HySPEC™
A Novel HyperSpectral Imager*

Identify • Quantify • Locate

- Spectral analysis of heterogeneous materials
- Over 80K spectra obtained simultaneously
- Illumination by a Tunable Laser

Testing of Skin-Care Products

Applications
- Product Development
- Process Monitoring
- QA/QC
- R&D Tool

Features
- High Spectral Resolution
- Complete Spectral scan in seconds
- Micro to Macro FOV
- Visible, NIR and Mid-IR
- No Sample Heating
- No Filters

Quantify Powder Mixture in Blender

Verify Cleaning Agent on Non-Woven Cloth

*US Patent 7,233,392

FACSS 2007
Please visit and see a demonstration at our booth #9

OPOTEK Inc.
2233 Faraday Avenue • Suite E • Carlsbad • California 92008
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Attention Presenters: Check this final program to verify the schedule of your talk or poster. Changes may have occurred since the preliminary program.

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FACSS International Office
2019 Galisteo Street, Building I-1, Santa Fe, NM 87505
(505) 820-1648 ☑ Fax: (505) 989-1073 ☑ facss@facss.org ☑ www.facss.org
Welcome! A warm welcome to all of you to the 34th annual Federation of Analytical Chemistry and Spectroscopy Societies (FACSS) from the Memphis organizing team, the FACSS Governing Board and our sponsoring organizations! We have a truly outstanding program this year with our format of top plenary speakers, poster and oral sessions and awards including the new Clara Craver award. Our exhibits and posters promise to capture your interest and intellectual curiosity. We have additional Hands-On workshops to enable you to learn what’s new in technology and enhance our workshop program. This year we have also added a web based employment bureau with many new features for both the prospective employers and job seekers. Finally, our Wednesday night networking event this year is at Graceland, home of Elvis Presley.

Plenary and Award Highlights - The keynote opening plenary session features Dr. Ira Levin of the National Institute of Health. The keynote closing plenary lecture is being given by the President-Elect of the American Chemical Society, Bruce Bursten. The Coblentz Society is introducing its first new award in many years, the Clara Craver award honoring young investigators. The Charles Mann award for achievements in Raman Spectroscopy will be presented, SAS will sponsor the Lester Strock & Meggers Awards, and ANACHEM will sponsor its annual award symposium. All this and our program of technical presentations and featured poster sessions make for another outstanding program. Celebrating our young investigators starts at the Sunday night student poster session sponsored by the Society of Applied Spectroscopy and including posters from the Coblentz Society student award winners.

Exhibits - The exhibits will be excellent; we had to make more room for exhibit space! The introduction of the Sunday Afternoon Hands-On workshop will be expanded to three this year, with topics including Imaging Science, Raman, and Mass Spectroscopy. On Monday there will be an exhibitor session that will introduce their new technologies. We will again have our Monday Night Exhibit opening reception to feature our exhibitors. Exhibitors will again have opportunities to sponsor student membership in our societies. Wireless internet will be available in the Exhibition area.

Workshops - a valuable component of FACSS, are conducted by leading experts. Topics include: Forensic, UV and NIR microscopy, Raman spectroscopy, Imaging, Infrared interpretation, Vibrational and TeraHertz imaging, Spectroscopy, basic and advanced Chemometrics, and ICP/MS and LCMS, along with NIR, SFC chromatography, and statistical design/applied mathematics. Procter and Gamble will present the Professional Analytical Chemistry short course for undergraduate students (no fee).

Employment Bureau - is yet another reason for excitement. We will offer a new on-line service that will enable pre and post conference capabilities for employers and job seekers. This service is provided free to all job seekers and employers. We are again going to have our employer panel during the lunch hour on Tuesday, and this year will include an additional seminar on Monday, covering job search strategies, interviewing and resume writing sponsored by Kelly Scientific Resources.

Wednesday Night Networking Event - Our Wednesday night networking event venue is Graceland (registration is required), and will include tours of the mansion, the car museum, the Elvis After Dark exhibit, and the airplanes used by Elvis and Priscilla. The Graceland grounds house a priceless collection of memorabilia.

Enjoying Memphis - In addition to the amenities of the conference hotel it is only a short streetcar ride to the world-renowned Beale Street Home of the Blues and the Birthplace of Rock ‘n’ Roll. Memphis offers a number of other destinations including Graceland, the Peabody Hotel and its ducks, the FedEx arena for Memphis Grizzly’s Basketball, the legendary Sun Studios where it all began, the Stax Museum of American Soul Music as well as other unique museums, grilled peanut butter and banana sandwiches, and more delicious barbeque per square mile than any place else. We invite you to be part of this week’s excitement that will be the 34th FACSS meeting.

JIM RYDZAK, 2007 Governing Board Chair and all of our Memphis team.
LOCATION: All conference symposia and the exhibit will be held at the Memphis Cook Convention Center. Workshops will be held at the convention center and the Memphis Marriott Hotel.

PROGRAM. This printed program contains titles and abstracts as submitted by the authors. It is not possible to edit these submissions.

SPEAKERS. There will be a LCD projector for each symposium. Speakers must supply their own computer with their presentation. Each speaker should adhere to the time allotted for the talk.

SPEAKER READY ROOM. A room is equipped with an LCD projector. The speaker ready room is 205.

POSTER SESSIONS. Authors are required to remain by their poster during their entire poster session.

Sunday SAS Sponsored Student Poster Session – Prefunction Foyer
  o Poster Session and Welcome Mixer 5:00 – 7:00 PM
Monday Poster Session – Prefunction Foyer
  o 9:00 – 10:30 AM poster session. Set up poster between 7:30 – 8:00 AM and remove between 4:30 – 5:00 PM
Tuesday Poster Session – Exhibit Hall
  o Morning Session 9:00 – 10:30 AM. Set up poster between 7:30 – 8:00 AM and remove at 12:30 PM
  o Afternoon Session 1:45 – 3:15 PM. Set up poster between 12:45 – 1:15 PM and remove by 5:00 PM
Wednesday Poster Session – Exhibit Hall
  o Morning Session 9:00 – 10:30 AM. Set up poster between 7:30 – 8:00 AM and remove at 12:30 PM
  o Afternoon Session 1:45 – 3:15 PM. Set up poster between 12:45 – 1:15 PM and remove by 5:00 PM
Thursday Poster Session – Prefunction Foyer.
  o Morning Session 9:30 – 10:30 AM and Afternoon Session 1:45 – 2:45 PM. Set up poster between 7:30 – 8:00 AM and remove after the PM poster session.

FACSS WORKSHOPS. A list of workshops, descriptions, and the locations begin on page 38. You must register for a FACSS workshop at the conference registration desk.

EMPLOYMENT BUREAU. The bureau is located in the Mississippi Room on the Mezzanine Level of the convention center. The center will be open Monday through Wednesday, 9:00 AM to 5:00 PM and 9:00 AM – 3:00 PM on Thursday. Registration forms are available at the employment bureau. See page 41 for additional information.

EXHIBITS. The exhibition is located in Ballroom A/B and will be open as follows: See page 27 for details.
  Monday (Opening Reception) 4:30 PM – 6:30 PM
  Tuesday – Wednesday 9:00 AM – 5:00 PM

BREAKS. Monday and Thursday breaks will be held in the Prefunction Foyer. Tuesday and Wednesday breaks will be held in the Exhibit Hall (Ballroom A/B).

INTERNET ACCESS. Complimentary wireless internet access will be available to all conference attendees. Access is located in the Exhibit Hall (Ballroom A/B) and the Prefunction Foyer, ballroom level.

REGULATIONS. The following regulations are in the best interest of the conference.
  1. There is no smoking in any conference area.
  2. An official name badge is required at all times.
  3. No advertising may be placed in the conference area.
  4. Only official exhibitors may display in the Exhibit Hall.
  5. No distribution of product/meeting literature will be allowed in the technical sessions.

SPECIAL EVENTS.

SUNDAY
  3:00 – 5:00 PM “What's Hot” Exhibitor Presentations, Room 201/202
  5:00 – 7:00 PM Welcome Mixer and SAS Sponsored Student Poster Session, SAS, FACSS, and Coblentz Student Award Presentations, Prefunction Foyer

MONDAY
  8:00 AM Plenary Lecture: Interdisciplinary Biophotonics: Molecular Domains to Organelles to Organs, Ira W. Levin, NIH, Ballroom C/D
  1:00 PM Working with Recruiters: The secrets that will help you achieve your career goals! Kelly Scientific Resources, Room 201, Sign up at conference registration desk
  1:30 – 2:30 PM “What's Hot” Exhibitor Presentations, Ballroom C/D
  4:30 – 6:30 PM Reception for Exhibit Opening (wine, beer, light hors d'oeuvres) Ballroom A/B

TUESDAY
  8:00 AM ANACHEM Award: An Analytical Chemist with a Focus on Separations Research: Separation of Photons and Separation of Molecules, Isiah M. Warner, Louisiana State University, Ballroom C/D
  8:30 AM Charles Mann Award: Confocal Raman Microscopy: Where are We Really Looking?, Neil Everall, Intertek MSG, Ballroom C/D
  12:30 PM SABIC Innovative Plastics sponsored Student/Professional Panel Discussion and Brown Bag Lunch. “I’m Graduating Soon. What’s Next?” Room 201, Sign up at conference registration desk

WEDNESDAY
  8:00 AM SAS Applied Spectroscopy William F. Meggers Award: Vibrational Spectroscopy, Microscopy and Imaging: Applications to Skin Pharmacology and Biochemistry, Richard Medelsohn, Rutgers University, Ballroom C/D
  8:30 AM Coblentz Society Clara Craver Award: Increased Process Understanding through Use of in-situ Vibrational Spectroscopy, Katherine A. Bakeev, GlaxoSmithKline, Ballroom C/D
  6:00 PM FACSS Wednesday Evening Networking Event, Graceland. Ticket required

THURSDAY
  8:00 AM SAS Lester Strock Award: Laser Ablation Inductively Coupled Plasma Spectrometry – Ready for Take Off, Detlef Günther, ETH Zurich, Ballroom C/D
  8:30 AM Plenary Lecture: The Centrality of Chemistry. Bruce Edward Bursten, President-Elect of the American Chemical Society, Ballroom C/D

COMPANION REGISTRATION. Companion registration is offered for persons accompanying conference registrants. Does not include access to symposia or exhibit hall other than for exhibit opening. Cost is $45 and includes the following:
  • Sunday Evening Welcome Mixer and SAS Student Poster Session
  • Monday, 4:30 – 6:30 PM, Exhibit Hall Opening Reception
  • Monday and Tuesday, 9:00 AM, coffee and pastries, Gatlinburg, Memphis Marriott Hotel
EVENTS OF SPECIAL INTEREST TO STUDENTS

Sunday Evening, Prefunction Foyer
• Welcome Mixer – 5:00- 7:00 PM
• SAS Sponsored Student Poster Session – 5:00 – 7:00 PM
  o SAS, FACSS and Coblenz Student Award presentations

Monday through Thursday
• FACSS Student Poster Awards will be presented.

Monday
• Employment Bureau in the Mississippi Room on Mezzanine Level
  Monday – Wednesday 9:00 AM – 5:00 PM; Thursday 9:00 AM – 3:00 PM
• Workshop – Professional Analytical Chemists in Industry: A Short Course for Undergraduate Students, Diane Parry, Procter and Gamble. No Charge. Register at the conference registration desk.
• 1:00 PM, Working with Recruiters: The secrets that will help you achieve your career goals! Kelly Scientific Resources, Room 201, Sign up at conference registration desk.

Tuesday
• 12:30 PM, SABIC Innovative Plastics Sponsored Student/Professional Panel Discussion and Brown Bag Lunch. “I’m Graduating Soon. What’s Next?, Room 201. Sign up at conference registration desk.

6:00 PM
WEDNESDAY EVENING NETWORKING EVENT - GRACELAND

After a full day of oral and poster presentations, join your colleagues for the Wednesday Evening Networking Event at Graceland. Catch up with friends on the motor coach ride from the convention center to Graceland. Experience life as Elvis did at Graceland with an audio-guided tour featuring commentary and stories by Elvis and his daughter, Lisa Marie. Decorated in the funky styles of the 50's, 60's and 70's, Graceland will lead you through Elvis's amazing journey to superstardom. See videos, photos, personal mementos and artifacts, and an impressive display of Elvis's gold and platinum awards. After touring the Mansion, you will enjoy a Barbeque dinner in Elvis's Car Museum featuring many of the vehicles once owned by Elvis. Highlights include the famous 1955 pink Cadillac and the 1973 Stutz Blackhawk along with many other cars, motorcycles and motorized toys. You will be able to board Elvis’s custom airplane the Lisa Marie, named after his daughter. The plane is equipped with gold plated seatbelts, suede chairs and leather-covered tables. Sincerely Elvis is currently displaying 55 of Elvis's jumpsuits worn during his Las Vegas tours. Don’t miss this opportunity to mingle with other conferees while exploring the life of Elvis Presley. Admission is limited, purchase your ticket at the conference registration counter. Cost for the event: $50

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### FACSS ORGANIZATION

**Member Organizations of FACSS**
- American Chemical Society, Analytical Division
- American Society for Mass Spectrometry
- ANACHEM
- Analysis Division of Instrument Society of America
- Coblentz Society
- Royal Society of Chemistry
- Society for Applied Spectroscopy

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**FACSS is the National Meeting for the Society for Applied Spectroscopy and the Coblentz Society**

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#### 2007 Chair Persons

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<td>James W. Rydzak</td>
<td>GlaxoSmithKline</td>
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<td></td>
<td>E-mail: <a href="mailto:james.w.rydzak@gsk.com">james.w.rydzak@gsk.com</a></td>
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<tr>
<td>Governing Board Chair Elect</td>
<td>Gary Brewer</td>
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<td>Mike Carrabba</td>
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<td>E-mail: <a href="mailto:mcarrabba@hachhst.com">mcarrabba@hachhst.com</a></td>
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<td>Paul Bourassa</td>
<td>Lifeblood Midsouth Regional Blood Ctr</td>
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<td></td>
<td>E-mail: <a href="mailto:paulb@lifeblood.org">paulb@lifeblood.org</a></td>
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<td>Program Chair</td>
<td>Ian R. Lewis</td>
<td>Kaiser Optical Systems, Inc.</td>
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<td>E-mail: <a href="mailto:lewis@kosi.com">lewis@kosi.com</a></td>
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#### 2007 Program Section Chairs

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<td>Mike Claybourn</td>
<td>AstraZeneca, Ltd</td>
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<td>Doug Gilman</td>
<td>Louisiana State University</td>
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<td>Bonnie Saylor and Victor Hutcherson</td>
<td>Society for Applied Spectroscopy</td>
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GOVERNING BOARD CHAIR

James Rydzak
GlaxoSmithKline

Jim Rydzak is a Manager of the Process Analytical and Chemometrics group within the Strategic Technology Division at GlaxoSmithKline, near Philadelphia, where he has worked for the past 8 years. Prior to working at GSK, he worked at Colgate-Palmolive for 16 years, first as a molecular spectroscopist, then started a Process Analytical Group in 1989 and later was a group leader and Analytical & Testing lab supervisor at the Mennen R&D site. Jim has a varied background as an analytical chemist with backgrounds in the Polymer (El Paso Polyolefins, Paramus N.J. 1981) and Electroplating (ROHCO, Cleveland, 1979) industries since 1979. Jim’s background in FT-IR, Raman and NIR spectroscopy led him into the field of Process Analytical. He has been a member of the Directors of Industrial Research Process Analytical round table, more recently Jim was one of the founding members of the ASTM E55 committee on the Pharmaceutical Application of Process Analytical Technology. Jim got his B.S. in Chemistry in 1976 from Mount Union College in Alliance, Ohio and his M.S. in Analytical Chemistry working for Peter Griffiths at Ohio University in 1978.

Jim attended his first FACSS conference in Philadelphia in 1982 and has presented numerous times. He has been active on the governing board of the FACSS since 1996, first as a Coblenz representative for several years, then as workshop and employment chair for the 2000-2002 conferences. Jim was the program chair for the 2003 FACSS conference and is the governing board chair for this year’s conference. Jim has also been a member of SAS for over 25 years, and has also served on the Coblenz board of managers for 3 years from 2002-2005. He also served as a Coblenz representative to the EAS governing board from 1998-2006. Jim has taught short courses in molecular spectroscopy with colleagues Paul Bourassa (our 2007 Memphis FACSS General Chair) and John Coates for the Center for Professional Advancement for eight years in Amsterdam and New Jersey in the 90’s. Jim has also teamed with Chris Hassell to run the Process Analytical Chemistry: Out of the Lab and into the Pipes course on PAT at the FACSS conference for several years.

GENERAL CHAIR

Paul Bourassa
Lifeblood Midsouth Regional Blood Ctr

Paul N. Bourassa has served FACSS in many roles. For the past ten years he has been the Treasurer of FACSS. In 1994 he served as Governing Board Chairman and in 1989 he served as the General Chairman for the FACSS conference in Chicago. He is also currently serving on the FACSS Long Range Planning Committee.

Paul is a member of the Society for Applied Spectroscopy, where is has just been elected to the post of Treasurer. He has previously served SAS as President of the Chicago Section in 1981 and twice as National Tour Speaker Chairman. Paul is a member of the Coblenz Society where he served as a delegate to FACSS for a number of years. He is also a member of the American Chemical Society. Having served on the Editorial Advisory Board of Spectroscopy, since the introduction of the journal, Paul has authored and coauthored a number of articles for the publication and served as editor of the Spectral Interpretation column. Paul has also served as a reviewer for the National Science Foundation. With colleagues Jim Rydzak and John Coates, Paul has taught courses in Molecular Spectroscopy for the Center for Professional Advancement in New Jersey and Amsterdam over a period of eight years.

After graduating from the Illinois Institute of Technology, in Chicago, Paul started his career in spectroscopy, with a mass spectrometer at the University of Chicago. After learning how to polish salt crystals, Paul began a long career in Infrared Spectroscopy. During his sixteen years at UOP, Paul widened his scope to include chromatography, NMR, UV-VIS-NIR, emission, x-ray and eventually became supervisor of the Spectroscopy Department at UOP. With his growing love of the art and science of the interpretation of spectral data, Paul established a company to provide consultation in this area.

As Director of Manufacturing and Distribution at Lifeblood Mid-South Regional Blood Center, in Memphis Tennessee for the past five years, Paul’s responsibilities cover departments involved in the making of blood components (red cells, plasma, platelets, Cryo, buffy coats, etc.) from whole blood donations, the testing of apheresis platelets for bacterial contamination and the distribution of blood products to area hospitals, clinics, secondary manufacturers and researchers.

Paul is also active in his community as the Clerk of Session at Farmington Presbyterian Church, a post he has served in for the past eleven years, as a member of the Germantown Ministers/Police Alliance and a member of the Germantown Coffee Club. There is no record of tenure with the Coffee Club.
Ian R. Lewis
Kaiser Optical Systems

Ian R. Lewis was born in 1968 in Weston-Super-Mare, Somerset, UK. He obtained his undergraduate degree in Chemistry and Chemical Technology at the University of Bradford in 1989 and his Ph.D. in 1992 in the field of infrared and Raman spectroscopic characterization of polydienes in the Interdisciplinary Research Center in Polymer Science and Technology under the joint direction of IRC associate director Professor Anthony Johnson and Professor Howell Edwards. Following his appointment as an Honorary Visiting Researcher to the IRC in 1992 he went to the University of Idaho to work as a postdoctoral research associate in the laboratories of Professor Peter Griffiths. During this time he also acted as a consultant on the application of Raman spectroscopy to several industrial companies. In 1996 he joined Kaiser Optical Systems as a Laser Spectroscopy Specialist and is currently global Marketing Manager.

He has been an active participant in past-FACSS conferences and has been the Program Section Chair for Raman in 2000, and from 2002 to the present. He has organized scientific sessions at several additional conferences including EAS. Ian is a board member of the Coblentz Society (2004-2008). He serves as the Chair of ASTM subcommittee E13.08 on Raman Spectroscopy (2002 to present), served as the secretary of E13.10 on Molecular Optic Imaging (2001-2003), and is the co-haiison from E13 to E55. During his career Ian has published approximately 45 scientific papers in refereed journals, has co-authored 6 book chapters, and is co-editor of Handbook of Raman Spectroscopy: From Research Laboratory to the Process Line (published in 2001). He serves on the editorial advisory board of Spectroscopy Magazine, and American Pharmaceutical Review. Ian is an active reviewer for a number of international journals and a member of several scientific societies.

Ian has been married since 1994 and has seven children, 4 girls and 3 boys. When not at work, participating in scientific activities, or engaged in his family’s numerous activities he can be found sleeping or enjoying any quiet moment he can find. Ian would like to take this opportunity to thank his family and particularly his wife, Mary, for giving him the time to organize the Program for this meeting.

Michael Carrabba
Hach Homeland Security Technology

Dr. Mike Carrabba is currently the Director of Hach Homeland Security Technologies Air Systems Division where he is working on using spectroscopy for the detection of biological hazards. He received his B.S. in Chemistry from Salem State College in 1981 and his Ph.D. from Tufts University in 1985. Mike’s graduate work was conducted under the tutelage of Dr. Jonathan Kenny and focused on the utilization of laser-induced fluorescence to examine ultra-cooled gas phase molecules in a supersonic jet molecular beam. After graduate school, Mike joined EIC Laboratories where he eventually became Vice-President for the Spectroscopy Division. He conducted a variety of research programs, including photoelectrochemical etching of semiconductors, fiber optic chemical sensors and state-of-the-art Raman spectroscopy. During this time, he introduced the use of holographic filters for Raman spectroscopy and developed numerous types of Raman instrumentation and techniques, several of which resulted in U.S. patents. After leaving EIC, Mike joined Chromex, Inc, a manufacturer of Raman spectroscopy systems, as Marketing Manager and most recently was the OEM Division Manager at Jobin Yvon, Inc. Mike has been very active in FACSS over the years serving as Governing Board Chair (2002), Program Chair (2000), Program Section Chair for Raman (1992-1999, 2001), Chairperson of the Long Range Planning Committee and as a member of the Governing Board. In 2003 he received the ASTM Award of Merit for his 12 years of service as the Chairman of the ASTM Subcommittee on Raman spectroscopy. In 2004, he received the FACSS Charles Mann Award for Applied Raman Spectroscopy and in 2007 the Williams Wright Award for Applied Spectroscopy. He is also a member of the Society for Applied Spectroscopy (SAS) and Coblentz Society. On the home front, his wife, Professor Mary Widmark Carrabba of Southern Oregon University, a highly skilled Infrared microscopist and the former treasurer for SAS, complements Mike’s Raman background.
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FLOOR PLANS

BALLROOM LEVEL – Registration, Plenary Sessions, Exhibits, Poster Sessions, Breaks

Plenary Sessions
Sunday, Monday, and Thursday, Poster Sessions
Exhibits and Tuesday and Wednesday Poster Sessions

LOBBY LEVEL
Room 11
Vibrational Spectroscopy
Environmental Applications of Analytical Chemistry
NIR Imaging
NIR Applications in the Pharmaceutical Industry
Advances in FTIR Imaging
Developments in Luminescence Spectroscopy
Novel Spectroscopic Instrumentation
Biovibrational Spectroscopy

Room 12
Instrumentation & Application of Process Analytical Chem.
Process Analytical Monitoring
ISA Analysis Division – Best of the Best
Applications of Fluorescence Spectroscopy
Initiative (NeSSi) to Improve Process Quality & Control
Novel Sensors and Instrumentation
Process Analysis
PAT Across the R&D

Room 13
Bioanalytical Applications of SERS
Quantitative Raman in Pharma
Current Analytical Tech for Drug Discovery
Charles Mann Award
Opportunities for Raman Spectroscopy
Evolving Dev. in the Use of Raman Spect.
Raman Spectral Imaging
Emerging Appl &Technologies in Raman Spect.

Room 14
Imaging & Spectroscopy in THz Region
Coherent 2-D Spectroscopy
Emerging Tech. for Homeland Security
Analysis & Modeling of Spectral Data
Surface Plasmon Resonance
Pharmaceutical Forensics
Recent Dev. In Explosive Detection Tech.

MEZZANINE LEVEL – Employment Bureau

SKYWAY TO MARRIOTT

LOBBY LEVEL – Monday through Thursday Symposia

Room 2
Hidden Isotope Ratio Information
Electrothermal Atomization vs. Electrothermal Vaporization Techniques
Current Advances in ICPMS
Biomedical Applications of Atomic Spectroscopy
Developments in Plasma Spectroscopy
Commemoration of Dr. Radu Mavrodineau
Fundamental Advances in Plasma Source MS

Room 3
Advances in Spectroscopy & MS in Forensic Sciences
Bioanalytical Electrochemistry
MS for Bioanalysis
Capillary Electrophoresis
Bioanalytical Microfluidics
Electrophoretic & Microfluidic Bioanalysis
Fabrication Strategies for Microfluidics
Surface Plasmon Resonance

Room 4
Chemometrics Applied to Expert Systems
Spectral and Multiway Pattern Recognition
Electrochemistry and Functional Nanomaterials
Nanotubes and Nanowires
Nanoscale Structures
Carbon Nanotube Separation

Room 5
Fundamentals of Electrospray Ionization
Molecular Spectroscopy in Forensic Science
Novel Methods for Biological MS
Particle MS
New Approaches to Environmental MS
Advances in Biomolecular Imaging MS
Direct Ionization Methods for High Throughput MS

Room 6
FACSS Young Investigators
ANACHEM Award
Student Awards
Coblentz Society Clara Craver Award
Meggars Award
Strock Award
Multivariate Curve Resolution
FACSS AWARDS

The Tomas Hirschfeld Scholars and the FACSS Student Award recognize outstanding contributions by individuals who are Ph.D. and M.Sc. candidates.

TOMAS HIRSCHFELD SCHOLAR

Matthew Schulmerich
University of Michigan

Presentation, Tuesday, 3:15 PM, Room L6

Matthew Schulmerich is a 4th year graduate student in the Chemistry Department at the University of Michigan where he is working with Professor Michael Morris. Prior to attending the University of Michigan, Matthew earned a B.S. in Chemistry and a B.A in Biology from St. John Fisher College in Rochester, New York. His research interests include subsurface Raman spectroscopy and imaging with an emphasis on musculoskeletal tissue. Matthew’s ground-breaking research has led to the development of instrumentation capable of resolving Raman spectra of samples located beneath more than two centimeters of light scattering materials, such as polyethylene. He has also demonstrated Raman mapping of material interfaces through light scattering media. This work earned him a graduate student poster award and an iPod Nano at FACSS 2005 and was featured on the cover of Applied Spectroscopy. Applying this novel technology to important problems in biomedical science, he became the first to demonstrate the recovery of bone Raman spectra through the skin at clinically relevant depths and with sufficient accuracy for diagnostic use. In addition to presenting his work at numerous national and international scientific meetings, Matthew has published in Applied Spectroscopy and The Journal of Biomedical Optics. He is currently developing Raman tomography in scattering media, including noninvasive imaging of bone structure, which is the topic of his FACSS 2007 paper. He also participates on a team that is investigating the genes responsible for bone mechanical properties where he is the lead Raman spectroscopist.

TOMAS HIRSCHFELD SCHOLAR

Junrong Zheng
Stanford University

Presentation, Monday, 3:10 PM, Room L14

Junrong Zheng is a postdoctoral associate in the Chemistry Department at Stanford University where he is working with Professor Michael D. Fayer, after he defended his PhD thesis from a 4-year graduate career in the same lab on August 13th 2007. Prior to attending Stanford University, Junrong earned a B.S. in Chemistry and a MS in Polymer Chemistry from Peking University in Beijing, China, and another MS in Polymer Physics from Rensselaer Polytechnic Institute in Troy, New York. His current research interests include 2D IR spectroscopy and its applications in the studies of molecular dynamics and reactions. Junrong’s ground-breaking research has led to the development of Ultrafast Chemical Exchange Spectroscopy. This work was credited by Chemical & Engineering News as “Spectroscopy’s New Era”. It earned him the Stanford Graduate Fellowship, and invited talks at the University of Maryland, the Physical Organic Chemistry Gordon Conference, and the Ultrafast Phenomena XV. Applying this novel technology to fundamental problems in physical chemistry, he systematically studied the correlation between the strengths and lifetimes of weak intermolecular interactions in liquids, and experimentally answered a more than 100 years old question – how fast does the C-C single bond of Ethane rotate in room temperature liquids. In addition to presenting his work at numerous national and international scientific meetings, Junrong has published 20 papers in Science, JACS, Acc. Chem. Res., JCP, Polymer, et al. He is currently developing new methods to push the 2D IR technique into wider applications.
FACSS STUDENT AWARD

Sen Li
Purdue University

Presentation, Tuesday, 3:35 PM, Room L6

Sen Li is a Ph.D. Candidate advised by Prof. Hilkka Kenttämaa in the Department of Chemistry at Purdue University. His main research focus is bioanalytical mass spectrometry. He has delineated mechanisms for radical-induced damage to peptides and developed methodologies for the identification of functionalities in mono- and polyfunctional analytes by using various mass spectrometry techniques. While obtaining a Bachelor Degree in Material Science and Engineering in China and a M.S. degree in Chemistry from Western Kentucky University (WKU) under Prof. Wei-ping Pan, he carried out research on mercury emission analysis from coal-combustion power plants, polymer and pharmaceutical materials characterization using thermal analysis and GC/MS techniques, and synthetic crystal process and characterization. Mr. Sen Li has received a number of awards and recognitions for his achievements in analytical chemistry research, including American Institute of Chemists Award, Eastman Chemical Company Fellowship, and Thomas W. Keough Award.

FACSS STUDENT AWARD - HONORABLE MENTION

William F. Pearman, University of South Carolina. Presentation: Wednesday 4:35 PM, Room L6

Germarie Sánchez-Pomales, University of Puerto Rico. Presentation: Wednesday 12:10 PM, Room L4

Luisa Theresa Maria Profeta, University of South Carolina. Presentation: Wednesday 11:30 AM, Room L14

TOMAS HIRSCHFELD AND FACSS STUDENT AWARDS

Call for Applications for 2008

The Tomas Hirschfeld Scholar(s) and the FACSS Student Awards recognize the most outstanding papers submitted to FACSS by a graduate student. Recipients will receive financial support to help them attend the 2008 FACSS meeting in Reno, NV (September 28 – October 2). In 2007 two Tomas Hirschfeld Scholars and one FACSS Student Award are being presented. In order to have your presentation considered for a Tomas Hirschfeld Scholar Award or FACSS Student Award, students should submit their abstract using the FACSS web site submission form and indicate on the dropdown menu on the form their interest in these awards.

The submission process involves submitting an abstract, completing the web site submission form, and submitting three sets of the following:

a) the form, available on the FACSS web site
b) a 250 word abstract of the work to be reported
c) two letters of nomination, one by the student's mentor. An explanation of the inventive contributions by the student to the work should be given. Creativity was a primary characteristic of Tomas's work, and thus should be a characteristic of the awardee
d) a copy of the candidates resumé
e) a copy of the candidate’s graduate transcript
f) copies of reprints and/or preprints of research accomplished.

The recipients will be included in a session highlighting young scientists and their work.

The FACSS Web site will begin accepting abstracts and applications for FACSS student awards in January 2008. Go to www.facss.org to submit an application.
Isiah M. Warner

**Louisiana State University**

*Presentation, Tuesday 8:00 AM, Ballroom C/D*

Isiah M. Warner received his B.S. in chemistry from Southern University (Baton Rouge) in 1968. He was a research chemist with Battelle Northwest for five years. He entered graduate school at the University of Washington in 1973 and received his Ph.D. in 1977. He was assistant professor of chemistry at Texas A&M University from 1977-82. He was awarded tenure and promoted to associate professor September 1982. He joined Emory University in 1982 as associate professor and was promoted to full professor in 1986. He was named Samuel Candler Dobbs Professor of Chemistry at Emory in September 1982. He joined Emory University in 1982 as associate professor and was promoted to full professor in 1986. He was named Samuel Candler Dobbs Professor of Chemistry at Emory in September 1987. He was on leave to the National Science Foundation (NSF) as Program Officer for Analytical and Surface Chemistry in 1988/89. In August 1992, Dr. Warner joined Louisiana State University as Philip W. West Professor of Analytical and Environmental Chemistry. He was Chair of the Chemistry Department from July 1994-97. He was appointed Boyd Professor of the LSU System in July 2000, Vice Chancellor for Strategic Initiatives in April 2001 and Howard Hughes Medical Institute Professor in 2002.

The primary emphasis of Dr. Warner’s research is development and application of improved methodology (chemical, mathematical, and instrumental) for studies of complex chemical systems. His research interests include fluorescence spectroscopy; chromatography; studies in organized media; guest/host interactions; environmental analyses; and mathematical analyses and interpretation of chemical data using chemometrics (chemical data analyses techniques).

Isiah Warner has more than 260 published or submitted refereed articles. He has been issued five patents for his work and has three others pending. He has chaired forty doctoral theses and is currently supervising fifteen others. Honors include: 2006 Southern Chemist Award, ACS – Memphis Section on December 7, 2006; Banneker Legacy Award, Benjamin Banneker Institute on November 17, 2006; Marquette University, honorary Doctor of Science degree on May 22, 2005; Charles E. Coates Award, ACS local section on May 12, 2005; Tuskegee University, George Washington Carver Achievement Award on January 27, 2005; University of Washington, College of Arts & Sciences, Distinguished Alumnus Award on May 20, 2004; ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences and Council for Chemical Research Diversity Award in 2003; elected to the status of Fellow of the American Association for the Advancement of Science in 2003; Howard Hughes Medical Institute Professor in 2002; CASE Louisiana Teacher of the Year, LSU Distinguished Faculty Award, AAAS Lifetime Mentor Award, Eastern Analytical Symposium Award for achievements in the Fields of Analytical Science, all in 2000; 1998 Fulbright Fellowship for Research/Teaching in Kenya; 1997 Presidential Award for Excellence in Science, Mathematics, and Engineering Mentoring from President Clinton; NOBCChE Award for "Outstanding Teacher" in 1993; and in 1988, the Percy Julian Award for Outstanding and Significant Contributions in Research, sponsored by NOBCChE; recipient of NOBCChE Outstanding Graduate Research Award in 1976; and other honors too numerous to mention.

Neil Everall

**Intertek MSG**

*Presentation, Tuesday 8:30 AM, Ballroom C/D*

Neil Everall gained his BSc in Chemistry in 1981 from the University of York, UK, and his PhD (researching picosecond Raman spectroscopy) in 1986 from the University of Durham, UK. After a Post Doctoral position at the Rutherford Appleton Laboratory (Oxford, UK), developing high power UV lasers, he joined ICI in 1988 to establish a Raman Spectroscopy facility at its Corporate Research Centre. For more than 13 years he led the infrared and Raman spectroscopy activity at ICI’s Measurement Science Group (MSG) at Wilton in the North East of England. He was appointed an ICI Company Research Associate in 2003, making him the Company’s senior measurement scientist. In 2007 ICI divested its Measurement Science Group in its entirety to Intertek PLC, and Everall is currently employed in the group which was formed, Intertek-MSG.

Everall’s research interests centre on the development and application of vibrational spectroscopy for characterising materials and industrial processes. In recent years this has included infrared and Raman studies of polymer structure (primarily polymerisation mechanisms, microstructure, crystallinity and molecular orientation), modelling the spatial response and depth resolution of the confocal Raman microscope, process analysis with Raman spectroscopy, and materials characterisation using infrared and Raman mapping/imaging. More recently he has been studying Raman photon migration in opaque media, in collaboration with workers at the Rutherford Appleton Laboratory, and has also been revisiting the issues that determine the working resolution of the Raman microscope. His most recent work has been focused on modelling and measuring the performance of infrared imaging spectrometers based on ATR optics.

Everall has published over 75 refereed articles, numerous book chapters, and 1 Patent, and is currently a European Associate Editor for *Applied Spectroscopy*. He also sits on the editorial advisory board for the *Asian Journal of Spectroscopy*, and was an Associate Editor of the Handbook of Vibrational Spectroscopy, a five-volume text edited by John Chalmers and Peter Griffiths and published in 2001. Everall is a member of the organising committee of the UK Infrared and Raman Discussion Group, and is a Fellow of the Royal Society of Chemistry. He is also a member of the EPSRC Peer review college.

In 2002 he was awarded, along with co-authors Hahn, Matousek, Parker and Towrie, the Meggers Award by the Society for Applied Spectroscopy, and in 2003 he received the Williams-Wright Award from the Coblenz Society. Most recently, he received, along with co-workers Matousek, Clark, Draper, Morris, Towrie, Finney, Goodship and Parker, the 2006 Meggers Award in recognition of continuing work on Raman photon migration.
DISTINGUISHED SERVICE AWARD
Recognizing members for their long-time service to the society

Laurence A. Nafie  
Syracuse University

Laurence A. Nafie received his Ph.D. from the University of Oregon in 1973, studying resonance Raman scattering, and from 1973 to 1975 he was a postdoctoral associate at the University of Southern California, working on the discovery and confirmation of infrared vibrational circular dichroism (VCD). In 1975 he joined the Chemistry faculty at Syracuse University to establish a research program in VCD and Raman optical activity (ROA). In 1978, he was named an Alfred P. Sloan Foundation Fellow and was promoted to Professor in 1982. In 1979 he proposed and carried out the first measurements of Fourier transform VCD, now the basis of all commercial VCD instrumentation. He was appointed Chairman of the Chemistry Department in 1984 and served until 2000. In 1988 he measured the scattered circular polarization (SCP) form of ROA for the first time that is now used in the only commercially available ROA spectrometer. In 1989 he predicted theoretically a new form of ROA called dual circular polarization (DCP) ROA that was confirmed experimentally in his laboratory in 1991. In 1995 he became founding Editor of the journal Biospectroscopy, published by John Wiley & Sons, and from 2001 to 2004 appearing as Biopolymers: Biospectroscopy. In 1996, he co-founded with Dr. Rina Dukor the company, BioTools, Inc., to market advanced vibrational spectroscopy instrumentation, including the ChiralIR VCD and ChiralRaman ROA spectrometers. In 2000, he was named Distinguished Professor of Chemistry at Syracuse University. He was awarded the Coblentz Award (1981), the Bomem Michelson Award (2001), and the William F. Meggers Award (2001). In 2003, he served as President of the Society of Applied Spectroscopy. He has over 250 publications and several patents awarded or pending.

GRADUATE STUDENT AWARD
Recognizing a graduate student for outstanding research in spectroscopy

Gary T. Dobbs  
Georgia Institute of Technology

Gary T. Dobbs Presentation, Tuesday 4:35 PM, Room L6

Gary T. Dobbs was born and raised in Russellville, AR. He received an academic scholarship to attend the University of Central Arkansas in Conway, AR, where he graduated cum laude in 2002 with a B.S. degree in chemistry with ACS certification. In 2001, he received an Energy Research Undergraduate Fellowship from the U.S. Department of Energy to investigate applications of glow discharge mass spectrometry at Oak Ridge National Laboratory under the guidance of Dr. Douglas C. Duckworth. Gary began his graduate studies at the Georgia Institute of Technology in 2002, where he was awarded the Institutes Presidential Fellowship. In addition, he received a fellowship to participate in the cross-disciplinary, Signals in the Sea: NSF IGERT program with joint cooperation between the Schools of Biology, Chemistry and Biochemistry, and Civil and Environmental Engineering. He is currently finalizing his doctoral research in the field of analytical chemistry under the advisement of Dr. Boris Mizaikoff. As a participant in the Gulf of Mexico Gas Hydrate Research Consortium through the Center for Marine Resources and Technology program at the University of Mississippi, his doctoral research has focused on the development of infrared spectroscopy as a tool for monitoring and examining oceanic gas hydrate ecosystems. His research has involved establishing the capability and first principles for monitoring simple, natural gas hydrates formed from aqueous solution in controlled laboratory experiments with mid-infrared fiber-optic evanescent wave spectroscopy, assessing the feasibility of implementing spectroscopic sensing strategies to monitor gas hydrate dynamics in seafloor sediments, and characterizing the diversity and origins of carbonate minerals characteristic of gas hydrate systems in the Gulf of Mexico. His current research interests include instrumental and application development for deep-sea chemical sensors.
Norman Colthup

Norman Colthup was born in Paris, France in 1924 of an American mother and an English father. He was brought to the United States in 1929 and eventually became an American citizen. After High School in New Canaan, CT, he went on to Antioch College in Ohio. This was interrupted by the war when he was drafted, but he was rejected because of an old injury.

In 1944, Colthup began his scientific career as a scientific assistant in the infrared group at American Cyanamid at the Stamford Connecticut laboratories. When the war ended, he returned to finish his interrupted studies for a B.S. degree at Antioch College. The college had a co-op plan where three month quarters at college alternated with three month quarters on a career related external job. Cyanamid agreed to this arrangement for Colthup, and after he graduated, in 1949, Cyanamid agreed to rehire him full time.

In 1937, the research lab scientists at Cyanamid at Stamford, CT had built one of the first industrial infrared spectrometers, and by 1944 they had made some start in discovering some group frequencies for vibrating molecules. The Cyanamid built IR spectrometers were single-beam types and the thermocouple signals were measured by coupled galvanometers and single-beam chaser recorder systems. Colthup worked as a technician starting in 1944 using this system and after some years he got interested in making his own group frequency correlations.

By 1949, Colthup had assembled a fairly extensive group frequency chart using entirely single-beam IR spectra, which was unprecedented at that time. Most people were unaware of the amount of data contained in this chart. His boss sent a copy to a journal editor, who asked for some text to go with it and saw to it that it was published. This chart came out just as easy to use double-beam IR spectrometers became available so a great many new people used IR for the first time. As a result, a great many chart reprints were distributed and the chart was reproduced in several IR books. Over the years, more data became available and eventually, Colthup’s IR group frequency chart extended to six pages long.

Fisk University in Nashville, TN gave a one week course in the use of IR in the chemical industry. Starting in 1959 with Cyanamid’s permission, Colthup became a frequent lecturer there on the interpretation of IR spectra. At first, he gave one lecture but eventually he lectured all week long.

In the 1960’s the American Chemical Society (ACS) had Colthup give a number of short courses, 2 or 3 days long, with Cyanamid’s permission, on the interpretation of IR spectra. The ACS also sponsored him to give brief talks on a tour of the east coast and a second tour of the pacific coast.

In 1971, the National Science Foundation in the US and the National Council for Science Education in India invited Colthup to visit India for a month to give a three day spectroscopy lecture session at each of five different Indian universities on the interpretation of infrared and Raman spectra. This included the University at Bangalore where Raman had resided. It was quite an experience for Colthup to see India close up.

At Cyanamid, he had gone through all the intermediate non-managerial levels to become finally a Principal Research Scientist in 1974. That same year, Fisk University decided to give Colthup an Honorary Doctor of Science degree. In 1979, the Coblentz Society awarded Colthup the Williams-Wright Award for outstanding contributions to the field of industrial infrared spectroscopy. In 1999, he received the coveted Maurice Hasler Award for outstanding contributions to infrared spectroscopy which have resulted in significant applications of broad utility.

Colthup has a number of publications in the IR and Raman fields. This includes the book Introduction to Infrared and Raman Spectroscopy that he co-authored with Daly and Wiberly. This book has been a best seller and is still popular and is now in its third edition. A similar book The Handbook of Infrared and Raman Characteristic Frequencies of Organic Molecules by Lin-Vien, Colthup, Fateley and Grasselli also has been a success. Colthup has a chapter in A Guide to Modern Methods of Instrumental Analysis® edited by Gouw.

He has some 40 or so articles in scientific journals. In a number of publications, he used molecular orbital calculations to evaluate many aspects of group frequencies, including C-H wag vibrations in olefins and aromatics, C-H bending in alkane groups, strained ring C=O force constants, interaction force constants in dicarbons, rotational isomers in anhydrides and CO/CS interactions in xanthates among others. Some aspects of mass spectra were also elucidated, giving information about relative energies of mass spec molecular fragments. In 1982, he used molecular orbital studies to reveal the theoretical basis for the success of the much used Q-e scheme (1947) of Alfrey and Price for calculating monomer content in free radical copolymerization reactions.

Norman Colthup has three fine sons, all with successful careers (not in science) and now has four grandchildren.
Sanford A. Asher
Sanford A. Asher, Distinguished Professor of Chemistry at the University of Pittsburgh received his B.A. in chemistry at the University of Missouri, St. Louis in 1971 and completed his Ph.D. in chemistry at the University of California, Berkeley in 1977. Dr. Asher was a Research Fellow in Applied Physics at Harvard University between 1977 and 1980. In 1980 he became Assistant Professor of Chemistry at the University of Pittsburgh. Dr. Asher’s research program at Pitt has involved development of new materials and the development of new spectroscopic techniques. His group developed UV resonance Raman spectroscopy as a new technique for fundamental and applied structural and trace studies of molecules in complex matrices. His group is using UV resonance Raman to examine the first stages in protein folding. In addition, Dr. Asher’s research group develops new photonic crystal optical devices and chemical sensing devices from self-assembling colloidal particles.

Dr. Asher has received numerous awards. He is the recipient of the Pittsburgh Spectroscopy Award which will be awarded at the 2008 PittCon meeting in New Orleans. He also became a Fellow of the Society of Applied Spectroscopy in 2007, received the Sigi Ziering Award from the American Society of Clinical Chemistry (2005), The University of Missouri, St. Louis Distinguished Alumni Award (2004), the ACS Pittsburgh Award (2002), the Ellis R. Lippincott Award from the Optical Society of America (2002), the Pittsburgh Technology Council Enterprize Award (2000), the Coblentz Society’s Bomem-Michelson Award (1999), the Society for Applied Spectroscopy’s Lester W. Stock Award (1998), the University of Pittsburgh’s Chancellor’s Distinguished Research Award (1996), the American Chemical Society Award in Spectrochemical Analysis (1994), the American Heart Association Established Investigator Award (1984) and an NIH Career Development Award (1984).

Professor Asher served as the Co-Director of the Materials Research Center of the University of Pittsburgh. He was the Chairman of the XV International Conference on Raman Spectroscopy held in Pittsburgh in 1996. He is Scientific Founder and Chairman of the Scientific Advisory Board of the startup company, Glucose Sensing Technologies, LLC, and is on the Scientific Advisory Boards of BioTools Inc. and Crystalplex Co. He consults for companies such as PPG Industries, ChemImage Corporation and Glucose Sensing Technologies, LLC.

He is the author of greater than 200 publications and has authored over twenty patents in the area of photonic crystals.

Ramon Barnes
Ramon Barnes is director of the University Research Institute for Analytical Chemistry, Professor Emeritus of Chemistry at the University of Massachusetts, editor of the ICP Information Newsletter (1975- ), and chairman of the Winter Conference on Plasma Spectrochemistry (1980- ). He received a Ph.D. in analytical chemistry from the University of Illinois, Champaign/Urbana, in 1966, an A.M. in chemistry from Columbia University, New York, in 1963, and was a post doctoral research fellow at Iowa State University, Ames, in 1968 and 1969. He served as an Army Captain at NASA Lewis Research Center, Cleveland, from 1966 to 1968. From 1969 to 2000 he taught analytical chemistry and maintained an international research program at the University of Massachusetts, Amherst. He has published more than 300 papers, edited four books, and continues an active research interest in fundamentals and applications of inductively coupled plasma (ICP) discharges for spectrochemical analysis. In 2003 he received the Lester W. Stock Award from the Society for Applied Spectroscopy for outstanding work in the development of the flow field-flow fractionation ICP technique. The University Research Institute for Analytical Chemistry (URIAC) is the research and development division of ICP Information Newsletter, Inc., a not for profit corporation established in 1997 to foster science education, research, and study in spectroanalytical chemistry. URIAC provides specialty plasma spectrochemical analysis, method development, training, consulting, and applied research with ICP atomic emission spectrometry and ICP mass spectrometry for ultratrace metal and stable isotope analyses in environmental forensics, drug development, medicine, public health, and semiconductor manufacturing.

Jeanette Grasselli Brown
Jeanette Grasselli Brown is the former vice president of research for Standard Oil and a 1950 graduate of Ohio University. Dr. Grasselli Brown served 38 years in industrial research, retiring in 1989 as Director of Corporate Research for BP America (formerly The Standard Oil Company ) where she was responsible for 250 people and a $40 million budget. She served as a Distinguished Visiting Professor and Director, Research Enhancement at Ohio University, Athens, Ohio. Appointed by Governor Voinovich to the Ohio Board of Regents a coordinating body for all higher education and reappointed by Governor Taft as Chair. She holds 1 patent, 80 publications and 9 books in the field of infrared and Raman spectroscopy. She received her B.S. in Chemistry from Ohio University and M.S. from Case Western Reserve University.

Norman B. Colthup
See page 15 for biographic information.
Robert S. Houk

Robert S. Houk, professor, received his undergraduate training at Slippery Rock University of Pennsylvania (B.S. 1974) and completed his doctoral work at Iowa State University (Ph.D. 1980). Following postdoctoral work at Ames Laboratory, he joined the Iowa State faculty in 1981. His awards include the Lester W. Strock Award, 1986; Maurice F. Hasler Award, 1993; ACS Award in Chemical Instrumentation, 1993; Wilkinson Teaching Award, 1993, and the Anachem Award, 2000. He serves on the Editorial Board of Spectrochimica Acta Acta Part B and the Journal of Analytical Atomic Spectrometry.

Ira W. Levin

See page 15 for biographic information.

Marvin Margoshes

I was born May 1925 in New York, NY. I attended New York Public Schools, and graduated from Brooklyn Technical High School January 1943. I worked as chemistry laboratory technician at the NYU Medical School, until I entered the U.S. Army in June 1943. After basic training at Keesler Field, Biloxi, MS, I entered the Army Specialized Training (ASTP) program at Kalamazoo College. When the ASTP Program was closed, March 1944, I was assigned to the 96th Infantry Division, then in Oregon, as a rifleman. After training in Oregon and California, we went to Hawaii, for further training. We made the landings on Leyte, in the Philippines, on November 20, 1944, and on Okinawa on April 1, 1945. I was wounded on both islands, and returned to duty after recovering.

I was discharged in January 1946, and started college at Mohawk College, Utica, NY (a temporary college set up to handle the flood of college applicants after WW II) in September 1946. I transferred to Brooklyn Polytechnic Institute (now New York Polytech) in September 1947, and completed the requirements for a B.S. in Chemistry in August 1950. (The degree was formally awarded in June 1951.) I entered Iowa State College as a graduate student in September 1950, and was assigned to Velmer Fassel’s group. I graduated with a Ph.D. in December 1953, with a thesis on infrared spectroscopy.

I joined Bert Vallee’s Biophysics Research Lab at the Harvard Medical School in January 1954. My first task was to complete the building of a flame spectrometer, built on a Jarrell-Ash Ebert spectrograph. I then used the instrument to study the interaction of Na and K in flame photometry, which was a matter of dispute among chemicalists. I found that the main effect was a strong background across the spectrum, due to recombination of sodium ions and electrons. The first automatic background correction method came out of this. A side project was to confirm a finding by the United Fruit Company of a low sodium content in bananas; as a side result, I found a high potassium content in the fruit. This rather trivial bit of research influenced more people than anything else I did in my career; it even led to the inclusion of dried bananas in the diet of astronauts in orbit, to correct for a loss of blood potassium in zero gravity. Another project was to develop a simple photometer to relieve the workload on our two spectrophotometers. Ralph Theirs and I built it specifically to measure the coenzyme NADH, a common end point in biochemical assays. Our design was a double-beam system with a black-light fluorescent lamp as the light source, a matched pair of detectors made by sawing a barrier-layer cell in half, and a sensitive microammeter. The instrument performed as well at its 350 nm wavelength as a Beckman DU, and it was marketed for several years as the Coenzmeter. My final project there was to isolate a cadmium- and zinc-containing protein named metallothionein. Cadmium was known to accumulate in the kidney, and the hope was that finding a specific protein containing the element would give a clue to its purpose. Fifty years, several thousand publications, and five international conferences later, the exact role of the protein is still unknown. A very important event during my stay in Boston was meeting Miriam Kagan, a Cantabrigian; we married in 1955, and have four children and seven grandchildren.

The stay at Harvard satisfied my inclination to pursue diverse areas of science, which was encouraged by George Hammond at Iowa State. But Harvard Medical was a dead end for me unless I went back to school to earn an MD. So in mid-1957, I joined Bourdon Scribben’s Spectrochemical Analysis Section at the NBS Division of Analytical Chemistry. Bourdon gave me almost total freedom to choose a research topic. In Vallee’s lab, Kei Fuwa had worked on a high-temperature cyanogen-oxygen flame source, and I decided to take the next step by making a DC-arc act like a flame. The result was the DC plasma jet. I began to use computers while defining the properties of this excitation source. When the first time-sharing computers became available, Stan Rasberry and I set up the first terminal in the Analytical Chemistry Division. The ability to use computers for common tasks, such as replacing the analog computation methods that had prevailed in spectrochemical analysis since the 1920s, soon proved to be a step forward; it not only saved time, it improved the accuracy and precision of analysis. I concentrated more on computer applications, which led me to think about what would be possible if one could measure the full UV/Vis spectrum photoelectrically, and how that could be done. The result was the idea to combine an echelle monochromator with a television-tube detector, connected to a computer. I could not get the support at NBS to pursue this idea.

Tomas Hirshfeld had similar thoughts at Block Engineering, and in 1969 I left NBS for that company. At the time, they were developing the FTS-14 IR spectrophotometer, and the echelle-TV spectrometer would be the next breakthrough product. Product design went smoothly, and the FTS-14 did attract a great deal of attention when it was introduced. But the initial sales were slow, in part because of the state of the economy at the time. Block Engineering was forced to put off building the prototype of the emission spectrometer indefinitely, and I decided not to hang around waiting. (They never were able to pick up the project again, and it was years before this kind of spectrometer was commercialized, with great success.)

My next, and last change of employment, was Technicon. The company had brought out the first automated clinical chemistry system in 1957, and Ralph Theirs bought one for the clinical chemistry lab at the Peter Bent Brigham Hospital, which he supervised in his spare time while he did research in Vallee’s lab. In the next twelve years, Technicon’s automated analyzers changed medical practice by providing accurate blood test results quickly.
Michael Morris

Michael Morris is professor of chemistry at the University of Michigan and an affiliated member of the university’s Biomedical Engineering faculty, its Comprehensive Cancer Center and its Core Center for Musculoskeletal Research. He presently serves on the editorial boards of Applied Spectroscopy, Journal of Biomedical Optics and Calcified Tissue International. His honors include the ACS Division of Analytical Chemistry Award in Spectrochemical Analysis, the ANACHEM Award, the Society for Applied Spectroscopy New York Section Gold Medal and Meggers Award, the Charles Mann Award in Applied Raman Spectroscopy, and several University of Michigan awards.

His research interests include Raman spectroscopy and Raman imaging. He is a pioneer in the analytical applications of Raman spectroscopy, particularly in its uses in microscopy and imaging. He has made important contributions to Raman spectroscopic instrumentation based on holographic and liquid crystal optics and has been a leader in development of computational techniques for multivariate Raman image processing and three-dimensional Raman imaging. He has worked on applications of Raman microspectroscopy and imaging to materials as diverse as mineralized tissue and synthetic polymer blends. He was also the first to do Raman-detected capillary electrophoresis and the first to do Raman-detected electrophoresis in a microchip. He was among the leaders of the first wave of coherent Raman spectroscopy and developed successful methods for coherent spectra free of non-resonant background.

Morris has been an active researcher in biomedical Raman spectroscopy for over 25 years. His contributions include physical biochemical studies of flavoproteins, bile pigments and neurotransmitters. In the last several years his laboratory has led the development of Raman spectroscopy for study of musculoskeletal tissues. He and his co-workers have published on bone biomechanics, structure/function relationships in mouse models for genetic disorders, mechanisms of tissue mineralization and non-invasive spectroscopic assessment of bone quality.

Kay Niemax

Prof. Dr. Kay Niemax is Director at ISAS - Institute for Analytical Sciences in Dortmund (Germany). He studied physics, chemistry and mathematics at the University of Kiel (Germany) and received his Diploma and Ph.D. in physics from the Institute of Experimental Physics at Kiel University in 1970 and 1972, respectively. In 1979 he became a lecturer in physics (Habilitation) and in 1984 professor in Kiel. 1979-1980 he was a Visiting Fellow at JILA in Boulder (Colorado), one of the worldwide leading research institutes in atomic and molecular physics. 1985 he became the head of the Elemental Analysis Department at Institute of Spectrochemistry and Applied Spectroscopy in Dortmund. In 1993 he moved to Stuttgart (Germany) where he took over the Chair in Physics of the University of Stuttgart-Hohenheim. Since 1997 he is a director at ISAS and professor for Physical-Chemical Analysis at the Faculty of Physics of the University of Dortmund.

From 1970 to 1985 the major research interests of Prof. Niemax were in the field of plasma and laser physics, laser spectroscopy of atoms and small molecules, spectral line broadening and atomic collisions. In particular, the laser spectroscopic technique to derive level isotope shifts of atoms from highly resolved Rydberg series lines and the investigations of pressure broadening and shift of Rydberg levels are well respected in the community. Since 1985 Prof. Niemax is working in the field of spectrochemistry and applied spectroscopy. He is developing new laser based techniques for chemical analysis of solid, liquid and gaseous samples. His name is closely connected with the development of new techniques for ultra trace analysis by diode laser absorption and laser ablation of solid samples.

Prof. Niemax has published over 220 papers in peer reviewed international journals and made numerous scientific contributions to proceedings and books. He gave more than 100 talks (plenary, keynote or invited) at international conferences and many invited talks at universities and research institutes in Germany and abroad. He is serving as reviewer for many funding agencies in Germany and abroad, such as DFG, EC, NSF and DOE, and the major scientific journals.
FELLOWS AWARD, continued
Recognizes individual members for their outstanding service to the field of spectroscopy.

Edward S. Yeung
Edward Yeung received his A.B. in chemistry from Cornell University and his Ph.D. in Chemistry from the University of California at Berkeley. Since then, he has been on the chemistry faculty at Iowa State University, where he is currently Robert Allen Wright Professor and Distinguished Professor in Liberal Arts and Sciences. His research interests span both spectroscopy and chromatography. He has published in areas such as nonlinear spectroscopy, laser-based detectors for chromatography, capillary electrophoresis, trace gas monitoring, single-cell and single-molecule analysis, DNA sequencing, and data treatment procedures in chemical measurements. He is an Associate Editor of Analytical Chemistry. He served on the editorial advisory board of Progress in Analytical Spectroscopy, Journal of Capillary Electrophoresis, Mikrochimica Acta, Spectrochimica Acta Part A, Journal of Microcolumn Separations, Electrophoresis, Journal of High Resolution Chromatography, Chromatographia and Journal of Biochemical and Biophysical Methods. He was awarded an Alfred P. Sloan Fellowship, was appointed Honorary Professors of Zhengzhou University, Zhongshan University, Xiamen University and Hunan University, and was elected Fellow of the American Association for the Advancement of Science. He received the ACS Division of Analytical Chemistry Award in Chemical Instrumentation, 4 separate R&D 100 Awards, the Lester W. Strock Award, the Pittsburgh Analytical Chemistry Award, the L. S. Palmer Award, the ACS Fisher Award in Analytical Chemistry, the Frederick Conference on Capillary Electrophoresis Award, the Eastern Analytical Symposium Award in Analytical Chemistry, the ACS Award in Chromatography, the International Prize of the Belgian Society of Pharmaceutical Sciences, the Eastern Analytical Symposium Award in Separation Science, the Ralph N. Adams Award in Bioanalytical Chemistry, the Golay Award, and the Chicago Chromatography Discussion Group Merit Award.

SAS Members are Cordially Invited to Attend the SAS Wine and Cheese Awards Reception
Tuesday, October 16, 2007 7:00 p.m.
Memphis Marriott Hotel Heritage Ballroom

This is a member’s only event.
To join the Society, please visit booths 17/18 in the convention center.
Richard Mendelsohn obtained his Ph.D. in 1972 in Biophysical Chemistry from MIT under the direction of Professor Richard C. Lord. His postdoctoral experience was with Professor Maurice Wilkins (Biophysics, King's College, London) and Dr. H. J. Bernstein (Spectroscopy, NRC-Ottawa, Canada). He moved to Rutgers University, Newark College in 1976 and is currently Professor of Chemistry. Dr. Mendelsohn has directed or currently directs 28 Ph.D. and 10 Masters students. He has published over 180 papers and 20 book chapters. His work has been funded for over 30 consecutive years by NIH, NSF, NATO, and PRF. In addition, he has received substantial industrial support, both from Europe and North America. He reviews extensively for most major Biochemistry, Biophysics and Spectroscopy Journals, and has consulted for several pharmaceutical and other companies. He has served on several NIH study sections, and presented over 100 invited lectures at meetings and Universities worldwide. His current research centers around two major themes as follows (i) the use of vibrational spectroscopy, microscopy and imaging to study skin pharmacology and biochemistry and (ii) IR spectroscopic studies of monolayer films related to pulmonary surfactant.

Bozena B. Michniak-Kohn obtained her Ph.D. in Pharmacology in 1980 from Leicester Polytechnic, Leicester, U.K now renamed the DeMontfort University. Postdoctoral experience was gained with Profs. N. Bodor (University of Florida) and B. Barry (University of Bradford, U.K). She returned in 1986 to the U.S. as Assistant Professor, College of Pharmacy, University of South Carolina, Columbia SC. In 1998 she became tenured full Professor and Director of the Transdermal and Topical Drug Delivery Laboratory. In 2000 she joined the Department of Pharmacology and Physiology at the University of Medicine and Dentistry of New Jersey-New Jersey Medical School, Newark, NJ as Associate Professor. In 2005 Dr. Michniak moved to a tenured position as Associate Professor in Pharmaceutics at the Ernest Mario School of Pharmacy, Rutgers-The State University of New Jersey, Piscataway, NJ and is the Director of the Laboratory for Drug Delivery of the New Jersey Center for Biomaterials (NJCBM). Dr. Michniak has directed over 25 Ph.D. students, 6 Masters students, and 200+ undergraduates and the work resulted in over 260 abstracts, 3 patents, 25 book chapters, and more than 85 papers. The work is funded from both federal (NIH/NSF/DoD/US Army Natick/DARPA) and industrial funds. She is a reviewer for over a dozen pharmaceutical and drug delivery journals, is a Consultant to over half a dozen pharmaceutical companies and is an expert in the area of transdermal and topical drug delivery.

David J. Moore is a research director in the global R&D group of International Specialty Products based in Wayne, New Jersey. His research interests are in membrane lipid biophysics, infrared spectroscopy of biological systems (from liposomes to intact cells), and the stabilization and delivery of biological active compounds. Most recently, Dr Moore has collaborated with Professor Mendelsohn's group at Rutgers University on the application of infrared spectroscopic imaging to research dermatology.

Ryan D. Pensack obtained a B.A. in Chemistry from Rutgers, The State University of New Jersey, in Newark, NJ in May of 2006. While at Rutgers he was granted the opportunity to perform experiments under the guidance of Dr. Richard Mendelsohn. These experiments included spectrometric measurements in the infrared region characterizing the kinetics of changes in a naturally occurring lipid system induced by different physical and chemical stresses. This experience led him to where he is currently - The Pennsylvania State University working towards a doctoral degree in Physical Chemistry. Motivated to remain in the field of spectroscopy, infrared in particular, he has recently been endowed with the opportunity to work under the supervision of Dr. John Asbury. Current experiments focus on developing new tools to examine charge carrier dynamics and to control the supramolecular assembly of organic electronic materials as a means to learn how to tailor the properties of the materials for the next generation of organic electronics which include organic solar cells, organic thin film transistors, and high energy density organic dielectrics for energy storage.
LESTER W. STROCK AWARD
Established by the SAS New England section to recognize an author(s) of an outstanding paper or series of papers

Detlef Günther
ETH Zurich

Presentation, Thursday, 8:00 AM, Ballroom C/D

Detlef Günther was born in Köthen, Germany in 1963. He obtained a Diploma degree in Chemistry in 1987 and a Ph.D. degree in Analytical Chemistry from the Martin-Luther-University Halle-Wittenberg under supervision of L. Moenke-Blankenburg in 1990. After carrying out a postdoctoral work in the Institute of Plant Biochemistry Halle (Development of analytical methods to characterize heavy metal-binding proteins using HPLC-ICP-MS) he joined the group of H.P. Longerich at the Memorial University of Newfoundland, Canada. From 1995 until 1998 he joined the group of C.A. Heinrich at the Institute of Isotope Geology and Mineral Resources at ETH Zürich. In 1998 he was appointed as Assistant professor in the Laboratory of Inorganic Chemistry at the ETH Zürich and since July 2003 he is Associate professor for Trace Element and Micro Analysis. He is recipient of the Ruzicka Award (2002), the European Award for Plasma Spectrochemistry (2003) and the Fresenius Award (2007).

His research program focuses on fundamental and applied studies in Inductively Coupled Plasma-Mass Spectrometry (ICP-MS) and Laser Ablation-Inductively Coupled Plasma-Mass Spectrometry (LA-ICP-MS), which includes studies on laser-sample interaction, aerosol transport, plasma-related excitation processes. The fundamental understanding of UV-ns and UV-fs laser ablation in combination with Q-ICP-MS, SF-ICP-MS, ICP-TOFMS and more recently MC-ICP-MS as well as alternative excitation sources has been demonstrated on a wide variety of applications, e.g. analyses of fluid inclusions, gemstones, metals, minerals, ceramic and other industrial materials.

ELLIS R. LIPPINCOTT AWARD
Given to honor the memory of Ellis R. Lippincott for significant contributions to vibrational spectroscopy. The medal is sponsored jointly by the Society for Applied Spectroscopy, the Coblentz Society, and the Optical Society of America.

Jonathan Tennyson
University College London

Jonathan Tennyson is Massey Professor of Physics and Head of the Department of Physics and Astronomy at University College London. He studied at the Universities of Cambridge and Sussex. He was a post-doc at the University of Nijmegen and Daresbury Laboratory before moving to UCL as a "New Blood" Lecturer. He Chairs the Chemical and Molecular Physics section of the European Physical Society and a IUPAC task group "A database of water transitions from experiment and theory". He was awarded the 2005 Sir David Bates Prize of the UK Institute of Physics.

Dr. Tennyson’s researches a range of topics in chemical physics dealing with both the underlying theory and applications of calculations of molecular spectra and collision problems. His group used first principles quantum mechanical calculations to assign an emission spectrum of H3+ in the Jovian ionosphere which led to a new observational handle on these systems. More recently he led to a major breakthrough in understanding the spectra of water and the assignment of a very congested and complicated spectrum of water recorded in sunspots, and the development of a comprehensive ab initio model predicting its spectrum.
COBLENTZ SOCIETY CLARA CRAVER AWARD

The Craver Award is presented annually to an outstanding young molecular spectroscopist whose efforts are in the area of applied analytical vibrational spectroscopy.

Recognizing a young individual under the age of 45, who has made significant contributions in applied analytical vibrational spectroscopy.

Katherine A. Bakeev
GlaxoSmithKline

Presentation, Wednesday, 8:30 AM, Ballroom C/D

Dr. Katherine A. Bakeev is currently a principal scientist with GlaxoSmithKline in King of Prussia, PA. There she is part of the Process Analytical Technology and Chemometrics group within Strategic Technologies, using spectroscopic tools for increased process understanding, and integrating their use within the development group. The scope of her work includes developing methods for process analysis from lab to manufacturing scale. Previously, she was a product specialist with Foss NIRSystems, Silver Spring, MD. In that role, she supported applications of NIR for the pharmaceutical and chemical markets on the Eastern US. She also did work in process analytical technology while working for International Specialty Products, Wayne, NJ from 1995-2000. Her post-graduate career started with AMP Incorporated in Harrisburg, PA. While still a student, she did internships with 3M in St. Paul, MN and for Dow Chemical Company while working on synthetic polymer chemistry research in the laboratory of Prof. Virgil Percec at Case Western Reserve University. Her education is in polymer science and engineering with a BS from Case Western Reserve University (1987) and PhD from the University of Massachusetts at Amherst (1993). Here graduate research under the direction of Prof. Shaw Ling Hsu was in studying polymorphic transitions of ferroelectric copolymers using vibrational spectroscopy, thermal analysis and X-ray analysis. Before starting her graduate studies she was the recipient of a Rotary Foundation Scholarship which allowed her to spend a year in the laboratory of Prof. Paul Rempp at the Institut Charles Sadron in Strasbourg, France where she worked on polymer synthesis and characterization. She also holds a Masters in Technology Management from Stevens Institute of Technology (2001).

Over the years, Katherine has published several papers and presented numerous presentations on the use of NIR. She has taught a course on Process Analytical Spectroscopy at EAS and at the IDRC. She is also the editor of the book “Process Analytical Technology: Spectroscopic Tools and Implementation Strategies for the Chemical and Pharmaceutical Industries.”

Katherine is the current president of the Council for Near Infrared Spectroscopy and a member of the Coblentz Society, the Society for Applied Spectroscopy and the American Chemical Society. She also actively participates in ASTM committees on Pharmaceutical Applications of PAT, and E13 for Molecular Spectroscopy and Separation Science.

FACSS 2009

October 18 – 22, 2009
Louisville Marriott Downtown Hotel
Louisville, KY

Governing Board Chair: Becky Dittmar – ramttidb@yahoo.com
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For many years, the Coblentz Society has encouraged young scientists to pursue studies in spectroscopy by seeking nominations of outstanding students for the Coblentz Student Awards. The awardees receive a copy of the Society’s Deskbook, a certificate, and a year’s membership in the Society. Their names, the names of their faculty advisors, and a brief description of their research appear in the Society’s Newsletter in the August issue of Applied Spectroscopy.

### Awardees

**Heather Brooke**

Heather Brooke began her interest in chemistry at a young age, when she took a chemistry mini-course in 3rd grade. She later earned a BS from Lander University where she received the Chemistry Discipline Award and did undergraduate research with Dr. Lynn DeAnhardt. Shortly after graduating, she obtained a position as a lab technician at Fujifilm in Greenwood, SC. After working there for 3 years, with both chemists and engineers, she decided to apply herself to a new challenge: graduate school. She began her academic adventure in May 2005, working under Dr. Michael Myrick as a Copenhaver Fellow at the University of South Carolina, and officially joined his research group in October 2005. In the past 2 years, she has attended and presented at both FACSS and PittCON, and received 2nd place at the Graduate Student Day Poster Competition (Physical Sciences & Engineering Division) at USC. In addition to her research, she has also been involved in the Society for the Advancement of Chemical Sciences (SACS) and served as treasurer this past year. She also has gained teaching experience by working as a lab instructor at Lander University (2004-2005) for Consumer Chemistry, and as a TA at USC for both General and Physical Chemistry labs.

**Christopher Fox**

My educational background includes a B.S. in biological engineering from Utah State University in 2003, after which I enrolled at the University of Utah in bioengineering where I am currently a Ph.D candidate scheduled for graduation in Fall 2007. Research experience, carried out in the lab of Joel Harris, involves using Raman microscopy to investigate lipid membrane structure and drug-membrane interactions in phospholipid vesicles as well as single-molecule detection of therapeutic peptide binding to lipid membranes using TIRF microscopy. In extracurricular activities, I maintain a strong interest in using science for global health and development: I have initiated a student chapter of Engineers Without Borders at the University of Utah, received a ‘commended essay’ designation from The Lancet/Global Forum for Health Research, and participated with a winning team in the international Mondialogo Engineering Award 2007. After graduation, I will begin employment with the Infectious Disease Research Institute in Seattle, WA to develop and characterize vaccine formulations for global health diseases.

**Brian Loudermilk**

“Mixture Selection Algorithms for Choosing Mixture Calibration Standards”,

*Presentation: Wednesday 10:30, Room L14*

Brian Loudermilk is currently a doctoral candidate at The University of Georgia working under the direction of Prof. James A. de Haseth. Before coming to graduate school, Brian completed his B.S. degree in chemistry at North Georgia College and State University. During his undergraduate career, Brian participated in research on synthesis and characterization of chromium complexes for medicinal applications. This research was under the direction of Profs. Noel A. P. Kane-Maguire and John Wheeler at Furman University. While at NGCSU, Brian earned a number of honors for his achievements in the chemistry program there including the Presidential Scholar Award. In his time in graduate school, Brian has worked on a number of collaborative research projects with Drs. David S. Himmelsbach and Franklin E. Barton II of the United States Department of Agriculture. Brian’s research has focused on application and development of chemometric methods for improved identification of cotton contaminants. His first research project was the development of novel search algorithms for a spectral library of cotton contaminants compiled by the USDA. Brian’s research since that time has focused on other chemometric methods for qualitative and quantitative identification of cotton contaminants. His current work is in the development of an algorithm for selection of mixture calibration standards. Brian’s research interests include chemometrics, vibrational spectrometry, multivariate regression, classification, spectral comparison, and computer programming. While at UGA, Brian has received from the UGA Graduate School a selective assistantship and travel award to present his research. Since entering graduate school, Brian has also been continuously awarded a research assistantship. He is a student member of The Coblentz Society and The Society for Applied Spectroscopy.
PREVIOUS FACSS BOARD AND MEETING CHAIRS

1973
Jeannette Grasselli  Governing Board Chair
1974 – Atlantic City
James White  Governing Board Chair
George Heinz  General
James White  Program
Edward Ruffing  Exhibit
1975 - Indianapolis
James Holcombe  Governing Board Chair
Gerald Wallace  General
James Holcomb  Program
Edward Ruffing  Exhibit
1976 - Philadelphia
Edward Brame  Governing Board Chair
Edward Brame  General
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Douglas Robinson  Arrangements
Edward Ruffing  Exhibit
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Sydney Fleming  Arrangements
Edward Ruffing  Exhibit
1980 - Philadelphia
L. Felix Schneider  Governing Board Chair
Sydney Fleming  General
Theodore Rains  Program
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Edward Ruffing  Exhibit
1981 - Philadelphia
Jack Katon  Governing Board Chair
Robert Barford  General
Mary Kaiser  Program
James Cavanaugh  Arrangements
Peter Keliher  Exhibit
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Sydney Fleming  Governing Board Chair
James Cavanaugh  General
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Matthew O’Brien  Arrangements
Peter Keliher  Exhibit
Mary Kaiser  Governing Board Chair
Matthew O’Brien  General
John LePhardt  Program
D. Bruce Chase  Arrangements
Peter Keliher  Exhibit
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D. Bruce Chase  General
Patricia Rouse Coleman  Program
Fred Corcoran  Arrangements
Peter Keliher  Exhibit
Robert Barford  Governing Board Chair
Fred Corcoran  General
Matthew Klee  Program
Marshall Fishman  Arrangements
Peter Keliher  Exhibit
Ronald Schroeder  Governing Board Chair
Marshall Fishman  General
Alexander Scheeline  Program
Terry Hunter  Arrangements
Edward Brame  Exhibit
Patricia Rouse Coleman  Governing Board Chair
David Coleman and L. Felix Schneider  General
John S. Beaty  Program
Edward Brame  Exhibit
James Cavanaugh  Governing Board Chair
Frank Plankey and John S. Beaty  General
Roger Gilpin  Program
Edward Brame  Exhibit
1989 - Chicago
Alexander Scheeline  Governing Board Chair
Paul Bourassa  General
Robert Michel  Program
Edward Brame  Exhibit
1990 - Cleveland
Nancy Miller-Ihli  Governing Board Chair
Charles Belle  General
Steven Hughes  Program
Edward Brame  Exhibit
1991 - Anaheim
David Coleman  Governing Board Chair
Richard Deming and Constance Sobel  General
James Holcombe  Program
Edward Brame  Exhibit
1992 - Philadelphia
Karmie Galle  Governing Board Chair
Matthew Klee  General
Barry Lavine  Program
Edward Brame  Exhibit
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SOCIETY AND COMMITTEE MEETINGS AND EVENTS

FACSS
All meetings will take place at the Marriott Hotel.

Saturday, October 13, Natchez
1:00 PM Long Range Planning committee

Sunday, October 14, Gatlinburg
7:00 PM Program Committee

Wednesday, October 17, Natchez
9:00 AM 2008 Planning/Budget Committee
10:00 AM Planning/Budget Committee for Reno (2008)
11:00 AM Planning/Budget Committee for Louisville (2009)
1:00 PM Budget and Finance Committee
1:00 PM Web Site Meeting, Memphis

Thursday, October 18, Natchez
1:00 PM Executive Committee
6:30 PM Governing Board Meeting

ASTM
All meetings will take place at the Marriott Hotel, Natchez

Monday, October 15
1:00 – 2:30 PM E13.08 Raman Spectroscopy
2:30 – 4:00 PM E13.10 Molecular Spectroscopic Optical Imaging
6:00 PM Raman Reception, Heritage Ballroom 1/2

COBLENTZ
All meetings will take place at the Marriott Hotel, Memphis

Monday, October 15
8:00 PM Board Meeting

SOCIETY FOR APPLIED SPECTROSCOPY
All meetings will take place at the Marriott Hotel

Sunday, October 14
7:30 AM – 6 PM SAS Executive Committee Meeting, Natchez
12:00 – 1:30 PM SAS Executive Committee Luncheon, Memphis

Monday, October 15
12:00 – 1:30 PM Editorial Committee Meeting/Lunch, Memphis

Tuesday, October 16
12:00 – 1:30 PM Publications Committee Meeting/Lunch, Memphis
4:30 – 6:30 PM SAS Governing Board Meeting, Natchez
7:00 – 9:00 PM SAS Wine and Cheese Reception, Heritage Ballroom 3/4 (members only)
### FACSS EXHIBITORS

<table>
<thead>
<tr>
<th>Company Name</th>
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<td>ICP Information Newsletter, Inc.</td>
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**Entrance**
ABB Analytical
585 boul. Charest E., Ste 300
Quebec, PQ, G1K 9H4 CANADA
Phone: 418-877-2944
www.abb.com/analytical

ABB Analytical capabilities embrace a large portfolio of laboratory, at-line and process FTIR and FTNIR analyzers, capable of performing real-time analysis of the chemical composition and/or physical properties of samples or process streams. The company is a market leader in FTIR and FTNIR in terms of technical innovation. Its knowledge has brought the new MB3000 FTIR spectrometer and Horizon MB™ software. The configuration of ABB’s MB3000 emphasizes simplicity at low cost while maintaining surprising versatility. There are two versions of the new general-purpose laboratory FTIR. The MB3000 is the MID-IR version and the MB3600 is the Near IR version. Combined with the new Horizon MB™ software, the MB3000 and MB3600 facilitate the acquisition, processing and analysis of samples as well as result management.

Advanced Chemistry Development Inc. (ACD/Labs)  Booth 2
110 Yonge Street, 14th FL
Toronto, ON, M5C 1T4 CANADA
Phone: 416 368 3435
www.acdlabs.com

Advanced Chemistry Development, Inc., (ACD/Labs) provides analytical scientists and managers with software for spectroscopic data handling and interpretation, chromatographic method development, impurity identification, material science studies, open-access laboratories, and more. Over the past decade, ACD/Labs has developed one of the most comprehensive integrated software for NMR, MS, HPLC, Raman, and IR on the market. Characterized by easy-to-use chemometric applications, processors, and managers, ACD/Labs’ molecular spectroscopy software is actively used in both industrial and academic research facilities around the world.

Ahura Corporation  Booth 48
46 Jonspin Road
Wilmington, MA 01887
Phone: 978 642 2547
www.ahurascientific.com

Ahura Scientific, Inc. develops rugged, ultra-compact optical systems for the detection, identification and authentication of unknown and suspect substances. Customers include the homeland security, life sciences, industrial and medical markets. Ahura’s TruScan is a handheld system for rapid, accurate material identity verification, offering incomparable ease of operation in a tough, lightweight form factor. TruScan was designed to meet the stringent requirements of pharmaceutical and industrial manufacturing operations. Using Raman spectroscopy, TruScan can be used to authenticate a variety of sample types, including incoming raw materials, intermediates and finished product. Ahura’s FirstDefender is used for immediate identification of unknown solid and liquid chemicals. It was designed to meet the needs of first responders who require accurate, fast identification to inform their remediation efforts. Hazmat and law enforcement teams, military organizations and government agencies use FirstDefender for identification of white powders, liquid spills, explosives, narcotics and more.

American Chemical Society, Analytical Division  Booth 74
1155 16th Street NW
Washington, DC 20036
Phone: 202 872 4544
www.acs.org

The American Chemical Society is a self-governed individual membership organization that consists of more than 160,000 members at all degree levels and in all fields of chemistry. The organization provides a broad range of opportunities for peer interaction and career development, regardless of professional or scientific interests. The programs and activities conducted by ACS today are the products of a tradition of excellence in meeting member needs that dates from the Society's founding in 1876. For more information, visit the ACS Website at www.chemistry.org.

Ametek Process Instruments  Booth 55
150 Freeport Rd.
Pittsburgh, PA 15238
Phone: 412 826 4433
www.ametikpi.com

AMETEK Process Instruments is a leader in process analyzers and measurement and control instruments. AMETEK manufactures the ProMaxion process mass spectrometers and the IPS-4 product line which is available in UV-VIS and NDIR configurations. AMETEK can customize process solutions based on specific application needs. These products are low maintenance and custom designed to improve product quality. Focused on a wide range of markets including PAT associated processes, AMETEK serves most of the world leaders in pharmaceutical development and manufacturing.

Analytik Jena USA, LLC  Booth 70
26009 Budde Rd, Ste D-100
The Woodlands, TX 77380
Phone: 281 367 6130
www.analytik-jena.com

Analytik Jena is the leading German manufacturer of analytical instrumentation in Spectroscopy. As a trusted vendor in industrial and scientific laboratories in more than 90 countries, Analytik Jena is a leading manufacturer of AAS, UV-VIS, TOC/TOX and Elemental analyzers. With more than 150 years of experience in the field of optical systems, Analytik Jena was also the first to launch a Continuum Source Atomic Absorption instrument. Our long tradition in developing high quality and precision analytical systems is what makes Analytik Jena one of today’s most innovative companies.
EXHIBITOR DESCRIPTIONS

Aspectrics, Inc. 
6900 Koll Center Pky. Ste 401
Pleasanton, CA 94566
Phone: 925 931 9270
www.aspectrics.com

Aspectrics Inc. manufactures rugged, reliable and sensitive At-line and On-line process Analyzers based on the patented Encoded Photometric Infrared (EP-IR) and Near Infrared (EP-NIR) technology. Aspectrics unique Encoded Photometric technology is used for at-line quality control, on-line process monitoring and remote field applications. Aspectrics MultiComponent™ analyzers were designed to scan at ultra-fast rates of 100 scan per second to provide real-time results for making critical process decisions. A small footprint, Ethernet connectivity and industry standard communication protocols enable quick and easy system integration in even the most demanding environments. Aspectrics EP-IR technology has been selected by R&D Magazine as one of the Top 100 most technologically significant products introduced in 2006. Markets Served: BioFuels Analysis•Specialty Gases•Petrochemical/Chemical•Continuous Emissions Monitoring (CEMS)•Kinetics•Environmental•Automobile Emissions Food / Beverage

B&W Tek, Inc. 
19 Shea Way, ste 301
Newark, DE 19713
Phone: 302 368 7824
www.bwtek.com

B&W Tek is a leader in developing and manufacturing biophotonic instrumentation. As a total solution provider, we serve Life Science and Biomedical communities by providing OED and OEM services. B&W Tek is dedicated to making the highest performance-to-cost products to meet customer's needs. Products include high power and broadband SLD/SLED sources, diode-pumped solid-state lasers, and high power diode/fiber lasers, UV/VIS/NIR/fluorescence/Raman spectrometers. ISO 9001 and ISO 13485 certified. For more information visit: www.bwtek.com

Bio-Rad Laboratories, Informatics Div 
Two Penn Center Plaza, Ste 800
1500 John F. Kennedy Blvd
Philadelphia, PA 19102-1737
Phone: 267 322 6937
www.knowitall.com

Leading provider of spectral databases & chemistry software. The company's KnowItAll Informatics System offers a fully integrated environment with flexible and expandable software and database solutions for spectroscopy (MS, NMR, IR, Raman, and spectral data management); cheminformatics; chemometrics, metabolomics. Award-winning solutions include:
- Spectral data management & mining, search, processing, analysis
- Bio-Rad/Sadtler™ Spectral Libraries
- Now includes Chemometrics & a patent-pending multi-spectrum visualization tool
- Desktop, department-wide, site-wide, global solutions
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<td>Iselin, NJ 08830</td>
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<td>Phone: 732-346-3026</td>
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<td><a href="http://www.spectroscopyonline.com">www.spectroscopyonline.com</a></td>
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<td>Spectroscopy is the only publication dedicated to the spectroscopic sciences, providing peer-reviewed technical and applications-oriented information to the largest audited circulation of influential spectroscopists in the United States. With its focus on cutting-edge techniques like Raman, X-ray, MS, ICP-MS, FT-IR, and the multitude of other hyphenated techniques that continue to grow in popularity, Spectroscopy’s unique editorial content enables substantial productivity improvement in the laboratory, while facilitating the exchange and flow of information throughout the scientific community.</td>
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<tr>
<td><strong>Thermo Scientific, Inc.</strong></td>
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<tr>
<td>5225 Vernona Road</td>
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<tr>
<td>Madison, WI 53711</td>
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<tr>
<td>Phone: 608 273 6822</td>
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<td><a href="http://www.thermo.com">www.thermo.com</a></td>
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<td>Count on Thermo Scientific for a range of high-end analytical instruments, chemistry and consumable supplies, reagents, laboratory equipment, software and services that enable integrated laboratory workflow solutions. Thermo Scientific is part of Thermo Fisher Scientific. Thermo Scientific instruments and solutions for elemental analysis range from AA and ICP to ICP-MS and high resolution inorganic mass spectrometry to Spark-OES and XRF. Our elemental analysis solutions combine reliability, superior performance, versatility and ease-of-use to solve even complex problems. In addition, we offer high performance FT-IR, IR microanalysis and imaging, and dispersive Raman technology that allow researchers the flexibility to build custom experiments and complete demanding analyses of molecular structures. Support this technology with our proven Laboratory Information Management Systems (LIMS) and Chromatography Data Systems (CDS) to help you lower costs, increase productivity and maximize uptime with our 24/7 worldwide support and service staff. For more information, visit <a href="http://www.thermo.com">www.thermo.com</a>.</td>
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<td><strong>Torsana Laser Technologies A/S</strong></td>
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<tr>
<td>Lyngbaekergade Alle 2A</td>
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<tr>
<td>Copenhagen 2990, Denmark</td>
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<td>Phone: 45 45560056</td>
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<td><a href="http://www.torsanalaser.com">www.torsanalaser.com</a></td>
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<td>Leaders in Light - Perfect for Raman Torsana Laser Technologies manufacture superior, application-specific laser systems for photonic analysis instruments. Our Starbright lasers are renowned for their unprecedented performance and quality. The lasers come in wavelengths ranging from 760 to 1080 nm, with various output powers up to 1 W. They are used in the most demanding research environments, particularly in Japan and the US, due to their low ASE, narrow line width, strong output power, and excellent wavelength stability.</td>
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<td><strong>Varian, Inc.</strong></td>
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<tr>
<td>3120 Hansen Way D-111</td>
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<tr>
<td>Palo Alto, CA 94304</td>
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<td>Phone: 650 424 4962</td>
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<td><a href="http://www.varian.com">www.varian.com</a></td>
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<td>Varian, Inc. is a world leader in scientific instruments' technologies and a major supplier of analytical solutions and nuclear magnetic resonance (NMR) systems. Varian, Inc. serves environmental, industrial, chemical / petrochemical, food / agricultural, metals / mining, pharmaceutical, life science, and heath care customers. We will be presenting our latest range of FTIR, UV, AA, ICP-OES, and ICP-MS products. To learn more about our exciting new products - the 700-ES series of simultaneous ICP-OES instruments, the 810/820-MS ICP-MS with unique CRI interference management technology, and the Varian FastImageIR FTIR Imaging system which produces thousands of full range FTIR spectra in seconds - Please visit us at Booth #28.</td>
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<td><strong>WITec GmbH</strong></td>
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<tr>
<td>101 Tomaras Ave.</td>
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<tr>
<td>Savoy, IL 61874</td>
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<tr>
<td>Phone: 217 351 9705</td>
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<td><a href="http://www.witec-instruments.com">www.witec-instruments.com</a></td>
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<td>WITec is a manufacturer of high resolution optical and scanning probe microscope solutions for scientific and industrial applications. A modular product line allows the combination of different microscopy techniques guaranteeing highest flexibility for a wide range of applications. WITec will showcase the alpha300 microscope generation. This series includes the Confocal Raman Imaging Microscope alpha300 R providing the ability to image the chemical properties of a sample at a resolution down to 200 nm. At each image pixel a complete Raman spectrum can be acquired in less than 10 ms. The resulting multi-spectrum file can then be analyzed with respect to various peak characteristics in order to generate high-resolution Raman images. Combined with the Atomic Force Microscopy capabilities of the alpha300 R, the chemical information can be linked with topographical surface structures. Images with an optical resolution beyond the diffraction limit can be easily obtained with the alpha300 S.</td>
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American Pharmaceutical Review, now in its 10th year, is a publication dedicated to bringing the latest trends and developments in the process of pharmaceutical and biopharmaceutical manufacturing. We regularly feature articles on the following topics, Polymorphism, Raman, NIR, PAT, and Chirality...just to name a few.

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Visit us at Booth #60

*Subscriptions are free to those within the United States and Canada. Subscriptions may be purchased for $135.00 USD ($85.00 for website access only) for anyone outside the United States and Canada.
ANALYTICAL RAMAN SPECTROSCOPY
See on site registration form for cost.
Sunday 8:00 – 11:30 AM, convention center Room 201/202
The course will provide an overview of modern Raman spectroscopy beginning with an introduction to Raman scattering and the differences between IR and Raman spectra. It will include discussion of sampling, calibration, data analysis methods (pre-treatments and modeling approaches), and successful application developments. Modern instrument configurations and configuration choices will be covered. The course will include a thorough introduction to the major approaches to sample illumination and spectrum collection, emphasizing fiber optic probes and Raman microprobes. Raman imaging will be briefly discussed. The applicability of and successes with Raman will be surveyed with numerous applications examples. This ½ day course will be split 50 / 50 between a) Raman practical considerations and theory and b) applications. Course attendees who wish to either receive a solid background in Raman and current applications information prior to or those who want a follow-up opportunity with hands-on instrument experience will be able to receive this by electing this course and the Hands-on Raman Workshop scheduled for Sunday afternoon. Attendees who elect to attend this course will be automatically registered for the Hands-on Raman Workshop held Sunday afternoon.

HANDS-ON RAMAN
Exhibitors, Instrumentation Company Representatives
Sunday, No charge
12:30 – 1:30 PM – overview, convention center – Room 201
1:30 – 4:00 PM – Hands On, convention center – Ballroom C
Class attendees will get a basic introduction to Raman Spectroscopy and Raman Spectroscopy techniques followed by hands-on experience with a variety of Raman instrumentation from FACSS exhibitors: HORIBA Jobin Yvon, WITec, Renishaw, B&W Tek, Kaiser Optical Systems, Ahura Scientific, Delta Nu; Ocean Optics, PerkinElmer, Centice, Lambda Solutions, Thermo Scientific, JASCO, Enwave Optronics, and Headwall Photonics.

HANDS-ON IMAGING
Exhibitors, Instrumentation Company Representatives
Sunday, No charge
1:30 – 2:30 PM – overview, convention center – Room 201
2:30 – 5:00 PM – Hands On, convention center – Ballroom C
Spectroscopic imaging, now more generally referred to as chemical imaging, has made tremendous strides in recent years on its path from a relatively novel technology through laboratory R&D instrument and more recently as a QA/QC tool and even as a process analytical technology. This workshop, taught by a number of experts in the field, will aim to introduce the concept of chemical imaging and demonstrate its value for understanding and quantifying a variety of spatially complex chemical and biological systems. We will discuss how a number of chemical imaging systems (Raman, NIR, IR, THz, etc.) work and the kind of information that can be derived from each technology platform. Part of the workshop will also include a ‘hands-on’ instrument demonstration during which a variety of chemical imaging systems and data processing software will be available from a variety of manufacturers. Participating companies include: Malvern Instruments, Varian, PerkinElmer, Witec, Bruker, Horiba Jobin Yvon

HANDS-ON MASS SPECTROMETRY
Exhibitors, Instrumentation Company Representatives
Sunday, No charge
1:00 – 4:30 PM – convention center – Room 204/205
Mass spectrometry continues to be one of the most widely applied analytical methods to identify, characterize, and quantify chemical species. Significant advances have been made in ways to study “biochemical” and “biologically important” molecules. New applications in process mass spectrometry, specialty gasses, biomarker discovery to microbial fingerprinting, continue to be announced. This workshop will begin with a 90 minute seminar which will review some basic principles of why/how MS works, ionization methods, principle analysis technologies, and the strengths/differences of each. A summary of both traditional and cutting edge mass spectrometry applications will be presented. The majority of the workshop time will be devoted to “hands-on” demonstrations by FACSS exhibitors.
CHEMOMETRICS IN MASS SPECTROMETRY
Barry M. Wise, Willem Windig, Jeremy M. Shaver; Eigenvector Research
See on site registration form for cost (includes computer use).
Monday, 9:00 AM – 5:00 PM, Marriott Hotel, St. Louis
Chemometrics in Mass Spectrometry covers methods for dealing with the discontinuous spectra produced by MS. Hyphenated instruments, such as GC/MS and LC/MS are also discussed. Participants will learn how overlapping peaks, such as resulting from GC/MS, can be resolved into separate peaks for each of the components and their associated single component spectra using self modeling mixture analysis. The newly developed technique has the same functionality as the well known SIMPLISMA method. Methods for extracting high quality mass chromatograms from complex data such as resulting from LC/MS with electro spray will also be covered. Methods that extract small differences between very similar samples, such as different batches of the same material, will also be discussed. The course includes hands-on computer time for participants to work example problems using PLS_Toolbox.
Self-modeling Mixture Analysis and Self-modeling Curve Resolution
• Pure variable method
• Pure spectrum method
• CODA (Component Detection Algorithm)
• the Durbin and Watson criterion
• extracting high quality mass chromatograms
• COMPARELCMS for Extracting Differences Between Similar Samples
• A new simpler algorithm
• Self modeling image analysis
• Conclusions
• Homework and Example Problems

PROFESSIONAL ANALYTICAL CHEMISTS IN INDUSTRY: A SHORT COURSE FOR UNDERGRADUATE STUDENTS
Diane Parry, The Procter & Gamble Company
Monday, 9:00 AM – 5:00 PM, No charge, Marriott Hotel, Knoxville
The objective of this workshop is to provide insight into the work of industrial analytical chemists. In a highly interactive forum, participants will explore the role of analytical chemist as problem solver using real problems encountered at Procter & Gamble. Participants have an opportunity to try their hand at solving real consumer product chemistry problems, and to get answers to some of their questions on industrial chemistry careers. The course is targeted at third-year undergraduates who have had some exposure to instrumental analysis; however, new undergraduate students, graduate students, and chemistry teachers have all reported that they found the short course highly beneficial. For additional information go to: www.pg.com/science/prof_chemists.jhtml.

INTRODUCTION TO SUPERCRITICAL FLUID CHROMATOGRAPHY
Jennifer L. Lefler, Thar Technologies, Inc.
See on site registration form for cost.
Monday, 9:00 AM – 1:00 PM, Marriott Hotel, Jackson
As the environment for discovering and developing potent pharmaceuticals becomes more competitive and more costly, companies are looking to identify potential lead compounds earlier in the process. Employing purification methods to facilitate the route to candidate selection is gaining in popularity. Technologies, such as preparative liquid chromatography (LC), have yielded in the isolation of impurities from potential lead molecules. Yet these techniques involve tremendous man hours and consume/generate large volumes of hazardous, liquid waste. An attractive alternative to preparative scale LC is a closely related technology, Supercritical Fluid Chromatography (SFC). The bulk of the mobile phase is carbon dioxide (CO2), which is highly tunable in its chromatographic properties and is easily removed from the collected fraction. Supercritical CO2 also demonstrates lower viscosity than traditional LC solvents, thereby enabling geometric scalability with reduced penalty of back pressure or pressure drop across a column, and follows the basic chromatographic principles understood by most end-users. This course will discuss the importance of pumping and regulating supercritical carbon dioxide in its chromatographic instrumentation and to demonstrate the scalability from conduct method development to purification for chiral and achiral matrices. We wish to demonstrate through several applications of the ease of use of the technology, as well as, demonstrate its economic and environmental attractiveness.

CHEMOMETRICS WITHOUT EQUATIONS (OR HARDLY ANY) – HANDS ON
Barry M. Wise, Jeremy M. Shaver, Willem Windig; Eigenvector Research, Inc.
See on site registration form for cost (includes computer use).
Tuesday and Wednesday, 9:00 AM – 5:00 PM, Marriott Hotel, St. Louis
Chemometrics without Equations concentrates on two areas of chemometrics: 1) exploratory data analysis and pattern recognition, and 2) regression. Participants will learn to safely apply techniques such as Principal Components Analysis (PCA), Principal Components Regression (PCR), and Partial Least Squares (PLS) Regression. Examples will include problems drawn from process monitoring and quality control, predicting product properties, and others. The target audience includes those who collect and/or manage large amounts of data that is multivariate in nature. This includes bench chemists, process engineers, and managers who would like to extract the most information from their measurements. The course will finish with a short section on how to apply these models for online predictions. Multivariate Statistical Process Control and inferential sensing. Students will work problems using MATLAB and PLS_Toolbox on computers provided (maximum of two students per computer).

PRACTICAL APPLICATIONS OF LCMS FOR SMALL MOLECULES
Michael P. Balogh, Waters Corporation
See on site registration form for cost.
Tuesday, 9:00 AM – 5:00 PM, Marriott Hotel, Knoxville
A one day course introduces the most commonly applied HPLC-to-mass spectrometry techniques and examines in detail the most widely used related technologies. High throughput, high sensitivity and ease-of-use considerations are illustrated with applications from industrial and environmental analyses as well as pharmaceutical interests. Course materials include video aids and a wide variety of practical applications to demonstrate ionization techniques and components while examining what makes an LC/MS method successful and where some of the common errors are made. An extensive Glossary as well as reference materials created specifically for LC/MS practice is included.
TERAHERTZ PULSED SPECTROSCOPY AND IMAGING
Phil Taday, TeraView Limited

See on site registration form for cost.

Tuesday, 9:00 AM – 1:00 PM, Marriott Hotel, Jackson

Working in the terahertz region has long been problematic due to weak sources and insensitive detectors. However, recent technological advances have brought working in this region of the electromagnetic spectrum into the spotlight again after many years of neglect. Companies like TeraView Ltd. are now developing instrumentation that can be used outside a terahertz research laboratory and that requires no user intervention. This course will cover the generation and detection techniques used in terahertz pulsed technology. It will also glimpse into the future by looking at developments in new areas, such as, terahertz quantum cascade lasers. The course will then cover the recent developments in spectroscopy, and will specifically look at the applications in the pharmaceutical industry. Of rapidity growing interest is the application of terahertz radiation in area of homeland security - the course will review developments in this area. Using the fact that terahertz beams are generated at point sources and are therefore easy to manipulate; the final part the course will cover recent advancements in medical mapping applications.

UV-VISIBLE-NIR AND IR MICROSCOPY FOR FORENSIC SCIENCE
Mary Carrabba, Southern Oregon University and Paul Martin, CRAIG Technologies

See on site registration form for cost.

Wednesday, 9:00 AM – 5:00 PM, convention center, Room 204

Most forensic laboratories use an FT-IR microscope for the analysis of trace evidence. In addition, many forensic labs also have (or are budgeting for) a UV-visible-NIR microspectrophotometer for the analysis of fibers and paints. There are, however, many more applications for molecular microspectroscopy in the forensic sciences. This workshop will cover the types of samples that can be analyzed, basic optics and spectroscopy, sample preparation techniques, advanced instrument usage techniques, and advanced data analysis techniques. While this class is designed for the forensic practitioner, others interested in molecular microspectroscopy will find the material of benefit as well.

ATTACK THE VARIANCE: AN INTRODUCTION TO ROBUST METHOD DESIGN
Drew Manica and Nancy Jestel; SABIC Innovative Plastics

See on site registration form for cost (includes computer use).

Wednesday, 9:00 AM – 5:00 PM, convention center, Room 202

This workshop will cover statistical design strategies (DOE & Robust Design) for building robust new methods and improving existing methods. Learn how critical experimental factors can be identified and controlled for measurement improvement as well as how deliberate experimental design can capture variability to produce a more robust measurement. Robust design methodologies accommodate variability present in the experimental factors themselves and in the measurement process in such a way that undesirable variation of the final result is minimized. Consequently, both an optimal and robust measurement system can be developed simultaneously. Hands-on breakout sessions will include the use of statistical software.

INDUCTIVELY COUPLED PLASMA-MASS SPECTROMETRY (ICP-MS): ADVANCED TOPICS
R. S. Houk, Ames Laboratory USDOE, Iowa State University

See on site registration form for cost.

Wednesday, 1:30 – 5:30 PM, convention center, Room 201

This course is meant for the experienced ICP-MS user, or someone who has completed the Introduction course.

Course Topics:
- Fundamentals of Ion Extraction
- Micronebulizers & Solvent Removal
- Droplets, Particles & Noise in the ICP
- Collision Cells
- Magnetic Sectors - Applications
- Multicollector Instruments for Isotope Ratio Measurements
- Quadrupoles in Alternate Stability Regions
- TOF Mass Analyzers
- Speciation by GC, LC and CE with ICP-MS
- Instrument Survey
FACSS EMPLOYMENT BUREAU

The FACSS Employment Bureau is now online so you can manage your employment efforts anywhere you can connect to the internet! The Employment Bureau is a free service to both job seekers and employers that provides job and applicant listings, message boards, and interviewing booths.

How to register: From the FACSS website (www.facss.org), click on Employment in the top menu. You can create a Job Target account to manage resumes, search employment opportunities and set up personal job alerts. Post your resume online, anonymously if desired, and create a job alert to email new postings directly to your in-box.

Before the conference:
Search available jobs and resumes, and contact the employer or candidate directly via your Job Target account. Employers (only) can pre-schedule interviews for the week of the conference by creating accounts to manage their on-line recruiting efforts and contact candidates in advance of the conference. All job descriptions will be posted free of charge until January 1, 2008, regardless of conference registration status. Please email erica.kylo@sabic-ip.com for additional information.

At the conference:
Location: The employment bureau is located on the Mezzanine Level, Mississippi Room
Hours: 9:00 AM – 5:00 PM, Monday – Wednesday and 9:00 AM – 3:00 PM on Thursday

Check your Job Target in-box to follow-up on your employment leads. Wireless internet access will be available in the Employment Bureau, the Exhibit Hall, and the Prefunction Foyer. Two desktop computers and a printer will also be available in the Employment Bureau to help you in your job/candidate search.

Interview booths will be available for 30-minute interviews during Employment Bureau hours. The employer is responsible for scheduling the use of interview booths by signing on a schedule posted in the Employment Bureau.

SPECIAL INVITATIONS TO STUDENT ATTENDEES:

Monday, 1:00 PM, Employment presentation by Kelly Scientific Resources. Title: “Working with Recruiters: The secrets that will help you achieve your career goals!” What are you doing in your job search? Are you surfing the right website, applying to the right companies, where does your resume go? Should you skip the job search process entirely and work with a recruiter? If you find any of these areas difficult, we invite you to join your FACSS colleagues to hear more about these questions. This presentation will offer scientists the essential skills needed in developing or enhancing their career. Interactive topics will include a PhD focus on job search strategies, how job searching has changed, interview / recruiter insight, and networking skills. Steve Holmes, Recruiting Manager, South Region Kelly Scientific Resources. Room 201

Tuesday, 12:30 PM, Student/Professional Panel Discussion and Brown Bag Lunch sponsored by SABIC Innovative Plastics. Topic: “I’m Graduating Soon. What’s Next?” Eat lunch and chat with professionals from a wide range of professional fields (academic, government, chemical industry, pharmaceuticals, goods and services, etc.). It’s a unique opportunity to ask questions, get helpful tips, and discuss topics that relate to your specific career-seeking situation within the current job market. Employers who are interested in participating in the employment panel, please email drew.manica@sabic-ip.com. Room 201.

Sign up at conference registration desk.
**PROGRAM HIGHLIGHTS**

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<td>FACSS Student Awards</td>
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<td>7:00 PM</td>
<td>SAS Reception</td>
<td>FACSS Networking Event</td>
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<td>Heritage Ballroom 3/4</td>
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## PROGRAM OVERVIEW

### SUNDAY

**3:00 PM**  
“What’s Hot” Symposium – oral presentations by FACSS 2007 exhibitors describing some of their latest products, page 47.  
*Room 201/202*

**5:00 PM**  
Welcome Mixer and SAS Sponsored Student Poster Session, Coblentz Student Awards and FACSS Student Awards, *Prefunction Foyer*

### MONDAY MORNING

**8:00 AM**  
PLENARY LECTURE, Ballroom C/D  
Interdiscilinary Biophotonics: Molecular Domains to Organelles to Organs; Ira W. Levin, page 48

**9:00 AM**  
SYMPOSIA AND POSTER SESSIONS  
**9:00 – 10:30, Posters**, *Prefunction Foyer*, page 48  
**10:30 – 12:30, Symposia**, page 49  
Hidden Isotope Ratio Information – Yours to Discover with MC-ICP-MS I, *Room L2*  
Advances in Spectroscopy and Mass Spectrometry in Forensic Sciences, *Room L3*  
Chemometrics Applied to Expert Systems for Identification of Materials, *Room L4*  
Fundamentals of Electrospray Ionization, *Room L5*  
FACSS Young Investigators I, *Room L6*  
Vibrational Spectroscopy: Advances in Instrumentation and Theory, *Room L11*  
Instrumentation and Application of Process Analytical Chemistry for Industrial Process Understanding and Control, *Room L12*  
Bioanalytical Applications of SERS, *Room L13*  
Imaging and Spectroscopy in the THz Region, *Room L14*

### MONDAY AFTERNOON

**1:30 PM**  
“What’s Hot” Symposium – oral presentations by FACSS 2007 exhibitors describing some of their latest products. *Ballroom C/D*, page 51

**2:30 PM**  
Symposia, page 51  
Hidden Isotope Ratio Information – Yours to Discover with MC-ICP-MS II, *Room L2*  
Bioanalytical Electrochemistry, *Room L3*  
Chemometrics Along Spatial and Chemical Dimensions, *Room L4*  
Fundamentals of Laser Desorption Ionization, *Room L5*  
FACSS Young Investigators II, *Room L6*  
Environmental Applications of Analytical Chemistry, *Room L11*  
Process Analytical Monitoring - SAS Technical Session, *Room L12*  
Quantitative Raman in Pharma, *Room L13*  
Coherent Two-Dimensional Spectroscopy I, *Room L14*

### TUESDAY MORNING

**8:00 AM**  
PLENARY LECTURES, Ballroom C/D  
ANACHEM Award, Isiah M. Warner, page 54  
Charles Mann Award, Neil Everall, page 54

**9:00 AM**  
SYMPOSIA AND POSTER SESSIONS  
**9:00 – 10:30, Posters**, *Ballroom A*, page 54  
**10:30 – 12:30, Symposia**, page 55  
Electrothermal Atomization vs. Electrothermal Vaporization Techniques, *Room L2*  
Mass Spectrometry for Bioanalysis, *Room L3*  
Spectral and Multiway Pattern Recognition, *Room L4*  
Molecular Spectroscopy in Forensic Science, *Room L5*  
Anachem Award Symposium in Honor of Isiah M. Warner, *L6*  
NIR Imaging, *Room L11*  
ISA Analysis Division – Best of the Best, *Room L12*  
Current Analytical Technologies for Drug Discovery, *Room L13*  
Coherent Two-Dimensional Spectroscopy II, *Room L14*

### TUESDAY AFTERNOON

**1:45 PM**  
SYMPOSIA AND POSTER SESSIONS  
**1:45 – 3:15, Posters**, *Ballroom A*, page 57  
**3:15 – 5:15, Symposia**, page 59  
Current Advances in ICPMS From Them That Knows, *Room L2*  
Capillary Electrophoresis, *Room L3*  
Electrochemistry and Functional Nanomaterials, *Room L4*  
Novel Methods for Biological Mass Spectrometry, *Room L5*  
Student Awards, *Room L6*  
NIR Applications in the Pharmaceutical Industry, *Room L11*  
Applications of Fluorescence Spectroscopy and Related Techniques, *Room L12*  
Professor Charles Mann Award to Neil Everall, *Room L13*  
Emerging Technologies for Homeland Security, *Room L14*
PROGRAM OVERVIEW

WEDNESDAY MORNING

8:00 AM PLENARY LECTURES, Ballroom C/D
SAS Applied Spectroscopy William F. Meggers Award, Richard Medelsohn, page 62
Coblentz Society Clara Craver Award, Katherine A. Bakeev, page 62

9:00 AM SYMPOSIA AND POSTER SESSIONS
9:00 – 10:30, Posters, Ballroom A, page 62
10:30 – 12:30, Symposia, Room L2
Biomedical Applications of Atomic Spectrometry
Bioanalytical Microfluidics, Room L3
Nanotubes and Nanowires for Sensing I, Room L4
Particle Mass Spectrometry: Techniques and Applications, Room L5
The Coblentz Society Clara Craver Award in Applied Vibrational Spectroscopy, Room L6
Advances in FTIR Imaging, Room L11
Initiative (NeSSI) to Improve Process Quality and Control, Room L12
Opportunities for Raman Spectroscopy, Room L13
Analysis and Modeling of Spectral Data, Room L14

WEDNESDAY AFTERNOON

1:45 PM SYMPOSIA AND POSTER SESSIONS
1:45 – 3:15, Posters, Ballroom A, page 66
3:15 – 5:15, Symposia, Room L2
Developments in Plasma Spectroscopy, organized by SAS Atomic Spectroscopy Technical Section, Room L2
Electrophoretic and Microfluidic Bioanalysis, Room L3
Nanotubes and Nanowires for Sensing II, Room L4
New Approaches to Environmental Mass Spectrometry, Room L5
Meggers Award Symposium – Richard Medelsohn, Room L6
Developments in Luminescence Spectroscopy and Instrumentation, Room L11
Novel Sensors and Instrumentation of Tomorrow, Room L12
Evolving Developments in the Use of Raman Spectroscopy, in Conjunction with Other Physical Measurements for the Characterization and Rational Design of Catalysts, Room L13
Surface Plasmon Resonance: Innovation and Application I, Room L14

THURSDAY MORNING

8:00 AM PLENARY LECTURE: Ballroom C/D
SAS Lester W. Strock Award, Detlef Günther, page 70
8:30 AM CLOSING PLENARY, Bruce Edward Bursten, President-Elect of the American Chemical Society, page 70

9:00 AM SYMPOSIA AND POSTER SESSIONS
9:30 – 10:30, Posters, Prefunction Foyer, page 70
10:30 – 12:30, Symposia, Room L2
Commemoration of Dr. Radu Mavrodineanu, Room L2
Fabrication Strategies for Microfluidics: Beyond the Cleanroom, Room L3
Nanoscale Structures and Their Application, Room L4
Advances in Biomolecular Imaging Mass Spectrometry, Room L5
Lester W. Stock Award – Detlef Günther, Room L6
Novel Miniature Spectroscopic Instrumentation, Room L11
Process Analysis for Food Quality and Safety, Room L12
Raman Spectral Imaging – Diversity in Applications, Room L13
Pharmaceutical Forensics, organized by the Forensic Technical Section of the Society for Applied Spectroscopy, Room L14

THURSDAY AFTERNOON

1:45 PM SYMPOSIA AND POSTER SESSIONS
1:45 – 2:45, Posters, Prefunction Foyer, page 70
2:45 – 4:45, Symposia, Room L2
Fundamental Advances in Plasma Source Mass Spectrometry, Room L2
Surface Plasmon Resonance: Innovation and Application II, Room L3
Carbon Nanotube Separation, Room L4
Direct Ionization Methods for High Throughput Mass Spectrometry, Room L5
Multivariate Curve Resolution, Room L6
Biovibrational Spectroscopy, Room L11
PAT Across the R&D and Manufacturing Interface, Room L12
Emerging Applications and Technologies in Raman Spectroscopy, Room L13
Recent Developments in Explosive Detection Technologies, organized by Forensic Technology Section of SAS, Room L14
## TECHNICAL PROGRAM OVERVIEW BY TOPIC

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<td>Charles Mann Award - Neil Everall (Awardee), Rm L13</td>
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<td>Student Awards, Rm L6</td>
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<tr>
<td>Coblentz Craver Award - Katherine Bakeev (Awardee), Rm L6</td>
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<td>Meggers Award - Rich Mendelsohn (Awardee), Rm L6</td>
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<td>Strock Award - Detlef Gunther (Awardee), Rm L6</td>
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<tr>
<td><strong>Monday PM</strong></td>
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<tr>
<td>Hidden Isotope Ratio Information - Yours to Discover with MC-ICP-MS II, Rm L2</td>
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<td><strong>Wednesday AM</strong></td>
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<td>Biomedical Applications of Atomic Spectroscopy, Rm L2</td>
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<td><strong>Wednesday PM</strong></td>
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<td>Developments in Plasma Spectroscopy organized by the SAS Atomic Spectroscopy Technical Section, Rm L2</td>
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<td><strong>Thursday AM</strong></td>
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<td><strong>Thursday PM</strong></td>
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<td>Bioanalytical Microfluidics, Rm L3</td>
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<td>Biomedical Applications of Atomic Spectroscopy, Rm L2</td>
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<td><strong>Wednesday PM</strong></td>
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<td>Electrophoretic and Microfluidic Bioanalysis, Rm L3</td>
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<td>Fabrication Strategies for Microfluidics: Beyond the Cleanroom, Rm L3</td>
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<td>Chemometrics Along Spatial and Chemical Dimensions, Rm L4</td>
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<td>Analysis and Modeling of Spectral Data, Rm L14</td>
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<td>Multivariate Curve Resolution, Rm L6</td>
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<td>Coherent Two-Dimensional Spectroscopy II</td>
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<td>Raman Spectral Imaging – Diversity in Applications, Rm L13</td>
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<td>Vibrational Spectroscopy: Advances in Instrumentation and Theory, Rm L11</td>
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<td>NIR Imaging, Rm L11</td>
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<td>NIR Applications in the Pharmaceutical Industry, Rm L11</td>
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<td>SAS Applied Spectroscopy Meggers Award – Rich Mendelsohn (Presenting Awardee), Rm L6</td>
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<td>Novel Miniature Spectroscopic Instrumentation, Rm L11</td>
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## TECHNICAL PROGRAM OVERVIEW BY TOPIC

### MASS SPECTROMETRY

**Monday AM**  
Fundamentals of Electrospray Ionization, *Rm L5*  
Advances in Spectroscopy and Mass Spectrometry in Forensic Science, *Rm L3*

**Monday PM**  
Fundamentals of Laser Desorption Ionization, *Rm L5*

**Tuesday AM**  
Mass Spectrometry for Bioanalysis, *Rm L3*

**Tuesday PM**  
Particle Methods for Biological Mass Spectrometry, *Rm L5*

**Wednesday AM**  
Fundamentals of Laser Desorption Ionization, *Rm L5*

**Wednesday PM**  
Particle Mass Spectrometry: Techniques & Applications, *Rm L5*

**Thursday AM**  
Advances in Biomolecular Imaging Mass Spectrometry, *Rm L5*

**Thursday PM**  
Direct Ionization Methods for High Throughput MS, *Rm L5*

### NANOSCIENCE, Room L4

**Tuesday PM**  
Electrochemistry and Functional Nanomaterial

**Wednesday AM**  
Nanotubes and Nanowires for Sensing I

**Wednesday PM**  
Nanotubes and Nanowires for Sensing II

**Thursday AM**  
Nanosciences and Nanotechnology

**Thursday PM**  
Carbon Nanotube Separation

### PHARMACEUTICAL

**Monday PM**  
Process Analytical Monitoring – SAS Technical Session, *Rm L12*  
Quantitative Raman in Pharma, *Rm L13*

**Tuesday AM**  
Current Analytical Technologies for Drug Discovery, *Rm L13*  
Pharmaceutical Forensics, *Rm L14*

**Tuesday PM**  
NIR Applications in the Pharmaceutical Industry, *Rm L11*

**Thursday AM**  
Process Analysis for Food Quality and Safety, *Rm L12*

**Thursday PM**  
PAT Across the R&D and Manufacturing Interface, *Rm L12*

### PROCESS, Room L12

**Monday AM**  
Instrumentation and Application of Process Analytical Chemistry for Industrial Process Understanding and Control

**Monday PM**  
Process Analytical Monitoring - SAS Technical Session

**Tuesday AM**  
ISA Analysis Division - Best of the Best

**Wednesday AM**  
Initiative (NeSSI) to Improve Process Quality and Control

**Wednesday PM**  
Novel Sensors and Instrumentation of Tomorrow

**Thursday AM**  
Process Analysis for Food Quality and Safety

**Thursday PM**  
PAT Across the R&D and Manufacturing Interface

### RAMAN

**Monday AM**  
Bioanalytical Applications of SERS, *Rm L13*

**Monday PM**  
Quantitative Raman in Pharma, *Rm L13*

**Tuesday AM**  
Molecular Spectroscopy in Forensic Science, *Rm L5*

**Tuesday PM**  
Charles Mann Award – Neil Everall (Awardee), *Rm L13*

**Wednesday AM**  
Opportunities for Raman Spectroscopy, *Rm L13*

**Wednesday PM**  
Evolving Developments in the Use of Raman Spectroscopy, in Conjunction with Other Physical Measurements for the Characterization and Rational Design of Catalysts, *Rm L13*

**Thursday AM**  
Raman Spectral Imaging – Diversity in Applications, *Rm L13*

**Thursday PM**  
Emerging Applications and Technologies in Raman Spectroscopy, *Rm L13*

### SEPARATIONS and MICROFLUIDICS

**Tuesday AM**  
ANAChem – Isiah Warner (Awardee), *Rm L6*

**Tuesday PM**  
Capillary Electrophoresis, *Rm L3*

**Wednesday AM**  
Bioanalytical Microfluidics, *Rm L3*

**Wednesday PM**  
Electrophoretic and Microfluidic Bioanalysis, *Rm L3*

**Thursday AM**  
Fabrication Strategies for Microfluidics: Beyond the Cleanroom, *Rm L3*

**Thursday PM**  
Carbon Nanotube Separation, *Rm L4*

### SPECIAL, Room L2

**Thursday AM**  
Commemoration of Dr. Radu Mavrodineau

### SURFACE PLASMON RESONANCE

**Wednesday PM**  
Surface Plasmon Resonance: Innovation and Application I, *Rm L14*

**Thursday PM**  
Surface Plasmon Resonance: Innovation and Application II, *Rm L3*

### TERAHERTZ, Room L14

**Monday AM**  
Imaging and Spectroscopy in the THz Region

### YOUNG INVESTIGATORS, Room L6

**Monday AM**  
Young Investigators I

**Monday PM**  
Young Investigators II
“What’s Hot” Symposium, Presider: Brian Dable, Room 201/202
3:00 Iridian Spectral Technologies, “More Signal, Less Background – Leading Edge Filters for Spectroscopy and Microscopy”
3:10 Opotek
3:20 Glass Expansion; “Benefits of Controlling Spray Chamber Temperature in ICP Spectrometry”
3:30 Millipore Labwater, “The New Milli-Q Advantage Ultrapure Water System”
3:40 Torsana Laser Technologies, Leaders in Light – Perfect for Raman
3:50 Photon Etc., “Top Notch™ Filters: Ultra Narrow and Tunable Notch Filters for Raman Spectroscopy”
4:00 JASCO Inc. “Mobile Research-Grade Raman Microprobe System”
4:20 Centice Corporation, “High Throughput Raman”
4:30 Delta Nu, “Universal Raman Detection – Dispersive NIR Raman (DNIR-Raman) above 1 Micron
4:40 HeadWall Photonics, Inc., “High Performance Spectral & Spatial Imaging Spectrometers”
4:50 Ametek Process Instruments

5:00 PM
SAS Sponsored Student Poster Session, Coblentz Student Awards, FACSS Student Awards
Prefunction Foyer

SAS Student Poster Showcase and Awards

Come join us in celebrating the shooting stars of science as SAS students showcase their research and compete for the annual SAS Student Poster Awards.

Sunday, October 14, 2007 5-7 p.m. (during the FACSS mixer)

Sponsored by
The Society for Applied Spectroscopy and FACSS
TECHNICAL PROGRAM – MONDAY
Plenary and Posters

8:00 AM, Plenary Session, Presider: James Rydzak, Ballroom C/D

Ira Levin

(1) Interdisciplinary Biophotonics: Molecular Domains to Organelles to Organs; Ira Levin1, Nicole Crane1, Tso-Ching Chen1, Zachary Schultz; 1National Institutes of Health

Dr. Levin received his B.S. from the University of Virginia and his Ph.D. from Brown University, as well as having had postdoctoral experience at the University of Washington. He is currently Deputy Director of the Division of Intramural Research in the National Institute of Diabetes and Digestive and Kidney Diseases, in addition to being Chief, of the Section on Molecular Biophysics, at the National Institutes of Health. His research interests lie primarily in the applications of vibrational infrared and Raman spectroscopic techniques toward the elucidation of the conformational, dynamical, thermodynamic, and functional properties of both intact and model membrane assemblies and related systems. Emphasis is placed on investigating the specific lipid-lipid and lipid-protein interactions governing biomembrane reorganizations. In particular, his efforts are directed toward defining and characterizing lipid microdomain formation as it pertains both to the existence of lateral heterogeneities and transverse asymmetries within biological membranes and to the ability and extent of these fluctuating microclusters, or domain motifs, to modulate integral membrane protein behavior. He has been at the forefront of developing spectroscopic infrared, Raman and viable reflectance imaging instrumentation. Specifically, his laboratory has provided pioneering technologies and studies in spectroscopic Fourier Transform Infrared and Raman microimaging. Current efforts are in translating laboratory research into clinical venues ranging from monitoring disease progression by means of spectroscopic histopathologic classifications to in vivo hyperspectral imaging for assessing tissue perfusion, vascular disease and endothelial dysfunction.

Dr. Levin has been honored with many awards including the Bome-Michelson Award by the Coblentz Society, the Meggers Award (three separate occasions) presented by the Society of Applied Spectroscopy, the Harold A. Iddles Lecture Series presented by the University of New Hampshire, and is a Fellow of the American Physical Society's Biophysical Division and, separately, a Fellow in the Division of Chemical Physics. He has also received the Lippincott Award in Vibrational Spectroscopy presented by the Optical Society of America. He has served on numerous boards and committees in various leadership capacities in the spectroscopy community and has published extensively over the course of his career. Dr. Levin is a member of the American Physical Society, the American Society for Biochemistry and Molecular Biology, the Biophysical Society, the Coblentz Society, the American Chemical Society, and the Society for Applied Spectroscopy.

MONDAY POSTER SESSION
9:00 – 10:30 AM
Prefunction Lobby

All Monday posters should be put up between 7:30 – 8:00 AM and removed between 4:30 – 5:00 PM. The presenting author is expected to be present at the poster during the poster session 9:00 – 10:30 AM.

<table>
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<tr>
<th>Board#</th>
<th>Title</th>
<th>Authors</th>
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<tbody>
<tr>
<td>1</td>
<td>(2) Regulatory Compliance Tools in ICP-OES Software to enable Fast Accurate Results for Method Driven Applications; Karen Harper1, Cassap Matthew1, Clavering Andrew1; 1Thermo Fisher Scientific</td>
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<tr>
<td>2</td>
<td>(3) Direct Determination of Trace Metal Elements in Diluted Quality Control Urine Materials Using a Collision Reaction Interface Equipped ICP-MS; Doug Shrader1, XueDong Wang1, Stephen Anderson1, Shane Elliott1; 1Thermo Fisher Scientific</td>
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<tr>
<td>3</td>
<td>(4) A Flexible, Easy to Use Platform for Analyzing Molecular Interactions on Arrays; Steve Weibel1, Voula Kodoiyanni1; 1GWC Technologies, Inc.</td>
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</table>
In the provided image, a page from a document is shown, containing a schedule for technical sessions, posters, and clinical sessions for FACSS 2008. The text is too small to transcribe accurately, but it appears to be part of a larger document that includes scientific abstracts and schedules. The document is hard to read due to the small font size and the layout, which seems to be a part of a conference program or a scientific publication.
### TECHNICAL PROGRAM – MONDAY
Orals 10:30 AM – 12:30 PM

### Monday Morning, Room L4
CHEMOMETRICS APPLIED TO EXPERT SYSTEMS FOR IDENTIFICATION OF MATERIALS
Organizers: Barry Lavine and Jerry Workman; Presider: Jerry Workman

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<th>Time</th>
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<th>Authors</th>
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<tr>
<td>10:30</td>
<td>(36) Wavelet Based Search Prefilters for Spectral Library Matching</td>
<td>Barry Laving1, Nikhil Mirjankar1, Kadambari Nuguru1, Oklahoma State University</td>
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<tr>
<td>10:50</td>
<td>(37) Automated Classification Techniques for Gemstones Using FTIR and Raman Spectroscopy; Stephen Lowry1, Jerry Workman1; Thermo Fisher Scientific Inc.</td>
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<tr>
<td>11:10</td>
<td>(38) The Role of Chemometrics in On-Line Chromatography; Brian Rohrbach1, Infometrix, Inc.</td>
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<tr>
<td>11:50</td>
<td>(39) Optimizing Chemometric Model Development and Robustness Evaluation for PAT Applications in the Pharmaceutical Industry; Bruce Thompson1; Merck &amp; Co., Inc.</td>
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<tr>
<td>12:10</td>
<td>(40) An Expert Spectroscopy System for Material Characterization; Jerry Workman1; Luminous Medical, Inc.</td>
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### Monday Morning, Room L5
FUNDAMENTALS OF ELECTROSPRAY IONIZATION
Organizer and Presider: Gary Van Berkel

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<th>Time</th>
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<th>Authors</th>
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<tr>
<td>10:30</td>
<td>(41) Multiple-electrode Electrospray Emitter Systems for Analytical Advantage in ES-MS; Vilmos Kertesz2, Gary J. Van Berkel1; Oak Ridge National Laboratory</td>
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<tr>
<td>10:50</td>
<td>(42) From Spray Stability to Ion Formation: Contorted Menisci and Ion Chemistry in Electrosprays; Akos Vertes1, Peter Nemes1, Joan Marginean1, Samita Goyal1; George Washington University</td>
<td></td>
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<tr>
<td>11:10</td>
<td>(43) Ultra-low Flow Electrospray: Equimolar Response and Small Molecule Analysis; Gary Valaskovic1, Lucas Utley2, Panos Hastis3, Mike Lee4, Jing-Tao Wu5; New Objective Inc.; AstraZeneca R&amp;D Boston; Millenium Pharmaceuticals; Millenium Pharmaceuticals</td>
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<tr>
<td>11:30</td>
<td>(44) Improving Sampling Efficiency for Electrospray Ionization – Mass Spectrometry; Bradley Schneider1, Hassan Javaheri1, Thomas Covey1; MDS SCIEX</td>
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<td>11:50</td>
<td>(45) Fundamentals of Desorption Electrospray Ionization; R. Graham Cooks1, Andre Venter1; Purdue University</td>
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<tr>
<td>12:10</td>
<td>(46) Electrospray in Ambient Air: The Oxygen Effect; Richard B. Cole1, Boguslaw P. Pozniak1; University of New Orleans</td>
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### Monday Morning, Room L6
FACSS YOUNG INVESTIGATORS I
Organizer: S. Douglass Gilman; Presider: Diane Parry

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<th>Time</th>
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<tr>
<td>10:30</td>
<td>(47) A Faster Method of Mass Spectrometry for Fast or Complex GC and LC Separations; Glen P. Jackson1, Ohio University</td>
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<tr>
<td>10:50</td>
<td>(48) Gas-Phase Ion-Electron Reactions for Structural Characterization of Acidic and Neutral Biomolecules; Kristina Hakansson1, Julie T. Adamson1, Hye Kyong Kwon1, Haichuan Liu1, Jiong Yang1, Hyun Ju Yoo1; University of Michigan</td>
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### Monday Morning, Room L11
VIBRATIONAL SPECTROSCOPY: ADVANCES IN INSTRUMENTATION AND THEORY
Organizer: Ian R. Lewis; Presider: E. Neil Lewis

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<th>Time</th>
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<tr>
<td>10:30</td>
<td>(53) Modeling Scattering in Vibrational Spectroscopy and Imaging; Anil Kodali, Rohit Bhargava; University of Illinois at Urbana-Champaign</td>
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<tr>
<td>10:50</td>
<td>(54) Quantitative Raman Spectroscopy in Turbid Media: Theory and Simulations; Wei-Chuan Shih1, Kate Bechtel1, Michael Feld1; Schlumberger-Doll Research; MIT Spectroscopy Laboratory</td>
<td></td>
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<tr>
<td>11:10</td>
<td>(55) Quantitative Raman Spectroscopy in Turbid Media: Experiment; Kate Bechtel1, Wei-Chuan Shih2, Michael Feld1; MIT Spectroscopy Laboratory; Schlumberger-Doll Research</td>
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<tr>
<td>11:30</td>
<td>(56) Comparison of Vibrational Circular Dichroism (VCD) Instruments. Development of a New Despersive VCD; Ahmed Lakhami, Peter Malon1, Timothy A. Kierdlerling1, Univ. of Illinois at Chicago; Univ. of Illinois at Chicago</td>
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### Monday Morning, Room L12
INSTRUMENTATION AND APPLICATION OF PROCESS ANALYTICAL CHEMISTRY FOR INDUSTRIAL PROCESS UNDERSTANDING AND CONTROL
Organizer and Presider: James Cronin

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<th>Time</th>
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<tr>
<td>10:30</td>
<td>(59) Ultra-Short Path Length UV-vis Spectroscopy for Process Control; Lewis Baylor1, Patrick O'Rourke1; Echtech Int'l Corp.</td>
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<td>10:50</td>
<td>(60) Application of Process Raman to Monitor Blending Efficiency; Wes Thompson1, Brian Marquardt1; University of Washington</td>
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<td>11:10</td>
<td>(61) The Use of Planar Array Infrared in Real-Time Studies of Structural Development in Polymeric Films; Bruce Chase1, John Rabolt1, Andreas Pesa1, Chris Snively1; DuPont Experimental Station</td>
<td></td>
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</tbody>
</table>
10:30 (65) SERS Nanosensors for Intracellular Applications; Janina Kneipp1, Harald Kneipp2, Margaret McLaughlin3, Dennis Brown1, Burghardt Wittig4, Katrin Kneipp5; 1Federal Institute for Materials Research (BAM); 2Wellman Center, Harvard Medical School; 3Program in Membrane Biology, Harvard Med; 4Charité Universitätsmedizin in Berlin

10:50 (66) Developing an Early Diagnosis Test for Pancreatic Cancer Using Surface-Enhanced Raman Spectroscopy (SERS); Gufeng Wang1, Robert J. Lipert1, Marc D. Porter2, Aaron R. Sasson3, Maneesh Jain4, Surinder K. Batra1, 1Ames Lab-U.S. DOE, Iowa State Univ.; 2Dept.Chem.& Biochem. Arizona State Univ.; 3Univ. of Nebraska Medical Center

11:10 (67) Multiplexed Detection of Infectious Diseases by SERRS; Karen Faulds1, Alastair Ricketts1, Fiona McKenzie1, W. Ewen Smith1, Duncan Graham1; 1University of Strathclyde

11:30 (68) Rapid, Direct Virus Classification via Surface-enhanced Raman Spectroscopy Fingerprinting with Novel Nanofabricated Silver Nanorod Arrays; Jeremy Driskell1, Saratchandra Shammuk1, Ralph Tripp1, Yiping Zhao1, Jabulani Barber2, Peter Dluy1, Lawrence Bottomley1, Richard Dluy1, University of Georgia; 2Georgia Institute of Technology

11:50 (69) Bioconjugated SERS Nanoparticle Tags for Cancer Detection and Imaging; Ximei Qian1, Dominic Ansari1, X. P. Peng1, Lily Yang1, Shuming Nie1; 1Emory University

12:10 (70) Overview of Time-Domain Terahertz Instrumentation and Applications; Jeffrey White1, David Zimdars1; 1Picometrrix LLC

10:50 (71) Aspects of Microwave and THz Spectroscopy in Pharmaceutical Analysis; Jonas Johansson1, Lubomir Gradinarsky1, Mike Claybourn1, Staffan Folestad1; 1AstraZeneca Pharmaceutical and Analytical R&D

11:10 (72) Understanding the Role of Terahertz Imaging in Pharmaceutical Analysis; Fiona Clarke1, Linda Jayes1; 1Pfizer

11:30 (73) Terahertz and MM-wave Imaging: Transmission and Reflection Capabilities and Needs; Joseph P. Dougherty1, William L. Koscr Jr1, Matthew R. Fettnerman1; 1Penn State University Electro-Optics Ctr.

11:50 (74) Lattice Dynamics Calculations of Phonon Spectra for Molecular Organic Crystals: Investigating the Polymorphism of Carbamazepine; Graeme M. Day1, Axel Zeiliger1, Mike Claybourn1; 1University of Cambridge; 2AstraZeneca

12:10 (75) Uses of Terahertz Pulsed Spectroscopy and Imaging in Industry; Philip Taday1, Alessia Portieri1, Yaochun Shen1, Louise Ho1; 1TeraView Limited, UK; 2University of Otago, New Zealand

Monday Afternoon, Room L13

BIOANALYTICAL APPLICATIONS OF SERS
Organizer and Presider: Duncan Graham

1:30 Thermo Scientific, “New Strategies for Cosmic Ray Rejection and the Implications for Common Raman Applications”

1:40 Bio-Rad Laboratories, “Cheminformatics Meets Chemometrics – A New Approach to Analyzing Spectral Data”


2:00 Renishaw, Inc.

2:10 Malvern Instruments, “The SyNIRgi – Rapid and Quantitative NIR Imaging”


Monday Afternoon, Room L2

HIDDEN ISOTOPE RATIO INFORMATION – YOURS TO DISCOVER WITH MC-ICP-MS
Organizers and Presiders: Ralph Sturgeon and Frank Wanhaecke

2:30 (76) SR and PB Isotopic Analysis using Multi-Collector ICPMS for Answering Archaeological Questions; Frank Vanhaecke1, David De Muynck1, Ghylaine Quitte1, Felix Oberli1, Elisabeth Smits1, Freerk de Wolff1, Ghent University; 2ETH - Zürich; 3Free University Amsterdam; 4Leiden University Medical Centre

2:50 (77) Isotopic Analysis of Bominerals by LA-ICP-MS: The Role of Ultra Short Pulse Width (Fs) Lasers; Brian Fryer1, Zhaoping Yang1, Sonia Melancon1, Joel Gagnon1; 1University of Windsor

3:10 (78) Extent of Matrix Effects between Zircon and Baddeleyite in Hf-isotope Analysis by Laser Ablation-MC-ICPMS; Paul Sylvester1, Rebecca Lam1; 1Inco Innovation Centre, Memorial University

3:30 (79) Use of MC-ICP-MS in Exploration Geochemistry; Kurt Kysor1, Quinn’s University

3:50 (80) Application of Multi-Collector ICP-MS (MC-ICP-MS) to Geochemistry: Aqueous and Solid Sampling; W. Ian Ridley1, Michael J. Pribil1, Stephen A. Wilson1; 1USGS, Denver Federal Center

4:10 (81) To Boldly Go – Measuring Fractionation of Mercury Isotopes in the Environment; Holger Hintelmann1, Delphine Foucher1, Wang Zheng1, Mark Dzurko1; 1Trent University
Monday Afternoon, Room L3
**BIOANALYTICAL ELECTROCHEMISTRY**
Organizer and Presider: Don Cannon

2:30  
(82) Micron-Scale Sensors for Detecting Reactive Oxygen Species Related to Noise Induced Hearing Loss *in situ* and *in vivo*; Alexander Scheel1, Rebekah Wilson1, Edward Chainani2; 1University of Illinois at Urbana-Champaign

2:50  
(83) Mediated and Direct Bioelectrocatalysis for Sensing Applications; Shelley D Minteer1, Tamara L Klotzbach1, Anne Blackwell1; 1Saint Louis University

3:10  
(84) Chemical Imaging of Single Cells with Scanning Electrochemical Microscopy; John Baur1; 1Illinois State University

3:30  
(85) Rapid Sample Preparation and Optimized Electrode Design for Dust Allergen Assays Integrated with Microelectrochemical Detection; Ingrid Fritsch1, Emily Anderson1, Andrea Henrichs2, Caitlin Williams1, Zoraida Aguilar1, 2University of Arkansas; 3Vegrandis, LLC

4:10  
(86) Enhanced Detection of H2O2 via Electrogenerated Chemiluminescence at Microelectrodes for Single-cell Systems; Perry Motsegood1, Donald M. Cannon1; 1University of Iowa Chemistry

Monday Afternoon, Room L4
**CHEMOMETRICS ALONG SPATIAL AND CHEMICAL DIMENSIONS**
Organizer and Presider: Frederick Koehler

2:30  
(88) Hyperspectral Confocal Fluorescence Imaging for Investigating Host-Pathogen Interactions; David Haaland1, Howland Jones1, Mark Van Benthem1, Michael Sinclair1, Catherine Branda1, Bryan Carson1, Jens Poschet1, Roberto Rebeil1, Diane Lidke1, Allan Brasier1, 1Sandia National Laboratories; 2University of New Mexico; 3University of Texas Medical Branch

2:50  
(89) Development of Image Data Analysis Tool for Pharmaceutical Applications; Lin Zhang1; 1Pfizer Global R&D

3:10  
(90) Chemometric Methods for Automating the Interpretation of Hyperspectral and Multispectral Infrared Imaging Data; Gary Small1; 1University of Iowa

3:30  
(91) Exploration and Resolution of Multilayer Spectroscopic Images; Anna de Juan1, Thomas Hancewicz1, Marcel Maeder2, Romà Tauler3; 1Universitat de Barcelona, Barcelona; 2The University of Newcastle, Australia; 3Unilever R & D, Trumbull, CT, U.S.; 4IQAB-CSIC, Barcelona

3:50  
(92) The Effects of Pre-Processing of Image Data on Self-Modeling Image Analysis; Willem Windig1, Mike Keenan1; 1Eigenvector Research, Inc.; 2Sandia National Laboratories

4:10  
(93) Interpretation of Support Vector Machines (SVMs) Model for Classification in Near Infrared (NIR) Spectroscopy; Olivier Devos1,2, Cyril Ruckebusch2; 1Ludovic Duponchel2, Jean-Pierre Huvenne1; 1Laboratoire de Spectrochimie Infrarouge et Raman; 2Univ. des Sci. et Tech. de Lille

Monday Afternoon, Room L5
**FUNDAMENTALS OF LASER DESORPTION IONIZATION**
Organizer and Presider: Gary R. Kinsel

2:30  
(94) The Relevance of Vacuum Ultraviolet Postionization of Laser Desorbed Neutrals to MALDI and DIOS Mass Spectrometry; Luke Hanley, Artem Akhmetov, Gerald Gaspar, Manshui Zhou, Peter Koin; 1University of Illinois at Chicago

2:50  
(95) Laser Desorption Ionization from Nanostructures; Akos Vertes1, Jessica Stolec1, Bennett Walker1; 1George Washington University

3:10  
(96) Recent Developments in Models of UV MALDI Ionization; Richard Knochenmuss1; 2Novartis

3:50  
(97) Experimental Probes of Equilibrium Conditions in Laser Desorbed Plumes of Material; Gary Kinsel1, Dennis Marynick2, Faten Yassin2, Ganga Fernando2; 1Southern Illinois University Carbondale; 2University of Texas at Arlington

4:10  
(98) The Role of Particulate in Laser Desorption/Ionization; Kermit Murray1; 1Louisiana State University

Monday Afternoon, Room L6
**FACSS YOUNG INVESTIGATORS II**
Organizer: S. Douglass Gilman; Presider: Mark Hayes

2:30  
(99) Analyte-loss Processes in Inductively Coupled Plasma Mass Spectrometry; Bodo Hattendorf1, Zhongke Wang1, Detlef Günther1; 2ETH Zurich, D-CHAB, Lab. for Inorg. Chem

2:50  
(100) Investigation of Reagent Gases for the Positive Chemical Ionization of the Polybrominated Diphenyl Ethers; Anne Vonderheide1, Thomas Hieber2, Peter Kauffman1, Jeffrey Morgan1, Lisa Jo Melynk1; 1United States Environmental Protection Agency; 2National Council of the Aging

3:10  
(101) Nanotube Based Lithography; Punit Kohli1, Rashid Zakeri1, Bojan Mitrovic1; 1University of Missouri

3:30  
(102) Direct Resolution of UV Resonance Raman Protein Secondary Structural Motifs using MCR-ALS; Renee Jiji1, John Simpson1; 1University of Missouri

3:50  
(103) Direct and Label-Free Detection of Solid-Phase Bound Compounds by SERS; Bernd Kuestner1, Carsten Schmuck1, Peter Wich1, Wolfgang Kiefer2, Sebastian Schlucker1; 1University of Wuerzburg

4:10  
(104) Multi-Color Electrophoretic Immunoassays; Michael Ropec1, Christelle Guillo1; 1Florida State University
Monday Afternoon, Room L11
ENVIRONMENTAL APPLICATIONS OF ANALYTICAL CHEMISTRY
Organizers: Ian R. Lewis and Adam Woolley; Presider: Paul Bourassa

2:30  (105) Boron in Environmental and Human Hair Samples from Argentina, South America; Sarah Hill1, Neil I. Ward1; 1University of Surrey, UK

2:50  (106) A Flow Injection Analysis-based Colorimetric Method for Determination of Trihalooracetic Acid Concentrations in Wastewaters; Paul Simon1, Gija Gemi2, Gary Emmert1; 1The University of Memphis; 2University of Central Missouri

3:10  (107) Improving Analytical Confidence in the Determination of PCBs in Complex Matrices by a Sequential GC-MS/MS Approach; Joseph H. Aldstadt1, Beth A. Ruddy1, Diab T. Qadah1, Harvey A. Bootsma2; 1CPACT, University of Wisconsin-Milwaukee; 2Center for Great Lakes Studies

3:30  (108) A Capillary Membrane Sampling Gas Chromatography-Mass Spectrometry Method for the Analysis of Trihalomethanes in Drinking Water; Michael Brown1, Meggan Larson1, Gary Emmert1; 1The University of Memphis

3:50  (109) Isolation and Quantification of Perfluorinated Compounds in Drinking Water Supply Samples using SPE Preconcentration and LC/MS Detection; Min Yoon1, Lee Lippencott2, Ill Yang1, Eileen Murphy1, Brian Buckley1, 1Environmental and Occupational Health Sciences Ins; 2NJ Dept of Environmental Protection

4:10  (110) Determination of Caffeine in Soft Drinks by LCMSD Trap; Zainah Al-Ballam1, Nisar Ahmed; 1Kuwait Institute for Scientific Research

Monday Afternoon, Room L12
PROCESS ANALYTICAL MONITORING SAS TECHNICAL SESSION
Organizers and Presiders: Edita Botonjic and Brandye Smith-Goettler

2:30  (111) The Opportunities and Roadblocks to Use of Multivariate Analysis Tools in PAT and Product Development; Andy Scott; 1GlaxoSmithKline

2:50  (112) Process Analytical Technology (PAT) – Reducing the Cost of Quality and a Whole Lot More; Deborah Peru; 1Colgate Palmolive

3:10  (113) Process Analytical Technology in API manufacturing, -Sustainable Systems for Process Control; John O'Reilly

3:30  (114) Utilization of Process Analytical Technology for Automated Process Control in Pharmaceutical Drug Substance Manufacturing; Frank Sistare1; 1Pfizer Inc.

3:50  (115) The Advantages of Trace Chemical Analysis using On-Line Intracavity Absorption Spectroscopy Compared to Conventional Absorption Techniques; Nichola Townshend1, David Littlejohn1, Alison Nordon1, John Girkin1, Unzuzu Elejalede2; 1CPACT, University of Strathclyde; 2IoP, University of Strathclyde

4:10  (116) Process Analysis of Soybean Oil Conversion to Biodiesel; Dale LeCaptain1, William Kelley1, Brian Hales1; 1Central Michigan University

Monday Afternoon, Room L13
QUANTITATIVE RAMAN IN PHARMA
Organizer and Presider: Manoharan Ramasamy

2:30  (117) Quantitative Transmission Raman Spectroscopy of Pharmaceutical Solids; Jonas Johansson1, Anders Sparén1, Olof Svensson1, Staffan Folestad1, Mike Claybourn2; 1AstraZeneca R&D Molndal; 2AstraZeneca R&D Macclesfield

2:50  (118) Determination of the Relative Stabilities of Pharmaceutical Polymorphs and Solvates by Vibrational Spectroscopy; CJ Pommier1, Raymond Scaringe1; 1Bristol-Myers Squibb

3:10  (119) Raman Spectroscopy: A Powerful Tool in Preformulation; Chad Dalton1, Sophie-D. Clas1, Rafik Naccache1; 1Merek

3:30  (120) Application of Raman in Biologics Drug Product Development; Tapan Das1; 1Pfizer Global Biologics

3:50  (121) In Process Monitoring of Morphonic Form Conversion Kinetics using Raman Spectroscopy; Susan Barnes1, Joanne Anderson1, Katherine Bakeev1, Jun Chen1, Darryl Ertl1, James Rydzak1; 1GSK UK; 2GSK RTP

4:10  (122) Use of Raman for API Processing Controls: Development, Implementation and Validation; Jonathan Haulenbeek1, Ming-Hsing Huang1, Charles Ray1, Robert Wethman1, John Wasylyk1; 1Bristol-Myers Squibb Co.

Monday Afternoon, Room L14
COHERENT TWO-DIMENSIONAL SPECTROSCOPY I
Organizer: Wei Zhao; Presider: John Asbury

2:30  (123) Coherent Two Dimensional Vibrational Spectroscopy; John Wright1, Mark Rickard1, Kathry Kornau1, Nathan Mathew1, Andrei Pakoulev1; 1University of Wisconsin- Madison

2:50  (124) Propagation and Detection Distortions in Coherent 2D FT Spectra; David Jonas1; 1University of Colorado at Boulder

3:10  (125) Ultrafast 2D IR Vibrational Echo Chemical Exchange Spectroscopy; Junrong Zheng1, Michael Fayer1; 1Stanford University

3:30  (126) Two Dimensional Spectroscopy of Photosynthetic Complexes; Gregory Engel1,2,3, Elizabth Read1, Tessa Calhoun1, Gabriela Schlau-Cohen1,2,2, Graham Fleming1; 1University of Chicago; 2University of California Berkeley; 3Lawrence Berkeley National Laboratory

3:50  (127) Structures of Peptides Probed with Ultrafast Two-Dimensional Infrared Spectroscopy; Nien-Hui Ge1, Hiroaki Maekawa1, Soo Hwan Sul1, Claudio Toniolo1; 1University of California, Irvine, USA; 2University of Padova, Italy

4:10  (128) CARS Imaging: Instrumentation and Applications; Brian Saar1, X. Sunney Xie1; 1Harvard University

4:30  (129) Non-equilibrium Dynamics of Peptides using Two-Dimensional Infrared Spectroscopy; Matthew Tucker1, Yan Jiang1, Jianxin Chen1, Robin Hochstrasser1; 1University of Pennsylvania
TECHNICAL PROGRAM – TUESDAY
Plenary Sessions, Presider: Greg Klunder

ANACHEM Award
8:00 AM Plenary Session, Ballroom C/D

Isiah Warner

(130) An Analytical Chemist with a Focus on Separations
Research: Separation of Photons and Separation of Molecules; Isiah Warner; 1Louisiana State University
Refer to page 13 for biographical information

Charles Mann Award
8:30 AM Plenary Session, Ballroom C/D

Neil Everall

(131) Confocal Raman Microscopy: Where Are We Really Looking?; Neil Everall; 1Intertek MSG
Refer to page 13 for biographical information

TUESDAY MORNING POSTER SESSION
9:00 – 10:30 AM
Exhibit Hall, Ballroom A

All Tuesday morning posters should be put up between 7:30 – 8:00 AM and removed at 12:30 PM. The presenting author is expected to be present at the poster during the poster session 9:00 – 10:30 AM.

Absorption

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<tr>
<td>1</td>
<td>(132) Determination of Lead in Green Tea by Graphite-Furnace Atomic Absorption Spectrometry; Amina Ali; Rabaa Al-Kandari; Kuwait Institute for Scientific Research</td>
<td>1Louisiana State University</td>
</tr>
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<td>2</td>
<td>(133) On the Orientation of the Isocyanate Group in the First Excited State of p-Fluorophenylisocyanate: Narasimha Ayachit; Neeraja Rani G; SDM Coll of Eng &amp; Tech., Dharwad, Karnataka, INDIA</td>
<td>1Louisiana State University</td>
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Atomic Spectroscopy

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<td>3</td>
<td>(134) Determination of Rare Earth Elements by Tungsten Coil Atomic Emission Spectrometry; George Donati; Ji Gu; Bradley Jones; Wake Forest University</td>
<td>1Wake Forest University</td>
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<tr>
<td>4</td>
<td>(135) Arsenic Speciation in Pteris Cretica cv Mayii (Moonlight Ferns) using X-ray Absorption Spectrometry; David J. Butcher; Youngsoo Cho; James Bolick; Amitava Roy; Western Carolina University</td>
<td>1Western Carolina University</td>
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<td>5</td>
<td>(136) Recent Developments of Compositional Depth Profiling of Nanometer Films with GD-OES; Arne Bengtson; James Oliver; KIMAB</td>
<td>1KIMAB</td>
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Bioanalytical

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<td>6</td>
<td>(137) A Critical Comparison of Positively and Negatively-Charged Ion Structures using Ion Mobility-Mass Spectrometry; Niki V. Arinzhe; Janel R. McLean; 1Department of Chemistry, Vanderbilt University</td>
<td>1Vanderbilt University</td>
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<td>7</td>
<td>(138) Biosensors Based on Fluorescence Resonance Energy Transfer using Conjugated Liposomes; Xuelian Li; Punit Kohli; Southern Illinois University</td>
<td>1Southern Illinois University</td>
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<td>8</td>
<td>(139) Computational Methods for Enhancing Infrared Spectroscopic Imaging; Rohith Reddy; Rohit Bhargava; University of Illinois at Urbana-Champaign</td>
<td>1University of Illinois at Urbana-Champaign</td>
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Chemometrics

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<td>9</td>
<td>(140) Calibration Transfer between Near-Infrared Spectrometers; Dongsheng Bu; Camo Software Inc.</td>
<td>1Camo Software Inc.</td>
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<tr>
<td>10</td>
<td>(141) Detection Band Minimization for Molecular Differentiability using Deep UV laser Induced Native Fluorescence; Rohit Bhartia; William Hug; Arthur Lane; Pamela Conrad; Ray Reid; Jet Propulsion Laboratory; Photon Systems Inc</td>
<td>1Jet Propulsion Laboratory; 2Photon Systems Inc</td>
</tr>
<tr>
<td>11</td>
<td>(142) Determination of the Pure Spectrum of Major Protein Secondary Structures through Multi-Excitation UV Resonance Raman Spectra; John Simpson; Renee Ji; University of Missouri</td>
<td>1University of Missouri</td>
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Chromatography

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<th>Board #</th>
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<tr>
<td>12</td>
<td>(143) Improved Conversion of Thiols to Disulfides with Electrodeposited Catalysts; Ricky Risley; Phillip Voegel; Southeastern Louisiana University</td>
<td>1Southeastern Louisiana University</td>
</tr>
<tr>
<td>13</td>
<td>(144) The Monitoring of Methylmercury in Abyssal Fish Species Marketed in Korea; Chun-Soo Kim; Sohee Kim; Yong-Seok Ko; Kwang-Soo Lee; Mi-Ok Kim; Seong-Cheol Kim; Jeong-Min Kim; Dae-Byoung Kim; Busan Regional KFDA</td>
<td>1Busan Regional KFDA</td>
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Education

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<th>Board #</th>
<th>Title</th>
<th>Authors</th>
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<tbody>
<tr>
<td>14</td>
<td>(145) Using Elemental Composition to Identify Forensic Soil Samples: A Lab Experiment That Uses ICP-AES and Multivariate Analysis; Scott Goode; Daniel Sullivan; Amelia Taylor; University of South Carolina</td>
<td>1University of South Carolina</td>
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Environmental

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<th>Board #</th>
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<th>Authors</th>
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<tr>
<td>15</td>
<td>(146) Application of FTIR-ATR on Characterization of Soil Organic Carbon and Nitrogen Humification Processes; Xianzhi (Amanda) Song; Western Carolina University</td>
<td>1Western Carolina University</td>
</tr>
</tbody>
</table>
16  (147) Application of Post Column Reaction-Ion Chromatography with Nicotinamide Fluorescence to Emerging Disinfection By-Products in Drinking Water; Paul Simone1, Patricia Ranaito2, Gary Emmert1; 1University of Memphis
17  (148) Polyanilines and Their Diao Dyes for the Development of Optical Sensors; Nasir Ahmad1, Ramaier Narayanawany3; 1School of Chemical Eng. and Analytical Science

Fluorescence
18  (149) Fluorescence Imaging of Exocytotic Release and Free Radical Distribution in PC12 Cells; Irma Nydegger1, Donald M. Cannon Jr.; 1University of Iowa
19  (150) XRF as a Tool Substituting IC and ICP in Additives Quantification in Polymers; Ihab Odhe1, Angelika Clark1; 1SABIC Innovative Plastics

Inductively Coupled Plasma
20  (151) Sample Preparation of Human Placenta for Trace Element Analysis; Pamela Kruger1, Patrick Parsons1,2; 1State Univ of New York at Albany; 2New York State Dept of Health
21  (152) Determination of Mercury in Blood and Urine by CVAAS and ICP-MS; Ela Bakowska1, Michael Kraky1, Lindsay Altenberger1; 1NMS Labs
22  (153) Determination of I- and IO3- in Fresh Water using CE-ICP-MS; Yuichi Takaku1, Yoshihito Ohtsuka1, Shun’ichi Hisamatsu1; 1Institute for Environmental Sciences

Infrared
23  (154) FTIR Assessment of Changes in the Infrared Spectrum of Dimethylsiloxyane Following Passive Aquous Contact; D. Radford Shanklin1, David L. Smalley1,2; 1University of Tennessee, Memphis; 2Tennessee Department of Health

Kinetics
24  (155) Kinetic Studies of Emerging Disinfection By-Products and Disinfectants with Nicotinamide; Gija Geme1, Gary L. Emmert2; 1University of Central Missouri; 2University of Memphis

Mass Spectrometry
25  (157) Stability and Internal Energy Deposition of a Venturi-assisted Micromachined Array of Ultrasonic Electroscops for Mass Spectrometry; Gija Gemen1, Gary L. Emmert2; 1University of Central Missouri; 2University of Memphis
26  (158) Understanding Complex Ion Motion in FT-ICR Cells; Jill Scott1, Timothy McJunkin1, David Dahl1; 1Idaho National Laboratory

Molecular Spectroscopy
27  (159) Optimization of Quartz-Enhanced Photoacoustic Spectroscopy Sensor for Isotopologue Analysis using ab initio Calculations; Blythe Ashcraft1, S. McWhorter1, A.A. Kosterev2, R. Lascola1, F.K. Tittel1; 1Savannah River National Laboratory; 2Rice University, Rice Quantum Institute
28  (160) Chemical Imaging versus X-ray Microtomography to Reveal Single Kernel Morphology Desirable for Commercial End Use; David L. Wetzel1, Hulya Dogan1; 1Kansas State University

Other
29  (161) Structure Activity Relationship Studies of Synthesized Urea Diamides on CNS Depression and Sleeping Time Potentiation Effect; Dipeshkumar Chaudhary1, Dhruvo Sen1; 1Shri Sarvajanik Pharmacy College

Raman
30  (162) Wood Cell Wall Characterization by Raman Microscopy and Atomic Force Microscopy; Antti Kivioja1, Paula Eronen1, Monika Österberg1, Anna-Stina Jääskeläinen1; 1Helsinki University of Technology
31  (163) FT-Raman Investigation of the Ability of PBI-Based Polymer Electrolyte Membranes to be Doped with an Amphoteric Agent; George Voviatzis1, Stamatina Roma1, Dimitra Peristeraki1, Eyrosini Vogli1; 1FORTH/ICE-HT

Separations
32  (164) Extraction, Separation, and Detection of Four Important Alkaloids; Christine Copper1, Carl Newman2, Greg Collins3; 1United States Naval Academy; 2Naval Research Laboratory

Spectral Analysis
33  (165) Estimation of Chemical Information in Latex Suspensions using Light Transport Theory to Remove Multiple Scattering Effects; Raimundas Steponavicius1, Suresh Thennadil1; 1Newcastle University

Surface Characterization
34  (166) A Spectroscopic Approach of the Interaction of the RuO4(g) with a Polyethylene Oxide Surface; Badia Amekraz1, Andrea Salvatones2, Christophe Moulin1, Frédéric Miserque1, Alex Chenuere1, Cécile Blanc1, Isabelle Bisi1, Pierre Blanc2; 1DEN/DPC, CEA-Saclay; 2DEN/DRCP, CEA-Valrhô

Surface Plasmon Resonance
35  (167) Study Binding Affinity between Insulin,Insulin Growth Factors and G-quartet Forming Oligonucleotide by Surface Plasmon Resonance; Junfeng Xiao1, Jennifer Carter1, Linda McGown1; 1Rensselaer Polytechnic Institute

Tuesday Morning, Room L2 ELECTROTHERMAL AUTOMIZATION VS. ELECTROTHERMAL VAPORIZATION TECHNIQUES Organizer and Presider: M. T. C. de Loos Vollebregt
10:30  (168) Features and Prospects of Continuum Source ET AAS with High Spectral Resolution; Uwe Heitmann1; 1ISAS - Institute for Analytical Sciences
10:50  (169) ETV-ICPMS: the Right Tool for Solid Sampling?; Martin Resano1, Maria T. Aramendia1,2, Miguel A. Belarra1, Frank Vanhaecke2; 1University of Zaragoza; 2Ghent University
11:10  (170) Determination of Cadmium in Blood and Urine by Electrothermal AAS: the Quest for a Universal Modifier with the THGA; Patrick Parsons1, Bong-Ki Jang1; 1New York State Department of Health; 2Soonchunhyang University
11:30  (171) Pyrolysis Curves in Electrothermal Atomic Absorption Spectrometry vs Electrothermal Vaporization Inductively Coupled Plasma Mass Spectrometry; Margaretha de Loos-Vollebregt1, Alessandra da Silva1; 1Delft University of Technology
TECHNICAL PROGRAM – TUESDAY
Orals 10:30 AM – 12:30 PM

Tuesday Morning, Room L3
MASS SPECTROMETRY FOR BIOANALYSIS
Organizer and Presider: Ryan Kelly

10:30 (174) Recent Developments in Ion/Ion Chemistry for Bioanalysis; Scott McLuckey1; Purdue University
11:10 (175) Residue Specific Site Directed Dissociation of Whole Proteins in the Gas Phase; Ryan Julian1; Tony Ly2; University of California Riverside
11:30 (176) Plasma Biomarker Discovery and Analysis using FT-ICR Mass Spectrometry; David Muddiman1, Adam Hawkridge1, Taufika Williams1, William Cliby2, John Burnett3; NC State University; 4Mayo Clinic College of Medicine
11:50 (177) Using Normalized Spectral Abundance Factors to Visualize Protein Complexes; Michael Washburn1; Stowers Institute for Medical Research
12:10 (178) Multiplexed Electrospray Sources for Improving the Sensitivity and Quantitation of Proteomics Measurements; Ryan Kelly1, Jason Page1, Keqi Tang1, Richard Smith1; Pacific Northwest National Laboratory

Tuesday Morning, Room L4
SPECTRAL AND MULTIWAY PATTERN RECOGNITION
Organizer and Presider: Frank Vogt

10:30 (179) Trilinear Analysis of Images Obtained with a Hyperspectral Imaging Confocal Microscope; Mark H. Van Benthem1, Michael B. Sinclair1, Rachel M. Noek1, Howland D. T. Jones1, David M. Haaland1, Allan R. Brasier1, Ping Liu2; Sandia National Laboratories; 3University of Texas Medical Branch
11:10 (180) Oriented Partial Least Squares: Theory and Application; William Rayens1, Yushu Liu1, Anders Andersen1, Charles Smith1; University of Kentucky
11:30 (181) Parallel Factor Analysis – Partial Least Squares Discriminant Analysis (PARAFAC-PLSDA) Applied to Third and Fourth Order Data Tensors; Karl Booksh1; 4University of Delaware; 5AFRL-APG Site
11:50 (182) Quantitative Results from Single Particle Characterization Data; Philip Hoppke1; Clarkson University
12:10 (183) Chemometrics Environmental Chemistry; Romá Tauler1; CSIC-IIQAB
12:10 (184) Wavelets and Genetic Algorithms Applied to Spectral Pattern Recognition; Barry Lavine1, Nikhil Mirjankar1, Kadambari Nuguru1; Oklahoma State University

Tuesday Morning, Room L5
MOLECULAR SPECTROSCOPY IN FORENSIC SCIENCE
Organized by the Forensic Technical Section of the Society for Applied Spectroscopy
Organizer and Presider: Mary Carrabba

10:30 (185) Forensic Investigation of Biological Threats; Kathryn Kalasinsky1; Armed Forces Institute of Pathology
10:50 (186) Colorimetric Analysis of Glass Fragments; Paul Martin1, Mike Eyring2, John Hoang3; 4CRAIC Technologies, Inc.; 5Micro Forensics, Ltd.; 6Arizona Dept. of Public Safety
11:10 (187) Pushing the Envelope for Fiber Analysis by UV/Visible and Fluorescence Microspectrophotometry; Stephen L. Morgan1, Edward G. Bartick2; 1University of South Carolina; 3Suffolk University
11:30 (188) The Merits and Pitfalls of the Forensic Analysis of Dyed Textile Fibers using Raman; Edward Bartick1, Brandi Vann1, Michael Angel1, Stephen Morgan1; 1University of South Carolina; 3Suffolk University
11:50 (189) Molecular Spectroscopy Coupled with Polarized Light Microscopy: Case History at FCC; John Crowe1, Mark Witkowski2; 1FDA Forensic Chemistry Center
12:10 (190) Validation Studies for Detection of Blood on Substrates of Forensic Relevance by Fourier-Transform Infrared (FT-IR) Spectroscopy; Anthony R. Trimboli1, Heather M. Taylor1, Stephen L. Morgan1; 1University of South Carolina

Tuesday Morning, Room L6
ANACHEM AWARD SYMPOSIUM IN HONOR OF ISIAH M. WARNER
Organizer and Presider: Victoria McGuffin

10:30 (191) Analytical Chemists' Best Friend: NIR Fluorescence Spectroscopy; Gabor Patonay1, L Strekowski1, JS Kim1, M Henary1; 4Georgia State University
10:50 (192) Isolating Interactions in Complex Fluids using Multivariate Optical Spectroscopy; Sharon Neal1; 1University of Delaware
11:10 (193) Carbon Micro and Nanomaterials Used in Separation Science; Susan Olesiak1, Justin Shearer1, Jeremy Steach1, Jonathan Clark2; 1Ohio State University
11:30 (194) Aptamers and Beyond: DNA Binding Ligands for Affinity Analysis; Linda McGown1, Jacqueline Cole1, Elizabeth Morgan1; 1Rensselaer Polytechnic Institute
11:50 (195) Spectroscopic Investigations of Chiral Recognition; Matthew McCarrol1; Jeremy Buckingham1, Irene Kimari1, Yafei Xu1; 1Southern Illinois University
12:10 (196) Mechanistic Studies of Chiral Separations; Victoria McGuffin1, Kaysab Gebre-Yohannes1; 1Michigan State University

Tuesday Morning, Room L11
NIR IMAGING
Organizer and Presider: Caroline Rodger

10:30 (197) “Processability” of Solids - The need to Understand the Matrix; Fiona Clarke1, Steve Hammond1; 4Pfizer
TECHNICAL PROGRAM – TUESDAY
Orals 10:30 AM – 12:30 PM and Poster Session 1:45 – 3:15 PM

Tuesday Morning, Room L12
ISA ANALYSIS DIVISION – BEST OF THE BEST
Organizer and Presider: Gary Brewer

10:30 (203) Field Experience with a Single NDUV and TCD Analyzer on A Mine Based Tail Gas Treating Units; Daniel Potter1, Kevin Harris1, Phil Harris2, Randy Hauer3, Byron Lewis4; 1AMETEK Process Instruments; 2ALON USA; 3HARITEC

11:10 (201) NIR Imaging and Quantitative Analysis of Inhomogeneous Pharmaceutical Formulations; Gary McGeorge1, John P. Bobiak2; 1Bristol-Myers Squibb

11:30 (200) Applications of Near Infra Red (NIR) Imaging for Understanding Pharmaceutical Performance; Caroline Rodger1, Mike Claybourn1, Vicki Woodward1; 1AstraZeneca, Macclesfield

11:50 (199) Approaches for Measuring the Micro and Macro Chemical and Physical Heterogeneity of Pharmaceutical Products and Their Intermediates; E. Neil Lewis1, Linda H. Kidder1, Suzanne J. Hudak1, Janie Dubois1, Kenneth S. Haber2; 1Malvern Instruments

Tuesday Morning, Room L13
CURRENT ANALYTICAL TECHNOLOGIES FOR DRUG DISCOVERY
Organizer and Presider: Bing Yan

10:30 (209) NMR in Drug Discovery; Michael Shapiro1; 1University of Maryland

11:10 (210) Automated LC/MS Purification of Lead Compounds using a Focused Gradient Approach; Jiang Zhao1, Thomas Swann1; 1BMS

11:30 (211) High-Throughput Bioanalysis of Drugs and Their Metabolites in Pharmaceutical Industry by LC/MS/MS; Perry Wang; 1Arrow International

12:10 (212) Strategies for Implementing Fast Liquid Chromatography in Pharmaceutical R&D in a GMP Environment; Zhong Li1; 1Merck Research Laboratories

Tuesday Morning, Room L14
COHERENT TWO-DIMENSIONAL SPECTROSCOPY II
Organizer: Wei Zhao; Presider: Nie-Hui Ge

10:30 (213) Applications of Multidimensional Vibrational Spectroscopies to Complex Materials; Dana Dilto1; 1University of Illinois at Urbana-Champaign

10:50 (214) Recent Advances and New Applications for 2D IR Spectroscopy; Martin Zanni1; 1University of Wisconsin-Madison

11:10 (215) Charge Transfer and Carrier Mobility in OPV Materials Examined with Ultrafast Multidimensional Infrared Spectroscopy; John Asbury1, Larry Barbou1, Maureen Hegadorn1, Ryan Pensack1; 2Penn State University

11:30 (216) Novel Relaxation-Assisted 2D IR Spectroscopy Method; Igor Ruchtsy1, Sri-Ram Naraharisetty1, Dmitry Kurochkin1, Valeriy Kasyanenko1; 1Tulane University

11:50 (217) Ultrafast IR Spectroscopy of Active Electronic Materials; Aaron Massari1, Andrei Eigner1, Jason Peterson1; 1University of Minnesota, Twin Cities

12:10 (218) Femtosecond Electronic Collinear 2D Spectroscopy; Ivan Piletic1, Martin Fischer1, Warren Warren1; 1Duke University

12:30 PM, Room 201, Ballroom Level
Student/Professional Panel Discussion and Box Lunch
I’m graduating soon. What’s Next?
Sponsored by SABIC Innovative Plastics

TUESDAY AFTERNOON POSTER SESSION
1:45 – 3:15 PM
Exhibit Hall, Ballroom A

All Tuesday afternoon posters should be put up between 12:45 – 1:15 PM and removed by 5:00 PM. The presenting author is expected to be present at the poster during the poster session 1:45 – 3:15 PM.

Absorption

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<tbody>
<tr>
<td>1</td>
<td>VCSEL Oxygen Spectroscopy for Structural Analysis of Pharmaceutical Tablets</td>
<td>Tomas Svensson1, Mats Andersson1, Jonas Johansson2, Sune Svanberg3, Stefan Andersson-Engels1, Staffan Folestad2; 1Dept. of Physics, Lund University, Sweden; 2Astra Zeneca R&amp;D, Mölndal, Sweden</td>
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Atomic Spectroscopy

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<tr>
<td>2</td>
<td>Determination of Mercury Utilizing Cold Vapor UV Photoreduction with in-Atomizer Trapping</td>
<td>Jillian Lennartz1, Jeremy Madden1, Neil Fitzgerald1; 1Marist College</td>
</tr>
<tr>
<td>3</td>
<td>SPE and Cd in Urine Determination using ICP-AES</td>
<td>Kathryn Pharr1, Brad Jones1; 1Wake Forest University</td>
</tr>
</tbody>
</table>
4 (222) Theoretical and Experimental Investigation of Laser Analytical Spectroscopy of Noble Metals(Au, Pt, Ag) by Method of Resonance Laser Ionization Spectroscopy; Atakam Khalmanov  
1Samarkand State University

Bioanalytical

5 (224) Investigation of Small Molecule Induced Global Secondary Structure Changes in the Beta-Amyloid Peptide using UV Resonance Raman; John Simpson 1, Mingjuan Wang 1, Patricia Joiner 1, Renee Jiji 1  
1University of Missouri

Biological

6 (225) Determination of Urinary Iodine by Inductively Coupled Plasma Mass Spectrometry; Amina Ali 1, Rabaa Al-Kandari 1, Kuwait Institute for Scientific

Chromatography

7 (226) On-Column Measurement of Density of a Compressible Fluid; L. Robert Baker 1, Marisa A. Stark 1, Steven R. Goates 1  
1Brigham Young University

Correlation Spectroscopy

8 (227) Structure Characterization of Human Surfactant Protein C Mutants Using Infrared Spectroscopy and 2D Correlation Analysis; Yu Zhu 1, Tharanga Diyunugala 1, John E Baatz 2, Richard A Dluhy 1  
1Univ of Georgia, Chemistry Dept.; 2Med Univ S Carolina, Dept Pediat

Education

9 (228) Applications of FTIR-ATR and X-ray Fluorescence (XRF) in the Art Conservation Program at Queen's University, Kingston, Canada; H. F. (Gus) Shurvell 1, Alison Murray 1  
1Queen's University

Environmental

10 (229) Extraction of Polycyclic Aromatic Hydrocarbons from Water Samples with Gold Nanoparticles; Huiyong Wang 1, Andres Campiglia 1  
1University of Central Florida

11 (230) Analysis of Condensed-Phase Aerosols using Infrared Photothermal Spectroscopy with Optical Beam Deflection (Mirage Effects); Ohuwatosin O Dada 1, Stephen E Bialkowski 1  
1Utah State University

12 (231) First Test Strip Approved for Regulatory Testing; Ivars Jaunakais 1, Maris Jaunakais 1, Howard Ray 1  
1Industrial Test Systems, Inc.; 2MJ Analytical Consulting

Fluorescence

13 (232) Fluorimetric Determination of Enoxacin using Tb Composite Nanoparticles; Mohammad Maimul Karim 1, Sang Hak Lee 1  
1Dept of Chemistry, Kyungpook National University

14 (233) Interaction of Lactoferricin B with Membranes: a Physico-Chemical Approach; Marijolaine Arseneault 1, Sarah Bedard 1, Maxime Boulet-Audet 1, Michele Auger 1, Michel Pezolet 1  
1CERSIM/CREFSIP, Chemistry Dept., Université

Forensic

15 (234) Drug Fingerprinting using Isotope Ratio Mass Spectrometry: Sourcing of Active Pharmaceutical Ingredients (APIs); Jonathan Litzau 1, Thomas Brueggemeyer 1  
1U.S. Food & Drug Administration

Inductively Coupled Plasma

16 (235) Determination of Titanium in High-Calcium Matrices using Multi-Component Spectrum Fitting with ICP-OES; Matthew Hanley 1, Steve Eckdahl 1, John Butz 1  
1Mayo Clinic

Infrared

17 (236) Analysis of Double-Strand Helix of Linear Polycrylonitrile by Infrared Multiple-Angle Incidence Resolution Spectrometry; Takeshi Hasegawa 1, Hiroyuki Kakuda 1, Tetsuo Okada 1  
1Tokyo Institute of Technology; 2JST PRESTO

18 (237) Attenuated Total Reflectance Infrared Spectroscopy (ATR-FTIR): a Quantitative Approach for Kidney Stone Analysis; Heather Golley-Stahl 1, Jenn Haas 1, Andrew Evans 1  
1Miami University; 2Indiana University School of Medicine

19 (238) Spatially Resolved FT-IR Microspectroscopy of the Nutritional Status of Stream Algae; David L. Wetzel 1, Justin N. Murdock 2, Walter Dodds 3  
1Microbeam Mol. Spec. Lab., Kansas State University; 2Div. of Biology, Kansas State University

20 (239) Application of ATR FT-MIR Spectroscopy for Rapid Identification of API in Pharmaceutical Drug Products; Jay Dodd 1  
1Abbott Laboratories

Instrumentation

21 (240) Kinetics in a Levitated Drop Microreactor and Related Myeloperoxidase Behavior; Alexander Scheeling 1, Christopher Field 1, Zakiah Pierre 1  
1University of Illinois at Urbana-Champaign

Laser Spectroscopy

22 (241) Evanescent-Wave Cavity Ring-Down Spectroscopy for Enhanced Detection of Surface Binding under Flow Injection Analysis Conditions; Freerk Ariese 1, Lineke van der Snepen 1, Joost B. Buijs 1, Cees Gooijer 1, Wim Ubachs 1  
1Laser Centre Vrije Universiteit Amsterdam

Mass Spectrometry

23 (242) Identification of Impurities in Choline Hydroxide in Water by LC/MS; Lilia Rousseva 1, Wayne Priitts 1  
1Abbott Laboratories

24 (243) Infrared Ablation/Ultraviolet Matrix-assisted Laser Desorption Ionization Mass Spectrometry; Fan Huang 1, Kermit Murray 1  
1Chemistry Dept, LSU

25 (244) High-throughput LDI MS Imaging using a Tunable High Repetition Rate IR Laser; Mark Little 1, Eli Margalith 1, Kermit Murray 1, Yohannes Rezenom 1  
1Louisiana State University

26 (245) Ion Signal Temporal Profiles in Pulsed Direct Current Glow Discharge Mass Spectrometry: Effects of Sampling Distance, Power, and Pressure; Megan DeJesus 1, James H. Barnes IV 2, Fred L. King 1  
1West Virginia University; 2Los Alamos National Laboratory

27 (246) Bioaerosol Ion Mobility Mass Spectrometry of Biological Agent Detection; Juaneka M. Hayes 1, Kermit K. Murray 1, Michael V. Ugarov 2, J. Albert Schultz 2, Juaneka Hayes 1, Juaneka Hayes 1, Juaneka Hayes 1, Juaneka Hayes 1, Louisiana State University; 2Ionwerks, Inc.
## TECHNICAL PROGRAM – TUESDAY

### Afternoon Poster Session 1:45 – 3:15 PM and Orals 3:15 – 5:15 PM

### Nanotechnology

| 28 | (247) Controlling the Organization of Porphyrins on Surfaces using Nanolithography; Zorabel M. LeJeune, Stephanie Daniels, Erhong Hao, Jie-Ren Li, M. Graca H. Vicente, Jayne C. Garmo; 1Louisiana State University |

### Raman

| 31 | (250) Surface-Enhanced Raman Spectroscopy Evidence for Hyaluronic Acid Polymer Entanglement at Nanoliter Volumes; Karen A. Esmonde-White, Gurjit S. Mandair, Michael D. Morris; 1University of Michigan, Biomedical Engin; 2University of Michigan, Chemistry |

| 32 | (251) New Tunable Notch Filter for Resonant Raman Spectroscopy; Matthieu Paillet, Marc Verhaegen, François Meunier, Richard Martel, Sébastien Blais-Ouellette; 1Université de Montréal; 2Photon etc. Inc. |

### Surface Enhanced Raman Spectroscopy

| 33 | (252) Plasmonic Tip Enhanced Raman Scattering of Strained Silicon with Single and Multiple Probes; Aaron Lewis, Rimma Dekhter, Hesham Taha; 1Nanonic Imaging Ltd. |

| 34 | (253) SERS on Mirror Substrates; George Chumanov, Mark Kinnan; 1Clemson University |

### Tuesday Afternoon, Room L2

**CURRENT ADVANCES IN ICPMS FROM THOSE THAT KNOWS**

Organizer and Presider: James A. Holcombe

| 3:15 | (254) Development of a Robust Method to Assess the Speciation of Arsenic in Seafood; Vincent Dufailly, Laurent Noël, Thierry Guérin, Jean-Marc Frémy; 1AFSSA-DERNS-UERPC; 2Queen's University |

| 3:35 | (255) Using ETV-Need for Preanalysis Separations ICP-MS for Sr/Rb Geochronological Dating without Preanalysis Separations; Adam Rowland, James Holcombe; 1Dept. of Chem. and Biochem. Univ. of Texas, Austin |

| 3:55 | (256) Multichannel Array Detection for Plasma Source Mass Spectrometry; Gregory D. Schilling, Francisco J. Andrade, James H. Barnes, IV, Roger P. Sperline, M. Bonner Denton, Charles J. Barinaga, David W. Koppennaal, Gary M. Hieftje; 1Indiana University; 2Los Alamos National Laboratory; 3University of Arizona; 4Pacific Northwest National Laboratory |

| 4:15 | (257) Spectroscopic Imaging of Argon Metastable Atoms between the Load Coil and the Sampling Cone of an ICP-MS; Haibin Ma, Paul Farnsworth; 1Brigham Young University |

### Tuesday Afternoon, Room L3

**CAPILLARY ELECTROPHORESIS**

Organizers: Adam Woolley and Ian R. Lewis; Presider: Isiah Warner

| 3:15 | (260) Electrophoretic Effects of the Adsorption of Anionic Surfactants to Poly(dimethylsiloxane)-Coated Capillaries; Maria Mora, Carla Giacomelli, Carlos Garcia; 1University of Texas at San Antonio; 2Universidad Nacional de Cordoba |


| 3:55 | (262) Investigation of Homocysteine Thiolactone-induced Protein Modification; Arthur Gates, Mark Lowry, Kristin Fletcher, Abitha Merugeshu, Oleksandr Rusin, James Robinson, Robert Strongin, Isiah Warner; 1Louisiana State University |

| 4:15 | (263) Diode-Laser Induced Fluorescence Capillary Electrophoresis for Fluorescamine-labeled Amino Acid Analysis from Biological Samples; Nikolay Kochevoy, Jeannita Pritchett, Scott A Shippy; 1University of Illinois at Chicago |

| 4:35 | (264) Development of a Portable Capillary Electrophoresis NMR System for Chemical Speciation; Julie Herber, Greg Klunder, Ysven Malba, Chris Harvey, Lee Evans, Vicky Demas; 1Lawrence Livermore National Laboratory |

| 4:55 | (265) The Development of a Non-Aqueous Capillary Electrophoresis-High Resolution Inductively Coupled Plasma Mass Spectrometry; Xiaodong Bu, Tiebang Wang, Qiang Tu; 1Merck Research Lab |

### Tuesday Afternoon, Room L4

**ELECTROCHEMISTRY AND FUNCTIONAL NANOMATERIALS**

Organizer and Presider: Shaowei Chen

| 3:15 | (266) In situ Microscope FTIR Spectroscopy and Its Applications in Nanomaterials Studies; Shi-Gang Sun, Zhi-You Zhou, Yan-Xia Jiang, Sheng-Pei Chen, Chun-Hua Zhen; 1Department of Chemistry, Xiamen University, China |

| 3:35 | (267) Synthesis and Characterization of Selective Electrocatalysts in the Nanoscale Length for Fuel Cell Reactions; Nicolas Alonso-Vante; 1University of Poitiers, UMR-CNRS 6503 |

| 3:55 | (268) Single-Walled Carbon Nanotubes Decorated with Pd Nanoparticles for High-Performance, Flexible Hydrogen Sensors; Yungang Sun; 1Argonne National Laboratory |

| 4:15 | (269) New-phased Nanostructures Designed for Lithium-ion Batteries Applications; Yi Xie; Changzheng Wu; 1University of Science and Technology of China |

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**Future Meetings:** FACSS 2008, September 28 – October 2, Reno, NV  •  FACSS 2009, October 18 - 22, Louisville, KY 59
## TECHNICAL PROGRAM – TUESDAY

**Orals 3:15 – 5:15 PM**

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<th>Time</th>
<th>Session</th>
<th>Title</th>
<th>Authors</th>
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<tr>
<td>4:35</td>
<td>(270) Novel Nanostructured, Composite Electrodes as Anodes Improved Anode Material for Direct Alcohol Fuel Cells</td>
<td>Diego Diaz; 1University of Central Florida</td>
<td></td>
</tr>
<tr>
<td>4:55</td>
<td>(271) Electronic Communication of Redox-Active Mieties on Ruthenium Nanoparticle Surfaces</td>
<td>Shaowei Chen; 1UC Santa Cruz</td>
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<td>3:15</td>
<td>(272) Electron Detachment Dissociation FTICR Mass Spectrometry for the Full Structural Characterization of Glicosaminoglycan Carbohydrates</td>
<td>J. Jonathan Amster, Jeremy J. Wolff, Tatiana Laremore, Robert J. Linhardt; 1University of Georgia; 2Renselaer Polytechnic Institute</td>
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<td>4:15</td>
<td>(275) Ionic Liquids as Matrices for MALDI Mass Spectrometry</td>
<td>Michael L. Gross; 1Washington University</td>
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<td>4:35</td>
<td>(276) Oligonucleotide-modified Fused Silica Surfaces for Affinity-MALDI-TOF-MS of Proteins</td>
<td>Jacquelyn Cole, Ashley Tennyck, Linda McGown; 1Rensselaer Polytechnic Institute</td>
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<td>4:55</td>
<td>(277) Large Scale Quantitative Analysis of Non-coding RNAs (ncRNAs) by their Signature Digestion Products using Stable Isotope Labeling and MALDI-MS</td>
<td>Mahmood Hassan, Patrick A. Limbach; 1University of Cincinnati</td>
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### Tuesday Afternoon, Room L5

**NOVEL METHODS FOR BIOLOGICAL MASS SPECTROMETRY**

Organizer and Presider: Kermit K. Murray

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### Tuesday Afternoon, Room L6

**STUDENT AWARDS**

Organizer: S. Douglass Gilman; Presider: James Rydzak

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<td>3:15</td>
<td>(278) Subsurface and Transcutaneous Raman Tomography using a Ring/Disk Fiber Optic Probe and Iterative Reconstruction</td>
<td>Matthew V. Schulmerich, Subhadra Srinivasan, Jaclynn M. Kreider, Jacqueline H. Cole, Ethan L. H. Daley, Katherine T. Dooley, Victoria Popescu, Steven A. Goldstein, Brian W. Pogue, Michael D. Morris; 1University of Michigan, Dept. of Chemistry; 2University of Michigan, Dept. of Orthopaedic Surgery; 3Dartmouth, Thayer School of Engineering</td>
</tr>
<tr>
<td>3:35</td>
<td>(279) Application of GC-Triple Quadrupole Mass Spectrometry for Rapid Functional Group Identification in Protonated Oxygen-containing Compounds and Their Mixtures</td>
<td>Sen Li, Penggao Duan, Michael Watkins, Brian Winger, Todd Gillespie, Hilkka Kenttamaa; 1Purdue University; 2Eli Lilly and Company</td>
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<td>3:55</td>
<td>SAS Poster Winner – TBA</td>
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<td>4:15</td>
<td>SAS Poster Winner - TBA</td>
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### Tuesday Afternoon, Room L11

**NIR APPLICATIONS IN THE PHARMACEUTICAL INDUSTRY**

Organizer and Presider: Katherine Bakeev

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<tr>
<td>3:15</td>
<td>(281) NearIR in the Process Lab: From Development to Validation</td>
<td>Jonathan Haulenbeck, Ming-Hsing Huang, Charles Ray, John Wasylyk; 1Bristol-Myers Squibb Co</td>
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<td>3:35</td>
<td>(282) Multiparameter Tablet Analysis By NIR Spectroscopy: From Dose Uniformity to Dissolution Testing</td>
<td>Manel Alcala, Marcelo Blanco; 1Universitat Autonoma de Barcelona</td>
</tr>
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<td>4:15</td>
<td>(284) Differentiation and Quantitative Determination of Surface and Hydrate Water in Lyophilized Mannitol Using NIR Spectroscopy</td>
<td>Wenjin Cao, Chen Mao, Wendy Chen, Hong Lin, Sampathkumar Krishnan, Nina Cauchon; 1Amgen Inc.; 2Purdue University</td>
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<td>4:35</td>
<td>(285) Efficacy of the Drug Tagitose Effected by Vibrational Microspectroscopy</td>
<td>David L. Wetzel, Robert A. Loder; 2Kansas State University; 3University of Kentucky</td>
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<td>4:55</td>
<td>(286) The Hard Facts: Spectral Effects of Relative Density and Radial Tensile Strength</td>
<td>Steven M. Short, Zhenqi Shi, Brian M. Zacour, Robert P. Cogdill, Peter L.D. Wildfong, Carl A. Anderson; 1Duquesne University</td>
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### Tuesday Afternoon, Room L12

**APPLICATIONS OF FLUORESCENCE SPECTROSCOPY AND RELATED TECHNIQUES**

Organizer and Presider: Andres D. Campiglia

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<th>Time</th>
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<td>3:15</td>
<td>(287) Wetting and Molecular Transport in Hydrophobic Pores at Nanometer Dimension Studied with Quantitative Confocal Fluorescence Imaging</td>
<td>M. Lei Geng, Zhenming Zhong, Reyan Freeynek, Mark Lowry; 1University of Iowa</td>
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<tr>
<td>3:35</td>
<td>(288) Excited State Dynamics in Conjugated Polymer Devices</td>
<td>Andre Guesquiere, Daeri Tenery, James Worden; 1University of Central Florida</td>
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<tr>
<td>3:55</td>
<td>(289) Excitation-Emission Matrix Fluorescence Spectroscopy to Differentiate Among Classes of Microorganisms as Vegetative or Spore</td>
<td>Karl Booksh, Burt Bronk, Jeffrey Cramer, Jozsef Czege; 1University of Delaware; 2AFRL-APG Site</td>
</tr>
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</table>
TECHNICAL PROGRAM – TUESDAY
Orals 3:15 – 5:15 PM

4:15 (290) Attenuation of Mediator Leakage in Biofuel Cell Polymer Modified Electrodes: Synthesis and Characterization of a Perfluoroalkyl-modified 2,2′-bipyridyl Ruthenium Complex; Paul Jelliss1, Shelley Minteer1, Mitesh Patel1, Michelle Watt1; 1Saint Louis University

4:35 (291) Luminescence Spectroscopy of Dye-doped Silica Nanoparticles and Quantum Dots; Swadshmukul Santra; 1University of Central Florida

4:55 (292) Artificial Nose Technology: Fluorescent Labeled DNA Optical Sensor Arrays with Enhanced Sensitivity and Selectivity for Detection of Biological Agents; Scott McWhorter1, C. Milliken1, R. Brignon1, A. Walker2, J. White2, J. Kauer2; 1Savannah River National Laboratory; 2Cogniscent, Inc.

Tuesday Afternoon, Room L14
CHARLES MANN AWARD IN HONOR OF NEIL EVERALL
Organizer and Presider: Michael D. Morris

3:15 (293) Numerical Simulations of Confocal Raman Spectroscopic Depth Profiles of Materials: A Photon Scattering Approach; Averil Macdonald1, Alun Vaughan2; 1University of Reading; 2University of Southampton

3:55 (294) Probing and Predicting Low Frequency, Raman-active Lattice Modes in Pharmaceutical Drug Polymorphs; Mike Claybourn1, Graeme Day2; 1AstraZeneca; 2Cambridge University

4:35 (295) Raman at 2200 m Below Sea Level: Challenges and Opportunities; Brian Marquardt; 1University of Washington

Tuesday Afternoon, Room L13
EMERGING TECHNOLOGIES FOR HOMELAND SECURITY
Organizer and Presider: Greg Klunder

3:15 (296) First-Principles Analyses of Solid-State Terahertz Spectra; Timothy Korter1, Damian Allis1; 1Syracuse University

3:35 (297) Standoff Raman HE Field Measurements: Issues Related to Standoff Detection; Chance Carter1, Mike Angel2, Joseph Kords1, Darron Nielsen1, Will Hunt1, Michael Chrisp1, Fred Howland1, Jim Hill1, Bruce Henderer1, Richard Whipple1, Del Eckels1, Christine Paulson1, Paul Steele1, Marion Lawrence-Snyder2, Jon Scaffidi2, Jasmine Erwin2; 1Lawrence Livermore National Laboratory; 2Dept. of Chem., Univ. of South Carolina

3:55 (298) A Piezoresistive Cantilever-Based Sensor for Gas-Phase Chemical Detection; Bradley Hart1, Timothy Ratto1, Albert Loui1, Thomas Wilson1, Erik Mukerjee1, Todd Sulchek1; 1Lawrence Livermore National Laboratory

4:15 (299) Gas phase Photoacoustic Spectroscopy in the long-Wave IR using Quartz Tuning Forks and Amplitude Modulated Quantum Cascade Lasers; Michael Wojcik1, Mark Phillips1, Elizabeth Golovich1, Bret Cannon1, Rich Ozanich1, Jay Grate1; 1Pacific Northwest National Laboratory

4:35 (300) Novel Method Development for Analysis of High Energy Peroxides by Raman Microscopy and Mass Spectrometry; Alvaro Peña-Quevedo1, Robert Cody1, Samuel Hernandez-Rivera1, 1University of Puerto Rico at Mayaguez; 2JEOL USA Inc.

4:55 (301) Examination of Forensic Evidence by Hyperspectral Imaging; Diane Williams1, Hina Ayub2; 1Federal Bureau of Investigation; 2Oak Ridge Institute of Science Education

FACSS 2008 ♦ September 28 – October 2 ♦ Grand Sierra Resort ♦ Reno, Nevada
Network with fellow scientists ♦ Experience and contribute new and exciting scientific developments in all areas of analytical chemistry and spectroscopy ♦ Plenary speakers and awards symposia from internationally recognized scientists
Come celebrate the 50th Anniversary of the Society for Applied Spectroscopy
Governing Board Chair: Gary Brewer (gary.brewer@us.abb.com); General Chair: John Hellgeth (john.w.hellgeth@hp.com)
Program Chair: Greg Klunder (klunder1@llnl.gov)
TECHNICAL PROGRAM – WEDNESDAY
Plenaries, Presider: Greg Klunder

William F. Meggers Award
8:00 AM Plenary Session, Ballroom C/D

Richard Mendelsohn

(302) Vibrational Spectroscopy, Microscopy and Imaging: Applications to Skin Pharmacology and Biochemistry; Richard Mendelsohn1, Guojin Zhang1, Andrew Chan1, David Moore2, Ryan Pensack1, Bozena Michniak1, Carol Flach1, 1Rutgers University; 2ISP Corporation
Refer to page 20 for biographical information

Coblentz Society Clara Craver Award
8:30 AM Plenary Session, Ballroom C/D

Katherine A. Bakeev

(303) Increased Process Understanding through Use of in-situ Vibrational Spectroscopy; Katherine Bakeev1, Susan Barnes1, Stacie Calad1, Jun Chen1, Robert Herrmann1, Juliet McComas1, James Rydzak1, Eric Voight1, 1GlaxoSmithKline
Refer to page 22 for biographical information

WEDNESDAY MORNING POSTER SESSION
9:00 – 10:30 AM
Exhibit Hall, Ballroom A

All Wednesday morning posters should be put up between 7:30 – 8:00 AM and removed at 12:30 PM. The presenting author is expected to be present at the poster during the poster session 9:00 – 10:30 AM.

<table>
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<th>Absorption</th>
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<tr>
<td>Board #</td>
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<tr>
<td>1  (304) Spectrophotometric Methods for Estimation of Acenocoumarol in Bulk and Its Pharmaceutical Dosage Forms; Sunil Makwana1, Dr.LakshamanBhai Patle1, Tejas Patle1, Tushar Patle1, Kirir Patle1, Timir Patle1, Amit Patle2, Ankita Mehta1; 1Faculty of Pharmacy,Dharmsinh Desai University; 2R.P.college of pharmacy, Changa; 2Department of Pharmaceutical Analysis</td>
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<th>Atomic Spectroscopy</th>
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<td>2  (305) Capabilities of a Desolvating Nebulizer System with Multicollector ICP-MS; Fred Smith1, 1CETAC Technologies</td>
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<td>3  (306) Analysis of Biodiesel and Petroleum Products Utilizing a Simultaneous CCD Detector ICP-OES System; Doug Shrader1, Steve Wall1, Andrew Ryan1; 1Varian, Inc.</td>
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<th>Bioanalytical</th>
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<tr>
<td>4  (307) Homogenous Fluorescence Resonance Energy Transfer Assays for Identification of Inhibitors of Angiogenesis and Anthrax Toxin Receptors using High Throughput Screening; Kenneth Christensen1, Michael Rogers23, Junhong He1, Nalini Anumula1; 1Clemson University; 2Children's Hospital Boston; 3Harvard Medical School</td>
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<tr>
<td>5  (308) Interchanging role of Donor and Acceptor in a Fluorescence Resonance Energy Transfer Experiment; Erastus Gatebe1, Punit Kohli1; 1Southern Illinois University</td>
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<tr>
<td>7  (310) Stability of Phosphorus in Stool Samples Measured by ICP-AES and ICP-MS; Ela Bakowska1, Anthony Costantino1, Anna Foror1, Gulo Gigolashvili1; 1NMS Labs</td>
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<th>Chromatography</th>
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<tr>
<td>8  (312) Application of 1H-NMR to Screen Cell-culture Media Additives: Evaluation of Data Pre-processing Methods and Selective Chemical Variation; Julie Wei1, Maureen Lanan1; 1Biogenidec Inc.</td>
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<th>Electrochemistry</th>
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<td>9  (313) Protein Separations Using Polyelectrolyte Multilayer Coatings with a Molecular Micelle: Optimization and Stability of Coatings; Candace Luces3, Sayo Fakayode3, Mark Lowry3, Isaiah Warner1; 1Louisiana State University</td>
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<th>Education</th>
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<tr>
<td>10 (314) New Spectroscopy Reference Tool for Academic Research and Teaching; Donald Tucker1, Leo Collins1, Gregory Banik1, Marie Scandone1; 1Bio-Rad Laboratories, Inc., Informatics Division</td>
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<th>Chemistry</th>
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<td>11 (315) Controlled Particle Deposition by Design of an Electrochemical Adsorption Cell; Fatemeh Ahmiki1, Ehsan Bakhshi2, Majid Mosalla3; 1Pardis group of National Petrochemical Co.&amp; Isfah; 2National Petrochemical Co. &amp; NIOC R&amp;D C; 3Materials Science Dept. of Shiraz University</td>
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### Technical Program – Wednesday

**Posters 9:00 – 10:30 AM**

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<td><strong>Environmental</strong></td>
<td>(316) Mass Spectrometric Speciation of Ultrafine Particulate Matter Formed by the Ozonolysis of Household Volatile Organic Compounds; Kara Huff Hartz¹, Hardik Amin¹, Meagan Hatfield¹; 2Southern Illinois University</td>
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<td>13</td>
<td><strong>Determination of Dissolved and Colloidal Silver in Water Using Colorimetric-Solid Phase Extraction</strong></td>
<td>Robert Lipert¹, April Hill¹, Marc Porter¹; 2Iowa State University; 3Arizona State University</td>
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<td>14</td>
<td><strong>Assessing the Impact of Hurricane Katrina on Nutrients and Algal Growth in Lake Maurepas</strong></td>
<td>Phillip Voegel¹, Kellie Silcio¹, Kristy Ball¹; 3Southeastern Louisiana University</td>
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<td>15</td>
<td><strong>Fluorescence</strong></td>
<td>(319) Ultra-Trace Beryllium Determination by a Fluorescence-Based Field-Portable Method; Kevin Ashley¹, Anoop Agravat², T. Mark McCleskey²; ¹CDC/NIOSH, Cincinnati, OH; 2Berylliant, Inc., Tucson, AZ; 3Los Alamos National Laboratory</td>
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<td>16</td>
<td><strong>Inductively Coupled Plasma</strong></td>
<td>(320) Macro ATR Imaging – Another Imaging Solution; David Drapcho¹, Ellen Misco¹; 3Varian, Inc</td>
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<td>17</td>
<td><strong>Infrared</strong></td>
<td>(321) Accurate Determinations of Ge Atom Fractions in SiGe Semiconductor Chips using High Performance ICP-OES; Savales Rabb¹, Michael Winchester¹, Lee Yu¹; 2National Institute of Standards and Technology</td>
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<td><strong>Fluorescence</strong></td>
<td>(322) Monitoring Changes in Protein Structure and Hydration in Food Materials with FT-IR, FT-Raman and Fluorescence Spectroscopy; Allen R Murosky¹, Douglas L Elmore¹, Sean A Smith¹, Carrie A Lendon¹, Janiece L Hope¹, Stefan K Baier¹, Jodi A Engleson¹, William R Aimutis¹; 1Cargill</td>
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<td>19</td>
<td><strong>An Infrared PLS Approach for Compositional Analysis of Polycarbonate, SAN, and Rubber Alloys</strong></td>
<td>Roger Hurst¹, Lei Li¹, James DeRudder¹, Yujian Liu¹; 1SABIC Innovative Plastics; 2WR Grace</td>
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<td>20</td>
<td><strong>Instrumentation</strong></td>
<td>(324) Development of a Portable Ringdown Spectrometer for CO2, CH4, and C-13 Isotope; Chuij Wang¹,², Nimisha Srivastava¹, John Cambre², Bryan Jones¹; 1Dept. Physics and Astronomy, MSU; 2ICET, MSU; 3Dept. of Electrical and Computer Eng, MSU</td>
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<td>21</td>
<td><strong>Laser Ablation</strong></td>
<td>(325) Improved in situ Measurements of Lead Isotopes in Silicate Glasses by LA-MC-ICPMS using Multiple Ion Counters; A. Kate Souders¹,², Paul Sylvestre¹,²; 1Micro-Analytical Facility, INCO Innovation Centre; 2Dept. of Earth Science, Memorial Univ</td>
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<td>22</td>
<td><strong>Mass Spectrometry</strong></td>
<td>(326) Direct Chromium Speciation in Solid State Materials - A GDMS Approach; Na Zhang¹, Jennifer Robertson-Honecker¹, Alex Pavkovich¹, Melissa Pabic¹, Fred King¹; 1West Virginia University</td>
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<td>23</td>
<td><strong>Drug Screening Applications Using NPC Spin Columns with HPLC/ESI-MS</strong></td>
<td>Marshall M. Siegel¹; 1Wyeth Research</td>
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<td>24</td>
<td><strong>Structural Characterization Strategies for Simultaneous Glycomics and Proteomics using Ion Mobility-Mass Spectrometry</strong></td>
<td>Larissa S. Fenn¹, John A. McLean¹; 2Vanderbilt University</td>
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<td>25</td>
<td><strong>Redistribution Behavior of Group IA and IIA Metals on Porous Oxide Surfaces Modified by Laser Irradiation</strong></td>
<td>Anita Gianotto¹, Recep Avci², Muhammed Deliorman³, Eric Williams³, Marnie Cortez³, Gary Groenewold³, Robert Fox³; 1Idaho National Laboratory; 2Montana State University</td>
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<td>26</td>
<td><strong>Microscopy</strong></td>
<td>(330) Measurement of Heterogeneous Rate Constants: Reaction of Allyl Bromide at Indium Surfaces; Walter Bowyer¹, Yessica Baez Sosa¹, Estefani Giordano¹, Anne Sessler¹, Isabel Olson¹; 2Hobart and W. Smith Colleges</td>
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<td><strong>Molecular Spectroscopy</strong></td>
<td>(331) Infrared and Raman Microscopy: Complimentary or Redundant Techniques?; Thomas Tague¹; 2Bruker Optics, Inc.</td>
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<td><strong>Imaging</strong></td>
<td>(332) Imaging of Organic Polymer Films Deposited on Infrared Reflecting Glass Reveals Heterogeneities; David L. Wetzel¹, Daniel A. Higgins¹, Corey R. Wetzel¹; 2Kansas State University</td>
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<td><strong>Nanotechnology</strong></td>
<td>(333) Progressive Stages of Crystal Growth of Porphyrin-Cobaltacarborane Conjugates Captured by AFM; Wilson K. Serem¹, Erhong Hao¹, Frank Froneczek¹, M. Graça H. Vicente¹, Jayne C. Garna¹; 1Louisiana State University</td>
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<td><strong>Optical Scattering</strong></td>
<td>(334) Nonlinear Spectroscopy of Cadmium Chalcogenide Quantum Dots; Seongmin Ma¹, William Yu¹, JaeTae Seo¹, Qiguang Yang¹, Bagher Tabibi¹, Vicki Colvin⁴, Jinhwa Heo¹, Wanjoong Kim¹, Sungsu Jung¹; 1Department of Physics, Hampton University, Hampton; 2Department of Chemistry, Rice University; 3Korea Research Institute of Standards</td>
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<td>31</td>
<td><strong>Raman</strong></td>
<td>(335) Rapid Measurements of optical Scattering using a Portable Photon Time-of-Flight Device; Francis Esmonde-White¹, David Burns¹; 2McGill University</td>
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<td><strong>High Speed Imaging Developments in Raman Spectroscopy</strong></td>
<td>(336) High Speed Imaging Developments in Raman Spectroscopy; Matthew Bloomfield¹, Ken Williams¹, Richard Bormett¹; 2Renishaw, plc; 3Renishaw, Inc</td>
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<td>33</td>
<td><strong>Wide Area Illumination (WAI) Raman Scheme</strong></td>
<td>(337) Wide Area Illumination (WAI) Raman Scheme for Reliable Quantitative Analysis of Etching Solution and Petrochemical Product; Hoeffl Chung¹, Jaejin Kim¹, Kyungtae Ryu¹, Yongdan Kim¹, Mark Kemper¹; 1Hanyang University; 2Kaiser Optical Systems</td>
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<td><strong>Analysis of the Composition of Biological Apatites by Raman Spectroscopy and Ion Chromatography</strong></td>
<td>(338) Analysis of the Composition of Biological Apatites by Raman Spectroscopy and Ion Chromatography; Mary Tecklenburg¹, Sh Rhonda Dennis¹, Adam Peral¹, Ayorinde Awonusi¹, Amy Marcotte¹, Robert Buckland¹, Monaliza Sirbecsu¹; 1Central Michigan University</td>
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<td>35</td>
<td><strong>Development of an Inductively Coupled Plasma/Electrospray Ionization Dual-Source Time-of-Flight Mass Spectrometer for Rapid Speciation and Metallomic Analysis</strong></td>
<td>(339) Development of an Inductively Coupled Plasma/Electrospray Ionization Dual-Source Time-of-Flight Mass Spectrometer for Rapid Speciation and Metallomic Analysis; Dianna A. Rogers¹, Steven J. Ray¹, Gary M. Hieftje¹; 1Indiana University</td>
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TECHNICAL PROGRAM – WEDNESDAY
Orals 10:30 AM – 12:30 PM

Wednesday Morning, Room L2
BIOMEDICAL APPLICATIONS OF ATOMIC SPECTROMETRY
Organizers: Mike Foulkes and Andy Fisher and Presiders: Patrick Parsons and Chris Harrington

10:30 (340) Arsenic and Mercury Speciation: Challenges and Successes; Carl Verdon1, Kathleen Caldwell2, Robert Jones1, Olga Piraner1, Mark Fresquez1, Christopher Freedman1, Cynthia Ward1, Graylin Miller1; 1Centers for Disease Control and Prevention

10:50 (341) Bone Lead Measurement by Non-Invasive KXRF: Results of an Interlaboratory Study and Traceability to ICP-MS; Patrick J. Parsons1, David J. Bellis1, Katherine M. Hetten1, Neeta R. Ginde1, Peter Mata1, Andrew C. Todd2; 1New York State Department of Health; 2Mount Sinai School of Medicine

11:10 (342) CDC Biomonitoring by ICP-DRC-MS, Enhancements to a More Efficient Autosampler and MoO Correction on Cd; Kathleen L. Caldwell1, Robert L. Jones1, Jeff Jarrett1, Ge Xiao1, Gulchekhra Shakirova1, Melanie Granlün1, Neva J Mullinix1; 1CDC/NECHE/DLS/IRAT

11:30 (343) Microdistribution of Trace Elements in Biological Tissues: a Comparison between LA-ICP-MS and Mj-XRF; David J. Bellis1, Zewu W. Chen1, Walter M. Gibson1, Dula Amarasiriwardena1, Patrick J. Parsons1; 1New York State Department of Health; 2X-ray Optical Systems; 3Hampshire College

11:50 (344) Intra- and Inters-Individual Variability of Copper, Selenium and Zinc in Serum and the Determination of Analytical Quality Specifications; Andrew Taylor1, 2, 12 other colleagues; 1University of Surrey; 2Network of EQAS Organisers

12:10 (345) The Determination of Platinum Containing Drug Adducts with DNA by a Combination of HPLC-ICP-MS and LC-ESI-MS/MS; Chris Harrington1, Rachel Le Pla1, Peter Farmer1; 1Biocentre, University of Leicester

Wednesday Morning, Room L3
BIOANALYTICAL MICROFLUIDICS
Organizer and Presider: Carlos Garcia

10:30 (346) Routine Monitoring of Ambient Aerosols using Microchip Electrophoresis; Charles Henry1, Scott Noblit1, Jeffery Collet, Jr1, Susanne Hering2; 1Colorado State University; 2Aerosol Dynamics, Inc

10:50 (347) Some low-Cost, Low-Resolution Microfabrication Alternatives for Electrophoresis Microchips and Bioanalytical Applications; Emanuel Carrilho1, Wendell Coltro1, Evandro Piccin1; 1University of Sao Paulo

11:10 (348) Barrowing Techniques from Microfluidics to Construct Miniaturized FIA Components and Devices; Gary Emmert1, Lucy Thurston1, Kyoo Dong Jo1; 1The University of Memphis

11:30 (349) Electroosmotic Flow Dynamics in Response to Biological Sample Adsorption; S. Douglass Gilman1, Funda Kizilkaya1, Jianhui Xiong1, Katie Blumssack1; 1Dept. of Chemistry, Louisiana State University

11:50 (350) Novel Valve Actuation and Applications in Microfluidics; Frank Gomez1, Attila Gaspar1, Menake Piyasena1, Schetema Stevens1, Marisol Salgado1; 1California State University, Los Angeles

12:10 (351) Development of Lab-on-a-Chip Biosensor for Glucose Based on a Packed Immobilized Enzyme Reactor; Carlos D. Garcia1, Lucas Blanes2, Maria F. Mora1, Claudimir Do Lago1, Arturo Ayon1; 1The University of Texas at San Antonio; 2Universidade de Sao Paulo

Wednesday Morning, Room L4
NANOTUBES AND NANOWIRES FOR SENSING I
Organizer: Jason Holt and Pehr Persson; Presider: Jason Holt

10:30 (352) Biochemical and Gas Sensing with a Novel Subwavelength Photonic Platform; Donald Sirbul1, Nicholas Fischer1, Timothy Ratto1, Jeff Tok1, Aleksandr Noy1; 1Lawrence Livermore National Laboratory

11:10 (353) The Sensitivity Limits of Nanowire Bio-Sensors; Xuan Gao1,2, Gengfeng Zheng1, Charles Lieber1; 1Harvard University; 2Case Western Reserve University

11:30 (354) Piezolectric Nanogenerators Based on Zinc Oxide Nanowire Arrays; Jimhui Song1, Z.L. Wang1; 1Georgia Tech

11:50 (355) Thermal Properties and Single Particle Tracking of Gold Nanoshells in Lipid Vesicles and Cell Membranes; Matthew Clark1, HyeongGon Kang1, Peter Yim1, Rani Kishore1, Kristian Helmerson1, Jeeseong Hwang1; 1NIST

12:10 (356) DNA-Assisted Purification and Assembly of Single-Walled Carbon Nanotubes; Germaric Sanchez-Pomales1, Nelson E. Rivera-Velez1, Lenibell Santiago-Rodriguez1, Carlos R. Cabrera1; 1University of Puerto Rico-Rio Piedras Campus

Wednesday Morning, Room L5
PARTICLE MASS SPECTROMETRY: TECHNIQUES AND APPLICATIONS
Organizer and Presider: Michael P. Tolocka

10:30 (357) Mass Spectrometry of Nanoparticles in the Atmosphere; Murray Johnston1, Melissa Reinard1, Christopher Zordan1, Matthew Dryfus1, Katherine Heaton1, Julie Lloyd1; 1University of Delaware

10:50 (358) Using Aerosol Chemical Ionization Mass Spectrometry (CIMS) to Study Radical-Initiated Oxidation of Organic Particles; Geoffrey Smith1, John Hearn1, Lindsay Renbaum1; 1University of Georgia

11:10 (359) Aerosol Mass Spectrometry: Aerosol Chemical and Microphysical Properties; Achim Trimborn1, Timothy Onasch1, Manjula Canagaratna1, Jesse Kroll1, Dagmar Tramborn1, Mike Cubison1, Jose Jimenez1, John Jayne1, Douglas Worsnop1; 1Aerodyne Research; 2University of Colorado

11:30 (360) High-Speed, Quantitative Analysis of Particle Chemistry using a Time-of-Flight Aerosol Mass Spectrometer; Joel Kimmel1, Peter DeCarlo1, Jose-Luis Jimenez1, Doug Worsnop2; 1University of Colorado; 2Aerodyne Research, Inc.

11:50 (361) Application of Photoelectron Resonance Capture Ionization Aerosol Mass Spectrometry to Internally Mixed Amino Acid-Lipid Particulate Proxies of Marine Organic Aerosols; Giuseppe Petrucci1, Scott Geddes1, James Zahardis1; 1University of Vermont

12:10 (362) Negative Ion Chemical Ionization Mass Spectrometry of Aerosol Organic Matter; Joel Thornton1, Reddy Yatavelli1, Faye McNeill1; 1University of Washington, Seattle
TECHNICAL PROGRAM – WEDNESDAY
Orals 10:30 AM – 12:30 PM

Wednesday Morning, Room L6
THE COBLENZSOCIETY CLARA CRAVER AWARD
SYMPOSIUM IN HONOR OF KATHERINE BAKEEV
Organizer and President: John Hellgeth

10:30 (363) Multidisciplinary Characterization of a Novel Anhydride and Amine Functionalized Polymer from Reactive Extrusion; Nancy Jestel¹, Mark Demnston¹, Mark Pietrafesa¹, Alex Sokolowski¹, Carl Strom¹, David Zoller¹; ¹SABIC Innovative Plastics
10:50 (364) Efficacy of Model NIR Calibrations for Determining Ethanol Content in Spirits; W.F. McClure; ¹NC State University

11:10 (365) Aquaphotomics: VIS – NIRS Absorbance Pattern of Water Matrix as Biological Marker; Roumiana Tsenkova; ¹Kobe University

11:30 (366) Comparison of NIR Instruments for Grain Analysis; David Himmelshab¹, Mireyong Sohn¹, Kevin Hicks², Franklin Barton, II²; ¹USDA-ARS-RRBRC, Athens, GA; ²USDA-ARS-ERRC, Wyndmorr, PA

11:50 (367) NIR Calibration Transfer – Tight Wavelength Control using a Rare-Earth Standard; William Muller¹; ¹FOSS NIRS, Inc.

12:10 (368) Intermediate-Frequency Raman Modes for the Lower Optical Transitions of Semiconducting Single-Walled Carbon Nanotubes; Fotios Papadimitrakopoulos¹, Zhentang Luo¹, Stephen K. Doorn²; ¹Nanomaterials Optoelectronics Laboratory, Department of Chemistry, Polymer Program, Institute of Materials Science, University of Connecticut; ²Chemistry Division, Los Alamos National Laboratory

Wednesday Morning, Room L11
ADVANCES IN FTIR IMAGING
Organizer and Presider: Rohit Bhardwaja

10:30 (369) The Role of FT-IR Spectral Imaging in Helping to Resolve a Pet Food Contamination Issue; Curtis Marcott¹, Gloria M. Story¹, Anthony E. Dowrey¹, Andrew S. Fix¹, Athlea Pullen¹, Adrienne Bigalow-Kern¹, R. Thomas Cambron²; ¹The Proctor & Gamble Company; ²Procter & Gamble Pharmaceuticals

10:50 (370) Spectral Imaging for Parallel High-Throughput Screening; Jochen Lauterbach; ¹University of Delaware

11:10 (371) Augmenting Spectroscopic Imaging for Analyses of Samples with Complex Surface Topographies; Michael Gilbert¹, Frank Vogt¹; ¹University of Tennessee

11:30 (372) Synchrotron Infrared Microspectroscopy Imaging using a Multi-Element Detector (IRMSI-MED) for Diffraction-Limited Chemical Imaging; Carol Hirschmug¹, Michael Nasse¹, Tim Kubala¹, Sebastian Janowski¹, Ruben Reininge¹; ¹Department of Physics, University of Wisconsin-Mil; ²Synchrotron Radiation Center, University; ³Scientific Answers & Solutions, Madison

11:50 (373) Implementing FT-IR Spectro-Imaging as a Biomedical Molecular Imaging Modality; Cyril Petibois¹,²; ¹University of Bordeaux 2; ²CNRS UMR 5084

12:10 (374) Practical Aspects of Automated Histopathology using FTIR Imaging; Rohit Bhardwaja¹, Rohith Reddy¹, Rong Kong¹, Frances Keith¹, Gokulakrishnan Srinivasan¹; ¹University of Illinois at Urbana-Champaign

Wednesday Morning, Room L12
INITIATIVE (NESSI) TO IMPROVE PROCESS QUALITY AND CONTROL
Organizer and Presider: Brian J. Marquardt

10:30 (375) NeSSI, Miniaturization, and Microminiaturization Benefits for Finer Control in Chemical Analysis; David Simku¹; ¹Swagelok Company

10:50 (376) NeSSI: An Enabling Platform for the Major Reduction in Total Cost of Ownership in Process Analytical Systems; Peter Van Vuuren; ¹Process Analytics Consultant

11:10 (377) Application of NeSSI at UOP: From Laboratory Applications to Commercial Process Monitoring; Falahah Falih¹; ¹UOP LLC

11:30 (378) NeSSI Generation 2: A New Initiative Creates New Opportunities for Smart Sampling Systems; Robert Farmer¹; ¹Siemens Energy & Automation, Inc.

11:50 (379) Analytics and Sample Handling; William Cost¹; ¹Parker Hannifin

12:10 (380) NeSSI Bus-based Intrinsically-safe Electromechanical Sample Conditioning System Component Developments; Robert E. Sherman; ¹CIRCOR International, Inc.

Wednesday Morning, Room L13
OPPORTUNITIES FOR RAMAN SPECTROSCOPY
Organizer: Ian R. Lewis; Presider: Jeri Timlyn

10:30 (381) Improved Probe Designs for Transcutaneous Raman Spectroscopy with Spatial Separation of Illumination and Collection Regions; Kathryn A. Douley¹, Matthew V. Schulerich¹, Ethan Daley¹, Steven A. Goldstein¹, Michael D. Morris¹; ¹Department of Chemistry, University of Michigan; ²Orthopaedics Research Laboratory, University of Michigan

10:50 (382) Raman Spectroscopic Studies of Surfactants Effects on Heme Protein Structure; Manliang Feng¹, Hiroyasu Tachikawa¹; ¹Jackson State University

11:10 (383) Low Power Deep UV Raman Spectroscopy; William Hug¹, Rohit Bhartia¹, Arthur Lane², Ray Reid; ¹Photon Systems; ²California Institute of Technology/JPL

11:30 (384) Total Internal Reflection Raman Spectroscopy in Paper and Print Analysis; Antti Kivioja¹, KaustavGuh¹, Eric Tyrode¹, Anna-Stina Jäskeläinen¹, Colin Bain¹, Tapani Vuorinen¹; ²Helsinki University of Technology; ³University of Durham

11:50 (385) A Small Volume Flow Cell for Raman Spectroscopic and Spectroelectrochemical Studies of Heme Proteins; Manliang Feng¹, Hiroyasu Tachikawa¹; ¹Jackson State University

12:10 (386) SERS Microscopy (µSERS): Selective and Sensitive Protein Localization in Tissue Specimens; Sebastian Schlücker¹, Bernd Küsten¹, Friedrich Schöppler¹, Carina Jahn¹, Alexander Marx², Philipp Ströbel¹; ¹Inst. of Phys. Chemistry, University of Wuerzburg; ²Inst. of Pathology, Clinics of Mannheim

Future Meetings: FACSS 2008, September 28 – October 2, Reno, NV • FACSS 2009, October 18 - 22, Louisville, KY

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TECHNICAL PROGRAM – WEDNESDAY
Orals 10:30 AM – 12:30 PM and Poster Session 1:45 – 3:15 PM

Wednesday Morning, Room L14
ANALYSIS AND MODELING OF SPECTRAL DATA
Organizers: Ian R. Lewis and Frederick Koehler
Presenter: Jeremy Shaver

10:30  (387) Mixture Selection Algorithms for Choosing Mixture Calibration Standards; J. Brian Loudenmilk1, Franklin E. Barton II2, David S. Himmelbach3, James A. de Haseth1; 1The University of Georgia; 2United States Department of Agriculture

10:50  (388) Automated Wavelength Selection for Spectroscopic Fuel Models by Symmetrically Contracting Repeated Unmoving Window Partial Least Squares; Jeffrey Cramer1, Kirsten Kramer1, Kevin Johnson1, Robert Morris1, Susan Rose-Pehrsson1; 1U.S. Naval Research Laboratory

WEDNESDAY AFTERNOON POSTER SESSION
1:45 – 3:15 PM
Exhibit Hall, Ballroom A
All Wednesday afternoon posters should be put up between 12:45 – 1:15 PM and removed by 5:00 PM. The presenting author is expected to be present at the poster during the poster session 1:45 – 3:15 PM.

Board #

Atomic Spectroscopy

1  (393) Real-time Measurement of Elemental Mercury Naturally Evaporating from Contaminated Samples Using Cavity Ringdown Spectroscopy; Susan Scherrer1, Chuij Wang1, F-X. Han1, Xiyang Yuan1; 1Department of Chemistry, Vanderbilt University

Bioanalytical

2  (394) Lead and Tin in Roman Bronze Coins by Atomic Absorption Spectrometry; Mary Kate Donais1, Ashley Dumas1, Kathleen Golden1, Holly Jakubowski1; 1Saint Anselm College

Biological

3  (395) Development of a High Performance Electrospray-Ion Funnel Interface for Biomolecular Ion Mobility-Mass Spectrometry; Sevugaran Sundarapandian1, John A. McLean1; 1Department of Chemistry, Vanderbilt University

Chemometrics

4  (397) FT-IR Microspectroscopic Detection of Gene Expression and Determining Its Extent in Wheat; David L. Wetzel1, Shilpa Sood2, Bikram S. Gill1; 1Kansas State University

5  (398) Introducing Chemometrics to the Analytical Curriculum—Combining Theory and Lab Experience; Frank Vogt1, Michael Gilbert1, Robert Luttrell1; 1University of Tennessee, Dept of Chemistry

Chemometrics

6  (399) Selection of an appropriate Chiral Selector for Chiral Analysis by Regression Modeling of Spectral Data; Selmor Modzabi1, Marianna A. Busch1, Kenneth W. Busch1; 1Baylor University

7  (400) Profiling Drugs by Fourier Transform Infrared/Affinitiye Total Reflectance Spectrometry and Principal Component Analysis; Huggins Z. Msimanga1, Robert Ollis2; 1Kennesaw State University; 2Georgia Bureau of Investigation

8  (401) Real-time Detection of Aerosolized Biological Compounds using a Fluorescence Based Detector; Brian Dable1, Geoff Wilson1, Jim Brady1, Mike Carrabba1; 1Hach Homeland Security Technologies

Education

9  (402) Open Access Education in the Analytical Sciences through the Analytical Sciences Digital Library; Alexander Scheeling1; 1University of Illinois at Urbana-Champaign

Electrochemistry

10  (403) Voltammetric Characterization and Optimization of Nanoscale Architectures for Bioanalysis; Timothy M. Paschkewitz1, Donald M. Cannon, Jr.; 1University of Iowa

Fluorescence

11  (404) Effect of pH on the Voltammetric Response of Cystiene at Chemically Modified Electrodes; Kristy Ball1, Ashley Hanna1, Phillip Voegel1; 1Southeastern Louisiana University

Forensic

12  (405) 3-D LIF for Trace Analysis; Lam Nguyen1, Eli Margalith1; 1OPOTEK, Inc.

Inductively Coupled Plasma

13  (406) A Highly Sensitive Method for the Determination of Dissolved Organics in Aqueous Media by Transfection FTIR; Ali Koek1, Amira Badan1, Susan Berets2, Joseph Lucania1; 1John Jay College of Criminal Justice; 2Harrick Scientific Products, Inc.

Future Meetings: FACSS 2008, September 28 – October 2, Reno, NV  •  FACSS 2009, October 18 - 22, Louisville, KY
### Infrared

16. (409) Application of Six Sigma DMAIC Methodology in Infrared Spectroscopy of Polymers; Eugene Galperin, \(^1\)SABIC Innovative Plastics

17. (410) FTIR Studies of Supported Lipid Layers Formed using Nanospheres and Cylindrical Nanopores; Todd Wells, \(^1\)Kristin Kryszak, \(^1\)Ignacio Garcia, \(^2\)Christine Stewart; \(^1\)University of Denver

### Laser Spectroscopy

19. (412) Nonlinear Spectroscopy Studies of Ultrafast Relaxation Dynamics in CdTe Quantum Dots; Marion Greene, \(^1\)Qiguang Yang, \(^1\)William Yu, \(^1\)SeongMin Ma, \(^2\)JaeTae Seo, \(^2\)Bagher Tabibi, \(^2\)Vicki Colvin, \(^3\)Wanjoong Kim, \(^3\)Seongsoo Jung; \(^1\)Department of Physics, Hampton University, Hampton; \(^2\)Department of Chemistry, Rice University; \(^3\)Korea Research Institute of Standards

### Mass Spectrometry

20. (413) Comparative Analysis of Phospholipid Profiles of Saccharomyces cerevisiae by Matrix Assisted Laser Desorption/Ionization Fourier Transform Mass Spectrometry (MALDI FTMS); \(^1\)S. Maricor Batoy, \(^1\)Sabine Borgmann, \(^2\)Jeffrey Jones, \(^3\)Peter Kaiser, \(^4\)Charles Wilkins; \(^1\)University of California, Irvine

21. (414) Development of an Automated Digestion and Deposition Chip Coupled to MALDI-TOF MS for Proteomics; \(^1\)Jeonghoon Lee, \(^1\)Steven A. Soper, \(^1\)Kermit K. Murray; \(^1\)Louisiana State University

22. (415) Laser Desorption Ion Mobility Mass Spectrometry for Biological Agent Detection; Juaneka M. Hayes, \(^1\)Kermit K. Murray, \(^2\)Michael V. Ugarov, \(^3\)J. Albert Schultz; \(^1\)Louisiana State University; \(^2\)Ionwerks, Inc.

23. (416) Rapid Screening for Functional Groups via Selective Ion-Molecule Reactions in a Linear Quadrupole Ion Trap Mass Spectrometer; \(^1\)Steven Habicht, \(^1\)Nelson Vinueza, \(^1\)Penggao Duan, \(^2\)Sen Li, \(^1\)Brian Winger, \(^2\)Todd Gillespie, \(^1\)Hilkka Kenttämaa; \(^1\)Purdue University; \(^2\)Eli Lilly and Company

### Materials Characterization

24. (417) Problems Arising Out of Impurities in Steam Turbines; Fatemeh Abniki, \(^1\)Ehsan Bahkshi; \(^2\)National Petrochemical Co.; \(^3\)Isfahan Univ. of Tech.; \(^4\)R&D Center of National Petrochemical Co.

25. (418) Studying Corrosion of Coated Titanium Anodes in a Corrosive Solution; \(^1\)Ehsan Bahkshi, \(^1\)Fatemeh Abniki; \(^2\)R&D Center of National Petrochemical Co.; \(^3\)Ghadir Petrochemical Company(NPC branch)

### Molecular Spectroscopy

26. (419) Excited State Electric Dipole Moment of two Tryptamine Derivatives through Solvatochromic Shifts; Neeraja Rani Gaddipati, \(^1\)Narasimha Ayachit; \(^1\)SDM College of Engg & Tech., Dharmaw, India

### Nanotechnology

27. (420) An Application of Graphs of Atomic Orbitals for QSAR Modeling of Toxicity of Metal Oxides; Bakhtiyor Rasuley, \(^1\)Andrey Toropov, \(^1\)Tomasz Puzyn, \(^1\)Danuta Leszczynska, \(^2\)Jery Leszczynski; \(^1\)CCMSI, Jackson State University, Jackson, MS 39217; \(^2\)Civil & Env. E, Jackson State University

### Nuclear Magnetic Resonance

28. (421) Assignment of High Resolved 13C NMR Spectra of Polycyanonitrile with Heptads; Yusong Wang, \(^1\)Fei Lu, \(^1\)Wenmin Pang, \(^1\)Qingren Zhu, \(^1\)Weitai Wu, \(^1\)Guoyong Xu, \(^1\)Lianghua Xu; \(^1\)University of Science and Technology of China; \(^2\)Beijing University of Chemical Technology

### Raman

29. (422) Universal Raman Detection – Dispersive NIR Raman (DNIR-Raman) above 1 Micron; Keith Carron, Rick Cox, Shane Boller; \(^1\)DeltaNu

30. (423) What is “Imaging” in Raman Spectral Imaging, and Why Should I Care?: Jay Zakrzewski; \(^1\)Headwall Photonics, Inc.

### Surface Characterization

31. (424) Thin Film Structure of Poly (2-perfluoro-octylethyl acrylate) Studied by Infrared Multiple-Angle Incidence Resolution Spectroscopy; \(^1\)Masaya Matsunaga, \(^1\)Kiyoshi Yamamoto, \(^1\)Takeshi Hasegawa; \(^1\)ASAHI Glass Co., LTD.; \(^2\)Tokyo Institute of Technology

### Surface Plasmon Resonance

32. (425) Surface Plasmon Resonance Optical Fiber Platform for Real-Time Oxygen Sensing; \(^1\)Veronica Rigo, \(^2\)Peter Geissinger; \(^1\)University of Wisconsin-Milwaukee

### Wednesday Afternoon, Room L2 DEVELOPMENTS IN PLASMA SPECTROSCOPY, Organized by SAS Atomic Spectroscopy Technical Section

3:15. (426) New Plasma Sources for Elemental, Molecular, and Metallomic Analysis; \(^1\)Gary Hieftje, \(^2\)Francisco Andrade, \(^3\)Gerardo Gamez, \(^4\)Steven Ray, \(^5\)Gregory Schilling, \(^6\)Jacob Shelley, \(^7\)Michael Webb; \(^1\)Indiana University

3:55. (427) True Comprehensive Speciation of Nutraceuticals through Liquid Chromatography-Particle Beam/Glow Discharge Mass Spectrometry; \(^1\)R. Kenneth Marcus, \(^2\)Joaumdir Castro, \(^3\)M. V. Balarama Krishna; \(^4\)Clemson University

4:15. (428) Gas Dynamics of an ICP Torch; \(^1\)Albert Gilmudtinov, \(^2\)Rinat Ibragimov, \(^3\)Mjakzjum Salakhov, \(^4\)Ila L. Tsvilskii; \(^1\)Kazan State University

4:35. (429) Laser Ablation-Inductively Coupled Plasma Mass Spectrometry – Ablation Characteristics of Zirconium and NIST Glass; \(^1\)Detlef G"unther, \(^2\)Barbara Kuhn, \(^2\)Yan Luo; \(^1\)Laboratory of Inorganic Chemistry, ETH Zurich, Wol; \(^2\)Department of Earth and Environmental Science
### TECHNICAL PROGRAM – WEDNESDAY

**Orals 3:15 – 5:15 PM**

**Wednesday Afternoon, Room L3**

**ELECTROPHORETIC AND MICROFLUIDIC BIOANALYSIS**

Organizer: Ian R. Lewis and Adam Woolley
President: Michael Sepaniak

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Title</th>
<th>Authors</th>
</tr>
</thead>
<tbody>
<tr>
<td>3:35</td>
<td>(432)</td>
<td>Automated Analysis of Amino Acids in Human Vitreous using a Low-Volume Sample Introduction Device</td>
<td>Eric Patterson, Sujeewa Pyankarage, Scott Shippy, University of Illinois-Chicago</td>
</tr>
<tr>
<td>3:55</td>
<td>(433)</td>
<td>Affinity Monolith Preconcentrators for Polymer Microchip Capillary Electrophoresis: Weichun Yang, Tao Pan, Xiuhua Sun, Adam Woolley, Dept of Chem and Biochem, Brigham Young University</td>
<td></td>
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<tr>
<td>4:15</td>
<td>(434)</td>
<td>Chemical and Biochemical Analysis using Microfluidic Platforms</td>
<td>Michael Sepaniak, Amber Wellman, Nahla Abu-Hatab, Joshy John, Maggie Connatser, University of Tennessee, Department of Chemistry</td>
</tr>
<tr>
<td>4:35</td>
<td>(435)</td>
<td>Measurement of Hemolymph Amino Acid Variations Due to Stress or Genotype from Individual Fruit-Flies</td>
<td>Sujeewa Pyankarage, Nikolay Kocherov, Hrvoje Augustin, David Featherstone, Scott Shippy, Department of Chemistry, UIC; Department of Biological Sciences, UIC</td>
</tr>
<tr>
<td>4:55</td>
<td>(436)</td>
<td>Affinity-Based Microdialysis Sampling using Heparin for Human Cytokine Collection</td>
<td>Yuexi Wang, Julie Stenken, Remselaar Polytechnic Institute</td>
</tr>
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**Wednesday Afternoon, Room L4**

**NANOTUBES AND NANOWIRES FOR SENSING II**

Organizers: Jason Holt and Pehr Pehrsson; President: Pehr Pehrsson

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Title</th>
<th>Authors</th>
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<tbody>
<tr>
<td>3:15</td>
<td>(437)</td>
<td>Carbon Supramolecular Assemblies in the Liquid Phase</td>
<td>Pa Chun Ke, Clemson University</td>
</tr>
<tr>
<td>3:55</td>
<td>(438)</td>
<td>Metal Oxide and Organometallic Nanowire Gas Sensors: Rational Tuning of Receptor / Transduction Functions and Prototype Devices</td>
<td>Andrei Kolmakov, SIU</td>
</tr>
<tr>
<td>4:35</td>
<td>(439)</td>
<td>Interactions between Functionalized Multi-Walled Carbon Nanotubes and Proteins</td>
<td>Bing Yan, Qinxin Mu, Wei Liu, Yuehan Xing, St. Jude Children's Research Hospital; Shandong University, China</td>
</tr>
<tr>
<td>4:55</td>
<td>(440)</td>
<td>GAS Preconcentration and Separation with Carbon Nanotubes</td>
<td>Michael Stadernmann, Adam McBrady, Vanessa Reid, Alex Noy, Rob Synovec, Olgica Bakajin, Lawrence Livermore National Lab; University of Washington, Seattle</td>
</tr>
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**Wednesday Afternoon, Room L5**

**NEW APPROACHES TO ENVIRONMENTAL MASS SPECTROMETRY**

Organizer: Kermit Murray; President: Jill Scott

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<th>Time</th>
<th>Session</th>
<th>Title</th>
<th>Authors</th>
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<tbody>
<tr>
<td>3:15</td>
<td>(441)</td>
<td>Coupling of Flow Injection with ICP-TOFMS to Increase Sample Throughput</td>
<td>William Balsanek, Christine Rivera, Andrew Saint, GBC Scientific Equipment (USA) LLC; MIBEN Tech, GBC Scientific Equipment Pty. Ltd.</td>
</tr>
<tr>
<td>3:35</td>
<td>(442)</td>
<td>Parametric Optimization of Electrochemically Modulated Separation for Pre-concentration of Uranium</td>
<td>Scott Lehn, Gregory Eiden, Martin Liezers, Douglas Duckworth, Pacific Northwest National Lab</td>
</tr>
<tr>
<td>3:55</td>
<td>(443)</td>
<td>Direct Solid Analysis of Coal Fly Ash Samples by Glow Discharge and Inductively Coupled Plasmas: an Integrated Approach</td>
<td>Alexandria M. Pavkovich, Melissa M. Public, Jennifer N. Robertson-Honecker, Fred L. King, West Virginia University</td>
</tr>
<tr>
<td>4:15</td>
<td>(444)</td>
<td>Simultaneous Analysis Method of 21 Pesticides in Tea by LC/ESI-MS-MS</td>
<td>Jae R. Scott, J. Michelle Kotler, Nancy W. Hinman, Beizhan Yan, Daphne L. Stoner, C. Doc Richardson, Idaho National Laboratory; University of Montana; University of Idaho</td>
</tr>
<tr>
<td>4:55</td>
<td>(446)</td>
<td>Exploring Biosignature-Mineral Associations using GALDI-FTMS</td>
<td>Jill R. Scott, J. Michelle Kotler, Nancy W. Hinman, Beizhan Yan, Daphne L. Stoner, C. Doc Richardson, Idaho National Laboratory; University of Montana; University of Idaho</td>
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**Wednesday Afternoon, Room L6**

**MEGGERS AWARD SYMPOSIUM**

Organizer and President Richard Mendelsohn

<table>
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<th>Time</th>
<th>Session</th>
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<th>Authors</th>
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<tbody>
<tr>
<td>3:15</td>
<td>(447)</td>
<td>Infrared Reflection-Adsorption Spectroscopy (IRRAS) of the Molecular Basis for Pulmonary Surfactant Function</td>
<td>Richard Mendelsohn, Joseph Brauner, Carol Flach, Rutgers University</td>
</tr>
<tr>
<td>3:35</td>
<td>(448)</td>
<td>Structural Polymorphism of a Membrane Protein Macromolecular Crystallography: The Filamentous Bacteriophage FF</td>
<td>George J. Thomas, Stacy A. Overman, Edward H. Egelman, University of Missouri-Kansas City; University of Virginia</td>
</tr>
<tr>
<td>3:55</td>
<td>(449)</td>
<td>Following Chemical Reactions in Protein and DNA Crystals by Raman Crystallography</td>
<td>Paul Carey, Case Western Reserve University</td>
</tr>
<tr>
<td>4:15</td>
<td>(450)</td>
<td>Study of Spider Silk Structure by Vibrational Spectroscopy</td>
<td>Michel Pezolet, Thierry Lefevre, Sarah Bedard, Jean-Francois Rioux-Dubé, Maxime Boulet-Audet, Marie-Eve Rousseau, Thierry Buffeteau; Laval University; Universite de Bordeaux</td>
</tr>
<tr>
<td>4:35</td>
<td>(451)</td>
<td>Surface Enhanced Raman Spectroscopy for in-situ Measurements of Signaling Molecules (e.g., Autoinducers) Relevant to Bacterial Chemical Communication – Quorum Sensing</td>
<td>William Pearman, Marion Lawrence-Snyder, S. Michael Angel, Alan Decho, University of South Carolina, Dept. of Chemistry and Biochemistry; Dept. of Environmental Health Science</td>
</tr>
<tr>
<td>4:55</td>
<td>(452)</td>
<td>Automated Breast Tissue Histopathology using Mid-IR Spectroscopic Imaging</td>
<td>Frances Nell Keith, Rohit Bhargava, University of Illinois at Urbana-Champaign</td>
</tr>
</tbody>
</table>
Wednesday Afternoon, Room L11
DEVELOPMENTS IN LUMINESCENCE SPECTROSCOPY AND INSTRUMENTATION
Organizer and Presider: Adres D. Campiglia

3:15 (453) Fluorescence and Scattering Detection of Individual Particles in Capillary Electrophoresis and Flow Cytometry; Edgar Arriaga1, Bobby Poe1, Dmitry Andreyev1, Marian Navratil1; 1University of Minnesota
3:35 (454) General Fluorescence Resonance Energy Transfer Assay for the Study of Cell Membrane Protein Clustering; Emily Smith1, Suzanne Sander1, Deepak Dibya1, Danny Brower2, Thomas Bunch2; 1Iowa State University; 2University of Arizona
3:55 (455) Surface Plasmon Enhancement at a Liquid-Metal Liquid Interface; Florencio Hernandez2, Arthur Thibert1, Carlos Toro1, Shengli Zou1, Ion Cohanoschi1; 1University of Central Florida
4:15 (456) Nanotubule Formation from Surface-Attached Liposomes using an Electric Field; Josemar Castillo1, Mark Hayes1; 1Arizona State University
4:35 (457) Development of Response Selective Fluorescence Sensors; Matthew McCarroll1, Daniel Dyer1, Lichang Wang1, Jeremy Buckingham1, Dan Brandys1, Rusong Xu, Irene Kimaru1; 1University of Central Florida; 2University of Washington
4:55 (458) Fabrication of Porous Optical Fiber Claddings for Crossed-Fiber Sensor Arrays using Microsphere Templating; Paul Henning1, Veronica Rigo1, Peter Geissinger1; 1University of Wisconsin Milwaukee

Wednesday Afternoon, Room L13
EVOLVING DEVELOPMENTS IN THE USE OF RAMAN SPECTROSCOPY, IN CONJUNCTION WITH OTHER PHYSICAL MEASUREMENTS FOR THE CHARACTERIZATION AND RATIONAL DESIGN OF CATALYSTS
Organizer and Presider: Frank Adar

3:15 (465) Smart Combinatorial Operando Spectroscopy Catalytic System; Israel Wachs1, 1Lehigh University
3:55 (466) Operando Spectroscopic Studies of the Methanol Conversion over Alumina-Supported Oxomolybdates Catalysts; Edmund Payen1, Sylvain Cristol1, Elise Berrier1, Gwenaële le Bourdon2, Sophie Morel2, Lionel le Bihan2, H. Vezin2; 1UCCS-UMR 8181; 2HORIBA JOBIN-YVON; 3LCOM, UMR 8009
4:15 (467) Operando and MultiOperando Raman Methodology: Rational Catalyst Discovery; Miguel A. Bañares1, José Prieto2, Consuelo Goberna-Selma2, M. Olga Guerrero-Pérez3, Anna E. Lewandowska1, Manuel García-Casado1; 1CSIC - Instituto de Catalysis; 2PID Eng & Tech
4:35 (468) Coupling Raman Spectroscopy to EPR, UV-vis and FTIR Spectroscopy for Deeper Insights in Selective Hydrocarbon Oxidation and Catalyst Synthesis; Angelika Brueckner1, Ursula Bentrup1; 1Leibniz Institute of Catalysis
4:55 (469) Raman Characterization Studies of TiO2 Supported Manganese Oxide Catalysts for Low Temperature SCR of NO with NH3; Sergey Mamedov1, Padmanabha Reddy2, Neeraja Ettireddy2; 1Arizona State University

Wednesday Afternoon, Room L12
NOVEL SENSORS AND INSTRUMENTATION OF TOMORROW
Organizer and Presider: Brian J. Marquardt

3:15 (459) Chip-based Liquid Chromatography for Online Process Monitoring; Scott Gilbert1, 2, 3, Ray Chrisman2, 3; 1Crystal Vision Microsystems LLC; 2Atodyne Technologies LLC; 3CPAC, University of Washington
3:35 (460) FT-IR Hollow Waveguide Gas Sensors for BTX Monitoring; Christina Young1, Neil Bruns2, Andy Riley3, John Martin1, Mark Disko2, Boris Mizaikoff2; 1Georgia Institute of Technology; 2ExxonMobil Research and Engineering Co.; 3ExxonMobil Biomedical Sciences, Inc.
3:55 (461) Process Sensing Utilizing Dielectric Spectroscopy; Shelley Begley1, Phil Bartley2; 1Agilent Technologies, Inc.; 2Innovative Measurement Solutions, Inc.
4:15 (462) Crystalline Ruthenium and Platinum Complexes for Measurement of Oxygen Concentrations in the Gas Phase and Aqueous Solutions by Emission Quenching; Kent Mamm1, Kari McGee1, Jason Burney1, David Veltkamp2, Brian Marquardt2; 1University of Minnesota; 2University of Washington
4:35 (463) A Single Process Technology Platform for NIR and Mid-IR Applications; Bertrand Lanher1; 1Aspectrics, Inc.
4:55 (464) Differential Mobility Spectrometry and Advantages of its Application for Chemical Process Monitoring/Control; Erkinion Nazarov1, Raanan Miller1, Quan Shi1; 1Sionex Corporation

Wednesday Afternoon, Room L14
SURFACE PLASMON RESONANCE: INNOVATION AND APPLICATION I
Organizer: Karl Booksh and Roger Terrill; Presider: Karl Booksh

3:15 (470) Pure Plasmons are Oscillations of the Free Carriers in Conducting Metal Oxides; Alina Efremenko1, Stefan Franzen1, Mark Losego1, Jon-Paul Maria1; 1North Carolina State University
3:35 (471) Integrated Label-Free Protein Detection and Separation in Real Time using Confined Surface Plasmon Resonance Imaging; Kyle Foley1, Nguyen Ly1, Nongjian Tao2; 1Arizona State University
3:55 (472) Nanoscale Building Blocks for Surface Plasmonic Resonance Biosensor Development; Amanda Haes1; 1University of Iowa
4:15 (473) Techniques to Improve Sensitivity in FT-SPR Measurements; Steve Lowry1, Eric Jiang1, Koichi Nishikida1, Steve Weibel1; 1Thermo Fisher Scientific; 2GWC Technologies
4:35 (474) Facilitated Detection of Small Molecules with Nanoparticle Bejeweled Swellable Polymers; Karl Booksh, Yoon-Chang Kim, Soame Banerji1, Wei Peng1; 1University of Delaware
4:55 (475) Controlled Assembly of ß-Mercaptoalkanoic Acid on Gold by Headgroup Electrostatic Interactions; Roger Terrill1, Arthur Cheng1, Paul Yong Nam Pak1, Shouwei Chen1; 1San Jose State University; 2University of California at Santa Cruz; 3Korea National University of Education

Future Meetings: FACSS 2008, September 28 – October 2, Reno, NV  •  FACSS 2009, October 18 - 22, Louisville, KY  69
**SAS Lester W. Strock Award**
8:00 AM Plenary Session, Ballroom C/D

**Detlef Günther**
(476) *Laser Ablation Inductively Coupled Plasma Spectrometry – Ready for Take Off: Detlef Günther*¹;
¹ETH Zurich, Laboratory of Inorganic Chemistry
*Refer to page 21 for biographical information.*

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**Bruce Edward Bursten**
President-Elect of the American Chemical Society
8:30 AM Closing Plenary Lecture, The Centrality of Chemistry, Ballroom C/D

Bruce E. Bursten was born in Chicago in 1954 and was raised in Milwaukee. He received his S.B. in Chemistry with Honors from the University of Chicago in 1974, and a Ph.D. in Chemistry from the University of Wisconsin-Madison in 1978 under the direction of Professor Richard F. Fenske. He was a National Science Foundation Postdoctoral Fellow at Texas A&M University from 1978-1980, conducting research with the late Professor F. Albert Cotton. He joined the faculty of The Ohio State University in 1980 as an Assistant Professor of Chemistry. In 1997 he was named Distinguished University Professor. In October, 1999 he became Chair of the Department of Chemistry at Ohio State, a position he held until October, 2003. In Fall, 2005 he moved to the University of Tennessee, Knoxville as Dean of the College of Arts and Sciences and Distinguished Professor of Chemistry. In 2006 he was elected to the Presidential succession of the American Chemical Society. He is President-Elect for 2007, and will be President and Immediate Past President in 2008 and 2009, respectively. Professor Bursten conducts research in inorganic chemistry. His research centers on the correlation of theoretical and experimental electronic structural data with the bonding and reactivity patterns of metal-containing molecules. He is the author or coauthor of 150 research papers, and he has presented more than 120 research seminars at other universities, national laboratories, and companies. He is also a coauthor of one of the leading textbooks in general chemistry. Professor Bursten has received numerous national and international honors for his academic accomplishments. Among these, in 1984 he received a Camille and Henry Dreyfus Foundation Teacher-Scholar Award and in 1985 he was named a Fellow of the Alfred P. Sloan Foundation. In 2001, he received the Catalyst Award from the American Chemistry Council, which is a national award for teachers of chemistry. He received the 2003 Spiers Medal and Prize from the Royal Society of Chemistry in the United Kingdom, he was elected a Fellow of the American Association for the Advancement of Science in 2004, and he received the Morley Medal of the Cleveland Section of the ACS in 2005.

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**THURSDAY POSTER SESSIONS**
9:30 – 10:30 AM and 1:45 – 2:45 PM
*Exhibit Hall, Ballroom A*

All Thursday posters should be put up between 7:30 – 8:00 AM and removed after the afternoon poster session (2:45 PM). The presenting author is expected to be present at the poster during both morning and afternoon sessions.

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<tr>
<th>Board #</th>
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<tr>
<td>1</td>
<td>(478) Simultaneous Spectrophotometric Estimation of Methocarbamol and Nimesulide in Tablet Dosage Form, Tushar Patel¹, LakshamanBhai Patel¹, Sunil Makwana¹, Tejas Patel¹, Kirit Patel¹, Timir Patel¹; ¹Faculty of Pharmacy, Dharmsinh Desai University</td>
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<tr>
<th>Atomic Spectroscopy</th>
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<td>(479) Total Arsenic Determination in Urine by Hydride Generation Atomic Fluorescence Spectrometry: Comparison between On-Line Microwave Assisted Heating and On-Line UV-Photooxidation; Kanna Ito¹, Christopher D. Palmer¹, Patrick J. Parsons¹², ¹University at Albany; ¹²New York State Dept. of Health</td>
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</table>
3 (480) Tungsten Coil Atomic Emission Spectrometry; Bradley Jones1, Clifton Calloway2, George Donati3, Jaquim Nobrega1; 1Wake Forest University; 2Winthrop University; 3Federal University of Sao Carlos

4 (481) High Resolution Continuum Source Atomic Absorption Spectrometry with Electrothermal Atomization: Panacea for Minimization of Spectral Interferences?; Gerhard Schlemmer1; 1Analytik Jena

Bioanalytical

5 (482) Characterization and Identification of Pollen by Vibrational Spectroscopy; Janina Kneipp1, Franziska Schulte1, Ulrich Panne2; 1Federal Institute for Materials Research and Testing (BAM)

6 (483) Following F. Novicida Infection with Multicolor Fluorescent Proteins and Spectral Imaging; Jerilyn Timlin1, Julie Kaiser1, Michael Sinclair1, Linda Nieman1, Todd Lane1; 1Sandia National Labs

7 (484) Development of a Nanomechanical Biosensor for Analysis of Endocrine Disrupting Chemicals; Kasey Hill1, Pampa Dutta1, Michael Sepaniak1; 1University of Tennessee, Department of Chemistry

8 (485) A New Liquid-Liquid Extraction Method for Determination of Montelukast in Small Volume Human Plasma Samples using HPLC withFluorescence Detector; Drashan Patel1; 1Darshan B. Patel, Sarvajanik Pharmacy College.; 2Hardik A. Prajapati, Sarvajanik Pharmacy.; 3Dr. C. N. Patel, Sarvajanik Pharmacy Co.

Biomedical

9 (486) Amperometric ATP Microbiosensors to Investigate the Maturation of the Carotid Body; Jean-Francois Masson1,2, Christine Kranz1, Estelle Gauda1, Boris Miziaikoff3; 1Georgia Institute of Technology; 2Johns Hopkins University; 3Univ. de Montreal

Chemometrics

10 (487) Application of Multivariate Curve Resolution in Pharmaceutical Process Understanding; Dongsheng Bu1, Martin Kermit1; 1Camo Software Inc

11 (488) Qualitative Interpretation of Regression Vectors in Multivariate Calibration; Christopher D. Brown1, Robert L. Green1; 1Aura Scientific

12 (489) Re-fitting PCA, MPCA and PARAFAC Models to Incomplete Data Records; Barry M. Wise1; 1Eigenvector Research, Inc.

13 (490) Multivariate Detection and Quantification Limits in the Analysis of Potent Drug Tablets by Transmission Near Infrared Spectroscopy; Manel Alcala1, Joshua Leon1, Jorge Ropero2, Rolodof J. Romañach1, Marcelo Blanco1; 1Univ. Puerto Rico - Mayagüez; 2Universitat Autònoma de Barcelona -Spain

Fluorescence

14 (491) Room-Temperature Fluorescence Analysis of Dye Extracts for Forensic Fiber Examination; Matthew Rex1, Andres Campiglia1; 1University of Central Florida

15 (492) Development of Robust and Inexpensive Optical Oxygen Sensor; Charles Branham1, Brian Marquardt2, Kent Mann3; 1CPAC; University of Washington; 2Applied Physics Lab, University of Washi; 3Dept. Chemistry,University of Minnesoate

Inductively Coupled Plasma

16 (493) Analysis of Gold in a Clinical Laboratory by Inductively Coupled Plasma - Mass Spectrometry; Michelle Wermers1, John Butz1, Gary Austin1; 1Mayo Clinic - Dept. of Lab Medicine and Pathology

Infrared

17 (494) Flavorful Compounds in Spirit Maturation by Infrared Spectroscopy and Multivariate Analysis; Powers Wolf1, Nicole Labbe1, John Collier1, Simon Petrovan1, Timothy Rials1; 1University of Tennessee; 2Florida State University

18 (495) Diffuse Reflectance Fourier Transform Mid-Infrared Spectral Properties of Forages with Varied Fatty Acid Content; Francisco Calderon1, James B. III Reeves1, Joyce Foster3, William Clapham1, James Fedders3, Merle F. Vigil1, W. Brien Henry4; 1USDA-ARS Central Great Plains Research Station, Ak; 2USDA-ARS Environmental Management and By; 3USDA-ARS Appalachian Farming Systems Res; 4USDA-ARS Corn Host Resistance Research

Analysis of Gaseous Samples with Sorbent Tube Preconcentration of Analytes Followed by Infrared Spectrometry and Gas Chromatography; Craig Lampert1, David Kofink1, Nge-Sing Chong2; 1Middle Tennessee State University

Ionization

20 (497) Analyte Mapping of Solid Samples by Laser Ablation Coupled with an Atmospheric-Pressure Glow Discharge Ionization Source; Jacob Shelley1, Joshua Wiley1, Francisco Andrade1, Steven Ray1, Gary Hiettje1; 1Indiana University; 2Unilever Corporation

Kinetics

21 (498) Ligand Substitution Kinetics as an Analytical Tool for Trace Analysis; Surendra Prasad1; 1The University of the South Pacific

Lab-on-a-Chip

22 (499) Integrated Protein Preconcentration and Separation Microdevices Prepared by Rapid Prototyping using solvent Imprinting; Xihuawun Sun1, Weichun Yang1, Tao Pan1, Adam Woolley1; 1Brigham Young University

Laser Spectroscopy

23 (500) Degenerate Four-Wave Mixing of Nanostructured Supramolecular Organic Semiconductor; Onguang Yang1, JaeTae Seo1, Russell Battle1, SeongMin Ma, Cheng Zhang2, Bagher Tabibi1, Sam-Shajing Sun2, Jinhwa Heo1, Wanjoong Kim1, Sungsoo Jung1; 1Department of Physics, Hampton University, Hampton; 2Department of Chemistry, Norfolk State U; 3Korea Research Institute of Standards

Mass Spectrometry

24 (501) Compatibility and Applicability of Novel Sampling Valve for Aerosol Time-of-Flight Mass Spectrometer; Totti Laitinen1, Kari Hartonen1, Markku Kulmala1, Marja-Liisa Riekkola1; 1University of Helsinki
TECHNICAL PROGRAM – THURSDAY

Poster Sessions 9:30 – 10:30 AM and 1:45 – 2:45 PM and Orals 10:30 AM – 12:30 PM

25 (502) Dynamic On-Chip Purification and Preconcentration/Focusing Targets for High Sensitivity Atmospheric Pressure Matrix-Assisted Laser Desorption Ionization (AP/MAI- DI) Peptidomics; Arti Navare1, Marcela Nouzova2, Salvador Hernandez-Martinez2, Fernando Norrega3, Facundo Fernandez4; 1Georgia Institute of Technology, Atlanta, GA; 2Florida International University, Miami,.; 3Instituto Nacional De Salud,Cuernavac

26 (503) Ion Mobility-Mass Spectrometry Shift Reagents for Multiplexed Peptide and Protein Characterization; Thomas Kerr1, John McLean1; Vanderbilt University

27 (504) Characterization of Dry Aerosol Particles and Solids using Desorption Electrospray Ionization and Electrospray-Assisted IR Laser Desorption Ionization Mass Spectrometry; Yohnnes H. Rezonov1, Jianan Dong1, Kermit K. Murray1; Louisiana State University

28 (505) Elemental Determinations in Coal Fly Ash Samples by Glow Discharge and Inductively Coupled Plasma Spectrometries: An Integrated Approach; Alexandria M. Pavkovich1, Jennifer N. Robertson-Honecker1,2; 1West Virginia University

Materials Characterization

29 (506) Studying Industrial Water Quality by Corrosion & Scaling Index with Changing the Method of Microorganisms Control; Ehsan Bakshis1, Fatemeh Abnik2; 1R&D Center of National Petrochemical Company; 2National Petrochemical Co.(Ghadir group)

30 (507) A New Type of Thermo-Associative Guanosine Gel: Yuehua Yu1, 2, Darren Nakamura1, Kevin DeBoyance1, Bonnie Lyon1, McGown Linda1; 1Rensselaer Polytechnic Institute

31 (508) Using FT-IR and UV-Vis Light Scattering to Examine the Effect of Tail Length on the Enthalpy of Bisurea Organogel Melting; Karla S. McCain1, Aaron M. Pierce1, Emily P.M. Kuo1, Paul E. Federick1, Andrew J. Carr1,2; 1Austin College

Microarrays

32 (509) Single Molecule Studies of Antibody-Antigen Binding: the Potential for Highly Quantitative Multiplexed Biosensors; Jamshid Temirov1, Andrew Bradbury1, James Werner1,2; 1Los Alamos National Laboratory

33 (510) Selective Deposition of Metals on Nanopatterns of n-alkylsilane Self-Assembled Monolayers; Iie-Ren Li1, Jayne C Garno1; 1Louisiana State University

Near Infrared

34 (511) Near-Infrared Model for Quality Evaluation of Flax Fiber; Miyeong Sohn1, Franklin Barton, II1, Danny Akin1, David Himmelshbach2; 1USDA-ARS

Other

35 (512) Structure Activity Relationship Studies of Synthesized Urea Diamides on CNS Depression andSleeping Time Potentiation Effect; Ravikumar Modi1, Dharbho Jyoti Sen1; 1Shri Sarvajamik Pharmacy College

Raman

36 (513) Rapid Method for Determination of Identity and Potency of Pharmaceutical Materials by FT Raman Spectroscopy; Robert Forbes1, Michael Dottitch1, Donald Hodges1, Richard Kattner1,2; 1Eli Lilly and Company

37 (514) Depth Profiling using Time-Resolved Raman Spectroscopy with a Fast-Gated Intensified CCD Camera; Freerk Ariese1, Marleen Kerssens1, Joost B. Buijs1, Cees Gooyer1; 1 Laser Centre Vrije Universiteit Amsterdam

38 (515) Development of a Submersible Raman Instrument for in-situ Analysis of Deep-Sea Hydrothermal Vents; Wesley J. Thompson1, Brian J. Marquardt1, Marvin D. Lilley2; 1University of Washington, APL; 2University of Washington, Oceanography

Speciation

39 (516) Determining Ingredient Speciation in a Complex Laundry Product Matrix; Bridget Becker1, David Eike2, Michael Rothgeb1, John Aiken1, William Laidig2, Bruce Murch1; 1HHC Analytical Sciences, P&G; 2Modeling and Simulation, P&G

Thursday Morning, Room L2

COMMEMORATION OF DR. RADU MAVRODINEANU

Organizer and Presider: Jerry Messman

10:30 (517) The Legacy of Dr. Radu Mavrodineau - Introductory Remarks; Jerry Messman1; 1Stranaska Scientific LLC

10:50 (518) The Spectroscopic Achievements of Radu Mavrodineau; Robert Watters1; 1NIST

11:10 (519) In Pursuit of Fluorescence Standardization – NIST Past and Present; Paul DeRose1; 1NIST

11:30 (520) Contributions of Radu Mavrodineau to the PBS/NIST Standard Reference Materials Program; Thomas Gills1

11:50 (521) NBS/NIST Optical Filters Program; Melody Smith1; 1National Institute of Standards and Technology

12:10 (522) The Legacy of Dr. Radu Mavrodineau - Concluding Remarks; Jerry Messman1; 1Stranaska Scientific LLC

Thursday Morning, Room L3

FABRICATION STRATEGIES FOR MICROFLUIDS: BEYOND THE CLEANROOM

Organizer and Presider: Aaron Wheeler

10:30 (523) Construction of Microfluidic Networks using Thermoplastic Elastomer Gels; Victor Uge2; 1Texas A&M University

10:50 (524) Polymeric Microdevices with Monolithic Columns for Bioanalysis; Adam Woolley1, Xiuhua Sun1, Weichun Yang1; 1Brigham Young University

11:10 (525) Fabrication of Unconventional Microfluidic Chips: Within or Outside the Cleanroom?; John Crabtree1,3; 1Micralyne Inc.

11:30 (526) Microfabrication in the Office; Claudimir Lucio da Lago1,2; 1Instituto de Quimica - Universidade de Sao Paulo

11:50 (527) Materials, Methods and Approaches to the Contact Liquid Photopolymerization-Based Fabrication of Polymeric Microfluidic Devices; Christopher Bowman1, Tommy Haraldsson1, Robert Sebra1, Brian Hutchinson1, Sirish Reddy1, Neil Cramer1, Kristi Anseth1, Robert Davis1,2; 1University of Colorado

12:10 (528) Digital Microfluidics Made Easy; Aaron Wheeler1,2, Mohamed Abdelgawad1, Michael Watson1,2; 1University of Toronto Department of Chemistry; 2Univ. Toronto Dept. Mechanical Eng.
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<th>Time</th>
<th>Session</th>
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<th>Organizers/Presiders</th>
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<tr>
<td>10:30</td>
<td>Thursday Morning, Room L4</td>
<td>NANO SCALE STRUCTURES AND THEIR APPLICATION</td>
<td>Organizer: Ian R. Lewis; Presider: Zorabel LeJeune</td>
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<tr>
<td>11:10</td>
<td>(549) Tuning Higher Hierarchical Nanopores in Anodic Aluminum Oxide</td>
<td>Rashid Zakerti1; Punit Kohli1; 1Southern Illinois University</td>
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<tr>
<td>11:10</td>
<td>(550) Optical Spectroscopy of Plasmonic Au Spherical Nanoparticles</td>
<td>Seongmin Ma1; Jinhwa Heo2; Wanjoo Kim2; JaeTae Seo1; Qiguang Yang1; Bagher Tabibi1; Wansoo Yun1; Sungsoo Jung1; Sangwoo Han1; William Yu1; 1Department of Physics, Hampton University; 2Hampton; 3Korea Research Institute of Standards an; 4Department of Chemistry, Gyeongsang Nati; 5Department of Chemistry, Rice University</td>
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<tr>
<td>11:30</td>
<td>(551) CTAB Stabilized Cubic and Spherical Gold Nanoparticles as Highly Sensitive Extrinsic Raman Labels for SERS Readout in Sandwich Immunoasays</td>
<td>Radha Narayanan1, Robert Liperi2, Marc Porteri; 1The Biodesign Institute, Arizona State University; 2Ames Laboratory, Iowa State University</td>
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<td>10:30</td>
<td>Thursday Morning, Room L5</td>
<td>ADVANCES IN BIOMOLECULAR IMAGING MASS SPECTROMETRY</td>
<td>Organizer and Presider: John A. McLean</td>
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<tr>
<td>10:50</td>
<td>(552) Surface Sampling Probe and Desorption Electrospray Approaches to Mass Spectrometry-Based Chemical Imaging of Tissue Sections</td>
<td>Gary Van Berkel, Vilmos Kertesz; 1Oak Ridge National Laboratory</td>
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<td>11:00</td>
<td>(553) Mass Spectrometric Imaging and Profiling of Single Cells and Tissues</td>
<td>Stanislav S. Rubakhin1, Jonathan V. Sweedleri; 1Beckman Institute, University of Illinois</td>
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<td>11:00</td>
<td>(554) Atmospheric Pressure IR-MALDI Imaging of Metabolites</td>
<td>Akos Vertesi1, Yue Li1, Bindesh Shrestha1, Peter Nemes1; 1George Washington University</td>
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<td>11:30</td>
<td>(555) Designing Nanoparticle Matrices for Enhanced Selectivity in Imaging Mass Spectrometry</td>
<td>David H. Russell1, Stacy D. Sherrold1, Edward T. Castellana; 1Department of Chemistry, Texas A&amp;M University</td>
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<td>11:50</td>
<td>(556) A Minimalist Approach to Imaging Lipids and Drugs in Rat Brain Sections, its Rewards and Pitfalls</td>
<td>Amina Sarah Woods1, Jeremy Post1, Shelley Jackson1; 1NIDA IRP, NIH</td>
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<tr>
<td>12:10</td>
<td>(557) Biomolecular MS Imaging with Ion Mobility-Mass Spectrometry</td>
<td>Imaging IM-MS Strategies; John A. McLean1; 1Department of Chemistry, Vanderbilt University</td>
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<tr>
<td>10:30</td>
<td>Thursday Morning, Room L6</td>
<td>LESTER W. STROCK AWARD SYMPOSIUM</td>
<td>Organizer and Presider: Paul Farnsworth</td>
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<tr>
<td>10:30</td>
<td>(558) The Effect of the Sampling Cone on Ion and Atom Distributions in an ICP-MS</td>
<td>Paul Farnsworth1; Haibin Ma1; 1Brigham Young University</td>
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<tr>
<td>10:50</td>
<td>(559) Progress in Laser Ablation ICP-MS: From Fundamental Intrigue to Routine Applications</td>
<td>Richard E Russo1, Jhansis Gonzalez1, Sy-Bor Wen1, Xianglei Mao1; 1Lawrence Berkeley National Lab</td>
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**Future Meetings:** FACSS 2008, September 28 – October 2, Reno, NV  •  FACSS 2009, October 18 - 22, Louisville, KY  

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**Thursday Morning, Room L11**

**NOVEL MINIATURE SPECTROSCOPIC INSTRUMENTATION**

Organizers and Presiders: Richard Crocombe and John Chalmers

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<tr>
<td>10:30</td>
<td>(560) Pharmaceutical Raw Materials ID Utilizing a Hand-Held Raman Spectrometer</td>
<td>Michael Longmire1, Brent Kuckkan1, Gary Thomas1, 1Eli Lilly and Company</td>
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<tr>
<td>11:30</td>
<td>(563) Portable Rapid-Scan FT-IR Spectrometer using Translational MOEMS Mirrors</td>
<td>Martin Kraft1, Werner Scherf1, Thilo Sandner2, Harald Schenk2, Andreas Kenda1; 1CTR Carinthian Tech Research AG, Villach, Austria; 2Fraunhofer IPMS, Dresden, Germany</td>
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<tr>
<td>11:50</td>
<td>(564) Bring the Spectrometer to the Sample - Plastics Identification using a Handheld NIR Spectrometer</td>
<td>Frederick Haibach1, Klevisha; 1Polychromix</td>
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<tr>
<td>12:10</td>
<td>(565) MEMS-scale Photoacoustic Sensor using an Interband Quantum Cascade Laser</td>
<td>David Heaps1, Paul Pellegrino1; 1Army Research Laboratory</td>
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**Thursday Morning, Room L12**

**PROCESS ANALYSIS FOR FOOD QUALITY AND SAFETY**

Organizer and Presider: Jens Petter Wold

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<tr>
<td>10:30</td>
<td>(566) Raman Spectroscopy for Characterization of Fatty Acid Composition in Foods</td>
<td>Nilos Kristian Afseth1, Vegard Herman Segtman1, Brian Marquardt1, Jens Petter Wold1; 1Matforsk - Norwegian Food Research Institute; 1CPAC - Center for Process Analytical Chemistry</td>
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<tr>
<td>10:50</td>
<td>(567) FTIR Microscopy as a Tool to Investigate Protein Secondary Structural Changes in Muscle Food Tissue</td>
<td>Achim Kohler1,2, Hanne Bertram1, Ulrike Böcker1,2, Ixasun Karton1,4, Zhiyun Wu1, Ragni Olsf; 1Matforsk, Norway; 2University of Life Science, Norway; 3Danish Institute of Agricultural Science; 4Department of Food Technology, Spain</td>
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<tr>
<td>11:10</td>
<td>(568) Representative On-Line Sampling of Heterogeneous Products by NIR Transflectance Imaging</td>
<td>Jens Petter Wold1, Vegard Segtman1, Martin Hoy1, Jon Tschudi2, Karl-Henrik Haugholt1, Jens T. Thielemann1; 1Matforsk; 2Sintef ICT</td>
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11:30 (555) Multivariate MR Imaging for Fruit Quality Assessment; Rebecca Milcerek1,2; Michael McCarthy1,2; 1University of California, Davis; 2Center for Process Analytical Chemistry

11:50 (556) Estimation of Pure Profiles with ICA, MCR and PARAFAC - Applications on NIR and Fluorescence Spectra from Food Systems; Frank Westad1,2; Jens Petter Wold1; 1CAMO Software; 2ABBON AS; 3Matforsk

12:10 (557) Monitoring of Pet Foods for Potentially Toxic Elements; Ela Bakowska1; Michael Rieders1; Joan Schemmer2; 3NM Labs

Thursday Morning, Room L13
RAMAN SPECTRAL IMAGING – DIVERSITY IN APPLICATIONS
Organizer and Presider: Eunah Lee

10:30 (558) Raman Imaging of Bacteria Cells Labeled with Metal Nanoprobes; Li-Lin Tay1; Jamshid Tanha1; Shannon Ryan1; 1National Research Council Canada

10:50 (559) Raman Imaging of Pharmaceutical Contaminants; David Exline1; RJ Lee Group, Inc.

11:10 (560) Carbon Nanotube Architectures: Synthesis and Characterization towards Functional Systems; Young Joon Jung1; Xugang Xiong1; Myung Gwan Hahn1; Ahmed Busnaina1; Pulickel Ajayan1; 1Northeastern University; 2Rensselaer Polytechnic Institute

11:30 (561) Raman Confocal Microscopy Imaging and the Use of Meso- and Nano-Structured Metallic Substrates; François Lagugné-Labarthet1; Nicolas Marquestaut2; Laurent Servant1; Valerie Guieu1; Meso Sojic1; 1University Of Western Ontario, Canada; 2Université Bordeaux 1, France

12:10 (562) Raman Hyperspectral Imaging of Cells, Cellular Components and Drug Uptake into Cells; Max Diem1; Christian Matthäus1; Tatjana Chernenko1; Miloš Miljkovic1; 1Northeastern University

Thursday Morning, Room L14
PHARMACEUTICAL FORENSICS
Organized by the Forensic Technical Section of the Society for Applied Spectroscopy
Organizer and Presider: Mark R. Witkowski

10:30 (563) Pharmaceutical Forensics: An Overview; Duane Mauzy1; 1Allergan

10:50 (564) DESI and DART Mass Spectrometry for Counterfeit Drug Fingerprinting: Application to Antimalarials, Oseltamivir, and Other Cases; Facundo Fernandez1; Leonard Nyadong2; Christina Hampton3; Kristin Johnson4; Sameer Late; Ajay Banga; Michael Green5; Paul Newton6; 1Georgia Institute of Technology, Atlanta; 2Mercer University, Atlanta; 3CDC Atlanta; 4Mahosot Hospital, Lao PDR.

11:10 (565) The Use of FT-IR and Raman Spectroscopy in Cases Involving Product Tampering; Mark Witkowski1; 1Jcinta Batson1; John Crowe1; 1FDA Forensic Chemistry Center Cincinnati Ohio

11:30 (566) Analysis of Suspected Counterfeit Pharmaceutical Products; Anthony Zook1; 2Merck & Co., Inc.

11:50 (567) Identification of Counterfeit Cialis, Levitra and Viagra Tablets by Open-Air Desorption Ionization Time-of-Flight Mass Spectrometry; Anthony Moffat1; Robert Cody2; Roger Jee1; Andrew O’Neil1; 1The School of Pharmacy, London; 2Jeol USA Inc, Peabody, MA
Thursday Afternoon, Room L4
CARBON NANOTUBE SEPARATION
Organizer and Presider: Paul Farnsworth

2:45 (581) Toward Quantitative Fluorimetric Analysis of Single-Walled Carbon Nanotubes; R. Bruce Weisman1
1Rice University
3:25 (582) Separating Carbon Nanotubes by Their Physical and Electronic Structure using Density Gradient Ultracentrifugation; Mark Hersam1, 2Northwestern University
3:45 (583) A Scanning Force Microscopy Assay for Metallic/Semiconducting Content in Mixed Single-Walled Carbon Nanotube Samples; Liwei Chen1, Wei Lu1, 2Ohio University
4:05 (584) Diameter and Chirality Dependent Aggregation of Single-Walled Carbon Nanotubes; Sandip Niyogi1, Sofiane Boukhalfa1, Satishkumar Chikkannanavar1, Stephen Doorn1, 2Los Alamos National Lab
4:25 (585) Enriching Individual (n, m) Carbon Nanotubes for Solution Chemistry; Wei Zhao1, Xiaomin Tu1, Yang Xu1, Satish Chikkannanavar1, Stephen Doorn1, 2Los Alamos National Lab

Thursday Afternoon, Room L5
DIRECT IONIZATION METHODS FOR HIGH THROUGHPUT MASS SPECTROMETRY
Organizer and Presider: Facundo Fernandez

2:45 (586) Applications of Desorption Electrospray Ionization; R. Graham Cooks1, 2Purdue University
3:05 (587) Development of Hybrid Atmospheric Ionization Sources for Direct Analysis of Macromolecules by FT-ICR-MS; David Muddiman1, Adam Hawkridge1, Jason Sampson1, Michael Bereman1, Brent Dixon1, 2NC State University
3:25 (588) Hitting the Bullseye More Often: Extending the Applications for the DART Ion Source; Robert Cody1, 2JEOL USA, Inc.
3:45 (589) Direct High-Throughput Analysis of Pathogenic Bacteria by DESI and DART; Facundo Fernandez1, Carrie Pierce1, 2, Leonard Nyadong1, John Barr2, Adrian Woolfitt1, Hercules Moura1, Robert Massung2, Robert Cody1, 2Georgia Institute of Technology; 2CDC; 2JEOL Inc
4:05 (590) Desorption Sonic Spray Ionization for (High) Voltage-Free Ambient Mass Spectrometry: Fast Fingerprinting Characterization of Drugs, Cosmetics and Food Products; Marcos N. Eberlin1, 2State University of Campinas, Brazil
4:25 (591) Geometry Independent Desorption Electrospray Ionization; Andre Venter1, 2Graham Cooks1, 2Purdue University

Thursday Afternoon, Room L6
MULTIVARIATE CURVE RESOLUTION
Organizer and Presider: Thomas Hancewicz

2:45 (592) Consideration of Measurement Uncertainties in Multivariate Curve Resolution by Alternating Least Squares; Roma Tauler1, 2CDC; 3JEOL
1Georgia Institute of Technology; 2CDC; 3JEOL
3:05 (593) Equation-Oriented System (EOS) as Tool to Multivariate Curve Resolution (MCR) with Multiple Constraints; Jihong Wang1, Marwood N. Ediger1, Thomas M. Hancewicz2, 2VeraLight Inc.; 2Unilever Research USA
3:45 (594) Confocal Fluorescence Hyperspectral Imaging of Biological Samples using Multivariate Curve Resolution Analysis Techniques; Howland Jones1, 2Purdue University
1David Haaland1, David Melgaard1, Michael Sinclair1, 2Sandia National Laboratories
4:05 (595) Band Target Entropy Minimization in Biomedical Raman Spectroscopy and Imaging: A User Report; Michael D. Morris1, 2University of Michigan
4:25 (596) Multivariate Curve Resolution in Advanced Process Modeling; Anna de Juan1, Romá Tauler2, 2University of Barcelona, Barcelona; 2IIQAB-CSIC

Thursday Afternoon, Room L11
BIOVIBRATIONAL SPECTROSCOPY
Organizer: Linda Kidder; Presider: Max Diem

2:45 (597) Raman Spectroscopic and Optical Characterization of Early Atherosclerotic Plaques; Lin-Ping Choo-Smith1, Mark Hewko1, Elicia Kohlenberg1, Michael Smith1, Saro Bascaramurty1, Michael Sowa1, 1NRC-Institute for Biodiagnostics
3:05 (598) Raman Spectroscopy of Biomimetic Polymers for Bone Tissue Engineering; Gurit S. Mandair1, Lihn N. Luong2, David H. Kohn2, Donghai Ho1, 2University of Louisville
3:25 (599) Temperature-Induced Conformational Changes in Human Tear Lipids Hydrocarbon Chains; Douglas Borchman1, 2University of Louisville
1Gary Foulks1, Marta Yappert1, Donghai Ho1, 2University of Louisville
4:05 (600) Applications of Attenuated Total Reflection FTIR Imaging to Skin; Ka Lung Andrew Chan1, Sergei Kazarin1, 2Imperial College London
1Marta Yappert1, Donghai Ho1, 2University of Louisville
4:25 (601) Infrared Spectroscopy of Individual Exfoliated Human Cells; Max Diem1, Benjamin Bird, Melissa Romeo1, 2Imperial College London
1Max Diem1, Benjamin Bird, Melissa Romeo1, 2Imperial College London

Future Meetings: FACSS 2008, September 28 – October 2, Reno, NV • FACSS 2009, October 18 - 22, Louisville, KY
Thursday Afternoon, Room L12
PAT ACROSS THE R&D AND MANUFACTURING INTERFACE
Organizer and Presider: Aaron W. Garrett

2:45  (603) Use of Raman Spectroscopy to Evaluate the API Crystal Form Stability in a Suspension; Aaron Garrett¹, David Reed¹, ²Eli Lilly and Company
3:05  (604) Use of In-Line Near-Infrared Spectroscopy to Monitor Segregation of a Pharmaceutical Powder Blend in a Tablet Press; David Reed¹, Marc Champagne¹, Aaron Garrett¹, Allen Steffler¹, Jimmy Engle¹, ²Eli Lilly & Company
3:25  (605) Chemometrics in Pharmaceutical Manufacturing: Feed Forward Control of Milling; Robert Roginski¹, Paul Collins²; ¹Eigenvector Research, Inc.; ²Eli Lilly and Company

Thursday Afternoon, Room L13
EMERGING APPLICATIONS AND TECHNOLOGIES IN RAMAN SPECTROSCOPY
Organizer and Presider: Neil Everall

2:45  (606) Polarized Raman as a Probe of Structural Development in Electrospun Fibers; Bruce Chase¹, John Rabolt¹, Meghana Kakade²; ¹DuPont; ²University of Delaware
3:05  (607) Raman Signal Enhancement in Deep Spectroscopy of Turbid Media; Pavel Matousek¹; ¹Rutherford Appleton Laboratory
3:25  (608) Multivariate Batch Monitoring – Is There a Right Way?; Marc Champagne¹, Aaron Garrett¹, David Reed¹, Allen Steffler¹, Ken Sorak¹, ²Eli Lilly and Company

Thursday Afternoon, Room L14
RECENT DEVELOPMENTS IN EXPLOSIVE DETECTION TECHNOLOGIES
Organized by the Forensic Technical Section of the Society for Applied Spectroscopy
Organizer and Presider: Mary Carrabba

2:45  (610) Developing a Capability to Detect and Identify Explosives Remotely; John Reaugh¹, Kambiz Salari¹, Gregory Klunder¹, Sorin Bastea¹, Richard Beherens, Jr.², Sean Maharrey²; ¹Lawrence Livermore National Laboratory; ²Sandia National Laboratory California
3:05  (611) Low Temperature Sublimation Rates of Explosive Constituents; Sean Maharrey¹, Richard Behrens¹; ¹Sandia National Laboratories
3:25  (612) Molecular Spectroscopic Measurements of VOC found in Explosive Vapors; Alan Ford¹, Scott W. Reeve¹, Tabetha Osborn¹, Sindhu Kaimal¹; ¹Arkansas State University

3:45  (613) Characterization of Chemical Vapor Signatures for Remote Detection of High Explosives; Marina L. Chiarappa-Zucca¹, Gregory L. Klunder¹, Richard A. Meissner¹, John E. Reaugh¹; ¹Lawrence Livermore National Lab
4:05  (614) Application of Sensor Fusion to Explosives Detection; Patrick Treado¹, Matthew Nelson¹, Jason Neiss¹, Robert Schweitzer¹, Charles Gardner¹; ¹ChemImage Corporation
4:25  (615) Enabling Field-Based Material Determination with Handheld Spectroscopy: Instrumental Advances and Applications in Public Safety and Security; Robert Green¹, Wayne Jalenak¹, Javier Santillan¹, Christopher Brown¹; ¹Ahura Scientific
With this in mind and the increasing number of micronutrients and guidelines are strictly adhered to in order to maintain compliance. Regulatory bodies such as the FDA, World Health Organisation and national drinking water authorities have introduced specific standard elemental analyses into regulatory compliance testing, as consumption, service requirements and of course, laboratory space. In today’s biomedical activities, significant emphasis is given both to interdisciplinary collaborations and to “translational research” in which laboratory methodologies are modified and rapidly adapted to clinical usage. We will introduce these general concepts first at the nuclear level of a eukaryotic cell in a discussion of the area of epigenetics; namely, the study of heritable changes in gene function that arise without changes in the DNA sequence. The repository of genetic information, the cellular chromosome, is comprised of chromatin which consists of tightly associated DNA and protein units termed histones. Since histone acetylation/deacetylation modifications dramatically effect cancer development and tumor progression, we collaborate with pathologists and oncologists in applying high-through-put vibrational spectroscopic imaging techniques to identify molecular biomarkers. These biomarkers are correlated with the efficacy of tumor responses to current drug treatments targeted specifically to histone deacetylation inhibition. As we progress from the cell nucleus to the cellular membrane, we next examine the structural elements of lipid bilayer assemblies and the putative roles of fluctuating lipid microdomains in regulating membrane behavior; we note that vibrational imaging techniques applied at these organizational levels add significant insights into biochemical processes as the spatial resolution approaches nanometer limits. Lastly, we describe our collaborations with transplantation surgeons in which we introduce visible reflectance imaging techniques to aid the surgeon in the performance of laparoscopic nephrectomies. Procedures will be described in which contrast enhancement of both partial laparoscopic and open abdominal images allows the accurate assessment of tissue oxygenation and multiple vessel differentiation by the surgeon despite significant visual limitations.

(2) Regulatory Compliance Tools in ICP-OES Software to enable Fast Accurate Results for Method Driven Applications. Karen Harper1, Cassap Matthew1, Clavering Andrew1; 1Thermo Fisher Scientific

ICP-OES is a long established multi element technique and is the routine workhorse in many laboratories. Advances in the optical layouts and charge transfer detectors such as CID (Charge Injected Device) enable simultaneous elemental analysis that provides fast and accurate sample throughput in remarkably compact instruments. These instruments have the advantages of reduced cost of ownership through careful design modelling that has reduced gas consumption, service requirements and of course, laboratory space. During the last decade, the workload of ICP-OES has moved from standard elemental analyses into regulatory compliance testing, as protection from potentially hazardous contaminants in our food, water and air has become a major topic of public interest. Regulatory bodies such as the FDA, World Health Organisation and national drinking water authorities have introduced specific methods to account for contaminants. These methods demand that guidelines are strictly adhered to in order to maintain compliance. With this in mind and the increasing number of micronutrients and contaminants requiring determination, it is critical that the method of testing is a rigorous and reliable one. Software development has been lead by this compliance, with the release of validation packages to aid 21 CFR, part 11 compliance for laboratories. Modern ICP systems are designed to aid with efficient method development by automating many of the optimisation procedures such as nebuliser gas, pump flow rate and RF Forward Power. These enhancements allow even the novice user to produce precise and accurate results, and coupled with intelligent accessories can enable the fastest most accurate results to date. The use of software and method development tools to aid and automate regulatory compliance will be discussed with supporting data. This paper will provide information relating to software validation, showcasing a new secure software package and intelligent accessories that were developed to enable regulatory compliance whilst maintaining cost efficiency.

(3) Direct Determination of Trace Metal Elements in Diluted Quality Control Urine Materials Using a Collision Reaction Interface Equipped ICP-MS. Doug Shroder1, XueDong Wang1, Stephen Anderson1, Shane Elliott1; 1Varian, Inc.

Interferences in ICP-MS can be problematic in complex matrices. In some biological analyses by ICP-MS it is possible to minimize the impact of spectroscopic interferences by matrix matching the standards to the samples. Blood and plasma are good examples of this. The composition of these fluids is highly regulated in the body, thus polyatomic interferences are relatively constant from one sample to the next. The composition of other biological matrices is not highly regulated and samples can vary greatly. Urine is a good example of this type of sample. In these circumstances the options available to analyze such materials are to either pre-treat the sample to eliminate the matrix before introduction to the ICP-MS or to eliminate the polyatomic interference in the ICP-MS. Sample pre-treatment is complex, expensive and time consuming, thus the preferred option is polyatomic removal using gas phase collision / reaction techniques. Design of the unique CRI-ICP-MS will be discussed along with principles of operation and performance attributes. It’s capability to handle polyatomic interferences in a complex urine matrix will be demonstrated. Sample preparation, instrument parameters, calibration and results for certified urine materials will be presented.

(4) A Flexible, Easy to Use Platform for Analyzing Molecular Interactions on Arrays. Steve Weibel1; Voula Kodoyianni1; 1GWC Technologies, Inc.

The SPRImager®II uses Surface Plasmon Resonance imaging (SPRI) to detect molecular binding (or dissociation) on arrays. To maximize its utility in array and biosensor development, the instrument’s design is open-platform: the gold-coated chips are completely accessible for full user control over attachment chemistry. Two types of sensor substrates are available. SpotReady™ substrates have 16 or 25 gold spots with a hydrophobic surround. This design facilitates manual fabrication of arrays on the bench, allowing for rapid methods development and easy setup of low-density arrays using submicroliter probe volumes. SPRChip™ substrates in contrast provide a uniform gold surface suitable for robotic spotting of denser arrays. Since SPRi can detect molecules regardless of chemical composition, the SPRImager®II platform is extraordinarily versatile. It has been used to analyze interactions involving antibodies, proteins, peptides, whole cells, RNA, DNA, transcription factors and aptamers. Here we show data illustrating the use of the SPRImager®II in analyzing (i) array quality prior to analyze exposure; (ii) sequential binding of DNA then proteins to the same nucleic acid array; (iii) antibody-antigen affinities and (iv) protein-protein interactions. The results show that the SPRImager®II
provides unique insights into array quality, and robust data for each type of array analysis. We also analyzed a 400-spot protein array fabricated on the SPRchip™. The results show specific binding of three analytes flowed consecutively over the same array, with good reproducibility for replicate probes. We conclude that the SPRimager®II is an ideal tool for biosensor development and for analysis of biomolecular interactions on arrays.

(5) A Novel Method of Analyzing Spectral and Chromatographic Data
Donald Tucker1, Leo Collins, Ph.D.2, Gregory Banik, Ph.D., Marie Scandone1; 1Bio-Rad Laboratories, Inc., Informatics Division
Traditionally, the visualization of multiple spectra or chromatograms takes place in an overlay, offset or stacked plotting form. A new technology known as Overlap Density (OD) Heatmaps reverses this situation by allowing comparative visualization of the overlap of large numbers of spectra or chromatograms so that trends and other useful information can be discerned. OD Heatmaps allows the user to explore data similarities and dissimilarities in large databases by providing information about the most and/or least commonly occurring spectral or chromatographic features in a data set(s). In this study, a new approach for spectral and chromatographic analysis that combines this new technology with chemometrics tools for multivariate analyses will be examined incorporating multiple analytical techniques in various application areas. The use of methods such as Principal Component Analysis (PCA) to perform multivariate analyses on spectral and chromatographic data has used for years in the field of analytical chemistry. This new approach for spectroscopic analysis will be examined in specific case studies. We will demonstrate the successful use of PCA and Overlap Density Heatmaps to analyze a query and the hit list from a spectral search and perform an overall analysis of a database.

(6) Spectral Imaging using Tunable Laser Source
Eli Margalith1, Lam Nguyen1; 1OPOTEK, Inc.
The use of OPO (Optical Parametric Oscillator) technology as a broadly wavelength-tunable laser light source offers decisive advantages in various spectral imaging applications. In this presentation we will discuss some of these advantages in obtaining reflection spectra of pharmaceutical samples. Specifically the ability to acquire high-resolution, calibrated hyperspectral data over the NIR range in a few seconds will be demonstrated. Actual wavelengths are measured and reflectance signal is calibrated and corrected for linearity at each wavelength in real-time for at each wavelengths are measured and reflectance signal is calibrated and corrected for linearity at each wavelength in real-time for at each wavelength in a few seconds will be demonstrated. Actual wavelengths are measured and reflectance signal is calibrated and corrected for linearity at each wavelength in real-time for at each wavelength, without the need for a pre-measuremen t calibration. The results show specific binding of three analytes flowed consecutively over the same array, with good reproducibility for replicate probes. We conclude that the SPRimager®II is an ideal tool for biosensor development and for analysis of biomolecular interactions on arrays.

(7) Comparing Resolution in IR Reflectance Imaging - NIR, mid-IR and ATR
Richard Spragg1, Jerry Sellers1, Robert Alexander1; 1PerkinElmer LAS
When images are measured in reflectance the observed structure is not necessarily just that of the sample surface. The 2-dimensional images produced by near and mid-IR imaging are representations of 3-dimensional objects. In reflectance images the effective spatial resolution is affected by how far the radiation penetrates into the sample as well as by diffraction and the pixel size. Although the penetration depth is likely to limit spatial resolution in NIR images, the boundaries between regions can appear more sharply defined than expected. Mid-IR reflectance images may contain both specular and diffuse components. These should have different spatial resolutions as the specular component shows purely surface structure. In ATR images the resolution has a component that depends on the distribution of components within a surface layer corresponding to the penetration depth, which is proportional to wavelength. These different contributions to the observed resolution can be investigated by imaging materials with known 2- and 3-D structure. We will show results obtained with a system that is capable of imaging in reflectance in both near and mid-IR as well as by ATR. The images obtained from the same regions of pharmaceutical tablets by the different approaches will be discussed.

(8) Extending the Range of Mercury Cadmium Telluride Focal Plane Arrays
Ellen Miseo1, David Drapcho1, John Leonard1; 1Varian, Inc.
Infrared Spectrochemical Imaging, the technology of coupling a focal-plane array to an FTIR to generate chemical specific images, has become an important tool in many areas of chemical research. The information derived from this technique has provided researchers with the ability to study the chemistries of spatially inhomogeneous samples. Initial development of focal-plane arrays in the mid-IR (2 to 15 um) was funded by the astronomy community and the U.S. Department of Defense. Theses researchers defined their devices based on their experiences and frames of reference and on the areas under investigation. Definitions of IR wavelength ranges differ, especially in the area of detector technology, between chemists and physicists (Table 1). Defense spending drove the technology toward military technical specifications and applications. The result is that cameras using focal plane arrays are designed with optical elements in them to limit the response to windows of interest to the physics and defense communities.

Wavelength Range Physicist Wavenumber Range Chemist
1.0 to 2.5 um Near-IR 10000 to 4000 cm-1 Near-IR
2.5 to 5 um Shortwave-IR 4000 to 2000 cm-1 Mid-IR
5 to 8 um Atmospheric window 2000 to 1250 cm-1 Mid-IR
8 to 14 um Long wave IR 1250 to 700 cm-1 Mid-IR
14 to 25 um 700 to 400 cm-1 Mid-IR
Greater than 25 um Far-IR

Table 1 – Differences in IR wavelength terminology

Mercury Cadmium Telluride (MCT) is capable of detecting infrared radiation from approximately 1 micrometer to approximately 25 micrometers dependent on the doping of the material. Most chemical spectroscopists are familiar with using MCT detectors into the near IR although the performance is not as good as Indium Antimonide. An MCT Focal Plane array is a photon counting device and to optimize performance in the region of interest, windows and anti-reflection coatings are chosen to selectively isolate the regions of interest. This limits the useful range for analytical spectroscopy. In this paper we will explore the use of an MCT focal plane array with specially designed optics to expand the regions of interest and enhance the performance in the (chemist defined) mid and near IR.

(9) An Ultra Sensitive Near-Infrared Camera for Chemical Imaging and Spectroscopy Applications
Ross Larue, Les Tack; 1Intevac
Transferred Electron (TE) photocathodes provide relatively high quantum efficiency between 950 and 1650 nm and recent design changes in cathode structure and processing techniques have improved tolerance to cooling, improved photocathode uniformity, cosmetics and reduced incidence of solid state emission points. The TE photocathode has recently been integrated with a back-thinned, multi-pin phase (MPP) CCD that is passivated to support electron-bombardment (EB) gain, analogous to EB-CCD sensors with GaAs photocathodes. The format of the sensor’s CCD is 1024 X 256 with 26 um square pixel pitch. The combination of high NIR quantum efficiency and EB gain offer a high-performance system for infrared imaging and spectroscopy applications.
ABSTRACTS

efficiency and Low noise gain (X100 gain is typical with an ENF < 1.1) provides exceptional low light sensitivity. The TE-EB-CCD sensor is can detect < 1 photoelectron under read noise limited operation. The Responsivity curve of the TE-EB-CCD sensor is provided in Fig. 2 and compared to an InGaAs focal plane array. InGaAs sensors have relatively high NIR quantum efficiency (~80%) but also have a very high noise floor from read noise and dark charge; these sensors do not support image intensification. TE-EB-CCD’s will have much higher Responsivity and SNR then InGaAs arrays for light levels typical for NIR Raman spectroscopy because of the relative sensor performance factors just discussed. The TE-EB-CCD sensor will support Raman applications using popular Diode and Nd:YAG lasers with excitation wavelengths between 976 1064 nm. The combination of laser excitation wavelengths in the“fluorescent free” zone coupled with low coupled with a sensor capable of detecting low light levels when integrated with a high resolution imaging spectrophotograph will facilitate NIR Raman applications previously performed with great difficulty with FT-NIR-Raman systems or dispersive Raman systems with CCD or InGaAs focal plane arrays. TE-EB-CCD’s will also be of great value for other low light NIR applications including Raman microscopy, photoluminescence, Raman chemical imaging, and NIR medical imaging. Configurations are also possible with CMOS sensors, which is expected to be of great value to Raman applications where size and power consumption have high priority.

(10) Complete ICP-AES Multi-Line Analysis Process: From Semi-Quantitative Analysis to Internal Standardization
Albert Brennstie1, Agnès Cosnier1, Sébastien Velasquez1, Sophie Leboull2, Catherine Wallerand2, Emmanuel Fretel1, Jean-Michel Mermet1; 1HORIBA Jobin Yvon Inc; 2HORIBA Jobin Yvon SAS; 3Spectroscopy Forever

In order to take full benefit of the information emitted by an ICP, it seems most useful and appropriate to perform multi-line analysis, i.e. the use of several lines per element, instead of using a single line, as usually conducted. Multi-line analysis makes it possible to cope with unexpected spectral interferences, as any outlier in a series of concentrations can be detected and rejected. The total process for method development includes a series of assistant software tools dedicated to the Horiba Jobin Yvon recently introduced ICP-AES system, the ACTIVA-M. Each tool aims at emphasizing multiple lines. The IMAGE tool allows the user to conduct semi-quantitative analysis so as to determine the list of elements and their concentration range. IMAGE is based on the entire acquisition of the sample spectrum. The S3-base is based on ICP experiments and consists of a collection of single-element spectra along with spectroscopic data such as wavelength, excitation energy, limit of detection, sensitivity and line width, resulting in a base with a double access. Using the S3-base, the MASTER tool facilitates multi-line selection, taking into account the list of elements and their concentrations. A filtering procedure suggests a list of possible lines based on relative sensitivities and potential spectral interferences, while an interactive display procedure permits the user to visualize the analyte lines and their vicinities, so as to validate the selection and to set up background corrections. A statistical tool, SOS, analyzes, for the set of lines of a given element, the various concentrations and their standard deviations, and rejects, if any, the outliers, so as to provide a single, reliable element concentration. When necessary, multi-line internal standard correction can be performed to improve accuracy. Using this logical step-by-step series of tools, any ICP user may become an expert. The ACTIVA-M, through its advanced CCD detector technology and the associated tools, is then perfectly dedicated and optimized to perform multi-line analysis, which results in improved concentration reliabilities. The complete multi-line analysis process will be illustrated with real data.

(11) New Interferometer for High-Resolution and Step-Scan FT-IR Spectroscopy.
Sergey Shilov1, Tom Tague2, Arno Simon2, Guenter Zachmann1; 1Bruker Optics

Bruker Optics introduces a new series of FTIR spectrometers based on the actively aligned UltraScan(TM) interferometer. The folding mirror is placed in the scanning interferometer arm to correct possible tiltts of the scanning mirror without introducing artifacts into the resultant spectrum. In contrast to the traditional “dynamic alignment”, the fixed interferometer is kept absolutely stable and precisely aligned. Therefore, the active alignment process generates no additional signal modulations. The friction free and high precision linear air bearing guarantees the ultimate sensitivity and stability for the high-resolution FTIR measurements from the UV to the terahertz spectral ranges. Advantages of the new patented TrueAlignment interferometer compare to traditional dynamically aligned Michelson interferometers will be discussed with reference to high-resolution and step-scan time-resolved FTIR spectroscopy applications.

(12) How Easy is FTIR to use Today.
Diane Errigo2, Josee Labrecque1, Henry Buijs1, Paul Chabot1; 1ABB Bomem; 2Biotools

Many years ago FTIRs required an expert operator who would be familiar with tweaking optical alignment to get the best spectroscopic results. The operator also needed considerable skill in viewing the spectral results to insure that the spectra were actually of good quality. Already since a number of years manufacturers have largely automated the optical alignment tweaking and a limited set of diagnostics would provide some assurance that at least the instrument was performing as expected for the current measurement. The next generation of FTIRs, as personified for example by the new ABB MB3000, go a step further and come with factory fixed optics that include permanent interferometer alignment as well as alignment concern for instrumental line shape conformity and overall reproducibility. Despite the invariability of the mechano-optical part of the modern FTIR, they are also provided with a more comprehensive health monitoring and overall diagnostic suite. The modern trend for FTIR is to achieve more reproducible spectroscopic results with much less specialized operator skill demands.

(13) HAPSITE Smart Plus, HAPSITE Viper, and HAPSITE ER Portable GC/MS Chemical Identification Systems
Bob Felty1, Ben Shultes1; 1INFICON, Inc.

INFICON produces the only truly portable Gas Chromatograph / Mass Spectrometer that can be taken directly onto the scene of a toxic organic chemical spill or chemical warfare agent attack and not have to be left outside at the edge of the hot zone. The instrument, dubbed the HAPSITE, is sealed to prevent contamination and the exterior can be easily decontaminated. It is designed for on-scene detection, identification and quantification of Volatile Organic Compounds (VOCs) such as Toxic Industrial Chemicals (TICs) and Chemical Warfare Agents (CWAs). GC/MS technology, the benchmark for the analysis of these and other organic compounds, is currently considered the most accurate analytical instrumentation in use for this purpose. Three new HAPSITE Models are scheduled for release in the third quarter of 2007. They are the HAPSITE Smart Plus, HAPSITE Viper, and HAPSITE ER. The HAPSITE Plus is an upgrade of the HAPSITE Smart model. Upgrade features include a color touch-screen for easy viewing and use. Improved Smart IQ software has also been redesigned for ease of use. The software is more automated which
will allow the operator to analyze, identify and quantify volatile compounds with a minimal amount of user interaction. The software also accommodates users who want more control of the HAPSITE for research or special applications. The HAPSITE Viper is a vehicle-mounted unit designed to test for both volatile and semi-volatile chemical warfare agents. The user can draw samples into the HAPSITE with an exterior sampling arm that is deployed from within the sealed vehicle. The HAPSITE can also be taken outside the vehicle and used in the same manner as other portable HAPSITE models. The HAPSITE ER is a portable unit that, like the Viper, contains a higher temperature sample path, which allows for the analysis of semi-volatile as well as volatile organic compounds. It is designed for the first responder market and has the same ease of use software and hardware contained in the HAPSITE Plus.

(14) GDOES - A Reliable and Economically Method to Analyze Conductive and Non Conductive Thin Layers
Ruediger Meinsner1, Michael Analytis1, Ludwig Adam1;
Spectrum Analytik GmbH
A glow discharge lamp which is used as sputtering and excitation source is the technical basis of any metal and surface analysis process. The area of degradation depends mainly on the anode used, which allows diameters of 1 mm, 2.5 mm, 4 mm, or 8 mm. The sputtering process is initiated by ionisation of the argon gas in the anode by applying a DC voltage. This ionises the argon atoms (plasma) and, because of an existing potential difference between anode and cathode, accelerates the ions with an average kinetic energy of up to 100 eV towards the cathode (sample). This bombardment forces atoms to leave the sample surface thus creating the characteristic sputtering crater in size of the anode diameter. In addition to the sample atoms some free electrons, called secondary electrons, are also generated during the sputtering process. The secondary electrons are accelerated towards the plasma and maintain the plasma activity through collisions with free electrons, Argon ions or meta-stable Argon atoms. The excited analyte atoms subsequently relax to the energetic ground state by emission of characteristic photons. These photons are then projected onto a holographic grating. Separation of wavelengths is done by an optical array according to Paschen/Runge on a Rowland circle which allows simultaneous analysis of all characteristic spectral lines of almost every element. Depth profiling analysis allows to detect concentration differences in a coating along a timeline. Typical depths vary, depending on the sample, from a few nanometers up to 200 µm Instruments using photomultiplier (PMT) technology are able to represent even the thinnest of layers because of their high sampling rate of 2000 measurements per second. The combination of high sensitive PMTs and sampling rate allows even the detection of elements present only in traces in a target sample. Usage of high resolution CCD modules offers additional element channel flexibility. Sensitivity of a CCD chip is significantly defined by its integration time, but in most cases a CCD is less sensitive than a PMT. CCD instruments not only offer a free choice of element channels and the option to analyse an almost unlimited amount of elements simultaneously, but also provide the option to define elements which do not produce emission lines in the spectrum projected onto the Rowland circle. Similarly to the CCD, a monochromator offers the possibility to freely choose any element channel and uses a fast PMT to determine the analytic results but may only define one element at a time. A combination of these technologies therefore provides the essential precision, speed and flexibility which is imperative in modern laboratories.

(15) Dendrimer Based NanoPhotonic Terahertz Source
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Dendrimer waveguide can generate a higher terahertz power via electro-optic rectification (EOR) that offers inherent power scalability because it is not limited by THz emission saturation or by heat dissipation. In an electro-optic dendrimer, the relationship between different material parameters, operating parameters, and the pump-THz conversion efficiency is of interest. In this note, the main factors that influence the efficiency will be discussed. An approximate model is used to estimate dendrimer waveguide’s EOR efficiency and power. Conventional photoductive devices produce average pulse train energy on the order of microwatts. For many practical applications, such as inspection and screening, detection of hidden weapons on humans, illicit materials, biological imaging, etc., the lack of power necessities long signal acquisition times, and is insufficient to divide among an array for parallel detection or synthetic aperture imaging. High power is also critical for sub-surface imaging and spectroscopy applications, where the THz beam may suffer considerable attenuation due to absorption and scattering it propagates through the medium. The crystalline semiconductors are the de facto materials for electronics and photonics devices because of their matured physics and technology that came a long way over the decades. However, polymeric materials are becoming an attractive alternative by virtue of their enhanced properties, cost-effectiveness, ease of fabrication, and ability to integrate with other on-chip functionalities. For terahertz generation, for instance, dendrimer materials remove the restrictions of directional and angular dependence of pump-THz conversion. Dendrimer allows creating a nanotechnology based photonic devices with attractive properties. An important aspect here is its multivalent molecular structure that allows boosting its electro-optic properties for enhanced EOR efficiency. This is important because the pump-THz conversion efficiency of an E-O material depends strongly on the 2nd order susceptibility which originates from its dipole concentration and their orientation that take direct part in the conversion mechanism. It is shown that average power > 100 mW per chip is expected with an efficiency of >1%. Details of the results and issues will be discussed.

(16) Reactive Spectrometers
Christopher D. Brown1, Robert L. Green1; 1Ahura Scientific
Spectroscopic platforms are being used for evermore complex tasks in increasingly varied circumstances. The extremely broad capabilities of spectroscopic technologies (e.g., Raman, FTIR, mass, NMR) often puts them in the first-tier of analytical choices for complex problems, but as deployed solutions they are usually configured to operate effectively in very restricted circumstances. The instruments are slaves to the analyst that developed the method -- usually a few low-level parameters are permanently set, and then the instrument is repeatedly triggered to collect data for some set period of time, with the instruments otherwise oblivious to the objective of the analysis. But as analytics move closer to the heart of the instruments, it becomes sensible to have the circumstances and objectives govern the instrument in real-time. In this paper we discuss the properties of several implementations of these systems, including quantitative devices adaptively optimizing confidence intervals, and field-portable Raman systems adaptively compensating for statistical power.

(17) Experimental Parameter Tradeoffs in High Throughput Polymorph and Salt Screening
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Chemical Imaging combines molecular spectroscopy and digital imaging, and has been demonstrated to be a powerful tool for molecular analysis of a wide range of materials. Chemical Imaging

ABSTRACTS
developed and introduced into the marketplace at logarithmic rates. Since the 1950’s new processes and new analyzers have been introduced. To demonstrate compliance to certifying agencies also requires research to insure the right throughput, linearity and efficiency. Topographic images of the surface can be correlated to the sample’s surface remains in the plane of the laser focus, optimising accuracy. Force microscope tip, feedback can be applied to ensure the laser spot size. When used in conjunction with an atomic force microscope tip, feedback can be applied to ensure the sample’s surface remains in the plane of the laser focus, optimising efficiency. Topographic images of the surface can be correlated with Raman images as the data are acquired simultaneously. This approach is likely to prove useful in the research of semiconductor and biological materials. A further development of the technique is to use specially-prepared metallised tips. Here, the SERS phenomenon is exploited, enhancing the Raman signal in the near-field; tip enhanced Raman scattering.

(18) Asset Management Can Control Time, Cost and Compliance
Gerry Hall1; 1; 1TimeKeeper America; 3Systea Scientific, LLC; 3Pasco County Environmental Lab
Since the 1950’s new processes and new analyzers have been developed and introduced into the marketplace at logarithmic rates. As equipment and instrumentation has become more sophisticated, more sensitive and more automated the challenges to purchase, certify and remain profitable escalates. Furthermore the requirements to demonstrate compliance to certifying agencies also escalate. As a lab manager how do you meet the challenges of today’s requirements? Equipment and instruments can cost from $25,000 to one million dollars. The instruments in your lab can have more value than the lab itself. The purchase of new equipment requires research to insure the right throughput, linearity and agency approvals are all in place. Next, qualified Chemists are required to run the analyzers. Keep in mind your staff is an integral part of your list of assets. Assets (equipment and people) control a lab’s reputation and the lab’s bottom line. Asset management needs to be integrated into your everyday operational mentality in the following ways. 1) Instruments must always be maintained to manufacturer’s recommendations. The first step in generating accurate data is to insure the analyzers always perform as if new. 2) A forward looking maintenance program must be in place. This can insure routine maintenance is completed on time even if a prime operator is on vacation. 3) Records must be maintained in a defensible manner. The quickest way to send the auditor to lunch early is to have “all your ducks in a row”. Records must be readily available (not misplaced), complete and legible. The entries should be time stamped and secure. 4) Management must personify, and champion, personnel empowerment. Chemists/technicians must become “experts” within their areas of responsibility. Training must never end. Ethics and other required programs must be fully endorsed – and practiced. Properly maintained instruments; and properly trained and motivated people facilitate the words in this abstract’s title. You will have a good start on asset management. Some new software companies are providing these tools on these devices the world of AFM and Raman have been separate and apart. Nanonics presents the first tool that combines the uniqueness of AFM for mechanical characterization with the capability of Raman to measure the chemical characteristics associated with local and highly defined silicon stress. This tool is an ideal integration of the worlds of AFM mechanics with the world of Raman material characterization and the specific application for MEMS device characterization highlights the importance of this combination.

(20) Nanoscale Imaging Techniques in Raman Spectroscopy
Matthew Bloomfield1; Ken Williams3; 2; 2; 2Systea Scientific, LLC; 2Renishaw, Plc; 2Renishaw, Inc.
Raman spectroscopy continues to provide analytical solutions in a variety of material science applications offering chemical specificity on a micrometer scale. The use of a piezoelectric-controlled sample stage permits accurate and repeatable sample movements in intervals significantly smaller than the diffraction limited laser spot size. When used in conjunction with an atomic force microscope tip, feedback can be applied to ensure the sample’s surface remains in the plane of the laser focus, optimising efficiency. Topographic images of the surface can be correlated with Raman images as the data are acquired simultaneously. This approach is likely to prove useful in the research of semiconductor and biological materials. A further development of the technique is to use specially-prepared metallised tips. Here, the SERS phenomenon is exploited, enhancing the Raman signal in the near-field; tip enhanced Raman scattering.

(21) Raman Chemical Imaging of Drug Loaded Polymers
Andrew Dennis1; Colin McCoy2; Robert Alexander1; John Cowley2; Jeffrey Taylor1; 1PerkinElmer; 2Queen's University of Belfast
Drug loaded polymers are now at the forefront of drug delivery technologies. They have found common use for several years in hormone replacement therapy (HRT) and contraception, but now their use is becoming more widespread in applications such as HIV prevention, prevention of infection, thrombocyte formation or cell proliferation in biomaterials, and dosage form design. The morphology of the polymer medium, and the drug loading characteristics dictate the drug release profile. A firm understanding of drug distribution, drug diffusion within the matrix, and drug release is required to optimize these systems and release their full potential. Drug release profiles are typically measured by soaking the drug loaded polymer matrix in solution and analyzing the drug concentration in solution over time using chromatographic techniques. Raman spectroscopy and Raman chemical imaging has been used to study drug loading and drug release in a range of drug loaded polymers. Automated chemical image generation using PCA techniques will be demonstrated. This “hands off” approach to chemical imaging allows for very high quality chemical images to be generated with no expert knowledge and minimal user effort. The detail rich Raman spectra and clear chemical images allow for a previously unseen level of understanding of the morphology and dynamics of drug release from these novel drug delivery systems.
Molecular and Microanalysis – Recent Advancements in Hybrid Instrumentation

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As the world leader in Raman, HORIBA Jobin Yvon has always been at the frontier of instrument innovations. The latest developments include hybrid instruments that combine two or more techniques in one instrument for enhanced material characterization. These hybrid instruments include Raman/PL, Raman/AFM, Raman/SEM, Raman/FT-IR, and Raman/PL/CL/SEM. The importance and advantage of these hybrid instruments will be discussed. Our Philosophy behind their designs and engineering will be explained. A few preliminary examples will be provided to demonstrate the benefits of not only multi-source data but also the enhancements due to the synergy of these microanalysis tools.

Spectral Data Management – LIMS, AIMS, PAT

David Joyce1, 1Thermo Fisher Scientific

At present many spectroscopists and chemometricians live in a world of flat files and multiple spreadsheets. Spectroscopy data is retained in isolation from lab chemistry and process histories. Convergence of these data streams will help accelerate the application of multivariate methods of data analysis. We propose the use of modern database and indexing tools coupled with non-proprietary data formats to aid compliance, provide data for in depth process analysis and to simplify day to day workflows.

MC-ICPMS: History and Applications

C.B. Douthitt2, 2Thermo Fisher Scientific

MC-ICPMS is unique among ICPMS instrumentation in that it is used almost exclusively for measurement of isotope ratios; measurement of concentrations and elemental ratios are the exception, not the rule. However, even with this restriction, the MC-ICPMS “bibliome” is now some 1200 papers in refereed journals, and the rate of publication has been steadily increasing. While the initial interest in MC-ICPMS was focused on measurements of radiogenic isotopes (Lu-Hf, U-Pb, Rb-Sr, Nd-Sm, applications where the new technique competed directly with TIMS), considerable interest has emerged in its use for the measurement of mass dependent fractionation of the stable isotopes of much of the periodic table. MC-ICPMS is being used to measure isotope ratios from Li to Pu. Recent reports of the detection of mass-independent-fractionation, especially of Hg, open up exciting new directions for research. The mass spectrometer hardware is, at this point, relatively mature and most of the current development work is focused on the use of high ohmic resistors (specifically 10e12 Ohms) for applications which had been thought to require multiple ion counting, on development of sample introduction systems which enhance sensitivity and stability, and exploration of laser ablation and chromatographic separations for sampling. The current market is about 15 units per year worldwide.

Isotope Fractionation: Happy Hunting Across the Periodic Table

Ariel Anbar1, 1Arizona State University; 2University of Frankfurt

The development and refinement of MC-ICP-MS techniques has revealed that mass fractionation in nature, once thought to be confined to light elements, is ubiquitous across the periodic table. From H to U, the isotopic composition of any element with two or more isotopes is measurably affected by chemical isotope fractionation. In many ways, the new “heavy” isotope systems can be thought of as analogous to traditional “light” stable isotopes, with fractionation arising from mass-dependent differences in vibrational frequencies and, hence, in bond strengths and reaction rates. This paradigm has been successfully applied to interpret variations in the isotopic compositions of elements like Cu, Fe, Zn and Mo, and the simple mass dependence it predicts provides guidelines useful in assessing data quality. However, it is suspected that some heavy isotopes can also be fractionated by other processes, such as the “nuclear field shift” effect, which is related directly to nuclear volume rather than to mass (Bigeleisen, 1996; Schauble, 2007). This effect manifests itself in fractionations that do not follow simple mass dependence, and which may have a direction opposite that expected from vibrational mass effects. Emerging MC-ICP-MS measurements of natural variations in 238U/235U provide very strong evidence that such novel effects are indeed important in nature. Hence, MC-ICP-MS makes possible the examination of novel physical processes, in addition to the effects of well-understood processes on heavy elements. Novel applications are likely to result.

Proof of Provenance by Isotopic and Elemental Fingerprinting

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Authenticity and provenance of agricultural goods and products are creating a lot of challenging questions to our scientific community. Currently, different approaches are used in order to cope with this task. Elemental fingerprinting and isotopic ratio analysis is widely applied in order to retrieve unique information of a sample. Whereas ‘light’ or ‘bio’ – isotopes (H, C, N, O or S) are commonly used, there is still a challenge and need to increase the number of isotopic systems in order to retrieve a unique set of information allowing a distinct mapping of provenance. ICP-MS technology has become a mature and widely applied analytical technique for a still increasing number of isotopic systems. Nonetheless, quick, reliable and accurate data has to be assessed on a large number of samples. Automated procedures are therefore of increased interest. Direct solid analysis by Laser ablation technology adds additional advantages. We have mainly focused on the investigation of Sr and Pb isotopes but are investigating the applicability of a number of additional isotopic systems in order to provide accurate and precise proof of provenance. Finally, the combinations of different sources of information have to provide a sound and robust statistical system for proof of authenticity. Still, we have to demonstrate the reliability of an isotopic fingerprint. Therefore, elemental sources and transfer pathways have to be considered in detail. Examples on the application of (LA)-MC-ICP-MS for authentication studies of agricultural products by different isotopic systems are discussed within this presentation.

Nu Plasma 1700: Design and Performance

Felix Oberli1, Philip A. Freedman2, Jamie Williams2, Simon Hollins3, Alex N. Halliday3; 1ETH Zurich; 2Nu Instruments Ltd.; 3University of Oxford

Nu Plasma 1700 is a large-geometry multi-collector ICPMS built by Nu Instruments Ltd (UK) for high-resolution, high-precision isotope ratio measurement. The prototype, installed at ETH Zurich in 2002, has successfully been used to study Li, Mg, Si, Ti, Cr, Fe, Ni, Sr, Hf and Pb isotopes by solution-desolvation and laser-ablation techniques. The double-focusing instrument uses a 943 mm radius, 70 degree electrostatic analyzer (ESA) followed by a 750 mm radius, 70 degree laminated sector magnet, whilst curved pole pieces and four multipole elements rotate the focal plane for right-angle intersection with the ion beams and ensure stigmatic focusing. These features result in the large mass dispersion of 1760 mm at an image demagnification of 0.8 unique to this instrument.
The ion source is operated at 6 kV, whereas the collector system is kept at ground potential. Ion signals are simultaneously recorded by up to 19 detectors. 10 Faraday collectors set at fixed dispersion are complemented by 6 mechanically adjustable cups (3 on either side of the fixed array), allowing for 16% overall mass dispersion at unit zoom magnification. Three discrete-dynode electron multipliers, one of them equipped with a retardation filter enhancing abundance sensitivity from 2 ppm to 0.2 ppm at mass 237, are interspersed with the fixed collector array. Multi-isotope beams are focused and matched to the dispersion of the fixed collector array by two electrostatic quadrupole zoom lenses. As opposed to other instruments operated in pseudo high-resolution mode, Nu Plasma 1700 simultaneously rejects interfering masses at both the low and high mass sides of the beams of interest. High-resolution tuning is achieved by means of a continuously adjustable source defining slit in combination with computer-controlled continuously adjustable collector slits at all 19 detectors. Aberration is minimized by selectable alpha restrictors and by higher-order functions applied to the four multiwells. With these provisions, the instrument achieves up to 40 000 resolving power (M/ΔM, 5-95% peak height), and a mass resolution of ~3'500 (10% valley convention) with flat peak tops over dM/M ~ 100 ppm at ~30% transmission relative to low (~700) mass resolution mode.

(28) Multiple-Ion Counting Inductively-Coupled Plasma and Thermal Ionization Mass Spectrometry for Analysis of Uranium and Plutonium Isotope Ratios

Lee Riciputi1, Deborah Bostick1, Stefan Bürger1, Edward McBay1; 1Oak Ridge National Laboratory

The use of simultaneous multiple-ion counting (MIC) for the analysis of small samples of uranium and plutonium has been investigated using the ThermoElectron Neptune inductively-coupled plasma mass spectrometer for IAEA environmental samples. More limited work has been done using multiple-ion counting on the ThermoElectron Triton thermal ionization mass spectrometer. Our results suggest that the performance of the MIC system varies between the two platforms, which we believe reflects both differences between plasma and thermal sources and the performance of the MICS themselves. These differences suggest that different analytical approaches to calibration of the multiple-ion counters may be required. Most of our long-term data using the MIC system if from the analysis of plutonium on the Neptune MIC-ICP-MS. Results from analysis of Pu QC samples over >18 months indicates that reproducibility of ~0.6% can be achieved for isotope ratios where both isotopes are present at the 10’s to 100’s of femtogram level, and reproducibilities of around 1% when the minor isotope is present at the 1’2 of femtogram level. Research sponsored by the Office of Nonproliferation and International Security (NA-24) and Office of Nonproliferation Research and Development (NA-22), National Nuclear Security Administration (NNSA), U.S. Department of Energy, under contract DE-AC05-00OR22725 with Oak Ridge National Laboratory, managed and operated by UT-Battelle, LLC. The submitted manuscript has been authored by a contractor of the U.S. Government under contract No. DE-AC05 00OR22725. Accordingly, the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes.

(29) Species-Specific Isotopic Fractionation of Mercury and Molybdenum during Physicochemical Reactions in Aqueous Solutions

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Recent advances in mass-spectrometric techniques, MC-ICPMS in particular, have allowed detection of variations in the isotopic composition of heavy stable elements, including Mo and Hg. These have spurred interest in unraveling isotopic fractionation mechanisms affecting these elements in natural geochemical, biochemical and other systems. This study focuses on quantification of isotopic fractionation of Mo and Hg during physicochemical reactions in solutions, including diffusion in water and water-octanol partitioning. Hg isotopic composition was determined by multiple-collector ICP-MS (Neptune, Thermo-Finnigan MAT) using solution nebulization for introduction of Hg into plasma. When necessary, a novel off-line Hg distillation procedure was used for purification of the element. Instrument mass discrimination for Hg isotope ratios was corrected with a TI element spike. External precision (1 STD) on measured 202Hg/199Hg ratios for the overall method was better than ± 0.2%. Experiments with water-octanol partitioning of Hg and Mo have been designed under variety of conditions in order to evaluate isotope signatures of hydrophobic (or lipophilic) fraction of these elements, which has the enhanced ability to cross biological cell membranes. Experiments modeling diffusion of Mo in aqueous solutions have been performed and the ratios of the diffusivities of Mo isotopes, D97Mo/D95Mo, in aqueous solutions have been determined. Diffusion of monomeric Mo oxanions in solution is concomitant with Mo isotopic fractionation with D97Mo/D95Mo = 0.99988±/−0.00004 (2 STD). In contrast, during diffusion of Mo polyanions, no measurable isotope fractionation has been found with D97Mo/D95Mo = 1.00000±/−0.00002 (2 STD). These results indicate the need for due consideration to Mo speciation when attempting to interpret the role of diffusive fluxes in the formation of Mo isotopic signatures in nature.

(30) Mass Spectrometry Applications in National Security and Forensic Science

Douglas Duckworth1, Helen Kreuzer1, Karen Wahl1, John Cliff1, Nancy Valentine1, Scott Lehn1, Martin Lierzens1, Gregory Eiden1; 1Pacific Northwest National Lab

Mass spectrometry is a proven tool in criminal forensics and its application to the detection, characterization, and attribution of materials associated with chemical, biological, and nuclear weapon materials continue to grow. Critical advancements in ancillary techniques related to processing now allow higher throughput, improved sensitivity, and specificity. The objective of this presentation is to provide an overview of select research and development activities within the Pacific Northwest National Laboratory, particularly as related to nuclear and biological materials characterization. Examples will be presented for a variety of mass spectrometric techniques — secondary ion mass spectrometry, stable isotope ratio mass spectrometry, inductively coupled plasma mass spectrometry (ICP-MS) — as well as hyphenated mass spectrometric approaches to specific analytical challenges. Advances in the use of electrochemically modulated separations to improve the elemental and isotopic analysis of nuclear materials will be presented as well as the use of stable isotope ratios in microbe forensics for cultures of B. subtilis spores produced on a total of 32 different culture media. Elemental characterization of culture media will be presented as well as an analysis of variation within individual samples grown between cultures produced in tandem, and between cultures produced in the same medium but at different times.

(31) Novel IMS Design for the Detection of Drugs and Explosives

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Successful detection of narcotics, explosives, or chemical warfare agents by ion mobility spectrometry (IMS) is instrument dependent.
Therefore, it is necessary to fully understand how well an instrument design can meet the resolution requirements for a specific detection problem. Previously, this type of understanding was only possible through empirical testing of an instrument. Now it is possible to evaluate an IMS instruments inherent capabilities to determine if it is adequate for the task via simulations. Modeling of IMS instrument performance can be accomplished using SIMION with the statistical diffusion simulations user program in conjunction with fluid dynamics from programs such as SolidWorks COMSOIFloWorks. Using this modeling approach, we have determined the theoretical resolution limitations for perfectly linear IMS designs. Based on the modeling, linear IMS designs are unlikely to meet both resolution requirements and the need for small compact form factors for instruments. Therefore, we have developed IMS designs that utilize nonlinear electrostatic fields in the drift regions for improved resolution in a compact design. Our modeling approach also allows us to determine whether a particular design can meet the detection challenge it is designed for before production to save costs.

(32) Capillary Electrophoresis/Mass Spectrometry for Analysis and Comparisons of Dyed Fibers

Stephen L. Morgan¹, Amy R. Stefan², Hartzell-Baguley Britany³, Brandi L. Vann¹; ¹University of South Carolina

Extraction and subsequent analysis of dye components from fibers offers the possibility for enhanced discrimination of trace fiber evidence. Microextraction methods have been developed for the removal of dyes from single fiber lengths as short as 2 mm. Extractions are performed on a liquid sampling handling robot using vials in 96-well plates. Extracts are subsequently analyzed by one of three different capillary electrophoresis (CE) methods. Diode array detection (DAD) is useful for fiber lengths of 5-10 cm, but mass spectrometric (MS) detection is necessary for shorter fiber lengths. Extraction and CE and CE/MS analyses will be presented for the separation and identification of dyes from six major textile dye classes: acid, direct, and reactive dyes from cotton and nylon fibers; vat dyes from cotton fibers; cationic dyes from acrylic fibers, and; hydrophobic disperse dyes. CE can separate most dye components and, coupled to DAD and MS, can provide semi-quantitative estimates of dye amounts as well as qualitative information to identify the dye(s) present. Although this approach is destructive to the sample, only an extremely small sample is required (about 1-2 mm of a single 15 micron diameter fiber). The time required for a typical fiber analysis might range from 10-30 min for extraction, followed by a 10 min CE run. Automated micro-extractions and CE offer the forensic analyst with % RSDs ranging from 5-25%, and limits of detection in the picogram range.

(34) Detection of Drugs, Explosives and Humans: Dogs vs Machines

Kenneth Furton¹, JoNell Aarons¹, Davia Hudson², Michael Macias¹, Samantha Tolliver¹; ¹Florida Int'l University

Laboratory and field studies identifying and quantifying the dominant odor signature chemicals used by certified law enforcement dogs are dogs and instruments to reliably locate forensic specimens including drugs, explosives and humans are presented. Laboratory studies include room temperature headspace Solid Phase Microextraction / Gas Chromatography / Mass Spectrometry. The results demonstrate that canines are generally not using the relatively low volatility parent substances but instead our characteristic volatile headspace components to accurately locate specimens. The implications of these results on the optimal selection of canine training aids and the tuning of instruments for these compounds are also discussed. In the case of drugs, detector dogs do not alert directly to the drugs cocaine and MDMA but rather methyl benzoate (1-10/Fg/kg spiked) and 3,4-methylenedioxybenzaldehyde (10-100 mg spiked). For the TNT and plastic explosives including C-4, detector dogs alert to DNT and 2-ethyl-1-hexanol as dominant odor signature chemicals. For living humans and human remains, there are a larger number of volatile target compounds including more than a dozen compounds from human remains including biological amines, alcohols/cresols, indoles, methyl sulfides and organic fatty acids. Human scent from living persons is comprised of hundreds of components with dozens of primary odor components which are stable over time regardless of diet or environmental conditions. Field studies have demonstrated the reliability of canines to match freshly collected human scent samples as well as those stored for long periods of time. Currently, there are scant optimized or standardized methods for the collection and storage of human scent evidence. Presently we present methods capable of preserving human scent samples for subsequent canine matching as well as for instrumental detection of the volatile organic compounds above human scent samples with characteristic volatile profiles observed between individuals. The detected compounds consist mainly of alcohols, aldehydes, amines, acid esters and ketones, and an instrumental analysis method has been developed that is capable of distinguishing individuals within a sampled group. The stability of primary odor components from hand scent samples has been studied under different environmental conditions including room temperature storage, -80°C, darkness and UV light exposure over 1-7 week storage periods.
(35) Forensic Applications of Laser Induced Breakdown Spectroscopy
Jose Almirall1; 1Florida International University
The chemical characterization of materials can provide important information as evidence in legal proceedings. The utility of trace elemental analyses for comparisons for glass, paint fragments, bullet lead and metal fragments has been demonstrated to offer a high degree of discrimination between different sources of these materials but the instrumentation required for the forensic analysis of these matrices (ie., LA-ICP-MS) is expensive, requires a high degree of operator sophistication and can be beyond the reach of many forensic laboratories. Scanning Electron Microscopy with an Energy Dispersive Spectrometer (SEM-EDX), X-Ray Fluorescence (XRF), Laser Ablation Inductively Coupled Plasma Atomic Emission Spectroscopy (LA-ICP-AES) and, more recently, LA-Inductively Coupled Plasma Mass Spectrometry (LA-ICP-MS) have been used in forensic laboratories for elemental analysis determinations. Single pulse and double pulse Laser Induced Breakdown Spectroscopy (LIBS) instruments have been evaluated as tools for the forensic elemental analysis of glass and compared in performance to other elemental methods in order to determine the utility of comparing casework sized glass samples. The figures of merit for the analysis of glass standards using single pulse and double pulse experiments with 1064 nm and 266 nm as excitation wavelengths is presented. Developments in the application of these LIBS systems for the forensic analysis of a variety of different matrices of interest to forensic scientists is also presented. The relatively low cost, ease and speed of operation and non-destructive nature of the LIBS analysis makes the technique a potentially viable forensic elemental analysis tool.

(36) Wavelet Based Search Prefilters for Spectral Library Matching
Barry Lavine¹, Nikhil Mirjankar¹, Kadambari Nuguru¹; ¹Oklahoma State University
A search prefilter is a quick test to spot dissimilar spectra, thereby avoiding a complete spectral comparison. Prefilters allow more sophisticated and correspondingly more time-consuming comparison algorithms to be used for spectral matching since the size of the library has been culled down for a specific match. Using the wavelet packet transform, IR library spectra are passed through two scaling filters: a high pass filter and a low pass filter. The decomposition process, which yields wavelet coefficients that represent the high and low frequency components of the signal are then iterated using successive wavelet packets until the required level of signal decomposition is achieved. Wavelet coefficients characteristic of functional groups are identified by a genetic algorithm for pattern recognition that uses both supervised and unsupervised learning to identify coefficients which optimize the clustering of the spectra by functional group in a plot of the two or three largest principal components of the data. Because the principal components maximize variance, the bulk of the information encoded by the selected coefficients is characteristic of a specific functional group. Spectral features encoded in the wavelet coefficients identified by the pattern recognition GA and containing detailed structural information will be used to develop response functions which will serve as substructure specific search prefilters.

(37) Automated Classification Techniques for Gemstones Using FTIR and Raman Spectroscopy
Stephen Lowry¹, Jerry Workman¹; ¹Thermo Fisher Scientific Inc.
FT-IR and Raman spectroscopy have proven to be excellent for detecting treatments and gem simulants and to provide key information for differentiating natural gems from their synthetic forms. FT-IR and Raman methods are often the first choice of advanced instrumentation techniques and provide a critical part of the gem certification process. This talk describes key applications of molecular spectroscopy in the analysis of gemstones and discusses sampling techniques for acquiring high quality infrared spectra from gemstones. Sampling is a significant challenge for cut or polished stones where the faceting process is designed to internally reflect the light as much as possible. Gemstones are generally crystal formations created from the atoms naturally occurring in the earth’s crust. They contain a broad range of metal and ions such as chromium, iron, magnesium, calcium, aluminum and beryllium. They generally also contain a negative group or ion such as silicates (SiO4), oxides (Al2O3), hydroxides (-OH) and occasionally borates (BO3), phosphates (PO3) and carbonates (CO3). The majority of gems with the exception of diamond contain oxygen in some form. Many gemstones consist of a major chemical composition that might be colorless such as corundum (Al2O3), but the presence of trace amounts of certain metal atoms can create bright colors. For example, sapphire and ruby are both corundum. The blue color in sapphires is caused by the presence of iron and titanium, and the red in ruby is due to chromium and iron. Although gemstones are complex natural products, many of the analytical techniques commonly used in industries such as pharmaceutical, polymer and semiconductor can provide valuable information on the composition and chemical structure of gems. Modern spectroscopic instruments have the sensitivity and reliability to routinely acquire high quality infrared spectra from gemstones. In this paper we will describe various applications of FT-IR and Raman to samples frequently encountered in a modern gemological laboratory. We will show specific examples where automated molecular spectroscopy has proven to be a valuable aid in the identification, not only of simulants but also of treated and synthetic materials.

(38) The Role of Chemometrics in On-Line Chromatography
Brian Rohrbach; 2Infometrix, Inc.
Chemometrics has long enjoyed use in research and quality assurance laboratories. Over the years, selected techniques have bridged the gap into process monitoring and control in areas such as signal processing, interpretation of on-line optical spectroscopy output, and the creation of inferentials. Implementation in on-line chromatography has lagged. Recent efforts have focused on identifying the role of chemometric technology during data acquisition and processing of chromatographic data. The impact is seen in several areas. •Preprocessing: All forms of chromatography are subject to retention time variability. In most process systems, this fluctuation forces the operator to review and occasional intervene to insure precise, reproducible peak identification and quantitation. Retention time variability is a significant source of variance in chromatographic data and confounds any subsequent analysis that is attempted. •Classification: Accurate identification and cataloging of ingredient changes, of process upsets and of instrument malfunction is critical. In some complex situations, we need to employ a combination of heuristics and chemometric model output to identify the process environment precisely. •Quantitation: This work extends beyond cataloging concentration values for individual analytes and begins to mirror the work that has long been done in on-line NIR. Fortunately, the transfer of calibration can be greatly simplified which enables prediction models to be deployed globally. •Data management: With hundreds or thousands of GCs performing identical analyses for a given user, the opportunity to simplify management of the data becomes strong. Here chemometrics plays the key role in identifying samples whose information content is unique and to vastly speed search techniques. Examples are drawn from the two-decades of experience with the Centers for Disease Control using HPLC and chemometrics to identify tuberculosis. Moving on-line
in the chemical and petroleum industries shows the impact of similar monitoring over the last 4 years and what is in store in the future.

(39) Optimizing Chemometric Model Development and Robustness Evaluation for PAT Applications in the Pharmaceutical Industry
Bruce Thompson1,2, Mercia & Co., Inc.
Process Analytical Technologies (PAT) are becoming an integral part of pharmaceutical manufacturing. The FDA’s PAT guidance and QbD initiative stresses the need for greater monitoring of process parameters and product chemical and physical properties during manufacturing. These initiatives encourage the use of multivariate tools, whether applied to spectroscopic data, like near infrared (NIR), or the collective body of process and analytical data. The use of multivariate tools to evaluate robustness metrics in calibration is demonstrated in this presentation. The example application of the techniques is in the development of an in-line NIR calibration for moisture measurement in a fluid bed dryer. The presentation will apply scientific theory and chemometrics to demonstrate multivariate model optimization and robustness of the implemented in-line NIR method. Model optimization evaluates the traditional parameters of pretreatments, wavelength range(s) and number of latent variables. This approach can generate a large number of suitable models. Various approaches to selecting optimum parameters include gradient methods, fuzzy logic and PCA techniques using either RMSEP or some other combination of accuracy and precision as performance metrics. Finally, the robustness of the optimized model parameters is evaluated through PCA and generating spectra that simulate likely failure modes of the analytical system. The result is a semi-automated process for developing multivariate models and demonstrating robustness.

(40) An Expert Spectroscopy System for Material Characterization
Jerry Workman1, Luminous Medical, Inc.
An expert system is recommended for classification, identification, interpretation, and possible semi-quantitation of components in neat or mixture conditions using vibrational spectroscopy. A key aspect to implementation of such a system is to codify the steps routinely used by the expert interpretive vibrational spectroscopist for identification of pure compounds, contaminants, and multicomponent mixtures. This exercise to codify the information and procedures (i.e., observations and thought processes) used by experts to perform spectral interpretation includes an outline of the rational steps taken during classification, collection of rules and advice provided by such experts, and additional references or sources of information referred to for accurate manual spectral interpretation. There are a wide variety of spectra and consideration of this fact should drive the choice of search options, especially for the initial search into any particular reference file. Additionally, the band shape and peak positions many be altered by the instrumentation used and by the physical state of the sample. Broadly speaking, most spectra would be encompassed using four basic search strategies. These include: (1) multiple searches to include strong and weak absorption peaks; (2) for the series of molecules with weak to medium key group frequency peaks, weighting factors are recommended as a pretreatment prior to searching; (3) For certain classes of materials, e.g. homologous series, polymers, copolymers, minerals, crystalline geological samples, etc. for which there are about 1-6 peaks and only much weaker; these few peaks are used exclusively for identifying characteristics; (4) Absorption peaks may be sharp or broad. Band widths of principal peaks within about the top 5% of the peak’s intensity may be as little as 2 cm^{-1} or as great as 10-30 cm^{-1} or more. Higher weight could be given to peaks that are a match for the reference spectra within ± 2 cm^{-1} width; and lower weight for matching within ± 5cm^{-1} for improved selectivity. These wide fluctuations suggest that clear separation of some categories of spectra is an optimal choice for long-term development of reference files. A good spectral search system needs to encompass strategies for all of these considerations.

(41) Multiple-Electrode Electrospray Emitter Systems for Analytical Advantage in ES-MS
Vilmos Kertesz1, Gary J. Van Berkel1, Oak Ridge National Laboratory
Control over the electrochemical reactions inherent to the operation of the electrospray ion source is critical in obtaining experimental results free from electrochemically-generated artifacts of the analyte or in utilizing the inherent electrochemistry to analytical advantage. Our recent efforts have focused on the use of alternative emitter electrode designs to control the electrochemistry of electrospray. The control of the working emitter electrode potential essential to electrochemistry control, was achieved by incorporating a three-electrode, controlled-potential electrochemical cell into the controlled-current ES emitter circuit. This potential control provided the ability to efficiently reduce analytes in positive ion mode and oxidize analytes in negative ion mode, in addition to the ability to control analyte oxidation in positive ion mode (or reduction in negative ion mode). Also, the system was used to selectively ionize analytes with different standard electrochemical potentials within mixtures to different charge states to overcome overlapping molecular ion isotopic clusters. Less precise control over the electrochemical reactions in electrospray was achieved with a battery-powered, controlled-current, two-electrode emitter cell. This cell system provided the ability to control the extent of analyte oxidation in positive ion mode in the electrospray emitter by simply setting the magnitude and polarity of the current at the working electrode. In addition, this cell provided the ability to effectively reduce analytes in positive ion mode and oxidize analytes in negative ion mode. The small size, economics, and ease of use of such a battery-powered controlled-current emitter cell was demonstrated by powering a single resistor and switch circuit with a small-size watch battery all of which might be incorporated on the emitter cell. The above mentioned systems both utilize an auxiliary electrode in the solvent flow path. This electrode may affect the solution composition via uncontrolled electrochemical reactions at lower flow rates due to more efficient mass transport to this electrode. A novel approach to eliminate these undesired Faradaic processes on the auxiliary electrode will be discussed.

(42) From Spray Stability to Ion Formation: Contorted Menisci and Ion Chemistry in Electrosprays
Akos Vertes1, Peter Nemes1, Ioan Marginean1, Samita Goyal2, George Washington University
Electrosprays exhibit a wide array of spraying regimes. They are characterized by large differences in the electrohydrodynamic disintegration of the liquid, in the droplet size and velocity distributions of the spray plume and in the nature and abundance of the produced ions. They also show different stability toward inherent changes in environmental and spraying conditions. Therefore, understanding spraying regimes and their transformations is of importance for analytical applications. We show that, in addition to the dripping, burst, pulsating, and cone-jet regimes, another ejection mode exists. In this astable regime the electrospray spontaneously switches between the pulsating and the cone-jet modes. With the introduction of this heretofore undescribed regime, a consistent view of the diverse axial regimes becomes possible, enabling their classification based on nonlinear dynamics. Electrosprays exhibit three main axial regimes, dripping,
pulsating, and cone-jet, potentially separated by two chaotic regimes, burst and astable, respectively. Of the axial spraying regimes the cone-jet mode appears to be most suited for ion production. Higher ion yields, a decreased extent of analyte fragmentation and oxidation are characteristic to this spraying mode. Thus in it the integrity of weak biologically relevant noncovalent complexes can also be preserved to a better degree. The effect of spraying mode changes is most prominent in the cone-jet mode, where the pH is expected to be lower than that of the bulk solution due to electrochemical oxidation of the solvent. In turn, proteins, sensitive to variations in the environment, undergo conformational changes, reflected by shifts in their charge state distributions. Our results suggest that improvements are achievable by the active control of the electrospray spraying regime.

(43) Ultra-low Flow Electrospray: Equimolar Response and Small Molecule Analysis
Gary Valaskovic1, Lucas Utley2, Panos Hastis3, Mike Lee4, Jing-Tao Wu5; 1New Objective Inc.; 2AstraZeneca R&D Boston; 3Millennium PharmaceuticalsMillennium Pharmaceuticals
Nanospray experiments were performed on an ensemble of drug molecules and their commonly known metabolites to compare performance with conventional ESI and to evaluate equimolar response capabilities. Drug-like molecules were analyzed, along with their well-known metabolites that formed via hydroxylation, dealkylation, hydrolysis, and glucuronidation. A variety of nanospray emitter designs (taper, diameter, length) were evaluated for robust operation at ultra-low flow rates (< 25 nl/min) on blood plasma prepared by protein-precipitation or liquid-liquid extraction. Nanospray exhibited a distinct trend toward equimolar response when flow rate was reduced from 25 nl/min to less than 10 nl/min. A more uniform response between the parent drug and the corresponding metabolites were obtained at flow rates of 10 nl/min or lower. Nanospray was used as a calibrator for conventional ESI LC-MS/MS; normalization factors were applied to the quantitation of an acyl-glucuronide metabolite of a proprietary compound in rat plasma. A nanospray correction and calibration method was developed to permit application of the standard curve for the parent drug to the metabolite compound. Quantitative results for drug metabolites were within ±20% of that obtained with reference standards and conventional ESI. An investigation of the equimolar phenomenon with respect to chemical diversity and choice of mass spectrometer platform and will be presented. Integration of the methodology into an automated flow-injection system will be highlighted.

(44) Improving Sampling Efficiency for Electrospray Ionization – Mass Spectrometry
Bradley Schneider1, Hassan Javaheri1, Thomas Covey1; 1MDS SCIEX
Substantial improvements in the sampling efficiency of electrospray ionization mass spectrometers have been achieved in the past decade. This presentation will describe some of the methods that have been used to improve sampling efficiency, with particular focus on the problem of electrospray beam divergence. Space charge effects, electric fields, and gas flows can all affect the shape of an electrosprayed plume, resulting in changes to the local ion density in the vicinity of a sampling aperture. The key to high sampling efficiency is to optimize the gas dynamics and electric fields such that a large fraction of the electrosprayed plume can be sampled into the mass spectrometer inlet. In the nanoflow regime, it is currently possible to design inlet systems such that the entire electrospray plume can be sampled into the instrument and desolvated properly for maximum ion liberation, providing sampling efficiencies as high as 80% for favorable compounds at solvent flows up to 500 nl/min. This indicates that the ionization efficiency of electrospray can be close to 100%, which has profound implications on the mechanism of ionization. This will be contrasted with proposed desorption/ionization mechanisms for matrix assisted laser desorption ionization (MALDI) and atmospheric pressure chemical ionization (APCI). However, there is a very significant reduction in electrospray sampling efficiency as the solvent flow rate increases up to approximately 1 ml/min, as a result of increased plume divergence and insufficient desolvation capability for ion liberation. Overcoming these difficulties is the key to designing ultra-high efficiency LC-MS systems. This presentation will discuss the relative merits of various approaches for increasing electrospray sampling efficiency throughout various flow regimes ranging from 50 nl/min to 1 ml/min.

(45) Fundamentals of Desorption Electrospray Ionization
R. Graham Cooks1, Andre Venter1; 1Purdue University
This presentation reviews and integrates what has been learned in the past 2 years on the fundamental processes involved in DESI, a powerful new ambient ionization method. The emphasis is on chemical reactions at the interface, physical phenomena including droplet sizes and velocities, and ion internal energies. Non-proximate detection and ion transfer through sampling "wands" gets special attention. Methods that relax the angular requirements of the technique are introduced. Fluid dynamics simulations explain the creation of microdroplets in the surface collision press and also the analyte "droplet pickup" mechanism. The coupling of DESI ion sources to miniature mass spectrometers is briefly addressed.

(46) Electrospray in Ambient Air: The Oxygen Effect
Richard B. Cole1, Boguslaw P. Pozniak1; 1University of New Orleans
Investigation of the influence of the ambient atmosphere on electrospray (ES) processes was conducted with the help of a small mobile platinum wire electrochemical probe placed inside the ES capillary. Electrochemical measurements of the potential difference between the wire probe and the ES capillary under open circuit conditions, and measurements of current branching between the probe and the ES capillary under constant potential conditions were mapped as a function of probe position to show the distribution of potentials and currents along the ES capillary. In traveling upstream, maps obtained under protective nitrogen showed a quasi-exponential decay with probe position. For maps obtained in the presence of oxygen, an anomalous dip is observed at positions close to the ES capillary exit. The effect was present in both positive and negative ion spraying modes. The total current drawn by ES remained constant throughout, regardless of the ambient gas, due to the self-regulating nature of electrospray. It was determined that the wire probe electrode response to a change in ambient gas is almost instantaneous when switching from nitrogen to oxygen; however, it takes tens of seconds to purge oxygen from the system. The influence of dissolved oxygen was assessed by comparing potential maps of regular and de-aerated solutions in the two different ambient atmospheres. It was shown that oxygen initially dissolved in solution, produces only a relatively minor effect. The "oxygen effect" is explained in terms of adsorption of gas through the skin of the electrospray meniscus (Taylor cone), and its "oxygen effect" is explained in terms of adsorption of gas through the skin of the electrospray meniscus (Taylor cone), and its subsequent upstream travel into the ES capillary interior, where it may become adsorbed onto the capillary walls, enter into electrochemical reaction at the metal-solution interface, or react chemically in the bulk solution with primary electrochemical reaction products. The ability of oxygen molecules to travel upstream is rationalized by recognizing the existence of turbulent liquid flow inside the Taylor cone that extends roughly two capillary diameters from the exit toward the interior.
(47) A Faster Method of Tandem Mass Spectrometry for Fast or Complex GC and LC Separations  
Glen P. Jackson; Ohio University

Tandem mass spectrometry offers a level of analyte specificity that enables lower detection limits and a higher degree of discriminatory power than conventional mass spectrometry. We have recently developed a method of fragmentation in quadrupole ion traps wherein excitation and fragmentation are deliberately accomplished during the mass acquisition scan of a quadrupole ion trap. The method is quite simple to achieve and enables a faster sampling rate for MS/MS than conventional CID. The faster acquisition rates are highly beneficial for fast or complex separation methods, as is demonstrated in three different applications: 1) confirmatory analysis of a mixture of high explosives in less than 3 minutes; 2) Identification of biomarkers in hair for substance abuse in less than five minutes, and 3) sequencing peptides in complex mixtures. The modified fast mass-acquisition scan with dynamic CID (DCID) was applied to a mixture a nine high explosives and to the analysis of 6 fatty acid ethyl esters, which are naturally occurring biomarkers for alcohol abuse that can be detected in hair. The high explosives can be separated and detected in selected reaction monitoring mode to around 5 pg on column; this is among the lowest reported detection levels for GC-MS of high explosives. The mixture of fatty acid ethyl esters were successfully separated and detected in fast GC-MS/MS mode at least 5 times faster than conventional separations. Detection limits are comparable to previously reported values. Finally, DCID and pulsed DCID are shown to be as effective as conventional CID in fragmenting small-to-large peptides such as leucine enkephalin and insulin chain A (~2.5 kDa). Pulsed DCID is similar to the pulsedQ experiment now available on the new Thermo range of 3D ion traps, and enables product ions below 1/3 of the precursor ion mass to be recaptured and mass analyzed. The combined benefits of faster sampling rate and better sequence coverage are expected to be beneficial for complex 2D LC proteomic separations.

(48) Gas-Phase Ion-Electron Reactions for Structural Characterization of Acidic and Neutral Biomolecules  
Kristina Hakansson¹, Julie T. Adamson¹, Hye Kyong Kweon¹, Haichuan Liu¹, Jiong Yang¹, Hyun Ju Yoo¹; ¹University of Michigan

The analytical advantages of electron capture dissociation (ECD) in proteomics research are well established and include the ability to localize labile modifications and to gather complementary sequence information compared to slow heating-based tandem mass spectrometric approaches, such as collision-activated dissociation (CAD) and infrared multiphoton dissociation (IRMPD). However, the applicability of ECD for other global analyses, including glycomics and metabolomics, is largely unexplored. One challenge is the requirement for at least doubly charged precursor ions. Multiple charging is only observed to a limited extent upon electrospray ionization (ESI) of many acidic, neutral, and small molecules, including sulfated species, oligosaccharides, and metabolites. We have explored two approaches for increasing the charge state of cationic species in ESI: zirconia-based enrichment of acidic molecules, and utilization of metal adducts and ion pairing reagents as charge carriers. Furthermore, we have explored the utility of electron detachment dissociation (EDD) and electron induced dissociation (EID) for characterization of anionic species. All experiments were performed with a 7 T quadrupole-FT-ICR hybrid mass spectrometer (Apex-Q, Bruker Daltonics). We have shown that zirconia-based enrichment provides selective isolation of phosphorylated peptides. ESI of isolated phosphopeptides results in higher charge states for improved ECD. Even a quadruply phosphorylated peptide could be characterized to determine the precise location of all four modification sites. We also found that metal addition can improve ESI response and yield improved structural characterization of acidic peptides, carbohydrates, and metabolites. For example, we observed complete sulfate loss in ECD of protonated sulfated peptides, however, sulfate groups were retained in ECD of metal-added peptides and oligosaccharides, thereby allowing their localization. For neutral metal-added oligosaccharides, sugar cross-ring cleavage, which provides carbohydrate linkage information, was dominant in some cases. In all cases, ECD provided complementary product ion spectra compared to IRMPD, thereby extending the amount of structural information gained about carbohydrates. Furthermore, both phosphoanhydride bond and sugar cross-ring cleavages were seen for metal-adducted nicotinamide adenine dinucleotide (NAD), neither of which was observed following sustained off-resonance irradiation-CAD. EDD and EID both yield complementary structural information compared to ECD, CAD, and IRMPD. However, their fragmentation efficiency is generally lower than for other MS/MS methods.

(49) Infrared Spectroscopy of Arginine Cation Complexes: The Stabilization of Gas-Phase Zwitterions  
Rebecca Jockusch¹, Matthew Forbes¹, Matthew Bush², Evan Williams³, Robert Dunbar³, Nick Polfer³, Jos Oomens³; ¹University of Toronto; ²University of California, Berkeley; ³Case Western Reserve UniversityFOM Institute for Plasma Physics

The structure of cationized arginine complexes [Arg+M]+, (M = H, Li, Na, K, Rb, Cs and Ag) and protonated arginine methyl ester [ArgOMe+H]+ have been investigated in the gas phase using calculations and infrared multiphoton dissociation (IRMPD) spectroscopy between 800-1900 cm-1 in a Fourier transform ion cyclotron resonance (FT-ICR) mass spectrometer. The structure of arginine in these complexes depends on the identity of the cation, adopting either a zwitterionic form (in salt-bridge complexes) or non-zwitterionic form (in charge-solvated complexes). A diagnostic band above 1700 cm-1, assigned to the carboxyl stretch, is observed for [ArgOMe+H]+ and [Arg+M]+, (M = H, Li and Ag), clearly indicating that Arg in these complexes is non-zwitterionic. In contrast, for the larger alkali metal cations (K, Rb and Cs) the measured IR-action spectra indicate that arginine is a zwitterion in these complexes. The measured spectrum for [Arg+Na]+ indicates that it exists predominantly as a salt bridge with zwitterionic Arg; however, a small contribution from a charge-solvated structure is also observed. While the silver cation lies between Li+ and Na+ in size, it binds as strongly or even more strongly to oxygen containing and nitrogen containing ligands than the smaller Li+. The measured IR action spectrum of [Arg+Ag]+ clearly indicates only the existence of non-zwitterionic Arg, demonstrating the importance of binding energy in conformational selection. The conformational landscapes of the Arg-cation species have been extensively investigated using a combination of conformational searching and electronic structure theory calculations [MP2/6-311++G(2d,2p)//B3LYP/6-31+G(d,p)]. Computed conformations indicate that Ag+ is di-coordinated to Arg, with the Ag+ chelated by both the N-terminal nitrogen and Nq of the side chain, but lacking a strong M+-carbonyl oxygen interaction that is present in the tri-coordinate Li+ and Na+ charge-solvation complexes. Experiment and theory show good agreement; for each ion species investigated, the global-minimum conformer provides a very good match to the measured spectrum.

(50) CARS Microscopy: Seeing the Invisible without Labeling  
Ji-Xin Cheng; ¹Purdue University

Coherent anti-Stokes Raman scattering (CARS) microscopy is a nonlinear optical imaging technique that allows high-speed
vibrational imaging. The integration of near IR picosecond pulse excitation, collinear beam geometry, epi-detection, and laser-scanning has produced a state-of-the-art CARS microscope with a detection sensitivity of 105 vibrational oscillators, sub-micron 3D resolution, and video-rate acquisition speed. The incorporation of spectral detection and other imaging modalities has added versatility to the CARS microscope. Advanced methods including polarization-sensitive detection, time-resolved detection, phase control, and interferometry were used for suppression of nonresonant CARS background. Although biological and biomedical applications are in an early stage, initial works have shown great potential of CARS microscopy in areas of membrane biophysics, cellular analysis, myelin sheath and demyelinating diseases, obesity and related health risks, skin and cosmetics. CARS microscopy is poised to become a powerful bio-imaging tool with continuous efforts in identifying unique applications that utilize the superior sensitivity and imaging speed of CARS over linear vibrational microscopy. The availability of a multifunctional, affordable, easy-to-operate CARS microscope will accelerate the development of new applications. The development of CARS endoscopy holds great promise for in vivo diagnosis.

(51) Increasing the Sensitivity of Carbon Fiber Microelectrodes for in vivo Applications

Jill Venton1; 1University of Virginia
Carbon-fiber microelectrodes have been used for in vivo measurements of neurotransmitters. Our lab is exploring a few different approaches to increasing the sensitivity of these electrodes. The first approach is to modify the surface of electrodes with carbon nanotubes. Applying a thin layer of carbon nanotubes resulted in a 2.5-fold increase in sensitivity for detection of dopamine and serotonin. Carbon nanotube modified electrodes also were more resistant to fouling by serotonin, so co-detection of dopamine and serotonin in vivo was possible. A second approach to increasing sensitivity is flame etching the microelectrodes. This results in electrodes with a 1-2 µm diameter as opposed to normal fibers with 7 µm diameters. These small electrodes have a higher signal per unit area and have higher S/N ratios than normal microelectrodes. The flame etched electrodes should cause less tissue damage and facilitate measurements in small places. The electrodes were used to measure dopamine release in anesthetized rats from very short stimulations.

(52) Using Carbon-Fiber Amperometry to Assess Nanoparticle Cytotoxicity

Christy Haynes1, Bryce Marquis1, Adam McFarland1, Katherine Braun1; 1University of Minnesota
Based on the unusual physical and chemical properties of nanoscale materials and their increasing use in medical and commercial applications, it is critical to develop and validate in vitro toxicity assays to aid in the safe implementation of emerging nanotechnologies. There are currently more than 450 commercial products that incorporate nanoscale materials of various size, shape, and composition. Upon intentional or unintentional introduction into the human body, the nanoparticle properties will determine the mechanism of cellular uptake and toxicity profile. Current cytotoxicity studies are largely limited to assays that measure average cell viability before and after exposure to nanoparticles instead of individual cell function even though live cells that have accumulated nanoparticles are likely to be functionally compromised. Here we show that microelectrode amperometry measurements reveal impaired exocytotic function in nanoparticle-exposed cells, giving insight into the disruption mechanism. In the case of mast cell exposure to 1 nM 25-nm-diameter spherical Au nanoparticles, there is a decrease of greater than 30% in the number of successful granule transport and fusion events, greater than 30% increase in the rate of intragranular matrix expansion, and greater than 15% increase in the number of secreted serotonin molecules. These results are in stark contrast to those achieved with traditional viability assays which detect little or no cytotoxicity. Our results suggest that nanoparticles interrupt the dense-core biopolymer matrix and present the potential for systematic studies showing how cell function is influenced by nanoparticle size, shape, and composition.

(53) Modeling Scattering in Vibrational Spectroscopy and Imaging

Anil Kodali1, Rohit Bhargava2; 1University of Illinois at Urbana-Champaign
Scattering processes in vibrational spectroscopy and optical imaging are important in defining structure, enhancing spectral response and for imaging. Here, we demonstrate a new model for scattering in biological materials that is based on Mie scattering theory and includes models of the scatterer to provide accurate field descriptions both in the near- and far fields. We demonstrate the scattering dependence of spectral response for non-absorbing frequencies for elastic scattering, convolution with absorption effects for IR linear absorption and enhancement for Raman spectroscopy. We discuss theoretically the utilization of enhanced scattering to develop new probes for biomedical applications.

(54) Quantitative Raman Spectroscopy in Turbid Media: Theory and Simulations

Wei-Chuan Shih1, Kate Bechtel2, Michael Feld2; 1Schlumberger-Doll Research; 2MIT Spectroscopy Laboratory
A limiting factor in non-invasive optical techniques is the variability of turbidity (absorption and elastic scattering) in the samples under investigation. The turbidity-induced spectral distortions and sampling volume variations, if left uncorrected, introduce additional non-specific variance into subsequent data analysis, e.g., multivariate calibration. Thus, quantification of an analyte-specific spectroscopic signal may be impaired. Using the photon migration framework developed previously, we derive an expression linking the measured Raman signal with the intrinsic Raman signal through diffuse reflectance and the total attenuation coefficient, mt. Intuitively, one would expect a one-to-one relationship between the Raman and diffuse reflectance signals for various turbidities. Indeed, this has been demonstrated in the literature, although in the special case where the scattering coefficient, ms, or the absorption coefficient, ma, is fixed while the other varies. For fluorescence spectroscopy in particular, fixed ms seems to be a good assumption. However, when both optical properties are allowed to vary, as is a more likely scenario for many applications, the one-to-one relationship does not hold. In these situations, the additional dependence on mt must be taken into account. Monte Carlo simulations have been employed to test the validity of the derived expression for semi-infinite and varying finite sample sizes. We also study the sensitivity of the expression with respect to the scattering anisotropy parameter, g. The dependence of the expression on sample size and anisotropy has important implications for in vivo studies.

(55) Quantitative Raman Spectroscopy in Turbid Media: Experiment

Kate Bechtel1, Wei-Chuan Shih2, Michael Feld2; 1MIT Spectroscopy Laboratory; 2Schlumberger-Doll Research
One of the central challenges in quantitative Raman spectroscopy is overcoming variability in sample turbidity (absorption and elastic scattering). The sample turbidity greatly influences the volume of tissue sampled by the excitation laser and the magnitude of the collected Raman signal. If narrow absorption features are present, turbidity also distorts the shape of the collected Raman spectra.
We have developed a correction method for turbidity-induced spectral distortions and sampling volume variability in Raman spectra, which relies on the recently derived relationship between Raman scattering, the total attenuation coefficient, and diffuse reflectance. Tissue phantoms were prepared in order to experimentally examine the effect of optical properties on the Raman signal and to demonstrate the applicability of the correction method. The tissue phantoms were composed of varying concentrations of Intralipid, an anisotropic scatterer commonly used to simulate tissue, India ink, and either creatinine or glucose to serve as an indicator of the Raman signal. Raman and diffuse reflectance spectra were collected sequentially via an integrated instrument. We find that prediction errors are significantly reduced using this simple method.

(56) Comparison of Vibrational Circular Dichroism (VCD) Instruments. Development of a New Despersive VCD Ahmed Lakhaniji, Peter Maloni, Timothy A. Kiederling; Univ. of Illinois at Chicago

We have designed and built a new dispersive vibrational circular dichroism (VCD) instrument, optimized for the measurement of mid IR bands such as the amide I and amide II vibrational modes of peptides and proteins (C=O stretching, and CN stretching NH bending, respectively) by maximizing sensitivity in the spectral range from 1800 cm−1 to 1400 cm−1. The major design factors were to make a compact VCD instrument for biological molecules, to increase signal to noise (S/N) ratio, to simultaneously collect the signals resulting from sample transmission and polarization modulation and to digitally normalize these signals following a design of Diem [1]. The design used a 0.3m monochromator, intense carbon-rod light source (~2500K) and a bandwidth limited (~ < 8/5m) MCT detector. The instrument uses 3 lock-in amplifiers whose outputs monitoring transmission and modulation are digitized and interfaced via RS232 to a personal computer which also controls the monochromator using LabView. The new dispersive VCD spectrometer will be compared with our previously constructed analogue-based dispersive VCD [2] and with some commercial Fourier Transform IR based VCD designs. We have collected spectra for peptides and proteins having different (alpha-helix, beta-sheet, and random coil) dominant secondary structures and for identical samples on several instruments, with comparable resolution and total measurement time. (1)Diem, M.; Roberts, G. M.; Lee, O.; Barlow, O. Appl. Spectrosc. 1988, 42, 20.(2)Kiederling, T. A.; Kubelka, J.; Hilario, J. Vibrational circular dichroism of biopolymers. Summary of methods and applications. In Vibrational spectroscopy of polymers and biological systems, Ed. Mark Braiman, Vasilis Gregoriou, Taylor & Francis Atlanta, 2006; pp 253.

(57) Dynamic Infrared Microspectroscopy using a Prism Based Spectrograph: Design and Optimization

Adam Lanzarotta; Miami University


(58) A Planar Array Infrared Reflection Spectrograph for Investigating the Dynamics of Poly(lactic acid) Stereocomplexation at the Air-Water Interface

Young Shin Kim1, Christopher Snively1, D. Bruce Chase2, John Rabolt3; University of Delaware; DuPont Experimental Station

Time-resolved infrared spectra of poly(D-lactic acid) (PDLA), poly(lactic acid) (PLLA), and their mixture (50/50 v/v) were obtained via a planar array infrared reflection spectrograph (PA-IRRS) in order to investigate the origin of stereocomplexation as well as the dynamics of the molecular conformational changes at the air-water interface during the compression of the monolayers. Features of the pressure-area (A−p) isotherm revealed that the mixed PDLA/PLLA film exhibited stronger intermolecular interactions than the pure polymer film, indicative of stereocomplexation in the mixture. In the bulk state, this intermolecular interaction of the mixed PDLA/PLLA sample was observed as a shift of certain IR bands in attenuated total reflection-Fourier transform infrared (ATR-FTIR) spectra when compared with those of the pure polymer. In solution, however, the IR band shift was not observed, indicating that both the pure PLLA and the mixture adopted the same conformation when prepared from a chloroform solvent. In the monolayer state at the air-water interface, time-resolved PA-IRRS spectra revealed that, during the compression of the films, the PLLA film adopted the 103-helical conformation while the polymer backbone in the mixed PDLA/PLLA film was found to be a 31-helical structure. These results suggest that the intermolecular interaction between PDLA and PLLA occurs when the two pure polymers are packed close enough to take on the characteristics of a solid film.

(59) Ultra-Short Path Length UV-vis Spectroscopy for Process Control

Lewis Baylor1, Patrick O'Rourke1; Equitech Int'l Corp.

A stumbling block to successful online spectroscopic analysis has been the requirement that the sample’s optical density fall in a range suitable for use with optical path lengths of at least 1 nm. In processes with high optical densities, samples are typically pulled and serially diluted prior to laboratory analysis. Equitech has developed online fiber-optic probes that allow for measurement at ultra-short path lengths using both transmission and attenuated total internal reflection designs. Examples of applications of these probes in the ink and plastics industries will be presented.

(60) Application of Process Raman to Monitor Blending Efficiency

Wes Thompson1, Brian Marquardt1; University of Washington

This presentation will discuss Raman spectroscopy as a process analytical tool for measuring blending and mixing of carbon nanotubes in a polymer matrix. Using a novel Raman probe the dispersion of the nanotubes can be followed in real-time, in a process-like environment with little interference from the sampling technique. This process provides a fast, non-invasive, information
rich, high-resolution monitoring technique that allows for collection of Raman data from all types of media (solid, liquid, gas, slurry, powder, etc.). Carbon nanotubes have promise as elements in electrically conducting polymers, however the distribution of nanotubes must be uniform to create an electrical path throughout the polymer. Maximum dispersion of these nanotubes is thus an important step in determining the point at which the polymer becomes conductive. In this presentation, Raman data will be presented indicating carbon nanotube dispersion into a polymer matrix. Early experiments indicate a possible correlation of increased Raman scattering efficiency with increased dispersion of nanotubes in the polymer matrix. In this presentation we will discuss the use of Raman spectroscopy as a process analytical tool for monitoring the degree of mixing and blending in various processes.

(61) The Use of Planar Array Infrared in Real-Time Studies of Structural Development in Polymeric Films

Bruce Chase1, John Rabolt2, Andreas Pes2, Chris Snively2; 1DuPont, 2University of Delaware

The development of infrared focal plane array detectors has made dispersive infrared spectroscopy a viable alternative to FT-IR in several areas. The sensitivity, speed and flexibility of Planar Array Infrared (PA-IR) instrumentation is comparable to FT-IR and the possibility for true double beam spectroscopic measurements is a real potential advantage in the area of process measurements. High S/N spectra can be obtained in milliseconds. When the full vertical dimension of the detector is utilized, true double beam measurements are possible, along with simultaneous parallel and perpendicular polarized measurements. Appropriate gating of the detector permits modulated studies such as dynamic measurements on stretched polymer films. These experiments, as well as potential limitations of the approach will be reviewed.

(62) Real Time Measurement of Propylene Oxide in Polyether Polys Via IR, Calibration via Calorimetry

Paul Weider1, André Buijs2, Dean Beerwinkle1, Remi de Groot2; 1Shell Global Solutions US Inc., 2Shell Global Solutions International

Shell Chemicals is among the leading global producers of polyether polyols. CARADOL polyether polyols, when combined with isocyanates, are used in urethane applications. Urethanes find use in products such as flexible and rigid foams, and in Coatings, Adhesives, Sealants & Elastomer (CASE) systems. As a result we may encounter them in a wide variety of goods including furniture, car seating, bedding, paints and coatings, artificial sports tracks, playground surfaces, ski suits and other waterproof leisure wear. Shell produces more than four hundred thousand metric tons per year of polyether polyols. Polyether polyols are produced by base or acid catalyzed polymerization of propylene Oxide (PO) with polyhydric alcohols and/or other functional initiators. An important aspect of safeguarding these exothermic reactions is to maintain a safe solution concentration of PO. Knowing exactly how much PO is in solution is difficult to ascertain due to the physical properties of the reacting mixture. Grab samples are hazardous to collect and difficult to analyze. In situ Infrared (IR) spectroscopy can readily detect the PO in solution, but how to calibrate the resulting IR spectra? We have accomplished this through reaction calorimetry. By adding pulses of PO to the reacting mixture and back integration across the pulse of the heat released, we can estimate the concentration of PO at any given time in the reaction. This is matched to the corresponding IR spectra to create calibration sets for the various grades. This work will also discuss moving these calibrations across platforms with different probes and detectors.

(63) A Case Study for Upgrading to Online NIR Measurement: Caustic Strength and Carbonate Content in Process Streams

Jessica L. Jarman1; SABIC Innovative Plastics

Near Infrared (NIR) Spectroscopy is rapidly gaining popularity in Quality Assurance/Quality Control (QA/QC) laboratories for several reasons, including commercially available robust instrumentation and decreased water sensitivity compared to mid-infrared analyses. Graphical interfaces supplied by instrument software companies are easy to use and usually switch between methods quickly. Additionally, the variety of available accessories on bench top instruments enables the analysis of a variety of material types such as solutions, powders, tablets, and pellets. Industrial businesses are increasingly challenged to produce faster results with fewer resources. Therefore, online analyses are also gaining popularity and NIR spectroscopy is already a commonly used technique for online testing. However, purchasing an instrument suitable for potentially harsh environments, installing fiber optic cables, and altering pipe configurations to accommodate probes can be costly and time consuming. Hidden and unattainable method requirements or lack of ownership and maintenance can easily destroy months of preparation and method development efforts. The case study presented here follows traditional caustic strength and carbonate measurements from a manual titration method, through NIR method feasibility studies, and into potential plant installation for online NIR measurements. All presented data and results were gathered during actual project investigation procedures in a polymer pilot plant in Mt. Vernon, Indiana. Statistical comparisons of each method type are included, as well as information on scoping out the project details and considerations for enhancing long term sustainability with minimized maintenance requirements.

(64) ReactIR™ for Hydrogenations and High Pressure Reaction Monitoring

Wes Walker1, 1Mettler Toledo

ReactIR™ has been applied to studies of hydrogenation and high pressure chemistry for more than 15 years. The range of chemical systems studied spans hydrogenations at slight overpressure to high-pressure supercritical carbon dioxide reactions. The presentation will consist of:

1. An introduction to ReactIR technology.
2. Four hydrogenation case studies, including the reduction of a nitrobenzene and pyrazine, a Rosenmund reduction, and a reductive amination.
3. Deployment of MonARC technology in the pilot plant and plant. This final segment will focus on integration of the attenuated total reflectance (ATR) sampling accessory to medium and large volume reaction vessels and strategies for coupling the MonARC to classified area distributed control systems via Modbus TCP/IP and digital to analog devices.

The specific advantages of in-situ analysis for high-pressure chemistry will be stressed. These advantages include; the detection of air or temperature sensitive intermediates and ease and safety of sampling without depressurization of the reaction vessel.

(65) SERS Nanosensors for Intracellular Applications

Janina Kneipp1, Harald Kneipp2, Margaret McLaughlin3, Dennis Brown1, Burghardt Wittig4, Katrin Kneipp5; 1Federal Institute for Materials Research (BAM), 2Wellman Center, Harvard Medical School, 3Program in Membrane Biology, Harvard MedCharité Universitätsmedizin in Berlin

Raman microspectroscopy has become an important tool for studies of various regular, induced or pathological processes in cultured cells. Although the method can deliver a high content of information on chemical composition and molecular structure, Raman measurements in individual cells remain a great challenge, in particular due to the extremely small cross sections for Raman
scattering, which often result in relatively long data collection times and therefore preclude from investigation of the dynamic processes of transport, trafficking, maturation or death in individual cells. In many cases, Raman or resonance Raman studies are performed at relatively high excitation intensities on fixed cells. In contrast, SERS enables the collection of excellent signal-to-noise Raman spectra in very short times (1 sec per spectrum and less) and low laser power (2 mW/1 µm spot) in individual living cells after gold nanoparticles are introduced into selected cellular compartments. The SERS effect has its origin in the favorable optical properties of metal nanostructures, and benefits from the enhanced local optical fields in their proximity. As these local fields are highly confined, we obtain strong and specific SERS spectroscopic signatures from nanometer-scaled volumes such as individual endosomes that are involved in uptake, transport and degradation of extracellular molecules. In the reported experiments, SERS signatures were measured from single living cells at different times after the uptake of gold nanoparticles. The spectral signatures were indicative of molecular changes in the environment of the nanostructures over time and provide information on the endosomal environment and key molecular players in its maintenance and regulation. Alteration of the SERS signal strength and parallel TEM studies indicate the formation of nanostructures providing optimum SERS enhancement for ultrasensitive probing inside the endosomal compartment. In addition to investigating the SERS signatures of cellular building blocks, we have been working on the development and application of nanorods, which, based on the SERS signature of a reporter molecule, can be used as stable and specific optical labels and also as nanosensors for one- and two-photon excitation. The reported results have implications in medical and biotechnology applications of SERS in cells.

(66) Developing an Early Diagnosis Test for Pancreatic Cancer Using Surface-Enhanced Raman Spectroscopy (SERS) 
Guifeng Wang1, Robert J. Lipert1, Marc D. Porter1, Aaron R. Sasson1, Maneesh Jain1, Surinder K. Batra1; 1Ames Lab-U.S. DOE, Iowa State Univ.; 2Dept.Chem.& Biochem. Arizona State Univ.; 3Univ. of Nebraska Medical Center
There is no specific tumor marker available for diagnosing pancreatic cancer. Recent research has suggested that the gene of MUC4 mucin, a member of the mucin family of proteins that is produced by secretory epithelial cells, is aberrantly expressed in pancreatic adenocarcinoma cell lines. Thus, the level of MUC4 in patient sera has potential as a diagnostic and possibly a prognostic marker for pancreatic cancer, but its measurement by conventional techniques such as PCR. This study demonstrates how SERRS can be a useful tool for rapid, direct virus classification via surface-enhanced Raman spectroscopy fingerprinting with novel Nanofabricated Silver Nanorod Arrays
Jeremy Driskell1, Saratchandra Shanmukh1, Ralph Tripp1, Yiping Zhao1, Jabilani Barber2, Peter Dluhy2, Lawrence Bottomley2; 1University of Georgia; 2Georgia Institute of Technology
Development of diagnostic methods for rapid and sensitive identification of viruses is essential for the advancement of therapeutic and preventive intervention strategies necessary to protect public health. Current diagnostic methods, including virus isolation, PCR, antigen detection and serology, are time-consuming, cumbersome, or lack the required sensitivity. We propose the use of aligned silver nanorod arrays, prepared by oblique angle vapor deposition (OAD), as surface-enhanced Raman scattering (SERS) substrates for the identification and quantitation of viral pathogens. The strength of a SERS-based biosensor is due to its simultaneous abilities to detect extremely low levels of material and to provide structural information as a result of narrow spectral features. The OAD method of substrate preparation facilitates the selection of nanorod size, shape, density, alignment, orientation, and composition, while the procedure is reproducible and relatively simple. The flexibility of this technique is advantageous for designing a nanostructured substrate with the greatest surface enhancement. Direct detection and classification of intact whole viruses, employing the OAD fabricated substrates, was achieved based on spectral differences in the SERS spectra of the viruses. Several viruses, including respiratory syncytial virus, HIV, and rotavirus, were chosen to assess the utility of this approach for viral biosensing. In addition to introducing this novel viral biosensor, this paper discusses and compares chemometric techniques used for virus classification.
(69) Bioconjugated SERS Nanoparticle Tags for Cancer Detection and Imaging
Ximei Qian1, Dominic Ansari1, X. P. Peng2, Lily Yang1, Shuming Nie1, 1Emory University
We report the spontaneous assembly of SERS nanotags with a durable, protective and versatile coating for bioanalytical and in vivo imaging applications. The imaging brightness levels for near infrared quantum dots (NIR QDs) and SERS nanotags have been determined at the single-particle level and in bulk colloidal solution with 633 nm laser excitation. Both measurements indicate that SERS nanotags are almost two orders of magnitude brighter than QD705. Bisfunctional polyethylene glycol (PEG) was employed to serve as a linker between the gold nanoparticle core and the targeting agents. To demonstrate the feasibility of this design for practical biomedical applications, we used the probe to measure the expression level of a protein biomarker on cancer cell surfaces. Cellular uptake studies have also been carried out by linking folic acid ligands to SERS nanotags through folate-receptor mediated endocytosis. In addition to surface-enhanced optical signals, gold nanoparticles are excellent contrast agents for transmission electron microscopy imaging of sub-cellular structure and X-ray endocytosis. The high sensitivity of NIR-SERS spectroscopy allows us to achieve noninvasive in vivo detection through the skin of tumor-bearing mice by using human single-chain fragment antibody epidermal growth factor receptor (ScFv EGFR) conjugated SERS tag for tumor targeting. To our knowledge, this is the first time one has achieved specific active tumor targeting in vivo using SERS sensors, which opens new possibilities for practical application of small tumor detection as well as ultra-sensitive biomedical diagnostics.

(70) Overview of Time-Domain Terahertz Instrumentation and Applications
Jeffrey White1, David Zimdars2, 1Picometrix LLC
This presentation will provide an overview of recent developments in Terahertz (THz) Time-Domain and Spectroscopic instrumentation and analysis. Numerous current and potential future applications will be considered. Most dielectric materials are quite transparent to THz radiation (0.05-3 THz, 0.0-1 mm, 1.7-100 cm⁻¹). Thus, transmission measurements through very thick (30cm² suitcase) are possible. This capability leads to many security inspection applications, especially imaging implementations. Another application is the inspection of thick foam materials. THz has been used to inspect the foam insulation on every NASA shuttle fuel tank since Columbia. However, highly polar materials (e.g., water, alcohols) are strongly absorbing. Thus, THz has been used to make bulk moisture measurements. The low energy of THz photons generally probes intermolecular interactions (e.g., polar material hydrogen bonding). Additional applications exist in morphology, crystallinity and polymerization measurements. To date, imaging is performed by raster scanning the THz sensor or sample object of interest. Multiplexed systems allowing a line scan have been developed. Typical measurement rates are 100 Hz with a S/N of 70dB at peak frequencies. This rate allows large size images to be obtained in reasonable times. Measurements in both transmission and reflection can be made. Reflection measurements appear similar to those made with ultrasound. Of course, THz measurements are made without sample contact. Another aspect of Time-Domain Terahertz is the radiation is emitted in an extremely short burst (~1 ps width). The THz time waveform collected provides the highest frequencies for which the electric field, as opposed to usual power detection, can be directly measured. Multiple applications measuring the electric field or the time delay of the pulse as it transmits through samples will be considered. Time-domain and spectroscopic information are always simultaneously available. Thus multiple simultaneous measurements, moisture content and sample thickness, can be made from the same measurement data. THz’s high measurement rate, ability to fiber optically couple the sensor, transmit through thick samples, provide imaging, make multiple parameter measurements simultaneously, and perform time-domain measurements all suggest manufacturing and control applications. Pharmaceutical, polymer / plastic / foam manufacturing and coating applications are example industrial measurement applications.

(71) Aspects of Microwave and THz Spectroscopy in Pharmaceutical Analysis
Jonas Johansson1, Lubomir Gradinarsky1, Mike Claybourn1, Staffan Folestad1, 1AstraZeneca Pharmaceutical and Analytical R&D
Spectroscopy using electromagnetic radiation in the frequency region from 300 MHz to 300 GHz and from 300 GHz to 3 THz referred to as microwave (MW) and terahertz (THz), respectively has not traditionally been used widely for pharmaceutical applications. The strong MWs interaction with the water molecule has been exploited mainly for drying applications, but the potential that exists in actually using this interaction for monitoring of moisture at different stages of the pharmaceutical manufacturing process or the moisture content of products has not been yet fully utilized. Nevertheless analyses of lab measurements of e.g. moisture behaviour inside microcrystalline cellulose (MCC) has been published as well as examples of MW systems able to provide moisture information for pharmaceutical and other applications mentioned. Here we demonstrate microwave spectroscopy for inline measurements of moisture during high-shear granulation of MCC based mixture. The application is not limited to only granulation, but could be extended to e.g. drying and coating using fluidized beds. Based on developments of new devices for emitting and detecting radiation in the THz region, new instrumentation for conducting spectroscopy of pharmaceutical materials is now available. THz spectroscopy compliments the established techniques of NIR spectroscopy, Raman spectroscopy, and mid IR spectroscopy, in terms of rapid and non-destructive analysis of solids and semi-solids, where polymorph identification, solid state characterisation of formulated products as well as imaging of layers and coatings has been already demonstrated. In this context we present a comparison of the established THz time-domain spectroscopy transmission mode of operation with a newly implemented Attenuated Total Reflection (ATR) mode. Effects of the particle size of the studied powder are analysed. The transmission measurements show a distinct dependence on particle size of the powder sample, while ATR measurements do not demonstrate any pronounced dependence. The latter fact, the comparable sensitivity of the two approaches, and the practicality of ATR puts it as the primary THz spectroscopic approach for rapid powder sample analyses, while the transmission mode could be utilized when more detailed studies of the sample behaviour under e.g. controlled temperature conditions is required.

(72) Understanding the role of Terahertz Imaging in Pharmaceutical Analysis
Fiona Clarke1, Linda Jayes1, 1Pfizer
The Terahertz region is currently a hot topic of discussion. This paper will look at the role of Terahertz imaging in support of pharmaceutical manufacturing. During the presentation examples will be shown of where Terahertz images have provided information of tablet coating processes, and how along with other chemical imaging methods can be used in the role of building process understanding.
(73) Terahertz and MM-Wave Imaging: Transmission and Reflection Capabilities and Needs
Joseph P. Dougherty¹, William L. Koser Jr², Matthew R. Fetterman³; ¹Penn State University Electro-Optics Ctr. Millimeter and terahertz frequencies have been demonstrated to be able to penetrate clothing to inspect for hidden weapons or explosive devices. Reliable data on the reflection and absorption of some common textiles is being obtained using a Teraview TPI Spectra 1000 transmission spectrometer, a Teraview TPI scan reflective spectrometer and a Thermo Nicolet FT-IR spectrometer. Our terahertz data covers the low frequency range from 1 wave number (1/cm) = 30GHz to the more absorbing range up to 100 wave numbers = 3 terahertz. Water can be a strong absorber in much of the terahertz and mm-wave bands. We will demonstrate imaging through both dry and wet textiles. It will be shown that, in spite of some water absorption, reasonable terahertz imaging is still possible through wet textiles. Bandages that are textile or polymer based are also very transparent to terahertz radiation. We have used this transparency to image burns though bandages. The changes in moisture content between heated and injured skin allows for high contrast in terahertz reflective imaging. This contrast difference could allow non-intrusive assessment of healing in cases where it is not possible to remove bandages or casts. Modeling of terahertz imaging can allow system designers to determine if there is an optimum frequency for a particular application. We are presently measuring the mm and terahertz optical/dielectric properties of a variety of materials in order to provide input data for our simulation efforts. Some image simulations will be shown.

(74) Lattice Dynamics Calculations of Phonon Spectra for Molecular Organic Crystals: Investigating the Polymorphism of Carbamazepine
Graeme M. Day¹, Axel Zeitler², Mike Claybourn²; ¹University of Cambridge; ²AstraZeneca
Spectroscopy in the terahertz frequency range has been shown to be a promising tool for the detection of crystal forms and for studies of phase transitions between structures. The power of terahertz spectra in studying molecular crystals stems from their providing a fingerprint of intermolecular interactions in the crystal structure, so that changes in packing of molecules often have dramatic effects on features of the spectra. However, our understanding of the influence of crystal packing on the resulting spectrum is relatively underdeveloped, limiting our ability to interpret observed spectral features. Atomistic lattice dynamics calculations are being developed to improve our understanding of the influence of specific intermolecular interactions on terahertz spectra and we present results of a study of the polymorphic pharmaceutical molecule carbamazepine. The calculations are used to characterize the lattice mode region of the spectra, providing a molecular-level understanding of the observed spectral features. The calculations are then used to explain the similarities and differences in the spectra of the various crystal forms of carbamazepine.

(75) Uses of Terahertz Pulsed Spectroscopy and Imaging in Industry
Philip Taday¹, Alessia Portieri¹, Yaochun Shen¹, Louise Ho²; ¹TeraView Limited, UK; ²University of Otago, New Zealand
Terahertz technology is can be utilized for solid-state pharmaceutical analysis, especially when applied as a spectroscopic technique. Examples of this include polymorphic differentiation, quantification; hydrate analysis and phase transition monitoring. When applied as an imaging technique, practices include chemical mapping and non-destructive solid dosage form analysis. Terahertz radiation – 3-333 cm-1 or 100 GHz-10THz – roughly coincides with the far-infrared region of the electromagnetic spectrum, where it is at its most sensitive to properties residing in the particulate (micron) and molecular (picometers) levels. Such properties include the crystalline phonon vibrations in solids and hydrogen-bonding stretches and torsions in gases and liquid. For both terahertz pulsed spectroscopy (TPS) and terahertz pulsed imaging (TPI) the core technology is the same, with the semiconductor emitter and receiver units playing a vital role in terahertz generation and detection. In this paper will highlight advancements in two areas:(1) the use variable temperature TPS to study the glass transition temperature in terahertz spectra and thus follow relaxation and crystallization processes in a solid matrix;(2) the use of TPI in understanding tablet coating performance especially when related to critical quantity attributes.

(76) Sr And Pb Isotopic Analysis Using Multi-Collector ICPMS For Answering Archaeological Questions
Frank van Haecke¹, David De Muynck², Ghylaine Quillet²; Felix Oberli³, Elisabeth Smits², Freek de Wolff³; ¹Ghent University; ²ETH - Zürich; ³Free University Amsterdam
Both Sr and Pb show natural variations in their isotopic composition as a result of decay of naturally occurring long-lived radioisotopes: 87Rb into 87Sr, 238U into 206Pb, 235U into 207Pb and 232Th into 208Pb. As these elements undergo no measurable isotopic fractionation upon industrial or biological processing, their isotopic analysis may shed light on the provenance of, e.g., ancient objects of art or human remains. In this presentation, the application of Sr and Pb isotopic analysis via multi-collector ICPMS in two case studies will be discussed. In a first case study, Pb isotopic analysis of skeletal tissue, excavated at a Roman cemetery, dating from the 1st – 3rd century AD, near Valkenburg (the Netherlands), sheds more light onto the presence of high contents of Pb in the bone tissue of stillborn and infants that have died at a very early age. By comparison of the isotopic composition of Pb present in femoral tissue on one hand and that of the graveyard soil on the other, the possible influence of diagenesis could be estimated. Via Pb isotopic analysis of, among other, amphorae and Pb objects, further information on the actual provenance of the bone Pb was derived. In a second case study, the Saint-Servatius basilica in Maastricht (the Netherlands), which testifies of 1600 years of history, was in the centre of attention. Sr isotopic analysis of the human remains discovered there was carried out to obtain some insight into the ‘heterogeneity’ of its past population. While the enamel is formed during early childhood and the isotopic composition of the Sr present herein reflects that of the food (and hence, the soil) where the individual lived at that time of his/her life, dentine shows a much faster Sr turnover and thus, its isotopic composition corresponds to that of the food consumed during the most recent years of a person’s life. Comparison of the isotopic composition of enamel and dentine Sr and further comparison with that of, among other, local soil and animal skeletal tissue, provides valuable information. Analytical aspects, such as appropriate sample preparation and correction for mass discrimination, will be discussed and (preliminary) conclusions concerning the archaeological questions posed will be presented.

(77) Isotopic Analysis of Bominerals by LA-MC-ICP-MS: The Role Of Ultra Short Pulse Width (Fs) Lasers.
Brian Fryer¹, Zhaoping Yang¹, Sonia Melancon¹, Joel Gagnon¹; ¹University of Windsor
LA-ICP-MS shows great promise for expanding the role of ин-situ isotopic studies of natural materials and allowing high spatial resolution analyses with precision and accuracy approaching TIMS methods. To achieve high precision and accuracy with LA-MC-ICP-MS requires the ability to consistently control mass bias and chemical fractionation in the ablation, transport and analysis of the sample and simultaneously to create the large ion beams in the MC-
ICP-MS, required for high precision analyses with Faraday detectors. Ultra short pulse width (Fs) lasers have been shown to minimize fractionation during ablation and produce the uniform and small particle size distributions required for high transport efficiencies and efficient and quantitative atomization and ionization in the ICP. To create large ion beams requires high laser power to ensure that the energy density over a significant area of the sample surface is well above the ablation threshold. We utilize the Quantrix Integra C® Fs laser to investigate sampling efficiencies and mass bias issues in the production of high precision Sr isotopic analyses of Ca-rich natural materials (otoliths, bones, teeth) of moderate Sr concentrations (300-1000 ppm). Results indicate that mass fractionation corrections for complete in-situ analyses are very similar to solution nebulization analyses of pure solutions and with comparable precisions on the isotopic ratios. The isotopic chemistry of otoliths, coupled with their trace element chemistry is becoming a major tool in fisheries management. Examples of data from fresh water fish species in the Laurentian Great Lakes will be presented.

(78) Extent of Matrix Effects between Zircon and Baddeleyite in Hf-Isotope Analysis by Laser Ablation-MC-ICPMS
Paul Sylvester1, Rebecca Lam1; 1Inco Innovation Centre, Memorial University

Isotopic ratios measured by laser ablation-multicollector-inductively coupled plasma mass spectrometry (LA-MC-ICPMS) may be biased by different amounts depending on the nature and composition of the sample matrix. Isotopic fractionation can be produced by material transformations at the ablation site, in a time-dependent manner, or by incomplete volatilization of ablated particles delivered to the ICPMS. Hafnium isotopic measurements of zircon (ZrSiO4) and baddeleyite (ZrO2) provide an excellent opportunity to quantify the nature and extent of matrix-dependent isotopic fractionation in silicate and oxide minerals of significant importance in the earth sciences. The hafnium isotope ratio of interest is the “initial” 176Hf/177Hf at the time of crystallization. The ratio is a tracer of magmas that formed the minerals because 176Hf is a radioactive decay product of 176Lu, and different reservoirs in the earth have different 176Hf/177Hf depending on their age and Lu/Hf ratio. To determine the initial 176Hf/177Hf, present-day 176Hf/177Hf is measured by LA-MC-ICPMS and corrected for instrumental mass discrimination effects by normalizing to the invariant 179Hf/177Hf ratio, also measured in the mineral. Isobaric interference of 176Yb on 176Hf is determined by normalizing measurements of the invariant 173Yb/171Yb ratio to the natural value, and using the derived fractionation factor to calculate 176Yb. For particularly old or high Lu/Hf grains, present-day 176Hf/177Hf will be significantly different than the initial ratio and must be corrected for in-growth of 176Hf formed by radioactive decay of 176Lu, using the 176Lu/177Hf ratio and age of the sample. Measurements of a wide range of zircon and baddeleyite illustrate that 179Hf/177Hf increases in a time-dependent manner as ablation proceeds until the laser pit reaches a critical depth. The scale of the increase (100-500ppm over 30 to 70 measurement cycles) far exceeds analytical precision of individual measurements. Both zircon and baddeleyite exhibit the increase, but it is more rapid in baddeleyite, which is softer and thus ablates more quickly. Because measured 176Hf/177Hf appears to fractionate in an analogous pattern as 179Hf/177Hf, mass bias corrections for the former ratio may be made effectively by normalizing to the latter ratio in each measurement cycle.

(79) Use of MC-ICP-MS in Exploration Geochemistry
Kurt Kyser; 1Queen's University

Isotopes are ideal tracers of both elements and processes in natural systems, particularly in environments characterized by redox conditions, fluid-mineral interactions or where processes involve phase changes of elements. As such, isotope ratios of many elements should show marked disparities near ore deposits where extreme redox environments abound, hydrothermal alteration is ubiquitous and select microbial consortia provide enhanced breakdown of the ores. Although exploration geochemistry has traditionally used elemental concentrations as a means for remotely sensing under cover ore deposits, isotope ratios of elements have been used only sparingly because of the expertise, time and resources required. The advent of MC-ICP-MS has made analysis of isotope ratios less time consuming and somewhat easier, depending on the elements of interest. We have developed protocols for the analysis of the isotope ratios of specific elements that are useful for detecting elements that have migrated from under cover ore deposits. Isotopic compositions of Li and B by MC-ICP-MS in soils record the extent of mineralizing fluids, Zn and Pb isotope ratios in soils and vegetation can be used to verify that these elements migrated from ores, Sr and S isotope ratios in groundwaters can reveal prospective areas for mineralization and U-Pb isotope systems can be used to evaluate specific areas in basins when the mineralizing fluid events were present. Separation of elements with masses less than Sr is required for precise analyses by MC-ICP-MS because of matrix-induced mass discrimination, but the isotope ratios of heavier elements can be analyzed with minimal effects from the character of the matrix. As the isotopic systems of other elements are explored with MC-ICP-MS, additional “fingerprints” of the source of elements in the near-surface environment should be revealed, including those that indicate under cover ore deposits.

(80) Application of Multi-Collector ICP-MS (MC-ICP-MS) to Geochemistry: Aqueous and Solid Sampling
W. Ian Ridley1, Michael J. Pribil2, Stephen A. Wilson2; 1USGS, Denver Federal Center

The purpose of this presentation is to provide an overview of the status of MC-ICP-MS studies in geochemistry. Particular emphasis is placed on studies at the USGS facility in Denver, Colorado. MC-ICP-MS instruments are being used with increasing frequency in geochemistry. This reflects the diversity of isotope systems that can be measured using this technique being applied, often for the first time, to problems in environmental geochemistry, economic geology, geologic hazards, climate change, and many other areas of geologic interest. Like most other isotope measurement techniques, e.g., thermal ionization mass spectrometry (TIMS), the separation of cations of interest from other matrix constituents is a necessary precursor to making precise and accurate isotopic measurements. This purification step is particularly critical in MC-ICP-MS methods development because of the substantial artificial mass bias effects (2-4% per amu) that are associated with plasma ionization and ion transport. Consequently, much effort has been applied by geochemists to understanding the mass bias laws that most accurately correct raw isotope ratio measurements. Based on these considerations the vast majority of MC-ICP-MS measurements involve liquid sampling, to facilitate ion chromatographic separations, and isotopic measurement using either wet (Peltier cooled aerosol) or dry (desolvated aerosol) plasma conditions. The latter, using desolvation nebulization, accounts for the majority of isotopic measurements because of enhanced sensitivity. Generally, isotopic measurements using in situ sampling of solids by laser ablation cannot produce the same degrees of accuracy and precision as liquid sampling, largely because of the uncertainties associated with additional matrix constituents. Nonetheless, if closely matrix-matched standards are available then useful measurements can be made with the advantage of preserving the spatial context of the analysis. The USGS Mineral Resources Program has focused on the development of MC-ICP-MS methods for analysis of non-
traditional isotope systems, such as Cu, Zn, Fe, Cr, Hg, S that are important in economic metallocgenesis and environmental geochemistry. In addition, the USGS has a program focused on the production of geochemical standard materials with a recent emphasis on micro analytical techniques, such as laser ablation ICP-MS. Some of these materials are well characterized for isotopic composition and are likely to prove useful in MC-ICP-MS studies that involve in situ sampling of solids. To date, the abiotic and biotic systematics of most non-tradition isotopes remains poorly understood. Consequently, whereas non-traditional isotopes can be measured with increasing precision and accuracy by MC-ICP-MS, there interpretation remains a challenge. This situation is common in isotope geochemistry when isotopic systems are at the infant stages of study.

(81) To Boldly Go – Measuring Fractionation of Mercury Isotopes in the Environment
Holger Hintelmann1, Delphine Foucher1, Wang Zheng1, Mark Dzurko1; 1Trent University
Analytical advances in the past decade and the recent advent of multicollector inductively coupled plasma mass spectrometry (MC-ICP/MS) have made it possible to measure fractionation of non-traditional elements, where mercury is still one of the more uncommon elements to study. We have developed a method for accurate and precise determination of Hg isotope ratios in a wide range of environmental samples. An on-line Hg cold-vapor technique, using stannous chloride as reductant, was coupled to MC-ICP/MS. All Hg isotope ratios were corrected for instrumental mass discrimination by simultaneously monitoring 205Tl/203Tl of MC-ICP/MS. All Hg isotope ratios were corrected for instrumental mass discrimination by simultaneously monitoring 205Tl/203Tl of a certified standard. The optimized method achieved a precision of better than 0.01 % RSD for mercury isotope ratios. Variations of the isotope composition of Hg were determined relatively to a standard (Mercury Standard Solution NIST SRM 3133) using the standard-sample bracketing approach. Mass-dependent fractionation was observed in cinnabar and coal samples and was also evident in dated sediment cores. We have successfully tracked plumes of Hg from mining activities in New Brunswick (Murray Brook mine) and the Gulf of Trieste (Idrija) and were able to distinguish anthropogenic from geogenic mercury. After preconcentration of mercury from aqueous samples having low, natural mercury levels, we show the first data of mercury isotope compositions for low level samples (< 10 ng/L).

(82) Micron-Scale Sensors for Detecting Reactive Oxygen Species Related to Noise Induced Hearing Loss in situ and in vivo
Alexander Scheeline1, Rebekah Wilson1, Edward Chainani2; 1University of Illinois at Urbana-Champaign
Noise-induced hearing loss limits life quality for approximately 9 million Americans and 180 million world-wide. Oxidative stress correlates with this cause of hearing loss, but whether causal or coincidental is unclear. Sensing of reactive oxygen species, specifically superoxide and hydrogen peroxide, during exposure to intense sound is a prerequisite to understanding the source of correlation. Sound transduction involves ion fluxes between the Scala of the inner ear, mediated by transducing hair cells. Thus, in order to achieve a complete picture of auditory transduction and changes during intense sound exposure, it is desirable to monitor not only reactive oxygen species but also to simultaneously monitor ion fluxes including at least sodium, potassium, calcium, and magnesium, and perhaps chloride and zinc. We are developing sensors for several of these species, based on enzyme-linked chronocoulometry (reactive oxygen species) and membrane conductance (ions). We report the performance of 200 micron wide reactive oxygen species sensors and initial steps in adapting potentiometric ion sensors to the spatio-temporal demands of the inner ear.

(83) Mediated and Direct Bioelectrocatalysis for Sensing Applications
Shelley D Minteer1, Tamara L Klotzbach1, Anne Blackwell1; 1Saint Louis University
There are many literature reports on employing dehydrogenase enzymes for bioelectrocatalysis for sensor applications. This research has focussed on the investigation of different mediator systems for dehydrogenase enzymes and different methods for mediator immobilization at electrode surfaces. Electropolymerized dyes (methylene green, methylene blue, azure C, etc.) have been investigated as mediators, along with binding of the mediator dye to existing chitosan polymeric backbones that are being employed for enzyme immobilization at the electrode. Secondly, we have been comparing these mediated bioelectrocatalysis systems to direct electron transfer electrocatalysis systems with dehydrogenase enzymes for sensor applications.

(84) Chemical Imaging of Single Cells with Scanning Electrochemical Microscopy
John Baur1; 1Illinois State University
Scanning electrochemical microscopy (SECM) is an important tool for making spatially-resolved measurements of chemical species at dynamic surfaces. Often, a redox mediator is added to the SECM cell to provide an electrochemical signal. Because such mediators can have toxic effects and interfere with the detection endogenous species, it is desirable to avoid their use when making measurements in biological systems. Two approaches for SECM imaging in biological systems without redox mediators will be presented. In the first, fast-scan cyclic voltammetry (FSCV) is performed at a carbon-fiber SEC hand tip. At fast scan rates (>100 V/s), the diffusion layer of the tip is small enough that it can be brought very close to the substrate (~2-3 µm) without appreciable diffusional interaction. Furthermore, FSCV permits simultaneous imaging of species having sufficiently different redox potentials. Chemical images of macrophage cells and model neurons using combined FSCV-SECM will be presented. In the second approach, tip impedance is used as a distance-dependent signal to maintain a constant tip-substrate separation. The impedance signal is modulated to a much higher frequency (200 kHz) than the current signal, permitting simultaneous and independent measures of distance and electrochemical activity. With this approach, topography and chemistry of the substrate can be imaged simultaneously. Images of model neurons recorded with this technique will be shown.

(85) Rapid Sample Preparation and Optimized Electrode Design for Dust Allergen Assays Integrated with Microelectrochemical Detection
Ingrid Fritsch1, Emily Anderson1, Andrea Henrichs2, Caitlin Williams1, Zoraida Aguilar2; 1University of Arkansas; 2Vegrandis, LLC
The National Institute of Allergy and Infectious Disease lists allergic diseases as one of the major causes of illness and disability in the U.S., affecting more than 50 million Americans. Avoidance of allergens is listed as the first step in treatment of disease related to allergies. There is a great need to be able to monitor indoor allergens in a regular fashion so that a better understanding of clinically significant amounts and extent of exposure to them is possible. We report progress toward developing an analysis for dust allergens that is simple, using a drastically improved sample preparation technique for the dust, and involves both molecular recognition with antibodies (in an immunoassay fashion) that are covalently immobilized and detection with self-contained
microelectrochemistry. Sample preparation times have been cut from several hours to minutes, and involve a much simplified dust extraction procedure than the ones used for commercial enzyme linked immunosorbant assays (ELISAs) so that analysis be performed on a regular basis in a allergist’s office. The microelectrochemical detection, which is performed within micrometers of the assay assembly site requires very small volumes and promises enhanced response times, sensitivity, and detection limits, compared to the commercial ELISAs. Different microelectrochemical electrode designs and separations of electrodes from the assay site will be discussed. The allergens that have been investigated include those for dust mite, cockroach, and cat. Steps toward analyzing all three in a panel on a single device will be discussed.

(86) Enhanced Detection of H2O2 via Electrogenerated Chemiluminescence at Microelectrodes for Single-cell Systems
Perry Motsegood1, Donald M. Cannon;1 University of Iowa Chemistry
Recent developments in neuroscience have suggested hydrogen peroxide, and other reactive oxygen species (ROS), show neuromodulatory behavior. Detection of these species is possible by electrochemistry, but has traditionally been limited to using enzyme-linked systems to gain reaction specificity. Unfortunately, these methods have been unable to provide spatial and temporal resolution necessary for single-cell analysis. Electrogenerated chemiluminescence (ECL) has the capability of combining optical data with electrochemical data resulting in a powerful tool for biological analysis. The luminol-H2O2 ECL reaction is typically performed with bulk solution conditions at high pH (9 or greater) to occur. Because of this restriction, detection of peroxide via luminol ECL is considered unsuitable for use in cellular systems. Although emission at pH 7.4 can be achieved, it is weaker, in comparison, to that at pH 10.5 and requires the concentration of the reactants to be orders of magnitude greater. Because signal intensity is directly related to pH new methods need to be developed for improved signal intensity. Microelectrodes, however, can be used to electrochemically alter reaction conditions near the electrode surface. Electrochemically generated hydroxide ions have been used in a variety of applications, including enhanced fluorescence emission, and shown a minimal impact on the bulk solution. Optical analysis has shown the ECL region is centered about the electrode with confinement being less than a radius unit (r = 5 um) from the electrode outer edge. Use of potential switching techniques has led to understanding the temporal capabilities of the solution kinetics and its effects on spatial distribution. Application of this technique at pH 7.4 will allow for improved ECL detection H2O2 resulting in emission intensities comparable to those observed at higher pH’s without effecting the bulk pH or adversely effecting any neighboring cells. Linking an electrochemical technique to an optical technique provides information not typically observed by comparable methods. The development of this technique poses the possibility of providing a sensitive yet maintaining spatial and temporal resolution. The information obtained by this method could provide insight into intracellular peroxide distribution and its potential implications within neuronal systems.

(87) Developing Nanoscale Electrode Systems for Electrogenerated Chemiluminescence Assays of Neuron and Glia Synergy
Donald Cannon1, Timothy Paschkeiwitz; Perry Motsegood1, Subbiah Alwarrapalan, Irma Nydegger; University of Iowa, Department of Chemistry
Through technological advances, such as miniaturization, bioanalytical investigations continue to advance our understanding of dynamic cellular functions. The analytical challenges arise in providing temporal analysis of short-lived species with sufficient sensitivity and spatial resolution to target cellular and subcellular processes. Specifically, we are investigating the underlying physical phenomena of nanoelectrode systems for enhanced electrogenerated chemiluminescence (ECL) biosensing. For instance, the high-frequency capability of nanoelectrodes permits faster oxidative / reductive cycling, thereby decreasing the area of light emission and ultimately increasing the spatial resolution for ECL probing. Initial ECL optimization experiments have been carried out at microelectrode structures. To further take advantage of miniaturized electrode structures, we have developed a focused-ion beam (FIB) milling protocol to form single nanowell architectures in insulating poly(methylmethacrylate) layers; thus exposing the underlying conductor substrate to form a nanowell electrode. More advanced preparation methods for unique nanoscale electrochemical architectures have also been investigated; such as metal deposition within the milled nanowells to form inlaid disk nanoelectrodes. Fabrication of nanoelectrode arrays has also been developed. With dimensional uniformity overcoming electric field non-uniformities, nanoelectrode arrays can operate with resolved radial diffusion to create ultra high current densities. While other nanoelectrode array fabrication methods have difficulties tailoring number and density, FIB milling allows individual electrode dimensions as well as interelectrode distances to be precisely established. Controlling the number, size and density of the nanoelectrodes is a powerful means for optimizing the cooperative effects between adjacent electroactive areas. Nanoelectrode array characterization is accomplished through traditional electroanalytical monitoring techniques integrated with ultrasensitive optical microscopy, with additional insight provided through multiphysics modeling. The development of simpler methods for the reproducible preparation of nanoelectrode structures of optimal number and density will enhance electrochemical-based biosensing interrogations.

(88) Hyperspectral Confocal Fluorescence Imaging for Investigating Host-Pathogen Interactions
David Haaland1; Howland Jones1, Mark Van Benthem1, Michael Sinclair1, Catherine Branda1, Bryan Carson1, Jens Poschet1, Roberto Rebei1, Diane Lidke2, Allan Brasier3; Sandia National Laboratories; 1University of New Mexico; 2University of Texas Medical Branch
We have developed a new 3D hyperspectral confocal fluorescence microscope that can optically section samples with diffraction-limited spatial resolution. At each voxel, the microscope records 512 wavelengths from the emission spectrum (500 to 800 nm) at a rate up to 8300 spectra/sec. When coupled with multivariate curve resolution (MCR) analyses, the microscope can resolve multiple spatially and spectrally overlapped emission components, thereby greatly increasing the number of fluorescent labels that can be monitored simultaneously. The MCR algorithm allows the “discovery” and relative concentrations of all emitting sources without cross talk. We have been using this system to investigate host-pathogen interactions. This presentation will focus on results from these studies when several mathematically equivalent solutions are possible from the MCR analysis of the spectral images. The interpretation of these equivalent results is enhanced with the appropriate selection of one of the solutions. Examples with two sources of autofluorescence in the cells or the sensitive detection of individual quantum dots will be presented to demonstrate the selection from several MCR solutions. As an example, we will show that when spectral shifts are present in the spectral images due to environmental interactions or size dependent spectral shifts in the case of quantum dots, the equivalent MCR results are either two spectral components located at the extremes of the possible spectral positions or a spectral component at the
center of the spectral component with the second component represented by a spectral derivative. We will demonstrate that the second representation listed above gives a more readily interpreted result. In the case of two sources of autofluorescence in a spectral image, we have found that interpretation of the data is straightforward with a main spectral component and a derivative component representing environmental effects on the peak position of the main autofluorescence component. Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

(89) Development of Image Data Analysis Tool for Pharmaceutical Applications
Lin Zhang1; Pfizer Global R&D
Spectroscopic imaging techniques are finding ever-increasing applications in pharmaceutical research and development due to their capability to provide spatial and chemical information about sample. One common data analysis approach in practice is the use of Partial Least Squares (PLS) to generate component distribution images. These images are reduced into binary images to extract component domain distribution statistics. Process understanding can further be obtained from these results. There exist a couple of challenges for image data analysis in practice. First, one crucial step is to threshold component distribution images to generate binary image. However, there is a lack of scientific guidance on how to set these thresholds properly. Second, sampling size is by a customer would be: how many images have to be measured (involving the number of tablets and slices within each tablet) to be statistically confident to make a decision? In this presentation, these questions will be answered through a case study for Active Pharmaceutical Ingredient (API) domain size comparison.

(90) Chemometric Methods for Automating the Interpretation of Hyperspectral and Multispectral Infrared Imaging Data
Gary Small1; University of Iowa
With the development and commercialization of mid-infrared multichannel detectors, the imaging capabilities of infrared spectroscopy have been significantly enhanced. These detectors are available in a variety of formats, including small linear or square arrays of 16 or 32 pixels, as well as larger scale focal plane arrays (FPA) with two-dimensional formats containing as many as 128x128 elements. A common issue encountered in the practical use of all of these detectors is the extremely high data rate, often producing hundreds or thousands of measurements per minute. This always an issue for imaging applications. A typical question asked presentation will focus on two applications of multichannel detectors in infrared spectroscopy and the development of chemometric methods to automate the interpretation of the acquired data. The first application focuses on the use of a multispectral infrared line scanner mounted in a downward-looking mode on an aircraft platform and used to make passive infrared measurements of ground scenes as the aircraft flies. This instrument can thus be used to interrogate the atmosphere between the ground and spectrometer, thereby allowing the detection of plumes of volatile organic compounds released from ground sources. The second application focuses on the coupling of an FPA detector, infrared microscope, and Fourier transform spectrometer to allow the collection of infrared microspectroscopic images. In both applications, the extremely high data rate requires automation of the data interpretation process. Digital filtering and pattern recognition methods are developed for both applications that help to accomplish the data interpretation task.

(91) Exploration and Resolution of Multilayer Spectroscopic Images
Anna de Juan1, Thomas Hancewicz2, Marcel Maeder3, Romà Tauler4; Universitat de Barcelona, Barcelona; The University of Newcastle, Australia; Unilever R & D, Trumbull, CT, U.S.IQAB-CSIC, Barcelona
Resolution of spectroscopic images is generally applied to a single scanned surface sample (2D image) or to the simultaneous analysis of independent 2D images with one or more compounds in common [1,2]. Preliminary exploration, based on repeated local pixel neighbourhood factor analyses, reveals the number of independent components overlapping around each pixel area. These results can be displayed together in a 2D local rank map that provides a global picture of the image complexity [3]. Resolution of the image measurement into pure component spectra and distribution maps is possible using alternating least squares resolution approaches [1,2]. The resolution results are substantially more robust if local rank information is implemented under the form of constraints. Local rank constraints, i.e., information about the presence or absence of certain image constituents in specific pixels, are coded combining the results of local pixel neighbourhood analysis and reference spectral information [4]. Multilayer image resolution poses new kinds of problems as compared with 2D image analysis. The first is the physical structure of the image itself, with three correlated spatial directions, the x- and y- coordinates of each surface layer scanned and the z-coordinate, indicative of the depth of the layer. Pixel neighborhood analysis should then be extended to 3-dimensional neighborhoods, resulting in appropriate local rank information, which can be implemented for resolution purposes in the same way as in 2D images. There are additional difficulties in 3D images: the quality of the data decreases with increasing depth of the measurement. Thus, the data become noisier, the spectral shape gets distorted and baseline problems escalate. To tackle these problems, suitable layer-specific baseline corrections and resolution strategies that take into account the layer-dependent signal-to-noise ratio have been developed. The application of all these features will be demonstrated on a real 3D emulsion image example. I.J.H. Wang, P.K. Hopke, T.M. Hancewicz, S.L.L. Zhang, Anal. Chim. Acta, 476 (2003): 93-109.2. A. de Juan, R. Tauler, R. Dyson, C. Marcolli, M. Rault, M. Maeder, TrAC-Trends in Anal. Chem., 23 (2004):70-793. A. de Juan, M. Maeder, T. Hancewicz, R. Tauler, Chemom. Intel. Lab. Sys., 77 (2005):64-74.A. de Juan, M. Maeder, T. Hancewicz, R. Tauler. J. of Chemom. (2007) (in press).

(92) The Effects of Pre-Processing of Image Data on Self-Modeling Image Analysis
Wilmeth Windig1, Mike Keenan1; Eigenvector Research, Inc.; Sandia National Laboratories
Chemical imaging is of increasing importance. One of the tools to reduce the massive amounts of data is self-modeling mixture analysis. This paper will focus on the pure variable approach. A pure variable (e.g., a m/e value, or a wave number) is a variable that has contributions from only one component in the mixture data set and thus can be used as a concentration estimate which can be used to resolve the mixture data into the pure component spectra and their contribution(“concentrations”). Similarly, pure pixels can be selected to resolve the mixture data. Image data are often of a noisy nature. Therefore, pre-processing of the data is often used to enhance the results. A popular pre-processing for TOF-SIMS data is based on the Poisson nature of the data. Another way to enhance data analysis is using the continuity present in images by checking spectral similarity of neighboring pixels. This paper will show how the data analysis results, as obtained with the pure variable/pixel approach, can be enhanced using the proper pre-processing tools, using data sets of actual samples. Sandia is a multiprogram...

(93) Interpretation of Support Vector Machines (SVMs) model for classification in Near Infrared (NIR) spectroscopy. Olivier Devo<i> </i>^2, Cyril Ruckebusch^1^2, Ludovic Duponchel^1^2, Jean-Pierre Huvenne^1^2, Laboratoire de Spectrochimie Infrarouge et Raman; ^1Univ. des Sci. et Tech. de Lille

Support vector machines (SVMs) are a new generation of learning algorithms used for classification and regression tasks. In the case of classification SVMs minimize simultaneously the empirical classification error and maximize the inter-class geometric margin. They operate in a Kernel-Induced Feature Space allowing non linear modeling. SVMs are of particular interest for classification based on spectroscopic measurement due to their good generalization ability even with relatively small training data set and their ability to deal with high dimensional space. SVMs have been introduced in chemometrics only recently and have proved to be powerful in NIR spectra classification in particular. Unfortunately the models obtained are quite difficult to interpret compare to other classification algorithms and SVMs are often used as “black box” methods. In this study we investigate the information than can be extracted from challenging classification with NIR spectroscopy datasets presenting overlapping class and/or multi-class prediction. First, the SVMs classification performance is compared to the ones obtained with classical classification methods. Second the influence of the SVMs parameters (kernel and trade-off parameters) on the classification performance is presented and a methodology for their optimization is proposed. Finally, as SVMs classification models rely only on small subsets of samples (the so called support vectors) we discuss their choice, number and distribution. This is performed in PCA subspace where a decision boundary is given too.

(94) The Relevance of Vacuum Ultraviolet Postionization of Laser Desorbed Neutrals to MALDI and DIOS Mass Spectrometry. Luke Hanley, Artem Akhmetov, Gerald Gaspar, Manshui Zhou, Peter Koin; ^1University of Illinois at Chicago

Matrix-assisted laser desorption ionization (MALDI) of low mass analytes is hindered by mass spectral interferences from the matrix material. Nanomaterials and nanostructures offer new ways to perform laser desorption ionization (LDI) for the analysis of small to moderately sized molecules by mass spectrometry (MS). We have recently reported a robust nanostructure, laser induced silicon microcolumn array (LISMA) as a particularly promising platform for matrix-free LDI MS of peptides and synthetic polymers. In this contribution we explore the fundamental ability of LISMA substrates for the matrix-free analysis of assorted analytes. Silicon wafers with low-resistivity were irradiated in an aqueous environment with a mode locked frequency tripled Nd-YAG laser. Repeated exposure of silicon wafers to Nd-YAG laser radiation produced a two dimensional array of microcolumns (LISMA) with an approximately 120 nm radii of curvature of the column tips. Mixtures were directly deposited from the solution phase on these surfaces. The soft laser desorption ionization (SLDI) experiments were conducted using a Kratos Axima III mass spectrometer with a nitrogen laser. At low fluence in SLDI, LISMA readily produced molecular ions for identification from a broad class of pharmaceuticals and peptides, such as pseudophedrine, propranolol, verapamil, loratadine, substance P, P14R, angiotensin and Bradykinin. Detection of analytes in the mass range from 150 to ~6000 amu was successful on the LISMA surface. Low detection limits of less than 1 femtomole were achievable with high mass resolution, sensitivity and semi-quantitation capabilities. At higher fluences the quasi-molecular ions produced at low laser energy were accompanied by structure specific fragmentation with minimum to no matrix or background ion interference. The versatility and robustness of the microcolumn arrays can be attributed to the submicrometer morphology and thermal, surface and optical properties of the processed silicon. Surface properties of the microcolumn arrays were systematically changed by altering the processing environment during their production. The unique structure of microcolumn arrays was analyzed using a scanning electron microscope. The combination of SLDI experiments and SEM imagery provided our initial insight into the fundamentals of this versatile technique.

(95) Laser Desorption Ionization from Nanostructures. Akos Vertes^2, Jessica Stolee^1, Bennett Walker^1, George Atwood^1, Washington University

Matrix-assisted laser desorption ionization (MALDI) of low mass analytes is hindered by mass spectral interferences from the matrix material. Nanomaterials and nanostructures offer new ways to perform laser desorption ionization (LDI) for the analysis of small to moderately sized molecules by mass spectrometry. We have recently reported a robust nanostructure, laser induced silicon microcolumn array (LISMA) as a particularly promising platform for matrix-free LDI MS of peptides and synthetic polymers. In this contribution we explore the fundamental ability of LISMA substrates for the matrix-free analysis of assorted analytes. Silicon wafers with low-resistivity were irradiated in an aqueous environment with a mode locked frequency tripled Nd-YAG laser. Repeated exposure of silicon wafers to Nd-YAG laser radiation produced a two dimensional array of microcolumns (LISMA) with an approximately 120 nm radii of curvature of the column tips. Mixtures were directly deposited from the solution phase on these surfaces. The soft laser desorption ionization (SLDI) experiments were conducted using a Kratos Axima III mass spectrometer with a nitrogen laser. At low fluence in SLDI, LISMA readily produced molecular ions for identification from a broad class of pharmaceuticals and peptides, such as pseudophedrine, propranolol, verapamil, loratadine, substance P, P14R, angiotensin and Bradykinin. Detection of analytes in the mass range from 150 to ~6000 amu was successful on the LISMA surface. Low detection limits of less than 1 femtomole were achievable with high mass resolution, sensitivity and semi-quantitation capabilities. At higher fluences the quasi-molecular ions produced at low laser energy were accompanied by structure specific fragmentation with minimum to no matrix or background ion interference. The versatility and robustness of the microcolumn arrays can be attributed to the submicrometer morphology and thermal, surface and optical properties of the processed silicon. Surface properties of the microcolumn arrays were systematically changed by altering the processing environment during their production. The unique structure of microcolumn arrays was analyzed using a scanning electron microscope. The combination of SLDI experiments and SEM imagery provided our initial insight into the fundamentals of this versatile technique.

(96) Recent Developments in Models of UV MALDI Ionization. Richard Knochenmuss^1, ^1Novartis

Within the 2-step framework for UV-MALDI ionization (primary ion generation followed by ion-molecule reactions), two numerical models have been developed. The rate equation approach allows rapid prediction or interpretation of MALDI mass spectra, but uses a simplified description of the early phase change and plume. The molecular dynamics model provides does not have this limitation, but is much slower, and limited in spatial and temporal scope. Extensions of and new results from these models will be reported. The rate equation model has been applied to thin samples interacting with surfaces, and MALDI from constrained spaces, corresponding to new MALDI variants. The molecular dynamics model has been extended to include secondary reactions with analytes, as well as external electric fields, and cluster-dependent thermodynamic properties. The results illuminate the complex interactions between physical and chemical processes in MALDI and aid in interpreting and planning MALDI experiments.
(97) Experimental Probes of Equilibrium Conditions in Laser Desorbed Plumes of Material
Gary Kinsel1, Dennis Marynick2, Faten Yassin2, Ganga Fernando1; 2Southern Illinois University Carbondale; 1University of Texas at Arlington

For the last several years our group has explored the equilibrium / non-equilibrium nature of the plume of material desorbed during a typical MALDI experiment. These investigations have been motivated primarily by our interest to develop a methodological approach to the discovery of new MALDI matrices. Initially, our investigations focused on the relationship between analyte thermochemistry and analyte ionization efficiency. In these experiments laser desorption of mixtures of a number of MALDI matrices (2,5-dihydroxybenzoic acid, sinapinic acid, etc.) or matrix analogs (the x,y-DHB isomers) with a series of amino acid analytes (or small peptides) were performed and the data obtained evaluated using an approach analogous to the kinetic method. For these studies the key issue was the linearity of the relationship between the natural log of the relative acceptor to donor intensity versus the amino acid gas-phase basicity (GB). Our studies clearly showed that analyze GB could be directly related to analyte ionization efficiency, supporting the equilibrium nature of the MALDI plume. Furthermore, evaluation of the slopes of these plots to determine the effective temperature of the desorption plume were consistent with other measures of this property. However, evaluation of the intercepts of these kinetic method plots, while in general agreement with the expected thermodynamic properties of the MALDI matrices, were not in as good agreement with the expected values based on experimental and calculated thermodynamic properties of the matrix derived proton donor species. Subsequent studies have focused on correlation of matrix performance with a range of quantifiable matrix properties including; matrix radical cation GA, matrix neutral GB, protonated matrix GA, matrix melting point, matrix sublimation temperature, matrix molar absorptivity, etc. No strong correlations between any of these measurable physical properties and matrix performance have been identified suggesting that neither isolated gas-phase, nor bulk matrix properties adequately describe matrix performance. Cumulatively, these studies suggest that while an equilibrium picture can adequately describe relative analyte ionization efficiency this picture is inadequate to the description of matrix performance.

(98) The Role of Particulate in Laser Desorption/Ionization
Kermit Murray; 1Louisiana State University

We are investigating the role of particles in laser desorption and ionization using both ultraviolet and infrared lasers. Recent studies of laser particle formation in our laboratory suggest that a large fraction of the material removed in MALDI is in the form of micrometer-sized particles. This is particularly true for infrared lasers that remove a large quantity of material as particulate. We are using several tools to investigate particle formation and the role of particles in ion formation. First, we are using aerodynamic particle sizing to measure the concentration and distribution of particles as a function of fluence and laser wavelength. Second, we are using laser ablation followed by post-ablation particle ionization to probe the dynamics of particle ablation. A tunable pulsed mid-IR OPO laser system is used for particle desorption and a UV excimer laser (248 or 351 nm) is directed at the plume of particles. The delay between these two lasers gives information about plume dynamics and the change in size distribution gives information about UV laser particle break-up. The third tool is UV irradiation of the plume to form ions in a TOF mass spectrometer. The IR laser ablates particles, neutrals and ions from the target and the UV excimer laser is directed above and parallel to the sample surface to break up the particles and create ions and also create ions by UV post-ionization. Ions are mass separated in a linear time-of-flight (TOF) mass spectrometer. A fourth tool is the entrainment of ablated particles in an electrospay of solvent. Ions are formed when the IR laser ablation plume interacts with the charged droplets in the electrospay. Using the combination of these tools, we are investigating ion formation with the ultimate goal of improving performance and expanding the applications of laser desorption mass spectrometry.

(99) Analyte-loss Processes in Inductively Coupled Plasma Mass Spectrometry
Bodo Hattendorf4, Zhongke Wang1, Detlef Günter1; 1ETH Zurich, D-CHAB, Lab. for Inorg. Chem

Analyte sensitivity is always of major concern when performing chemical analysis. Especially with the desire to steadily improve spatial resolution in direct solid analysis, the instrumentation used has to be able to detect ever smaller quantities of material reproducibly and accurately. Inductively coupled plasma mass spectrometry (ICPMS) is probably one of the most versatile and sensitive detectors for direct solid sample analysis, when coupled to laser ablation (LA) sampling. Nonetheless, the detection efficiency of current ICPMS instruments (ppm to per mil, depending on analyte and instrumentation) would only allow major element analysis in the per mil range when spatially resolved sampling in the sub-micrometer range shall be achieved (e.g. using near field methods for laser ablation (1)). It is thus of major concern to determine to which extent the detection efficiency of ICPMS - especially in combination with LA-sampling - can be raised in order to facilitate lower limits of detection at high spatial resolution. Ours studies aim at identifying dominating processes that cause analyte loss in an ICPMS and the influence of operating conditions on analyte sensitivities with a special focus on laser ablation for sample introduction. Is can be shown that detection efficiency is affected by vaporization of the aerosol, the particle size distribution of the laser generated aerosol and the operating parameters of the ICP. Since vaporization efficiency is furthermore dependent on the chemical composition of the aerosol particles, matrix dependent variations in the absolute and relative elemental sensitivities are observed. Additionally, diffusion of neutral and ionic species out of the region sampled by the vacuum interface of the MS reduces detection efficiency. The degree of analyte loss through diffusion does not only depend on the species mass and gas temperature but also the kinetics of the evaporation and the gas composition of the ICP. Finally, a change of the gas temperature in the ICP changes the ion kinetic energy. This in turn affects the transmission of analyte through the ion optics if matrix effects occur during the analysis.1: E.L. Gurevich, R. Hergenröder, 2007 Winter Conference on Plasma Spectrochemistry, Taormina, Italy, Poster TuPo 20

(100) Investigation of Reagent Gases for the Positive Chemical Ionization of the Polybrominated Diphenyl Ethers
Anne Vonderheide1, Thomas Hieber2, Peter Kauffman2, Jeffrey Morgan1, Lisa Jo Melnyk1; 1United States Environmental Protection Agency; 2National Council of the Aging

Polybrominated diphenyl ethers (PBDEs) fall into the class of compounds known as brominated flame retardants (BFRs) and their incorporation in a multitude of products is responsible for saving numerous lives. However, toxicology studies have alerted researchers to the potential adverse health effects that may develop as a result of prolonged or extreme exposure to these compounds. Frequent disposal and subsequent leaching has focused concern on environmental concentrations and current reports cite increasing levels. Analytical method development continues in support of this research and the present work examines the feasibility of utilizing gas chromatography (GC) ion trap mass spectrometry (IT-MS), operating in the positive chemical ionization (CI) mode, to gain

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both the high specificity and the high sensitivity necessary in the analysis of environmental samples. Extending this instrumental scheme to incorporate MSn analysis was investigated to provide both molecular ion and fragmentation data. Several reagent gases were evaluated, including methane, methanol and acetonitrile; comparative results demonstrated more difficult protonation as the number of bromine atoms increased. Methane, possessing the lowest proton affinity, provided the highest sensitivity for the analytes. Additional CI parameters, such as ionization and reaction times, were studied to optimize sensitivity and excitation amplitude was established to obtain sufficient fragmentation while maintaining maximum signal. The developed method provides a rugged and efficient procedure with the potential to analyze PBDEs in environmental samples with both high selectivity and high sensitivity. Although this work was reviewed by EPA and approved for publication, it may not necessarily reflect official Agency policy.

(101) Nanotube Based Lithography
Punit Kohli1, Rashid Zakeri1, Bojan Mitrovic1; 1Southern Illinois University
We will describe the design and fabrication of a novel programmable nanotube array-based lithography. In this technique, individually addressable conical nanotubes are embedded in a glass chip are used as “nanopens” for the deposition of molecules onto flat surfaces. Unlike some passive deposition systems, such as AFM based deposition of molecules, our deposition is an “active” deposition system because we can control the deposition of the molecules through an appropriate sign and magnitude of the applied electric field. Many hundreds to thousands of nanotubes in a glass chip can be easily prepared; therefore, it is possible to produce massively parallel “nanopens” at a lower cost. With this method, it is also possible to deposit nanoparticles (semiconducting quantum dots, metallic and magnetic nanoparticles etc.) on flat surfaces. The main advantages of the proposed system over existing technologies are fast, inexpensive and controlled massive-parallel deposition of molecules at the submicron level on surfaces. In particular, we will demonstrate the deposition of nucleic acids and protein molecules on to mica and glass slides using nanotubes-based lithography. Also, we will describe various parameters that control the deposition of molecules and nanoparticles using proposed technique.

(102) Direct Resolution of UV Resonance Raman Protein Secondary Structural Motifs using MCR-ALS
Renee Jiji2, John Simpson1; 1University of Missouri
UV resonance Raman (UVRR) is a promising method for protein structural studies. However, association of resolved spectral components with discrete secondary structures can be problematic, especially in the highly informative amide III region. It has previously been shown that cross sections and Raman scattering profiles may be resolved from 2D multi-excitation UVRR spectra, a priori, by incorporation of hard model constraints within an alternating least squares algorithm. However, structural assignments must still be made by the user based upon values, often correlative in nature, found scattered throughout the literature. We are attempting to combine this deconvolution with an extension of the data array to include spectra of several proteins with known crystal structures, essentially creating a secondary structural library. This endeavor should allow unambiguous assignment of discrete spectral components. Recent results from these studies will be presented.

(103) Direct and Label-Free Detection of Solid-Phase Bound Compounds by SERS
Bernd Kuestner1, Carsten Schmuck1, Peter Wich1, Wolfgang Kiefer1, Sebastian Schluecker2; 1University of Wuerzburg
Solid-phase synthesis of DNA, peptides and carbohydrates is nowadays widely used in chemistry, for example, in the design of combinatorial libraries containing structurally related compounds. In most cases a modified polystyrene resin with a typical loading of about 100 pmol per bead is used as solid support. Any spectroscopic attempt to directly detect molecules bound to a single bead has to cope with the low loading and the presence of a significant excess of the solid support itself. Therefore, techniques combining both high sensitivity and chemical specificity are required. Surface-enhanced Raman scattering (SERS) is an ultrasensitive Raman technique enabling the identification of molecules nearby metallic nanostructures. We established a methodology for the direct and label-free detection of solid-phase bound compounds by SERS microspectroscopy. In this context, we were able to characterize solid-phase bound peptide receptors on a single polystyrene bead. A comparison with the conventional Raman spectrum of the neat receptor in aqueous solution indicates that no spectral contributions from the polystyrene matrix are observed. The reproducibility of this new vibrational microspectroscopic approach for the detection of solid-phase bound compounds was demonstrated by mapping experiments. Future studies will focus on monitoring the complexation of the receptor molecules with target peptides directly on single beads.Acknowledgement: This work is supported by the German Research Foundation (Deutsche Forschungsgemeinschaft, SFB 630/ A3 and C1). C. Schmuck, P. Wich, B. Küstner, W. Kiefer, S. Schlücker, Angew. Chem. Int. Ed., 2007, 46, 4786 - 4789.

(104) Multi-Color Electrophoretic Immunoassays
Michael Roper1, Christelle Guillo1; 1Florida State University
One method by which cells communicate is via secretion of ions, small molecules, peptides, and proteins. To understand these communication processes, analytical techniques are needed that can provide simultaneous monitoring of multiple molecules which may be at much different concentrations and on a timescale of the biological process. We have developed a capillary electrophoresis immunoassay method to simultaneously detect insulin and glucagon, two peptides released from islets of Langerhans that control glucose homeostasis. Using a two-color electrophoretic immunoassay, both analytes were quantified simultaneously although there was a 20-fold difference in the concentrations of these peptides. We will utilize this methodology on a microfluidic device to monitor the secretory relationships of the peptides released from islets of Langerhans utilizing multiple fluorophores.

(105) Boron in Environmental and Human Hair Samples from Argentina, South America
Sarah Hill1, Neil I. Ward1; 1University of Surrey, UK
Boron is a ubiquitous but variable element in the global environment. Cases of deficiency are often reported in agriculture leading to supplementation as boron is essential for normal plant development. However, regions of high concentrations are rare and usually limited to semi-arid or arid areas, such as the southern states of the USA, Turkey and southern Australia. San José de Uchú in San Juan, Argentina has an arid climate and a preliminary study has shown higher than expected levels of boron compared with literature data in various media, e.g. sediments, water and human hair. For example, typical values for fresh water range from 0.01-0.5 mg/l B whereas the levels found ranged from 3-5 mg/l B. The toxic effects of high levels of boron on plants and foodstuffs are well documented, whereas in mammals there is confusion over the ramifications. However, importantly, little is known about...
ABSTRACTS

(106) A Flow Injection Analysis-based Colorimetric Method for Determination of Trichloroacetic Acid Concentrations in Wastewaters

Joseph H. Aldstadt1, Gija Geme2, Gary Emmert1; 1The University of Memphis; 2University of Central Missouri

The United States Environmental Protection Agency (USEPA) has developed methods for analyzing haloacetic acids (HAA) in drinking water and also wastewaters. USEPA method 552.3, the current method for HAA analysis, uses liquid-liquid microextraction of HAAs into methyl-tert-butyl ether followed by acidic methanol derivatization to their corresponding methyl esters for two hours at 50 °C. The HAA methyl esters are then analyzed by GC-ECD. These methods work quite well in compliance monitoring for drinking water samples where nine HAA species could be present. When only one HAA species must be reported at mg/L concentrations (trichloroacetic acid, TCAA), analysis by EPA 552.3 is labor intensive and can be inefficient. A solution to this would be an inexpensive automated method selective for TCAA. The Hach Company has developed a batch method for analysis of total trihalomethanes (TTHMs) in drinking water, in which TCAA was an interferent. The TTHM batch analysis was then used to analyze TCAA concentrations. The batch analysis is carried out by reacting TCAA with N,N-diethylnicotinamide under alkaline conditions at 100 °C. The pH of the solution is then lowered to ~2.5 and powdered G-Amido Acid is added to form a color with absorbance detection at 515 nm using a 10 cm quartz cell. The batch-analysis method detection limit was 0.04 mg/L. The mean % recovery, an estimate of accuracy, is 64 % and % relative standard deviation, an estimate of precision, is 11 %. The goal of this research is to automate the TCAA batch method using flow injection analysis for determination of TCAA concentrations in wastewater. Preliminary MDL, accuracy and precision estimates for TCAA will be reported as well as preliminary interference studies with other HAA species that could be present.

(107) Improving Analytical Confidence in the Determination of PCBs in Complex Matrices by a Sequential GC-MS/MS Approach

Joseph H. Aldstadt1, Beth A. Rudy2, Diab T. Qadah1, Harvey A. Bootsma3; 1Univ. of Wisconsin-Milwaukee; 2Center for Great Lakes Studies

A method is described for achieving increased confidence in the selective determination of PCBs using capillary gas-liquid chromatography with electron impact ionization tandem mass spectrometry (GC-MS/MS). It is well known that quantitation of PCBs by MS is susceptible to a false positive interference that arises from the co-elution of a higher PCB homolog with a lower PCB homolog (i.e., M-Cl+ from a higher homolog is M+ for a lower homolog). Because the elution order of the PCB congeners is not exactly proportional to increasing Cl content, frequent switching from MS/MS windows for specific homologs must take place. This can yield significant errors when matrix-induced retention time shifts occur. We therefore explored an approach involving repetitive analyses of a single extract. We optimized a method that required three injections, with homolog classes sequentially monitored as: 1-4-7-10, 2-5-8, and 3-6-9, respectively. The sequential design of the method entails the use of separate, broad MS/MS windows for each homolog class, thereby minimizing adverse matrix effects on retention variability. However, a consequent tripling of overall analysis time is incurred for each sample. The homolog classes are determined with high confidence (99%) that overlapping higher homolog fragments do not interfere with the quantitation of lower homologs. The method was demonstrated for extracts in small samples (~750-1000 mg) from a variety of freshwater biota (n = 20). Application of the method resulted in more accurate quantitation, correcting an average 31% relative error (false positive bias) in observed concentrations.

(108) A Capillary Membrane Sampling Gas Chromatography-Mass Spectrometry Method for the Analysis of Trihalomethanes in Drinking Water

Michael Brown1, Meggan Larson1, Gary Emmert1; 1The University of Memphis

Water chlorination is a very successful disinfection process; however, there is formation of disinfection by-products such as the trihalomethanes (THM4). Since the THM4 are possible carcinogens, the United States Environmental Protection Agency (USEPA) regulates their total concentration in finished drinking water. Currently, the maximum contaminant level set by the USEPA for total THM4 is 0.080 mg/L. USEPA methods for THM4 analysis, while suitable for quarterly compliance monitoring would be expensive or difficult to use for regular monitoring. A capillary membrane sampling-gas chromatography-mass spectrometry (CMS-GC-MS) method was developed for analysis of THM4 in drinking water. This method uses a capillary membrane sampling device (CMS), which has a “tube-within-a-tube” design whereby silicone membrane tubing is inserted into Tefzel tubing. During sampling, drinking water is flowed around or through the length of silicone membrane tubing and to waste. THM4 present in the sample will pervaporate through the silicone membrane tubing and into a gas stream. The THM4 laden gas stream is then flowed through an adsorbent trap, thus collecting the THM4. The trap is heated and the THM4 are flowed to an injection valve system coupled to a GC-MS. GC-MS allows for characterization of other compounds besides THM4 that may be present in drinking water samples. Optimization, MDL, accuracy, and precision studies for THM4 were performed and the results will be presented. Following these studies, drinking water grab samples from various locations were analyzed and the concentrations of THM4 were determined.

(109) Isolation and Quantification of Perfluorinated Compounds in Drinking Water Supply Samples Using SPE Preconcentration and LC/MS Detection

Min Yoon1, Lee Lippencott2, Ill Yang1, Eileen Murphy2, Brian Buckley1; 1Environmental and Occupational Health Sciences Ins; 2NJ Dept of Environmental Protection

Perfluorinated compounds (PFCs) are used for thousands of important manufacturing and industrial applications such as fluoropolymers and liquid repellents for paper, textile, leather, surfactant additives, coating and firefighting goods. Most notably,
PFOA is a principal precursor in the manufacture of Teflon. However, these compounds have been found to be rather detrimental to in environment and human health, especially, PFOA. It has just recently been declared as “a likely carcinogen” by an EPA SAB review panel [1]. PFOA and other PFCs have been found in multiple drinking water sites throughout the state of New Jersey and are thought to create a potential health risk. In this study, a method for determining perfluorinated compounds (PFCs) in water samples was developed and optimized. The focus of this work was on the most prevalent PFCs, perfluorooctanoic acids (PFOA) and perfluorooctane sulfonate (PFOS) in aqueous environmental matrices: Method development was concentrated on three main areas: 1) pre-concentration 2) identification and 3) quantification of these target analytes. For the pre-concentration step, the compounds were isolated by the solid-phase extraction (SPE) using C-18 as the sorbent. The analytes were then identified and quantified using high-performance liquid chromatography coupled to negative electrospray ionization - ion trap mass spectrometry (LC-ESI-IT-MS) with a background subtraction method and single ion monitoring (SIM). Previous studies have focused on GC/MS methods [2]. With SPE-LC/MS, method detection limits (MDLs) of PFOA and PFOS are currently less than or equal to 25 parts per trillion (ng/L) for 1L of water samples. The recovery of PFOA was excellent (88%) under acidic condition (pH = 2) with a precision of less than 10% (RSD). In order to improve the identification and quantification of PFCs, HPLC and ESI-MS conditions were optimized for trace levels of PFOA analysis. Selected ion monitoring (SIM), tandem mass (MS2) and triple mass (MS3) were compared for better sensitivity and selectivity of our method. This presentation will focus on the successful LC-ESI-IT-MS optimized methods for identification and quantification of PFOA and PFOS in ground water samples. [1] EPA Science Advisory Board Panel Report on PFOA , May 2006. http://www.epa.gov/sab/pdf/sab_06_006.pdf[2] B. F. Scott, C. Spencer, S. A. Mabury, D. C. G. Muir, Poly and Perfluorinated Carboxylates in North American Precipitation. Envir. Sci. & Technol. Vol. 40 (2006) 7167-7174.

(110) Determination of Caffeine in Soft Drinks by LC/MSD Trap
Zainab Al-Ballam, Nisar Ahmed; 1Kuwait Institute for Scientific Research
Caffeine is a stimulant that is commonly found in many foods and drinks that we consume. Caffeine has a mild addictive effect on the body; it is therefore interesting to know exactly how much caffeine is in a variety of energy and regular drinks samples import into Kuwait. The analysis is made by Liquid Chromatography - Mass Spectrometry. The level of caffeine in samples analyzed was in the range of (1-350) ug/ml. Energy soft drinks samples showed high caffeine level.

(111) The Opportunities and Roadblocks to Use of Multivariate Analysis Tools in PAT and Product Development
Andy Scott; 1GlaxoSmithKline
Multivariate analysis (MVA) is a developing area of interest and activity within the pharmaceutical industry and regulatory agencies; particularly in light of guidance on process analytical technologies (PAT) and quality by design (QbD). MVA is a very powerful tool though is not a panacea. To realize value the tools should be properly used within pharmaceutical development and manufacturing, a number of hurdles must be overcome and the possible outcomes should be clearly understood. An insight to these hurdles and brief examples of the use and outcomes of the use of MVA, at differing phases of development and within manufacturing, is presented.

(112) Process Analytical Technology (PAT) – Reducing the Cost of Quality and a Whole Lot More.
Deborah Peru; 1Colgate Palmolive
The cost of quality is largely controlled by two factors; 1) process variability and 2) product/process understanding. By shifting the responsibility of quality testing from the Quality laboratory to the Making Operators, we can begin to reduce process variability by obtaining near-real time information that is important in process understanding and quality control. The ease in making a quantitative at-line spectroscopic measurements provides the opportunity to measure in-process samples quickly thus providing information necessary to make corrections to the process without the need for elaborate engineering resources upfront. Moving beyond rapid at-line spectroscopic methods are in-line and on-line methods that begin to automate the measurement & control process by eliminating the need for Operators to pull grab samples for analysis. The main benefits of automating these methods include the ability to use the information in real-time for better process control which ultimately improves overall process capability and significantly tightens up the variability in critical ingredients and other performance attributes. While the justification for implementing PAT generally comes from the “realized cost savings”, we also find other important benefits of PAT that are difficult to quantify as “realized cost savings” but are in many instances, even more important to the bottom line. This area includes the product and process learnings that you gain when implementing these methods. This talk discusses the traditional benefits of using PAT in manufacturing as well as some additional learnings gained from the implementation of PAT in manufacturing.

(113) Process Analytical Technology in API Manufacturing. - Sustainable Systems for Process Control
John O Reilly
Roche Ireland manufactures active pharmaceutical ingredients (APIs) for Roche Pharma division. Roche Ireland has applied process analytical technology in key manufacturing operations over the past 20 years particularly in the control of solvent recovery. The ultimate goal for a PAT application is to satisfy a business need. In API manufacturing this need can arise from financial, safety, regulatory or environmental demands. A PAT application must be built on solid scientific principles, must be integrated into the production systems and must provide real-time information for process control and must be sustainable. A holistic approach to the design, development and implementation of a real PAT example is presented. The roadmap to a successful process analytical application that is sustainable in an API manufacturing environment is described.

(114) Utilization of Process Analytical Technology for Automated Process Control in Pharmaceutical Drug Substance Manufacturing
Frank Sistare; 1Pfizer Inc.
Process Analytical Technology (PAT) has been traditionally defined as any instrument application that is inserted into a process to obtain data. This encompasses many analytical applications including simple PAT such as on line pH and redox measurements to, the current modern, spectroscopic and chromatographic techniques. The definition of PAT has been further defined by the FDA. The 21st Century cGMP definition of PAT, Implementing PAT for characterization only is not real process analytics unless it is used for process control, must be considered when developing PAT applications. To be considered a Process Analytical Technology application under the current definition, the application must provide process control measurements such that it predicts or trends process data enabling direct process control. Further, the PAT instrument should be connected to the process controller to...
(115) The Advantages of Trace Chemical Analysis using On-line Intracavity Absorption Spectroscopy Compared to Conventional Absorption Techniques
Nichola Townshend1, David Littlejohn1, Alison Nordon1, John Girk1, Untiziu Elejalede1; 1CPACT, University of Strathclyde; 2IoP, University of Strathclyde
Techniques based on molecular absorption spectrometry are important in many areas of analysis. By increasing the absorption path length of a system, the sensitivity of the resulting absorption measurement can be increased. A novel way of achieving this is via the use of Intracavity Laser Absorption Spectroscopy (ICLAS), a technique which has been recognised as one of the most sensitive detection methods for absorption and has been applied in a number of spectroscopic studies. ICLAS requires the sample to be placed inside a laser cavity rather than outside resulting in a much larger effective absorption path length due to multipasses and vital control over the laser gain and intracavity absorption. Consequently, drastic enhancements in sensitivity can be achieved when ICLAS replaces conventional absorption techniques. When working close to the threshold current of the system, the cavity becomes very sensitive and in turn exhibits a small dynamic range allowing small changes in analyte concentration to be detected. Conversely, when working further away from the threshold of the system, a large dynamic range can be utilised but sensitivity to smaller concentration changes is sacrificed. Experiments were carried out to compare the sensitivity achieved when dye standards were analysed using both conventional UV-visible spectrometry and ICLAS using a low cost laser diode. The effect of working at different multiples of the diode laser threshold current was investigated in order to assess the limit of detection at different pump powers; the repeatability of the ICLAS measurements was also assessed at each chosen pump power. Factors affecting the stability of the system were also investigated to identify potential sources of variation and in turn achieve the optimum set-up and working conditions for the system. Data has shown that significant sensitivity enhancements can be achieved when using ICLAS instead of conventional UV-visible absorption. Furthermore, it has been shown that mg/L concentrations can be determined using ICLAS and that the ability to reliably detect such low concentrations is dependent upon the pump power chosen. Clear differences in the obtainable dynamic range have been identified from data acquired at different threshold multiples.

(116) Process Analysis of Soybean Oil Conversion to Biodiesel
Dale LeCaptain1, William Kelley1, Brian Hales1; 1Central Michigan University
International political instability and finite supply are only two factors that raise huge question marks about the future of US energy demands. Biodiesel is a renewable energy source that is produced in the US and is proposed here to be produced at CMU. Using the campus dining ‘waste’ cooking oil, this project is to research and develop analytical methods for monitoring the chemical synthesis of biodiesel. The novel analysis proposed will enable effective monitoring of the process, which is key to efficient chemical production.

(117) Quantitative Transmission Raman Spectroscopy of Pharmaceutical Solids
Jonas Johansson1, Anders Sparén1, Olof Svensson1, Staffan Folestad1, Mike Claybourn2; 1AstraZeneca R&D Molndal; 2AstraZeneca R&D Macclesfield
The increasing demand for efficient control of quality in both pharmaceutical manufacturing and during pharmaceutical development calls for faster and more robust analytical techniques. Most spectroscopic techniques are non-destructive and solid samples can be analysed in their native state without any sample preparation. The importance of this has received recent attention with the growing awareness of the importance of solid-state properties of pharmaceutical compounds and the need for solid-state characterisation. Raman spectroscopy has lately received much interest and is now considered as the first choice in many applications. In spite of the many advantageous features of Raman spectroscopy, a significant disadvantage of pharmaceutical Raman spectroscopy is the sub-sampling of solid samples, such as tablets. In this work, quantitative analysis of pharmaceutical formulations using the new approach of transmission Raman spectroscopy has been investigated. For comparison, measurements were also made in conventional backscatter mode. The experimental set-up consisted of a Raman probe-based spectrometer with 785 nm excitation for measurements in backscatter mode. In transmission mode the same system was used to detect the Raman scattered light, while an external diode laser of the same type was used as excitation source. Quantitative partial least squares models were developed for both measurement modes. The results for tablets show that the prediction error for an independent test set was lower for the transmission measurements with a relative root mean square error of about 2.2 % as compared with 2.9 % for the backscatter mode. Furthermore, the models were simpler in the transmission case where only a single PLS component was required to explain the variation. The main reason for the improvement using the transmission mode is a more representative sampling of the tablets, compared with the backscatter mode. Capsules containing mixtures of pharmaceutical powders were also assessed by transmission only. The quantitative results for the capsules’ contents were good, with an RMSEP of 3.6 w/w % for an independent test set. The advantage of transmission Raman over backscatter Raman spectroscopy has been demonstrated for quantitative analysis of pharmaceutical formulations and the prospects for reliable, lean calibrations for pharmaceutical analysis is discussed.

(118) Determination of the Relative Stabilities of Pharmaceutical Polymorphs and Solvates by Vibrational Spectroscopy
CJ Pommier1, Raymond Scaringe1; 1Bristol-Myers Squibb
In the Quality by Design (QbD) paradigm, a thorough understanding of the crystallization process of an active pharmaceutical ingredient (API) is central to the control of polymorphic form and critical to ensure product performance. When a crystallization is performed in a solvent system where solvates could be formed, it is possible to elucidate the relative thermodynamic stabilities of all of the known crystal forms as a function of temperature and solvent composition. This information can be utilized to design a process that ensures isolation of the desired crystal form independent of scale. Here we describe a...
study to determine the relative stabilities of three solvates and one neat form, all relevant to the process under consideration, thereby determining the thermodynamic safe zone for the crystallization. In this work the ability of Raman spectroscopy to distinguish between the various crystal forms was established by examining samples with crystal structure/composition verified by PXRD. Raman spectroscopy was then utilized to perform the crystal form identifications in slurry, which reduced the time required to perform the analyses as compared to the traditional approach of PXRD.

(119) Raman Spectroscopy: A Powerful Tool in Preformulation

Chad Dalton1, Sophie-D. Clas1, Rafik Naccache2, Merck

In recent years, Raman spectroscopy has matured into an indispensable tool for preformulation scientists due to its speed, sensitivity and selectivity. The technique's most significant advantage over other, more common spectroscopic methods is its ability to discriminate between aromatic API (active pharmaceutical ingredient) and typical aliphatic excipients. This enables phase detection and quantitation down to very low levels in drug product when the appropriate spectral region is selected. Additionally, such changes may also be monitored in early dosing suspensions in cases where a drug's stability may be questionable. The talk will focus predominantly these aspects including some practical considerations regarding the generation of calibration curves.

(120) Application of Raman in Biologics Drug Product Development

Tapan Das1, Pfizer Global Biologics

The past decade has seen tremendous growth in protein-based drug development. One of the major issues in biologics development is the formation of aggregates and particulates. Detection and characterization of aggregates and particulates in an injectable dosage form is important to establish safety and stability, and key to this is use of orthogonal technologies. This presentation will highlight application of Raman to characterize aggregate and foreign particles in protein formulations.

(121) In Process Monitoring of Polymorphic Form Conversion Kinetics using Raman Spectroscopy

Susan Barnes2, Joanne Anderson3, Katherine Bakeev4, Jun Chen5, Darryl Ertl6, James Rydzak7, GSK UP, GSK RTP

Raman can play a significant role in the in-situ monitoring of solvates and polymorphs in the Pharmaceutical industry. This presentation will cover the spectroscopic aspects of developing process understanding that could lead ultimately to process control for a compound. In addition to the use of Raman, the presentation will include examples of the use of in-situ monitoring tools such as NIR and near line tools such as ATR mid-IR and how they may be used to confirm the Raman analysis and present a complete picture of the in-situ process.

(122) Use of Raman for API Processing Controls: Development, Implementation and Validation

Jonathan Haulenbeck1, Ming-Hsing Huang2, Charles Ray3, Robert Wethman4, John Wasylyk5, Bristol-Myers Squibb Co.

During the production of pharmaceutical ingredients, product concentration is typically monitored analytically by HPLC. Where a sample from a reaction mixture cannot be obtained in a representative and reproducible manner, other alternatives must be pursued. Here we outline a strategy for monitoring a critical processing parameter using an in-line Raman probe. An overview of the validation parameters used and challenges faced in scaling up lab and at-line models to a large scale processing environment will be presented.

(123) Coherent Two Dimensional Vibrational Spectroscopy

John Wright1, Mark Rickard1, Kathryn Komai1, Nathan Mathew2, Andrei Pakoulev3, University of Wisconsin-Madison

Coherent multidimensional vibrational spectroscopy is a new approach for obtaining more detailed information about vibrational spectrum. It is analogous to multidimensional NMR. It is based on exciting multiple transitions on a molecule within the dephasing time so coherence is maintained between the multiple transitions. This talk will focus on the characteristics of frequency domain approaches to multidimensional spectroscopy. Here, three 900 fs excitation pulses excite three vibrational transitions to create an output beam by four wave mixing. The measurements can be made in the frequency or time domain. The frequency domain methods resolve phase coherence only during the dephasing time of molecular coherences and thus avoid the need for long term phase coherence between the three excitation pulses that time domain methods require. We will show that frequency domain methods have a number of useful characteristics: • They allow implementation of multiple quantum coherences like the HMQC methods of NMR;• Unlike pump-probe spectroscopy, they isolate specific coherence pathways so one can avoid the complications of having simultaneous bleaching, stimulated emission, and excited state absorption pathways;• They isolate coherence transfer effects. We will show examples of these effects and how they can be used to isolate the states that are coupled by interactions and how they can provide the complete dynamics of the coherences and populations of coupled quantum states.

(124) Propagation and Detection Distortions in Coherent 2D FT Spectra

David Jonas1, University of Colorado at Boulder

Coherent 2D FT spectra correlate spectroscopic transitions on a single chromophore, allowing spectroscopic separations without physical separations. Theory borrowed from NMR treats only optically thin samples, a limit in which the signal vanishes. A recent solution of Maxwell’s equations for coherent four-wave mixing in the three-dimensional frequency domain provides a nonlinear analog of Beer’s law (more precisely, the Fresnel equations). We discuss distortions of coherent 2D FT spectra resulting from pulse propagation inside the sample and interference detection of the nonlinear optical signal. 1D treatments of propagation distortions are useless; 2D treatments are exact but require the full nonlinear response; and 2D treatments are about as accurate as current experiments up to an absorbance of about one, where the signal strength is typically maximized.

(125) Ultrafast 2D IR Vibrational Echo Chemical Exchange Spectroscopy

Junrong Zheng1, Michael Fayer2, Stanford University

Ultrafast 2D IR vibrational echo chemical exchange spectroscopy is applied to the study of dynamics of weakly hydrogen bonded solute-solvent complexes in liquid solutions. The 2D IR vibrational echo technique obtains full phase information through heterodyne detection and is akin the 2D NMR methods. The strengths of the solute-solvent hydrogen bonds are adjusted by modifying the chemical structures of the solutes (donors) and solvents (acceptors). For the eight samples studied, the formation enthalpies vary from -0.6 kcal/mol to -2.5 kcal/mol, and the dissociation time constants vary from 3 ps to 32 ps. The dissociation rates of the hydrogen bonds are found to be strongly correlated with their formation enthalpies. The correlation can be described with an equation similar to the Arrhenius equation. As another example of chemical exchange spectroscopy, the rate of carbon-carbon single bond rotational isomerization of an ethane derivative in room temperature liquid solution is measured. The results are compared to simulations of a similar compound and the simulations are in
good agreement with the experiments. Based on the experimental results and density functional theory calculations, the time constant for the ethane internal rotational isomerization under the same conditions is about 12 ps.

(126) Two Dimensional Spectroscopy of Photosynthetic Complexes
Gregory Engel1,2, Elizabeth Read1,2, Tessa Calhoun1,2, Gabriela Schlu–Cohen1,2, Graham Fleming2,3, University of Chicago; 2University of California Berkeley; 3Lawrence Berkeley National Laboratory
Two dimensional electronic spectroscopy provides detailed information about electronic structure and electronic dynamics on ultrafast timescales. Probing chromophores embedded within photosynthetic complexes with this technique, we are able to observe the underlying design principles that drive photosynthesis. In particular we see strong evidence for long lived coherences after excitation, coherence transfer as well as population transfer. New techniques leveraging novel polarization schemes to isolate individual response pathways will be presented along with further evidence for quantum beating and coherence transfer within photosynthetic protein complexes.

(127) Structures of Peptides Probed with Ultrafast Two-Dimensional Infrared Spectroscopy
Nien-Hui Ge1, Hiroaki Maekawa1, Soo-hwan Sul1, Claudio Toniolo2; 1University of California, Irvine, USA; 2University of Padova, Italy
Ultrafast two-dimensional infrared (2D IR) spectroscopy is a very powerful technique for probing molecular structures and their equilibrium dynamics. We will report investigations of peptide structures using multiple pulse sequences and polarization configurations. Experimental results will be presented for a model dipeptide that serves as a paradigm for studying backbone conformations in proteins. The diagonal line shapes and cross peak patterns are compared to simulations based on multiple conformations obtained from DFT structural optimization and free energy calculations in the gas phase. Two-dimensional IR spectra of several Aib-homopeptides will also be presented. These peptides serve as a model for the 310-helix that may be involved as a folding intermediate in the coil-helix formation. The evolution of 2D spectral features as a function of chain length is observed and simulated using a vibrational exciton model that takes into account vibrational couplings, diagonal frequency shifts, and inhomogeneous structural distributions.

(128) CARS Imaging: Instrumentation and Applications
Brian Saar1, X. Sunney Xie1; 1Harvard University
Microscopy based on coherent anti-Stokes Raman scattering (CARS) has grown dramatically in popularity in recent years. CARS imaging offers contrast with chemical selectivity based on intrinsic Raman-active vibrations in the sample. Unlike fluorescence microscopy, CARS does not require staining or labeling with dyes or fluorophores, and it offers major advantages over spontaneous Raman microscopy in terms of sensitivity and image acquisition speed. Our group's recent research involves both technical developments to make CARS microscopy more sensitive and easier to use, and biological/biomedical applications, such as brain and skin imaging or the structural characterization of plant degradation. We will discuss the state-of-the-art in CARS instrumentation, including frequency modulation techniques for suppression of the nonresonant background, and present several recent applications of CARS imaging.

(129) Non-equilibrium Dynamics of Peptides using Two-Dimensional Infrared Spectroscopy
Matthew Tucker1, Yan Jiang1, Jianxin Chen1, Robin Hochstrasser1; 1University of Pennsylvania
The 2D IR approach can be used for direct studies of conformational dynamics of peptides. Understanding the structural changes involved in the kinetics of protein folding and misfolding is one of the most significant questions of non-equilibrium dynamics. In order to address this question, we have developed some new infrared probes that involve Fermi resonances. Furthermore, we utilize fast phototriggers to initiate the folding of small single state or ‘downhill’ folding peptides and then measure the structural changes by 2D IR. In addition, peptides can be isotopically labeled to identify the role of specific regions of these systems in folding and tracking their structures and their distributions as a function of time. Therefore, specific pathways leading to intermediates could also be derived from 2D IR non-equilibrium experiments on these peptides.

(130) An Analytical Chemist with a Focus on Separations Research: Separation of Photons and Separation of Molecules
Isiah Warner; 1Louisiana State University
My research has always focused on the solution to a broad spectrum of chemical problems through improved analytical measurements. This research has been quite diverse, beginning with my early studies focusing primarily in the area of molecular spectroscopy and leading to my current studies focusing primarily in the area of separation science. In more recent years, my research has reached a defined equilibrium with distinct components in both analytical separations and analytical spectroscopy. In an effort to present a broad scope of my current and ongoing research, this talk will focus in these two distinct areas of analytical chemistry. In the area of separations, this talk will focus on the utility of molecular micelles as reagents for separations in capillary electrophoresis, particularly in the area of chiral and protein separations. In the area of spectroscopy, this talk will focus on my more recent work in collaboration with Professor Robert Strongin, formerly of the chemistry department at LSU and now at Portland State University. These latter studies focus on the development and characterization of a new class of fluorescent dyes, some of which emits white light as a result of emission of multiple bands of light. The analytical utility of both of these areas of research (separations and spectroscopy) will be discussed in detail.

(131) Confocal Raman Microscopy: Where Are We Really Looking?
Neil Everall; 1Intertek MSG
Confocal Raman microscopy is a powerful tool for characterising the structure of materials and biological systems, but the spatial resolution which is attained in practice falls somewhat short of the nominal "cubic micrometre" which one often reads in both elementary texts and research papers. Over the last seven years or so it has become increasingly recognised that the metallurgical objectives which are provided as the default with most commercial Raman instruments introduce severe spherical aberration, which causes blurring of the laser focus, severe loss of signal, and a contraction of the apparent depth scale. Fortunately, use of corrected objectives can minimise all these effects [1]. However, what is less well appreciated is the extent to which, even in the absence of spherical aberration, the “out of focus” light can be transmitted via the confocal pinhole to register a signal at the detector. So, for example, one can detect appreciable Raman signals from material located tens of microns above, below or to the side of the nominal focal volume. These residual signals are an entirely predictable consequence of the confocal Raman collection geometry [2], but one which remains largely unappreciated in the
current literature. The importance of this effect depends on the relative scattering efficiencies of the material which lies within the optimum focal volume, compared with the more distant sample regions. It is a far from negligible contribution in many situations, as will be shown in this work. This presentation will discuss the quantitative ramifications of this phenomenon on the axial and lateral spatial resolution of the confocal Raman microscope, using polymer laminates as idealized samples. Conclusions are drawn regarding the optimum geometry and sample form which is required to minimize image distortions.[1] N Everall, J Lapham, F Adar, A Whitley, E Lee and S Mamedov, Appl. Spectrosc. 61 (3), pp. 251-259 (2007).[2] A Macdonald and A Vaughtn, J Raman. Spectrosc., in press.

(132) Determination of Lead in Green Tea by Graphite-Furnace Atomic Absorption Spectrometry
Amina Ali; Rabaa Al-Kandari; Kuwait Institute for Scientific Research
The main objective of this study was to evaluate the existence of lead in green tea samples. The samples were prepared in two ways: acid digestion and steeping in hot water. The results showed that hot water does not leach lead in the green tea samples whereas the preparation by acid digestion showed the existence of lead. The highest value was 7.245 mg/kg and the lowest value was 0.1 mg/kg.

(133) On the Orientation of the Isocynate Group in the First Excited State of P-Fluorophenylisocynate
Narasinga Ayachit, Neeraja Rani G.; SDM Coll of Eng & Tech., Dharwad, Karnataka, India
The orientation of amino group in aniline was considered to change to 180 degrees in the excited state from 38 degrees in the ground state by Suppan[1], to determine the excited electric dipole moment using solvatochromic shifts. Ayachit[2] freed the problem of assumption of considering the orientation in the excited state. This method led to not only to the better calculation of excited state dipole moments also gave a novel method of calculating the orientation of substituents in mono substituted benzenes in their excited states. This method was shown to work successfully in some other cases [3, 4]. In this paper the method after improvement, has been applied to p-fluorophenylisocyanate and the orientation of the substituent isocynate in the first excited state is shown to change considerably affecting the symmetry of the molecule.

(134) Determination of Rare Earth Elements by Tungsten Coil Atomic Emission Spectrometry
George Donati, Ji Gu; Bradley Jones; Wake Forest University
The fourteen lanthanides are determined by tungsten coil atomic emission spectrometry. Twenty-five microliter sample aliquots are placed directly on the coil. A simple constant current power source carefully dries the sample prior to analysis. During this dry step, the voltage is monitored to prevent over heating. This allows for shorter atomization cycles while improving sensitivity and coil lifetime. During the 5 s high temperature atomization step, the emission signals for as many as seven lanthanides are determined simultaneously in the same 55 nm spectral window. The analytical figures of merit for all 14 natural lanthanides are reported and compared with nitrous oxide flame atomic emission spectrometry. Tungsten coil atomic emission concentration detection limits are in the range 0.8 (Yb) to 600 (Pr) µg/L, and are lower than those for the flame in most cases. The absolute detection limits are near or below the ng level: significantly lower than the flame detection limits due to the smaller sample volume required. A three fold improvement in detection limit may be realized by combining the signals for multiple emission lines for a single element. The accuracy of the method is demonstrated for the determination of seven lanthanides in a standard reference soil sample. After a simple acid extraction, the measured values agree with the reported values with 95% confidence in all cases but one, Yb. Finally, a conditioning program for new tungsten coils enhances reproducibility and maximizes the emission signal.

(135) Arsenic Speciation in Pteris cretica cv Mayii (Moonlight Ferns) using X-ray Absorption Spectrometry
David J. Butcher; Youngsoo Cho; James Bolick, Amitava Roy; 1Western Carolina University; 2Louisiana State University
Pteris cretica cv Mayii (moonlight fern) has been demonstrated to be an efficient arsenic hyperaccumulating plant, suitable for phytoremediation of this toxic element. In this work, moonlight ferns were grown hydroponically in solutions containing various arsenic compounds. The arsenic species present in the foliage were characterized by x-ray absorption spectroscopy. In freshly-cut leaves, arsenic was present as arsenic (III), while drying induced oxidation to arsenic (V). The concentration of arsenic in foliage exposed to different chemical forms of arsenic was measured by inductively coupled plasma – optical emission spectrometry. Higher arsenic concentrations were measured in plants exposed to arsenic (III) and arsenic (V) compared to monomethyl arsenate, suggesting preferential accumulation by the inorganic species.

(136) Recent Development of Compositional Depth Profiling of Nanometer Films with GD-OES
Anne Bengston, James Oliver; KIMAB
Modern surface technology includes an ever increasing variety of very thin surface coatings in the nanometer range. Therefore, there is an increasing need for cost-effective techniques for characterisation of such coatings. GD-OES is an established for very rapid compositional depth profiling (CDP) of thin films, also quantitatively. However, performing such analysis correctly is far from trivial. While it is well established that both direct current (DC) and radio frequency (RF) sources can reach stable discharge conditions within milliseconds, it is also necessary that these conditions closely matches those used for calibration of the analytical method. If this is not the case, large errors in the quantification of the depth profiles can easily result. Since the actual discharge conditions are material-dependent, and the thin film may have very different electrical properties from the calibration samples, great care must be taken in setting up the source parameters. In this work, examples of such effects are shown. Methods to deal with these effects in order to improve the analytical accuracy are described and discussed.

(137) A Critical Comparison of Positively and Negatively-Charged Ion Structures using Ion Mobility-Mass Spectrometry
Niki V. Arinze; Janel R. McLean; Larissa S. Fenn; John A. McLean; 1Department of Chemistry, Vanderbilt University
Ion mobility-mass spectrometry (IM-MS) combines a gas-phase separation based on collision cross section (apparent surface area) with mass analysis and provides a means to study anhydrous ion structures. Most singly-charged, gas-phase peptides adopt a charge-solvated, globular structure that minimizes exposure to the low dielectric environment and maximizes intramolecular charge solvation. The relationship between collision cross section and mass-to-charge delineates the average globular mobility-mass correlation. The mobility-mass correlation for positively-charged, protonated peptide ions has been characterized. Here, we will critically evaluate the mobility-mass correlation of negatively-charged ions and compare it to that of positively-charged ions.
analyzed on the same IM-MS instrument. The differences in the collision cross sections of the positively and negatively charged peptide ions will be critically evaluated. Peptide ions can be generated by using matrix-assisted laser desorption ionization (MALDI) and electrospray ionization (ESI). We will report data from MALDI and ESI generated ions (on the same instrumental platform) to gain insight into the effect of the ionization mechanism on the ultimate structure of the peptides in vacuo.

(138) Biosensors Based on Fluorescence Resonance Energy Transfer Using Conjugated Liposomes
Xuelian Li1, Punit Kohli2,1 Southern Illinois University
We describe here a generic approach for highly-sensitive sensors based on fluorescence resonance energy transfer (FRET) between fluorophore and polydiacetylene (PDA). These novel FRET based systems utilize primarily changes in J (the spectral overlap between the emission of the donor and absorption of the acceptor) for the rate of energy transfer between donor and acceptor. The UV/Vis spectra, the steady-state fluorescence emission, and anisotropy analysis of the conjugated polymerized liposomes consisted of sulfonhodamine-tagged-diacetylene and receptors-linked diacetylene in different molar ratios were investigated. The receptor molecules that can interact with biologically-interested molecules/particles were chosen. The liposome solution has a very weak fluorescence from donor (sulforhodamine 101) after polymerization of PDA with UV light due to energy transfer from donor to back-bone of the PDA (acceptor). Some of the stress-induced due to interactions between ligands and receptors resulted in the chromatic shift in the absorption spectrum of PDA. These changes in the PDA absorption spectrum leads to decrease in the spectral overlap between the emission spectra of donor and the absorption spectra of acceptor resulting in decrease in the FRET efficiency. These sensors, thus, show an “On-Off” optical sensor based on FRET between fluorophore and PDA where the fluorescence is highly quenched in turned “Off” state but are turned “On” due to receptor-ligand interactions. Finally, we will discuss our latest results on novel reversible FRET sensors which show FRET response for many “On-Off” cycles. Keywords: Biosensors, FRET, Conjugated Liposomes.

(139) Computational Methods for Enhancing Infrared Spectroscopic Imaging
Rohit Bhartia1, Rohit Bhargava1, Pamela Conrad1, Ray Reid2, Jet Propulsion Laboratory; 2Photon Systems Inc.
Native fluorescence spectroscopy is a very sensitive method of detection for biological and chemical compounds and has recently been shown to provide molecular specificity. To show this, we have acquired high-resolution fluorescence spectra of a wide variety of chemicals and biological material and processed it using Principal Component Analysis and cluster analysis. After determining the effect of excitation the wavelength on the ability to differentiate compounds, the spectra were binned into a fewer number of discrete, non-contiguous, bands such that spectral features contributing to the molecular specificity found in the high resolution data were retained. This approach of using discrete, non-contiguous, bands provides a significant enhancement in sensitivity as compared to spectrometer based systems as they reduce the number of optical surfaces and typically have a better etendue. Now, with newer ion-beam sputtered filters, filters in the deep UV with >60% transmission with out-of-band rejection of OD 5 or greater are commercially available. Another issue resolved with the use of fewer numbers of discrete detection bands is the insensitivity to optical alignment and chromatic aberrations that plague emission detection over wide spectral ranges typically ranging from the deep UV (~250nm) to the Vis-Red (~900nm). We will demonstrate the discrimination capability of deep UV native fluorescence spectroscopy with high resolution and discrete band data and how of noise reduction. This scheme has been used to de-noise over 500 data samples and the SNR results are comparable to that obtained when factors are hand picked. We also explore the use of wavelet transform in de-noising, which, unlike MNF transform is image independent and computationally efficient algorithms to compute wavelet coefficients are known. Computation time for de-noising can be reduced by a factor of about N/log2(N) (N being the number of data points in a sample) by making use of these techniques, while achieving similar SNR levels. We also analyze the relation between SNR and tissue classification accuracy by examining prostate tissue samples. Based on optimized SNR, we then optimized classification using efficient algorithms and cost models. Last, we demonstrate the utilization of computational and optical theory approaches to correct aberrations in imaging large tissue sections that lead to improved fidelity with conventional morphologic images.

(140) Calibration Transfer between Near-Infrared Spectrometers
Dongsheng Bu1, Camo Software Inc.
A calibration transfer method was evaluated by transferring multivariate models between two equivalent near-infrared (NIR) instruments. The method includes selecting a few representative samples to build the transfer equation, and the Direct Standardization algorithm. Both NIR analyzers have spectral and reference data available for calibrating tablet assay of the active within an intact pharmaceutical product. Two calibration transfer routines were compared, 1) transfer the second analyzer’s spectra and use original multivariate model built on first analyzer; 2) transfer the first analyzer’s spectra and rebuild the multivariate model for the direct usage by the second analyzer’s spectra. The prediction results of before and after calibration transfer were compared by the use of two analyzers' data. A practical approach is proposed to maintain multivariate model for an instrument and estimate if the model is obsolete. A general validation approach was discussed to ensure a calibration successful deployed to multiple instruments in a network.

(141) Detection Band Minimization for Molecular Differentiability using Deep UV Laser Induced Native Fluorescence
Rohit Bhartia1, William Hug2, Arthur Lane1, Pamela Conrad1, Ray Reid2, Jet Propulsion Laboratory; 2Photon Systems Inc.
Native fluorescence spectroscopy is a very sensitive method of detection for biological and chemical compounds and has recently been shown to provide molecular specificity. To show this, we have acquired high-resolution fluorescence spectra of a wide variety of chemicals and biological material and processed it using Principal Component Analysis and cluster analysis. After determining the effect of excitation the wavelength on the ability to differentiate compounds, the spectra were binned into a fewer number of discrete, non-contiguous, bands such that spectral features contributing to the molecular specificity found in the high resolution data were retained. This approach of using discrete, non-contiguous, bands provides a significant enhancement in sensitivity as compared to spectrometer based systems as they reduce the number of optical surfaces and typically have a better etendue. Now, with newer ion-beam sputtered filters, filters in the deep UV with >60% transmission with out-of-band rejection of OD 5 or greater are commercially available. Another issue resolved with the use of fewer numbers of discrete detection bands is the insensitivity to optical alignment and chromatic aberrations that plague emission detection over wide spectral ranges typically ranging from the deep UV (~250nm) to the Vis-Red (~900nm). We will demonstrate the discrimination capability of deep UV native fluorescence spectroscopy with high resolution and discrete band data and how
these bands were chosen for our instrumentation. Examples of fluorescence data pertaining to biological and chemical samples will be illustrated.

(142) Determination of the Pure Spectrum of Major Protein Secondary Structures through Multi-Excitation UV Resonance Raman Spectra.
John Simpson1, Renee Jiji1; 1University of Missouri
The ultraviolet resonance Raman (UVRR) spectra of proteins contain a wealth of information including their secondary structural composition. However, it is difficult to unambiguously resolve the UVRR spectral signatures arising from discrete secondary structures as each amide region often contains numerous overlapping components. This limitation is compounded by the presence of aromatic side chains, which introduce many additionally overlapped vibrational modes. Although chemometric methods have been used to determine the secondary structural composition of model proteins, they are limited in their accuracy by the quality of the pure secondary structure spectra with which the composition calculation is based on. Furthermore, large errors can be expected for proteins containing larger degrees of non-standard protein conformations. An alternative is direct deconvolution of 2D multi-excitation UVRR spectra. This may be achieved through the incorporation of chemically relevant constraints within a multivariate curve resolution-alternating least squares (MCR-ALS) algorithm. ‘Pure’ secondary structure spectra are re-constructed post-analysis.

(143) Improved Conversion of Thiols to Disulfides with Electrodeposited Catalysts
Ricky Risley1, Phillip Voegel1; 1Southeastern Louisiana University
The ability of electrodeposited cobalt(II)-phthalocyanine, cobalt(II)-tetra-2,3-pyridinoporphyrazine, and cobalt(II)-tetra-3,4-pyridinoporphyrazine to catalyze the conversion of thiols to disulfides is examined. Electrodeposition of catalysts leads to improved conversion rates for these catalysts compared to the use of catalysts dispersed into the highly alkaline reaction mixture. Specifically, over a thirty minute reaction time with electrodeposited cobalt(II)-tetra-2,3-pyridinoporphyrazine as catalyst, the removal of octanethiol by conversion to dioctyldisulfide increased by 12% compared to the same reaction conditions employing the dispersed catalyst. The effectiveness of cobalt(II)-tetra-3,4-pyridinoporphyrazine as a dispersed catalyst for the oxidation of octanethiol is 46% and 71% greater than that of cobalt(II)-phthalocyanine and cobalt(II)-tetra-2,3-pyridinoporphyrazine respectively. It is expected that similar increases in effectiveness will be observed when the 3,4-derivative is employed as an electrodeposited catalyst for this reaction. The clean conversion of thiols directly to disulfides is verified by mass spectrometry following gas chromatographic separation. The only product of significant concentration following the reaction is the expected disulfide.

(144) The Monitoring of Methylmercury in Abyssal Fish Species Marketed in Korea
Chun-Soo Kim1, So-Hee Kim1, Yong-Seok Ko1, Gwang-Soo Lee1, Mi-Ok Kim1, Seong-Cheol Kim1, Jeong-Min Kim1 and Dae-Byoung Kim1; 1Busan Regional KFDA
The monitoring of methylmercury in abyssal fish species marketed in Korea. Busan Regional Korea Food & Drug Administration, Test & Analytical Center, Hazard Substance Analysis TeamSo-Hee Kim, Yong-Seok Ko, Gwang-Soo Lee, Chun-Soo Kim*, Mi-Ok Kim, Seong-Cheol Kim, Jeong-Min Kim and Dae-Byoung Kim
Abstract Mercury is a well-known environmental pollutant that exist three major forms, elemental Hg0, inorganic Hg2+ and organic Hg. Methylmercury is the most toxic form of mercury present in the environmental and its bioaccumulation in fish provides the major route of exposure for humans. The aim of this study was to investigate the methylmercury (MeHg) level of abyssal fish species marketed in Korea. Fish sample was extracted with hydrochloric acid and toluene, clean up using L-cystein solution. MeHg (as methylmercury chloride) was analysed by gas chromatography-electron capture detection (GC-ECD) using Thermon HG-capillary column. Detection limit and recovery of the method were reported 0.02 mg/kg (as mercury), 87–113 (average 98 %), respectively. MeHg was detected in all analysed samples of Inshore hagfish, Mako shark, Oil fish, Opah, Patagonian toothfish, and Sawedged perch. MeHg levels ranged up to 4.80 mg/kg and 0.31 mg/kg respectively. Oilfish contained highest levels, followed by Paragonian toothfish, Mako shark, Opah, Inshore hagfish and Sawedged perch.

(145) Using Elemental Composition to Identify Forensic Soil Samples: A Lab Experiment that uses ICP-AES and Multivariate Analysis
Scott Goode1, Daniel Sullivan1, Amelia Taylor1; 1University of South Carolina
We present a laboratory exercise that demonstrates the unique multi-element capability of the ICP-AES at a level that is interesting to undergraduate students. A forensic scenario was chosen to spark the students’ interest and to provide an example of real-world application of a laboratory instrument. The widely varying composition of soil from one location to the next is ideal for forensic identification, allowing elemental concentrations to serve as means of comparison between control samples and unknown samples. The need for multi-elemental determination, as well as its high sensitivity, low detection limit, and overall simplicity are just a few advantages of analysis by inductively coupled plasma-atomic emission spectroscopy (ICP-AES). Introduction to ICP-AES instrumentation, optimization of instrumental parameters, and statistical handling of experimental data are emphasized. Students collect soil samples from various locations and digest them in nitric acid. The filtered solutions are then analyzed by ICP-AES for Al, Ca, Fe, Mg, and Mn. A multivariate statistical analysis of the resulting data is used to determine whether or not the elemental contents of the known samples are distinguishable enough to warrant a possible match with any of the unknowns.

(146) Application of FTIR-ATR on Characterization of Soil Organic Carbon and Nitrogen Humification Processes
Xianzhi (Amanda) Song1; 1Western Carolina University
Preliminary evidences suggest that the long – term stability of soil organic carbon is associated with the amounts and structural components of lignin, polysaccharides, aromatic C, and nitrogen in soils. Determination of such structural components has been not easy due to the extreme complexity of soil systems. This paper was an attempt to obtain such knowledge by using FTIR coupled with ATR to measure the functional groups of lignin, polysaccharides, aromatic C and nitrogen as a function of the extent of soil organic matter decomposition and humification, which was carried out through physical size fractionation. The result of such research can be used as a reference in determining the possibility of applying FTIR directly on soil organic carbon and nitrogen analyses; also a reference in improving soil carbon sequestration and reducing anthropogenic N pollution.
The halocetic acids (HAAs) are disinfection by-products (DBPs) in drinking water distribution systems. The United States Environmental Protection Agency (USEPA) currently regulates five HAAs in drinking water due to possible health concerns. The five regulated HAAs are: monochloroacetic acid (MCAA), dichloroacetic acid (DCAA), trichloroacetic acid (TCAA), monobromooacetic acid (MBAA), and dibromooacetic acid (DBAA). The current maximum contaminant level (MCL) for the total concentration of these five HAAs (HAA5) is 0.060 mg/L. There are four unregulated HAAs that are commonly present: bromochloroacetic acid (BCAA), bromodichloroacetic acid (BDCAA), dibromochloroacetic acid (DBCAA) and tribromooacetic acid (TBA). The HAA5 species in addition to the four chlorinated and brominated unregulated HAAs are called HAA9. An on-line automated method has been previously developed for analysis of HAA9 in drinking water using a post-column reaction ion chromatography method with nicotinamide fluorescence (PCR-IC). The method detection limits (MDL) for the HAA9 species were at the single microgram/L level with relatively good mean % recoveries and % relative standard deviations. Recently, emerging DBPs such as iodinated HAs, iodinated trihalomethanes, halocetaldehydes, haloketones, halocetonitriles, and halocetamides have all been identified in drinking water distribution systems. These compounds could be possible interferences for the PCR-IC method and the focus of this work is to identify and possibly resolve selected emerging DBP interferences with the HAA9 species.

(148) Polyamelines and their Diazo Dyes for the Development of Optical Sensors
Nasir Ahmad1, Ramaier Narayanaswamy1; 1School of Chemical Eng. and Analytical Science Polyamelines and their diazo dyes for the development of Optical Sensors. Polyamelines and their diazo dyes have been synthesized and prepared through a process of derivatization to form their diazo dyes. The derivatization and diazo dyes have been synthesized and modified through derivatization to form their diazo dyes. The derivatization with sulphanilic and anthranilic diazonium ions results in increased solubility in polar solvents including water. They exhibit stable and reversible optical (UV-VIS) pH response. Results show that diazonium ions decomposed during coupling reaction but the resulting carbononium ion react with electron rich nitrogen atoms of the polyameline backbone. Very interestingly, this resulted in luminescent polyamelines having emission wavelength around 428 nm and excitation wavelength around 310 nm. The fluorescence intensity is pH dependent and maximum in the range of pH 6 to 8 and is very sensitive to the presence of heavy metal ions in its solution. For example, the detection limits for Cu 2+ ions in solution with polyameline (TiO2) diazo sulphanilic acid were evaluated as 0.03 ppm. This poster will present characterization results of some diazo dyes of polyamelines and their use in optical sensing of metal ions, pH, gases and vapours.

(149) Fluorescence Imaging of Exocytotic Release and Free Radical Distribution in PC12 Cells
Irma Nydegger1, Donald M. Cannon Jr.1, 3; 1University of Iowa Neurotransmitter exocytotic release dynamics and degradation have been implicated in many major neurological disorders such as: stroke, Alzheimer’s, Parkinson’s and dementias. Exocytosis is the process by which intracellular vesicles fuse with the cell membrane and release their contents. In neuronal networks, exocytosis gives rise to synaptic transmission, more specifically the release of neurotransmitters in the synaptic cleft. To develop advanced analytical methods to study exocytosis, Pheochromocytoma (PC12) cells have been used as a well-established neuronal model cell line. When stimulated with elevated K+ (100mM) solution, they undergo vesicular exocytosis in a Ca2+-dependent manner and release dopamine. These cells also differentiate to form neurites (neuronal-like extensions) when exposed to nerve growth factor (NGF). PC12 cells have shown exocytotic release in both undifferentiated and differentiated phenotype states. Electrochemistry has been primarily used to study PC12 cell exocytotic release due to its high sensitivity. Fluorescence assays for the study of PC12 exocytosis have not been as thoroughly investigated. Fluorescence microscopy offers an attractive ancillary view to electrochemical techniques, which are severely limited in their selectivity. Multiple fluorescent dyes (structural, functional-Reactive Oxygen Species and exocytosis dyes) can be coupled together to provide higher selectivity and spatial resolution during exocytosis. We have developed an advanced fluorescent microscopy protocol with the necessary sensitivity and resolution to distinguish between functional differences of single PC12 cells at various stages of differentiation. These differences were primarily associated with the amount and spatial location of release sites and were dependent on the time of NGF treatment (0, 5 and 14 days). To monitor exocytotic release at these differentiation stages, a membrane potential dye, FM 1-43, was utilized. FM 1-43 preferentially binds to lipid membranes and undergoes fluorescence enhancement after binding. Upon cell stimulation with elevated K+-solution, vesicle fusion and subsequent internalization was visually observed. Our control experiments have allowed us to view the appearance of brightly lit vesicles by removing background interferences from unbound dye. These experiments support the hypothesis that PC12 cells treated with NGF for a varying amount of time express different phenotypes, allowing for a more thorough understanding of the differentiation process in eukaryotic cells.

(150) XRF as a Tool Substituting IC and ICP in Additives Quantification in Polymers
Jhab Odeh1, Angelika Clark1; 1SABIC Innovative Plastics X-ray fluorescence (XRF) is a great tool to use in manufacturing settings where semi-quantitative methods are needed. Traditional analysis of inorganic fire retardants and glass fillers in polymers requires ion chromatography (IC), Inductively-Coupled Plasma (ICP), ashing (glass/mineral content). Antimony, bromine, calcium, and titanium were the main elements of interest. The current work describes a DoE approach to bundling IC, ICP, and ashing methods into one wavelength XRF method. The quality of the standards prepared for this process have a direct effect on the final method developed. The advantages of utilizing this method include faster analysis, lower solvent use, and a drop in waste disposal needs.
Future Meetings: FACSS 2008, September 28 – October 2, Reno, NV • FACSS 2009, October 18 – 22, Louisville, KY

(151) Sample Preparation of Human Placenta for Trace Element Analysis
Pamela Kruger1, Patrick Parsons1, 2; 1 State Univ of New York at Albany; 2 New York State Dept of Health
The goal of this project is to analyze 167 archived human placentae that were collected between 1992 and 1999 as part of an NIH-funded study focused on lead and pregnancy. In this study, inductively coupled plasma mass spectrometry (ICP-MS) is used to analyze the placenta for select essential traces (e.g., Mn, Co, Cu, Zn, Se, Mo) and non-essential toxic elements (e.g., As, Cd, Hg, Pb), as well as a number of rare earth elements of the lanthanide series. Successful chemical analysis of placental tissue is only possible following careful attention to sample handling and preparation. Here we describe some of the key preanalytical variables associated with collecting and analyzing placenta. Issues such as placenta inhomogeneity and contamination concerns are addressed, along with long-term archival storage of biological tissues. Two different digestion techniques are investigated for the successful determination of all analytes of interest: microwave-assisted (MW) digestion with HNO3, and room temperature (RT) digestion with tetramethylammonium hydroxide (TMAH) and ethylenediaminetetraacetic acid (EDTA). From our preliminary data, the MW method proves suitable for all elements except Hg, which requires TMAH. Method validation is accomplished using certified reference materials (CRMs) and spiked recovery experiments. Analytical results and simple descriptive statistics for samples of placenta body, myometrium, and the umbilical cord are presented and compared. Future goals include studies that examine associations between the analytical data and human subject variables such as age, nutritional status, and various health outcome parameters.

(152) Determination of Mercury in Blood and Urine by CVAAS and ICP-MS
Ela Bakowska1, Michael Kraky1, Lindsay Altenberger1; 1 NMS Labs
Metallic Mercury is used in thermometers, barometers, devices used to test blood pressure, wall thermostats, fluorescent light bulbs, batteries, electric light switches, indoor gas meter regulators, and for a variety of other purposes. Metallic Mercury is also used in some ethnic religious and cultural practices. Some middle and high school chemistry lab experiments involve use of metallic Mercury. Exposure to very high levels of metallic Mercury vapor can cause brain, kidney, and lung damage and may seriously harm a developing fetus. Exposure to lower levels of airborne Mercury for prolonged periods of time could produce irritability, sleep disturbances, tremors, coordination problems, changes in vision or hearing, and memory problems. Most of the effects of Mercury resulting from low level exposure are reversible, once exposure is terminated. Blood or urine samples are used to test for Mercury exposure. Once exposure has stopped, the Mercury level in the blood drops rapidly, so blood tests are useful only for very recent exposures. The metallic Mercury that is absorbed into the body is excreted mainly in the urine. This presentation will present analytical challenges associated with measuring Mercury in blood and urine. The issue of stability of Mercury in samples during the collection and storage will be addressed. Addition of sulfonic acid and urine samples, in order to stabilize Mercury was evaluated. Two most commonly used analytical techniques: Cold Vapor Atomic Absorption Spectroscopy (CVAAS) and Inductively Coupled Plasma Mass Spectrometry (ICP-MS) will be compared for precision and accuracy of the measurements. Additional aspects of sample-to-sample analysis time, ease of sample preparation and ease of analysis will be presented.

(153) Determination of I- and IO3- in Fresh Water using CE-ICP-MS
Yuichi Takaku1, Yoshihito Ohtsuka1, Shun’ichi Hisamatsu1; 1 Institute for Environmental Sciences
The method for the determination of two valence states of inorganic iodine, I and IO3, was developed using a capillary electrophoresis system coupled with an ICP-MS system, and successfully applied to fresh water samples. A standard capillary column (150 μm inner φ and 75 cm length) was adopted applying 30 kV as the extraction voltage. Buffer solution of 5 mM TRIS-HNO3 (pH 3.0) was used for the mobile phase. The results of analysis of surface water samples in Lake Towada and rivers surrounding the lake indicated that the chemical form of inorganic iodine in all samples was IO3. Additional lake water samples were collected from Lake O-ike-higashi-ko in the Juni-ko area at the Shirakami-Sanchi. The lake has a strong thermocline during almost all seasons; its bottom layer is in a highly reductive state. Depth profiles of I and IO3 clearly showed that I was not detected in the surface layer, but it was predominant in the bottom layer, and vice versa for IO3. Because this separation method is rapid and sensitive, it will be widely used in future. This work was supported by contract with the Government of Aomori Prefecture.

(154) Ftr Assessment of Changes in the Infrared Spectrum of Dimethylsiloxane Following Passive Aqueous Contact
D. Radford Shanklin1, David L. Smalley1; 1 University of Tennessee, Memphis; 2 Tennessee Department of Health
Sequential study of interactions between implanted silicone and surrounding tissues is difficult in part due to cellular reactions confounding the chemical events at the interface. The possibility of siloxane and aqueous interaction is due to (a) mixed ionic-covalent nanometer films on the surface of selected solutions. 1.0 ml Dow Corning MDX-4-4011 (Lot HHH0001) was layered on the 5.0 cm2 surface of test solutions in 50 ml Kimax beakers: (1) normal saline, 0.85% NaCl; (2) 1.0 N KCl in water as potassium equivalent; (3) 10% Betadine, USP. Siloxane infrared spectra have a distinctive signature range, wave numbers 1020-1100; a third center on wave number 1262. Betadine was tested because it is used to irrigate surgical wounds wherein silicone devices might be implanted. Aliquots (0.05 ml) were drawn from the siloxane layer into the lumen of a 27 gauge needle on insulin syringes and transferred as a fluid layer between two 13 mm BaF2 disks (Wilmad Glass, Buena, NJ). Spectra were read by a Perkin Elmer Model 1605 FT-IR and stored and printed through the PE Spectrum LiteTM program on a Packard Bell LG-1510 computer to Epson Stylus Color 500 and Epson C60/C62 inkjet printers. Post treatment samples were obtained at 12 hours and at 13 and 66 days. All aqueous solutions resulted in changes in per cent transmission at all standard peaks and a shift to higher wave numbers, likely due to silanolization. Maximum transmission change was achieved at 12 hours from saline and Betadine; maximum change from KCl was at 13 days; all showed some pattern reversal later which varied but did not return to the baseline for MDX-4-4011 fluid, even after 66 days. Further study will be needed to show whether these changes are due to layer solvation or molecular restructuring with the addition of silanol groups at sites of oxygen-silicon bond-breakage, the latter implied by wave number shift.
(152) Understanding Complex Ion Motion in FT-ICR Cells

Jill Scott1, Timothy McJunkin1, David Dahl1; 1Idaho National Laboratory

Based on the theoretical foundation for Fourier transform ion cyclotron mass spectrometry (FT-ICR-MS), several features should be inherent to the FT-ICR-MS measurement. For example, the mass range should be greater than 1000 u because every ion should reach the same radius regardless of its mass-to-charge (m/z) ratio; however, in practice the useful m/z window for a given set of parameters is usually only around 500 u. In addition, quantification of ions within the cell, including isotope ratios, should be more accurate than acquired in practice. The reason FT-ICR-MS performance does not match with the theoretical predictions is that the ion motion in a real FT-ICR cell is highly complicated. While analytical solutions for various ion motion issues have been reported in the literature, modeling the ion motion within an FT-ICR cell with SIMION provides a comprehensive view of ion trajectory issues. FT-ICR cells reported to date suffer from trapping and excitation phenomena that lead to ions of the same m/z not being excited to the same radius as well as ions of different m/z values being excited to different radii. Lessons learned from the modeling exercise are necessary to determine how to simplify the ion motion so that FT-ICR-MS can function as predicted by theory.

(153) Optimization of Quartz-Enhanced Photoacoustic Spectroscopy Sensor for Isotopologue Analysis using Ab Initio Calculations

Blythe Ashcraft1, S. McWhorter1, A.A. Kosterev2, R. Lascola1, F.K. Tittel2; 1Savannah River National Laboratory; 2Rice University, Rice Quantum Institute

The Savannah River Site (SRS) has a long history of hydrogen isotopic processing and analysis. Real-time monitoring of trace impurity formation is vital to optimization of the hydrogen processing conditions. Isotopologues of ammonia, methane, and water are known or expected impurities in the processing of hydrogen isotopes. Researchers at the Savannah River National Laboratory (SRNL) and Rice University have been developing quartz enhanced photoacoustic spectroscopy (QEPAS) sensors for trace gas sensing in a hydrogen process stream. QEPAS is a variation of conventional PAS which utilizes a piezo-electric tuning fork coupled with a quartz resonator. Given the lack of readily available literature concerning the vibrational spectra of the impurity isotopologues, computational modeling was utilized to determine an optimal laser tuning range for the experiments. This presentation will outline the principles of QEPAS and recent experimental results including detection of ammonia and methane in a hydrogen gas stream along with results from computational calculations.

(155) Kinetic Studies of Emerging Disinfection By-Products and Disinfectants with Nicotinamide.

Gija Geme1, Gary L. Emmert2; 1University of Central Missouri; 2University of Memphis

Water chlorination is the most common form of drinking water disinfection used in the United States. The major problem with water chlorination is that it leads to the production of chlorinated disinfection by-products (DBPs). Other disinfectants are used either alone or combined with FAC. Ozone (O3), chlorine dioxide (ClO2), and chloramines have all been used to help minimize the production of these DBP species. More importantly, recent research indicates that the halogenated-nitrogenated DBPs that result from chloramination may be a more pressing public health concern than the original halogenated DBPs. Recently we reported a new method for on-line monitoring of halogenated drinking water DBPs. The chemical basis of the method is the reaction of the halogenated DBPs with nicotinamide (NCA) in basic solution to form fluorescent products. We also proposed the chemical kinetic rate law and possible mechanism associated with the reaction. We will present more fundamental studies of the reaction of NCA with emerging DBPs and drinking water disinfectants. The rate law will be reported for the reaction of NCA with the emerging DBP species and disinfectants under the conditions of the analysis. The rate law has been proposed by measuring the rate as a function of hydrogen ion concentration. Preliminary studies show that rate for the emerging DBP increases as the concentration of hydrogen ion increases. Preliminary studies have shown that reaction of NCA with disinfectants follow different rate law.

(157) Stability and Internal Energy Deposition of a Venturi-assisted Micromachined Array of Ultrasonic Electrosprays for Mass Spectrometry

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The increasing use of mass spectrometry (MS) in proteomics and metabolomics, has generated an urgent need for the development of high throughput ionization sources. Conventional ionization sources such as nanospray ionization (NSI) provide invaluable information about a particular sample but are limited not only in throughput, but also in the need to use high voltages (1-5 kV) to produce liquid atomization. Furthermore, conventional electrospray methods suffer from limited dynamic range due to charge transport limitations. We have shown that the Array of Micromachined UltraSonic Electrosprays (AMUSE), invented and developed by Fedorov and Degertekin [1], and demonstrated on a mass spectrometry system jointly with our group [2], has the potential of overcoming these limitations. The AMUSE decouples the processes of droplet formation and droplet charging by acoustically forcing the ejection of micron-sized droplets from an array with 400 1-5 um diameter nozzles using an RF potential, while applying a low voltage (100 V) DC potential directly to an aqueous analyte solution. A Venturi device incorporated into the setup increases the linear velocity of the droplet flow causing a corresponding increase in the ion transfer efficiency. In previous studies, we demonstrated the effectiveness of AMUSE for ionizing standard compounds prepared in acidified aqueous solvent mixtures, even in the absence of DC potentials. We here present further characterization of the Venturi-assisted AMUSE device coupled to a quadrupolar ion trap. The effect of varying the applied DC potential used to charge the analyte in both of these devices is explored. Comparative studies using thermometer compounds are also presented with the goal of determining the internal energy deposition during ionization by the Venturi-assisted AMUSE device as compared to that obtained using Venturi-assisted electrospray ionization and nanospray ionization.[1] Fedorov, A. G. and Degertekin, F. L., “Electrospray Systems and Methods”, U.S. Patent 7,208,727 (04/24/2007) and U.S. Patent App. 11/594,489 (10/25/2006).[2] Aderogba, S., et al., Appl. Phys. Lett., 86, 203110-203113 (2005). The mass spectrometric characterization of a novel 20x20 array of micromachined electrosprays is presented.
The presence of two amide linkages andLabel out of which the thio urea were found longer duration of sleep inducing property due to the urea/thio urea linkage and the urea/thio urea diamide derivatives compounds have sleep inducing property due to the presence of determine the sleeping time. It has been found that all the test mice using propylene glycol as an inert vehicle. The loss of carried out by administering intraperitoneally the various doses of CNS depression study of all the synthesized compound were substituted as bond energy in ortho is higher than para substitution: than urea linkages and 2-substituted derivatives are lesser than 4-substitution.

(161) Structure Activity Relationship Studies of Synthesized Urea Diamides on CNS Depression and Sleeping Time Potentiation Effect Dipeshkumar Chaudhary1, Dhrubo Sen2; Shri Sarvajanik Pharmacy College The urea derivatives as barbiturates are closed ring trioxopyrimidine heterocyclic molecule whereas benzodiazepines have also closed ring biososteric azeine heterocyclic molecule consisting of two nitrogen atoms as hetero element possessing CNS depression activity. The proposed plan is based on the open chain urea derivatives having same number of nitrogen atoms in the synthesized molecule to show the CNS depression action either by individually and by synergistically with the reference standard of barbiturates as well as with benzodiazepines. Four series of compounds were synthesized by replacing the variable X as O=Oxygen and S=Sulphur to form the urea and thiourea derivatives of antranilic acid as well as of p-amino benzoic acid and finally the free carboxylic acid of series-2 and series-4 were converted to the carboxamide. Compound-1: 2-carboxy-phenyl urea Compound-5: 4-carboxy phenyl ureaCompound-2: 2-carboxamido-phenyl urea Compound-6: 4-amido phenyl ureaCompound-3: 2-carboxy-phenyl thiourea Compound-7: 4-carboxy phenyl thioureaCompound-4: 2-carboxamido-phenyl thiourea Compound-8: 4-amido phenyl thioureaNow two different categories of compounds were formed at substitutions at 2 and 4 positions of the phenyl rings to produce total eight urea derivatives having open chain having free carboxylic and carboxamide functional groups. All the synthesized compounds were characterized by their m.p., solubility parameters for their polarity, elemental microanalysis by N%, and spectral studies by UV, IR and NMR for structural confirmation. The acute toxicological studies of the compounds were done by determination of LD50 intraperitoneally by mg/kg dose in propylene glycol in 18 hours fasting mice and found that LD50 was as follows in between 400-950 mg/kg, which shows that thiourea derivatives are more toxic than urea linkages and 2-substituted derivatives are lesser than 4-substitution as bond energy in ortho is higher than para substitution: Compound-1 < Compound-2 < Compound-5 < Compound-6 < Compound-3 < Compound-4 < Compound-7 < Compound-8. The CNS depression study of all the synthesized compound were carried out by administering intraperitoneally the various doses of the test compounds in mg/kg dose in 18 hours fasting male albino mice using propylene glycol as an inert vehicle. The loss of righting reflex and regaining of it was noted for each compound to determine the sleeping time. It has been found that all the test compounds have sleep inducing property due to the presence of urea/thio urea linkage and the urea/thio urea diamide derivatives were found longer duration of sleep inducing property due to the presence of two amide linkages and out of which the thiourea derivative and thiourea diamide derivatives showed lesser duration than urea and urea diamide linkage. (162) Wood Cell Wall Characterization by Raman Microscopy and Atomic Force Microscopy Antti Kivioja1, Paula Eronen1, Monika Österberg1, Anna-Stiina Jääskeläinen1; Helsinki University of Technology The wood cell wall has a unique composite structure containing mainly three types polymers, cellulose, hemicelluloses and lignin. The cell wall has a layered structure in which the outermost layer has relatively high lignin content and the cellulose microfibrils are randomly located, while the inner layers have much lower lignin content and the cellulose microfibrils are highly ordered. The ultimate structure of the wood cell wall defines its properties and behavior in wood-based materials, such as timber, paper and cellulose-based composites. For several years, our laboratory has utilised separately Raman microspectroscopy and atomic force microscopy (AFM) to investigate the structural features of wood cells. AFM gives information on sample surface topography in nanometer scale and especially phase imaging has been widely applied. On the other hand, Raman spectroscopy reveals information on the chemical composition of the wood cells and mapping technique provides spatial distribution of different wood components. Only recently, it has been possible to collect AFM images and Raman spectra simultaneously from the same position of the sample. In this way more information is attained than when using these techniques separately. This paper shows how Raman spectroscopy provides an unambiguous chemical interpretation of certain AFM images of wood fibres. Earlier, this has been done indirectly which has left space for speculations. In addition, we show that AFM facilitates the interpretation of Raman spectra of cellulose. This is because the Raman spectra are dependent on the microfibril orientation and when AFM image illustrates the microfibril orientation it is easy to correlate the orientation with the spectral features. (163) FT-Raman Investigation of the Ability of PBI-based Polymer Electrolyte Membranes to be Doped with an Amphoteric Agent George Voyiatzis1, Stamata Maria Roma1, Dimitra Peristeraki1, Erynnisi Vogli1; 1FORTH/ICE-HT A polymer electrolyte membrane fuel cell, PEMFC, is a “sandwich” of an acid-doped PEM between two electrodes; it produces water, electrical energy and a small amount of heat. It is a silent device with direct conversion of chemical energy into the electrical without intermediate step of mechanical work. Due to its minimal negative impact on the environment, it is suited to renewable fuels. High-temperature (120-200oC) polymer electrolyte membranes have been developed and studied because of their advantages; high CO tolerance, simple thermal and water management. Polybenzimidazole, PBI, is a promising proton conducting membrane for high temperature PEMFCs. It exhibits excellent thermal stability, low methanol crossover rate, and high ionic conductivity when doped with an amphoteric agent (i.e. phosphoric acid or a base). However, the long term stability of the high temperature PEMFCs suffers due to the leaching out of the doping agent, mainly the phosphoric acid. The aim of the present study is to understand via vibrational FT-Raman spectroscopy the ability of the PBI-based PEMs to be doped with an amphoteric agent and eventually get valuable information how to hamper the leaching out of the doping agent. PBI can be either protonated by an acid or deprotonated by a base; FT-Raman spectroscopy allows the monitoring of both protonation & deprotonation of the imidazole groups of PBI. In the acid-doped PBI, the Raman band of the imidazole group at 1540-cm-1 is decreasing, while, among other spectral changes, a new peak appearing at 1570-cm-1 is
attributed to the protonated imidazole group. Moreover, the benzene trigral ring deformation i6 mode at 1000-cm-1 is insensitive to the doping procedure and it constitutes an intrinsic calibration peak. In the FT-Raman spectra, no spectral changes occur above a certain doping level for H3PO4 85% doped PBI. Likewise, the intensity ratio of a doping-sensitive Raman band over an insensitive-one remains constant above the same doping level. FT-Raman monitors very well the protonation step of the PBI-based PEMS and it might be proved very useful to handle the acid uptake, the “Achilles heel” of the high temperature PEMS. Acknowledgement: The financial support of the present work by the Appolon-B FP6-2004-NMP-TI-4-028473 and the NOE NanoMemPro (NMP3-CT-2004-500623) CEU projects is greatly acknowledged.

(164) Extraction, Separation, and Detection of Four Important Alkaloids
Christine Copper, Carl Newman, Greg Collins; United States Naval Academy; Naval Research Laboratory

Alkaloids can be isolated from various natural products and can be used for purposes that are helpful or harmful to humans. Previously, high-performance liquid chromatography (HPLC) with absorbance detection has been the favored method to separate and detect alkaloids in assorted matrices. In this work, we present an alternative to HPLC for the separation of several highly toxic alkaloids. A method comprised of a simple solid-phase extraction procedure followed by micellar electrokinetic chromatographic separation (MEKC) is demonstrated for the detection of four toxic alkaloids: colchicine, aconitine, strychnine, and nicotine in a procedure followed by micellar electrokinetic chromatographic detection system. With the exception of aconitine, the detection of these alkaloids is obtained using an on-column diode array detection system. In this work, we present an alternative to HPLC for the separation of several highly toxic alkaloids. A method comprised of a simple solid-phase extraction procedure followed by micellar electrokinetic chromatographic separation (MEKC) is demonstrated for the detection of four toxic alkaloids: colchicine, aconitine, strychnine, and nicotine in a procedure followed by micellar electrokinetic chromatographic detection system. With the exception of aconitine, the detection of these alkaloids is obtained using an on-column diode array detection system. With the exception of aconitine, the detection of these alkaloids is obtained using an on-column diode array detection system. With the exception of aconitine, the detection of these alkaloids is obtained using an on-column diode array detection system.

(165) Estimation of Chemical Information in Latex Suspensions using Light Transport Theory to Remove Multiple Scattering Effects
Raimundas Steponavicius, Suresh Thennadi; Newcastle University

Effective control of latex quality needs accurate information about chemical properties of the latex (concentrations and composition) throughout polymerization process and therefore, availability of online measurements is often an essential requirement for implementation of advanced process and quality optimization schemes. On-line spectroscopic measurements have the potential for providing such information, but accurate calibration models are needed. The heterogeneous nature of polymer latex complicates the extraction of the information contained in spectroscopic measurements using conventional calibration techniques because of variations arising from multiple light scattering [1], [2], [3], [4]. The idea of the proposed approach is to separate absorption and scattering effects using radiative transfer theory and then to apply classical chemometrics on the absorption part to extract concentrations of chemical components from spectral data. Firstly, we examine the impact of the multiple light scattering on conventional calibration models (partial least squares PLS). Their predictions are then compared with the results of PLS models built using absorption spectra obtained after removing the scattering effects (i.e., bulk absorption coefficient fya) by use of light transport theory (inverse adding-doubling method). The information content, in the extracted absorption and scattering coefficients, is examined. Calibration models were built using different NIR measurements made on polystyrene samples of 5 different particle sizes (100 to 500 nm) at 7 different concentrations (0.1-2.3%) for each particle size. Keywords: NIR calibration models, estimation of concentrations, suspensions1. Gossen, P.D., J.F. MacGregor, and R.H. Pelton, Composition and Particle Diameter for Styrene/Methyl Methacrylate Copolymer Latex Using UV and NIR Spectroscopy. Applied Spectroscopy, 1993. p. 1792-1870.2. Vieira, R.A.M., et al., In-line and in situ monitoring of semi-batch emulsion copolymerizations using near-infrared spectroscopy. Journal of Applied Polymer Science, 2002. 84(14): p. 2670-2682.3. Reis, M.M., et al., Correlation between polymer particle size and near-infrared spectroscopy. Macromolecular Rapid Communications, 2003. 24(10): p. 620-624.4. Reis, M.M., et al., In situ near-infrared spectroscopy for simultaneous monitoring of multiple process variables in emulsion copolymerization. Industrial and Engineering Chemistry Research, 2004. 43(23): p. 7243-7250.

(166) A Spectroscopic Approach of the Interaction of the RuO4(g) with a Polyethylene Oxide Surface.
Badia Ame-kraz, Andrea Salvatore, Christophe Moulin, Frédéric Miserque, Alex Cheniere, Cécile Blanc, Isabelle Bisel, Pierre Blanc; DEN/DPC, CEA-Saclay; DEN/DRCP, CEA-Valrhô

Spectroscopic techniques have been used to study the complex surface chemistry of the Ruthenium tetroxide when it contacted polymer surfaces. Polyethylene oxide (PEO) films supported on aluminium disks were exposed to a RuO4(g) plasma generated in situ at ambient pressure and temperature. The surface chemistry has been investigated by means of X-Ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), scanning electron microscopy (SEM) equipped with an energy-dispersive spectrometry (EDS) system, and electrospray ionization mass spectrometry (ESI-MS). Polymer surface chemistry is a growing field with a variety of technological applications such as metallization and fabrication of composites. For metal coatings application, the accurate determination of the ruthenium chemical states present on polymer surfaces has considerable importance. Detailed understanding of the spectroscopic patterns of the Ru-containing metal oxides is also of fundamental interest in that spectra of metal oxides tend to be considerably more complex than those of the associated pure metal. Commercially available species (anhydrous RuO2, hydrous ruthenium dioxide RuO2.2H2O, potassium perruthenate K2RuO4 and potassium ruthenate K2RuO4) have been used to characterize the XPS pattern of these oxides which are suspected and to determine if they exist as stable surface species on POE films. XPS data show that RuO4(g) reacts with PEO functional groups present at the surface to give predominantly hydrous ruthenium dioxide (RuO2.xH2O). XRDR analysis was also used to confirm that all of the metal substrates present on the polymer film are amorphous, as observed for the bulk material with the composition RuO2.2H2O. The XRDR signature of the anhydrous RuO2 with the tetragonal rutile structure has not been detected. SEM-EDS data revealed that ruthenium deposition was enhanced on thin polymer films. Surface “damage” of polyethylene oxide, including conversion of alcohols and ethers into aldehydes and esters functional groups respectively and formation of low molecular weight PEO chains has been examined by ESI-MS.

(167) Study Binding Affinity between Insulin, Insulin Growth Factors and G-Quartet Forming Oligonucleotide by Surface Plasmon Resonance
Junfeng Xiao, Jennifer Carter, Linda McGown; Rensselaer Polytechnic Institute

The insulin-linked polymorphic region (ILPR) of the human insulin gene promoter region contains tandem repeats of a G-rich 14-15 base pair repeat unit that has been shown to form G-quadruplex structures in vitro [1-3]. Previous research has discovered that insulin exhibits high affinity binding in vitro to G-quadruplexes...
formed by an oligonucleotide comprised of two repeats of the ILPR tandem repeat sequence (ILPR2) that is immobilized onto a fused silica surface, leading to the hypothesis that binding of insulin to the ILPR in vivo may play a role in regulation of insulin transcription [4]. Here we report on real-time monitoring of binding interactions of ILPR2 with insulin, and insulin growth factors (IGF-I and IGF-II) using surface plasmon resonance on a Biacore 3000 system. Surface charge switch strategy is employed for the DNA immobilization and a DNA oligonucleotide that does not exhibit a well-defined secondary structure is used as a control surface. Results show that affinity binding of ILPR2 is greater for IGF-II than insulin, and lowest for IGF-I. KD values of these three interactions fall in the range of 10-7-10-8 M. Binding interactions between ILPR2 and other proteins, including neutravidin and thomrin, were much smaller than the affinity interactions with insulin and IGFs. The thornbin result is particularly important when thornbin exhibits high affinity binding with another DNA G-quadruplex structure by means of the thornbin binding aptamer[5]. These studies have significance in both the potential biological implications for insulin in formation of its own gene and the potential analytical uses for a new, high affinity binding ligand for insulin proteins.[1] Catasti, P.; Chen, X.; Moyzis, R. K.; Bradbury, E. M.; Gupta, G. J. Mol Biol. 1996, 264, 534.[2] Bell, G. I.; Karam, J. H.; Rutter, W. J. Proc. Natl. Acad. Sci. U.S.A. 1981, 78, 5759.[3] Lew, A.; Rutter, W. J.; Kennedy, G. C. Proc. Natl. Acad. Sci. U.S.A. 2000, 97, 12508.[4] Adam C. Connor, Elizabeth J. Morgan, Linda B. McGown. J. AM. CHEM. SOC. 2006, 128, 4986.[5] Lawrence W. Dick, Jr. Linda B. McGown. Anal. Chem. 2004, 76, 3037.

(168) Features and Prospects of Continuum Source ET AAS with High Spectral Resolution
Uwe Heitmann; 1ISAS - Institute for Analytical Sciences

High-resolution continuum source atomic absorption spectrometry (HR-CS AAS) has been successfully introduced into the analytical market in 2005. Since then it attracts more and more attention (HR-CS AAS) has been successfully introduced into the analytical equipment available in the laboratories at ISAS Berlin. In addition, as conventional atomic lines in order to determine the concentration rotational lines of diatomic molecules can be used in the same way availability of all wavelengths between 189 and 900 nm and the elements, especially of non-metals, which are normally not interferences but also useful alternatives for the determination of method development process. On the other hand, molecular sampling should be another domain of HR-CS ET AAS and should based systems (LS AAS) due to its multitude of information and dramatic reduction of spectral interferences. Thus, direct solid sampling should be another domain of HR-CS ET AAS and should result in a more accurate analyte determination and a time-saving method development process. On the other hand, molecular structures are not only potential troublemaker causing spectral interferences but also useful alternatives for the determination of elements, especially of non-metals, which are normally not accessible to LS AAS instrumentation. Using HR-CS AAS, rotational lines of diatomic molecules can be used in the same way as conventional atomic lines in order to determine the concentration of the corresponding element. [2]This lecture gives a status of the features and prospects of HR-CS ET AAS, and insight into the equipment available in the laboratories at ISAS Berlin. In addition, practical examples for the determination of real samples and non-metals will be given. Literature:[1] B. Welz, H. Becker-Ross, S. Florek, U. Heitmann, High-Resolution Continuum Source AAS – The Better Way to Do Atomic Absorption Spectrometry, Wiley-VCH, Weinheim, Germany, 2005.[2] U. Heitmann, H. Becker-Ross, S. Florek, M.D. Huang, M. Okruss, Determination of Non-Metals via Molecular Absorption Using High-Resolution Continuum Source Absorption Spectrometry and Graphite Furnace Atomization, Journal of Analytical Atomic Spectrometry, 21, 1314-1320 (2006).

(169) ETV-ICPMS: the Right Tool for Solid Sampling?
Martin Resano1, Maria T. Aramendia1,2, Miguel A. Belarra1, Frank Vanhauwe2; 1University of Zaragoza; 2Ghent University

Among the different methods that permit carrying out the direct elemental analysis of solid samples, graphite furnace-based methods have proven to be very suitable. These methods show interesting features such as a high sample throughput, excellent sensitivity and a reduced risk of suffering from analyte losses or contamination issues. Moreover, in latest years, due to the generalized use of peak area as the measurement mode (in the case of GFAAS), the advances in instrumentation and the possibilities for chemical modification, most of the recent papers have reported reliable results by using straightforward calibration approaches with aqueous standard solutions. This is an important advantage when comparing the performance of these techniques with that of other successful solid sampling approaches that usually rely on the use of matrix-matched solid standards for calibration, such as XRF, LA-ICPMS, GD-MS, et al... For this reason, we believed that solid sampling-graphite furnace-based methods show enough potential to be more widely used in real-life applications. This work tries to critically evaluate the current possibilities of solid sampling-electrothermal vaporization-ICPMS and establish those situations for which the use of this technique may offer an advantageous performance. Several applications from the authors’ lab, which would be difficult to implement by means of traditional dissolution approaches, will be discussed in order to illustrate the strengths and weaknesses of this technique. In particular, the topics presented will include: i) direct multi-element analysis of high-tech materials; ii) the development of mono-elemental but challenging applications related with the determination of complex analytes (e.g., Cr, Si) by means of ETV coupled to sector field-ICPMS.

(170) Determination of Cadmium in Blood and Urine by Electrothermal AAS: The Quest for a Universal Modifier with the THGA
Patrick Parsons1, Bong-Ki Jang2; 1New York State Department of Health; 2Soonchunhyang University

Measurement of cadmium (Cd) in whole blood and/or urine is used to assess occupational exposure to this toxic metal. While many clinical laboratories use electrothermal atomic absorption spectrometry (ETAAS) for this analysis, most resort to separate analytical methods for urine and blood matrices. The transversely-heated graphite atomizer (THGA) would seem to be a natural choice for such an analysis, but experience suggests that a common method for both blood and urine matrices may be quite difficult to achieve. The principal aim of this study was an evaluation of the THGA platform for determining Cd in blood and urine, including a comparison between standard and “end-capped” graphite tubes, permanent and conventional modifiers, and calibration based on aqueous Cd standards. We used a Perkin-Elmer Model 4100ZL ETAAS instrument equipped with longitudinal Zeeman background correction. We evaluated conventional modifiers such as NH4H2PO4, both with and without Mg(NO3)2, and Pd(NO3)2, as well as a permanent modifier (250µg W + 200µg Rh). The results suggest that treating an end-capped tube with 250 µg of W plus 200 µg of Rh makes calibration against aqueous standards possible and yields acceptable results for Cd in both urine and blood matrices. If one is using a standard THGA tube, then adding
0.2% (w/v) NH4H2PO4 modifier to the diluent for samples and standards is sufficient to achieve acceptable results.

(171) Pyrolysis Curves in Electrothermal Atomic Absorption Spectrometry vs Electrothermal Vaporization Inductively Coupled Plasma Mass Spectrometry
Margaretha de Loos-Vollebregt1, Alessandra da Silva1; 1Delft University of Technology

Traditional pyrolysis curves in electrothermal atomic absorption spectrometry (ETAAS) show us the maximum temperature that can be used to remove most of the sample matrix without losing part of the analyte(s), whereas chemical modifiers are widely used in the optimisation of such pyrolysis conditions. This approach has also been adopted in Electrothermal vaporization (ETV) sample introduction of solutions, slurries and solid samples in inductively coupled plasma mass spectrometry (ICP-MS). However, in ETV-ICP-MS the situation is more complicated because the transport efficiency for the analyte depends on the amount of vaporized substance and therefore removal of the sample matrix may influence the sensitivity. Non-linear calibration curves are frequently observed with low-matrix or matrix-free standard solutions. If chemical modifiers co-vaporize with the analyte, their effect is manifested in increased transport efficiency for the analyte, which can be explained by considering that the vapor of the modifier nucleates to a higher extent than the analyte vapor and the latter can condense onto the modifier nuclei. In addition to this, chemical condensation can often be the case with complex matrices, when a less volatile compound is formed by a chemical reaction in the vapor phase. The resulting aerosol carrier effects have been observed for several analytes when using a Pd/Mg-nitrate modifier. We have extensively studied the different behavior of pyrolysis curves for As, Se, Cd, Pb and Hg in biological materials (slurries with TMAH) in the presence of Pd / Mg modifier and permanganate modifier, using the same graphite furnace unit in both systems. Preliminary conclusion is that selective matrix removal should be considered in ETV-ICP-MS, which is far more complicated than optimization of the temperature program in ETAAS. In addition, ETV-ICP-MS has proven to be a useful tool for the study of vaporization and atom formation processes in the graphite furnace.

(172) Parallel ETV and Nebulizer Introduction into an ICPMS
James Holcombe1, Thomas Kreschollek1; 1University of Texas at Austin

Complex matrix components can present isobaric problems for nebulizer-based determinations in ICPMS and/or can raise questions whether other isobaric interferences exist. ETV sample introduction has been shown to remove these matrix interferences via temperature programming or to differentiate between them because of the time dependent signal profile. To take advantage of this temporal information while continuing to use the nebulizer for analysis, a simple coupling of an ETV to a nebulizer system was devised. The device shows no impact on nebulizer performance, but allows the ETV to act as a supplement to the nebulizer without the need to change equipment. Various optimization techniques are used to demonstrate the range of capabilities of the ETV/nebulizer combination. The ETV introduction is shown to have a linear response and detection limits for a variety of elements in both HNO3 and HCl matrices. For example, in a 1% HCl matrix, the detection limits for 51V+ (51ClO interference), 56Fe (ArO interference), 75As (75ArCl interference), and 78Se were found to be 0.008 ppb, 1.1 ppb, 0.088 ppb, 0.063 ppb, respectively. The nebulizer detection limits in 1% HCl for 51V, 56Fe, 75As and 78Se were found to be 0.60 ppb, 8.5 ppb, 1.5 ppb and 1.2 ppb, respectively.

(173) Overview of Speciation in the Field by Electrothermal, In-torch Vaporization (ITV) Sample Introduction System for Inductively Coupled Plasma Spectrometry
Vassili Karanassios; 1University of Waterloo

In this presentation, electrochemical and separation methods we are developing for pre-concentration and speciation in the field and analysis in the lab by ITV-ICP-AES (in-torch vaporization-inductively coupled plasma-atomic emission spectrometry) will be described in detail.

(174) Recent Developments in Ion/Ion Chemistry for Bioanalysis
Scott McLuckey1; 1Purdue University

The emergence of electrospray ionization and electrospray ion traps in the 1980s has enabled the study of the reactions of oppositely charged ions within the context of an MSn experiment. Since the mid-1990s, attention has been devoted to understanding fundamental aspects of the reactions of multiply-charge ions derived from biomolecules, applications of bio-ion/ion reactions, and the development of instrumentation to facilitate ion/ion chemistry studies. A wide range of applications have been developed and tools to implement ion/ion reactions for bioanalysis have become commercially available. This presentation emphasizes the range of ion/ion reaction applications that rely on either proton transfer, electron transfer, or metal ion transfer. Some applications involve the use of multiple ion/ion reaction steps orion/ion reactions in conjunction with collision-induced dissociation. Proton transfer reactions have been used primarily for charge state manipulation. They have been employed for protein mixture analysis, product ion analysis following either collision-induced dissociation or electron transfer dissociation, protein or oligonucleotide ion concentration via ion parking, and charge inversion. Two steps of charge inversion have been shown to be capable of increasing the absolute charge of an ion. Electron transfer has been used foremost as a primary structure probe through its propensity to lead to cleavage of amide linkages. Metal transfer has been used to alter the cations associated with a biopolymer. Significant advances in instrumentation for ion/ion reactions have recently been reported. These include the adaptation of linear ion traps for ion/ion reactions and the coupling of linear ion traps with other analyzers to form hybrid instruments. Hybrid instruments, in particular, offer important potential performance improvements because they allow for the ion/ion reaction conditions and mass analysis conditions to be completely decoupled. They also facilitate transmission mode ion/ion reactions that do not require mutual ion storage. Examples of novel ion/ion reaction experiments implemented on hybrid instruments will be illustrated.

(175) Residue Specific Site Directed Dissociation of Whole Proteins in the GasPhase
Ryan Julian1; Tony Ly1; 1University of California Riverside

A method for initiating fragmentation at a specific residue for whole proteins is presented. The general method relies on photodissociation to site selectively generate a radical which then facilitates cleavage of the protein upon collisional activation. Interference from native chromophores such as tryptophan and tyrosine is not found to be problematic. Results are presented for several proteins, suggesting that the technique is generally applicable. Considerations for database searching are presented in relation to the type of data that can be obtained with this kind of experiment. In addition, experiments with peptides have been utilized to explore the chemical mechanism that leads to the site selective dissociation.
Sensitivity and Quantitation of Proteomics Measurements

Michael Washburn1, Stowers Institute for Medical Research
Spectrum counting is an appealing and relatively straightforward approach for quantitative proteomics. Since the spectrum count of a protein in a proteomic analysis is the total number of peptides, not just unique peptides, detected and identified for a given protein, searching criteria and false positive minimization is important. There are several different versions of spectral counting currently in use, but each approach has shared core characteristics. We use spectral counting as the basis for the normalized spectral abundance factor (NSAF), which takes into account the length of a protein and the total spectral count intensity of a given run. An additional important consideration for quantitative proteomic analysis is the use of replicates for statistical analysis and determining the proper statistical test to use based on the overall structure of the datasets. We routinely use the NSAF approach for quantitative analysis of protein complexes, which will be the focus of this presentation.

Multiplexed Electrospray Sources for Improving the Sensitivity and Quantitation of Proteomics Measurements

Ryan Kelly1, Jason Page1, Keqi Tang1, Richard Smith1, Pacific Northwest National Laboratory
The field of proteomics has benefited tremendously from the greater throughput enabled by liquid chromatography-electrospray ionization mass spectrometry (LC-ESI-MS) relative to conventional techniques. Improving the sensitivity of LC-ESI-MS is key to increasing proteome coverage and analyzing smaller sample sizes. To this end, we have significantly increased the sensitivity of LC-ESI-MS analyses by constructing an array of individual ES emitters, which divides the ≈1–2 µL/min flow rate from robust capillary LC separations into 10-fold increase in sensitivity relative to experiments that employed a single emitter under the same conditions. Also, because ion suppression is reduced at lower flow rates, signal intensities from the multi-emitter devices better reflect analyte concentrations in solution. Efforts to adapt the multi-ESI arrays to a high density microfabricated platform, as well as performance of the emitters for specific proteomics applications will be discussed.

Trilinear Analysis of Images Obtained with a Hyperspectral Imaging Confocal Microscope

Mark H. Van Benthem1, Michael B. Sinclair1, Rachel M. Noe1, Howland D. T. Jones1, David M. Haaland1, Allan R. Brasier1, Ping Liu2, Sandia National Laboratories; 1University of Kentucky
Hyperspectral imaging confocal microscopy (HSI-CM) is a powerful tool for the analysis of cellular processes, such as the immune response. HSI-CM is a data rich technique that routinely generates two-way data having a spectral domain and an image or concentration domain. We typically produce images with dimensions of 200 × 200 image pixels by 512 wavelength elements. Using a variety of modifications to the instrument or experimental protocols, one can readily produce three-way data with HSI-CM. These data are often amenable to trilinear analysis. For example, we have used a time series of 18 images acquired during photobleaching of the fluorophores in an effort to identify fluorescence resonance energy transfer (FRET). The resulting images now represent intensity as a function of concentration, wavelength and photodegradation in time, to which we apply our techniques of trilinear decomposition. We have successfully employed trilinear decomposition of photobleaching data. These data include images of fixed HEK 293 cells transfected with yellow and green fluorescent proteins as molecular probes of cellular proteins involved in the cellular immune response. While very useful in the interpretation of biological processes, the size of the data generated with the HSI-CM can be difficult to manage computationally. Given dimensions like 200 × 200 × 512 × 18 elements, these data sets require careful processing and efficient analysis algorithms. Accordingly, we have implemented novel fast algorithms that can quickly perform the trilinear decomposition. In this presentation we will describe how three-way data are produced and the methods we have used to process them.

Oriented Partial Least Squares: Theory and Application

William Rayens1, Yushu Liu1, Anders Andersen1, Charles Smith1, University of Kentucky
In this talk we address optimal discrimination for problems where dimension reduction is a necessary first step. Such problems are common in chemometrics as well as in the neurosciences owing to the relative ease of generating features and the expense of recruiting subjects or running samples. A typical approach is to first reduce the dimension of the data (e.g. with principal components) and then follow up with a linear discriminant analysis on the scores. Liu and Rayens (2007) have shown that using partial least squares (PLS) to accomplish the first step will reduce misclassification probabilities. They also showed that a particular ridge class of “oriented” PLS (OrPLS) models will do even better. We will review these results and mention new ones that deal with the more difficult problem of unequal group covariances. Our primary application will be the use of fMRI to study differences in cortical activation between women with a family history of Alzheimer’s disease and a control group of women lacking important risk factors. While excellent separation is possible with the ridge class mentioned above, some interesting insights emerge concerning the choice of the ridge parameters.

Parallel Factor Analysis – Partial Least Squares Discriminant Analysis (PARAFAC-PLSDA) applied to Third and Fourth Order Data Tensors

Karl Boosk1, University of Delaware; 2AFRL-APG Site
Presented here is the application of PARAFAC-PLSDA to the classification of gram positive and gram negative bacteria and vegetative bacteria spores. Fourth order data arrays are collected by excitation – emission matrix fluorescence spectroscopy of different cultures both prior and following UV photolysis. The data arrays are highly non-linear; UV irradiation causes the weakly fluorescing calcium dipicolinic acid to blue-shift and increase in fluorescence intensity. Similarly, differences in the tryptophan spectrum can be seen following irradiation. PARAFAC is employed to extract seven spectral profiles that relate to intrinsic chemical constituents or the local environment surrounding these constituents. Following normalization of the extracted profiles to account for sample size variations, PLSDA is capable of distinguishing among the 4 classes of bacteria, spores, or background samples.
and apportionment problems will be presented. Adaptive resonance theory (ART) neural networks and Density-based Spatial Clustering of Application with Noise (DBSCAN) are used to identify decomposition of the sampled aerosol. In this presentation, the approaches to particle classification including adaptive resonance theory (ART) neural networks and Density-Based Spatial Clustering of Application with Noise (DBSCAN). Applications of these approaches to specific source identification and apportionment problems will be presented.

Environmental monitoring studies often produce huge amounts of measured physical parameters and chemical concentrations evaluated at distant geographical sites and during different time periods. Moreover, these parameters and chemical concentrations are also estimated at different environmental compartments (i.e. air, water, sediments, biota...). All these data sets are difficult to handle and evaluate in a simple and fast way using simple univariate statistical and modeling tools, especially due to their large size and to their multicomponent and multivariate nature. In order to recognize relevant patterns of variation in these large environmental data sets, the application of modern chemometric methods based in statistical multivariate data analysis and in factor analysis is proposed. The basic assumption of these methods is that each of the parameters or chemical concentrations measured in a particular sample is mostly affected by different contributions coming from independent sources. By using these methods, specific point sources and diffuse sources of contaminants in the environment and their origin (natural, anthropogenic, industrial, agricultural...) may be investigated and their relative distribution among samples (geographical, temporal, among different environmental compartments distributions) can be evaluated. At each sampling site, relative source quantitative apportionment is estimated allowing an assessment of their environmental impact, distribution and time evolution. In this presentation, the use of different chemometric methods in the analysis of environmental monitoring data sets will be evaluated. Special attention will be paid to the different encountered data structures and to the different data pretreatment methods usually used to facilitate environmental pattern recognition and resolution. Examples of application of air and water contamination studies will be given.

A two-step procedure for analyzing complex infrared and near infrared spectral data has been developed. First, the wavelet packet transform is used to denoise and deconvolute vibrational spectra by decomposing each spectrum into wavelet coefficients, which represent the sample’s constituent frequencies. Second, a genetic algorithm (GA) for pattern recognition analysis is used to identify wavelet coefficients characteristic of the sample’s class label. The pattern recognition GA employs both supervised and unsupervised learning to identify coefficients that optimize clustering of the samples by class in a plot of the two or three largest principal components of the data. Because principal components maximize variance, the bulk of the information encoded by the selected features is about differences between wheat types in the data set. The principal component analysis routine embedded in the fitness function of the pattern recognition GA served as an information filter, significantly reducing the size of the search space since it restricted the search to feature sets whose principal component plots show clustering on the basis of class. In addition, the algorithm focused on those samples and or classes that are difficult to classify as it trains, using a form of boosting. Samples that consistently classify correctly were not as heavily weighted as samples that were difficult to classify. Over time, the algorithm learned its optimal parameters similar to a neural network. The pattern recognition GA integrates aspects of artificial intelligence and evolutionary computations to yield a “smart” one pass procedure for feature selection, classification, and prediction. Analyzing diffuse reflectance spectra of durum wheat and infrared spectra of paint chips from stolen automobiles, we will demonstrate the efficacy and advantages of this approach for genotyping and forensic analysis.

Environmental monitoring studies often produce huge amounts of measured physical parameters and chemical concentrations evaluated at distant geographical sites and during different time periods. Moreover, these parameters and chemical concentrations are also estimated at different environmental compartments (i.e. air, water, sediments, biota...). All these data sets are difficult to handle and evaluate in a simple and fast way using simple univariate statistical and modeling tools, especially due to their large size and to their multicomponent and multivariate nature. In order to recognize relevant patterns of variation in these large environmental data sets, the application of modern chemometric methods based in statistical multivariate data analysis and in factor analysis is proposed. The basic assumption of these methods is that each of the parameters or chemical concentrations measured in a particular sample is mostly affected by different contributions coming from independent sources. By using these methods, specific point sources and diffuse sources of contaminants in the environment and their origin (natural, anthropogenic, industrial, agricultural...) may be investigated and their relative distribution among samples (geographical, temporal, among different environmental compartments distributions) can be evaluated. At each sampling site, relative source quantitative apportionment is estimated allowing an assessment of their environmental impact, distribution and time evolution. In this presentation, the use of different chemometric methods in the analysis of environmental monitoring data sets will be evaluated. Special attention will be paid to the different encountered data structures and to the different data pretreatment methods usually used to facilitate environmental pattern recognition and resolution. Examples of application of air and water contamination studies will be given.

(184) Wavelets and Genetic Algorithms Applied to Spectral Pattern Recognition
Barry Lavine1, Nikhil Mirjankar2, Kadambari Nigam2; 1Oklahoma State University

(182) Quantitative Results from Single Particle Characterization Data
Philip Hopke1; 1Clarkson University

(185) Forensic Investigation of Biological Threats
Kathryn Kalasinsky; 1Armed Forces Institute of Pathology

(186) Colorimetric Analysis of Glass Fragments
Paul Martin1, Mike Eyring2, John Hoang3; CRAIC Technologies, Inc.; Micro Forensics, Ltd.; Arizona Dept. of Public Safety

Glass fragments are commonly found at crime scenes and can be from a number of different sources including windshields, mirrors, headlamps, broken windows and containers, and even eyeglasses. In recent years, plastics have supplanted glass, as they tend to be more resistant to breakage. However, under energetic conditions,
plastics shatter just as easily as glass and yield similar types of microscopic evidence. While they can be readily differentiated from glass, they are more difficult to separate from one another and as such represent important evidence. Due to the multitude of uses found for this type of material, glass is formed in many different ways and in many different colors. And because it shatters so easily, it is commonly found as microscopic shards at the crime scene and as such can be very difficult to obtain accurate colorimetric information. This is because the randomness of the shape of the glass fragments leads to refraction and diffraction of light passing through it. These optical effects can make the glass evidence appear to be one color when observed from one angle and change colors as it is rotated. When analyzed with a UV-visible microspectrophotometer using standard techniques, refraction and diffraction cause spectral artifacts to appear. These artifacts appear in a number of different forms and include peak shifting, reshaping of peaks and dramatic changes in intensity. To date, it has been very difficult to get accurate and quantifiable color data on microscopic glass fragments because of these effects. The purpose of this paper is to describe a technique that eliminates the spectral artifacts and allows for the microspectroscopic analysis of glass and plastic trace evidence. These techniques include sample preparation, methods of spectral data acquisition and, of course, spectral analysis and interpretation. This talk will also review data from a number of glass samples in order to provide examiners with representative data to aid them with casework. This includes microscopic samples of glasses of different colors and from a multitude of sources. Micro-spectra have been acquired and are compared in order to educate the audience on the pertinent features of the spectra.

(187) Pushing the Envelope for Fiber Analysis by UV/Visible and Fluorescence Microspectrophotometry

Stephen L. Morgan, Edward G. Bartick, University of South Carolina, Suffolk University

Identification of patterns in analytical chemical data and interpretation of observed differences is a frequent task for forensic chemists. A fiber examiner might perform UV/visible microspectrophotometry on known and questioned fibers to evaluate possible associations between source and location. However, fiber evidence is class evidence (i.e., not unique) because many fibers from different sources could be indistinguishable. The discovery of a fiber and its identification as a particular fiber type (e.g., acrylic, cotton, nylon, polyester) may not, of itself, provide much support for a forensic investigation. The probative value of particular fibers found at a crime scene depends on their uniqueness relative to the background of fibers normally encountered at that location in the absence of the crime. What is often required is information that makes the trace evidence more specific and discriminating. Our current database of dyed textile fibers consists of more than 1,500 fibers collected from commercial sources and over 15,000 UV-visible, fluorescence, and Raman spectra. This talk will demonstrate the use of this database in conjunction with software developed for forensic comparison on spectra by principal component analysis and linear discriminant analysis. These techniques enable confirmation of statistical validity of discrimination between different polymer classes and dyed textile fibers, visualization of significant differences between groups of spectra discrimination, and tracking of spectral changes with environmental changes. The fibers and associated spectra in the database, in combination with validated computer programs, represent an extensible tool for fiber comparisons in forensic casework.

(188) The Merits and Pitfalls of the Forensic Analysis of Dyed Textile Fibers using Raman

Edward Bartick, Brandi Vanni, Michael Angel, Stephen Morgan, University of South Carolina, Suffolk University

Raman microspectroscopy provides a rapid and non-destructive tool for the forensic identification of single fibers with little to no sample preparation. Typically, FT-IR microscopy has been used in both forensic fiber identification and in industrial analysis because of its sensitivity to minor variations in polymer structure. However, fibers having thick diameters transmit infrared light poorly, and the cross-section of fibers can act as a lens to refract light thus changing relative band intensities. Therefore, fibers are normally flattened which is a laborious task and distorts sample morphology. In Raman microspectroscopy, most of the concerns cited above are inconsequential. A Raman microscope can be used to measure spectra on small samples with high spatial resolution and little to no sample preparation. Raman microspectroscopy has been used in our laboratories to characterize and discriminate among various undyed polyamide fibers from different structural subclasses. We have also employed multivariate statistical analysis, namely linear discriminant analysis (LDA). The Raman spectra of different classes and subclasses were found to be visually different and LDA was employed to assess the discrimination among various polyamide fibers from different structural subclasses. Spectra of polyamide fibers are characteristic of the fibers and the assigned Raman bands correlated well with the known structures. Spectral differences between the fiber subclasses were visually distinguishable and statistically significant. On titanium doped nylon fibers, Raman microspectroscopy was used to distinguish between rutile and anatase forms of the inorganic pigment titanium dioxide (TiO2) and to make quantitative measurements of titania loading. The pitfalls come into play with dyed fibers. The dye Raman scatters and masks the polymer structure which is advantageous when the interest lies with identifying the dye composition. However, the dye responses vary with the dyes and the underlying polymer materials. Additionally, fluorescence can interfere, making it more difficult to obtain predictable spectra. These problems can be overcome, but the analysis becomes more complex. Because Raman spectroscopy is not straight forward, less interest is displayed by forensic examiners when conducting textile fiber analysis.

(189) Molecular Spectroscopy Coupled with Polarized Light Microscopy: Case History at FCC

John Crowe, Mark Witkowski, FDA Forensic Chemistry Center

Optical microscopy and molecular micro spectroscopic analysis of trace evidence is an important function in forensic science. Until recently most optical observations (PLM) and subsequent Fourier transform infrared (FT-IR) and Raman microscopic measurements were performed on two separate instruments. The two instruments being a dedicated PLM microscope and a commercial FT-IR and/or Raman microscope. This can lead to problems and issues when transferring samples between the two different microscopic set ups. The recent coupling of a microscope with greater optical capabilities (PLM) and FT-IR and Raman microscopes now allows for both optical and chemical information to be collected on a single instrument. The coupling of these two techniques (Optical microscopy and molecular micro spectroscopy) has greatly expedited the routine samples encountered at the FDA’s Forensic Chemistry Center (FCC). Fibers, pharmaceuticals, foods, and tampering cases are just a few of the examples of the samples that the Polarized Light Microscope-Infrared Spectroscopy (PLM-IR) and Polarized Light Microscope-Infrared Spectroscopy-Raman spectroscopy (PLM-IR-Raman) systems handle on a daily basis. Over the past five years hundreds of cases have been solved using this orthogonal approach to sample analysis. Four specific cases
will be discussed. The coupling of these two orthogonal techniques makes for a rapid, yet powerful tool for the forensic chemist.

(190) Validation Studies for Detection of Blood on Substrates of Forensic Relevance by Fourier-Transform Infrared (FT-IR) Spectroscopy
Anthony R. Trimboli1, Heather M. Taylor1, Stephen L. Morgan1; 1University of South Carolina
Blood is a critical piece of evidence frequently discovered at crime scenes. Improved detection methods are needed because small traces of blood may be obscured by surrounding backgrounds. Attempts to clean up blood may also prevent visual or chemical detection of blood. Common chemical detection methods involve toxic chemicals, such as luminol, which can also compromise DNA integrity. Infrared (IR) spectroscopy used in a real-time mode would address these issues and reduce analysis time. Hemoglobin, the major protein in hematocrit, and albumin, the chief component in plasma, produce a distinctive IR absorbance (amide I and amide II bands in the 1650-1540 cm⁻¹ spectral range). This research is designed to validate forensic applicability of IR spectroscopy for rapid detection/visualization of blood. Our hypothesis is that IR spectroscopy possesses sufficient specificity to exhibit a low false positive detection rate for blood on a variety of possible background materials (e.g., clothing, carpets, wood, or other surfaces). Replicate spectra of neat and bloodstained substrates were collected using two different approaches: diffuse reflectance and attenuated total reflectance. Multiple substrates including olefin, nylon, and polyester polymers, coated with Scotchguard™ and other stain release treatments, were tested with varying levels of blood contamination. Discrimination of bloodstained substrates from clean surfaces was achievable in most cases. However, because nylon (commonly in carpets) is a polyamide, similar bands are seen in nylon spectra. This potential interference may complicate determination of the presence of blood on nylon-containing substrates. Principal component (PCA) and linear discriminant analysis (LDA) were employed to validate the ability to distinguish the vibrational bands of blood from that of the substrates. Further investigation using partial least squares (PLS) analysis was also performed to determine the limit of detection for each method on the various materials.

(191) Analytical Chemists' Best Friend: NIR Fluorescence Spectroscopy
Gabor Patonay1, L. Strekowski1, J.S. Kim1, M. Henary1; 1Georgia State University
During the last two decades near-infrared (NIR) absorbing chromophores have been used extensively in analytical and bioanalytical chemistry, in areas such as determination of properties of biomolecules including DNA sequencing, immunoassays, capillary electrophoresis (CE) separations, etc. It was recognized early on that this spectral region is in the range where interference is limited. The part of the NIR region where most NIR fluorophores are available (i.e., the 700-1200 nm range) has several advantages for bioanalytical chemists and affords very low detection limits due to the high molar absorptivities of NIR fluorophores. Specially designed NIR fluorophores open up new bioanalytical detection possibilities. By moving detection from a visible region to the longer wavelengths, the background interference from the complex matrix is greatly lowered, thereby reducing scatter and shifting of the Raman line even further from the spectral region of interest. Advanced dye synthesis has allowed the design of highly stable NIR chromophores. Carbocyanines are especially good candidates for analytical purposes. They are relatively easy to synthesize and variations in their structures allow for designing dyes that fit a particular application. This presentation will focus on how carbocyanines can be tailored to particular applications. Analytical and bioanalytical applications include biomolecule characterizations and quantitative and qualitative determinations of biologically important analyses (e.g., intracellular Ca²⁺, etc.). Carbocyanines recently moved into medical applications and to a degree much wider in scope than the original cardiogreen (or ICG) made possible. Recently, our research group has introduced bis-cyanines as novel NIR indicators for analytical and bioanalytical applications. Depending on their microenvironment, bis-cyanines can exist as an intramolecular dimer with the two cyanines either in a stacked form or in a linear conformation in which the two subunits do not interact with each other. These unique carbocyanines further extend the analytical and bioanalytical utility of the dye class.

(192) Isolating Interactions in Complex Fluids using Multivariate Optical Spectroscopy
Sharon Neal1; 1University of Delaware
One of the interesting trends in analytical methodology has been the development of multivariate measurements. While the power of hyphenated separations measurements such as GCMS are well known, expansion to multivariate formats has increased the utility of many other types of measurements including the quantification of hybridized probes on cDNA microarrays and resolution of photosynthetic processes in bacteria. In this presentation, a short overview of this trend will be presented, followed by a description of how multivariate spectral analysis is contributing to the study of complex fluids based on mixtures of lipids. These intriguing soft materials are finding applications in a variety of fields, but improved methods to characterize them are needed to capitalize on their unique properties fully.

(193) Carbon Micro and Nanomaterials Used in Separation Science
Susan Olesik, Justin Shearer, Jeremy Steach, Jonathan Clark; 1Ohio State University
Glassy carbon is both chemical and mechanically robust. We have recently synthesized unique precursor molecules that form carbon media. These precursor molecules are capable of self-assembly and self-polymerized. The polymers are effective for the production of unique formats of separation science. Progress on the development of micro and nano-scaled carbon-based separation science will be described in this talk.

(194) Aptamers and Beyond: DNA Binding Ligands for Affinity Analysis
Linda McGown1, Jacquelyn Cole1, Elizabeth Morgan1; 1Rensselaer Polytechnic Institute
Affinity binding reagents have played a crucial role in analytical methods for detection, separation, purification, isolation and quantitation of molecules of interest. Antibodies have been unrivaled as affinity reagents due to their strong and selective binding; however, drawbacks associated with their production, stability and manipulation have prompted researchers to seek alternatives. Foremost among alternatives are DNA binding ligands such as aptamers and related oligonucleotides that offer affinity on par with monoclonal antibodies, but with important advantages. Once a DNA binding ligand to a target molecule has been identified, it can be readily synthesized without a living host, and chemically modified and manipulated with ease. DNA binding ligands are chemically stable and can be reversibly folded and unfolded for capture and release of the target molecule indefinitely. We have been using DNA binding ligands immobilized at fused silica surfaces for affinity MALDI-mass spectrometry and affinity capillary electrophoresis. These surfaces offer a robust, simple, reusable platform for isolation, preconcentration and specific detection of difficult analytes such as low abundance proteins or...
peptides in biological samples. In recent work we have extended the concept of DNA binding ligands beyond the combinatorial approach to aptamer discovery in the design of oligonucleotides with sequences derived from genomic DNA. In a variation on the aptamer concept, we have introduced the idea of using DNA binding ligands with sequences derived from genomic DNA as candidates for affinity binding reagents. In addition to the analytical significance of genomic-inspired binding ligands, their discovery may offer insight into the role of secondary structures in genetic processes such as gene regulation.

(195) Spectroscopic Investigations of Chiral Recognition
Matthew McCarroll1, Jeremy Buckingham1, Irene Kimaru1, Yafei Xu1; 1Southern Illinois University
Efforts in our laboratory have resulted in the development of fluorescence anisotropy based methods for the evaluation of chiral recognition. The technique has proven to be an effective method for both fundamental and applied investigations of chiral discrimination. Specifically, novel quantitative methods have been developed to determine enantiomeric composition and the thermodynamics of enantioselective binding. Recent efforts have focused on the feasibility of using fluorescence anisotropy to study chiral recognition on chromatographic interfaces, especially the possibility of screening chiral selectors and the a priori prediction of optimum separation conditions. The talk will give a broad overview of our efforts, accomplishments and future directions in this area of research.

(196) Mechanistic Studies of Chiral Separations
Victoria McGuffin1, Kahsay Gebre-Yohannes1; 1Michigan State University
In liquid chromatography, thermodynamics and kinetics are equally important for any successful separation. Thermodynamic parameters provide an understanding of the energetic interactions between the solute and the mobile and stationary phases, which are intrinsically related to the aspects of retention and selectivity. Kinetic parameters provide an understanding of the rates of mass transport processes, which are intrinsically related to the efficiency or plate height. Both thermodynamic and kinetic information is necessary in order to optimize resolution. While many studies have focused on the comprehensive thermodynamic and kinetic characterization of traditional reversed-phase separations, limited information is available for chiral separations. In this study, a series of coumarin-based solutes is separated using a beta-cyclodextrin stationary phase with a polar-organic mobile phase. Temperature and pressure are varied in order to observe the effects and determine important thermodynamic and kinetic parameters. The retention factor, together with the concomitant changes in molar enthalpy and molar volume, are used to elucidate the thermodynamic behavior. The rate constants, together with the concomitant activation energy and activation volume, are used to elucidate the kinetic behavior. In addition, the differential changes in thermodynamic and kinetic parameters provide a detailed examination of the chiral contributions to retention. An increase in temperature decreases the retention and chiral selectivity, but increases the mass transfer rates for all coumarin-based solutes. An increase in pressure decreases the retention, but does not significantly affect the chiral selectivity. Van’t Hoff plots of the natural logarithm of retention factor versus inverse temperature are linear with positive slopes, indicating an enthalpically favorable transfer from mobile to stationary phase. The second eluted enantiomer has a more negative change in molar enthalpy than the first, suggesting an enthalpically more favorable transfer. For all solutes, both the differential change in molar enthalpy and the differential change in molar entropy between the two enantiomers are negative. From these values, the compensation temperature is determined and is above ambient temperature, indicating an enthalpically-driven separation. Although the solutes have similar structures, different compensation temperatures are determined and enthalpy-entropy compensation is not observed. This suggests that the retention mechanism is distinctly different. The change in molar volume is positive, indicating that the compounds occupy more space in the stationary phase than in the mobile phase. This suggests that inclusion in the cyclodextrin cavity does not occur to a significant extent, as expected in the polar-organic mode. With regard to the kinetic behavior, the rate constants generally increase with increasing retention factor for the coumarin-based solutes. However, the second eluted enantiomer has a surprisingly faster rate constant than the first enantiomer. The activation energy is positive, and the second eluted enantiomer always has larger activation energy than the first enantiomer. These thermodynamic and kinetic measurements provide a detailed and comprehensive view of the chiral retention mechanism.

(197) “Processability” of Solids - The Need to Understand the Matrix
Fiona Clarke1, Steve Hammond1; Pfizer
The matrix of pharmaceutical solid dosage forms can be evaluated using instrumentation which allows for chemical images to be obtained. These chemical images are generated based on spectral information collected across a specific sample area. Chemical images allow the distribution and size of components to be examined, once in the final dosage form. Therefore matrix exploration can be used to understand the impact of a change in material properties on the final dose, as such variations in input particle size of materials or a variation in the process parameters can be visualised. Having the ability to examine the matrix distribution of components within the final solid dosage form, provides a means to identify critical to quality attributes. This allows greater understanding of what the impact is on the dosage form following a change to input raw materials. It is therefore necessary to pair good material characterisation tools with chemical images to be able to predict process performance. This presentation will examine a number of different case studies. One example will determine the impact to the tablet matrix upon changing the input particle size of a key excipient. A second example will focus on the variability in the hydration state of magnesium stearate and the impact to its distribution in the final solid dosage form. The presentation will then move on to look at the impact on dissolution performance on changing the age of the input raw materials – with the age impacting the final distribution in the solid dosage form. API supplier change and the impact on the final drug product will then be examined with the final example looking at how terahertz spectroscopy could be utilised to assess variation in tablet coating thickness. This presentation will show how chemical imaging methods, paired with material characterisation tools can assess the impact of a change in material properties, along with the possibility of prediction of product performance.

(198) Near-Infrared Spectral Imaging: a Systematic Approach to Sample Comparison via Spectro-Spatial Analysis
Thomas Brueggemeyer1; 1Forensic Chemistry Center, U.S. Food & Drug Admin.
A common task in a forensic laboratory is to distinguish between a product which is “normal”, and one which is counterfeit, adulterated, tampered with, or somehow sub-standard. Near-infrared spectral imaging has proven quite useful in producing striking visualizations of complex matrices in pharmaceutical and food products. While “a picture is worth a thousand words” may hold true, there is a need in a forensic setting to supplement visualized data with numbers. In addition to providing objectivity, quantitative results can potentially provide sensitivity to sample...
characteristics which may be missed with visualization alone. In traditional spectral comparisons, a distance measure or metric is used to represent the degree of difference between samples. However, in spectral imaging, a sample is represented by a data cube of many thousands of spectra, each from a particular spatial location. Thus, a single distance measure cannot fully characterize all the possible differences between two data cubes. In one scenario, two samples may differ completely in that the anticipated product is replaced with a totally different material. Any number of inter-cube distance measures may suffice in this “easy” situation. Or, the same components may be present in the two samples, but the relative proportions may differ. In some situations, the basic sample blends may be very similar, but a minor adulterant is found in only the suspect sample. Finally, the two chemical compositions may be identical, but spatial discrepancies might exist—differing particle sizes, or the extent of blending. It would be very useful for a library search algorithm to return not one, but several inter-cube distances, each corresponding to a fundamental way in which data cubes may differ. The work to be described will demonstrate how the scenarios above—ways in which samples can differ—call for the use of various distance measures. Both artificial and real pharmaceutical and food examples will be used to demonstrate the utility of these metrics.

(199) Approaches for Measuring the Micro and Macro Chemical and Physical Heterogeneity of Pharmaceutical Products and their Intermediates
E. Neil Lewis3, Linda H. Kidder1, Suzanne J. Hudak1, Janie Dubois3, Kenneth S. Haber1, 1Malvern Instruments
A variety of imaging technologies have become commonplace in the pharmaceutical industry for assessing a wide range of the physical and chemical properties of both finished products and pharmaceutical raw materials (excipients and active ingredients). The technologies breakdown into two main groupings which may be termed morphological imaging, in which the impact of the size and shape of the raw materials (particles) are scrutinized, and chemical imaging in which the spatial relationships of these components are assessed after one or more manufacturing steps. Chemical imaging is employed typically to measure blends, granulations, time release granules or finished products. In this presentation we will present data derived from several different imaging technologies, both morphological and chemical. We will present data from a technique which seeks to bridge the gap between these methodologies. This implementation may be described as a “statistical spectroscopic approach” that measures heterogeneity, both chemical (on micro- and macro- spatial levels) and physical. Because the technique is non-destructive and the performance of samples can later be evaluated through additional assays, the impact of these characteristics on the performance of pharmaceutical products can be determined.

(200) Applications of Near Infra Red (NIR) Imaging for Understanding Pharmaceutical Performance
Caroline Rodger1, Mike Claybourn1, Vicki Woodward1; 1AstraZeneca, Macclesfield
The application of Near Infra Red (NIR) Imaging in the Pharmaceutical Industry is becoming wide spread. Information available from a NIR image, including domain distribution, agglomeration, segregation etc coupled with down field data can help understand and improve a pharmaceuticals performance. This presentation discusses statistical representation of NIR images coupled with down field data such as dissolution, stability etc in order to distill information on understanding and controlling a pharmaceuticals key quality parameters. Chemometric and statistical evaluation of NIR Images will be presented and related to applications including tablet compression, uniformity of content and blend time.

(201) NIR Imaging and Quantitative Analysis of Inhomogeneous Pharmaceutical Formulations
Gary McGeorge4, John P. Bobiah1, 1Bristol-Myers Squibb
Chemical imaging technologies can provide quantitative compositional and spatial information at microscopic levels. In this work, we will present the application of NIR imaging for the identification and classification of API-rich agglomerates in a series of pharmaceutical tablet formulations. Precise compositional information for each pixel in the image was established through chemometric methods. API-rich agglomerates in the compressed tablet were classified in terms of their apparent particle size; the resulting particle size distributions were comparable to those attained by light scattering prior to compaction. Correlation of the particle size distributions before and after compaction confirms the survivability of the API agglomerates. The presence of large spatial heterogeneities (API-rich agglomerates) poses an analytical challenge that is seldom addressed quantitatively: how best to objectively characterize the spatial distribution of a dispersed phase? A variety of approaches were applied in order to classify the distribution of the API-rich agglomerates- the pros and cons of each measure are briefly highlighted.

(202) Field Experience with a Single NDUV and TCD Analyzer on Amine Based Tail Gas Treating Units
Daniel Potter1, Kevin Harris1, Phil Harris2, Randy Hauer1, Byron Lewis3, 1AMETEK Process Instruments; 2ALON USA; 3HARITEC
The paper describes the initial installation and subsequent improvements of a gas analyzer installed on a SCOT (Shell Claus Off-gas Treating) tail gas treating unit (TGTU) for Claus SRU (Sulfur Recovery Unit) tail gas. The process requires the measurement of H2 (Hydrogen) to control the reduction gas to a CoMo (Cobalt Molybdenum) catalytic reactor and the measurement of H2S + COS (Hydrogen Sulfide and Carbonyl Sulfide) to monitor the efficiency of the amine contactor and CoMo reduction reactor. The analyzer combines a non-dispersive ultraviolet (NDUV) optical bench with a thermal conductivity detector (TCD) for the simultaneous measurement of H2S, COS and H2 from the sample point at the overhead of the amine absorber. This measurement has previously been performed by a gas chromatograph or using discrete cold / dry analyzers. The innovation comes from combining the detection techniques, electronics and sample system into a single integrated continuous analyzer for a specific application. A significant reduction in cost and maintenance is realized. The sample system was given special attention in this application. The toxicity of H2S is well known and therefore the sample system was designed so the sample could be returned to the process at the same point as the sample take off. A heated sample probe was designed which has sample wetted parts fabricated from stainless steel and an aluminum heater for temperature control.

(203) In-Line Turbidity Measurements for Industrial Processes
John Groetsch1, David Bigalke1; 1Mettler Toledo Ingold, Inc.
In-line turbidity analyzers have been successfully used for many years to measure the suspended solids and/or emulsions levels in liquid process streams in real time. The technique employed is the measurement of light scattering at various angles from the light source and at various wavelengths. The data from these in-line analyzers has helped to optimize and reduce upsets in industrial processes. This paper gives an overview of the light scattering turbidity techniques used and why certain methods perform best in specific applications. Sensor fouling or coating can be a concern, therefore automatic in-place cleaning will be discussed. Calibration
(205) Alternative On-Line Hydrogen Measurement
Ulrich Gokeler1; Siemens Energy & AUtomation
Hydrogen is one of the most widely used reaction gas in the hydrocarbon processing industry. On-line compositional measurement is used to determine and control hydrogen concentrations in various process streams. An often applied gas measurement technology is continuous thermal conductivity which depends on the large thermal conductivity difference between Hydrogen and most other gases present. This measurement technology typically provides adequate precision under stable process conditions when impurities are at low and stable concentrations. However, increased and changing concentrations of impurities can have an adverse impact on the hydrogen measurement precision and consequently have an impact on process control. This is especially evident during process changes. By utilizing an alternative analyzer technology to speciated and quantify Hydrogen, high precision can be achieved under any process conditions without complicating the measurement configuration significantly. This paper discusses measurement requirements, variables impacting quantification at various process conditions as well as comparing alternative system configuration and economical aspects.

(206) An Ultra-Sensitive, Multi-Species Trace Gas Analyzer for Process Analysis and Control
Eric Crosson1; Kathleen Hartnett1; Picarro
The need for multi-species, trace gas analysis in industries ranging from petrochemical process control to combustion analysis to environmental monitoring is driving the development of process analyzers with both high sensitivity and high speed. Cavity Ring-Down Spectroscopy (CRDS) is a laser-based, all-optical technique capable of parts-per-billion sensitivity and fast 1 Hz measurement rates in even the most complex gas streams, without long term drift or periodic calibration requirements. With a high finesse optical cavity coupled to a high precision wavelength monitor, the CRDS analyzer has a spectral resolution 1000 times better than a Fourier Transform Infrared Spectrometer (FTIR) thus allowing CRDS to distinguish individual absorption features. Picarro has developed a next-generation CRDS gas analyzer that can measure up to four separate species with the same performance, inherent stability, and reliability of the standard single-species gas analyzers. The modular broadband design enables configuration of the multi-species platform to any four of a variety of target species. With an innovative precision wavemeter and operation below atmospheric pressure, the analyzer makes extremely accurate measurements of the target species without cross-talk from optically absorbing background species. Available target species include but are not limited to ammonia, hydrogen sulfide, methane, carbon dioxide, carbon monoxide, water vapor, ethylene, ethanol, methanol, acetylene, and nitrous oxide. We present results obtained with a four-species CRDS analyzer measuring four important atmospheric contaminants (hydrogen sulfide, ammonia, nitrous oxide, and methane) in the vicinity of Concentrated Animal Feeding Operations (CAFOs).

(207) On-Line Liquid Chromatography’s Role in Process Analytics
Rick Cosley1; Mike Doyle1; Dionex Corporation
The use of liquid chromatography (LC) has grown rapidly since it was first introduced in the late 1960’s to become one of the most widely used techniques in the analytical laboratory. Since LC does not require the analyte to be vaporized prior to analysis, LC based methods can be applied to a broad range of molecules from inorganic ions to proteins. This presentation will provide a brief review of the attributes of LC that make it an attractive technology to consider for on line applications, the general capabilities of a typical commercial on line LC analyzer, an overview of the types of applications where on line LC has been successfully applied in multiple industry segments, closing with a more detailed discussion of application examples from the chemical and pharmaceutical industries.

(208) High-Temperature Multi-Point Sampling Mass Spectrometry
Peter Traynor; Robert Wright; Thermo Fisher Scientific
Mass Spectrometers have been deployed for the purpose of optimizing chemical processing units for 20 years or more. When the appropriate technology is used, MS provides the advantage of rapid and complete analysis of multiple process streams. This fast and comprehensive analysis can be used to provide better product yields and more efficient use of energy and materials. Some process streams present special challenges, however. These often require that relatively high temperatures are maintained throughout the analyzer stream sequencing device in order to prevent polymerization or condensation of the sample. This presentation will cover the analyzer design features that can lead to extremely reliable operation in spite of the challenges presented by some of the more difficult process streams. Acrylonitrile, hydrogen cyanide and vinyl acetate will be presented as examples.

(209) NMR in Drug Discovery
Michael Shapiro; University of Maryland
The drug discovery process often involves the screening of compound libraries to identify drug candidates capable of binding to target macromolecules. New approaches in biological and chemical research are driving a change in the pharmaceutical industry. Recent advances in NMR spectroscopy such as affinity NMR techniques, which detect binding of a small molecule with a “receptor”, have been shown to be valuable tools to perform rapid screening of compounds for biological activity. These NMR observable events include using relaxation, chemical shift perturbations, translational diffusion, and magnetization transfer. These one and 2- dimensional NMR methods increase both the throughput of screening and yield crucial data on the mode of binding. The practical utility of these techniques will be described.

(210) Automated LC/MS Purification of Lead Compounds Using a Focused Gradient Approach
Jiang Zhao1; Thomas Swann1; BMS
N/A

(211) High-Throughput Bioanalysis of Drugs and Their Metabolites in Pharmaceutical Industry by LC/MS/MS
Perry Wang; Arrow International
Bioanalysis is a technique, which is used for the quantitative determination of drug and their metabolites in biological matrices. Hyphenated instrumentation, such as liquid chromatography-mass spectrometry (LC-MS) is an essential tool in pharmaceutical industries. Due to its high selectivity and sensitivity, it plays a crucial roll for drug discovery and development. Reducing timeline is one of the most important factors for drug discovery and development, which require high-throughput analytical approaches. The introduction and implementation of automated 96-well and even 384-well extraction techniques has made the approaches more realistic. The automated extraction techniques can be protein precipitation, solid-phase extraction, and liquid-liquid extraction. Additional high-throughput techniques include on-line extraction,
the application of pierceable caps for biological tubes, and so-called nano-stream technique, which has recently been introduced into the pharmaceutical industries. Combination of automated 96-well sample preparation with the application of liquid chromatography coupled with tandem mass spectrometry (LC/MS/MS) has enabled bioanalysts to face the high-throughput challenges. High-throughput assay can be also improved by using a parallel system, such as dual system – two HPLC systems are connected to one MS system. A real study comparison will be presented for the dual system. Most recent advances in the bioanalytical field will be reviewed in this presentation.

(212) Strategies for Implementing Fast Liquid Chromatography in Pharmaceutical R&D in a GMP Environment
Zhong Li, 1, 1Merck Research Laboratories
Genomic revolution, the advent of combinatorial chemistry and computational modeling, and high-throughput screening (HTS) have dramatically accelerated the discovery of molecules as precursory to drug development. The vast number of PCCs necessitates an increasing need for faster, simpler, higher performance, and more cost effective analytical tools for characterizing and testing bulk drug substances and finished formulation products. High-performance liquid chromatography (HPLC) has been the work-horse of pharmaceutical laboratories and is among the most powerful and versatile tools for the detection and quantitation of chemical components in complex matrices frequently encountered during pharmaceutical R&D processes. Currently, there is a revived interest in the development and implementation of fast liquid HPLC methods. This presentation aims to summarize the latest developments and to critically review the current approaches for achieving fast liquid chromatography including: (1) use of short HPLC columns; (2) small-particle liquid chromatography; (3) ultra-high pressure liquid chromatography (UHPLC); (4) high-temperature liquid chromatography (HTLC); (5) monolithic liquid chromatography. It is evident that each technology has its own strengths and limitations and should be used only when the individual advantages can be best leveraged for the specific analytical needs. No single strategy will fit all situations. From the perspective of pharmaceutical application in a GMP working environment, there is clearly a need to strike a judicious balance of speed, resolution, sensitivity, reproducibility, and ruggedness. Several important practical aspects relevant to the implementation of fast-LC technologies in pharmaceutical labs, such as method development, method validation, method transfer, and instrumental requirements will be discussed. Applications of the various fast LC methods in support of pharmaceutical research and development will be presented to demonstrate the applicability and benefits of fast LC.

(213) Applications of Multidimensional Vibrational Spectroscopies to Complex Materials
Dana Dlott, 1University of Illinois at Urbana-Champaign
In this talk I will discuss recent results obtained using multidimensional vibrational spectroscopy to study the dynamics of molecular materials. Two techniques will be described that use a combination of ultrashort IR and visible pulses to probe molecules in bulk materials and on surfaces. Studies of vibrational energy flow through molecules, across molecules and across interfaces will be described.

(214) Recent Advances and New Applications for 2D IR Spectroscopy
Martin Zanni, 1University of Wisconsin-Madison
In the past few years several new advances have taken place that are revolutionizing the ease and applicability of 2D IR spectroscopy. This talk will describe an advance made by our group to automate the collection of 2D IR spectra using a mid-IR pulse shaper that we have recently built. With this shaper, we can now programmably create various pulse sequences to optimize the data collection efficiency and resolution of the experiment. Applications of our new approach to various membrane peptide systems will be given.

(215) Charge Transfer and Carrier Mobility in OPV Materials Examined with Ultrafast Multidimensional Infrared Spectroscopy
John Asbury, 1Larry Barbour, 1Maureen Hegadorn, 1Ryan Pensack, 1Penn State University
Two-dimensional infrared and ultrafast visible pump-infrared probe spectroscopy are used to examine charge transfer and carrier mobility in organic photovoltaic materials by probing their native vibrational modes. Mixtures of electron donating polymers and electron accepting fullerene materials that represent prototypical organic solar cells are examined. By studying the carbonyl (C=O) stretch of both electron donor and acceptor materials, we directly time resolve charge transfer on the few picosecond and circa one nanosecond time scales. The slower time scale results from excitons that must diffuse to the interface before charge transfer can occur. The carbonyl frequency is sensitive to the local bonding environment. The sensitivity allows us to time resolve the diffusion of electrons and holes within the materials over a range of time scales covering picoseconds to nanoseconds. The experiments provide sensitive probes of carrier dynamics that are useful for designing the next generation of efficient organic photovoltaic materials.

(216) Novel Relaxation-Assisted 2D IR Spectroscopy Method
Igor Rubtsov, 1Sri-Ram Naraharisetty, 1Dmitry Kurochkin, 1Valeriy Kasyanenko, 1Tulane University
A novel method of 2DIR spectroscopy, relaxation-assisted 2DIR (RA 2DIR), is proposed that utilizes vibrational relaxation and intramolecular vibrational energy redistribution and permits measuring structural constraints using modes separated by larger distances. The utility of RA 2DIR for measuring bond connectivity patterns is demonstrated on several examples. About 20-fold amplification of the CN / CO cross-peak amplitude is shown for the modes spatially separated by ca. 11 Å using RA 2DIR.

(217) Ultrafast IR Spectroscopy of Active Electronic Materials
Aaron Massari, 1Audrey Eigner, 1Jason Peterson, 1University of Minnesota, Twin Cities
We present recent results of the application of multidimensional infrared spectroscopy to active electronic materials (AEM). Specifically, we describe the ultrafast dynamics observed in organic conducting polymers and small molecules under electrical bias.

(218) Femtosecond Electronic Collinear 2D Spectroscopy
Ivan Piletic, 1Martin Fischer, 1Warren Warren, 1Duke University
Ultrafast nonlinear 2D spectroscopy has advanced rapidly over the last decade. A majority of the work has incorporated phase matching schemes whereby multiple pulses are combined in a non-collinear fashion in a sample with signal intensity being emitted in a unique direction. We have recently implemented multiple collinear pulses to generate the photon echo pulse sequence that are used to excite coherences and populations in a sample. This sequence is achieved using a pulse shaper containing an acousto-optic crystal capable of diffracting near-IR light when driven by radiofrequency waves. The main advantages of this strategy are high detection sensitivity, fast spectral acquisition, and simplicity in implementation. (J. Chem. Phys. 126, 164307 (2007))
photon echo signals are detected in the rotating frame thereby dramatically reducing the amount of data that needs to be taken in order to construct 2D spectra. The acousto-optic crystal is capable of being updated at MHz frequencies implying that a 2D spectrum may be collected in less than a second when the laser repetition rate is set to these frequencies. In this work collinear 2D spectroscopy is used to study the dynamics of dyes and quantum dots pertinent in imaging applications. New features appear in these spectra that are not observed in 2D NMR. Off-diagonal peaks occur that are the result of a dynamic Stokes shift effect. This effect is pronounced and may be utilized in imaging applications to examine spatially heterogeneous environments such as living cells. This type of application is only feasible using collinear pulses since it would be difficult to cross several beams and detect signals using the phase matching scheme in highly scattering samples.

(219) VCSEL Oxygen Spectroscopy for Structural Analysis of Pharmaceutical Tablets
Tomas Svensson1, Mats Andersson1, Jonas Johansson1, Sune Svanberg1, Stefan Andersson-Engels1, Staffan Folestad2; 1Dept. of Physics, Lund University, Sweden; 2Astra Zeneca R&D, Mölndal, Sweden
Techniques for characterization of highly light scattering pharmaceutical solids (e.g. tablets) are of great interest to the pharmaceutical industry. Non-destructive and fast techniques are of particular interest, especially due to the growing importance of process monitoring. This work deals with the study of tablet structure and porosity by employing high resolution diode laser oxygen spectroscopy. The use of this technique for detection of gases dispersed within highly scattering materials is referred to as gas in scattering media absorption spectroscopy (GASMAS). The technological key is the contrast between narrow gas phase absorption and broadband bulk absorption. We use the optical absorption of molecular oxygen, located around 760 nm. Very recently, we have constructed a compact and simple system based on wavelength modulation spectroscopy (WMS). We use VCSEL diode laser technology, PN photodiodes and coherent sampling and are now able producing good data in about 1 second. The system exhibit excellent absorption linearity and reproducibility. We show that the observed WMS oxygen signal is highly sensitive to differences in tablet compression and granule particle size. We have also studied gas re-invasion after having stored our samples in a nitrogen environment, and are able to resolve diffusion processes occurring on a second timescale. Our results are correlated with relevant techniques such as mercury porosimetry. We also perform time-of-flight spectroscopy to determine actual photon pathlengths. The average pathlength for a 3 mm thick tablet is on the order of 100 mm, and our WMS oxygen signal corresponds to the absorption of 5-60 mm pathlength through ambient air (depending on compression and particle size). In conclusion, a highly compact system for on-line porosity determination on a second scale is presented.

(220) Determination of Mercury Utilizing Cold Vapor UV Photoreduction with In-Atomizer Trapping
Jillian Lennartz1, Jeremy Madden1, Neil Fitzgerald1; 1Marist College
The determination of mercury in environmental samples is typically accomplished by vapor generation using a chemical reductant prior to introduction to atomic spectrometry. Although these methods are low cost and achieve low detection limits, they usually require the fresh preparation of a chemical reductant (e.g. sodium borohydride), relatively large volume gas liquid separators due to frothing and droplet formation, and the use of significant amounts of chemicals with subsequent generation of waste. Alternative methods, based of total combustion of samples to generate mercury vapor, overcome many of these problems and require no sample preparation while maintaining good detection limits, however, these methods necessitate the purchase of a dedicated instrument. Recently we have investigated a method for the determination of mercury utilizing cold vapor generation via UV photoreduction. In this method, mercury vapor is generated by UV irradiation of a sample in the presence of a low molecular weight organic acid in lieu of a chemical reductant. Detection of the mercury is achieved using a conventional Graphite Furnace Atomic Absorption Spectrometer after in-situ trapping onto a palladium coated graphite furnace. This method can be considered a ‘greener’ technique due to a reduction in chemicals used and can be applied relatively easily in any laboratory with a graphite furnace instrument for very little additional cost. The system significantly improved the detection limit compared to a previously reported UV photoreduction system using a quartz tube atomization cell. Variables were optimized individually and gave a detection limit of 0.12 µg L-1 (3s) with a precision of 9.0% relative standard deviation for a 20 µg L-1 mercury standard. Environmental samples were used to validate the method.

(221) SPE and Cd in Urine Determination using ICP-AES
Kathryn Pharr1, Brad Jones1; 1Wake Forest University
A new method for determining cadmium in urine samples using ICP-AES has been explored. The amount of Cd in urine samples is near the limit of detection. Therefore, sample preparation was necessary. The samples were concentrated using a solid phase extraction (SPE) method. First, the solid phase disk was washed with 3M nitric acid and rinsed with distilled, deionized water. Then the disk was chelated with 2M NH4OH and rinsed again with DDI water. Next, 100 mL of the sample was washed through. The Cd chelated to the disk and the rest of the matrix flushed through the system. Another addition of 3M HNO3 to the disk resulted in Cd being eluted. The product was then determined using a standards with the ICP-AES. To ensure reproducibility, Bi was used as an internal standard before the SPE procedure. The LOD for standards for the Cd 226.502 nm was 0.673 ppb.

(222) Theoretical and Experimental Investigation of Laser Analytical Spectroscopy of Noble Metals(Au,Pt,Ag) by Method of Resonance Laser Ionization Spectroscopy
Akmat Khalmanov1, Samarkand State University, The Laboratory of Laser Analytical Spectroscopy of Noble Metals (Au, Pt, Ag) by Method of Resonance Laser Ionization Spectroscopy Akmat Toskhatovitch Khamanov1, Samarkand State University 703004, 15 Univ.Blvd, Samarkand Abstract At present work we have proposed a new effective stepwise excitation schemes for gold (Au), platinum (Pt) and silver (Ag) atoms and have experimentaly studied with resonance laser ionization was also studied. Two types of atomizers, for example rod-flame and graphite furnace were applied for investigations. Maximum ionization signals of Au atoms were observed for principal quantum numbers n=8 and n=9. In the case for Ag atoms, the wavelengths 272.0 nm and 282.0 nm from 5p states have shown two strong auto-ionization states. It is observed that the increase in the selective ionization signal is several order higher than one stepwise excitation. Analytical potentiality of laser-enhanced ionization (LEI) spectrometry is demonstrated by determining gold, platinum and silver content in standard water solutions. The low limits of detection for Au,Pt and Ag were 5pg/mL, 50pg/mL and 0.2pg/mL, respectively, in the graphite furnace. Theoretical calculations were performed for Au,Pt and Ag atoms. There is a good agreement between theoretical and experimental results for this atomizers.
The beta-amyloid peptide is a major component of senile plaques associated with Alzheimer's disease. The peptide is intrinsically disordered in its monomeric form, while larger aggregates adopt a secondary sheet structure. Several small molecules have been identified that inhibit this conformation change. Spectroscopic evidence, including circular dichroism and UV resonance Raman, indicate that the peptide undergoes a small shift in secondary structure in the presence of these small molecules. However, the nature of this change is obscured somewhat by the highly overlapped nature of the spectral signatures for the various geometric constraints imposed by each secondary structure. Thus, we are investigating the use of chemometric methods, which are ideal for resolving overlapping spectral components in multivariate data to resolve and identify the spectral signatures associated with small molecule induced conformation changes.

(225) Determination of Urinary Iodine by Inductively Coupled Plasma Mass Spectrometry

Amina Ali, Rabaa Al-Kandari; 1Kuwait Institute for Scientific Research, Kuwait

Urinary iodine is an essential element which is utilized by the thyroid gland for the biosynthesis of the thyroid hormones. These hormones strongly influence an extended range of biochemical reactions. Immune defense and antibody production depend on reliable thyroid function. Iodine is obtained only through the diet and is mainly absorbed by the gastrointestinal tract as the inorganic anion, iodide. The status of iodine nutrition for any population is determined by measurements of iodine concentration in the urine, and that equilibrium is established between the most ingested iodine, such as sodium or potassium iodide, is excreted in the urine, and that equilibrium is established between dietary iodine intake and UI excretion. Inductively coupled plasma mass spectrometry (ICP-OES) was chosen for UI determination because of its highly sensitive and rapid screening analytical technique that requires minimal sample preparation and manipulation, with low limits of detection, and reliable, precise results. Results were found to be in accordance with World Health Organization (WHO) criteria; i.e.; greater than 100µg/l which is considered normal. Not more than 7% of the population had UI less than 50µg/l which is considered moderate. Only one sewer case with a UI of less than 10µg/l was observed.

(227) Structure Characterization of Human Surfactant Protein C Mutants Using Infrared Spectroscopy and 2D Correlation Analysis

Yu Zhu1, Tharanga Diyunugala1, John E Baatz2, Richard A Dluhy1; 1Univ of Georgia, Chemistry Dept.; 2Med Univ S Carolina, Dept Pediat

Surfactant protein C (SP-C) is a small (4.2KDa) unique hydrophobic protein presenting in pulmonary surfactant and has been shown to be important for normal lung breathing functionalities, such as reducing surfactant potential, promoting adsorption, spreading and stability of the lipid lining in lung. Amyloid fibril formation of mature SP-C has been detected under pathological conditions and is believed to contribute to the failure in proper lung functioning. The molecular structure of mature SP-C consists of 1) two palmitoylated Cysteine residues surrounded by two Prolines at the N-terminus, 2) a positively charged Lys-Arg pair, 3) a very hydrophobic poly-valine alpha-helix segment, and 4) a heptapeptide C-terminus. The poly-valine segment is metastable and has an intrinsic tendency to form beta-sheet. Palmitoylation at the N-terminus of mature SP-C appears to stabilize the alpha-helix from aggregating into beta-sheets. [1] Work done previously by our group revealed a pH-dependent mechanism of amyloid fibril formation of deacylated bovine SP-C (dSP-C). [2] Further investigations on a series mutants of the deacylated human SP-C (dhSP-C) were carried on using infrared spectroscopy (IR) combined with 2D IR correlation analyses. Recombinants of dhSP-C at the N-terminus (C5S/C6S, K11Q/R11Q) and within the poly-valine segment (V21P) respectively showed distinctive secondary structure changes in response to pH titration. Compared to the wild type dhSP-C, which showed a similar alpha to beta conformational change with increasing pH as reported previously [2], mutagenesis at the N-terminus resulted in increasing of beta-conformations, whereas mutagenesis within the poly-valine segment resulted in increasing of random coils. Model-based 2D analysis developed in our lab [3, 4] unambiguously revealed the rate changes in intensity of each conformation. The results indicated that the unfolding proceeds from the N-terminus to the C-terminus and the poly-valine segment is essential for a stable hydrophobic alpha-helix structure.
conservation science. The second group of students trains to be conservators; their background can be in the humanities or the sciences and engineering. These students undertake scientific research projects in the second year of their two-year program. Students in this group must choose one of the treatment streams: conservation of paintings, artifacts, or paper. XRF has been used for in situ pigment analysis of paints in paintings and metals in archaeological objects have been identified. Identification of some materials proved more difficult for example the identification of silver in old photographs. Using FTIR-ATR, students have analysed varnishes, pigments and grounds in paintings, surface coatings on paper, and ancient ceramic objects and have monitored the degradation of objects such as a contemporary latex sculpture. Conservation treatments have been evaluated, for example by analyzing the leached materials removed during the aqueous cleaning of contemporary paintings.

(229) Extraction of Polycyclic Aromatic Hydrocarbons from Water Samples with Gold Nanoparticles

Huiyong Wang1, Andres Campiglia1; 1University of Central Florida

The fact that several polycyclic aromatic hydrocarbons (PAH) can induce cancer has been documented in numerous epidemiological studies. Their omnipresence in the environment results from incomplete combustion of organic materials involved in countless natural processes or human activities. Because a primary route of potential human exposure to PAH is the ingestion of contaminated drinking water, the Environmental Protection Agency (EPA) has included sixteen PAH in its priority pollutants list and recommends their routine monitoring in water samples taken from municipal wells. Reported methods for PAH extraction include liquid-liquid and solid-phase extraction, solid-phase micro-extraction, supercritical-fluid extraction, microwave-assisted extraction and accelerated solvent extraction. The driving force is to achieve sample clean-up and PAH pre-concentration via simple, rapid and inexpensive experimental procedures. The approach presented here takes advantage of the strong affinity between PAH and gold nanoparticles (Au NPs). Our literature search reveals no reports on the use of Au NPs for the purpose at hand. We demonstrate efficient PAH extraction - i.e. above 90% - for the sixteen EPA-PAH via an environmentally friendly procedure without the need of sophisticated instrumentation. 0.5 micro-liters of organic solvent (1-pentanethiol) per water sample are sufficient to release the extracted PAH from the surface of Au NPs. This new extraction method is interfaced here to Laser-Excited Time-Resolved Shpol’skii Spectroscopy to demonstrate the ability of determining EPA-PAH at the concentrations found in tap water samples.

(230) Analysis of Condensed-Phase Aerosols Using Infrared Photothermal Spectroscopy with Optical Beam Deflection (Mirage Effects)

Oluwatosin O Dada1, Stephen E Bialkowski1; 1Utah State University

Analysis of atmospheric aerosols tends to be complex and difficult. The potential of mid-infrared photothermal spectroscopy for the analysis of aerosols is demonstrated. Ammonium Nitrate aerosols generated in the laboratory were deposited on a flat surface substrate by the use of Micro-Orifice Uniform Deposits Impactor (MOUDI). Photothermal spectroscopy using optical beam deflection (Mirage effect) was used to analyze the deposited aerosols. Mirage effects from aerosols was measured by using pulsed infrared laser light to heat up aerosols collected on plates, and observing the deflection of light as it passes near the heated surface. Concentration measurement from the impactor was used as standards for the photothermal measurements. Photothermal deflection signals of deposited aerosols show a linear relationship with aerosols concentrations. Finite element analysis modeling was used to investigate the subsequent temperature change when absorption and relaxation of electromagnetic radiation occurs. The model proves useful in understanding the profile of the thermal propagation through the aerosols into the surrounding air.

(231) First Test Strip Approved for Regulatory Testing

Ivars Jaunakais1, Maris Jaunakais2, Howard Ray1; 1Industrial Test Systems, Inc.; 2MJ Analytical Consulting

Chlorine in the public drinking water supply must be monitored carefully. Of several methods used to monitor Free Chlorine, N,N-Diethyl-p-phenylenediamine (DPD) is commonly used. This method can be time consuming and technique dependent. Another method is available. The method uses a test strip impregnated with 3, 3'5, 5' Tetramethylbenzidine (TMB). The method requires a 20 second dip in a 50ml water sample. After a 20 second wait time the concentration of free chlorine is determined by comparison to a calibrated, pre-printed color chart. After extensive random and blinded studies the method is shown to have acceptable false positive and false negative rates, method sensitivity, and correlation to AWWA Standard Method 4500-CI G. The method has false positive and false negative rates of 0-1%. Method sensitivity is > 0.1ppm free chlorine, with a stated method range of 0ppm to about 2.0ppm. Correlation with AWWA standard method 4500-CI-G is greater than 97% (R2 = 0.9736).In a rulemaking at 40 CFR Part 122, as printed in the Federal Register (Vol.72, No. 47, Monday, March 12, 2007, p.11204) the USEPA approved ITS Method D99-003 for use in regulatory monitoring. With the printing in the Federal Register the patented Industrial Test Systems, Inc. Free Chlorine Test Strip becomes the first test strip method approved for use in regulatory monitoring.

(232) Fluorimetric Determination of Enoxacin Using Tb Composite Nanoparticles

Mohammad Mainul Karing1, Sang Hak Lee1; 1Dept of Chemistry, Kyungpook National University

Enoxacin (ENX), the second generation drug of the quinolone antibiotics is used in the treatment of systemic infections including urinary tract, respiratory, gastrointestinal and skin infections. It kills bacteria through inhibiting cell DNA-gyrase and prohibiting DNA replication. Fluorimetric method is useful for the determination of various drugs.Determination of enoxacin was reported in several articles. In our study, terbium-acetyl acetone (acac) composite nanoparticles have been prepared under vigorous ultrasonic radiation. The nanoparticles synthesized are water-soluble, stable and have extremely narrow emission bands. They were used as fluorogenic probe for the determination of enoxacin. The fluorescence intensity of Tb3+ in composite nanoparticles is synergistically enhanced by the addiction of enoxacin. The observed synergism could be due to the energy transfer from the enoxacin to Tb3+acac composites. The enhancement is directly proportional to concentration of enoxacin concentrations. Under the optimum experimental conditions, the linear working curve was obtained over the concentration range of 1×10-4-2×10-6 M with a correlation coefficient of 0.9987. The detection limit is 2.5×10-7 M. The relative standard deviation is 1.75% for 1×10-5  M (n=10). The proposed method has been applied to the determination of enoxacin in pharmaceutical tablet. The method reported here is interference free.

(233) Interaction of Lactoferrin B with Membranes: A Physico-Chemical Approach

Mariolaine Arsenault1, Sarah Bedard1, Maxime Boulet-Audet1, Michele Auger1, Michel Pezolet1; 1CERSIM/CREFSIP, Chemistry dep., University

The disruption of the phosphatidylglycerol (PG) membrane has been followed by the release of fluorescent probes encapsulated in
Difficulties due to relatively low concentrations in most human preparations were also studied. Analytical approaches using IRMS delta values among different lots and among materials produced at different locations and manufacturers. Carbon, nitrogen, hydrogen, binding to the different model membranes. 

The increasing sophistication and quality of these products demand advanced analytical tools to combat the problem. Isotope testing. The order parameter of the amide band. The order parameter of the amide was calculated from ATR IR results. The molecular orientation of the peptide carbonyl groups depends on the surface pressure as detected from the amide I band. The order parameter of the amide groups indicates that LfcinB interacts differently with the DPPG monolayer depending whether the peptide is inserted in the monolayer or only adsorbed at the monolayer surface. Results obtained by IR spectroscopy and solid state NMR on large monolayer or only adsorbed at the monolayer surface. 

Adsorption studies provide evidences that the peptide could insert into the DPPG monolayer only below 30mN/m. Images obtained by atomic force microscopy and Brewster angle microscopy also shows a different organisation below and over 20mN/m. The molecular orientation of the phospholipids chains and LfcinB were calculated from ATR IR results. The molecular orientation of the peptide carbonyl groups depends on the surface pressure as detected from the amide I band. The order parameter of the amide groups indicates that LfcinB interacts differently with the DPPG monolayer depending whether the peptide is inserted in the monolayer or only adsorbed at the monolayer surface. Results obtained by IR spectroscopy and solid state NMR on large unilamellar vesicles of DOPG, POPG and DPPG also indicates different behavior of the lipid bilayer in the presence of the peptide (10:1 lipid/peptide ratio) and a variation of the secondary structure from disordered to fβ-sheet of the antimicrobial peptide upon binding to the different model membranes.

(234) Drug Fingerprinting Using Isotope Ratio Mass Spectrometry: Sourcing of Active Pharmaceutical Ingredients (APIs)

Jonathan Litzen1, Thomas Brueggemeyer1; 1U.S. Food & Drug Administration

Counterfeit or diverted finished dosage forms and active pharmaceutical ingredients (APIs) present a challenge to both law enforcement and to laboratories performing drug authenticity testing. The increasing sophistication and quality of these products demand advanced analytical tools to combat the problem. Isotope ratio mass spectrometry (IRMS) is a potentially powerful weapon in efforts to source APIs and attribute fake products to specific criminal operations. Unlike current analytical methods which establish the identifications of particular APIs and related substances, isotopic fingerprinting can potentially answer the question of whether two APIs came from the same source. IRMS was used to examine various known APIs to study variations in delta values among different lots and among materials produced at different locations and manufacturers. Carbon, nitrogen, hydrogen, and oxygen delta values were evaluated and a comparison of their specificity will be presented. Data handling and aspects of sample preparation were also studied. Analytical approaches using IRMS to test finished dosage forms will be discussed.

(235) Determination of Titanium in High-Calcium Matrices Using Multi-Component Spectrum Fitting with ICP-OES

Matthew Hanley1, Steve Eckdahl1, John Butz1; 1Mayo Clinic

Analysis of titanium in biological samples presents numerous difficulties due to relatively low concentrations in most human specimens and to significant analytical problems on most potential platforms. Atomic Absorption methods are plagued by poor sensitivity and rapid degradation of graphite rods, ICP-MS exhibits multiple polyatomic and isobaric interferences and Neutron Activation is extremely costly and time consuming. For these reasons ICP-OES is a favored method for analysis, but even this exhibits significant problems related to background peak broadening. Of particular difficulty is quantifying titanium in high calcium matrices such as digested bone due to interference from a minor calcium peak at 335.036 nm which can engulf the entire titanium analytical region. Clinically, this is of interest due to use of titanium as an alloy component in implants and artificial joints. Titanium bone, serum and fluid measurements have been used as measures of implant leaching and catastrophic wear. Methods to physically remove calcium through chelation and titanium complexation are time-consuming and require considerable effort. A direct analysis method is desirable over significant specimen work-up or filtration for reasons of safety and time savings. Therefore, a mathematical correction for the calcium background was developed using Multicomponent Spectrum Fitting (MSF) in conjunction with ICP-OES and tested against a Zeeman correction Graphite Furnace (ZGFAA) method with an extended pre-analytical char to volatilize calcium. These methods were applied to quantify titanium in aqueous and biological matrices of high calcium concentration. Values collected using the correction-based methods were compared to baseline values obtained using calcium-free matrix with a routine ICP-OES method along with comparison to NIST certified values and in-house controls. The MSF calcium correction showed superior selectivity and peak resolution compared to the baseline ICP-OES method (detection limits improved to 20 ng/mL from over 200 ng/mL without correction) as well as better detection limits and faster analysis than the ZGFAA method. Successful recovery of titanium in high (~30,000 mg/L) calcium matrices using the MSF ICP-OES methodology as well as good agreement with expected values shows that use of this correction is a simple and effective way to eliminate calcium background interferences in analysis of titanium.

(236) Analysis of Double-Strand Helix of Linear Polylethyleneimine by Infrared Multiple-Angle Incidence Resolution Spectrometry

Takeshi Hasegawa1, Hiroyuki Kakuda1, Tetsuo Okada1; 1Tokyo Institute of Technology; 2JST PRESTO

Infrared multiple-angle incidence resolution spectrometry (IR MAIRS) has been employed to analyze structure of double-strand helix in a thin layer of linear polyethyleneimine (LPEI). LPEI is known to form a double-strand helix in crystal when it is dehydrated, which was revealed by X-ray diffraction technique. We have prepared a dried thin film of LPEI by dipping method from an aqueous solution of LPEI. IR MAIRS is powerful to reveal anisotropic structure in thin films. It yields a set of two (IP and OP) spectra that correspond to the conventional transmission and reflection-absorption (RA) spectra, but an important point is that the MAIRS spectra are both from an identical sample deposited on an infrared transparent substrate. The conventional technique requires different substrates for the transmission and RA techniques, which may have different influences on structure of the two thin layers. In our present case, the aqueous LPEI solution is repelled by a metallic surface, which means that the RA spectrometry cannot be employed to analysis of the dipped thin film. In addition, IR MAIRS has a benefit of infrared spectroscopy that anisotropic structure can be discussed even if the layer has unorganized molecular arrangement, which is not suitable for X-ray analysis. Before the MAIRS analysis, temperature-induced IR spectra of the dipped LPEI film was subjected to alternative least squares (ALS) analysis. The ALS analysis clearly revealed that a dehydrated LPEI thin film comprises two kinds of ordered...
molecular aggregates and a disordered part. IR MAIRS analysis was also readily performed for another aged thin film, a surprisingly large anisotropic structure was found in the thin film. In particular, the methyl wagging (1247 cm-1) and the methylene twisting (1281 cm-1) vibrations exhibited a remarkable MAIRS dichroism, which strongly suggests that the double-strand helices are highly oriented probably because of the aggregation forces among the helices. Of another great interest was the N-H stretching vibration band, which was split at 3222 and 3212 cm-1 in the IP and OP spectra, respectively. This is understandable if these bands are due to the Davydov splitting after the robust structure formation of the double-strand helix.

(237) Attenuated Total Reflectance Infrared Spectroscopy (ATR-FTIR): a Quantitative Approach for Kidney Stone Analysis
Heather Gulley-Stahl1, Jenn Haas1, Andrew Evan2; 1Miami University; 2Indiana University School of Medicine
Urolithiasis, or kidney stone disease, is common throughout the world and affects approximately 10% of the US population. Calcium oxalate monohydrate (COM) is the most frequent constituent in urinary stones appearing about 50% of the time. Hydroxyapatite (HAP) is the second most prevalent appearing in about 12% of stones. Current methods for quantifying kidney stone components are lacking. While urolithiasis treatment depends on stone composition, approximately 40% of stones are misdiagnosed due to qualitative analyses currently used. Previous studies have used FTIR as a quantitative approach to kidney stone analysis, but require extensive sample preparation. This research has investigated the use of ATR which requires significantly reduced sample preparation while at the same time providing high sensitivity. Since most stones contain at least two different constituents, the samples were analyzed as binary ratios ranging from 0 to 100% HAP in COM. Calibration curves were constructed and analyzed using a linear fit. The limits of detection using this technique are 0.0867% COM and 0.2634% HAP. 1.) L. Estepa and M. Daudon, Biospectroscopy 3, 347-369 (1997). 2.) F. Cohen-Solal, B. Dabrowsky, J. Boulou, B. Lacour and M. Daudon, Appl. Spec. 58, 671-789 (2004). L. Estepa, P. Levillain, B. Lacour and M. Daudon, Clin. Chim. Acta 298, 1-11 (2000).

(238) Spatially Resolved FT-IR Microspectroscopy Of The Nutritional Status Of Stream Algae
David L. Wetzel1, Justin N. Murdock2, Walter Dodds2; 1Microbeams, Mol. Spec. Lab., Kansas State University; 2Div. Of Biology, Kansas State University
FT-IR microspectroscopy can be used to localize nutritional differences in algal mats at the spatial resolution of individual cells, allowing the illumination of species specific responses to nutrient additions in natural, mixed assemblages. Algae growing on stream bottoms develop in a three-dimensional matrix (mats) consisting of interacting species which respond rapidly, and uniquely, to changes in environmental nutrient conditions. Nutrient pollution can significantly alter the structure and physiology of algal mats as different species can dominate depending on nutrient availability. These changes can further affect whole ecosystem dynamics such as dissolved oxygen availability, toxin production, and nutritional value of the mat for grazers. In the past, FT-IR has been used to analyze the nutritional status of stream algal mats, but has been limited to examining homogenized, multispecies samples. Simultaneous spatially resolved image analysis of levels indicative of protein, lipid, carbohydrate, and phosphodiester provide a multidimensional response pattern to perturbations of the normal nutritive environment. Data are presented to demonstrate individual algal species’ responses to manipulations of ambient nitrogen and phosphorus concentrations.

(239) Application of ATR FT-MIR Spectroscopy for Rapid Identification of API in Pharmaceutical Drug Products
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POSTER Identification of Active Pharmaceutical Ingredients (API) in a drug product has become increasingly important in pharmaceutical industry at various phases of clinical trials and marketed products especially for receiving laboratories. A rapid analytical technique for the identification of drug products is of utmost importance. In this work the feasibility of Attenuated Total Reflectance Fourier Transform Mid-Infrared Spectroscopy (ATR-FTMIR) to identify the API in a solid and parenteral drug formulation is investigated. Historically, MIR spectroscopy of solids was done by KBr dispersions and analyzing either by KBr pellet or Diffuse Reflectance techniques. The KBr pellet or diffuse reflectance method involves a tedious and careful sample preparation and long purge times. Where as ATR analysis is rapid and the samples are analyzed in their native state with little or no sample preparation. In the case of parenteral liquid samples, a drop of the liquid is placed on the internal reflection element (IRE) and allowed to evaporate. For solids samples, tablet cores can either be placed directly on the IRE or a small amount of the ground tablet can be placed on the IRE with added pressure using a pressure device to establish good contact. Presence of unique API bands in the drug product demonstrates specificity of API in the drug product. In this work ATR spectra were shown to be equivalent to the KBr pellet preparation or KBr dispersion spectra. Three different dosage forms of the drug product was evaluated, namely, tablets, capsules and parenteral dosage form. Comparison of KBr pellet or KBr dispersion spectra and Ge-ATR spectra for various samples demonstrated to be equivalent. Therefore, ATR technique is rapid, with little or no sample preparation, reproducible, easily transferable and reliable technique for the identification of pharmaceutical products.

(240) Kinetics in a Levitated Drop Microreactor and Related Myeloperoxidase Behavior
Alexander Scheeling1, Christopher Field1, Zakiah Pierre1; 1University of Illinois at Urbana-Champaign
Reactor walls can act as recombination catalysts for free radicals. A problem under some circumstances for milliliter and larger reactors, walls can have a profoundly perturbing effect on reaction kinetics in microfluidic systems. We approach the problem of studying kinetics catalyzed by nanogram and smaller quantities of enzymes by carrying out reactions in ultrasonically-levitated drops. Our initial focus is on the chemistry of myeloperoxidase as a source and sink of reactive oxygen species and a component of the immune system. We present the design and optimization of the drop levitator and diagnostic systems including optical absorption, chemiluminescence, fluorescence, and chronoamperometry. Characterization of drop mixing time as measured by chemiluminescence is shown, as is data on redox chemical kinetics as observed in a microliter drop. Related measurements using mass spectrometry to characterize suicide chlorination of myeloperoxidase are also discussed.

(241) Evanscent-Wave Cavity Ring-Down Spectroscopy for Enhanced Detection of Surface Binding Under Flow Injection Analysis Conditions
Freek Ariese1, Lineke van der Steen2, Jost B. Buijs3, Cees Gooijer4, Wim Ubachs5; 1Laser Centre Vrije Universiteit Amsterdam
The feasibility of liquid-phase evanescent-wave cavity ring-down spectroscopy (EW-CRDS) for surface-binding studies under flow-injection analysis (FIA) conditions is demonstrated. The EW-CRDS set-up consists of an anti-reflection coated Dove prism (with or without custom polishing of the total internal reflective (TIR))
surface) inside a linear cavity. A teflon spacer with an elliptical hole clamped on the surface of the prism acts as a 20-microliter sized flow cell, which is probed ca. 80 times by the 532-nm laser pulses. The baseline noise of this system is of the order of 10-4 absorbance units; the baseline remains stable over a prolonged time and the prism surface does not become contaminated during repeated injections of the reversibly adsorbing test dyes Crystal Violet (CV) and Direct Red 10 (DR10). At typical FIA or liquid chromatography (LC) flow rates, the system has sufficient specificity to discriminate between species with different surface affinities. For CV a much stronger decrease in ring-down time was observed than calculated based on its bulk concentration and the effective depth probed by the evanescent wave, indicating binding of this positively charged dye to the negatively charged prism surface. An enrichment factor of 60 was calculated for CV; for the poorly adsorbing dye DR10 it was 5. The extent of adsorption can be influenced by adjusting the flow rate or the eluent composition. For CV we find a detection limit of 3 micromolar for the unpolished surface; less binding occurs on the polished surface: LOD = 5 micromolar. The setup shows great promise for the development of a detection system for antigens binding to surface-linked antibodies.

(242) Identification of Impurities in Choline Hydroxide in Water by LC/MS
Lilia Rousseva2, Wayne Pritts1, Abbott Laboratories
Identification of Impurities in Choline Hydroxide in Water by LC/MS Lilia A. Rousseva, Wayne A. Pritts/Abbott Laboratories, Analytical Process Development, 1401 Sheridan Road, North Chicago, IL 60064-4000 Choline derivatives have been broadly used in the pharmaceutical and chemical industries. They have been used as a starting material or intermediate for drug compounds. The purpose of this study was to develop a LC/MS method for identification of impurities in choline hydroxide in water. Different analytical techniques have been evaluated and applied for testing of choline hydroxide in water, such as HPLC, IC (Ion Chromatography), and capillary electrophoresis (CE) with detection by refractive index (RI), conductivity and evaporative light scattering (ELSD). However, the technique of LC/MS is one of the most sensitive and accurate methods for detection and characterization of impurities. A 45% solution of choline hydroxide in water was obtained from several vendors. Two LC/MS systems with an electrospray ion source were used for identification and confirmation of choline hydroxide impurities. Columns with different selectivity and several chromatographic conditions were evaluated. Mass spectra were recorded by both a single quadrupole and quadrupole ion trap MS system. The ion source parameters were optimized to obtain better ionization of the impurities in choline hydroxide. For the ion trap, parameters were optimized for the fragmentation of the impurities. By using mass spectrometry for detection, impurities such as choline hydroxide dimer and choline hydroxide trimer, and ethylene glycol were detected in the choline hydroxide from different vendors. The obtained mass spectra and m/z (mass to charge) ratio confirmed the existence and the identity of these impurities. The results suggest that LC/MS is a sensitive and accurate technique for identification and confirmation of impurities present in choline hydroxide in water.

(243) Infrared Ablation/Ultraviolet Matrix-assisted Laser Desorption Ionization Mass Spectrometry
Fan Huang1, Kermit Murray1, Chemistry Dept, LSU
A study of two laser-matrix-assisted laser desorption ionization (MALDI) mass spectrometry is described. A tunable pulsed infrared (IR) optical parametric oscillator (OPO) laser system was set to directly irradiate the sample target to ablate particles, neutrals and ions. A pulsed 351 nm ultraviolet (UV) excimer laser that is 1.4 mm above and parallel to the sample surface acted as the post ablation ionization laser to break up the particles and create ions. The compound 2, 5-dihydroxybenzoic acid (DHB) was used as an IR/UV matrix, and mass spectra of peptides and protein molecular weight standards, such as bradykinin, bovine insulin, and cytochrome c were recorded with a linear time-of-flight (TOF) mass spectrometer. Under these conditions, two mass spectra were generated, an IR MALDI mass spectrum from the OPO and a UV laser generated spectrum generated by irradiating the IR laser generated plume. Several factors that can affect bradykinin ion yield were studied, such as delay time, IR laser fluence and UV laser fluence. The implications of the results of this two laser MALDI study will be discussed in relation to the mechanisms of IR laser ablation and UV and IR MALDI.

(244) High-throughput LDI MS Imaging Using a Tunable High Repetition Rate IR Laser
Mark Little1, Eli Margalith1, Kermit Murray2, Yohannes Rezemon2; 1Optek, Inc.; 2Louisiana State University
The recent commercial development of MALDI ion source tandem mass spectrometers has led to the demand for higher repetition rate lasers for high throughput applications such as off-line LCMS and tissue imaging. Although these applications can benefit from a high repetition rate laser, none is commercially available. IR lasers can directly ionize biomolecules, which eliminates matrix addition and solves problems associated with UV MALDI tissue imaging. The larger penetration depth of IR lasers over UV lasers can also benefit tissue imaging as material below the tissue surface can be ionized. Increased ablation over UV lasers makes IR lasers ideal for MALDESI and IM MALDI MS where a larger amount of material is free from the bulk sample deposit aids analysis. We are developing a high repetition rate tunable IR laser system based on optical parametric oscillator (OPO) technology. The system is selectively tunable from 2.85 to 3.45 micrometers depending on the optical materials used and generates pulse energies greater than 1 mJ over the entire tunable range. The ability to tune the laser wavelength allows signal optimization based on the absorption of the sample. The system is being tested on a custom-built reflectron mass spectrometer. An interface with an orthogonal extraction MALDI source using a fiber optic input coupling is also being developed. Data has been obtained with a prototype high repetition rate tunable IR laser system demonstrating intact ionization of small molecules as well as peptides and proteins with and without an added matrix. Ionization of analytes at different wavelengths shows a change in ion signal over a 300 nm range. Further testing will include tissue imaging experiments without matrix addition as well as demonstrating that IR ionization of samples without matrix addition is comparable to UV MALDI for a wide variety of molecular classes in the 0.1 to 6 kDa range. The final goal for the high repetition rate IR laser system will be the combination of simplified sample preparations through the elimination of matrix addition, greater ablation potential of IR lasers and atmospheric pressure ion sources to achieve high-throughput direct analysis of sample materials at ambient conditions.

(245) Ion Signal Temporal Profiles in Pulsed Direct Current Glow Discharge Mass Spectrometry: Effects of Sampling Distance, Power, and Pressure
Megan DeJesus1, James H. Barnes IV2, Fred L. King1, Cris L. Lewis1; 1West Virginia University; 2Los Alamos National Laboratory
Ion signal temporal profiles for a pulsed direct current glow discharge have been measured for both discharge and sputtered species using time time-of-flight mass spectrometry. The effects of sampling distance, pulse power, and discharge gas pressure on the profiles are examined independently as other parameters are held
constant. The temporal ion signal profiles presented here illustrate the differences between ions of discharge gas species and ions of sputtered atoms. The ion signals from discharge gas species drop to baseline intensities within 0.02 ms of discharge power termination, whereas the temporal profile for ionized sputtered atoms was found to maximize approximately 0.2 ms following discharge power termination due to an increase in Penning ionization. In addition to using time-gated acquisition, it is possible to further influence the ionization mechanisms within the plasma through the careful selection of plasma parameters; in doing so, one can maximize analytical signals while suppressing ion signals from interfering species. In this research, we conduct a comparative investigation of ion signal temporal profiles through the variation of discharge parameters to better refine the method and to gain a better understanding of the processes taking place in the discharge.

(246) Bioaerosol Ion Mobility Mass Spectrometry of Biological Agent Detection
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We are developing an on-line interface for MALDI of collected bioaerosols that is coupled to an ion mobility time of flight mass spectrometer. The detection of biological agents presents significant challenges for analytical instrument technology due to the need for rapid analysis coupled with the complex nature of potential sample contaminants. Biological warfare (BW) agents are typically dispersed as aerosol particles and therefore detection instrumentation must be fast, sensitive, and selective for positive detection with minimal false alarms. Furthermore, portable instruments that can function in harsh environments with minimal operator intervention are required. We are developing bioaerosol ion mobility mass spectrometry (BIMMS) for near real time detection and analysis of collected bioaerosols. Particles are collected on a target and prepared for BIMMS analysis. Ions are formed by 337 nm UV or 3 μm IR MALDI. Separation occurs in an ion mobility cell at 10 Torr helium buffer gas. An IR and UV transparent sapphire vacuum window is used for laser entry into the instrument and gold first-surface mirrors direct the beam into the IM cell. Laser desorbed ions drift for 20 cm in the mobility cell and then pass through a 0.5 mm orifice into a differentially pumped region before being extracted into a 20 cm orthogonal time-of-flight mass spectrometer for analysis. Initial studies are focused on the detection and identification of the biological warfare simulants Bacillus subtilis (BG) Bacillus thuringiensis (BT) and Erwinia herbicola (EH) against a background of dust, salt and pollen. Mass spectra of collected bacteria show distinct trend lines associated with different components of bacteria and complex mixtures with little interference. These particular fingerprints can be use for the detection of BW agents in near real-time.

(247) Controlling the Organization of Porphyrins on Surfaces using Nanolithography
Zorabel M. LeJeune1, Stephanie Daniels1, Erhong Hao1, Jie-Ren Li1, M. Graca H. Vicente1, Jayne C. Garno1; 1Louisiana State University.

The self-assembly of porphyrins is mediated by complex intermolecular interactions, such as pi-pi stacking between macrocycles or by the binding interactions between peripheral groups and surfaces. We are applying the tools of AFM characterization and nanolithography to investigate and control the assembly of porphyrins on various surfaces. Our goal is to construct nanoscale test platforms for measurements of surface properties to gain insight into structure/function relationships. Porphyrins and metalloporphyrins are practical materials for developing molecular electronics due to oxidative, thermal and chemical stability; however, the limited solubility in most solvents poses problems for preparing regular and organized thin films and nanostructures. Deposition methods and the nature of organic solvents influence the formation of porphyrin clusters on surfaces. For example, at high concentration porphyrins link together to form stacks. We have overcome these difficulties by controlling the drying parameters and by using mixtures of solvents to achieve desired surface coverage during self-assembly. The basic porphyrin structures used for these studies are tetra-substituted porphyrins containing pyridyl and phenyl groups. Modification of the macrocycle such as addition of peripheral or tethering groups on various positions on the molecule and chelation of various metals affects the structure and properties of the porphyrins. We will present results with porphyrin nanostructures which were prepared using scanning probe lithography (nanoshaving and nanografting) and particle lithography approaches. Nanoshaving can be applied to measure the thickness of molecular layers by referencing uncovered areas of the substrate as a baseline for height measurements. Nanografting can be used to determine the thickness of porphyrin layers by comparing the well-known heights of n-alkanethiol nanostructures inscribed within a matrix layer of porphyrins. Characterizations of arrays of designed porphyrin nanostructures with force modulation imaging and current-sensing AFM provide insight for the properties, molecular orientation and assembly of porphyrins.

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The study deals with the modeling solubility of fullerene C60 in organic solvents using QSAR/QSPR tool. A Genetic Algorithm and multiple regression analysis (MLRA) were applied to select the descriptors and to generate the correlation models. As additional descriptors for QSAR/QSPR analysis the parameters from quantum-chemical calculations at DFT (B3LYP/ LANL2DZ) level have been applied. The models were evaluated according to their statistical values i.e. so-called model performances (r, R2, s, F, Q2) after splitting sets of organic solvents to training and test sets. The GA-MLRA approach with application of quantum-chemical calculations showed good results in this study, which allows to build simple, interpretable and transparent models that can be used for future predictions of C60 solubility in organic solvents.

(249) Thermal Cracking Studies by Design of a Pilot Plant
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Thermal cracking of hydrocarbons from ethane up to gasoil is one of the most important processes for production of olefins, the basic feedstock for the petrochemical industry. The key to successful process control in the manufacture of ethylene, is temperature control of thermal cracking furnaces. This paper studies a computerized thermal cracking pilot plant and its capabilities for experimental activities. A computer program was developed for the monitoring and control purposes. The effect of temperature on ethylene yield is investigated by simulation and experimental studies. The results show good agreement between Comparison of these results with industrial data, show that, they have the same trends. Coil Outlet Temperature (COT) is an important parameter affecting yield of ethylene production and therefore it should be controlled. Since furnaces are the first step in the production
process, disturbances that occur due to the furnace operation will affect the entire process. COT is controlled by measuring the cracked gas temperature in the coil outlet and manipulating the heat input to the furnace. This loop is one of the most important loops in the control of thermal cracking furnaces. Fluctuations on COT is caused by the coke deposited on the COT measuring thermocouple. Furnace temperature tracks the furnace set point. Increasing the oscillation at higher set points, are due to nonlinear plant dynamic and using constant controller tunings. Based on the kinetic model a computer program for simulating the plant is developed. The software program is used to investigate the effects of temperature on the product yields. Simulation results indicate that increasing COT, increases the ethylene yield. Simulation results was tested experimentally by the pilot. Comparison of simulation, experimental and industrial results show, those have the same trends. The discrepancies between industrial and simulation results refer to the reactor configuration and the discrepancies between simulation and experimental results are due to the nonlinear and unknown furnace dynamic model, and some measurement errors in experiments.

(250) Surface-Enhanced Raman Spectroscopy Evidence for Hyaluronic Acid Polymer Entanglement at Nanoliter Volumes
Karen A. Esmonde-White1, Gurjit S. Mandair2, Michael D. Morris*1, University of Michigan, Biomedical Engin.; 2University of Michigan, Chemistry
Surface enhanced Raman spectroscopy (SERS) is used to determine the entanglement threshold of the viscoelastic biopolymer, hyaluronic acid (HA), which is known to play a crucial role in the normal function of vitreous humor and the lubrication of synovial joint space. By using droplet deposition techniques, we could apply nanoliter volumes of dilute, overlapped, and entangled HA solutions onto gold-coated SERS substrates. SERS spectra of the dried deposits were collected using a 785 nm laser. These measurements were correlated with specific viscosity measurements obtained from bulk HA solutions at clinically relevant concentrations (0.25-3 mg/mL) and volumes (0.5-1 mL). The effects of HA viscosity modifiers, such as sodium chloride and molecular weight on polymer chain entanglement were also investigated. Our studies showed that changes to the HA 899 cm-1 and 945 cm-1 band intensities could be correlated with two transitions in the polymer concentration regimes: from dilute to overlapped (0.5-1 mg/mL) and overlapped to entangled (~3.5 mg/mL). The HA 899 cm-1 and 945 cm-1 band intensities appeared higher at low concentrations, owing to more efficient collection of Raman scattering from thinner, less entangled HA deposits. This dilution effect indicated that the SERS spectrum is sensitive to the elongation or shrinkage of the HA polymer chain. These results were supported by light microscopy studies in which there was a positive relationship between concentric ring shape and HA concentration. In conclusion, we show that SERS is an invaluable technique for examining the entanglement properties of this weakly scattering biopolymer.

(251) New Tunable Notch Filter for Resonant Raman Spectroscopy
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1Photon etc. Inc.
Resonance Raman spectroscopy is a powerful tool for the characterization and investigation of the vibrational and electronic properties of a wide range of systems. While the excitation wavelength matches an electronic transition of the studied system, a selective enhancement of its Raman signal by several orders of magnitude is achieved. Thus, RRS has been used as a major probe in various fields of biology, chemistry and physics. We have developed new equipment for Resonance Raman spectroscopy studies: tunable notch filters based on volume Bragg gratings. For this application, we used narrow bandwidth diffracting elements with high diffraction efficiencies and out-of-band transmission higher than 90%. The notch filter is continuously tunable over 300 nm and exhibits a bandwidth below 10 cm-1, one order of magnitude narrower than notch filters on the market. The laser attenuation of the filter is close to 104. Designed to operate in conjunction with a commercial tunable Ti:Sapphire, the Bragg tunable filter allowed the measurement of Raman signal below 50 cm-1 with a single monochromator spectrometer. This new promising device should allow researchers to explore new areas in the field of Raman spectroscopy. In this paper, we will first present the characteristics and performances of these Bragg tunable filters. Their integration in our micro-Raman experiment will be shown. We will then discuss RRS results obtained with this set-up on different systems such as carbon nanotubes.

(252) Plasmonic Tip Enhanced Raman Scattering of Strained Silicon with Single and Multiple Probes
Aaron Lewis1, Rimma Dekhter2, Hesham Taha2; 1Nanonic Imaging Ltd.
Raman spectroscopy is an effective tool for the identification and analysis of molecular components of complex materials. The spatial resolution of Raman spectroscopy is limited by the wavelength of the light. One approach to overcome this drawback is Surface Enhanced Raman Scattering (SERS). This technique uses nanometric interactions between metal structures and surfaces to effect enhancement of the Raman signals. An important mechanism for enhancement originates from an electrostatic lensing effect due to the excitation of localized surface plasmon resonances. This is accomplished in a scanned probe microscopy context by employing an ultra-sharp metalized tip that is brought into a focused laser spot on the sample surface thereby enhancing the Raman signal. In this technique also known as Tip Enhanced Raman Scattering (TERS) the electrical field is locally enhanced near the sharp metalized tip. Rastering the sample should then allow for Raman imaging with nanometric resolution. Experimentally this imposes certain difficult constraints both in terms of the polarization of the light and the nature of the scanned probe imaging platform that is required. Our work demonstrates that a combination of a unique SPM platform (Nanronics MultiViev System) with a Confocal Raman microscope (Renishaw Ltd) and a patented cantilevered glass metalized probe allows for high resolution topographical data with nanometric online Raman spectral imaging without any silicon probe background. This abstract will focus on selectively imaging a thin film of strained silicon on silicon. These developments which have considerable significance to semiconductor device analysis have shown strong with enhancement factors of ∼ 104 with specialized single gold particle cantilevered glass probes developed by our group [Inna Barsegova, et al, “Controlled Fabrication Of Silver Or Gold Nanoparticle Atomic Force Probes: Enhancement Of Second Harmonic Generation,” Applied Physics Letters 81, 3461-63 (2002) 1] Within this context it will be shown that multiple probe scanned probe microscopes have considerable potential in such tip enhanced applications.

(253) SERS on Mirror Sandwich Substrates
George Chumanov1, Mark Kinnan1; 1Clemson University
Surface-enhanced Raman scattering (SERS) is a powerful analytical tool used for structure-functional characterization and detection of a variety of small and large molecules. SERS originates from molecules adsorbed on nanostructured Ag and Au surfaces. The two types of mechanisms responsible for the effect include (1) the enhancement of the local EM field due the
(254) Development of a Robust Method to Assess the Speciation Of Arsenic in Seafood

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The exposure to arsenic is primarily due to contaminated water and food ingestion. The toxicity of arsenic is dependent on its speciation i.e. chemical form. Yet, at the moment, government agencies assess the safety of food items based solely on the total concentration of Arsenic. Foods that contain a level higher than the total concentration guidelines are declared unsafe, irrespective of the actual form of the element, which may be non-toxic. In any case, such assessment method must be robust (i.e. applicable to a wide variety of sample types) so that it can be used cost-effectively by government agencies for risk assessment i.e. the continuous monitoring of food safety. High performance liquid chromatography (HPLC) coupled to inductively coupled plasma mass spectrometry (ICP-MS) is a widely used technique for the determination of arsenic species. The goal of this project is to develop a relatively rapid HPLC/ICP-MS method to determine the speciation of arsenic in seafood. A multivariate optimization of the chromatographic separation of 7 arsenic species that are commonly found in seafood was carried out by the experimental design methodology. Indeed, this approach allowed us, in a minimum of experiments: (1) to study and evaluate the influence on various factors and their possible interactions on separation; (2) to determine the optimum conditions of this separation on an Dionex IonPac AS 7 anion-exchange column with a nitric acid gradient eluent. The results show a better separation and in a shorter time than achieved by previously published methods. The 7 species are indeed baseline separated within 11 min in a single chromatographic run. A focused-microwave extraction method was also developed to solubilize As species from solid food. The analytical figures of merit will be reported, including the stability of retention times, linear dynamic range, quantitation limit, trueness, fidelity and reproducibility. This method was also combined to a fast continuous leaching method to allow the determination of bio-accessible arsenic species.

(255) Using ETV-Need for Preanalysis Separations ICP-MS for Sr/Rb Geochronological Dating without Preanalysis Separations

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Analysis of Rb and Sr isotopes can serve as a useful geochronometer and indicator of geological history, but mass spectrometric isotopic analysis currently requires significant effort to separate the isobars at mass 87 (generally via ion exchange chromatography) prior to measurement since a MS resolving power of 286,000 is needed for the 87Sr/87Rb separation. It is shown that careful control of the temperature program using electrothermal vaporization (ETV) of the sample can provide an alternate means of thermally and temporally separating the Rb and Sr prior to introduction to the mass spectrometer, reducing sample preparation requirements and time. This is achieved by taking advantage of the fact that Rb is significantly more volatile than Sr in the ETV furnace. Isotopic analysis of the vaporized material is carried out ICP-MS. Using this more rapid approach, ETV-ICP-MS analysis of NIST feldspar SRM 607 revealed an age of 1,339 +/- 99 Ma, which is in agreement with the value of 1,409 Ma. Details of the development and features of the method and utilizing a multicollector system as well as a time-of-flight MS will be presented.

(256) Multichannel Array Detection for Plasma Source Mass Spectrometry

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An array detector, based on Faraday ion collection, has been developed and coupled to a Mattauch-Herzog mass spectrograph (MHMS) to enable the simultaneous and continuous detection of a range of mass-to-charge (m/z) values. Such a system offers several key advantages over traditional scan-based mass spectrometers. First, the duty cycle is greatly improved and can theoretically reach 100%. This advantage provides improved limits of detection, reduced sample sizes, and shorter analyses times. A second advantage is the ability to remove correlated noise between two or more analyte channels through ratioing, thereby yielding very accurate and precise isotope ratio analyses. A final advantage that is obtained through simultaneous detection is the elimination of spectral skew that can arise when several analytes must be monitored within time-dependent signals such as those from chromatographic separations or single-shot laser ablation events. The current version of the array detector contains 128 Faraday-strip collectors that are 45-im wide and spaced on 50-im centers. Each collector is connected to its own charge-integrating amplifier to offer fast simultaneous destructive or non-destructive readout at rates of over 2 kHz frequencies for all channels. Furthermore, two levels of gain are available and individually selectable for each collector. Most recently, the MHMS-array detector combination has been coupled to a new atmospheric-pressure glow-discharge plasma ionization source (APGD). The flowing afterglow of the APGD has been shown to efficiently ionize samples in the liquid, gaseous, and solid states and to generate simple mass spectra that usually contain only the molecular or protonated molecular ion peaks. Use of the APGD makes possible the first molecular ion detection with the MHMS-array detector combination. This presentation will provide an overview of the abilities of the array detector, including experimental demonstration of the advantages of using such a device along with general figures-of-merit for ICP ionization. These figures of merit include limits of detection in the parts-per-quadrillion range for most isotopes, and isotope-ratio.
accuracies and precision levels of better than 1% and 0.01% RSD, respectively. In addition, recent studies using the APGD as an ionization source will be presented.

(257) Spectroscopic Imaging of Argon Metastable Atoms Between the Load Coil and the Sampling Cone of an ICP-MS
Haibin Ma1, Paul Farnsworth1; 1Brigham Young University
Changes in sample matrix affect the spatial distributions of analyte species in an inductively coupled plasma in ways that are not yet clearly understood. Fluorescence images of analyte species have provided valuable insights into the nature of the changes in analyte distributions between the load coil and sampling cone of an ICP-MS [1]. Images of plasma species would help complete the picture. Among possible plasma species, only argon atoms in the 4s levels are viable candidates for imaging by conventional laser techniques. The planar laser induced fluorescence technique used for analyte species proved to be ineffective for the argon 4s atoms. A combination of high emission backgrounds and low fluorescence quantum yields made it impossible to produce images with acceptable signal-to-noise ratios. An alternative imaging approach was developed that relied on changes in absorption images induced by a sheet of bleaching radiation. In this paper we will present the initial images of argon 4s density obtained by the new bleaching technique, and discuss the strengths and weaknesses of the technique as a tool for diagnostics in the ICP.[1] A. A. Mills, J. H. Macedone, P. B. Farnsworth, Spectrochimica Acta Part B 61 (2006) 1039-1049.

(258) ICPMS Collision Cell: Novel Applications Using Xeon Gas
Kirk Lokits1, Joseph Caruso1; 1University of Cincinnati
Over the past ten years, ICPMS instrumentation has adapted to the constant occurrence of polyatomic and isobaric interferences relative to the m/z of interest. One such adaptation for dealing with this predicament is the octopole collision/reaction cell. Fundamentally, the cell is pressurized with a gas which removes interferences by two mechanisms: reaction or collision with the interfering polyatomic species. Hydrogen and helium gases are universally utilized in the collision cell for the majority of applications. However, xenon has recently been introduced as an optional gas. This overview of current research capitalizes on the ability of xenon to simultaneously detect sulfur, phosphorous, arsenic and other elements in a variety of sample matrices.

(259) Analysis of "New" ICP-OES Emission lines between 800-1100 nm
Eric Merkel1, Bradly T. Jones1; 1Wake Forest University
New developments in microarray detector technology in commercial Inductively Coupled Plasma-Optical Emission Spectroscopy (ICP-OES) instruments have resulted in an increased range of detectable emission wavelengths (800-1100nm). One common problem in simultaneous multi-element determination in ICP-OES is interference between emission lines of similar wavelengths, making new usable emission lines desirable. New emission lines above 800nm are being explored using the appropriate spectral subtraction of the full eschelle images for elements of interest. New emission lines for Na, Cs, Hf, and other elements have been found, and various analytical figures of merit have been reported. Comparisons to the performance of these new analytical lines to traditional sub-800nm emission lines have also been reported.

(260) Electrophoretic Effects of the Adsorption of Anionic Surfactants to Poly(dimethylosiloxane)-Coated Capillaries
Maria Mora1, Carla Giacomelli1, Carlos Garcia1; 1University of Texas at San Antonio; 2Universidad Nacional de Cordoba
Poly(dimethylosiloxane) (PDMS) is one of the most convenient materials to fabricate capillary electrophoresis microchips. Even though PDMS has many advantages; its use is limited by its hydrophobicity. Although it is well known that the surface properties of PDMS can be modified by anionic surfactants, very little is known regarding the driving forces or the electrophoretic consequences of the adsorption of anionic surfactants. In this work, the adsorption of alkyl surfactants on PDMS was studied by performing electroosmotic flow (EOF) measurements. In order to mimic the behavior of PDMS microchannels, fused silica capillaries were coated with PDMS and used for the EOF measurements. This approach allows measuring the EOF using standard CE instrumentation obtaining very reproducible results. The adsorption isotherms were obtained using alkyl surfactants with different chain length and head groups. According to our results, the interaction of alkyl surfactants with the PDMS surface is determined by a combination of hydrophobic and electrostatic interactions, where the former is more significant than the latter. The affinity of each surfactant for the PDMS surface was calculated by fitting the adsorption profiles with a Langmuir equation and, in the case of alkyl sulfates, correlated to the corresponding CMC value. Financial support for this project was provided by The University of Texas at San Antonio.

(261) Deep UV Laser Induced Native Fluorescence Detectors for Gel Plane and Capillary Electrophoresis and CapLC
William Hug1, Rohit Bhartia2; 1Pharmaceutical Research, 2Purdue University
Most laser induced fluorescence (LIF) detectors employ visible lasers that can be applied to separated analytes that have been chemical derivatized with a suitable fluorescent label matching the laser excitation wavelength. Derivatization with fluorescent labels or tags is normally performed prior to separation for gel plane and capillary electrophoresis and after separation for capillary electrophoresis. Derivatization is a complex and sometimes unreliable process that limits the types of molecules that can be studied and is often responsible for perturbing the very cellular chemistry being studied. The use of deep UV lasers that match the maximum absorption band of aromatic amino acids allows detection of a wide range of peptides, proteins and other biomolecules with very high sensitivity. Deep UV lasers allow detection of the native fluorescence characteristics of analytes. The process is laser induced native fluorescence (LINF). We will demonstrate that employing excitation at 224nm enables very low limits of detection without the need for sample staining, and further enables differentiation of biomolecules with similar molecular weight using a small number of spectral detection bands during analyte separation using gel plane or capillary electrophoresis or capillary liquid chromatograph. Limits of detection of 2 pg to 5 pg for chicken albumin will be shown for an off-the-shelf planar gel from BioRad using a simple, breadboard, DUV-LINF detector without staining or sample post processing. The amount of material detected is actually much less since the above LOD loads are the total amount of protein loaded into a lane and not the amount detected in a particular band. We believe a gel-plane scanner designed for the specific purpose of scanning gels can achieve 100 fg LOD or less. Results will also be shown of DUV-LINF detectors for capillary electrophoresis and capillary liquid chromatograph using 224nm laser excitation of a broad range of biomolecules. Limits of detection without the use of dye tags will be demonstrated below 1nM.
(262) Investigation of Homocysteine Thiolactone-induced Protein Modification
Arther Gates1, Mark Lowry1, Kristin Fletcher1, Abitha Merugesu1, Oleksandr Rusin1, James Robinson1, Robert Strongin1, Isaiah Warner1; 1Louisiana State University
We report the first demonstration of rapid electrophoretic monitoring of homocysteine thiolactone-induced protein oligomerization (HTPO), a unique form of protein damage that may have clinical significance as an indicator of cardiovascular and neurovascular diseases. HTPO of the model protein bovine cytchrome c was initiated in vitro. The relative monomer and aggregate levels of the resultant protein mixtures were determined following separation using capillaries coated with the cationic polymer, poly (diallyldimethylammonium chloride). UV monitoring allowed sensitive detection of higher order species present at low concentration. Separations performed under standard injection conditions were optimized on the basis of applied voltage and sample denaturation conditions. Separations performed using short-end injection allowed for more rapid analyses, typically in less than 70 seconds. Relative errors for run-to-run migration times were less than 0.5%. This novel oligomeric system provides a rapid and straightforward in vitro method for screening therapeutic agents for ability to inhibit HTPO. Changes in peak area for monomer and aggregate species were used to assess HTPO inhibition as a function of pyridoxal-5-phosphate (PLP) concentration. PLP was shown to effectively inhibit HTPO in vitro. Rapid analysis times of approximately 1.5 minutes were achieved for inhibition screening. In addition, we have also designed a novel nanoparticle-based biosensor for the colorimetric detection of HTPO in human sera.

(263) Diode-Laser Induced Fluorescence Capillary Electrophoresis for Fluorescamine-labeled Amino Acid Analysis from Biological Samples
Nikolay Kocherov1, Jeanita Pritchett1, Scott A Shippy1; 1University of Illinois at Chicago
Amino acids play important neurochemical and physiological roles. The ability to better understand their involvement in normal and dysfunctional tissues requires fast analysis of amino acid content in nanoliter volumes of in vivo samples. Fluorescamine is a fluorogenic derivatizing reagent that provides a fast reaction (<1s) and readily reacts even at sub-micromolar analyte concentrations. Despite all these advantages, fluorescamine is not a widely-used derivatizing reagent due to a lack of optimal excitation sources. Recently, blue diode lasers (405-nm) have been introduced and these match well with the reacted dye absorption spectral maxima. This paper discusses the use of a blue diode-laser induced fluorescence (LIF) detector for fluorescamine-labeled compounds for a capillary-based electrophoresis system (CE). The LIF system was built in-house using a commercial 10-mW 411-nm diode laser module as excitation source, and a photon-counting photomultiplier tube (PMT) as the detector. Laser light was filtered by a narrow passband interference filter followed by a broadband filter, and fluorescence was separated from excitation light using a long-pass filter and a broadband filter. System control and data acquisition was achieved via the LabView environment. The limit of detection was found to be as low as 40-nM for serine, and calibration curves for 15 amino acids demonstrated a linear range from 1-20µM. Separation conditions for fluorescamine-labeled amino acids were optimized, and three sets of conditions were developed. One condition was optimized for resolution showing 20 standard amino acids separated. Another condition was developed for speed with 12 amino acid resolved in <4 minutes. The third condition was a balance of resolution and speed with a separation of 15 standard amino acids in 6.5 minutes. To demonstrate the applicability of this system for a “real world” sample, 250-nL rat vitreous perfusate samples were analyzed with this system. The separation showed 35 amine peaks, 18 of which were identified. Overall, the blue diode-laser induced fluorescence detector was shown to be a good choice for fluorescamine-labeled amines analysis and it appears widely applicable to the study of amino acids from samples collected from biological systems.

(264) Development of a Portable Capillary Electrophoresis NMR System for Chemical Speciation
Julie Herberg1, Greg Klunder1, Vince Malba1, Chris Harvey1, Lee Evans1, Vicky Demas1; 1Lawrence Livermore National Laboratory
Capillary electrophoresis (CE) is a simple rapid separation method that can be used to identify species in solution. The most common method of detection for metal species by CE is to use complexing agents and background electrolytes for indirect UV absorbance detection. However, this can perturb the original distribution of species in the sample and is non-specific. Nuclear magnetic resonance (NMR) has also been used to directly identify species that are coordinated with F, P, or C in aqueous solutions. Previous investigators have demonstrated coupling NMR to CE using small hand-wound coils around the capillary. LLNL is developing a new portable CE system that will include a compact on-line NMR spectrometer. CE is very amenable to compact and portable design with the biggest limitations being the high voltage power supply and detection. Optical detection will be included, although it is rather non-specific. Shrinkage the NMR spectrometer has been more of a challenge, the current design can fit into a briefcase. This includes the control electronics and a 1 tesla permanent magnet that has demonstrated 8ppm resolution. We are also developing separation protocols to determine speciation of uranyl complexes in solutions with minimal perturbation to the original sample equilibrium. Separations have been demonstrated with indirect UV absorption using a background electrolyte. Experimental results and detection capabilities will be presented.

(265) The Development of a Non-Aqueous Capillary Electrophoresis-High Resolution Inductively Coupled Plasma Mass Spectrometry
Xiaodong Bu1, Tiebang Wang1, Qiang Tu1; 1Merck Research Lab
In this work, a non-aqueous CE-ICP-MS has been established as an efficient and reliable technique for the elemental speciation study with potential applications for pharmaceutical compound analysis. The newly designed sheath flow with PFA micro flow nebulizer interface provided stable and versatile connection between non-aqueous CE and ICP-MS, and functions as an on-line diluter to dilute the non-aqueous CE elute to aqueous system before it reaches the plasma. The benefits of non-aqueous capillary electrophoresis have been discussed in two aspects. The wide selection of organic solvents, with their very different physicochemical properties, broadens our scope to manipulate separation selectivity. The lower currents present in non-aqueous solvents allow the use of high electric field strengths and wide bore capillaries, the latter in turn allowing larger sample load. In many cases detection sensitivity can also be enhanced. Organic solvents offer the ability to alter the electrophoretic mobility of the ions and control of the EOF are essential to improve resolution and separation speed. Significant changes in selectivity among anions are observed by using up to 100% methanol in the running buffer. The ability to move peaks selectively using different percent of methanol demonstrates the flexibility of this technique. Overall highly charged ions show the largest decrease in mobility upon addition of methanol due to experience stronger dielectric friction and ionic strength effects than the lower charged ions. Peak area based limits of detection were either better or comparable with
aqueous CE, and sub ppb limits of detection were illustrated. Limits of detection can be further improved using wide-bore capillary methods which can transfer relatively large volumes of dilute sample into plasma. This method can improve limits of detection by as much as three orders of magnitude which would make the limits of detection for CE-ICPMS as good as conventional ICP-MS analyses.

(266) In situ Microscope FTIR Spectroscopy and Its Applications in Nanomaterials Studies
Shi-Gang Sun1, Zhi-You Zou1, Yan-Xia Jiang1, Sheng-Pei Chen1, Chun-Hua Zhen1; 1Department of Chemistry, Xiamen University, China
Electrochemical in situ microscope FTIR spectroscopy (MFTIRS) was developed and applied in studies of nanomaterials. Further combination of the in situ MFTIRS with an individually addressable array of microelectrodes allowed carrying out combinatorial analysis. The adsorption of CO on nanostructured electrode surfaces was studied by the newly developed techniques. Anomalous IR properties of nanostructured materials, especially the dependence on surface structure, were investigated by combinatorial surface analysis. The study demonstrated the advantages of employing an IR microscope in nanomaterials studies, and revealed that the anomalous IR properties of nanostructured film materials have undergone a transition from enhanced IR absorption effect to Fano-like effect, and further to abnormal IR effects along with the increase in size of islands inside film as well as in thickness of the film.

(267) Synthesis and Characterization of Selective Electrocatalysts in the Nanoscale Length for Fuel Cell Reactions
Nicolas Alonso-Vante, 1University of Poitiers, UMR-CNRS
Tolerance and reactivity can be promoted via a chemical route of the catalyst synthesis by designing the “real” chemical precursor in such a way as to tailor novel materials by arranging individual transition metals to form cluster-like compounds. Thus, following this line of reasoning, the fact of using molecular cluster compounds as precursors emerges as an attractive alternative since the cluster may predetermine the proper stoichiometry of the metal atoms. Thus, the organizational effect of such molecular precursors to tailor novel materials opens a variety of interesting phenomena for physics and chemistry, and constitute the basis for the development of electrochemical energy converters (fuel cells) working in mild conditions, such as e.g., PEMFC (proton exchange membrane fuel cells) or DAFC (direct alcohol fuel cells). Significant progress has been achieved with cluster-like mono-, bi-, metallic and chalcogenide materials, in the nanometer scale range. Platinum, as cathode for the oxygen reduction reaction (ORR), has no inertness to crossover of methanol in a direct methanol fuel cell (DMFC). However, alloying this noble metal with other non-noble transition metals, such as, e.g., Ni, Cr, has increased the tolerance to this phenomenon. Although the target, in the near future, is to develop materials based essentially on non-noble metals, it was, however, illustrative to explore the advantage or disadvantage of chalcogenes to tailor novel platinum-based materials. Earlier works showed, indeed, that a full tolerance of methanol is obtained for the oxygen reduction reaction by means of ruthenium-chalcogenide. All data reported up to date points that the energy efficiency of related interfaces is particularly influenced by the composition and the electronic state of the catalyst. We believe that tolerance and reactivity can be promoted via a chemical route of the catalyst synthesis by designing the “real” chemical precursor. We will discuss this aspect based on recent electrochemical and structural data obtained on platinum-, and ruthenium-based nanoparticulate materials.

(268) Single-Walled Carbon Nanotubes Decorated with Pd Nanoparticles for High-Performance, Flexible Hydrogen Sensors
Yugang Sun1, 1Argonne National Laboratory
Hydrogen sensing represents an important technique in a wide range of applications for ‘hydrogen economy’ such as industrial processing, fuel cells, hydrogen storage and separation, etc. Conventional hydrogen sensors are fabricated, in general, on rigid substrates (e.g., glass, quartz, silicon wafers) by using thin palladium films with continuous or discontinuous morphologies as well as nanowires and nanotubes made of pure palladium or alloys. The rigidity (and/or fragility) of these devices somehow limits their application in systems with curvilinear surfaces that require conformal lamination and mechanical shock-resistance. In contrast, hydrogen sensing devices fabricated on flexible polymeric substrates can find applications complementary to that of the conventional sensors on rigid substrates. We have recently found that nanoparticles of palladium deposited on the support of networks of single-walled carbon nanotubes significantly change the transport property of carbon nanotubes when the composites are exposed to hydrogen. The unique behavior enables us to fabricate flexible hydrogen sensors with the use of nanotube/palladium hybrid building blocks on poly(ethylene terephthalate) (PET) sheets. The as-fabricated devices have excellent performance which is comparable to (even higher than) the conventional sensors. For example, these sensors can detect hydrogen with concentration as low as 30 ppm in air at room temperature. The response time is as short as 1.5 seconds when the devices are exposed to 1% hydrogen in air.

(269) New-phased Nanostructures Designed for Lithium-ion Batteries Applications
Yi Xie1, Changzheng Wu1; 1University of Science and Technology of China
It is well known that the rechargeable Li-ion batteries now dominate the portable electronic market. Compared with other secondary batteries such as the nickel-cadmium and nickel metal hydride cell, the lithium-ion batteries have obvious advantages, such as high cell voltage, high energy density, long cycle lifetime, low maintenance, low self-discharge and no memory effect. For a qualified electrode material, cathode and anode, the basic demands include high reversible capacity, high rate capability, satisfactory cyclic performance, good performance at low and high temperature, good electrolyte compatibility, process compatibility, safety and low cost. Now the key problems needed to solve is that electrode materials approach to the fully utility of theoretical capacity and the low electronic conductivity, and thus the capacity and the high-rate capability of lithium ion battery is significantly limited for the further battery applications. One solution to overcome this limitation is that the development of new inorganic functional materials with excellent electronic conductivity and lithium ion diffusion coefficient will be expected to improve the battery capacity, cyclic performance and high rate capability. Driven by this motivation, our research focuses on looking for new-phased candidate electrode materials and constructing their nanoarchitectures to improve electrode capacity, cyclic and high rate performance. In this talk, several examples such as Cu2SnS3, C9N5H3, and VOOH have been given on the designed new-phased electrode nanomaterials and nanoarchitectures, which may find potential applications in lithium-ion batteries. Besides these new nanomaterials and nanoarchitectures are fully characterized by various techniques, their performances on electrochemical lithium ion storage were systemically studied. In addition, some novel strategies were proposed to design the new nanoarchitectures possibly applied as lithium-ion battery electrodes.
Novel Nanostructured, Composite Electrodes as Anodes Improved Anode Material for Direct Alcohol Fuel Cells

Diego Diaz; 1University of Central Florida

There is a great deal of concern about finding alternative energy sources to power our living and transportation demands. Although a great deal of interest has been based on hydrogen and on photovoltaics, the need to power smaller devices can not been neglected. Direct alcohol fuel cells (DAFCs), especially direct methanol (DMFC) or direct ethanol (DMEC) fuel cells have shown great promise to power smaller transportation and electronic devices and to help alleviate energy demands for such devices. Direct Alcohol Fuel Cells (DMFCs) appeared as a promising alternative to hydrogen fuel cells, and are being actively developed due to their ease of preparation, safe handling and storage, low cost and high-energy density. Unfortunately, DAFCs suffer easy poisoning, require expensive Pt-based anodes and have relatively low performance due to the many possible intermediate processes to the alcohol fuel oxidation and to membrane and design problem of the cell. In order to improve the oxidation of the alcohol at the anode, we have focused on the preparation of novel, nanostructured electrodes that reduce the amount of Pt on the electrode, and that incorporate novel catalysts that can compete in performance with the commercially available Pt/Ru and Pt/Ru/C anodes. Current efforts involve the utilization of nanocrystalline ceria and other metal oxide particles as catalyst for the complete oxidation of the alcohol to carbon dioxide and novel electrode arrangements based on the Pt functionalization of nanotemplated electrodes. The combination of these approaches offer a viable, cost-effective alternative to fuel cells that rival or exceeds the performance of the traditional Pt/Ru bifunctional catalysts. These electrodes offer enhanced surface area and better tolerance to CO poisoning. Studies dealing with the performance of the catalysts and electrode composites will be presented. A preliminary mechanism for the alcohol oxidation based on ceria’s oxygen storage capacity is presented. Results show there is a great promise on DAFCs and that a great deal of improvement can be achieved to bring DAFCs as an alternative to power generation.

Electronic Communication of Redox-Active Moieties on Ruthenium Nanoparticle Surfaces

Shaowei Chen; 1UC Santa Cruz

Intervalance electron transfer was observed with ferrocene moieties that were bound to ruthenium nanoparticle surface by the ruthenium-carbene pi linkages. Electrochemical measurements exhibited two pairs of voltammetric peaks with the difference of the formal potentials very comparable to those observed with biferrocene derivatives. Electronic communication between the particle-bound metal centers was further evidenced in near-infrared measurements which showed a strong absorption at 1930 nm. The paradigm demonstrated in this report offers a novel prospective in the investigation of nanoscale electron transfer involving nanoparticles and redox-active functional groups.

Electron Detachment Dissociation FTICR Mass Spectrometry for the Full Structural Characterization of Glycosaminoglycan Carbohydrates

I. Jonathan Amster1, Jeremy J. Wolff2, Tatiana Laremore3, Robert J. Linhardt4; 1University of Georgia; 2Renselaer Polytechnic Institute

Dissociation of multiply-charged ions by electron-capture and electron transfer has attracted considerable interest for the structural characterization of labile biomolecules. These methods produce a radical site in an ion which leads to dissociation via pathways that are complementary to the types of fragmentation observed for closed shell ions. There are many biomolecules which are acidic in nature, and which do not yield cations by electrospray ionization, but rather form multiply-charged anions. For such compounds, electron detachment dissociation (EDD) provides the means to generate a radical ion which yields fragmentation products that are considerably different from those produced from the even electron anionic species. Here we demonstrate the effectiveness of EDD for the structural characterization of anionic carbohydrates. The complementary nature of EDD versus infrared multiphoton dissociation (IRMPD) and collisionally activated decomposition (CAD) for heparan sulfate oligomers is shown to provide a more complete characterization of these complex biomolecules than by any single one of these dissociation methods.

Investigation of Unusual Fragmentation Routes of Protonated Prodiginines Using Electrospray Mass Spectrometry and Computer Modeling

Richard B. Cole1, Ken Chen2, Pat Lane3, Yang Cai4, Bernard Rees4, Gregory L. Challis5; 1University of New Orleans; 2Children's Hospital of New Orleans; 3University of Warwick

Many Gram-positive and Gram-negative bacteria can produce bright-red pigmented prodigiones that contain a tripyrrole backbone. These compounds have stimulated much current interest as they have shown the ability to target and kill cancer cells, as well as exhibiting immunosuppressive properties. Because they are difficult to chemically synthesize in the lab, employing microorganisms to produce them is a promising alternative route. Although the absorbance maxima at 535 and 470 nm allow visible region detection of these red pigments, the characterization and identification of novel prodigiones are still largely dependent on NMR, requiring labor-intensive sample purification steps. Few applications of mass spectrometry for the analysis of prodigiones have been reported, and those consisted mainly of providing molecular weight confirmations. Here we present an electrospray tandem mass spectrometry study of protonated prodigiosin, undecylyprodigine and butyl-meta-cycloheptylprodigine, that explores fragmentation pathways to explain the unusual observance of radical fragment ions in CID spectra. The presence of these odd-electron ions produced by decompositions of the even-electron precursors violates the “even-electron rule” of mass spectrometry. Structures of, and decomposition pathways leading to, observed fragment ions have been proposed, and the underlying basis for the competition between even-electron producing vs radical cation generating decomposition pathways has been rationalized. Computational studies using GAUSSIAN 2003 have been performed to optimize the structures of reactants and products. These studies indicate that the nitrogen atom on ring C and the methoxy oxygen effectively chelates the proton to form a seven-member ring that renders loss of methyl radical from the methoxy function favorable. In competition with this pathway is loss of a methanol molecule from the same site leading to even-electron fragment ions. Additionally, the characteristic and unusual loss of methyl radical from each prodigine can be useful for performing a constant neutral loss scan to quickly and efficiently identify prodigine compounds in a complex biological mixture without purification steps.

Identification and Structure Determination of Using Q-Trap and Chip-based Nanoelectrospray Ionization with Hybrid Q-TOF Tandem Mass Spectrometry

Cameron Sullards1, Jeremy Allegood1, Alfred Merrill, Jr.1, 1GA Tech

Organisms usually contain a diverse variety of sphingolipid subspecies (see www.sphingomap.org) and knowledge about the types and amounts is imperative because they influence membrane structure, interactions with the extracellular matrix and neighboring cells, vesicular traffic and the formation of specialized structures such as membrane rafts, phagosomes and autophagosomes, as well
as participate in intracellular and extracellular signaling. Fortunately, “sphingolipidomic” analysis is becoming feasible for important subsets such as all of the backbone “sulfing” subspecies (ceramides, ceramide 1-phosphates, sphingoid bases, sphingoid base 1-phosphates, inter alia) using mass spectrometry. 1-3 The next challenge is to develop equally robust methods for more polar sphingolipids such as sphingomyelins, globoisides, and gangliosides. This has been accomplished for several of these species using both a hybrid quadrupole / linear ion trap (QTrap) and chip-based nanoelectrospray (nanoESI) in conjunction with Q-TOF tandem mass spectrometry. The QTrap provides alternative fragmentation mechanisms and MS3 for detailed structural information. The chip-based nanoESI provides much greater sensitivity while using extremely small sample volumes. Here sample consumption is on the order of a few hundred nL/min, therefore, MS and multiple MS/MS analyses may be performed with only a few ul of sample. Additionally, the high resolution and accurate mass measurement of the Q-TOF in both MS and MS/MS modes allows unequivocal identification of specific headgroup, fatty acid, and sphingoid base combinations. This research was supported by NIH-GM069338 (Lipid MAPS Consortium).

(275) Ionic Liquids as Matrices for MALDI Mass Spectrometry
Michael L. Gross1; 1Washington University
The reproducibility of signals and the ability to quantify by MALDI mass spectrometry can be improved by the use of ionic liquids, as was first shown in this lab in collaboration with the D. Armstrong group. With some time-of-flight instruments, quantification can only be done by using an internal standard that is a congener of the analyte or an isotopically labeled variant of the analyte. By using ionic liquids as matrices, the dynamic range and the reproducibility of the signals can be improved by at least an order of magnitude. Although the uniformity of the presentation has significant advantages for improving precision and ability to quantify, the sensitivity is reduced because no regions of high concentration (normally call “sweet spots”) exist. One way to improve the signal intensity without increasing the sample amount is to make MALDI spots smaller, affording higher concentrations while using the same amount of material. We are employing a technique by which nanoliter volume spots (10-300 nL) can be made for MALDI-TOF detection. The nanoliter syringe and induction-based fluidics (IBF) insure precise volume deposition. Use of ionic liquid matrices gives better homogeneity and reproducibility of signals than would be generated from MALDI spots made by using solid matrices. In some experiments, the ability to detect a limited amount of analyte is improved by approximately an order of magnitude. This use of ionic liquids with nanoliter deposition methods has the potential use for analyzing proteins and other biological samples at levels comparable to what can be achieved by conventional MALDI with solid matrices but with considerably improved reproducibility and capacity for quantification. The presentation will emphasize recent results obtained for peptides, proteins, and complex lipids.

(276) Oligonucleotide-Modified Fused Silica Surfaces for Affinity-MALDI-TOF-MS of Proteins
Jacquelyn Cole1, Ashley Tennyck1, Linda McGowin,1; 1Rensselaer Polytechnic Institute
Affinity binding reagents have played a crucial role in the translation of proteomic discoveries to clinical diagnostics due to their ability to isolate target proteins from complex protein mixtures. Antibodies have been unrivaled as affinity reagents for proteins due to their strong and selective binding; however, drawbacks associated with their production, stability, and manipulation have prompted researchers to seek alternatives. We

(277) Large Scale Quantitative Analysis of Non-coding RNAs (ncRNAs) by their Signature Digestion Products using Stable Isotope Labeling and MALDI-MS
Mahmud Hossain1, Patrick A. Limbach1; 1University of Cincinnati
Escherichia coli (E. coli) non-coding RNAs (ncRNAs) includes 3 ribosomal RNAs (rRNAs) (5S, 16S, and 23S rRNAs) and inconsistently-distributed 46 isoaccepting transfer RNAs (tRNAs) for 21 amino acids, among others. rRNAs have long been recognized as fulfilling a structural role and tRNAs as performing an adapter in the conversion of genetic message to protein. Considering the cellular dynamics of ncRNAs, different methods, e.g., RP-HPLC, northern blotting, microarray, etc. have been developed for their analysis; however, these techniques are time-consuming, complicated, and are generally insensitive to the posttranscriptional modification status of RNAs. Here we present a ribonuclease-mediated cleavage and 18O-labeling approach coupled with MALDI-MS for the quantitative analysis of E. coli ncRNAs by their signature digestion products. A comparison of an organism’s complete complement of RNA digestion products of ribonuclease yields a set of unique or “signature” digestion product(s) that ultimately enable the detection as well as quantification of cognate RNAs from a total ncRNA pool. E. coli was cultured in different MOPS media which reflects its diverse growth rates. For relative quantification of RNA abundances, selectively isolated ncRNAs were labeled with either 16O- (control cultures) or 18O-labeled H2O (enhanced growth cultures) during RNase digestion and the quantification is realized by comparing the ion intensity ratios (16O- vs. 18O-) of relevant signature digestion products for any particular RNA in MALDI-MS. For absolute quantification, isotopically labeled synthetic oligonucleotide analogs of signature digestion products are used. It was found from our preliminary experiments that 35 isoaccepting tRNAs could be used for quantification due to the non-overlapping masses of the digestion products from about 40 isoaccepting tRNAs detected so far by the use of three individual ribonucleases (RNase T1, A and U2). Similarly, multiple digestion products were found appropriate for the quantification of large rRNAs. Optimized methods will then be used to examine the effect of light-induced transformations of etioplasts from C. sativus in order to elucidate pathways important in rRNA synthesis and light-induced posttranscriptional modifications, and for the analysis of large cytoplasmic rRNAs of cold-sensitive mutants of Neurospora crassa, a multicellular filamentous fungus, which was found defective in ribosome formation at low temperatures.
Future Meetings: FACSS 2008, September 28 – October 2, Reno, NV • FACSS 2009, October 18 – 22, Louisville, KY

(278) Subsurface and Transcutaneous Raman Tomography using a Ring/Disk Fiber Optic Probe and Iterative Reconstruction
Matthew V. Schulmerich1, Subhadra Srinivasan2, Jaclynn M. Kreider3, Jacqueline H. Cole4, Ethan L. H. Daley2, Katherine T. Dooley1, Victoria Popescu5, Steven A. Goldstein2, Brian W. Pogue6, Michael D. Morris5, 1U of Mich., Dept. of Chemistry; 2U of Mich., Dept. of Orthopaedic Surgery; 3Dartmouth, Thayer School of Engineering

We report the use of a fiber optic probe with ring illumination and an array of 50 collection fibers to obtain resolved, three dimensional distributions of Raman spectral components located below the surface of a material or tissue that scatters the incident light. The previously reported ring/disk fiber optic probe(1) is used to collect light in the center of the illumination ring. Multiple acquisitions with different spatial separations between the illumination ring and the field of view of the collection fibers are used to increase the number of projections to be used in the restoration. From the spatial distribution of collected signals, the distribution of sources (i.e. the shape of the Raman scattering object) can be recovered. Blind reconstruction can be used to give a rough approximation to object shape and position in the absence of independent knowledge of spatial position. It is expected that improved reconstructions will be obtained if the shape of the object is independently known. We will discuss the application of this technique to tissue phantoms - embedded objects in gels with light scattering properties similar to those of soft tissue. We will also discuss the latest results in bone tissue, in which the shape and position of the bone is accurately known from micro-computed tomography. 1. M. V. Schulmerich, K. A. Dooley, M. D. Morris, T. M. Vanasse and S. A. Goldstein, "Transcutaneous fiber optic Raman spectroscopy of bone using annular illumination and a circular array of collection fibers," J. Biomed. Optics 11, 060502 (2006)

(279) Application of GC-Triple Quadrupole Mass Spectrometry for Rapid Functional Group Identification in protonated Oxygen-containing Compounds and Their Mixtures
Sen Li1, Penggao Duan1, Michael Watkins2, Brian Winger2, Todd Gillespie2, Hilkka Kettunen3; 1Purdue University; 2Eli Lilly and Company

Rapid identification of functional groups in drug degradation products and other pharmaceutical mixtures is important to the development of new drugs. Mass spectrometric methods provide a sensitive and fast solution for the analysis of compounds directly in mixtures. We have developed methods based on ion-molecule reactions with neutral boron-containing reagents for the identification of the functional groups in protonated oxygen-containing analytes in an Fourier transform ion cyclotron resonance (FT-ICR) mass spectrometer. The derivatized analytes are easily identified based on the natural isotope ratio of boron (25%, 10B to 11B). We report here the implementation of this methodology to a triple quadrupole (QqQ) mass spectrometer. The combination of GC-QqQ the ion-molecule reactions accomplished in the ion source of the triple quadrupole mass spectrometer. The combination of GC-QqQ and this methodology has been demonstrated to separate and derivatize each component in the mixture of several oxygen functionalities.

(280) Infrared Spectroscopy for Exploring Complex Oceanic Gas Hydrate Ecosystems
Gary Dobbs1, An Nguyen2, Yulia Luzinova3, Yosef Raichlin2, Christine Kranz2, Abraham Katzir2, Roger Sassen3, Boris Mizaikoff2; 1Georgia Institute of Technology; 2Tel-Aviv University; 3Texas A&M University

Substantial amounts of hydrocarbons are sequestered in naturally occurring ice-like formations known as gas hydrates. In particular, oceanic gas hydrates are globally distributed in complex heterogeneous ecosystems that typically occur at depths exceeding 500 m and at temperatures below 10 C. Gas hydrates have received attention for their potential as an alternative energy resource as well as to further understand their role in cycling of greenhouse gases, such as methane, at a molecular level. In the presented work, we will describe fundamental strategies for monitoring gas hydrate growth utilizing infrared fiberoptic evanescent field spectroscopy by exploiting state-responsive infrared absorption features of water. Furthermore, we will highlight key application areas where IR optical sensing strategies can be integrated to advance geophysical exploration and evaluation of oceanic gas hydrate occurrences. Complementary to investigating the dynamics of gas hydrate formation, it is well established that microbial processes substantially affect carbon cycling within oceanic gas hydrate ecosystems. Specifically, sulfate reducing bacteria shift pore water alkalinity to favor authigenic carbonate formation, which traps enormous amounts of carbon dioxide generated by microbial anaerobic oxidation of methane. Extensive spectroscopic studies evaluating seafloor sediments substantiates that IR evanescent field sensing provides the additional capability of identifying patchy origins and distributions of carbonate mineral polymorphs within these complex ecosystems. We present spectroscopic evidence enabling carbonate polymorph speciation and origin assessment within biogeochemical and geophysical frameworks extending from the photic zone to anoxic seafloor sediments.

(281) NearIR in the Process Lab: From Development to Validation
Jonathan Haulenbeek1, Ming-Hsing Huang1, Charles Ray1, John Wasylyk1; 1Bristol-Myers Squibb Co.

Near infrared spectroscopy has become a widely used analytical technique for evaluation of powder blends, solvent compositions and tablet coating in the pharmaceutical arena. The successful application of NearIR in a process control laboratory includes critical instrument documentation and certification, the development of robust methods, evaluation of key validation characteristics, and a secure method and data handling system to meet compliance requirements. We will present several NearIR methods used for routine analyses in a process analytical lab which replace traditional analytical methods such as Karl Fisher moisture determinations and gas chromatography.

(282) Multiparameter Tablet Analysis by NIR Spectroscopy: From Dose Uniformity to Dissolution Testing
Manel Alcala1, Marcelo Blanco1; 1Universitat Autonoma de Barcelona

The use of Process Analytical Technologies (PAT) by the pharmaceutical industry is a response to its growing need for
improved productivity and quality in order to face the increasing competition in this field. Near Infrared Spectroscopy (NIR) has become one of the most powerful PAT tools, as a nondestructive analytical technique that enables simultaneous measurements of chemical composition (viz. the content in Active Principle Ingredient, API) and various physical properties (viz. particle size, tablet compaction and dissolution testing) in pharmaceutical samples. Multivariate techniques, including calibration or classification models, allow to extract the relevant information from big amounts of data and subsequently to develop analytical methods for the monitoring of critical parameters. Partial Least Squares (PLS1 & PLS2) and Discriminant Partial Least Squares (DPLS) models have been developed for the determination of API content, compaction and dissolution testing in intact tablets. Calibration sets were built with laboratory samples consisting by mixtures of API and excipients that were compacted. Different strategies of sample preparation and model development are presented. Based on the results, the proposed NIR method is an effective alternative to current methods for the intended purpose. The proposed method is simple and robust—they involve minimal analyst intervention—, clean—they use no toxic reagent and produce no toxic waste—, and fast—the results can be obtained within a few seconds.

(283) Monitoring of Film Formation and Coating Thickness in Small-Scale by In-Line Near Infrared Spectroscopy
Meike Römer1, Jyrki Heinämäki1, Jouko Yliruusi1; 1University of Helsinki, Faculty of Pharmacy

Aqueous film coatings are widely used for pharmaceutical solid dosage forms. These coatings are mainly applied for taste masking, but can also be used to prevent drug degradation in the stomach (enteric coating) or to modify the drug release. To monitor the film coating process a novel small-scale coating approach has been set up. It consists of a rotating plate made of Teflon rotating at constant speed. This plate has 20 moulds in which tablets of a diameter between 9 to 11 mm fit. The set up can also be used to prepare free films at the same time. A spray unit is applied which uses a common spraying nozzle with pressurized air in order to imitate the coating process during an industrial process. After spraying the tablets pass a heating unit (infrared light) and then an in-line near infrared (NIR) spectrometer. This NIR spectrometer uses a magnetic trigger to monitor the same two tablets during the whole process. Flat-faced tablets of 9 mm diameter containing high-density polyethylene have been prepared to test this set up. A coating solution for a sustained release coat containing Kollicoat SR30D and Kollicoat IR (2.5:1) was sprayed onto the tablets. For each tablet the weight and thickness (digital micrometer) was individually measured before and after the coating process. Depending on the film coating solution one coating process took about 60 min in order to achieve a thickness of 300 µm. A calibration curve of predicted film thickness determined by NIR spectra versus real film thickness was developed. The use of these results is currently being tested as a calibration set for a rotating plate set up to prepare a robust calibration set of tablets with great coating thickness variation in a short time.

(284) Differentiation and Quantitative Determination of Surface and Hydrate Water in Lyophilized Mannitol Using NIR Spectroscopy
Wenjin Cao1, Chen Mao2, Wendy Chen1, Hong Lin1, Sampathkumar Krishnan1, Nina Cauchon1; 1Amgen Inc.; 2Purdue University

Mannitol hydrate is a metastable form produced during lyophilization. It is unstable, and therefore can undergo dehydration to release water to the surrounding environment at room temperature. The analysis of this form is challenging due to its thermodynamic instability. This study describes the development of a fast and non-invasive method to determine the mannitol hydrate and surface water content in a lyophilized product using near-infrared spectroscopy (NIR). The mannitol hydrate was produced through lyophilization and characterized using XRPD, TGA and NIR spectroscopy. Quantitative methods for hydrate and surface water were developed for NIR spectra with curve fitting and partial least square (PLS) regression models. The curve-fitting method deconvoluted the NIR spectra into hydrate and surface water peaks and generated a calibration model by correlating pure spectra peak area to concentration. The standard error of prediction (SEP) for hydrate and surface water content were 0.65% and 0.40%, respectively. The PLS model developed for the same sample set was better than the curve fitting model; SEP = 0.50% for hydrate water and 0.22% for surface water, respectively. The methods can be used to monitor the formation and stability of mannitol hydrate in mannitol-containing formulations during the lyophilization process.

(285) Efficacy of the Drug Tagitose Effected by Vibrational Microspectroscopy
David L. Wetzel1, Robert A. Lodder2; 1Kansas State University; 2University Of Kentucky

Deposition of lipid on the walls of the aorta presents a serious hazard leading to atherosclerosis. This condition can be result of high glucose levels in the blood. Spongy lipid deposition on the inside of the aorta wall of an ApoE− mouse fed a sucrose diet was dramatically revealed with synchrotron infrared microspectroscopic imaging of aorta sections. Both mid-IR and near-IR instruments were used. The aorta section of a similar mouse on a control diet microspectroscopically exhibited essentially no lipid present. Regions within the aorta cell wall that visually appeared suspect were probed and no lipid was found. Tagitose has been suggested as a sweetener substitute for sucrose. Unlike the depositions on the sucrose fed mice that were attached to as much as 75% of the circle of the aorta, sections from the mouse ingesting Tagitose had only a few sparsely distributed spongy areas. When these areas were probed microspectroscopically a relatively low lipid concentration was found. This study although related to the efficacy of Tagitose to persuade lipid formation on the aorta walls induced by high glucose levels has analytical implications applicable to medical spectroscopic diagnosis. Various medical imaging techniques available clinically are briefly presented showing the need for spectrochemical analysis that will detect the presence of lipid on the aorta or on arterial walls, in general.

(286) The Hard Facts: Spectral Effects of Relative Density and Radial Tensile Strength
Steven M. Short1, Zhenqi Shi1, Brian M. Zacour1, Robert P. Coghill1, Peter L.D. Wildfong2, Carl A. Anderson3; 1Duquesne University

Solid oral dosage forms are the predominate route of administration for pharmaceutical substances. Consequently, it is important to understand the metrics that address the critical quality attributes of the dosage form. One attribute commonly evaluated for tablets is hardness or radial tensile strength (RTS). By definition, RTS is a destructive test. Near-infrared spectroscopy (NIRS) has been demonstrated to nondestructively predict RTS. Despite the numerous accounts of successful calibration, the precise mechanism(s) of calibrations between near-infrared (NIR) response and RTS has not been extensively described. In this work, 174 4-component (anhydrous theophylline, lactose monohydrate, MCC (PH 200), and starch) compacts covering a wide concentration range in all constituents were compacted at 67.0, 117.3, 167.6,
Wetting and Molecular Transport in Hydrophobic Pores at Nanometer Dimension Studied with Quantitative Confocal Fluorescence Imaging

M. Lei Geng1, Zhenming Zhong1, Reygan Freeney1, Mark Lowry1; 1University of Iowa

Nanometer-sized hydrophobic pores play crucial roles in many fields of chemistry and biology: the interaction interface in chemical separations, the nanocontainers in drug delivery, and the channels in cell membrane, for example. Understanding of the properties of hydrophobic pores at nanometer dimension is thus desirable in these fields and in the fundamental studies of hydrophobic interactions. In this work, we investigate the wetting and molecular transport in 10-nm pores in silica particles that are surface-modified with a hydrophobic C18 monolayer. Using quantitative confocal fluorescence imaging, it is observed that the mesopores are not wettable by an aqueous solution. Interestingly, an apolar molecule can still partition into the pores in the absence of any solvent wetting. Wetting occurs when a fraction of organic solvent is added to the solution. Using ratiometric imaging, we measure the polarity inside the nanometer pores while increasing the volume composition of the organic solvent. Surprisingly, the microenvironmental polarity in the hydrophobic pores increases with a decrease in solvent polarity before wetting and decreases after the solution fills the pores. These observations by confocal fluorescence imaging shed new light on our understanding of nanometer wetting and transport.

Excited State Dynamics in Conjugated Polymer Devices

Andre Gesquiere1, Daeri Tenery1, James Worden1; 1University of Central Florida

Interactions between excited state and charged (polaron) species in conjugated polymers can play a significant role in electroluminescent organic light emitting diodes (OLED) and organic photovoltaic devices (OPV). Unfortunately, it has become exceedingly difficult to unravel the complex processes and related heterogeneous kinetics of a functioning conjugated polymer device due to three factors: (i) the large number of different excitonic and polaronic species in the device, (ii) the potential for large spatial variations and fluctuations in the concentration of these species, and (iii) the large morphological heterogeneity of the conjugated polymer material itself. For OPVs the added complexity of the morphological structure of the organic materials at the molecular and mesoscale in these devices and the lack of understanding of solar energy conversion processes is significantly hampering progress in the field. Attempts to better understand these issues had limited success. These studies mostly involved current-voltage (I-V) device characterization and photocurrent measurements under solar spectrum air mass 1.5 (AM1.5) simulating conditions. These are bulk methods that give an averaged and sometimes misleading set of information, due to slow charge detrapping from deep traps for example. New techniques called F-V/SMS (Fluorescence-Voltage Single Molecule Spectroscopy) and FV-TR-SMS (Fluorescence-Voltage Time-Resolved Single Molecule Spectroscopy) have recently been introduced as tools for measuring the chemical and physical state of single fluorescent nanoparticles in a functioning device. In these experiments rates and mechanisms for singlet exciton quenching by hole polarons, triplet exciton quenching by hole polarons, singlet quenching by triplets and interfacial charge transfer were determined for conjugated polymer nanoparticles in a functioning device. This is a new direction in materials spectroscopic research that opens opportunities for the design and optimization of functional organic materials by providing fundamental mechanistic understanding and structure function relationships at the molecular and mesoscale level.

Excitation-Emission Matrix Fluorescence Spectroscopy to Differentiate Among Classes of Microorganisms as Vegetative or Spore

Karl Booksh1, Burt Bronk2, Jeffrey Cramer1, Jozsef Czege2; 1University of Delaware; 2AFRL-APG Site

Excitation-emission matrix (EEM) fluorescence spectroscopy is employed to distinguish among cultures of gram positive and gram negative bacteria and vegetative bacteria, spores, and other background samples. Irradiation of the microorganisms with UV light induced changes in the EEM spectral fingerprints. For example, UV irradiation causes the weakly fluorescing calcium dipicolinic acid to blue-shift and increase in fluorescence intensity. Similarly, differences in the tryptophan spectrum can be seen following irradiation. Employing both pre- and post-irradiated EEM spectra for analysis by Parallel factor Analysis (PARAFAC) and subsequent partial least squares discriminant analysis (PLS-DA) shows the ability to differentiate among the four classes of microorganisms.

Attenuation of Mediator Leakage in Biofuel Cell Polymer Modified Electrodes: Synthesis and Characterization of a Perfluoroalkyl-modified 2,2′-bipyridyl Ruthenium Complex

Paul Jelliss1, Shelley Minteer2, Mitsesh Patel1, Michelle Watt; 2Saint Louis University

In biofuel cells where enzyme-electrode communication depends on mediated electron transfer, leaching of electronic mediator species from the immobilizing polymer membranes coating modified anodes and/or cathodes is problematic and can significantly diminish the running time of the device. Using standard methodology, we have synthesized the complex [Ru(2,2′-N2C10H6{(CH2)3(CF2)5CF3}2-4,4′)(k2-2,2′-bipyridyl ruthenium congener. Paul Jelliss1, Shelley Minteer2, Mitsesh Patel1, Michelle Watt; 2Saint Louis University

In biofuel cells where enzyme-electrode communication depends on mediated electron transfer, leaching of electronic mediator species from the immobilizing polymer membranes coating modified anodes and/or cathodes is problematic and can significantly diminish the running time of the device. Using standard methodology, we have synthesized the complex [Ru(2,2′-N2C10H6{(CH2)3(CF2)5CF3}2-4,4′)(k2-2,2′-N2C10H10)2], where one of the 2,2′-bipyridyl ligands bears terminal perfluorinated alkyl chains, in an attempt to exploit ‘like-dissolves-like’ intermolecular forces as an anchoring mechanism for the complex in Nafion membranes. Nafion thin films were cast or spin-coated onto electrodes and glass microscope slips, exposed to solutions of the complex and then examined by cyclic voltammetry and fluorimetry in a comparative study with tris-2,2′-bipyridyl ruthenium. Despite the fluorimetric verification of significant uptake of the ruthenium complex by the Nafion film, potentiometric analysis indicated drastically diminished charge transport properties in phosphate buffer solutions. Closer analysis of the electronic spectroscopic data suggests very different behavior of the fluorinated complex in Nafion compared with the standard tris-2,2′-bipyridyl ruthenium congener.

Luminescence Spectroscopy of Dye-doped Silica Nanoparticles and Quantum Dots

Swadeshmukul Santra; 1University of Central Florida

During the past couple of decades, nanoparticle based luminescent probes such as dye-doped nanoparticles, quantum dots have become quite popular for various bioimaging applications including cell/tissue imaging, imaging of intracellular components, cell tracking etc. It has been successfully demonstrated that these luminescent probes are much brighter and photostable than traditional organic dyes. Development of such luminescent probes requires robust nanoparticle design as well as appropriate synthesis.
techniques. For bioimaging applications, there is an additional but crucial synthesis step i.e. nanoparticle surface modification. In many cases, it becomes quite challenging to keep photophysical characteristics of these luminescent nanoparticles intact during the surface modification procedure. In this presentation, I will primarily focus on synthesis, characterization and photoluminescence characteristics of dye-doped silica nanoparticles and ultra-small CdS:Mn/ZnS quantum dots. However, this presentation will cover a systematic approach for the nanoparticle design, synthesis, surface modification and bioconjugation. In addition, future perspectives of nanoparticle based luminescent probes for bioimaging and sensing applications will be discussed.

(292) Artificial Nose Technology: Fluorescent Labeled DNA Optical Sensor Arrays with Enhanced Sensitivity and Selectivity for Detection of Biological Agents

Scott McWhorter1, C. Milliken1, R. Brigmon1, A. Walker2, J. White2, J. Kauer2; 1Savannah River National Laboratory; 2Cogniscent, Inc.

Events surrounding the attacks of 9-11 have led to increased efforts to prepare the US against potential biological terrorism, including agents that may be of unknown or recombiant microbiological threat (RMT) which also underscore the need for new technologies to selectively sense a broad array of traces of microbes and toxins. Researchers at the Savannah River National Laboratory along with Cogniscent Inc. have been studying a novel DNA detection technology which consists of single-stranded oligonucleotides with lengths of tens of nucleotide bases which exhibit different cross-reactive affinities towards defined recognition targets (i.e., flexible but selective). These DNA sequences are created from random sequences (non-specific) of about 20 nucleotides, and then labeled with a fluorescent dye which acts as the transduction mechanism. The advantages of such an approach are the ability to exert rational control over design, development, and deployment of sensing materials that can be uniquely specified, mass produced, have large combinatorial potential, and can be screened using high-throughput methods. This presentation will discuss the application of this novel DNA sensor technology to detect and distinguish among several Bacillus bacterial species.

(293) Numerical Simulations of Confocal Raman Spectroscopic Depth Profiles of Materials: A Photon Scattering Approach

Averil Macdonald1, Alun Vaughan2; 1University of Reading; 2University of Southampton

Confocal Raman Spectroscopy has long been the subject of considerable interest with the expectation that vibrational spectroscopic data could be obtained at high spatial resolutions (lateral ~1 mm: vertical ~2 mm) from within optically transparent media. Based on this assertion, the Raman response of many laminated polymer systems was reported, some of which suggested that the interface between even immiscible polymers is indistinct. This conclusion is not easy to understand on thermodynamic grounds. Consequently, the nature of the confocal response in Raman depth profiling came under scrutiny and, several models based upon geometrical optics have been proposed with the objective of explaining the forms of the Raman depth profiles that are obtained when focusing below the surface of transparent, single component materials. We set out to investigate the Raman depth profiles obtained from a series of semi-crystalline polymers that were chemically similar, but morphologically different. Since all our samples had equivalent refractive indices, and all were examined using identical optical instrumentation, all existing theories, would predict an identical depth profile response. Not surprisingly, the optical signal from high clarity materials is extinguished much less rapidly that that obtained from systems that are highly scattering. The implication is that, geometrical optical models are lacking in some fundamental physical respect that relates to the processes that occur within the specimen. We, therefore, present a very different approach to the problem which is based upon the concept of Raman photon generation from within an extended volume. We show that, despite its inherent simplicity, the physics behind our model is able successfully to predict the form of the depth profile for each material, something that has not been achieved by any model previously proposed, and that the parameters used in the model scale with independent physical measurements. Finally the model is used to account for the fact that useful Raman spectra can be obtained when the laser is focused as much as 40 mm above the sample surface.

(294) Probing and Predicting Low Frequency, Raman-active Lattice Modes in Pharmaceutical Drug Polymorphs

Mike Claybourn1, Graeme Day2; 1AstraZeneca; 2Cambridge University

Normal mode Raman spectroscopy has been successfully used for polymorph identification and quantification of pharmaceutical drug substances. The success of the analysis is based on the strength of perturbation of internal vibrational modes by structural changes in the crystal lattice. Published data shows peak shifting or intensity changes are the general observations. However, the effects are difficult to predict and invariably an intuitive approach is used for interpretation. In many cases, the effect is weak and limits the application for quantitative analysis. A more direct approach, and one that allows prediction and assignment of the spectral bands is to probe the lattice vibrational modes (phonons). These modes are sensitive to intermolecular interactions in the crystal lattice resulting from, for example, molecule orientation, packing, stacking and hydrogen bonding. For crystals of organic molecules such as pharmaceuticals, the energies for these modes are in the far infrared (typically 10 to 300cm-1) and can therefore, be probed using near-laser line Raman measurements. Generally, the temperature behaviour of phonons is different to normal modes and so they can be discriminated in the data analysis. Currently, there are a number of methodologies for the prediction of phonon modes characteristic of a polymorph. For the pharmaceutical systems described here, the approach is based on rigid body type calculations, either using observed or lattice energy minimised unit cell dimensions. This assumes separation between the inter- and intra-molecular modes. For many systems this may be a limitation.

(295) Raman at 2200 m Below Sea Level: Challenges and Opportunities

Brian Marquardt1; 1University of Washington

This presentation highlights the successful design, development and deployment of a fully submersible Raman instrument to depths greater than 2200m (7200 feet). The Raman instrument was designed and built for deployment to the ocean bottom by way of the Deep Submersible Alvin submarine for the in-situ analysis of hydrothermal vents. The submersible Raman system was completely designed and built from the ground up utilizing commercial hardware in the laboratory. It consists of a high resolution, high sensitivity commercial Raman instrument coupled to a Raman ballprobe immersion optic specially engineered for analysis at high pressure and temperature. Hydrothermal vents or “black smokers” are located over 2000 m below the surface of the ocean, which exist in a wildly turbulent state at high pressures (300 bar) and extreme temperatures (2-400° C). Hydrothermal vent fluid is also quite acidic (pH 2) compared to the surrounding ocean water; this combined with the depth, high temperature and pressure makes the study of this corrosive environment extremely difficult. Our current research involves the exploration of this environment to identify and quantify chemical species within hydrothermal
Future Meetings: FACSS 2008, September 28 – October 2, Reno, NV  •  FACSS 2009, October 18 – 22, Louisville, KY

vent fluid. Raman spectroscopy was chosen for this study due to minimal spectral interference from seawater and the ease of identifying unknown species by their characteristic vibrational frequencies. This presentation will describe the submersible Raman instrument design, the optical sampling requirements for vent deployment and present the Raman data from our most recent deployment in September 2007.

(296) First-Principles Analyses of Solid-State Terahertz Spectra
Timothy Korter1, Damian Allis1; 1Syracuse University
The investigation of advanced theoretical methods to model and predict the terahertz (THz) spectra of molecular solids (e.g. explosives) will be described with the goal of understanding the underlying chemical origins of experimental spectral features. Terahertz spectroscopy of solid-state samples has been utilized in a diverse number of fields, ranging from security applications to the pharmaceutical industry. These experimental THz investigations have demonstrated that many compounds have distinct absorption spectra that can be used for their detection, identification, and characterization. While the origins of these absorption features are generally attributed to intermolecular vibrations, intramolecular torsions, or even crystal lattice vibrations, the actual assignment of particular observed spectral features to specific atomic motions is rare. The assignment of these spectral features is crucial in understanding these characteristic THz spectra. The difficulty in assigning low-frequency THz spectra derives from the very nature of the vibrational motions. Broadly speaking, these motions can no longer be considered as localized atomic motions, like those encountered in the mid-infrared (e.g., O-H stretching modes). The THz frequency vibrational motions must be considered in a global sense where all of the atoms in the entire molecule are participating in the intramolecular or intermolecular motion. This global motion, particularly the intermolecular coordinates, leads to a complete failure of familiar single-molecule-based modeling approaches. A typical calculation treats the molecule of interest in isolation with no environmental interactions present. Our research group has directly addressed the limitations of isolated-molecule calculations by applying density functional theory (DFT) with periodic boundary conditions (PBC) in recent publications on the complete first principles analyses of the THz spectra of the high explosives HMX and PETN. These DFT calculations allow for the complete simulation of all internal and external vibrational motions and enable the explicit assignment of the THz absorption features in these spectra. In addition to these high-energy materials, details of the assignment of the THz spectra of biomolecules such as biotin and lactose will also be discussed.

(297) Standoff Raman HE Field Measurements: Issues Related to Standoff Detection
Chance Carter1, Mike Angel2, Joseph Kordas1, Darron Nielsen1, Will Hunt1, Michael Chrisp1, Fred Howland1, Jim Hill1, Bruce Henderer1, Richard Whipple1; 1Lawrence Livermore National Laboratory; 2Dept. of Chem., Univ. of South Carolina
Fieldable standoff Raman systems are being developed for a variety of applications including planetary measurements and forensic analyses (e.g. high explosives). We have designed and field tested such a system for detecting a variety of forensic-related materials at intermediate distances (10s of meters) in ambient light conditions. In the system to be described light is collected using a telescope which is fiber-coupled to an f/1.8 spectrograph with a gated ICCD detector and a pulsed laser source is used for excitation. The instrument development will be discussed along with specific issues related to standoff detection.

(298) A Piezoresistive Cantilever-Based Sensor for Gas-Phase Chemical Detection
Bradley Hart1, Timothy Ratto1, Albert Loui1, Thomas Wilson1, Erik Mukerjee1, Todd Sulcek1; 1Lawrence Livermore National Laboratory
A compact and low-power cantilever-based sensor has been developed and used to detect various vapor analytes including chemical warfare agents. This device is based on the static deflection of microcantilevers, which is measured via changes in piezoresistance rather than with a conventional beam-deflection method. By incorporating the signal transducer into the microcantilevers themselves, reliance on external optics is eliminated and the size and power consumption of the sensor is significantly reduced. The sensor elements currently consist of thermoplastic polymer coatings applied to the backside of each microcantilever. To ensure sensitivity to a diversity of analytes, a series of polymers have been selected with a range of physical and chemical characteristics, including polarity, glass transition temperature, and elastic modulus. The current device consists of an array of eight piezoresistive cantilevers with silicon nitride surfaces, six of which are functionalized and two assigned as references. Characteristic response patterns of differential deflection voltages were measured for a number of organic compounds, including ethyl acetate, methylene chloride, and sulfur mustard. Principal components analysis (PCA) was applied to the data. This qualitative analysis, which we have performed in real time, demonstrates that analytes can be rapidly distinguished based on their chemical identity and concentration.

(299) Gas Phase Photoacoustic Spectroscopy in the Long-Wave IR Using Quartz Tuning Forks and Amplitude Modulated Quantum Cascade Lasers
Michael Wojdik1, Mark Phillips1, Elizabeth Golovich1, Bret Cannon2, Rich Ozanich1, Jay Grate1; 1Pacific Northwest National Laboratory; 2JEOL USA Inc.
We demonstrate the performance of a novel long-wave infrared photoacoustic laser absorbance spectrometer for gas-phase species using an amplitude modulated (AM) quantum cascade (QC) laser and a quartz tuning fork microphone. Photoacoustic signal was generated by focusing the output of a Fabry-Perot QC laser operating at either 8.41 μm or 10.1 μm between the legs of a quartz tuning fork which served as a transducer for the transient acoustic pressure wave. The QC laser was modulated at the resonant frequency of the tuning fork (32.8 kHz). This sensor was calibrated using the infrared absorber Freon-134a by performing a simultaneous absorption measurement using a 35 cm absorption cell. The NEAS of this instrument was determined to be 2 x 10^-8 W cm / Hz^1/2, and the fundamental sensitivity of this technique is limited by the noise floor of the tuning fork itself. Sensitivity in excess of 1 ppbv to diisopropyl methylphosphonate was also demonstrated.

(300) Novel Method Development for Analysis of High Energy Peroxides by Raman Microscopy and Mass Spectrometry
Alvaro Peña-Quevedo1, Robert Cody2, Samuel Hernandez-Rivera3; 1University of Puerto Rico at Mayaguez; 2JEOL USA Inc.; 3TAMU
Characterization and detection of Triacetone Triperoxide (TATP) and hexamethene triperoxide diamine (HMTD) using Direct Analysis in Real Time Mode of Flight (DART-TOF) Mass Spectrometer. This study also presents the first method of detection for Tetramethylene Diperoxide Dicarbamide (TMDD) and other nitrogen based peroxides using Vibrational Spectroscopy and Mass Spectrometry. Analysis of acetone peroxides by GC-MS was also conducted. HMTD showed a clear peak of 209 m/z [M+H]^+ and small adduct peak of 226 m/z [M+NH4]^+ that allowed its detection in standards solution and lab made standards.
Method development for trace detection will be compared with studies conducted to compare results with DART-TOF. All samples were analyzed to compare results that could differentiate from HMTD absent. TATP samples with deuterium enrichment are being [M+NH4]+, and the peak of 223 m/z or 222 m/z is completely m/z [M+NH4]+. TATP showed a single peak at 240 m/z [M+NH4]+, and the peak of 223 m/z or 222 m/z is completely m/z [M+NH4]+. TMDD presented mixture of peaks with a base peak of 101 m/z, and the peak of 223 m/z or 222 m/z is completely m/z [M+NH4]+. TATP showed a single peak at 240 m/z [M+NH4]+, and the peak of 223 m/z or 222 m/z is completely m/z [M+NH4]+. TMDD presented mixture of peaks with a base peak of 101 m/z, and the peak of 223 m/z or 222 m/z is completely m/z [M+NH4]+. TATP showed a single peak at 240 m/z [M+NH4]+, and the peak of 223 m/z or 222 m/z is completely m/z [M+NH4]+.

(301) Examination of Forensic Evidence by Hyperspectral Imaging
Diane Williams1, Hina Ayub2; 1Federal Bureau of Investigation; 2Oak Ridge Institute of Science Education
The detection and visualization of obliterated writings that were undecipherable using traditional techniques, have been accomplished through the use of visible-near infrared and short wave infrared hyperspectral imaging systems and thermal video imaging systems. The results will be presented in the context of relevance to forensic examinations as well as application of the techniques to analyze additional samples types.

(302) Vibrational Spectroscopy, Microscopy and Imaging: Applications to Skin Pharmacology and Biochemistry
Richard Mendelsohn1, Guojin Zhang2, Andrew Chan3, David Moore4, Ryan Pensack5, Bozena Michniak6, Carol Flach7; 1Rutgers University; 2ISP Corporation
Vibrational Microscopy and Imaging: Applications to Skin Pharmacology and Biochemistry: Richard Mendelsohn, Guojin Zhang, K. L. Andrew Chan, David J. Moore, Ryan Pensack, Bozena B. Michniak-Kohn and Carol R. Flach Vibrational microscopy and imaging are now poised to address important biomedical issues, including the diagnosis of pathological states. Skin provides a unique opportunity for extending vibrational spectroscopic imaging to diverse areas including drug delivery, drug metabolism, and single cell biochemistry. Recent studies from our laboratory that auger well for vibrational microscopy applications to a variety of tissues will be discussed as time permits, and include the following: 1) Liposomes have long been touted as potential drug delivery vehicles, with some success in practice. Both IR imaging and Raman microscopy have been used to monitor the extent of permeation into skin of several preparations of phosphatidylcholine vesicles, which differ in vesicle size and in lipid physical state. 2) Pro-drugs are used to enhance the delivery of therapeutic agents into skin, where they are hydrolyzed by enzymes and converted to the chemically active form of the drug. We have demonstrated the feasibility of tracking and spatially imaging, via confocal Raman microscopy, the prodrug-to-drug inter-conversion for a derivative of 5-fluorouracil, a well-known anti-cancer agent and for a derivative of resveratrol, the main anti-oxidant from red wine. 3) Proper wound healing entails a complex spatial and temporal series of events. Preliminary vibrational microscopy measurements provide evidence for the spatial evolution of a variety of collagen structures and orientation that appear during the sequence of the healing process. Our goal is to correlate phenotypes with the sequence of genes that regulate the healing events.

(303) Increased Process Understanding through use of in-situ Vibrational Spectroscopy
Katherine Bakeev1, Susan Barnes1, Stacie Calad1, Jun Chen1, Robert Herrmann1, Juliet McComas1, James Rydzak1, Eric Voight1; 1GlaxoSmithKline
In development of new processes, there are many opportunities in applying various tools for process understanding – be it the formation of side products, consumption of reagents, degradation of product, reaction kinetics, polymorphic transitions, etc. As industry faces increasingly aggressive development timelines, and demands higher quality products, the application of in-situ tools for analysis during development becomes more widespread. We have used in-situ monitoring by FTIR, NIR and Raman spectroscopy to gain better insight into some of our processes. For development of new synthetic routes, FTIR has been used to understand the reaction kinetics and achieve better reaction control. In other experiments we have been able to elucidate the decomposition of a key reagent whose inconsistent performance was ill-understood. Raman and NIR spectroscopy have been used as tools to monitor a polymorphic transition of a drug substance and verify not only that the process is very rapid, but that the kinetics of undesired transformations is different from the formation of the desired polymorphic form.

(304) Spectrophotometric Methods for Estimation of Acenocoumarol in Bulk and its Pharmaceutical Dosage Forms
Sunil Makwana1, LakshamanBhai Patel1, Tejas Patel1, Tushar Patel1, Kirit Patel1, Timar Patel1, Amit Patel1, Ankita Mehta2; 1Faculty of Pharmacy, Dharmsinh Desai University; 2R.P.College of Pharmacy, Changa; 3Department of Pharmaceutical Analysis, University of Western Ontario
Four simple, sensitive, accurate and precise visible spectrophotometric methods (A, B, C and D) have been developed for the quantitative estimation of acenocoumarol in bulk drug and pharmaceutical formulations (tablets). Method A is based on the reaction of reduced acenocoumarol with aromatic aldehyde, paradimethylamino cinnamaldehyde (PDACA) producing colored Schiff’s bases at the ëmax (nm) 527.5 nm and. Method B is based on the reaction of reduced acenocoumarol with aromatic aldehyde, paradimethylamino benzaldehyde (PDBA) in acidic condition producing colored Schiff’s bases having ëmax(nm) at 441.5 nm. Method C is based on the oxidation followed by coupling reaction of reduced acenocoumarol with 3-methyl-2-benzothiazolinone hydr azone (MBTH) in presence of Ceric ammonium sulphate to form green colored chromogens at ëmax(nm) 585.0 nm. Method D is based on the reaction of reduced acenocoumarol with folin’s (1, 2-naphthoquinone-4-sulphonate) reagent to form brown colored chromogens at ëmax (nm) 480.0 nm. Beer’s law is obeyed in the concentration range of 2-10 µg/mL for Method A, 5-25 µg/mL for method B, 20-100 µg/mL for Method C and 2-12 µg/mL for Method D. The reduction of acenocoumarol is carried out with zinc dust and hydrochloric acid at room temperature in methanol. The results obtained with proposed are in good agreement with labeled amounts when marketed pharmaceutical formulations are analyzed. The results of analysis have been validated statistically and by recovery studies.

(305) Capabilities of a Desolvating Nebulizer System with Multicollector ICP-MS
Fred Smith1, CETAC Technologies
Multicollector ICP-MS instruments are specialized devices for high-precision isotope ratio measurements. For the introduction of liquid samples, there are a number of essential features for the sample introduction system: low-flow capability (< 100 microliters/min), enhanced ICP-MS sensitivity, reduced solvent-based interferences, and resistance to hydrofluoric (HF) acid. In addition, fast analyte washout is desirable, particularly for memory-
prone elements such as thorium. This paper will describe a desolvating nebulizer system that couples an adjustable PFA (perfluoroalkoxy) low-flow nebulizer with a PFA spray chamber and an inert membrane desolvator. This system will be applied with multicollector ICP-MS for U-Th dating studies. A new rapid washout feature will be described. Important figures of merit will include enhancement of Th and U signal and reduction of ThF⁺ and UH⁺ interferences.

(306) Analysis of Biodiesel and Petroleum Products Utilizing a Simultaneous CCD Detector ICP-OES System
Doug Shraden, Steve Wall, Andrew Ryan; Varian, Inc.
Over the last few years, the production and use of biodiesel has increased dramatically. Pure biodiesel (B-100) contains no petroleum diesel but is blended with petroleum diesel in some cases. It can be used in conventional diesel engines without significant modifications. Biodiesel is biodegradable, non-toxic and provides significant reduction of pollutants such as sulfur and aromatics. It is considered an important alternative fuel source. ASTM has adopted a specification for pure biodiesel (ASTM D 6751) that is to be used in blends up to 20% with diesel. Some state's are also requiring total Ca, Mg and Na/K to be determined. Concentration of these six inorganic components can effectively be determined using ICP-OES techniques. Current requirements and methods for biodiesel products will be reviewed. The simultaneous CCD detector ICP-OES system utilized and method parameters developed for the analysis of these products will be discussed. Results for biodiesel and petroleum based samples will be presented.

(307) Homogenous Fluorescence Resonance Energy Transfer Assays for Identification of Inhibitors of Angiogenesis and Anthrax Toxin Receptors Using High Throughput Screening
Kenneth Christensen, Michael Rogers, Junhong He, Nalini Anumula; Clemson University; Children's Hospital Boston; Harvard Medical School
We have developed, optimized, and performed pilot screening using homogeneous fluorescence resonance energy transfer assays to identify small molecules that inhibit the protein-protein interactions between anthrax protective antigen (PA) and the anthrax toxin receptors capillary morphogenesis gene protein 2 (CMG2) or tumor endothelial protein 8 (TEM8) using high throughput screening. Competitive binding of PA to these receptors has recently been shown to inhibit angiogenesis and tumor growth. As a result, identification of inhibitors will provide leads for valuable therapeutics against angiogenesis-dependant diseases such as cancer, macular degeneration, and others. The first step in anthrax intoxication involves the binding of PA, an otherwise non-toxic component of the multimeric anthrax toxin, to the cell surface receptors TEM8 and CMG2 with high affinity. Our assay takes advantage of these specific interactions. A cysteine mutant of PA (PA E733C) was labeled with a donor fluorophore (Alexa Fluor 488) while soluble receptor binding domain truncation mutants were labeled with an acceptor fluorophore (Alexa Fluor 546). When mixed at equimolar ratios, significant energy transfer was observed. These assays have been converted to work in a 384-well format and optimized for reproducibility, robustness, stability, and sensitivity. Typical \( z^2 \) values for these assays under screening conditions were >0.90. We have pilot this assay using a library of ~3000 bioactive compounds at the New England Research Center of Excellence (NERCE). Three compounds showed activity in this assay and have been tested in various secondary assays. A detailed analysis of assay performance and pilot assay results will be presented.

(308) Interchaining role of Donor and Acceptor in a Fluorescence Resonance Energy Transfer Experiment
Erasus Gatehe1, Punit Kohli; Southern Illinois University
The stress-induced electronic absorption transition of polydiacetylene (PDA) offers a unique opportunity to investigate interchanging roles of donors and acceptors in fluorescence energy transfer (FRET) without violating the law of nature that the energy flows “down hill”. Using PDA and lissamine rhodamine (LR) pair, we have demonstrated the energy donor and energy acceptor molecules can interchange their roles. We have shown that when the PDA is in red form, it acts as a donor, whereas LR acts as an acceptor. However, in its blue-PDA form, PDA acts as an acceptor whereas LR is an donor. LR utilizes its absorption and emission properties to reversibly acts as donor and acceptor depending on the nature of PDA. To our best of knowledge, this is the first example demonstrating the interchanging roles of donor-acceptor and offers a unique and fast way of studying FRET systems. We have also investigated the effect of donor-acceptor ratios on the FRET efficiency, and the experimental FRET efficiency is compared with theoretical FRET efficiency. Finally, we will describe reversible interchanging roles of donors and acceptors over many thermo-chromatic cycles in an modified-PDA-LR liposomal system.

(309) Light Activated Switch for Artificial Ion Channels
Our target is the engineering of a light sensitive gate for artificial ion channels. To design a rigid but reversible switch mechanism is crucial because most of the artificial ion channels known so far miss any control mechanism. The absence of control severely limits their applications in technical environments. The designed gate will drive the artificial ion channels to operate successfully as molecular switch in microfluidic systems, in biomimetic sensors and various technical devices. Our entered system is divided in two regions: the gate part and the body part. The gate part is based on light-responsive azo groups. These groups are attached to the transmembrane artificial ion channel body part formed by calix[4]resorcinarene. Key of controlling mechanism is the conformational change between cis and trans isoforms, which is translated into movement of the gate. The switch is quite resistant and can block or can let the ions to pass through artificial ion channel. Channel activity will be suppressed and reversibly revived by UV-Vis irradiations. Informations about artificial channel activity are provided by the Patch Clamp technique, commonly used for electrophysiological analysis.

(310) Stability of Phosphorus in Stool Samples Measured by ICP-AES and ICP-MS
Ela Bakowska, Anthony Costantino, Anna Foror; Gulo Gigolashvili; NMS Labs
Phosphorus is crucial in maintaining strong, healthy bones and teeth. It is important for the cells for energy storage and nerve function. The amount of phosphorus (as phosphate) in blood is regulated by the parathyroid hormone (PTH) and by controlling phosphate absorbed from the food and excreted in urine and stool. People with severe malnutrition, impaired kidney function, or who use diuretics or aluminum-containing antacids, suffer severe alcohol intoxication, or severe burns have depleted phosphate levels (hypophosphatemia). People with kidney failure have excess phosphate build up in blood (hyperphosphatemia). Phosphorus levels in blood can be controlled through diet, dialysis and phosphate binders. Phosphate binders help to pass excess phosphate into stool by combining with phosphate to form compounds that are...
not absorbed by blood. Phosphorus in hundreds of stool samples was measured by Inductively Coupled Plasma – Atomic Emission Spectroscopy (ICP-AES). The measurements of Phosphorus in stool by ICP-AES were compared with the results obtained by Inductively Coupled Plasma – Mass Spectrometry (ICP-MS). In their standard configurations, ICP-AES and ICP-MS can only handle liquid samples. The homogenized stool specimens were acid digested prior to the analyses. A dedicated microwave digestion system (ETHOS 1200 with Teflon micro inserts) facilitated high throughput of samples: 60-90 per day. The concentrations of Phosphorus as determined by the method of standard additions were compared with the results obtained against external calibration (aqueous standards). Accuracy and precision data will be presented. The short-term (days and weeks) stability of phosphorus in stool samples and the long-term (6-15 months) stability of phosphorus in stool samples were evaluated. Also the stability of phosphorus in digestates will be presented.

(312) Application of 1H-NMR to Screen Cell-culture Media Additives: Evaluation of Data Pre-processing Methods and Selective Chemical Variation
Julie Wei1, Maureen Lanan1; 1Biogenidec Inc
Metabolomic techniques using NMR are investigated for the comparison of complex media additives used in commercial cell-culture processes. Data pre-processing is found to be critical to facilitate spectral interpretation by reducing noise caused by variations in the sample pH and age and slight variations in the magnetic field. In this presentation, data preprocessing methods such as line broadening, binning, local peak alignment and orthogonal signal correction (OSC) are evaluated in light of our knowledge of cell-culture variations due to a media additive. The combination of selective chemical variation and OSC is found to be a simple and robust method to reduce misleading chemical variation and noise.

(313) Protein Separations Using Polyelectrolyte Multilayer Coatings with a Molecular Micelle: Optimization and Stability of Coatings
Candace Luces1, Sayo Fakayode1, Mark Lowry1, Ishia Warner1; 1Louisiana State University
Novel polyelectrolyte multilayer (PEM) coatings were constructed for the enhancement of protein separations in open tubular capillary electrophromatography (OT-CEC). The effects of four different cationic polymers (poly-L-lysine, poly-L-ornithine, poly-L-lysineserine, and poly-L-glutamic acid-lysine), and three anionic polymers, the molecular micelles sodium poly(N-undecanoyl-L-leucyl-alanine) (poly-L-SULA), sodium poly(N-undecanoyl-L-leucyl-valinate) (poly-L-SULV), and sodium poly(undecylencyl sulfate) (poly-SUS) were investigated as potential PEM coatings for protein separations. The simultaneous effects of cationic polymer concentration, number of bilayers, temperature, applied voltage and pH of background electrolyte on the separation of four basic proteins (α-chymotrypsinogen, lysozyme, ribonuclease A and cytochrome c) were analyzed using a Box Behnken experimental design. The results indicated that the optimal coating types were very dependent on the cationic and anionic polymers used in the PEM coating. Also, the two chiral molecular micelles (poly-L-SULA and poly-L-SULV) resulted in higher protein resolution as compared to the achiral molecular micelle, poly-SUS. The highest resolution was obtained using rinse times between 5 and 15 minutes suggesting optimal interactions with the wall coating. Furthermore, studies involving the interactions of denatured proteins with PEM coatings resulted in greater PEM-protein interactions. In addition, the influence of NaCl on the run to run reproducibility of the PEM coatings for the protein separations was investigated for each cationic polymer. All cationic polymers exhibited excellent reproducibilities with a %RSD of the EOF of less than 1% in the presence of NaCl in PEM coatings. Confirmation that these separations involve wall interactions, and thus a CEC process, is also provided.

(314) New Spectroscopy Reference Tool for Academic Research and Teaching
Donald Tucker1, Leo Collins1, Gregory Banik1, Marie Scandone1; 1Bio-Rad Laboratories, Inc., Informatics Division
The role of spectroscopy in academic research and teaching is clear and long-standing. Spectral reference sources began in the 1950’s with the publication of print handbooks of IR, NMR, and other spectral and chromatographic data. The hardcopy era gave way to the electronic age with the advent of personal computers and the digitization of spectral data in the 1980’s. Since then, the number of available spectral collections as well as the power of the informatics tools required to manage the collections have continued to grow. In order to satisfy the scientific community’s need for information, we are presenting spectral databases and software tools for academic research and teaching. This presentation will describe a powerful combination of reference data, tools, and technology that will assist faculty and students in their scholarly research as well as train students in the skills and technologies that they will utilize once they leave academia.

(315) Controlled Particle Deposition by Design of an Electrochemical Adsorption Cell
Fatemeh Abniki1, Ehsan Bakhshi2, Majid Mosalla3; 1Pardis group of National Petrochemical Co. & Isfah; 2National Petrochemical Co. & NIOC R&D C; 3Materials Science Dept. of Shiraz Unive Deposition of colloidal particles substrate is encountered in a variety of naturally occurring processes such as particulate fouling of heat exchangers, thrombus formation in vascular prostheses and other artificial organs and aerosols entering the lungs. Deep bed filtration of waste waters is perhaps the most prominent example of importance to industry. Design of an electrochemical adsorption cell utilizing reticulated vitreous carbon (R.V.C.) as the working electrode, stainless steel as the counter electrode and a cellulose acetate membrane, for separating the anodic and cathodic, is described for the separation of 5.4 μm polystyrene latex colloidal particles from a KCl solution. The experimental results are compared with Derjaguin-Landau-Verwey-Ovdrbeek (D.L.V.O.) prediction for the occurrence of favorable and unfavorable deposition conditions. In the theoretical section of this work it will be assumed that the main energies contributing adsorption interaction between the surfaces will be due to electrical double layer to Van der Waals attraction. The some of these energies provides the total interaction energy between surfaces and this constitutes the underlying assumption for the classical D.L.V.O. theory of colloidal stability. In order to observe solely the effect of these forces the effect of hydrodynamic interactions has to be kept at a minimum. Therefore experiments carried out were directed mainly at finding out the dividing line between hydro dynamically-controlled and electro statically-controlled processes. In this way, for the present experimental conditions the main forces contributing to deposition process are the surface forces and hydrodynamics. At the highest flow rate of 34 cm3/min the colloidal forces were shown to be negligible compared to the hydrodynamics. Indeed the effect of surface at the KCl concentration of 0.001 mol/dm3 apparently only become significant at flow rate of 1.7 cm3/min. At this flow rate and KCl concentration of 0.001 mol/dm3 experimental results show clear evidence of conditions governing the of favorable and unfavorable deposition conditions. The variation of collector potential under unfavorable deposition condition does not produce large changes in the deposition rate whereas variation collector
potential under favorable condition produce significant change in
the deposition state.

(316) Mass Spectrometric Speciation of Ultrafine Particulate Matter Formed by the Ozonolysis of Household Volatile Organic Compounds
Kara Huff Hartz1, Hardik Amin1, Meagan Hatfield1; 1Southern Illinois University

Particulate matter (PM) pollution is detrimental to public health and indoor air quality. The toxicology of PM is not known, and the myriad of sources and chemical components of PM require investigation. One source of PM in indoor environments is the reaction of ozone with household volatile organic compounds (VOCs), where some of the products have reduced volatility and partition into PM. Recent work has shown that some household air fresheners and cleaners contain VOCs such as monoterpenes, which react with ozone and produce PM at levels that degrade air quality. The reaction products from this PM source are not known. To address this issue, PM is generated in 5.5 m³ Teflon reaction chamber by exposing individual household products to ozone. The mass concentration of PM generated by the ozonation reaction is measured by scanning mobility particle size spectrometry. PM samples are collected onto quartz filters. Solvent extraction removes PM from the filters, the extracts are concentrated, and the analytes are converted to their trimethyl silyl ester and ether products. The extracts are analyzed by a Varian gas chromatograph with mass spectrometric detection using electron impact and chemical ionization. The analysis of the ion fragments produced in the ion trap enable the identification and quantification of the chemical species found in PM. The product characterizations are used in conjunction with measures of the concentration of PM to determine which household VOCs are prone to PM formation and predict their toxicity.

(317) Determination of Dissolved and Colloidal Silver in Water Using Colorimetric-Solid Phase Extraction
Robert Lipert1, April Hill1, Marc Porter2; 1Iowa State University; 2Arizona State University

The increased antibiotic resistance exhibited by many bacteria today has led to resurgence in the use of silver as an antibacterial agent in a wide range of applications, e.g., in food-storage containers, air fresheners, washing machines and the drinking water treatment system on International Space Station (ISS). However, there are growing concerns that the colloidal silver in wastewater may pose risks to human health and to beneficial bacteria and aquatic organisms, which has led to recent regulation of colloidal silver by the FDA and EPA. As a possible approach to meet the resultant monitoring needs, we have developed a rapid, simple method for determining silver in both dissolved and colloidal forms. The technique can measure dissolved silver in aqueous solution at concentrations between 0.1 and 1.0 ppm, which spans range mandated by the ISS Medical Operations Requirements Document. The method is based on colorimetric solid-phase extraction (C-SPE) and involves the extraction of silver(I) from water samples onto a solid-phase membrane that has been impregnated with the selective colorimetric reagent dimethylaminobenzylidene rhodanine (DMABR). Silver(I) exhaustively reacts with DMABR to form a colored compound, the amount of which is measured by a handheld diffuse reflectance spectrophotometer. Total silver is determined by first passing the sample through an inline cartridge containing Oxone, which converts colloidal silver to dissolved silver(I). The method, which requires less than 2 min per analysis, has been validated through comparison with ICP-MS analysis of water from the Russian segment of ISS, which contains colloidal silver.

(318) Assessing the Impact of Hurricane Katrina on Nutrients and Algal Growth in Lake Maurepas
Phillip Voegel1, Kellie Silcio1, Kristy Ball1; 1Southeastern Louisiana University

Following Hurricane Katrina, human population density surrounding Lake Maurepas and its associated rivers has increased. The stress of additional human population on water treatment facilities may lead to higher levels of nutrients in Lake Maurepas and ultimately to increasing levels of algal growth. During summer months, warm temperatures may, in conjunction with increased algal growth, lead to decreasing dissolved oxygen concentrations. Low oxygen concentrations for extended periods of time are likely to adversely affect commercial and recreational fishing in the lake. Current levels of phosphate, nitrate, and dissolved oxygen will be compared to pre-Katrina levels and correlated with the amount and types of algae present in the lake. Algal speciation is completed using both traditional light microscopy and by mathematical analysis of liquid chromatography of algal pigments.

(319) Ultra-Trace Beryllium Determination by a Fluorescence-Based Field-Portable Method
Kevin Ashley1, Anoop Agrawal2, T. Mark McCleskey3; 1CDC/NIOSH; 2Berylliant, Inc.; 3Los Alamos National Laboratory

A highly sensitive molecular fluorescence method for measuring ultra-trace levels of beryllium in workplace samples has been developed. The procedure has been validated and published in the NIOSH Manual of Analytical Methods and as an ASTM International standard. Extremely low detection limits for beryllium in air filter and surface wipe samples will be necessary in view of expected decreases in applicable occupational exposure limits (OELs) for this element. The overall analytical method entails extraction of beryllium workplace samples by dilute ammonium bifluoride (NH₄HF₂, aqueous), followed by filtration and fluorescence detection using the high-quantum yield fluorophore, hydroxybenzoquinoline sulfonate (HBQS). This work will present an overview of the method development, interlaboratory evaluation, interference tests, detection limit estimations, uncertainty calculations, etc., to which the method was subjected. Attributes of the NH₄HF₂ extraction — HBQS fluorescence technique include method detection limits (MDLs) of <0.8 ng to ≤2 ng Be/sample (depending on the fluorometer used), quantitative recoveries from beryllium oxide, a dynamic range of several orders of magnitude, and freedom from interferences. Other key advantages of the technique are field portability, low cost, ease of use, and high sample throughput. The method performance compares favorably with that of inductively coupled plasma-mass spectrometry (ICP-MS).

(320) Macro ATR Imaging – Another Imaging Solution
David Drapcho1, Ellen Miseo1; 1Varian, Inc

Infrared imaging using a focal plane array detector is now a mainstream spectroscopic technique. The method provides both spatial and spectral information on a variety of samples. Traditionally, attenuated total reflectance (ATR) methods have extended the power of infrared spectroscopy to samples that are neither reflective nor thin enough to be examined in transmission. ATR imaging (using an ATR crystal with a spectrochemical imaging system, US Patent #6141100) is a relatively new technique that has the same ease of use and sampling capabilities as ATR does for single point analysis. In addition, ATR imaging provides increased spatial resolution. In a macro accessory and coupled with a focal plane array detector, spectral and spatial information of a sample with micrometer size domains can be obtained. A recent advance in this technique is the introduction of the Specac Imaging Golden Gate ATR accessory. This accessory, designed to preserve
the infrared image to the focal plane array, makes analysis of samples not amenable to transmission or specular reflection easy. ATR provides an enhancement in spatial resolution. This image shows a calibration sample with lines of photot resist on glass. Each line is 10 micrometers wide. The large sample accessory, where the Imaging Golden Gate is used, is designed to image 1:1. In normal transmission mode the spatial resolution on the system is 40 microns per pixel. With the imaging Golden Gate there is an enhancement in the spatial resolution due to the effect of the refractive index of the ATR crystal in the accessory. Examples of samples analyzed using the imaging Golden Gate will be presented and we will discuss the ease of use of the system.

(321) Accurate Determinations of Ge Atom Fractions in SiGe Semiconductor Chips Using High Performance ICP-OES
Savelas Rabb1, Michael Winchester1, Lee Yu1; 1National Institute of Standards and Technology
Silicon germanium (SiGe) technology has played a significant role in the development and success of the wireless and computer industries. The fabrication process using this technology is very similar to that for silicon-based chips. Therefore, only small changes in production are required, allowing for lower costs. Also, SiGe devices can be smaller, with reduced noise and higher frequencies, while maintaining the same low power requirements as Si devices. These favorable qualities make SiGe technology competitive with more expensive counterparts based on group III-V semiconductors, such as gallium arsenide (GaAs) and indium phosphide (InP). As the popularity of SiGe technology continues to advance in today’s electronics market, characterization of these semiconductors becomes more vital. We have developed an inductively coupled plasma optical emission spectroscopic (ICP-OES) method that can be used to determine accurately and precisely the Ge atom fractions in SiGe alloys. This approach eliminated the need to measure the mass of the chip, thereby avoiding a potentially significant source of uncertainty. Digestions of the chips occurred in the presence of HF/HNO3 at room temperature in closed vessels to prevent the loss of Si as volatile SiF4. Recoveries of both Si and Ge in these digests were observed to be effectively 100%. For the Si determinations, NaOH was introduced to reduce Si background and memory. Expanded uncertainties (95% confidence) associated with the determined Ge atom fractions, accounting for all significant components of uncertainty, were observed to be ~ 0.2 %.

(322) Monitoring Changes in Protein Structure and Hydration in Food Materials with FT-IR, FT-Raman and Fluorescence Spectroscopy
Allen R Muroski1, Douglas L Elmore1, Sean A Smith1, Carrie A Lendon1, Janiece L Hope1, Stefan K Baier1, Jodi A Engleson1, William R Aimutis1; 1Cargill
High protein nutritional bars are popular sources of supplemental protein. At the time of preparation, the bars have a relatively soft texture that is appealing to most consumers. Unfortunately, with time the bars become firmer – a trait that limits the product’s shelf life. The firming process is poorly understood – although it is known that protein-water interactions play a key role. To better understand the firming process at the molecular level, we performed an accelerated shelf life study using infrared, Raman and fluorescence spectroscopy. In this study, experiments were performed on simple model protein bars that contained soy protein isolate, glycercel (as a texturizer), fructose (as a sweetener) and water. Experiments were performed with and without low-level additions of sodium sulfate. Sulfite is a common food additive used to inhibit Maillard reactions, which can influence color, flavor and texture. After preparation, the bars were stored at three different relative humidities at 37°C for 14 days. We used Infrared and Raman spectroscopy to obtain information about protein secondary structure, hydrogen-bonding and water content, and fluorescence spectroscopy to obtain information about the tryptophan side chain environment. Results will be presented and discussed. Our group has developed a variety of methods for monitoring molecular level events associated with protein-water interactions. Some of the methodologies used in this study will be presented and discussed in terms of utility, strengths and limitations.

(323) An Infrared PLS Approach for Compositional Analysis of Polycarbonate, SAN, and Rubber Alloys
Roger Hurst1, Lei Li1, James DeRudder1, Yuyuan Liu2; 1SABIC Innovative Plastics; 2WR Grace
The demands for hydrolytic stability and improved impact resistance of polymer alloys have greatly expanded their compositional complexity, presenting new challenges for infrared compositional analyses. Traditional mid-infrared approaches have used band ratios to calculate the relative amounts of each structural element. These were converted to polymer amounts using a unique structural element followed by serial subtractions from the composite. The new polymer systems contain polycarbonate (PC), styrene acrylonitrile resin (SAN), and two rubber components. These components have several common elements: three of the components contain styrene and two contain butadiene. Butadiene in the components exists as three different microstructures (cis, trans, and vinyl) where their relative amounts can be controlled with the polymerization conditions. These common elements contribute to uncertainty associated with serial subtractions; therefore, the traditional approaches are not readily applicable to the new polymer systems. The current work describes a partial least squares (PLS) approach that calculates the polymer percent composition directly instead of using prediction of monomer/microstructure contents. Following development at one plant site, the procedure was tested at multiple sites. A statistically designed subset of samples was used for correction of the main calibration at each site so that recalibration was not required. Data will be presented demonstrating its robustness to translation and correction.

(324) Development of a Portable Ringdown Spectrometer for CO2, CH4, and C-13 Isotope
Chuji Wang1,2, Nimisha Srivastava1, John Cambre2, Bryan Jones3; 1Dept. Physics and Astronomy, MSU; 2ICET, MSU; 3Dept. of Electrical and Computer Eng. MSU
Development of a Portable Ringdown Spectrometer for Greenhouse Gases and Carbon. Carbon sequestration (capture, transport, and storage of CO2) will play a significant role in the reduction and control of greenhouse gas (GHG) emissions. One of the technological challenges in the measurement, monitoring, and verification of CO2 in the process of capture, transport, and storage of CO2 is to rapidly quantify small variations of CO2 concentrations over a high concentration base, e.g., 380 ppm and to confidently discriminate the source of CO2 from its surroundings. This paper discusses the development of a portable spectral analyzer capable of simultaneously detecting CO2, CH4, and C-13 isotope with high sensitivity and accuracy using diode laser cavity ringdown spectroscopy. Several novel approaches in the instrumentation, such as optical configuration, instrument case, and electronic packaging, will be discussed.
ABSTRACTS

(325) Improved in situ Measurements of Lead Isotopes in Silicate Glasses by LA-MC-ICPMS using Multiple Ion Counters
A. Kate Souders1,2, Paul Sylvester1,2,3Micro-Analytical Facility, INCO Innovation Centre; 4Dept. of Earth Science, Memorial Univ.
A new technique that improves the spatial resolution and detection limits of the measurement of lead isotope ratios in silicate glasses with 15 ppm total Pb by laser ablation-multicollector magnetic sector-inductively coupled plasma mass spectrometry (LA-MC-ICPMS) is presented. The method allows for the concurrent, static measurement of 204Pb, 206Pb, 207Pb, 208Pb, along with 202Hg and 235U, in six Multi-Ion Counters (MICs) fitted on a Finnigan NEPTUNE MC-ICPMS. Use of a collector array consisting only of MICs eliminates the need for cross calibration between Faraday cups and ion counters, as employed in previous methods reporting 204Pb values by LA-MC-ICPMS. Standard-sample-standard bracketing using BCR-2G as the calibrant is used to correct for instrumental mass bias. Accuracy and precision of the method was evaluated by replicate analyses of various MPI-DING reference glasses, with low Pb concentrations (1.38 to 11.6 ppm total Pb) and well-determined isotopic ratios. Typical spot sizes for in situ analyses ranged from 40-69 microns, providing better spatial resolution than previous LA-MC-ICPMS reporting 204Pb. Due to the high sensitivity of the MICs, the Hg-correction of the measured 204-mass was significant, especially for samples with < 5 ppm total Pb. Two different methods were used to correct for Hg on the 204-mass with the results agreeing within error for each method on all lead isotope ratios. Measured lead isotope ratios for the MPI-DING reference glasses T1G (11.6 ppm Pb) and ATHO (5.67 ppm Pb) agree within 0.10% and 0.16% respectively of the accepted values. For MPI-DING KL2G (2.9 ppm Pb) and ML3B (1.38 ppm Pb), measured Pb ratios involving 204Pb agree within 1% of the accepted values with typical precisions of < 2.9 % RSD (2 sigma). The results for KL2G and ML3B demonstrate improvement over previous LA-MC-ICP-MS data in terms of both detection limits and spatial resolution, while retaining similar levels of accuracy and precision. This new method provides the capability of making quantitative in situ lead isotope measurements on tiny objects of geologic interest such as mineral growth bands, melt inclusions, and accessory minerals, even where they are lead poor.

(326) Direct Chromium Speciation in Solid State Materials - A GDMS Approach
Na Zhang1, Jennifer Robertson-Honecker1, Alex Pavkovich1, Melissa Pablic1, Fred King1, West Virginia University
The toxicity of Chromium is closely related to its oxidation state. Chromium V1 (CrVI) is toxic and a possible carcinogen, whereas chromium III (CrIII) is an essential trace element for living organisms. A pulsed glow discharge time-of-flight mass spectrometry method was developed for the direct speciation of chromium in solid state samples. The millisecond pulsed glow discharge is a versatile ion source that can provide elemental, structural and molecular information. By tuning the operating parameters, the plasma chemistry is adjusted to favor cluster ion formation. Similar to prior results reported by others for secondary ion mass spectrometry, unique cluster ions are identified that permit the differentiation between CrV1 and CrIII in chromium oxide samples. Specifically, signals at 104 and 120m/z, corresponding to C2+ and C2O+ cluster ions, are indicative of CrVI, whereas signal at 160m/z, attributable to CrO3+, is indicative of CrIII. The impact of glow discharge operating conditions on the appearance of these characteristic cluster ions and speciation of Manganese oxides is also discussed.

(327) Drug Screening Applications Using GPC Spin Columns with HPLC/ESI-MS
Marshall M. Siegel1, Wyeth Research
The high throughput screening HTS methodology has been the technique of choice of pharmaceutical companies to initially screen corporate libraries for exploratory drug leads by developing methods that mimic the cellular function of a target protein. HTS methods generally take considerable time to develop and are unique for each biological system of interest. We will describe and review the use of gel permeation chromatography (GPC) in the spin column mode with HPLC electrospray ionization mass spectrometry detection (ESI-MS) as a reliable structural screening methodology that can be performed at high speed and high sensitivity with large numbers of compounds, especially when analyzed as mixtures, requiring nearly no development time. This structurally based method relies on the ability to observe non-covalent bonding between a protein (or any biomolecule) of therapeutic interest and members of a compound library in the condensed phase, the chromatographic separation of the protein-ligand complex and the analysis of the ligand in the denatured complex under optimal mass spectrometric conditions. A primary drug screen will be illustrated for RG54 protein and secondary drug screens will be illustrated for MMP-1 Protein, Estrogen Receptor Protein and DNA/RNA targets. Additional GPC Spin column ESI/MS methods illustrated will be competition experiments between inhibitor mixtures and a protein target to identify the strongest binder and methods to determine the binding site of the ligand in the protein target.

(328) Structural Characterization Strategies for Simultaneous Glycomics and Proteomics using Ion Mobility-Mass Spectrometry
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Proteomic studies using mass spectrometry (MS) based techniques have demonstrated great potential in life sciences research. However, technological challenges remain in the rapid and accurate characterization of peptide and protein post-translational modifications (PTMs, e.g. phosphorylation, glycosylation, etc.). It is imperative to characterize PTMs because variations from their normal abundance and changes in PTM patterns can be highly indicative of specific disease states. For example, protein glycosylation patterns have been associated with diseases including prostate and ovarian cancer, Alzheimer’s, HIV/AIDS, and diabetes. The characterization of protein glycosylation is particularly difficult by MS-methodologies because of the intricate branching of carbohydrates and the large number of potentially isobaric glycan positional isomers. Typically, glycosylation studies are performed in two-steps: (i) characterization of the protein (i.e. proteomics), and (ii) characterization of the carbohydrates (i.e. glycans). Unfortunately, this separates the glycomics information from that of the positional context of the carbohydrate on the protein (viz. glycoproteomics). In this report, we describe simultaneous glycomics and proteomics by using ion mobility-mass spectrometry (IM-MS) separation strategies. Ion mobility-MS provides rapid (is-ms) two-dimensional separations on the basis of analyte structure and m/z in the IM and MS dimensions, respectively. Simultaneous glycomics and proteomics can be performed because carbohydrates and peptides of similar mass preferentially adopt different gas-phase structures, i.e. carbohydrates are generally more compact compared to peptides. Furthermore, isobaric glycans that differ in the branching ratio of individual carbohydrate moieties are readily separated due to the alkali-metal charge carrier (typically sodium) preferentially coordinates at the highest branching site of the molecule. In the analysis of carbohydrate positional isomers, this results in higher-order branched species adopting more compact structures by enhanced intramolecular coordination to the alkali metal. Further
glycan structural details are obtained by performing in-source decay (ISD) with subsequent structural analysis of the fragment ions. In MALDI based ISD experiments, we obtain carbohydrate fragmentation patterns that provide complementary structural information in that specific fragment ion channels are preferred depending on the branching ratio and composition of the glycan. This report will describe both MALDI and ESI-based IM-MS strategies for simultaneous glycomics and proteomics characterization of model systems and complex biological samples.

(329) Redistribution Behavior of Group IA and IIA Metals on Porous Oxide Surfaces Modified by Laser Irradiation

Anita Gianotto1, Recep Avci2, Muhammed Deliorman2, Eric Williams2, Marnie Cortez1, Gary Groenewold1, Robert Fox1,*
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Removal of cationic metals from inorganic oxides is complicated by strong binding and highly porous surfaces. Aggressive retention of metals may occur via cation exchange with anionic sites, formation of organic complexes, surface precipitates, or incorporation into the oxide matrix. In many of these cases, the resultant surface species have proven to be difficult or impossible to remove using chemical or even physical approaches. Metals can be redistributed from the subsurface to the surface using laser irradiation. Marble, granite, and concrete were exposed to aqueous solutions of Cs and Co, allowed to equilibrate and then analyzed using imaging secondary ion mass spectrometry, but only low abundances of the metals were detected. Samples were then irradiated (337 nm, 0.05 to 1.3 J/cm²), and subsequent analysis showed marked enhancement of the metal ions. Transmission electron microscopy did not reveal ablation at low fluences, however SIMS depth profiling showed that the metal cations had originally been distributed into the subsurface. Taken together, these results indicate that the metals had partitioned substantially into the ‘bulk’ of the oxide samples, and were moved to the surface by photo-irradiation, which occurred without substantial surface ablation. Surface imaging showed that Cs⁺ or Co₂⁺ mobilized from the pores and cracks. Additional experiments using 284 nm, 318 nm, 345 nm, 532 nm, and 1064 nm irradiation showed an effect due to wavelength irradiation, suggesting that the effect was primarily thermal in nature. The spectra contained significant Na⁺, Al⁺, Si⁺, K⁺, Ca₂⁺ signals; after laser irradiation the Ca⁺, K⁺, and Na⁺ signals were enhanced, while Al⁺ and Si⁺ signals were not. The imaging capability of the TOF-SIMS permitted the matrix composition of the materials to be investigated for preferential binding to ionic exchange sites for the contaminant metals. Comparison of individual ion images suggested that Cs⁺ preferred cation exchange sites occupied by K⁺, consistent with the similarities in charge and ionic radii of the two cations. Sites occupied by Na⁺ were substituted less extensively by Cs⁺. Trends observed for preferential binding of Cs⁺ and Co₂⁺ on porous mineral oxide surfaces in granite, marble and cement mediums will be discussed.

(330) Measurement of Heterogeneous Rate Constants: Reaction of Allyl Bromide at Indium Surfaces

Walter Bowyer1, Yessica Baez Sosa1, Estefanie Giordano1, Anne Sessler1, Isabel Olson1; 1Hobart and W. Smith Colleges

We have developed a photomicroscopic method for measurement of heterogeneous reactions that involve loss of atoms from metal surfaces. For example, we have published kinetic measurements for the formation of Grignard reagents from magnesium and organobromides including rate constants and Arrhenius parameters. We have now modified and extended that strategy. Indium mediated allylation is an extremely versatile reaction that offers regio- and stereoselectivity. Furthermore, it proceeds in aqueous solutions, which are much safer than the solvents used for alternative reactions. However, the patterns of reactivity are different on indium surfaces than on magnesium surfaces. Recently, we described a novel cell combined with photomicroscopy to measure the rates of the heterogeneous reaction (probably an electron transfer) at the indium surface. We provide compelling evidence that under our conditions the reaction is diffusion controlled and report minimum values of the heterogeneous rate constant. Finally, we report a combination of strategies, including NMR spectroscopy, photomicroscopy, and electrochemical measurements to determine the structure of the organometallic intermediate, a contentious issue in the literature on indium mediated allylations. The potential for broader application of our technique to determining rate constants of other heterogeneous reactions is discussed.

(331) Infrared and Raman Microscopy: Complimentary or Redundant Techniques?

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In comparing infrared and Raman microscopes, the following differences are readily evident. For infrared microanalysis, the spatial resolution is limited by the wavelength of light and the numerical aperture of the conventionally used reflecting objectives to about 10 microns. MicroATR infrared measurements achieve 4x better spatial resolution, when employing a germanium internal reflection element, than reflection and transmission measurements, thereby achieving ~3 micron resolution. For dispersive Raman microscopy, the numerical aperture of refraction-based lenses is larger and the excitation wavelength is short resulting in at least 3 times better spatial resolution. The analysis area for Raman microanalysis is defined by the laser spot size and the analysis area for infrared is selected by positioning a remote mask (aperture). Examples of each case will be presented. Another important consideration is coverage of spectral range. A typical infrared microscope is limited to 650-4000 cm⁻¹ for typical measurements. Moving to a wide-band MCT detector with longer wavelength detectability results in an undesirable loss in sensitivity. Raman microscopes typically collect data from 3600-70 cm⁻¹. The allows the characterization of inorganic compounds and well as solid state modes of vibration. Examples of inorganic and polymorphic compounds will be shown to demonstrate the benefit of low wavenumber data collection. Atmospheric interference from CO₂ and H₂O infrared bands can reduce the quality of infrared spectra, where these molecules have very weak Raman cross-sections. Modern spectroscopic software can very effectively remove infrared bands from atmospheric water and bands resulting from CO₂ appear in a region of the spectrum that is usually free of absorption bands. Infrared microscopes are unable to perform confocal depth analysis, where modern Raman microscopes incorporate a confocal design to allow depth profiling of materials. Spectral interpretation is an important consideration in evaluating how Raman and infrared microscopes can be employed. Because infrared spectrometers are so widely utilized, extensive spectral libraries are readily available. In addition, most chemist are considerably more familiar with infrared band positions and therefore able to more readily identify unknown species.

(332) Imaging of Organic Polymer Films Deposited on Infrared Reflecting Glass Reveals Heterogeneities

David L. Wetzel1; 1Kansas State University

Organic polymer films designed to include various chromophores are deposited on glass substrates to allow selective transmission for industrial end use. Of the various organic polymers formulated deposition takes place one at a time. A film build is achieved starting with a monolayer. Considering that the art of film deposition may be a factor microspectroscopic imaging of
the frequency of known bands within the film. Also any chemical heterogeneity is evidenced from examining individual spectra.

(333) Progressive Stages of Crystal Growth of Porphyrin-Cobaltacarborane Conjugates Captured by AFM
Wilson K. Serem, Erhong Hao, Frank Frongzek, M. Graça H. Vicente, Jayne C. Ganno, Louisiana State University

The progressive evolution of meso-substituted porphyrin-cobaltacarborane crystals can be viewed with high-resolution AFM images. The crystalline aggregation of porphyrins and metalloporphyrins on surfaces is influenced by the nature of the peripheral substituents and their position on the macrocycle. A series of porphyrin-cobaltacarborane conjugates were prepared in high yields (70-95%) via a ring-opening reaction of zwitterionic cobaltacarborane. Investigation of aggregation properties was accomplished by fluorescence spectrophotometry, UV-vis and atomic force microscopy. Evidence of aggregation as demonstrated by fluorescence measurements appears to be time-dependent over intervals of days to weeks. Changes in the propensity to form crystals or aggregates were investigated at the nanoscale using AFM, for a series of meso-substituted macrocycles containing 2 to 8 cobaltacarborane clusters per porphyrin [333-Co(S-C4H8O2-1,2-C2B8H10)(1,2-C2B9H11)]. Structures spanning a range of sizes evolved as the crystals mature and grow into fractal microcrystallites. The progressive stages of crystal growth on mica(0001) were captured with high-resolution AFM topography images for samples which were dropcast on atomically flat surfaces and dried in ambient conditions. The crystals of porphyrin-cobaltacarborane first form small seed particles, which align into columnar structures. The linear columns grow laterally to generate rectangular planar sheets. Branching of the sheets originates from the centers of the planes as the sheets grow into larger crystallites. Both UV/Vis and DLS investigations provided evidence that crystals had already formed in solution. Amplitude and phase images display homogeneous contrast for the crystalline sheets, which suggests an ordered and regular self-assembly. The thickness of the layered sheets of assembled porphyrins corresponds to the thickness of a single molecular layer, revealing unconfined areas of the substrate as a baseline for cursor measurements. The amphiphilic and fluorescent properties of this class of dendrimer-like compounds show promise for application as novel drug carriers in boron neutron capture therapy (BNCT) treatment of tumors.

(334) Nonlinear Spectroscopy of Cadmium Chalcogenide Quantum Dots
Seongmin Ma, William Yu, JaeTae Seo, Qiguang Yang, Bagher Tabori, Vicki Colvin, Jinhua Heo, Wanjoo Kim, Sungsoo Jung, Department of Physics, Hampton University, Hampton; Department of Chemistry, Rice University; Korea Research Institute of Standards

The third-order nonlinear susceptibilities of cadmium chalcogenide (Te, Se, S) quantum dots (QDs) were investigated using concentration- and polarization-resolved degenerate four-wave mixing (DFWM) in a nonresonant region. Degenerate four-wave mixing is the interaction between four light waves with the same frequency in an optical nonlinear medium via the third-order nonlinear polarization. The sizes of the QDs were near bulk Bohr radius. The first exciton absorption peaks of CdTe, CdSe, and CdS QDs were ~698 nm, ~565 nm, and ~387 nm, respectively. The excitation light source was a 6-nm pulse laser with 10-Hz repetition rate at 1064-nm wavelength for CdTe and CdSe QDs, and was the nanosecond laser at 532-nm wavelength for CdS QDs. The polarization dependent third-order nonlinear susceptibilities of QDs were measured as a function of concentration and the second hyperpolarizability were extracted from the slope of the susceptibility versus concentration. The ratios of the hyperpolarizabilities for CdTe, CdSe, and CdS QDs were ~0.26, ~0.34, and ~0.29, which indicate a large contribution of an electronic polarization process to the cubic nonlinearity of QDs.

(335) Rapid Measurements of Optical Scattering using a Portable Photon Time-of-Flight Device
Francis Esmonde-White, David Burns, McGill University

We present continuing research into the development of a novel photon time-of-flight device for the rapid measurement of scattering in optically turbid media. Quantification of optical scattering and absorption properties in situ is an area of wide interest in biomedical optics. Near-infrared diffuse reflectance is an attractive method for quantification in tissue because it is non-invasive and does not require extensive specimen preparation. However, scattering caused by tissue alters the optical path length and limits practical quantification of bioanalytes. We hypothesize that measurements of the absorption and scattering coefficients by photon time-of-flight will improve the accuracy of near-infrared diffuse reflectance measurements. A clinically practical time-of-flight device was constructed in-house. Optical scattering is measured at two wavelengths, 850 and 905 nm, in the therapeutic window of 700-1300 nm. Aqueous solutions of Intralipid and ink were prepared and used as optical standards with known scattering and absorption properties. This device is functional in ambient light conditions, and does not require a constrained dark-room setting. Time-dependent intensity profiles were recorded, and the optical pulse shape was processed in Matlab to estimate the optical scattering and absorption coefficients.

(336) High Speed Imaging Developments in Raman Spectroscopy
Matthew Bloomfield, Ken Williams, Richard Bormett, Renishaw, Pte; Renishaw, Inc

The ability to create chemical images by acquiring Raman spectra from an array of positions and then processing them to reveal the parameter of interest is a powerful chemical imaging technique. Traditionally, these spatially-related data have been collected by raster scanning the sample beneath the incident laser focused to a point or a line, typically in micrometer intervals. A new method of sample scanning combined with the static laser line focus has been developed that dramatically increases the image acquisition speed without compromising Raman image or spectrum quality. This innovative approach allows the Raman imaging to be applied to small and large areas where it had previously been impractical due to time constraints that would otherwise produce poor spectral signal-to-noise. Raman imaging is now possible for large and small areas at speeds much greater than possible with traditional methods. With clear advantages to the pharmaceutical industry in particular, examples will be shown from a variety of materials to illustrate the benefits of this method.

(337) Wide Area Illumination (WAI) Raman Scheme for Reliable Quantitative Analysis of Etching Solution and Petrochemical Product
Hoeil Chung, Jaejin Kim, Kyungtaeg Ryu, Yongdan Kim, Mark Kemper, Hanyang University; Kaiser Optical Systems

A novel and reliable Raman collection system for on-line analysis of etchant solutions and naphtha has been proposed. The principal
idea was to develop a means to effectively utilize the wide area illumination (WAI) scheme for Raman collection, which covers a large sample area (coverage area: 28.3 mm2) to improve the reliability in sample representation and the reproducibility of sampling. The latter is due to the reduced sensitivity of sample placement with regard to the focal plane. Etchant solutions, composed of hydrogen peroxide, sulfuric acid and water, were successfully measured using the WAI Raman scheme. Raman spectra were collected directly through Teflon tubing that is currently being used at wet stations; therefore, the resulting Raman spectra contained information from both Teflon and the sample. This allowed a unique calibration strategy to be employed because the Teflon tubing served as an effective intensity correction standard in addition to serving as a sample cell. The non-overlapping Teflon band at 732 cm-1 was used as a reference peak to correct any Raman intensity changes resulting from laser power variations. Hydrogen peroxide and sulfuric acid concentrations were accurately measured by using principal component regression (PCR) after an intensity correction, using the Teflon peak. Using the WAI scheme, the compositional analysis of simulated naphtha samples was attempted. Near-infrared (NIR) spectroscopy, widely adopted in the field of petroleum refining, was also employed to compare with the prediction results obtained with the WAI scheme. Since the Raman spectral features are more distinct and selective, it was hypothesized that the resulting calibration accuracy could be improved if reproducible Raman spectra could be collected. The overall predictions using Raman spectroscopy were indeed shown to be superior to those resulting from NIR spectroscopy.

(338) Analysis of the Composition of Biological Apatites by Raman Spectroscopy and Ion Chromatography
Mary Tecklenburg1, ShaRhonda Dennis1, Adam Peralta1, Ayorinde Awonusi1, Amy Marcotte1, Robert Buckland1, Monaliza Sirbecsuc1, 1Central Michigan University

The mineral apatite is present naturally in geological formations and in biological tissue. In bone and teeth it resembles calcium hydroxyapatite [Ca10(PO4)6(OH)2] with significant substitution. In bone, carbonate substitutes for 6-8% of the phosphate and very little hydroxide is present. In teeth, dentine has a similar composition to bone while enamel has low levels of carbonate and fluoride substitutes for hydroxide. In addition, minor amounts of sodium, potassium, calcium, monohydrogen phosphate, chloride and other ions may substitute into apatite. The composition is also known to change with age, stress, and structural features. The ion composition of bone and other apatite minerals has been analyzed by standard techniques but several grams of sample were needed as well as a significant time investment as separate tests were required for each ion. We have investigated the use of ion chromatography (IC) and Raman spectroscopy to quickly and efficiently determine apatite ion composition of small (20 mg) samples of synthetic apatite and bone. The concentrations of Ca2+, Na+, Mg2+, Cl-, and PO4– measured by IC chromatography were compared with values obtained by atomic absorption for cations, a colorimetric test for phosphate, and an ion selective electrode for chloride. The ion chromatography method required just two runs (anion and cation mode) of a single sample to measure all of the ions. In addition, Raman spectroscopy was used to measure carbonate concentration which is not available by IC since it is an integral part of the solvent.

Duane A. Rogers1, Steven J. Ray1, Gary M. Hieftje1, 1Indiana University

In recent years the importance of chemical speciation, i.e. the determination of an element amongst its various oxidation states and molecular or complex forms, has been recognized as more relevant than total elemental concentration. Although the total elemental concentration is often easier to evaluate, the bioavailability and toxicological information it yields are inherently limited. For this reason, researchers have begun employing multiple instruments to obtain the elemental and the molecular information from biological samples. However, employing multiple instruments for the analysis of a given sample produces several disadvantages. In the work presented here, a single time-of-flight mass spectrometer (TOFMS) will be described that utilizes two sources to obtain comprehensive atomic and molecular information simultaneously. The dual-source TOFMS has been designed and constructed in our laboratory. The current arrangement for the instrument utilizes an inductively coupled plasma to obtain elemental, isotopic, and quantitative information. Concomitantly, an electrospray source is operated to provide molecular information. Due to the wide mass range and high spectral-generation rate of TOFMS, ions from both sources can simultaneously be sampled by a single mass analyzer to provide excellent temporal resolution of transient signals, while simultaneously simplifying peak assignment from a chromatographic separation.

(340) Arsenic and Mercury Speciation: Challenges and Successes
Carl Verdon1, Kathleen Caldwell2, Robert Jones3, Olga Piraner3, Mark Fresquez1, Christopher Freedman1, Cynthia Ward1, Graylin Miller1, 1Centers for Disease Control and Prevention

We present two hyphenated HPLC-ICP-DRC-MS methods for the speciation of arsenic and mercury. The arsenic speciation method separates seven As species in urine: arsenobetaine (AB), arsenocholine (AC), trimethylarsine oxide (TMAO), arsenate (As(V)), arsenite (As(III)), monomethylarsonate (MMA) and dimethylarsonate (DMA). This robust method utilizes an anion-exchange column (PRP-X100™, Hamilton Company, Reno NV), connected to an ICP-DRC-MS (ELAN® DRCII™, PerkinElmer Life and Analytical Sciences, Shelton CT) that monitors 75As++ using 10% hydrogen / 90% argon as the DRC gas. Method LOD's for the various species range from 0.4-1.7 μg As/L. The As speciation method meets our requirement for sample throughput of 2000-3000 sample analysis per year per instrument. This As speciation method is now being used in a production mode for the analysis of a U.S. population survey, National Health and Nutrition Examination Survey, (NHANES) as well as for other biomonitoring studies of As exposure. Mercury speciation has been a component of the National Health and Nutrition Survey (NHANES) survey from 1999 to the present (www.cdc.gov/exposurerreport). The analytical methods used to date consists of a total and an inorganic methods using ICP-MS and CVAAS, respectively. Together, these methods gives inorganic and total mercury information in whole blood, from which the organic fraction is derived by calculation. Due to the increased public health interest in ethyl mercury, it is critical that we are able to simultaneously measure these three forms of mercury in human blood using one method with high specificity and sensitivity without sacrificing throughput. We have developed an HPLC-ICP-DRC-MS method that uses an Apex™ Q system with a micro-flow nebulizer that enhances desolvation efficiency and boosts
sensitivity for Hg. The 202Hg+ ion signal is further improved using argon for collisional focusing in the Dynamic Reaction Cell™ (DRC). The Hg speciation method will be used in a production mode for the analysis of a U.S. population survey, National Health and Nutrition Examination Survey, (NHANES) as well as for other biomonitoring studies of Hg exposure.

(341) Bone Lead Measurement by Non-Invasive KXRF: Results of an Interlaboratory Study and Traceability to ICP-MS
Patrick J. Parsons1, David J. Bellis1, Katherine M. Hetter1, Neeta R. Ginde2, Peter Mata1, Andrew C. Todd1; 1New York State Department of Health; 2Mount Sinai School of Medicine

K-shell x-ray fluorescence (KXRF) spectrometry is used for non-invasive, in vivo measurements of Pb in bone. Typically, the KXRF instrumentation is calibrated via plaster-of-Paris phantoms doped with Pb. The calibration standards have Pb concentrations that are based on units of µg/g dry weight plaster. The fluoresced K-shell Pb X-ray peaks are normalized to the coherent scatter peak because the latter arises from interactions between the incident photons and the bone matrix. Since plaster-of-Paris is different from bone, a matrix conversion factor, called the coherent correction factor (CCF), is applied to computed concentrations in order to transform them into units of µg/g bone mineral (b.m.). In this study, we describe an inter-laboratory study of bone Pb measurements that was conducted among 12 laboratories that use KXRF instrumentation. We circulated 9 tibiae that were obtained post mortem from Pb-dosed goats. The tibiae had been cleaned of adhering tissues and marrow, leaving the intact bare bones for the interlaboratory study. Twelve laboratories returned data from a total of 15 KXRF systems. Each laboratory measured each bone five times, enabling us to assess and compare intra- and inter-laboratory precision. After the study, the bones were analyzed for Pb content using inductively coupled plasma – mass spectrometry (ICP-MS), after digestion in nitric acid. Thus, a second aim was to compare the results for bone Pb obtained by KXRF to those obtained by ICP-MS. Results showed a substantial spread in the concentrations obtained with the 15 KXRF systems; the SD of the repeated measurements ranged from 0.9 to 6.1 µg/g b.m. for the lowest Pb concentration bone, to 0.6 to 4.6 µg/g b.m. for the highest Pb concentration bone. For ICP-MS analysis, each tibia was subdivided into surface and core components and Pb content determined. We back-converted the reported KXRF concentrations by the CCF to yield concentration units of µg/g dry weight for the comparison with the ICP-MS-measured concentrations. We found that the Pb concentration in the tibia “surface” (via ICP-MS) was greater than that found in the bone core. Qualitatively, the KXRF-measured Pb concentrations are between the ICP-MS-measured surface and core concentrations.

(342) CDC Biomonitoring by ICP-DRC-MS, Enhancements to a More Efficient Autosampler and MoO Correction on Cd
Kathleen L. Caldwell1, Robert L. Jones1, Jeff Jarrett1, Ge Xiao1, Gulechekha Shakirova1, Melanie Granklin1, Neva J Mullinix1; 1CDC/NCEH/DLS/IRAT

This talk will describe enhancements to our whole blood and urine multi-element methods performed routinely in our laboratory as part of the National Health and Nutrition Examination Survey (NHANES) which, among other uses, supplies data for the National Report on Human Exposure to Environmental Chemicals [1]. This work provides important information as to the normal levels of these elements in the U.S. population. We will look at the use of a more efficient sample introduction procedure and the implications this has had on our sample throughput workflow. Additionally we will look at our newly optimized urine method which operates in ‘mixed-mode’ to analyze thirteen elements in urine using a PerkinElmer ELAN® Inductively Coupled Plasma Dynamic Reaction Cell Mass Spectrometer (ICP-DRC-MS). Eleven elements are measured in “Standard mode” with no gas in the reaction cell. The remaining elements, arsenic and cadmium, are measured in independent “DRC modes” where the reaction cell is pressurized with gas. When analyzing for cadmium, the reaction cell is pressurized ('DRC mode') with oxygen and the quadrupole mass filter in the reaction cell prevents 98Mo from entering the oxygen-rich environment of the cell. The 98Mo16O+ ions which have been found to interfere with detection of 114Cd at m/z 114 react with the oxygen in the cell creating 98Mo16O2+ and 98Mo16O3+ at masses which no longer represent an interference to 114Cd analysis. Since the quadrupole in the reaction cell prevents 98Mo+ from entering the cell, no additional interfering 98Mo16O+ is formed in the oxygen-rich environment of the cell. The need for removal of this interference was observed when evaluating historical NHANES urine cadmium results, though the need was not apparent from historical proficiency testing results (where cadmium results were typically high relative to the molybdenum concentration). During this presentation, the recent modifications to the method and recent data from the Third National Report on Human Exposure to Environmental Chemicals will be discussed. [1] Third National Report on Human Exposure to Environmental Chemicals, http://www.cdc.gov/exposurerreport/, Centers for Disease Control and Prevention, 2005.

(343) Microdistribution of Trace Elements in Biological Tissues: A Comparison between LA-ICP-MS and μ-XRF
David J. Bellis1, Zewu W. Chen2, Walter M. Gibson2, Dula Amarasingawarde1, Patrick J. Parsons1; 1New York State Department of Health; 2X-ray Optical Systems; 3Hampshire College

Laser ablation - inductively coupled plasma mass spectrometry (LA-ICP-MS) is currently the analytical technique of choice for the determination of the microdistribution of trace elements in biological tissues since it combines the micrometer-scale precision of the LA system with the low limits of detection (LODs), and multi-element capability of ICPMS. Until now, determination of the microdistribution of trace elements at low concentrations in biological tissues by X-ray fluorescence (XRF) has required high-energy synchrotron source radiation, as laboratory-based, low-power sources have not achieved the necessary LODs. Here we demonstrate the determination of trace element microdistribution at low concentrations in bone by focused monochromatic microbeam (μ-) XRF with a low power source (45 W molybdenum tube). This system uses the newly-developed doubly curved crystal optic (DCC) (X-ray Optical Systems (XOS) Inc., East Greenbush, NY). The DCC optic focuses the exciting X-rays to a micrometer-sized point on the sample surface providing spatial resolution as low as 20 μm, and increases the energy flux thus lowering the resulting LOD. We compare the data obtained via μ-XRF to those obtained from the same bone sample via LA-ICP-MS. The two methods recorded the same general trace element distribution, but the stability of μ-XRF was superior to that of LA-ICP-MS.

(344) Intra- and Inter-Individual Variability of Copper, Selenium and Zinc in Serum and the Determination of Analytical Quality Specifications
Andrew Taylor1; 1DNA Marker Services, 12 other colleagues; *University of Surrey; *Network of EQAS Organisers

Measurements of intra- and inter-individual variability were taken to define total allowable error (TEa) for copper, selenium and zinc in serum. These calculations were used to propose the following quality specifications (QS) for the determination of these elements so that results can be demonstrated to be fit for the purpose to which they are applied. Cu in serum ± 0.84 μmol/L or ±12%,
from blood taken from patients treated with these agents; and cell lines known to have high and low resistance to CP. The developed sample types including: a calf thymus DNA model; DNA extracted the development of an HPLC-ICP-MS method for measuring GG adducts, DNA-protein adducts and interstrand crosslinks. We report the determination of platinum containing drug adducts with DNA by a combination of HPLC-IAP-MS and LC-ESI-MS/MS

Chris Harrington1, Rachel Le Pla1, Peter Farmer1; 1Biocentre, University of Leicester

Cisplatin (CP) is a highly successful cancer treatment which in combination with other chemotherapy agents has achieved cure rates of up to 90% against testicular cancer and is also active against other tumours including ovarian cancer. Unfortunately CP also exhibits a range of side-effects including sickness, nausea and other problems. Along with these side effects some tumours are inherently resistant to the drug or can acquire resistance. For this reason second (carboplatin) and third (oxaliplatin) generation drugs have been developed in an attempt to overcome these drawbacks. Oxaliplatin (OP) is less toxic than CP and has demonstrated anti-tumour activities in CP resistant cell lines and also in tumour types that are intrinsically resistant. Furthermore this drug is the only platinum drug effective in colorectal cancer and is frequently used against other tumours including ovarian cancer. Unfortunately CP combination with other chemotherapy agents has achieved cure rates of up to 90% against testicular cancer and is also active against other tumours including ovarian cancer. Unfortunately CP also exhibits a range of side-effects including sickness, nausea and other problems. Along with these side effects some tumours are inherently resistant to the drug or can acquire resistance. For this reason second (carboplatin) and third (oxaliplatin) generation drugs have been developed in an attempt to overcome these drawbacks. Oxaliplatin (OP) is less toxic than CP and has demonstrated anti-tumour activities in CP resistant cell lines and also in tumour types that are intrinsically resistant. Furthermore this drug is the only platinum drug effective in colorectal cancer and is frequently used as a first line treatment for this disease. Both CP and OP are currently used to treat various cancers in the UK. Both drugs bind to the N7 position of the purine DNA bases forming DNA-drug adducts. These are mainly intramolecular crosslinks between adjacent guanines (GG) (~65%) and between an adjacent adenine and guanine (AG) (~25%) and a small percentage of monofunctional adducts, DNA-protein adducts and interstrand crosslinks. We report the design and produce both channel and metal electrodes, used for separation and detection (amperometric and contactless conductivity detection). With ease of fabrication, we can rapidly design and produce integrated microchips for all kinds of analytes and samples. To increase the number of applications and sensitivity, we have also designed a confocal laser-induced fluorescence detection system.

Gary Emmert1, Lucy Thurston1, Kyoo Dong Jo1; 1The University of Memphis

We have borrowed from the techniques of polymeric microfabrication to construct miniaturized devices for use in drinking water monitoring. In particular, we have developed a series of simple techniques that can be used to construct components that can be assembled together to yield relatively simple and inexpensive, but very useful analyzers for measuring the concentrations of drinking water disinfectants and disinfection by-products. In particular, two analyzers will be presented. The first uses a LED-based spectrophotometer that was constructed from simple components with portions of the flow cell and missing parts being made from PDMS. The PDMS is used to construct channels with a simple template approach. Designs are made in a Petri plate or other vessel using wires of different dimensions glued to the surface. PDMS is poured into the mold, cured and then carefully removed to create miniaturized channels. Dimensions of 100 to 400 microns are easily made and these structures can be characterized using a common digital scanner and commercially available photo-software. Ultimately, a simple flow injection analyzer was constructed that was capable of on-line monitoring of chlorine concentrations directly from drinking water systems. Additional studies involved constructing a slightly more complicated LED-based fluorescence detector from PDMS. This device was capable of method detection limits for fluorescein of 400 pM. Studies applying this detector in a method designed to monitor total trihalomethanes and total haloacetic acids gave method detection limits of 0.50 micrograms/L with good accuracy and precision. Further applications of these simple techniques will be discussed.
also be presented. While there should be no confusion that these techniques, as we apply them, cannot make high resolution, truly microfluidic devices, they can be used to make smaller channels and other structures that can be assembled into more complicated designs. Their advantage is that they provide simple procedures for fabrication that can be useful for those who might want to construct flow injection analyzers that are roughly \( \frac{1}{4} \) the scale of more traditional systems. Moreover, they do not require any specialized facilities or expertise to accomplish this goal of miniaturization.

(349) Electroosmotic Flow Dynamics in Response to Biological Sample Adsorption

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Migration time reproducibility is a major limitation for capillary electrophoretic separations, and variable electroosmotic flow is the major factor causing this problem. We have developed an experimental method for accurately and precisely monitoring fluid flow rates in capillaries and microchip devices with a time resolution of up to 2 Hz. We are using this technique to study electroosmotic flow as a function of time when biological sample components adsorb to a fused-silica capillary surface. Electroosmotic flow dynamics are being measured immediately after injections of purified proteins, lipids and carbohydrates as well as after injection of biological fluids and cultured cells. Such samples are known to alter electroosmotic flow. The goal of this study is to understand better understand how electroosmotic flow changes as a function of time due to adsorption of biological sample components. This information will enable us to understand how best to apply marker methods to correct for electroosmotic flow variability and improve capillary electrophoresis reproducibility. This experimental approach also will be applied to evaluate surface treatments designed to minimize sample adsorption and electroosmotic flow variability. Finally, our method for electroosmotic flow monitoring will be used to correct electropherograms for variable electroosmotic flow, and the reproducibility obtained using this approach will be compared to results obtained using marker-based methods.

(350) Novel Valve Actuation and Applications in Microfluidics

Frank Gomez\(^2\), Attila Gaspar\(^2\), Menake Piyasena\(^2\), Schetema Stevens\(^2\), Marisol Salgado\(^2\); \( ^2 \)California State University, Los Angeles

We describe the development of a simple, external in-line magnetic valve and its use in the design of a disposable and inexpensive microfluidic chip, fabricated from poly(dimethylsiloxane) (PDMS), incorporating conventional chromatographic reversed-phase silica beads (C18) without the use of frits or permanent physical barriers, tapers or restrictors. The actuation of the valve is based on the principle that flexible polymer walls of a liquid channel can be pressed together by the aid of a permanent magnet and a metal bar. In the presence of a small NdFeB magnet lying below the channel of interest, the metal bar is pulled downward simultaneously pushing the thin layer of PDMS down thereby closing the channel stopping any flow of fluid. The operation of the valve is dependent on the thickness of the PDMS layer, the height of the channel, the gap between the chip and the magnet and the strength of the magnet. The microfluidic channels are completely closed to fluid flows commonly used in microfluidic applications. The packing of C18 modified silica beads into the microfluidic channels is made possible by the hydrophobic nature and excellent elasticity of PDMS. Separation of dyes, small drugs and other compounds have been performed utilizing the microchips and reproducible and high resolution separation results have been obtained. A fiber optics assembly is incorporated onto the chip for detection of products resulting from on-chip reactions. Detailed construction and characterization of the fritless microfluidic chips are discussed. We expect that this fritless chip will allow for high-throughput separations of many different types of materials including proteins and DNA and enable multiplexing of multiple chromatographic process on a single chip.

(351) Development of Lab-on-a-Chip Biosensor for Glucose Based on a Packed Immobilized Enzyme Reactor

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In this work, the development of a packed immobilized enzyme reactor (IMER) and its integration to a capillary electrophoresis - microchip is described. The present microchip design differs from others, in the fact that the same chip could be used for with or without the particles and, just by changing the material used to pack the IMER, different analytes can be detected. The applied procedure involves the separation of the target analyte by capillary electrophoresis, which is then coupled to a post-column IMER that produces H2O2. The H2O2 produced is finally detected downstream at the surface of a working electrode. By packing particles modified with glucose oxidize at the end of the separation channel, glucose was detected above 0.1 mM. The analytical performance of the microchip-CE has been demonstrated by performing the separation and detection of glucose and noradrenaline. Additions of fructose showed no effect on the peak position or the peak magnitude of glucose. The microchip-CE-IMER was also applied to quantify glucose in carbonated beverages. Details of the preparation, performance and advantages of the new microchip-CE-biosensor will be discussed.

(352) Biochemical and Gas Sensing with a Novel Subwavelength Photonic Platform

Donald Sirbuly\(^1\), Nicholas Fischer\(^1\), Timothy Ratto\(^1\), Jeff Tok\(^1\), Aleksandr Noy\(^1\); \( ^1 \)Lawrence Livermore National Laboratory

Compact, reusable biochemical and gas sensors are highly desirable for rapid on-site analytical analysis of vapor and liquid mixtures in the field. A key to miniaturizing devices and providing reliable quantitative chemical identification of small sample volumes hinges on the development of novel materials capable of multiple complementary sensing modalities. Here we demonstrate an optical sensing platform that utilizes the evanescent field of a subwavelength semiconductor nanowire waveguide to detect gas vapors (e.g. hydrogen) and biochemical species (e.g. oligonucleotides). To promote local chemical functionalization, multiplex sensing, and reusability, the optical cavities are integrated into polymeric flow cells. Gas concentration is quantitatively detected by submersing high dielectric nanoparticles within the propagating evanescent field. Upon exposure to vapor the optical properties of the nanoparticles changes and causes attenuation or enhancement of the guided optical energy. For biochemical detection we have developed a rapid means of coating the optical surface of the waveguides with functional lipid membranes. Real-time biological sensing (e.g. DNA hybridization) was tested and achieved by anchoring single-stranded oligonucleotides within the supported bilayer and reading out the optical signatures as complimentary strands annealed within the exposed optical field. With the advantage of carrying out multiple spectroscopy techniques such as absorbance, fluorescence and surface enhanced Raman spectroscopy (SERS) on sub-picoliter probe volumes, these evanescent field sensors offer a unique design for portable all-optical detection systems. This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under Contract W-7405-Eng-48. For Official Use Only - Patent Information Pending
(353) The Sensitivity Limits of Nanowire Bio-Sensors

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Nanowire field effect transistors (NWFTs) are emerging as powerful tools for biological studies such as bio-molecule detection, yet their sensitivity limits are not understood at a fundamental level. I will discuss the interplay of device parameters such as gate bias and NW diameter on the operating modality and sensitivity of NWFT sensors. pH and cancer marker detections are studied as silicon-NWFTs are tuned from linear to subthreshold regimes by electrochemical gating. First, pH sensing data show that NWFT has the strongest response and the best signal to noise ratio in the subthreshold regime. Operating in the subthreshold regime also reduces the detection limit for prostate specific antigen down to ~fM for a device with ~pM detection limit in the linear regime. This sensitivity improvement is due to the reduced screening ability of carriers in NW. A quantitative model describing these results and the intrinsic charge detection limit of NWFT sensors will be discussed.

(354) Piezoelectric Nanogenerators Based on Zinc Oxide Nanowire Arrays

Jinhui Song1, Z.L. Wang1; 1Georgia Tech

We demonstrate an innovative approach for converting nano-scale mechanical energy into electric energy by piezoelectric zinc oxide nanowire (NW) arrays. By deflecting the aligned NWs using a conductive atomic force microscopy (AFM) tip in contact mode, the energy that was first created by the deflection force and stored in zinc oxide nanowire. Thus the mechanical energy converted into electricity by piezoelectric effect has been measured for demonstrating nano-scale power generator. The operation mechanism of the electric generator relies on the unique coupling of piezoelectric and semiconducting dual properties of ZnO as well as the elegant rectifying function of the Schottky barrier formed between the metal tip and the NW. The connection between NW and outer circuit is silver, where the metal-semiconductor ohmic contact is formed. The connection between the NW and Pt tip is metal-semiconductor schottky contact. This unique design combined with piezoelectric effect of ZnO nanowire produces a novel device: nanogenerator. Potential on the stretched side of NW increases as the AFM tip bends the NW. Reverse biased Schottky barrier prevents the neutralization of the polarized charges. As tip moves to the negative potential side of NW, the schottky barrier is forward biased. The polarized charges of NW are neutralized, then the electrical energy is released to outer circuit. The efficiency of the NW based piezo-electric power generator is ~ 17-30%. The output power volume density of the NW is ~ 80 MW/cm3, about 450 times higher than that of bulk PZT. The approach presented has the potential of converting biological mechanical energy, acoustic/ultrasonic vibration energy, and biofluid hydraulic energy, into electricity, demonstrating a new path way for self-powering of wireless nanodevices and nanosystems.

(355) Thermal Properties and Single Particle Tracking of Gold Nanoshells in Lipid Vesicles and Cell Membranes

Matthew Clarke1, Hyoeng-Gon Kang2, Peter Yin1, Rani Kishore1, Kristian Helmersson1, Jeeseong Hwang1, 2NIST

The potential of nanomaterials as therapeutic agents holds great promise. Indeed, sufficient local heating using carbon nanotubes, gold nanoshells, or cages has been shown to affect cell health. While important research has focused on the net effects of these materials in biological environments, understanding the local environment of these materials during the thermal excitation is crucial for the development of quantitative techniques towards many biomedical and clinical applications. Here, we present our results on the examination of local thermal properties of single gold shell nanocrystals. These nanoshells consist of a silica core with an outer coating of gold. The absorption profile depends on the thickness of these layers. In this research, particles with a 60 nm silica core and 20 nm gold layer were used, which exhibit an absorption maximum near 785 nm. We modified our total internal reflectance fluorescence microscope to simultaneously perform differential interference contrast (DIC) microscopy using a 785 nm illumination source. This approach enables multi-modal imaging of the nanocrystals for both simultaneous multiplexed fluorescence and DIC contrast while they are exposed under a thermal excitation source. Ratiometric fluorescence microscopy is used to determine the nanoshell’s local heating profile, while the 785 nm DIC is used for thermally exciting them and following their positions to conduct single particle tracking microscopy. The effects of local heating in biological and biomimetic environments were studied either in lipid vesicle systems or in cells. In the lipid system, the nanoshells were mixed with 1,2-Dimyristoyl-sn-Glycero-3-Phosphocholine (DMPC). Temperature driven lipid transitions were then monitored as a function of gold nanoshell excitation. For measurements in cells, antibody-labeled nanoshells targeted to membrane proteins were incubated with mammalian fibroblast cells. Subsequently, the diffusion of these particles as a function of 785 nm excitation and nanoparticle density was determined. Additionally, cellular uptake of nanoshells and effects on cellular behavior will also be reported.

(357) Mass Spectrometry of Nanoparticles in the Atmosphere

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Airborne nanoparticles, defined as particles with diameters under several tens of nanometers, have important consequences for human health and the environment. Particles in this size range can be emitted directly into air by energetic processes such as combustion, or they may be formed in situ by gas phase oxidation.
of precursors such as sulfur dioxide or volatile organic compounds. As the use of nanomaterials in common products and processes increases, new avenues for nanoparticle release into air may become important especially in the workplace. We have developed several aerosol mass spectrometers for characterizing airborne nanoparticles. One uses laser desorption ionization to analyze single particles that have been aerodynamically size selected. Another uses a laser induced plasma to perform elemental analysis of individual particles that have been size-selectively captured in an ion trap. A third uses various two-step desorption ionization sequences to characterize the organic composition of nanoparticles. Each of these instruments has been deployed for ambient nanoparticle measurements. Ambient measurements provide an opportunity to investigate the sources of nanoparticles in the atmosphere and assess the level of human exposure to them. Instrumental performance and ambient data from two air quality monitoring sites, urban and coastal marine, will be presented.

(358) Using Aerosol Chemical Ionization Mass Spectrometry (CIMS) to Study Radical-Initiated Oxidation of Organic Particles

Geoffrey Smith1, John Hearn2, Lindsay Renbaum1; 1University of Georgia

While ozonolysis reactions of organic aerosols have received much attention recently, there have been relatively few studies of radical reactions with organic films or particles despite their importance for oxidation in the troposphere. We are exploring such radical-initiated reactions using CI and OH radicals with organic particles by monitoring changes in particle composition. The Aerosol CIMS technique is used to analyze liquid and solid aerosol particles by first thermally vaporizing them at temperatures up to 300 °C and then chemically ionizing the particle vapor. The ions are then detected with a quadrupole mass spectrometer. The soft ionization and variety of ionization reactions make it possible to detect many types of organic species with little or no fragmentation. The measured rates of reaction within the particles and identification of oxidation products will be presented. These experiments provide insight into the oxidative processing which may potentially alter many critical properties of organic aerosol, including hygroscopicity and their ability to act as cloud condensation nuclei.

(359) Aerosol Mass Spectrometry: Aerosol Chemical and Microphysical Properties

Achim Trimborn1, Timothy Onasch1, Manjula Canagaratna1, Jesse Kroll1, Dagmar Trimborn1, Mike Cubison1, Jose Jimenez2, John Jayne1, Douglas Worsnop1; 1Aerodyne Research; 2University of Colorado

The Aerosol Mass Spectrometer (AMS) is a widely used instrument for measuring the size-resolved chemical composition of non-refractory aerosol particles. In the standard AMS, particles are flash vaporized and ionized by standard 70 eV electron impact. This ‘hard’ ionization of organic molecules results in extensive fragmentation and makes it difficult to determine the molecular composition of complex mixtures. The introduction of a high resolution time of flight mass spectrometry to the AMS provides the ability to distinguish unambiguously between oxidized (secondary) and “hydrocarbon-like” (primary) aerosol. The resolution of m/Δm ~ 5000 is sufficient to resolve the elemental composition of all ions at nominal masses below m/z = 100. This allows for the quantitative determination of important chemical characteristics of the aerosol, such as the oxygen to carbon ratio of the organics. Large organic molecules generally cannot be directly measured with the AMS due to the high level of fragmentation caused by electron impact. To improve speciation of the organic aerosol, “softer” ionization methods, such as low energy electron impact (LEEI), vacuum ultra violet photo ionization (VUV) and Li ion attachment, were developed. In LEEI mode, the electron energy is reduced to ~14 eV. This results in spectra showing fragments in a higher mass range than with standard electron impact but still has significant fragmentation. VUV is softer than the LEEI approach and provides a universal ionization scheme for organic aerosols. VUV still shows significant fragmentation, though it preserves the parent ion, allowing for better speciation of the molecules. In contrast, Li ion attachment leads to almost no fragmentation of the organics, with the parent + lithium [M+6] ion exhibiting the strongest signal in the mass spectrum. While this approach is not a universal ionization technique, it is sensitive towards organics which are not highly oxidized (i.e., hydrocarbon-like aerosol). We will discuss these various ionization schemes, with a particular emphasis on the applications of Li ion attachment.

(360) High-speed, Quantitative Analysis of Particle Chemistry using a Time-of-flight Aerosol Mass Spectrometer

Joel Kimmel1, Peter DeCarlo1, Jose-Luis Jimenez1, Doug Worsnop2; 1University of Colorado; 2Aerodyne Research, Inc.

The Aerodyne time-of-flight aerosol mass spectrometer (ToF-AMS) is a portable instrument, which determines particle size by measuring velocity after expansion into vacuum and analyzes chemical composition by electron-impact (EI) mass spectrometry. Data for 35-nm to 1.2-um, non-refractory aerosols are acquired with mass resolving power up to 5000. 1-minute detection limits range between 1 and 20 ng m-3. Quantitative characterization of complex aerosols requires broad dynamic range. And, because particles create intense bursts of ions, data acquisition routines must be based on analog detection, rather than the simpler method of ion counting. The ToF-AMS uses a unique digitally thresholded analog-to-digital converter that can discard low-intensity signals. By selectively eliminating electronic noise, this process can lead to notable improvements in sensitivity. But, significant non-linearity can be introduced by threshold settings that reject portions of single ion signals. Thus, comprehensive characterization of signal waveforms is required for proper implementation of this strategy. Methods will be presented for adjusting detector gain and quantifying the degradative effects of threshold setting in order to maximize dynamic range in the ToF-AMS. The monitoring of certain dynamic processes requires the ability to track changes in aerosol chemistry with sub-second time resolution. Using recently developed software routines, the ToF-AMS can record high-resolution mass spectra at rates up to 100 Hz. As demonstration, data will be presented from both eddy covariance flux measurements in the canopy of the Blodgett Forest (California) and controlled biomass burning experiments. Because EI induces fragmentation of nearly all analyte molecules, MS information content is potentially limited by redundancies in the fragmentation of analyte and background molecules. In an effort to better identify molecular tracers for particular aerosol sources, we have recently constructed a prototype metastable atom bombardment (MAB) ionization source. In MAB ionization, energy is transferred to analyze molecules through interaction with excited-state molecules of a neutral reagent gas that are produced in a low-pressure discharge. The quantity of energy transferred depends on the reagent gas used, and the gas can be selected in order to yield ionization without fragmentation. Preliminary data characterizing the functionality and sensitivity of this source will be presented.
(361) Application of Photoelectron Resonance Capture Ionization Aerosol Mass Spectrometry to Internally Mixed Amino Acid-Lipid Particulate Proxies of Marine Organic Aerosols
Giuseppe Petrucci, Scott Geddes, James Zahardis; 'University of Vermont

Marine aerosols contribute significantly to the global organic aerosol burden and there is strong recent evidence of a direct correlation between peaks in biological activity and emission of organic compounds into the marine troposphere. Little is known however, about the partitioning of amino acids and other proteinaceous matter, between the marine monolayer (i.e. sea-air interface) and the marine boundary layer. This contributes to uncertainty in describing the fate of organic nitrogen in the oceanic biogeochemical cycle. As of late, free amino acids and other types of proteinaceous matter (e.g. combined amino acids, transparent, stainable proteins, etc) have been detected in marine aerosols. Both of the aforementioned studies have sampled onto filters with subsequent storage, extraction and analysis. We have recently applied photoelectron resonance capture ionization aerosol mass spectrometry (PERCI-AMS) to the analysis of amino acids, including serine, glutamic acid and phenylalanine in proxies of marine organic aerosols and their heterogeneous reaction products in the presence of ozone. Preliminary results indicate that ozonolysis of serine and oleic acid amides converts a fraction of the amino acid to its nitrate analogue, suggesting that organic nitrogen from amino acids may exist in the nitrated form. This in turn may impact transport, reactivity and possibly detection, thus meriting further investigations with other amino acids that have been detected in the marine troposphere under realistic ozone concentrations (< 100 ppb). We are also exploring conditions that may favor the formation of high molecular weight products in these lipid-amino acid amides including polyamides and alpha-acyloxyalkyl hydroperoxides. We are currently adapting PERCI-AMS to sample both free amino acids and hydrolyzed proteinaceous matter (e.g. bovine serum albumin) from above the marine microlayer. It is our hope to adapt these laboratory aerosol simulations using PERCI-AMS to field studies.

(362) Negative Ion Chemical Ionization Mass Spectrometry of Aerosol Organic Matter
Joel Thornton1, Reddy Yatavelli2, Faye McNeill1; 'University of Washington, Seattle

To measure the complex, highly oxidized nature of organic matter in atmospheric particles will require a number of complementary analytical techniques. I will report on progress towards utilizing selected negative ion chemical ionization mass spectrometry coupled to a novel aerosol impactor with a low cut-point diameter and capable of rapidly volatilizing non-refractory organic material. I discuss the utility of negative reagent ions, such as the halides, as a means to distinguish between carboxylic acid containing species from those of aliphatic character. We have employed the impact-ionization technique in a range of chamber and flow tube studies of aerosol growth and aging to study the partitioning of organics between the gas and particle phases and heterogeneous oxidation kinetics. I will also discuss the viability of such instrumentation for use in field campaigns to study ambient particulate organic matter.

(363) Multidisciplinary Characterization of a Novel Anhydride and Amine Functionalized Polymer from Reactive Extrusion
Nancy Jestel1, Mark Denniston1, Mark Pietrafesa1, Alex Sokolowski2, Carl Strom1, David Zoller1; 'SABIC Innovative Plastics

Polymers with reactive functional groups are readily available commercially. The reaction of these groups during polymer extrusion provides a cost-effective means to combine immiscible polymers to produce new classes of polymer blends. Reactive extrusion of such materials also is used to promote the adhesion of filler materials to the polymer matrix. These post-polymerization reactions often involve by-products and degradation compound formation and side reactions. This field presents a rich area of analytical study and requires a multidisciplinary characterization approach. There are several categories of functionalized polymers, but maleic anhydride groups are one of the most common. These commonly are reacted with polyamides to form copolymers. However, in many cases, an amine-functionalized polymer would be useful, but these have been challenging to produce via extrusion. This study focuses on the characterization of efforts to produce such a polymer by extending a maleic anhydride group with an amine group via reactive extrusion. The solution reaction of fumaric acid and hexamethylene diamine produces a white precipitate, which can be isolated and subsequently extruded with thermoplastics, such as polyethylene. Maleimide and primary and secondary amine structures are hypothesized to form. The characterization of the precipitate via Fourier transform infrared spectroscopy (FTIR) and nuclear magnetic resonance (NMR) will be discussed, as will the use of fast FTIR, differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), and thermal desorption gas chromatography-mass spectrometry (TD GCMS) to understand its thermal behavior. The precipitate was extruded with linear low-density polyethylene (LLDPE) and with an aromatic-based polymer under a variety of conditions. FTIR spectra were analyzed to determine if the precipitate behaves the same in the presence of polymer as alone. Spectral band interpretation was aided by studying several model compounds and systems, particularly since the presence of aromatic species complicates the system. There is evidence of the formation of a cyclic aliphatic primary amine upon heating, but the bonding between polymer and this compound was neither proven nor disproved.

(364) Efficacy of Model NIR Calibrations for Determining Ethanol Content in Spirits
W. F. McClure, 'NC State University

Near infrared spectroscopy (NIRS) calibrations based upon mixtures of neat constituents are not known their robustness, exception being pharmaceutical applications where the final product is a blend of any number of rather pure raw materials. Numerous examples where mixture calibrations fail to live up to expectations can be found in agriculture. For example, calibrations for predicting protein in plant tissue, derived from known mixtures of pure protein, starch and cellulose – the primary constituents in plant tissue, are destined to fail. Quite the contrary, acceptable protein calibrations must be based on spectra acquired from plant-tissue samples and a reference analysis of the protein content of those samples. Furthermore, the predictions of future samples utilizing calibrations from the “training” process insist that the samples be similar to the ones making up the training set. Nonetheless, researchers remain challenged by the concept of a model calibration. Although the literature contains papers that demonstrate the efficacy of NIR spectrometry for determining alcohol content, it seems that none address the model calibration challenge. In a recent study of the qualitative features of the spectra of both ethanol/water mixtures and commercially available alcoholic beverages certain striking similarities were revealed. For example, ethanol absorption bands from a 40% ethanol/water mixture appeared congruent with the same bands in whiskies containing the same levels of ethanol. Recognizing the similarities between mixtures and certain spirits, this paper reports work to determine the extent to which model calibrations, based on ethanol/water mixtures, can be used to estimate ethanol in commercial spirits.
(365) Aquaphotomics: VIS – NIRS Absorbance Pattern of Water Matrix as Biological Marker

Roumiana Tsenkova; "Kobe University

When analyzing biological systems using conventional IR spectroscopy, the aqueous component has always been considered somewhat of a nuisance in that it strongly absorbs across the entire frequency range. It therefore tends to mask the more subtle features arising from the materials of interest. Moreover, as water is a not very well understood system, it is difficult to calculate the specific contribution made by the aqueous phase. Water as a natural biological matrix containing only small molecules and hydrogen bonding changes its absorbance pattern, accordingly, when adapting to physical or chemical change in biological systems. Recent work on mammary gland inflammation diagnostics with NIRS, has shown that the spectra of bio fluids, such as raw milk, blood, urine, rumen juice are very similar. These samples are dominated by water that absorbs near infrared light energy in a specific way depicting respective water absorbance patterns (WAP) according to the rest of the elements in the system. Therefore, each biological system under various perturbations could be presented by its water matrix coordinates, WAMACs. Further study proved that loadings and regression vectors developed for various constituents in these fluids depend on the health of the respective animal. They had a substantial number of common wavelengths with high impact to each model. Most of these wavelengths were found to be well-known water absorbance bands or overtones of assigned in IR range specific water configurations, eg dimers, trimers, solvation shells etc. As these configurations are very sensitive to the configuration and charges of the solvated molecules or clusters, the NIR spectrum of the solvent has been found to contain significant information about the solutes. This has opened a whole new area, aquaphotomics, to develop non-destructive, real time spectrophotometry of water and biosystems under various perturbations to study the influence of water on the structure and functioning of biological systems and for disease diagnosis and understanding.

(366) Comparison of NIR Instruments for Grain Analysis

David Himmelsbach1, Miryeong Sohn1, Kevin Hicks2, Franklin Barton, II3; 1USDA-ARS-RRRC, 2USDA-ARS-ERRC

Three different near-infrared (NIR) spectroscopic instruments were compared for use in the analysis of barley grain for the development of a rapid method of analysis for 6 components of the grain. One Fourier-transform and two dispersive instruments were utilized and evaluated for the prediction of: moisture, starch, protein, oil, ash and α-glucan in both intact and ground grain. One hundred forty-three samples of barley grains of 3 types (hulled, hullless and malt) collected over 2 growing seasons and from various locations in the United States were utilized in the study. Samples could be classified using PCA by type and growing season. Good PLS correlations (R2=0.9) were obtained to moisture, starch, protein and oil compositional data with lower correlations (R2=0.8-0.6) to ash and α-glucan. Results on ground samples were better than for whole kernels. There was no apparent predictive advantage in using a high-resolution FT-NIR instrument over a dispersive system for ground samples. The high-resolution FT system only proved superior for the assessment α-glucan in whole kernels. A high signal-to-noise ratio is apparently the important factor for prediction of most components of grains like barley. The selection which type of instrument to use for analysis depends on the nature of the sample and the type of analysis desired.

(367) NIR Calibration Transfer – Tight Wavelength Control Using a Rare-Earth Standard

William Muller1; 1FOSS NIRSSystems, Inc.

Calibration transfer between diffuse reflectance NIR instruments sometimes presents a challenge. Multiple instrumental factors contribute to this difficulty. This paper focuses on wavelength control between like instruments, which is addressed to achieve successful calibration transfer between instruments. Previous papers have described the benefit of Reference Standardization, which virtually eliminates spectral baseline (Y-Axis) differences attributable to reflectivity differences between ceramic reflectors, polymer reflectors, and other NIR background reflectance references. Once the baseline reference is standardized to 100% reflectance, the next major spectral improvement in a diffuse NIR instrument is accomplished by tight control over the wavelength response of instruments. Wavelength response, measured on the X-axis, is reported in either nanometers or reciprocal centimeters. Because NIR spectra are composed of overlapping absorbances, wavelength control using an absorber with sharp peaks is somewhat complicated with a diffuse instrument. Though each useful peak of a rare-earth standard has a sharp absorbance, the effect of adjacent peaks can skew the shape of that peak. Further, instrument bandwidth may have a minor effect upon the reported position of the peak. The peak-finding algorithm must ignore the shoulders of the peaks, and view the highest-absorption part of the peak. Early NBS (National Bureau of Standards) work on rare-earth NIR reflectance standards used a proportional-divider bisection technique. Center of gravity methods are sometimes used, though these are affected by peak shape. Current polynomial peak-finding methods are considerably more precise. Production batches of rare-earth materials appear to have some slight differences in measured peak position. Though differences are typically only a few hundredths (or tenths) of a nanometer, and only on certain peaks, this issue determines whether the standard can be used for wavelength control (calibration) on NIR instruments. Lastly, wavelength response on reflectance rare-earth wavelength standards should fall within the NIST uncertainty limits for this type of standard. Therefore, each instrument must pass a Wavelength Certification test to NIST peak nominals to be qualified for use. This paper describes methods used to characterize and standardize instrument wavelength-scale response, to assure that calibration transfer is easily accomplished between similar NIR diffuse reflectance instruments.

(368) Intermediate-Frequency Raman Modes for the Lower Optical Transitions of Semiconducting Single-Walled Carbon Nanotubes: Fotios Papadimitrakopoulos1, Zhengtang Luo1, Stephen K. Doorn2; 1Nanomaterials Optoelectronics Laboratory, Department of Chemistry, Polymer Program, Institute of Materials Science, University of Connecticut, 2Chemistry Division, Los Alamos National Laboratory

A new class of intermediate-frequency modes IFMs associated with the E22s and E11s optical transitions of bundled HiPco single-walled carbon nanotubes SWNTs have been investigated via tunable laser 700-985 nm resonance Raman spectroscopy. "Steplike" dispersive behavior was observed for these IFMs, along with associated clusters of radial breathing mode RBM overtones at higher frequencies. While the excitation profiles of both RBM and RBM overtones follow a classical behavior predicted by resonance Raman theory, significant differences are observed for the IFM excitation profiles. The observed IFM maxima were found to obey a resonance behavior based on a combination of the E22s and E11s S transition energies, scaled by the inverse diameter of the respective nanotube. Only IFMs for the mod(n-m,3)=2 nanotubes are visible, with intensities found to obey the family-
(369) The Role OF FT-IR Spectral Imaging in Helping to Resolve a Pet Food Contamination Issue
Curtis Marcott¹, Gloria M. Story¹, Anthony E. Doyrey¹, Andrew S. Fix¹, Aletha Pullen², Adrienne Bigelow-Kern², R. Thomas Cambron²; ¹The Procter & Gamble Company; ²Procter & Gamble Pharmaceuticals
The use of contaminated wheat gluten as an ingredient in pet food led to renal toxicity in a number of cats and dogs. Melamine, cyanuric acid, and related compounds were identified as the contaminants by mass spectrometry. The role Fourier transform infrared (FT-IR) spectral imaging played in identifying melamine cyanurate as the insoluble precipitate in kidney tubules, will be discussed.

(370) Spectral Imaging For Parallel High-Throughput Screening
Jochen Lauterbach; ¹University of Delaware
In the past few years, high-throughput screening (also commonly called “combinatorial catalysis”) has become a routine technology for the development of heterogeneous catalysts for many chemical applications. Spectral imaging approaches are truly parallel high-throughput screening techniques, where the screening time is not proportional to the number of samples, as it is with sequential approaches, but is independent of the number of samples in the field of view of the instrument. We employ asynchronous rapid-scan FTIR hyperspectral imaging, which combines the ability to study multiple samples in a combinatorial library in real time in a quantitative fashion. The IR imaging system employs a 128 x 128 pixel mercury cadmium telluride Focal Plane Array (FPA) detector, which is sensitive in the mid-IR range. We can collect one interferogram in each pixel of the detector every ~1s in an asynchronous fashion. The end results are spectral images with 16384 interferograms for each scan, where each pixel contains a full infrared spectrum. We currently use two reactors, one for 16 powder samples (high-surface area support) and one for 8 monoliths, such as core samples from automotive exhaust aftertreatment catalysts. Examples from our recent work will be presented, including the discovery and optimization of novel Nitrogen Storage and Reduction catalysts for lean burn automotive applications, the study of K/Ru supported catalysts for ammonia decomposition, and the optimization of ethylene epoxidation catalysts.

(371) Augmenting Spectroscopic Imaging for Analyses of Samples with Complex Surface Topographies
Michael Gilbert¹, Frank Vogt¹; ¹University of Tennessee
Spectroscopic imaging has become a widely used tool for analyses of heterogeneous samples. By utilizing focal plane array detectors in spectrometers a large number of spectra are acquired from different sample locations in parallel. This enables studies of analyte distributions in an X-Y plane. One example focused here is chemical sensing of biological material. However, in many cases samples need to be analyzed in three spatial dimensions (X-Y-Z). This requires the acquisition of both spectroscopic (X-Y) and topographic (Z-dimension) information. Spectroscopic imaging sensors cannot achieve this because 2-dimensional (2D) images are taken from 3-dimensional (3D) samples. Consequently, depth information is inherently lost. We have augmented a spectroscopic imaging system that not only determines X-Y distributions of chemical information but also probes sample topographies. This is achieved by a custom-made illumination optics that generates and projects a regular light pattern onto a sample. Due to a sample’s 3D topography, the regular light pattern is distorted according to the sample’s surface structure. In other words, the topography is encoded into the distortions of the light pattern. In order to relate distortions of this light pattern to physical heights, the setup must be calibrated using objects of precisely known dimensions. Based on distortions produced by these calibration objects a transform from distortion to physical heights/topography can be derived. Because the analysis of the topography must not affect spectroscopic measurements, two different wavelength ranges are used. An example will be presented utilizing mid-IR spectroscopy for chemical analyses and a light pattern generated in the visible region to probe the topography. This measurement technique is being applied to analyze and classify different tissue types obtained from mouse organs. This novel sensing technique is compared to a conventional pathological approach that can only analyze thin slices of laboriously prepared tissue samples.

(372) Synchrotron Infrared Microscopy Imaging Using a Multi-Element Detector (IRMISH-MED) for Diffraction-Limited Chemical Imaging
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Examining kinetics of living cells (phytoplankton), fungi and bacteria-mineral interactions requires the ability to image sufficiently large sample areas encompassing even large whole cells quickly on biological time scales. A new facility based at the Synchrotron Radiation Center is being presently being developed and commissioned by the University of Wisconsin-Milwaukee for infrared studies of these systems. The brilliance of the synchrotron is critical to provide sufficient flux density to obtain diffraction limited images on such short time scales (in under a minute). Multiple overlapping beams will be used to homogenously illuminate the sample area, imaged onto a multi-element detector (MED). The beamline will consist of 12 25 x 25 mm2 beams, that will be demagnified and independently steered to fill a 40 micron2 sample area at the sample plane of a commercial infrared microscope, a Bruker Hyperion Microscope with a 64 x 64 pixel focal plane array detector. It will be equipped with a 15x Schwarzschild condenser and a 74x Schwarzschild objective achieving effective geometric pixel sizes of 0.54 x 0.54 micron2 at the detector. This pixel size is equal to 1/2.8 for even the shortest wavelengths of 2 micrometer, providing adequate information for point spread function (PSF) deconvolutions of the chemical images to obtain high quality diffraction-limited (or higher) resolution. This project has a potential to impact a wide variety of research areas ranging from soft matter condensed physics, nanoscience, biology, chemistry, veterinary science, engineering, environmental science and geology.

(373) Implementing FT-IR Spectro-Imaging as a Biomedical Molecular Imaging Modality
Cyril Petibois¹²; ¹University of Bordeaux; ²CNRS UMR
FT-IR spectro-imaging instrumentation is coming of age to envisage its routine utilization in the biomedical field. Clinicians tackle this imaging modality as a molecular probe for disease pattern recognition, notably for diagnosing cancers, but also for pathologies implying alterations of tissue morphology and functions. However, if the FT-IR imaging technique now provides high quality images of tissues, the offer of data treatment tools remain very poor in softwares proposed by the manufacturers of FT-IR instruments. Consequently, the current scientific effort is mostly devoted on the implementation of chemometrics specifically applied to FT-IR spectro-imaging. A convergence is clearly required between spectroscopists, chemometrists, and clinicians to grab the opportunity at positioning FT-IR spectro-imaging.
biomedical imaging context. With its 6 µm spatial resolution, its micromolar sensitivity, the global organic information provided, and the possibility to analyze samples without pre-treatments, this technique offers critical advantages regarding the most popular modalities currently in use. Through several examples from recent studies, the aim of this report is to show how FT-IR imaging might play a role in clinics and for laboratory research.

(374) Practical Aspects of Automated Histopathology using FTIR Imaging
Rohit Bhargava1; Rohit Reddy1; Hong Kong1; Frances Keith1; Gokulakrishnan Srivivasan1; University of Illinois at Urbana-Champaign

FTIR imaging is a strongly emerging technology for the analysis of biomedical samples. In particular, its use for automated histopathology has gained considerable importance. We demonstrate, first, the effects of experimental parameters on tissue classification and provides quantitative measures of the effects of each. Strategies to find optimal operating points are discussed. Next, the entire classification process is described mathematically and important statistical considerations are enumerated. In particular, a model is provided to predict how results may change with study design. Several examples from different tissue types are provided to illustrate the classification process and the effect of experimental parameters. We demonstrate that similar approaches can successfully classify several types of tissue with the same underlying performance measures. We conclude that designing a robust classifier is the key exercise and is insensitive to variations in biological or experimental parameters. Last, an integrative protocol to understand and analyze the classification process in quantitative terms is suggested.

(375) NeSSI, Miniaturization, and Microminiaturization Benefits for Finer Control in Chemical Analysis
David Simko1; Swagelok Company

Institutional, governmental, and industrial research communities are under pressure to reduce the cost of R&D, improve the timeliness and productivity of the R&D effort, address safety in the lab, and pack more equipment and systems into confined space. Important trends in analyzers and analyzer systems are miniaturization, moving analytical instruments from large rack-mounted devices to an instrument-on-a-card eventually to a lab-on-a-chip, and implementation of intelligent closed loop control of analyzer systems. The New Sampling and Sensor Initiative (NeSSI) released in August 2000 by the Center for Process Analytical Chemistry (CPAC), a joint an academic-industry research consortium at the University of Washington in Seattle, is a response to these trends. Initially conceived as a method to improve process analyzer sample systems, the modular components developed in response to the Initiative have become platforms for miniaturized systems that support the laboratory and R&D effort, such as gas and liquid handling, pure water, and basic utility systems. These systems are easy to configure, using software developed for the purpose, and easy to assemble. Valves, filters, regulators, and other functional fluid control components surface mount on a 1½ in. square position on a substrate that defines the flow path through the system. The interface seal is defined by a consensus standard, ANSI/ISA 76.00.02. Manifolding facilitates the connection of multiple supply, sample, calibration, and purge streams. Sensors have also been configured to surface mount to the system substrate. The technology also provides a platform for standard sensor arrays and interface with microanalytical devices and micro reactors. Proven applications using miniature modular technology exist in process and pilot plants and in laboratories in both manual and automated systems. A goal is to employ more automation with miniature modular systems populated with intelligent devices that can communicate with each other via an intrinsically safe open-architecture communications bus. This paper discusses miniature modular technology; what it is; where and how it is applied in process and pilot plants, laboratories, and by the instrument manufacturers; and its impact on costs.

(376) NeSSI: An Enabling Platform for the Major Reduction in Total Cost of Ownership in Process Analytical Systems
Peter van Vuuren; Process Analytics Consultant

This paper will describe the real potential of NeSSI as a sensor platform which combined with fiber-optic based on-line spectroscopic techniques could have a major impact on the total cost of ownership for process analytics installations. NeSSI was originally designed to allow for smart sampling systems which when integrated with on-line analyzers would result in an overall reliability and maintainability improvement as sampling systems have been implicated as the weakest link in a majority of on-line process analytical applications. However, NeSSI was always also projected as a platform for a new generation of mini or micro-analyzers or sensors which should enable easy access to a process sample and easy connectivity to associated process control systems. Properly designed and implemented, this new generation of analyzers or sensors is expected to bring a new level of application specific, reliability and cost-effectiveness to the business of on-line analytics. The cost of “unreliability” is of course mainly manifested in the total cost of ownership as the cost of spare parts and the cost of additional manpower to support the analyzer. However, when analyzing the overall total cost of ownership for analyzer intensive manufacturing plants, it came as no surprise that the major cost of the analytical installation is the infrastructure cost, i.e. analyzer shelters, sample transport lines, support for consumables etc. Recently, spectroscopic techniques such as Raman and Tunable Diode Laser Absorption Spectroscopy which use remote fiber-optic based sensors have been poised to make inroads as alternative measurement techniques to traditional analyzers such as process chromatographs. The presentation will highlight a more detailed analysis of Total Cost of Ownership (TCO) and use a typical ethylene/propylene manufacturing process as an example how such fiber-optic probes/sensors in combination with NeSSI as a smart sampling platform can replace traditional analyzers and as a bonus, significantly reduce the infrastructure and operations costs, both of which make up the bulk of the TCO for a process analytics installation.

(377) Application of NeSSI at UOP: From Laboratory Applications to Commercial Process Monitoring
Falah Falih1; UOP LLC

Commercial needs are consistently increasing pressure on researchers to develop more compact and modular tools that can be constructed easily, and modified to help improve and speed up testing capabilities at UOP. An integral part of addressing these needs is the implementation of the NeSSI systems at UOP. Using the NeSSI technologies at UOP offers greater flexibility and saves time in constructing and modifying many of our advanced characterization tools. This talk will present several advanced characterization tools that were constructed at UOP, using NeSSI, and some of our compact and portable commercial process monitoring tools that were constructed using NeSSI.

(378) NeSSI Generation 2: A New Initiative Creates New Opportunities For Smart Sampling Systems
Robert Farmer1; Siemens Energy & Automation, Inc.

Sample conditioning systems used in process analytics have the undesirable distinction of being the one part of a total process analysis system that requires the most maintenance. At the same time, it is traditionally expensive or prohibitively complex to use
hand, surfactants have been evaluated. The anionic surfactant SDS shows the least effect on the heme structure. Only a slight increase of the v2 band, the emerging of the v2 band at 1583cm-1, and a significant disruption to the protein’s structure as evidenced by a shift of the v4 band, the emerging of the v2 band at 1583cm-1, and a significant disruption to the protein’s structure as evidenced by a shift of the v4 band. Our recent work indicates that proteins exhibit different electrochemical behaviors on CNT prepared using various surfactants. The present study is devoted to explore the surfactant effects on the active site structures of heme proteins using Raman spectroscopic method. Three types of surfactant including anionic, cationic and non-ionic surfactants have been evaluated. The anionic surfactant SDS shows a significant disruption to the protein’s structure as evidenced by the shift of the v4 band, the emerging of the v2 band at 1583cm-1, and the changes of spectral features at the lower frequency region. The band at 1583 cm-1 indicates the presence of a low-spin component which may be responsible for the ambiguous Faradic current of the CV. The cationic surfactant CTAB also shows a considerable effect on the protein structure. However, the Raman spectrum at the lower frequency region is similar to that of the native protein with all the bands at the same frequencies. A new band at 1489 cm-1 indicates that the heme is at a 5 coordinated high spin state implying the loss of the distal water molecule. This change, caused by the hydrophilic interaction of CTAB with the heme pocket, favors the electron transfer in that both the ferric and ferrous hemes have the same spin state and no re-organizational energy is involved during the electron transfer process. Among three surfactants tested, the non-ionic surfactant Triton X-100 has the largest effect on the heme structure. Only a slight increase of the v2 band at 1582 cm-1 is observed implying the presence of a low spin component. The low spin component, which mediates the electron transfer, may account for the Faradic response of the protein at the CNT-Triton X-100 modified electrode. Since the protein retains a nearly native structure, the adsorption of unfolded proteins at the electrode surface is avoided and a higher Faradic current is observed. Acknowledgement: This work was supported by the National Institutes of Health (Grant S06G008047and NIH-RCMII1G12RR12459-01).

(383) Low Power Deep UV Raman Spectroscopy
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Deep UV Raman spectroscopy with excitation below 250nm has long been demonstrated as the best way to avoid native...
fluorescence background interference for essentially all target and background materials and can provide a Raman method with the most universal applicability. However, excitation in the deep UV offers challenges both for minimizing photochemical and thermal sample damage which require low power, low dose, excitation to achieve Raman spectra. This, in turn, requires a rethinking of the traditional ways of doing deep UV Raman spectroscopy. A new class of miniature deep UV lasers that have output at 224nm and 248nm offer the prospect for new, miniature UV Raman spectrometer systems. These new lasers have natural linewidths less than 3 GHz, corresponding to less than 0.5pm or 0.07 cm-1. The laser transitions are CW transitions so that CW operation is theoretically possible. The output power of a 56 cm long laser tube is over 80mW at 224nm, and 1 W at 248nm. In order to sustain this level of output the lasers would consume many kW of electrical power and require water cooling, etc. Because these lasers are transverse excited hollow cathode devices, the rise and fall time of the gain can be accomplished in less than about 10 ms. This allows the commutation of the input power to enable the laser tube and power supply to be made in very small and low average power configurations and enables miniature instruments that do not require high average laser power levels. We will demonstrate an inexpensive, new, fully integrated, miniature UV Raman spectrometer with an overall size of 6”x7”x14” including laser, laser power supply/controller, monochromator, detector, manual or motorized XYZ stage, and all optical and mechanical components. This instrument has a spectral resolution of 34 cm-1 and has an overall line power consumption less than 15 W. We will demonstrate the abilities of this instrument to measure a wide range of materials. And we will describe the next generation of this instrument with a spectral resolution less than 15 cm-1.

(384) Total Internal Reflection Raman Spectroscopy in Paper and Print Analysis

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Confocal Raman spectroscopy has been commonly applied to investigate papers and printed products. Technological improvements in lasers, optical filters and charge-coupled device (CCD) detectors have improved the sensitivity of Raman microscopy to analyse volumes of only a few femtolitres. However, in surface analysis of papers and prints even this depth resolution is not high enough and therefore more sensitive techniques are needed. Total internal reflection (TIR) spectroscopy offers a rapid and nondestructive technique to study sample surfaces. The basics of TIR-Raman spectroscopy lies on the evanescent wave which is caused by total internal reflection. Typically the evanescent wave penetrates to a depth of ca. 50 nm and therefore it offers a remarkably improved depth resolution compared to confocal Raman spectroscopy. TIR-Raman technique makes also possible improvements in the strength of the incident field due to evanescent electric field effects. In this technique, it is possible to use relatively large laser spot, high laser power and wide entrance aperture on the spectrometer which results in high-quality spectra, short acquisition time and minimum sample damage. The objective of this work is to investigate the applicability of TIR-Raman spectroscopy to characterise printed papers. Theoretically, it is possible to analyse the thickness of paper coating layers and ink films with extremely high sensitivity. In addition, it might be possible to follow the binder degradation in paper. In this technique, it is possible to use larger size of measurement area due to larger excitation laser spots. This means that quantitative depth profiling from a large sample area is less time consuming than with confocal Raman spectroscopy. In this paper, we will report the success of these analyses in practise. The results from TIR Raman spectroscopy will be compared to those obtained by confocal Raman spectroscopy.

(385) A Small Volume Flow Cell for Raman Spectroscopic and Spectroelectrochemical Studies of Heme Proteins

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One challenge of Raman spectroscopy for studying heme proteins is that some of these proteins and their reaction intermediates are photolabile. The samples either change their structures through light induced transformations or photo-decompose in the laser beam. Protein samples can also be denatured due to local heat produced by the intense laser irradiation. A flow-cell has been introduced to minimize these effects. However, the reported flow system requires a large volume of sample, which is not practical for precious protein samples, and can not perform Raman spectroelectrochemical studies. In this study, a micro flow system was designed in an effort to solve these problems. The flow system consists of a capillary cell, electrochemical flow cell, and a peristaltic pump that is connected to and controlled by a computer. The feasibility of this system has been tested with photolabile heme protein samples including a novel diheme protein MauG and other proteins adsorbed on nanoparticles. Results indicate that the new flow cell can effectively obviate the laser damage to the sample. The flow system can also be easily connected to an electrochemical cell for controlling the redox state of heme proteins and for monitoring the redox potential during Raman spectrochemical titration. Since the biological functions of heme proteins are closely related to their redox states, this system provides an effective approach to explore the redox state induced structural changes and their biological importance. In summary, the new flow system offers the following advantages. First, it uses a small volume sample (as low as 100 μL). Secondly, it can be easily coupled to an electrochemical cell, chemical reaction cell or other type of chemical module for real time monitoring of a reaction process.

Acknowledgement: This work was supported by the National Institutes of Health (Grant S06GM08047 and NIH-RCMI 1G12RR12459-01)

(386) SERS Microscopy (μSERS): Selective and Sensitive Protein Localization in Tissue Specimens

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In immunohistochemistry and immunofluorescence, proteins are localized in cells and tissue specimens with labeled antibodies. Using either dyes or fluorophores as labels, however, limits the number of simultaneously detectable target molecules because of the spectral overlap of the corresponding label/marker signals. In contrast to electronic transitions, the line width of vibrational transitions is significantly smaller. This offers unique capabilities for a highly multiplexed detection of target molecules, in particular by Raman scattering. In order to meet the sensitivity requirements for bioanalytical applications such as immunooassays, surface-enhanced Raman scattering (SERS) from Raman markers on noble metal nanoparticles is employed.[1] We present the first realization of SERS microscopy (μSERS), also called immuno-Raman microscopy.[2] Specifically, the localization of prostate-specific antigen (PSA) in prostate tissue specimens is demonstrated.[2] Because of the SERS distance dependence, the SERS selection rules and the specific electronic resonance conditions employed, only very few Raman bands from the marker moiety close to the nanoparticle surface are detected. For μSERS experiments, formalin-fixed and paraffin embedded tissue specimens from patients undergoing prostatectomy for prostate cancer were prepared by standard protocols. After paraffin
removal, rehydration and antigen retrieval, tissue sections were incubated with the immuno-SELS marker/labeled antibody and finally thoroughly washed with PBS buffer. Characteristic Raman signals of the marker were detected in the PSA(-) epithelial tissue as expected for this proof of principle.[2] As negative controls, Raman spectra in the PSA(-) stroma and lumen were recorded: they do not exhibit spectral contributions from the immuno-SELS marker.[2] Applications and future directions for this novel and innovative Raman technique in cell and tumor biology will be discussed. References[1] D. S. Grubisha, R. J. Lipert, H. Y. Park, J. Driskell, M. D. Porter, Anal. Chem. 75 (2003), 5936–5943.[2] S. Schlücker, B. Küstner, A. Punge, R. Bonfig, A. Marx, P. Ströbel, J. Raman Spectrosc. 37 (2006), 719–721.

(387) Mixture Selection Algorithms for Choosing Mixture Calibration Standards

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When building a spectroscopic calibration model to predict the composition of mixtures, it is desirable to build the model with actual samples from the process being studied. These samples can be analyzed via a primary method and then a calibration based on some method of spectrometry can be built. If these samples are chosen judiciously, one can be confident that the samples used to build the calibration are representative of the population of samples the model will be used to analyze. In some cases, though, it is impossible or difficult to use actual samples from the process of interest, so simulated mixture samples must be used. In this case, it is important that the range of mixture samples cover the entire mixture space and that the number of mixture samples be large enough to provide adequate coverage of the mixture space. For a two component mixture, this task is trivial, but for three or more components the task of choosing which mixtures to make becomes increasingly difficult. The practical difficulty lies not in determining the boundaries of the mixture space, but in dealing with the large number of possible mixtures. Mixture selection algorithms capable of recommending sets of mixtures that will appropriately cover the concentration range of interest for three or more components mixtures have been developed. The algorithms receive as inputs the upper and lower concentration limits for each component, and the algorithms output a suggested set of mixtures to representatively cover the concentration ranges of interest.

(388) Automated Wavelength Selection for Spectroscopic Fuel Models by Symmetrically Contracting Repeated Unmatched Window Partial Least Squares

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The correlation of near infrared (NIR) and Raman spectroscopic data to jet and diesel fuel properties is benefited by the deliberate selection of continuous wavelength sub-ranges. An automatic wavelength selection strategy would allow for the unsupervised construction of partial least squares (PLS) regression models of increased predictive utility when supervised model construction and maintenance is not feasible. Unfortunately, measuring the predictive utility of a model through “leave-one-out” (or full) cross-validation unacceptably hinders one of the most thorough operations suited for this task, changeable size moving window partial least squares (CSMWPLS), due to an automated version of the algorithm’s necessarily large number of PLS model constructions. Presented is a restricted version of the CSMWPMLS algorithm in which the initial information range selection is accomplished multiple times through interval PLS (iPLS) analysis windows no longer move, and the size changes consist of symmetric attenuations. It is shown that the proposed algorithm can provide significant PLS model improvements during the course of a fully automated analysis of jet and diesel fuel data sets in less time than an automated CSMWPMLS algorithm.

(389) Selection of an Appropriate Chiral Selector for Chiral Analysis by Regression Modeling of Spectral Data

Selmor Modzabi1, Marianna A. Busch1, Kenneth W. Busch1; 1Baylor University

With the current emphasis in the pharmaceutical industry on single enantiomer drugs, there is a need for rapid analytical methods to assess the enantiomeric purity of emerging drugs. Recently, a new technique, known as chiral analysis by regression modeling of spectral data (CARMSD), has been developed by our group and used successfully to predict the enantiomeric composition of unknown samples of chiral analytes. With the CARMSD method, a fixed amount of chiral analyte is mixed with a fixed amount of some chiral auxiliary. Under these conditions, it is found that the UV-visible spectra of the solutions vary with the enantiomeric composition of the samples, and these spectral variations can be correlated with the enantiomeric composition of the samples by multivariate regression modeling. Once a multivariate regression model has been developed with a calibration set of samples, the mathematical model can then be used to predict the enantiomeric composition of future samples solely from their UV spectra. As a key aspect of this approach is the selection of an appropriate chiral selector. A premise behind the CARMSD approach is that the chiral selector associates in some way with the enantiomeric pair of the chiral analyte producing diastereomeric interactions that lead to small differences in the UV spectra of samples with different enantiomeric compositions. An ideal chiral selector would have a center of chirality as close as possible to the functional group involved in the association between the chiral analyte and the chiral selector so as to provide maximum diastereomeric effects. In addition, the chiral selector should be as rigid as possible to limit the number of possible conformations of the analyte-selector adduct. This paper will report our efforts in developing appropriate chiral selectors for CARMSD that maximize the spectral differences in the UV spectra of the samples.

(390) Non-Linear Spectral Effects in Multivariate Optical Computing

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Prior applications of multivariate optical computing (MOC) have intrinsically presumed that all samples follow the Beer-Lambert law in relation to analyte property of interest, for example, concentration. The process of developing a multivariate optical element (MOE), the component which performs an optical regression in MOC, relies on this assumption, thereby articulating the design process towards a system that presumes a linear result. Realistically though, few spectroscopic applications possess perfectly linear analyte properties. In situations where non-linear effects present complications to the calibration of a chemical system, understanding the underlying causes of the non-linearity is crucial for planning appropriate compensation in calibration systems. Multivariate optical computing, as with most calibration techniques, is susceptible to problems due to non-linearity in an analyte system. Thus, for the continued development of this technology, it is necessary to explore what restrictions evolve from non-linear affects, and remedies for them. Potential treatments for handling non-linearity in MOC include adjusting analyte input parameters, modifying the design algorithm and changing system specifications. In this presentation, solutions for coping with spectral non-linearity in MOC will be presented, along with analogous methods using traditional chemometric methods for comparison.
ABSTRACTS

(391) Advancing Kernel Principal Component Analysis (KPCA) by Utilizing 2-Dimensional Wavelet Compression: A Means to Enhance Spectroscopic Imaging
Robert Luttrell1, Frank Vogt1; 1University of Tennessee
Multivariate image analysis (MIA) is a standard tool for visualizing spectroscopic imaging data. MIA is based on a principal component analysis (PCA) and combines three user-selected scores into one image resulting in a red-green-blue image. Such an image provides distributions of spectroscopic signatures represented by different colors. However, PCA can only discriminate a number of factors that are either equal to the number of variables (wavelengths) or the number of samples; whichever is smaller. In spectroscopic imaging of complex biomedical samples, a large number of influences determine the spectroscopic signatures. Consequently, linear algorithms like PCA do not enable straightforward and comprehensive investigations for these types of studies. In order to overcome such limitations, Kernel Principal Component Analysis (KPCA) is introduced to spectroscopic imaging. KPCA transforms measured spectra into a so-called feature space that has a much higher dimensionality. Due to this, more factors can be derived and used for classification. Further, KPCA has been developed to model nonlinear behavior and thus can be applied in situations where Beer’s Law is not applicable. Simulated data as well as imaging data acquired from different tissue types are used to demonstrate KPCA applications. In spectroscopic imaging thousands (64 x 64 pixels = 4096 spectra) or even tens of thousands of spectra (256 x 256 pixels = 65536 spectra) are acquired. At one point in the KPCA algorithm a covariance matrix of dimensions \#spectra x \#spectra is needed which requires hundreds to thousands of megabytes of storage space. Because KPCA has to compute all eigenvalues and eigenvectors of this covariance matrix, its routine application to spectroscopic imaging is inhibited. In order to avoid this restriction, a compression algorithm based on wavelet transforms has been developed. This compression is applied during the calculation of the covariance matrix. Thus the full matrix is never held in memory and only the compressed matrix is diagonalized. The eigenvectors are calculated in the compressed wavelet domain and a decomposition step derives approximations of the true eigenvectors. Computation time for compression is not an issue here since the main goal of this approach is to make KPCA on large data sets feasible.

(392) Characterization of Chemical Imaging Data with Robust Statistical Tools
Frederick Koehler1, Kenneth Haber1, E. Neil Lewis1; 1Malvern Instruments
In performing on-line or at-line characterization of heterogeneity in samples relevant to statistical process control, root cause analysis, blend uniformity, and other applications, summarizing the content of a stream of chemical imaging data sets characterizing the process has become a requirement. After appropriate spectral pre-processing, univariate or multivariate chemometric methods such as PLS or PCR are often employed to produce a chemical map which describes the spatial distribution of each chemical species of interest in the chemical image data set. In many applications where distinct domains or particles are available, quantitative analysis of the spatial heterogeneity of the resulting images has been performed through the determination of key metrics such as particle size, as well as morphological characteristics such as circularity, elongation, etc. However, applications lacking discrete domains or particles are often encountered where a similar quantitative metric of overall heterogeneity is desirable. New tools, including the use of robust statistical methods applied to chemical image data providing an overall summary of spatial heterogeneity and another which can quantitate the preferential affinity of one chemical component for another will be described.

(393) Real-time Measurement of Elemental Mercury Naturally Evaporating from Contaminated Samples Using Cavity Ringdown Spectroscopy
Susan Scherrer1, Chuji Wang1, F-X. Han1, Yixiang Duan2, Christopher Winstead1; 1Mississippi State University; 2Los Alamos National Laboratory; University of Southern Mississippi
We are exploring the feasibility of developing a portable mercury sensor using cavity ringdown spectroscopy (CRDS) to directly detect and measure trace amounts of elemental mercury evaporating out of contaminated soil and solution samples. Considerable amounts of mercury have been released into the environment by anthropogenic as well as natural sources, and this mercury, which can be found in the atmosphere, groundwater, and soil, is a significant environmental concern, impacting all aspects of the food chain. Monitoring and remediation of mercury-contaminated sources requires on-site and real-time information regarding mercury concentrations, transfer rates, and fate (dynamic behavior). To date, the majority of commercially available tools and methods to accurately monitor mercury, such as cold vapor atomic absorption spectroscopy and ICP-MS, require some type of sample manipulation in order to measure mercury. We report a demonstration of CRDS in which elemental mercury vaporized from actual mercury-spiked soils and solutions is measured without any sample preparation, such as pre-concentration or heating. Contaminated samples were placed directly below the ringdown cavity and various parameters, such as distance from the laser beam and sample container geometry as well as simulated field conditions, such as wind, were investigated. Elemental mercury from soils contaminated by HgCl2, HgS, and Hg(NO3)2 was briefly explored; and, in accordance with the literature, the results indicate that HgCl2 is less stable in soils than the other two mercury compounds. These soils were then spiked with various concentrations of the standard mercury solution in order to observe the temporal behavior of the elemental mercury vapor from soils. Detection limits in the pptv range were readily measured in the headspace above the samples. A laboratory ringdown system is utilized in this proof-of-concept research. This study demonstrates that the CRDS technique is not only a powerful tool for mercury monitoring/measurement but also provides a potential technique to study mercury dynamics with high temporal resolution in mercury contaminated sources due to the rapid, real-time response and relative ease of sample exploration. Preliminary results, experimental considerations, and future direction will be presented.

(394) Lead and Tin in Roman Bronze Coins by Atomic Absorption Spectrometry
Mary Kate Donais1, Ashley Dumas1, Kathleen Golden1, Holly Jakubowski1; 1Saint Anselm College
Roman bronze coins collected by students at archaeological dig sites in Crete and Italy were analyzed for lead and tin content by atomic absorption spectrometry. Due to corrosion, the coins could not be visually identified so chemical characterization was instead used to aid in the determination of age and geographic area where the coins were originally minted. A simple method utilizing a programmable block digestion system, acid matched standards, and atomic absorption analysis was successfully used by both research students and non-science majors in an archaeology class. External calibration was used for the lead determinations, whereas standard additions was used for tin. Through comparisons of the data to previously published data it was possible to determine the approximate time and provenance from which the coins originated.
(395) Development of a High Performance Electrospray-Ion Funnel Interface for Biomolecular Ion Mobility-Mass Spectrometry
Sevugarajan Sundarapandian1, John A. McLean1; 1Department of Chemistry, Vanderbilt University

Ion mobility spectrometry coupled with mass spectrometry (IM-MS) has become an important bioanalytical tool that is used to characterize complex samples such as protein digests on the basis of both analyte structure and m/z. In fundamental biophysical studies, IM separations are interpreted with molecular mechanics simulations, which oftentimes can elucidate potential molecular structures that give rise to the experimental IM profiles. By using weak electrostatic field separation conditions in the IM drift cell, the separation is directly related to the ratio of the ion charge-to-mass cross section (or apparent surface area), but it is presently poorly understood whether the measured ion structures are influenced by the ion source that is used to produce them (e.g. MALDI versus ESI derived ions). Our present IM-MS instrument was constructed to use moderate pressure MALDI (2-5 Torr) as the ion source. In this report we describe the design and integration of an ESI ion source that can be rapidly interfaced to the IM-MS for studies of both MALDI and ESI generated ions. The interface uses an hour glass ion funnel design similar to that described by Smith and coworkers [1], with a continuous dc-bias and rf-fields to focus ions to the center of the funnel. In this arrangement, the ion funnel is utilized for high ion transmission efficiency from the atmospheric pressure ESI to the entrance of the IM drift cell and as an ion trap to store ions between IM-MS separations. This interface design can also be readily combined with high pulse repetition rate atmospheric pressure MALDI (upto 5000 Hz), which emulates a hour glass ion funnel design similar to that described by Smith and coworkers [1], with a continuous dc-bias and rf-fields to focus ions to the center of the funnel. In this arrangement, the ion funnel is utilized for high ion transmission efficiency from the atmospheric pressure ESI to the entrance of the IM drift cell and as an ion trap to store ions between IM-MS separations. This interface design can also be readily combined with high pulse repetition rate atmospheric pressure MALDI (upto 5000 Hz), which emulates a continuous ion source such as ESI, so that a critical comparison of MALDI versus ESI derived peptide and protein ions can be made with minor differences in the instrumental arrangement that is used.[1] K. Tang et al., Anal. Chem. 77, 3330-3339 (2005).

(396) Assessments of Sandwich-Type Immunoassay Kinetics using Rotated Capture Substrates and Surface-Enhanced Raman Scattering (SERS)
April Hill2,3, Guifeng Wang2, Robert Lipert1,3, Marc Porter1,2,3

A systematic examination of sandwich-type immunoassay kinetics has been carried out using substrate rotation to control mass transfer and surface-enhanced Raman scattering (SERS) as a readout modality. Heterogeneous immunoassays typically rely on diffusion-limited mass transfer to deliver both the antigen and the labeled antibody to the solid capture substrate. Although the rate of antigen-antibody binding is usually fast, these assays often require long incubation times for both binding steps because the analytes (e.g., proteins, viruses, and bacteria) and the labels (e.g., tagged antibodies) are large species with small diffusion coefficients (i.e., slow rates of diffusional transfer). We recently introduced capture substrate rotation as a means to enhance sample and label flux, thereby decreasing assay time from 24 h to 25 min. Building on these studies, the current work is aimed at a detailed investigation of the kinetics involved in sandwich-type immunoassays using substrate rotation rate to manipulate flux and examine the impact of other parameters (i.e., size and concentration of both antigen and label) on assay kinetics. We examined the effect of rotation rate and time on the antigen binding step and determined the optimum conditions for binding various types of antigens. The effect of these parameters on the label binding step, which used gold nanoparticles coated with both a Raman reporter molecule for detection via SERS and an antibody for biorecognition, was also investigated. These results, which indicate that the use of substrate rotation can significantly reduce the time required to perform SERS-based immunoassays while simultaneously increasing assay sensitivity by reducing the amount of non-specific binding, are presented.

(397) FT-IR Microspectroscopic Detection of Gene Expression and Determining its Extent in Wheat
David L. Wetzel1, Shilpa Sood1, Bikram S. Gill1; 1Kansas State University

In wild wheats a tough glume has endured but in domesticated cultivars used for commercial production in the Great Plains of the United States this trait is absent. The toughness of this part of the plant that protects the kernel is related to the prevalence of lignin along with the cellulose that constitutes the glume. Infrared microspectroscopy in the 4000 cm-1 to 800 cm-1 region enables determination of this trait in relative amounts in experimental lines resulting from the breeding process. Spectra from spatially resolved pixels obtained in an imaging procedure what fraction of the glume is lignified. Ratiosing of the peak areas from lignin to the peak areas of cellulose provides a measure of the relative amount of lignin in the lignified part of the glume. As a measure of the extent of gene expression semiquantitative microspectroscopic imaging data provides selection criteria for the process of reintroducing the tough glume trait into domesticated lines.

(398) Introducing Chemometrics to the Analytical Curriculum—Combining Theory and Lab Experience
Frank Vogt1, Michael Gilbert1, Robert Luttrell1; 1University of Tennessee, Dept of Chemistry

In a typical analytical curriculum, spectroscopic measurement techniques are introduced in conjunction with Beer’s Law. Quantification is often restricted to single-component samples because data evaluation at one selected wavelength position is very straightforward. However, in real-world applications Beer’s Law can often not be applied directly because features from different analytes are superimposed. This is a typical situation which requires chemometric data analysis techniques to preserve analyte selectivity. Students are better prepared for future careers by introducing such methods into the analytical curriculum. Chemometrics achieves optimum concentration predictions from error affected data by means of least-squares regression. Basic principles of univariate least-squares can be introduced along with calibration curves. Beer’s Law is then expanded to multivariate Classical Least-Squares (CLS) by measuring and evaluating absorbances at different wavelengths. CLS is introduced first because it is based on Beer’s Law and students can straightforwardly gain an understanding of data evaluation. However, CLS can only be applied in well-defined situations and for many real-world applications Principal Component Regression (PCR) is required. We observed that teaching chemometrics is greatly enhanced by hands-on experiences. An experiment utilizing FTIR spectroscopy has been designed which can be performed in most teaching labs. In this experiment, students are required to prepare samples, measure spectra, build chemometric calibration models and predict the concentrations in unknown mixtures. In order to demonstrate the capabilities and limitations of both algorithms two scenarios are investigated during this experiment: (1) Students are given the identity and concentrations of each analyte in all calibration samples; only these analytes are present in the unknown samples. (2) An unknown amount of an additional absorber is included in some of the calibration and unknown samples. Situation (2) violates the requirements of CLS but simulates many real-world applications. Consequently, the CLS-algorithm only predicts correct concentrations in situation (1). PCR, however, can handle both situations. In the classroom, 3-4 one hour lectures are required to cover the material. As a homework set, students applied basic linear algebra and derived a solution to a
Chemical techniques used to provide profile information of a finished product (medicines, illicit drugs, pesticides, beverages, etc) are crucial since they give feedback on the quality of the product, and in investigative cases, information can be used to track the origin of batches of illicit drugs. Standard methods commonly used for profiling products include separation techniques (thin layer, gas, and liquid chromatography, and capillary electrophoresis). One inherent disadvantage of these clean-up techniques is low throughput. A quick approach that is gaining some momentum in its applications is the use of infrared spectrometry in combination with attenuated total reflectance element (FTIR/ATR). In this study we have obtained spectra of various mixtures of a drug and an inactive material (sorbitol) as our test samples. We have further obtained spectra of various brands of over-the-counter medicines (Tylenol, migraine formula). These formulations contain similar active ingredients (aspirin, caffeine, and acetaminophen) and excipients that are combinations of cellulose, stearic acids, glycols, providone, among others. The spectra were obtained on the solid powders, with no attempt to isolate the drug. The acquired spectra were analyzed by principal component analysis (Simca ver 5.1b). Results for both the test mixtures and over-the-counter formulations showed distinct classifications of the spectra, with Euclidean distances more than unity between the formulation brands.

(401) Real-time Detection of Aerosolized Biological Compounds using a Fluorescence Based Detector
Brian Dahlen1, Geoff Wilson1, Jim Brady1, Mike Carrabba1, Hach Homeland Security Technologies
This presentation will show results generated with a fluorescence-based bio-aerosol monitor to detect the presence of low concentration levels of pathogens amid the ambient aerosol. Using an ultraviolet beam of light, the monitor records specific physical properties about individual particles that pass through the beam, such as size and fluorescence intensities. The information learned about the particles detected during a fixed time interval are combined and processed using a real-time chemometric algorithm to determine the probability that a stipulated pathogen concentration was present. Using algorithm results recorded during field tests of the bio-aerosol monitor, the quantitative performance of the detection algorithm can be shown using by Receiver-Operating Characteristic (ROC) curves. ROC curves may be used to compare operation factors such as level of detection, the probability of a false negative, and false positive probability; to determine the optimal operating parameters of the monitor.

(402) Open Access Education in the Analytical Sciences through the Analytical Sciences Digital Library
Alexander Scheeline1, University of Illinois at Urbana-Champaign
The Analytical Sciences Digital Library (www.asdlib.org) is an NSF-sponsored web collection of peer-reviewed websites and original publications whose purpose is to facilitate learning about analytical measurements. Co-sponsored by the Analytical Division of the American Chemical Society, content includes student posters, a professional directory, and links to related digital libraries in environmental sciences, the Southern and East African Network of Analytical Chemists, and the Journal of Chemical Education. The FACSS presentation focuses on Open Access Publishing, peer-reviewed original, archival publications. The slowly-growing collection is approaching critical mass, the minimum size that will warrant indexing by the mainstream chemical indices. Because the publication is purely electronic, formats appropriate to pedagogical material rather than constrained by convention or the limitations of the printed page allow for great flexibility and creativity. Open Access means that all potential readers can use the material at no cost. Difficulties in achieving the full potential of publishing through ASDLib are attracting a sufficient manuscript stream and getting sufficiently rapid response from reviewers. Should these difficulties be overcome, one hopes for the day when editorial volume will present different challenges.

(403) Voltammetric Characterization and Optimization of Nanoscale Architectures for Bioanalysis
Timothy M. Paschkewitz1, Donald M. Cannon, Jr.1; University of Iowa
Recent efforts to improve electrochemical analyses through the miniaturization of sensing architectures have resulted in the improved ability to study complex biological systems. Unique behavior within neuronal systems can be more thoroughly investigated when the length scales of the sensing element (r = 50-100 nm electrodes) approaches size scales of the system under investigation (typical neuron ca. 15-20 µm with synaptic clefts of ca. 50 nm). The ability to directly probe properties, functions and fundamentally new phenomena involved in neuronal communication is made possible when using nanoelectrodes. In addition, reduced IR drop and capacitive currents contribute to increased sensitivity when electrode areas are of nanometer sizes. The motivation of this research is to develop nanoscale electrode architectures to elucidate unique chemical dynamics among single cells in neural systems with improved spatial and temporal resolution. Using Ga+ focused-ion beam (FIB) to mill through ca. 5-µm layers of poly(methylmethacrylate) (PMMA), we have fabricated films with nanometer pores. FIB milling offers stable and facile control over nanoscale fabrication. Such control has allowed for fabrication of single nanopore electrodes and multiple pore arrays. The flexibility of this technique for nanoelectrode fabrication is that architectures can be tailor-made to fit specific applications. In situ physical characterization of the resulting nanopore has been achieved using SEM, confocal, AFM, and brightfield imaging. A construct that tightly seals PMMA to an electroactive substrate (Au) has been designed allowing easy electrochemical interfacing. Electrochemical characterization has been performed using standard redox couples ([Fe(CN)6]3-/ [Fe(CN)6]4-), [IrCl6]2- / [IrCl6]3-, and [Cp2FeTMA]2+ / [Cp2FeTMA]+) with cyclic (CV) and square wave voltammetry (SWV). Resulting electroanalytical data deviates from classical functions that describe measured current responses (neither limiting current plateaus nor diffusive peaks are observed, however somewhat of an intermediate). Initial fluorescence assays to explore interfacing PMMA nanopore electrodes with PC12 model neuronal cells have indicated that the cells will adhere to PMMA without the need for classical adhesion agents (poly-L-lysine, collagen). Concomitant use of FDA and DAPI fluorescent dyes has shown that adhered cells are viable for further in vitro analysis. Further design will include ways to control cell distribution on PMMA for bioelectroanalysis.

(404) Effect of pH on the Voltammetric Response of Cystiene at Chemically Modified Electrodes
Kristy Ball1, Ashley Hanna1, Phillip Voegel1; Southeastern Louisiana University
Glassy carbon electrodes are modified with cobalt phthalocyanine, cobalt-tetra-2,3-pyridinoporphyrine, and cobalt-tetra-3,4-pyridinoporphyrine by scanning from -0.2 to +0.9 volts vs Ag/AgCl for 10 minutes. The resulting electrodes are employed for
the oxidation of cysteine at pH values ranging from 5 - 10. At low pH, the oxidation current is low and increases with increasing pH up to about pH 7 for both cobalt phthalocyanine and cobalt tetra-3,4-pyridinophorphazene. At higher pH values, the level of oxidation current decreases. For reactions involving cobalt tetra-2,3-pyridinophorphazene as catalyst when preparing chemically modified electrodes, the oxidation current consistently decreases over the range of pH examined. Cobalt(II)tetra-3,4-pyridinophorphazene provides the most sensitive detection of cysteine at low pH (pH < 6) while 2,3-pyridinophorphazene provides higher sensitivity at high pH (pH>8). The products of the reactions are analyzed by GC/MS.

(405) 3-D LIF for Trace Analysis
Lam Nguyen1, Eli Margalith1; 1OPOTEK, Inc.

Fluorescence detection can be a powerful analytical technique for the detection and quantification of trace species. The high detection sensitivity of the technique derives from the fact that the fluorescence signal from the target molecule often appears from a condition of virtually no background signal. A proof-of-principle prototype fluorescence spectrometer instrument utilizing an optical parametric oscillator (OPO) has been built and tested on several model analyte systems. The instrument enables continuous scanning of the excitation wavelength while recording the emission spectra. This 3-D fluorescence technique provides unique advantages such as a high sensitivity, highly selective, and non-destructive analytical technique for a variety of pharmaceutical-related applications, including reaction monitoring, process impurity analysis, and blend monitoring for verification of final drug content and homogeneity. Detection sensitivity and chemical selectivity for multi-component mixtures utilizing fluorescence detection can be significantly higher than for competing non-destructive techniques such as NIR or UV spectroscopy. An initial demonstration of these capabilities was made in the liquid phase for selection of active pharmaceutical ingredients (API) at trace quantities solvated in water. As a further demonstration of the capabilities provided by the high power OPO light source, analysis of a contaminated solid surface was performed at a stand-off distance of 15 cm.

(406) A Highly Sensitive Method for the Determination of Dissolved Organics in Aqueous Media by Transflectance FTIR
Ali Kokalç1, Amira Badaan1, Susan Berets2, Joseph Lucania; 1John Jay College of Criminal Justice; 2Harrick Scientific Products, Inc.

Transflectance is that form of reflection spectroscopy which uses a diffusely reflecting substrate for liquid and solid samples. The sensitivity of this technique allows samples to be run in the near-infrared without any preparation. It is seldom used in the mid-infrared, however. Intense peaks in this latter region require sample dilution and solvent peaks frequently interfere with the determination of unknown solutes. In this study, transflectance is used in the mid-infrared analysis of dilute organic compounds in water, where further sample dilution is not required. Solvent interference is eliminated by evaporation. Precise volumes of sample are used, enabling determinations of the concentrations of the original solutions. Less than ten microliters of sample per analysis is required. The equipment consists of the Harrick Praying Mantis diffuse reflection accessory, installed in an FTIR spectrometer, with a special removable sample holder for a transflectance substrate. This holder allows the substrate to be easily and repeatedly replaced in the same position. The substrate is a bead-blasted aluminum disk, 2.7mm thick and 9.1mm in diameter with a central spherical indentation 0.5mm deep and 2.9mm in diameter. A syringe is used to introduce liquid sample into the indentation. The solvent is evaporated using a special heating stage at a controlled 90 degrees C. The substrate is then placed in the holder to obtain the FTIR sample spectrum. The same substrate without sample is used for the background. Calibration curves for two organic compounds are given, showing practical concentration ranges. Precision, sensitivity increases, internal standards, and applicability to non-aqueous solutions are discussed. The use of an alternate, flat transflectance substrate for qualitative analysis of the solvent is demonstrated. Finally, future technique and equipment improvements are outlined.

(407) A New Versatile Programmable Temperature Spray Chamber for ICP
Jerry Dulude1, Vesna Dolic1, Ron Stux1; 1Glass Expansion

The IsoMist Programmable Temperature Spray Chamber has a range of 70 degrees going from -10 to 60C and is programmable in 1 degree increments. Temperature is controlled via an external PC using a standalone proprietary software application. Once programmed, the PC connection is no longer required unless temperature modification is required or temperature monitoring is desired. The unit houses a baffled cyclonic spray chamber which minimizes noise and carryover. Applications of the IsoMist will be described demonstrating its utility across the temperature range. Set at -10C, the analysis of straight naphtha demonstrates its ability to achieve low detection limits in a volatile matrix. Set at 60C, the IsoMist can be used to enhance sample transport for microsamples so that detection limits are not compromised. For analyses demanding long-term stability, the IsoMist maintains a stable ambient temperature dramatically reducing temperature related sensitivity drift. Lastly, an ICP-MS application will be described showing the ability of the IsoMist to reduce oxide interferences.

(408) Increased Instrument Efficiency on PerkinElmer ELAN® DRC II ICP-MS, via Utilization of an ESI SC-FAST Equipt Autosampler.
Jonathan Good1, John Butz2, Gary Priester2; 1Mayo Foundation; 2Elemental Scientific Inc.

A novel autosampler and sample introduction system was applied to a routine analytical procedure for five toxic elements, in urine and whole blood: arsenic, lead, cadmium, mercury and thallium. Extensive validation was then performed to determine if analytical time could be decreased while maintaining or improving analytical sensitivity and robustness. After making necessary adjustments to the procedure, timings were collected to determine if there was a significant time savings with the application of the ESI SC-2 autosampler combined with the SC-FAST sample injection system. Analytical comparisons and precision experiments were run to determine any changes in procedural performance. When data collection was complete, timings showed a 30% reduction of the analytical time, or forty seconds per sample analysis, and the experimental data showed increased performance relative to the method utilizing the old autosampler and sample introduction system.

(409) Application of Six Sigma DMAIC Methodology in Infrared Spectroscopy of Polymers
Eugene Galperin1, 1SABIC Innovative Plastics

Nuclear Magnetic Resonance (NMR) is frequently an instrument of choice for compositional analysis of new co-polymers. However NMR is costly and impractical to use in manufacturing environment. Therefore, there is a need of transferring NMR methods to at-line techniques such as Mid-IR, Near-IR and Raman. In this example several tools, such as GR&R, PLS, and Fishbone diagram were used to transfer NMR compositional method for the new High Heat Lexan polymer (XHT) to solution Near-IR. The new Near-IR method decreased analysis time, thereby enabled reduction in off-spec material production.
We studied temperature effects on nanopore-confined and nanosphere supported, 1,2-dipalmitoyl α-glycero-3-phosphocholine (DPPC). Supported phospholipid bilayers have a great potential for the design and construction of biochips, biosensors and microarrays. Knowledge of the behavior of these supported lipids is essential for future design of sensors and sensor arrays. Lipids self-assembled in rigid nanoporous aluminum oxide have a large surface area and are protected from contamination and degradation. The phase transition of unsupported vesicles in the cooling direction is substantially more cooperative than for anodic aluminum oxide, AAO, supported lipids. However, in the heating direction the relative cooperativity appears unaffected. What is more, the van’t Hoff enthalpy is reduced for both heating and cooling directions. Since the gel to fluid phase transition is mainly entropy-driven due to trans-gauche isomerization at the expense of van der Waals interactions, the reduced ∆H likely results from a smaller cooperative unit and possibly less conformational disorder in the liquid crystalline phase. Although the symmetric CH stretching mode has a narrower width for gel phase confined lipids vs unconfined, both have similar widths in the liquid crystalline state. Since peak width is proportional to acyl chain mobility, the overall order of the liquid crystalline state appears to be unaffected by nanopore-confinement. While planar-supported phospholipid bilayers have been used as sensor platforms, they do not adequately mimic the native membrane environment. Furthermore, flow of aqueous solutions over a typical untethered planar-supported lipid film results in rapid removal of lipids. Likewise, the use of ATR-FTIR as an experimental approach to the study of biological membranes is dependent on strong adhesion of membrane films on the internal reflection element (IRE). We have discovered, the addition of a layer of close-packed nanospheres effectively decouples the membrane from the surface while increasing adhesion. We have investigated the stability and behavior of lipids bonded to this nanosphere adhesion layer. A clear pretransition is observed which is unusual for substrate-supported bilayers. Additionally, the nanosphere supported lipids have fewer end gauche and more kink rotomers in the liquid crystalline state.
order to inactivate Met30. The yeast cells were lysed in isopropanol. The supernatant was stored in dark tubes under nitrogen and analyzed within 2 days by MALDI FTMS. A saturated solution of 2,5-dihydroxy-benzoic acid (DHB) was used as a matrix. Phospholipid mass analysis was performed using the positive ion mode of a 9.4 Tesla FTMS with an external ion source and Nd-YAG laser operating at 1 = 355 nm. Phospholipid assignments were accomplished via an optimized windows version 3.8.25 of the lipid database and search software, utilizing a previously published assignment algorithm2. Following methodology described above, reproducible MALDI-FTMS spectra were obtained from yeast lysates. After assigning the phospholipids, a statistical analysis was performed in order to determine the significant differences in the phospholipid profile of S. cerevisiae. During the inactivation of Met30, the mutant Met4DMet30D, is more abundant in phosphatidic acid and phosphatidyl choline between 10-25% compared to the wt. These results show that performing comprehensive comparative phospholipid screenings by MALDI FTMS helps to identify the impact of mutations on the lipid content of S. cerevisiae.

(414) Development of an Automated Digestion andDeposition Chip Coupled to MALDI-TOF MS forProteomics
Jeonghoon Lee1, Steven A. Soper1, Kermit K. Murray1, 1Louisiana State University
We report on the development of an automated digestion and deposition microfluidic chip platform for the identification of proteins using MALDI-TOF mass spectrometry. In proteomics, the main limitation to identifying proteins is the labor-intensive stages of digestion and separation. Also, achieving high sensitivity with low sample consumption while maintaining high protein sequence coverage is still challenging. Microfluidic systems are a promising approach to increasing throughput and to reducing time-consuming preparation steps in proteomics. An automated proteolytic digestion and droplet deposition system was constructed based on a plastic microfluidic device for off-line MALDI analysis. The microfluidic chip channels were fabricated on a poly(methyl methacrylate) plate with a micromilling machine and using the hot embossing method. The bioreactor is an open channel 100 µm wide and 100 µm deep, and has a 4 cm effective channel length. The microfluidic chip was assembled by thermally annealing a cover slip after UV-modification of the chip. Trypsin was then covalently immobilized on the surfaces of the microchip using coupling reagents. The chip was operated by pressure-driven flow and mounted on a robotic fraction collector system. The digest peptides were coaxially mixed with a solution of MALDI matrix and deposited as discrete spots on MALDI targets. The microreactor provided efficient digestion of cytochrome c at a flow rate of 1 µL/min, producing a residence time of approximately 24 s within the reaction bed. Various proteins were evaluated including cytochrome c, bovine serum albumin (BSA), myoglobin, and phosphorylase b. The efficiency of the digestion was evaluated by monitoring the sequence coverage, which was 64, 35, 58, and 47%, respectively. In the second approach to deposit digested peptides onto a MALDI targets, we evaluated a micro-post structured chip that was operated by an electrokinetically-driven flow. The micro-post structured chip can provide increased digestion efficiency due to a high surface area-to-volume ratio geometry. Also, the chip driven by electrokinetic flow can eliminate mechanical pumping systems and provide flat flow profile in the microchannel. The fabricated bioreactor consisted of a 4 cm x 200 µm x 50 µm microfluidic channel with trypsin immobilized on an array of 50 µm in diameter round-shaped micro-post support structures with a 50 µm edge-to-edge inter-post spacing. Cytochrome c was used as a model protein for evaluating the performance of the automated tryptic digestion and droplet deposition system operated by an electrokinetically-driven flow.

(415) Laser Desorption Ion Mobility Mass Spectrometry for Biological Agent Detection
Juaneka M. Hayes1, Kermit K. Murray1, Michael V. Ugarov2, J. Albert Schultz2, 1Louisiana State University; 2Ionwerks, Inc.
The detection of biological agents presents significant challenges for analytical instrument technology. Biological agents are commonly disseminated as aerosol particles, either sprayed over a wide area or covertly distributed, therefore detection instrumentation must be fast, sensitive, and selective for positive detection with minimal false alarms. Portable instruments that can function in harsh environments with minimal operator intervention are required. Mass spectrometers are exceptionally well suited as detection systems for chemical and biological agents. The challenges for mass spectrometer design are to develop instruments with analysis time in the range of seconds to minutes that can identify specific compounds against a complex background of organic and inorganic compounds. In the ion mobility time-of-flight mass spectrometer (IM-TOFMS), ions are formed by laser desorption in the mobility cell that is held at a pressure of 10 Torr helium. The instrument is operated with a 337 nm UV laser or 3 µm mid-IR OPO laser system. An IR and UV transparent sapphire vacuum window is used for laser entry into the instrument and gold first-surface mirrors direct the beam into the IM cell. Laser desorbed ions drift for 20 cm in the mobility cell and then pass through a 0.5 mm orifice into a differentially pumped region before passing into the mass spectrometer. Mass selection is performed in a 20 cm reflectron TOF mass spectrometer.

(416) Rapid Screening for Functional Groups via Selective Ion-Molecule Reactions in a Linear Quadrupole Ion Trap Mass Spectrometer
Steven Habich1, Nelson Vinueza1, Penggao Duan1, Sen Li1, Brian Winger2, Todd Gillespie2, Hilkka Kenttämaa1, 1Purdue University; 2Eli Lilly and Company.
The ability to rapidly identify degradation products and impurities in drug product mixtures is of great importance to the pharmaceutical industry. Tandem mass spectrometry has provided a partial solution to this problem—analytes ionized, for example, by electrospray ionization (ESI) can be separated in the first mass analysis stage and then subjected to collision-induced dissociation (CID) in order to obtain structural information. However, these CID experiments usually cannot provide unambiguous information on the elemental connectivity of unknown analytes and thus only inferences can be drawn about the structure of the analytes. Recently, our group has developed methodology that involves the use of selective ion-molecule reactions to probe the structures of protonated analytes for the presence and number of specific functional groups in an FT-ICR mass spectrometer. We report here on the implementation of this methodology to a commercially available linear quadrupole ion trap (LIT) mass spectrometer. An external reagent mixing manifold has been developed that allows a selective neutral reagent of interest to be mixed with the helium buffer gas used in the trap. The protonated analyte of interest is isolated in the trap and allowed to react with the neutral reagent for a specified amount of time before being ejected and detected. Preliminary results indicate that the diagnostic reaction products observed in the LIT match those expected based on our previous results obtained using other types of mass spectrometers. The variety of charged species created by the ESI source has also allowed us to probe the reactions of ammoniated and sodiated ions with neutral reagents as opposed to only protonated ions. This is especially useful for certain monofunctional oxygen-containing compounds (e.g., carboxylic acids), since the protonated ions are not always easily generated by positive mode ESI.
source, this methodology is readily applicable to liquid chromatography–mass spectrometry (LC–MS) methods.

(417) Problems Arising out of Impurities in Steam Turbines
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Different impurities are transported into the steam turbine from the Preboiler cycle in the feedwater and the boiler as a total carryover. Their major sources include condenser leak, make up water, and improperly operated condense polishers. The turbine environment is controlled through a control of impurity ingress and various feedwater, boiler water, and steam chemistry limits. The corrosiveness of the steam turbine environment is caused by one or more of following: 1) Concentration of impurities from low part per billion levels in steam to percent levels on surfaces and the formation of concentrated aequous solutions (concentration by deposition or evaporation of moisture) 2) Insufficient pH control (in both acid and alkaline regions) 3) High-velocity, high-turbulence, and low-pH moisture. The steam impurities that are of most concern include chlorides, sulfates, fluorides, carbonates, hydroxides, organic and inorganic acids, oxygen, and CO2. Their behavior in turbine steam and deposits is well documented. There are strong synergistic effects and interactions with metal oxides. In addition to corrosion during operation, turbines can be corroded during: 1-Manufacture (machining fluids and lubricants), 2-Storage (airborne impurities and preservatives), 3- Erection (airborne impurities, preservatives, and cleaning fluids), 4-Nondestructive testing (cleaning and testing fluids), 5- Lay up (deposits plus wet air) Many of the above substances may contain high concentrations of sulfur and chlorine, which could form acids upon decomposition. Decomposition of typical organic for example, carbon tetra-chloride (CCl4), occurs at about 150 °C, there fore, the composition of all of the above substances should be controlled and most of them should be removed before operation.

(418) Studying Corrosion of Coated Titanium Anodes in a Corrosive Solution
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Titanium anodes contain base metal made from titanium that was coated with thin layers of different oxides such as RuO2, IrO2, TiO2. These anodes mainly used in related technology with Electro-chemical process especially in chlorine-electrolysis systems. In this research, since coated anodes samples charged under fixed amperage. Thus Galvano Statistic Graphs was used for studying and observing corrosion and coating dissolution as well as studying their stability. For this reason, activated tests were elected (using diluted solution of NaCl instead of industrial and concentration solutions thereof) so that corrosion phenomena shall be observed in very low period of the samples life. The relative graphs reveals this fact that corrosion and dissolution of coatings shall be done in three stages. It should be noted that by passing short period of time after dissolution, potential of base metal will be exceed for pitting potential. Therefore titanium base metal shall face with sever local corrosion and the coated samples will be total corroded. In this regard, Electro-active elements such as Ru and Ir shall leave from coat in gradual dissolution manner. What remains on the surface of titanium metal is titanium oxide accompany with little contents of RuO2 and IrO2. In other words, with gradually dissolution of coatings the existing chain of electrical conductivity in the said coating will find high separation and conducts the same as non-coated titanium, that make resistance oxide layer on the surface. Also the effect of some different factors are mentioned hereunder. 1) By increasing concentration of Cl Ions, the life of coated titanium anodes as well as corrosion period will be increased. 2) By increasing imposed current density, the life of samples as well as corrosion period will be decreased. 3) High concentration and acid solutions have no significant changes in comparison with neutral solutions. But in alkaline solution, in addition to observing picks in Cathode branches, there is slope change in Anode branch. Finally by increasing pH the life of anodes decreased and dissolution reactions will be occurred in lower potentials.

(419) Excited State Electric Dipole Moment of Two Tryptamine Derivatives through Solvatochromic Shifts
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The determination of excited state electric dipole moment through solvatochromic shifts is one of the easiest approaches to understand the molecular structure in the excited state. These studies have gained importance due to their application in photo science, especially if they are of biological importance. In view of this the excited state electric dipole moments of two Tryptamine derivatives which are of biological importance are determined and reported here. The fluorescence shifts have been used and the results found seems to be more consistent in comparison with the one calculated through absorption shifts. The results presented are also discussed. A qualitative estimate of the orientation of the dipole moments in ground and excited state are also presented and discussed. Of the several methods proposed, the one proposed from N.H.Ayachit1, N.H.Ayachit et al [2] and N.H.Ayachit & G.Neeraja Rani[3] is used in view of the several advantages it has. References: 1. N.H.Ayachit, Chemical Physics Letters 164, 272(1989) 2. N.H.Ayachit, D.K. Deshpande, M.A. Shashidhar & K. Suryanarayana Rao, Spectrochimica Acta, 42A, 585, 1405(1986). 3. N.H.Ayachit & G. Neeraja Rani, Physics and Chemistry of Liquids, 45, 41(2007).

(420) An Application of Graphs of Atomic Orbitals for QSAR Modeling of Toxicity of Metal Oxides
Bakhtiyor Rasulev1, Andrey Toropov1, Tomasz Puzyn1, Danuta Leszczyńska1, Jerzy Leszczyński1; 1CCMSI, Jackson State University, Jackson, MS; 2Civil & Env. E, Jackson State University

Toxicity of fifteen metal oxides towards rats has been modeled using optimal descriptors calculated with molecular graphs and graphs of atomic orbitals. A graph of atomic orbital represents an attempt to take into account structure of chemical element for QSRR/QSAR analysis (i.e., replacing one vertex of chemical element by group of vertexes which represent images of the atomic orbitals). The derived here graphs of atomic orbitals optimize descriptors reasonable predict the toxicity of the studied metal oxides. Statistical characteristics are n=11, r^2=0.911, s=0.179, F=92 (training set); n=4, r^2=0.877, s=0.216, F=14 (test set). In future, when appropriate experimental data will be available, this approach could be used for QSAR analysis of nano-particles of metal oxides, which are important component of modern nanotechnologies. Key words: QSAR, Graph of atomic orbitals, metal oxides, nano oxides, toxicity towards rats.

(421) Assignment of High Resolved 13C NMR Spectra of Polyacrylonitrile with Heptads
Yusong Wang1, Fei Lu1, Wemin Pang1, Qingren Zhu1, Weitai Wu1, Guoyong Xu1, Lianghua Xu1; 1University of Science and Technology of China; 2Beijing University of Chemical Technology

Higher resolved 13C NMR spectra of atactic polyacrylonitrile (PAN) and isotactic-rich PAN than that in previous articles [1,2] were obtained under optimized solution concentration and experimental temperature. Assignments of part nitride carbon spectra with heptads were quantitatively confirmed that are different from the existing views [2]. The methine carbon spectra
were first assigned partly with pentads and heptads, respectively. Atactic PAN obeyed Bernoullian statistics. First-order Markov statistics, Second-order Markov statistics were applied to calculate the content of the n-ads of isotactic-rich PAN. Meanwhile, the number-average lengths of the isotactic and syndiotactic sequences, which were calculated by “block” statistics, identified the above assignment of heptads from other side. References:1. Katsuraya K, Hatano K, Matsuzaki K, Minagawa M. Polymer 20012: 6323-6326. 2. Minagawa M, Yamada H, Yamaguchi K, Yoshii F. Macromolecules 1992; 25; 503-510.

(422) Universal Raman Detection -- Dispersive NIR Raman (DNIR-Raman) above 1 Micron
Keith Carron, Rick Cox, Shane Buller; DeltaNu
DNIR-Raman (Dispersive NIR –Raman) data and characteristics will be presented. The ease of sampling that is found with Raman spectroscopy makes it ideal as a material identification method. However, in spite of the advantages in Raman sampling, many samples are plagued with either inherent fluorescence or fluorescence from impurities. Automated baseline correction routines can sometimes remove backgrounds that do not contain too much structure. For example, Fourier transform techniques can remove the low frequency components of a Raman spectrum and correct for some fluorescence features. However, it is often the case that fluorescence can produce features that fall into the frequency of Raman bands. This leads to distortion of the Raman spectrum and leads to poor library correlations. A solution is to eliminate fluorescence by using an excitation that does not produce fluorescence. Examples can be found using very short wavelengths that produce Raman scattering at wavelengths shorter than relaxed fluorescence is exhibited or long wavelengths using FT-Raman. UV excitation requires complex laser systems that limit its practical use as a material identification method. FT-Raman has laid the groundwork for > 1 micron Raman spectroscopy. It has clearly demonstrated that most fluorescence is removed with 1.064 nm Nd:YAG excitation. Noisy InGaAs or germanium detectors were ideal for multichannel FT-Raman detection. DNIR-Raman maintains all of the advantages of FT-Raman, except it includes the no moving part advantage of a fixed grating spectrometer. We will present data using an Intevac MOSIR 950 InGaAs detector with Transfer Electron (TE) and Electron Bombardment (EB) gain technology. The DNIR system has excellent range, resolution, and stability characteristics. 1064 nm and 980 nm excitation will be compared.

(423) What is “Imaging” in Raman Spectral Imaging, and Why Should I Care?
Jay Zakrzewski; Headwall Photonics, Inc.
Raman spectroscopy is experiencing a rapid increase in commercial and military application integration. There has been frequent discussion regarding relatively low cost, low resolution single point (single fiber) spectrometers for handheld transportable applications, although only limited advancement of higher performance designs. Applications which require maximum signal collection and dynamic range, including those which require multi-channel or full input aperture free optic imaging capability, will benefit if one can fill the entire height of the tallest spectroscopy CCD with minimal distortion of the input image. Most commercially available dispersive spectrometer designs have difficulty imaging all field points of the full Raman spectral bandwidth onto large area spectroscopy CCD’s. Czerny-Turner designs typically have throughput limitations of f/4 - f/6.5, and exhibit relatively high image distortions as one moves further away from the central input axis. Toroidal mirrors are often employed to minimize this effect, although this provides optimized correction for only one point on the focal plane. Others, which are based on axial-transmissive designs suffer at short focal lengths from chromatic aberrations, smile, and keystone. For best results, these often require the use of curved input apertures, non-standard refractive lens material selection, and wavelength optimized anti-reflective coatings on each lens surface to compensate for chromatic aberrations, reflection losses, and potential ghost images. This paper will describe a novel aberration corrected high reciprocal dispersion retro-reflective concentric imaging spectrograph design which produces minimal image blur over the full CCD focal plane with exceptionally high signal to noise efficiency and f/2.4 throughput. This design provides non-magnified 1:1 imaging of straight slit or stacked linear arrays of optical fibers covering the full height of spectroscopy CCD’s with optimal channel separation.

(424) Thin Film Structure of Poly (2-perfluoro-octhylethyl acrylate)Studied by Infrared Multiple-Angle Incidence Resolution Spectroscopy
Masaya Matsunaga1, Kiyoshi Yamamoto1, Takeshi Hasegawa2;
1ASAHI Glass Co., LTD.; 2Tokyo Institute of Technology
Some poly(fluoroalkyl acrylate)s and poly(fluoroalkyl methacrylate)s are known to exhibit excellent oil and water repellency, which are widely used in industry for manufacturing oil-and water-repellent materials. Thin film structure of these polymers have been studied by X-ray analytical techniques, reporting that the perfluoro alkyl (Rf) group contributed to crystallization to form the lamellar structure consisted of single- or double-layer packing of the side chain when the number of CF2 moieties is larger than six, which has a apparent relation to the repellency. Most of these studies were focused on the crystalline regions only, however, and amorphous regions were left unanalyzed because X-ray diffraction techniques require crystalline structure. In the present study, the infrared multiple-angle incidence resolution spectroscopy (MAIRS) has been employed to study the molecular orientation of poly(2-perfluoro-octylethyl acrylate; C8FA) in a thin film on a Si substrate. Infrared MAIRS yields two spectra of the surface-parallel and -perpendicular vibrational modes in optically thin films on an infrared transparent substrate, which is powerful for analysis of polymer orientation irrespective of degree of crystallization. The thin film was prepared by the dipping the Si substrate in a solution of poly C8FA dissolved in HCFC-225 (dichloro pentafluoropropane) with a concentration of 0.5 wt%, and the withdrawn substrate was thermally treated at ca. 120 C. The infrared MAIRS spectra suggested a schematic model: the RF group is straight and oriented perpendicular to the substrate. The side chain was found to be twisted at an ethyl spacer between RF group and carbonyl group due to the hydrogen bonding between H-F. The carbonyl group was suggested to face to the main chain or to the silanol group of the substrate. This schematic model is consistent with a rough image in our previous study by X-ray analysis, and the detailed structure revealed in the present study is reasonable to understand the surface property. In addition, we have also performed the density functional theory calculation to find the optimized structure of the molecules. The calculated results agreed with the schematic structure suggested by the infrared MAIRS technique.

(425) Surface Plasmon Resonance Optical Fiber Platform for Real-Time Oxygen Sensing
Veronica Rigo1, Peter Geissinger1; 1University of Wisconsin-Milwaukee
We describe the development of a novel generic approach to optical-fiber oxygen sensing based on metal-enhanced fluorescence. This effect leads to an increase in fluorescence quantum yield and a reduction in fluorescence lifetime of weakly emitting fluorophores that are held in close proximity to noble metal surfaces with nanometer-scale surface roughness. This sensor
is based on fluorescence quenching of a fluorophore, dichlorotris(1,10-phenanthroline) ruthenium (II). To take advantage of the metal-enhancement effects in our arrays, a thin silver film was deposited by vacuum evaporation onto the core of one of the optical fibers. Subsequently, SiO2 was deposited as an optically transparent spacer layer between the metal and the fluorosensor that is embedded in a photo-polymerized hydrogel matrix. The sensor was tested using a two-crossed-fiber sensor array with two regions excited by a ND:YAG (532.1 nm) laser, with the second region used as intensity reference. The sensor was mounted in a home-built flow chamber where both oxygen and nitrogen were pumped into the chamber at different partial pressures. The fluorescence emitted by the sensor molecules was captured by a second fiber at right angle to the fiber carrying the excitation light. A pass filter and a detector were employed to monitor the sensor fluorescence emission. The output current from the detector (PMT) was analyzed with an oscilloscope. The second part of this study involves the fabrication of different nanostructured surfaces using chemical deposition routes. We used high-resolution TEM imaging and optical spectroscopy to study the relationship of geometrical features of individual silver nanostructures and their optical plasmon resonant properties. This allows matching of the plasmon resonance frequencies to the fluorosensors spectral properties, which is crucial to successfully employ the MEF effect, and to develop ultra-sensitive chemical sensors.

(426) New Plasma Sources for Elemental, Molecular, and Metallic Analysis
Gary Hieftje1, Francisco Andrade2, Gerardo Gamez1, Steven Ray1, Gregory Schilling1, Jacob Shelley1, Michael Webb1; 1Indiana University

In this presentation, the focus will be on new plasma sources for optical and mass spectrometry. The sources are largely based on glow-discharge approaches, with some at reduced (conventional) pressure and others at atmospheric pressure. They offer new possibilities not only for sample fragmentation, atomization, excitation and ionization, but also for sampling. The first new source is intended for the simultaneous emission-based examination of spots on a two-dimensional (planar) chromatographic plate, such as one from thin-layer chromatography or two-dimensional gel electrophoresis. Coupled with a monochromatic imaging spectrometer, the glow-discharge source enables the simultaneous detection and quantification of spots that hold metal-containing proteins or those stained with silver, gold nanoparticles, or metal-containing affinity tags used to identify functional groups. The device is anticipated to be an important tool in the emerging area of “metallomics”. Another new source, also based on a glow discharge, samples metallic species directly from solution, and at atmospheric pressure. Similar to the “ELCAD” device described by others, this source offers a simplified design, extremely rapid throughput, and outstanding detection limits. It requires no gas flow and operates at low power levels; it is therefore attractive for field applications. Fundamental characteristics of the discharge will also be outlined. A third glow discharge, also operated at atmospheric pressure, is intended for ionizing species directly from solid or gaseous samples for mass-spectrometric detection. This discharge is uncomplicated, unusually stable, and generates simple spectra that consist principally of the molecular ion or protonated molecular ion. The potential impact of these new sources in several areas will be assessed.

(427) True Comprehensive Speciation of Nutraceuticals Through Liquid Chromatography-Particle Beam/Glow Discharge Mass Spectrometry
R. Kenneth Marcus1, Joaudimir Castro1, M. V. Balarama Krishna2; 1Clemson University

This laboratory has been following a line of research looking to provide tools for what we have termed “comprehensive speciation”. As such, we look to couple a chromatographic separation (typically LC) with a single ionization source capable of producing both elemental and molecular mass spectra of various organometallics and organics. A secondary criterion is the ability to sample LC effluents under a variety of elution modes. To this end, we have chosen to use a particle beam (PB) LC/MS interface to convert the solute/solvent mixtures to dry analyte particles for delivery into a low-pressure ion source. Glow discharge (GD) ion sources have a long history of effective use in the elemental analysis of solids. The low pressure, inert gas plasma provides an environment where thermal degradation of molecular species takes place, yet with sufficient energetics to yield meaningful molecular and elemental mass spectra. The development of the LC/PB-GDMS instrument has been funded specifically for use in the characterization of botanical extracts (i.e., nutraceuticals). One must distinguish between toxic, carcinogenic, adventitious, and benign forms of the elements (i.e. metals). Finally, one should perform these analyses across the spectrum of sample forms, including raw materials, ethanolic and aqueous extracts, and a number of solid tablet matrices. We will describe here the operation aspects of the LC/PB-GDMS system as is applied to a variety of botanical materials including echinacea, green tea, echinacea, green tea, kelp, and bladderwrack. The ability to perform comprehensive speciation will be demonstrated in the case of arsenic components in the kelp and bladderwrack. Identification and quantification of active ingredients in green tea will be presented in light of the now cult-like sales of the drink. It is believed that the coupling of HPLC, the PB interface, and GDMS analysis is a powerful approach that can indeed deliver comprehensive speciation.

(428) Gas Dynamics of an ICP Torch
Albert Gilmudinov1, Rinat Ibragimov1, Mjakzjum Salakhov1, Ilia Tsivilskii1; 1Kazan State University

Operation of a conventional ICP torch is based on the use of 3 independent gas flows: outer and intermediate gas flows entering the torch tangentially and the central injector flow entering the system axially. The three gas flows are mixed in the plasma region and leave the system as a single complex-structured vortex. Three dimensional nonstationary consideration of gas flow dynamics in an ICP torch is developed in this work. All the fine details of the torch geometry are taken into account, gas flows are considered from the inlet till they leave the system without any simplifications. The model is based on numerical solution of a full set Navier-Stokes equations and allows prediction of temporal behavior of 3 dimensional distributions of gas flow velocities, pressure and temperature. It is shown that in the conventional ICP torch a steady state in flow motion is never reached, so the system is dynamic by its nature. Complex-structured jet leaving the torch and entering the still environment induces a set of vortices in the region adjacent to the torch. Destruction of the vortices results in generation of self-induced oscillations at a frequency of several hundreds Hertz. A principally new effect of gas back flow in the torch near axis region is predicted and investigated. A computer animated presentation of the flow dynamics will be given. Variety of gas flow velocities and torch geometries are studied. Comparison of computed data with available experimental results will be discussed.
(429) Laser Ablation-Inductively Coupled Plasma Mass Spectrometry – Ablation Characteristics of Zircons and NIST Glass
Detlef Günther1, Barbara Kuhn1, Yan Luo2; 1Laboratory of Inorganic Chemistry, ETH Zurich, Wol; 2Department of Earth and Environmental Sciences
206Pb/238U geochronology is becoming one of the most prominent applications of LA-ICP-MS due to the precision and accuracy achievable when using matrix matched standards and the related high throughput age determinations. A collision cell can be used with practical. Magnetic sector instruments provide a means to mass ICP-MS. Within the last several years, approaches to reduce the spectral overlaps have long been one of the major challenges in overcoming spectral overlaps using these approaches and an ion/molecular ion signal ratios. This talk will focus on progress in ratiometric biomarker of oxidative stress. Despite numerous methods reported for glutathione analysis, reliable measurement of GSH/GSSG in biofluids is challenging due to its chemical lability, which is often exacerbated by time-consuming off-line sample pretreatment steps. On-line sample preconcentration with chemical derivatization by capillary electrophoresis offers a versatile single-step method for direct analysis of GSH and related metabolites since sample pretreatment is seamlessly integrated during separation. The optimized method was applied to red blood cell lysates derived from a single-drop of blood, which demonstrated sub-micromolar detection limits relevant for rapid yet reliable analyses of low abundance GSH species, including GSSG and S-nitroso-GSH.

(436) On-line Sample Preconcentration with Chemical Derivatization by Capillary Electrophoresis: A Single-step Strategy for Analysis of Glutathione Metabolism
Adam Ptolemy1, Mohamed Al Husseiny2, Philip Britz-McKibbin1; 1McMaster University
Glutathione metabolism is a major intracellular antioxidant defense mechanism against reactive oxygen and nitrogen species. This has prompted researchers to quantify the relative amounts of the reduced and oxidized states of glutathione (GSH/GSSG) as a ratiometric biomarker of oxidative stress. Despite numerous

(440) Overcoming Spectral Overlaps in ICP-MS
John Olesik1, Patrick Gray1; 1The Ohio State University
Spectral overlaps have long been one of the major challenges in ICP-MS. Within the last several years, approaches to reduce the impact of spectral overlaps after the ions are sampled have become practical. Magnetic sector instruments provide a means to mass spectrally resolve most, but not all, overlaps. Highly efficient ion-molecule reactions can be used to reduce spectral overlap ion signals by orders of magnitude. A collision cell can be used with ion kinetic energy discrimination to improve elemental ion/molecular ion signal ratios. This talk will focus on progress in overcoming spectral overlaps using these approaches and an assessment of remaining issues.

(434) Affinity Monolith Preconcentrators for Polymer Microchip Capillary Electrophoresis
Weichun Yang1, Tao Pan1, Xiuhua Sun1, Adam Woolley1; 1Dept of Chem and Biochem, Brigham Young University
The purification and preconcentration of trace proteins are crucial steps in many biological and clinical applications. Microfluidic techniques, with small sample input requirements, high speed and potential for process integration, can be advantageous in such analyses. We are evaluating monoliths as analyte-selective sample preconcentrators in polymer microdevices to improve the sensitivity and selectivity in protein analysis. Monolithic materials are formed within poly(methyl methacrylate) (PMMA) microchannels by in situ photopolymerization of a mixture of acrylate monomers, initiator, and porogens. Flow experiments

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using either hydrodynamic or electrokinetic pumping in these monoliths demonstrate retention and enrichment of amino acids, and elution is feasible by rinsing with solutions of pH ~2 or lower. We are presently evaluating antibody-based affinity monoliths to enhance analyte selectivity. Experiments are also ongoing to couple sample preconcentration with capillary electrophoresis (CE) in these microchips. To reduce nonspecific analyte adsorption during microchip CE, we have developed methods for attaching poly(ethylene glycol) (PEG) groups on the channel walls. Fast and reproducible CE of fluorescently labeled amino acids and proteins was achieved in our PEG-modified microdevices. These affinity monolith integrated microchips should provide a simple and effective platform for trace analysis in complex biological samples.

(434) **Chemical and Biochemical Analysis Using Microfluidic Platforms**

Michael Sepaniak1, Amber Wellman1, Nahla Abu-Hatab1, Joshy John1, Maggie Connatser1; 1University of Tennessee, Department of Chemistry

Microfluidics (MFs) offer advantages of multiplexed analysis on small, inexpensive platforms. We describe herein two distinctly different MF-based optical detection techniques that have the common point of sequestering and measuring analyte signals in highly localized EM fields. The first technique seeks to integrate a passively-pumped, MF platform and planar waveguide technology, utilizing magnetic beads as solid supports for fluoro-arrays with direct detection of bound analyte within the sample mixture accomplished by selectively driving functionalized beads to a localized evanescent field. Because analyte binding occurs in free solution, the reaction is not diffusion limited and once beads are magnetically delivered to the evanescent wave, the analyte can be detected with fewer complications arising from non-optically homogeneous biological matrices. Initial optimization, calibration and regeneration were performed using a model sandwich immunoassay system for the detection of rabbit IgG, with which we demonstrate a LDR of 3 orders of magnitude and physiologically relevant detection limits of 0.1 ng/mL. The second technique mutes a MF platform with colloidal-based surface enhanced Raman scattering (SERS) to perform parallel, high throughput vibrational spectroscopy. Spectra are acquired for analytes localized in surface plasmon fields associated with passively-pumped conventional and uniquely synthesized cubic silver colloids under non-destructive flow conditions. Technique optimization studies will be described and a SERS response reproducibility of better than 7% demonstrated. Utilization of a very high numerical aperture, long working distance Raman spectrometer microscope objective results in very high sensitivity with ease of alignment. Calibration curves of the dye crystal violet and the drug mitoxantrone (resonant enhanced) were generated, and the major SERS peaks were observable down to concentrations of low-nM and sub-pM, respectively.

(435) **Measurement of Hemolymph Amino Acid Variations due to Stress or Genotype from Individual Fruit-Flies**

Sujeewa Piyankarage1, Nikolay Kocherov2, Hrvoje Augustin2, David Featherstone2, Scott Shippy1; 1Department of Chemistry, UIC; 2Department of Biological Sciences, UIC

Chemical information from exceedingly small organisms such as Drosophila melanaster (fruit fly) is usually accomplished through using populations to attain larger sample volumes. A method is described that is capable of obtaining in vivo hemolymph samples of 50-300 nL volumes from individual Drosophila larvae. The work also demonstrates qualitative and quantitative analyses of amino acid levels of hemolymph of several fruit-fly genotypes and amino acid variations based upon larval stress. Individual larvae were isolated in a dish and a narrow incision in its cuticle was made with a dissection pin. The leaking hemolymph was then collected into a Tygon-tube sampling probe by reduced pressure. Once collected, 50-300 nL samples were diluted and derivatized with fluorescamine for analysis by capillary electrophoresis with laser induced fluorescence detection. More than 12 amino acids were resolved from the hemolymph using two optimized run buffer conditions in a 50-µm inner diameter fused silica capillary at applied field strengths of 600 Vcm-1 and 380 Vcm-1. Samples were collected under zero evaporation and at intervals from 30 to 120 sec after piercing the larva to show that the effect of hemolymph evaporation on the amino acid measurements. Evaporation is insignificant when the hemolymph collection was completed within 60 sec. Significant increases in hemolymph arginine and glutamate levels were observed when the larvae were stressed prior to sampling. However, a significant difference was not observed for most of the amino acids when the larvae were anesthetized prior to sampling. Five mutant genotypes with modified gene expression for xCT and JHI-21 proteins were analyzed with three other control types. Significantly lower levels of hemolymph glutamate were observed for the xCT “genderblind” mutants compared to the control types. Three JHI-21 mutants showed significantly higher hemolymph glutamate levels in spite of the fact that the modified genes come from the same genotypic superfamily. The developed sampling technique, which collects hemolymph from individual larva, is efficient and enables accurate organism level chemical information. It also minimizes errors associated with possible sample contaminations, estimations and effects of evaporation compared to the traditional hemolymph sampling techniques.

(436) **Affinity-Based Microdialysis Sampling using Heparin for Human Cytokine Collection**

Yuexi Wang1, Julie Stenken1; 1Rensselaer Polytechnic Institute

Cytokines are transient signaling proteins produced by inflammatory cells and are of significant biomedical importance. Microdialysis sampling is a widely used sample collection method. The large molecular weights for cytokines (~8-80 kDa) cause low relative recovery. Heparin binds some cytokines with high affinity since under in vivo conditions heparin sulfate maintains chemical gradients for some cytokines. The inclusion of heparin in the perfusion fluid as an affinity agent was performed to improve the relative recovery of human cytokines. Five human cytokines (IL-4, IL-6, IL-7, MCP-1 and TNF-a) were collected with and without heparin in the perfusion fluid. The relative recoveries of five cytokines have all been improved with heparin in the perfusion fluid. For these five cytokines, the control and enhanced relative recoveries at 0.5 µl/ml flow rate are (n=3): IL-4, 4.2±0.5% and 7.2±1.7%; IL-6, 1.4±0.8% and 3.6±2.6%; IL-7, 1.3±0.8% and 4.8±3.5%; MCP-1, 1.9±1.6% and 19.5±2.1%; TNF-a, 7.3±1.3% and 16.9±2.3%. Human MCP-1 was chosen as the model protein to further quantify the relation between infused heparin concentration and increases in MCP-1 recovery. The presence of heparin in the cytokine samples does not interfere with cytokine quantification. Less than 5% free heparin was lost through the dialysis probe and was measured by high performance liquid chromatography coupled with pulsed amperometric detection (HPLC-PAD) system. The inclusion of dextran or sulfated-β-CD as negative controls in the microdialysis sampling perfusion fluid caused no statistically significant change in the relative recovery for MCP-1. Thus, the known binding affinity between heparin and these human cytokines is the driving force behind the increase in cytokine relative recovery across the microdialysis sampling membrane. The enhanced recoveries meet the prerequisites of the detection and quantification of cytokines, in which we could better understand the mode of activities of...
(437) **Carbon Supramolecular Assemblies in the Liquid Phase**  
**Pu Chun Ke**\(^1\), \(^1\)Clemson University  
Supramolecular assembly utilizes the workings of noncovalent interactions (hydrophobic, van der Waals, pi-stacking, etc.) and offers tremendous opportunities for enhancing the biocompatibility and bioavailability of nanomaterials in biological systems and in the environment. One significant advantage of these noncovalent schemes is their ability to preserve the desirable physical properties of the nanomaterials. In this talk I will present our recent experiments and simulations on the solubilization of fullerenes and carbon nanotubes using naturally occurring lysophospholipids and gallic acids. These carbon nanoassemblies were formed via hydrophobic interactions and pi-stacking. They were found to possess interesting morphology and rich optical properties which can be utilized for monitoring their translocation across cell membranes. Towards understanding the toxicity of nanomaterials I will show the biomodification of carbon nanoassemblies by Daphnia magna (water flea), a living organism commonly used for toxicological studies. Finally I will present the binding of carbon nanomaterials and natural organic matter and elaborate the significance of this study for environmental protection.

(438) **Metal Oxide and Organometallic Nanowire Gas Sensors: Rational Tuning of Receptor / Transduction Functions and Prototype Devices**  
**Andrei Kolmakov**\(^1\), \(^1\)SIU  
The recent developments in nanotechnology induce the changes in the current paradigms in sensors. Namely, the search for new materials and morphologies of the sensing elements along with their receptor and transduction principles is a frontier of this field. Among the most promising new sensing platforms are quasi-1 dimensional (1D) semiconducting nanostructures which electronic properties sensitively respond to the processes on their surfaces. In our report we will concentrate on fabrication of the sensing elements out of single crystal metal oxide and metallophthalocyanine nanostructures. The current understanding of the receptor and transduction functions of single wire and multiwire devices will be considered. The array of methods which allow one to rationally functionalize and characterize chemiresistors and chemi-FETs will be reported. In particular we have developed and tested experimental approaches to tune sensitivity and selectivity of these sensors as well as implemented new methods to monitor the surface processes on individual nanostructures. Quasi 1-D chemiresistors made of metal oxides are close to occupy their specific niche in the real world solid state sensors. The prototypes of nanowire electronic noses and real world nanowire micromachined devices will be presented and their excellent performance will be demonstrated.

(439) **Interactions between Functionalized Multi-Walled Carbon Nanotubes and Proteins**  
**Bing Yan**\(^1\), **Qingxin Mu**\(^2\), **Wei Liu**\(^2\), **Yuehan Xing**\(^2\), \(^1\)St. Jude Children's Research Hospital; \(^2\)Shandong University, China  
Various functionalized nano materials have the potential to be applied in medicine and diagnostics. However, their potential effects on biological systems need to be investigated. In this work, we used spectroscopic methods to investigate interactions between functionalized multiwalled carbon nanotubes (f-MWNT) with BSA, trypsin, henoksinase, ovalbumin, carboxydrase and hemoglobin. The surface of MWNT was first chemically modifies to produce carboxyl-, Fmoc-tyrosine-, isobutyl-MWNts. Using Bradford method and HPLC, we first quantified the protein adsorption ability of each f-MWNT and the specific adsorption of each f-MWNT to protein. Carboxyl-MWNT showed strongest protein adsorption ability. The binding of f-MWNT with proteins was also studied by steady state and time resolved fluorescence spectroscopy. Addition of f-MWNT into protein induced quenching of the protein intrinsic fluorescence. Carboxyl-MWNT induced largest fluorescence quenching and Fmoc-tyrosine-MWNT induced the second largest change. Based on CD studies, nanotube/protein binding induced small changes in protein secondary structure in case of carboxyl-MWNT, but even less so in other f-MWNts. F-MWNT can interact with proteins by electrostatic, π-π, and hydrophobic interactions. Our results showed that the electrostatic interaction is stronger than other binding forces. Such f-MWNT-protein interactions may trigger partial protein conformational changes and cause the formation of cryptic epitopes that have the potential to cause inappropriate cellular responses and result in cellular toxicity.

(440) **GAS Preconcentration and Separation with Carbon Nanotubes**  
**Michael Stadermann**\(^1\), **Adam McBrady**\(^2\), **Vanessa Reid**\(^2\), **Alex Noy**\(^1\), **Rob Synovec**\(^2\), **Olgica Bakajin**\(^1\), \(^1\)Lawrence Livermore National Lab; \(^2\)University of Washington, Seattle  
Separation and characterization of substances has been restricted to laboratory operations in the past, and the instruments performing the tasks are bulky and power-hungry. In today’s world, there is an increased demand for the capability of doing rapid separation and analysis of chemical substances in the field. This requires small, portable units that consume little power, but have the separation capacity of larger desktop systems. The key to reducing dimensions and power consumption lies in microfabrication, combined with the development of novel materials that can be used for separation. We are investigating the use of carbon nanotubes as gas preconcentrators, separators and detectors for portable detection systems. Their high surface-to-volume ratios make nanotubes an ideal adsorption phase for gas preconcentration, as well as a separation phase gas chromatography. I will present our results with microfabricated nanotube-coated preconcentrators and separators types of devices and show that nanotubes provide a promising alternative to existing technologies. This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under Contract W-7405-Eng-48 and supported by the DARPA Micro Gas Analyzers program.

(441) **Coupling of Flow Injection with ICP-TOFMS to Increase Sample Throughput**  
**William Balsanek**\(^1\), **Christine Rivera**\(^2\), **Andrew Saint**\(^2\), \(^1\)GBC Scientific Equipment (USA) LLC; \(^2\)MIBEN Tech; \(^2\)GBC Scientific Equipment Pty. Ltd.  
Inductively coupled plasma mass spectrometers, “due to their multi-element capability and superior detection limits,” are the instrument of choice when performing environmental methods such as US EPA method 200.8. Commercially available instruments which perform these methods are generally equipped with quadrupole mass analyzers. While quadrupole based mass spectrometers have many benefits, they do suffer limitations in terms of speed of spectral acquisition and multi-element transient signal capability. In this study, an inductively coupled plasma time-of-flight mass spectrometer (ICP-TOFMS) was used with flow injection sample introduction to run US EPA method 200.8. Due to the ICP-TOFMS’s ability to conduct full mass scans (e.g. 2-260 amu) in approximately 30 is, sample analysis can be accelerated without comprising accuracy, precision or limit of detection for US EPA 200.8.
(442) Parametric Optimization of Electrochemically Modulated Separation for Pre-concentration of Uranium
Scott Lehn1, Gregory Eiden1, Martin Liezers1, Douglas Duckworth1; 1Pacific Northwest National Lab
Inductively coupled plasma mass spectrometry (ICP-MS) is a tool that is routinely used for trace elemental analysis. Technological advances are such that analysts can be fairly readily detected at the femtogram level. However, for analysts such as uranium, detection of the uranium at trace and ultra-trace levels is insufficient, as isotope ratios of the sample are also important. One way to achieve the capability of measuring isotope ratios at ultra-trace levels is to pre-concentrate the uranium. Electrochemically modulated separation has been shown to be a viable technique to perform the pre-concentration. There are still many parameters that need to be optimized to achieve the necessary performance. Among these parameters are sample flow rates, both for pre-concentration and analysis by ICP-MS; electrode preparation, electrochemical cell geometry and size; solvent; and other variables. The coupling of the electrochemical cell to the ICP-MS will also be a critical component of the studies. The results of the parametric optimization will be presented.

(443) Direct Solid Analysis of Coal Fly Ash Samples by Glow Discharge and Inductively Coupled Plasmas: An Integrated Approach
Alexandria M. Pavkovich1, Melissa M. Pabic1, Jennifer N. Robertson-Honecker1, Fred L. King1; 1West Virginia University
Increasingly, coal utilization byproducts (CUB) are used in various applications ranging from landfill lining to wallboard production. With the growth in their use, the concentration of toxic elements in both CUB and CUB-derived products is becoming an environmental concern. Here, we report the analysis of the most ubiquitous coal utilization byproduct (CUB), coal fly ash, by pulsed glow discharge plasma (GDP) and inductively coupled plasma (ICP). The GDP source was coupled with time-of-flight mass spectrometry (ToF-MS), while the ICP source utilized atomic emission spectrometry (AES) coupled to a laser ablation unit. In addition, a Grimm-type GDP interface was designed for operation with a commercial ICP-MS instrument. Each of these instruments allow for atomization, excitation, and ionization directly from a solid sample. Preliminary studies are reported regarding the utility of these instruments for the determination of potentially trace elements in coal fly ash.

(444) Simultaneous Analysis Method of 21 Pesticides in Tea by LC/ESI-MS-MS
Jae Chun Choi, Jong Sup Jeon1, Hyun Kyung Woo1, Hana Lee1, Chan Soon Kang, Hwa Jung Lee; 1KFDA
Rapid and sensitive simultaneous analytical method based on LC/ESI-MS-MS method has been developed for determination of tebufenpyrad-a, fluoroxuron-b, pyraclofos-c, difenoconazole-d, cyhalothrin-e, amitraz-f, hexythiazox-g, fluazinam-h, chlorpyrifos-i, hexaflumuron-j, chlorfluazuron-k, tebuconazole-l, triflumizole-m, fenpyroxam-n, cyhalothrin-o, thiamethoxam-p, hexythiazox-q, fluazinam-r, chlorpyrifos-s, hexaflumuron-t, chlorfluazuron-m, tebuconazole-n, triflumizole-o, fenpyroxymate-p, cyhalothrin-i, amitraz-j, azoxystrobin-k, carbendazim-l, tebufenpyrad-a, flufenoxuron-b, pyraclofos-c, difenoconazole-d, LC/ESI-MS-MS has been developed for determination of Rapid and sensitive simultaneous analytical method based on ammonium acetate and methanol as mobile phase the method was optimized to achieve the necessary performance. Among these parameters are sample flow rates, both for pre-concentration and analysis by ICP-MS; electrode preparation, electrochemical cell geometry and size; solvent; and other variables. The coupling of the electrochemical cell to the ICP-MS will also be a critical component of the studies. The results of the parametric optimization will be presented.

(445) Determination of Selenium Content in White Flour, White Bread, and Local Bread by Inductively Coupled Plasma Mass Spectrometry (ICP-MS)
Amina Ali1; 1Kuwait Institute for Scientific Research
Selenium (Se) is an essential nutrient for humans and animals. The key role of selenium in mammalian metabolism is attributed to the presence of four selenocysteine residues in the enzyme glutathione peroxidase. This enzyme protects human cell membranes and structure from oxidative injury. Selenium, functioning as part of glutathione peroxidase, has been recognized as a cellular antioxidant. In addition, the element is also known, to mention only the most important properties, a protecting agent against heavy metal toxicity, cancer, and cardiovascular diseases. Lack of selenium or disturbance in the metabolism by metals may promote free radical production. The Results was found in accordance with Status of Selenium in using inductively coupled plasma Optical Emission Spectroscopy (ICP-OES).

(446) Exploring Biosignature-Mineral Associations using GALDI-FTMS
Jill R. Scott1, J. Michelle Kotler2, Nancy W. Himman2, Beizhan Yan2, Daphne L. Stoner1, C. Dov Richardson3; 1Idaho National Laboratory, 2University of Montana; 3University of Idaho
Unambiguous detection of biosignatures in extraterrestrial and ancient terrestrial materials would have a profound impact on current understanding of the origins of life. Laser desorption Fourier transform mass spectrometry (LD-FTMS) has been used to detect various biological and organic compounds associated with different minerals. For natural samples, LD-FTMS requires no sample preparation and offers high sensitivity to acquire spectra with a single laser shot for heterogeneously distributed biosignatures. Some organics compounds (i.e., polyaromatic hydrocarbons) self-ionize for easy detection, but most organic compounds require ionization assistance. Therefore, we are exploring how well different minerals assist in ionization, a process called geomatrix-assisted laser desorption/ionization (GALDI). Some minerals are capable of ionizing biological compounds by the expected cationization; however, other minerals produce complex cluster ions that could lead to false positives (i.e., assigning a biosignature identity to an ion formed by interactions of a prebiotic with the mineral). Other minerals totally fail to produce any biosignature, which would lead to false negatives. The effectiveness of GALDI appears to depend not only on the composition of the biological molecule and mineral moity, but also on how they are associated. Biological or organic signatures are more easily obtained from minerals if the organic compound is closely integrated with the mineral matrix. Organic compounds have successfully been detected in natural, terrestrial minerals. The organics in the natural samples are in low concentration and unevenly dispersed through out the samples; thus, presenting a major detection challenge that requires high sensitivity and the ability to search through the sample.

(447) Infrared Reflection–Absorption Spectroscopy (IRRAS) of the Molecular Basis for Pulmonary Surfactant Function
Richard Mendelsohn1, Joseph Brauner1, Carol Flach1; 1Rutgers University
Pulmonary surfactant is a thin lipid/protein film lining the air-alveolar interface in the mammalian lung. An approach to the molecular basis of two essential functions carried out by the surfactant constituents determined by (IRRAS) and ancillary
technologies will be described. First, the film functions to reduce 
the work of breathing and to prevent alveolar collapse during 
expansion-compression cycles. The hydrophobic surfactant-
specific proteins SP-C and SP-B enhance the spreading of surfactant lipids across the air/water interface in vitro, are excluded 
from the monolayer film to endure film stability under the high 
pressures of compression, but must remain sufficiently close to the 
monolayer to be recruited for successive cycles. The reversible 
formation of multilayers is thought to provide the molecular basis 
for removal and re-insertion of these proteins. We have used 
combined pressure-area isotherm, IRRAS, and AFM measurements 
to characterize the SP-C-induced reversible monolayer-multilayer 
transition. The orientation of SP-C is altered during this process, 
from preferentially perpendicular to the interface in multilayers to a 
much more parallel orientation in monolayers. Second, the 
hydrophilic surfactant collectins SP-A and SP-D provide the first 
line of defense against airborne pathogens. These proteins interact 
with lipopolysaccharides (LPS) from the outer membrane of Gram-
negative bacteria to promote membrane lysis. We have developed 
an IRRAS assay for calcium-dependent collectin/LPS binding. In 
addition, using simulations for the Amide I contour and for the 
orientation dependence of IRRAS intensities, we determined the 
geometry of the interaction between a truncated construct (neck + 
carbohydrate recognition domain of SP-D) with an Rd LPS mimic 
of the bacterial outer membrane lipids from Gram-negative 
bacteria. These data provide a model for lipid-protein recognition 
occurring in host defense.

(448) Structural Polymorphism of a Membrane Protein 
Macromolecule: The Filamentous Bacteriophage Ff 
George J. Thomas, Stacy A. Overman, Edward H. Egelman; 
1University of Missouri-Kansas City; 2University of Virginia 
All filamentous bacteriophages consist of a single-stranded DNA 
genome encapsidated by several thousand copies of a small helical 
coat protein (pVIII), plus several copies of four minor proteins at 
the filament ends. The filamentous phages are important as cloning 
vehicles and vectors for peptide display. The most extensively 
studied phage (Ff) also serves as a tractable model of membrane-
associated nucleoprotein assembly and is considered a potentially 
valuable tool for pharmaocotherapy and nanotechnology applications. To understand the assembly architecture of the native 
Ff virion we have employed methods of Raman, ultraviolet-
resonance Raman and polarized Raman spectroscopies of aqueous 
samples, as well as electron microscopy of specimens in vitreous 
ice. The latter investigations allow image reconstructions of the 
native viral capsid at a nominal resolution of ~8 Å. The results 
demonstrate polymorphism as a general principle of filamentous 
phage morphology in the native aqueous environment. Analysis of 
the spectroscopic and cryo-EM results will be described.

(449) Following Chemical Reactions in Protein and RNA 
Crystals by Raman Crystallography 
Paul Carey, 1,2 Case Western Reserve University 
By using a Raman microscope single crystals of proteins or nucleic 
acids provide Raman spectra of unprecedented quality and 
stability. Thus, the crystals provide ideal platforms for performing 
Raman difference spectroscopy. In a typical experiment a single 
crystal of an enzyme is prepared and its Raman spectrum is 
obtained via the microscope. Substrate molecules are infused into 
the crystal and these react with the enzyme inside the crystal. 
Raman spectra are recorded as a function of time and the difference 
spectrum [enzyme-substrate complex] minus [enzyme] provides the 
Raman spectra of intermediates on the reaction pathway. This 
provides information on the identity of the intermediates, their 
kinetic properties and a strong synergistic link to X-ray 
crystallography. The spectroscopist can inform the crystallographer 
about the status of events in the crystal enabling the 
crystallographer to flash freeze the crystal and obtain the structure 
of a desired intermediate. The approach allows us to determine, for 
example, the molecular basis of drug resistance in bacterial 
enzymes - a very important area in contemporary medicine. Similarly 
the method provides a rich vein of novel information on chemical 
changes in RNA crystals, eg, on the titration of active site bases, on 
RNA-metal interactions and on reactions occurring within the 
crystals.

(450) Study of Spider Silk Structure by Vibrational 
Spectroscopy 
Michel Pezole1, Thierry Lefèvre1, Sarah Bedard1, Jean-François 
Roux-Dubé2, Maxime Boulet-Audet1, Marie-Eve Rousseau1, 
Thierry Buffeteau2; 1Laval University; 2Université de Bordeaux I 
Spider silk is among nature’s most highly engineered structural 
materials, achieving, in some cases, combinations of strength and 
toughness that are still unmatched by other high-performance 
synthetic fibers. Spiders produce several different silks, each with a 
specific range of mechanical properties. Dragline silk exhibits high 
toughness that comes from a good trade-off between stiffness and 
tensility. Such properties are due to the peculiar block 
copolymer structure of dragline silk that is composed of alternating 
alanine-rich hard segments containing beta-sheets and glycine-rich 
soft segments. On the other hand, flagelliform silk of the capture 
spirals of the web is highly elastic due to the presence of proline 
and glycine residues.Raman spectromicroscopy is a very powerful 
technique to investigate the conformation and orientation of 
proteins of different native silk fibers. The main advantage of this 
technique is that the laser beam can be focused to about 1 
micrometer in diameter in the sample, therefore allowing the in situ 
recording of high quality spectra of single silk filaments. Our 
laboratory has recently made significant advances on the use of 
polarized Raman spectromicroscopy to study quantitatively the 
conformation and orientation of spider silk proteins. This technique 
has been used to characterize different types of silk produced by 
spiders including dragline, capture spiral, prey capture and cocoon 
silk fibers. In addition, by taking advantage of the confocality of the 
Raman microscope the structure of the highly concentrated 
aqueous solution (spinning dope) has studied for the first time in situ 
in the intact major ampulate gland of spiders. Finally, high 
quality attenuated total reflectance polarized spectra of single 
spider silk filaments have been using the Specac Golden Gate 
accessory.

(451) Surface Enhanced Raman Spectroscopy for in-situ 
Measurements of Signaling Molecules (e.g., Autoinducers) 
Relevant to Bacterial Chemical Communication – Quorum 
Sensing 
William Pearman, 1 Marion Lawrence-Snyder1, S. Michael Angel1, 
Alan Decho2; 1University of South Carolina Dept. of Chemistry 
and Biochemistry; 2Dept. of Environmental Health Science 
Autoinducer (AI) molecules are used by Quorum Sensing (QS) 
bacteria to communicate information about their environment, and 
are critical to their ability to coordinate certain physiological 
activities. Studying how these organisms react to environmental 
stresses could provide invaluable insight into methods to control 
these activities. To this end, we are investigating spectroscopic 
methods of analysis that allow in-situ measurements of these AI 
molecules under different environmental conditions. We found that 
for one class of AI's, N-acyl homoserine lactones (AHLs), Surface 
Enhanced Raman Spectroscopy (SERS) is a method capable of 
performing such measurements in-situ. SERS spectra of several 
different AHLs with acyl chain lengths from 4 to 12 carbons were 
collected for the first time using Ag colloidal nanoparticles 
synthesized via both citrate and borohydride reduction methods.
(452) Automated Breast Tissue Histopathology Using Mid-IR Spectroscopic Imaging
Frances Nell Keith1, Rohit Bhargava2; 1University of Illinois at Urbana-Champaign

Molecular techniques to aid in conventional morphologic diagnosis of breast cancer are rapidly emerging. Fourier transform infrared (FTIR) molecular spectroscopy, widely used in the chemical industry, is now being applied widely to pathology. An IR spectrum is a quantitative measurement of the molecular composition of the examined material. Therefore, it can give a numerical measurement of breast tissue composition that can be related to both the histology and pathology of the tissue. To visualize microscopic tissue structure in the manner of clinical practice, however, FTIR imaging is required to provide information on spatial tissue heterogeneity. We have correlated corresponding tissue images from FTIR imaging with hematoxylin and eosin (H&E) and immunohistochemical (IHC) staining. We demonstrate here that IR images can provide significant biochemical tissue information without the use of molecular probes or contrast agents but may be limited in some cases. This study employs a high-throughput approach based on the application tissue microarrays (TMAs) to rapidly collect data from a large and varied selection of malignant and benign tissue to build a prediction algorithm. A large set of spectral metrics is selected by examination of spectra from distinct tissue classes denoted on stained and infrared images. Probability distribution profiles are then generated for each metric. Objective computer algorithms, based on a modified Bayesian classifier, are employed for rapid and automated histopathology. The accuracy of this supervised pattern recognition method is assessed by using receiver operating characteristic (ROC) analysis and optimized by varying the metric classification parameters. Validation is conducted on separate TMAs to evaluate the performance of the developed classifier. Results demonstrate effective breast tissue histology classification and progress towards pathologic classification. This computerized technique for breast pathology could reduce problems associated with inter-observer variability in breast biopsy interpretation and will help establish IR pathology could reduce problems associated with inter-observer variability. The SERS method shows promise for monitoring both the amount and changes in AI molecules in-situ, within biofilms containing QS bacteria as the biofilm environment (e.g. salinity, temperature, UV exposure) is changed. This new capability offers the ability to “listen in” on chemical communications between bacteria in their natural environment as that environment is stressed.

(453) Fluorescence and Scattering Detection of Individual Particles in Capillary Electrophoresis and Flow Cytometry
Edgar Arriaga1, Bobby Poe1, Dmitry Andreyev1, Marian Navratil1; 1University of Minnesota

Both flow cytometry (FCM) and capillary electrophoresis with post-column laser-induced fluorescence detection (CE-LIF) have been used to detect individual particles. However, their performance has not been directly compared. Here, we report on: (i) a comparison of a commercial FCM instrument with an in-house built CE-LIF instrument using fluorescently labeled microspheres and isolated mitochondria and (ii) a simple side scattering detector for capillary electrophoresis. While FCM offers offer two-fold better relative standard deviations than CE-LIF for individual fluorescent measurements of microspheres, CE-LIF produces S/N ratios that are >25 times higher than FCM. When 10-nonyl acridine orange (NAO) labeled mitochondria are analyzed, the S/N ratios of both techniques are similar. Most detection schemes for individual particle CE-LIF analysis have been based on fluorescence. Here, we report a detector capable of simultaneously monitoring scattering and fluorescence signals of individual microsphere particles and mitochondria, separated by CE. Fluorescence versus scattering (FVS) plots made it possible to identify particle subtypes and to detect changes associated with cryogenic storage of mitochondria. Other points of comparison between CE-LIF and FCM such as sample consumption and throughput will be presented within the context of subcellular analysis.

(454) General Fluorescence Resonance Energy Transfer Assay for the Study of Cell Membrane Protein Clustering
Emily Smith1, Suzanne Sander2, Deepak Dibya2, Danny Brower2; 1Iowa State University; 2University of Arizona

Fluorescence Resonance Energy Transfer (FRET) is being used to study the microclustering of a class of cell membrane receptors called integrins. Integrins are proteins involved in bidirectional signaling across the membrane, and are critical for cell adhesion, motility, and growth. The FRET studies are performed in live cells without modifying the protein of interest. FRET donor and acceptor protein constructs consist of fluorescent proteins fused to suitable transmembrane and cytoplasmic domains. The constructs are expressed by the cell and reported on the micro-scale clustering of the integrins. These studies are used to screen protein mutants, and can be combined with other genetics techniques to identify the molecular mechanism of protein clustering within the cell membrane.

(455) Surface Plasmon Enhancement at a Liquid-Metal-Liquid Interface
Florencio Hernandez1, Arthur Thibert1, Carlos Toro1, Shengli Zou1, Ion Cohanischii1; 1University of Central Florida

In this talk will show the first experimental evidence of surface Plasmon enhancement at a liquid-metal-liquid interface on a pseudo-Kretschmann geometry. Pumping gold nanoparticle clusters at the interface of a hexane-water mixture, we are able to measure a fluorescence enhancement of three orders of magnitude in Rose Bengal. The emission augmentation, due to the electric-field enhancement and the reduction of the fluorescence lifetime of dye molecules is visible to the naked eye. Theoretical modeling of the electric-field intensity enhancement of emulated surfaces will be presented as a support the experimental results. This new approach will open a new road for the study of dynamic systems using plasmonics.

(456) Nanotubule Formation from Surface-Attached Liposomes Using an Electric Field
Josemar Castillo1, Mark Hayes1; 1Arizona State University

The spontaneous formation of long range (millimeters) membrane-bound nanotubules is possible by the application of modest electric fields (2-20 V/cm) to immobilized liposomes. Nanotubules exhibit characteristic radial dimensions of tens of nanometers. Various experimental techniques are now available to create lipid nanotubules; including the use of microfluidic devices and microinjection protocols such pipette aspiration and electroinjection techniques. This contribution introduces a new technique for preparing nanotubules from immobilized liposomes. Current immobilization is performed by electrostatic interaction between the bilayer and a microscope glass slide using a polybrene coating. Tubes up to several centimeters in length and generally...
aligned with the applied electric field were created from the immobilized liposomes prepared with various ratios of phosphatidycholine (PC), phosphatidic acid (PA) and phosphatidylethanolamine (PE). The effect of the applied field in nanotubular formation is examined in terms of tubular length and average number of tubules per liposome for different compositions. Nanotubules were examined by fluorescence microscopy using fluorescent phospholipids to study structure and stability of the lipid nanotubules in the substrate. These new, diverse and potentially useful structures can create and extend micro and nanoscale device function as well as provide novel fabrication strategies. The formation of nanotubules under low intrinsic fields suggests that mechanical electrostatic interaction play a role in the morphology and functionality of membrane-bound structures found in biological membranes and networks.

(457) Development of Response Selective Fluorescence Sensors
Matthew McCarroll1, Daniel Dyer1, Lichang Wang1, Jeremy Buckingham1, Dan Brandys1, Ruisong Xu, Irene Kimaru1, 2Southern Illinois University
Fluorescent probes offer much promise as sensitive and selective sensors. Sensor development has focused primarily on using binding selectivity to obtain a selective response. Herein we describe an approach to the development of photoinduced electron-transfer (PET) based sensors that utilizes an additional and orthogonal mode of discrimination we term response selectivity. The approach relies on the computational and theoretical prediction of electron-transfer kinetics based on Rehm-Weller and Marcus theories, which allows evaluation of the photophysical behavior of a prototype fluorescent probe/sensor prior to the synthesis of the molecule. The transduction mechanism of a PET sensor is based on the perturbation of the HOMO/LUMO electronic energy system of the electron receptor in response to binding of the analyte. In our approach we take advantage of the fact that a target analyte and an interferent may both bind to the sensor, yet selectivity may be observed if only the analyte perturbs the electronic structure properly to register a sensing event. Recent work (J. Phys. Chem. B, 110 (46), 22991-22994, 2006) has shown the approach to be successful at predicting the behavior of a sensor that is sensitive and selective to Zn (II). This work will be presented as a proof-of-concept. Additionally, the results of recent and ongoing work using the approach to develop sensors for small carboxylate molecules will be discussed in detail.

(458) Fabrication of Porous Optical Fiber Claddings for Crossed-Fiber Sensor Arrays Using Microsphere Templating
Paul Henning1, Veronica Rigo1, Peter Geissinger1; 1University of Wisconsin Milwaukee
Optical fiber sensing allows for remote spectroscopic measurements to be carried out in harsh environments. The entire fiber length may be used for sensing by locating sensor molecules outside of the fiber core; light propagating in the core interacts with the sensor molecules through evanescent fields, which may also capture the sensor-molecule fluorescence and guide it to the detector. Large sensor arrays can be built, with the location of a particular sensor determined by the arrival time of the corresponding fluorescence pulse at the fiber end with respect to the exciting laser pulse. Thus, many different parameters may be monitored simultaneously. Adjacent sensor regions must be spaced meters apart along a single fiber because the spatial resolution is constrained by the sensor fluorescence lifetimes. Forming an orthogonal junction with an additional fiber, with the second fiber capturing through evanescent fields, the sensor fluorescence pulses, allows for greatly reducing the spacing between adjacent regions. Small displacements, however, between the fibers can result in large signal changes due to the exponential decay of evanescent fields away from the fiber core/cladding interface. Thus, hydrogel resins are unsuitable for sensing in aqueous environments as polymer swelling causes separation of the junction, resulting in weak, inconsistent signals. Here, microsphere templating was used to create pores in a hydrophobic polymer that allow analyte passage to the evanescent region. Rigid fiber junctions were created from commercial latex microspheres and Norland optical adhesives. Microsphere coverages and pore sizes were investigated with SEM imaging for comparison of deposition techniques. Fluorescence measurements show an approximate response time of one second and improved consistency for replicate measurements. Also, pH sensing was demonstrated using fluorescein emission.

(459) Chip-based Liquid Chromatography for On-line Process Monitoring
Scott Gilbert1,2,3, Ray Chrisman2,3, 1Crystal Vision Microsystems LLC; 2Atodyne Technologies LLC; 3CPAC, University of Washington
The focus of this presentation will be lab-on-chip liquid chromatographic (LC) systems designed specifically for on-line reaction monitoring and sampling. The miniaturized instrumentation utilizes interchangeable chips where sample pretreatment and chromatographic components are microfabricated on a single substrate. The sampling component is designed for flow-through circulation of the process stream, and has been optimized for continuous stream monitoring. Sample pretreatment is handled by microfluidic mixing and extraction elements to provide dilution and clean-up of sample aliquots prior to LC analysis. Furthermore, rapid chromatographic separations achieved by judicious use of both highly porous monolithic stationary phases and open tubular-like channels provide real-time chromatographic process analysis. We will present analytical and performance obtained data for these devices, as well as discussing the sampling and pretreatment methods developed during the course of this work.

(460) FT-IR Hollow Waveguide Gas Sensors For BTX Monitoring
Christina Young1, Neil Brons2, Andy Riley2, John Martin3, Mark Disko2, Boris Mizaikoff2; 1Georgia Institute of Technology; 2ExxonMobil Research and Engineering Co.; 3ExxonMobil Biomedical Sciences, Inc.
Industry today requires robust in-situ gas sensors capable of online continuous monitoring selective and sensitive for carcinogenic compounds in the workplace and in particular, benzene, toluene, and xylene (BTX). Current methods such as GC face challenges relative to real-time detection, robustness, and selective detection of these compounds outside of the laboratory and within concentration ranges pertinent to health regulation standards. The study presented here utilizes multivariate lab and field gas calibration of FT-IR hollow waveguide (FT-IR HWG) gas sensors for selective low ppm to ppb detection of BTX in complex environmental matrices. The FT-IR HWG gas sensors offer a new alternative to in-situ environmental gas monitoring by taking advantage of unique mid-infrared molecular signatures of BTX in the fingerprint range through utilization of custom-made IR transparent gas cells coupled to an Ag/AgI internally coated hollow waveguide thus allowing for simultaneous probing of gas absorption through increased pathlength with very low sample volumes. Fast and selective thermal desorption of sorbent materials as a precursor to FT-IR HWG gas sensors push detection limits of BTX even further for sensitive and selective workplace and environmental monitoring with representative figures of merit being introduced here.
(461) Process Sensing Utilizing Dielectric Spectroscopy
Shelley Begley, Phil Bartley; Agilent Technologies, Inc.; Innovative Measurement Solutions, Inc.
The dielectric properties of a material are one of the factors that determine how a material interacts with an applied electromagnetic field. The knowledge of the dielectric properties of materials and their frequency and temperature dependence is of great importance in various areas of science and engineering in both basic and applied research. It has always been an important quantity to electrical engineers and physicists involved in the design and application of circuit components and stealth vehicles. This knowledge has become increasingly important to agricultural engineers, biological engineers, chemists, medical researchers and food scientists. The accurate measurement of dielectric properties can provide these scientists and engineers with valuable information that allows them to properly incorporate the material into its intended application or to monitor a process for improved quality control. Dielectric properties often can be related to a physical parameter of interest. It has been demonstrated that properties such as moisture content, fruit ripeness, bacterial content, mechanical stress, and other seemingly unrelated parameters are related to the dielectric properties of the material. The reason is that a material’s dielectric properties are determined by its molecular structure. If the molecular structure changes it dielectric properties changes. Measurement techniques are often non-destructive and can be made in near real-time. Because of these attributes the measurement of dielectric properties, dielectric spectroscopy, can be implemented as process sensors. This paper reviews measurement techniques and published applications. A process for correlating dielectric measurements to physical properties is also presented.

(462) Crystalline Ruthenium and Platinum Complexes for Measurement of Oxygen Concentrations in the Gas Phase and Aqueous Solutions by Emission Quenching
Kent Mann, Kari McGee, Jason Burney, David Veltkamp; University of Minnesota; University of Washington
Several highly emissive, crystalline salts ruthenium and platinum complexes lumophore have been tested as oxygen sensors. Oxygen detection by luminescence quenching correlates with the void space in the crystalline lattice. The emission intensity and lifetime quenching of a ruthenium complex displayed strictly linear Stern-Volmer behavior with a slope of 2.43. A single exponential (\(k = 640\) nsec, pure nitrogen; 190 nsec, pure oxygen) is observed for the emission intensity decay for all oxygen concentrations. The time dependence of the emission caused by a step function air pressure drop is significantly affected by changing the light penetration depth when different excitation wavelengths are used. These experiments are consistent with the diffusion of oxygen molecules in and out of the crystals with a diffusion coefficient on the order of 10-7 - 10-8 cm2/s. The technological significance of these crystalline oxygen sensors was demonstrated by long term stability experiments and by the successful calibration of a ballprobe coated sensor against a dissolved oxygen Clark electrode using a partial least squares (PLS) model with a single principal component.

(463) A Single Process Technology Platform for NIR and Mid-IR Applications
Bertrand Lanher; Aspectrics, Inc.
Encoded Photometric Infrared technology relies upon the modulation of a full spectral range into 128 segments at various frequencies, allowing to recombine all spectrum information into an encodagram at a rate of 100 scans per second. The technology is independent of the spectral range taken into consideration. The advantages of co-adding 100 scans per second are inherent to the technology. Analytical results pertaining to the application of such technology to data collected in both the mid and near infrared regions of the electromagnetic spectrum are proposed. More specifically, a study of stability of the calibration developed for the measurement of ethane and propane in a methane stream (LNG) over a period of 3 months is proposed to illustrate the gas phase and Mid-IR capabilities of this single process technology platform. Simultaneous measurement of several compounds (including methanol, water and glycerins) in biodiesel are presented to illustrate the liquid phase and Near IR capabilities of the technology.

(464) Differential Mobility Spectrometry and Advantages of its Application for Chemical Process Monitoring/Control
Erkinjon Nazarov, Raanan Miller; Sionex
The trend in Process Analytical Chemistry (PAC) of moving the chemical analysis from the laboratory to the process plant can significantly improve product quality, operation efficiency, and safety. However, novel technical approaches involving chemical engineering and analytical chemistry are needed. These may utilize lab-on-a-chip type micro-analytical analyzers, or sensors, with automatic sample introduction from process lines. Such sensors have to provide high sensitivity, be able to work over a wide range of temperatures, be robust and easily replaceable, small in size, and relatively low cost. In addition, it is desirable that the analyzers operate as a “smart” diagnostic tool to provide on-line information simultaneously tracking variations in compositions of several chemicals in single or multiple chemical streams. This presentation explores adapting Sionex mobility based gas analyzer systems for PAC applications. The Sionex mobility based gas analyzers, Differential Mobility Spectrometers (DMS) and Ion mobility spectrometers (IMS) have traditionally been deployed in Homeland Security applications detecting trace levels of chemical warfare agents and explosives. An advantage of this class of analyzers is their excellent sensitivity and selectivity and their ability to operate at ambient pressure. This makes them suitable for miniaturization and for field deployment. Over the past several years Sionex Corporation has developed a new miniature microfabricated chip-type differential mobility sensor which is used as the engine for a number of sensitive analytical devices: standalone gas detectors, gas analyzers, and GC detectors. Currently two additional systems with enhanced chemical discrimination abilities have been developed. The first system is the Sionex microAnalyzer a miniature instrument that combines a DMS with a fast chromatographic pre-separation. It has been successfully used to detect sulfur contained chemicals and odorants in natural gas, as well as BTEX and Toxic Industrial Chemicals in various gas mixtures. The second system is a portable tandem DMS-IMS system. It includes a DMS for rapid separation of positive and negative ions, and two short (1.5cm) IMS drift tubes for further resolution of DMS pre-filtered ions. The sensor system is compact; measuring only 2”\(\times\)2.5”\(\times\)3”. In this work we will present designs and analytical characteristics of a number of these advanced analytical systems.

(465) Smart Combinatorial Operando Spectroscopy Catalytic System
Israel Wachs; Lehigh University
With the recent introduction of the operando spectroscopic methodology that involves simultaneous spectroscopic characterization of catalysts and reaction product analysis to develop molecular structure-activity/selectivity relationships, there is currently a strong desire to obtain real-time catalyst spectroscopic and performance information under relevant reaction conditions. The operando spectroscopic approach requires that the spectroscopic and catalytic information be able to provide the following:• Real-time generation of spectroscopic and catalytic
The partial oxidation of methanol is of great interest for industrial applications and Raman spectroscopy is a powerful spectroscopic technique allowing us to follow the evolution of the catalyst during the first step of the reaction, which lead to a fine interpretation of the mechanisms occurring on the catalyst surface. Moreover computation of the spectroscopic signatures (Raman and XANES) permits the confirmation of the structural model leading to a detailed picture of the catalyst in working conditions.

(467) Operando and MultiOperando Raman Methodology: Rational Catalyst Discovery
Miguel A. Bañares1, José Prieto3, Consuelo Goberna-Selma2, M. Olga Guerrero-Pérez2, Anna E. Lewandowska1, Manuel García-Casado1, 1CSIC - Instituto de Catalisis; 2PID Eng & Tech.

The reaction environment changes the catalyst surface as compared with its structure under vacuum, ambient or in situ dehydrated conditions, which makes it critical to characterize the catalyst surface and bulk structures during operation. A particularly powerful in situ approach is the operando methodology, i.e., combination of reaction in situ spectra and activity measurement in a single experiment. The term operando started to be used during 2002 [1-5]. “Operando” is Latin for “working”. To truly assess structure-activity relationships, it is critical that the operando reaction cells be designed like catalytic reactors [3-6]; most operando methodology [3-6] to an automated multi-reactor array provides a new tool for understanding the structure-activity/selectivity relationships in catalysis at a molecular level, as one of us disclosed in 2000 [7].

Among the different spectroscopic techniques, Raman spectroscopy is particularly suited to study catalysts under controlled temperature, gas flow and pressure. The spectra were simultaneously measured by GC. Raman spectra recorded during the methanol oxidation reaction over Al2O3 supported polyoxomolybdate catalysts were collected at different temperatures and under various catalytic conditions. All the data indicates that, in the absence of oxygen, methanol reacts with the active polyoxomolybdate phase to give oxidation products until all accessible centers are reduced. The reduction of the catalyst has also been monitored by the XANES spectra. Indeed the oxidized state shows a characteristic pre-edge peak that drastically decreases upon reduction along with a shift of the absorption edge towards lower energies (c.a. 3eV) indicating reduction of the metallic centers. The EXAFS region of the XAS spectra leads to complementary informations and shows that the oxygen environment around the molybdenum is a distorted tetrahedron as suggested by LRS. In order to assess the oxidation degree of the molybdenum centers combined Operando Raman/EPR experiments was performed, which was completed by a quantitative XPS characterization. Moreover ESEE and HYSCORE EPR studies give a better insight into the structure of the reduced supported oxomolybdate phase. Thus Operando combined spectroscopic techniques allows us to follow the evolution of the catalyst during the first step of the reaction, which lead to a fine interpretation of the mechanisms occurring on the catalyst surface. Moreover computation of the spectroscopic signatures (Raman and XANES) permits the confirmation of the structural model leading to a detailed picture of the catalyst in working conditions.

(466) Operando Spectroscopic Studies of the Methanol Conversion over Alumina-Supported Oxomolybdates Catalysts
Edmond Payen1, Sylvain Cristol1, Elisé Berrière1, Gwenaelle le Bourdon2, Sophie Morel2, Lionel le Bihan2, H. Vézian1, UCSC-UUMR; 2HORIBA Jobin-Yvon; 1COM, UMR

The partial oxidation of methanol is of great interest for industrial applications and Raman spectroscopy is a powerful spectroscopic technique that can give insights into catalytic systems enabling to obtain information at the molecular scale on the active phase under reaction conditions. Complementary atomic information can be obtained by other techniques such as XANES, EPR and XPS, although the vacuum is required by this later one preventing its use in operando conditions. The oxidation of methanol in the catalytic condition has therefore been characterized by these physical techniques. Whatever the techniques used, dedicated flow type reactor-cells have been designed and the catalytic performances were simultaneously measured by GC. Raman spectra recorded during the methanol oxidation reaction over Al2O3 supported polyoxomolybdate catalysts were collected at different temperatures and under various catalytic conditions. All the data indicates that, in the absence of oxygen, methanol reacts with the active polyoxomolybdate phase to give oxidation products until all accessible centers are reduced. The reduction of the catalyst has also been monitored by the XANES spectra. Indeed the oxidized state shows a characteristic pre-edge peak that drastically decreases upon reduction along with a shift of the absorption edge towards lower energies (c.a. 3eV) indicating reduction of the metallic centers. The EXAFS region of the XAS spectra leads to complementary informations and shows that the oxygen environment around the molybdenum is a distorted tetrahedron as suggested by LRS. In order to assess the oxidation degree of the molybdenum centers combined Operando Raman/EPR experiments was performed, which was completed by a quantitative XPS characterization. Moreover ESEE and HYSCORE EPR studies give a better insight into the structure of the reduced supported oxomolybdate phase. Thus Operando combined spectroscopic techniques allows us to follow the evolution of the catalyst during the first step of the reaction, which lead to a fine interpretation of the mechanisms occurring on the catalyst surface. Moreover computation of the spectroscopic signatures (Raman and XANES) permits the confirmation of the structural model leading to a detailed picture of the catalyst in working conditions.

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(468) Coupling Raman Spectroscopy to EPR, UV-vis and FTIR Spectroscopy for Deeper Insights in Selective Hydrocarbon Oxidation and Catalyst Synthesis

Angelika Brueckner1, Ursula Bentrup2, Leibniz Institute of Catalysis

Raman spectroscopy as a tool for monitoring working transition metal oxide catalysts during the selective oxidation of hydrocarbons such as lower alkanes has received much attention in heterogeneous catalysis. While valuable information on the structure of different metal-oxygen bonds and their role in the catalytic cycle can be derived from Raman spectra when the metal species are in their highest oxidation state, it revealed often difficult to detect such moieties when they are reduced during reaction. Simultaneous coupling of Raman spectroscopy with spectroscopic techniques that are particularly sensitive for the detection of reduced (paramagnetic) transition metal ions can markedly widen the information potential obtainable from catalytic redox processes. This will be illustrated by two examples using operando-EPR/UV-vis/Raman spectroscopy: 1) monitoring supported vanadia catalysts during oxidative propane dehydrogenation and 2) monitoring polypyrrolometallate catalysts containing molybdenum and vanadium during formation and selective oxidation of isobutane. In the first case, various vanadium sites with different structure and catalytic activity could be identified on the same catalyst. In the second case, Raman spectroscopy provided information on phase changes. Additionally, coupled in situ-Raman/FTIR/UV-vis spectroscopy was used to follow the stepwise synthesis of MoVNBTeOx catalysts by a slurry procedure. In these systems, Raman spectroscopy provided specific information on changes of molybdate anions by interaction with V and Te species while FTIR was particularly sensitive to sulfate, oxalate and ammonium components of the synthesis mixture. It was found that the sequence of adding the different components to the synthesis mixture did not influence the product structure. In contrast, the nature of the vanadium component appeared to be of crucial importance.

(469) Raman Characterization Studies of TiO2 Supported Manganese Oxide Catalysts for Low Temperature SCR of NO with NH3.

Sergey Mamedov1, Padmanabha Reddy Ettireddy2, Neeraja Ettireddy3, Punit Boolchand4, Panagiotis G. Simmriotis5, Horiba John Yvon Inc; 1University of Cincinnati

A series of TiO2 supported manganese oxide catalysts were prepared by wet-impregnation method for the low temperature selective catalytic reduction (SCR) of NO with ammonia as a reductant. A combination of various physico-chemical techniques such as N2 physisorption, O2chemisorption, TPR, X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and Raman were used to characterize the chemical environment of these catalysts. The Raman studies acted as complimentary tool to XPS in order to characterize the manganese oxides (MnO, Mn2O3, Mn3O4, MnO2) on the surface. Raman data show that there is a strong interaction between the Mn oxides and the support, which is responsible for the impressive catalytic performance in comparison with other systems we investigated.

(470) Pure Plasmons are Oscillations of the Free Carriers in Conducting Metal Oxides

Alina Efremenko1, Stefan Franzen1, Mark Losego1, Jon-Paul Maria1; North Carolina State University

In this talk the plasmons of the noble metals are contrasted with those of conducting metal oxides. The surface plasmon polaritons (SPP) of noble metals are observed in the visible range because of the fact that the d-band is coincident in energy with the conducting band for these metals. Thus, the plasmons observed in silver and gold have a significant contribution from bound electrons in addition to the free electron contribution predicted by the Drude theory for conduction. Other metals such as aluminum, gallium, nickel, palladium and the remainder of the transition metals have plasmons that are significantly higher in energy and consequently are not easily observed in the visible part of the electromagnetic spectrum. Conducting metal oxides have a lower charge carrier density than metals by around one to two orders of magnitude. Therefore, the surface plasmons in conducting metal oxides is observed in the near-infrared region. We demonstrate that SPPs can be observed in indium tin oxide, which is a representative of conducting metal oxides. Moreover, we demonstrate that the Drude theory can be used to predict novel plasmonic effects not observed in the noble metals due to the interference of the bound electrons. Moreover, we demonstrate that the number of free carriers can be controlled by thin film technology such that there is a range of novel plasmonic materials is now accessible.

(471) Integrated Label-Free Protein Detection and Separation in Real Time Using Confined Surface Plasmon Resonance Imaging

Kyle Foley1, Nguyen Ly1, Nongjian Tao1; Arizona State University

Surface plasmon resonance is a powerful tool used to detect chemical and biological interactions without the use of labels. A novel use of the technique is using it to measure protein separations. Using an electrically isolated gold surface, fluid and proteins are electrokinetically driven through a channel. Protein separation is monitored using SPR imaging in a new method involving microfluidic channels and sensing surface modification. Ultrathin fluidic channels are fabricated on a SPR imaging sensor surface. Real-time monitoring of protein separation is demonstrated.

(472) Nanoscale Building Blocks for Surface Plasmon Resonance Biosensor Development

Amanda Haes1; University of Iowa

The development of new technologies based on nano- and microscale phenomenon is important and significant for many reasons. One of the most prominent of these is biological sensors for the diagnosis of diseases, detection of environmental toxins, and drug discovery. This talk will focus on the microscopic and spectroscopic analysis of the optical properties of nanostructures and their integration with microfluidic devices with applications in biological sciences. We will show results for an optical sensor based on localized surface plasmon resonance spectroscopy. It will be demonstrated that this nanoparticle based sensor can be used to detect a variety of ligands, including a biomarker for Alzheimer's disease.
Techniques to Improve Sensitivity in FT-SPR Measurements

Steve Lowry, Eric Jiang, Koichi Nishikida, Steve Weibel; Thermo Fisher Scientific; GWC Technologies

The use of Fourier Transform spectroscopy to acquire surface plasmon resonance data has proven very valuable in studying biological binding experiments. Although FT-SPR is a very sensitive technique, a number of applications require lower detection levels due to low molecular weights or limited binding sites. In this paper we will describe some data acquisition and signal processing techniques that greatly improve the sensitivity of the experiment. We will also describe some results of FT-SPR to specific bioanalytical applications.

Facilitated Detection of Small Molecules with Nanoparticle Bejeweled Swellable Polymers

Karl Booksh, Yoon-Chang Kim, Soame Banerji, Wei Peng; University of Delaware

Embedding layers of gold nanoparticles into a swellable polymer overlayer provides three to four orders of magnitude increased sensitivity for selective detection of ammonia and glucose in two separate examples. A bare fiber optic sensor is sensitive to parts-per-thousand changes in vapor phase ammonia and percent changes for aqueous phase glucose concentration. Coating the sensor with polyallylamine improves the detection limit to the mid-parts-per-million. Including gold nanoparticles further enhances the SPR shift and lowers detection limits to the low-ppm regime. Similarly, a multilayer, molecular-imprinted polystyrene-sulphonate-polyallylamine with embedded nanoparticles decreases the detection limit from the percent range to below 100 ppm. Both of these polymer transduction layers are shown to be robust. The ammonia sensor is unresponsive to methane, hydrogen sulfide and humidity changes. The glucose sensor was applied to detection of glucose in urine and is robust to fructose and phosphate.

Controlled Assembly of Fe-Mercaptoalkanoic Acid on Gold by Headgroup Electrostatic Interactions

Roger Terrill, Arthur Cheng, Paul Yong Nam Pak, Shaowei Chen; San Jose State University; University of California at Santa Cruz; Korea National University of Education

Monolayers and submonolayers of 11-mercaptopundecanoic acid (MUA) and 3-mercaptopropionic acid (MPA) were prepared on gold surfaces from a range of phosphate buffer solutions (90% aqueous, 10% ethanol) to examine the influence of headgroup charge on monolayer formation. Buffers were either pH 2 (> pKa) and buffer concentrations ranged from 1 to 0.0001 M in even decades. Surface plasmon resonance measurements of the surface coverage revealed substantial dependences, of approximately equal magnitudes for both MUA and MPA on solution composition. At pH 2 dense layers formed and the formation was independent of ionic strength. At pH 7 submonolayers formed those were between 20 and 30% less dense. It was also observed that at pH 7 there was a substantial sensitivity to ionic strength - 1M buffers yielded roughly 20% denser layers than 0.001 M ones. Cyclic voltammetry experiments of Fe(CN)64-/3- redox chemistry at MUA coated electrode surfaces fully corroborate the above observations showing the substantial permeability of MUA layers formed from anionic precursors, but dense, blocking layers from neutral MUA.

Laser Ablation Inductively Coupled Plasma Spectrometry – Ready for Take Off

Detlef Günther; ETH Zurich, Laboratory of Inorganic Chemistry

The introduction of laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) by A. Gray in 1985 initiated immediately a vast interest in this direct solid sampling technique, due to the micro-local access to qualitative and quantitative information about the elemental composition as well as isotope ratios. A large number of studies on the laser-solid interaction, aerosol transport and the vaporization and ionization of particles within the ICP contributed significantly to the improvement of this technique towards a “quantitative tool”, which is currently applied in a wide variety of laboratories. However, even the increased number of applications can not hide remaining problems of this technique, which are partially laser and strongly ICP-related. The presentation will highlight applications “ready for take off” and will discuss processes where permission for “take off” is still denied.

Simultaneous Spectrophotometric Estimation of Methocarbamol and Nimesulide in Tablet Dosage Form

Tushar Patel, LakshamanBhai Patel, Sunil Makwana, Tejas Patel, Kirit Patel, Timir Patel; Faculty of Pharmacy, Dharmsinh Desai University

A simple, accurate and precise spectrophotometric method has been developed for the simultaneous estimation of Methocarbamol and Nimesulide in combined dosage form. The method is based on absorbance measurement of both the drugs at wavelength of absorbance maxima. Methocarbamol has two absorbance maxima at 223 nm and at 274 nm whereas Nimesulide has an absorbance maximum at 393 nm. The solvent used was Methanol. Beer-Lambert’s law was followed in the concentration ranges 5-100µg/ml and 1-40µg/ml for Methocarbamol and Nimesulide, respectively. Limit of detection of Methocarbamol was found 0.66µg/ml and for Nimesulide it was 0.75µg/ml. The results of analysis have been validated statistically and recovery studies have been performed.

Total Arsenic Determination in Urine by Hydride Generation Atomic Fluorescence Spectrometry: Comparison between On-Line Microwave Assisted Heating and On-Line UV-Photooxidation

Kanna Ito, Christopher D. Palmer, Patrick J. Parsons; University at Albany; New York State Dept. of Health

The principal aim of this work is to develop a simplified method for determination of seven arsenic (As) species in urine. The approach we are taking is to utilize hydride generation atomic fluorescence spectrometry (HG-AFS) coupled with microwave assisted heating (MW) or UV-photooxidation (UV). The continuous flow manifold was set for maximum As(V) sensitivity by optimizing the HCl and NaBH4 concentrations. The on-line oxidation of seven As species to As(V) was accomplished by optimizing the K2S2O8 concentration. Final optimized conditions were 15% (v/v) HCl, 1.0% (m/v) NaBH4, and 3.0% (m/v) K2S2O8 for MW, and 3.5% (m/v) K2S2O8 for UV. The MW method had higher % conversion efficiency for most As species than did UV. The conversion to As(V) under MW conditions ranged from 96% (AsIII, AsB, AsC) to 105% (MMA), while the conversion with UV ranged from 95% (TMAO, AsB) to 106% (MMA). The assay will be validated by analyzing certified reference materials such as NIST 2670; Toxic metals in urine, NIES No.18; human urine, and by analyzing archived urine proficiency testing materials from the New York State Department of Health.

Tungsten Coil Atomic Emission Spectrometry

Bradley Jones, Clifton Calloway, George Donati, Jaoquim Nobrega; Wake Forest University; Winthrop University; Federal University of Sao Carlos

A novel tungsten coil atomic emission spectrometer is described and evaluated. The system employs a single tungsten coil as a combined atomizer and excitation source for the determination of metals by atomic emission spectrometry. The tungsten coil is extracted from a 150 W, 15V commercial slide projector light bulb.
A 25 microliter sample aliquot is applied directly to the coil in a reducing atmosphere. A simple, laboratory constructed, computer-controlled power supply provides a constant current to the coil. A small charge coupled device spectrometer renders the system light and portable. Simultaneous multi-element detection is possible with limits of detection similar to those observed for inductively coupled plasma atomic emission spectrometry. The average tungsten coil lifetime is approximately 300 heating cycles. Matrix modification, especially as it affects the surface of the coil will be described. Simple sample preparation techniques are employed. The internal standard method is used for quantitation. Application to environmental field analyses will be discussed.

(481) High Resolution Continuum Source Atomic Absorption Spectrometry with Electrothermal Atomization: Panacea for Minimization of Spectral Interferences?

Gerhard Schlemmer; 1 Analytik Jena

High resolution-continuum source AAS makes use of a single radiation source to cover the spectral range from 190-900 nm. The high spectral resolution in the range of about 2 pm, required in AAS, is provided by an Echelle-monochromator. The analytical line selected as well as the spectral environment of about 100 pm on both sides of the spectral line is recorded on a detector array. HR-CSAAS therefore is the only technique in AAS which provides highly resolved information on the analytical line and its spectral vicinity simultaneously. Complex matrices selected from typical real-life analytical situations are used to compare the performance of state-of-the-art background correction techniques, i.e. Zeeman-effect background correction and background correction off-line using a high resolution continuum source AAS-spectrometer. Examples include high and fast background originating from light scattering as well as structured background originating from atomic and molecular absorption. Arsenic absorption on the primary resonance line 193.7 nm in the presence of Aluminium compounds at concentrations higher than 50 mg/L serves as a typical example to prove the superiority of HR-CSAAS over Zeeman-effect background correction in a so far not completely solved application problem of ET-AAS. Under optimized conditions a limit of determination of about 1 µg/L As can be achieved in model solutions containing up to 200 mg/L aluminum. Scientifically new information: Simultaneous background correction in AAS with high spectral resolution for structured background. Comparison of HR-CSAAS vers. Zeeman-AAS.

(482) Characterization and Identification of Pollen by Vibrational Spectroscopy

Janina Kneipp1, Franziska Schulte1, Ulrich Panne1; 1 Federal Institute for Materials Research (BAM)

The Raman or infrared spectrum of a complex biological sample is brought about by spectral contributions from all Raman or IR-active molecular groups contained in the sample and hence can serve as a fingerprint-like identifier for a specific biomaterial. The vibrational spectroscopic investigation of pollen has been reported in a few studies, but so far no systematic work has been carried out regarding the application of Raman and FTIR for identification purposes and the investigation of allergologic mechanisms. We have been working towards the goal of a spectroscopy-based characterization of natural bioaerosols, and in particular the identification of pollen contained therein, a matter of increasing interest not only to people suffering from allergies. In microspectroscopic approaches we investigated pollen of several plant species, such as willow, birch, hazel and many others. Raman microspectra were obtained under a variety of sampling conditions and with different excitation wavelengths. We also compared the results of different sample preparation procedures. As complementary method to Raman spectroscopy, synchrotron FTIR microspectroscopy is employed, which permits the acquisition of high-quality spectra from very small sample volumes containing very few or even single pollen grains. Apart from the application of multivariate data analysis methods for the identification of species-specific spectral signatures, we also collected spectra from purified pollen compounds, such as sporopollenin, the major constituent of the exine. By closer examining pollen fractions, we hope to learn more about the main contributors to a complex spectral fingerprint of pollen and their fragments. Vibrational spectroscopy on purified pollen compounds permits an investigation of molecular alteration due to changes in the ambient conditions (e.g. of water content or presence of trace gases) and will hopefully improve our understanding of important allergologic mechanisms.

(483) Following F. Novicida Infection with Multicolor Fluorescent Proteins and Spectral Imaging

Jerilyn Timlin1, Julie Kaiser1, Michael Sinclair1, Linda Nieman1, Todd Lane1; 1 Sandia National Labs

The ever-growing assortment of fluorescent proteins with divergent spectral properties has enabled biological researchers to easily visualize expression patterns of multiple proteins in vivo. We report our development and use of multicolor fluorescent protein fusions and a custom confocal spectral imaging microscope to explore spatio-temporal protein expression during host-pathogen interaction with Francisella novicida (F. novicida). F. novicida is surrogate for the highly virulent Francisella tularensis, a gram-negative bacterium that causes tularemia and is a potential bioterrorist agent. In experiments where murine macrophages are infected with F. novicida we use confocal spectral imaging to visualize the expression of IglA and IglB, two cytoplasmic proteins required for growth of F. novicida in a host macrophage cell. We will present results that demonstrate the importance of using advanced spectral unmixing methods to isolate and remove the confounding effect of the overlapping host cell autofluorescence spectrum in order to accurately detect the naturally weak expression levels of the fluorescent proteins present in vivo. Using this sensitive analytical imaging technology, we will map protein expression within the host cell with high spatial resolution at various timepoints post-infection. We will detail the spectroscopic imaging and multivariate analysis approach, including its potential for elucidating weak and possibly transient signals in real-time via live cell imaging. This method is unique because it allows direct visualization of the spatial location of multiple species (the pathogen, the host, and labeled proteins for example) in intact cell systems – a feat which is not possible with current biological assays such as western blots.

(484) Development of a Nanomechanical Biosensor for Analysis of Endocrine Disrupting Chemicals

Kasey Hill1, Pampa Dutta1, Michael Sepaniak1; 1 University of Tennessee, Department of Chemistry

The use of bioreceptor functionalized microcantilevers (MCs) to detect and screen endocrine disrupting chemicals (EDCs) is demonstrated. EDCs’ adverse affects on the endocrine system of humans, livestock, and wildlife provides strong motivation for advances in analytical detection and monitoring techniques. The interaction between EDCs and protein receptors or antibodies immobilized on a MC surface induces an apparent surface stress. This surface stress leads to static bending of the MC, which is detected by an optical beam bending technique. The combination of protein receptor, which include estrogen receptor alpha and estrogen receptor beta, as well as monoclonal antibodies (Ab), with MC systems employing modified nanostructured surfaces provides for excellent response sensitivity and the inherent selectivity of biospecific receptor-EDC interactions. Optimization of the MC nanostructured surface, linking chemistry, and protein conditions...
has been accomplished with model systems, anti-IgG and IgG, as well as anti-biotin and biotin. A comparison of responses of three EDCs, which include 17-beta-estradiol, 17-beta-estradiol, and 2- OH-estrone, with ER-alpha and ER-beta illustrates which estrogen receptor subtype provides the greatest sensitivity. Antibodies specific to a particular EDC can also be used for analyte specific screening. Calibrations plots for a MC functionalized with anti-17-beta-estradiol Ab show responses in the range of 1 x 10^-11 through 1 x 10^-7 M for 17-beta-estradiol with a linear portion extending over two orders of magnitude in concentration.

(485) A New Liquid-Liquid Extraction Method for Determination of Montelukast in Small Volume Human Plasma Samples Using HPLC with Fluorescence Detector

Drashan Patel¹; ¹Darshane B. Patel, Sarvajanik Pharmacy College; ²Hardik A. Prajapti, Sarvajanik Pharmacy; ³C. N. Patel, Sarvajanik Pharmacy Co.

Montelukast is a potent orally active cyssteinyl leukotriene receptor antagonist that significantly improves parameters of asthmatics. A new liquid-liquid extraction based reverse phase liquid chromatography method has been developed and subsequently validated for the determination of montelukast in human plasma. The separation was achieved with C8 column (150x4.6 mm, 5 micron) and a mobile phase comprising of a mixture of 10 mM ammonium acetate buffer (pH 3.0) and acetonitrile in a ratio of 35:65 v/v. Montelukast was extracted from human plasma using a liquid-liquid extraction technique with ter-butylmethylether. The limit of detection and lowest limit of quantification were 5 and 10 ng/ml respectively. This method was found to be linear over the range of 10 to 1000 ng/ml with a recovery of 53 to 62%.

(486) Amperometric ATP Microbiosensors to Investigate the Maturation of the Carotid Body

Jean-Francois Masson¹,², Christine Kranz³, Estelle Gauda³, Boris Mizaikoff⁴; ³Georgia Institute of Technology; ²Johns Hopkins University; ⁴Univeristé de Montreal

Clinical studies to determine the age-dependent release of ATP stimulated at the rat carotid body will be presented for potassium depolarization, hypoxia (Low O2), and hypercapnia (High CO2) conditions. Laterally resolved release of ATP was measured at the carotid body using a miniaturized dual-enzyme biosensor based on the co-immobilization of glucose oxidase and hexokinase under various stimuli to establish the dose-response of the carotid body from rat pups. Optimization of the ATP biosensor using polymer entrapment or covalent immobilization of the enzymes in the sensing scheme results in a microbiosensor sensitive enough to detect minute amount, between 5 and 10 uM, of ATP released by the carotid body. The presented ATP microbiosensor can detect micromolar ATP concentrations. Selective detection of ATP in presence of catecholamines, co-released with ATP under various stimuli, is achieved using dual barrel microelectrodes. One electrode modified with a biosensing layer to measure ATP and the second electrode as a background monitoring electrode were used to determine ATP release and co-released neurotransmitter molecules from the carotid body. The background monitoring electrode detected catecholamines release at both the carotid body and the superior cervical ganglion in the concentration range of approx. 1 uM for potassium depolarization and hypercapnia. Selection of the biological media is critical to the determination of ATP. Interference of HEPES-containing biological medium with the amperometric biosensor was observed due to the photooxidation of HEPES forming hydrogen peroxide. Hence all measurements to study the ATP release from the carotid body were performed in Ringer’s solution.

(487) Application of Multivariate Curve Resolution in Pharmaceutical Process Understanding

Dongsheng Bu¹; Martin Kermit; ¹Camo Software Inc

Multivariate Curve Resolution (MCR) method is intended for the recovery of concentrations and spectral profiles of the components in unresolved mixtures using a minimal number of assumptions about the nature of these mixtures. We are currently applying MCR in the pharmaceutical industry to understand and monitor process. One of the major applications is to detect the reaction end point of active ingredient synthesis monitored by on-line mid-infrared spectrometer. In this case, reference sampling is difficult and there is possible intermediate during the synthesis. MCR is applied to obtain relative concentration of a major reagent where a steady state of the synthesis is achieved. Principal Component Analysis (PCA) score plots of different batches are useful in following the changes of measured spectra and to study batch-to-batch difference. The application of MCR in wavelength selection for building quantitative model, and the effect of common spectral pre-treatments on MCR analysis will be discussed.

(488) Qualitative Interpretation of Regression Vectors in Multivariate Calibration

Christopher D. Brown; ¹; Robert L. Green; ¹; Ahura Scientific

The qualitative interpretation of regression vectors determined with multivariate calibration is rather frequent in the analytical literature. Many put forth that the presence (or absence) of certain features in the regression vector is suggestive of the chemical sensitivity and selectivity of the resulting chemometric model. In this paper we will review statistical and chemometric interpretations of regression coefficients, including the early work of Lorber [1], Seasholtz and Kowalski [2] and others that followed. Much of this work is derived from the properties of classical (or K-matrix) calibration methods and net analyte signal theory. After highlighting the more complex properties of inverse calibration methods [3], we systematically examine the primary factors that make regression vector interpretation extremely difficult in most real-world applications. These factors include the contravariance constraint, the latent structure of the chemical system and calibration design, and the errors-in-variables nature of most calibration problems. In concluding we show that, while method sensitivity and selectivity is difficult to prove by qualitative examination of the regression vector, current quantitative figures of merit can be extremely instructive.[1] A. Lorber, Analytical Chemistry 58:1167 (1986)[2] M.B. Seasholtz and B.R. Kowalski, Applied Spectroscopy 44:1337 (1990)[3] C.D. Brown, Analytical Chemistry 76:4364 (2004)

(489) Re-fitting PCA, MPCA and PARAFAC Models to Incomplete Data Records

Barry M. Wise; ¹; Eigenvector Research, Inc.

Many processes and analytical methods generate multivariate or multiway data sequentially. In calibration mode this is not generally a problem, one just waits until all the data is in, then sets about modelling. Often, particularly in process applications, it is desired to know how well the model represents the incoming data before the complete record is available. Several options have been proposed to deal with this problem. Some of the methods are based on in-filling the missing data so that the models may be applied in the usual way. This approach, however, suffers from all the problems associated with missing data. How does one fill in the record, particularly when the missing parts are systematic, not random? An alternative approach is considered here. Models are fit to partial data records by simply truncating the model loadings to coincide with the available data and fitting the partial factors using a classical least squares (CLS) approach. The estimated scores and residuals are found to converge to those of the entire record quite rapidly in the data sets considered. In fault detection applications
the implies that it is often possible to detect a bad batch well before its completion. The partial refit method is compared to the method for in-filling missing data in PCA developed previously.

(490) Multivariate Detection and Quantification Limits in the Analysis of Potent Drug Tablets by Transmission Near Infrared Spectroscopy

Manel Alcala1, Joshua Leon1, Jorge Ropero1, Rodolfo J. Romañach1, Marcelo Blanco2; 1Univ. Puerto Rico - Mayaguez; 2Universitat Autònoma de Barcelona -Spain

The determination of detection and quantitation limits for potent drug tablets using NIR transmission spectroscopy will be reported. The drug distribution in a pharmaceutical tablet batch is critical in formulations where the active pharmaceutical ingredient (API) is a potent drug at low concentration levels. For example, a 0.1 mg drug aggregate may double the drug content in a potent drug formulation. However, current regulations only require that 10 tablets from a batch that may contain several million tablets be analyzed. Several methodologies for the estimation of detection and quantification limits are in the bibliography. Nevertheless, both limits were determined by a multivariate method based on the sample-specific standard error for PLS regression, which gives limits were determined by a multivariate method based on the sample-specific standard error for PLS regression, which gives similar results to the univariate method endorsed by ISO 11483. This simple strategy defines the best calibration range for the PLS model and subsequently minimizes the prediction error during routine analysis. The preliminary results obtained by this strategy confirm that Multivariate Detection and Quantification Limit (MDL and MQL) correspond to 0.006 and 0.019 % (w/w), respectively. Its demonstrated the ability of NIR spectroscopy to effectively work with low drug content formulations. At this moment, no bibliographic report has been found where MDL and MQL have been obtained from low drug content tablets using NIR spectroscopy. NIR spectroscopy, in transmission mode, can be used for quantification of solid dosage formulations with less than 1% (w/w) API concentration. Because the method does not require sample preparation, and its non-destructive, it could be used to analyze a large number of tablets during process development, detect drug agglomeration problems and facilitate process development and optimization.

(491) Room-Temperature Fluorescence Analysis of Dye Extracts for Forensic Fiber Examination

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Dye analysis has long been recognized as an important feature for forensic fiber comparisons due to the diversity of visually and microscopically indistinguishable dye materials. Numerous methods have been reported for isolating dyestuffs from fibers and for comparing dyes and dye mixtures, including ultraviolet, visible and infrared absorption spectrometry, thin-layer chromatography and high-performance liquid chromatography. This presentation focuses on forensic fiber investigation via Room-Temperature Fluorescence (RTF) spectroscopy. Fluorescence Microscopy has been reported for forensic fiber analysis but the full potential of RTF has not been explored yet. Wavelength selection in Fluorescence Microscopy was carried out with band-pass filters that take no advantage of the wealth of information provided by data formats such as excitation-emission matrices (EEM), wavelength-time matrices (WTM) and time-resolved excitation-emission matrices (TREEM). This presentation compares multidimensional data formats recorded from dye extracts of fibers pre-dyed with both fluorescent and non-fluorescent commercial dyes. Intrinsic fluorescent impurities co-extracted with the dyes bare evaluated as reliable sources for fiber examination. The potential interference of environmental impurities is evaluated as well.
The maturation of spirits in white oak barrels involves compounds that are naturally present in the wood and also produced during the manufacturing of the barrel. Thermal treatment (charring and toasting processes) is usually applied to the white oak material to breakdown and caramelize the different compounds such as lignin, cellulose, and hemicellulose which results in the formation of chemicals vital to the flavoring, aroma, and overall quality of the spirits. Therefore, it is essential to assess the material before and after treatment in order to select the best conditions and materials specific to the type of spirit. In this work, infrared spectroscopy coupled with multivariate analysis is used to rapidly assess the thermal treatment and to develop models to predict the concentration of some of the most important compounds that are involved in the quality of the spirit. In order to build the model, thermal treated white oak samples were analyzed using near infrared spectroscopy (NIR). These samples were then subjected to a “maturation” step and analyzed by High Performance Liquid Chromatography (HPLC). Partial least squares regression (PLS) was then used to correlate the NIR spectra with the data generated by HPLC creating a model for the quick identification of the concentration compounds found in the spirit after maturation.

(495) Diffuse Reflectance Fourier Transform Mid-Infrared Spectral Properties of Forages With Varied Fatty Acid Content
Francisco Calderon1, James B. Reeves II2, Joyce Foster1, William Clapham1, James Fedders2, Merle F. Vigil1, W. Brian Henry2, USDA-ARS Central Great Plains Research Station, Ak; USDA-ARS Environmental Management and By; USDA-ARS Appalachian Farming Systems Res USDA-ARS Corn Host Resistance Research U

Ruminant diet can affect the fatty acid (FA) content of meat and dairy products, which indicates that managing forage consumption is important in determining the quality of the animal products. Mid-infrared spectroscopy is sensitive to changes in forage FA and has been used successfully to quantify FA in forages using chemometrics. However, few studies have attempted to identify the specific spectral changes that occur due to fatty acid variability in plant materials low in lipid content, where spectral differences may be subtle. A total of 182 samples from eleven forage species, including 13 varieties, were sampled at three growth stages. Samples were scanned using Fourier transform mid-infrared spectroscopy (FTMIR) and analyzed by gas chromatography for lauric, myristic, palmitic, stearic, palmitoleic, oleic, linoleic, and alpha-linolenic acids. Principal components analysis shows that forbs, legumes and grasses form separate clusters according to their fatty acid profiles. Grasses have low C18:0 and high C14:1 relative to the other forage types. Forbs have relatively low amounts of C18:2 and C14:1, and high amounts of C14:0. Forage samples from the first harvest tend to have high C16:0, C16:1 and C18:3, but lower C14:1. The principal components analysis of the FTMIR spectra shows that there was a clear separation between the spectra from the first harvest and those of the last two harvests because absorbances in 3320-3615 cm-1, 3245 cm-1, 2892 cm-1, and 1150-1170 cm-1 increased with harvest time. Partial least squares analysis showed that bands at 1678 cm-1, 1536 cm-1, 1397 cm-1, 825 cm-1, and 536 cm-1 were positively correlated with C16:0, C16:1 and C18:2 concentration in forages, while a wide band at 3501 cm-1 was negatively correlated.

(496) Analysis of Gaseous Samples with Sorbent Tube Preconcentration of Analytes Followed by Infrared Spectrometry and Gas Chromatography
Craig Lampert1, David Kofink1, Ngee-Sing Chong1, Middle Tennessee State University

Toxic compounds are frequently found at trace concentrations and hence their direct analysis can be challenging. Analyte preconcentration using sorbent tubes followed by their thermal desorption to transfer the analytes either into a long pathlength gas cell for infrared (IR) spectrometry or a gas sampling loop for gas chromatography (GC). The objectives of this study are to evaluate the analytical performance of both techniques for gaseous analysis. The reliability of IR analysis is influenced by water vapor and carbon dioxide in air samples. Therefore, their background IR absorbances were reduced by scrubbing the samples with NaOH and molecular sieve materials, respectively. The concomitant preconcentration of analytes with the rejection of water vapor was achieved via the use of hydrophobic sorbent materials such as Carbobox™ 1000, Carbopack™ X, Carbotrap™, and Carbopack™ Y. Commercially available sorbent tubes containing Tenax TA and Anasorb CMS were also tested. By carefully avoiding analyte breakthrough, preconcentration factors of 20 to 500-fold were achieved for trace gas analysis in the low parts-per-billion levels. The optimal parameters of thermal desorption in terms of desorption temperature and flow rate of desorbing gas were also characterized. The accuracy of the IR analysis depended on both the selection of wavenumber regions for quantitative analysis and the efficient removal of water vapor from the samples. For the GC analysis, quantitative calibration of C1-C6 alkanes, alkenes, and aromatic compounds was performed with a flame ionization detector for sample loop volumes of 250 mL, 2.0 mL, and 5.0 mL. In terms of analytical sensitivity, the 5.0-mL loop provided the best detection limits. It was found that more efficient heating and insulation of the loop and the injector area is especially critical for preventing the adsorption or condensation of aromatic compounds inside the sample loop so that optimal detection is achieved. The retention time for both C1-C6 and aromatic compounds are generally reproducible even though there is a small shift of about 0.1 minute for C6-C8 aromatic compounds. The relative merits of this technique will be discussed in terms of sensitivity, selectivity, accuracy, and ease of analysis for both heated and unheated loops.

(497) Analyte Mapping of Solid Samples by Laser Ablation Coupled with an Atmospheric-Pressure Glow Discharge Ionization Source
Jacob Shelley1, Joshua Wiley1, Francisco Andrade2, Steven Ray1, Gary Hieftje1; 1Indiana University; 2Unilever Corporation

Many modern applications of mass spectrometry require that chemical information be collected as a function of spatial location on a sample surface. The analyze map that is generated can yield important information about the sample. However, a major complication of most methods of imaging mass spectrometry is the need for the ionization source to operate under vacuum. For this reason, the use of recently developed atmospheric-pressure ionization sources would be attractive. In the present study, a 266 nm laser was used to ablate a section of solid sample. The resulting aerosol and vapor mixture was transported by a nitrogen stream to a novel atmospheric-pressure glow discharge (APGD) for subsequent ionization. This APGD, which is operated with helium as the discharge gas, can ionize the sample vapor in two different ways: directly into the helium glow discharge or into the flowing afterglow which contains a stream of excited species and reagent ions. The ionized sample was then analyzed with a time-of-flight (TOF) mass spectrometer. By raster scanning the laser beam across the sample surface, a two-dimensional mass-spectral image was generated. With this method, the spatial resolution of the...
image is limited by the spot size of the laser (~25 μm). By increasing the power density of the laser such that the surface of the sample is ablated, as opposed to desorbed, a depth profile of the sample can also be obtained. The resulting combination of laser ablation and APGD has been used to examine several sample surfaces, including metals, plastics, biological specimens, gels, and liquids. For example, the spatial distribution of caffeine within green tea leaves has been successfully mapped, as well as the distribution of pharmaceutical agents within a tablet. Analytical figures of merit and optimization of laser/ionization cell configurations will also be presented.

(498) Ligand Substitution Kinetics as an Analytical Tool for Trace Analysis
Surendra Prasad1; The University of the South Pacific
An ever increasing awareness of the important and critical role of extremely small concentration of some chemical species when present in chemical, physical and environmental samples has greatly stimulated interest in research aimed at determination of such species in trace level in a variety of complex matrices. The refinement and extension of analytical requirements imposed by the presence of trace amount of elements or compounds led to the development of same new micro-analytical techniques of chemical analysis. One of them is “Kinetic Methods of Analysis”, which is now emerging as a young area of research in the field of analytical chemistry. This is a ‘rate-based technique’ rather than equilibrium based one. The ‘Kinetic Catalytic Methods (KCM)’ continued to be the most popular method in the literature of kinetic methods of analysis. Their growing popularity and gradual acceptance is due to high specificity, sensitivity and precision combined with simple procedure and economy compared to the other methods of comparable analytical merit. Several reactions such as redox reactions, ligand substitution reactions and metalloporphyrin formation have been utilised as indicator reactions for the development of kinetic catalytic methods of trace analysis. Potassium hexacyanoferrate(II) is known to be among the least labile cyano-complexes of transition metal ions. Exchange of labeled cyanide between [Fe(CN)6]4- and free cyanide or aminopyridine is extremely slow, but under the action of u.v. light reversible auration takes place with the formation of [Fe(CN)5H2O]3- and CN-. The aquapentacyanoferrate(II) produced has been reported to react with nitrogen heterocycles giving intensely coloured products. Metal ions, such as mercury(II), which readily form complexes with cyanide, strongly catalyse the exchange reactions of hexacyanoferrate(II). Mercury is a potent environmental pollutant and we were looking for a kinetic method for its determination in trace concentrations. The search has resulted in an investigation of the kinetics and mechanistic anatomy of the mercury(II)-catalyzed reaction between hexacyanoferrate(II) and Mpz+ which gives an intense blue product, [Fe(CN)5Mpz]2-. The kinetics behavior of such reactions have been thoroughly studied and plausible mechanisms have been proposed, and are utilised for development of methods for trace determination of Hg(II). This presentation describes how to design catalytic kinetic methods of analysis. The mechanisms of the reactions are particularly important in establishing the methods, and will be briefly discussed for two specific cases in the present talk.

(499) Integrated Protein Preconcentration and Separation Microdevices Prepared by Rapid Prototyping using Solvent Imprinting
Xiuhua Sun1, Weichun Yang1, Tao Pan1, Adam Woolley1; Brigham Young University
Microfluidic analysis devices offer high throughput, and low consumption of sample and reagents relative to conventional assays. Microchip systems made of polymers, such as poly(methyl methacrylate) (PMMA), are potentially advantageous in analytical chemistry because of low-cost, rapid, scalable and simple fabrication. We have devised an approach for fabrication of PMMA microchips by solvent imprinting and bonding. SU-8 patterned templates were used to create microstructures on PMMA surfaces after treatment with acetonitrile. The imprinted channels were readily sealed using solvent bonding. This fabrication method is simple and fast, and yields good separation performance [1]. We are applying solvent imprinting methods in making microchips for protein preconcentration and analysis. These microdevices include a small length of glycidyl methacrylate based monolith; and reservoirs and channels are provided for sample injection, standard loading, rinsing, analyte elution and separation. We have covalently attached antibodies onto the monolith through the reaction between amine and epoxy groups. We are presently evaluating the selective enrichment of these microdevices, coupled with on-chip electrophoretic separation. These integrated systems should offer rapid analysis, flexible solution handling and complex sample pretreatment, providing an important step toward lab-on-a-chip analysis of biomolecules. Reference:[1] X. Sun, B. A. Peeni, W. Yang, H. A. Becerril, A. T. Woolley, J. Chromatogr. A, in press (2007).

(500) Degenerate Four-Wave Mixing of Nanostructured Supramolecular Organic Semiconductor
Qiguang Yang1, JaeTae Seo2, Russell Battle1, SeongMin Ma3, Cheng Zhang3, Bagher Tabibi1, Sam-Shajing Sun1, JinHwa Heo1, Wanjoo Kim1, Sungsoo Jung2; 1Department of Physics, Hampton University, Hampton; 2Department of Chemistry, Norfolk State U; 3Korea Research Institute of Standards
A novel class of photovoltaic nanostructured block copolymers, where conjugated donor and acceptor blocks are covalently linked by nonconjugated chains, has been synthesized and characterized. Both linear and nonlinear optical properties of this type of nanostructures may be improved greatly if perfect nanoscale ordered morphology can be achieved. Our block copolymer exhibited better processability than the corresponding blends of individual blocks and it did not have a large scale phase separation problem during the film forming process; therefore, it was expected to have higher performance in solar cell device applications. On the other hand, the quantum confinement effect of the photo-generated carriers in the periodical nanostructures may enhance the third-order nonlinearity of the copolymer significantly. In this work, we report the experimental investigations of the third-order nonlinearity of our block copolymer at both resonant and non-resonant wavelengths by using a 6 ns Nd:YAG laser. The forward degenerate four-wave mixing was used to characterize both the 1111 and 1221 components of the third-order nonlinear susceptibility tensor. The hyperpolarizability of the copolymer was about 10-43 m2/V2 at 532 nm while it reduced to about 10-46 m2/V2 at 1064 nm. The physical origin of the nonlinearity was attributed to electronic process as well as other processes.

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Over the past decade, the formation and growth of nanometre-size atmospheric aerosol particles have been observed at a number of sites around the world. The particles have a significant effect on climate change and on human health, which mainly depends on the size and chemical composition of aerosol particles. Chemical analysis of particles can be based on various techniques, where mass spectrometry (MS) is one of the most commonly used techniques. Nowadays aerosol sampling systems allows particle collection straight to the analyzer or first collecting aerosol sample.
to the aerosol filter, which can then be analyzed by means of other methods, e.g., MS. Generally, problem has been reliable ultrafine aerosol particle chemical analysis in real-time or even near real-time. Our goal was to design a sampling system, which can be used for near real-time ultrafine aerosol particle chemical analysis in conjunction with time-of-flight (TOF) mass spectrometer. The idea of the sampling valve is to collect charged and size separated aerosol particles by electrostatic precipitation through nitrogen sheath gas for relatively large platinum surface. At the ms-side, the collected compounds are released from the sampling surface by laser desorption (Nd:YAG 1064 nm) and right after desorption, one UV-laser pulse (Eximer ArF 193 nm) is used to ionize the plume. Then ions are accelerated to the time-of-flight mass spectrometer and analyzed according to their mass to charge ratios with micro channel plate detector. Valve operation has been tested in conjunction with self-constructed aerosol time-of-flight mass spectrometer with several chemical compounds like alkenes, PAH’s, weak acids and inorganic salts. Performance and efficiency of the valve during the collection and desorption have been tested and the valve was confirmed to be suitable inlet system for nanoparticle analysis. In future, work is going on to integrating size selective collection to the system by controlling aerosol flow rate to the surface of the valve and valve collection voltage

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The diverse nature of peptides gives emphasis to their involvement in multiple regulatory processes in living systems. For this reason, peptides have been identified as ideal biomarkers in various diseases. A detailed profiling and sequence study of peptides have been identified as ideal biomarkers in various regulatory processes in living systems. For this reason, irreversible binding, or due to irreproducible flow paths, causing used for sample clean-up purposes may result in sample loss due to solid-phase extraction on-tip columns (C18, C4 ZipTips, Millipore) per spot, the purity of the crystallized samples, and instrumental MS, the data quality depends upon the analyte density deposited through the sample. A throughput study of complex peptidomes is therefore essential. One complex biological matrices. The development of more sensitive can sometimes hamper the breadth of detectable peptides in spectrometry. However, limitations in current MS methodologies over the past decade due to advancement in the modern mass studies, where the focus is on proteins. Peptidomics has flourished involves systemic polypeptide analysis by mass spectrometry, covering the lower mass range, and complementing proteomic studies, where the focus is on proteins. Peptidomics has flourished over the past decade due to advancement in the modern mass spectrometry. However, limitations in current MS methodologies can sometimes hamper the breadth of detectable peptides in complex biological matrices. The development of more sensitive and robust mass spectrometric peptide profiling tools for the high throughput study of complex peptidomes is therefore essential. One of the preferred tools in Peptidomics is MALDI MS. In MALDI MS, the data quality depends upon the analyte density deposited per spot, the purity of the crystallized samples, and instrumental figures of merits such as sensitivity, resolving power and limit of detection. A commonly overlooked step, also crucial for ensuring high quality MALDI MS data, is sample preparation. Conventional solid-phase extraction on-tip columns (C18, C4 ZipTips, Millipore) used for sample clean-up purposes may result in sample loss due to irreversible binding, or due to irreproducible flow paths, causing poor quality mass spectral data. Polymer contamination from these pipette tips can also significantly suppress analyte signal. To overcome these issues, an on-chip dynamic preconcentration/focusing sample preparation method was investigated. We here demonstrate, for the first time, the successful adaptation of desalting/focusing targets with atmospheric pressure MALDI mass spectrometry, to combine the advantage of AP/MALDI ion sources to perform MSn when mounted on a quadrupolar ion trap, with the advantages of on-chip purification and pre-concentration. A comparison between conventional AP/MALDI targets and focusing plates showed 300 to 600 fold S/N ratio gains with 6-10 %RSD reproducibility. Results for the de novo sequencing of standard peptides and protein digestions strongly suggest that this approach will bring significant breakthroughs for enabling new experiments in the field of comparative peptidomics.

(503) Ion Mobility-Mass Spectrometry Shift Reagents for Multiplexed Peptide and Protein Characterization
Thomas Kerr1, John McLean1; 1Vanderbilt University
The characterization of peptides and proteins is greatly facilitated by targeted increases in the information content in MS spectra. Two-dimensional separations using ion mobility-MS (IM-MS) approaches provide enhanced information content in that separations are performed on the basis of ion structure (i.e. apparent surface area, Å2) and m/z in the IM and MS dimensions, respectively. For example, in the analysis of complex biological samples, IM-MS approaches have demonstrated that specific m/z signals can be assigned to the molecular class to which they belong (e.g. lipids, peptides, carbohydrates, etc.). This assignment is based on the observation that molecules of different molecular class preferentially adopt structures which yield correlated collision cross sections vs. m/z. Within a specific molecular class, e.g. peptides, signals are predicted to occur only in a small region of conformation space. For over 600 singly-charged peptides that have been measured, over 98 % of these signals were found to occur within +/- 7 % of the average IM-MS correlation. This report describes the utility of high density and low surface area tags, for the selective labeling of specific amino acids or chemical functionality (sulfhydryl groups of cystine in these studies). Thus, the covalent tag-modification shifts the peptide signals to locations of conformation space that are not predicted to contain peptide signals. The selective tag consists of a chemically reactive end group, a linker, and metal-chelating moiety. The linker exhibits high specificity for lanthanide metals, which provides the desirable traits of high density and low surface area. Furthermore, different lanthanide metals can be coordinated with the tags which allow multiplexed labeling strategies to be used. For example, similar to isotope-coded affinity tag (ICAT) strategies to map the relative quantitiation of protein expression profiles of two samples, the present strategy is suitable for labeling multiple samples (e.g. at different points in the cell cycle) by utilizing either different lanthanides or isotopically enriched lanthanides, respectively. Using a suite of model cystine containing peptides, IM-MS shifts on average of >15 % are observed. The utility of this approach for tagging protein digestes for high-confidence level protein identification and multiplexed relative quantitation is described.

(504) Characterization of Dry Aerosol Particles and Solids using Desorption Electrospray Ionization and Electrospray-Assisted IR Laser Desorption Ionization Mass Spectrometry
Yohannes H. Rezennom1, Jianan Dong1, Kermit K. Murray1; 1Louisiana State University
We report direct analysis of dry aerosol particles and aqueous samples under ambient conditions. Dry aerosol particles dispersed into the air using a fluidized bed powder disperser and directed at an angle of 45º with respect to the skimmer cone of ion trap mass spectrometer. Ions are formed by interaction with an electrospray source held at an angle of 90º with respect to the particle flow and 45º with respect to the skimmer cone. To demonstrate this technique, samples of powdered caffeine and erythromycin were analyzed. In addition, mixtures of powders from real-world samples including artificial sweeteners, powdered beverage, and over-the-counter medications were characterized. Mass spectra obtained from the interaction of the electrospray with the dispersed particles show an intense peak from the protonated molecule or sodium adduct. In further developing particle-spray source, we
incorporated an infrared laser for desorbing droplets or neutral molecules from aqueous samples to take advantage offered by IR laser. In this setup, a stainless steel sample plate placed on an XYZ positioner was positioned in front of the ion trap mass spectrometer. A pulsed IR laser was directed at 45° with respect to the surface of the sample for desorption. Desorbed analyte droplets or molecules were continuously ionized using a nanoelectrospray source directed towards the orifice of the ion trap mass spectrometer. Standard aqueous peptides, proteins, and other real-world samples were characterized directly without sample pretreatment using this technique. The spectra obtained from these samples resemble multiply-charged ESI spectra.

(505) Elemental Determinations in Coal Fly Ash Samples by Glow Discharge and Inductively Coupled Plasma Spectrometry: An Integrated Approach
Alexandria M. Pavkovich1, Jennifer N. Robertson-Honecker2; 1West Virginia University

Increasingly, coal utilization byproducts (CUB) find wide application ranging from landfill lining to wallboard production. As the use of this material, CUB, increases so does concern over the potential environmental impact of toxic elements that it may contain at trace levels. The development of glow discharge plasma (GDP) and inductively coupled plasma (ICP) spectrometry methods for the trace element characterization of the most ubiquitous coal utilization byproduct (CUB), coal fly ash, is reported. The GDP source was coupled with time-of-flight mass spectrometry (ToF-MS) to provide direct determination of trace elements, whereas, ICP atomic emission spectrometry (AES) was employed with laser ablation for comparison. Each of these techniques allows direct determination of the elements of interest from solid state samples with minimal sample preparation. Preliminary results focusing on selected elements of interest are presented.

(506) Studying Industrial Water Quality by Corrosion & Scaling Index with Changing the Method of Microorganisms
Ehsan Bakhshi1, Fatemeh Abniki2; 1R&D Center of National Petrochemical Company; 2National Petrochemical Co.(Ghadir group)
The use of biocides in water cooling towers, specially in open recirculating systems to prevent problems arising from the microorganisms is an important subject. With the aim of removing non oxidizing biocides in these towers, a research project was started. During the 16 months period, sodium hypochlorite was injected in to the basins of cooling towers. During the 16 months period, sodium hypochlorite was injected to the systems. Production of sodium hypochlorite in the complex made its selection as a substitute for biocides, logical and economical.

(507) A New Type of Thermo-Associative Guanosine Gel
Yuehua Yu1, Darren Nakamura2, Kevin DeBoyance2, Bonnie Lyon1, McGown Linda1; 1Rensselaer Polytechnic Institute

Guanosine gels (G-gels) are self associated networks of guanine derivatives. The building blocks of these gels are “G-quartet” structures that are formed through Hoogsteen hydrogen bonding between four neighboring nucleobases. Further association of G-quartets results in formation of “G-wires” and at even higher concentrations, highly ordered cholesteric or hexagonal liquid crystalline gel phases. Although G-quartet structures are well known and studied, their understanding and applications are based on single guanosine derivatives or G-rich oligonucleotides. Here we introduce binary guanosine gels, or “G-gels”, that are formed in mixtures of hydrophobic guanosine (GUO) and hydrophilic 5’-guanosine monophosphate (GMP). Under appropriate conditions of GUO/GMP ratio, the binary G-gels exhibit interesting thermosassociative gelation properties. This property has been applied on cell growth. Circular dichroism (CD) spectroscopy, thermal melt experiments and fluorescence spectroscopy were applied to further understand the behavior.

(508) Using FT-IR and UV-vis Light Scattering to Examine the Effect of Tail Length on the Enthalpy of Bisurea Organogel Melting
Karla S. McCain1, Aaron M. Pierce1, Emily P.M. Kuo1, Paul E. Frederick1, Andrew J. Carr1; 1Austin College

Organogelators are low molecular weight molecules which self-assemble in organic solvents to produce solid-like materials and have potential applications in areas including safer petroleum product transportation and drug delivery. The bisurea organogelators used in this study contain two ureas separated by a six carbon alkane linker and contain four n-alkyl tail groups ranging from six to twenty-two carbons in length. The goal of this project was to better understand the relationship between organogelator molecular structure and organogel properties. The amide II band was used to determine the relative amount of hydrogen bonding between urea groups and the methylene bending region was used to determine the relative number of conformational defects in the n-alkyl tails. Previous work has shown that conformational defects in these n-alkyl tails, and thus their entanglement, are important for the formation of strong junction zones and solid gels. As organogelators melted, the amide II band showed a relatively sharp transition from hydrogen bound to non-hydrogen bound urea groups and the conformational defect bands showed a sharp decrease in the relative number of defects over the same temperature range. Because FT-IR methods were not precise enough to measure a change in the melting temperature with organogelator concentration, UV-vis light scattering was used to determine the enthalpy change for organogelator melting by the application of the Shroeder - van Laar equation. Changes in enthalpy were dependent on the number of carbons in the alkyl tail and were on the order of several hundred kJ/mol. These very large changes in enthalpy are attributed to the energy required to rotate C-C bonds in order to untangle the n-alkyl tails which hold junction zones together.
(509) Single Molecule Studies of Antibody-Antigen binding: The Potential for Highly Quantitative Multiplexed Biosensors

Jamshid Temirov1, Andrew Bradbury1, James Werner1; 1Los Alamos National Laboratory

Ultrasonic affinity (antibody based) biosensors with the capability of measuring multiple analytes simultaneously (multiplexing) are of great importance in disease diagnosis, biological warfare agent detection and drug discovery (especially development of therapeutic antibodies). We have been studying the binding of individual fluorescently labeled antigens to surface immobilized antibodies using wide-field fluorescence imaging. The fluorescence time history at an individual binding site is used to calculate a binding affinity. Our single molecule approach to biosensing could have distinct advantages, which include:- Since individual antigens are literally counted, these measurements are highly quantitative. Unlike Enzyme-Linked Immuno Sorbent Assays (ELISAs), there is no need for signal amplification (which introduces both noise and measurement uncertainty).- Fluorescent labeling of the antibodies and cross-correlated two-color imaging practically eliminates the non-specific binding to biosassay, as only antigens that are spatially co-localized with known antibody locations are counted.- As these single molecule affinity measurements are based upon kinetic properties (on/off times) and not total fluorescence intensities, they are not subject to limitations in dynamic range customary of most fluorescent methods.- A different antibody (that recognizes a distinct target) could be located in every 1 by 1 micron square of a surface, meaning that a 1x3 slide could have 10^9 different recognition elements. For a standard 100 by 100 micron field-of-view of a high NA microscope objective this still leads to potentially 10^4 different recognition elements imaged simultaneously.Here we report 2-D images of individual antibody-antigen binding events, fluorescence time history of these binding events and computation of a binding affinity distribution. This work is funded by Exploratory Research (ER) grant from the Los Alamos National Laboratory Directed Research and Development (LDRD) program (20050377ER).

(510) Selective Deposition of Metals on Nanopatterns of n-Alkylsilane Self-Assembled Monolayers

Jie-Ren Li1, Jayne C Garmo2; 1Louisiana State University

Metal and semiconductor nanomaterials exhibit quantized electrical and optical properties that can be applied in the design of future nanodevices. To achieve these prospects, it would be a great advantage to develop nanofabrication capabilities which not only provide nanoscale control of the geometry and arrangement of nanomaterials, but also enable control of surface chemistry and reactivity with spatial selectivity. We have developed new methods to produce nanopatterns of n-alkylsilane thin films with designed surface functionalities using particle lithography combined with vapor deposition. A close-packed film of monodisperse polystyrene latex or colloidal silica beads serves as an evaporative mask to direct the binding of silane self-assembled monolayers. The silane nanopatterns are then used as a foundation for the adsorption of metals. Either deposition of synthesized nanoparticles or electroless deposition was successful for constructing nanopatterned surfaces of metals such as gold, copper, cobalt and iron. The spacing between metal deposits can be tuned with different sizes of silane nanoparticles, which are determined by the diameter of the template particles. The thickness of the metal deposits can be controlled with chemistry parameters by changing the concentration of metal solutions and immersion intervals. The AFM views of hundreds of nanostructures produced by particle lithography display exquisitely uniform geometry and periodicity at the nanoscale. The high density and high throughput advantages of self-assembly can be used to rapidly manufacture tens of thousands of metal deposits with few defects, for areas spanning centimeters.

Compared to competing lithographic methods, our approach does not require expensive or complex instrumentation such as electron or ion beams, lasers, or UHV equipment. Instead, traditional bench chemistry approaches with centrifuging, drying, mixing, heating and rinsing are the simple steps needed for nanofabrication. Our results demonstrate that particle lithography is a reproducible and robust approach for manufacturing two-dimensional arrays of n-alkylsilane nanopatterns which can be used to selectively adsorb metals. Combining metal deposition and lithographic approaches offers a viable, practical and inexpensive alternative for fabricating nanostructures. The designed nanostructures may provide test platforms for surface properties measurements or as metal-molecule-semiconductor heterojunctions in molecular electronic devices.

(511) Near-Infrared Model for Quality Evaluation of Flax Fiber

Miryeong Sohn1, Franklin Barton, II1, Danny Akin1, David Himmelsbach1; 1USDA-ARS

We have been working on a near-infrared (NIR) calibration model for determining fiber and trash (shive) content in flax for several years. This is an extremely arduous task since there are no real reference methods for either assay. We created a reference method with pure samples of ground fiber and shive materials and developed a model. The NIR method was accepted as a standard test method by ASTM International in 2005. This is the first such chemometric assay developed for agricultural products with a spectral reference method. This paper will discuss the work for development and improvement of the robust calibration model, and for evaluation the equation transfer with various sets of new samples including multi-cleaned flax fiber.

(512) Structure Activity Relationship Studies of Synthesized Urea Diamides on CNS Depression and Sleeping Time Potentiation Effect

Ravikumar Modi1, Dhurbo Jyoti Sen1; 1Shri Sarvajanik Pharmacy College

The urea derivatives as barbiturates are closed ring trioxopyrimidene heterocyclic molecule whereas benzodiazepines have also closed ring biosisosteric azepine heterocyclic molecule consisting of two nitrogen atoms as hetero element possessing CNS depression activity. The proposed plan is based on the open chain urea derivatives having same number of nitrogen atoms in the synthesized molecule to show the CNS depression action either by individually and by synergistically with the reference standard of barbiturates as well as with benzodiazepines. Four series of compounds were synthesized by replacing the variable X as O=Oxygen and S=Sulphur to form the urea and thiourea derivatives of anthranilic acid as well as of p-amino benzoic acid and finally the free carboxylic acid of series-2 and series-4 were converted to the carboxamide. Compound-1: 2-carboxy-phenyl urea Compound-5: 4-carboxy phenyl urea Compound-2: 2-carboxamido-phenyl urea Compound-6: 4-amido phenyl urea Compound-3: 2-carboxy-phenyl thiourea Compound-7: 4-carboxy phenyl thiourea Compound-4: 2-carboxamido-phenyl thiourea Compound-8: 4-amido phenyl thiourea Now two different categories of compounds were formed at substitutions at 2 and 4 positions of the phenyl rings to produce total eight urea derivatives having open chain having free carboxylic and carboxamide functional groups. All the synthesized compounds were characterized by their m.p., solubility parameters for their polarity, elemental microanalysis by N% and spectral studies by UV, IR and NMR for structural confirmation. The acute toxicological studies of the compounds were done by determination of LD50 intraperitoneally by mg/kg dose in propylene glycol in 18 hours fasting mice and found that LD50 was as follows in between 400-
950 mg/kg, which shows that thio urea derivatives are more toxic than urea linkages and 2-substituted derivatives are lesser than 4- substitution as bond energy in ortho is higher than para substitution: Compound-1 < Compound-2 < Compound-5 < Compound-6 < Compound-3 < Compound-4 < Compound-7 < Compound-8. The CNS depression study of all the synthesized compound were carried out by administering intraperitoneally the various doses of the test compounds in mg/kg dose in 18 hours fasting male albino mice using propylene glycol as an inert vehicle. The loss of righting reflex and regaining of it was noted for each compound to determine the sleeping time. It has been found that all the test compounds have sleep inducing property due to the presence of urea/thio urea linkage and the urea/thio urea diamide derivatives were found longer duration of sleep inducing property due to the presence of two amide linkages and out of which the thio urea derivative and thio urea diamide derivatives showed lesser duration than urea and urea diamide linkage. Sleeping time potentiation effect was studied for the test compounds by using pentobarbitone as barbiturates and alprazolam as benzodiazepines on male albino mice. The 2-sustituted derivatives were found less active than 4- substituted derivatives due to the steric hindrance and ortho effect. All the observations were noted for four groups of mice and the bioassay result was tabulated after statistical parameters for significance of pharmacological screening: Student’s-t-test and P-value. All the test results were found significant to a high extent for the structure activity relationship studies of the synthesized molecules.

(513) Rapid Method for Determination of Identity and Potency of Pharmaceutical Materials by FT Raman Spectroscopy
Robert Forbes1, Michael Dotlich1, Donald Hodges1, Richard Kattner1, Elf Lilly and Company

Ft-Raman is evaluated as a technique for rapid quantitation of the potency of pharmaceutical materials while performing identification simultaneously. Solid samples are dissolved in an organic solvent and an FT-Raman spectrum obtained. The intensities of bands characteristic of the analyte are compared to a reference standard prepared and analyzed in the same way to generate a potency result. The Raman potency method was evaluated for a set of pharmaceutical samples. Linearity, specificity, precision, and accuracy were evaluated and compared to validation results obtained with HPLC methods for the compounds. The advantages and disadvantages of the Raman method versus HPLC will be discussed. Raman spectroscopy affords a rapid and relatively simple method for potency and identity determination.

(514) Depth Profiling using Time-Resolved Raman Spectroscopy with a Fast-Gated Intensified CCD Camera
Freek Ariese1, Marleen Kerssens1, Joost B. Buigs1, Cees Goojers1;
1Laser Centre Vrije Universiteit Amsterdam

Depth profiling is demonstrated in diffusely scattering media, making use of the time difference between Raman photons emitted from the top layer and Raman photons stemming from a deeper layer. Time-resolved detection is carried out with an intensified CCD camera that can be gated with a 300-ps gate width. Excitation is with a 3-ps frequency doubled Ti-sapphire laser at 400 nm; the repetition rate is 76 MHz. The test system is a 1-mm layer of powdered PMMA (first), and a 2-mm layer of fine trans-stilbene crystals (second). By gradually increasing the delay of the detector gate, photons from greater depths are collected. The net difference in path length between the two layers is 2 mm, which would in clear media correspond with 10 ps and which would be too fast for our detection system. However, because of the multiple-scatter effect the actually observed time difference between the intensity maxima of the first and second layer was 200 ps, and each layer could be probed selectively. The setup is relatively straightforward and easily implemented. The performance will be compared to that of other depth profiling approaches such as Kerr-gated detection.

(515) Development of a Submersible Raman Instrument for in-situ Analysis of Deep-Sea Hydrothermal Vents
Wesley J. Thompson1, Brian J. Marquardt1, Marvin D. Lilley2;
1University of Washington, APL; 2University of Washington, Oceanography

We have developed a submersible Raman instrument and successfully deployed it in one of the harshest environments on the planet. Hydrothermal vents can be located 2200m below the surface of the ocean at pressures of 300 bar and temperatures of 2-400 °C. Our objective in this endeavor was to create a robust commercial Raman instrument for in-situ analysis of the chemical species being released from these hydrothermal vents. The instrument consists of a custom designed high resolution, high sensitivity Raman instrument coupled to a Raman ballprobe immersion optic. These components were encased in a rugged aluminum pressure casing for deep submersion and coupled to an oil filled fiber optic cable assembly for mobility and analysis in the deep ocean environment. This instrument was successfully deployed using the Deep Submersible Vehicle, DSV/Alvin to multiple vent sites on the Juan de Fuca Ridge, an area of very active hydrothermal venting off the coast of Washington. Communication between the submarine and the instrument was conducted via a serial connection and an onboard computer in the instrument. This allowed for real time viewing of the data and changes to the collection technique of the instrument. A variety of both high (300 °C) and low (25 °C) temperature vents were sampled. Currently we are seeking to identify and quantitate the chemical species in the Raman data collected and redesign the instrument for multiple month deployment when connected to an underwater networked fiber optic observatory.

(516) Determining Ingredient Speciation in a Complex Laundry Product Matrix
Bridget Becker1, David Eike2, Michael Rotherg1, John Aiken1, William Laidig2, Bruce Murch2; 1HHC Analytical Sciences, P&G; 2Modeling and Simulation, P&G

In an endeavor to better understand the chemistry of liquid laundry products, we have developed a method to explore ingredient speciation in neat product. High viscosity, many chemical entities, and complex fluid behaviors are all examples of factors which complicate measurements in laundry product matrix. Boric acid, which evolves as a result of dissolving borax in water, is involved in multiple equilibria that encompass both self-association as well as association with other product ingredients. This paper will illustrate the results obtained by using multiple equilibrium calculations to simulate results of 1H and 1H NMR experiments. This method serves as a way to avoid large scale equilibrium constant determination in the complex product matrix with extensive equilibrium network among ingredients.

(517) The Legacy of Dr. Radu Mavrodineanu - Introductory Remarks
Jerry Messman, 1Stranaska Scientific LLC

The opening presentation of this honorary symposium provides a brief overview of the distinguished professional career and life of the late Dr. Radu Mavrodineanu, a renowned analytical scientist and spectroscopist of international reputation. In addition to his own personal commentary, the speaker will present contributed personal/professional remembrances and anecdotal memories of Radu Mavrodineanu on behalf of several of Radu’s close friends and scientific colleagues.
(518) The Spectroscopic Achievements of Radu Mavrodineanu

Robert Watters; 1NIST

Dr. Radu Mavrodineanu emigrated from Romania and started his work in the U.S. in the area of chemical uptake of plants. Fortunately for atomic spectroscopy, he turned his attention to flame spectroscopy and became world-famous by the time he wrote the definitive book, Flame Spectroscopy, Parts 1 & 3 in 1965. Radu joined the Analytical Chemistry Division of what was then known as the National Bureau of Standards (NBS) in April, 1969. There, he developed a special high accuracy spectrophotometer that could measure transmission data with known accuracy. The use of this instrument to develop several Standard Reference Materials (SRMs) for calibrating the photometric scale will be described in another talk in this session. In this presentation, Radu’s contributions to the field of spectroscopy including his work at collecting and editing key compendia of the time will be described.

(519) In Pursuit of Fluorescence Standardization – NIST Past and Present

Paul DeRose; 1NIST

For more than 30 years, NIST/NBS has played a leading role in the standardization of fluorescence. It built a high accuracy fluorescence spectrometer in the 1970s, which enabled the first, commercially-available, certified reference materials (CRMs) for fluorescence to be produced. NIST has continued to develop other CRMs to help meet the current needs of the fluorescence community. The development of past, present and future fluorescence standard reference materials (SRMs) by NIST will be discussed.

(520) Contributions of Radu Mavrodineanu to the NBS/NIST Standard Reference Materials Program

Thomas Gills

This paper provides personal commentary and insight into the scientific contributions of Radu Mavrodineanu to the NBS/NIST Standard Reference Materials Program.

(521) NBS/NIST Optical Filters Program

Melody Smith; 1National Institute of Standards and Technology

The Optical Filters program was initiated at the National Bureau of Standards (NBS) by Dr. Radu Mavrodineanu in 1970 with the construction of a reference spectrophotometer and the introduction of Standard Reference Material (SRM) 930, “Glass Filters for Spectrophotometry.” It continues in operation today at the renamed National Institute of Standards and Technology (NIST). Although Dr. Mavrodineanu generally followed an existing model pioneered by the British National Physical Laboratory in his design for the NBS High Accuracy Spectrophotometer (HAS) and in the selection of the initial SRM material, his personal stamp is evident in many features of the program’s infrastructure and its evolution under his guidance. Notable among reference material developments he led are SRM 2031 UV/visible transmittance filters and SRM 2034 for wavelength calibration. Well into its fourth decade, the program has largely fulfilled its original purpose of establishing accuracy benchmarks and quality control tools for commercial spectrophotometers used for chemical and pharmaceutical measurements. SRM production is being curtailed as comparable Certified Reference Materials (CRMs) become available in the private sector. The program continues to provide recertification of NBS/NIST SRM neutral density filters to support traceability to a recognized national scale for CRM suppliers and end users of SRMs or CRMs.

(522) The Legacy of Dr. Radu Mavrodineanu - Concluding Remarks

Jerry Messman; 1Stranaska Scientific LLC

The closing presentation of this honorary symposium provides unique insight into the legacy of the late Dr. Radu Mavrodineanu, a renowned analytical scientist and spectroscopist of international reputation. As a namesake tribute to the “founding father” of NIST’s contemporary high-accuracy spectrophotometry program, the speaker describes his company’s commemorative Vintage MAVRO Artifact Series and Recalibration Service. The establishment of the Radu Mavrodineanu Memorial Award for Analytical Metrology is also discussed.

(523) Construction of Microfluidic Networks using Thermoplastic Elastomer Gels

Victor Ugaz; 1Texas A&M University

Currently, poly(dimethylsiloxane) (PDMS) is one of the most widely used substrates for fabrication of microfluidic networks owing to a variety of favorable properties including optical and UV transparency, biocompatibility, gas permeability, and general ease of fabrication. While a number of rigid polymer materials have been investigated for use in microfluidic applications, there has been much less progress toward identifying viscoelastic substrates that could serve as alternatives to PDMS. In this paper, we explore fabrication of microchannel networks using thermoplastic elastomer gels consisting of polystyrene-(polyethylene/polybutylene)-polystyrene (SEBS) triblock copolymers in hydrocarbon extender oils for which the ethylene/butylene midblocks are selectively miscible. The insoluble styrene endblocks microphase separate into distinct domains with characteristic size scales on the order of 10-20 nm while the soluble midblocks interpenetrate into the oil to form a viscoelastic gel network that exhibits many of the same favorable properties as PDMS. But unlike PDMS where gels are cast by a chemical crosslinking process, thermoplastic elastomer gels are melt processable at temperatures in the vicinity of 100 °C. Melt processability allows microfluidic channels to be fabricated in minutes by simply making impressions of the negative relief structures on heated master molds. Multiple impressions to be made against different masters to construct complex geometries incorporating multi-height features within the same microchannel. Interconnected multilayered structures are also straightforward to fabricate owing to the ability to bond and seal multiple layers by briefly heating the material at the bond interface. Thermal, viscoelastic, and permeability properties can be tuned over a wide range through proper selection of gel composition.

(524) Polymeric Microdevices with Monolithic Columns for Bioanalysis

Adam Woolley1; Xiuhua Sun1; Weichun Yang1; 1Brigham Young University

Microfluidic systems have excellent potential to improve methods for biomolecular analysis. However, microchip devices have two disadvantages relative to conventional techniques: (1) the separation distance is typically shorter, so analysis of complex mixtures can be difficult; and (2) smaller amounts of sample are loaded, making detection of trace analytes challenging. We are working to address these limitations through the use of on-chip monolithic columns for sample cleanup and preconcentration in polymer microdevices. We have fabricated monolithic columns from glycidyl methacrylate (GMA) and ethylene dimethacrylate monomers, using cyclohexanol/dodecane as the porogen. In these monoliths, the GMA moieties provide reactive epoxy groups for covalent immobilization of affinity species like antibodies. Alternatively, the GMA groups can be reacted with an amine-containing compound (e.g., Tris) to provide a solid-phase...
ABSTRACTS

(525) Fabrication of Unconventional Microfluidic Chips: Within or Outside the Cleanroom?  
John Crabtree; Micralyne Inc.

Micralyne is a manufacturer of microfabricated components and has grown into one of the only private, independent and profitable OEM MEMS foundries in the world. Micralyne has collaborated on microfluidic research with numerous pioneers in the area over the last decade. MEMS and microfluidic devices made at our foundry are made from silicon, glass and quartz with traditional lithographic techniques. The presentation will examine the need for cleanroom facilities for the different fabrication steps involved in making microfluidic devices. First, a brief introduction to Micralyne will be given, showing examples of microfluidic devices we make, as well as the methods and equipment used to make them, both inside and outside the cleanroom. The body of the talk will focus on the rationale that substantiates costly cleanliness criteria, and evaluate its applicability to various device paradigms. Several specific device + application examples that have been investigated collaboratively with researchers at the Universities of Alberta, Calgary and Toronto as well as the National Research Council of Canada will be highlighted: plastic device microfabrication; SU-8/glass hybrid chips for DEP cell analysis; and acoustic jet machining as an effective microfabrication tool.

(526) Microfabrication in the Office  
Claudimir Lucio do Lago; Instituto de Quimica - Universidade de Sao Paulo

Despite the promising possibilities of microfluidics, the number of research groups around the world would be very small without the dissemination of alternative techniques for fabrication and use of microfluidic devices. Among a myriad of approaches, there is the laser printer toner, which can be used for patterning or as structural material. We anticipate that these new techniques will increase the accessibility and usability of microfluidic devices, both inside and outside the cleanroom. The body of the talk will focus on the rationale that substantiates costly cleanliness criteria, and evaluate its applicability to various device paradigms. Several specific device + application examples that have been investigated collaboratively with researchers at the Universities of Alberta, Calgary and Toronto as well as the National Research Council of Canada will be highlighted: plastic device microfabrication; SU-8/glass hybrid chips for DEP cell analysis; and acoustic jet machining as an effective microfabrication tool.

(527) Materials, Methods and Approaches to the Contact Liquid Photopolymerization-Based Fabrication of Polymeric Microfluidic Devices  
Christopher Bowman, Tommy Haraldsson, Robert Sebra, Brian Hutchison, Sirish Reddy, Neil Cramer, Kristi Anseth, Robert Davis; University of Colorado

Here, we will present results associated with the development and application of living radical photopolymerizations (LRP) for the manufacture of microfluidic devices (MFDs). The LRP method enables facile materials modification and dramatically improved layer-to-layer coupling within devices. This approach facilitates the development and manufacture of prototype devices in which it is possible to (i) fabricate complex three-dimensional devices, (ii) control surface chemistry in all three dimensions and with a wide range of well-adhered surface chemistries possible, (iii) fabricate complex fluid control elements including mixers, reactors, channels, valves, and pumps, (iv) manufacture electrical elements in three dimensions to control field and temperature, (v) synthesize devices that contain prefabricated elements or materials produced by other techniques, (vi) create thermally and chemically resistant ceramic devices by utilizing thiol-ene based polymer derived ceramic materials, and (vii) culture cells on microfabricated wells and modify surfaces with cell cleavable molecules. These developments have built a foundation through which our group and others can now fabricate complex three-dimensional MFDs that are suitable for a wide range of detection and analysis functions. Further, we have developed several new materials strategies, including the use of thiol-ene photopolymerizations that circumvent several other issues associated with photopolymerization-based microfluidic device manufacture. Here, we will present results associated with the device manufacture, materials design and the application of these prototype devices. Detection and analysis will focus on three-dimensional cell culture assays, antigen/antibody detection, cell type detection, and high sensitivity DNA microarray analysis.

(528) Digital Microfluidics Made Easy  
Aaron Wheelè; Mohamed Abdelgawad; Michael Watson; University of Toronto Department of Chemistry; Univ. Toronto Dept. Mechanical Eng.

Digital microfluidics (DMF) is a novel fluid handling technique used to transport discrete droplets of liquid across the surface of an array of electrodes. There is currently much enthusiasm for applying DMF to biochemical applications; however, it is currently used in only a few laboratories, world-wide. This is largely a function of accessibility: most researchers do not have access to the clean-room facilities that are required for device fabrication. Here, we present two new strategies, not requiring clean-rooms, for rapid prototyping of DMF chips: a micro contact printing-based approach, and another relying on printed circuit board (PCB) substrates. We anticipate that these new techniques will increase the accessibility of digital microfluidics, and will significantly expand the innovations and applications of DMF.

(529) Tuning Higher Hierarchal Nanopores in Anodic Aluminum Oxide  
Rashid Zakert; Punit Kohli; Southern Illinois University

Controlled template synthesis of anodic aluminum oxide is an area of extreme importance for many applications in nanoscience and nanotechnology. To date, most of the research has focused on creating linear hexagonally packed pores in alumina matrix. Controlling the formation of non-linear and branched nanopores would open up many new exciting opportunities in different areas including nano-device fabrication (nano-optics, nano-electronic and nano-fluidics), separation science, and medicine. We will present here a novel method of creating higher hierarchal nanopores such as
as multi-branched and non-linear pores in anodically grown alumina with controlled pore size, porosity and length. In this technique, we use simultaneous oxidation of a single aluminum substrate in two different electrolytes and/or applied potential that provides us handles to tune different processing parameters for alumina growth. Since properties of nanopores are strongly dependent upon electrolytes and voltages applied, we are able to tune the properties of nanopores by simultaneously adjusting the applied potential in different electrolyte solutions.

(530) Optical Spectroscopy of Plasmonic Au Spherical Nanoparticles
Seongmin Ma1, Jinhwa Heo2,3, Wangjoong Kim2, JaeTae Seo1, Qiguang Yang1, Bagher Tabibi1, Wansoo Yun2, Sungsoo Jung2, Sangwoo Han2, William Yu3; 1Department of Physics, Hampton University; 2Korea Research Institute of Standards; 3Department of Chemistry, Gyeongsang NatiDepartment of Chemistry, Rice University

The third-order nonlinear optical properties of Au nanoparticles (NPs) in water with ~21.5 nm size were investigated using Z-scan and degenerate four-wave mixing (DFWM) techniques in a surface plasmon resonant region. The absorption peak of Au NPs was around 526 nm, which was attributed to surface plasmon resonance. The nonlinear refraction and nonlinear absorption coefficients of Au NPs with concentration ~2×10-6 mol/m3 were ~1.2×10-9 m/W and ~1.69×10-16 m2/W at 532-nm wavelength and 6-ns pulse width using the closed and open aperture Z-scan techniques, respectively. The polarization- and concentration-resolved DFWMs were utilized to evaluate the cubic nonlinearities of Au nanomaterials. The cubic nonlinearities with parallel and orthogonal excitations were estimated to be ~5.3×10-21 – 2.41×10-21 m2/V2, and ~0.34×10-21 – 1.98×10-21 m2/V2, respectively, for various concentrations of Au NPs ~6.51×10-7 – 2.55×10-6 mol/m3. The average hyperpolarizabilities of Au NPs were extracted to be ~3.60×10-40 m5/V2 and ~2.52×10-40 m5/V2, respectively from the cubic nonlinearity as a function of concentration. The origin of optical nonlinearity is mainly from the electronic process of surface plasmon bleaching effect.

(531) CTAB Stabilized Cubic and Spherical Gold Nanoparticles as Highly Sensitive Extrinsic Raman Labels for SERS Readout in Sandwich Immunoassays
Radha Narayanan1, Robert Lipert2, Marc Porter1; 1The Biodesign Institute, Arizona State University; 2Ames Laboratory, Iowa State University

This presentation describes results from the first application of particle shape in the construction of Extrinsic Raman Label (ERLs) in sandwich immunoassays. ERLs, applied in the last step of the assay, are sensitive tags for captured antigens, with detection limits at low femtomolar levels in early disease detection (cancer biomarkers) (1) and bioterrorism prevention (viruses) (2). The findings herein compare the detection limit obtained for ERLs based on standard spherical citrate capped gold nanoparticles (sp-cit-Au) with those for CTAB-stabilized spherical (sp-CTAB-Au) and cubic gold nanoparticles (cu-CTAB-Au) in the SERS readout for human IgG protein. With respect to sp-cit-Au, the detection limit is 41 times lower with sp-CTAB-Au and 336 times lower with the cu-CTAB-Au. These findings, along with assessments of underlying factors that contribute to these differences, will be discussed.(1) D. Grubisha, R. Lipert, H.Park, J. Driskell, M. Porter, Anal. Chem. 2003 75, 5936.(2) J. Driskell, K. Kwarta, R. Lipert, M. Porter, J. Neill, J. Ridpath, Anal. Chem. 2005, 19, 6147.

(532) Redox Chemistry of HPLC Purified Single-Stranded DNA Encased Single-Walled Carbon Nanotubes
Xiaomin Tu1, Wei Zhao1,2; 1University of Arkansas Little Rock

Intensive research is being done on exploiting efficient separation techniques for single-walled carbon nanotubes (SWNTs) with defined chirality. The development of chromatographic separation of has made a breakthrough in purifying SWNTs according to the single electronic types. Ion-exchange chromatography (IEC) can separate SWNTs by their metallic or semiconducting nature, while size-exclusion chromatography (SEC) is able to isolate SWNTs via their lengths. However, there is limited work on the chemical properties of purified SWNTs. In our previous work, we found that pre-HPLC purified ss-DNA-SWNTs are optically sensitive to hydrogen peroxide (H2O2). Here, we found that the redox properties of HPLC purified ss-DNA-SWNTs change dramatically and become insensitive to H2O2. However, with addition of AgNO3, the reaction can be reactivated. On the other hand, the purified nanotubes remain the reactivity with iodine and a reversible reaction behavior is observed. The investigation foretells the importance of the surface functionalization on the tunable redox properties of SWNTs and affords insights for the development of a versatile class of SWNT-based optical sensors.

(534) Surface Sampling Probe and Desorption Electrospray Approaches to Mass Spectrometry-Based Chemical Imaging of Tissue Sections
Gary Van Berkel, Vilmos Kertesz,1 Oak Ridge National Laboratory

Several new sampling/ionization techniques have emerged that enable the sampling and ionization of analytes from surfaces under ambient conditions with subsequent mass spectrometric interrogation of the ions. Two of these techniques under study in our lab are the liquid microjunction surface sampling probe (SSP) and desorption electrospray ionization (DESI). Each of these analysis techniques presents the possibility to spatially resolve the distribution of different molecules in/on a surface. In this presentation the basics of these two techniques for imaging will be covered and issues such as read out resolution, analysis time, analyte ionization specificity, etc., will be examined. Imaging of endogenous and dosed small molecules in organ and whole body tissue sections will be emphasized.

(533) Mass Spectrometric Imaging and Profiling of Single Cells and Tissues
Stanislav S. Rubakhin1, Jonathan V. Sweedler1; 1Beckman Institute, University of Illinois

Chemical imaging has been propelled by rapid technological advances within the past decade that now allow the investigation of tissues and cells with unprecedented chemical information content, limits of detection, dynamic range, and spatial resolution. This progress is certainly notable in the field of mass spectrometry imaging (MSI) where two-dimensional and three-dimensional maps of vast numbers of molecules and atoms located in tissues and organ systems can be generated. Peptides and proteins present in the brain are among the compounds studied by MSI and specifically by matrix-assisted laser desorption/ionization mass spectrometry imaging (MALDI MSI). Driven by the needs of biomedical research, MALDI MSI has become a fully developed subfield of chemical imaging with its own specialized approaches, instrumentation and software, as well as sample preparation and signal acquisition methods. Despite the significant progress in development of MALDI MSI, there are several challenges currently facing this methodology in achieving high throughput analyses and analyses at single cell resolution. Single cell spatial resolution can be important for probing samples made up of the mosaic of biochemically and functionally heterogeneous cells in the nervous system. To address these challenges, we are developing a new
strategy which integrates several approaches. This strategy includes investigation of nervous tissues specimens with MSI, followed by high throughput MS profiling of the samples prepared using the stretched sample array method, and, after determination of regions of interest, isolation and investigation of individual cells and subcellular structures with single cell MALDI MS. Such integration of MSI, MS profiling and single cell MS methods forms a flexible and powerful analytical platform which increases the chemical information content of measurements and improves their effective spatial resolution. Our newest achievements using this strategy for investigation of cell-cell signaling in the nervous system are described.

(536) Atmospheric Pressure IR-MALDI imaging of Metabolites
Akos Vertes1, Yue Li1, Bindesh Shrestha1, Peter Nemes1; 1George Washington University
Most cells and biological tissues are rich in water. Thus, they are amenable to laser ablation at ~2.94 µm, the absorption band of OH vibrations. The ablation process exhibits two partially overlapping phases. During the first ~1 µs, a dense plume develops as a consequence of phase explosion in the target. This plume contains ions, neutrals and some particulate matter, and exhibits a shock front at the plume-air interface. Its expansion is slowed by the pressure of the background gas (air), so it eventually comes to a halt and collapses back onto the target. The second phase is induced by the recoil pressure in the target and results in the ejection of mostly particulate matter. Depending on laser fluence and target properties, this phase lasts for up to ~300 µs. We followed two strategies to harness these two ejection modes for analytical applications. First, we extracted ions from the initial plume by an external electric field and pulsed dynamic focusing. This enabled atmospheric pressure (AP) infrared (IR) matrix-assisted laser desorption ionization (MALDI) analysis of biological specimens and in vivo investigations of plants in both positive and negative ion modes. Unknown metabolite ions were identified using tandem mass spectrometry and collision activated dissociation. This AP IR-MALDI approach exhibited a high mass limit of 1,000 to 2,000 Da. In the second approach, we utilized the neutral species and particulate matter produced during later phase of IR laser ablation through a post-ionization strategy. Intercepting the ejected particulates with an electrospray plume gave rise to abundant ions and enabled the detection of large proteins (e.g., human serum albumin with a molecular weight of 66,556 Da) and other species directly from biological samples. This method, termed laser ablation electrospray ionization (LAESI), showed electrospray-like ionization, producing a series of multiply charged ions. LAESI yielded excellent ion signal and enabled the in vivo profiling of a petite marigold seedling with minimal damage. We demonstrated that both AP IR-MALDI and LAESI were capable of imaging and depth profiling of biomedical samples with substantial water content. They provided complementary information on the composition of the ablated target.

(537) Designing Nanoparticle Matrices for Enhanced Selectivity in Imaging Mass Spectrometry
David H. Russell1, Stacy D. Sherrod1, Edward T. Castellana1; 1Department of Chemistry, Texas A&M University
We are designing novel laser desorption ionization (LDI) matrices and developing laser patterning strategies to improve spatial resolution, increase sensitivity, and elevate throughput in imaging mass spectrometry. Our matrix design efforts have focused on the use of gold nanoparticles (AuNPs) which can be tailored through surface chemistry to provide both selectivity and enhanced ionization capabilities. We have demonstrated that optimum matrix to analyte ratios for AuNP are very different from that for MALDI, and that conjugated AuNP offers an added element of selectivity, i.e., analyte pull down capabilities, targeted binding to cell surfaces. The imaging MS system under development in our laboratory utilizes spatially dynamic laser patterning. The laser patterning optics consists of three major components: beam conditioning optics, a digital micromirror array (DMA), and an imaging lens system. The beam conditioning optics expands, homogenize and collimate the laser beam, thus optimizing the beam profile that is incident upon the DMA. Individual mirrors in the digital micromirror array are addressed by software to be either in an “on” or “off” state depending on the uploaded pattern. Laser light reflected from individual mirrors in the DMA is focused on the sample plate by the imaging lens system resulting in a patterned image. This arrangement provides a rapidly adjustable ionizing beam for the LDI experiment, and the LDI irradiation can be rapidly (~16 us) patterned into regular or complex shapes of variable dimensions. The union of these two technologies allows for the selective targeting and analysis of desired analytes from complex samples in a high throughput label free fashion. By using selective nanoparticles in imaging mass spectrometry, one can both screen for known and hunt for unknown biomarkers of disease in tissue biopsies. No other single instrument platform provides the capability for spatially selective molecular studies of complex samples in biomedicine today.

(538) A Minimalist Approach to Imaging Lipids and drugs in Rat Brain Sections, its Rewards and Pitfalls
Amina Sarah Woods1, Jeremy Post1, Shelley Jackson2; 1NIDA IRP, NIH
Lipidomics is the new frontier in biomolecular structural studies. Not only are lipids the main components in membranes that define the contours of the cell and its organelles, they also form stable noncovalent complexes with proteins and organic biomolecules such as drugs, are a storage depot for many therapeutic compounds and certain types of organic molecules and play an important role in signaling. To study lipid composition and distribution, complex and time-consuming techniques are used. However, recent advances in mass spectrometry, mainly matrix-assisted laser desorption/ionization (MALDI) have made it possible to directly probe tissue to study structural components, drugs localization and biomolecules distribution. Direct tissue imaging is a powerful tool as it gives a more complete and accurate structural picture and can trace and follow where drugs localize in tissue with minimal anatomical disruption and a minimum of manipulations. Hence, we believe that in addition to its accuracy and efficiency, this new approach will lead to a better understanding of physiological processes as well as the pathophysiology of disease.

(539) Biomolecular MS Imaging with Ion Mobility-Mass Spectrometry: Imaging IM-MS Strategies
John A. McLean1; 1Department of Chemistry, Vanderbilt University
In contrast with optical imaging methodologies, imaging MS provides a highly multiplexed means for generating unique images corresponding to the spatial coordinates of each analyte present in the sample on the basis of mass. However, selective MS images are challenging to obtain in cases where multiple endogenous species may occur at isobaric m/z, or in congested regions of the mass spectrum (e.g., for low molecular weights). Two-dimensional post-ionization separations using imaging ion mobility-MS (IM-MS) provides a means for overcoming these limitations by dispersing specific signals in conformational space on the basis of ion-neutral collision cross section (i.e., apparent surface area) vs. m/z. Advantages of the imaging IM-MS approach include: (i) qualitative identification of the analyte molecular class, (ii) separation of chemical noise from the analytes of interest, and (iii) enhanced concentration dynamic range by attenuation of ion suppression.
effects in the TOFMS source. A present challenge to IM-MS approaches is the concomitant increase in data handling capabilities that accompanies the additional IM separation dimension. The present state-of-the-art and future directions for imaging mode IM-MS instrumentation and emerging biological and pharmaceutical applications will be addressed.

(540) The Effect of the Sampling Cone on Ion and Atom Distributions in an ICP-MS
Paul Farnsworth1, Haibin Ma1; 1Brigham Young University
Lehn et al. have demonstrated that the sampling cone of an inductively coupled plasma mass spectrometer causes significant changes in the plasma several mm upstream from the sampling cone [1]. The quantitative scattering measurements reported by the Hieftje group give detailed information through selected plasma cross sections, but do not provide a comprehensive spatial picture of how the sampling cone is affecting the plasma. In this paper we will present comparisons of analyte density images collected in the presence and in the absence of the sampling cone. The images were collected using planar laser induced fluorescence. The comparisons will include images of ground-state atom density, ground-state ion density, and excited state ion density under a range of plasma operating conditions. [1] S. A. Lehn, K. A. Warner, M. Huang, G. M. Hieftje, Spectrochimica Acta Part B, 57B (2002) 1739-1751

(541) Progress in Laser Ablation ICP-MS: From Fundamental Intrigue to Routine Applications
Richard E Russo1, Jhans Gonzalez1, Sy-Bor Wen1, Xianglei Mao1; 1Lawrence Berkeley National Lab
Laser ablation ICP-MS has been studied for over 30 years with tremendous gains in our understanding of the fundamental processes. Coupled with the advances in instrumentation, LA-ICP-MS now can be used for many routine chemical analysis applications. The benefits of real time direct solid sampling without chemical dissolution justify the long term investment to bring this technology to fruition. Once troublesome issues like fractionation, for the most part, can be mitigated by the use of appropriate standards, as required for all analytical technologies. The use of UV wavelengths and short laser pulses (nanosecond to femtosecond) relaxes matrix matching, as well as allows absolute detection sensitivity on the femtogram level and micron spatial resolution. The talk will provide a general overview of current fundamental research in the laser ablation with an example of general applications.

(542) Fs-LA-ICP-MS – Towards Solid Sample Analysis without Matrix Matched Standards
Niemax Kay1, Helmut Lindner1, Carmen Cecilia Garcia1, Joachim Koch1; 1ISAS – Institute for Analytical Sciences, Dortmund
There are three Achilles heels in laser ablation ICP-MS for accurate analysis of solid samples, namely (i) possible changes of sample composition due to fractional evaporation from the laser crater, (ii) mass losses during the transport of laser generated particles, and (iii) incomplete atomization of particles in the ICP. Fractional evaporation may affect the analysis of volatile elements and occurs particularly if the laser is producing melt in the ablation process. Transport losses by diffusion and inertial effects are increasing the risk of systematic errors because the element composition of laser produced particles is often strongly dependent on particle size. Finally, the particles transported into the ICP should not be too large since incomplete, i.e. fractional, atomization can also be a source of error. It will be demonstrated that these effects have to be taken into account, in particular, if the pulse lengths of the lasers are long. Systematic investigations of particle production, characterization and transport at femtosecond laser ablation (fs-LA) of solid samples have revealed exceptional advantages versus sampling with longer laser pulses in LA-ICP-MS. It has been shown that heat transfer to the sample is very small at pulse lengths < 1 ps and fractional evaporation can be neglected. Furthermore, the particles are very small. The main part of the ablated mass is represented by particles with diameters between 5 and 500 nm which can be transported over large distances without significant losses. Particles of such size are usually also small enough to be completely atomized in an ICP. The considerable advantages of fs-LA over ablation with longer laser pulses have been demonstrated by measurements of the mass transport efficiency and the elemental composition of all transported particles, as well as by analyses of minor and major elements applying fs-LA-ICP-MS.

(543) Aerosol and Particle Sample Introduction and Vaporization for ICP-MS
John Olesik1, Josh Dettman1, Noel Casey1; 1The Ohio State University
Aerosol generation from solutions or laser ablation, transport into the ICP and vaporization in the ICP remain incompletely understood, with potentially huge implications on practical analysis. For solution samples, we will focus on the fundamental processes that control sample aerosol transport at small sample flow rates (< 50 uL/min), evaporation prior to entering the ICP and conversion to ions in the ICP. The effect of the spray chamber on transport efficiency, ICP loading, sensitivity and band broadening for sub microliter sample flows will be discussed. For solid samples, laser ablation sampling and subsequent vaporization of particles in the ICP will be considered. New insight from time resolved signals produced from single laser pulses and from individual vaporizing particles will be described.

(544) Insights into Excitation Mechanisms and Matrix Effects in ICP-AES
George Chan1, Gary M. Hieftje1; 1Department of Chemistry, Indiana University
Despite assertions of some manufacturers and the belief of many users, matrix interferences are common in ICP-AES and are likely responsible for errors in reported concentrations of 20% or more. There are three basic kinds of matrix interference: those arising in the sample-introduction process, those that happen in the plasma, and those stemming from spectral overlaps. Many procedures have been devised for coping with matrix interference, revealing that at least some users recognize the problems they cause. The most common such methods are matrix matching, standard additions (spiking) and internal standardization. Unfortunately, all require extra sample handling (thereby increasing the likelihood of contamination), at least some prior knowledge of the approximate sample composition, and all compromise full multielement analysis. What would be ideal is a technique that can detect the presence of an interference when it exists, so these extra steps are taken only when they are necessary. Such a technique should ideally also not require that dopants or other reagents be added to the plasma in order to provide the warning signal. They should also not require specialized diagnostic instrumentation. Instead, the flag should arise either from plasma signals or those intrinsic to each sample; it should also be available from emission signals acquired from commercial ICP-AES instrumentation. Lastly, the warning signal should itself be amenable to use in correcting the interference directly, again without extra steps, specialized instrumentation, or the addition of reagents. In this presentation, several potential diagnostic flags, derived directly from ICP emission signals, will be evaluated. In diagnosing plasma-based matrix interferences, they are understandably tied to the mechanism by which atoms are ionized and excited in the ICP. One of the diagnostic flags, in particular, will be shown capable of signaling
the presence of matrix interferences that arise in the plasma, in the sample-introduction process, or from spectral overlap. The same approach can also be used to correct for many matrix interferences, without time-consuming and troublesome additional measurements or apparatus.

(545) Photographic Studies of Laser Ablation ICP-MS
R.S. Houk¹, Dan Zamzow¹, Stan Bajie¹, David Baldwin¹; ¹Ames Lab USDOE
High speed movies with a fast framing rate are obtained for particles traveling through an ICP. This paper follows the fate of particular large particles. Vaporization, atomization and ionization events can be seen visually from emission of yttrium, calcium and other elements. Effects of laser type, characteristics of the original solid sample (e.g., particle size in pellets), use of helium or argon carrier gas, and particle size selection will be presented.

(546) Pharmaceutical Raw Materials ID Utilizing a Hand-Held Raman Spectrometer
Michael Longmire¹, Brent Kuckkam¹, Gary Thomas¹; ¹Eli Lilly and Company
With guidance and encouragement from the FDA, pharmaceutical manufacturers are increasingly relying upon the concepts of Quality by Design (QBD) and Process Analytical Chemistry (PAT) for a risk-based approach to quality manufacturing. The foundation of this approach is an in-depth understanding of the critical parameters in the process that must be controlled and measured. Control and analysis of raw materials, solvents, and starting materials is of critical importance and is typically an area of much less emphasis because the analyses are often time-consuming or lack specificity. Technologies such as Raman and Near Infrared (NIR) spectroscopy offer enhanced specificity with minimal or no sample preparation. Raman offers the additional advantage that portable, robust, hand-held systems are commercially available for use in remote locations. This presentation will describe a strategy for identity screening of incoming materials for pharmaceutical manufacturing, in which the analyses are conducted with a hand-held Raman spectrometer, in the warehouse or loading dock. This approach offers improved release time of materials while maintaining necessary quality.

(547) The Application of Variable Filter Array (VFA) Mid-Infrared Spectrometers in Process Monitoring
Sandy Rintoul¹, Dylan Wilks¹; ¹Wilks Enterprise, Inc.
Mid-IR Fourier Transform spectrometers (FTIR) are widely used in quality control laboratories for many applications related to process management. However, these instruments tend to be large and environmentally sensitive and are typically not suited for installation onsite or along process streams. Fixed wavelength, IR filter analyzers have been used both in-line (i.e. beverage monitors) and at line (i.e. hydrocarbon-in-water analyzers) for many years. The recent introduction of linear variable filters (LVF) and mid-IR detector arrays allow for a spectral range to be analyzed much like an FTIR. With an active measurement area of 12.8 x ½ mm coupled with the detector array for a total size of 22 x 22 x 4 mm, a mini spectrometer greatly broadens the applicability of mid infrared analysis for process monitoring. Adding a source, sample stage and electronics, the total package size can be under 12 x 16 x 4 cm. The additional advantage of having no exposed air path or moving parts allows for operation in rugged plant environments. Specific applications of VFA spectrometers such as alcohol in wine and gasoline, biodiesel in diesel fuel, trans fatty acid in vegetable oil and others will be described in detail. With a simplified computer interface, displays can be modified for a specific application to make it friendly to non-technical operators by giving either a numeric readout or a pass/fail message.

Robert G. Messerschmidt; ¹Aspectrics, Inc.
Encoded Photometric Infrared Spectrometry (EP-IR) is a new way of encoding and multiplexing wavelengths for vibrational spectroscopy. It allows instrument designs that are much more rugged than those employing a classical Michelson type interferometer. In an FT-IR, wavelengths are encoded interferometrically by moving a mirror precisely over a linear distance of several millimeters. Small errors of movement, on the order of a fraction of a wavelength, can cause considerable loss of contrast, and SNR. In EP-IR, the modulation of light is accomplished with an encoding disc that is orders of magnitude less sensitive to positional errors. This disc rotates rapidly, encoding up to 100 complete spectral records per second. Just like in FT-IR, the spectral waveform hitting the detector is the Fourier transform of the spectrum. This is a key advantage, since all of the well-developed Fourier processing methods can be used with EP-IR. In this paper, an analysis of the benefits of EP-IR in a series of industrial applications requiring ruggedness and compactness will be shown.

(548) Portable Rapid-Scan FT-IR Spectrometer using Translational MOEMS Mirrors
Martin Kraft¹, Werner Scherf², Thilo Sandner², Harald Schenk², Andreas Kenda¹; ¹CTR Carinthian Tech Research AG, Villach, Austria; ²Fraunhofer IPMS, Dresden, Germany
Portable spectrometers, mostly based on gratings in combination with detector arrays, are available up to the near-IR. Yet, this technology is not a viable solution for the mid-IR. One grating can cover only a part of the mid-IR and suitable detector arrays, if available at all, are costly. FTIR spectrometers thus remain the standard. To be suitable for on-site application, an FT spectrometer would not only have to satisfy the spectroscopic requirements but also need to be compact, robust and preferably cost-effective. FT spectrometers are typically rather bulky and vulnerable against shock and vibrations, due to the moving mirror. Designing fully portable FT-spectrometers would now require replacing the inert scanning mirrors with something both smaller and less susceptible to external influences. These requirements can be met by resonantly driven translational micro-opto-electro-mechanical (MOEMS) mirrors developed by the Fraunhofer IPMS. The MOEMS mirror used in the initial experiments was a 2mm² rectangular mirror element suspended on two springs. Electrostatically driven by voltages less than 50V this device is capable of a resonant sinusoidal forward-backwards oscillation in the kHz range with mechanical amplitudes up to ±100µm. The resulting prototype covers a spectral range of 4500 1/cm to 1500 1/cm at a spectral resolution better than 30 1/cm. A new micro-mirror design using a bearing spring layout has a circular mirror area of 7mm² with an amplitude exceeding ±200µm, allowing to build FT spectrometers with spectral resolution better than 16 1/cm. Based on a classical Michelson layout and equipped with a three-stage Peltier-cooled MCT detector, the resulting spectrometer prototype has a footprint of 150x120x100mm³ and a weight less than 1.5 kg. At a mirror modulation frequency of e.g. 950Hz, a 1000 scan spectrum can be acquired in about one second. This allows acquiring spectra with signal-to-noise characteristics comparable to many standard laboratory spectrometers. Foreseen applications include (process) analysis of major and minor components, exploiting the compact size, low weight and good robustness of these instruments. A second application field is high-speed reaction monitoring, making use of the rapid scanning capabilities and ms time resolution of the instruments.
(550) Bring the Spectrometer to the Sample - Plastics Identification Using a Handheld NIR Spectrometer

Frederick Haibach1, Klevisha;2 Polychromix

New technologies have allowed miniaturization of spectrometers. Smaller spectrometers provide instrument manufacturers opportunities for component integration, as well as reductions in weight and power consumption. Miniaturization, together with onboard spectral interpretation (libraries, chemometric models) results in an analyzer that provides customers with new applications and new opportunities for optimizing workflows. NIR has long been seen as a solution for materials identification challenges in plastic recycling. Identifying and sorting material can turn waste into a high value product. Most waste material has a poorly documented or even unknown history. Carpet fiber, one source of recyclable material, is relatively straightforward. Most carpets are made of one of a few plastics. Contamination presents the greatest non-material variation. The environment is demanding on handheld instrumentation, simple result presentation, robust chemometric models, rapid analysis and immunity to shock are critical requirements. NIR has not been used at the recycling collection point to identify plastics. Handheld instruments provide a nearly instantaneous assessment of the material. The analysis, in contrast to carpet, is a much more complex problem. Samples of a single material may vary in size, shape, and adjuvant content. The reliability of different types of NIR spectral identification will be discussed in this context.

(551) MEMS-scale Photoacoustic Sensor Using a Interband Quantum Cascade Laser

David Heaps1, Paul Pellegrino1; Army Research Laboratory

Photoacoustic spectroscopy is a useful monitoring technique that is well suited for trace gas detection applications. A sensitive and compact differential photoacoustic method for trace gas measurements is proposed. The technique possesses favorable detection characteristics which suggest that the system dimensions can be scaled to a micro-system design. The objective of present work is to incorporate two strengths of the Army Research Laboratory (ARL), Interband Quantum Cascade Laser (ICL) source development and chemical and biological sensing into a monolithic micro-electromechanical systems (MEMS) photoacoustic trace gas sensor. Previous data have shown that reducing the size of the photoacoustic cell can produce a very sensitive sensor using a CO2 laser. Recent work has shown that with further reduction in the size of the photoacoustic cell in combination with an ICL as the source produces favorable detection limits for Dimethyl Methyl Phosphonate (DMMP) a precursor to a nerve agent. These studies involve the incorporation of an ICL source operating at ~3.45 μm. This experimentation is expected to culminate in the creation of an extremely versatile MEMS photoacoustic sensor.

(552) Raman Spectroscopy for Characterization of Fatty Acid Composition in Foods

Nils Kristian Afsæth1, Vegard Herman Segtman1, Brian Marquard2, Jens Petter Wold1; Matforsk - Norwegian Food Research Institute; CPAC - Center for Process Analytical Che

There is an increasing interest in methods for rapid and reliable characterization of the fatty acid composition of fish and meat products. In the food processing industry there is a need for rapid characterization of raw and end products in order to meet increasing consumer demands of food labeling. And in the field of animal sciences rapid methods for characterizing fatty acid profiles would be beneficial both in breeding programs and in the control of the effects of different feeding regimes. Raman spectroscopy has been recognized as a promising tool for rapid and non-destructive analysis of food systems, and the technique has shown its feasibility in the fat compositional analysis of fats and oils. There are, however, few studies dealing with Raman and the characterization of fatty acid composition of adipose tissue of fish and meat, and the present talk will focus on the potential of using Raman spectroscopy to characterize fatty acid profiles of fish and meat products. Through Raman studies on food matrices like salmon adipose tissue and minced salmon muscle the feasibility of Raman spectroscopy for the characterization of fatty acid unsaturation and other average fatty acid parameters will be illustrated. The potential of using Raman spectroscopy for prediction of single fatty acids will also be addressed.

(553) FTIR Microscopy as a Tool to Investigate Protein Secondary Structural Changes in Muscle Food Tissue

Achim Kohler1,2, Hanne Bertram3, Ulrike Böcker2,1, kaksun Carton1,2, Zhiyun Wu4, Ragni Ofstad1; Matforsk, Norway; University of Life Science, Norway; Danish Institute of Agricultural Science

Department of Food Technology, Spain


(554) Representative On-Line Sampling of Heterogeneous Products by NIR Transflectance Imaging

Jens Petter Wold1, Vegard Segtman1, Martin Høy1; CPAC - Center for Process Analytical Chem

Most solid foods are heterogeneous in some way. There are typically three main types of heterogeneity encountered in foods: 1. Random region heterogeneity, 2. Layer heterogeneity, and 3) Gradient heterogeneity. In quality analysis and process control we are normally more interested in the bulk composition of a batch of food or a discrete food product, than in the local chemical characteristics achieved by a point measurement. Thus, the way we choose to approach a heterogeneous food sample with our spectroscopic device, is crucial for the relevance of the measurement. In general, we need to measure as much as possible of the heterogeneous sample in order to get the best estimate of the true average content of the analyte. In this presentation we describe how non-contact VIS/NIR transflectance measurements is combined with multi spectral imaging to obtain representative sampling of very heterogenous samples. This technology allows
relatively deep penetrating optical sampling as well as large flexibility in spatial sampling patterns and calibration approaches. Practical examples will be given for fish fillets, meat trimmings, as well as packed products. Aspects connected to optical properties of the material, how deep we are actually measuring, and robust calibration regimes between multispectral images (X) and continuous varying analytes (y), will be discussed.

(555) Multivariate MR Imaging for Fruit Quality Assessment
Rebecca Milczarek1,2, Michael McCarthy1,2; 1University of California, Davis; 2Center for Process Analytical Chemistry
In-line assessment of external fruit quality using machine vision is a mature field, but assessment of internal fruit quality at production line speeds has only recently become feasible. Advances in magnetic resonance imaging (MRI) hardware have facilitated this development. However, optimal use of MRI in a process environment is an open problem. To work toward optimization in a fruit sorting application, the chemometric technique of multivariate image analysis was performed with a data set of MR images of mandarin oranges. The goal of the sorting process is to separate seeded and unseeded fruit, so the image parameter of interest was contrast between seeds and pulp. Congruent images of seeded fruit were obtained using a Turbo Fast Low Angle Shot (FLASH) imaging sequence on a 1 Tesla industrial-grade system. Inversion time was varied at 15 levels, from 100 ms to 1500 ms, holding all other scan parameters constant. The resulting image data set was analyzed with Principal Components Analysis (PCA). Separation between seeds and pulp was seen in the first three principal components; the loading patterns on these principal components indicated that an inversion time of 500 ms resulted in the highest contrast between seeds and pulp. This work demonstrates that multivariate image analysis is a valuable objective tool for optimization of scan parameters in MRI. The technique will enable optimal use of MRI in a processing environment.

(556) Estimation of Pure Profiles with ICA, MCR and PARAFAC - Applications on NIR and Fluorescence Spectra from Food Systems
Frank Westad1,2, Jens Petter Wold2; 1CAMO Software; 2ABBON AS; 3Matforsk
One of the common objectives in data analysis is to extract "pure sources" from a complex set of signals, e.g. how to find the pure spectra from a number of objects with mixtures of the chemical compounds. Principal Component Analysis (PCA) is often applied in chemometrics for exploratory data analysis, and is sometimes combined with a rotation of the axes to interpret underlying structures, e.g. Varimax. However, the extraction of pure and statistically independent spectra from a set of mixtures can not be expected by the use of PCA. Independent Component Analysis (ICA) has the past years drawn attention due to the potential to extract components that are independent, so-called “blind source separation”. Such applications range from NIR spectroscopy, processing of medical signals, and compression of images. ICA attempts to recover the original signals by finding a linear transformation that provides statistical independence between the sources, under the assumption that the data does not follow a Gaussian distribution. By the use of higher-order statistical information from the densities of the data, this goal may be achieved. However, ICA requires uncorrelated pure profiles, which is not the case in many chemical systems. Validation is critical to find the correct rank of ICA models, and the order of the components may change when cross-validation is applied. This is handled by re-ordering and reflecting the components for the individual models. Jack-knifing is applied to find the significant regions of the estimated spectral profilesMultivariate Curve Resolution (MCR) is another method where the objective is to find the pure spectra. A two-step procedure with ICA and MCR will also be presented. When data are present as "3-way", like in fluorescence spectra, with excitation and emission spanning two variable dimensions, PARAFAC may be used as a benchmark. The methods are compared on applications from Near-Infra Red spectra of water obtained at different temperatures, and fluorescence spectra of butter.

(557) Monitoring of Pet Foods for Potentially Toxic Elements
Ela Bakowska1, Michael Rieders1, Joan Schemmer1; 1NMS Labs
Recent extensive recalls of pet foods raised awareness of importance of screening of food products (for pets as well as for people) for potentially toxic substances. Currently, when the food products are questioned - they are usually screened mostly for contamination caused by bacteria and some organic compounds like pesticides. The screening for some potentially toxic elements (Arsenic, Cadmium, Lead and Mercury) is sometimes performed, when food products are questioned. However, many more elements are usually not determined at all. Those elements include known toxic elements like Beryllium and Thallium, as well as elements which at lower concentrations are considered essential, however at higher concentrations are considered toxic (for example Selenium). All the elements of interest (up to 70) are measured utilizing a variety of analytical techniques: Atomic Absorption (Flame, Graphite Furnace and Cold Vapor), Inductively Coupled Plasma Atomic Emission Spectroscopy and Inductively Coupled Plasma Mass Spectrometry (ICP-MS). ICP-MS allows not only for the quantitative determination of individual elements, but also allows for fast screening of more than 70 elements in a single analytical measurement. The semi-quantitative analysis of pet food products provided almost quantitative results for over 70 elements. The pet food products were acid-digested (in a microwave digestion system) and subsequently screened for elemental composition. The sample-to-sample analysis time was less than 5 minutes. Several NIST Standard Reference Materials (SRMs) were used as quality controls.

(558) Raman Imaging of Bacteria Cells Labeled With Metal Nanoprobes
Li-Lin Tay1, Jamshed Tanha1, Shannon Ryan1, 1National Research Council Canada
Detection of pathogenic bacteria bares great importance in public health. Raman spectroscopy and microscopy have been utilized to detect and classify different types of bacterial cells based on their unique vibrational signatures. Bulk Raman detections are plagued by sensitivity issues due to the nature of low scattering cross-section. Surface enhanced Raman spectroscopy (SERS) is a popular alternative which offers great improvement in detection sensitivity through the use of metal nanoprobe. In this study, we utilize the metal nanostructures (colloidal silver nanoparticles) labeled with novel single domain antibody (sdAb) specifically engineered to target the protein naturally expressed on the surface of Staphylococci aureus cells. The sdAb contains only the heavy chain variable domain yet fully retains the antigen recognition site. The sdAb is conjugated to colloidal silver nanoparticles (Ag-NP) through the exposed lysine or cystine residue. We rely on the binding specificity between the naturally expressed protein A on the surface of the S. aureus cells and sdAb to achieve specific pathogen recognition. Incubating the sdAb functionalized silver nanoparticles with different types of pathogens; we observed that only S. aureus cells were well decorated with Ag nanoparticles thus exhibits excellent SERS signals. This demonstrated the unique selectivity of the functional nanoprobe towards the targeted pathogen. Rapid detection of the silver nanoprobe labeled pathogen cells can be achieved by monitoring the strong SERS response of the various vibrational modes from the targeted cells. In this
presentation, we will demonstrate the detection of S. aureus cells using SERS microscopy.

(559) Raman Imaging of Pharmaceutical Contaminants
David Exline; 1RJ Lee Group, Inc.
The pharmaceutical and biomedical industries are often faced with particulate contamination issues relating to process development, raw materials and final product. In-depth analytical characterization of single particulate contaminants is often time consuming and expensive. Raman microprobe analysis of contaminants is used affectively to characterize particles, but is not efficient when dealing with hundreds of particles in a single sample. This presentation will discuss the evaluation of sample preparation and Raman imaging for the overall characterization of particle contaminant populations present in pharmaceutical products and the potential of increased testing efficiency.

(560) Carbon Nanotube Architectures: Synthesis and Characterization towards Functional Systems
Yung Joon Jung1, Xingang Xiong1, Myung Gwan Hahn1, Ahmed Busnaina1, Pulickel Ajayan1; 1Northwestern University; 2Rensselaer Polytechnic Institute
Carbon nanotubes (CNTs) have been investigated actively due to their excellent mechanical, electrical and thermal properties as well as nanometer scale one-dimensional structures. However, to build highly organized and integrated functional systems with CNTs, it is required to arrange them into well-defined configurations in a large scale. In this presentation, I will present two major synthetic methods, chemical vapor deposition and directed self-assembly, for building of diverse nanotube (both SWNT and MWNT) based organized functional systems. Also the characterization of fabricated nanotube based structures and tuning their property using Raman Spectroscopy will be discussed. Produced micro- and sub-microscale nanotube based architectures and systems can be directly used as interconnect wires in future semiconducting devices, diverse sensing elements, and other active components in flexible electronics.

(561) Raman Confocal Microscopy Imaging and the Use of Meso- and Nano-Structured Metallic Substrates
François Laguéné-Labarthe1, Nicolas Marquestaut2, Laurent Servant1, Valérie Guieu2, Meso Sojic2; 1University Of Western Ontario, Canada; 2Université Bordeaux 1, France
Due to the inherently weak Raman scattering cross section, the signal of diluted solutions or monolayer films is often difficult to measure or need long acquisition times. However when combined with metallic nanostructured surfaces with gold or silver patterns, the Raman signal can be enhanced by several order of magnitude leading to short acquisition times even for monolayers adsorbed on these structures. We present here results conducted on nanostructured surfaces made of gold and prepared by electron-beam lithography techniques or conventional chemical preparation. The Raman mapping of these nanotopographies is performed under a confocal Microscope (Horiba-Jobin-Yvon) and simultaneous topography is obtained with an atomic force microscope (Veeco).

(562) Raman Hyperspectral Imaging of Cells, Cellular Components and Drug Uptake into Cells
Max Dietz1, Christian Matthäus1, Tatjana Chenko1, Miloš Mitkovic1; 1Northeastern University
Modern Raman Micro-spectroscopic instrumentation permits the acquisition of confocal hyperspectral data sets of individual human cells at a spatial resolution of the diffraction limit. Using green or blue excitation wavelengths (514.5 or 488 nm at about 30 mW), data sets were collected at 300 nm resolution in the X-Y plane, and just less than a micrometer in the Z direction. Given the size of a human cell – typically about 60 micrometer in diameter, the number of spectra that need to be collected approaches about 40,000. Thus, short data integration times (250-500 msec/point) are essential; further-more, immersion of the cell in an aqueous environment (and the use of a water immersion objective) is highly desirable to prevent damage to the cellular material. The short integration times result in spectra of relatively poor S/N ratio. Extensive data processing, using three-dimensional de-noising and spike filter algorithms developed in house, followed by unsupervised methods of multivariate statistics (hierarchical cluster analysis) yields spectral map of cells of unrivaled quality. We have used this methodology to track mitochondria in cells, to monitor the uptake of perdeuterated liposomes into cells, to follow cell differentiation – induced hormone accumulation and other cell biological effects. Raman hyperspectral imaging, as compared to the more commonly used techniques such as confocal fluorescence microscopy, offers the advantage that cells are being studied without stains and label, and in an aqueous environment.

(563) Pharmaceutical Forensics: An Overview
Duane Mauze1; 1Allergan
Pharmaceutical forensics is the study of suspected counterfeit prescription drugs. Typically, the counterfeit prescription drugs include only high value drugs such as LipitorTM, CrestorTM, and ViagraTM. As both the drug product and its packaging are counterfeit, forensic examinations of questioned prescription drugs include the techniques of questioned document examination as well as both qualitative and quantitative drug and excipient analysis. International criminal organizations are involved in the trafficking of counterfeit drugs, including the Russian mafia and Latin American drug cartels. The total estimated dollar volume of this trafficking is in excess of $15 billion annually. Most counterfeit drugs originate in India or China, and are distributed world-wide. It is estimated that 1 to 3 percent of US prescription drugs are counterfeit, but the number rises to 25% in Latin America, and 50% in Africa and parts of Asia. A number of deaths in the U.S. have been attributed to counterfeit drugs. Examples of counterfeit drugs will be used to illustrate the analytical approach to demonstrating that a prescription drug is counterfeit.

(564) DESI and DART Mass Spectrometry for Counterfeit Drug Fingerprinting: Application to Antimalarials, Oseltamivir, and Other Cases
Facundo Fernandez1, Leonard Nyadong1, Christina Hampton1, Kristin Johnson1, Sameer Late1, Ayaj Banga2, Michael Green2, Paul Newton2; 1Georgia Institute of Technology, Atlanta; 2Mercer University, Atlanta; 2CDC AtlantaMahosot Hospital, Lao PDR.
The counterfeiting of pharmaceuticals is a well-recognized public health problem. Pharmaceutical quality is most commonly assessed using high performance liquid chromatography (HPLC). However, the sample preparation and chromatographic separation required are time-consuming. In this study, Desorption Electrospray Ionization Mass Spectrometry (DESI-MS), and Direct Analysis in Real Time (DART) accurate mass MS are compared for the high-throughput screening of solid pharmaceuticals. We present DESI and DART results for three case studies. First, we present the quantitative analysis of counterfeit artesunate antimalarials by DESI. Malaria, caused by Plasmodium falciparum parasites causes an estimated 1-3 million deaths per year. In SE Asia, counterfeit artemisinin tablets have become widespread, seriously endangering malaria control. This criminal trade is now threatening to expand to Africa. The second case refers to the analysis of Tamiflu® (oseltamivir) by reactive DESI. Due to the recent outbreaks of avian influenza, the demand for antivirals has increased tremendously, with stockpiling leading to shortage of supply. With
Tamiflu® as the leading antiviral in the market, its high cost and demand, have made it a preferred target for counterfeiters. Reports of counterfeit Tamiflu® samples, which have been shown to not contain the active ingredient, have already appeared. The third case describes the DART survey of low quality drugs collected in the Thailand-Myanmar border. Multi-drug resistant Plasmodium falciparum malaria is a severe public health problem in the Thailand-Myanmar border. Antimalarial drugs such as chloroquine and sulphadoxine-pyrimethamine are no longer effective. Quinine and mefloquine, if used alone, have very low efficacy. Many Thai villagers and migrant workers from Myanmar buy small packets of drugs over-the-counter from grocer shops and small pharmacies as their first line of treatment for fever and malaria. These small plastic bags, which contain 4-5 tablets and capsules are called ‘yaa chud’ in Thai, or literally ‘combination medicine’, and are sold to patients without prescription or medical assessment. The identification by DART MS of the drugs present in these “informal” pharmaceuticals is of critical importance, as they may contain drugs that are not efficacious for malaria and other causes of fever, may cause confusing adverse clinical events and/or contraindicated in pregnancy or childhood.

(565) The Use of FT-IR and Raman Spectroscopy in Cases Involving Product Tampering
Mark Witkowski1, JaCinta Batson1, John Crowe1; 1FDA Forensic Chemistry Center Cincinnati Ohio
The Food and Drug Administration (FDA) is responsible for the regulation of a large number of products which include foods, pharmaceuticals, biology, medical devices and cosmetics. As a result, the type of forensic evidence received at the Forensic Chemistry Center (FCC) for analysis can vary greatly from case to case. A portion of the evidence received for analysis at the FCC includes cases involving product tampering. Fourier transform infrared (FT-IR) spectroscopy and Raman spectroscopy are two instrumental techniques which can be applied to the examination of evidence related to product tampering. Both techniques can be applied to examination of the product packaging as well as the product contents. FT-IR and Raman microspectroscopic techniques can be used very effectively to examine trace evidence isolated from evidence from a product tampering case. The techniques can provide specific information on the identification and characterization of materials used to tamper with a product such as adhesives, tapes, dyes and pigments. The techniques are rapid and when coupled with sample preparation methodologies (e.g. microex Extractions, small particle analysis), a large amount of information can be obtained from a piece of forensic evidence. This presentation will discuss the FT-IR and Raman spectroscopic methods used by the FCC in the analysis of evidence from cases involving product tampering. Examples of data obtained from the application of these methods to actual case studies will be presented.

(566) Analysis of Suspected Counterfeit Pharmaceutical Products
Anthony Zook1; 1Merck & Co., Inc.
Counterfeit pharmaceutical products are an increasing global problem with significant public safety concerns. The ability to detect counterfeit products and packaging components is critical to protecting patients and supporting enforcement actions against the counterfeiters. Full characterization of counterfeit specimens further supports enforcement actions by demonstrating linkages between seemingly different counterfeit events. Case studies utilizing forensic analyses for the identification and characterization of counterfeit pharmaceutical products will be presented. This will include applications of digital image analysis, topomicroscopy, and molecular spectroscopy.

(567) Identification of Counterfeit Cialis, Levitra and Viagra Tablets by Open-Air Desorption Ionization Time-of-Flight Mass Spectrometry
Anthony Moffat1, Robert Cody2, Roger Jes1, Andrew O’Neil1; 1The School of Pharmacy, London; 2Jeol USA Inc
With counterfeit medicines becoming a growing problem in the USA and Europe, there is a need for their fast and easy identification for forensic purposes. This is also needed for the authentication of genuine pharmaceutical products in wholesale and retail outlets serving the public. Lifestyle drugs such as Cialis, Levitra and Viagra appear to be the most targeted products by counterfeiters, especially those obtained from Internet sources. New mass spectrometric techniques such as Direct Analysis in Real Time (DART) time-of-flight mass spectrometry can easily differentiate authentic and counterfeit Cialis, Levitra and Viagra tablets from their film coat and core compositions. The technique is minimally destructive, has high resolution and gives accurate mass measurements to allow molecular formulae of the ingredients to be identified within minutes. For example, by just presenting a suspect Cialis tablet to the source for five seconds the absence of triacetin from the film coat of counterfeit tablets can be identified. Reconstructed ion chromatograms also easily demonstrate the lack of triacetin in counterfeit tablets. When the scrapings of the cores of tablets are presented to the source, good quality chemical ionisation mass spectra can be obtained for the actives in authentic tablets corresponding to [tadalafil + H]+ or [vardenafil + H]+ or [sildenafil + H]+ in Cialis, Levitra and Viagra tablets respectively. None of the counterfeit samples of Cialis tested contained tadalaflu; they gave instead a large peak due to sildenafil. Similarly, the counterfeit Levitra tablets contained sildenafil and tadalaflu instead of vardenafu. The mass spectra of the core of the tablet also gives a profile of the excipients used in the tablets and this can also be used to differentiate authentic from counterfeit tablets. The identification of other contaminants on the surface of the film coats is another method of discriminating tablets and the profiles of these contaminants may be used to link suspected cases of common manufacture. All of these methods are fast and can be performed with minimal destruction of the tablets to allow the high throughput screening of medicines suspected of being counterfeit without the need for authentic drug samples.

(568) Raman Mapping of Tablet Dosage Formulation as a Means for Detecting and Sourcing Counterfeit Pharmaceuticals
Frans Adat1, Eunah Lee1, Andrew Whitley1, Mark Witkowski2; 1Horiba Jobin Yvon; 2FDA
As a means to determine if confiscated tablets are counterfeit and entering the pharmaceutical delivery outlets, Raman and FTIR dosage maps are being recorded. These maps are showing that even though the API (active pharmaceutical ingredient) is included in the formulation, the tablets can be classified as counterfeit from the identity and distribution of the excipients. The derivation of the Raman molecular maps requires multivariate tools to separate the contributions from the various components because of their substantial spectral overlap. Factor Analysis with Alternating Least Squares, Score Segregation and Binary Rotation have provided the ability to separate the components and create maps representing their distribution. In at least one of the examples the presence of stearate was determined even though it was present at low levels. In another, high fluorescent levels were found to be associated with microcrystalline cellulose, a material that is often observed to carry impurities. These types of observations is proving helpful in classifying confiscated material to different sources of manufacture.
one of the major drawbacks of atmospheric-pressure ionization sources is that reproducibility, and thus quantitation, are difficult to achieve because of the necessity of precisely positioning the sample with respect to the source. In the current study, the cold (−200 °C) flowing afterglow of a helium atmospheric-pressure glow discharge (APGD) is investigated as a novel ionization source for gas-phase organic mass spectrometry. By positioning the afterglow in front of a time-of-flight (TOF) mass spectrometer, an entire mass spectrum of reagent and analyte ions can be obtained. The vapor-phase analyte was introduced into the afterglow via an external stream of helium. Calibration curves for a variety of organic compounds were generated using a well-stirred tank exponential-dilution method. With this method, detection limits on the order of 1 to 100 fmol/s were achieved. In addition, the problem of sample positioning will be addressed through spatial characterization of the afterglow by temperature mapping and analyte signal analysis. The use and characterization of the APGD in the flowing afterglow mode as a potential ionization source for gas chromatography will also be presented.

(570) Three-Dimensional Nonstationary Model of an ICP-MS Interface

Albert Gilmutdinov1, Rinat Ibragimov1, Mjakzjum Salakhov1; Kazan State University

Spectroanalytical Induction Coupled Plasma (ICP) represent an extremely complicated physical phenomenon that includes interrelated gas dynamics and electromagnetic effects: two highly swirled outer and intermediate gas flows are mixed in the plasma region with axial injector flow creating a complex-structured plasma jet containing analyte atoms and ions. The overall gas dynamics is driven by highly spatially nonuniform and rapidly changing in time electromagnetic fields. Long time ago direct experiments have revealed that the plasma is not axially symmetrical and is highly dynamic in time. However, only recently a four dimensional description of free running ICP was developed in the author’s laboratory. The theory accounts for the true three dimensional geometry of the torch and the plasma is considered to be nonstationary. It is based on simultaneous solution of Navier-Stokes equations describing the gas flow dynamics (pressure, velocity and temperature distributions) and the set of Maxwell equations that predicts temporal behaviour of spatial structure of electromagnetic fields. In ICP-MS spectrometry the situation is further complicated: the plasma jet is directed to the interface that has complex geometry and significant pressure drop occur within the interface. The four dimensional approach of the authors is further extended in this work to include the interface into the consideration. The first results of modeling of the whole plasma-sampler-skimmer system will be presented in this talk.

(571) A Novel Cold Plasma Source for the Soft Ionization of Organic Molecules

Jacob Shelley1, Francisco Andrade2, Steven Ray1, Joshua Wiley1, Gary Hieftje1; Indiana University; Unilever Corporation

Recently, a group of atmospheric-pressure ionization sources has emerged onto the mass spectrometry scene. These sources, including desorption electrospray ionization (DESI) and direct analysis in real time (DART), have led to a new field known as “ambient mass spectrometry.” These ambient sources have numerous advantages over conventional ionization sources, such as high ionization efficiency (10-5-3·10-1) and direct analysis of solid samples. Furthermore, soft ionization generally occurs, mostly through proton-transfer mechanisms, thereby yielding simple mass spectra containing predominantly the protonated molecular-ion peak. For these reasons, ambient mass spectrometry fits the role of a nearly ideal method for organic mass spectrometry. However,

(572) Phosphorous/Sulfur Detection by ICPMS - from Spinal Fluid to Warfare Agents

Joseph Caruso; University of Cincinnati

Metals and metal-containing compounds are known to play important roles in many biological processes. Important human metabolic processes may be studied using the metallomics approach. For example, it is possible to study cerebrospinal fluid (CSF) metabolites from stroke patients with and without the further complication of vasospasm – a seriously life threatening condition. Our first studies in this area are to compare phosphopeptides from low abundance and lower M.W. proteins in hopes of finding particular metabolites that may predict the onset of vasospasm. 31P was the elemental target to screen for P containing peptides by ICPMS. Studies were done both with and without capillary LC-ICPMS and with a newly designed capillary LC-ICPMS interface to allow much stronger solvent for LC, while retaining a low solvent load to the plasma. Following this screening for phosphorous, we were able to utilize nano-CHIP-LC-IonTrap MS to identify some of these metabolites. With other agents have agents have ongoing studies using S and P as elemental tags to determine particular agents from the vesicant and nerve agent groups. Using ICPMS detection with collision/reaction cell, the detection levels are excellent and chromatographic resolution by LC and GC is excellent. Commonly expected interferences such as from pesticides may be overcome. This talk will describe the progress in these areas using chromatographically coupled mass spectrometric methods.

(573) Analysis of B-Supplements and Pharmaceutical Compounds by Reverse Phase HPLC with Sequential PDA and ICP-MS Detection

Timothy Shelbourn1, Leah Williamson2, Todd Gillespie1, Robert Montgomery3; Eli Lilly and Company; University of Georgia-Athens

A series of method development experiments have been conducted using reverse phase HPLC with sequential UV/Vis detection using a photodiode array (PDA) and elemental detection using inductively coupled plasma mass spectrometry (ICP-MS). Mixtures of vitamin B supplements cyanocobalamin (B12), thiamin (B1), and biotin, were investigated using isotropic separation. For the B-supplement experiments, UV absorbance by PDA and the elements cobalt, phosphorus and sulfur were monitored simultaneously by ICP-MS. It was demonstrated that co-eluting peaks can be resolved by monitoring different heteroatoms simultaneously. A related substances analysis of a proprietary pharmaceutical compound and its associated degradation products was performed using a gradient separation while monitoring UV absorbance by
PDA, along with bromine, chlorine and sulfur simultaneously by ICP-MS. The addition of elemental detection provided high specificity for compounds that contain heteroatoms and metals without requiring the interpretation of mass spectra. Molecules containing a heteroatom that lack a chromophore, or do not have strong UV/Vis absorbance, can be monitored in the chromatograph by elemental detection.

(574) Plant Metabolism Studies by ICPMS - Informing As and Se Phytoremediation
Joseph Caruso: 1University of Cincinnati
Metals and metal-containing compounds play important roles in many biological processes. Plant studies involve informing the metabolic processes in wild type and genetically enriched plants, as such studies can provide fundamental information on generating a better phytoremediating plant. The approach involved the overexpression of a gene isolated from the Se hyperaccumulator, A. bisulcatus, which encodes for selenocysteine methyltransferase (SMT) to methylate SeCys and form Se-(methyl)-selenocysteine (MeSeCys), a non-proteinogenic amino acid, thus diverting the Se flow away from SeCys and subsequent production of SeMet, both of which can be mis-incorporated into proteins. Decreasing SeCys levels represents an important Se tolerance strategy. A second genetic modification allows enhanced Se uptake when grown on selenium-containing media. In genetically modifying a plant, the transgene is introduced with the intent it will integrate into the genome. Further studies have been undertaken with other plant types that have implication for arsenic soil remediation as well as Se. This talk will describe the progress in these areas using the approach of coupling chromatography with ICPMS add selectivity to the chromatography/ molecular MS experiment.

(575) Fabrication of Tethered Lipid Membrane Arrays on Nanoglassy Substrates with SPR
Quan Cheng1, Joseph Taylor2; 1University of California Riverside
Biosensor technology is already exploiting the exceptional characteristics of tether bilayer membranes. These membranes can be functionalized by incorporating anchor or receptor molecules into the bilayer framework, thus expanding their use in chip-based biosensing and studies of cell-surface communication and interactions. In this talk, we will report the microfluidic fabrication of robust and fluid tethered bilayer arrays within a poly(dimethylsiloxane) (PDMS) chip, and demonstrate its addressability and biosensing by incorporating the monosialoganglioside (GM1) receptor into the bilayer framework for detection of cholera toxin. Rapid optimization of the experimental conditions has been achieved by using the nanoglassified surfaces in combination with surface plasmon resonance (SPR). This ultrathin glassy film on gold mimics glassy carbon-on-metal thin film substrates employed in microfluidics, allowing real-time monitoring of multiple assembly steps, and therefore permitting rapid prototyping and development of microfluidic arrays. The development of the tethered bilayer membrane arrays with high mobility provides an ideal host environment for membrane-associated proteins and thus opening new avenues for high-throughput analysis of these proteins.

(576) Nanoscale Carbon-on-Metal Films as Stable Substrates for Combinatorial Chemistry, SPR Imaging, and Mass Spectrometry
Matthew R. Lockett1, Margaret F. Phillips1, Michael R. Shortreed1, Steven C. Wei1, Lloyd M. Smith1; 1University of Wisconsin; 2GWC Technologies
Array-based technologies have become an essential tool for screening large numbers of molecular interactions in a parallel and multiplexed format. A major deciding factor in the versatility of any array is the substrate and support chemistry employed. The substrate should offer stability under various reaction conditions, support a large number of chemical functionalities, and be reproducibly created. Carbon-based substrates covalently modified with the proper attachment chemistry afford the stability necessary for combinatorial chemistry conditions and can be functionalized with a wide-variety of molecules. The fabrication of a carbon-on-metal thin film substrates are proven robust enough to support combinatorial oligonucleotide synthesis, fluorescence and SPR imaging modalities, and MALDI mass spectrometric analysis. The ability to support multiple analytical modalities offers an advantage over many of the substrates currently in use. The current work will demonstrate the ability of the carbon-on-metal thin film substrates to provide a combinatorial method for analyzing bio-affinity interactions.

(577) Nanometer-Scale Spatiotemporal Control of Environmentally-Responsive Materials Probed by Surface Plasmon Resonance Imaging
Paul W. Bohn1, Xuejun Wang1, Ping Shi1; 1University of Notre Dame
Recently there has been a great deal of interest in generating and utilizing gradient polymer surfaces due to potential applications, as substrates for selective adsorption, templates for cell migration, and tools for combinatorial chemistry studies. Furthermore, spatially graded physical structures are of interest, because the strength of interaction with the environment, $f_{Gint}$, can be continuously varied in space, providing a useful alternative to the more common practice of temporally varying the interaction strength along a spatially invariant structure. A key goal of work in this laboratory is to develop laterally graded surfaces and thin films, in order to utilize active control strategies and externally applied perturbations in conjunction with molecular and supramolecular architectures to control transport. An electrochemical-potential-gradient-based method to generate chemical composition and physical property gradients on thin Au electrodes is applied to the formation of spatiotemporally controlled polymer gradients. Polymerization reactions are of particular interest and utility, because they can be used as a route to environmentally-responsive materials. Environmentally-responsive polymers may be gradient-templated by using an initially-formed small molecule gradient as a template for atom transfer radical polymerization, ATRP, or by desorbing oligomers directly. The preparation and characterization of these novel materials and structures benefits enormously from surface plasmon resonance imaging studies which have the capacity to monitor sub-nm scale changes in thickness over fYm-scale lateral distances.

(578) Optical Flocculation of Bio-inspired self-assembly of Gold Nanoparticles
Jasmine Austin1, Marion Greene1, Wanjoong Kim1, William Yu2, JaeTae Seo2, Qiguang Yang2, Bagher Tabibi1, SeongMin Ma1, Wansoo Yun2, Seongsoo Jung2; 1Department of Physics, Hampton University, Hampton; 2Korea Research Institute of Standards an; 3Department of Chemistry, Rice University
The surface plasmon resonance spectra of gold nanomaterials are tunable, from visible to near infrared region, by controlling the individual morphologies and structures that determine their dielectric properties. Interband transition and free conduction electron scattering processes are directly related to the dielectric properties. The electron scattering rate is inversely proportional to the particle morphology or engineered-surface conditions, which allows optical tunability or spectral modification of nanomaterials. A combination of the optical tunability and bio-inspired self-assembly of Au nanomaterials through a biospecific interaction of proteins functionalizes the nanomaterials as optical biosensors. The interaction
of (strept)avidin and the biotin-attached gold nanoparticles inspired self-assembly between the nanoparticles, that created surface plasmon coupling between neighboring particles, and modified their optical properties. Maximum changes of absorbance and SPR peaks between Au, Au-biotin, and Au-biotin-avidin were 0.3 and 1.2, and 6 nm and 53 nm, respectively, with concentrations of ~0.1 μM 8.30×10⁻5 mol/mL for the nanoparticles of ~4.5 μV 23.1 nm. Analytical and numerical modeling of static or discrete dipole approximation and finite difference time domain supported the optical spectra and microscopic image of functionalized Au bio nanomaterials systems.

(579) Fiber Optic Surface Plasmon Resonance Sensor for Monitoring Oceanographic Variance
Karl Booksh1, Yoon-Chang Kim2, Jeffrey Cramer3, Michelle Keighan4; 1University of Delaware
SPR spectroscopy is applied to monitor changes in dissolved organic carbon and salinity across a Puget Sound transect and in the vicinity of a deep sea hydrothermal vent. Here we will discuss the different types of environmental information that can be obtained by using SPR in concert with conductivity for determining changes in dissolved organic carbon and salinity. The SPR spectrometer was field calibrated to eliminate the effect of temperature changes. In locations where the DOC level increases, a red shift in the SPR in dissolved organic carbon and salinity. The SPR spectrometer by using SPR in concert with conductivity for determining changes of optically calibrated emissi on intensity measurements from extrinsic factors relevant to SWNT fluorimetry. By compiling a set agents. Progress will be reported in studying both intrinsic and extrinsic factors relevant to SWNT fluorimetry. Since the discovery of structure-dependent near-IR emission from semiconducting single-walled carbon nanotubes (SWNTs), fluorimetric analysis has emerged as a valuable tool for characterizing SWNT samples. Recently, specialized hardware and sophisticated data analysis programs have been developed and commercialized to provide impressive analytical speed and sensitivity. Because the wavelengths of visible absorption and near-IR emission are known for all (n,m) structures, fluorimetry provides secure qualitative analysis of the semiconducting species present in a bulk sample. But as is the case for all structure-sensitive spectroscopic methods, quantitative determination of relative or absolute species concentrations remains far more challenging. Two types of information are needed to make fluorimetric analysis quantitative. One concerns the intrinsic differences in photophysical parameters (absorptivities and emission quantum yields) in perfect nanotubes as a function of (n,m), or equivalently as a function of diameter, chiral angle, and mod 1 vs. mod 2 character. The second concerns extrinsic factors, or imperfections, that can influence fluorescence intensities. These extrinsic factors may include the presence of quenching sites (structural defects, ends, or chemical derivatizations), the extent of sample aggregation, and the influence of specific suspending agents. Progress will be reported in studying both intrinsic and extrinsic factors relevant to SWNT fluorimetry. By compiling a set of optically calibrated emission intensity measurements from individual (n,m)-identified nanotubes under a fluorescence microscope, we have deduced their absolute fluorimetric efficiencies. This quantity is the product of 222 absorptivity times fluorescence quantum yield. Expressed per carbon atom, the results show systematic but relatively mild variations (spanning a factor of ~2.5) that correlate mainly with emission wavelength. One of the most unavoidable extrinsic influences is probably length-dependent quantum yields resulting from exciton quenching at the ends of SWNTs. We will present results from fluorescence measurements on individual SWNTs in aqueous suspensions in which the fluorescence intensity of each nanotube is correlated directly with its physical length as determined from its diffusional motions. By elucidating the extrinsic effects influencing emission efficiency and understanding how these relate to sample preparation and handling, it will soon be possible to apply near-IR fluorimetry as the only bulk method capable of quantitative (n,m)-resolved analysis.

(581) Toward Quantitative Fluorimetric Analysis of Single-Walled Carbon Nanotubes
R. Bruce Weisman1; 1Rice University
Since the discovery of structure-dependent near-IR emission from semiconducting single-walled carbon nanotubes (SWNTs), fluorimetric analysis has emerged as a valuable tool for characterizing SWNT samples. Recently, specialized hardware and sophisticated data analysis programs have been developed and commercialized to provide impressive analytical speed and sensitivity. Because the wavelengths of visible absorption and near-IR emission are known for all (n,m) structures, fluorimetry provides secure qualitative analysis of the semiconducting species present in a bulk sample. But as is the case for all structure-sensitive spectroscopic methods, quantitative determination of relative or absolute species concentrations remains far more challenging. Two types of information are needed to make fluorimetric analysis quantitative. One concerns the intrinsic differences in photophysical parameters (absorptivities and emission quantum yields) in perfect nanotubes as a function of (n,m), or equivalently as a function of diameter, chiral angle, and mod 1 vs. mod 2 character. The second concerns extrinsic factors, or imperfections, that can influence fluorescence intensities. These extrinsic factors may include the presence of quenching sites (structural defects, ends, or chemical derivatizations), the extent of sample aggregation, and the influence of specific suspending agents. Progress will be reported in studying both intrinsic and extrinsic factors relevant to SWNT fluorimetry. By compiling a set of optically calibrated emission intensity measurements from individual (n,m)-identified nanotubes under a fluorescence microscope, we have deduced their absolute fluorimetric efficiencies. This quantity is the product of 222 absorptivity times fluorescence quantum yield. Expressed per carbon atom, the results show systematic but relatively mild variations (spanning a factor of ~2.5) that correlate mainly with emission wavelength. One of the most unavoidable extrinsic influences is probably length-dependent quantum yields resulting from exciton quenching at the ends of SWNTs. We will present results from fluorescence measurements on individual SWNTs in aqueous suspensions in which the fluorescence intensity of each nanotube is correlated directly with its physical length as determined from its diffusional motions. By elucidating the extrinsic effects influencing emission efficiency and understanding how these relate to sample preparation and handling, it will soon be possible to apply near-IR fluorimetry as the only bulk method capable of quantitative (n,m)-resolved analysis.

(582) Separating Carbon Nanotubes by Their Physical and Electronic Structure using Density Gradient Ultracentrifugation
Mark Hersam1; 1Northwestern University
The utilization of single-walled carbon nanotubes (SWNTs) in large quantities for molecular electronics, optoelectronics, biosensors, and medical applications will require SWNTs of the same physical structure, electronic type, and band gap. Since current methods of synthesis produce mixtures of nanotubes with different physical structures and electrical properties, the development of strategies for the post-production separation of these one-dimensional materials is highly desirable. In this work, we demonstrate a scalable method for separating SWNTs by their diameter and electronic type (i.e., semiconducting versus metallic) using density gradient ultracentrifugation (DGU). Since DGU is a technique commonly utilized to separate and isolate different sub-cellular components, DNA from RNA, and even different sequences of DNA by their compositions, we initially focused on the bulk sorting of DNA wrapped SWNTs in aqueous density gradients [1]. This process led to enrichment of SWNTs by diameter - especially in the small diameter regime (i.e., SWNT diameter = 0.7 - 1.0 nm). However, DNA wrapping possessed several undesirable characteristics including prohibitive expense in large scale production, irreversible wrapping, and inefficient wrapping for SWNTs with diameters exceeding 1 nm. Consequently, subsequent work has focused on DGU of surfactant encapsulated SWNTs [2]. In particular, bile salt surfactants, such as sodium cholate (SC), have overcome the drawbacks of DNA. Furthermore, additional control over the density-structure relationship has been achieved by using co-surfactant mixtures of SC and sodium dodecyl sulfate (SDS). For example, highly efficient metal versus semiconductor separation has been achieved with SDS:SC co-surfactant ratios ranging from 1:4 to 3:2. Characterization of the resulting sorted SWNT samples includes optical absorption spectroscopy, photoluminescence spectroscopy, Raman spectroscopy, scanning probe microscopy, and direct charge transport measurements. Since DGU produces relatively large quantities of monodisperse SWNTs, this talk will conclude with our most recent efforts to realize enhanced performance in SWNT devices, such as thin-film field effect transistors and transparent conductors, using SWNTs sorted by DGU.[1] M. S. Arnold, S. I. Stupp, and M. C. Hersam, Nano Letters, 5, 713 (2005).[2] M. S. Arnold, A. A. Green, J. F. Hulvat, S. I. Stupp, and M. C. Hersam, Nature Nanotechnology, 1, 60 (2006).

(583) A Scanning Force Microscopy Assay for Metallic/Semiconducting Content in Mixed Single-Walled Carbon Nanotube Samples
Liwei Chen1, Wei Li2; 1Ohio University
Single-walled carbon nanotubes (SWNTs) can be either metallic or semiconducting depending on their diameter and chirality. This amazing richness in structure and properties provides a great opportunity for nanoelectronics. However, as-synthesized SWNTs are always mixtures of a variety of tubes that include both metallic and semiconducting species and it is an enormous challenge to separate these SWNTs before they can be assembled into functional devices. In fact, there is not a readily available assay to characterize the metallic/semiconducting content in SWNTs mixtures. For semiconducting tubes, their (n,m) distribution can be obtained by using co-surfactant mixtures of SC and sodium dodecyl sulfate (SDS). For example, highly efficient metal versus semiconductor separation has been achieved with SDS:SC co-surfactant ratios ranging from 1:4 to 3:2. Characterization of the resulting sorted SWNT samples includes optical absorption spectroscopy, photoluminescence spectroscopy, Raman spectroscopy, scanning probe microscopy, and direct charge transport measurements. Since DGU produces relatively large quantities of monodisperse SWNTs, this talk will conclude with our most recent efforts to realize enhanced performance in SWNT devices, such as thin-film field effect transistors and transparent conductors, using SWNTs sorted by DGU.[1] M. S. Arnold, S. I. Stupp, and M. C. Hersam, Nano Letters, 5, 713 (2005).[2] M. S. Arnold, A. A. Green, J. F. Hulvat, S. I. Stupp, and M. C. Hersam, Nature Nanotechnology, 1, 60 (2006).
tubes can be detected with resonance Raman spectroscopy but tunable Raman laser source is needed to cover the wide tube diameter range and Raman cross-section for (n,m) specific tubes has not been established to quantify the metallic content in a mixture. We recently reported a scanning force microscopy based method to measure the static dielectric polarization of individual SWNTs. We show that the difference in longitudinal dielectric constants between metallic and semiconducting SWNTs results in detectable signal difference in the dielectric channel. Here we further develop this approach to improve the contrast between metallic and semiconducting tubes. We use this method to assay the content of metallic tubes in a mixture.

(584) Diameter and Chirality Dependent Aggregation of Single-Walled Carbon Nanotubes

Sandip Niyogi1, Sofiane Boukhalfa1, Satishkumar Chikkannavar2, Stephen Doorn1; 1Los Alamos National Lab. Single-walled carbon nanotubes dispersed in water using sodium dodecylsulfate allows the study of properties of individual nanotubes. Nanotube isolation is maintained in the dispersions by the electrostatic repulsion between the dodecylsulfate groups adsorbed on the nanotube surface. We present data showing changes in SWNT absorbance and emission spectra in response to titrating the dispersion with salt solutions. The results show an ability to manipulate surface charge density on the SWNTs through changes in surfactant equilibria and charge screening. The diameter dependence of these effects allows diameter-selective aggregation of SWNTs and some specific cases of chirality-dependent stability have been observed.

(585) Enriching Individual (n, m) Carbon Nanotubes for Solution Chemistry

Wei Zhao1, Xiaomin Tu1, Yang Xu1, Satishkumar Chikkannavar2, Stephen Doorn2; 1University of Arkansas-Little Rock; 2Los Alamos National Lab. Single-walled carbon nanotubes (SWNTs) have attracted much attention as a new generation material for nanoelectronics and nanophotonics. However, their structural heterogeneity containing different chiralities is a big challenge for their applications. Methods mainly based on the geometry-selectivity for nanotubes have been developed as promising ones for easily scaling up for enriching individual (n, m) nanotubes. Among them, HPLC assisted separation and purification of SWNTs show great promises because a HPLC system can combine with versatile chromatographic methods for purification. It has been reported that metallic and semiconducting nanotube separation for HiPco nanotubes can be achieved when combining with ion-exchange chromatography (IEC). Here we show that the IEC method provide additional enrichment of individual semiconducting (n, m) nanotubes from starting HiPco nanotubes. The redox properties of the selected individual (n, m) nanotubes have been studied with various oxidants and will be discussed in this presentation.

(586) Applications of Desorption Electrospray Ionization

R. Graham Cooks1, Purdue University
This paper delineates applications of DESI currently being investigated at Purdue with emphasis on those involving high speed analysis. The applications all depend on the chemical specificity of the method. They include (i) analysis of inks in forensics, (ii) analysis of drugs of abuse in bioligical fluids, (iii) metabolicomics studies of biological fluids and (v) lipid analysis directly from untreated biological tissue, especially in the context of bacterial typing. The work covered also includes high throughput pharmaceutical analysis and applications in which the sample and mass spectrometer are well-separated in space. Instances in which DESI is combined with a miniature mass spectrometer get particular attention. Practical issues are treated including sample matrix effects, substrate effects and analytical performance characteristics of DESI and other ambient ionization methods. Experiments in which DESI is used in conjunction with a miniature mass spectrometer are also discussed. A shoebox sized, 10 kg handheld miniature mass spectrometer, the Mini 10, based on a rectilinear ion trap mass analyzer is shown to allow immediate determination of biomolecules and drugs in the real environment. The use of this instrument for protein characterization is also shown.

(587) Development of Hybrid Atmospheric Ionization Sources for Direct Analysis of Macromolecules by FT-ICR-MS

David Muddiman1, Adam Hawrakie1, Jason Sampson1, Michael Bereman1, Brent Dixon1; 1NC State University
This presentation will detail our efforts at the development and application of hybrid ionization sources - DESI and MALDESI with FTICR-MS and interfaces for ESI-MS for the direct analysis of biological molecules with implications for tissue imaging.

(588) Hitting the Bullseye More Often: Extending the Applications for the DART Ion Source

Robert Cody1; 1JEOL USA, Inc. It has been almost five years since the DART open-air ion source was first constructed. The initial mechanisms based on proton-transfer or oxygen anion reactions have shown broad application to small-molecule analysis, and DART has found use in a growing number of laboratories. However, no single analytical technique is ideal for every application and some compound classes are not desorbed or ionized efficiently under standard DART conditions. Recently, new ionization modes have been found for the DART ionization of "difficult" compounds such as saturated alkanes and aromatic compounds. These spectra offer clues to the chemistry involved in DART and provide information that is complementary to current DART analysis, including conditions for forming electron-ionization-like mass spectra by DART. Techniques will be discussed for the rapid analysis of compounds that are not easily desorbed. Developments in quantitative DART analysis and prospects for DART imaging will be discussed.

(589) Direct High-throughput Analysis of Pathogenic Bacteria by DESI and DART

Facundo Fernandez1, Carrie Pierce1,2, Leonard Nyadong1, John Barr1, Adrian Woolfitt2, Hercules Moura2, Robert Massung2, Robert Cody1; 1Georgia Institute of Technology; 2CDC; 3JEOL Inc. Direct analysis in real time (DART) and Desorption Electrospray Ionization (DESI) are versatile, new ionization techniques for mass spectrometry that allow the direct detection of chemicals on a variety of surfaces, without sample preparation. In this study, DART coupled to time-of-flight mass spectrometry (TOF MS), and DESI coupled to quadrupolar ion trap (QiT) MS are applied to the identification and classification of pathogenic bacteria. This approach capitalizes on the ability of TOF MS to provide improved selectivity through exact mass measurements, and of QiT to provide added layers of statistical identification confidence via MS(n). Three separate strains (Nine Mile I, Nine Mile II, RSA 514) of Coxiella burnetii, the causative agent of Q-fever, were analyzed by direct ionization methods. In the case of DART, direct in-situ thermal hydrolysis, methylation, and ionization of the bacterial membrane fatty acids was used to increase the sensitivity in generating fatty acid methyl ester (FAME) profiles for each bacterial strain. For each isolate, a data set was generated from three replicates prepared on two different days. Results show that FAME intensity profiles are unique for each strain. Clustering of the DART TOF MS data via Parallel Factor Analysis (PARAFAC) allowed to unequivocally distinguish between strains. DESI
Ionization (DESI) is performed demonstrating. This novel DESI
A major improvement in the way Desorption Electrospray
signal strength. Advantages include improvements in the ease of
geometries, currently the most critical parameters in obtaining good
interface removes the need to optimize the spray and collection
rates and enclosure material were investigated.

small molecules. The effects of various operating parameters for
results were obtained in all cases for typical proteins, peptides and
conventional optimized-geometry open DESI source. Comparable
collection capillaries set at various angles were compared to the
independent of the geometrical configuration of the spray and inlet.

interface now also allows for the direct analysis of 96 well plates
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DART TOF MS and DESI QIT MS hold promise as rapid,
providing information complementary to DART. In summary,
ionization (DeSSI). When DeSSI is applied, efficient desorption
ionization of analytes occur at ambient conditions by using a
supersonic cloud of charged droplets to bombard the surface
containing the analyte. A major advantage of DeSSI-MS is the use
of neither heating nor high voltages at the sonic spray capillary.
DeSSI-MS usually provides clean mass spectra with little solvent
cluster ions and with enough abundant analyte signals for DeSSI-
MS/MS. These features facilitate therefore the detection of light
components or impurities, or both. The high-velocity supersonic
DeSSI spray also facilitates deep matrix penetration thus providing
quite homogenous sampling and long-lasting ion signals. DeSSI
offers therefore a friendly environment in which to perform
ambient mass spectrometry. In this talk we will discuss, as
examples of the many applications envisaged for DeSSI-MS, its
use for the analysis of drug on tablets and explosives on variable
surfaces, for typification and counterfeiting detection of perfumes,
vegetable oils and biofuels, and for "sample-preparation free" on-
site ambient analysis of environmental samples and body fluids
using semi-permeable membranes (DeSSI-MIMS).

Geometry Independent Desorption Electrospray Ionization
André Venter1, Graham Cooks2; 1Purdue University
A major improvement in the way Desorption Electrospray Ionization (DESI) is performed is demonstrated. This novel DESI
interface removes the need to optimize the spray and collection geometries, currently the most critical parameters in obtaining good
signal strength. Advantages include improvements in the ease of implementation, robustness and safety of the technique. This
interface now also allows for the direct analysis of 96 well plates by DESI. The new configuration provides improved ionization
efficiency, safety, and ease of use and performance largely independent of the geometrical configuration of the spray and inlet.

Geometry independent DESI sources with the incident and collection capillaries set at various angles were compared to the
conventional optimized-geometry open DESI source. Comparable results were obtained in all cases for typical proteins, peptides and
small molecules. The effects of various operating parameters for the new source such as applied spray potential, liquid and gas flow
rates and enclosure material were investigated.

Consideration of Measurement Uncertainties in Multivariate Curve Resolution by Alternating Least Squares
Roma Tauler1, Peter Wentzell2; 1IFQAB-CSIC, Spain; 2Dalhousie
University, Canada
In this presentation, the effects of non-uniform measurement errors on traditional alternating least squares strategies in multivariate
curve resolution are investigated and compared with new strategies where measurement uncertainties are considered in weighted least
squares procedures. Examples of applications in the resolution of environmental patterns in air and water contamination studies will
be presented. Results show that unweighted MCR-ALS strategies have a higher inclination to overfit the data and to incorrectly
resolve minor source contributions and that new weighted MCR-
ALS strategies produce better results. The extent of the improvement is dependent on the particular situation and the
measurement error structure of the data.P.D. Wentzell, T.K.
Karakah, S. Roy, M.J. Martinez, C.P. Allen and M. Werner-
Washburne, "Multivariate Curve Resolution of Time Course

Equation-Oriented System (EOS) as Tool to Multivariate Curve Resolution (MCR) with Multiple Constraints
Jihong Wang1, Marwood N. Ediger1, Thomas M. Hancewicz2;
VeraLight Inc.; 1Unilever Research USA
Constrained models are crucial to the success of Self-Modeling
Curve Resolution (SMCR). Convergence of constrained alternating
least squares (ALS) models may be elusive and the situation
worsens with multiple constraints. An alternative approach is to
design special algorithms and programs for unique combinations of
constraints. Since constrained models are important in numerous
applications, a generalized method was sought to implement
constrained models. Models and constraints can be transferred into a
problem of solving over-defined systems of multivariate
polynomial equations. The problem of solving systems of
multivariate polynomial equations arises naturally in mathematics
and computer science. The Equation-Oriented System (EOS)
provides an effective approach to the problem of solving polynomials
used in chemometrics. EOS has a conventional interface to represent different equations using Einstein summation
convention, and the algorithm can be conveniently and completely
coded in scripting languages like MATLAB. Simulated examples
will be presented to demonstrate the power of EOS in solving MCR
problems with multiple constraints. The jagged three-dimensional
array of Fluorescence excitation-emission-matrix (EEM) example
shows the benefit of using EOS in industrial application.

Confocal Fluorescence Hyperspectral Imaging of Biological Samples using Multivariate Curve Resolution
Analysis Techniques
Howland Jones1, David Haaland1, David Melgaard1, Michael
Sinclair1, Mark Van Benthem1; 1Sandia National Laboratories
Sandia has designed and developed a hyperspectral confocal
fluorescent microscope for imaging and studying biological
samples (live biological cells, various plant related materials,
bacteria and biofilms). To analyze the image data generated from
this microscope, we have developed fast and efficient Multivariate
Curve Resolution (MCR) algorithms and software to extract pure
component spectra and the associated relative quantitative
concentrations from these hyperspectral images. MCR is a
powerful technique when dealing with our relatively unknown
biological samples because it can provide quantitative analysis of
the image data without the need for standards, and it can discover
all the emitting species present in an image, even those about which
we have no a priori information, making it an invaluable tool when
researching unknown biological samples. Another research
advantage of hyperspectral imaging with the use of our MCR
algorithms is that it allows us to separate many overlapping
fluorophores and create interpretable images, once again making it
an ideal research tool for the biologist. One challenge that we have
faced with our image datasets is dealing with several noise sources
associated with our hyperspectral microscope (Poisson distributed,
structured and read noise) which complicates the ability to extract
the pure-component spectra and their associated concentrations
with MCR from these image datasets. In the past, we have found
that weighting our image datasets for Poisson distributed noise
improves our ability to extract weakly emitting fluorophores which
may get buried in the noise. However, since our image data
are composed of more than Poisson distributed noise, we should
weight the data appropriately for all noise sources present prior to
analyzing these data with MCR. In this presentation, I will demonstrate different weighting schemes on simulated and real image data taken from biological images explored in our laboratory and discuss the benefits of properly weighting our image data prior to MCR analyses. I will also discuss methods to estimate the statistical significance of the concentration estimates for minor spectral components resulting from these analyses. Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

Michael D. Morris; 1University of Michigan
Band target entropy minimization (BTEM) is a powerful and often-overlooked approach to self-modeling curve resolution. In effect, the method finds all bands correlated with a target band or bands using as a criterion minimization of information entropy or a related function. Unlike most other targeting methods, BTEM searches small magnitude eigenvectors in as well as those retained by the standard criteria. Although low magnitude eigenvectors look like noise, they do contain determinate signal and may contain much of the information about minor components in the system. Because it extracts information from these eigenvectors, BTEM usually provides greater signal/noise ratio for minor components than other methods. In this talk, the theory of BTEM will be briefly sketched and its advantages and problems outlined. Applications to problems in musculoskeletal tissue biology and clinical diagnostics will be illustrated with data sets from Raman microprobe scans, Raman hyperspectral images and fifty point Raman maps made with a multi-fiber fiber optic probe.

(596) Multivariate Curve Resolution in Advanced Process Modeling
Anna de Juan1, Romà Tauler2; 1Universitat de Barcelona, Barcelona; 2IQAB-CSIC
Multivariate curve resolution offers many possibilities for modeling of complex processes. The underlying bilinear model of curve resolution, which expresses the raw data collected during process monitoring as the composition-weighted sum of pure component signal contributions, allows for the description of processes collected with a variety of spectroscopic techniques and with a partially or completely unknown mechanism. Curve resolution can easily handle multitechnique and/or multieexperiment data structures. The analysis of these data sets can provide a very robust structural information to characterize the compounds involved in a process (multitechnique monitoring) or can allow for the simultaneous study of a set of designed experiments that can allow for the detection of minor or intermediate compounds, changing the experimental conditions of process development, or for the assessment of the effect of different inducing agents or process control variables in the process mechanism. An interesting feature of curve resolution methods is the possibility of introducing external information related to properties of the signal recorded or to the shape of the process profiles under the form of constraints. Whereas soft-modeling constraints (non-negativity, closure,...) are the most generally applied, process profiles can also be fitted according to a hard model, if the mechanism of the process is partially or totally known. Unlike pure hard-modeling approaches, where the total mechanism of the process should be known and a global model is needed in multieperiment analysis, hard-modeling constraints can fit only some of the components contributing to the signal recorded during a process and can handle sets of experiments with a non-common model or structures with model-free and model-based experiments. All these possibilities will be shown with real examples.

(597) Raman Spectroscopic and Optical Characterization of Early Atherosclerotic Plaques
Lin-Ping Choo-Smith1, Mark Hewko1, Elicia Kohlenberg1, Michael Smith1, Saro Bascamurty1, Michael Sowa1; 1NRC-Institute for Biodiagnostics
Atherosclerosis is the process by which fatty material, cholesterol, calcium and other substances are deposited in the inner lining of an artery leading to the development of plaques. Significant deposition results in reduced blood flow as the lumen is narrowed, with unstable plaques eventually rupturing to form clots triggering a heart attack or stroke. Using current diagnostic techniques such as angiography and intravascular ultrasound, it is difficult for clinicians to assess the nature of the plaque composition and its propensity to rupture. This information would be valuable in assisting interventional cardiologists in the planning of intravascular procedures such as balloon angioplasty to restore blood flow thorough an artery. The myocardial infarction-prone Watanabe heritable hyperlipidemic rabbit strain naturally develops atherosclerotic plaques due to high levels of cholesterol in the blood and is a useful model for investigating atherosclerosis progression. Using Raman spectroscopy and optical coherence tomography (OCT), arterial tissue from rabbits at various ages were investigated. Conventional white light angioscopy showed that even at the early age of 6 months, there was evidence of lumen narrowing with raised regions on the surface. OCT investigation of longitudinally sectioned arteries showed that control areas had smooth continuous and homogeneous transitions as the OCT signal penetrated the vessel surface. In contrast, the images of the raised regions showed significant heterogeneity on the surface as well as in the axial direction. Raman measurements from bulk tissue revealed that the raised regions had spectra characterized by numerous peaks across the spectra. The biochemical origins of these spectral peaks and a comparison of OCT and histological investigations will be discussed with respect to the pathogenesis of atherosclerosis.

(598) Raman Spectroscopy of Biomimetic Polymers for Bone Tissue Engineering
Gurjit S. Mandair1, Lihn N. Luong2, David H. Kohn2, Michael D. Morris3; 1University of Michigan, Department of Chemistry; 2University of Michigan, Biomedical Eng.
In bone tissue engineering, poly(lactic-co-glycolic acid) (PLGA) polymers are widely used to deliver bone or serum-derived growth factors to the injured site in order to promote bone regeneration. The osteoinductive and osteoconductive properties of PLGA films can be improved through biomimetic engineering in which a bone-like apatitic layer is co-precipitated with one or more growth factors onto the polymer surface. However, the effect of protein co-precipitation on crystal morphology is not yet fully understood. In this study, Raman spectroscopy is used to examine the effect of a model protein, bovine serum albumin (BSA) on crystal morphology, mineral spatial distribution, and its retention within the nucleated mineral layer. Biomimetic polymers were prepared by incubating the model protein and PLGA film in a mineral-inducing simulated body fluid (SBF) for a period of six days at 37 C. Mineralized controls without protein incorporation were also prepared. Previous HRTEM and power diffraction studies have showed that protein co-precipitation resulted in changes to the plate-like crystal morphology compared to mineralized controls [1]. These results were subsequently confirmed by Raman spectroscopy in which the intensity of the asymmetric phosphate bands appeared to change with protein incorporation. These bands are known indicators of biological apatites in bone inorganic salts and thus we show how phosphate band profiles obtained from protein-modified biomimetic apatites resemble those of mouse bone apatites. In conclusion, we show that Raman spectroscopy is an invaluable tool for studying the inorganic mineral phases of biomimetic materials.

(599) Temperature-Induced Conformational Changes in Human Tear Lipids Hydrocarbon Chains
Douglas Borchman¹, Gary Foulks¹, Marta Yappert¹, Donghai Ho¹;
¹University of Louisville

As a first step to characterize human meibum and tear lipids, infrared spectroscopy was applied to characterize the molecular structure/conformation and packing of hydrocarbon chains. Lipid phase transitions were described by a two state sigmoidal equation consisting of four parameters: minimum order, magnitude of change, transition temperature and cooperativity. Temperature-induced phase transitions were experimentally reproducible and were similar for multiple samples collected from the same person. No hysteresis was observed. Hydration of polar tear lipids increased their phase transition cooperativity, enthalpy and entropy. Hydrophobic interactions in meibum lipid (ML) were stronger than in tear-fluid lipids (TL), as reflected by the higher entropy and enthalpy of the gel to liquid crystalline phase transition of ML. The results of this study provide further evidence of the differences in the composition and structure of ML and TL. The conformational changes observed in the hydrocarbon chains of ML with temperature suggest that the observed therapeutic increased delivery of ML with eye lid heating could be related to the increased disorder in the packing of the hydrocarbon tails. This work also highlights the power of infrared spectroscopy to characterize molecular structure/conformation, and packing of human tear lipids and provides a basis to be applied next to study tear film lipid composition-structure-function relationships and lipid-protein interactions in relation to age, sex and dry eye symptoms.

(600) Applications of Attenuated Total Reflection FTIR Imaging to Skin
Ka Lung Andrew Chan¹, Sergei Kazarian¹; ¹Imperial College London

Infrared spectroscopy is a recognized powerful material characterisation tool. The development of infrared array detectors that enable the rapid capture of 2D chemical images has widened the applications of this technology to a wide range of materials. It makes both the spectral (molecular) and spatial information available. In particular, Fourier transform infrared (FTIR) imaging in Attenuated Total Reflection (ATR) mode provides the opportunity to study samples in a quantitative manner in the mid-IR region without the need of microtoming. In addition, sampling depth in ATR measurements can be controlled by changing the angle of incidence, enabling depth profiling up to a few micrometers. This poster reports two new applications of FTIR-ATR imaging to obtain 1) a 3-dimensional depth profile of skin samples (human stratum corneum) by the combination of variable angle ATR with imaging and 2) the chemical composition and distribution of different substances in human stratum corneum under a controlled humidity environment. Univariate analysis as well as principle component analysis (PCA) were applied for the data treatment.

(601) Infrared Spectroscopy of Individual Exfoliated Human Cells
Max Diem, Benjamin Bird, Melissa Romeo; ¹Northeastern University

We have collected thousands of high quality images and infrared spectra from individual exfoliated cells. In general, cells were imaged first at low magnification (10X or 15X) using an infrared micro-spectrometer, while single cell infrared spectra were collected. These images are of insufficient quality to allow a cell-by-cell cytological diagnosis. After infrared data acquisition (ca. 2-4 sec/cell, resulting in a S/N ratio > 200:1), cells were stained using standard cytological staining procedures, and re-imaged at 40X magnification. To this end, the coordinates of each cell, stored during infrared data acquisition, were used to re-identify the cells after staining. For each of a number of cell types, we have collected hundreds of cells with corresponding high quality images. Whereas cytologists or cytotechnicians will not render a diagnosis of unstained cell images, the stained images of the majority of cells obtained in this fashion are of sufficient quality to get positive diagnoses. However, the cell preparation procedures used in large cytolgy laboratories differ substantially from the methods originally used by us. Thus, we have adapted cytolgical procedures such that spectra can be obtained that do not show effects of sample preparation (fixation). We have shown that very similar epithelial cells from different species (human and canine) can be reliably distinguished using principal component analysis (PCA) of the spectra. To this end, data sets containing about 1000 spectra were analyzed, and the mechanism of spectral distinction was investigated. Furthermore, we were able to distinguish three different cell types commonly found in human urine by PCA of the cell spectra, and could even use this procedure for blind identification of unknown cells.

(602) FTIR Characterization of Tumors in Woodchuck Liver. A Comparative Study.
Eric Pellerin¹, Eilean McKenzie¹, Mike Jackson¹; ¹National Research Council Canada

With the human hepatitis B virus, it is estimated that there are currently 350 million carriers worldwide who can transmit the virus throughout their lifetime. About 25 to 35 % of those with chronic carrier status will eventually die from complications of the infection, either from cirrhosis or hepatocellular carcinoma (HCC). Hepatocellular carcinoma is the 5th most common malignant tumor to be diagnosed. The eastern American woodchuck (Marmota monax) is an excellent model for the study of hepatitis and liver carcinoma, as the woodchuck hepatitis virus and the human hepatitis B virus are very similar in morphology, genome, methods of transmission, course of infection and progression to HCC. But with the exception that the progression from infection to HCC occurs only in 3 years in woodchucks compared to 30 years in man. As part of this project at the Institute for Biodiagnostic, the use of Infrared Spectroscopy was considered to analyze the chemistry of liver tumors. Since the infrared spectrum of a tissue sample provides a molecular fingerprint of the tissue, differences have been seen between the infrared spectra of normal and diseased tissues, because of changes in the disease process. The results shown will try to characterize these differences by mapping different liver sections, both normal and diseased, using a point-by-point method with a MCT detector and a globar source, a synchrotron source, as well as with the use of a FPA detector. An emphasis will be made on these three methods to try and compare the advantages and disadvantages of each one.

(603) Use of Raman Spectroscopy to Evaluate the API Crystal Form Stability in a Suspension
Aaron Garrett¹, David Reed¹; ¹Eli Lilly and Company

PAT is frequently used to efficiently explore the design space of new processes in R&D, but it can also be leveraged post-launch to better understand the control space of commercial processes. This presentation will highlight results obtained from the use of Raman spectroscopy to investigate the crystal form stability of a suspension as a function of time, API particle size, and temperature. The objective of this study is to determine if the
manufacturing hold-time of an intermediate can be increased without impacting product quality.

(604) Use of In-Line Near-Infrared Spectroscopy to Monitor Segregation of a Pharmaceutical Powder Blend in a Tablet Press

David Reed1, Marc Champagne1, Aaron Garrett1, Allen Steffler1, Jimmy Engle1; 1 Eli Lilly & Company

A method for real-time in-line near-IR (NIR) monitoring of dry powder blends for segregation within a tablet press is reported. A strategy was implemented to monitor and map potential areas where segregation is likely to occur by placing separate NIR probes in two different locations within a tablet press used for direct compression. One NIR probe was positioned at the bottom of the powder transfer chute located just prior to the tablet press gear box. The other NIR probe was positioned further downstream in the gear box where powder is pushed into the dye for tablet compression. A study design was established to strategically vary the drug concentration (i.e., API) at defined intervals to simulate segregation events. The trajectory of the varying API concentration through the entire tablet press was captured by both NIR probes and correlated back to the offline HPLC content uniformity of the stratified final ejected tablets. Good agreement was observed between the two NIR probe predictions of API content uniformity for the flowing powder relative to HPLC results of the ejected tablets. Feasibility results indicate that continuous in-line NIR measurement of powder uniformity within the tablet press is demonstrated to be a viable alternative to the traditional off-line HPLC content uniformity analysis. The potential to monitor a larger fraction of the entire blended sample preparation relative to the usual HPLC approach of testing a much smaller portion as whole tablets (via ICH stratified sampling approach) is very attractive. The in-line NIR method also provides an additional tool to understand and relate powder properties (such as particle size, shape, density, surface texture, cohesiveness, etc.) to powder uniformity and segregation. The potential use of the method for real-time monitoring of a running production process is now being explored.

(605) Chemometrics in Pharmaceutical Manufacturing: Feed Forward Control of Milling

Robert Roginski1, Paul Collins2; 1 Eigenvector Research, Inc.; 2 Eli Lilly & Company

In the FDA's Process Analytical Technology Initiative, the term "analytical" is viewed broadly so as to encompass chemical, physical, and microbiological measurements in addition to mathematical treatments and risk analysis of process data. Implementing such approaches - both for existing processes and for those currently in development - is highly encouraged so as to ensure quality and efficiency in manufacturing with less reliance upon end product testing. We present here a feed forward approach to controlling ultimate particle size distribution of a crystalline material. This approach, which combines multivariate laboratory analyses with process parameters is used to successfully meet targets in the final particle size, thereby minimizing batch-to-batch variability.

(606) Implementing PAT in R&D and Contract Manufacturing Environments

Andrew Lange1, Kevin Bittorf2, Ben Littler1, Tapan Sanghvi1, Jeff Katstra1, Sreedhar Shapally1, Nuno Matos2; 1 Vertex Pharmaceuticals, Inc.; 2 Iovione FarmaCiencia SA

Case studies will be presented regarding several specific PAT applications applied during development and transferred into the manufacturing environment. These examples will demonstrate the importance of a systematic approach to choosing the correct PAT tools for the correct unit operations. Perspective will be given regarding the similarities and differences in the use of PAT in two different environments: fully integrated development and manufacturing operations, and in the development environment with subsequent transfer to a contract manufacturer. The number and kind of PAT tools implemented will be different between the R&D and manufacturing sides of the business. The method for prioritizing PAT applications will be described as a combination of risk analysis and an investigation of the costs/benefits of implementation, yielding a stage appropriate method for implementation and long-term use.

(607) Application of a Tunable Diode Laser Absorption Spectroscopy (TDLAS) based PAT Sensor for Monitoring Vial Product Temperature during Lyophilization

William Kessler1, Stefan Schneider3, Henning Gieseler2, Michael Pikal1; 1 Physical Sciences Inc.; 2 University of Erlangen-Nuremberg; 3 University of Connecticut

An optically based TDLAS water vapor mass flux sensor was used to demonstrate real time, non-intrusive vial product temperature measurements during lyophilization. Experiments were performed using an FTS LyoStar II laboratory scale lyophilizer outfitted with a LyoFlux tunable diode laser absorption spectroscopy based mass flux monitor. The LyoFlux monitor continuously and non-intrusively measured the water vapor concentration and gas flow velocity in the duct connecting the lyophilizer chamber and condenser using Doppler-shifted near infrared absorption spectroscopy. The concentration (molecules/cm^3) and gas velocity (cm/second) measurements were combined with the knowledge of the duct cross sectional area (cm^2) to determine the water vapor mass flow rate (grams/second). The rate measurements were integrated to provide a determination of total water removed throughout the process. Through water sublimation experiments position dependent vial heat transfer coefficients (Kv) were determined and compared to gravimetric based determinations. The TDLAS and gravimetric based vial heat transfer coefficients were in good agreement. The calculated heat transfer coefficients for edge vials were approximately 20% higher than that of center vials. The heat transfer coefficients were combined with a heat and mass transfer model to determine average product temperatures during partial and full load freeze drying of sucrose, mannitol and glycine. Product temperatures calculated using the average Kv for all drying runs were in excellent agreement with “center vial” thermocouple data. As expected, thermocouple temperature data for “edge vials” were consistently higher than “center vial” data due to wall radiation effects. The TDLAS based non-intrusive temperature measurements demonstrate the potential to achieve enhanced process monitoring and control during laboratory scale lyophilization and during scale-up to manufacturing scale lyophilization were thermocouple data are often inaccurate and unreliable.

(608) Multivariate Batch Monitoring – Is there a Right Way?

Marc Champagne1, Aaron Garrett1, David Reed1, Allen Steffler1, Ken Sorak1; 1 Eli Lilly and Company

Within the chemometric community there are discussions about the unfolding of the batch data cube. The traditional chemometric approach has been unfolding variable wise for the observation layer and then using the scores of these results for building batch to batch multivariate model. The newer process engineering approach is to unfold along the batches using one model. Is one way better than the other or are they equivalent? This talk will show the results of batch projects case studies done at Lilly.
(609) Polarized Raman as a Probe of Structural Development in Electrospun Fibers
Bruce Chase1, John Rabolt2, Meghana Kakade3; 1DuPont; 2University of Delaware
Raman scattering is a powerful tool for the determination of structure and orientation in polymers, where the chemical structure is already known. Polymeric macroscopic properties such as tenacity, modulus, elasticity, etc. are determined by molecular level effects such as conformational state populations, orientation, and intermolecular interactions. Significant changes occur at the molecular level as a molten or solution phase polymer is spun into fiber form. The polymer goes from an unoriented, amorphous state to an oriented, semi-crystalline material via the deformations imposed by spinning and drawing. Raman spectroscopy can potentially provide information on both structure and orientation. Changes in band intensities can be related to conformational populations and to formation of crystalline regions. Changes in relative intensities as a function of incident and scattered polarization yields information on chain orientation. Electro-spinning, currently undergoing a renaissance, is a solution process whereby small diameter fibers (100s of nanometers) can be produced. With such small diameter fibers, small stresses during the spinning process can potentially have a very large effect of the mechanical properties of the final product. The issues of shear and tensile deformation in electro spinning are still largely unanswered. Electro spinning of nylon, polyethylene oxide fibers and synthetic spider silk provide examples where both conformational state populations and chain orientation can be perturbed by the process itself. The basics of electro-spinning and the use of vibrational spectroscopy to probe structure and orientation in such materials will be discussed.

(610) Raman Signal Enhancement in Deep Spectroscopy of Turbid Media
Pavel Matousek1; 1Rutherford Appleton Laboratory
A simple method for the enhancement of signals in transmission Raman and Spatially Offset Raman Spectroscopy (SORS) for non-invasive analysis of turbid samples is presented. The enhancement, which is typically several-fold, is achieved using a multilayer dielectric optical element acting as a unidirectional mirror preventing the loss of laser photons at the critical point of their entry into the sample. This leads to a substantial increase of the dielectric optical element acting as a unidirectional mirror which is typically several-fold, is achieved using a multilayer. The resulting increased Raman signal strength leads to a higher data quality and consequently higher sensitivity or penetration depth, features important in many analytical applications. Potential uses include the sensitive non-invasive disease diagnosis in vivo and the quality control of pharmaceutical products. The concept is also applicable in an analogous manner to other types of analytical methods such as fluorescence spectroscopy or it can be used to enhance the effectiveness of the coupling of laser radiation into tissue in applications such as photodynamic cancer therapy.

(611) Non-Invasive Raman Spectroscopy for Human and Animal Studies.
Michael D. Morris; 1University of Michigan
The development of fiber optic Raman probes specifically designed for highly scattering systems have enabled through-the-skin measurement in human and animal tissues at unprecedented depths. In these probes the exciting laser light is incident on the tissue at a point or points spatially separated from the collection point(s). Spatial separation of injection and collection zones emphasizes signals from below the skin and also has the important benefit of minimizing fluorescence background, which in the near-infrared arises mostly from skin melanin. Using a probe design in which a ring of laser light surrounds the field of view of a close-packed circular array (disk) of about 50 fibers, we have been able to measure bone tissue constituents at depths exceeding 5 mm with an accuracy of a few percent, sufficient for several proposed clinical applications. We will describe the latest results obtained in several animal models that are useful in the study of disease and genetic defects or that are useful as models of human tissue optics at clinically important sites. We will also describe new probe geometries adapted for small animal use and will summarize progress in Raman tomography.

(612) Analysis of Electronic vs. Geometric Parameters in Ligand-Receptor Binding using Raman Spectroscopy
Don Pivonka; 1AstraZeneca Pharmaceuticals
An application of vibrational spectroscopy has been developed as a tool with which to gain further understanding of how both the physical structure and the electronic properties of a molecule are related to activity within a biological assay, i.e., the structure-activity relationship (SAR). In that context, vibrational spectroscopy was first developed as a tool for identification of the molecular subcomponents, within a compound series, which play an active role in binding kinetics. Secondarily, vibrational spectroscopy has exhibited utility in uncovering electronic trends within both pendant functional groups and within the molecular backbone scaffold, which foster the binding process. The ability of this technique to differentiate electronic from geometric parameters of the ligand-receptor interaction will be specifically addressed. The success of this technology opens the door to a much broader investigation of ligand-receptor interaction.

(613) Attenuated Total Internal Reflection Raman Microspectroscopy
André Sommer; 1Miami University
Attenuated total internal reflection (ATR) infrared spectroscopy is a routine analytical tool that enables one to collect infrared spectra from very thin surface layers of highly absorbing samples. When coupled with an infrared microscope and a hemispherical internal reflection element, the method provides the additional benefit of high spatial resolution in the x-y plane. The resultant volumetric resolution of the method is excellent allowing volumes of less than one femto-liter to be probed (1). Since all spatial characteristics are fundamentally limited by the wavelength of light, the probed volume can be reduced to sub atto-liter volumes by reducing the wavelength by a factor of 10. However, in order to maintain the molecular information content of the method ATR Raman microspectroscopy must be employed. ATR Raman spectroscopy and ATR–SNOM (Scanning Near Field Microscopy) - Raman spectroscopy have previously been reported but the systems studied included highly scattering samples (2, 3). This paper will present an overview of the potential of ATR Raman microspectroscopy and investigate the use and technical limitations of the method for the analysis of conventional samples. References: 1. B. M. Patterson, N. D. Danielson and A. J. Sommer, Anal. Chem., 75(6), 1418-1424 (2003). 2. M. Yoshikawa, T. Gotoh, Y. Mori, M. Iwamoto and H. Ishida, Appl. Phys. Lett., 64 (16), 2096-2098 (1994). 3. M. Futamata and A. Bruckbauer, Chem. Phys. Lett. 341 (5-6) 425-430 (2001).

Paul Pudney1, James Day1,2, Jeroen Bongaerts3; 1Measurement Science Unit Unilever Research, Colworth; 2Durham University; 3Corporate Research P&ES Unilever Research
Lubrication is ubiquitous in the human body and we would like to try and understand how this influences ‘feel’, especially on the skin and in the mouth and also how it might change delivery of actives.

ABSTRACTS
To help us understand these effects we have been using and developing soft tribology methods. However direct information on the shape and content of the rubbing contact from these measurements have, so far, been missing. To answer these questions we have developed a unique tribology-Raman instrument that allows optical and spectroscopic experiments of lubricated rubbing contact and simultaneous lubrication measurements. It consists of a confocal Raman instrument coupled with a modified ‘Mini Traction Machine’. The contact consists of a quartz window shear rates, and film thickness to the lubricating properties. We are now in a position to start linking lubricant composition, does change from the bulk composition under certain conditions. the rubbing contact and when breakdown of emulsions occurs Raman measurements. This allows us to show what is entrained in demonstrate that we can determine what is in the gap from the Raman measurements. This allows us to show what is entrained in the rubbing contact and when breakdown of emulsions occurs under shear. We show that an emulsion composition in the gap does change from the bulk composition under certain conditions. We are now in a position to start linking lubricant composition, shear rates, and film thickness to the lubricating properties.

(615) Developing a Capability to Detect and Identify Explosives Remotely

John Reaugh1, Kambiz Salari1, Gregory Klunder1, Sorin Bastea1, Richard Beherens, Jr.2, Sean Maharrey2,1 Lawrence Livermore National Laboratory; 1Sandia National Laboratory California

The goal of our program is to develop the capability to detect and identify explosives at a distance of 50 meters or more downwind. To do so, we characterize the vapor and small particulate plume that is emitted by a quantity of chemical so that we can utilize or develop methods to detect the relevant species. It is well known that the vapor pressures of RDX, HMX, and other high performance explosive crystals are too low to be detected. We are characterizing the volatiles emitted from an explosive, both composition (what chemical species are present) and concentration (how much) as the plume evolves and is transported through the atmosphere. Solid Phase Microextraction (SPME) has been used at our laboratory and elsewhere to collect the volatiles in the head-space surrounding explosives. In published work, the volatiles have included chemical feed stock for explosive synthesis, co-products made in the synthesis, solvents used in either synthesis or purification/recrystallization steps, taggants introduced by international agreement, and in some cases the parent explosive. The technique is well established for determining the composition, but the concentration cannot be quantitatively established. The Sandia Simultaneous Thermogravimetric Modulated Beam Mass Spectrometer (STMBMS) technique measures the specific evolution rate and concentrations of the various species that were identified with SPME, and checks for the appearance of other species as well. The evaporation rates per unit area and partial pressures of each species are used to develop a source term for Computational Fluid Dynamics (CFD) simulations. These simulations of turbulent flow are used to computationally transport the species from the explosive to plausible detector locations over the operational distance (50 to 80 meters). We present results of our experiments and simulations as applied to a particular case of explosive emplacement. This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under Contract W-7405-ENG-48.
using these fibers. Therefore, other coatings will be investigated to address the lower vapor pressure explosives.

(619) Application of Sensor Fusion to Explosives Detection
Patrick Treado¹, Matthew Nelson¹, Jason Neiss¹, Robert Schweitzer¹, Charles Gardner¹; ¹ChemImage Corporation
Atomic and molecular spectroscopy, especially when performed in conjunction with hyperspectral imaging, are well suited to the detection of explosives in both close-contact (proximity) and standoff detection modes. In this presentation, we will describe efforts to combine laser induced breakdown spectroscopy (LIBS), Raman spectroscopy and hyperspectral imaging to the detection of explosive hazardous materials in complex backgrounds. We will emphasize the use of objective figures of merit, including probability of detection (Pd), probability of false alarms, and receiver operator characteristics (ROC) curves to assess sensor performance.

(620) Enabling Field-Based Material Determination with Handheld Spectroscopy: Instrumental Advances and Applications in Public Safety and Security
Robert Green¹, Wayne Jalenak¹, Javier Santillan¹, Christopher Brown¹; ¹Ahura Scientific
There is an increasing demand for rapid analytical test procedures that can be performed outside of the laboratory at the point of need by scientists and non-scientists alike. Fieldable solutions for determination of materials used in improvised explosive devices (IEDs), chemical warfare agents, and illegal drug manufacture and trade are of particular interest. Vibrational spectroscopy is expressly useful for material identification and screening due to inherent analytical selectivity and the range of analytes that can be measured. Furthermore, recent technological advances have transformed spectroscopic systems from expensive, delicate, laboratory devices requiring careful operation and maintenance to ruggedized, miniaturized (< 4lb) handheld systems designed to be operated by non-experts. In this presentation, we discuss handheld chemical identification systems that bring together ultra compact laser packaging, state-of-the-art microfabrication, and advances in analytical intelligence including probability based decision making. These unique hardware and software modifications allow for reliable performance over a range of operating conditions including temperature, humidity, and transit shock. The utility of vibrational techniques for determination of IEDs including peroxide based explosives that can be prepared from relatively innocuous household chemicals will be presented. In addition, the use of handheld spectroscopy in the remediation of clandestine drug manufacturing operations will be described. Finally, tactical issues will be illustrated through the use of case studies and real-world experiences.
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<td>Zou, Shengli</td>
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