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Attention Presenters: Check this final program to verify schedule of your talk or poster. Changes may have occurred since the preliminary program.

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FACSS National Office
2019 Galisteo Street, Building I-1, Santa Fe, NM 87505
(505) 820-1648  Fax: (505) 989-1073  facss@facss.org  www.facss.org
On behalf of the FACSS Governing Board and the FACSS Executive Committee it is our pleasure to welcome you to Portland for the the 31st annual meeting of the Federation of Analytical Chemistry and Spectroscopy Societies.

FACSS is a special conference in the analytical community in that it brings together researchers from a variety of scientific disciplines. The goal of the FACSS meeting has always been to facilitate communication between researchers in all the analytical sciences. In our view, sharing work with people in other, sometimes unrelated disciplines stimulates new thinking about how their own work is generated and disseminated. In contrast to many highly topical conferences, the atmosphere and program at FACSS promotes fresh, lateral thinking.

For several years, the organizing committee has listened to the constructive comments from attendees at past meetings. In response to that feedback, a new format for the technical program was implemented at the 2004 conference. This format is designed to provide more time to bring together the attendees to encourage, mixing, discussion, and exchange of ideas. For this new format, each day will begin with ‘wake-up coffee’ followed by plenary presentations by an internationally acclaimed speaker and FACSS award winner. The technical program will consist of only nine, highly focused, concurrent sessions per AM and PM period, and each of those sessions will be comprised of both poster and oral presentations. Ample time will be allotted to the poster presentations to maximize their visibility and impact. We welcome your feedback on the changes.

This year’s technical program features thematic symposia in the topical areas of Atomic Spectroscopy, IR and Near IR, Raman Spectroscopy, Education, Forensics, Chemometrics, Nanoscience and Nanomaterials, Process Analytical Chemistry, special sessions in recognition of FACSS award winners, and an expanded emphasis on Bioanalytical Chemistry. Sessions devoted to emerging areas include Metallomics, advanced data acquisition strategies and data analysis, popular areas such as Sample Handling techniques for IR characterization, imaging, long distance education, weapons of mass destruction, and week-long emphasis on Proteomics by Mass Spectrometry, Nanotechnology for carbon tubes and Bioanalytical research. Plenary lecturers include William Schopf from the Department of Earth and Space Sciences, and Center for the Study of Evolution and the Origin of Life, University of California, Los Angeles. Dr. Schopf’s Monday morning address is titled 'Earth’s Earliest Fossils: Solution to Darwin’s Dilemma.’ Tuesday morning lectures will be by Walt Jennings, Anachem Award winner and Mike Carrabba, the Charles Mann Award Winner. A Wednesday plenary lecture will be given by Boris Mizaikoff, the Meggers Award Winner. Thursday’s plenary will be by Richard A. Mathies, the Lippencott Award Winner.

However, FACSS is more than scientific presentations and symposia. There is a wide collection of workshops to choose from, an Employment Bureau, and of course a state-of-the-art research tools and instruments exhibit.

If you are a visitor to Portland, make sure you take time to enjoy the "City of Roses". Portland is a beautiful blend of urban parks, internationally acclaimed attractions, world-class shopping and dining, and a thriving arts community offering a colorful palette of art galleries, local theater and Broadway performances! Outside magazine voted Portland one of the "10 Greatest Places to Live". On Wednesday, October 6 join your colleagues at the Portland Classical Chinese Garden a classical Chinese garden where you will enjoy hundreds of rare and unusual shrubs, perennials, water plants, bamboo and orchids amidst a landscape of pavilions, stone, and poetry. At this event you will enjoy Chinese influenced cuisine as well as a sampling of Oregon's fine wines and reserve beers. Ask at the FACSS registration desk for ticket information.

Finally, the excellence of FACSS is the result of the hard work of a large group of individuals who selflessly volunteer their time and energy. When you see someone wearing a "Committee Ribbon" on their name tag please take the time to thank them for their efforts. Better yet, offer to become involved in the organization of next years FACSS meeting. We can always use more help.

Michael Blades  David Trimble  George Agnes
2004 Governing Board Chair  2004 General Chair  2004 Program Chair
EVENTS OF INTEREST TO STUDENTS

Sunday Evening, Holladay Lobby
• Welcome Mixer
• SAS Student Poster Session

Monday
• Employment Bureau in Rooms B117 – B118 opens at 8:30 AM
  Monday – Thursday 8:30 AM – 5:00 PM

Tuesday
• 12:00 AM – 1:15 PM, Student/Professional Panel Discussion and brown bag lunch, Room B118

Wednesday
• 8:30 AM – 5:00 PM, Professional Analytical Chemists in Industry: A Short Course for Undergraduate Students; Diane Parry, instructor, No charge
• 4:00 – 5:00 PM, Strategies for Career Development, Room B113

STUDENT POSTER AWARD SPONSORS

Society for Applied Spectroscopy (SAS)
  Analytical Chimica Acta
  CRC Press
  IM Publication
  John Wiley & Sons
  Meinhard Glass Products
  Spring-Verlag

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GENERAL INFORMATION

LOCATION: All conference symposia and exhibits will be held at the Oregon Convention Center, 777 NE Martin Luther King Jr. Blvd, Portland, OR 97121. Saturday and Sunday Workshops will be held at the Doubletree Hotel Lloyd Center, 1000 NE Multnomah, Portland, OR. Monday through Thursday workshops will be held at the convention center.

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 carefully adhere to the time allotted for the talk.

SPEAKER READY ROOM. A room is equipped with an LCD projector. The speaker ready room is A102.

POSTER SESSIONS.
Sunday Poster Session: There will be a Sunday evening SAS Student poster session during the welcome mixer from 5:00 – 7:00 PM in the Holladay Lobby of the convention center.

Monday - Thursday Poster Sessions will take place in the Exhibit Hall. The morning poster session is scheduled for 9:00 – 10:30 AM and the afternoon poster session is scheduled for 2:00 – 3:30 PM. Your poster should remain up all day. Odd numbered posters present in the morning session and even numbered posters present in the afternoon session.

FACSS WORKSHOPS. A list of workshops, descriptions, and the locations begins on page 28. You must register for a FACSS workshop at the conference registration desk.

EMPLOYMENT BUREAU. The bureau will be located in Rooms B117-B118 at the convention center. The center will be open Monday through Thursday, 8:30 AM to 5:00 PM. Registration forms are available at the employment bureau. See page 33 for additional information.

INTERNET CAFÉ. Internet access will be available in Exhibit Hall A-1 Tuesday and Wednesday 9:00 AM – 4:00 PM and Thursday 9:00 AM – 2:00 PM

EXHIBITS. The exhibition is located in Hall A-1 and will be open as follows: See page 20 for details.

BREAKS. All conference refreshment breaks will be located in the Exhibit Hall

REGULATIONS. The following regulations are in the best interests of the conference.
1. There is no smoking in any conference area.
2. An official name badge is required for admission to any session or the Exhibit Hall.
3. No advertising may be placed in the conference area.
4. Only official exhibitors may display in the Exhibit Hall.

SPECIAL EVENTS.

SUNDAY
5:00 – 7:00 PM Welcome Mixer and SAS Student Poster Session, FACSS and SAS Award Presentations, Holladay Lobby

MONDAY
8:00 AM Plenary Lecture: Earth's Earliest Fossils: Solution to Darwin's Dilemma, J. William Schopf, University of California, Los Angeles

5:30–7:30 PM Reception for Exhibit Opening (wine, beer, snacks), Hall A

TUESDAY
8:00 AM ANACHEM Award, Brief History of Developments in GC Columns, Walter Jennings, Agilent Technologies, Inc.

8:30 AM Charles Mann Award; Raman Spectroscopy: How Did We Get Here and Where Are We Going?, Michael Carrabba, Hach Homeland Security Technologies

12:00 – 1:15 PM Student/Professional Panel Discussion and brown bag lunch, Room B118

Noon Lunch for conference, Room B118
(Tickets required)

WEDNESDAY
8:00 AM Plenary Lecture: Semiconducting and Piezoelectric Nanobelts, Nanorsprings and Nanorings; Zhong Lin Wang, Georgia Institute of Technology

8:30 AM Meggers Award; Mid-Infrared Chemical Sensors - From the Bench into the Deep Sea, Boris Mizaikoff, Georgia Institute of Technology

4:00 PM Strategies for Career Development, all students welcomed, Room B113

6:30 PM FACSS Gala, Portland Classical Chinese Garden, Ticket required

THURSDAY
8:00 AM Lippencott Award; Femtosecond Stimulated Raman Spectroscopy, Richard A. Mathies, University of California, Berkeley

Noon Farewell luncheon for exhibitors and guests.

COMPANION REGISTRATION. Companion registration is offered for persons accompanying conference registrants and includes a designated name badge and the activities listed below. Cost is $45.

MONDAY
9:00 AM Introduction to Portland, Coffee and pastries, Room A 109

5:30–7:30 PM Reception for Exhibit Opening. Wine, beer, snacks, Hall C

TUESDAY and WEDNESDAY
9:00-11:00 AM Coffee and pastries, Room A 109
FACSS ORGANIZATION

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

2004 Chair Persons

Governing Board Chair  Michael Blades, University of British Columbia
                      E-mail:  blades@chem.ubc.ca
Governing Board Chair Elect Mark Hayes, Arizona State University
Past Governing Board Chair  Michael Carrabba, Hach Homeland Security Technologies
Second Past Governing Board Chair  Ron R. Williams, Saginaw Valley State University
Secretary  John Graham, Hercules Inc.
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Exhibit Chair  Scott McGeorge, Transition Technologies, Inc.
                E-mail:  mcgeorge@transition.ca
General Chair  David Trimble, Swarthmore College
                E-mail:  dtrimbl1@swarthmore.edu
Program Chair  George Agnes, Simon Fraser University
                E-mail:  gagnes@sfu.ca
Workshops Chair  Christine Wehlburg, MITRE Corporation
Employment Chair  Randy Bishop and Drew Manica, GE Plastics
Local Support  Gary Beck, ATI Wah Chang

2004 Program Section Chairs

Atomic Spectroscopy  George Agnes, Simon Fraser University
Awards  Paul Farnsworth, Brigham Young University
Bioanalytical  Dana Spence, Wayne State University
Chemometrics  Paul Gemperline, East Carolina University
Education  Pam Mabrouk, Northeastern University
Forensics  Greg Klunder, Lawrence Livermore National Lab.
IR and Near IR  John Hellgeth, Hewlett-Packard
Mass Spectrometry and Proteomics  Liang Li, University of Alberta
Nanoscience and Nanomaterials  Wei Zhao, University of Arkansas and Stephen K.
                                      Doorn, Los Alamos National Laboratory
Process Analytical  James Rydzak, GlaxoSmithKline
Raman  Ian Lewis, Kaiser Optics
SAS Student Poster Session  Bonnie Saylor and Victor Hutcherson, Society for Applied Spectroscopy

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Michael W. Blades  
*University of British Columbia*

Michael Blades was born in 1951 in Barrington Passage, Nova Scotia, Canada. He attended Barrington Passage Municipal High School and in 1971 obtained a diploma in Electronic Engineering Technology from the Nova Scotia Institute of Technology and worked for a brief period as an electronic technician at the Defense Research Establishment - Atlantic in Dartmouth, Nova Scotia. He received his undergraduate degree at St. Marys University (Halifax, Nova Scotia) in 1975 and his PhD at the University of Alberta in 1980 under the supervision of Dr. Gary Horlick. He subsequently went to Indiana University to work as a postdoctoral research associate in the laboratory of Dr. Gary Hieftje (1980-81). He has been at the University of British Columbia since 1981 and since September 2003 has been Acting Head of the Chemistry Department. 

His current research interests are in the areas of ion-trap mass spectrometry coupled with laser desorption/resonant laser photoionization and fluorescence spectroscopy, development and application of ultraviolet resonance Raman spectroscopy (UVRRS) and visible Raman microscopy for biophysical and bioanalytical measurements including the study of protein adsorption, protein structure/function relationships, protein-protein interactions of interest in immunology and enzymology, assays for steroids and other small biomolecules. Blades has published approximately 95 scientific papers in refereed journals. He has received a number of honours and awards including the 1987 Canadian Society for Chemistry McBryde Medal, a University of British Columbia Killiam Research Prize (1988-89), a Senior Killiam Fellowship (1991-92), the Canadian Society for Chemistry 1994 Fisher Lecture Award, the 1995 Royal Society of Chemistry Analytical Spectroscopy Award, and the 2004 Spectroscopy Society of Canada Smith Detection Award. He has served on the editorial advisory boards of *Spectrochimica Acta B*, *Applied Spectroscopy*, and the *Journal of Analytical Atomic Spectrometry* and is currently the Canadian Editor for *Applied Spectroscopy*. 

In 1999 Blades was the General Chair of the FACSS meeting, which marked the first joint meeting with the International Conference on Analytical Sciences and Spectroscopy (ICASS) and the first time the FACSS meeting had been held outside of the United States. In addition to his role as Governing Board Chair for the FACSS for 2004 he is the zone representative and Analytical Chemistry convenor for the joint Pacific Basin Societies Chemistry Conference (Pacifichem 2005). 

Blades likes to play hockey with his colleagues at UBC, ride his windsurfer and snowboard, play guitar, and drink the beer with his friends.
George R. Agnes  
*Simon Fraser University*

George is an associate professor in the Department of Chemistry at Simon Fraser University. He joined the faculty there as an assistant professor in 1995, following a postdoctoral fellowship at Indiana University in 1994 (Supervisor G. Hieftje) and his doctoral training at the University of Alberta (Supervisor G. Horlick).

The program of research that he has developed has evolved to become exclusively centered on the use of levitation technologies to investigate fundamental and applied phenomena. This line of research was initiated following receipt of a Young Investigator Award from the American Society for Mass Spectrometry in 1998. Current areas of study include developing strategies for the preparation of picoliter aliquots of solution for subsequent analysis using instrumental methods, such as MALDI-MS. Fundamental studies being performed by his group include chemistry in media that have net charge, imaging of biomacromolecule distributions in materials, ion generation processes in Electrospray, and research at the interface between atmospheric particle chemistry and lung cell biology to address longstanding questions concerning particulate air pollution. He has trained 7 graduate students and 1 postdoctoral fellow, published 20 refereed manuscripts, 2 patents, and he filed 3 provisional patents within the past year.

George is an active outdoor enthusiast and he enjoys living in the greater Vancouver, BC area solely because it is a well-located jumping off point for a multitude of sporting activities such as hiking, surfing, skiing, kayaking, fishing, scuba diving, and mountain biking. When away from the city (which he feels is not often enough), he obsessively pursues high-wind windsurfing and alpine skiing depending on the season. When confined to the city, he cycles year round each morning up a small mountain to his office and laboratory at SFU.

---

Scott W. McGeorge  
*Transition Technologies Inc.*

Scott founded Transition Technologies in 1994 and focused on scientific product distribution and consulting to meet the demands for laboratory productivity enhancements in the Canadian marketplace. In 1999 the Company expanded into the life science arena and currently expends a significant effort servicing the medical genetics community providing solutions for mutation detection and nucleic acid analysis using denaturing HPLC methods.

Scott received his B.Sc. degree in chemistry from the University of Waterloo with a minor in computer science in 1980. He was able to combine aspects of these disciplines at McGill University in Montreal where he studied with Dr. Eric D. Salin. He received his Ph.D. in 1985 for applications of image sensor technology for ICP-AES.

After graduate school, Scott worked for a small instrumentation company with funding from an Industrial Research Fellowship. He later managed a corporate group assigned to the development of multiple dispersion ICP spectrometer systems employing echelle optics and photodiode array detection. He founded Transition Technologies in the summer of 1994 and currently enjoys serving a client base with wide ranging interests and problems. He has authored or co-authored 13 publications. He has served as Exhibit Chair for FACSS since 1996 and continues to enjoy this involvement.

Research interests include novel methods for DNA heteroduplex analysis to enhance the accuracy and throughput for genetic mutation screening and scoring. New directions for the business include contract laboratory services targeting niche applications associated with the company’s core competencies. Scott is active in the martial arts earning a black belt in Goju Jitsu Ryu (Renshi Michael Neville, 5th Dan) last October and shortly afterward a black belt in conventional Jiu Jitsu (Shihan Robert Krantsz, 7th Dan). Yoi.
### PROGRAM SPONSORS

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- Dorothy Mann, on behalf of the Mann Family

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- Springer-Verlag
LEVEL 1
Session Rooms, Employment Bureau, Exhibits, Posters, Workshops

Exhibit Hall A1
Exhibits
Internet Café
Breaks
Award Posters

Exhibit Hall A
Poster Sessions

Exhibit Hall B

Sunday Welcome Mixer and SAS Poster Session
Holladay Lobby, Level 2

PLENARY SESSIONS
Ballroom 201, Level 3
FACSS AWARDS

The Tomas Hirschfeld Award and the FACSS Student Award recognizes outstanding contributions by individuals who are Ph.d. and M.Sc. candidates

TOMAS HIRSCHFELD AWARD

Ryan J. Priore
University of South Carolina

Ryan Priore received his Bachelor of Science degree in Chemistry from the University of Pittsburgh in May 2001. During his undergraduate studies, his research focused on measuring the elastic modulus differences between benign and malignant breast cancer tissue under the direction of Dr. Gilbert Walker. He also interned at ChemImage Inc. (Pittsburgh, PA) where he was introduced to the field of chemical imaging. In his two-year internship, Ryan used Raman microspectroscopy as a materials characterization tool.

Ryan is currently pursuing his doctoral studies at the University of South Carolina with an emphasis on chemical imaging via multivariate optical computing under the direction of Dr. Michael Myrick. His research interests lie broadly in the design and fabrication of thin films for predictive imaging spectroscopy and the development of real-time chemical imaging techniques. Currently he is applying thin film based optical computing to the IR using photoacoustic detection schemes.

Ryan was the recipient of the Raymond Davis Scholarship from the Society for Imaging Science & Technology in 2003. He received the Bouknight Outstanding Teaching Award and the Durig Travel Award from the University of South Carolina in 2002. His graduate research commenced in the summer of 2001 with the Copenhaver Research Fellowship. Ryan has been an author on 7 publications and conference proceedings and has presented his research at over 10 international conferences.

FACSS STUDENT AWARD

Lawrence W. Dick, Jr.
Duke University

Lawrence (Larry) is pursuing his Ph.D. in Chemistry from Duke University. He graduated from the University of Scranton, Scranton PA in 2001 with a B.S. in Biochemistry. As an undergraduate, Larry performed independent research under the supervision of Dr. Joe Vinson on the effects of cranberries and cranberry juice on formation of atherosclerosis in a normal hamster model. Larry's dissertation research at Duke, under the direction of Dr. Linda B. McGown, is focused on the use of aptamers in analytical chemistry. He has published two papers and made three conference presentations on this work. His most recent work is on a new approach to affinity MALDI that uses aptamer arrays as the affinity platform.

Larry is currently living in Clifton Park, NY and finishing his Duke University degree as a Visiting Researcher at Renssleer Polytechnic Institute, Troy, NY with Dr. McGown. He is a member of the American Chemical Society and Phi Lambda Upsilon.
**DISTINGUISHED SERVICE AWARD**
Recognizing members for their long-time service to the society.

Kathryn S. Kalasinsky

Kathryn S. Kalasinsky received her B.S., M.S., and Ph.D. degrees from the University of South Carolina. She has over 25 years experience in the fields of environmental and forensic toxicology. She recently entered the field of microbiology where she is currently exploring spectroscopic methods of biothreat detection. After many years of service in state government and industry, Dr. Kalasinsky began working for the federal government at the Armed Forces Institute of Pathology in 1991 where she became Chief of Research and Education for the Division of Forensic Toxicology in the Office of the Armed Forces Medical Examiner. Dr. Kalasinsky is well known for her many applications of spectroscopy to solving forensic problems primarily for drugs of abuse questions. She is currently the Chief of Optical Spectroscopy in the Division of Microbiology in the Department of Infectious and Parasitic Diseases Pathology at the Armed Forces Institute of Pathology. She has over 200 publications and presentations in the field and is currently serving on the editorial boards of two spectroscopy journals. Dr. Kalasinsky has served as President of the Coblentz Society and the Society for Applied Spectroscopy. She is the recipient of the 1995 Irving Sunshine Award for Outstanding Research in Forensic Toxicology from the American Academy of Forensic Sciences.

**HONORARY MEMBERSHIP AWARD**
Recognizing those individuals who have made exceptional contributions to spectroscopy

Mitsuo Tasumi

Mitsuo Tasumi was born on January 23, 1937 in Nishinomiya, Japan. He received his B.Sc., M.Sc., and D.Sc. From the University of Tokyo. His postdoctoral training was at the University of Michigan under Professor S. Krimm and at the Politecnico di Milano, Italy under Professor G. Natta. He is currently President and Professor Emeritus at Saitama University. He is also Professor Emeritus at the University of Tokyo, a member of the Board of Directors of ASIA SEED, a member of the Senate of Shibaura Institute of Technology, Visiting Professor at the College of Chemistry at the University of California at Berkeley.

Dr. Tasumi is an expert in the field of vibrational spectroscopy and is currently interested in the developments in computer capabilities and theoretical treatments of molecular potential functions to simulate accurately vibrational spectra of molecules in various environments.

Dr. Tasumi has received numerous awards including Fellow of the Optical Society of America, the TRVS Award from the International Conference on Time-Resolved Vibrational Spectroscopy, the Purple Ribbon Medal from the Japanese Government, the Ellis R. Lippincott Award, the Prize of the Spectroscopical Society of Japan, the Prize of the Chemical Society of Japan, the Prize of the Society of Polymer Science of Japan, and the Fulbright Scholarship for Researchers. He has published extensively over the course of his distinguished career. Dr. Tasumi has served as a member of the Editorial Boards of the *Journal of Molecular Structure, Vibrational Spectra and Structure, Spectrochimica Acta, Journal of Raman Spectroscopy, Vibrational Spectroscopy, Section of Analytica Chimica Acta, Comprehensive Polymer Science, and Biopolymers/Biospectroscopy*. He is a member of numerous professional organizations and has been involved with a vast array of international conferences and meetings.
LESTER W. STROCK AWARD
Established by the SAS New England section to recognize an author(s) of an outstanding paper or series of papers.

James D. Winefordner
James D. Winefordner was born on December 31, 1931 in Geneseo, IL, USA. He received his B.S., M.S., and Ph.D. degrees in chemistry from the University of Illinois in 1954, 1955, and 1958, respectively. His research advisor was Professor H.V. Malmstadt. From September 1958 to September 1959, he served as a post doctoral fellow at the University of Illinois. In September 1959, he was appointed Assistant Professor of Chemistry at the University of Florida. In September 1965, he was promoted to Full Professor. He was appointed Graduate Research Professor of Chemistry at the University of Florida in September 1976. He was Chairman of the Analytical Division of the Department of Chemistry for 30 years.

His research interests include: atomic and molecular emission, absorption, and fluorescence in flames and other hot gases; molecular fluorescence and phosphorescence of species in the condensed phase; development of sensitive, selective gas and liquid chromatographic detectors; and development of spectroscopic instrumentation for analysis. He has published over 850 scientific papers, 10 chapters, and 40 refereed reviews on the above topics and given over 400 invited talks and seminars at international and national conferences and symposia and at universities, colleges, and industries. Since coming to the University of Florida, 155 of his graduate students received Ph.D. degrees and 37 more M.S. degrees. He has also had 95 post doctoral associates work with him.

He is a member of the American Chemical Society, Society of Applied Spectroscopy, Phi Lambda Phi, Alpha Chi Sigma, and American Association for Advancement Sciences. He has generated over 22 million dollars in individual grant funds. He has been a member of the Advisory Boards of Journal of Pharmaceutical and Biomedical Analysis, Analytical Sciences, the Analyst, Progress in Analytical Spectroscopy, Analytical Chemistry, Analytical Letters, and Chemical Instrumentation and currently is Chairman of the Advisory and Editorial Boards of Talanta, Spectrochimica Acta B, Polycyclic Aromatic Hydrocarbons, and on the Advisory Board of Canadian Journal of Spectroscopy. He is Editor of the Wiley Chemical Analysis Series and was the 1983 President of Society of Applied Spectroscopy (SAS). Dr. Winefordner is a past chairman of the Analytical Division of the American Chemical Society (ACS) and was a member of the NBS Evaluation Panel, 1975-1978, and was a member of the NSF Advisory Board in Chemistry (1977-1979).

He received the 1971 Sigma Xi University of Florida Research Award, the 1968 Meggers Award, the 1973 ACS Award in Analytical Chemistry (Fisher Award), the 1973 Pittsburgh Society of Applied Spectroscopy award, and the 1978 ACS Chemical Instrumentation Award co-sponsored by the Division of Analytical Chemistry and the Instrumentation Specialties Company. He was also the recipient of the 1980 ANACHEM Award, the 1981 Theophilus Redwood Lecture Award, the 1982 ACS Florida Section Award, the 1982 Southern Chemist Award, the 1983 SAS Honorary Membership Award, the 1984 University of Florida Teacher/Scholar of the Year Award, the 1984 Golden Key Honorary Membership, the 1985 Blue Key Distinguished Faculty Award, 1986 Honorary Member Japan Society of Analytical Chemistry, 1987 Torbern Bergman Award, 1987 ACS Analytical Division Spectroscopy Award, Spectrochimica Acta B Best Paper Awards for both 1988 and 1997, the 1989 New York Section Eastern Analytical Symposium Spectroscopy Award, the 1991 Pittsburgh Analytical Chemistry Award, the 1993 Cincinnati Section of ACS Oesper Award, the 1993 Talanta Gold Medal, the November/December 1994 issue of Spectrochimica Acta B (which was an honor issue for J.D.W.), the 1995 ACS Analytical Division Award for Teaching, the 1996 Eastern Analytical Symposium Award for Outstanding Research in Analytical Chemistry, 1996 Robert Boyle Award, 1997 and 2001 Pergamon Spectrochimica Acta B Best Paper Awards, the 2001 University of Florida Foundation Professorship, the 2002 UF Doctoral Dissertation Advisor and Mentoring Award, and the 2003 Colloquium Spectroscopicum Internationale Award for Outstanding Contributions to Analytical Spectroscopy.

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.

Richard A. Mathies
Richard A. Mathies received his B. S. Degree in Chemistry in 1968 at the University of Washington. He earned the M. S. Degree in 1970 and the Ph. D. in 1973 in Physical Chemistry at Cornell University from Andreas Albrecht. Following two years of study as a Helen Hay Whitney Postdoctoral Fellow at Yale with Lubert Stryer, he moved to the Chemistry Department at the University of California at Berkeley in 1976 where he is Professor of Chemistry.

Mathies has used resonance Raman spectroscopy to elucidate the structure and reaction dynamics of energy and information transducing photoactive proteins. His work on the photochemistry of the visual pigment rhodopsin has established the structure of the primary photoproduct, demonstrated that the primary cis-to-trans photoisomerization in vision is complete in only 200 fs, and analyzed the nuclear evolution that governs the excited state isomerization. His recent development of femtosecond stimulated Raman spectroscopy provides a new way to study structural dynamics of reaction intermediates and transition states with high resolution vibrational spectra and sub-100 fs time resolution.
MEGGERS AWARD
Recognizing the author(s) of an outstanding paper appearing in Applied Spectroscopy

Presented to Markus Janotta, Abraham Katzir, and Boris Mizaikoff for the paper entitled
“Sol-Gel-Coated Mid-Infrared Fiber-Optic Sensors.” Volume 57 Number 7

Marcus Janotta
Dr. Marcus Janotta was born in Austria. His PhD thesis: “Chemical Modifications for improved Mid-Infrared Evanescent Field Sensing Systems” was performed at the Institute for Analytical Chemistry / TU Vienna and the School of Chemistry and Biochemistry / Georgia Tech (Dr. Boris Mizaikoff). His Master Thesis “Molecularly Imprinted Polymers for Optical Chemical Sensors” was performed at the Institute for Analytical Chemistry / TU Vienna (Dr. Boris Mizaikoff) and at the Institute for Applied and Pure Chemistry / Lund, Sweden (Dr. Klaus Mosbach). Dr. Janotta is currently in a research and teaching position at the University of Applied Sciences Wr. Neustadt/Tulln.

Abraham Katzir
Biographical sketch not available

Boris Mizaikoff
Dr. Boris Mizaikoff received his Ph.D. in Analytical Chemistry at the Vienna University of Technology in 1996. Heading the Chemical Sensor Laboratory (CSL), he has been responsible for numerous research projects in the field of chemical IR sensors, including 5 multinational projects funded by the European Union. In 1997, he joined the University of Texas, Austin as a postdoctoral fellow. In October 2000 he finalized his Habilitation (Assoc. Prof. For Analytical Chemistry) at the Vienna University of Technology. Today his research interests focus on optical sensors, biosensors and biomimetic sensors operating in the mid-infrared spectral range, novel IR light sources (e.g. quantum cascade lasers), system miniaturization and integration based on micro- and nanofabrication, multifunctional scanning nanoprobes (e.g. combination AFM-SECM, SNOM-SECM), scanning probe tip integrated nano(bio)sensors, development of chemical recognition layers and sensing membranes (e.g. molecularly imprinted polymers, functionalized sol-gels), chemometric data evaluation, and advanced vibrational spectroscopic techniques including SEIRA and SERS.

Dr. Mazaikoff is author/co-author of over 70 refereed publications, 9 international patents and numerous contributions at scientific conferences. Since fall 2000 he has been a faculty member at the Georgia Institute of Technology, School of Chemistry and Biochemistry, heading the Applied Sensors Laboratory (ASL). His research at ASL is currently supported by the NIH, NSF, DOE, USGS, EU and ARO.

GRADUATE STUDENT AWARD
Recognizing a Graduate Student for Outstanding Research in Spectroscopy

Juris Meija
Juris Meija was born in the Republic of Latvia. During high-school Juris was invited to study in a specially established physics school in order to participate in the International Physics Olympiads. However, he soon escaped physics in favor of chemistry which resulted in two bronze medal awards in the 29th and 30th International Chemistry Olympiads (1997 and 1998). In 2001 he obtained his bachelor’s degree in chemistry from the University of Latvia (summa cum laude) and after that he joined the research group of Professor Joseph A. Caruso at the University of Cincinnati (Cincinnati, OH) to pursue doctoral studies in the field of selenium speciation. His research now is mainly focused on the exploitation of molecular and atomic mass spectrometry to understand the selenium metabolites in plants, their biochemical transformations and chemical properties. The main relevance of Juris’ work to analytical chemistry is to show how elemental speciation techniques, molecular modeling, chromatography, atomic and molecular spectrometry are crucial to unraveling some complex problems on the bio-metals/bio-analytical chemistry. Juris has a rather multidisciplinary approach to solve science problems demonstrating the complimentary of knowledge obtained from the various scientific fields. His research interests cover disciplines such as theoretical studies on isotope dilution method and statistics, applied quantum chemistry in mass spectrometry, rare fatty acid research in plants, chemical education problems and lately, art-science relationships. Juris has authored and co-authored 17 publications, 2 books and 10 popular scientific articles. In his free time he devotes himself to the world of symphonic and opera music.
Walter Jennings
Emeritus Professor Walter Jennings completed a thirty-five year career on the Davis Campus of the University of California, where he constructed his first gas chromatograph in 1954, authored a number of books on gas chromatography, served as Editor for several multi-author books, and published some 300 scientific papers. His laboratory at the University served as a chromatographic Mecca, attracting graduate students, postdoctoral scholars, and other research collaborators from over twenty-five different countries. Their foci included characterization and elucidation of the biosynthetic pathways of volatiles isolated from natural products, techniques of sample preparation, the design and modification of instruments and accessories, studies on fundamental chromatographic relationships, and developments in column deactivation and manufacture. Efforts in window diagramming, combined with research into stationary phase chemistry, led to the first WCOT columns containing a bonded, crosslinked stationary phase designed to maximize the resolution of all solutes in a given mixture. Walt was also the first to demonstrate computer-generated van Deemter plots and their use in evaluating the effects of column and operational parameters. Many scientists who worked with Dr. Jennings during this period are now well known academicians, others occupy responsible positions in instrument companies, and some direct research efforts in areas as diverse as flavor, forensic, petrochemical, pharmaceutical, and environmental analysis.

He was awarded sabbatical leaves in Austria, Germany, and Switzerland, and spent considerable time working in Bulgaria and Poland under the auspices of the International Atomic Energy Agency. He was one of the first to be awarded the prestigious “Humboldt-Preis” from the Alexander von Humboldt Foundation, consisting of a substantial endowment (then tax-free in both Germany and the U.S.) and a one-year appointment as a Senior American Scientist in Germany.

In 1974, collaborating with one of his completing doctoral students, he founded J&W Scientific, Inc., which became the world's largest supplier of fused silica columns. The company was sold to Fisons in 1986, resold to Saratoga Partners in 1996, and to Agilent Technologies in 2000. Through all of these changes, Professor Jennings continued as a Consultant.

Professor Jennings has received the Founders Award in Gas Chromatography administered by the Beckman Corporation, the M.J.E. Golay Award, the Keene Dimick Award, the A.J.P. Martin Gold Medal, and the Silver Jubilee Award at the 19th International Symposium on Capillary Chromatography at Riva del Garde, Italy. In 1999, Professor Jennings was honored by his alma mater by the bestowal of their highest award to individuals, the Award of Distinction. At the 2002 Pittsburgh Conference in New Orleans, he received the Dal Nogare Award for his contributions to Separation Science.

His other awards include the L.S. Palmer Award of the Minnesota Chromatography Forum, the Award of Merit from the Chicago Chromatography Discussion Group, the National Chromatography Award of the Northeast Regional Chromatography Discussion Group, and others from the French Association of Analytical Chemists, the University of Bologna, the Taiwanese Food Chemists Society, and the Society of Flavor Chemists.

Professor Jennings is a Past Chairman of the American Chemical Society's Subdivisions of Flavor Chemistry, and of Chromatography and Separation Science, and has always been an active supporter of chromatography discussion groups. In each year since the early 1970s, he has instructed an average of thirty extra-curricular courses in gas chromatography at points all over the world, and is still very active on the world-wide seminar circuit. At eighty-two years of age, he continues these latter activities. He presently resides in El Dorado Hills, California, and functions as a Consultant for Agilent Technologies and for AirToxics, both in Folsom, California.

MANN AWARD
For Achievements in the Field of Applied Raman Spectroscopy

Michael Carrabba
Mike Carrabba is currently a Principal Scientist for Hach Homeland Security Technologies where he is working on 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 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. He is also a member of the Society for Applied Spectroscopy (SAS) and Coblentz Society. On the home front, his wife, Dr. Mary Widmark Carrabba, a highly skilled Infrared microscopist and the former treasurer for SAS, complements Mike’s Raman background.
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<td>Edward Ruffing</td>
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<td>1976 - Philadelphia</td>
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<td>1978 - Boston</td>
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<td>1979 - Philadelphia</td>
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<td>Mary Kaiser</td>
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<td>1989 - Cleveland</td>
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<td>1990 - Philadelphia</td>
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<td>1991 - Anaheim</td>
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<td>1992 - Philadelphia</td>
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<td>1995 - Philadelphia</td>
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<td>Edward Brame</td>
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L. Felix Schneider and Dave Coleman General
Julian Tyson Program
Mildred Barber Exhibit

1994 - St. Louis
Paul Bourassa Governing Board Chair
Terry Hunter General
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Mildred Barber Exhibit

1995 – Cincinnati
Jon W. Carnahan Governing Board Chair
Joseph A. Caruso General
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1996 – Kansas City
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O. Karmie Galle General
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1997 - Providence
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Chris Brown General
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1998 - Austin
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1999 - Vancouver
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2000 - Nashville
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2001 – Detroit
David A. Laude Governing Board Chair
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2002 – Providence
Michael Carrabba Governing Board Chair
Robert G. Michel General Chair
Mark A. Hayes Program Chair
Scott McGeorge Exhibits

2003 – Fort Lauderdale
Ronald Williams Governing Board Chair
Rina Dukor General Chair
James Rydzak Program Chair
Scott McGeorge Exhibit

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Chemistry
### FACSS

**Saturday, October 2**  
8:30 AM  FACSS Retreat, Cascade 1, Doubletree Hotel  
**Sunday, October 3, Broadway, Doubletree Hotel**  
7:00 PM Web Site Meeting  
7:30 PM Program Committee

**Wednesday, October 6, Room B112, Convention Center**  
9:00 AM  2005 Planning/Budget Committee  
10:00 AM Budget Committee for Quebec City  
11:00 AM Budget Committee for Orlando  
11:30 AM Budget Committee for Memphis  
1:00 PM  Budget and Finance Committee

**Thursday, October 7**  
8:30 AM  Executive Committee, Room A104, convention center  
7:00 PM  Governing Board, Idaho Room, Doubletree Hotel

### ASTM

**Monday, October 4**  
10:30 AM–12:00 PM  E13.10 Molecular Spectroscopic Optical Imaging, Room B112, convention center

**Tuesday, October 5**  
4:00 – 5:30 PM  E13.08 Raman Spectroscopy, Room B112 convention center  
6:00 PM  Raman Reception, Multnomah Room, Doubletree Hotel

### COBLENTZ

**Monday, October 4**  
8:00 PM  Board Meeting, Idaho Room, Doubletree Hotel

### SOCIETY FOR APPLIED SPECTROSCOPY

**Sunday, October 3**  
7:30 AM – 6:00 PM  SAS Executive Committee Meeting, Weidler Room, Doubletree Hotel  
12:00 PM – 1:30 PM  SAS Executive Committee Luncheon, Broadway Room, Doubletree Hotel

**Monday, October 4**  
12:00 – 1:30 PM  Publications Committee Meeting/Lunch, Room B119 convention center

**Tuesday, October 5**  
6:00 – 8:00 PM  SAS Wine and Cheese Reception, Holladay/Broadway, Doubletree Hotel (members only)  
8:00 - 11:00 PM  SAS Governing Board Meeting, Ross Island/Morrison

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[Diagram of Exhibition Hall A-1]

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<td><strong>Advanced Chemistry Development Inc.</strong></td>
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<tr>
<td>90 Adelaide St W, Ste 702</td>
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<tr>
<td>Toronto, ON, M5H 3V9 CANADA</td>
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<tr>
<td><strong>Phone</strong>: 416 368 3435</td>
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<tr>
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www.facss.org

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ICP Information Newsletter, Inc. is a not for profit corporation established in 1997 to foster science education, research, and study in spectroanalytical chemistry. The corporation comprises three divisions: the ICP Information Newsletter, a monthly newsletter with international distribution that gathers all conference and published information related to plasma spectrochemistry; the Winter Conference on Plasma Spectrochemistry, a biennial meeting with international participation featuring state-of-the-art research developments in plasma spectrochemistry, and the University Research Institute for Analytical Chemistry, the research and development division that provides specialty plasma spectrochemical analysis, method development, training, consulting and applied research with ICP atomic emission spectrometry and ICP mass spectrometry. The 2004 Winter Conference on Plasma Spectrochemistry is scheduled for Fort Lauderdale, Florida, January 4-10, 2004. See www-unix.oit.umass.edu/~wc2004/WinterConf2004.htm for program and registration details. The ICP Information Newsletter now in its twenty-ninth year of publication is currently distributed to subscribers in computer-readable format on CD-ROM.

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<tr>
<td>371 Parkland Plaza</td>
</tr>
<tr>
<td>Ann Arbor, MI 48103</td>
</tr>
<tr>
<td>Phone: 734 665 8083</td>
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<tr>
<td><a href="http://www.kosi.com/raman">www.kosi.com/raman</a></td>
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<td><strong>Lambda Solutions, Inc.</strong></td>
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<tr>
<td>411 Waverley Oaks Rd, Ste 335</td>
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<tr>
<td>Waltham, MA 02452</td>
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<td>Phone: 781 478 0170</td>
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<td><a href="http://www.lambdasolutions.com">www.lambdasolutions.com</a></td>
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<td>Lambda Solutions Inc. (LSI), a photonics solution company, introduces its Dimension-P1 and Dimension-M1 Raman Systems. Each system incorporates LSI’s innovative optics and software solutions to provide unsurpassed resolution and sensitivity, bringing this level of technology to a wide range of analytical and industrial users. The Dimension-P series features LSI’s high light-throughput RamanVector fiber probe, and variable power, narrow linewidth 785nm laser integrated with a high sensitivity TE-cooled CCD to yield 3cm-1 resolution and 2500cm-1 bandwidth. The Dimension-M1 Raman microscope is equipped with either a 532 or 785nm laser coupled to a Nikon Model L150 microscope for easy expansion of microscopic studies to Raman spectral analysis. The systems include LSI’s proprietary RamanSoft with its automated background removal algorithm and user-friendly interfaces for data processing and display. LSI also introduces its next generation software solution, LSI SpectralSoft, for critical discriminant and database analysis in quality assurance, and process control applications.</td>
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<td><strong>Light Diagnostics, Inc.</strong></td>
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<tr>
<td>6620 South 400 West</td>
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<tr>
<td>Murray, UT 84107</td>
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<tr>
<td>Phone: 801 293 9266</td>
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<td>Light Diagnostics is a developer of LED based metrology instrumentation. This includes custom spectroscopy, and analytical instrumentation using diffuse reflectance, fluorescence, absorption and Raman spectroscopy for condensed phase analysis in the field, lab, and clinic. New Product: Fluorescence Excitation Ratiometry</td>
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*Phone: 608 273 6822*
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A world leader in high-tech instruments, Thermo Electron Corporation helps life science, laboratory, and industrial customers advance scientific knowledge, enable drug discovery, improve manufacturing processes, and protect people and the environment with instruments, scientific equipment and integrated software solutions. Products include sample preparation equipment, liquid handling and automation systems and analytical instruments for chromatography, mass spectrometry, molecular and elemental spectroscopy and microanalysis. These are integrated with information solutions and supported by professional and financial services.

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Varian, Inc. is a world leader in scientific instruments and consumable laboratory products serving environmental, industrial, chemical, life science and pharmaceutical customers. At the FACCSS conference we will be presenting our latest range of spectroscopy products. To learn more about the latest in ICP-AES, ICP-MS and AA technology, visit us at Booth #124/126

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The VICI (Valco Instruments Co Inc) family of companies offers a wide range of products for analytical application. Valco manufactures valves, fittings, detectors, and other equipment for the general analytical market. VICI Gig Harbor Group offers a complete line of GC capillary columns. VICI Metronics makes a full line of gas permeation devices for Gas Standard generation. VICI Mat/Sen produces a line of Gas Purifiers for a variety of applications. VICI Precision Sampling offers a broad range of analytical gas and liquid syringes, Mininert TM valves, sampling probes and ready-to-use tubing products

**Wah Chang**
Booth 408
Analytical Services
1600 Old Salem Road NE
Albany, OR 97321
*Phone: 541 917 6774*
www.corrosionsolutions.com

The Laboratories of Wah Chang have been providing Analytical Chemistry, Metallurgical and Corrosion Evaluation services for over 50 years. Using a diverse array of modern equipment and procedures, the laboratories have consistently met and exceeded customer expectations in a wide variety of industries with complete client confidentiality. The Analytical Services Laboratory has Nadcap (National Aerospace Defense Contractors Accreditation Program) certification and is certified in accordance with the ISO 17025 and ISO 9002 standards. The Laboratories are staffed around the clock to provide services that include: -Inductively Coupled Plasma -Mass Spectrometry (ICP-MS) -Plasma emission Spectroscopy -Atomic Absorption Spectrometry -Interstital Gases Analysis -Scanning Electron Microscopy -Particle Size Analysis -Radiometric Analysis -Hardness and Tensile Analysis -Corrosion Testing

**WITec GmbH**
Booth 307
Hoefvessinger Weg 6
Ulm D 89081, GERMANY
*Phone: 49 700 9483236*
www.WITec.de

WITec is a manufacturer of high performance equipment for scientific and industrial applications focused on new solutions for Optical and Scanning Probe Microscopy (Scanning Near-field Optical Microscopes, Confocal Scanning Microscopes, Raman-CSM, Atomic Force Microscopes, Pulsed Force Mode AFM). WITec offers the AlphaSNOM using unique cantilever technology, the Confocal Raman Microscope CRM 200 designed for highest sensitivity and resolution and the Mercury 100 AFM with the integrated Digital Pulsed Force Mode for material research and nanotechnology. Modular design guarantees high flexibility and easy upgrade possibilities.
FACSS/SAS WORKSHOPS

Workshops are a valuable component of FACSS and are conducted by leading experts. There is an additional charge for workshops. Saturday and Sunday workshops will be held at the Doubletree Hotel and Monday through Thursday workshops will be held at the convention center.

Following are the rates for workshops unless otherwise indicated.

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ATTACK THE VARIANCE: STATISTICAL DESIGN STRATEGIES FOR ANALYTICAL METHOD DEVELOPMENT

Randy Bishop and Drew Manica, GE Advance Materials
Saturday, October 2 – Sunday, October 3, 8:30 AM – 5:00 PM
Willamette 2 – Selwood, Doubletree Hotel

The workshop will cover statistical design strategies (DOE) for both improving existing methods and building robust new methods. Learn how important factors can be identified and controlled for measurement improvement. Further, robust design methodologies accommodate variability present in operational factors, thereby yielding a practically robust and optimal measurement output. Hands-on breakout sessions will include the use of statistical software.

FT-IR SAMPLE HANDLING - METHODS AND ACCESSORIES

Clara Craver, Craver Chemical Consultants and Richard A. Larsen, Jasco, Inc.
Saturday, October 2 – Sunday, October 3, 8:30 AM – 5:00 PM
Willamette 1 – Hawthorne, Doubletree Hotel

This intensive 2-day workshop will introduce infrared spectroscopy, outline the various sample handling methods and provide the fundamentals for the interpretation of infrared spectra. Invited speakers will present lectures on advanced topics of interest such as imaging, step-scan spectroscopy, or other molecular spectroscopy techniques. Several interpretation lectures will cover the basic group frequencies and their use in identifying a variety of infrared samples including polymers and most major chemical functional groups. Interpretation exercises will provide practice in identifying molecular structures in real-world samples. Examples will be given of major pitfalls in interpretation of spectra of mixtures and in evaluating the certainty of a match of an unknown with results from spectral searching of library databases. Additional workshop lectures will discuss Fourier Transform Infrared (FT-IR) sample analysis methods and the accessories used to obtain representative infrared spectra of analytical samples. Methods for obtaining the 'ideal' spectrum and how to get the most out of the large variety of available FT-IR sampling accessories will be reviewed in addition to the common pitfalls to avoid during sample preparation and spectral interpretation of the results. Sampling techniques such as transmission measurements, FT-IR Microscopy, Multiple Internal Reflectance (MIR, HATR), Diffuse Reflectance (DRIFTS), Specular Reflectance and Reflection-Absorption Spectroscopy (RAIRS) will be examined to determine which method, or accessory, can provide the infrared data required of specific samples. The benefits and limitations of FT-IR sampling methods, library Search procedures and data manipulation methods will also be explored. A working familiarity with Organic chemistry and knowledge of molecular functional groups is highly advisable.

PROCESS ANALYTICAL FOR FACULTY, sponsored by the NSF/CWCS and industry

Lynn Melton, University of Texas, Dallas
Saturday, October 2 – Sunday, October 3, 8:30 AM – 5:00 PM
Willamette 3 – Ross Island, Doubletree Hotel, No Charge

Process Analytical Chemistry is an important growth area in industry but is rarely discussed in academic analytical chemistry courses. This workshop is intended to help faculty with no prior industrial experience learn the basics of process analytical chemistry so that they can provide introduce this area to their students. It is based on teaching materials used in a short course at Dow Chemical Company, which the presenter co-organized in 1999. Each faculty participant will receive a copy of the Practical Aspects of Process Analytical Chemistry CD-ROM, which contains the PowerPoint presentations and a license to adapt the material for use in their own classrooms. During the two days of the workshop, participants will learn about:

- the context of process analytical chemistry – the foundation for the economics-based decisions that determine whether a company should invest in a process analytical project;
- the role of teams in process analytical chemistry projects;
- process control strategies (without equations);
- the adaptation of familiar spectrometric and chromatographic instrumentation to meet the demands of rapid, reliable online measurements; and
- the development of sampling systems to bring a representative, timely, conditioned sample from the process to the analyzer

The last portion of the workshop will focus on ways that faculty can adapt the course materials for use in their classes. Participation in this workshop is limited to faculty or soon-to-be-faculty (postdocs, grad students, etc). There is no registration fee. Costs for the course are being sponsored by NSF/CWCS and industry.

ANALYTICAL RAMAN SPECTROSCOPY

Michael Morris, University of Michigan
Sunday, October 3, 8:30 AM – 12:30 PM
Cascade 1 – 3 Sisters, Doubletree Hotel

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 resonance and surface enhancement of spectra, polarization and the advantages of working with different excitation wavelengths. Modern instrument configurations will be covered, with emphasis on single stage spectrographs and CCD array detectors. 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. Calibration and data reduction topics covered will include Raman shift and intensity standards, white light correction, polarization corrections and signal/noise ratios. Multivariate calibration and 2D Raman spectroscopy will be briefly described. Important applications areas will be surveyed. Attendees will be briefed on recent developments including time-gated Raman spectroscopy and CARS.
BIOLOGICAL INFRARED AND RAMAN SPECTROSCOPY
Rina Dukor, BioTools, Inc.
Sunday, October 3, 8:30 AM – 5:00 PM
Cascade 2 – Mt. Bachelor, Doubletree Hotel
The Society for Applied Spectroscopy is pleased to offer a course designed to introduce both bioscientists and spectroscopists to the rapidly expanding use of IR in the biosciences. It will enable bioscientists to ascertain if IR can provide solutions to their biological problems and help them learn how to use IR for their experiments. The course will aid spectroscopists in finding out what biological experiments are possible or needed, how to handle biological samples, and what techniques and accessories yield the most biological information.

INDUCTIVELY COUPLED PLASMA- MASS SPECTROMETRY (ICP-MS): INTRODUCTION
R. S. Houk, Ames Laboratory USDOE, Iowa State University
Sunday, October 3, 8:30 AM – 12:30 PM
Cascade 4 – Mt. St. Helens, Doubletree Hotel
This course is meant for the beginner in ICP-MS. Course Topics The ICP as an Ion Source Ion Extraction and Beam Formation Operating Principles of Ion Lenses, Quadrupole Mass Analyzers, and Detectors Magnetic Sector Mass Analyzers with the ICP Causes of and Corrections for Spectral Interferences and Matrix Effects Survey of Methods to Remove Polyatomic Ions - Cool Plasma, Collision Cells, Solvent Removal Survey of Applications and Designing a Sound Analytical Strategy Using ICP-MS

PROCESS ANALYTICAL CHEMISTRY: OUT OF THE LAB AND INTO THE PIPE
Christian Hassell, Los Alamos National Lab and James W. Rydzak, GlaxoSmithKline
Sunday, October 3, 8:30 AM – 5:00 PM
Cascade 3 – Mt. Hood, Doubletree Hotel
Process analyzers are becoming more important to the manufacturing industry by providing improved process quality, yields, uptimes and safety, while reducing hazards and environmental impact. This course will answer a question frequently posed by laboratory analytical chemists: “What is process analytical chemistry and how does it differ from more traditional laboratory-based analysis?” It will introduce basic relevant engineering concepts, and compare process analyzers with laboratory instrumentation. The course will primarily focus on online and in-line applications of optical and mass spectrometry, gas chromatography, and titrimetry as they are applied in the refining, chemicals, petrochemicals, food, personal care, pharmaceuticals, and life science industries.

INFRARED CHEMICAL IMAGING
E. Neil Lewis, Spectral Dimensions, Inc.
Sunday, October 3, 1:00 – 5:00 PM
Cascade 1 – 3 Sisters, Doubletree Hotel
The coupling of digital imaging and optical spectroscopy has traditionally proceeded through two distinct pathways either utilizing imaging detectors in concert with discreet optical filters, or coupling high-resolution spectrometers with point mapping approaches. Fixed bandpass optical filters provide high image quality with little or no spectral information, while mapping approaches emphasize spectral performance over image quality. More recently, technologies that completely integrate these modalities have emerged and matured. The application of continuously tunable optical filters, step-scan interferometers, rapid-scan interferometers, high-performance 2D infrared focal-place array detectors (FPA’s), infrared line-arrays, and powerful data processing methods have all contributed to the feasibility and ease of completely integrating spectroscopy and imaging. However, the value and utility of infrared and near-infrared chemical imaging is its ability to non-invasively visualize chemical heterogeneity, and to provide both a qualitative and quantitative assessment of the molecular composition and architecture of a diverse array of heterogeneous materials. As a result, it can be used to assess the quality and performance of new and existing complex materials and products. Topics covered in this half-day course will include: imaging spectrometer technologies, focal-plane array detectors and data processing methods and software. We will frame the instrumentation discussion with a strong emphasis on the value and practical applications of the technology for biological, polymeric and pharmaceutical problem solving.

INDUCTIVELY COUPLED PLASMA - MASS SPECTROMETRY (ICP-MS): ADVANCED TOPICS
R. S. Houk, Ames Laboratory USDOE, Iowa State University
Sunday, October 3, 1:00 – 5:00 PM
Cascade 4 – Mt. Helens, Doubletree Hotel
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 and 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
CHEMOMETRICS IN ANALYTICAL CHEMISTRY AND SPECTROSCOPY
Charles, E. Miller, DuPont Engineering
Monday, October 4, 8:30 AM – 5:00 PM, A 104 convention center
Conferences $350, Students $100, Non-Conferences $450
(includes use of PC)
An introductory course for those who are interested in efficiently and safely applying basic chemometric "tools" to their analytical data. After a short review of the history, philosophy and rationale for these tools, the most commonly used tools (including Multiple Linear Regression, Principal Components Analysis, Partial Least Squares and SIMCA classification) are discussed. Actual case studies are used to demonstrate their utilization for (i) the development of qualitative and quantitative analytical methods, (ii) exploratory analyses of multivariate analytical data, and (iii) safe implementation and maintenance of chemometrics-enhanced analytical methods in the field. The utilization of Six-Sigma methodologies for optimal development and implementation of chemometric models will also be discussed. Although the main emphasis will be on applications in instrumental analysis and spectroscopy, other applications will be used as needed to illustrate the subject matter.

CHEMOMETRICS WITHOUT EQUATIONS
(or Hardly Any) - HANDS ON!
Barry M. Wise, Eigenvector Research, Inc.
Monday, October 4 – Tuesday, October 5, 8:30 AM – 5:00 PM
A 103 convention center
Conferences $550, Students $150, Non-conferences $750
(includes use of PC)
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).

LC/MS: INTRODUCTION TO PRINCIPLES AND APPLICATIONS
Michael P. Balogh, Waters Corporation
Monday, October 4, 8:30 AM – 5:00 PM, A 108 convention center
A one day course introduces the most commonly applied HPLC-to-mass spectrometry interfaces and examines in some detail the most widely used mass spectrometry technologies. Small molecule, high throughput and high sensitivity interests are covered along with more complex molecules and accurate mass considerations. 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.

NEAR-INFRARED: A VERSATILE, RAPID, & NON-DESTRUCTIVE ANALYTICAL TECHNIQUE I
Donald A. Burns, NIR Resources, Emil W. Ciureczak, Integrated Tech. Solutions, and Howard L. Mark, Mark Electronics
Monday, October 4, 8:30 AM – 5:00 PM, A 107 convention center
This session covers the basic tenets of NIR, particularly for newcomers and people who would like a solid review of the subject: e.g., principles & theory, overtones & combination bands, calibration & wavelength selection, search strategies, hidden information, and on-line analysis. Also discussed will be the hardware (who make what) and basic algorithms used in NIR (chemometrics). A basic bibliography (over 2500 references) will be provided on a take-home disk; use it to display, sort, search, add, and print the entries.

INFRARED AND RAMAN MICROSPETROSCOPY
André Sommer, Miami University
Tuesday, October 5, 8:30 AM – 12:30 PM
A 107 convention center
The workshop will present an overview on the fundamentals of molecular microspectroscopy and will provide specifics regarding current instrumentation and current applications. Topics to be covered include: elements of optical microscopy and how they relate to the design and performance of infrared and Raman microscopes, sample preparation for each method and problem solving using the combined techniques. The instructor has over 23 years of industrial problem solving experience using the featured methods and has taught at 15 Molecular Microspectroscopy Short Courses held at Miami University.

INDUSTRIAL PROBLEM SOLVING USING THERMAL ANALYSIS
Joseph Marcinko and Anthony A. Parker
Polymer Synergies LLC
Tuesday, October 5, 8:30 AM – 5:00 PM
A 108 convention center
This course is designed to give an appreciation of the problem solving situations in which thermal analysis can add value. A brief background of the instrumentation will be given. Differential Scanning Calorimetry (DSC), Differential Thermal Analysis (DTA), Dynamic Mechanical Analysis (DMA), Thermomechanical Analysis (TMA) and Thermogravimetric Analysis (TGA) and TGA coupled with Mass Spectrometry (TGA/MS) will be covered. Case studies of investigating how these techniques have been utilized to solve industrial process questions and problems will be presented.

Course Objectives
- Learn the basics of the techniques – DSC, DTA, TGA, TGA-MS, TMA, DMA
- Learn how to use multiple thermal analysis techniques in tandem to solve process and performance problems in product development – examples including composites, coatings, elastomer development, and process studies
- Learn how to identify the nature of transitions in polymeric materials
- Understand the principles of temperature equivalence and applications, i.e. learn how to use thermal analysis data to develop models for time-temperature dependent mechanical behavior
- Develop an appreciation for when to use a particular TA technique
NEAR-INFRARED: A VERSATILE, RAPID, & NON-DESTRUCTIVE ANALYTICAL TECHNIQUE II
Donald A. Burns, NIR Resources, Emil W. Ciurczak, Integrated Tech Solutions, and Howard L. Mark, Mark Electronics

Tuesday, October 5, 8:30 AM – 5:00 PM
A 104 convention center

This session continues with more detailed discussions of the strengths and shortcomings of types of equipment, logical approaches to method development, spectral pre-treatments and how they affect equations. The course also covers qualitative and quantitative analysis, both lab and process applications. The course ends with how you can learn more: groups to join, books/journals to read, meetings to attend, courses to take, and use of the Internet.

INTRODUCTION TO MULTIVARIATE IMAGE ANALYSIS
Barry M. Wise, Eigenvector Research

Wednesday, October 6 – Thursday, October 7
8:30 AM – 5:00 PM, A 103 convention center
Conferees $550, Students $150, Non-Conferencees $750
(includes use of PC)

Designed to give the student practical experience. Before the course, students will be sent a pre-course reading assignment covering some of the basic background and principles of MIA. The course will start with a brief review of principal components analysis (PCA) and partial least squares (PLS) regression and how they are used in image analysis. Additional topics to be covered include multivariate image regression, and preprocessing to capture textual information. Methods to mitigate the effects of background interference, e.g., clutter, will also be discussed. Students will work problems using MATLAB and PLS_Toolbox on computers provided (maximum of two students per computer).

FDA GUIDELINES AND EXPECTATIONS FOR VALIDATION OF PAT METHOD
Emil W. Ciurczak, Integrated Tech Solutions

Wednesday, October 6, 8:30 AM – 5:00 PM
A 107 convention center

Much has been said about the FDA’s PAT (Process Analytical Technologies) initiative. Numerous meetings have been held where the benefits and pitfalls have been discussed. This course will condense the applications, advantages, and potential difficulties of the PAT approach. We will examine the guidelines published by FDA and expectations for Validation under cGMP and 21CFR11.

TECHNICAL WRITING FOR INDUSTRIAL SCIENTISTS AND MANAGERS
Joseph Marcinko and Anthony Parker, Polymer Synergies, LLC

Wednesday, October 6, 8:30 AM – 5:00 PM
A 104 convention center

The goal of the technical writer is to convey information in a manner that allows the audience to easily glean important concepts, messages, and data. Upon completion, participants will have the skills needed to plan and prepare high-quality technical, scientific, and business documents.

Who Should Attend:
- Scientists, technicians, and managers who would like to improve their technical writing skills.
- Persons who are new to a scientific or technical role and would like to improve their technical writing skills.
- Managers who would like to improve the writing skills of their employees.
- Individuals for whom English is not their first language, and who wish to improve their written communication skills.

WORKSHOP SPONSORS

Mettler Toledo
Smith Detection
The FACSS Employment Bureau will be available during the 2004 FACSS Conference to both job applicants and employer representatives. The Employment Bureau is a free service that provides job and applicant listings, message boards, and interviewing booths. Participants must be registered for the conference. Separate files will be available for job opportunities and applicant resumes. Registered participants may review these files during Employment Bureau hours. Either applicants or employers may request on-site interviews.

LOCATION. The employment bureau is located in Rooms B117 – B118 at the convention center.

HOURS. 8:30 AM – 5:00 PM, Monday – Thursday

- **Applicants** should submit the FACSS Employment Bureau Applicant Form and a personal one-page resume. The Applicant Form is designed to allow easy review by employer representatives. Applicants also should include a formal resume. Applicants who wish to exclude their resume from the resume book should check the appropriate box on the registration form.
- **Employers** should submit the Employer Form. Books containing all applicant approved resumes will be available for purchase and will be mailed after the conference.

ON-SITE REGISTRATION. Applicants and employer representatives must sign in with the Employment Bureau upon arrival at the meeting. Applicant Resumé forms and Employer forms will be available for review. Interview booths will be available during Employment Bureau hours. The Employment Bureau will schedule 30-minute interviews upon request from either employers or applicants. Interview notices and messages will be posted on message boards. It is recommended that Employment Bureau participants check the message boards at approximately two-hour intervals during the day.

SPECIAL INVITATION TO STUDENT ATTENDEES: Please plan to attend the Student/Professional Panel Discussion and brown bag lunch sponsored by SAS on Tuesday at 12:00 – 1:15 PM in the Employment Bureau. Panelists from various segments of academia and industry will be available to answer questions regarding careers in their fields. Lunch will be provided for students attending this panel discussion.

ORDER FORM FOR BOOK OF APPLICANT RESUMÉS

Resumé books will be prepared containing all applicant resumes received (unless an applicant has requested to be excluded). Books will be mailed after the conference. The cost of each book is $100. Please fill out the information below if you wish to purchase applicant resumé books.

Number of books requested _______ x $100  Total Amount:  $ ______________________

This form must be accompanied by full payment for the total amount. Checks must be in U.S. dollars and payable through a U.S. bank. We regret that we do not accept purchase orders.

☐ Check is enclosed. Make payable to FACSS

☐ Charge total amount to VISA, MasterCard, or Amex

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Mailing address:
Company/Institution ____________________________
Address __________________________________________

City State Zip Country ____________________________

Representative’s Name ____________________________

SEND TO: FACSS Registration, PO Box 24379, Santa Fe, NM 87506 (USA)
FAX: (505) 989-1073 • Faxed orders must be charged to VISA or MasterCard

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**SAS Student Poster Showcase and Awards**

Come aboard and join us for food and fun as SAS students showcase their research and compete for the annual SAS poster awards.
Sunday, October 3
5-7 p.m. Holladay Lobby, Oregon Convention Center during the FACSS mixer.

**ICP-MS & ICP-AES**

- Nebulizers
- Spray Chambers
- Torches
- Cones
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- AND MUCH MORE

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### PROGRAM OVERVIEW

#### SUNDAY EVENING
Welcome Mixer and SAS Student Poster Session, 5:00 – 7:00 PM, Holladay Lobby

#### MONDAY MORNING

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<tr>
<td>8:00 AM</td>
<td><strong>PLENARY LECTURE:</strong> Earth's Earliest Fossils: Solution to Darwin's Dilemma, J. William Schopf, <em>Ballroom 201</em>, page 40</td>
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#### MONDAY AFTERNOON

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#### TUESDAY MORNING

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<tr>
<td>8:00 AM</td>
<td><strong>PLENARY LECTURES</strong>, <em>Ballroom 201</em>&lt;br&gt; • ANACHEM Award, Walter Jennings, page 48&lt;br&gt; • Charles Mann Award, Michael Carrabba, page 48</td>
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<tr>
<td>9:00 AM</td>
<td><strong>SYMPOSIA AND POSTER SESSIONS</strong>&lt;br&gt; 9:00 – 10:30 Posters, <em>Exhibit Hall</em>, page 48&lt;br&gt; 10:30 – 12:30 Symposia, page 51&lt;br&gt; • LIBS, <em>Room C123</em>&lt;br&gt; • ANACHEM GC1, <em>Room B116</em>&lt;br&gt; • The Role of Analytical Chemistry in Human Disease, <em>Ballroom 201</em>&lt;br&gt; • General Chemometrics, <em>Room B114</em>&lt;br&gt; • Advances in Forensic Analytical Techniques, <em>Room B113</em>&lt;br&gt; • Coherent 2D Vibrational Spectroscopy, <em>Room C124</em>&lt;br&gt; • Ion Trap MS for Proteomics, <em>Room A105</em>&lt;br&gt; • Carbon Nanotube Separation, <em>Room B115</em>&lt;br&gt; • Charles Mann Award, <em>Room A106</em></td>
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#### TUESDAY AFTERNOON

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<tr>
<td>2:00 PM</td>
<td><strong>SYMPOSIA AND POSTER SESSIONS</strong>&lt;br&gt; 2:00 – 3:30 Posters, <em>Exhibit Hall</em>, page 48&lt;br&gt; 3:30 – 5:30 Symposia, page 53&lt;br&gt; • Advances in Plasma Spectrometry, <em>Room C123</em>&lt;br&gt; • ANACHEM GC2, <em>Room B116</em>&lt;br&gt; • Biomarkers-Analytical Applications in the Research and Assessment of Human Disease, <em>Ballroom 201</em>&lt;br&gt; • Chemometrics in Pharmaceutical Process Analytical Technology, <em>Room B114</em>&lt;br&gt; • Anytime/Anyplace Access to Instrumentation Over the Internet: Changing the Way Science is Taught, <em>Room B113</em>&lt;br&gt; • Coherent 2D Vibrational Spectroscopy, <em>Room C124</em>&lt;br&gt; • Ion Trap MS for Proteomics II, <em>Room A105</em>&lt;br&gt; • Nanomaterials for Photonics, <em>Room B115</em>&lt;br&gt; • Novel Vibrational Techniques for Biology: In Recognition of Richard Mathies 2004 Lippencott Award Recipient, <em>Room A106</em></td>
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## PROGRAM OVERVIEW

### WEDNESDAY MORNING

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<td>Semiconducting and Piezoelectric Nanobelts, Nanosprings and Nanorings;</td>
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<td>Zhong Lin Wang, page 56</td>
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<td>9:00 AM</td>
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#### SYMPOSIA AND POSTER SESSIONS

**9:00 – 10:30 Posters, Exhibit Hall, page 56**
- Important Aspects of Elemental Speciation, Sample Preparation, Separation, Sample Introduction, Room C123
- Biological Analysis Enabled by Micromachining Technologies, Room B116
- Multivariate Analysis of Hyperspectral Images, Room B114
- New Ideas in Teaching Analytical Chemistry, Room B113
- Vibrational Spectroscopy Coupled with Combinatorial Chemistry, Room C124
- FTMS for Proteomics, Room A105
- Nanomaterials for Photonics, Room B115
- Raman in Process Analytical, Room A106

### WEDNESDAY AFTERNOON

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<td>3:30 – 5:30 Symposia, page 60</td>
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<td>Molecular Inorganic and Organometallic Mass Spectrometry, Room C123</td>
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<td>Probing Cellular Properties and Function with Microchip Devices, Room B116</td>
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<td>Multivariate Curve Resolutions: Recent Advances and Applications, Room B114</td>
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<td>IR Microspectroscopy, Instrumentations and Applications, Room C124</td>
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<td>FTMS for Proteomics, Room A105</td>
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<td>Nanotubes and Nanowires for Sensing, Room B115</td>
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<td>Raman in Pharma, Room A106</td>
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### THURSDAY MORNING

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<td>8:00 AM</td>
<td>PLENARY LECTURE: Lippencott Award, Femtosecond Stimulated Raman Spectroscopy, Richard A. Mathies, Ballroom 201, page 63</td>
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**9:00 AM** SYMPOSIA AND POSTER SESSIONS

**9:00 – 10:30 Posters, Exhibit Hall, page 63**
- Metallomics I, Room C123
- Apatmers in Analysis, Ballroom 201
- Chemometrics Applications of Cluster Analysis and Pattern Recognition, Room B114
- Research Supportive Curricula in Environmental Chemistry, Room B113
- New Techniques in Sampling for IR Spectroscopic Data, Room C124
- MS Front-End Devices and New Methodology for Proteomics, Room A105
- Nanotubes and Nanowires for Sensing, Room B115
- State of the Art Infrastructure for PAT Spectroscopy in Industry, Room B116
- Raman Microscopy and Imaging, Room A106

### THURSDAY AFTERNOON

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<td>MS Front-End Devices and New Methodology for Proteomics, Room A105</td>
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<td>Nanotubes and Nanowires for Sensing, Room B115</td>
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<td>Emerging Technologies for Process Analysis, Room B116</td>
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<td>Raman Spectroscopy in Art and Archaeology, Room A106</td>
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# TECHNICAL PROGRAM OVERVIEW BY TOPIC

## AWARD SESSIONS, Room B116 and A106

**Tuesday AM**
- ANACHEM, Room B116
- Charles Mann, Room A106

**Tuesday PM**
- ANACHEM, Room B116
- Lippencott, Room A106

## ATOMIC SPECTROSCOPY, Room C123

**Monday AM**
- Sample Introduction

**Monday PM**
- Laser Ablation

**Tuesday AM**
- LIBS

**Tuesday PM**
- Advances in Plasma Spectrometry

**Wednesday AM**
- Important Aspects of Elemental Speciation, Sample Preparation, Separation, Sample Introduction

**Wednesday PM**
- Molecular Inorganic and Organometallic Mass Spectrometry

**Thursday AM**
- Metallomics

**Thursday PM**
- Metallomics

## BIOANALYTICAL, Ballroom 201, B116, and A106

**Monday AM**
- Analytical Methods to Characterize the Nervous System, Ballroom 201
- Biological Application of Nanoparticles for Surface Enhanced Raman Scattering, Room A106

**Tuesday AM**
- The Role of Analytical Chemistry in Human Disease, Ballroom 201

**Tuesday PM**
- Biomarkers-Analytical Applications in the research and Assessment of Human Disease, Ballroom 201

**Wednesday AM**
- Biological Analysis Enabled by Micromachining Technologies, Room B116

**Wednesday PM**
- Probing Cellular Properties and Function with Microchip Devices, Room B116

**Thursday AM**
- Aptamers in Analysis, Ballroom 201

## CHEMOMETRICS, Room B114

**Tuesday AM**
- General Chemometrics

**Tuesday PM**
- Chemometrics in Pharmaceutical Process Analytical Technology

**Wednesday AM**
- Multivariate Analysis of Hyperspectral Images

**Wednesday PM**
- Multivariate Curve Resolutions: Recent Advances and Applications

**Thursday AM**
- Chemometrics Applications of Cluster Analysis and Pattern Recognition

**Thursday PM**
- Multiway Analysis and Multiway Method Development

## CHEMOMETRICS, Room B114

**Tuesday PM**
- Anytime/Anyplace Access to Instrumentation Over the Internet: Changing the Way Science is Taught

**Wednesday AM**
- New Ideas in Teaching Analytical Chemistry

**Thursday AM**
- Research Supportive Curricula in Environmental Chemistry

## FORENSICS, Room B113

**Monday AM**
- Detection of Weapons of Mass Destruction

**Monday PM**
- New Developments in Mass Spectrometry for Forensics

**Tuesday AM**
- Advances in Forensic Analytical Techniques

## IR and NEAR IR, Room B114 and Room C124

**Monday AM**
- Near IR, Room C124
- 2D Correlation Spectroscopy, Room B114

**Monday PM**
- Near IR, Room C124
- 2D Correlation Spectroscopy, Room B114

**Tuesday AM**
- Coherent 2D Vibrational Spectroscopy, Room C124

**Tuesday PM**
- Coherent 2D Vibrational Spectroscopy, Room C124

**Wednesday AM**
- Vibrational Spectroscopy Coupled with Combinatorial Chemistry, Room C124

**Wednesday PM**
- IR Microspectroscopy Instrumentation and Applications, Room C124

**Thursday AM**
- New Techniques in Sampling for IR Spectroscopic Data, Room C124

**Thursday PM**
- IR Microspectroscopy Imaging, Room C124

## MASS SPECTROMETRY AND PROTEOMICS, Room A105

**Monday AM**
- TOF MS for Proteomics

**Monday PM**
- TOF MS for Proteomics

**Tuesday AM**
- Ion Trap MS for Proteomics

**Tuesday PM**
- Ion Trap MS for Proteomics

**Wednesday AM**
- FTMS for Proteomics

**Wednesday PM**
- FTMS for Proteomics

**Thursday AM**
- MS Front-End Devices and New Methodology for Proteomics

**Thursday PM**
- MS Front-End Devices and New Methodology for Proteomics
### NANOSCIENCE AND NANOMATERIALS, Room B115

**Monday AM**
- Carbon Nanotube Separation

**Monday PM**
- Carbon Nanotube Separation

**Tuesday AM**
- Carbon Nanotube Separation

**Tuesday PM**
- Nanomaterials for Photonics

**Wednesday AM**
- Nanomaterials for Photonics

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

**Thursday AM**
- Nanotubes and Nanowires for Sensing

**Thursday PM**
- Nanotubes and Nanowires for Sensing

### PROCESS ANALYTICAL TECHNOLOGY, Room B116

**Monday AM**
- Process Analytical Technologies in Pharma

**Monday PM**
- Miniature Spectroscopic Sensors

**Thursday AM**
- State of the Art Infrastructure for PAT Spectroscopy in Industry

**Thursday PM**
- Emerging Technologies for Process Analysis

### RAMAN, Room A106

**Monday AM**
- Biological Applications of Nanoparticles for Surface Enhanced Raman Scattering

**Monday PM**
- Data Analysis and Raman Spectra

**Tuesday AM**
- Charles Mann Award Symposium

**Tuesday PM**

**Wednesday AM**
- Raman in Process Analytical

**Wednesday PM**
- Raman in Pharma

**Thursday AM**
- Raman Microscopy and Imaging

**Thursday PM**
- Raman Spectroscopy in Art and Archaeology
TECHNICAL PROGRAM – MONDAY
Plenary and Posters

7:30 Wake Up Coffee, Ballroom Lobby

8:00 AM, Plenary Session, Ballroom 201

J. William Schopf

(1) Earth's Earliest Fossils: Solution to Darwin's Dilemma; J. William Schopf, University of California, Los Angeles

MONDAY POSTER SESSIONS and BREAKS
9:00 – 10:30 AM and 2:00 – 3:30 PM
Exhibit Hall A

All Monday posters should be put up between 7:30 – 8:00 AM and removed between 5:30 – 6:00 PM. Odd numbered posters present between 9:00 - 10:30 AM and even numbered posters present between 2:00 – 3:30 PM

Sample Introduction

(2) Ultra High Throughput Microwave Digestion ; 40 Samples per batch - A Novel Breakthrough Approach for Pressurized Dissolutions; Bob Lockerman1, Cindy Condrey1,1 CEM Corporation

(4) Determination of Cadmium at Ultratrace Levels by Flow Injection Vapor Generation With a Tetrahydroborate-Form Anion-Exchange with In-Atomizer Trapping by ETAAS; Julian F. Tyson; University of Massachusetts


(6) Analysis of Various Difficult Sample Matrices Using High Resolution ICP-OES; Geoff Tyler1, Agnès Cosnier2, Sébastien Velasquez1; 1Glass Expansion, Inc., Pocasset, MA; 2Jobin Yvon SAS

(7) Fraunhofer Effect: Tungsten Coil Atomic Absorption Spectrometry; Jennifer A. Rust1, Joaquim A. Nobrega1, Clifton P. Calloway, Jr.1, Bradley T. Jones1; 1Wake Forest University; 2Winthrop University; 3Universidad Federal de Sao Carlos

(8) ETV-ICP-TOFMS: An Ideal Coupling of Sample Introduction and Detection2; Guay Ertas1, James A. Holcombe1; 1Department of Chemistry and Biochemistry, The University of Texas at Austin

(9) New Developments in RF Glow Discharge Optical Emission Spectrometry Extend the Range of Applications; Patrick Chapon1, Philippe Hunault2, Celia Olivero-Tauziede1; 1Jobin Yvon SAS; 2Jobin Yvon Inc

(10) An Improved Model for Aerosol Desolvation in Inductively Coupled Plasmas; Daniel Mittelberger1, Kaveh Kahan1, Deborah Levin2, Akbar Montaser3; 1The George Washington University; 2Pennsylvania State University

(11) An Improved Liquid Sample Introduction Method for Chemical Reaction Interface Mass Spectrometry; Kaveh Jonabchi1, Kaveh Kahan1, Paolo Lacchi1,2, Akbar Montaser3; 1Department of Chemistry, George Washington University; 2Department of Pharmacology, George Washington University

(12) In Atomizer Trapping for Determination of Mercury in Urine by Cold Vapor and W-Coil Electrothermal Atomic Absorption Spectrometry; Fernando Barbosa Jr4, Samuel deSouza1, Francisco Krug5, UFSCAR; 6Faculdade de Medicina - USP Ribeirao Pre; 7CEN-USP

(13) New Ways to Improve the Power of Detection in Flame Atomic Absorption Spectrometry; Harald Berndt1, Erika Pulvermacher1, ISAS-Institute for Analytical Sciences

(14) A New Pneumatic Nebulizer for ICP Spectroscopy; Hsiaoming Tan1, Hidekazu Miyahara1, Yoichi Mizuwa1, Takayuki Doi1, Goro Ohba2, Masato Watanabe1, Eiki Hotta1, Tokyo Institute of Technology

(15) Performance of an Inert Self-aspirating Micro flow Nebulizer; Jerry Dulude1, Bobby Brezni2, Salar Samii3, Jonathan Levine4, Kaveh Kahan5, Akbar Montaser6; 1Glass Expansion; 2George Washington University

(16) Development and Evaluation of a New Direct Injection Multi-gas ICP Source; Akitoshi Okino1, Hidekazu Miyahara1, Yoichi Mitsuwa1, Takayuki Doi1, Goro Ohba1, Masato Watanabe1, Eiki Hotta1, Tokyo Institute of Technology

Laser Ablation

(17) Preliminary Study of Hydrogen Emission Characteristics on Solid samples Using Laser-Ablation Technique; Koo Hendrik Kurniawan1, Tjung Jie Lie1, Nasrullah Idris2,kiichiro Kagawa3, Tadashi Maruyama4, Tadashi Maruyama3, 1Research Center of Maju Makmur Mandiri Foundation; 2Department of Fiber Amenity; 3Department of Physics, Faculty of Education; 4The Wakasa Wan Energy Research Center

(18) Laser Ablation Mass Spectrometry Technique for Analyzing Aluminosilicates : Characterization Data Using Both Positive and Negative Ion Mode; Jean Jacques Gaumet1, Jérémie Castello1, Jean François Muller1, Gérard Friour4, Olivier Poncelet1, Jean Guilmet2, 1Laboratoire de Spectrométrie de Masse et de Chimie; 2Kodak Research Labs, CRT 60-3, Z.I. Nord
(78) A Miniaturized Analyzer Design for Process and Handheld Chemical Composition Measurements; Thomas Hagler; 1Advanced Photometrics Inc.

Biological Applications of Nanoparticles for Surface Enhanced Raman Scattering

(79) Conductive Inks for Sensors: High Conductivity through Particle Alignment; Alexander Scheel1, April Schrickler1, Ewa Kirkor1; 1University of Illinois at Urbana-Champaign Departm; 2University of Texas at Austin

(80) Surface Plasmon Resonance Sensor by Evanscent Wave Cavity Ring-Down Spectroscopy; Hsiu-Fang Fan1, King-Chuen Lin1; 2National Taiwan University

(81) Dispersion and Stability Studies of Gold Nanoparticles in Organic Solvents; Jeffrey M. McMahon1, Steven R. Emory2; 1Western Washington University

(82) Spatially Resolved Depth Profiling Analysis of Single Small Polymeric Particles by Confocal Raman Microscopy; Travis Bridges1, Joel Harris1; 1University of Utah (83)

(83) Variations and Changes of Photoinducted Luminescence Bands of Surface-Enhanced Raman Active Single Ag Nano-aggregates; Tami Take Inok1, Kazuhiro Hashimoto1, Yasuo Kikkawa1, Akifumi Ikehuta1, Yukihiro Ozaki1; 1Kwanse-Gakuin University

Data Analysis and Raman Spectra

(85) Rapid pesticide residue analysis on imported fruits by SERS; Chetan Shende1, Frank Incore2, Alan Gift3, Paul Maksymuk4, Stuart Farquharson5; 1Real-Time Analyzers

Monday Morning, Room C123

SAMPLE INTRODUCTION

Organizer and Presider: Akbar Montaser

10:30 (86) Small Sample Volume ICP-MS using a Reaction Cell or Sector Mass Spectrometer; John Olesik1; 1Ohio State University

10:50 (87) Spatial Mapping of Droplet Velocity and Size for Direct and Indirect Nebulization in Plasma Spectrometry; Kaveh Kahen1, Kaveh Jorabchi1, Callum Gray1, Akbar Montaser1; 1The George Washington University, Department of Chemistry

11:10 (88) In-situ Visualization and Characterization of Aerosol Droplets in an Inductively Coupled Plasma; Kaveh Jorabchi1, Kaveh Kahen1, Callum Gray1, Akbar Montaser1; 1George Washington University

11:30 (89) A New Pneumatic Nebulizer for Sample Introduction in ICP Spectrometry - Miniaturized Pneumatic Extension Nozzle; Harald Berndt1, Sascher Groom1, Gerhard Schaldach2, Peter Walzel2; 1ISAS - Institute for Analytical Sciences, 2University of Dortmund - Chair of Mechat

11:50 (90) Tunable Direct Injection High Efficiency Nebulizer for Inductively Coupled Plasma Mass Spectrometry; Cristina Necita1, Kaveh Kahen1, Craig Westphal1, William Ruckwski1, Akbar Montaser1; 1George Washington University, Department of Chemistry

12:10 (91) Application of Micronebulization in Inductively Coupled Plasma Mass Spectrometry and Laser Ablation ICP-MS; J. Sabine Becker1, D. Schumloeffel1, M. V. Zorii1, P. Giusti1, C. Pickhardt1, R. Lobinski1; 1Central Division of Analytical Chemistry, Research, 2Group of Bio-Inorganic Analytical Chemistry

Monday Morning, Room B114

2D CORRELATION SPECTROSCOPY

Organizers and Presiders: Wei Zhao and Isao Noda

10:30 (92) Characterizing Brain Chemistry with Electrochemical Techniques; Adrian Michael1; 1University of Pittsburgh

11:10 (93) Neuroepidemiological Analysis of a Small Nervous System Using Multidimensional MS-Based Approaches; Liming Li1, Kimberly Kutz1, Joshua Schmidt1, Yu Wanga1, Qiang Fu1; 1University of Wisconsin-Madison

11:50 (94) Characterizing the Chemical Environment of the Mammalian Central Nervous System; Scott Shippy1; 1University of Illinois at Chicago

12:10 (95) Sensitive Neurotransmitter Monitoring Using Biosensors; Wei-Hong Tan1; 1University of Florida

12:30 (96) Monitoring D-Serine in the Rat Striatum Using Online Microdialysis Capillary Electrophoresis; Michael Bowser1, Chanda Ciriack1; 1University of Minnesota

Monday Morning, Room B113

DETECTION OF WEAPONS OF MASS DESTRUCTION

Organizer and Presider: Greg Klunder

10:30 (97) Two-Dimension Infrared (2D) Correlation Spectroscopy Study of Biodegradable Polymers; Isao Noda1, Tony Dowrey1, Curt Maricott1, Mike Satkowski1; 1Procter & Gamble Co.

10:50 (98) Two-Dimensional Infrared Correlation Spectroscopy Study of Crystallization Dynamics of Poly(L-lactic acid) during Cold-Crystallization; Yukihiro Ozaki1, Jianming Zhang1, Hideko Tsuji2, Isao Noda1; 1Kwanse-Gakuin University; 2Toyoohashi University of Technology; 3The Procter & Gamble Company

11:10 (99) Use of Two-dimensional Vibrational Correlation with Near-, Mid-infrared and Raman Spectroscopy to Study Agricultural Problems; David Himmelsbach1, Franklin Barton1, II, James de Haseth1; 1USDA-ARS-Richard B. Russell Research Center; 2Department of Chemistry, The University of Georgia

11:30 (100) 2D-IR Correlation and Principal Component Analysis of Ice Melting; Hug Richard1, 2K. Dendrism1, Martin Kordes1; 1Ohio University

11:50 (101) Introduction of New Correlation Indices Independent of the Band Shifting Phenomena in Generalized Two-Dimensional Correlation Infrared Spectroscopy; Shin-ichi Mort1, Yasuhiro F. Miura1, Michio Sug1, Yukihiro Ozaki1; 1Faculty of Engineering, Toh University of Yokoham; 2School of Science and Technology, Kwanse

12:10 (102) Infrared Study of the Solvation of Amino Acids; Feng Gai1; 1University of Pennsylvania

Monday Morning, Room B111

ANALYTICAL METHODS TO CHARACTERIZE THE NERVOUS SYSTEM

Organizer and Presider: Scott Shippy

10:30 (92) Characterizing Brain Chemistry with Electrochemical Techniques; Adrian Michael1; 1University of Pittsburgh

11:10 (93) Neuroepidemiological Analysis of a Small Nervous System Using Multidimensional MS-Based Approaches; Liming Li1, Kimberly Kutz1, Joshua Schmidt1, Yu Wanga1, Qiang Fu1; 1University of Wisconsin-Madison

11:50 (94) Characterizing the Chemical Environment of the Mammalian Central Nervous System; Scott Shippy1; 1University of Illinois at Chicago

12:10 (95) Sensitive Neurotransmitter Monitoring Using Biosensors; Wei-Hong Tan1; 1University of Florida

12:30 (96) Monitoring D-Serine in the Rat Striatum Using Online Microdialysis Capillary Electrophoresis; Michael Bowser1, Chanda Ciriack1; 1University of Minnesota
11:10 (105) A Transportable, High Resolution FT Mass Spectrometer for Analysis of Chemical Warfare Agent Surrogates, Corrosive Materials, and Incendiary Materials; Dean Davis¹, Kenneth Gallaher¹, Wayne Rimkus¹, Siemens Applied Automation

11:30 (106) Chemical Incident Response System; James Crabtree², Samuel Reighley², Leonard Buettner³, Agilent Technologies, Inc.; 2South Carolina Law Enforcement Division; 3US Army, RDECOM, ECBC

11:50 (107) Detection of Chemical Weapons using an ES/SIMS Ion Trap Mass Spectrometer; Anthony Appelhans¹, Gary Groenewold¹, John Williams², Mark Jeffery³, Idaho National Engineering and Environmental Labor; 2West Desert Test Center, Dugway Proving

12:10 (108) Chemical Odour Signatures of Powder Explosives and Their Implications upon Biological Detection of Explosives by Canis Familiaris; Ross Harper¹, Stefan Rose¹, Jose Almirall¹, Kenneth Fulton¹, International Forensic Research Institute; 1University of Medicine and Forensic Consulting

Monday Morning, Room C124
NEAR IR
Organizer and Presider: Katherine Bakeev

10:30 (109) NIR Characterization of Gun Propellants; Lewis Kansas¹, Erin hardmeyer¹, Susan Gorine², Thomas DeAngelis¹, 1Geo-Centers, Inc.; 2U.S. Army ARDEC

10:50 (110) Embedding Covert Anticounterfeit Spectral Features into Pharmaceutical Formulations to authenticate pharmaceutical products; James Polli¹, Stephen Hoag¹, University of Maryland School of Pharmacy

11:10 (111) An Optical Near Infrared Assessment of Arterial Island Epigastric Free Flaps; Distinguishing between Arterial, Venous, and Total Occlusion; Michael Sowa¹, Jeri Payette¹, Elicia Kohlenberg¹, Arone Chichak¹, Robert J A Ramirez¹, Alexander Star¹, 1CNSI/UCLA; 2Nanomix Inc.

11:30 (112) Maintaining Near-IR Calibration Models in Unstable Media; Cliona M. Fleming¹, Christopher D. Brown¹, Stephen J. VanSlyke¹, InLight Solutions, Inc.

11:50 (113) On-Line Monitoring of the Density of LLDPE, and Ethylene Content of Polypropylene in Melt States by Near-Infrared Spectroscopy and Chemometrics; Masahiro Watari¹, Yukihiro Ozaki¹, Yokogawa Electric Corporation; 1Kwansei-Gakuin University

12:10 (114) NIR and Multivariate Statistics for Determination of DVD Adhesive Composition; Randy Bishop¹, 1GE Advanced Materials
### Monday Morning, Room B116
**PROCESS ANALYTICAL TECHNOLOGIES IN PHARMA**  
Organizer and Presiders: James Rydzak

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<th>Time</th>
<th>Session</th>
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<tr>
<td>10:30</td>
<td>(127) Process Analytical Technology for Pharmaceutical Unit Operations: Andrew Lange¹; ³Pfizer Global Research</td>
</tr>
<tr>
<td>10:50</td>
<td>(128) A Novel Approach to Determining Particle Size Distributions of Pharmaceutical Powders by NIR: Chun Cai¹, David Radspinner¹; ³Aventis Pharmaceuticals</td>
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<tr>
<td>11:10</td>
<td>(129) Monitor Pharmaceutical Drying Processes in Fluid Bed Dryer by Using Infrared and Near Infrared Spectroscopies: Chi-Shi Chen¹, Martin Warman¹, Joep Timmermans¹; ³Pfizer Inc.</td>
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<tr>
<td>11:30</td>
<td>(130) Raman and ATR-FTIR Spectroscopic Monitoring of the Polymorphic Transformations of Acetaminophen: Kris Berglund¹,², Lili Feng²; ³Luleå University of Technology; ²Michigan State University</td>
</tr>
<tr>
<td>11:50</td>
<td>(131) Application of Mid-IR Spectroscopy for Pharmaceutical Process Monitoring: Mike Claybourn¹; ³AstraZeneca</td>
</tr>
<tr>
<td>12:10</td>
<td>(132) The Use of Chemometrics To Understand Chemistry: Duncan Thompson¹; GlaxoSmithKline</td>
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### Monday Morning, Room A106
**BIOLOGICAL APPLICATIONS OF NANOPARTICLES FOR SURFACE ENHANCED RAMAN SCATTERING**  
Organizers and Presiders: Michael Natun and Griff Freeman

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
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<tbody>
<tr>
<td>10:30</td>
<td>(133) Biological Applications of Single-Molecule Surface-Enhanced Raman Spectroscopy: Steven Emory¹, Teresa Wenda¹, Haley Pugsley¹, Rebecca Jensen¹, Rebecca Newhouse¹; ²Western Washington University</td>
</tr>
<tr>
<td>10:50</td>
<td>(134) Design of Surface Enhanced Raman Tags for Low Level Biolyte Detection: Marc D. Porter¹, Robert J. Lipert¹, Hye-Young Park¹, Jeremy Driskell¹, Jill Uhlenkamp¹, Betsy Jean Yakes¹; ³Iowa State University</td>
</tr>
<tr>
<td>11:10</td>
<td>(135) Nanoparticle SERS Beacons: Griff Freeman¹, William Doering¹, Michael Natan¹, Michael Sha¹, Sharron Penn¹; ³Nanoplex Technologies, Inc.</td>
</tr>
<tr>
<td>11:30</td>
<td>(136) Detection and Identification of Bacteria Using Surface Enhanced Raman Spectroscopy: Ranith Premasiri¹, Gilford Jones¹, Larry Zeigler¹; ³Photonics Center, Boston University; ²Department of Chemistry, Boston University</td>
</tr>
<tr>
<td>11:50</td>
<td>(137) Rapid Detection of Chemical Warfare Agent Hydrolysis Products by Surface-Enhanced Raman Spectroscopy: Frank Inscore¹, Alan Gift¹, Stuart Farquharson¹; ³Real-Time Analyzers</td>
</tr>
<tr>
<td>12:10</td>
<td>(138) Metal Nanostructures for Surface-enhanced Raman Spectroscopy: Rebecca A. Jensen¹, Rebecca Newhouse², Haley R. Pugsley², Steven R. Emory²; ³Western Washington University</td>
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### Monday Afternoon, Room B114
**2D CORRELATION SPECTROSCOPY**  
Organizers and Presiders: Wei Zhao and Isao Noda

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
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<tbody>
<tr>
<td>3:30</td>
<td>(139) Femtosecond Laser Ablation Mass Spectrometry: Roland Hergenroeder¹, Vanja Marjetic¹, Joachim Koch¹, Ota Samek¹, Kay Niemax¹; ²ISAS-Institute for Analytical Sciences</td>
</tr>
<tr>
<td>3:50</td>
<td>(140) UV-Femtosecond and Nanosecond Laser Ablation-ICP-MS: Repeatability and Reproducibility During the Ablation of Transparent Materials: Jhanis González¹, Siv. Dunders¹, Chunyi Liu¹, Samuel Mao¹, Xianglei Mao¹, Richard Russo¹; ³Lawrence Berkeley National Laboratory</td>
</tr>
<tr>
<td>4:10</td>
<td>(141) Resonant Laser Ablation of Metals Detected by Atomic Emission in a Microwave Plasma, and By Inductively Coupled Plasma Mass Spectrometry: Danielle Cleveland¹, Peter Stchur¹, Xiandeng Dan Hou¹, Karl Xiaodong Yang¹, Robert G. Michel¹; ²Department of Chemistry, University of Connecticut</td>
</tr>
<tr>
<td>4:30</td>
<td>(142) Laser Ablation Inductively Coupled Plasma Mass Spectrometry of Human Hair: Kevin Bemben¹, Eric Salín¹; ³McGill University</td>
</tr>
<tr>
<td>4:50</td>
<td>(143) Laser Ablation and Ionization Mass Spectrometry for the Chemical Analysis of Glasses: Greg Kluunder¹; ²Lawrence Livermore National Laboratory</td>
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<tr>
<td>5:10</td>
<td>(144) Laser Ablation ICP Optical Spectrometry of Vitreous Waste Surrogates: A New Model for Hazardous Waste QC Analysis: Lawrence Neufeld¹, Pete Brown¹, Gary Kunselman¹; ²New Wave Research, Inc.; ³Teledyne Leeman Labs</td>
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### Monday Afternoon, Room C123
**LASER ABLATION**  
Organizer and Presider: Greg Klunder

<table>
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<tr>
<th>Time</th>
<th>Session</th>
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<tbody>
<tr>
<td>3:30</td>
<td>(145) Quantitative 2D IR Correlation Analysis: Richard Dhuly¹; Saratchandra Shammukh¹; ³University of Georgia</td>
</tr>
<tr>
<td>3:50</td>
<td>(146) 2-D Correlation Analysis and Multivariate Chemometric Data Treatment of Time-Resolved Vibrational Spectra: Heinz W. Siessler¹, Peiyi Wu¹, Markus Fueleborn¹; ²Department of Physical Chemistry, University of Du; ³Department of Macromolecular Science</td>
</tr>
<tr>
<td>4:10</td>
<td>(147) Two-Dimensional Correlation for Peak Identification in DNA Analysis: Lei Geng¹, Gufeng Wang¹; ³University of Iowa;</td>
</tr>
<tr>
<td>4:30</td>
<td>(148) Using Perturbation Domain Decomposition to Reveal System Dynamics and Enhance Cross Peak Discrimination in Two-Dimensional Correlation Spectroscopy: Andrew Jirasek¹,², Georg Schulze¹, Michael W. Blades¹,², Robin F. B. Turner¹,²; ²Biotechnology Laboratory, University of British Columbia; ³Department of Chemistry, University of British Columbia; ³Department of Electrical and Computer Engineering</td>
</tr>
<tr>
<td>4:50</td>
<td>(149) Two-Dimensional Correlated Spectroscopic Studies on the Fine Structure of the Fluorescent Bands from Conjugated Organic Compounds: Yizhuang Xu¹, Wei He¹, Di Miao¹, Jinguang Wu¹; ³Department of Chemistry, Peking University, Beijing</td>
</tr>
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### MONDAY POSTER SESSIONS and BREAK  
2:00 – 3:30 PM, See pages 40-43  
*Exhibit Hall A*
Monday Afternoon, Room B113
NEW DEVELOPMENTS IN MASS SPECTROMETRY FOR FORENSICS
Organizer: Greg Klunder • Presider: Relchel Lowe

3:30 (151) Desorption/Ionisation on Chemically Modified Porous Silicon for the Identification of Small Analyte Molecules relevant in Forensic Investigations.; Rachel Lowe1,2, Nico Voelcker2, Paul Kirkbride2, Robert Blackledge1, Nathan Salazar4, Eden Go3, Gary Siuzdak1; 1The Scripps Research Institute, Center of Mass Spectrometry; 2The Flinders University of South Austral; 2, BioAnalyte, Melbourne, Australia; 3, Flinders Medical Center, SA, Australia; 4USDA-ARS Russell Research Center, Beltsville, MD
3:50 (152) Culture Dependent Variability in Bacillus Spore Protein Composition Observed by Capillary Liquid Chromatography and Mass Spectrometry; David Liu1, Karen Wahl1, John Bernert1; 1USDA-ARS Russell Research Center, Beltsville, MD
4:10 (153) Simultaneous Screening for Multiple Categories of Drugs of Abuse by LC/MS/MS; June Feng1, Yingkun Dai1, Lanqing Wang1, John Bernert1; 1USDA-ARS Russell Research Center, Beltsville, MD
4:30 (154) HPLC-MS and HPLC-FTIR Analysis of Inks for Forensic Purposes; Roger Jones1, Anthony Wagner1, John McClelland1, Carol Hurd1; 1Institute of Physical Research and Applications For a New Series of NIR Spectrometers; 2Division of Parasitic Diseases, Centers; 3Centre for Tropical Medicine, Oxford University; 4Institute for Physical Research and Applications For a New Series of NIR Spectrometers; 2Division of Parasitic Diseases, Centers; 3Centre for Tropical Medicine, Oxford University

Monday Afternoon, Room C124
NEAR IR, II
Organizer and Presider: David Himmelsbach

3:30 (157) End User Specification and Justification of a New Field-Ready NIR Spectrometer Design; James de Haseth1, Trad A. Brown1, II, David Himmelsbach2; 1University of Georgia; 2US Department of Agriculture
3:50 (158) Applications For a New Series of NIR Spectrometers; Franklin Barton1, II, James de Haseth2, David Himmelsbach1; 1USDA-ARS Russell Research Center; 2Department of Chemistry, University of Georgia
4:10 (159) ALERT! Code (Near Infra) RED!…..A New, Non-Scanning, Multiplexing Spectrometer Design: Can it Pass the Throughput/SNR Challenge?; Richard DeVerse1, Andreas Coppi1, Frank Geshwind2, Robert Hammaker1, Bill Fateeley1, Ronald Coifman1; 1Plain Sight Systems
4:30 (160) Design Challenges for a Fourier Transform Spectrometer in Non-Invasive Blood Glucose Monitoring; Ben VerSteeg1, John Maynard2, Alan Ross3, Russell Abbink4; 1InLight Solutions, Inc.

Monday Afternoon, Room B115
CARBON NANOTUBE SEPARATION II
Organizers: Wei Zhao and Steven Doorn • Presider: Stephen Doorn

3:30 (161) Technology Beyond the Laboratory: From Customized Instruments to Low-Cost Spectral Sensors; John Coates1, 2Coates Consulting
3:50 (162) A High-Resolution, MEMS-based, Miniature NIR Spectrometer; Richard Crocombe1, Larry McDermott1, Matthew Smith1; 1Axsun Technologies
4:10 (163) Single Cell Profiling with Mass Spectrometry for Neuropeptide Discovery; John Jurchen1, Stanislav Rubakhin1, Nathan Hatcher1, Eric Monroe2, Jonathan Sweedler1; 1Department of Chemistry, University of Illinois
4:30 (164) Recent Developments in TOF/TOF; Jennifer M. Campbell1; 2Applied Biosystems
5:10 (165) A Proteomics Approach to BioAgent Detection; Robert Cotter1, 2Johns Hopkins University
5:30 (166) Quantitative Proteomic Analysis of Inorganic Phosphate Treatment of Osteoblast Cells Using a Combined ESI/MALDI-MS/MS Approach; Li-Kong Yu1, Kelly A. Conrads2, David A. Lucas3, King C. Chan4, Brian L. Hood5, Carl F. Schaefer6, Hailem J. Issaq1, George R. Beck Jr.7, Thomas P. Conrads1, Timothy D. Veenstra1; 1Laboratory of Proteomics and Analytical Technologies; 2Laboratory of Cancer Prevention, Center; 3Center for Bioinformatics
6:30 (167) Aptamer-Enhanced Matrix Assisted Laser Desorption/Ionization for Affinity Mass Spectrometry; Lawrence Dick1, 2, Linda McGown1; 1Duke University
5:10 (168) Clustering of Counterfeit Antimalarial Tablets using Accurate Mass Measurements in an Orthogonal Time-of-Flight Mass Spectrometer; Facundo Fernandez1, Krystyn Alter1, Leonard Arthur2, Michael Green2, Paul Newton1; 1School of Chemistry and Biochemistry, Georgia Institute; 2Division of Parasitic Diseases, Centers; 3Centre for Tropical Medicine, Oxford University

Monday Afternoon, Room A105
TOF MS FOR PROTEOMICS
Organizer and Presider: Robert Cotter

3:30 (169) Amine-Assisted Separation of Single Wall Carbon Nanotube by Type; Fotios Papadimitrakopoulos1, 2University of Connecticut
3:50 (170) Separation of Semiconducting from Metallic Carbon Nanotubes by Noncovalent Engineering of Walled Carbon Nanotubes; John Chen1, Rajagopal Ramasubramaniam1, Haiying Liu2; 1Zyvex Corporation; 2Department of Chemistry, Michigan Technology
4:10 (171) Extinction Coefficients and Purity of Single-Walled Carbon Nanotubes; Bin Zhao1, Mikhail E. Itkis2; 1University of California
4:30 (172) Optical Trapping of Water-Soluble Single-Walled Carbon Nanotubes; Yuegang Zhang1, 2Intel Corporation

Monday Afternoon, Room B113
NEW DEVELOPMENTS IN MASS SPECTROMETRY FOR FORENSICS
Organizer: Greg Klunder • Presider: Relchel Lowe

3:30 (150) Probing Sonication-induced Spectral Changes in HiPco Carbon Nanotubes by using 2D Correlation Spectroscopy; Wei Zhao1, Brian Benedict1; 1Department of Chemistry, University of Arkansas
4:10 (151) A Taxonomy-Based Decision Tree for Forensic Fiber Dye Analysis by LC-MS; June Feng1, Yingkun Dai1, Lanqing Wang1, John Bernert1; 1USDA-ARS Russell Research Center, Beltsville, MD
4:30 (152) Recent Developments in TOF/TOF; Jennifer M. Campbell1; 2Applied Biosystems
5:10 (153) A Proteomics Approach to BioAgent Detection; Robert Cotter1, 2Johns Hopkins University
5:30 (154) A Proteomics Approach to BioAgent Detection; Robert Cotter1, 2Johns Hopkins University
6:30 (155) A Proteomics Approach to BioAgent Detection; Robert Cotter1, 2Johns Hopkins University

Monday Afternoon, Room CE24
NEAR IR, II
Organizer and Presider: David Himmelsbach

3:30 (156) End User Specification and Justification of a New Field-Ready NIR Spectrometer Design; James de Haseth1, Franklin Barton1, II, David Himmelsbach2; 1University of Georgia; 2US Department of Agriculture
3:50 (157) Recent Developments in TOF/TOF; Jennifer M. Campbell1; 2Applied Biosystems
4:10 (158) A Proteomics Approach to BioAgent Detection; Robert Cotter1, 2Johns Hopkins University
4:30 (159) A Proteomics Approach to BioAgent Detection; Robert Cotter1, 2Johns Hopkins University
5:10 (160) A Proteomics Approach to BioAgent Detection; Robert Cotter1, 2Johns Hopkins University
6:30 (161) A Proteomics Approach to BioAgent Detection; Robert Cotter1, 2Johns Hopkins University

Monday Afternoon, Room B115
CARBON NANOTUBE SEPARATION II
Organizers: Wei Zhao and Steven Doorn • Presider: Stephen Doorn

3:30 (162) A High-Resolution, MEMS-based, Miniature NIR Spectrometer; Richard Crocombe1, Larry McDermott1, Matthew Smith1; 1Axsun Technologies
3:50 (163) Single Cell Profiling with Mass Spectrometry for Neuropeptide Discovery; John Jurchen1, Stanislav Rubakhin1, Nathan Hatcher1, Eric Monroe2, Jonathan Sweedler1; 1Department of Chemistry, University of Illinois
4:10 (164) Recent Developments in TOF/TOF; Jennifer M. Campbell1; 2Applied Biosystems
4:30 (165) A Proteomics Approach to BioAgent Detection; Robert Cotter1, 2Johns Hopkins University
5:10 (166) A Proteomics Approach to BioAgent Detection; Robert Cotter1, 2Johns Hopkins University
6:30 (167) A Proteomics Approach to BioAgent Detection; Robert Cotter1, 2Johns Hopkins University
4:50 (173) Fabrication and Assembly of Single-Walled Carbon Nanotubes by Dielectrophoresis; Jie Tang1,2, Guang Yang2, Huazhi Geng2, Jian Zhang2, Qi Zhang2, Lu-Chang Qin2, Otto Zhou2; 1National Institute for Materials Science, Tsukuba; 2Department of Physics and Astronomy, University of North Carolina at Chapel Hill

5:10 (174) Load Transfer in Functionalized SWNT/polymer Nanocomposites; Viktor Hadjiev1, Dimitris Lagoudas2, Ramanan Krishnamoorti1, James Tour1, Leonard Yowell2, Sivaram Arepalli1, 1University of Houston; 2Texas A&M University; 1University of Puerto Rico - Mayaguez Campus; 2NASA Johnson Space Center

Monday Afternoon, Room B116
MINIATURE SPECTROSCOPIC SENSORS
Organizer and Presider: Michael Myric

3:30 (175) Development of Small Raman Systems for Stand-off and In-situ Measurements; S. Michael Angel; 1Department of Chemistry & Biochemistry, The University of South Carolina

3:50 (176) Compact Spectrometers in Modern Analytical Spectroscopy; Harry Forsyth1; 1Ocean Optics

4:10 (177) Design of Miniature Spectrometers Based on Light Emitting Diodes; Kevin Cantrell1; James D. Igle2; 1University of Portland; 2Oregon State University

4:30 (178) Miniaturization of Industrial Photometric Analyzer; Mike Ponsinol1; 1Custom Sensors & Technology

4:50 (179) MEMS Technology Moves Process Spectroscopy Into A New Dimension; Richard Crocombe1, Larry McDermott1, Matthew Smith2; 1Axsun Technologies

5:10 (180) Development of Compact Instrumentation for at Line Metal Analysis; James Barnes1, Cris Lewis1, Ruth Waddell1, Christian Hassell1; 1Los Alamos National Laboratory

Monday Afternoon, Room A106
DATA ANALYSIS AND RAMAN SPECTRA
Organizer and Presider: Mark Kemper

3:30 (181) Multivariate vs. Univariate Quantitation of Polymorphs in Drug Product by Raman Spectroscopy; Fred LaPlant1, Mario Fabiilli1, Steve Arrivo2; 1Pfizer, Inc.

3:50 (182) Raman and Near Infrared Spectroscopic Studies of Compounds Dissolved in Methanol and Water Solvent systems; Rodolfo Romañach1, Zainette Rivera1, Ciser Cabarcas1, Maria Guardiola2, Mark Kemper3; 1University of Puerto Rico - Mayaguez Campus; 2Kaiser Optical Systems

4:10 (183) Raman Analysis of Concentrated Salt Solutions Using Robust Modeling and Data Fusion; Jeremy M. Shaver1, Samuel A. Bryan2, Tatiana G. Levitskaia3, Serguei I Sinkov2; 1Eigenvector Research, Inc.; 2Pacific Northwest National Laboratory

4:30 (184) Development and Implementation of an On-Line Quantitative Raman Method for Pharmaceutical In-Process Reaction Analysis; Robert Wethman1, Charles Ray1; 1Bristol-Myers Squibb

4:50 (185) Algorithms and Preprocessing Techniques to Automatically Classify Samples in a Microtiter Plate by Raman Spectroscopy; Steve Lowry1, Dave Dalrymple1, Dick Wieboldt1; 1Thermo Electron Corporation

5:10 (186) Data Reduction Methods in Dynamic Raman Spectroscopy of Tissue Specimens; Michael D. Morris1, William F. Finney2, Nicole Crane3, Andrew Callender4; 1University of Michigan

5:30 (187) Challenges of Qualitative Data Analysis in Raman Microspectroscopy of High-throughput Crystallization Wellplates; CJ Pommier1, Gary McGeorge2, Victor Rosso3, Anne Song3; 1Bristol-Myers Squibb
TECHNICAL PROGRAM – TUESDAY
Plenary and Posters

7:30 Wake Up Coffee, Ballroom Lobby

ANACHEM Award
Presented by Colin Poole
8:00 AM Plenary Session, Ballroom 201

Walter Jennings

(188) Brief History of Developments in GC Columns; Walter Jennings
1,2; 1University of California, Davis; 2Agilent Technologies, Inc

Charles Mann Award
8:30 AM Plenary Session, Ballroom 201

Michael Carrabba

(189) Raman Spectroscopy: How Did We Get Here and Where Are We Going?; Mike Carrabba1; 1Hach Homeland Security Technologies

TUESDAY POSTER SESSIONS and BREAKS
9:00 – 10:30 AM and 2:00 – 3:30 PM
Exhibit Hall A/A-1

All Tuesday posters should be put up between 7:30 – 8:00 AM and removed between 5:30 – 6:00 PM. Odd numbered posters present between 9:00 - 10:30 AM and even numbered posters present between 2:00 – 3:30 PM

LIBS
(190) Determination of Chromium in Solids and Liquids by Laser-Enhanced Ionization Spectrometry in the Nitrous Oxide/Acetylene Flame; Isabelle Poulin1, Denis Boudreau1; 1Université Laval

(191) Utilization of Confinement Effect and Sub-target Effect in Spectrochemical Analysis using TEA CO2 Laser-Induced Plasma; Kiichiro Kagawa1,2, Nasrullah Idris1, Takao Kobayashi1, Hendrik Kurniawan3, Kenichiro Tsuyuki4, Satoru Miura4; 1Department of Fiber Amenity Engineering, Faculty; 2Department of Physics, Faculty of Education; 3Research Center of Maju Makmur Mandiri; 4Kajima Technical Research Institute

Advances in Plasma Spectrometry
(193) Semi Quantitation Mode in Modern Inductively Coupled Plasma Mass Spectrometry for the Determination of Trace Elements in Routine Laboratories; Heidi Chen1, Ewa Dabek-Zlotorzynska1, Nouri Hassan2, Monique Lanouette2, Pat E. Rasmussen2; 1AAQD, Environmental Technology Centre, Environment; 2Safe Environments Programs, HECS Branch

(194) Evaluation of Semi Quantitation Mode Combined with Collision Cell in Routine Analysis of Environmental Samples using ICP-MS; Heidi Chen1, Ewa Dabek-Zlotorzynska1; 1AAQD, Environmental Technology, Environment Canada

(195) New Array Detector ICP-OES Design Criteria; Geoff Tyler1, Cendrine Dubuisson1, Emmanuel Fretel1, Alain Le Marchand1, Yves Danthez1, Olivier Rogerieux1; 1Jobin Yvon SAS

(196) Investigation of Hydroxyl-mediated Spectral Interference From Easily Ionized Elements in Laser-enhanced Ionization Spectrometry in the 281-285 nm Range.; Karine Herreyre1, Denis Boudreau1; 1Université Laval

(197) Relationship of Plasma Rotational Frequency and Plasma Temperature in a New Multi-plasma Gas ICP; Hidekazu Miyahara1, Takayuki Doi1, Yoichi Mizusawa1, Yasushi Hayashi1, Eiki Hotta1, Akitoshi Okino1; 1Department of Energy Sciences Tokyo Institute of Technology

(198) A New Concentric PFA Nebulizer for ICP-MS Spectrometry; Fred Smith2, Joe Brady1; 1CETAC Technologies

(199) Cost Effective Clinical Elemental Analysis; Graphite Furnace AAS or ICP-MS?; Simon Nelms1, Phil Shaw1, Bill Spence1, Martin Nash1; 1Thermo Electron

(200) Considerations on the Connection of a Glow Discharge Ion Source to a Fast Scanning Sector Field ICP-MS; Lothar Rottmann1, Joachim Hinrichs1, Wolfgang Schoettger1, Meike Hamester1; 1Thermo Electron

(201) Optimizing ETV-ICP(TOF)MS and Mass Transport to the Plasma; James Holcombe1, Nikhilesh Desai1, Gulay Ertas1, William Balsanek1; 1University of Texas at Austin

(202) Online Standard Additions Calibration of Transient Signals for Inductively Coupled Plasma Mass Spectrometry; Eric D. Salin1, E. Jane Maxwell1, Margaret Antler1; 1McGill University
TECHNICAL PROGRAM – TUESDAY  
Posters 9:00 – 10:30 AM and 2:00 – 3:30 PM

(203) Revisiting Traditional Methods for Determination of Trace Metals in Clinical Samples by Graphite Furnace AAS; Doug Shradler, Christine Rivera, Jean-Pierre Lener; iVarian Inc.

(204) Sector Field ICP-MS for the Direct Determination of Semiconductor Relevant Inorganic Contaminants and Matrices; Meike Hamster, Julian Wills, Lothar Rottmann; Thermo Electron

(205) Determination of Micro-inclusions – a New Dimension in OES Analysis of Metallic Samples; Arne Bengtson, Miroslava Sedlakova; 1Swedish Institute for Metals Research

(206) Imaging of Ion Densities in the Sampling Cone of an ICP-MS by Planar Laser Induced Fluorescence; Paul Farnsworth, Jeffrey Macdowen, Andrew Mills; iBrigham Young University

(207) Development of Sampling Geometry for Monitoring Ion Concentrations in RF Plasma Induced Deposition Reactions by Quadrupole Mass Spectrometry; Jeff Anderson, Rene Rodriguez; iISU Chemistry

(208) Enhanced Security Software for Inductively Coupled Plasma Mass Spectrometry (ICP-MS); Peter Cop, Mihauela Geaman; iPerkinElmer SCIEX

The Role of Analytical Chemistry in Human Disease

(209) Separation and Determination of Semi-Volatile Organics in Fine Particles; Jimmy Pau; iU. S. EPA

(210) Stability Investigation of CRL1005 Polymer Adjuvant for HIV DNA Vaccine Using Traditional and Spectroscopic Methods of FT-IR/ATR, NMR and MALDI-MS; Joyce Sweeney, Steven Cohen, Tsang-Lin Hwang, Pei-Kuo Tsai; iMerck & Co., Inc.;

(211) Precision and Control of Linoleic Acid/Ferric Thiocyanate Assay for Antioxidants; Alexander Scheeline, Laurel Luckey, Mark Mulliner, Mark Rundell, Elizabeth Wagner, Michael Plewa; 1University of Illinois at Urbana-Champaign Departm; 2University of Illinois at Urbana-Champaign

(212) Reversed Phase Retention on Porous Polymer Monoliths Used in Capillary Electrochromatography; Michelle Bushey, Brent Waguespack, Slade Hodges, Lindsay Sondergeld, Meghan Bush; i Trinity University

(213) Chemometric Tools for Noise and Background Reduction of Complex Liquid Chromatography/Mass Spectrometry and Extraction of Minor Sample Differences; Willem Windig; iEigenvector Research Inc


(215) Separation of Racemic 2,4-Dinitrophenyl Amino Acids on 9-O-(phenyloxycarbonyl)quinine-bonded Carbon-Clad Zirconia in Reversed-Phase Liquid Chromatography; Jung Hae Park; i In Whan Kim; 1Yeungnam University; 2Daegu University

(216) GC x GC - TOFMS and Metabolomics; Janiece L. Hope, Amanda E. Sinha, Bryan J. Prazen, Robert E. Synovec; 1University of Washington

(217) Applications of Small Surface Plasma Resonance Sensors for Biochemical Monitoring; Jean-Francois Masson, Tina Battaglia, Margaret Barnhardt, Ronald Nieman, Stephen Beaudoin, Karl Booksh; 1Department of Chemistry and Biochemistry, Arizona; 2School of Chemical Engineering, Purdue University

(218) Application of the Aluminum Substrate in NIR-Raman Spectroscopy: Quantitative Analysis of Methyl Parathion Pesticide Microdroplets; Roberto Sato, Cirilo Medina, Claudio Frausto; 1Universidade de Guadalajara, Campus Los Lagos; Centro de Investigaciones en Optica

(219) Hyperpolarized Xenon For NMR Signal Enhancement of Surface Species; Kevin Knagge, Daniel Raftery, Jonathan Prange, Carl Murphy; i Purdue University

(220) Can Breast Cancer Be Caused by Active or Passive Smoking?; Gus Miller; iEdinboro University of Pennsylvania

(221) Fluorescence Detector for Capillary Electrophoresis using Violet Light Emitting Diode and Labeling Reagent; Riichiro Nakajima, Takayoshi Tanaka, Keiichi Noda, Yuki Matsui, Takashi Tamura, Kazuhiro Tsukagoshi; iDoshisha University

(222) Characterization of an Electroactive Metal Chelator using in situ Raman Microscopy; James Holcombe, Ashley Johnson; 1The University of Texas at Austin

(223) Removal of the Effect of Skin Pigmentation in Tissue Spectra: Demonstration with Tissue Mimicking Phantoms; Olusola Soyemi, Michelle Landry, Babs Soller, Patrick Idwasi, Ye Yang; iUniversity of Massachusetts Medical School

(224) High-Pressure NMR and Raman Spectroscopy for Studying Solvation Thermodynamics; Jeanette D. Hanna, Dor Ben-Amotz; iPurdue University

(225) Accelerator Mass Spectrometry Method for Quantification of Beryllium in Biological Samples: Application for Studying Chronic Beryllium Disease; Marina Chiarappa-Zucca, Robert Finkel, Roger Martinelli, Jeffery McAninch, Kenneth Turkeltaub; iLawrence Livermore National Laboratory

(226) The Characterization of Azophenol Analogues for Use as Fluorescent Ion Selective Probes; Richard Williams, Yosef Hijji; 1Morgan State University, Chemistry Department

(227) New Approaches for the Efficient Fabrication and High-Spatial Resolution Readout of Large Arrays of Optical Fiber Sensors; Peter Geissinger, Barry Prince, Maureen Prince, Alan Schwabacher; 1Department of Chemistry & Biochemistry, University of Wisconsin; 2Department of Chemistry, University of Canterbury

(228) A Novel Method for Particle Synthesis and Their Controlled Deposition onto Individual Lung Cells; Allen Haddrell, George Agnes, Stephen van Eeden; 1Simon Fraser University; 2University of British Columbia

(229) Biomarkers-Analytical Applications in the Research and Assessment of Human Disease Arena Pharmaceuticals

(230) Nanoparticle-Enhanced Fluorescent Detection of Biomarkers; Scott Reed; iPortland State University

(231) Chemometrics in Pharmaceutical Process Analytical Technology

(232) Determination of the Enantiomeric Composition of Guest Molecules by Chemometric Analysis of the Fluorescence Spectra of Cyclodextrin Guest-host Complexes; Kenneth Busch, Sayo Fakayode, Marianna Busch; 1Baylor University
(234) Fluorescence Investigation of Factors Which Affect the Chloride Sensing Ability of 6-methoxyquinoline; Anindya Darra1, Apurba Lal Koner1, Padmaja Prasad Mishra1, Smita Jha1; 1Indian Institute of Technology, Bombay

(235) Spectroscopic Studies of Goat Diets in Arid Environments; Gary Rayson1, Dean Anderson2, Kris Havstad2, Y. S. Landau2, Tzach Glasser2, John Walker2; 1Department of Chemistry and Biochemistry, New Mexico State University; 2United States Department of Agriculture; 3State of Israel Ministry of Agriculture; 4Texas A&M University System Extension

(236) PCB Contamination in an Asphalt-Coated Storm Sewer: An Environmental and Materials Investigation; Eileen M. Skelly Frame1, Anthony J. Kriech2, Kenneth R. Pike3; 1Full Spectrum Analytical Consultants, Halfmoon, NY; 2Heritage Research Group, Indianapolis; 3Earthworks Environmental, Brockport, NY

(237) Characterization of Nuclear Fuel “Particles” by Micro-COLUMN Gas Pressurized Extraction Chromatography and Inductively Coupled Plasma Mass Spectrometric Detection (ICP-MS); Jeffrey Giglio1, Daniel Cummings1, Kevin Canney1, Marianne Noy1, Mary Adamic1; 1Argonne National Laboratory-West

(238) Measurement of Aerosol Optical Properties Using Cavity Ring Down Spectroscopy; Hossein Bazargan1, Dean Atkinson1; 1Portland State University, Chemistry Department

(239) Water Only HPLC with FID Detection; Dale Felix1, Stephanie Marin1, Brian Jones1; 1Solarity Technologies

(240) How Toxic is Asbestos? An Analysis of the Research; Gus Miller1; 1Edinboro University of Pennsylvania

(241) Optimization of an Automated SPME-GC/ITMS Method for Analysis of a Broad Range of Water Contaminants; Robert Stiles1; 1Portland State University, Chemistry Department

(242) Chlorine Detection at EPA Regulatory Limits by Use of a Test Strip; Howard Ray1; 1Industrial Test Systems, Inc.

(243) Membrane Introduction Tandem Mass Spectrometry (MIMS-MS/MS) for Real Time Measurement of Atmospheric Contaminants; Chris Gill1, Skye Creba1, Janet Nelson1, Alexander Thompson1, Chris Simpson1, Erik Krogh1; 1Malaspina University-College; 2University of Washington

(244) Cyanide Detection ug/L to mg/L with Great Precision Using Reagent Strip Colorimetric Method; Ivars Jaunakais1; 1Industrial Test Systems, Inc.

(245) Algorithm Development for Automated Raman Spectral Searching; Brian Eckenrod1, Valerie Cavet1, Anthony Kearsley1; 1FBI; 2NIST

(246) High-precision Uranium Isotopic Analysis for Environmental Forensics Using MC-ICPMS; Demonstration Studies at the Hanford Site, Washington; John N. Christensen1, 2, P. Evan Dresel3, Mark E. Conrad2, Donald J. DePaolo1, 3, 4, 5; 1Lawrence Berkeley National Laboratory; 2Pacific Northwest National Laboratory; 3Department of Energy and Planetary Science

(247) The Intramolecular Interactions during the Melt Crystallization of PLLA and PLLA/PDLLA Stereocomplex Investigated by Infrared and 2D IR Spectroscopy; Jianming Zhang1, Yukihiro Ozaki1, Hideko Tsuji1, Isao Noda2, Kwansai Gakuen University; 2Toyohashi University of Technology; 3The Procter & Gamble Company

(248) Terahertz Spectroscopy of High-energy Materials; Philip Taday1, William Tribe1, David Newnham1, Yaochen Shen1, Michael Kemp1; 1TeraView Limited

(249) VCD Spectroscopic Determination of Absolute Stereochecmy as a Complimentary Technique for Investigation of Chiral Drugs; Mike Claybourn1, Helen Turner1, Christopher Frampton2, Ron Roberts3, Andrea Russell4; 1AstraZeneca; 2Southampton University; 3Bruker Noyon

(250) Absolute Configuration and Solution Conformation Determinations by Vibrational Circular Dichroism; Teresa B. Freedman1, David Dunmore1, Xiaolin Cao1, Laurence A. Nafie1; 1Department of Chemistry, Syracuse University

(251) Wavelength Modulation Spectroscopy for Simultaneous Temperature and H2O Concentration Measurement in a Flame; Mohammadreza Gharayi1, Steven Buckley1; 1University of California, San Diego

(252) Quantitation of Metallothionein by Using CID Mass Spectrometry; Yuchen Lu1; 1West Virginia University

(253) Evaluation of Dual Use Direct to Metal (DTM) Primers for U.S. Department of Defense (DOD) Tactical Vehicles; William Lum1, James Kidd1, Chris Miller1, John Escarsrega, Brian Placzankis1; 1Army Research Laboratory, Materials Applications Branch

(254) Design of Two-dimensional Photonic Crystal Slab with Complete Bandgap for Infrared Spectroscopy; Hitoshi Kitagaw1, 2, Takashi Asano1, Susumu Noda1; 1Kyoto University; 2ALPS Electric Co., Ltd

(255) Field Portable Raman Probe for in-situ Analysis of Hydrothermal Vents; Tina Battaglia1, Eileen Dunn1, John Holloway1, Marvin Lilley2, Brian Dable2, Brian Marquardt2, Karl Booksh1; 1Arizona State University; 2Center for process Analytical Chemistry; 3University of Washington

(256) Exploration of Molecular Orientation in Polymers Fibers Using Novel Raman Spectroscopy Methods; Simon Frisk1, Richard M. Ikeda1, D. Bruce Chase2, John F. Rabolt2; 1Dept. Materials Science and Engineering; 2DuPont Central Research and Development

(257) Raman Spectroscopic Markers for Osteoarthritis: Collagen Amide Vibration; Nicole Cranef1, Michael Morris1, Blake Roessler1, Abigail Smukler1; 1University of Michigan, Department of Chemistry; 2University of Michigan Medical School

(258) Rapid Saliva Analysis for Clinical Trials; Chetan Shende1, Alan Gift1, Frank Inscore1, Stuart Farquharson1; 1Real-Time Analyzers

(259) Terahertz Spectroscopy in Proteomics; Philip Taday1, Thomas Lo1, David Newnham1, Michael Pepper1; 1TeraView Limited; 2University of Cambridge

(260) Monitoring Astronaut Health: Urinalysis by Surface-enhanced Raman Spectroscopy; Frank Inscore1, Chetan Shende1, Alan Gift1, Stuart Farquharson1; 1Real-Time Analyzers

(261) LSI’s Intelligent Software: New Tools for Raman Spectra-Informatics; Yongguo Yang1, Canwen Liu1, Shaoqing Peng1, Wanglong Zhou2, Victor Sapirstein1; 1Lambda Solutions, Inc.
<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
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</table>
<pre><code>  | 1University of California, San Diego; 2University of Maryland, College Park              |
</code></pre>
| 11:10  | (270) LIBS at Low Pressure: Application to planetary surface exploration; David Cremers, Béatrice Sallé, Roger Wiens, Sylvestre Maurice, CEA Saclay, France;  
      | 1Los Alamos National Laboratory, Los Alamos; 2Observatoire Midi-Pyrénées, Laboratoire     |
| 11:30  | (271) Temperature Effects in ns/ns Dual Pulse Laser Induced Breakdown Spectroscopy; Jonathan Scaffidi, William Pearman, J. Chance Carter, William Colston, Jr.;  
      | 1University of South Carolina; 2United States Military Academy; 3Lawrence Livermore National Lab |
| 11:50  | (273) Compact Echelle Spectrograph with High Resolution Intensified CCD for Laser Induced Breakdown Spectroscopy (LIBS); Marc Neglia, Bruce True, Ryan Sullivan;  
      | 1Princeton Instruments (a division of Roper Scientific)                                     |
### TECHNICAL PROGRAM – TUESDAY
Orals 10:30 AM – 12:30 PM

**Tuesday Morning, Room B114**

**GENERAL CHEMOMETRICS**
Organizer and Presider: Barry Wise

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
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<tbody>
<tr>
<td>10:30</td>
<td>(284) A Novel Spectroscopic Method for Determining the Enantiomeric Purity of Samples Without the Need of a Chiral Auxiliary; Dennis Rabbé, Mariana Busch, Kenneth Busch; Baylor University</td>
</tr>
<tr>
<td>10:50</td>
<td>(285) Analysis of Jet Fuel Properties based on Raman Spectroscopy; Stuart Farquharson, Alan Gift, Wayne Smith; Real-time Analysts 11:10 (286) The Use of Raman Spectroscopy to Characterize Hydrogenation Reactions; Mark Kenner, Ian Lewis, Sri Venkata Tumuluri, Bonnie Avery, Mitchell Avery; Kaiser Optical Systems; University of Mississippi</td>
</tr>
<tr>
<td>11:30</td>
<td>(287) Photoacoustic Multivariate Optical Computing: Ethanol and Water in the MIR; Ryan Priore, Michael Myrick; University of South Carolina</td>
</tr>
<tr>
<td>11:50</td>
<td>(288) Chiral Analysis by Regression Modeling of UV Absorption Spectral Data—the Use of Modified Cyclodextrins as Chiral Auxiliaries; Mariana Busch, Sayo Fakayode, Isabel Swamidoss, Kenneth Busch; Baylor University</td>
</tr>
<tr>
<td>12:10</td>
<td>(289) A Review of Multi-way Models and Their Use in Monitoring Batch and Continuous Processes; Barry M. Wise, Neal Gallagher; Eigenvector Research, Inc.</td>
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**Tuesday Morning, Room B113**

**ADVANCES IN FORENSIC ANALYTICAL TECHNIQUES**
Organizer: Greg Klunder  Presider: Rachel Lowe

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
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<tbody>
<tr>
<td>10:30</td>
<td>(290) Comparison of instrumental and Biological Field Detection of Accelerants and Explosives; Kenneth Fortun, Shirley Chin, Laura Conner, Ross Harper, Jeannette Perr, Douglas Heller, Jose Almirall; Florida Int'l Univ.</td>
</tr>
<tr>
<td>10:50</td>
<td>(291) SPME-GC/MS Investigations Into the Uniqueness of Human Scent; Allison Curran, Kenneth Fortun; Florida International University</td>
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<td>10:50</td>
<td>(291b) Application of Fluorescence Line Narrowing Spectroscopy to Forensic Fiber Examination; Andres Campiglia, Michael Sigman; Univ. of Central Florida</td>
</tr>
<tr>
<td>11:30</td>
<td>(292) Analysis of Children's Latent Fingerprint Residues by Infrared Microspectroscopy; Diane Williams, Justine Brucker-Serrano, Rebecca Schwartz, Edward Bartick; Oak Ridge Institute of Science Education; FBI Counterterrorism/Forensic Science Research</td>
</tr>
<tr>
<td>12:10</td>
<td>(294) Use of FT-IR and EDXRF to Characterize Counterfeit Inkjet Inks; Gene Hall, Jeannine Matuzza; Rutgers University</td>
</tr>
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**Tuesday Morning, Room C124**

**COHERENT 2D VIBRATIONAL SPECTROSCOPY I**
Organizers: Wei Zhao & Peter Hamm  Presider: David Jonas

<table>
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<tr>
<th>Time</th>
<th>Session</th>
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<tr>
<td>10:30</td>
<td>(295) Ultrafast Infrared Vibrational Echo Correlation Spectroscopy; Michael D. Fayer, John B Asbury, Tobias Steinel; Stanford University</td>
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<tr>
<td>11:10</td>
<td>(296) Multidimensional Ultrafast IR-Raman Spectroscopy; Dana Drott; University of Illinois at Urbana</td>
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<td>11:30</td>
<td>(297) Third and Fifth-Order Two-Dimensional Infrared Spectroscopy; Martin Zanni; University of Wisconsin-Madison</td>
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<tr>
<td>11:50</td>
<td>(298) Phase-Stabilized Two-Dimensional Femtosecond Spectroscopy; Tobias Brixner, Igor V. Stiopkin, Graham R. Fleming; Department of Chemistry, University of California</td>
</tr>
<tr>
<td>12:10</td>
<td>(299) Coherent Two-Dimensional Infrared Spectroscopy of Small Peptides; Nien-Hui Ge, Denis Karaiskaj, Hiroaki Maekawa, Soohwan Sul, Jiang Ying; University of California, Irvine</td>
</tr>
</tbody>
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**Tuesday Morning, Room A105**

**ION TRAP MS FOR PROTEOMICS I**
Organizer and Presider: Gary Glish

<table>
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<tr>
<th>Time</th>
<th>Session</th>
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<tr>
<td>10:30</td>
<td>(300) Enzyme Kinetics and Mechanisms; Julie Leary; UC Berkeley</td>
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<tr>
<td>10:50</td>
<td>(301) Studying Metalloporphyrin-Ligand Binding by Quadrupole Ion Trap Mass Spectrometry; Victor Ryzhov; Northern Illinois University</td>
</tr>
<tr>
<td>11:10</td>
<td>(302) Discovering and Characterizing Drug Fragments Using Ion Trap Mass Spectrometry; Mark Cancilla, Daniel Erlanson, Andrew Braisted, Jun Wang, Michelle Arkin, James Wells; Sunesis Pharmaceuticals</td>
</tr>
<tr>
<td>11:30</td>
<td>(303) Structural Analysis of the Glycosylation in Luteinizing Hormone Using a Quadrupole Ion Trap Mass Spectrometer; Heather Desaire; University of Kansas</td>
</tr>
<tr>
<td>11:50</td>
<td>(304) Comparative Performance of Linear and Three-dimensional Quadrupole Ion Trap Mass Spectrometers for the MS/MS Analysis of Peptides; David Burinsky, Connell Cunningham Jr, Gary Glish; GlaxoSmithKline, University of North Carolina - Chapel Hill</td>
</tr>
<tr>
<td>12:10</td>
<td>(305) Unsupervised Clustering of a Large Truth Set of Ion Trap Peptide MS/MS Spectra; Vicki H. Wysocki, Yingying Huang, George Tseng, Shinsheng Yuan, Lijilana Pasa-Tolic, Mary S. Lipton, Richard D. Smith; University of Arizona, University of Pittsburgh, UCLA, Pacific Northwest National Laboratory</td>
</tr>
</tbody>
</table>
Tuesday Morning, Room B115
CARBON NANOTUBE SEPARATION III
Organizers: Wei Zhao & Steven Doorn • Presider: Michael Strano

10:30 (306) Fullerenes and Nanotube Characterization; Robert Hauge1, Zhenming Gu1, Haiping Peng1, Kirk Zigler1, Ya-Qiong Xu1, Anil Sadana1, W.E. Billups1, Al Schultz2, Michael Ugarov2, Richard Smalley1; 1Rice University; 2IonWorx
10:50 (307) Controlled and Reversible Doping of SWNTs; Michael O’Connell1, Ezra Eibergen1, Steve Doorn1; 1Los Alamos National Lab

11:10 (308) Ultra-Long Carbon Nanotubes by Chemical Vapour Deposition; Lianxi Zheng1, Michael O’Connell1, Stephen Doorn1, Xiaozhou Liao1, Yonghao Zhao1, Mark Hoffbauer1, Quanxi Jia1, Dean Peterson1, Jie Liu2, Yuntian Zhu1; 1Los Alamos National Laboratory; 2Chemistry Department, Duke University

11:30 (309) AFM-Nanofinder Composite System and Its Application to Characterization of Single Walled Carbon Nanotubes; Nobukata Nagasawa1,2, Yasushi Morihira1, Jin-Ting Ye1, Pavel Rukovskiy1, Zhi-Kang Tang2, Igor Kudryashov1, Jack Roberts1, Shoji Suruga1; 1Tokyo Instruments, Inc.; 2Department of Physics and Institute of Nano Science and Technology, Hong Kong Univ. of Science and Technology; 3Sympathic TI, Corp.

11:50 (310) Novel Soft Materials Composed of Single-walled Carbon Nanotubes and Ionic Liquids; Takanori Fukushima1, Takuzo Aida1,2, ERATO Aida Nanospace Project, IST; 2Department of Chemistry and Biotechnology

12:10 (311) Direct Growth of Long and Aligned Single Walled Carbon Nanotubes for Nanoscale Electronic Applications; Jie Liu1; 1Duke University

Tuesday Morning, Room A106
CHARLES MANN AWARD
Organizer and Presider: Michael Pelletier

10:30 (312) Status of Deep UV Semiconductor Sources for Laser Induced Native Fluorescence and Resonance Raman Spectroscopy; William F. Hug1, D. Reid1, A. Bhattacharyya1, T. D. Moustakas2, R. Treece2, J. R. Smith1, J. I. Pankove1; 1University of Hawaii; 2Department of Electrical Engineering; 3Astralux Incorporated, Boulder, CO; 4Oregon State University

10:50 (313) A High Performance, Low cost, Very Flexible Raman Spectrometer As A Microscope Attachment; Jun Zhao; 1Bruker Optics

11:10 (314) SERS of Chemical Agents in Water - Determining Limits of Detection; Steven Christensen1, Kevin Spencer2, James Sylvia1, Kristina Gonser1; 1US Army Edgewood Chem Bio Center; 2EIC Laboratories

11:30 (315) Quantitative Process Monitoring Utilizing Raman Spectroscopy; Brian J. Marquardt1, Brian K. Dable1, David Veitkamp1; 1Center for Process Analytical Chemistry

11:50 (316) Development of a Raman Fiber Optic Probe for Monitoring Corrosion Species in High-Level Nuclear Waste; Job M. Bello1, David T. Hobbs; 1EIC Laboratories; 2Savannah River Technology Center

12:10 (317) Fieldable Raman Systems for Trace Analysis; Kevin Spencer1, James Sylvia1, Susan Clauson2, Peter Marren1, Jane Bertone1, Steven Pullins1; 1EIC Laboratories, Inc.

TUESDAY POSTER SESSIONS and BREAK
2:00 – 3:30 PM, See pages 48 - 51

Tuesday Afternoon, Room C123
ADVANCES IN PLASMA SPECTROMETRY
Organizer and Presider: Akbar Montaser

3:30 (318) Recent Advances in ICP Optical Emission Instrumentation; Peter Brown; 1Teledyne Leeman Labs

4:10 (319) Current Status of Laser Ablation ICP-AES: Applications integrating a large beam, short wavelength laser with a simultaneous optical detection system; Lawrence M. Neufeld; 1New Wave Research

4:30 (320) Elemental and Speciation Sample Preparation for Environmental and Forensic Analysis; H.M. Skip Kingston1, Mizanur Rahman1, John Kern1, Matt Patamok2, Theodore Towns1; 1Duquesne University; 2Applied Isotope Technologies (AIT)

5:10 (321) Direct Solution Introduction with Conventional Nebulizers for Inductively Coupled Plasma Mass Spectrometry Using a Short Torch Configuration; Craig Westphal1, Kaveh Kahlen1, Akbar Montaser1; 1George Washington University

Tuesday Afternoon, Room B116
ANACHEM
Organizer: ANACHEM • Presider: Colin Poole

3:30 (322) Chromatography and the Controversy on Kava-Liver Toxicity Association; Chung-Shih Tang1, Klaus Dragull1; 1University of Hawaii

3:50 (323) TBA; Jim Settleidge

4:10 (324) Gas Chromatographic Analysis of Reactive Carbonyl Compounds; Taka Shibamoto; 1University of California

4:30 (325) Tracking Color and Pigment Changes in Anthocyanin Products; Ronald Wrolstad1; 1Oregon State University
Tuesday Afternoon, Room C124
COHERENT 2D VIBRATIONAL SPECTROSCOPY
Organizers: Wei Zhao and Peter Hamm • Presider: Martin Zanni

3:30 (340) Chemical Measurement in the Terawatt Regime; John Wright; 'University of Wisconsin

4:10 (341) Femtosecond 1D and 2D Fourier Transform Spectroscopy of Vibrational and Electronic Motions; David Jonas; 'Dacie Farrow; 'Wei Qian; 'Ryan Smith; 'Allison Ferro; 'University of Colorado

Tuesday Afternoon, Room B115
NANOMATERIALS FOR PHOTONICS I
Organizers and Presiders: Guokui Liu and Gary Wiederrecht

3:30 (351) Nanophotonics with Single Molecules and Small Metallic Nanostructures; W. E. Moerner; 'Department of Chemistry and Chemical Engineering, Stanford University

4:10 (352) Biological Imaging with Quantum Dots; David Norris; 'University of Minnesota

4:50 (353) Single Metal Particle Sensor and Interferometer; Xiao-Min Lin; 'Sang-Kee Eah; 'Gary Wiederrecht; 'Department of Chemistry, University of Wisconsin

5:10 (354) Sensitive RNA Detection in vitro and in vivo; Jianwei Li; 'Paul Choi; 'Benjamin Lee; 'Mark Stanisz; 'Charles Kulwin; 'Xiaoliang Xie; 'Harvard University
<table>
<thead>
<tr>
<th>Time</th>
<th>Title</th>
<th>Presenters</th>
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<tbody>
<tr>
<td>3:30</td>
<td>Biophysical and Bioanalytical Ultraviolet Resonance Raman Spectroscopy Using Fiber-Optics</td>
<td>Michael Blades, Andrew Jirasek, Georg Schulze, R. F. B. Turner, Geoff Horsman, Fred Vaillancourt, Chris Barbosa, Lindsay Eltis</td>
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<td>Organizer and Presider: Glen Loppnow</td>
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<tr>
<td>3:50</td>
<td>Vibrational Spectroscopy of Functional Proteins on Surfaces</td>
<td>Stefan Franzen, Scott Brewer, Simon Lappi, Selina Moses, Jennifer Belyea, NC State Univ.</td>
</tr>
<tr>
<td>4:10</td>
<td>Deep UV Raman Spectroscopic Characterization of Self Assembling Biomaterials</td>
<td>Igor Lednev, Autumn Carlsen, Vladimir Ermolenkov, Wei He, Sei Higashiya, Natalya Topilina, Christopher Wells, John Welch, Ming Xu</td>
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<td></td>
<td>Department of Chemistry, University at Albany, SUNY</td>
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<tr>
<td>4:30</td>
<td>Nonlinear Interferometric Vibrational Imaging</td>
<td>Stephen Boppart, Daniel Marks, Jeremy Bredfeldt, Claudio Vinegoni, University of Illinois</td>
</tr>
</tbody>
</table>
Zhong Lin Wang

(360) Semiconducting and Piezoelectric Nanobelts, Nanosprings and Nanorings; Zhong Lin Wang; Georgia Institute of Technology

Boris Mizaikoff

(361) Mid-Infrared Chemical Sensors - From the Bench into the Deep Sea; Boris Mizaikoff; Georgia Institute of Technology

**WEDNESDAY POSTER SESSIONS and BREAKS**

9:00 – 10:30 AM and 2:00 – 3:30 PM

**Exhibit Hall A/A-1**

All Wednesday posters should be put up between 7:30 – 8:00 AM and removed between 5:30 – 6:00 PM. Odd numbered posters present between 9:00 - 10:30 AM and even numbered posters present between 2:00 – 3:30 PM

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**Important Aspects of Elemental Speciation, Sample Preparation, Separation, Sample Introduction**

(362) X-Ray Fluorescence for Trace Analysis and Environmental Applications Using X-Ray Optics: Thomasin Miller1, Ning Gao1, Zewu Chen1, Walter Gibson1; 1X-ray Optical Systems, Inc.

(363) Determination of Metals in Urban Dust Samples Using Inductively Coupled Plasma Mass Spectrometry: Influence of Microwave Digestion Procedures; Heidi Chen1, Nouri M. Hassan1, Monique Lanouette1, Pat E. Rasmussen1, Valbona Celo1, Ewa Dabek-Zlotorzynska2; 1Safe Environments Program, HECS Branch, Health Canada; 2AAQD, Environmental Technology Centre

(364) Application of a New Commercial GC-ICP-MS Interface for the Analysis of Organotin and Organomercury Species; Martin Nash1, Phil Shaw1, Bill Spence1, Simon Nelms1, Eva Krupp1; 1Thermo Electron Corp., Ion Path; 2LCABIE, HELIOPARC Pau

(365) The Separation and Determination of Iodinated Haloacetic Acids by Gas Chromatography Time of Flight Mass Spectrometry; Hans Mentzen1, David Reckhow1, Julian Tyson1; 1University of Massachusetts, Department of Analytical Chemistry; 2University of Massachusetts

(366) Capabilities of Perfluorinated Carboxylic Acids as Ion-pairing Agents for Arsenic Speciation Analysis by Reversed Phase-LC-ESI-MSn; Jorgelina C. A. Wuilloud1, Rodolfo G. Wuilloud1, Douglas T. Heitkemper1; 1US-Food and Drug Administration/Forensic Chemistry

(367) Advances in Speciation Analysis Using HPLC-ICP-MS: Kenneth Neubauer1, Pamela Perrone1, Wilhad Reuter1, Zoe Grosser1, Ruth Wolf1; 1PerkinElmer Life and Analytical Sciences

(368) Transport of Lead and Arsenic in Plants Used in Phytoremediation; David Butcher1, Joshia Liebschutz1, Patrick Baldwin1; 1Western Carolina University

(369) Determination of Selenium Species by Flow Injection Inductively Coupled Plasma Optical Emission spectrometry (FI-ICP-OES); Princess Hernandez1, Julian Tyson1, Peter Uden1, Dennis Yates1; 1Department of Chemistry, University of Massachusetts; 2PerkinElmer Life & Analytical Sciences

(370) Investigation of Arsenic Species in Hizikia Fusiforme Algae Using Highly Efficient Gradient Ion-Exchange LC-ICP-MS and LC-ESI-MSn; Rodolfo G. Wuilloud1, Jorgelina C. A. Wuilloud1, Douglas T. Heitkemper1; 1US-Food and Drug Administration/Forensic Chemistry

(371) Determination of Fe Species in Cooked Meats; James Harnly1, Edith Blackwell1, Charmonte Watkins1; 1U. S. Department of Agriculture

(372) Determination of Total Mercury in Biological Tissues using Flow Injection CVAAS Following Formic Acid Solubilization; Masahiko Kan1, Scott Willie1, Christine Scriver1, Ralph Sturgeon1; 1Environmental Information Measurement Sciences, Ho; 2Institute for National Measurement Standards

(373) The Investigation of Fertilizer Analyses from Start to Finish Utilizing Microwave Digestion Preparion and Simultaneous ICP-OES with Axial Viewing; Christine Rivera1, Elaine Hasty2; 1Varian, Inc.; 2CEM Corp.

**Molecular Inorganic and Organometallic Mass Spectrometry**

(374) Surface Analysis of Zn coated Steel; Do-Hyung Lee1; 1Research Institute of Industrial Science and Technology

(375) Characterization of Uranyl Ioin Binding by Datura innoxia; Debbie Serna1, Dr. Gary Rayson2; 1New Mexico State University

(376) Determination of Trace Inorganic Mercury by Cold Vapor Generation from Tin Immobilized on an Anion-Exchange; Julian F. Tyson1; 1University of Massachusetts
Biological Analysis Enabled By Micromachining Technologies

Liposomes As Model Systems for Biological Particles: Characterization by Capillary Electrophoresis; Michele Pscher1, Mark Hayes1, 1Arizona State University

Analysis of Liposome Incorporated Intrinsic and Extrinsic Membrane Proteins Via Capillary Electrophoresis; Michele Pscher1, Mark Hayes1, 1Arizona State University

An LC-MS Method for the Quantification of Triglycerides using Metabolically-derived 13C Triglycerides as Internal Standards; April Lachance1, Jason Evans1, 1University of Massachusetts Boston

Development of High-Performance Electromobility Focusing for Protein Analysis; Ryan Kelly1, Paul Humble1, Milton Lee1, Adam Woolley1, 1Brigham Young University

Control of Non-specific Protein Adsorption to Surfaces for Biochemical Monitoring; Jean-Francois Masson1, Tina Battaglia1, Stephen Beaudoin1, Karl Booksh1, 1Department of Chemistry and Biochemistry, Arizona; 2School of Chemical Engineering, Purdue University

Studies of Chiral Recognition Using Fluorescence Anisotropy; Matthew McCarroll1, Yafei Xu1, Irene Kiragu1, 1Southern Illinois University

Polymerized liposomes specifically fabricated for protein sensing; Andres Campagna1, Sanku Mallik1, 1University of Central Florida; 2North Dakota State University

Development of a Polymer-based Optical Sensor for the Ultra-sensitive and Sequence-specific Detection of DNA Material; Kim Dorr1, Sébastien Dubus1, Mario Leclerc1, Denis Bouord1, 1Université Laval

“Smart Sensor” Design: Optical Computations; Jeff Cramer1, Soane Banerji1, Frank Vogt1, Karl Booksh1, Matthew Johnson2, Lisa Hansen2, Denise Wilson1, 1Arizona State University; 2University of Washington

Accelerating Discovery Analytical Chemistry Using Micro Parallel Liquid Chromatography; Surekha Vajihala1, 1Nanostream

High Efficiency Separation of Proteins in Poly(methyl methacrylate)-Based Microchips: Application of a New Optimization Technique; Hamed Shadpour1, Steven A. Soper1, 1Louisiana State University

Lead Content in Ancient Bronze Coins; Mary Kate Donais1, Ashley Dumas1, Gregory Whissel1, 1Saint Anselm College

Elemental Imaging with a Confocal X-ray Fluorescence; George Havrilla1, Ning Gao1, 1Los Alamos National Laboratory; 2XOS

Formation of Dioxygen Complexes with Reduced Uranyl Cations; Anna Gianotto1, Kevin Cossel1, Garold Gresham1, Michael Van Stipdonk2, Garo Groenewold1, 1Idaho National Engineering and Environmental Labor; 2Wichita State University

Formation of Dioxygen Complexes with Reduced Uranyl Cations; Anna Gianotto1, Kevin Cossel1, Garold Gresham1, Michael Van Stipdonk2, Garo Groenewold1, 1Idaho National Engineering and Environmental Labor; 2Wichita State University

Covalent Oxo-Uranium Cluster Ions in the Gas Phase; Gary S. Groenewold1, Michael J. Van Stipdonk2, Garold Gresham, Victor Anbalagan1, Anna K. Gianotto1, Anthony D. Appelhans1, 1Idaho National Engineering and Environmental Labor; 2Wichita State University

Direct Thermal Vaporization for Metals Speciation in Soil; Eric D. Salin1, Rebecca Lam1, Josiane Lafleur1, 1McGill University

Determination of As, Se and Various Trace Metals in Rain Waters; Hakan Gurleyuk1, Crystal R. Howard1, Robert Brunette1, 1Frontier Geosciences

Probing Cellular Properties and Function With Microchip Devices

Development of Analytical Tools in Capillary Systems for Metabolic Analysis at Single Cell Volumes and Concentrations; J. M. Draygon1, L. W. Burgess1, A. C. Young1, A. K.-Y. Jen1, T. J. Hankins1, J. B. Callis1, T. J. Strovas1, M. E. Lidstrom1, 1Microscale Life Sciences Center, University of Washington

Dielectrophoretic Force Microscopy of Biological Interfaces; Brian Lynch1, Al Hilton1, Garth Simpson1, 1Purdue University

The Use of Design in Experiment in Release Rate Robustness Testing; Danford Lee1, June Liu1, Vicky Jimenez1, Steve Fields1, Jason Xin Zhang1, 1ALZA

Multivariate Analysis of Hyperspectral Images

Understanding the Limitations of Multivariate Curve Resolution when Applied to Hyperspectral Images; Howland Jones1, David Haaland1, Edward Thomas1, Jerilyn Timlin1, 1Sandia National Laboratories

New Ideas In Teaching Analytical Chemistry

A Unifying Approach to the Description of Chemical Instrumentation in a Course on Instrumental Methods of Analysis; Gary Rayson1, 1New Mexico State University

An Overview of Two NSF-CCLI Projects at Trinity University: Philosophy, Interdisciplinary Ventures, Outcomes; Michelle Bushey1, 1Trinity University

Development of a CDrom Resource to Support the Undergraduate Teaching of Sampling and Sample Preparation; Brian Woodgett1, Alexis Holden1, Irene Mueller-Harvey1, 1UK Analytical Partnership; 2University of Central Lancashire, UK; 3University of Reading, UK

Student Projects with Oxygen Binding Proteins: Spectroelectrochemical Results; Scott Dorman1, Clare Kenny2, Melinda Martin2, Eduardo Ramos1, Timothy Johnson1, Justin Weinstein1, 1Birmingham-Southern College; 2University of South Alabama

Incorporating Analytical Thinking Into An Introductory Course in Chemistry; David Harvey1, 1DePauw University

Analysis of Lithia Water: Instilling a Historical and Community Perspective into the Quantitative Analysis Laboratory; Steven Petrovic1, 1Southern Oregon University

Using Cyberspace for Teaching Analytical Science: The Analytical Science Digital Library and Beyond; Cameron Dreyer1, 1University of Central Arkansas
Vibrational Spectroscopy Coupled With Combinatorial Chemistry

(415) Use of Multivariate Curve Resolution (MCR) in the Analysis of FT-IR Step Scan Photo-Acoustic Depth Profiled Data of Aged Polyurethane; Dion Rivera, M. Kathleen Alam, Sandia National Laboratories

(416) Simulation Model Using PLS and Numerical Analysis Method: Conversion Rate and Diffusion Motion in Heterogeneous Reaction; Hsu-Fang Fan, Thou-Long Chin, King-Chuen Lin, Taiwan University, IAM-SINICA

(417) Applications of Chemometrics for the Analysis of Temperature Dependent Infrared Spectra of Hydrogen Bonded Polymers; Shigeki Morita, Serge Kokot, Yukihiro Ozaki, QWa; 3Kwansei Gakuin University, Australia; 4Queensland University of Technology

(417a) Infrared Microscopy – An Alternative Method for Probing Resin Bead Site Distributions?; Gurjit Manda1, Andrea Russell1, Zhanhu Yu2, Nicola Galaffu1, Mark Bradley2; 1University of Southampton

(417b) Getting More from IR-Microscopy of Resin-bound Libraries; Gurjit Manda, Andrea Russell, Gavin Aston, Mark Bradley2; 1University of Southampton, 2PerkinElmer Instruments

(417c) Micro-Flow Cells for Infrared Microscopy: a New Tool in the Vibrational Analysis of Drug Libraries; Gurjit Manda, Andrea Russell, Mark Bradley, Terry Finn, Keith Burton, Ian Clemens; 1University of Southampton; 2Eli Lilly & Co.

IR Microspectroscopy Instrumentation and Applications

(418) Probing Ice Nucleation on a Self-Assembled Monolayer of 11-Mercapto-1-Undecanol Using Infrared Microscopy; Kady Dendrmas, Hugh Richardson; 1Ohio University

(419) New Fabrication Technology for Multivariant Optical Fibers; Ryan Priora, Michael Myrick; 1University of South Carolina

(420) Application of Far-Ultraviolet Absorption Spectroscopy to a Highly Sensitive Quantitative and Qualitative Analysis for Aqueous Solutions; Noboru Higashi, Yukihiro Ozaki; 1Kurabo Industries Ltd., 2Kwansei Gakuin University

(421) FT-IR Spectroscopic Characterization of Polymer Nanocomposites; Vasillis Gregorius, Stavros Bollas, Athina Korakianiti, Spyros Tzavalas, Georgia Kandilioti; 1FORTH-ICEHT

(422) Synchrotron Infrared Microspectroscopic Characterization of Cox II Genetic Mouse Aorta that Produces Aneurysms without Atherosclerosis; David L. Wetzel, Lisa A. Cassis, Robert A. Ladd; 1Microbeam Molecular Spectroscopy Laboratory, Kansas; 2Graduate Center for Nutritional Studies; 3Chemistry Department, University of Kent

(423) Localized Chemical Analysis of Treated Stored Grain Insects via Synchrotron Infrared Microspectroscopy; David L. Wetzel, Bhadriraju Subramanyam, Tiffany L. Fisher; 1Microbeam Molecular Spectroscopy Laboratory, Kansas; 3Department of Grain Science and Industry

(424) Solid State Analysis of Polymorphic Drug Forms Using the Combined Techniques of Visible Image Analysis and Infrared Microspectroscopy; David Schiering, John Seelenbinder, Christina Tobler; 1SensIR Technologies, LLC

(425) Assessment of Performance Increases Obtained With a Novel Ge Detector Design As Applied to FT-Raman spectroscopy; Francis Deck; 1Thermo Electron Corp

(426) Applications for a Unique Spectrophotometer with 3-D Optics and Far UV to NIR Capability; John Monti, Shannon Richard, Timothy Alt, Thermo Scientific Instruments

(427) Optical Response of Single-Walled Carbon Nanotubes to Various Acids; Wei Zhao, Chulho Song; 1Department of Chemistry, University of Arkansas

(428) Mid and Far IR characterization of materials using the Smart Orbit(TM) Diamond ATR; Michael Bradley, Federico Izzia; 1Thermo Electron Corporation

(429) FT-IR Microimaging of Wood Composites, Stephen S. Kelley, Timothothy G. Rials, Nicole Labbe; 2National Renewable Energy Laboratory; 3University of Tennesse, Forest Products

Raman In Process Analytical

(431) Simultaneous Single-molecule Optical and Electrical Recording of DNA Interactions with Nanopores and Lipid Membranes; Emily L. Chandler, Alyssa L. Smith, Lisa M. Burden, John J. Kasiomaniczak, Daniel L. Burden, 1Wheaton College; 2Helmleon of Molecular Nanotechnologies and Measuring, National Institute of Standards and Technology

(432) Development of Novel Magnetic Nano-composites for A High Throughput Measurement of Partition Coefficient of Drug Candidates; Edman SC Tsang, Xin Gao, Kin Tam; 1University of Reading, UK; 2AstraZeneca, Macclesfield, UK

(433) New Applications of Raman Spectroscopy; Hugh Gottes, Saya Gamsey, Bakthan Singaram; 1University of California at Santa Cruz, 2Analytical Services Group

(434) Field Portable Raman Flow Cell Using a Polymer Waveguide for in-situ Environmental and Industrial Process Monitoring; Tina Battaglia, Jean-Francois Masson, Eileen Dunn, John Holloway, Karl Booksh; 1Arizona State University

(435) Application of Raman Chemical Imaging to Wood Cell Walls; Umesh Agarwal; 1USDA F.S. - Forest Products Laboratory

(435a) Remote Sensing with an Auto-focusing Raman Fiber Optic Probe; Nancy Kawai, Robert Forney; 1InPhotonics, Inc.

(435b) Performance Testing of a Raman Spectrometer Optimized for Mars Mineral Studies; Bruce McIntosh; 1Hamilton Sundstrand

(436) Humidity Induced Hydration State Changes of Active Pharmaceutical Ingredients Elucidated with Raman Spectroscopy; Helen Jervis, Sarah Williams, Patrick Tampkins; 1Surface Measurement Systems Ltd.; 2Renishaw plc

(437) A Study of Sulfamerazine Single Crystals Using Atomic Force Microscopy and Complementary Techniques; Xiaoping Cao, Changquan Sun, Thomas Thamann; 1Pfizer Inc.
**TECHNICAL PROGRAM – WEDNESDAY**

**Orals 10:30 AM – 12:30 PM**

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
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<tbody>
<tr>
<td>10:30</td>
<td>(438) Sample Preparation For Trace Element Speciation; Ralph Sturgeon¹, Zoltan Mester¹, Lu Yang¹, Paulette Maxwell¹, Christine Savriër¹, Scott Willie¹; NRC-INMS</td>
</tr>
<tr>
<td>10:50</td>
<td>(439) Sample Introduction Considerations for Elemental Speciation; John Olesik; Ohio State University</td>
</tr>
<tr>
<td>11:10</td>
<td>(440) Separations for Elemental Speciation with ICP-MS Detection; Joseph Caruso¹; University of Cincinnati</td>
</tr>
<tr>
<td>11:30</td>
<td>(441) ICP Detectors for Speciation Studies; Norbert Jakubowski¹, Michael Edler¹, Ingo Feldmann¹; Institute for Analytical Sciences (ISAS)</td>
</tr>
<tr>
<td>11:50</td>
<td>(442) Continued Developments in the Analysis of Polybrominated Diphenyl Ethers by GC-ICP-MS; Steven Wilbur¹, Emmett Soffey¹; Agilent Technologies</td>
</tr>
<tr>
<td>12:10</td>
<td>(443) Speciation Studies in Large Biomolecules; I Sabine Becker¹, J Susanne Becker², Miroslav V. Zor¿¹, Carola Pickhardt¹, Michael Przybylski²; Central Division of Analytical Chemistry Centre Juelich; Laboratory of Analytical Chemistry</td>
</tr>
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</table>

**Wednesday Morning, Room C123**

**IMPORTANT ASPECTS OF ELEMENTAL SPECIATION, SAMPLE PREPARATION, SEPARATION, SAMPLE INTRODUCTION**

Organizer and Presider: Joseph Caruso

**Wednesday Morning, Room B116**

**NEW IDEAS IN TEACHING ANALYTICAL CHEMISTRY**

Organizer and Presider: David Harvey

<table>
<thead>
<tr>
<th>Time</th>
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<tbody>
<tr>
<td>10:30</td>
<td>(444) Microfluidics for Genetic Analysis, Pathogen Detection and Space Exploration; Richard Mathies¹; University of California, Berkeley</td>
</tr>
<tr>
<td>11:10</td>
<td>(445) Miniaturized Electrically Driven Systems for Protein Analysis; Adam Woolley¹; Brigham Young University</td>
</tr>
<tr>
<td>11:30</td>
<td>(446) Metabolic Analysis by Microchip Electrophoresis/Electrochemistry; Charles Henry¹, Carlos García¹, Yan Liu¹; Colorado State University; University of Texas-San Antonio</td>
</tr>
<tr>
<td>11:50</td>
<td>(447) Deciphering the Role of Nitric Oxide in Vessel Relaxation using a Microchip-based Endothelium; Dana Spence¹, Nicholas Torrence², Alexander Price²; Wayne State University; Saint Louis University</td>
</tr>
<tr>
<td>12:10</td>
<td>(448) Chemical Analysis of Subcellular Structures Enabled by Micro and Nano Fluidics; Daniel T. Chiu¹; University of Washington</td>
</tr>
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</table>

**Wednesday Morning, Room B114**

**BIOLICAL ANALYSIS ENABLED BY MICROMACHINING TECHNOLOGIES**

Organizer and Presider: Adam Woolley

**Wednesday Morning, Room C124**

**VIBRATIONAL SPECTROSCOPY COUPLED WITH COMBINATORIAL CHEMISTRY**

Organizer and Presider: John Chalmers

<table>
<thead>
<tr>
<th>Time</th>
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<tr>
<td>10:30</td>
<td>(451) New Approaches for Understanding Multivariate Curve Resolution Applied to Hyperspectral Images; David Haaland¹, Jerilyn Timlin¹, Howland Jones¹, Michael Keenan¹, Christopher Stork¹, David Melgaard¹, Michael Sinclair¹; Sandia National Laboratories</td>
</tr>
<tr>
<td>12:10</td>
<td>(452) Multivariate Curve Resolution of Hyperspectral Images: Initialization and Functional Constraints; Neal Gallagher¹, Jeremy Shaver¹, Barry Wise¹; Eigenvector Research, Inc.</td>
</tr>
<tr>
<td>10:30</td>
<td>(453) Teaching Efficient Experimental Design and Multiple Approaches to Data Interpretation in the Analytical Chemistry Laboratory Curriculum; Richard Stolzberg¹; University of Alaska Fairbanks</td>
</tr>
<tr>
<td>10:50</td>
<td>(454) Integration and Assessment of Service-Learning into Introductory and Analytical Chemistry; Joan Esson¹; Kalamazoo College</td>
</tr>
<tr>
<td>11:10</td>
<td>(455) Critical Thinking and Problem Based Learning via Complementary Instrumentation Laboratory Exercises; Douglas Klarup¹, Jonathan Blitz¹, David McCurdy¹; Eastern Illinois University; Truman State University</td>
</tr>
<tr>
<td>11:30</td>
<td>(456) A Literature-Based Senior Level Instrumental Course; Jason Evans¹; University of Massachusetts</td>
</tr>
<tr>
<td>11:50</td>
<td>(457) Multiple Instruments, Courses, Users, and Disciplines: An Overview of Two NSF-CCLI Projects at Trinity University; Michelle Bushey; Trinity University</td>
</tr>
<tr>
<td>12:10</td>
<td>(458) Environmental Chemistry Design Projects in the Analytical Chemistry Curriculum; Robert Hamers, Pamela Doolittle, Robert McClain¹; University of Wisconsin-Madison</td>
</tr>
<tr>
<td>10:30</td>
<td>(459) Realising the Potential of Infrared Microscopy for Combinatorial Chemistry; Andrea Russell¹, Gurjit Mandair¹, Mark Bradley¹; University of Southampton</td>
</tr>
<tr>
<td>11:10</td>
<td>(460) Mapping Inside Solid Supports: Scanning Confocal Raman Spectroscopy; Jeremy Frey¹, Mark Bradley¹, Jurgen Kress¹, Abbe Rose¹, Helen Stanford¹; School of Chemistry, University of Southampton</td>
</tr>
<tr>
<td>11:30</td>
<td>(461) The Contribution of Vibrational Spectroscopy in Addressing the Critical Quality Issue in Combinatorial Chemistry; Biny Yan¹; DPI</td>
</tr>
<tr>
<td>12:10</td>
<td>(462) IR and Raman Tag Strategy for Monitoring Solid Phase Oligosaccharide Synthesis; Mike George¹, Mike Hargreaves¹, Barrie Bell¹, Jerilyn Timlin¹; University of Nottingham</td>
</tr>
</tbody>
</table>

**Wednesday Morning, Room B111**

**MICROMACHINING TECHNOLOGIES**

Organizer and Presider: Adam Woolley

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
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<tbody>
<tr>
<td>10:30</td>
<td>(449) Discriminant Image Resolution: MCR Analysis of Multivariate Image Utilizing Both Spatial and Spectral Information; Thomas Hanczewicz², Ji-hong Wang³; Unilever R&amp;D; JHW Consulting</td>
</tr>
<tr>
<td>11:10</td>
<td>(450) Spectral Unmixing of Remotely Sensed Thermal Infrared Hyperspectral Images Using Multivariate Curve Resolution; Chris Stork¹, Michael Keenan¹, David Haaland¹; Sandia National Laboratories</td>
</tr>
</tbody>
</table>
Wednesday Morning, Room A105
FTMS FOR PROTEOMICS
Organizer and Presider: Carlito Lebrilla

10:30 (463) Application of FTICR Mass Spectrometry in High Throughput Quantitative Proteomics; Richard Smith1, David Camp1, Jon Jacobs1, Weijun Qian1, Mary Lipton1, Harold Udseth1, Lijilana Pasa-Tolic1, Gordon Anderson1, Yufeng Shen1, Matthew Monroe1, 2Pacific Northwest National Laboratory


11:30 (465) Precise Characterization of Intact Proteins Using a Top Down Strategy with a High-Resolution Q-FTMS; Michael J. Roth, Andrew J. Forbes, Yi Du1, Steven M. Patrice, Michael T. Boyne III1, Lihua Jiang1, Jim Pesavento1, Jon Ferguson1, Rich LeDuc1, Neil L. Kelleher1; 1University of Illinois

11:50 (466) Incorporating FTICRMS into a shotgun proteomics process; David Goodlett1, Scott Shaffer1, Byren Gallis1, Jinshi Chen1; University of Washington

12:10 (467) NanoLC-FTMS Based Mapping of Protein Oxidation Sites Using Element-Coded Affinity Mass Tags; Nicolas L. Young1, Susan Lee2, Paul A. Whetstone2, Nathaniel G. Butlin1, Todd M. Cornillie1, Sarah M. Cheal1, Christopher G. Bailey1, Lori C. Zeller1, Whetstone2, Nathaniel G. Butlin2, Todd M. Cornillie2, Tags; 1, 2University of Washington

Wednesday Morning, Room B115
NANOMATERIALS FOR PHOTONICS
Organizers and Presiders: Guokui Liu and Gary Wiederrecht

10:30 (468) 3D Nanophotonic Structures Fabricated with Rubber Stamps and Conformable Phase Masks; John Rogers1; University of Illinois

11:10 (469) Rare-Earth-Doped Nano-Structured Materials for Optical Fiber Amplifiers; Bernard Jacquier1, Anne Marie Jurdye1, Laurent Bigot1, Bruno Gallais3, Dominique Bayart4, Laurent Gasca1; Laboratoire de Physico-Chimie des Matériaux Lumineux; 1Laboratoire de Physique des Lasers Atome; 2Laboratoire d’Optique du Solide; University of California, Davis

11:50 (470) Photoluminescent Diblock Copolymers - Structure and Optical Property; Hau Wang; 1Argonne National Laboratory

12:10 (471) Collective Plasmonic Behavior of Metal Nanoparticle Structures; Gary Wiederrecht1, Gregory Wurtz2, Alexandre Bouhelier2, Jasmina Hranisavljevic2, Stephen Gray1, Renaud Bachelot1, Jin Seo Im1; 1Argonne National Laboratory

Wednesday Morning, Room A106
RAMAN IN PROCESS ANALYTICAL
Organizer and Presider: Brian Marquardt

10:30 (472) Analysis of Dyed Fibers by Raman Microscopy; S. Michael Angel1, Brandy L. Clelland1, James E. Hendrix1, Stephen L. Morgan1, Edward G. Bartick1; 1Department of Chemistry & Biochemistry, The University of South Carolina; 2Counterterrorism and Forensic Science Research

10:50 (473) Novel Strategies for Sampling Processes with Raman Spectroscopy; Brian Dable1, Brian Marquardt1, 2, David Veltkamp1, 2, Brooke Love2, Marvin Lilley2, Sylvie Theas2; 1Center for Process Analytical Chemistry; 2University of Washington

11:10 (474) Raman Spectroscopy for Quantification of Fat Composition in High-protein Whey Emulsions; Nils Kristian Alseth1; 1Vegard Herman Segtnam1, Jens Petter Wold1, 2University of Washington, 1National Laboratory

11:30 (475) Development of Raman-Based Methods for Waste Analysis at the Savannah River Site; Robert Lascola1, Charles Coleman1, David Hobbs1, Savannah River National Laboratory

11:50 (476) Process Raman Chemical Imaging; Matthew Nelson1, Julianne Wolfe1, Laura Marks1, Patrick Treado1; ChemImage Corporation

12:10 (477) Advanced Control of Manufacturing Processes Using Raman-Based Gas Analysis; Ronald Rich1; Atmosphere Recovery, Inc.

Wednesday Afternoon, Room C123
MOLECULAR INORGANIC AND ORGANOMETALLIC MASS SPECTROMETRY
Organizers and Presiders: Gary Goenewold and Anita Gianotto

3:30 (478) Heterogeneous Catalysis in the Gas Phase: Size-Specific Reactions of Iron Cluster Cations with Ammonia; Petter Armentrout1, 2, Rohana Liyanage1, 2, Charles Coleman1, 2, David Hobbs1, 2, Savannah River National Laboratory

3:50 (479) Cu+-Ligand Interactions: Structures and Bond Dissociation Energies, Solvation, Chenlation, and Hydrogen Bonding Interactions; Mary T. Rodgers1, Nalaka S. Rannulu1; 1Wayne State University

4:10 (480) Metal Complex Coordination Structure from Gas-Phase Ion-Molecule Reactions in a Quadrupole Ion Trap Mass Spectrometer; Richard W. Vachet1, Mariany Y. Combariza1, Angela M. Fahey1; University of Massachusetts

4:30 (481) Exploration of Gas-Phase Uranium Complex Reactions Using Electrospray Ionization and Ion-Trap Mass Spectrometry; Michael Van Stipdonk1, Gary Groenewold2, Gary Gresham2, Winnie Chien1, Victor Anbalagan1; 1University of Cincinnati, Department of Chemistry & Biochemistry; 2Idaho National Engineering and Environment Environment

4:50 (482) Molecular Nanoboxes with Metal Ion Lids; David Dearden1, Jon Willes1, Kevin Walker1, Haizhen Zhang1, Krzysztof Krakowiak1; 1Brigham Young University Department of Chemistry & Biochemistry; 2IBC Advanced Technologies, Inc.

5:10 (483) Host-Guest Interactions of Uranyl Carbonate Probed by Mass Spectroscopy; Jason Telford1, Nathan Lien1; 1University of Iowa

5:30 (483b) Se and S Trichalcogenides: Facts from Artifacts; Juris Meija1, Joseph A. Caruso1; 1University of Cincinnati, Department of Chemistry
Wednesday Afternoon, Room B114
PROBING CELLULAR PROPERTIES AND FUNCTION WITH MICROCHIP DEVICES
Organizer and Presider: R. Scott Martin

3:30 (484) Microanalytical Separations to Track Cellular Signal Transduction; Nancy Allbritton1,3,4, Jim Palmer1, G.P. Li1,2,5, Mark Bachman1,2, Chris Sims1; 1Department of Physiology and Biophysics, University of California; 2Department of Electrical and Computer Engineering; 3Center for Biomedical Engineering; 4Integrated Nanosystems Research Facility

4:10 (485) Rapid Prototyping of Micro and Nanofluidic Systems for Subcellular Analysis; Daniel Chu1; 1University of Washington

4:30 (486) Manipulating Membrane Bound Bioparticles with Channel Structures and Electric Fields; Mark Hayes1, Timothy Crowley1, Michele Pysher1; 1Arizona State University

4:50 (487) Exploring Mitochondrial Properties Using Microfluidic Devices; Edgar Arriaga1, Chris Whiting1, Karen Olson1; 1University of Minnesota

5:30 (488) An Integrated PC 12 Cell Reactor/Analysis System; Michelle W. Li1, Michelle L. Kovarik1; 1Saint Louis University

Wednesday Afternoon, Room B114
MULTIVARIATE CURVE RESOLUTIONS: RECENT ADVANCES AND APPLICATIONS
Organizer and Presider: Scott Ramos

3:30 (489) Application of MCR Methods in Environmental Forensics; Glenn Johnson1; 1University of Utah

4:10 (490) Process Analysis, Imaging and Environment: Challenging Fields for Multivariate Curve Resolution; Anna de Juan1, Romà Tauler1; 1Chemometrics group. Dept. of Analytical Chemistry; 2Department of Environmental Chemistry

4:50 (491) Application of Multivariate Curve Resolution to the Analysis of FT-IR Hyperspectral Images; Bosana Budevska1; 1DuPont

5:10 (492) Analysis of NMR Data using Multivariate Curve Resolution Techniques; Kathleen Alam1, Todd Alam1; 1Sandia National Laboratories, Chemical and Bio; 2Sandia National Laboratories, Organic

Wednesday Afternoon, Room C124
IR MICROSCOPIC IMAGING INSTRUMENTATION AND APPLICATIONS
Organizer and Presider: John Hellgeth

3:30 (493) Developments in Infrared Microscopy; John A. Reffner1; 1SensIR Technologies

3:50 (494) Infrared Microscopy Analysis of Isolated Particles Significantly Below the Diffraction Limit; Milo Overbay1; 1Hewlett Packard Corporation

4:10 (495) ATR Microscopy for Chromatographic Detection; André Sommer1, Brian Patterson1, Neil Danielson1; 1Miami University

Wednesday Afternoon, Room B115
NANOTUBES AND NANOWIRES FOR SENSING
Organizers and Presiders: Peter Pehrsson and Jie Liu
Presider: Pehr Pehrsson

3:30 (504) Nanotube Thin Film Devices and Sensors; Jie Liu1; 1Duke University

4:10 (505) Carbon Nanotubes as Chemical Sensors: Shu Peng1, Kyeongjae Cho1; 1Stanford University

4:50 (506) Moving and Sensing Biomolecules Using Nanotube Membranes; Punit Kohli1, C. Chad Harrell1, Zuzanna Siwy1, Charles R. Martin1; 1University of Florida
Wednesday Afternoon, Room A106
RAMAN IN PHARMA
Organizer and Presider: Lynne Taylor

3:30  (507) Raman Mapping in Support of Pharmaceutical Solid Dosage Form Development; Mark Henson¹;
       ¹Pfizer Global R&D
3:50  (508) Raman Spectroscopy: a PAT Tool for Quantitative Assessment of Tablet Potency; Jonas Johanson¹, Jonas Eriksson¹, Staffan Folestad¹;
       ¹AstraZeneca R&D Molndal, Sweden
4:10  (509) Application of Raman and IR Spectroscopy in Pharmaceutical Development; Sabine Pfeffer-Hennig¹, Miriam Bellus¹;
       ¹Novartis Pharma AG, Chemical & Analytical Development
4:30  (510) The Use of Raman Spectroscopy in the Detection of Counterfeit and Adulterated Pharmaceutical Products; Mark Witkowski¹, Thomas Brueggemeyer¹, JaCinta Batson¹, Jill Loeliger¹;
       ¹FDA / Forensic Chemistry Center
4:50  (511) Raman Spectroscopy for the Characterization of Solid-state Forms During Pharmaceutical Manufacturing; Robert Cambron; ¹Procter & Gamble
5:10  (512) Monitoring the Kinetics of Solvent Mediated Phase Conversions of Pharmaceutical Solids; Lynne Taylor¹, Håkan Wikstöm¹, Jukka Rantanen¹;
       ¹Purdue University; ¹University of Helsinki
7:30 Wake Up Coffee, Ballroom Lobby

8:00 AM Plenary Session, Lippencott Award, Ballroom 201

Richard Mathies

(513) Femtosecond Stimulated Raman Spectroscopy; Richard Mathies\(^1\); \(^1\)University of California, Berkeley

### THURSDAY POSTER SESSIONS and BREAKS

9:00 – 10:30 AM and 2:00 – 3:30 PM

**Exhibit Hall A/A-1**

All Thursday posters should be put up between 7:30 – 8:00 AM and removed between 5:30 – 6:00 PM. Odd numbered posters present between 9:00 - 10:30 AM and even numbered posters present between 2:00 – 3:30 PM

**Metallomics**

(515) Protein Determination by Monitoring Phosphorous Atomic Emission; Tim M. Brewer\(^1\), Fuxia Jin\(^1\), R. Kenneth Marcus\(^1\); \(^1\)Clemson University

(517) Immobilized Short-Chain Peptides for use in Metal Preconcentration and Remediation; Jacqueline L. Stair\(^1\), James A. Holcombe\(^1\); \(^1\)University of Texas at Austin

(518) The Use of Gallium Matrices to Study Proteins by Pulsed Glow Discharge Time-of-Flight Mass Spectrometry; Na Zhang\(^1\), Megan DeJesus\(^1\); \(^1\)West Virginia University

(519) Synthesis and Characterization of a Copolymer Hydrogel for Environmental Analysis of Heavy Metals; Maury Howard\(^1\), William Snee\(^1\); \(^1\)Southeastern Louisiana University

**Chemometrics Applications of Cluster Analysis and Pattern Recognition**

(520) Is there a Difference in Life Expectancy between Overweight Men and Women?; Gus Miller; \(^1\)Edinboro University of Pennsylvania

(521) Maximum Likelihood Principal Component Analysis with Equal Row Error Covariance: A Dramatic Improvement in Algorithmic Speed and Efficiency; Chris Stork\(^1\), Michael Keenan\(^1\); \(^1\)Sandia National Laboratories

**Multiway Analysis and Multiway Method Development**

(522) A Finite Mixture Model for Quantitative Analysis of Two-dimensional Comprehensive Gas Chromatograms (GCxGC); Alan Wills\(^1\), Blandina Valenzuela\(^1\), Jon Wahl\(^1\), George Preti\(^2\), Peter Yang\(^2\), Jae Kwak\(^2\), Kunio Yamazaki\(^2\), Gary Beauchamp\(^2\); \(^2\)Battelle; \(^2\)Monell Chemical Senses Center

**Research Supportive Curricula In Environmental Chemistry**

(523) Problem Based Learning and Environmental Projects for Analytical Chemistry Courses; Preetha Ram\(^1\); \(^1\)Emory University

**New Techniques In Sampling for IR Spectroscopic Data**

(524) FTIR Analysis of Contamination by Searching Difference Spectra Against Libraries of Difference Spectra; Kenneth Laughlin\(^1\); \(^1\)Rohm and Haas Company

(525) An Infrared Study of C-H\_\_\_\_O Hydrogen Bondings and Thermal Behavior of Poly(3-hydroxybutyrate-co-3-hydroxyhexanoate); Yukihiro Ozaki\(^1\), Harumi Sato\(^1\), Rumi Murakami\(^1\), Fuminoohu Hirose\(^1\), Kenichi Senda\(^1\), Isao Noda\(^1\); \(^1\)Kwansei Gakuin University; \(^2\)Kaneka Corporation; \(^3\)The Procter & Gamble Company

(526) Infrared Complex Refractive Index Measurements and Simulated Reflection Mode Infrared Absorption Spectroscopy of Shock Compressed Polymer Thin Films; David Moore\(^1\), Shawn McGrane\(^1\); \(^1\)Los Alamos National Laboratory

(528) Spectroscopic and Microscopic Analysis of Protein Adsorption on Passivated Porous Silicon; Li-Lin Tay\(^1\), Nelson Rowell\(^1\), Daniel Poitra\(^2\), David Lockwood\(^1\), Rabah Boukherroub\(^2\); \(^1\)National Research Council, Ottawa, Ontario, Canada; \(^2\)Interdisciplinary Research Institute

(530) Identification of the Polymorphs of Sulfathiazole Using Terahertz Pulsed Spectroscopy; Philip Taday\(^1\), David Newham\(^1\), Yoaohun Shen\(^1\), Clare Strachan\(^1\); \(^1\)TeraView Limited; \(^1\)School of Pharmacy and Department of Chemistry

(531) Infrared Investigation of Organosilane Films on Silicon-Coated Germanium ATR Plates; David Tallant\(^1\), David Adams\(^1\), Manuel Garcia\(^1\), Michael Kent\(^1\), Hyun Yim\(^1\); \(^1\)Sandia National Laboratories

(532) Evaluation of Two Types of Infrared Methods to Characterize Soil Organic Carbon; Douglas D. Archibald\(^1\), Amy L. Shofer\(^1\), Rupinder K. Randhawa\(^1\); \(^1\)Crop & Soil Sciences Department, The Pennsylvania State University; \(^1\)Department of Plant and Soil Sciences

(533) Local Optical Axis Resolved Spectroscopy (LOARS); Isao Noda\(^1\), William Allen\(^1\), Anthony Dowrey\(^1\), Curtis Marcott\(^1\); \(^1\)Procter & Gamble Co.

(534) FT-IR spectroscopic investigation on the origin of the low energy PL emission bands in fluorones used for OLED applications; Vasilis Gregoriou\(^1\), Christos Chochos\(^1\), Ioannis Kallitasis\(^1\); \(^1\)FORTH-ICEHT; \(^1\)University of Patras
(535) Organic Monolayer Vibrational Spectroscopy Using Single Reflection ATR; Nelson Rowell1, Li-Lin Tay1, David Lockwood1, Rabah Boukherroub2, 1National Research Council, Ottawa, Ontario, Canada; 2Interdisciplinary Research Institute, IE

(536) On The Photooxidation of a Crude Iranian Petroleum Maltenic Fraction as a Film over Seawater; Babak Nahinknafs1, A.S.S.C

(537) Optical Diagnostics for the Iodine Sulfur Cycle; Denis Doizi1, Vincent Dauvois1, Jean Luc Roujou1, Vincent Delanne1, Bruno Larousse1, Olivier Hercher1, Pierre Fauvet1, Christophe Moulin1, CEA

(538) Determination of the Absolute Configuration and Dimeric Liquid-State Conformation of a Chiral Acetylenic Carboxylic Acid; Richard W. Duerst1, Teresa B. Freedman1, Rina K. Dukor1, Kerry Swift1, Rodger F. Henry1, Laurence A. Nafie1, 2Syracuse University, Department of Chemistry; 2BioTools, Inc.; 3Abbott Laboratories

(539) Metrological Characterization of Didymium Oxide Wavelength Reference Materials in the Short-Wave Near Infrared Region; Jerry Messman1, Stranaska LLC

IR Microspectroscopy Imaging

(540) A Faster Approach to Infrared Rheo-Optics using Planar Array Infrared Spectroscopy; Christian Pellerin1, Simon Frisk1, John Rabolt1, Bruce Chase2, 1University of Delaware; 2DuPont Inc.

(541) A Sampling Methodology to Overcome Optical Anomalies and Thickness Dependence in FT-IR Imaging and Combined Automated Polarized Light/Raman Microscopy; Douglas Elmore1, Chad Leverette1, Sean Smith1, Brian Anderson1, Allen Muroski1, Var St. Jeor1, Cargill, Inc.

(542) Real Time Study of the Branching Effect in Phospholipids at the Air/Water Interface Using Planar Array Infrared (PA-IR) Spectroscopy; Yuiyan Liu1, Isabelle Pelletier1, Christian Pellerin1, Bruce Chase2, John Rabolt1, 1University of Delaware, Department of Materials Science; 2Central Research and Development, DuPont

(543) Characterization of Nafion Membrane Conversion Using IR and MXRF Imaging; George Havrilla1, Matthew Stanton1, Richard Ames1, Los Alamos National Laboratory

(544) Hyperspectral Imaging for Endogenous and Exogenous Fluorophore Differentiation in Live Cells; Jerilyn Timlin1, David Haaland1, Michael Sinclair1, Michael Keenan1, Sandia National Laboratories

(545) Microscopic FT-IR Imaging: Spatial Resolution and the Diffraction Limit; Jonathan Tarr1, Koichi Nishikida1, William J. McCarthy1, N. Simon Nunn1, Thermo Electron Corporation

(546) Objective Data Cube Comparison Following Near-Infrared Spectroscopic Imaging; Thomas W. Brueggemeyer1, Mark R. Witkowski1, Jacinta S. Batson1, Jill R. Loeliger2, U.S. Food & Drug Administration–Forensic Chemistry

(547) Spread Spectrum Image Steganography; Srinivasan Allimuthu1, 1Crescent Engineering College

(548) Real-Time Detection of Chemical Agents Using Planar Array Infrared Spectroscopy; Christian Pellerin1, John F. Rabolt1, Bruce Chase2, University of Delaware; DuPont Inc.

MS Front-End Devices and New Methodology for Proteomics

(549) Electrowetting-on-Dielectric for Analysis of Peptides and Proteins by Matrix Assisted Laser Desorption/Ionization Mass Spectrometry; Robin L. Garrell1, Aaron R. Wheeler1, Hyejin Moon2, Chang-Jin Kim3, Joseph A. Loo1, 1UCLA Department of Chemistry; 2UCLA Department of Mechanical Engineering

(550) Statistical Tools for Microorganism Identification Using Matrix-assisted Laser Desorption/Ionization Mass Spectrometry.; Nathaniel Beagley1, Kristin H. Jarman1, Nancy B. Valentine1, Catherine E. Petersen1, Karen L. Wahl1, Pacific Northwest National Laboratory

(551) Silica Sol-gels for MALDI-MS Application; Noemi Nagy1, Suzanne Ackloo1, Sanela Martic2, Vladimir Baranov3, John D. Brennan2, 1MDS Sciex; 2McMaster University

(552) Differential Chemistry as a Function of Droplet m/z using a Variation of the tandem MS Theme (EDB+MALDI-MS); George Agnes1, Samuel Bakhous1, Mike Bogan1, Simon Fraser University

(553) The Use of Gallium and MALDI Matrices to Study Proteins by pulsed Glow Discharge Time-of-Flight Mass Spectrometry; Na Zhang1, Megan DeJesus1, Jennifer Robertson1, Lei Li1, Yuchen Lu1, Fred King1, 1Virginia University

(554) Survey of Purification Methods for the Analysis of Proteins by pulsed Glow Discharge Time-of-Flight Mass Spectrometry.; Robert Robertson1, lei li1, Yuchen Lu1, Fred King1, 1Virginia University

(555) Evaluation of Gallium and MALDI Matrices for Pulsed Glow Discharge; Na Zhang1, Megan DeJesus1, Jennifer Robertson1, lei li1, Yuchen Lu1, Fred King1, 1Virginia University

(556) A Closed System Digestion and Purification Procedure for the Accurate Assay of Chlorine in Fossil Fuels; Maury E. Howard1, Robert D. Vocke2, 1Southeastern Louisiana University; 2National Institute of Standards and Technology

Nanotubes and Nanowires for Sensing

(557) Confocal Raman-ASF, a New Tool for Materials Research; Olaf Hochbruck1, Ute Schmidt1, Wolffram Ibach1, Sabine Hild1, Joerg Mueller1, Joachim Koenen1, Klaus Weisshaup1, 1Witec GmbH; 2Department of Experimental Physics

State of the Art Infrastructure for PAT Spectroscopy in Industry

(558) Analysis of Petrochemical Liquid Samples by Process Mass Spectrometry via a Programmable Temperature Vaporiser Interface; Andrew Owen1, J. Steven Lancaster2, David Littlejohn1, Thomas Lynch2, Robert Wright1, 1Department of Pure and Applied Chemistry/CPACT, Un; 2 Hull Research & Technology Centre, BP Ch; 3Thermo ONIX, Winsford, Cheshire, UK

(559) Visualizing Vortex Sheddng >From a Square Cylinder using Pressure Sensitive Paint; Christina McGraw1, Gamal Khalil1, James Callis1, University of Washington Department of Chemistry
(561) Identification and Characterization of Process Impurities and Oxidative Degradate Products in Ivermectin; Chris Beasley¹, Kyle Fliszar¹, Andreas M. Abend¹, Robert A. Reed¹, ¹Mercer Research Laboratories, Mercer & Co., Inc.

(562) HPLC at High Temperature and High pH with a New, Highly Stable Silica Column; Dale Felix¹, Stephanie Marin¹, Brian Jones¹, ²Selerity Technologies

(563) Non-Invasive Determination of Porosity in Solids by Diode Laser Oxygen Spectroscopy: Application to Pharmaceutical Tablets; Tomas Svensson¹, Jonas Johannson², Stefan Andersson-Engels¹, Sune Svanelg¹, Staffan Folestad², ²Department of Physics, Lund Institute of Technology, Lund; ³Astra Zeneca R&D, Molndal, Sweden

(564) Development/Validation of a New Reversed-Phase Ion-Pair HPLC Method for Detection/Quantification of New Insulin Related Substances in Purification Processes in Development; Warren Rowland¹, Xiangli Zhang¹, Renee Rieke¹, ²Eli Lilly

(565) The Use of Thermal Desorption GC/MS To Monitor the Weight Loss During Thermal Gravimetric Analysis; Charles Pan¹, Marilyn Alvine³, Frances Liu¹, Richard Vivieleechua¹, ²Novartis Pharmaceuticals Corporation

(566) Calibration Transfer in Near-infrared Spectroscopy; Mike Clavybour¹, Mark Smith¹, Anthony Moffat¹, David Rees¹, ²School of Pharmacy, University of London; ³AstraZeneca

(567) Development of an Automated Protocol for Preparation of Samples for Silicone Functionality Analysis by Gas Chromatography; Herbert Brothers¹, Cynthia Gould¹, Tanya Habitz¹, Ronda Grosse¹, ²Dow Corning Corporation

Raman Microscopy and Imaging

(569) Raman Analysis of Diamonds and Gemstones; Amanda Jenkins¹, Richard Larsen¹, ²Jasco Inc.

(570) A New Triple Additive/Subtractive Monochromator Design Provides the Ultimate Flexibility; Ryan Sullivan¹, Bruce True¹, Ravi Guntupalli¹, ²Princeton Instruments (a division of Roper Scientific)

(571) The Combination of Automated Polarized Light Microscopy and Raman Microscopy for the Analysis of Chemical Systems; Chad Leverette¹, Sean Smith¹, Douglas Elmore¹, ²Cargill, Incorporated

(572) Elastic Deformation of Bone Probed by Raman Spectroscopy; Apparatus and Results; Andrew Callender¹, William Finney¹, Michael Morris¹, ²University of Michigan

(573) Micro Raman Spectroscopic Investigation of Solvent and Dye Diffusion in Polymers; Andres Gupper¹, Jaap van der Weerd¹, Sergei G. Kazarin¹, ²Imperial College London

(574) High Brightness Lasers in Confocal Raman Spectroscopy; Kelly Cox¹, ²Thermo Electron Corporation

(575) An Ex Vivo Study of Early Dental Caries by Multi-Modal Optical Methods; Alex C.-T. Ko¹, Lin-Ping Choo-Smith¹, Mark Hewko¹, Larry Leonardi¹, Cecilia Dong¹, Peter Williams¹, Claire Cleghorn¹, ²Institute for Biodiagnostics, National Research Council; ³Department of Restorative Dentistry; ⁴Department of Dental Clinic Sciences

(576) Raman Study of GaAs1-xBix/GaAs Epilayers Grown by Molecular Beam Epitaxy; Li-Lin Tay¹, David Lockwood¹, Erin Young¹, Tom Tielde², ³National Research Council, Ottawa, Ontario, Canada; ³Department of Physics, University of British Columbia

(577) Effect of Reactant Gas Velocity and Geometry on CARS Monitored Pulsed rf Pulsed PECVD Silicon Nitride Thin Films; Barjean Phillips¹, Rene Rodriguez¹, Lisa Lau¹, Shane Steidley¹, ²Idaho State University; ³AMI Semiconductor

(578) Contributions to BioDefense and Pathology Utilizing Molecular Chemical Imaging; Patrick Trezado¹, Steve Vanni¹, John Maier¹, Matthew Nelson¹, ²ChemImage Corp.

(579) Raman Microspectroscopy: an Efficient Technique to Determine Quantitatively the Orientation of Protein Fibers; Thierry Lefèvre¹, Marie-Eve Rousseau¹, Michel Pézzelet¹, ²Univiersité laval - CERSIM

(580) Performance of Raman Mapping and Imaging Systems in the Analysis of Solid Dosage Pharmaceuticals; Slobodan Sasie¹, Don Clark¹, John Mitchell¹, Martin Snowden¹, ²Pfizer, Analytical R & D, Rampsgate Road, Sandwich;

(581) Development of an Automated Protocol for Preparation of Samples for Fractionation Analysis by Gas Chromatography; Herbert Brothers¹, Cynthia Gould¹, Tanya Habitz¹, Ronda Grosse¹, ²Dow Corning Corporation

Emerging Technologies for Process Analysis

(582) CE-SELEX - In Vitro Selection of Functional Oligonucleotide Aptamers; Sergey Krylov¹, Berezovski Maxim¹, Drabovich Andrei¹, Svetlana Krylova¹, Musheev Michael¹, Okhnon Victor¹, Petrov Alexander¹, ²Department of Chemistry, York University

Posters 9:00 – 10:30 AM and 2:00 – 3:30 PM and Orals 10:30 AM – 12:30 PM

Thursday Morning, Room C123

MELLOMICS

Organizer and Presider: Dave Koppenaal

10:30 (583) Metallomics - Overview and Analytical Opportunity Prognosis; David W. Koppenaal¹, ²Pacific Northwest National Laboratory

10:50 (584) Microorganisms and the Chemical Elements; Lawrence Wackett¹, ²University of Minnesota

11:30 (585) Metal isotopes in metallomics; Ariel Anbar¹, ²Arizona State University

11:50 (586) High Throughput ICP-MS Analysis of the Arabidopsis Ionome; David E Salt¹, D.J. Eide², J.F. Harper³, J.I. Schroeder³, J.M. Ward³, M.L. Guerinot³, ⁴Purdue University; ⁵University of Missouri; ⁶University of Nevada-Reno; ⁷UC-San Diego

Thursday Morning, Ballroom 201

APTAMERS IN ANALYSIS

Organizer and Presider: Mike Bower

10:30 (587) Aptamer Biosensors; Andrew D. Ellington¹, ²University of Texas, Austin

10:50 (588) Kinetic CE Methods for Selection, Characterization, and Analytical Utilization of Oligonucleotide Aptamers; Sergey Krylov¹, Berezovski Maxim¹, Drabovich Andrei¹, Svetlana Krylova¹, Musheev Michael¹, Okhnon Victor¹, Petrov Alexander¹, ²Department of Chemistry, York University

11:10 (589) Progress Towards a High-Throughput, Aptamer-Based Nanoeextractor; Vincent Remcho¹, Angela Doneanu¹, Jack Rundel¹, Yolanda Tennico¹, ²Oregon State University

11:30 (590) Molecular Engineering of Nucleic Acids for Bioanalysis and Bionanotechnology; Weihong Tan¹, ²University of Florida

11:50 (591) Novel Analytical Aptamer Reagents for Microfluidic Chips; Nils Walter¹, Robert Kennedy¹, Jens-Christian Meiners¹, Phillip Sekelia¹, Jennifer Willard¹, Katherine Korbiak¹, Meredith Lambert¹, ²Department of Chemistry, University of Michigan; ³Department of Physics and Biophysics Research

12:10 (592) CE-SELEX - In Vitro Selection of Functional DNA using Capillary Electrophoresis; Michael Bowser¹, Shaun Mendonsa¹, Renee Mosing¹, ²University of Minnesota
<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
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<tr>
<td>10:30</td>
<td>(593) Genetic Algorithms for Pattern Recognition: Feature Selection, Classification, Clustering, and Prediction in a Single Step; Barry Lavine, Charles Davidson, 1Clarksion University</td>
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<td>11:10</td>
<td>(594) Multivariate Curve Resolution as a Chemical Classification Tool; Thomas Hanacewicz, Ji-hong Wang, David Budac, 1Unilever R &amp; D; 2JHW Consulting</td>
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<td>11:30</td>
<td>(595) New Approaches to Classification using Wavelets and Trees; Steven Brown, Anthony Myles, Nathaniel Woody, 1University of Delaware; 2Glaxo-SmithKline, RTP, NC</td>
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<td>11:50</td>
<td>(596) The Development of UV Resonance Raman Spectroscopy for Bacterial Identification; E. Consuelo Lopez Diez, Royston Goodacre, 1UMIST, Department of Chemistry</td>
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<td>12:10</td>
<td>(597) UV Spectroscopy in Conjunction with Chemometrics Analysis: A Simplified Approach for Differentiation of Functional Foods; Dave Luthria, Sudarsan Mukhopadhyay, James Hamry, John Finley, David Burns, Food Composition Lab, USDA; 2Grand Forks Human Nutrition Research Center, 3Department of Chemistry, McGill University</td>
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<tr>
<td>10:30</td>
<td>Outcomes of the Undergraduate Research Summit: Developing Research-Supportive Curricula; Thomas Wenzel, Bates College</td>
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<td>11:10</td>
<td>Atomic Absorption Spectroscopy in Undergraduate Teaching and Research; David Goodney, Willamette University</td>
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<td>11:30</td>
<td>Integrating Environmental Analytical Research Throughout the Curriculum; Kevin Cantrell, University of Portland</td>
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<td>11:50</td>
<td>Enhancing Research and Service Learning Opportunities in Environmental Chemistry; Anna Cavinato, Ronald Kelley, Eastern Oregon University</td>
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<td>10:30</td>
<td>With Diamond, Anything is Possible; John A. Relfner, SensIR Technologies</td>
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<td>11:10</td>
<td>Direct Analysis of Condensed Samples Using Photoacoustic and Transient Infrared Spectroscopies; John McClelland, Roger Jones, Anthony Wagner, Ames Laboratory-USDOE; 2MTEC Photoacoustics, Inc.</td>
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<td>11:50</td>
<td>Attenuated Total Reflection Direct-Deposition Nanosampler; James de Haseth, Shelly Seerley, University of Georgia</td>
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<td>12:10</td>
<td>Mid-Infrared Diffuse Reflection Spectroscopy of Species In and On Absorbing Substrates; Lacey Averett, David Heaps, Peter Griffiths, Univ. of Idaho</td>
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<td>10:30</td>
<td>Imaging MALDI with an Orthogonal TOF Mass Spectrometer; Werner Ems, Gamini Pyiadasa, James R McNabb, Victor Spencer, Kenneth G Standing, Dept. of Physics and Astronomy, University of Manitoba</td>
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<td>10:50</td>
<td>Evaluating Large Proteomics Datasets from HPLC-ESI-MS/MS Experiments; Daniel Figueys, University of Ottawa</td>
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<td>11:10</td>
<td>Analysis of the Ciliome of the Protozoan Tetrahymena Thermophila Using Translated and Unannotated Genomic Information; K.W. Michael Siu, Jeffrey C. Smith, Ronald E. Pearlman, Department of Chemistry, York University; 2Department of Biology, York University; Centre for Research in Mass Spectrometry</td>
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<td>11:30</td>
<td>Alternative Separation Strategies for Shotgun Proteomics; Ron Orlando, James Atwood, Cameron Cavola, Brent Weatherly, Todd Minning, Rick Tarleton, Complex Carbohydrate Research Center, University of Georgia; 2Department of Cellular Biology, University of Georgia</td>
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<td>11:50</td>
<td>Improvement of N-terminal Sulfonation Procedures for MALDI PSD Peptide Sequencing and Its Application in Determining Protein Ubiquitination; Dongxia Wang, Robert J. Cotter, Johns Hopkins University School of Medicine</td>
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<td>12:10</td>
<td>Electrodynamic Charged Droplet Processing to Couple Low Flow Rate Separations with MALDI-MS; George Agnes, Michael J. Bogdan, Simon Fraser Univ.</td>
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<td>10:30</td>
<td>Modulating the Optical Response of Single Walled Carbon Nanotubes to Specific Molecular Adsorption: Tissue Implantable Biosensors; Michael Strano, Seunghyun Baik, Paul Barone, Daniel Heller, Department of Chemical and Biomolecular Engineering</td>
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<td>10:50</td>
<td>Chemical and Bio Sensors Based on nanowires and Nanotubes; Chongwu Zhou, University of Southern California</td>
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<td>11:30</td>
<td>Optical pH Sensing Based on Surface-Modified Single-Walled Carbon Nanotubes; Wei Zhao, Chulho Song, Pehr Pehrsson, Kristy Kelley, Brian Benedict, Department of Chemistry, University of Arkansas; 2Chemistry Division, Naval Research Labor</td>
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<td>11:50</td>
<td>Carbon nanotubes based nanoelectrode arrays: fabrication, evaluation, and chemical &amp; biosensing applications; Yuehe Lin, Yi Tu, Fang Liu, Wassana Yantasoe, Zhifeng Ren, Pacific Northwest National Laboratory; 2Boston College</td>
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Thursday Morning, Room B116
STATE OF THE ART INFRASTRUCTURE FOR PAT
SPECTROSCOPY IN INDUSTRY
Organizer and Presider: Terry Todd

12:10 (618) Tailored Assembly of Carbon Nanotubes by Chemical Vapor Deposition; Pulickel Ajayan1, Anyuan Cao1, Yong Jung1, Guowen Meng1; ‘Rensselaer Polytechnic Institute

10:30 (619) Process Analysis Technology at Roche Ireland Limited, a Holistic Approach; John O’Reilly1; ‘Roche Ireland Limited

10:50 (620) Collaborations and Teaming for Successful PAT Projects; Christian Hassell; ‘Los Alamos National Lab

11:10 (621) Successful Process Analyzer Implementation; Ann M. Brearley1, ‘Ann M. Brearley Consulting


11:50 (623) Validation of a Near-Infrared Transmission Spectroscopic Procedure for Measuring Assay in Pharmaceutical Tablets; Howard Mark1, ‘Mark Electronics

Thursday Morning, Room A106
RAMAN MICROSCOPY AND IMAGING
Organizer and Presider: Rich Bornett

10:30 (625) Hot stage-Raman Microscopy as a Hyphenated Technique for Investigation of the Thermodynamics of Samples: a Feasibility Study; Dirk Cleeren1, Sigrid Stokbroeka1, Jef Peeters1, Marcus E. Brewster1, ‘Johnson & Johnson Pharmaceutical R&D Belgium

10:50 (626) Raman Imaging Spectroscopy and Molecular Modeling Methods for Assessing the Intracellular Distribution of Pharmacologic Agents; Michael Miller1, Jian Ling1, ‘Southwest Research Institute

11:10 (627) Process Monitoring of Paintable Display Production Using Confocal 3D Raman Spectroscopy and Chemometrics; Peter de Peinder1, Inge Vorstenbosch1, Arjan Manik1, ‘Philips Electronics

11:30 (628) Raman Microscopy and Imaging Applications to Nanostructures and Single Molecule Detection; Ricardo Aroca1; ‘University of Windsor

11:50 (629) Characterization of Phthalocyanine Printing Inks by Micro Raman Spectroscopy; Gene Hall1, ‘Rutgers University

12:10 (630) Extending the Capabilities of Drop Coating Deposition Raman (DCDR); Dongmao Zhang1, Yong Xie1, Corasi Ortiz1, Don Ben-Amotz1; ‘Purdue University

Thursday Afternoon, Room B114
MULTIWAY ANALYSIS AND MULTIWAY METHOD DEVELOPMENT
Organizer and Presider: Karl Booksh

1:30 (631) New Mass-Spectrometric Systems for Metallomics; Gary Hieflie1, Steven Ray1, Duane Rogers1; ‘Indiana University

3:30 (632) Collision/Reaction Cell ICP-MS: Enhancements to Elemental Speciation Studies; Joseph Caruso1, ‘University of Cincinnati

3:50 (633) Particle Beam/Glow Discharge Mass Spectrometry: Simultaneous Acquisition of Molecular, Fragment, and Atomic Mass Spectra; Robert Kenneth Marcus1, Jakob L. Venzie1, W. Clay Davis1; ‘Clemson University; ‘National Institute of Standards and Technology

4:10 (634) LC Sector Field ICP-MS for Simultaneous Speciation analysis of P and S in Proteins; Meike Hamester1, Torsten Lindemann1, Lothar Rottmann1; ‘Thermo Electron

4:50 (635) Detection of Heteroelements in Proteins by ICP-MS; Norbert Jakubowski1, Wolf D. Lehmann1, Michael Edler1, Ingo Feldmann1; ‘Institute for Analytical Sciences (ISAS); ‘German Cancer Research Institute

5:10 (636) Chemical Imaging of Biological Materials by NanoSIMS; Peter Weber1, Julie Smith1, Ian Hutchison1; ‘Lawrence Livermore National Laboratory

THURSDAY POSTER SESSIONS and BREAK
2:00 – 3:30 PM, See pages 63 - 65
Exhibit Hall A

Thursday Afternoon, Room C123
METALLOMICS
Organizer and Presider: Dave Koppenaal

3:30 (637) Guidelines to Choose Multivariate Data Analysis Methods for Multivariate Resolution of Chemical Data Sets; Anna de Juan1, Romá Tauler2; ‘Chemometrics Group, University de Barcelona; ‘Department of Environmental Chemistry, Institute of Chemistry and Environmental Research, CSIC

3:50 (638) Purity Applied to PARAFAC; Neal Gallagher; ‘Eigenvector Research, Inc

4:10 (639) Study the Process of Refining Wood Using 3-Way PLS Regression Analysis of Fluorescence Spectra; Valerie Lengard1, Dongsheng Bu1, Charu Mati1, Zala Vijay1, Waltraud Kessler2; ‘Cam Smart Inc; ‘Institut für Angewandte Forschung

4:30 (640) Characterization of Drug Metabolism Using Chemometric Methods; Sarah Rutan1, Raymundo Sanchez-Ponce1, Sarah Graham1, Dennis Thekkudan1, Shom Paul1; ‘Virginia Commonwealth University

4:50 (641) 3-Way and 4-Way PARAFAC Applied to Analysis of Pesticides and PAHs, Karl S. Booksh1, Yoon-Chang Kim1, Michelle L. Nahorniak1, James A. Jordan1, and Gary A. Cooper1; ‘Department of Chemistry and Biochemistry, Arizona State University

5:10 (642) Utilizing 3-Dimensional Wavelet Transforms (3D WT) for Accelerated Evaluation of Hyperspectral Image Cubes; Frank Vogt1, Karl Booksh1; ‘Arizona State University

Thursday Afternoon, Room C124
IR SPECTROSCOPY IMAGING
Organizer and Presider: Christine Wellburg

3:30 (643) Applications of Infrared Spectroscopic Imaging Utilizing Different-sized MCT Focal Plane Arrays; Gloria Story1, Curtis Marcott1; ‘The Procter & Gamble

3:50 (644) Near-Infrared Imaging in Food Safety; Jamie Dubois1, Frederick S. Fry1, Elizabeth M. Calvey1, E. Neil Lewis1; ‘JIFSAN, Food and Drug Administration and Universit; ‘CFSAN, Food and Drug Administration; ‘Spectral Dimensions Inc.
Thursday Afternoon, Room A105
MS FRONT-END DEVICES AND NEW METHODOLOGY FOR PROTEOMICS
Organizer and Presider: Liang Li

3:30 (649) Development of Microfluidic Devices for Proteomics; Jed Harrison; University of Alberta

3:50 (650) Microfluidic Chip Front-ends for MALDI Mass Spectrometry; Kermit Murray1, Steve Soper1, Harrison Musyimi1, Damien Narcisse2, Xia Zhang1, Mark Little1, Yichuan Xu1; Louisiana State University

4:10 (651) New Surface Enhanced Neat Desorption SELDI Protein Biochip for Proteomic Analysis; Scott Weinberger2,1; Ciphergen Biosystems, Fremont, CA, USA

4:30 (652) Liquid Chromatography Coupled to UV-MALDI Using Off-Line Sample Spotting; Robert Brown1, Ron Orlando2; Utah State University; University of Georgia

4:50 (653) Protein and Peptide Analysis By Very High Throughput MALDI-TOF Mass Spectrometry of Liquid Chromatography Effluent; James Reilly1, Kirk Boraas2, Noah Christian1, Sean Stryker1, Matthew Thompson1, Weidong Cui1; Indiana University

5:10 (654) Development and Applications of LC/MALDI MS for Comprehensive Proteome Analysis; Liang Li1,2; Department of Chemistry, University of Alberta

Thursday Afternoon, Room B115
NANOTUBES AND NANOWIRES FOR SENSING
Organizers: Peter Pefrsson and Jie Liu • Presider: Shu Peng

3:30 (665) Silver Nanowire for SERS applications; Andrea Tao1, Peidong Yang1; UC Berkeley

4:10 (666) DNA Sensing Based on Silicon Nanowires; Zhiyong Li1, Yong Chen2, Xuema Li1, Ted Kamins1, Stan Williams2; HP Labs; UCLA

4:50 (667) Self-Assembly of Colloidal Nanostructures for Nanoelectronics and Nanoplasmonics; Yi Cui1, Alexander Liddle2, Paul Alivisatos1,2; University of California, Berkeley; Lawrence Berkeley Lab

5:10 (668) Electron-Transfer Chemistry of Octadecylamine-Functionalized Single-Wall Carbon Nanotubes; Shaowei Chen1, Yiyun Yang1, Wei Zhao2; University of California - Santa Cruz; University of Arkansas - Little Rock

Thursday Afternoon, Room B116
EMERGING TECHNOLOGIES FOR PROCESS ANALYSIS
Organizer and Presider: Brian Marquardt

3:30 (659) Portable Integrated UV Resonance Fluorescence and Raman Chemical Sensor for in situ, autonomous, detection; William Hug1, Ray Reid1, Pamela Conrad2, Arthur Lane2, Rohit Bhartia1; Photon Systems; Jet Propulsion Laboratory, Caltech

3:50 (660) MicroNMR Systems for Process Control; Michael McCarthy1, Jeffrey Walton1, Jeffrey de Ropp1, Artem Goloshevsky1, Scott Collins1; University of California Davis; University of Maine

4:10 (661) Portable Surface Plasmon Resonance Sensors; Alexei Naimushin; Seattle Sensors Systems, Inc.

4:30 (662) Vapochromic Detection and Quantification of Relative Humidity and Organic Solvent Vapors; Kent Mann1, Brian Marquardt2, Daron Janzen1, Stephen Drew1; University of Minnesota, Department of Chemistry; Center for Process Analytical Chemistry, 1,2; Carlton College

4:50 (663) The Theory and Application of RF/microwave Dielectric Spectroscopy; Philip Bartley1, Shelley Begley1; Innovative Measurement Solutions; Agilent Technologies

5:10 (664) Analytical Applications of Modular Sampling Systems (NeSSI); Dave Veltkamp1, Brian Marquardt2, University of Washington