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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
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WELCOME TO FACSS 2004

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 destrction, 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.

Monday (Opening Reception)	**5:30 – 7:30 PM**
Tuesday – Wednesday	**9:00 AM – 4:00 PM**
Thursday	**9:00 AM – 2:00 PM**

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 conferees,** *Hall A* ***(Tickets required)***

WEDNESDAY

8:00 AM **Plenary Lecture:** Semiconducting and Piezoelectric Nanobelts, Nanosprings 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 exhibitiors 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

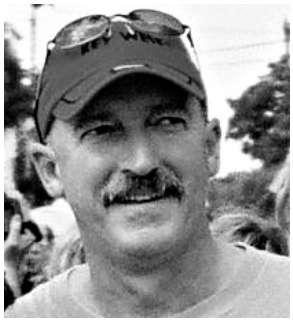
Governing Board Chair	**Michael Blades,** *University of British Columbia* E-mail: blades@chem.ubc.ca
Governing Board Chair Elect	Mark Hayes, *Arizona State University*
Past Governing Board Chair	**Michael Carrabba,** *Hach Homeland Security Technologies*
Second Past Governing Board Chair	**Ron R. Williams,** *Saginaw Valley State University*
Secretary	**John Graham,** *Hercules Inc.*
Treasurer	**Paul N. Bourassa,** *Lifeblood Mid-South Regional Blood Center*
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,** *Simor 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*

FACSS CHAIRS

GOVERNING BOARD CHAIR



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.

GENERAL CHAIR

David S. Trimble

Swarthmore College

David Trimble is currently the Scientific Instrument Coordinator for the Department of Chemistry at Swarthmore College. He received his B.S. in Chemistry from Denison University with a concentration in computer science. He was able to utilize aspects of both these disciplines at the University of Tennessee, Knoxville under the mentorship of Dr. Gleb Mamantov. He received his Ph.D. in Analytical Chemistry for the Raman spectroscopic and spectroelectrochemical characterization of transition metal complexes in molten chloroaluminates. David conducted post-doctoral studies under the mentorship of Dr. Arlene Garrison at the University of Tennessee Measurement and Controls Engineering Center. He demonstrated the usefulness FT-Raman as a method to study a variety of industrially interesting chemical systems, and in particular fiber optic-based FT-Raman measurements for the on-line control of chemical distillation columns.

After completing his post doctoral studies David joined Union Camp Corporation, Franklin, Virginia. As a staff chemist in the Technical Department David served many roles in the on-line, at-line and central laboratory measurements associated with product and process quality and environmental compliance issues associated with the manufacture of bleached printing papers. As a Senior Chemist he became deeply involved in the root cause analysis of production upsets and finished product customer complaint resolution. David left, what had become by acquisition International Paper, as Team Leader of Analytical Services.

In the course of his career David has authored or co-authored 14 publications and presentations. The paper “Environmental Benefits of Ozone-Based Bleaching” presented at the 1993 TAPPI Environmental Conference received the best paper award within the water category.

David has been an active member of the Coblentz Society and serves as delegate for the society on the governing boards for the EAS and FACSS organizations. He has served as co-chair of the 2002 and 2003 FACSS Workshops Committee. David is also a member of the Society for Applied Spectroscopy, the American Chemical Society, and served as Secretary to ASTM subcommittee E13.03 on Infrared Spectroscopy from 1994-1996. When in the industry he was a member of the Technical Association for the Pulp and Paper Industry.

FACSS CHAIRS

PROGRAM CHAIR

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 referred 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.

EXHIBITS CHAIR

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

ATOMIC SPECTROSCOPY

Burgener Research
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Perkin Elmer/Sciex
Teledyne Leeman Labs
Thermo Electron Corp
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FOSS NIRsystems, Inc.
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FORENSICS

Agilent Technologies

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John Wiley & Sons
Kaiser Optical Systems, Inc.
Renishaw, Inc.
Spectroscopy Magazine
Thermo Electron Corp.

WORKSHOPS

Mettler Toledo
Smith Detection

MANN AWARD

Dorothy Mann, on behalf of the Mann Family

STUDENT POSTER AWARD SPONSORS

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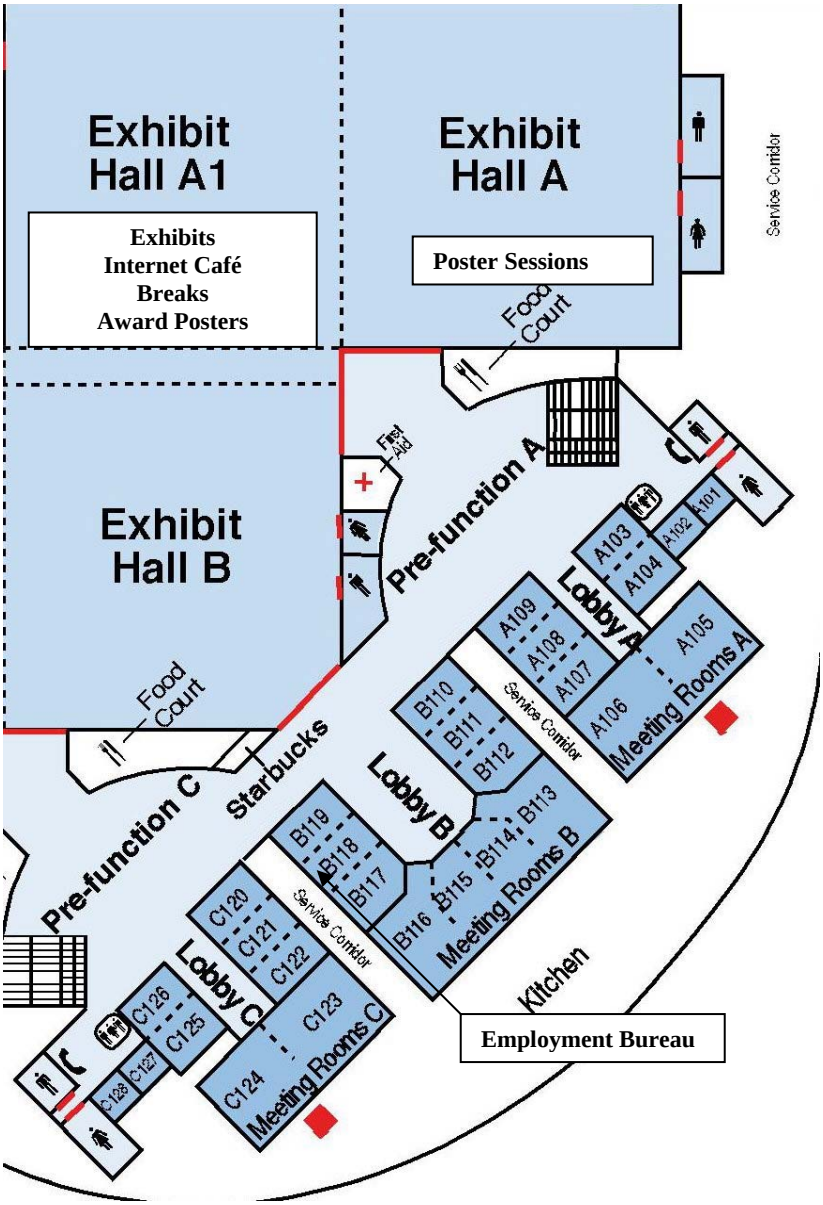
IM Publication
John Wiley & Sons
Meinhard Glass Products
Springer-Verlag

FLOOR PLANS

LEVEL 1

Session Rooms, Employment Bureau, Exhibits, Posters, Workshops



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 Rensselear Polytechnic Institute, Troy, NY with Dr. McGown. He is a member of the American Chemical Society and Phi Lambda Upsilon.

SOCIETY FOR APPLIED SPECTROSCOPY AWARDS

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 of array of international conferences and meetings.

SOCIETY FOR APPLIED SPECTROSCOPY AWARDS

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.

SOCIETY FOR APPLIED SPECTROSCOPY AWARDS

MEGGERS AWARD

Recognizing the author(s) of an outstanding paper appearing in Applied Spectroscopy

Photo Not Available

Markus Janotta **Abraham Katz**ir **Boris Mizaikoff**

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 avaialable

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

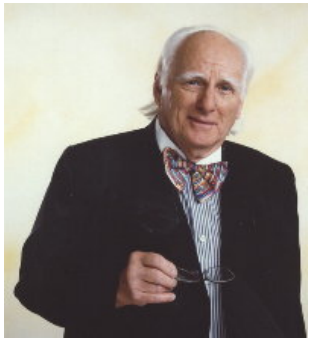
Recognizing a Graduate Student for Outstanding Research in Spectroscopy

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 science problem solving demonstrating the complimentarity 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 the free time he devotes himself to the world of symphonic and opera music.

ANACHEM AWARD

Presented to an outstanding analytical chemist based on activities in teaching, research, administration or other activity which has advanced the art and science of the field.



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 using spectroscopy for the detection of biological hazards. He received his B.S. in Chemistry from Salem State College in 1981 and his Ph.D. from Tufts University in 1985. Mike's graduate work was conducted under the tutelage of Dr. Jonathan Kenny and focused on the utilization of laser-induced fluorescence to examine ultra-cooled gas phase molecules in a supersonic jet molecular beam. After graduate school, Mike joined EIC Laboratories where he eventually became Vice-President for the Spectroscopy Division. He conducted a variety of research programs, including photoelectrochemical etching of semiconductors, fiber optic chemical sensors and state-of-the-art Raman spectroscopy. During this time, he introduced the use of holographic filters for Raman spectroscopy and developed numerous types of Raman instrumentation and techniques, several of which resulted in U.S. patents. After leaving EIC, Mike joined Chromex, Inc, a manufacturer of Raman spectroscopy systems, as Marketing Manager and most recently was the OEM Division Manager at Jobin Yvon, Inc. Mike has been 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

PREVIOUS FACSS BOARD AND MEETING CHAIRS

1973	
Jeannette Grasselli	Governing Board Chair
1974 - Atlanta	
James White	Governing Board Chair
George Heinz	General
James White	Program
Edward Ruffing	Exhibit
1975 - Indianapolis	
I. James Holcombe	Governing Board Chair
Gerald Wallace	General
I. James Holcomb	Program
Edward Ruffing	Exhibit
1976 - Philadelphia	
Edward Brame	Governing Board Chair
Edward Brame	General
Edward Dunlap	Program
Douglas Robinson	Arrangements
Edward Ruffing	Exhibit
1977 - Detroit	
Edgar Peck	Governing Board Chair
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Jeannette Grasselli	Program
L. Felix Schneider	Arrangements
Edward Ruffing	Exhibit
1978 - Boston	
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James Cornwell	Arrangements
Edward Ruffing	Exhibit
1979 - Philadelphia	
Peter Keliher	Governing Board Chair
Douglas Robinson	General
Philip LeFleur	Program
Sydney Fleming	Arrangements
Edward Ruffing	Exhibit
1980 - Philadelphia	
L. Felix Schneider	Govering Board Chair
Sydney Fleming	General
Theodore Rains	Program
Robert Barford	Arrangements
Edward Ruffing	Exhibit
1981 - Philadelphia	
Jack Katon	Govering Board Chair
Robert Barford	General
Mary Kaiser	Program
James Cavanaugh	Arrangements
Peter Keliher	Exhibit
1982 – Philadelphia	
Sydney Fleming	Governing Board Chair
James Cavanaugh	General
Andrew Zander	Program
Matthew O'Brien	Arrangments
Peter Keliher	Exhibit
1983 - Philadelphia	
Mary Kaiser	Governing Board Chair
Matthew O'Brien	General
John Lephardt	Program
D. Bruce Chase	Arrangements
Peter Keliher	Exhibit
1984 - Philadelphia	
Theodore Rains	Governing Board Chair
D. Bruce Chase	General
Patricia Rouse Coleman	Program
Fred Corcoran	Arrangements
Peter Keliher	Exhibit
1985 - Philadelphia	
Robert Barford	Governing Board Chair
Fred Corcoran	General
Matthew Klee	Program
Marshall Fishman	Arrangements
Peter Keliher	Exhibit
1986 - St. Louis	
Ronald Schroeder	Governing Board Chair
Marshall Fishman	General
Alexander Scheeline	Program
Terry Hunter	Arrangements
Edward Brame	Exhibit
1987 - Detroit	
Patricia Rouse Coleman	Governing Board Chair
David Coleman and L. Felix Schneider	General
John S. Beaty	Program
Edward Brame	Exhibit
1988 - Boston	
James Cavanaugh	Governing Board Chair
Frank Plankey and John S. Beaty	General
Roger Gilpin	Program
Edward Brame	Exhibit
1989 - Chicago	
Alexander Scheeline	Governing Board Chair
Paul Bourassa	General
Robert Michel	Program
Edward Brame	Exhibit
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Nancy Miller-Ihli	Governing Board Chair
Charles Belle	General
Steven Hughes	Program
Edward Brame	Exhibit
1991 - Anaheim	
David Coleman	Governing Board Chair
Richard Deming and Constance Sobel	General
James Holcombe	Program
Edward Brame	Exhibit
1992 - Philadelphia	
Karmie Galle	Governing Board Chair
Matthew Klee	General
Barry Lavine	Program
Edward Brame	Exhibit

PREVIOUS FACSS BOARD AND MEETING CHAIRS

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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
John Koropchak	Program
Mildred Barber	Exhibit

1995 – Cincinnatti

Jon W. Carnahan	Governing Board Chair
Joseph A. Caruso	General
Richard F. Browner and R. Kenneth Marcus	Program
Mildred Barber	Exhibit

1996 – Kansas City

Rachael Barbour	Governing Board Chair
O. Karmie Galle	General
William Fateley	Program
Scott McGeorge	Exhibit

1997 - Providence

Mildred Barber	Governing Board Chair
Chris Brown	General
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Scott McGeorge	Exhibit

1998 - Austin

John Graham	Governing Board Chair
David Laude	General
Isiah Warner and Linda McGown	Program
Scott McGeorge	Exhibit

1999 - Vancouver

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Michael Blades	General
Ronald Williams	Program
Scott McGeorge	Exhibit

2000 - Nashville

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Arlene Garrison	General
Michael Carrabba	Program
Scott McGeorge	Exhibit

2001 – Detroit

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David Coleman and L. Felix Schneider	General Co-Chairs
David J. Butcher	Program
Scott McGeorge	Exhibit

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

SOCIETY AND COMMITTEE MEETINGS

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*

FACSS EXHIBITORS

Advanced Chemistry Development Inc.	Booth 109
Advanced Photometrics	Booth 325
Avalon Instruments	Booth 418
B&W Tek, Inc.	Booth 107
BioTools, Inc.	Booth 320
Bruker Optics, Inc.	Booths 301/303
CETAC Technologies	Booths 412/414
Coblentz	Booth 324
Critical link, LLC	Booth 322
Digilab, LLC	Booths 400/402
Eigenvector Research, Inc.	Booth 410
Elsevier	Booth 425
FACSS	Booth 106
FernCreek Technologies	Booth 407
Fibertech Optica, Inc.	Booth 223
Glass Expansion	Booth 203
High Purity Standards, Inc.	Booth 113
Hinds Instruments, Inc.	Booth 220
HORIBA Jobin Yvon	Booths 300/302/304/306
ICP Information Newsletter, Inc.	Booth 123
IonSpec Corporation	Booth 111
John Wiley & Sons	Booth 205
Kaiser Optical Systems, Inc.	Booth 221
Lambda Solutions, Inc.	Booth 305
Light Diagnostics, Inc.	Booth 406
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Newport Corporation	Booth 121
Ocean Optics, Inc.	Booth 120
Olis, Inc.	Booth 222
OPOTEK, Inc.	Booth 404
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Pittsburgh Conf of Analytical Chem	Booth 225
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Russell Publishing LLC	Booth 103
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Shimadzu Biotech	Booths 102/104
Shimadzu Scientific	Booth 100
Siemens Applied Automation	Booth 403
Smith Detection	Booth 201
Society for Applied Spectroscopy	Booth 321
Solutions Plus	Booth 207
Spectral Dimensions	Booth 119
Spectroscopy Magazine	Booth 122
Springer-Verlag New York, Inc.	Booth 416
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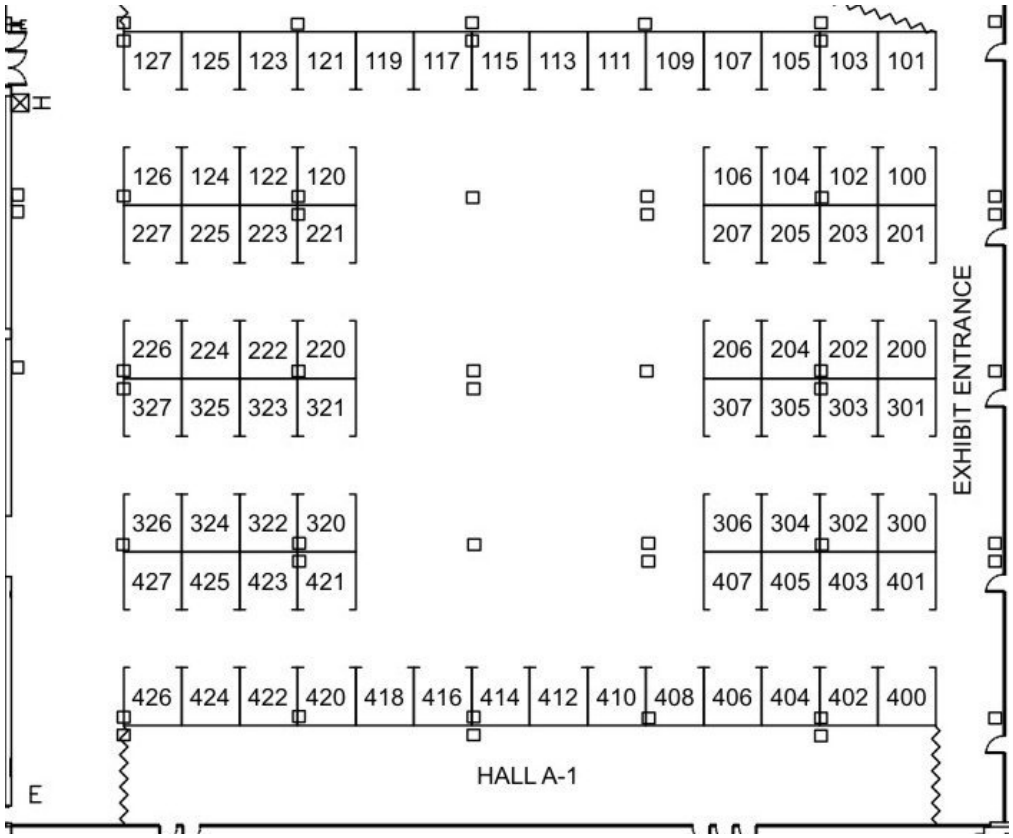

EXHIBITOR DESCRIPTIONS

Advanced Chemistry Development Inc. **Booth 109**
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Toronto, ON, M5H 3V9 CANADA
Phone: 416 368 3435
www.acdlabs.com

Advanced Chemistry Development, Inc., (ACD/Labs) is a chemistry software company offering solutions that truly integrate chemical structures with analytical chemistry information to produce ChemAnalyticsTM. ACD/Labs creates innovative software packages that aid chemical research scientists worldwide with spectroscopic validation of structures, elucidation of unknown substances, chromatographic separation, medicinal chemistry, preformulation of novel drug agents, systematic nomenclature generation, and chemical patenting and publication. Combined, ACD/Labs' solutions create an analytical informatics system that provides dramatic feed-forward effects on the chemical and pharmaceutical research process. Founded in 1993, and headquartered in Toronto, Canada, ACD/Labs employs a team of over 100 dedicated individuals whose continual efforts carry ACD/Labs' innovative technologies into pharmaceutical, biotech, chemical, and materials companies throughout the world. Information about Advanced Chemistry Development and its products can be found at www.acdlabs.com. For more information contact Daria Jouravleva at 416-368-3435 or e-mail at daria.jouravleva@acdlabs.com.

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www.coblentz.org

The Coblentz Society is an association dedicated to fostering the understanding and application of vibrational spectrometry such as Fourier transform and dispersive infrared spectroscopy and raman scattering spectroscopy. The Society, founded in 1954, promotes communication amongst vibtational spectroscopists. Information about the Society's awards, Spectral Database Products and other functions are available at the exhibit.

EXHIBITOR DESCRIPTIONS

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Elsevier plays an integral part within the analytical science community delivering quality research and information via reputable journals, books and electronic products. Our new and latest edition is the *Encyclopedia if Analytical Science*, second edition which will be publishing in December 2004. From Activation Analysis to Zone Broadening, this ten volume set has 568 articles on analytes, samples, and instrumental techniques that provide various approaches to solving analytical chemistry problems. Topics ranging from food science to forensics, environmental science to medicine are covered, as are important characterization techniques such as microscopy and surface analysis. The online version of this work will also be available in spring 2005 on ScienceDirect. For more information on the Encyclopedia and our extensive selection of analytical chemistry books, journals and electronic resources please visit the Elsevier booth. www.elsevier.com

FACSS **Booth 106**
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www.facss.org

FACSS 2005 will be held October 9 – 13 in Quebec City, Canada. Quebec City offers a strong cultural flavor uniques to North America. A famous history, the Old City, and unparalleled fine dining will provide FACSS conferees with an excellent meeting venue. Be sure to watch the web site for abstract submission information for the next FACSS conference.

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FiberTech Optica designs and manufactures specialty multimode step-index UV-VIS and VIS-NIR fused silica fibers, plastic clad silica (PCS) and hard plastic silica (HCS) fibers as well as fiber optic assemblies. Do you want to improve the signal-to-noise ratio of your systems? Many choices of numerical apertures, core to clad ratios and diameters and various types of buffers and coatings are available. Low solarization fibers are also available. We also design and manufacture custom bundles, reflectance and immersion probes and single fiber assemblies used in harsh industrial and scientific environments. Applications include remote spectroscopy, on-line process control analysis, remote sensing, illumination, chemical analysis, non invasive testing laser marking, cutting, welding and soldering. We address all of your fiber optic needs.

Glass Expansion **Booths 203**
4 Barlows Landing Rd, Unit 2
Pocasset, MA 02559
Phone: 508 563 1800
www.geicp.com

Sample introduction components for ICP-AES and ICP-MS sprectrometers, including nebulizers, spray chambers, torches, injectors, RF coils, cones, tubing, and accessories. At FACSS, we will be showcasing our Eluo nebulizer cleaner, new line of silver and gold plated RF coils, and Capricorn argon humidifier. Other significant products include the new Helix O'ring-free spray chambers and a line of HF resistant nebulizers and spray chambers.

EXHIBITOR DESCRIPTIONS

High Purity Standards, Inc. **Booths 113**
P.O. Box 41727
4741 Franchise Street
Charleston, SC 29418
Phone: 843 767 7900
www.hps.net

High-Purity Standards is a manufacturer of high-purity spectrometric standard solutions for the calibration, interference check, quality control and method development of analytical methods for AAS, ICP, ICP-MS, IC, and CNS elemental analysis. Metal standards are directly certified against NIST 3100 Series Standard Reference materials. High-Purity Standards offers a line of certified reference materials that range from soils, sludge, coal, to foods such as soybean meal, dog food, and cottonseed meal. These materials are certified for major, minor and trace metals including carbon, sulfur and nitrogen by two different methods. We manufacture custom blends to meet our customers' specific laboratory needs. Free consultation available to answer customer questions in the use of the product and related laboratory preparations and analyses.

Hinds Instruments, Inc. **Booth 220**
3175 NW Aloclek Drive
Hillsboro, OR 97124
Phone: 503-690-2000
www.hindspem.com

Hinds Instruments manufactures photoelastic modulator (PEM) systems for a broad range of polarization modulation applications. These include FTIR spectroscopy, IRRAS, birefringence measurements, polarization modulation, linear and circular dichroism, VCD and MCD, chopping a light beam, ellipsometry, and polarimetry. PEMs operate by changing or detecting the polarization state of light at a fixed frequency (20 kHz – 84 kHz).

HORIBA Jobin Yvon **Booths 300/302/304/306**
3880 Park Avenue
Edison, NJ 08820-3012
Phone: 732 494 8660
www.jyhoriba.com
HORIBA Jobin Yvon provides high performance instrumentation for spectroscopy and other scientific and analytical applications. We are the World Leader in Raman spectroscopy. At FACSS we will be introducing the LabRAM ARAMIS a revolutionary fully automated confocal Raman microscope, which switches automatically between up to four lasers, notch filters, and gratings. Our Emission Division manufactures ICP, Glow Discharge optical emission spectrometers, and elemental analyzers for C, S, O, N, & H. We will also demonstrate our award winning EDXRF Microscope - the XGT 5000. Horiba will present the OMA-300 an online/in-situ process analyzer that applies UV/VIS/NIR diode array principles and fiber optics technology to perform multi-component analysis of liquid or gas samples. The Fluorolog, the world's most sensitive Spectrofluorometer, now has both TCSPC and phase capability. We will also be showing selections from our range of CCDs, gratings, and spectrographs, and our Spectroscopic Ellipsometers and Optical Emission Spectrometers. Come and talk to our team of experts and see what HORIBA Jobin Yvon can do for you.

ICP Information Newsletter, Inc. **Booth 123**
85 N. Whitney Street
Amherst, MA 01002-1869
Phone: 413 256 8942
www.chem.umass.edu/winterconf2000

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

IonSpec Corporation **Booth 111**
20503 Crescent Bay Drive
Lake Forest, CA 92630-8825
Phone: 949 305 3867
www.ionspec.com

IonSpec is the leading manufacturer of Fourier transform mass spectrometers, including the ultra-high performance QFT-7 hybrid FTMS for LC/MS/MS. IonSpec has over 21 years of experience in FTMS and maintains an outstanding reputation for technical service and support.

John Wiley & Sons **Booth 205**
111 Rivert Street 4-02
Hoboken, NJ 07030
Phone: 212 850 6758
http:www.wiley.com

Want to know the latest in analytical chemistry and spectrometry? Then come and visit Wiley at booth 205 for a wide range of books, reference works, journals, online products and resources. Or visit www.wiley.com. Come and collect the journal sample copies, view articles online at Wiley InterScience and sign up for your FREE Content Alerts at www.interscience.wiley.com. See spectroscopyNOW.com, Wiley's highly regarded spectroscopy portal or visit www.spectroscopyNOW.com. For Wiley's complete product portfolio, visit www.wiley.com

EXHIBITOR DESCRIPTIONS

Kaiser Optical Systems, Inc. **Booth 221**
371 Parkland Plaza
Ann Arbor, MI 48103
Phone: 734 665 8083
www.kosi.com/raman

Kaiser Optical Systems, Inc., a Rockwell Collins Company, is a world leader in the production of high-performance holographic optical elements (HOEs) for spectroscopic, aerospace, and military applications. Our holographic notch filters for laser line rejection have revolutionized Raman spectroscopy. Our innovative fiber optic probe, imaging spectrograph, and transmission grating technologies provide a solid foundation for a complete family of compact, high-performance, extremely reliable instrumentation: the RamanRxn Systems™ family of Raman analyzers. RamanRxn Systems analyzers are at work wherever analyses need to be fast and non-invasive. RamanRxn1™ analyzers are in the R&D lab probing the behaviors of enzymes, exploring the structures of new materials with microscopy, and screening drug candidates with HTS. RamanRxn2™ and RamanRxn3™ process analyzers are in the process line monitoring reactions, polymerizations, and polymorph transformations—all in situ. And they're at the process line analyzing moving polymeric films and fibers, semiconductors, and DLC films with non-contact optics.

Lambda Solutions, Inc. **Booth 305**
411 Waverley Oaks Rd, Ste 335
Waltham, MA 02452
Phone: 781 478 0170
www.lambdasolutions.com

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.

Light Diagnostics, Inc. **Booth 406**
6620 South 400 West
Murray, UT 84107
Phone: 801 293 9266

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

Mettler Toledo AutoChem Inc. **Booth 101**
8223 Cloverleaf Drive
Millersville, MD 21108
Phone: 410 987 3222
www.mt.com

Newport Corporation **Booth 121**
1791 Deere Avenue
Irvine, CA 92606
Phone: 949 253 1468
www.newport.com
Newport introduces the OSM-400 spectrometer - a fully self-contained instrument enabling real-time spectroscopic analysis, with user-friendly operation via its touch screen. On-board memory enables storage of 100 graphs, which can be downloaded to a PC. Newport is a global leader in photonic instrumentation and integrated systems to the Research, Industrial and Aerospace and Defense markets.

Ocean Optics, Inc. **Booth 120**
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Dunedin, FL 34698
Phone: 727 733 2447
www.oceanoptics.com

Olis, Inc. **Booth 222**
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Phone: 706 353 6547
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Move to the modern with Olis, Inc! (1) Research spectrophotometers for dual beam absorbance, fluorescence, and circular dichroism for best data during steady-state and kinetic studies. (2) Accessories for temperature ramping, titration, stopped-flow, and photolysis. (3) Brand-new fiber-optic spectrometers plus Olis accessories and software for great lower cost workstations. (4) Modernizations of Perkin-Elmer 983 IRs, Cary 14 UV/Vis/NIR, SLM 8000, Aminco DW-2 and other 'upgrade worthy' models, too! All Olis hardware compatible with Olis Windows 2000/ XP compatible software.

OPOTEK, Inc. **Booth 404**
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Carlsbad, CA 92008
Phone: 760 929 0770
www.opotek.com
Mfr. of efficient, compact, and widely tunable solid state laser systems based on its Optical Parametric Oscillators (OPO). These systems are used in photochemistry, photobiology, medical diagnostics and environmental monitoring, They are computer controlled and simple to use. Contact Eli Margalith, President, emargalith@opotek.com

PerkinElmer Life &Analytical Sciences **Booth 405**
710 Bridgeport Avenue
Shelton, CT 06484
Phone: 203 402 6878
www.perkinelmer.com/instruments

EXHIBITOR DESCRIPTIONS

Photon Systems **Booth 115**
1512 Industrial Park Street
Covina, CA 91722-3417
Phone: 626 967 6431
www.photonsystems.com

Photon Systems will exhibit a new family of 224nm and 248nm lasers that are the size, weight and power consumption of HeNe lasers yet emit at a variety of wavelengths in the deep UV. The lasers demonstrated have quasi-cw output power up to 50mW at 224nm and 250mW at 248nm. We will also exhibit and demonstrate a Targeted Ultraviolet Chemical Sensor (TUCS) based on deep UV laser induced native fluorescence and UV Raman capable of detection of aromatic amino acids and other organic molecules down to the 100 molecule level. The TUCS is also capable of detecting and classifying microorganisms down to the single microbe level at a working distance of 45cm.

Pittsburgh Conference of Analytical Chem **Booth 225**
300 Penn Center Blvd., Ste 332
Pittsburgh, PA 15235
Phone: 412 859 0818
www.pittcon.org

The Pittsburgh Conference and Exposition on Analtyical Chemistry and Applied Spectroscopy is the greatest scientific program and instrumentation show held anywhere in the world. We embrace life sciences, genomics, proteomics, forensics, nanotechnology, pharmaceutical sciences and modern food sciences. More than 1200 companies occupying more than 2500 booths display the very latest technologies. The program consists of 2500 papers and 60 symposia.Visit us at www.pittcon.org for a complete description of all facets of Pittcon

Renishaw, Inc. **Booths 420/422**
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www.renishaw.com

Get chemical/molecular information from your SEM using the power of Raman spectroscopy. Renishaw Raman Microscopes provide chemical information confocally at sub-micron spatial resolution with auto-alignment, internal calibration & performance validation. Renishaw Raman spectrometers are configurable to include multiple excitation sources from the UV through NIR with automated laser switching and alignment, quick-launch fiber-optic probes, AFM/NSOM/Raman, SEM-Raman, hot/cold cells, macrosampling, global Raman imaging, near excitation analysis, 2D/3D mapping and depth-profiling.

Retsch Inc. **Booth 117**
74 Walker Lane
Newtown, PA 18940
Phone: 267 757 0351
www.retsch-us.com

Retsch manufactures quality laboratory equipment for solid sample preparation: mills, pulverizers, crushers as well as sample dividers, sieves, sieve shakers, optical particle sizers, feeders and cleaners. Products shown will include the new high energy bench top planetary ball mills PM 100 and 200. The products are used in many industries for research and development, quality control and small- scale production. Retsch provides application/technical support and full service facilities.

RoMack, Inc. **Booth 423**
105 Edward Wyat Drive
Williamsburg, VA 23188
Phone: 757 258 4805
www.romackfiberoptics.com

RoMack,Inc. manufacturers fiberoptic assemblies, components and related products specifically tailored for spectroscopic, laser, pharma and medical applications. Products include probes, fiberoptics, connectors, adapters, patchcords, bundles, arrays, imagers, collimators, couplers, tapers and filter packages. Romack, Inc. routinely takes concept to product, creating solutions to the most difficult problems.

Royal Society of Chemistry **Booth 224**
Thomas Graham House
Science Park, Milton Road
Cambridge, UK CB4 0WF
Phone: 44 1223420066
www.rsc.org

The RSC is the largest organisation in Europe for advancing the chemical sciences. Supported by a network of 45,000 members worldwide and an internationally acclaimed publishing business, our activities span education and training, conferences and science policy, and the promotion of the chemical sciences to the public. Visit the booth to enquire about membership, browse though our catalogue or collect a sample copy of one of our internationally renowned journals; including The Analyst, JAAS, JEM, Lab-on-a-Chip, and Analytical Abstracts.

Russell Publishing LLC **Booth 103**
9200 Keystone Crossing, Suite 475
Indianapolis, IN 46240
Phone: 317 816 8787

On display will be our new publication PAT - The Journal of Process Analytical Technology and our other premier publication for the pharmaceutical industry American Pharmaceutical Review. Visit our booth to sign up for your FREE subscription to these publications.

SCP Science **Booth 421**
348 Route 11
Champlain, NY 12919-4816
Phone: 800 361 6820
www.scpscience.com

A manufacturer and distributor of analytical equipment and supplies for the inorganic chemical laboratory market. Products include DigiPREP family of graphite block digestion systems and accessories; PlasmaCAL ICP-AES/MS Calibration standards, available for all elements and now offering up to 21 months shelf-life; PlasmaTEST Instrument Control Standards, the only commercial product available for tracking the analytical performance of your ICP-AES or ICP-MS Spectrometer; PlasmaCAL Skimmer and Sampler cones for ICP-MS Spectrometers

EXHIBITOR DESCRIPTIONS

Shimadzu Biotech **Booths 102/104**
7102 Riverwood Drive
Columbia, MD 21046
Phone: 800-477-1227
www.shimadzu-biotech.net

Shimadzu Biotech is a new strategic global business unit of Shimadzu Corporation, focused on the biotechnology and pharmaceutical sectors. It has been created to bring together a strong solutions-based offering to accelerate the progress of biotechnology research and development. Shimadzu Biotech offers a wide range of key products, covering technologies from DNA sequencing to high performance mass spectrometry, to provide an integrated approach to the fast growing proteomics and genomics markets. It also supports other applications, including micro-satellite DNA and SNP analysis for drug discovery.

Shimadzu Scientific **Booth 100**
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Columbia, MD 21046
Phone: 410 381 1227
www.ssi.shimadzu.com

Shimadzu offers a full line of analytical instrumentation, including UV Visible and Fluorescence Spectrophotometers; FTIR Spectrometers; Automated FTIR Microscope; HPLC systems and components; LC/MS; Gas Chromatography; GC/MS; Data Stations for Spectroscopy and Chromatography; Thermal Analyzers, TOC, Atomic Absorption Spectrometers, Particle Size Analyzers, Balances, Arc-Spark Optical Emission Spectrometers, Capillary Rheometers, Mooney Viscometers, Universal Testing Equipment and more.

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www.sea.siemens.com/quantra

QUANTRA - a compact, high-resolution FTMS based on a 1 Tesla permanent magnet. QUANTRA boasts extremely good performance as a universal detector. Under $70,000, High Resolution MS is now affordable for general analytical and process analysis.

Smith Detection **Booth 201**
14 Commerce Drive
Danbury, CT 06810
Phone: 203 207 9726
www.smithdetection.com

Smith Detection is a company dedicated to simplicity in sampling. The TravelIR is the first portable FT-IR system that delivers lab-quality analysis on-site/in the field. The IlluminatIR accessory for light microscopies expands a microscope's capabilities to do molecular analysis. Unlike complex FT-IR microscopes, the IlluminatIR retains all of the functions of the original microscope such as polarized light, fluorescence, and image analysis. Spectral data is provided which allows the microscopist to identify specimens even when there is no optical contrast. The FuraSampleIR II and DuraScope are unique, in-compartment diamond ATR systems that transform commercial spectrometers into complete analysis systems. The DuraSampleIR II is an integral reflection accessory for FT-IR analysis of liquid and solid samples. The DuraScope brings capability to in-compartment analysis through DuraVision(TM). DuraVision provides the user a video-magnified image of the sample, seen through the diamond ATR element

Society for Applied Spectroscopy **Booth 321**
201B Broadway Street
Frederick, MD 21701-6501
Phone: 301-694-8122
www.s-a-s.org

The Society for Applied Spectroscopy is an association of scientific professionals who have organized to advance and disseminate knowledge and information concerning spectroscopy and other allied sciences. We've served the scientific community for over 40 years and are the publishers of Applied Spectroscopy. Visit our booth for membership information.

Solutions Plus **Booth 207**
2275 Cassens Drive, S-147
Fenton, MO 63026
Phone: 618 458 6991
www.riccachemical.com

Since 1983, standards, reagents and solutions for your environmental and analytical requirements, prepared with the utmost care and rigorous adherence to a strict quality system. Products are tested directly against NIST standards where those are available. Spectroscopy standards (AA, ICP, ICP-MS, etc) are a specialty and the product offering has been greatly expanded in a newly released 2004 catalog. Custom manufacturing and private-label requests are welcome.

Spectral Dimensions **Booth 119**
3416 Olandwood Court #210
Olney, MD 20832
Phone: 301 260 0290
www.spectraldimensions.com

Spectral Dimensions, Inc., will exhibit its range of Chemical Imaging Instruments and Software including ISys Chemical Imaging Software. ISys software is the premier imaging package with full chemometric and visualization tools. It handles image cubes from most imaging and microscopy techniques including mid-IR, NIR, and Raman.

Spectroscopy Magazine **Booth 122**
485 Route 1 South, Bldg F, 1st Fl
Iselin, NJ 08830
Phone: 732 346 3081
www.spectroscopyonline.com

Spectroscopy is the only publication dedicated to delivering a complete information solution to the largest circulation of spectroscopists in North America. By providing peer-reviewed, technical and applications-oriented information in every issue, Spectroscopy enables substantial productivity improvement in the laboratories of the spectroscopists leading the way in all areas of spectroscopy.

EXHIBITOR DESCRIPTIONS

Springer-Verlag New York, Inc. **Booth 416**
175 Fifth Avenue
New York, NY 10010
Phone: 212 460 1577
www.springer-ny.com

Teledyne Leeman Labs Inc. **Booth 401**
6 Wentworth Drive
Hudson, NH 03051
Phone: 603 886 8400
www.leemanlabs.com

Thermo Electron Corp. **Booths 200/202/204/206**
5225 Vernona Road
Madison, WI 53711
Phone: 608 273 6822
www.thermo.com

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 informatics solutions and supported by professional and financial services.

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Phone: 925 942 4889
www.varianinc.com

Varian, Inc. is a world leader in scientific instruments and consumable laboratory products serving environmental, industrial, chemical, life science and pharmaceutical customers. At the FACSS 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

VICI Valco Instruments Co., Inc. **Booth 105**
7811 Westview Drive
Houston, TX 77055
Phone: 713-688-9345
www.vici.com

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 braod 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**
Hoevelsinger 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.

	half day	**full day**	**2 day**
Conferees:	$150	$300	$500
Students:	$25	$50	$100
Non-Conferees	$250	$400	$700

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.

FACSS/SAS WORKSHOPS

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 on-line 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

FACSS/SAS WORKSHOPS

CHEMOMETRICS IN ANALYTICAL CHEMISTRY AND SPECTROSCOPY

Charles, E. Miller, ***DuPont Engineering***

Monday, October 4, 8:30 AM – 5:00 PM, A 104 convention center

Conferees $350, Students $100, Non-Conferees $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

Conferees $550, Students $150, Non-conferees $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. Ciurczak,** ***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 MICROSPECTROSCOPY

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 illustrating 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 time-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

.

FACSS/SAS WORKSHOPS

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-Conferees $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 included multivariate image regression, and preprocessing to capture textural 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 transfer of complex information from one individual to another, or to a group, is an important competency for those working in technical and industrial environments. Poor writing can devalue even the best technical work. Good writing skills convey more than just data; they communicate the technical abilities and professionalism of the author.

We believe this short course to be the most unique of its kind, designed by industrial scientists and managers, for industrial scientists and managers. Our objective is to improve corporate communications by providing employees with the tools that they need to effectively communicate their ideas to any audience. We accomplish this by combining our lectures with "hands-on" activities that help to reinforce and develop important writing skills such as defining and understanding the needs of a writer's audience, and communicating ideas through "parallel structure" (the most commonly used yet least understood of all writing techniques).

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 some tools and guidelines to help 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.

PROFESSIONAL ANALYTICAL CHEMISTS IN INDUSTRY: A SHORT COURSE FOR UNDERGRADUATE STUDENTS

Diane Parry, ***The Procter & Gamble Co.***

Wednesday, October 6, 8:30 AM – 5:00 PM

A 108 convention center, No charge

The objective of this workshop is to provide insight into the work of industrial analytical chemists. In a highly interactive forum, participants will explore the role of analytical chemist as problem solver using real problems encountered at Proctor & Gamble. Participants have an opportunity to try their hand at solving real consumer product chemistry problems, and to get answers to some of their questions on industrial chemistry careers. The course is targeted at third-year undergraduates who have had some exposure to instrumental analysis; however, new undergraduate students, graduate students, and chemistry teachers have all reported that they found the short course highly beneficial.

WORKSHOP SPONSORS

Mettler Toledo

Smith Detection

FACSS EMPLOYMENT BUREAU

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 resumés will be available for purchase and will be mailed after the cnference.

ON-SITE REGISTRATION. Applicants and employer representatives must sign in with the Employment Bureau upon arrival at the meeting. Applicant Resuméforms 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 INVITIATION 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 resumés 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

_____

Visa/MasterCard/Amex Number **Exp. Date** **Cardholder's Signature**

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

PROGRAM HIGHLIGHTS

SUNDAY	MONDAY	TUESDAY	WEDNESDAY	THURSDAY
	7:30 Wake up coffee	7:30 Wake up coffee	7:30 Wake up coffee	7:30 Wafe up coffee
8:30 AM – 5:00 PM FACSS/SAS Workshops	8:00 – 9:00 AM Plenary Session	8:00 – 9:00 AM Plenary Session	8:00 – 9:00 AM Plenary Session	8:00 – 9:00 AM Plenary Session
	8:30 AM – 5:00 PM Workshops	8:30 AM – 5:00 PM Workshops	8:30 AM – 5:00 PM Workshops	8:30 AM – 5:00 PM Workshops
	9:00 – 10:30 AM Poster Session and Break	9:00 – 10:30 AM Poster Session and Break	9:00 – 10:30 AM Poster Session and Break	9:00 – 10:30 AM Poster Session and Break
		9:00 – 4:00 PM Exhibits Open	9:00 – 4:00 PM Exhibits Open	9:00 – 2:00 PM Exhibits Open
	10:30 AM – 12:30 PM Oral Symposia	10:30 AM – 12:30 PM Oral Symposia	10:30 AM – 12:30 PM Oral Symposia	10:30 AM – 12:30 PM Oral Symposia
	12:30 – 2:00 PM Lunch Break	12:30 – 2:00 PM Lunch for Conferees in Exhibit Hall	12:30 – 2:00 PM Lunch Break	12:30 – 2:00 PM Lunch Break
	2:00 – 3:30 PM Poster Session and Break	2:00 – 3:30 PM Poster Session and Break	2:00 – 3:30 PM Poster Session and Break	2:00 – 3:30 PM Poster Session and Break
	3:30 – 5:30 PM Oral Symposia	3:30 – 5:30 PM Oral Symposia	3:30 – 5:30 PM Oral Symposia	3:30 – 5:30 PM Oral Symposia
5:00 – 7 00 PM Welcome Mixer and SAS Student Poster Session *Holladay Lobby*	5:30 – 7:30 PM Exhibit Opening Reception *Exhibit Hall A-1*	6:00 PM SAS Reception *(SAS members only) Holladay/Broadway, Doubletree Hotel*		
		6:00 PM Raman Reception *Multnomah, Doubletree Hotel*	6:00 PM FACSS Gala *Portland Classical Chinese Garden*	

PROGRAM OVERVIEW

SUNDAY EVENING

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

MONDAY MORNING

8:00 AM **PLENARY LECTURE: Earth's Earliest Fossils: Solution to Darwin's Dilemma**, J. William Schopf, *Ballroom 201*, page 40

9:00 AM **SYMPOSIA AND POSTER SESSIONS**

9:00 – 10:30 Posters, *Exhibit Hall*, page 40

10:30 – 12:30 Symposia, page 43

- Sample Introduction, *Room C123*
- Analytical Methods to Characterize the Nervous System, *Ballroom 201*
- 2D Correlation Spectroscopy, *Room B114*
- Detection of Weapons of Mass Destruction, *Room B113*
- Near IR, *Room C124*
- TOF MS for Poteomics, *Room A105*
- Carbon Nanotube Separation, *Room B115*
- Process Analytical Technologies in Pharma, *Room B116*
- Biological Applications of Nanoparticles for Surface Enhanced Raman Scattering, *Room A106*

MONDAY AFTERNOON

2:00 PM **SYMPOSIA AND POSTER SESSIONS**

2:00 – 3:30 Posters, *Exhibit Hall*, page 40

3:30 – 5:30 Symposia, page 45

- Laser Ablation, *Room C123*
- 2D Correlation Spectroscopy, *Room B114*
- New Developments in Mass Spectrometry for Forensics, *Room B113*
- Near IR , *Room C124*
- TOF MS for Proteomics, *Room A105*
- Carbon Nanotube Separations, *Room B115*
- Miniature Spectroscopic Sensors, *Room B116*
- Data Analysis and Raman Spectra, *Room A106*

TUESDAY MORNING

8:00 AM **PLENARY LECTURES,** *Ballroom 201*

- **ANACHEM Award**, Walter Jennings, page 48
- **Charles Mann Award,** Michael Carrabba, page 48

9:00 AM **SYMPOSIA AND POSTER SESSIONS**

9:00 – 10:30 Posters, *Exhibit Hall*, page 48

10:30 – 12:30 Symposia, page 51

- LIBS, *Room C123*
- ANACHEM GC1, *Room B116*
- The Role of Analytical Chemistry in Human Disease, *Ballroom 201*
- General Chemometrics, *B114*
- Advances in Forensic Analytical Techniques, *Room B113*
- Coherent 2D Vibrational Spectroscopy, *Room C124*
- Ion Trap MS for Proteomics, *Room A105*
- Carbon Nanotube Separation, *Room B115*
- Charles Mann Award, *Room A106*

TUESDAY AFTERNOON

2:00 PM **SYMPOSIA AND POSTER SESSIONS**

2:00 – 3:30 Posters, *Exhibit Hall*, page 48

3:30 – 5:30 Symposia, page 53

- Advances in Plasma Spectrometry, *Room C123*
- ANACHEM GC2, *Room B116*
- Biomarkers-Analytical Applications in the Research and Assessment of Human Disease, *Ballroom 201*
- Chemometrics in Pharmaceutical Process Analytical Technology, *Room B114*
- Anytime/Anyplace Access to Instrumentation Over the Internet: Changing the Way Science is Taught, *Room B113*
- Coherent 2D Vibrational Spectroscopy, *Room C124*
- Ion Trap MS for Proteomics II, *Room A105*
- Nanomaterials for Photonics, *Room B115*
- Novel Vibrational Techniques for Biology: In Recognition of Richard Mathies 2004 Lippencott Award Recipient, *Room A106*

PROGRAM OVERVIEW

WEDNESDAY MORNING

8:00 AM **PLENARY LECTURES,** *Ballroom 201*
Semiconducting and Piezoelectric Nanobelts, Nanosprings and Nanorings; Zhong Lin Wang, page 56
Meggers Award, Boris Mizaikoff, page 56

9:00 AM **SYMPOSIA AND POSTER SESSIONS**
9:00 – 10:30 Posters, *Exhibit Hall*, page 56
10:30 – 12:30 Symposia, page 59

- 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*

WEDNESAY AFTERNOON

2:00 PM **SYMPOSIA AND POSTER SESSIONS**
2:00 – 3:30 Posters, *Exhibit Hall*, page 56
3:30 – 5:30 Symposia, page 60

- Molecular Inorganic and Organometallic Mass Spectrometry, *Room C123*
- Probing Cellular Properties and Function with Microchip Devices, *Room B116*
- Multivariate Curve Resolutions: Recent Advances and Applications, *Room B114*
- IR Microspectroscopy, Instrumentations and Applications, *Room C124*
- FTMS for Proteomics, *Room A105*
- Nanotubes and Nanowires for Sensing, *Room B115*
- Raman in Pharma, *Room A106*

THURSDAY MORNING

8:00 AM **PLENARY LECTURE: Lippencott Award, Femtosecond Stimulated Raman Spectroscopy**, Richard A. Mathies, *Ballroom 201,* page 63

9:00 AM **SYMPOSIA AND POSTER SESSIONS**
9:00 – 10:30 Posters, *Exhibit Hall*, page 63
10:30 – 12:30 Symposia, page 65

- Metallomics I, *Room C123*
- Aptamers 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

2:00 PM **SYMPOSIA AND POSTER SESSIONS**
2:00 – 3:30 Posters, *Exhibit Hall*, page 63
3:30 – 5:30 Symposia, page 67

- Metallomics, *Room C123*
- Multiway Analysis and Multiway Method Development, *Room B114*
- IR Microspectroscopy Imaging, *Room C124*
- MS Front-End Devices and New Methodology for Proteomics, *Room A105*
- Nanotubes and Nanowires for Sensing, *Room B115*
- Emerging Technologies for Process Analysis, *Room B116*
- Raman Spectroscopy in Art and Archaeology, *Room A106*

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 Applicationsof 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

EDUCATION, *Room B113*

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

TECHNICAL PROGRAM OVERVIEW BY TOPIC

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

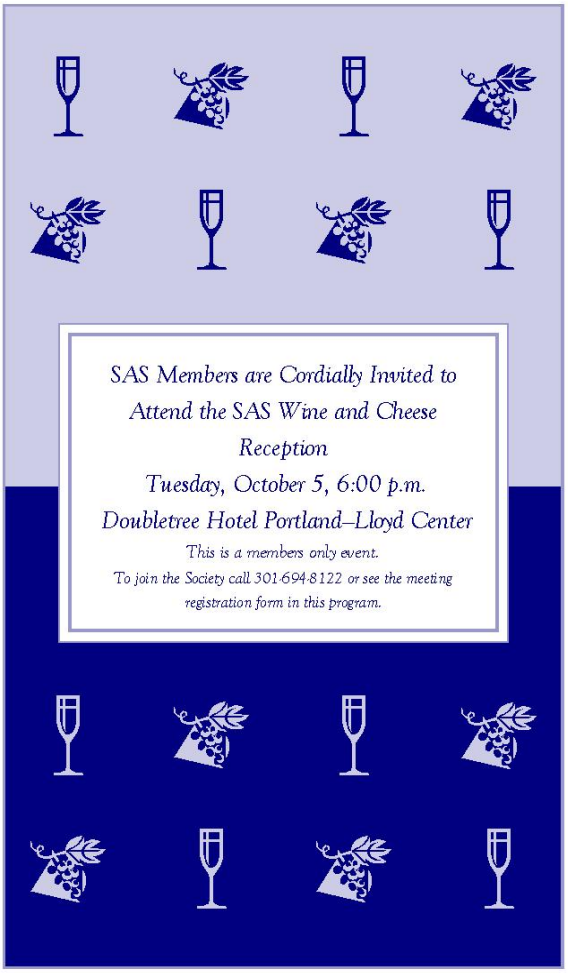
Tuesday PM
- Novel Vibrational Techniques for Biology: In Recognition of Richard Mathies, 2004 Lippencott Awardee

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 Lockerman[1], Cindy Condreay[1]; [1]*CEM Corporation*

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

(5) **Characterization of Tertiary Aerosols in ICP-AES**; Jerry Dulude[1], Robert Brezni[2], Salar Samii[3], Jonathan Levine[3], Kaveh Kahen[3], Akbar Montaser[3]; [1]Glass Expansion, Inc., Pocasset, MA; [2]Glass Expansion, Pty, Ltd., Melbourne, A; [3]George Washington University

(6) **Analysis of Various Difficult Sample Matrices Using High Resolution ICP-OES**; Geoff Tyler[1], Agnès Cosnier[1], Sébastien Velasquez[1]; [1]Jobin Yvon SAS

(7) **Fraunhofer Effect: Tungsten Coil Atomic Absorption Spectrometry**; Jennifer A. Rust[1], Joaquim A. Nobrega[3], Clifton P. Calloway, Jr.[2], Bradley T. Jones[1]; [1]Wake Forest University; [2]Winthrop University; [3]Universidade Federal de Sao Carlos

(8) **ETV-ICP-TOFMS: An Ideal Coupling of Sample Introduction and Detection?**; Gulay Ertas[1], James A. Holcombe[1]; [1]Department 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 Chapon[1], Philippe Hunault[2], Celia Olivero-Tauziede[1]; [1]Jobin Yvon SAS; [2]Jobin Yvon Inc

(10) **An Improved Model for Aerosol Desolvation in Inductively Coupled Plasmas**; Daniel Mittelberger[1], Kaveh Kahen[1], Deborah Levin[2], Akbar Montaser[1]; [1]The George Washington University; [2]Pennsylvania State University

(11) **An Improved Liquid Sample Introduction Method for Chemical Reaction Interface Mass Spectrometry**; Kaveh Jorabchi[1], Kaveh Kahen[1], Paolo Lecchi[2], Akbar Montaser[1]; [1]Department of Chemistry, George Washington University; [2]Department 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 Jr[2], Samuel deSouza[1], Francisco Krug[3]; [1]UFSCAR; [2]Faculdade de Medicina - USP Ribeirao Pre; [3]CENA-USP

(13) **New Ways to Improve the Power of Detection in Flame Atomic Absorption Spectrometry**; Harald Berndt[1], Erika Pulvermacher[1]; [1]ISAS -Institute for Analytical Sciences

(14) **A New Pneumatic Nebulizer for ICP Spectroscopy**; Hsiaoming Tan;

(15) **Performance of an Inert Self-aspirating Micro flow Nebulizer**; Jerry Dulude[1], Bobby Brezni[1], Salar Samii[2], Jonathan Levine[2], Kaveh Kahen[2], Akbar Montaser[2]; [1]Glass Expansion; [2]George Washington University

(16) **Development and Evaluation of a New Direct Injection Multi-gas ICP Source**; Akitoshi Okino[1], Hidekazu Miyahara[1], Yoichi Mizusawa[1], Takayuki Doi[1], Goro Ohba[1], Masato Watanabe[1], Eiki Hotta[1]; [1]Tokyo Institute of Technology

Laser Ablation

(17) **Preliminary Study of Hydrogen Emission Characteristics on Solid samples Using Laser-Ablation Technique**; Koo Hendrik Kurniawan[1], Tjung Jie Lie[1], Nasrullah Idris[2], Kiichiro Kagawa[3], Tadashi Maruyama[4]; [1]Research Center of Maju Makmur Mandiri Foundation; [2]Department of Fiber Amenity; [3]Department of Physics, Faculty of Education; [4]The 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 Gaumet[1], Jérémie Castello[1], Jean François Muller[1], Gérard Friour[2], Olivier Poncelet[2], Jean Guilment[2]; [1]Laboratoire de Spectrométrie de Masse et de Chimie; [2]Kodak Research Labs, CRT 60-3, Z.I. Nord

(19) **Use of Sol-Gels as Solid Matrices for Trace Analysis by UV Laser Ablation and Laser-Enhanced Ionization Detection**; Mathieu Viger[1], Jean-François Y. Gravel[1], Denis Boudreau[1]; [1]Laval University

(20) **Potentialities of Laser Ablation and Laser Desorption Mass Spectrometry to Characterized Organic and Inorganic Environmental Pollutants on Dust Particles**; Frederic Aubriet[1], Vincent Carre;[1], Paul T. Scheepers[2], Jean-Francois Muller[1]; [1]University of Metz; [2]University of Nijmegen

(21) **Application of a New Dual Mode Sample Introduction System for Routine LA-ICP-MS Analyses**; Martin Nash[1], Phil Shaw[1], Bill Spence[1], Simon Nelms[1], [1]Thermo Electron Corp., Ion Path, Road 3, Winsford

(22) **Studies on Vaporization Characteristics in a Graphite Furnace Electrothermal Vaporizer Sample Introduction System for Plasma Source Spectrometry**; Greet de Loos[1], Tibor Kantor[2], Salvador Maestre[3]; [1]Delft University of Technology; [2]Eotvos University Budapest; [3]University of Alicante

(23) **Aerosol Phase Digestion in Atomic Spectrometry**; Lori Allen[1], Joseph Topczewski[1]; [1]University of Wisconsin - Parkside

(24) **Internal Standardization for Lead Determination in Coal Samples by LA-LEI**; Jean-François Y. Gravel[1], Mathieu L. Viger[1], Philippe Nobert[1], Denis Boudreau[1]; [1]Chemistry Department, Université Laval

(25) **Investigation of Vapor Generation Methods for the Determination of Cadmium**; Neil Fitzgerald[1], Ryan Bendl[1], Eric Ritschdorff[1]; [1]Marist College

(26) **Study on Applications of dc Voltage Modulation Technique for a Thin Film Analysis**; Hyunkook Park[1], Kazuaki Wagatsuma[1]; [1]Institute for Materials Research

(27) **Determination of Particulate Matter and Particle Size Effects in a Sol-gel Matrix by Radio Frequency Glow Discharge Optical Emission Spectrometry**; Tim M. Brewer[1], W. Clay Davis[2], Julia Cooper[1], Wandee Luesaiwong[1], Bryan Spraul[1], R. Kenneth Marcus[1]; [1]Clemson University; [2]NIST Hollings Marine Laboratory

(28) **Gas Phase Reactions From UV Laser Ablation of the Ca4GdO(BO3)3 Ceramic Target Studied by Mass Spectrometry.**; Eric Millon[1], Rachel Chety-Gimondo[1], Frederic Aubriet[1]; [1]LSMCL, Institut de Physique et Chimie, University of Metz

(29) **Laser Ablation Inductively Coupled Plasma – Mass Spectrometry: Dependence of Particle Size and Laser Pulse Width**; Richard Russo[1], Jhanis González[1], Chunyi Liu[1], Samuel Mao[1], Xianglei Mao[1]; [1]Lawrence Berkeley National Laboratory

(30) **Influence of Particle Size on Laser Ablation Inductively Coupled Plasma – Mass Spectrometry**; Chunyi Liu[1], Samuel Mao[1], Sy-Bor Wen[1], Jhanis González[1], Xianglei Mao[1], Richard Russo[1]; [1]Lawrence Berkeley National Laboratory

(31) **Solids Sampling Using Double-Pulse Laser Ablation Inductively Coupled Plasma Mass Spectrometry**; Jhanis González[1], Chunyi Liu[1], Jong Yoo[1], Xianglei Mao[1], Richard Russo[1]; [1]Lawrence Berkeley National Laboratory

(32) **Alternative Uses for Geological Data Reduction Software: Simplifying Isolation of Changing LA-ICP-MS Data Sets Within a Heterogeneous Sample Matrix**; Lawrence Neufeld; [1]New Wave Research, Inc.

(33) **High Sensitivity ICP-MS for Advanced Laser Ablation Performance**; Michael Plantz[1], Michelle Cree[1], Steve Wall[1]; [1]Varian Inc.

(34) **Sample Preparation and Analysis of Toxic Metals in Consumer and Industrial Products**; Jean-Pierre Zajac[1], George Feilders[1], Ranjan Roy[1]; [1]SCP SCIENCE

(35) **Investigation of Cold-Vapor Atomic Spectrometry for Mercury by UV Photoreduction**; Ryan Bendl[1], Neil Fitzgerald[1]; [1]Marist College

(36) **Tungsten Coil Electrothermal Vaporization in Inductively Coupled Plasma Atomic Emission Spectrometry**; Amanda Davis[1], Bradley Jones[1]; [1]Wake Forest University

(37) **Spectral, Spatial and Temporal Characteristics of a Millisecond Pulsed Glow Discharge: Electron Density and Temperature**; Jennifer Robertson[1], Na Zhang[1], Megan DeJesus[1], Vishal Vaghela[1], Lei Li[1], Amy Keesee[2], Earl Scime[2], Fred King[1]; [1]West Virginia University, C. Eugene Bennett Department; [2]West Virginia University

Analytical Methods to Characterize the Nervous System

(38) **Chemotherapy Drug Analyzer: Fast Chemical Analysis by Surface Enhanced Raman Spectroscopy**; Alan Gift[1], Chetan Shende[1], Frank Inscore[1], Paul Maksymiuk[1], Stuart Farquharson[1]; [1]Real-time Analyzers

(39) **Identifying bacterial spores and as hoax materials by Raman Spectroscopy**; Stuart Farquharson[1], Wayne Smith[1]; [1]Real-time Analyzers

2D Correlation Spectroscopy

(41) **Two-Dimensional, High Resolution Shear Measurements from Temperature Sensitive Paint and Imaging Polarimetry**; Fletcher Kimura[1], Werner Kaminsky[1], Gamal Khalil[1], James Callis[1]; [1]University of Washington

(42) **Application of 2D Correlation Spectroscopy for the Characterization of Wood**; Nicole Labbé[1], Nicolas André[1], Timothy G. Rials[1], Stephen S. Kelley[2]; [1]Forest Products Center, University of Tennessee; [2]National Renewable Energy Laboratory

Detection of Weapons of Mass Destruction

(43) **Analysis of Bacilli Spores in Nasal Swabs by Surface-enhanced Raman Spectroscopy**; Stuart Farquharson[1], Alan Gift[1], Frank Inscore[1]; [1]Real-time Analyzers

(44) **An Improved Ionization Probe for Detecting Explosives Residues By Surface Laser Photofradmentation-Fragment Detection Spectroscopy at Ambient Conditions**; Rosario Sausa, Jerry Cabalo; [1]US Army Research Laboratory

(45) **Improving the Detection of Explosive Compounds Before and After Detonation**; Jeannette Perr[1], José R. Almirall[1], Kenneth G. Furton[1]; [1]Florida International University

Near IR

(46) **Application of near-infrared sepctroscopy for determining linen content in linen/cotton blend fabrics**; Miryeong Sohn[1], David Himmelsbach[1], Danny Akin[1], Franklin Barton, II[1]; [1]USDA-ARS

(47) **Near-IR Spectroscopic and Kinetic Studies of Simple Alkyl Peroxy Radicals Using CW-Cavity Ring-Down**; Dean Atkinson[1], Jason Farmer[1]; [1]Portland State University - Chemistry Department

(48) **Time-Resolved NIR Spectroscopy for Quantitative Analysis of Intact Pharmaceutical Tablets.**; Christoffer Abrahamsson[1], Jonas Johansson[2], Stefan Andersson-Engels[1], Sune Svanberg[1], Staffan Folestad[2]; [1]Department of Physics, Lund Institute of Technolog; [2]AstraZeneca R&D Mölndal, SE-431 83 Mölnd

(49) **Time-Resolved NIR Spectroscopy for Analysis of Solid Pharmaceuticals**; Jonas Johansson[1], Staffan Folestad[1], Mats Josefson[1], Christoffer Abrahamsson[2], Stefan Andersson-Engels[2], Sune Svanberg[2]; [1]AstraZeneca R&D Molndal, Sweden; [2]Div. of Atomic Physics, Lund Institute

(49a) **Photothermal Lens Spectrometry In SubNanoliter Sample Cells**; Stephen Bialkowski; [1]Utah State University

(50) **Seamless Calibration Transfer with Process Near-Infrared Spectrometers**; Katherine Bakeev[1], Robert Mattes[1], Tim Kelly[1]; [1]FOSS NIRSystems

(51) **Surface Plasmon Resonance-Near-Infrared Spectroscopy for Quantitative Analysis**; Akifumi Ikehata[1], Tamitake Itoh[1], Yukihiro Ozaki[1]; [1]Kwansei-Gakuin University

(52) **Classification of Gender and Maturity Status in Chinook salmon by Short Wavelength Near Infrared spectroscopy**; Calvin Davis[1], Heather Peters[1], Anna Cavinato[1], Timothy Hoffnagle[2]; [1]Eastern Oregon University; [2]Oregon Department of Fish and Wildlife

(53) **Near-IR Vibrational Circular Dichroism in Polypeptides, Proteins, Pharmaceuticals and Terpenes**; Teresa B. Freedman[1], Taiping Zhao[1], Shengli Ma[1], Changning Guo[1], Xiaolin Cao[1], Laurence A. Nafie[1]; [1]Department of Chemistry, Syracuse University, Syra

(54) **Surface Pressure Measurement Using Singlet Oxygen Emission**; Alvin Chang, Gamal Khalil, Martin Gouterman; [1]University of Washington

(55) **Monitoring the Epimerization of 2,2-Dimethyl-1,3-Dioxolane-4-Methanol Using Near-Infrared Vibrational Circular Dichroism Spectroscopy**; Laurence A. Nafie[1,3], Changning Guo[1], Rekha D. Shah[2], John Mills[2], Rina K. Dukor[3], Xiaolin Cao[1], Teresa B. Freedman[1]; [1]Department of Chemistry, Syracuse University, Syra; [2]Johnson & Johnson Pharmaceutical Researc; [3]BioTools Inc.

(56) **Monitoring Wood-Filled Polyolefin Composite Properties By Near Infrared Spectroscopy**; Timothy G. Rials[1], Stephen S. Kelley[1,2], Nicole Labbé[1], Douglas J. Gadrner[3]; [1]Forest Products Center; [2]National Renewable Energy Laboratory; [3]Advanced Engineering Wood Composites Center

(57) **Wood Load Prediction by Near Infrared (NIR) Spectroscopy**; Nicolas André[1], Nicole Labbé[1], Timothy G. Rials[1], Stephen S. Kelley[1,2]; [1]Tennessee Forest Products Center; [2]National Renewable Energy Laboratory

(58) **Filter Infrared Spectroscopy for Coating and Cleanliness Measurement**; Paul Shelley[1], Martin Szczesniak[2]; [1]Boeing; [2]Surface Optics Corp

(59) **Evolution in NIST Reference Materials for Molecular Spectrometry**; Steven Choquette[1], John Travis[1], Melody Smith[1], Paul DeRose[1]; [1]National Institute of Standards and Technology

(60) **Optically Reflective Thin Layer Electrode for Infrared Micro-Spectroelectrochemical Measurements**; D. L. Perkins[1], M. V. Schiza[1], P. G. Miney[1], M. L. Myrick[1]; [1]Dept. of Chemistry and Biochemistry, Univesity of South Carolina

(61) **The Variable Filter Array Spectrometer - A New Concept in Mid-IR Spectral Analysis**; Sandra Rintoul[1], Paul Wilks[1], [1]Wilks Enterprise, Inc.

(62) **Towards the Characterization Biological Toxins using Field-Based FT-IR Spectroscopic Instrumentation**; David Schiering[1], Robert Walton[2], Chris Brown[3], Joseph Brewer[4], James Scott[4], Mark Norman[1]; [1]SensIR Technologies; [2]United States Air Force AFIOH; [3]University of Rhode Island; [4]Southwest Research Institute

(63) **Computer Assisted Structure Verification and Interpretation of Infrared and Raman Spectra**; Michael Boruta[1], Michel Hachey[1], Antony Williams[1]; [1]Advanced Chemistry Development, Inc.

(64) **Infrared and Raman Spectroscopy - How to Capture and Retain the Knowledge We Acquire**; Michael Boruta[1], Michel Hachey[1], Antony Williams[1]; [1]Advanced Chemistry Development, Inc.

(65) **On-line Determination of Water in Dried Salted Cod - From Feasibility Study to Prototype**; Jens Petter Wold[1], Vegard Segtnan[1], Erik Wold[2], Ib-Rune Johansen[3], Karl Henrik Haugholt[2], Jon Tschudi[2], Alain Ferber[2]; [1]Matforsk - Norwegian Food Research Institute; [2]Sintef ICT, Norway; [3]Tomra, Norway

(66) **Reagent-free Infrared Clinical Chemistry and Diagnostics: Enhanced Sensitivity via Microfluidic Sample Preconditioning of Blood and Urine**; R. Anthony Shaw[1], Angela Man[1], Sarah Low-Ying[1], Colin Mansfield[1]; [1]Institute for Biodiagnostics, National Research Council

(67) **Quantitative Clinical Analytical Infrared Spectroscopy: Improved Preparation Technique for Film Creation and its Application to Microfluidic Preconditioned Samples**; Angela Man[1], R. Anthony Shaw[1], Sarah Low-Ying[1], Colin Mansfield[1]; [1]Institute for Biodiagnostics, National Research Council

(68) **Real Time Mid-Infrared Monitoring of Protecting Groups in Synthesis**; Robert Brush[1], Francis Van der Eycken[1]; [1]METTLER TOLEDO AutoChem

TOF MS for Proteomics

(69) **Extending Atmospheric Pressure MALDI: Liquid Matrices and Secondary Ionization Techniques**; Kevin Turney[1], W. W. Harrison[1]; [1]University of Florida

Process Analytical Technologies in Pharma

(70) **Analyisis of Chiral Pharmaceuticals using HPLCwith CD Detection**; Amanda Jenkins[1], William Hedgepeth[1]; [1]Jasco Inc.

(71) **Second Generation Humidity and Temperature Control for Spectroscopy**; Helen Jervis; [1]Surface Measurement Systems Ltd.

(72) **The Use of a Large-Spot Probe for Accurate Quantification of a Degradant in an Intact Tablet by Raman Spectroscopy**; Mark Kemper[1], David Strachan[1], Ian Lewis[1], Robbe Lyon[2], Ajaz Hussain[2], Patrick Faustino[2], Christopher Ellison[2], Everett Jefferson[2]; [1]Kaiser Optical Systems; [2]USFDA

(73) **FDA PAT Guidance 2003 Feedback and Final PAT Guidance 2004**; James Rydzak[1]; [1]GlaxoSmithKline

(74) **A Pragmatic Tool for Process Analytics**; Kenneth Fredeen[1], David Schiering[1], John Corbett[1], Mark Norman[1], John Seelenbinder[1]; [1]Smiths Detection, Inc.

Miniature Spectroscopic Sensors

(75) **Key Design Considerations for a Low Cost Quality Control Raman Spectrometer**; Mike Fuller[1]; [1]Digilab LLC

(76) **A New Compact, High-Performance, Scattered Circular Polarization Raman Optical Activity Spectrometer**; Laurence A. Nafie[1,2], Rina K. Dukor[2], Laurence D. Barron[3], Lutz Hecht[3], Gilbert Hangartner[4], Werner Hug[4]; [1]Department of Chemistry, 1-014 CST, Syracuse University; [2]BioTools, Inc. 950 N. Rand Road, Unit 12; [3]Chemistry Department, Glasgow University; [4]Institute of Physical Chemistry

(77) **Miniature Instruments Based on Multivariate Optical Computing**; Michael Myrick[1], Luisa Profeta[1], Ryan Priore[1], Maria Schiza[1], Michael Simcock[1], [1]University of South Carolina

(78) **A Miniaturized Analyzer Design for Process and Handheld Chemical Composition Measurements**; Thomas Hagler[1]; [1]Advanced Photometrics Inc

Biological Applications of Nanoparticles for Surface Enhanced Raman Scattering

(79) **Conductive Inks for Sensors: High Conductivity through Particle Alignment**; Alexander Scheeline[1], April Schricker[1,2], Ewa Kirkor[1]; [1]University of Illinois at Urbana-Champaign Departm; [2]University of Texas at Austin

(80) **Surface Plasmon Resonance Sensor by Evanscenct Wave Cavity Ring-Down Spectroscopy**; Hsiu-Fang Fan[1], King-Chuen Lin[1]; [1]National Taiwan University

(81) **Dispersion and Stability Studies of Gold Nanoparticles in Organic Solvents**; Jeffrey M. McMahon[1] Steven R. Emory[1]; [1]Western Washington University

(82) **Spatially Resolved Depth Profiling Analysis of Single Small Polymeric Particles by Confocal Raman Microscopy**; Travis Bridges[1], Joel Harris[1]; [1]University of Utah (83) **Variations and Changes of Photoinduced Luminesence Bands of Surface-Enhanced Resonance Raman Active Single Ag Nano-aggregates**; Tamitake Itoh[1], Kazuhiro Hashimoto[1], Yasuo Kikkawa[1], Akifumi Ikehata[1], Yukihiro Ozaki[1]; [1]Kwansei-Gakuin University

Data Analysis and Raman Spectra

(85) **Rapid pesticide residue analysis on imported fruits by SERS**; Chetan Shende[1], Frank Inscore[1], Alan Gift[1], Paul Maksymiuk[1], Stuart Farquharson[1]; [1]Real-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 Olesik[1]; [1]Ohio State University

10:50 (87) **Spatial Mapping of Droplet Velocity and Size for Direct and Indirect Nebulization in Plasma Spectrometry**; Kaveh Kahen[1], Kaveh Jorabchi[1], Callum Gray[1], Akbar Montaser[1]; [1]The George Washington University, Department of Chemistry

11:10 (88) **In-situ Visualization and Characterization of Aerosol Droplets in an Inductively Coupled Plasma**; Kaveh Jorabchi[1], Kaveh Kahen[1], Callum Gray[1], Akbar Montaser[1]; [1]George Washington University

11:30 (89) **A New Pneumatic Nebulizer for Sample Introduction in ICP Spectrometry - Miniaturized Pneumatic Extension Nozzle**; Harald Berndt[1], Sascher Groom[2], Gerhard Schaldach[2], Peter Walzel[2]; [1]ISAS - Institute for Analytical Sciences; [2]University of Dortmund - Chair of Mechan

11:50 (90) **Tunable Direct Injection High Efficiency Nebulizer for Inductively Coupled Plasma Mass Spectrometry**; Cristina Nechita[1], Kaveh Kahen[1], Craig Westphal[1], William Rutkowski[1], Akbar Montaser[1]; [1]George Washington University, Department of Chemistry

12:10 (91) **Application of Micronebulization in Inductively Coupled Plasma Mass Spectrometry and Laser Ablation ICP-MS**; J. Sabine Becker[1], D. Schaumloeffel[2], M. V. Zoriy[1], P. Giusti[2], C. Pickhardt[1], R. Lobinski[2]; [1]Central Division of Analytical Chemistry, Research; [2]Group of Bio-Inorganic Analytical Chemistry

Monday Morning, Ballroom 201
ANALYTICAL METHODS TO CHARACTERIZE THE NERVOUS SYSTEM
Organizer and Presider: Scott Shippy

10:30 (92) **Characterizing Brain Chemistry with Electrochemical Techniques**; Adrian Michael[1]; [1]University of Pittsburgh

11:10 (93) **Neuropeptidomic Analysis of a Small Nervous System Using Multidimensional MS-Based Approaches**; Lingjun Li[1], Kimberly Kutz[1], Joshua Schmidt[1], Yun Wang[1], Qiang Fu[1]; [1]University of Wisconsin-Madison

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

12:10 (95) **Sensitive Neurotransmitter Monitoring Using Biosensors**; Weihong Tan[1]; [1]University of Florida

12:30 (96) **Monitoring D-Serine in the Rat Striatum Using Online Microdialysis Capillary Electrophoresis**; Michael Bowser[1], Chanda Ciriacks[1]; [1]University of Minnesota

Monday Morning, Room B114
2D CORRELATION SPECTROSCOPY
Organizers and Presiders: Wei Zhao and Isao Noda

10:30 (97) **Two-Dimension Infrared (2D IR) Correlation Spectroscopy Study of Biodegradable Polymers**; Isao Noda[1], Tony Dowrey[1], Curt Marcott[1], Mike Satkowski[1]; [1]Procter & Gamble Co.

10:50 (98) **Two-Dimensional Infrared Correlation Spectroscopy Study of Crystallization Dynamics of Poly(L-lactic acid) during Cold-Crystallization**; Yukihiro Ozaki[1], Jianming Zhang[1], Hideto Tsuji[2], Isao Noda[3]; [1]Kwansei Gakuin University; [2]Toyohashi University of Technology; [3]The Procter & Gamble Company

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

11:30 (100) **2D-IR Correlation and Principal Component Analysis of Ice Melting**; Hugh Richardson[1], K. Dendramis[1], Martin Kordesch[1]; [1]Ohio University

11:50 (101) **Introduction of New Correlation Indices Independent of the Band Shifting Phenomena in Generalized Two-Dimensional Correlation Infrared Spectroscopy**; Shin-ichi Morita[1], Yasuhiro F. Miura[1], Michio Sugi[1], Yukihiro Ozaki[2]; [1]Faculty of Engineering, Toin University of Yokoham; [2]School of Science and Technology, Kwanse

12:10 (102) **Infrared Study of the Solvation of Amino Acids**; Feng Gai[1]; [1]University of Pennsylvania

Monday Morning, Room B113
DETECTION OF WEAPONS OF MASS DESTRUCTION
Organizer and Presider: Greg Klunder

10:30 (103) **Investigating the Affinities and Persistence of VX Nerve Agent**; Adam Love[1], Andy Vance[1], John Reynold[1], Lee Davisson[1]; [1]LLNL

10:50 (104) **New Method for Attachment of Biomolecules to Porous Silicon: Platform for enzyme-Based Chemical Warfare Agent Detection**; John G. Reynolds[1], Sonia E. Letánt[1], Bradley R. Hart[1], Staci R. Kane[1], Sharon J. Shields[1], Masood Z. Hadi[2], Tu-Chen Cheng[3], Vipin K. Rastogi[3]; [1]Lawrence Livermore National Laboratory; [2]Sandia National Laboratory; [3]U. S. Army Edgewood

11:10 (105) **A Transportable, High Resolution FT Mass Spectrometer for Analysis of Chemical Warfare Agent Surrogates, Corrosive Materials, and Incendiary Materials**; Dean Davis[1], Kenneth Gallaher[1], Wayne Rimkus[1]; [1]Siemens Applied Automation

11:30 (106) **Chemical Incident Forensic Response System**; James Crabtree[1], Samuel Reighley[2], Leonard Buettner[3]; [1]Agilent Technologies, Inc.; [2]South Carolina Law Enforcement Division; [3]US Army, RDECOM, ECBC

11:50 (107) **Detection of Chemical Weapons using an ES/SIMS Ion Trap Mass Spectrometer**; Anthony Appelhans[1], Gary Groenewold[1], John Williams[2], Mark Jeffery[2]; [1]Idaho National Engineering and Environmental Labor; [2]West 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 Harper[1], Stefan Rose[2], Jose Almirall[1], Kenneth Furton[1]; [1]International Forensic Research Institute; [2]University Medical and Forensic Consulting

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

10:30 (109) **NIR Characterization of Gun Propellant**; Lewis Kansas[1], Erin hardmeyer[1], Susan Gorine[2], Thomas DeAngelis[1]; [1]Geo-Centers, Inc.; [2]U.S. Army ARDEC

10:50 (110) **Embedding Covert Aniticounterfeit Spectral Features into Pharmaceutical Formulations to authenticate pharmaceutical products**; James Polli[1], Stephen Hoag[1]; [1]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 Sowa[1], Jeri Payette[1], Elicia Kohlenberg[1], Arone Pabbies[2], Paul Kerr[2], Kan-Zhi Liu[1], Angela Man[1], Lorenzo Leonardi[1]; [1]Institute for Biodiagnostics, National Research Co; [2]Department of Otolaryngology, University of Manitoba

11:30 (112) **Maintaining Near-IR Calibration Models in Unstable Media**; Cliona M. Fleming[1], Christopher D. Brown[1], Stephen J. VanSlyke[1]; [1]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 Watari[1,2], Yukihiro Ozaki[2]; [1]Yokogawa Electric Corporation; [2]Kwansei-Gakuin University

12:10 (114) **NIR and Multivariate Statistics for Determination of DVD Adhesive Composition**; Randy Bishop[1]; [1]GE Advanced Materials

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

10:30 (115) **Understanding Protein Structure using Stepwise Fragmentation on a MALDI QIT TOF MS**; Rachel Martin[1], Shaun Bilsborough[1], Kathryn Jackson[1], Matt Openshaw[1]; [1]Shimadzu Biotech

10:50 (116) **A New Paradigm for Proteomics: Combining MALDI Imaging-MS and Ion Mobility-MS/MS**; David H. Russell[1]; [1]Laboratory for Biological Mass Spectrometry

11:10 (117) **High Sequence Coverage of 2-D Liquid Separated Proteins Using CE-QIT-TOF**; David Lubman[1], Kan Zhu[1], Chul Yoo[1]; [1]The University of Michgan

11:30 (118) **Measurement of Peptide Dissociation Kinetics in Surface-induced Dissociation TOF Experiments**; Vicki H. Wysocki[1], Chaminda M. Gamage[1], Xiujuan Wen[1]; [1]University of Arizona

11:50 (119) **The Search for Serum Biomarkers – Comparison of Multiple Proteomic Approaches**; Jennifer Van Eyk[1], Qin Fu[1], Rebecah Gundrey[2], Simon Sheng[1], Robert Cotter[2]; [1]Dept. Medicine, Johns Hopkins University; [2]Dept Pharmacology, Johns Hopkins University

12:10 (120) **(Off-line HPLC)/MALDI/QqTOF Measurements on Proteins and Peptides**; Kenneth Standing[1], Oleg Krokhin[1], Werner Ens[1]; [1]University of Manitoba

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

10:30 (121) **Single-Walled Carbon Nanotubes Under the Influence of Dynamic Coordination and Supramolecular Chemistry**; J Fraser Stoddart[1], Kelly S Chichak[1], Robert J A Ramirez[1], Alexander Star[2]; [1]CNSI/UCLA; [2]Nanomix Inc.

10:50 (122) **Studies of SWNT Bangap Emission Quenching**; Stephen Doorn[1], Michael O\'Connell[1], Ezra Eibergen[1]; [1]Los Alamos Nationa Laboratory

11:10 (123) **Manipulating Carbon Nanotubes with Nucleic Acids**; Ming Zheng[1], [1]DuPont CR&D

11:30 (124) **Electric Field Separation and Directed Assembly of Functionalized SWNTs and Other Nanowires**; Pehr Pehrsson[1], Lars Ericson[1]; [1]Naval Research Laboratory

11:50 (125) **Using Chemical Functionalization to Control the Electrophoretic Mobility of Single Walled Carbon Nanotubes**; Michael Strano[1], Seunghyun Baik[1], Monica Usrey[1], Lolita Rotkin[2]; [1]Department of Chemical and Biomolecular Enginee; [2]Beckman Institute, University of Illinois

12:10 (126) **Selective Metallic Tube Reactivity in the Solution-Phase Osmylation of Single-walled Carbon Nanotubes**; Stanislaus Wong[1,2]; [1]State University of New York at Stony Brook; [2]Brookhaven National Laboratory

TECHNICAL PROGRAM – MONDAY
Orals 10:30 AM – 12:30 PM and 3:30 – 5:30 PM

Monday Morning, Room B116
PROCESS ANALYTICAL TECHNOLOGIES IN PHARMA
Organizer and Presider: James Rydzak

10:30 (127) **Process Analytical Technology for Pharmaceutical Unit Operations**; Andrew Lange[1]; [1]Pfizer Global Research

10:50 (128) **A Novel Approach to Determining Particle Size Distributions of Pharmaceutical Powders by NIR**; Chun Cai[1], David Radspinner[1]; [1]Aventis Pharmaceuticals

11:10 (129) **Monitor Pharmaceutical Drying Processes in Fluid Bed Dryer by Using Infrared and Near Infrared Spectroscopies.**; Chi-Shi Chen[1], Martin Warman[1], Joep Timmermans[1]; [1]Pfizer Inc.

11:30 (130) **Raman and ATR-FTIR Spectroscopic Monitoring of the Polymorphic Transformations of Acetaminophen**; Kris Berglund[1,2], Lili Feng[2]; [1]Luleå University of Technology; [2]Michigan State University

1150 (131) **Application of Mid-IR Spectroscopy for Pharmaceutical Process Monitoring**; Mike Claybourn[1]; [1]AstraZeneca

12:10 (132) **The Use of Chemometrics To Understand Chemistry;** Duncan Thompson[1]; [1]GlaxoSmithKline

Monday Morning, Room A106
BIOLOGICAL APPLICATIONS OF NANOPARTICLES FOR SURFACE ENHANCED RAMAN SCATTERING
Organizers and Presiders: Michael Natan and Griff Freeman

10:30 (133) **Biological Applications of Single-Molecule Surface-Enhanced Raman Spectroscopy**; Steven Emory[1], Teresa Wenda[1], Haley Pugsley[1], Rebecca Jensen[1], Rebecca Newhouse[1]; [1]Western Washington University

10:50 (134) **Design of Surface Enhanced Raman Tags for Low Level Biolyte Detection**; Marc D. Porter[1], Robert J. Lipert[1], Hye-Young Park[1], Jeremy Driskell[1], Jill Uhlenkamp[1], Betsy Jean Yakes[1]; [1]Iowa State University

11:10 (135) **Nanoparticle SERS Beacons**; Griff Freeman[1], William Doering[1], Michael Natan[1], Michael Sha[1], Sharron Penn[1]; [1]Nanoplex Technologies, Inc.

11:30 (136) **Detection and Identification of Bacteria Using Surface Enhanced Raman Spectroscopy.**; Ranjith Premasiri[1], Gilford Jones[2], Larry Zeigler[2]; [1]Photonics Center, Boston University; [2]Deparment of Chemistry, Boston University

11:50 (137) **Rapid Detection of Chemical Warfare Agent Hydrolysis Products by Surface-Enhanced Raman Spectroscopy**; Frank Inscore[1], Alan Gift[1], Stuart Farquharson[1]; [1]Real-Time Analyzers

12:10 (138) **Metal Nanostructures for Surface-enhanced Raman Spectroscopy**; Rebecca A. Jensen[1], Rebecca Newhouse[1], Haley R. Pugsley[1], Steven R. Emory[1], [1]Western Washington University

MONDAY POSTER SESSIONS and BREAK
2:00 – 3:30 PM, See pages 40-43
Exhibit Hall A

Monday Afternoon, Room C123
LASER ABLATION
Organizer and Presider: Greg Klunder

3:30 (139) **Femtosecond Laser Ablation Mass Spectrometry**; Roland Hergenroeder[1], Vanja Margetic[1], Joachim Koch[1], Ota Samek[1], Kay Niemax[1]; [1]ISAS-Institute for Analytical Scienes

3:50 (140) **UV-Femtosecond and Nanosecond Laser Ablation-ICP-MS: Repeatability and Reproducibility During the Ablation of Transparent Materials**; Jhanis González[1], Siv Dundas[1], Chunyi Liu[1], Samuel Mao[1], Xianglei Mao[1], Richard Russo[1]; [1]Lawrence Berkeley National Laboratory

4:10 (141) **Resonant Laser Ablation of Metals Detected by Atomic Emission in a Microwave Plasma, and By Inductively Coupled Plasma Mass Spectrometry.**; Danielle Cleveland[1], Peter Stchur[1], Xiandeng Dan Hou[1], Karl Xiadong Yang[1], Robert G. Michel[1]; [1]Department of Chemistry, University of Connecticut

4:30 (142) **Laser Ablation Inductively Coupled Plasma Mass Spectrometry of Human Hair**; Kevin Bemben[1], Eric Salin[1]; [1]McGill University

4:50 (143) **Laser Ablation and Ionization Mass Spectrometry for the Chemical Analysis of Glasses**; Greg Klunder[1]; [1]Lawrence Livermore National Laboratory

5:10 (144) **Laser Ablation ICP Optical Spectrometry of Vitreous Waste Surrogates: A New Model for Hazardous Waste QC Analysis**; Lawrence Neufeld[1], Pete Brown[2], Gary Kunselman[2]; [1]New Wave Research, Inc.; [2]Teledyne Leeman Labs

Monday Afternoon, Room B114
2D CORRELATION SPECTROSCOPY
Organizers and Presiders: Wei Zhao and Isao Noda

3:30 (145) **Quantitative 2D IR Correlation Analysis**; Richard Dluhy[1], Saratchandra Shanmukh[1]; [1]University of Georgia

3:50 (146) **2D-Correlation Analysis and Multivariate Chemometric Data Treatment of Time-Resolved Vibrational Spectra**; Heinz W. Siesler[1], Peiyi Wu[2], Markus Fuelleborn[1]; [1]Department of Physical Chemistry, University of Du; [2]Department of Macromolecular Science

4:10 (147) **Two-Dimensional Correlation for Peak Identification in DNA Analysis**; Lei Geng, Gufeng Wang,; [1]University of Iowa;

4:30 (148) **Using Perturbation Domain Decomposition to Reveal System Dynamics andEnhance Cross Peak Discrimination in Two-Dimensional Correlation Spectroscopy**; Andrew Jirasek[1,2], Georg Schulze[1], Michael W. Blades[1,2], Robin F. B. Turner[1,3]; [1]Biotechnology Laboratory, University of British Columbia; [2]Department of Chemistry, University of British Columbia; [3]Department of Electrical and Computer Engineeering

4:50 (149) **Two-Dimensional Correlated Spectroscopic Studies on the Fine Structure of the Fluorescent Bands from Conjugated Organic Compounds**; Yizhuang Xu[1], Wei He[1], Di Miao[1], Jinguang Wu[1]; [1]Department of Chemistry, Peking University, Beijing

5:10 (150) **Probing Sonication-induced Spectral Changes in HiPco Carbon Nanotubes by using 2D Correlation Spectroscopy**; Wei Zhao[1], Brian Benedict[1]; [1]Department of Chemistry, University of Arkansas

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

3:30 (151) **Desorption/Ionisation on Chemically Modified Porous Silicon for the Identification of Small Analyte Molecules relevant in Forensic Investigations.**; Rachel Lowe[1,2], Nico Voelcker[2], Paul Kirkbride[3], Robert Blackledge[4], Nathan Salazar[4], Eden Go[1], Gary Siuzdak[1]; [1]The Scripps Research Institute, Center of Mass Spectrometry; [2]The Flinders University of South Austral; [3]Forensic Science South Australia, 21 Div; [4]Naval Criminal Investigative Service Reg

3:50 (152) **Culture Dependent Variability in Bacillus Spore Protein Composition Observed by Capillary Liquid Chromatography and Mass Spectrometry**; David Wunschel[1], Karen Wahl[1], Jon Wahl[1], Alan Willse[1], Nancy Valentine[1]; [1]Pacific Northwest National Laboratory, Richland WA

4:10 (153) **Simultaneous Screening for Multiple Categories of Drugs of Abuse by LC/MS/MS**; June Feng[1], Yingkun Dai[1], Lanqing Wang[1], John Bernert[1]; [1]Centers for Disease Control and Prevention

4:30 (154) **HPLC-MS and HPLC-FTIR Analysis of Inks for Forensic Purposes**; Roger Jones[1], Anthony Wagner[1], John McClelland[1]; [1]Institute for Physical Research and Technology, Iowa State University

4:50 (155) **Forensic Fiber Dye Analysis by LC-MS**; Michael Sigman[1], Min Huang[1]; [1]University of Central Florida, National Center for Forensic Science

5:10 (156) **A Taxonomy-Based Decision Tree for Microorganism Identification Using Matrix-assisted Laser Desorption/Ionization Mass Spectrometry**; Kristin Jarman[1], Dale Anderson[1], Karen Wahl[1]; [1]Pacific Northwest National Lab

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 Haseth[1], Franklin Barton, II[2], David Himmelsbach[2]; [1]University of Georgia; [2]US Department of Agriculture

3:50 (158) **Applications For a New Series of NIR Spectrometers**; Franklin Barton[1], James de Haseth[2], David Himmelsbach[1]; [1]USDA-ARS Russell Research Center; [2]Deptartment 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 DeVerse[1], Andreas Coppi[1], Frank Geshwind[1], Robert Hammaker[1], Bill Fateley[1], Ronald Coifman[1]; [1]Plain Sight Systems

4:30 (160) **Design Challenges for a Fourier Transform Spectrometer in Non-Invasive Blood Glucose Monitoring**; Ben VerSteeg[1], John Maynard[1], Alan Ross[1], Russell Abbink[1]; [1]InLight Solutions, Inc.

4:50 (161) **Technology Beyond the Laboratory: From Customized Instruments to Low-Cost Spectral Sensors**; John Coates[1], [1]Coates Consulting

5:10 (162) **A High-Resolution, MEMS-based, Miniature NIR Spectrometer**; Richard Crocombe[1], Larry McDermott[1], Matthew Smith[1]; [1]Axsun Technologies

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

3:30 (163) **Single Cell Profiling with Mass Spectrometry for Neuropeptide Discovery**; John Jurchen[1], Stanislav Rubakhin[1], Nathan Hatcher[1], Eric Monroe[1], Jonathan Sweedler[1]; [1]Department of Chemistry, University of Illinois

3:50 (164) **Recent Developments in TOF/TOF**; Jennifer M. Campbell[1], [1]Applied Biosystems

4:10 (165) **A Proteomics Approach to BioAgent Detection**; Robert Cotter[1]; [1]Johns Hopkins University

4:30 (166) **Quantitative Proteomic Analysis of Inorganic Phosphate Treatment of Osteoblast Cells Using a Combined ESI/MALDI-MS/MS Approach**; Li-Rong Yu[1], Kelly A. Conrads[2], David A. Lucas[1], King C. Chan[1], Brian L. Hood[1], Carl F. Schaefer[3], Haleem J. Issaq[1], George R. Beck Jr.[2], Thomas P. Conrads[1], Timothy D. Veenstra[1]; [1]Laboratory of Proteomics and Analytical Technologies; [2]Laboratory of Cancer Prevention, Center; [3]Center for Bioinformatics

4:50 (167) **Aptamer-Enhanced Matrix Assisted Laser Desorption/Ionization for Affinity Mass Spectrometry**; Lawrence Dick Jr.[1], Linda McGown[1]; [1]Duke University

5:10 (168) **Clustering of Counterfeit Antimalarial Tablets using Accurate Mass Measurements in an Orthogonal Time-of-Flight Mass Spectrometer**; Facundo Fernandez[1], Krystyn Alter[1], Leonard Arthur[1], Michael Green[2], Paul Newton[3]; [1]School of Chemistry and Biochemistry, Georgia Institute; [2]Division of Parasitic Diseases, Centers; [3]Centre for Tropical Medicine, Oxford University

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

3:30 (169) **Amine-Assisted Separation of Single Wall Carbon Nanotube by Type**; Fotios Papadimitrakopoulos[1]; [1]University of Connecticut

3:50 (170) **Separation of Semiconducting from Metallic Carbon Nanotubes by Noncovalent Engineering of Carbon Nanotube Surfaces;** Jian Chen[1], Rajagopal Ramasubramaniam[1], Haiying Liu[2]; [1]Zyvex Corporation; [2]Department of Chemistry, Michigan Technology

4:10 (171) **Extinction Coefficients and Purity of Single-Walled Carbon Nanotubes**; Bin Zhao[1], Mikhail E. Itkis[1], Hui Hu[1], Sandip Niyogi[1], Robert C. Haddon[1]; [1]University of California

4:30 (172) **Optical Trapping of Water-Soluble Single-Walled Carbon Nanotubes**; Yuegang Zhang[1]; [1]Intel Corporation

4:50 (173) **Fabrication and Assembly of Single-Walled Carbon Nanotubes by Dielectrophoresis**; Jie Tang[1,2], Guang Yang[2], Huaizhi Geng[2], Jian Zhang[2], Qi Zhang[2], Lu-Chang Qin[2], Otto Zhou[2]; [1]National Institute for Materials Science, Tsukuba; [2]Department of Physics and Astronomy, University of North Carolina at Chapel Hill

5:10 (174) **Load Transfer in Functionalized SWNT/polymer Nanocomposites**; Viktor Hadjiev[1], Dimitris Lagoudas[2], Ramanan Krishnamoorti[1], James Tour[3], Leonard Yowell[4], Sivaram Arepalli[4]; [1]University of Houston; [2]Texas A&M University; [3]Rice University; [4]NASA 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; [1]Department of Chenistry & Biochemistry, The University of South Carolina

3:50 (176) **Compact Spectrometers in Modern Analytical Spectroscopy**; Harry Forsyth[1], [1]Ocean Optics

4:10 (177) **Design of Miniature Spectrometers Based on Light Emitting Diodes**; Kevin Cantrell[1], James D. Ingle[2]; [1]University of Portland; [2]Oregon State University

4:30 (178) **Miniturization of Industrial Photometric Analyzer**; Mike Ponstingl[1]; [1]Custom Sensors & Technology

4:50 (179) **MEMS Technology Moves Process Spectroscopy Into A New Dimension**; Richard Crocombe[1], Larry McDermott[1], Matthew Smith[1]; [1]Axsun Technologies

5:10 (180) **Development of Compact Instrumentation for at Line Metal Analysis**; James Barnes[1], Cris Lewis[1], Ruth Waddell[1], Christian Hassell[1]; [1]Los 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 LaPlant[1], Mario Fabiilli[1], Steve Arrivo[1]; [1]Pfizer, Inc.

3:50 (182) **Raman and Near Infrared Spectroscopic Studies of Compounds Dissolved in Methanol and Water Solvent systems**; Rodolfo Romañach.[1], Zainette Rivera[1], Ciser Cabarcas[1], Maria Guardiola[1], Mark Kemper[2]; [1]University of Puerto Rico - Mayaguez Campus; [2]Kaiser Optical Systems

4:10 (183) **Raman Analysis of Concentrated Salt Solutions Using Robust Modeling and Data Fusion**; Jeremy M. Shaver[1], Samuel A. Bryan[2], Tatiana G. Levitskaia[2], Serguei I Sinkov[2]; [1]Eigenvector Research, Inc.; [2]Pacific Northwest National Laboratory

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

4:50 (185) **Algorithms and Preprocessing Techniques to Automatically Classify Samples in a Microtiter Plate by Raman Spectroscopy**; Steve Lowry[1], Dave Dalrymple[1], Dick Wieboldt[1]; [1]Thermo Electron Corporation

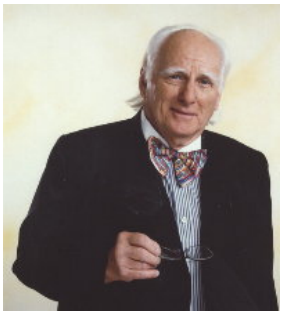
5:10 (186) **Data Reduction Methods in Dynamic Raman Spectroscopy of Tissue Specimens**; Michael D. Morris[1], William F. Finney[1], Nicole Crane[1], Andrew Callender[1]; [1]University of Michigan

5:30 (187) **Challenges of Qualitative Data Analysis in Raman Microspectroscopy of Jigh-throughput Crystallization Wellplates**; CJ Pommier[1], Gary McGeorge[1], Victor Rosso[1], Anne Song[1]; [1]Bristol-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]; [1]University of California, Davis; [2]Agilent 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 Carrabba[1]; [1]Hach 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 Poulin[1], Denis Boudreau[1]; [1]Université Laval

(191) **Utilization of Confinement Effect and Sub-target Effect in Spectrochemical Analysis using TEA CO2 Laser-Induced Plasma**; Kiichiro Kagawa[2], Nasrullah Idris[1], Takao Kobayashi[1], Hendrik Kurniawan[3], Kenichiro Tsuyuki[4], Satoru Miura[4]; [1]Department of Fiber Amenity Engineering, Faculty; [2]Department of Physics, Faculty of Education; [3]Research Center of Maju Makmur Mandiri; [4]Kajima 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 Chen[1], Ewa Dabek-Zlotorzynska[1], Nouri Hassan[2], Monique Lanouette[2], Pat E. Rasmussen[2]; [1]AAQD, Environmental Technology Centre, Environment; [2]Safe Environments Programs, HECS Branch

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

(195) **New Array Detector ICP-OES Design Criteria**; Geoff Tyler[1], Cendrine Dubuisson[1], Emmanuel Fretel[1], Alain Le Marchand[1], Yves Danthez[1], Olivier Rogerieux[1]; [1]Jobin 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 Herreyre[1], Denis Boudreau[1]; [1]Université Laval

(197) **Relationship of Plasma Rotational Frequency and Plasma Temperature in a New Multi-plasma Gas ICP**; Hidekazu Miyahara[1], Takayuki Doi[1], Yoichi Mizusawa[1], Yasushi Hayashi[1], Eiki Hotta[1], Akitoshi Okino[1]; [1]Department of Energy Sciences Tokyo Institute of Technology

(198) **A New Concentric PFA Nebulizer for ICP-MS Spectrometry**; Fred Smith[1], Joe Brady[1]; [1]CETAC Technologies

(199) **Cost Effective Clinical Elemental Analysis: Graphite Furnace AAS or ICP-MS?**; Simon Nelms[1], Phil Shaw[1], Bill Spence[1], Martin Nash[1]; [1]Thermo Electron

(200) **Considerations on the Connection of a Glow Discharge Ion Source to a Fast Scanning Sector Field ICP-MS**; Lothar Rottmann[1], Joachim Hinrichs[1], Wolfgang Schoettger[1], Meike Hamester[1]; [1]Thermo Electron

(201) **Optimizing ETV-ICP(TOF)MS and Mass Transport to the Plasma**; James Holcombe[1], Nikhilesh Desai[1], Gulay Ertas[1], William Balsanek[1]; [1]University of Texas at Austin

(202) **Online Standard Additions Calibration of Transient Signals for Inductively Coupled Plasma Mass Spectrometry**; Eric D. Salin[1], E. Jane Maxwell[1], Margaret Antler[1]; [1]McGill University

(203) **Revisiting Traditional Methods for Determination of Trace Metals in Clinical Samples by Graphite Furnace AAS**; Doug Shrader[1], Christine Rivera[1], Jean-Pierre Lener[1]; [1]Varian Inc.

(204) **Sector Field ICP-MS for the Direct Determination of Semiconductor Relevant Inorganic Contaminants and Matrices**; Meike Hamester[1], Julian Wills[1], Lothar Rottmann[1]; [1]Thermo Electron

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

(206) **Imaging of Ion Densities in the Sampling Cone of an ICP-MS by Planar Laser Induced Fluorescence**; Paul Farnsworth[1], Jeffrey Macedone[1], Andrew Mills[1]; [1]Brigham Young University

(207) **Development of Sampling Geometry for Monitoring Ion Concentrations in RF Plasma Induced Deposition Reactions by Quadrupole Mass Spectrometry**; Jeff Anderson[1], Rene Rodriguez[1]; [1]ISU Chemistry

(208) **Enhanced Security Software for Inductively Coupled Plasma Mass Spectrometry (ICP-MS)**; Peter Cop[1], Mihaela Geaman[1]; [1]PerkinElmer SCIEX

The Role of Analytical Chemistry in Human Disease

(209) **Separation and Determination of Semi-Volatile Organics in Fine Particles**; Jimmy Pau[1]; [1]U. 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[1], Steven Cohen[1], Tsang-Lin Hwang[1], Pei-Kuo Tsai[1]; [1]Merck & Co., Inc.;

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

(212) **Reversed Phase Retention on Porous Polymer Monoliths Used in Capillary Electrochromatography**; Michelle Bushey[1], Brent Waguespack[1], Slade Hodges[1], Lindsay Sondergeld[1], Meghan Bush[1]; [1]Trinity University

(213) **Chemometric Tools for Noise and Background Reduction of Complex Liquid Chromatography/Mass Spectrometry and Extraction of Minor Sample Differences**; Willem Windig[1]; [1]Eigenvector Research Inc

(214) **Determination of Sensitivity and Precision Limits in a Fourier Transform Surface Plasmon Resonance Instrument**; Steve Lowry[1], Eric Jiang[1], Koichi Nishikida[1], Alastair Wark[2], Voula Kodoyianni[2], Stephen Weibel[2], Tim Burland[2]; [1]Thermo Electron Corp.; [2]GWC Technologies 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 Hag Park[1], In Whan Kim[2]; [1]Yeungnam University; [2]Daegu University

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

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

(218) **Application of the Aluminum Substrate in NIR-Raman Spectroscopy: Quantitative Analysis of Methyl Parathion Pesticide Microdroplets**; Roberto Sato[1], Cirilo Medina[1], Claudio Frausto[2]; [1]Universidad de Guadalajara, Campus Los Lagos; [2]Centro de Investigaciones en Optica

(219) **Hyperpolarized Xenon For NMR Signal Enhancement of Surface Species**; Kevin Knagge[1], Daniel Raftery[1], Jonathan Prange[1], Carl Murphy[1]; [1]Purdue University

(220) **Can Breast Cancer Be Caused by Active or Passive Smoking?**; Gus Miller; [1]Edinboro University of Pennsylvania

(221) **Fluorescence Detector for Capillary Electrophoresis using Violet Light Emitting Diode and Labeling Reagent**; Riichiro Nakajima[1], Takayoshi Tanaka[1], Keiichi Noda[1], Yuki Matsui[1], Takashi Tamura[1], Kazuhiko Tsukagoshi[1]; [1]Doshisha University

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

(224) **Removal of the Effect of Skin Pigmention in Tissue Spectra: Demonstration with Tissue Mimicking Phantoms**; Olusola Soyemi, Michelle Landry, Babs Soller, Patrick Idwasi, Ye Yang; [1]University of Massachusetts Medical School

(225) **High-Pressure NMR and Raman Spectroscopy for Studying Solvation Thermodynamics**; Jeanette D. Hanna[1], Dor Ben-Amotz[1]; [1]Purdue University

(226) **Accelerator Mass Spectrometry Method for Quantification of Beryllium in Biological Samples: Application for Studying Chronic Beryllium Disease**; Marina Chiarappa-Zucca[1], Robert Finkel[1], Roger Martinelli[1], Jeffery McAninch[1], Kenneth Turteltaub[1]; [1]Lawrence Livermore National Laboratory

(227) **The Characterization of Azophenol Analogues for Use as Fluorescent Ion Selective Probes**; Richard Williams[1], Yousef Hijji[1]; [1]Morgan State University, Chemistry Department

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

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

(230) **Quantitation of Particulate Matter Toxicity on a Per Particle Per Cell Basis**; Alen Haddrell[1], George Agnes[1], Stephen van Eeden[2]; [1]Simon Fraser University; [2]University of British Columbia

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

(231) **Nanoparticle-Enhanced Fluorescent Detection of Biomarkers**; Scott Reed[1]; [1]Portland State University

Chemometrics in Pharmaceutical Process Analytical Technology

(233) **Determination of the Enantiomeric Composition of Guest Molecules by Chemometric Analysis of the Fluorescence Spectra of Cyclodextrin Guest-host Complexes;** Kenneth Busch[1], Sayo Fakayode[1], Marianna Busch[1]; [1]Baylor University

TECHNICAL PROGRAM – TUESDAY
Posters 9:00 – 10:30 AM and 2:00 – 3:30 PM

Advances in Forensic Analytical Techniques

(234) **Fluorescence Investigation of Factors Which Affect the Chloride Sensing Ability of 6-methoxyquinoline**; Anindya Darra[1], Apurba Lal Koner[1], Padmaja Prasad Mishra[1], Smita Jha[1]; [1]Indian Institute of Technology, Bombay

(235) **Spectroscopic Studies of Goat Diets in Arid Environments**; Gary Rayson[1], Dean Anderson[2], Kris Havstad[2], Y.S. Landau[3], Tzach Glasser[3], John Walker[4]; [1]Department of Chemistry and Biochemistry, New Mexico State University; [2]United States Department of Agriculture; [3]State of Israel Minstry of Agriculture; [4]Texas A&M University System Extension

(236) **PCB Contamination in an Asphalt-Coated Storm Sewer: An Environmental and Materials Investigation**; Eileen M. Skelly Frame[1], Anthony J. Kriech[2], Kenneth R. Pike[3]; [1]Full Spectrum Analytical Consultants, Halfmoon, NY; [2]Heritage Research Group, Indianapolis; [3]Earthworks 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 Giglio[1], Daniel Cummings[1], Kevin Carney[1], Marianne Noy[1], Mary Adamic[1]; [1]Argonne National Laboratory-West

(238) **Measurement of Aerosol Optical Properties Using Cavity Ring Down Spectroscopy**; Hossein Bazargan[1], Dean Atkinson[1]; [1]Portland State University, Chemistry Department

(239) **Water Only HPLC with FID Detection**; Dale Felix[1], Stephanie Marin[1], Brian Jones[1]; [1]Selerity Technologies

(240) **How Toxic is Asbesstos. An Analysis of the Research**; Gus Miller; [1]Edinboro University of Pennslyvania

(241) **Optimization of an Automated SPME-GC/ITMS Method for Analysis of a Broad Range of Water Contaminants;** Robert Stiles[1]; Ill Yang[1]; Brian Buckley[1]; [1]Environmental and Occupational Health Science Institute

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

(243) **Membrane Introduction Tandem Mass Spectrometry (MIMS-MS/MS) for Real Time Measurement of Atmospheric Contaminants**; Chris Gill[1], Skye Creba[1], Janet Nelson[1], Alexander Thompson[1], Chris Simpson[2], Erik Krogh[1]; [1]Malaspina University-College; [2]University of Washington

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

(245) **Algorithm Development for Automated Raman Spectral Searching**; Brian Eckenrode[1], Valerie Cavett[1], Anthony Kearsley[2]; [1]FBI; [2]NIST

(246) **High-precision Uranium Isotopic Analysis for Environmental Forensics Using MC-ICPMS: Demonstration Studies at the Hanford Site, Washington**; John N. Christensen[1], P. Evan Dresel[2], Mark E. Conrad[1], Donald J. DePaolo[1, 3]; [1]Lawerence Berkeley National Laboratory; [2]Pacific Northwest National Laboratory; [3]Department of Earth and Planetary Science

Coherent 2D Vibrational Spectroscopy

(247) **The Intermolecular Interactions during the Melt Crystallization of PLLA and PLLA/PLLA Stereocomplex Investigated by Infrared and 2D IR Spectroscopy**; Jianming Zhang[1], Yukihiro Ozaki[1], Hideto Tsuji[2], Isao Noda[3]; [1]Kwansei Gakuin University; [2]Toyohashi University of Technology; [3]The Procter & Gamble Company

(248) **Terahertz Spectroscopy of High-energy Materials**; Philip Taday[1], William Tribe[1], David Newnham[1], Yaochen Shen[1], Michael Kemp[1]; [1]TeraView Limited

(249) **VCD Spectroscopic Determination of Absolute Stereochemistry as a Complementary Technique for Investigation of Chiral Drugs**; Mike Claybourn[1], Helen Turner[2], Christopher Frampton[3], Ron Roberts[1], Andrea Russell[2]; [1]AstraZeneca; [2]Southampton University; [3]Bruker Nonius

(250) **Absolute Configuration and Solution Conformation Determinations by Vibrational Circular Dichroism**; Teresa B. Freedman[1], David Dunmire[1], Xiaolin Cao[1], Laurence A. Nafie[1]; [1]Department of Chemistry, Syracuse University

(251) **Wavelength Modulation Spectroscopy for Simultaneous Temperature and H2O Concentration Measurement in a Flame**; Mohammadreza Gharavi[1], Steven Buckley[1]; [1]University of California, San Diego

Ion Trap MS for Proteomics

(252) **Quantitation of Metallothionein by Using CID Mass Spectrometry**; Yuchen Lu[1]; [1]West Virginia University

Nanomaterials for Photonics

(253) **Evaluation of Dual Use Direct to Metal (DTM) Primers for U.S. Department of Defense (DOD) Tactical Vehicles**; William Lum[1], James Kidd[1], Chris Miller[1], John Escarsega[1], Brian Placzankis[1]; [1]Army Research Laboratory,Materials Applications Branch

(254) **Design of Two-dimensional Photonic Crystal Slab with Complete Bandgap for Infrared Spectroscopy**; Hitoshi Kitagawa[1,2], Takashi Asano[1], Susumu Noda[1]; [1]Kyoto University; [2]ALPS Electric Co.,Ltd

Charles Mann Award

(255) **Field Portable Raman Probe for in-situ Analysis of Hydrothermal Vents**; Tina Battaglia[1], Eileen Dunn[1], John Holloway[1], Marvin Lilley[3], Brian Dable[2], Brian Marquardt[2], Karl Booksh[1]; [1]Arizona State University; [2]Center for process Analytical Chemistry; [3]University of Washington

Novel Vibrational Techniques for Biology

(256) **Exploration of Molecular Orientation in Polymers Fibers Using Novel Raman Spectroscopy Methods**; Simon Frisk[1], Richard M. Ikeda[1], D. Bruce Chase[2], John F. Rabolt[1]; [1]Dept. Materials Science and Engineering; [2]Dupont Central Reseach and Development

(257) **Raman Spectroscopic Markers for Osteoarthritis: Collagen Amide Vibrations**; Nicole Crane[1], Michael Morris[1], Blake Roessler[2], Abigail Smukler[2]; [1]University of Michigan, Department of Chemistry; [2]University of Michigan Medical School

(258) **Rapid Saliva Analysis for Clinical Trails**; Chetan Shende[1], Alan Gift[1], Frank Inscore[1], Stuart Farquharson[1]; [1]Real-Time Analyzers

(259) **Terahertz Spectroscopy in Proteomics**; Philip Taday[1], Thomas Lo[1], David Newnham[1], Michael Pepper[1,2]; [1]TeraView Limited; [2]University of Cambridge

(260) **Monitoring Astronaut Health: Urinalysis by Surface-enhanced Raman Spectroscopy**; Frank Inscore[1], Chetan Shende[1], Alan Gift[1], Stuart Fraquharson[1]; [1]Real-Time Analyzers

(261) **LSI's Intelligent Software: New Tools for Raman Spectra-Informatics**; Yongwu Yang[1], Canwen Liu[1], Shaoqing Peng[1], Wanglong Zhou[1], Victor Sapirstein[1]; [1]Lambda Solutions, Inc.

(262) **A Spectroscopic Investigation of Bovine Serum Albumin Protein Solution Aggregation and Conformation**; Charbel Tengroth[1], Fredrik Andersson[1], Sven P. Jacobsson[1]; [1]Analytical Development

(263) **Raman Detection of Protein, Peptide and Amino Acid Phosphorylation**; Yong Xie[1], Dongmao Zhang[1], Dor Ben-Amotz[1]; [1]Purdue University

(264) **Elucidation of the Atherosclerotic Disease Process by Raman Microscopy**; Fran Adar, Coralie Naudin[1], Andrew Whitley[1], Syun-ru Yeh[2], Linda Jellicks[2], Denis Rousseau[2]; [1]Jobin Yvon, Inc.; [2]Albert Einstein School of Medicine

(265) **Raman Spectroscopy of Insulin Revisited: Conformational Dynamics and Transitions Reflected from the Main-Chain Amide I Band**; Jian Dong [1], Zhuli Wan[1], Maxim Popov[1], Nelson Phillips[1], Michael Weiss[1], Paul Carey [1]; [1]Case Western Reserve University

(266) **Raman Spectra of Carbonated Apatites: Effect of Biologically Relevant Ion Substitution**; Mary Tecklenburg[1], Ayorinde Awonusi[1], ShaRhonda Dennis[1]; [1]Central Michigan University

(267) **Differential UV and Thermally Induced Effects Observed in DNA Using UV Resonance Raman Spectroscopy**; Michael Blades[2], Georg Schulze[1], Robin Turner[1,3], Andrew Jirasek[1,2]; [1]Biotechnology Laboratory, The University of British Columbia; [2]Dept. of Chemistry, The University of British Columbia; [3]Dept. of Electrical and Computer Engineering

Tuesday Morning, Room C123
LIBS
Organizer and Presider: Greg Klunder

10:30 (268) **Sequential Pulse LIBS Measurements in High Pressure Aqueous Solutions**; S. Michael Angel[1], Jon Scaffidi[1], Marion Lawrence[1], William Pearman[2], J. Chance Carter[3], Bill W. Colston Jr.[3]; [1]Department of Chemistry & Biochemistry, The University of South Carolina; [2]Department of Chemistry, United States Military Academy; [3]Medical Technology Program, Lawrence Livermore National Lab

10:50 (269) **Measurement of Gas-Phase Hydrocarbon Concentrations Using Laser-Induced Breakdown Spectroscopy**; Francesco Ferioli[2], Steven G. Buckley[1]; [1]University of California, San Diego; [2]University of Maryland, College Park

11:10 (270) **LIBS at Low Pressure: Application to planetary surface exploration**; David Cremers[2], Béatrice Sallé[1], Roger Wiens[2], Sylvestre Maurice[3]; [1]CEA Saclay, France; [2]Los Alamos National Laboratory, Los Alamos; [3]Observatoire Midi-Pyrénées, Laboratoire

11:30 (271) **Temperature Effects in ns/ns Dual Pulse Laser Induced Breakdown Spectroscopy**; Jonathan Scaffidi[1], William Pearman[2], J. Chance Carter[3], William Colston, Jr.[3], S. Michael Angel[1]; [1]University of South Carolina; [2]United States Military Academy; [3]Lawrence Livermore National Lab

11:50 (273) **Compact Echelle Spectrograph with High Resolution Intensified CCD for Laser Induced Breakdown Spectroscopy (LIBS)**; Marc Neglia[1], Bruce True[1], Ryan Sullivan[1]; [1]Princeton Instruments (a division of Roper Scientific)

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

10:30 (274) **Meeting Today's Analytical Challenges for the Analysis of Air Toxics using Time-of-Flight Mass Spectroscopy**; Wade Bontempo[1], Diane Benton[1], Sandia Kao[1], Linda Freeman[1]; [1]Air Toxics Limited

10:50 (275) **The Wine is Bottled Poetry: Using Analytical Chemistry to Understand the Poetry of Wine Flavor**; Susan Ebeler[1]; [1]University of California

11:10 (276) **Advances Toward Low Bleed AND Inert Capillary GC Columns for Improved Inertness GC/MS Systems**; Jason Ellis[1], Mitch Hastings[1]; [1]Agilent Technologies

11:30 (277) **Measuring Residue Levels in Citrus Oils: Analysis of Limonene Chlorohydrins and Pesticides by Capillary Gas Chromatography with Atomic Emission Detection**; Matthias Guentert[1], Carlos Macku[1], Lauren A. Johnson[1], John P. Walradt[1]; [1]Symrise Inc.

11:50 (278) **Characterization of a Novel Anthocyanin From Beluga Black Lentils (Lens culinaris)**; Gary Takeoka[1], Lan Dao[1], Hirotoshi Tamura[2]; [1]Western Regional Research Center, Agricultural Res; [2]Department of Biochemistry and Food Science

Tuesday Morning, Room 201
THE ROLE OF ANALYTICAL CHEMISTRY IN HUMAN DISEASE
Organizer and Presider: Dana Spence

10:30 (279) **Analytical Chemists and the Diagnosis of Cancer**; Douglas Demetrick[1,2,3]; [1]University of Calgary; [2]Calgary Laboratory Services; [3]Tom Baker Cancer Center

11:10 (280) **An Emerging Role for Red Blood Cells in Human Disease**; Dana Spence[1]; [1]Wayne State University

11:30 (281) **Microelectrodes for Studies of Brain Chemistry**; Adrian Michael; [1]University of Pittsburg

11:50 (282) **Separation-based Microanalytical Devices for the Study of Neurological Disorders**; Walter Vandaveer[1], Susan Lunte[1], Brian Huynh[1], Pradyot Nandi[1], Barbara Fogarty[1], Matthew Rosebraugh[2], Celeste Frankenfeld[1], Scott Martin[3]; [1]University of Kansas; [2]Drake University; [3]Saint Louis University

12:10 (283) **Using Novel Analytical Techniques to Probe Metabolism and Insulin Secretion in Islets of Langerhans**; Gabriella Dahlgren[1], Robert Kennedy[1]; [1]University of Michigan

TECHNICAL PROGRAM – TUESDAY
Orals 10:30 AM – 12:30 PM

Tuesday Morning, Room B114
GENERAL CHEMOMETRICS
Organizer and Presider: Barry Wise

10:30 (284) **A Novel Spectroscopic Method for Determining the Enantiomeric Purity of Samples Without the Need of a Chiral Auxiliary**; Dennis Rabbe[1], Marianna Busch[1], Kenneth Busch[1]; [1]Baylor University

10:50 (285) **Analysis of Jet Fuel Properties based on Raman Spectroscopy**; Stuart Farquharson[1], Alan Gift[1], Wayne Smith[1]; [1]Real-time Analyzers11:10 (286) **The Use of Raman Spectroscopy to Characterize Hydrogenation Reactions**; Mark Kemper[1], Ian Lewis[1], Sri Venkata Tumuluri[2], Bonnie Avery[2], Mitchell Avery[2]; [1]Kaiser Optical Systems; [2]University of Mississippi

11:30 (287) **Photoacoustic Multivariate Optical Computing: Ethanol and Water in the MIR**; Ryan Priore[1], Michael Myrick[1]; [1]University of South Carolina

11:50 (288) **Chiral Analysis by Regression Modeling of UV Absorption Spectral Data—the Use of Modified Cyclodextrins as Chiral Auxiliaries**; Marianna Busch[1], Sayo Fakayode[1], Isabel Swamidoss[1], Kenneth Busch[1]; [1]Baylor University

12:10 (289) **A Review of Multi-way Models and Their Use in Monitoring Batch and Continuous Processes**; Barry M. Wise, Neal Gallagher; [1]Eigenvector Research, Inc.

Tuesday Morning, Room B113
ADVANCES IN FORENSIC ANALYTICAL TECHNIQUES
Organizer: Greg Klunder • Presider: Rachel Lowe

10:30 (290) **Comparison of instrumental and Biological Field Detection of Accelerants and Explosives**; Kenneth Furton, Shirley Chin[1], Laura Conner[1], Ross Harper[1], Jeannette Perr[1], Douglas Heller[1], Jose Almirall[1]; [1]Florida Int'l Univ.

10:50 (291) **SPME-GC/MS Investigations Into the Uniqueness of Human Scent**; Allison Curran, Kenneth Furton; [1]Florida International University

10:50 (291b) **Application of Fluorescence Line Narrowing Spectroscopy to Forensic Fiber Examination**; Andres Campiglia[1], Michael Sigman[1]; [1]Univ. of Central Florida

11:30 (292) **Analysis of Children's Latent Fingerprint Residues by Infrared Microspectroscopy**; Diane Williams[1,2], Justine Brucker-Serrano[1,2], Rebecca Schwartz[2], Edward Bartick[2]; [1]Oak Ridge Institute of Science Education; [2]FBI Counterterrorism/Forensic Science Research

11:50 (293) **The Characterization of Microchemical Test Resultant Crystalline Formations using Polarized Light Microscopy, Infrared and Raman Spectroscopy.**; John Crowe[1], Mark Witkowski[1]; [1]US FDA/FCC

12:10 (294) **Use of FT-IR and EDXRF to Characterize Counterfeit Inkjet Inks**; Gene Hall[1], Jeannine Matuza[1]; [1]Rutgers University

Tuesday Morning, Room C124
COHERENT 2D VIBRATIONAL SPECTROSCOPY I
Organizers: Wei Zhao & Peter Hamm • Presider: David Jonas

10:30 (295) **Ultrafast Infrared Vibrational Echo Correlation Spectroscopy**; Michael D. Fayer[1], John B Asbury[1], Tobias Steinel[1]; [1]Stanford University

11:10 (296) **Multidimensional Ultrafast IR-Raman Spectroscopy**; Dana Dlott; [1]University of Illinois at Urbana

11:30 (297) **Third and Fifth-Order Two-Dimensional Infrared Spectroscopy**; Martin Zanni[1]; [1]University of Wisconsin-Madison

11:50 (298) **Phase-Stabilized Two-Dimensional Femtosecond Spectroscopy**; Tobias Brixner[1], Igor V. Stiopkin[1], Graham R. Fleming[1]; [1]Department of Chemistry, University of California

12:10 (299) **Coherent Two-Dimensional Infrared Spectroscopy of Small Peptides**; Nien-Hui Ge[1], Denis Karaiskaj[1], Hiroaki Maekawa[2], Soohwan Sul[1], Jiang Ying[1]; [1]University of California, Irvine

Tuesday Morning, Room A105
ION TRAP MS FOR PROTEOMICS I
Organizer and Presider: Gary Glish

10:30 (300) **Enzyme Kinetics and Mechanisms**; Julie Leary[1]; [1]UC Berkeley

10:50 (301) **Studying Metalloporphyrin-Ligand Binding by Quadrupole Ion Trap Mass Spectrometry**; Victor Ryzhov[1]; [1]Northern Illinois University

11:10 (302) **Discovering and Characterizing Drug Fragments Using Ion Trap Mass Spectrometry**; Mark Cancilla[1], Daniel Erlanson[1], Andrew Braisted[1], Jun Wang[1], Michelle Arkin[1], James Wells[1]; [1]Sunesis Pharmaceuticals

11:30 (303) **Structural Analysis of the Glycosylation in Luteinizing Hormone Using a Quadrupole Ion Trap Mass Spectrometer**; Heather Desaire[1]; [1]University of Kansas

11:50 (304) **Comparative Performance of Linear and Three-dimensional Quadrupole Ion Trap Mass Spectrometers for the MS/MS Analysis of Peptides**; David Burinsky[1], Connell Cunningham Jr[2], Gary Glish[2]; [1]GlaxoSmithKline; [2]University of North Carolina - Chapel Hill

12:10 (305) **Unsupervised Clustering of a Large Truth Set of Ion Trap Peptide MS/MS Spectra**; Vicki H. Wysocki[1], Yingying Huang[1], George Tseng[2], Shinsheng Yuan[3], Ljiljana Pasa-Tolic[4], Mary S. Lipton[4], Richard D. Smith[4]; [1]University of Arizona; [2]University of Pittsburgh; [3]UCLA; [4]Pacific Northwest National Laboratory

TECHNICAL PROGRAM – TUESDAY
Orals 10:30 AM – 12:30 PM and 3:30 – 5:30

Tuesday Morning, Room B115
CARBON NANOTUBE SEPARATION III
Organizers: Wei Zhao & Steven Doorn • Presider: Michael Strano

10:30 (306) **Large Fullerene and Nanotube Characterization**; Robert Hauge[1], Zhenning Gu[1], Haiqing Peng[1], Kirk Zigler[1], Ya-Qiong Xu[1], Anil Sadana[1], W.E. Billups[1], Al Schultz[2], Michael Ugarov[2], Richard Smalley[1]; [1]Rice University; [2]IonWerks

10:50 (307) **Controlled and Reversible Doping of SWNTs**; Michael O'Connell[1], Ezra Eibergen[1], Steve Doorn[1]; [1]Los Alamos National Lab

11:10 (308) **Ultra-Long Carbon Nanotubes by Chemical Vapour Deposition**; Lianxi Zheng[1], Michael O'Connell[1], Stephen Doorn[1], Xiaozhou Liao[1], Yonghao Zhao[1], Mark Hoffbauer[1], Quanxi Jia[1], Dean Peterson[1], Jie Liu[2], Yuntian Zhu[1]; [1]Los Alamos National Laboratory; [2]Chemistry Department, Duke University

11:30 (309) **AFM-Nanofinder Composite System and It's Application to Characterization of Single Walled Carbon Nanotubes**; Nobukata Nagasawa[1,2], Yasushi Morihira[1], Jian-Ting Ye[2], Pavel Rutkovski[1], Zi-Kang Tang[2], Igor Kudryashov[1], Jack Roberts[3], Shoji Suruga[1]; [1]Tokyo Instruments, Inc.; [2]Department of Physics and Institute of Nano Science and Technology, Hong Kong Univ. of Science and Technology; [3]Symphotic TII, Corp.

11:50 (310) **Novel Soft Materials Composed of Single-walled Carbon Nanotubes and Ionic Liquids;** Takanori Fukushima[1], Takuzo Aida[1, 2]; [1]ERATO Aida Nanospace Project, JST; [2]Department of Chemistry and Biotechnology

12:10 (311) **Direct Growth of Long and Aligned Single Walled Carbon Nanotubes for Nanoscale Electronic Applications**; Jie Liu[1]; [1]Duke 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. Hug[1], D. Reid[1], A. Bhattacharyya[2], T. D. Moustakas[2], R. Treece[3], J. R. Smith[3], J. I. Pankove[3]; [1]Photon Systems, Inc., Covina, CA; [2]Department of Electrical Engineering; [3]Astralux Incorporated, Boulder, CO; [4]

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

11:10 (314) **SERS of Chemical Agents in Water - Determining Limits of Detection**; Steven Christesen[1], Kevin Spencer[2], James Sylvia[2], Kristina Gonser[1]; [1]US Army Edgewood Chem Bio Center; [2]EIC Laboratories

11:30 (315) **Quantitative Process Monitoring Utilizing Raman Spectroscopy**; Brian J. Marquardt[1], Brian K. Dable[1], David Veltkamp[1]; [1]Center 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. Bello[1], David T. Hobbs[2]; [1]EIC Laboratories; [2]Savannah River Technology Center

12:10 (317) **Fieldable Raman Systems for Trace Analysis**; Kevin Spencer[1], James Sylvia[1], Susan Clauson[1], Peter Marren[1], Jane Bertone[1], Steven Pullins[1]; [1]EIC Laboratories, Inc.

TUESDAY POSTER SESSIONS and BREAK
2:00 – 3:30 PM, See pages 48 - 51
Exhibit Hall A/A-1

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; [1]Teledyne 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; [1]New Wave Research

4:30 (320) **Elemental and Speciation Sample Preparation for Environmental and Forensic Analysis**; H.M. Skip Kingston[1], Mizanur Rahman[1], John Kern[1], Matt Pamuku[1,2], Theodore Towns[1]; [1]Duquesne University; [2]Applied Isotope Technologies (AIT)

5:10 (321) **Direct Solution Introduction with Conventional Nebulizers for Inductively Coupled Plasma Mass Spectrometry Using a Short Torch Configuration**; Craig Westphal[1], Kaveh Kahen[1], Akbar Montaser[1]; [1]Gerorge 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 Tang[1], Klaus Dragull[1]; [1]University of Hawaii

3:50 (323) **TBA;** Jim Settledge

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

4:30 (325) **Tracking Color and Pigment Changes in Anthocyanin Products**; Ronald Wrolstad[1]; [1]Oregon State University

Tuesday Afternoon, Ballroom 201
BIOMARKERS-ANALYTICAL APPLICATION IN THE RESEARCH AND ASSESSMENT OF HUMAN DISEASE
Organizer and Presider: Michael Martin

3:30 (326) **Current State of Biomarker Discovery and Development**; Stephen Naylor[1]; [1]MIT and Boston University School of Medicine

4:10 (327) **Performance Evaluation of Biomarker in Cancer Detection and Diagnosis;** Sudhir Srivstava[1], [1]National Cancer Institute

4:50 (328) **Design and Mechanism of Action of Neuronal Nicotinic Acetylcholine receptor Compounds**; Amina S. Woods[1], Hay-Yan J. Wamg[1], Andrew E. Taggi[2]; [1]NIDA IRP, NIH; [2]Cornell University

5:10 (329) **Nanocluster MALDI Matrices combined with MALDI-Ion Mobility-oTOFMS (MALDI-IM-oTOF) for Analysis of Biological Tissue Surfaces**; J. Albert Schultz[1], Michael Ugarov[1], Agnès Tempez[1], Thomas Egan[1], Jack Wang[2], Shelley Jackson[2], Amina S. Woods[2]; [1]Ionwerks Inc; [2]NIDA-IRP

Tuesday Afternoon, Room B114
CHEMOMETRICS IN PHARMACEUTICAL PROCESS ANALYTICAL TECHNOLOGY
Organizer and Presider: Paul Gemperline

3:30 (330) **Modeling of Batch Processes With in-situ Spectroscopic and Calorimetric Measurements**; Paul Gemperline[1], Maryann Ehly[1], Heather Teague[1], Graeme Puxty[2], Marcel Maeder[2], R. Russell Rhinehart[3]; [1]East Carolina University; [2]Newcastle University, Australia; [3]Oklahoma State University

4:10 (331) **Development of Chemometrics Tools for Process Analytical Technology: Some Case Studies**; Lin Zhang[1], S. Sonja Sekulic[1]; [1]Pfizer Inc

4:30 (332**) In-line FTIR and Raman Spectroscopy Supporting Process Development for Active Pharmaceutical Ingredients**; Zhihao Lin[1], Zhihong Ge[1]; [1]Merck & Co., Inc.

4:50 (333) **Challenging FT-NIR Transmission Spectroscopy with Low Drug Content Tablets**; Rodolfo Romañach; [1]University of Puerto Rico - Mayaguez Campus

Tuesday Afternoon, Room B113
ANYTIME/ANYPLACE ACCESS TO INSTRUMENTATION OVER THE INTERNET:
CHANGING THE WAY SCIENCE IS TAUGHT
Organizer and Presider: Devon Cancilla

3:30 (334) **Western's Integrated Laboratory Network (ILN): Instrumental Science Anytime/Anyplace**; Devon Cancilla; [1]Western Washington University

3:50 (335) **Introducing the ILN into the Pharmacy Program at UBC**; Simon Albon[1]; [1]UBC Faculty of Pharmaceutical Sciences

4:10 (336) **Teaching with Technology: How the ILN Fits into the Curriculum**; Samia Khan, University of British Columbia

4:30 (337) **An Institutional Perspective to Development of an ILN**; Larry Gilbert[1]; [1]Western Washington University

4:50 (338) **Stories from the Trenches: Using the ILN in High School Science**; John Stockman[1]; [1]Bellingham High School

5:10 (339) **Interfacing Science and Policy through the ILN: Science Across the Curriculum**; Jean Melious[1]; [1]Western Washington 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; [1]University of Wisconsin

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

4:30 (342) **Multidimensional Orientational Spectroscopy**; Mark Berg[1]; [1]Department of Chemistry and Biochemistry, University of South Carolina

4:50 (343) **CARS Microscopy: Coming of Age**; Xiaolin Nan[1], Eric Potma[1], Conor Evans[1], Wei Y. Yang[1], X. Sunney Xie[1]; [1]Department of Chemistry and Chemical Biology, Harvard

5:10 (344) **Doubly Vibrationally Enhanced Four Wave Mixing Spectroscopy for Metal Ion-Acetonitrile Complexes**; Wei Zhao[1]; [1]Department of Chemistry, University of Arkansas

Tuesday Afternoon, Room A105
ION TRAP MS FOR PROTEOMICS
Organizer and Presider: Gary Glish

3:30 (345) **Infrared Atmospheric Pressure Matrix-Assisted Laser Desorption/Ionization of Biological Molecules**; Christopher Von Seggern[1], Robert Cotter[1]; [1]Johns Hopkins University School of Medicine

3:50 (346) **Parallel MS/MS on a Quadrupole Ion Trap via Differential Ion Accumulation**; Richard W. Vachet[1], Jonathan Wilson[1]; [1]University of Massachusetts

4:10 (347) **Strategies for Intact Protein Sequence Analysis Using Gas-Phase Ion/Ion Reactions in Electrodynamic Ion Traps**; Gavin Reid[1]; [1]Michigan State University

4:30 (348) **Top-down Proteomics in a Quadrupole Ion Trap: Prospects and Challenges**; Gary Glish[1]; [1]University of North Carolina

4:50 (349) **Isotope-Coded Affinity Tag Approach to Study Gene Regulation by Antisense Inhibition: Cellular Response to Target Protein Reduction**; Gregory Barrett-Wilt[1], Thomas Vincent[2], Jeremy Graff[3], Steven Hofstadler[1], Eric Marcusson[2]; [1]Ibis Therpeutics, a Division of Isis Pharmaceutica; [2]Isis Pharmaceuticals; [3]Lilly Research Labs, Cancer Research Div

5:10 (350) **Application of a Hybrid Linear Ion Trap / Fourier Transform Mass Spectrometer for Biomarker Discovery**; Nathan Yates[1], Chrissina Burns[2], John Cummings[1], Ekaterina Deyanova[1], Adi Ganz[2], Linda Kochanski[1], Anita Lee[1], John Mehl[1], Fanyu Meng[1], Cloud Paweletz[1], Ellen Rohde[1], Jeff Sachs[2], Priyanka Verma[2], Matt Wierner[2], Ronald Henderickson[1]; [1]Department of Molecular Profiling, Merck Research; [2]Applied Computer Science and Mathematics

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[1], David Fromm[1], Arvind Sundaramurthy[2], P. James Schuck[1], Katharine Willets[1], Gordon Kino[2]; [1]Stanford University Department of Chemistry; [2]Stanford University

4:10 (352) **Biological Imaging with Quantum Dots**; David Norris[1]; [1]University of Minnesota

4:50 (353) **Single Metal Particle Sensor and Interferometer**; Xiao-Min Lin[1], Sang-Kee Eah[2], Gary Wiederrecht[1], Heinrich Jaeger[2], Norbert Scherer[2]; [1]Argonne National Laboratory; [2]University of Chicago

5:10 (354) **Sensitive RNA Detection in vitro and in vivo**; Jianwei Li[1], Paul Choi[1], Benjamin Lee[1], Mark Stanisz[1], Charles Kulwin[1], Xiaoliang Xie[1]; [1]Harvard University

Tuesday Afternoon, Room A106
NOVEL VIBRATIONAL TECHNIQUES FOR BIOLOGY: IN RECOGNITON OF RICHARD MATHIES 2004 LIPPINCOTT AWARDEE
Organizer and Presider: Glen Loppnow

3:30 (355) **Biophysical and Bioanalytical Ultraviolet Resonance Raman Spectroscopy Using Fiber-Optics**; Michael Blades[2], Andrew Jirasek[1,2], Georg Schulze[1,2], R. F. B. Turner[1], Geoff Horsman[3], Fred Vaillancourt[4], Chris Barbosa[2], Lindsay Eltis[3]; [1]Biotechnology Laboratory, University of British Columbia; [2]Dept. of Chemistry, University of British Columbia; [3]Dept. of Microbiology, University of British Columbia; [4]Dept. of Biological Chemistry and Molecular Biology, University of British Columbia

3:50 (356) **Vibrational Spectroscopy of Functional Proteins on Surfaces**; Stefan Franzen[1], Scott Brewer[1], Simon Lappi[1], Selina Moses[1], Jennifer Belyea[1]; [1]NC State Univ.

4:10 (357) **Deep UV Raman Spectroscopic Characterization of Self Assembling Biomaterials**; Igor Lednev[1], Autumn Carlsen[1], Vladimir Ermolenkov[1], Wei He[1], Sei Higashiya[1], Natalya Topilina[1], Christopher Wells[1], John Welch[1], Ming Xu[1]; [1]Department of Chemistry, University at Albany, SUNY

4:30 (358) **Nonlinear Interferometric Vibrational Imaging**; Stephen Boppart[1], Daniel Marks[1], Jeremy Bredfeldt[1], Claudio Vinegoni[1]; [1]University of Illinois

4:50 (359) **Structure-Function-Dynamics Relationships from Resonance Raman Spectroscopy of Homologous Biomolecules**; G. R. Loppnow[1], S. Yarasi[1], M. A. Webb[1], E. Fraga[1]; [1]Dept of Chemistry, Univ. of Alberta

TECHNICAL PROGRAM - WEDNESDAY
Plenary and Posters

7:30 Wake Up Coffee, *Ballroom Lobby*

8:00 AM Plenary Session, Ballroom 201

Zhong Lin Wang

(360) **Semiconducting and Piezoelectric Nanobelts, Nanosprings and Nanorings**; Zhong Lin Wang[1] Georgia Institute of Technology

Meggers Award
8:30 AM Plenary Session, Ballroom 201

Boris Mizaikoff

(361) **Mid-Infrared Chemical Sensors - From the Bench into the Deep Sea**; Boris Mizaikoff; [1]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

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 Miller[1], Ning Gao[1], Zewu Chen[1], Walter Gibson[1]; [1]X-ray Optical Systems, Inc.

(363) **Determination of Metals in Urban Dust Samples Using Inductively Coupled Plasma Mass Spectrometry: Influence of Microwave Digestion Procedures**; Heidi Chen[2], Nouri M. Hassan[1], Monique Lanouette[1], Pat E. Rasmussen[1], Valbona Celo[2], Ewa Dabek-Zlotorzynska[2]; [1]Safe Environments Program, HECS Branch, Health Can; [2]AAQD, Environmental Technology Centre

(364) **Application of a New Commercial GC-ICP-MS Interface for the Analysis of Organo-Tin and Organo-Mercury Species**; Martin Nash[1], Phil Shaw[1], Bill Spence[1], Simon Nelms[1], Eva Krupp[2]; [1]Thermo Electron Corp., Ion Path; [2]LCABIE, Helioparc Pau

(365) **The Separation and Determination of Iodinated Haloacetic Acids by Gas Chromatography Time of Flight Mass Spectrometry**; Hans Mentzen II[1], David Reckhow[2], Julian Tyson[1]; [1]University of MAssachusetts, Department of Analytical Chemistry; [2]University 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. Wuilloud[1], Rodolfo G. Wuilloud[1], Douglas T. Heitkemper[1]; [1]US-Food and Drug Administration/Forensic Chemistry

(367) **Advances in Speciation Analysis Using HPLC-ICP-MS**; Kenneth Neubauer[1], Pamela Perrone[1], Wilhad Reuter[1], Zoe Grosser[1], Ruth Wof[1]; [1]PerkinElmer Life and Analytical Sciences

(369) **Transport of Lead and Arsenic in Plants Used in Phytoremediation**; David Butcher[1], Joshua Liebschutz[1], Patrick Baldwin[1]; [1]Western Carolina University

(370) **Determination of Selenium Species by Flow Injection Inductively Coupled Plasma Optical Emission spectrometry (FI-ICP-OES)**; Princess Hernandez[1], Julian Tyson[1], Peter Uden[1], Dennis Yates[2]; [1]Department of Chemistry, University of Masachusetts; [2]PerkinElmer Life & Analytical Sciences

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

(373) **Determination of Fe Species in Cooked Meats**; James Harnly[1], Edith Blackwell[1], Charmonte Watkins[1]; [1]U. S. Department of Agriculture

(374) **Determination of Total Mercury in Biological Tissues using Flow Injection CVAAS Following Formic Acid Solubilization**; Masahiko Kan[1], Scott Willie[2], Christine Scriver[2], Ralph Sturgeon[2]; [1]Environmental Information Measurement Sciences, Ho; [2]Institute for National Measurement Stand

(375) **The Investigation of Fertilizer Analyses from Start to Finish Utilizing Microwave Digestion Prepration and Simultaneous ICP-OEs with Axial Viewing**; Christine Rivera[1], Elaine Hasty[2]; [1]Varian, Inc.; [2]CEM Corp.

Molecular Inorganic and Organometallic Mass Spectrometry

(376) **Surface Analysis of Zn coated Steel**; Do-Hyung Lee[1]; [1]Research Institute of Industrial Science and Technology

(377) **Characterization of Uranyl Ion Binding by Datura innoxia**; Debbie Serna[1], Dr. Gary Rayson[1]; [1]New Mexico State University

(378) **Determination of Trace Inorganic Mercury by Cold Vapor Generation from Tin Immobilized on an Anion-Exchanger**; Julian F. Tyson[1]; [1]University of Massachusetts

(380) **Lead Content in Ancient Bronze Coins**; Mary Kate Donais[1], Ashley Dumas[1], Gregory Whissel[1]; [1]Saint Anselm College

(381) **Elemental Imaging with a Confocal X-ray Fluorescence**; George Havrilla[1], Ning Gao[2]; [1]Los Alamos National Laboratory; [2]XOS

(382) **Formation of Dioygen Complexes with Reduced Uranyl Cations**; Anita Gianotto[1], Kevin Cossel[1], Garold Gresham[1], Michael Van Stipdonk[2], Gary Groenewold[1]; [1]Idaho National Engineering and Environmental Labor; [2]Wichita State University

(383) **Covalent Oxo-Uranium Cluster Ions in the Gas Phase**; Gary S. Groenewold[1], Michael J. Van Stipdonk[2], Garold Gresham, Victor Anbalagan[2], Anita K. Gianotto[1], Anthony D. Appelhans[1]; [1]Idaho National Engineering and Environmental Labor; [2]Wichita State University

(384) **Direct Thermal Vaporization for Metals Speciation in Soil**; Eric D. Salin[1], Rebecca Lam[1], Josiane Lafleur[1]; [1]McGill University

(385) **Determination of As, Se and Various Trace Metals in Rain Waters**; Hakan Gurleyuk[1], Crystal R. Howard[1], Robert Brunette[1]; [1]Frontier Geosciences

Biological Analysis Enabled By Micromachining Technologies

(386) **Liposomes As Model Systems for Biological Particles: Characterization by Capillary Electrophoresis**; Michele Pysher[1], Mark Hayes[1]; [1]Arizona State University

(387) **Analysis of Liposome Incorporated Intrinsic and Extrinsic Membrane Proteins Via Capillary Electrophoresis**; Michele Pysher[1], Mark Hayes[1]; [1]Arizona State University

(389) **An LC-MS Method for the Quantification of Triglycerides using Metabolically-derived 13C Triglycerides as Internal Standards**; April Lachance[1], Jason Evans[1]; [1]University of Massachusetts Boston

(390) **Development of High-Performance Electromobility Focusing for Protein Analysis**; Ryan Kelly[1], Paul Humble[1], Milton Lee[1], Adam Woolley[1]; [1]Brigham Young University

(391) **Control of Non-specific Protein Adsorption to Surfaces for Biochemical Monitoring**; Jean-Francois Masson[1], Tina Battaglia[1], Stephen Beaudoin[2], Karl Booksh[1]; [1]Department of Chemistry and Biochemistry, Arizona; [2]School of Chemical Engineering, Purdue University

(392) **Studies of Chiral Recognition Using Fluorescence Anisotropy**; Matthew McCarroll[1], Yafei Xu[1], Irene Kiragu[1]; [1]Southern Illinois University

(393) **Polymerized liposomes specifically fabricated for protein sensing**; Andres Campiglia[1], Sanku Mallik[2]; [1]University of Central Florida; [2]North Dakota State University

(394) **Development of a Polymer-based Optical Sensor for the Ultrasensitive and Sequence-specific Detection of DNA Material**; Kim Doré[1], Sébastien Dubus[1], Mario Leclerc[1], Denis Boudreau[1]; [1]Université Laval

(395) **"Smart Sensor" Design: Optical Computations**; Jeff Cramer[1], Soame Banerji[1], Frank Vogt[1], Karl Booksh[1], Matthew Johnson[2], Lisa Hansen[2], Denise Wilson[2]; [1]Arizona State University; [2]University of Washington

(397) **Accelerating Discovery Analytical Chemistry Using Micro Parallel Liquid Chromatography**; Surekha Vajjhala; [1]Nanostream

(398) **High Efficiency Separation of Proteins in Poly(methyl methacrylate)-Based Microchips: Application of a New Optimization Technique**; Hamed Shadpour[1], Steven A. Soper[1]; [1]Louisiana State University

(399) **Rapid Prototyping of Thermoset Polyester Microfluidic Devices**; Gina S. Fiorini[1], Robert M. Lorenz[1], Jason S. Kuo[1], Daniel T. Chiu[1]; [1]University of Washington

(400) **The Use of a Microchip Laser for Two-photon Excitation of Native Fluorescence in Proteins**; Li LI[1], Uchenna Paul[1], Milton Lee[1], Paul Farnsworth[1]; [1]Brigham Young University

(401) **Bioanalytical Applications of Microchip-CE with Pulsed Electrochemical Detection**; Carlos D. Garcia[1], Charles S. Henry[2]; [1]The University of Texas at San Antonio; [2]Colorado State University

(402) **Speciation of Pt and Se for Mechanism Characterization of Chemotherapeutic Agents Using SEC-ICPMS**; Rumin Xei[1], Murugesan Gounder[2], Lorna Rodriguez[2], Eric Rubin and Brian Buckley Rubin[2], Brian Buckley[1]; [1]EOHSI Rutgers University; [2]New Jersey Cancer Institute

(403) **Mechanisms of Dopant-Assisted Atmospheric Pressure Photoionization (DA-APPI) for LC/MS. Part II: Reactions Following Photoion Production.**; Michael Blades[1], Damon Robb[1]; [1]University of British Columbia

Probing Cellular Properties and Function With Microchip Devices

(404) **Development of Analytical Tools in Capillary Systems for Metabolic Analysis at Single Cell Volumes and Concentrations**; J. M. Dragavon[1], L. W. Burgess[1], A. C. Young[1], A. K.-Y. Jen[1], T. J. Hankins[1], J. B. Callis[1], T. J. Strovas[1], M. E. Lidstrom[1]; [1]Microscale Life Sciences Center, University of Washington

(405) **Dielectrophoretic Force Microscopy of Biological Interfaces**; Brian Lynch[1], Al Hilton[1], Garth Simpson[1]; [1]Purdue University

(406) **The Use of Design of Experiment in Release Rate Robustness Testing**; Danford Lee[1], June Liu[1], Vicky Jimenez[1], Steve Fields[1], Jason Xin Zhang[1]; [1]ALZA

Multivariate Analysis of Hyperspectral Images

(407) **Understanding the Limitations of Multivariate Curve Resolution when Applied to Hyperspectral Images**; Howland Jones[1], David Haaland[1], Edward Thomas[1], Jerilyn Timlin[1]; [1]Sandia National Laboratories

New Ideas In Teaching Analytical Chemistry

(408) **A Unifying Approach to the Description of Chemical Instrumentation in a Course on Instrumental Methods of Analysis**; Gary Rayson[1]; [1]New Mexico State University

(409) **An Overview of Two NSF-CCLI Projects at Trinity University: Philosophy, Interdisciplinary Ventures, Outcomes**; Michelle Bushey; [1]Trinity University

(410) **Development of a CDrom Resource to Support the Undergraduate Teaching of Sampling and Sample Preparatione**; Brian Woodget[1], Alexis Holden[2], Irene Mueller-Harvey[3]; [1]UK Analytical Partnership; [2]University of Central Lancashire, UK; [3]University of Reading, UK

(411) **Student Projects with Oxygen Binding Proteins: Spectroelectrochemical Results**; Scott Dorman[1], Clare Kenny[2], Melinda Martin[2], Eduardo Ramos[1], Timothy Johnson[1], Justin Weinstein[1]; [1]Birmingham-Southern College; [2]University of South Alabama

(412) **Incorporating Analytical Thinking Into An Introductory Course in Chemistry**; David Harvey[1]; [1]DePauw University

(413) **Analysis of Lithia Water: Instilling a Historical and Community Perspective into the Quantitative Analysis Laboratory**; Steven Petrovic; [1]Southern Oregon University

(414) **Using Cyberspace for Teaching Analytical Science: The Analytical Science Digital Library and Beyond**; Cameron Dorey[1]; [1]University of Central Arkansas

TECHNICAL PROGRAM – WEDNESDAY
Posters 9:00 – 10:30 AM and 2:00 – 3:30 PM

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[1], M. Kathleen Alam[1]; [1]Sandia National Laboratories

(416) **Simulation Model Using PLS and Numerical Analysis Method: Conversion Rate and Diffusion Motion in Heterogeneous Reaction**; Hsiu-Fang Fan[1], Thou-Long Chin[2], King-Chuen Lin[1]; [1]Nation Taiwan University; [2]IAMS-SINICA

(417) **Applications of Chemometrics for the Analysis of Temperature Dependent Infrared Spectra of Hydrogen Bonded Polymers**; Shigeaki Morita[1], Serge Kokot[2], Yukihiro Ozaki[1]; [1]Kwansei Gakuin University; [2]Queensland University of Technology

(417a) **Infrared Microscopy – An Alternative Method for Probing Resin Bead Site Distributions?;** Gurjit Mandair[1], Andrea Russell[1], Zhanru Yu[1], Nicola Galaffu[1], Mark Bradley[1]; [1]University of Southampton

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

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

IR Microspectroscopy Instrumentation and Applications

(418) **Probing Ice Nucleation on a Self-Assembled Monolayer of 11-Mercapto-1-Undecanol Using Infrared Micrscopy**; Kady Dendramis[1], Hugh Richardson[1]; [1]Ohio University

(419) **New Fabrication Technology for Multivariate Optical Elements**; Ryan Priore[1], Michael Myrick[1]; [1]University of South Carolina

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

(421) **FT-IR Spectroscopic Characterization of Polymer Nanocomposites**; Vasilis Gregoriou[1], Stavros Bollas[1], Athina Korakianiti[1], Spyros Tzavalas[1], Georgia Kandilioti[1]; [1]FORTH-ICEHT

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

(423) **Localized Chemical Analysis of Treated Stored Grain Insects via Synchrotron Infrared Microspectroscopy**; David L. Wetzel[1], Bhadriraju Subramanyam[2], Tiffany L. Fisher[1]; [1]Microbeam Molecular Spectroscopy Laboratory, Kansa; [2]Department 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[1], John Seelenbinder[1], Christina Tobler; [1]SensIR Technologies, LLC

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

(426) **Applications for a Unique Spectrophotometer with 3-D Optics and Far UV to NIR Capability**; John Monti[1], Shannon Richard[1], Timothy Alt[1]; [1]Shimadzu Scientific Instruments

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

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

(429) **FT-IR Microimaging of Wood Composites**; Stephen S. Kelley[1,2], Thimothy G. Rials[2], Nicole Labbé[2]; [1]National Renewable Energy Laboratory; [2]University of Tennesse, Forest Products

Nanotubes and Nanowires For Sensing

(431) **Simultaneous Single-molecule Optical and Electrical Recording of DNA Interactions with Nanopores and Lipid Membranes**; Emily L. Chandler[1,2], Alyssa L. Smith[1], Lisa M. Burden[1,2], John J. Kasianowicz[3], Daniel L. Burden[1,2]; [1]Wheaton College (IL); [2]Biomolecular Nanotechnologies and Measur; [3]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[1], Xin Gao[1], Kin Tam[2]; [1]University of Reading, UK; [2]AstraZeneca, Macclesfield, UK

Raman In Process Analytical

(433) **New Applications of Raman Spectroscopy**; Josh Goldman[1], Hugh Gotts[2], Soya Gamsey[1], Bakthan Singaram[1]; [1] University of California at Santa Cruz; [2] Analytical Services Group

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

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

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

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

Raman in Pharma

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

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

TECHNICAL PROGRAM – WEDNESDAY
Orals 10:30 AM – 12:30 PM

Wednesday Morning, Room C123
IMPORTANT ASPECTS OF ELEMENTAL SPECIATION, SAMPLE PREPARATION, SEPARATION, SAMPLE INTRODUCTION
Organizer and Presider: Joseph Caruso

10:30 (438) **Sample Preparation For Trace Element Speciation**; Ralph Sturgeon[1], Zoltan Mester[1], Lu Yang[1], Paulette Maxwell[1], Christine Scriver[1], Scott Willie[1]; [1]NRC-INMS

10:50 (439) **Sample Introduction Considerations for Elemental Speciation**; John Olesik; [1]Ohio State University

11:10 (440) **Separations for Elemental Speciation with ICP-MS Detection**; Joseph Caruso[1]; [1]University of Cincinnati

11:30 (441) **ICP Detectors for Speciation Studies**; Norbert Jakubowski[1], Michael Edler[1], Ingo Feldmann[1]; [1]Institute for Analytical Sciences (ISAS)

11:50 (442) **Continued Developments in the Analysis of Polybrominated Diphenyl Ethers by GC-ICP-MS**; Steven Wilbur[1], Emmett Soffey[1]; [1]Agilent Technologies

12:10 (443) **Speciation Studies in Large Biomolecules**; J. Sabine Becker[1], J. Susanne Becker[2], Miroslav V. Zoriy[1], Carola Pickhardt[1], Michael Przybylski[2]; [1]Central Division of Analytical Chemistry Centre Juelich; [2]Laboratory of Analytical Chemistry

Wednesday Morning, Room B116
BIOLOGICAL ANALYSIS ENABLED BY MICROMACHINING TECHNOLOGIES
Organizer and Presider: Adam Wooley

10:30 (444) **Microfluidics for Genetic Analysis, Pathogen Detection and Space Exploration**; Richard Mathies[1]; [1]University of California, Berkeley

11:10 (445) **Miniaturized Electrically Driven Systems for Protein Analysis**; Adam Woolley[1]; [1]Brigham Young University

11:30 (446) **Metabolic Analysis by Microchip Electrophoresis/Electrochemistry**; Charles Henry[1], Carlos Carcia[1, 2], Yan Liu[1]; [1]Colorado State University; [2]University of Texas-San Antonio

11:50 (447) **Deciphering the Role of Nitric Oxide in Vessel Relaxation using a Microchip-based Endothelium;** Dana Spence[1], Nicholas Torrence[2], Alexander Price[2]; [1]Wayne State University; [2]Saint Louis University

12:10 (448) **Chemical Analysis of Subcellular Structures Enabled by Micro and Nano Fluidics**; Daniel T. Chiu[1]; [1]University of Washington

Wednesday Morning, Room B114
MULTIVARIATE ANALYSIS OF HYPERSPECTRAL IMAGES
Organizer and Presider: David Haaland

10:30 (449) **Discriminant Image Resolution: MCR Analysis of Multivariate Image Utilizing Both Spatial and Spectral Information**; Thomas Hancewicz[1], Ji-hong Wang[2]; [1]Unilever R&D; [2]JHW Consulting

11:10 (450) **Spectral Unmixing of Remotely Sensed Thermal Infrared Hyperspectral Images Using Multivariate Curve Resolution**; Chris Stork[1], Michael Keenan[1], David Haaland[1]; [1]Sandia National Laboratories

11:50 (451) **New Approaches for Understanding Multivariate Curve Resolution Applied to Hyperspectral Images**; David Haaland[1], Jerilyn Timlin[1], Howland Jones[1], Michael Keenan[1], Christopher Stork[1], David Melgaard[1], Michael Sinclair[1]; [1]Sandia National Laboratories

12:10 (452) **Multivariate Curve Resolution of Hyperspectral Images: Initialization and Functional Constraints**; Neal Gallagher[1], Jeremy Shaver[1], Barry Wise[1]; [1]Eigenvector Research, Inc.

Wednesday Morning, Room B113
NEW IDEAS IN TEACHING ANALYTICAL CHEMISTRY
Organizer and Presider: David Harvey

10:30 (453) **Teaching Efficient Experimental Design and Multiple Approaches to Data Interpretation in the Analytical Chemistry Laboratory Curriculum**; Richard Stolzberg[1]; [1]University of Alaska Fairbanks

10:50 (454) **Integration and Assessment of Service-Learning into Introductory and Analytical Chemistry**; Joan Esson[1]; [1]Kalamazoo College

11:10 (455) **Critical Thinking and Problem Based Learning via Complementary Instrumentation Laboratory Exercises**; Douglas Klarup[1], Jonathan Blitz[1], David McCurdy[2]; [1]Eastern Illinois University; [2]Truman State University

11:30 (456) **A Literature-Based Senior Level Instrumental Course**; Jason Evans[1]; [1]University of Massachusetts

11:50 (457) **Multiple Instruments, Courses, Users, and Disciplines: An Overview of Two NSF-CCLI Projects at Trinity University**; Michelle Bushey; [1]Trinity University

12:10 (458) **Environmental Chemistry Design Projects in the Analytical Chemistry Curriculum**; Robert Hamers, Pamela Doolittle, Robert McClain; [1]University of Wisconsin-Madison

Wednesday Morning, Room C124
VIBRATIONAL SPECTROSCOPY COUPLED WITH COMBINATORIAL CHEMISTRY
Organizer and Presider: John Chalmers

10:30 (459) **Realising the Potential of Infrared Microscopy for Combinatorial Chemistry**; Andrea Russell[1], Gurjit Mandair[1], Mark Bradley[1]; [1]University of Southampton

11:10 (460) **Mapping Inside Solid Supports: Scanning Confocal Raman Spectroscopy**; Jeremy Frey[1], Mark Bradley[1], Jurgen Kress[1], Abbe Rose[1], Helen Stanford[1]; [1]School of Chemistry, University of Southampton

11:30 (461) **The Contribution of Vibrational Spectroscopy in Addressing the Critical Quality Issue in Combinatorial Chemistry**; Bing Yan; [1]DPI

12:10 (462) **IR and Raman Tag Strategy for Monitoring Solid Phase Oligosaccharide Synthesis**; Mike George[1], Mike Hargreaves[1], Barrie Kellam[1]; [1]University of Nottingham

TECHNICAL PROGRAM – WEDNESDAY
Orals 10:30 AM – 12:30 PM and 3:30 –5:30 PM

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 Smith[1], David Camp[1], Jon Jacobs[1], Weijun Qian[1], Mary Lipton[1], Harold Udseth[1], Ljiljana Pasa-Tolic[1], Gordon Anderson[1], Yufeng Shen[1], Matthew Monroe[1]; [1]Pacific Northwest National Laboratory

11:10 (464) **Rapid Proteomic Analysis Using Accurate Mass Data and HPLC/MALDI/FTMS**; I Jonathan Amster, Bryan A Parks, Jeremy Wolff, Hilda Hernandez, Iris Porat, William B Whitman; [1]University of Georgia

11:30 (465) **Precise Characterization of Intact Proteins Using a Top Down Strategy with a High-Resolution Q-FTMS**; Michael J. Roth[1], Andrew J. Forbes[1], Yi Du[1], Steven M. Patrie[1], Michael T. Boyne III[1], Lihua Jiang[1], Jim Pesavento[1], Jon Ferguson[1], Rich LeDuc[1], Neil L. Kelleher[1]; [1]University of Illinois

11;50 (466) **Incorporating FTICRMS into a shotgun proteomics process**; David Goodlett[1], Scott Shaffer[1], Byron Gallis[1], Jinzhi Chen[1]; [1]University of Washington

12:10 (467) **NanoLC-FTMS Based Mapping of Protein Oxidation Sites Using Element-Coded Affinity Mass Tags**; Nicolas L. Young[1], Susan Lee[2], Paul A. Whetstone[2], Nathaniel G. Butlin[2], Todd M. Corneillie[2], Sarah M. Cheal[2], Christopher G. Bailey[1], Lori C. Zeller[1], W. Henry Benner[1], Claude F. Meares[2]; [1]Lawrence Livermore National Laboratory, Biosecurit; [2]University of California, Davis

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 Rogers; [1]University of Illinois

11:10 (469) **Rare-Earth-Doped Nano-Structured Materials for Optical Fiber Amplifiers**; Bernard Jacquier[1], Anne Marie Jurdyc[1], Laurent Bigot[2], Bruno Gallas[3], Dominique Bayart[4], Laurent Gasca[4]; [1]Laboratoire de Physico-Chimie des Matériaux Lumine; [2]Laboratoire de Physique des Lasers Atome; [3]Laboratoire d'Optique du Solide University; [4]Alcatel Research & Innovation

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

12:10 (471) **Collective Plasmonic Behavior of Metal Nanoparticle Structures**; Gary Wiederrecht[1], Gregory Wurtz[1], Alexandre Bouhelier[1], Jasmina Hranisavljevic[1], Stephen Gray[1], Renaud Bachelot[1], Jin Seo Im[1]; [1]Argonne National Laboratory

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

10:30 (472) **Analysis of Dyed Fibers by Raman Microspectroscopy**; S. Michael Angel[1], Brandi L. Clelland[1], James E. Hendrix[1], Stephen L. Morgan[1], Edward G. Bartick[2]; [1]Department of Chemistry & Biochemistry, The University of South Carolina; [2]Counterterrorism and Forensic Science Research

10:50 (473) **Novel Strategies for Sampling Processes with Raman Spectroscopy**; Brian Dable[1,2], Brian Marquardt[1,2], David Veltkamp[1,2], Brooke Love[2], Marvin Lilley[2], Sylvie Theas[2]; [1]Center for Process Analytical Chemistry; [2]University of Washington

11:10 (474) **Raman Spectroscopy for Quantification of Fat Composition in High-protein Whey Emulsions**; Nils Kristian Afseth[1], Vegard Herman Segtnan[1], Jens Petter Wold[1], Brian J. Marquardt[2]; [1]Matforsk - Norwegian Food Research Institute; [2]CPAC University of Washington

11:30 (475) **Development of Raman-Based Methods for Waste Analysis at the Savannah River Site**; Robert Lascola[1], Charles Coleman[1], David Hobbs[1]; [1]Savannah River National Laboratory

11:50 (476) **Process Raman Chemical Imaging**; Matthew Nelson[1], Julianne Wolfe[1], Laura Marks[1], Patrick Treado[1]; [1]ChemImage Corporation

12:10 (477) **Advanced Control of Manufacturing Processes Using Raman-Based Gas Analysis**; Ronald Rich[1]; [1]Atmosphere Recovery, Inc.

WEDNESDAY POSTER SESSIONS and BREAK
2:00 – 3:30 PM, See pages 56 - 58
Exhibit Hall A/A-1

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**; Peter B. Armentrout[1], Rohana Liyanage[1], Xiao-Guang Zhang[1]; [1]University of Utah

3:50 (479) **Cu+-Ligand Interactions: Structures and Bond Dissociation Energies. Solvation, Chelation, and Hydrogen Bonding Interactions**; Mary T. Rodgers, Nalaka S. Rannulu[1]; [1]Wayne State University

4:10 (480) **Metal Complex Coordination Structure from Gas-Phase Ion-Molecule Reactions in a Quadrupole Ion Trap Mass Spectrometer**; Richard W. Vachet[1], Marianny Y. Combariza[1], Angela M. Fahey[1]; [1]University of Massachusetts

4:30 (481) **Exploration of Gas-Phase Uranium Complex Reactions Using Electrospray Ionization and Ion-Trap Mass Spectrometry**; Michael Van Stipdonk[1], Gary Groenewold[2], Gary Gresham[2], Winnie Chien[1], Victor Anbalagan[1]; [1]Wichita State University; [2]Idaho National Engineering and Environment

4:50 (482) **Molecular Nanoboxes with Metal Ion Lids**; David Dearden[1], Jon Willes[1], Kevin Walker[1], Haizhen Zhang[1], Krzysztof Krakowiak[2] ; [1]Brigham Young University Department of Chemistry & Biochemistry; [2]IBC Advanced Technologies, Inc.

5:10 (483) **Host-Guest Interactions of Uranyl Carbonate Probed by Mass Spectroscopy**; Jason Telford[1], Nathan Lien[1]; [1]University of Iowa

5:30 (483b) **Se and S Trichalcogenides: Facts from Artifacts;** Juris Meija[1], Joseph A. Caruso[1]; [1]University of Cincinnati, Department of Chemistry

TECHNICAL PROGRAM – WEDNESDAY
Orals 3:30 – 5:30 PM

Wednesday Afternoon, Room B116
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 Allbritton[1,3,4], Jim Palmer[1], G.P. Li[2,3,4], Mark Bachman[2,3,4], Chris Sims[1]; [1]Department. of Physiology and Biophysics, University of California; [2]Department of Electrical and Computer Engineering; [3]Center for Biomedical Engineering; [4]Integrated Nanosystems Research Facility

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

4:30 (486) **Manipulating Membrane Bound Bioparticles with Channel Structures and Electric Fields**; Mark Hayes[1], Timothy Crowley[1], Michele Pysher[1]; [1]Arizona State University

4:50 (487) **Exploring Mitochondrial Properties Using Microfluidic Devices**; Edgar Arriaga[1], Chris Whiting[1], Karen Olson[1]; [1]University of Minnesota

5:30 (488) **An Integrated PC 12 Cell Reactor/Analysis System**; Michelle W. Li[1], Michelle L. Kovarik[1]; [1]Saint 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 Johnson[1]; [1]University of Utah

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

4:50 (491) **Application of Multivariate Curve Resolution to the Analysis of FT-IR Hyperspectral Images**; Boiana Budevska; [1]DuPont

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

Wednesday Afternoon, Room C124
IR MICROSPECTROSCOPY INSTURMENTATION AND APPLICATIONS
Organizer and Presider: John Hellgeth

3:30 (493) **Developments in Infrared Microspectroscopy**; John A. Reffner[1]; [1]SensIR Technologies

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

4:10 (495) **ATR Microspectroscopy for Chromatographic Detection**; Andre' Sommer[1], Brian Patterson[1], Neil Danielson[1]; [1]Miami University

4:30 (496) **The Role of Infrared and Raman Imaging in Biological Warfare Detection**; Kathryn Kalasinsky[1], Victor Kalasinsky[2]; [1]Divsion of Microbiology, Armed Forces Institute; [2]Division of Environmental Toxicology

4:50 (497) **The Contribution of Dipicolinic Acid and Calcium Dipicolinate in the Mid-infrared Absorbance of Bacillus subtilis studied by FT-IR Reflectance Microspectroscopy**; D. L. Perkins[1], C. R. Lovell[1], B. V. Bronk[2], B. Setlow[3], P. Setlow[3], M. L. Myrick[1]; [1]University of South Carolina; [2]Air Force Research Laboratory at U.S.A; [3]Univ of Connecticut Health Center

5:10 (498) **Robust Microanalysis Methods in the Semiconductor Foundry**; Stephen Hill[1], Paul Swain[1]; [1]WaferTech LLC

Wednesday Afternoon, Room A105
FTMS FOR PROTEOMICS
Organizer and Presider: Carlito Lebrilla

3:30 (499) **Fourier Transform Ion Cyclotron Resonance for Proteomics: High Resolution, Accurate Mass, MS/MS, and Speed**; Christopher Hendrickson[1,2], Greg Blakney[1], Michael Chalmers[1], Mark Emmett[1,2], Logan Mackay[1,2], Melinda McFarland[1], Carol Nilsson[1], John Quinn[1], Matthew Renfrow[1], Alan Marshall[1,2]; [1]National High Magnetic Field Laboratory; [2]Department of Chemistry and Biochemistry

4:10 (500) **Analysis of Clathrin Coated Vesicles by LC-FTMS**; Daniel Boismenu; [1]Réseau Proteomique de Montréal Proteomics Network

4:30 (501) **Top Down and Bottom Up Analysis of the Human Ribosome use FTICR**; Julie Leary[1]; [1]UC Berkeley

4:50 (502) **An Integrated Biomarker Discovery Platform Based on nanoLC-dual-ESI-FT-ICR Mass Spectrometry**; Adam M. Hawkridge[1], Christopher J. Mason[1], Kenneth L. Johnson[1], H. Robert Bergen III[1], David C. Muddiman[1]; [1]Mayo Clinic College of Medicine

5:10 (503) **A Glycomics Approach to Proteomics**; Carlito Lebrilla, Hyunnjoo An; [1]University of California, Davis

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 Liu[1]; [1]Duke University

4:10 (505) **Carbon Nanotube as Chemical Sensors**; Shu Peng[1], Kyeongjae Cho[1]; [1]Stanford University

4:50 (506) **Moving and Sensing Biomolecules Using Nanotube Membranes**; Punit Kohli[1], C. Chad Harrell[1], Zuzanna Siwy[1], Charles R. Martin[1]; [1]University 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 Henson[1]; [1]Pfizer Global R&D

3:50 (508) **Raman Spectroscopy: a PAT Tool for Quantitative Assessment of Tablet Potency**; Jonas Johansson[1], Jonas Eriksson[1], Staffan Folestad[1]; [1]AstraZeneca R&D Molndal, Sweden

4:10 (509) **Application of Raman and IR Spectroscopy in Pharmaceutical Development**; Sabine Pfeffer - Hennig[1], Miriam Bellus[1]; [1]Novartis Pharma AG, Chemical & Analytical Development

4:30 (510) **The Use of Raman Spectroscopy in the Detection of Counterfeit and Adulterated Pharmaceutical Products**; Mark Witkowski[1], Thomas Brueggemeyer[1], JaCinta Batson[1], Jill Loeliger[1]; [1]FDA / Forensic Chemistry Center

4:50 (511) **Raman Spectroscopy for the Characterization of Solid-state Forms During Pharmaceutical Manufacturing.**; Robert Cambron ; [1]Procter and Gamble

5:10 (512) **Monitoring the Kinetics of Solvent Mediated Phase Conversions of Pharmaceutical Solids**; Lynne Taylor[1], Håkan Wikström[1], Jukka Rantanen[2]; [1]Purdue University; [2]University of Helsinki

TECHNICAL PROGRAM – THURSDAY
Plenary and Posters

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 Willse[1], Blandina Valenzuela[1], Jon Wahl[1], George Preti[2], Peter Yang[2], Jae Kwak[2], Kunio Yamazaki[2], Gary Beauchamp[2]; [1]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], Fuminobu Hirose[2], Kenichi Senda[2], Isao Noda[3]; [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[1], David Lockwood[1], Rabah Boukherroub[2]; [1]National Resarch Council, Ottawa, Ontario, Canada; [2]Interdisciplinary Research Institute

(529) **High Sensitivity Ammonia Monitor Based on Cavity Ringdown Spectroscopy**; Bernard Fidric[1], Steve Sanders[1], Sze Tan[1], Hoa Pham[1], Alexander Kachanov[1], Edward Wahl[1], Eric Crosson[1], Barbara Paldus[1]; [1]Picarro, Inc.

(530) **Identification of the Polymorphs of Sulfathiazole Using Terahertz Pulsed Spectroscopy**; Philip Taday[1], David Newnham[1], Yaochun Shen[1], Clare Strachan[2]; [1]TeraView Limited; [2]School of Pharmacy and Department of Che

(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. Shober[2], Rupinder K. Randhawa[1]; [1]Crop & Soil Sciences Department, The Pennsylvania State University; [2]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 fluorenes used for OLED applications**; Vasilis Gregoriou[1], Christos Chochos[1], Joannis Kallitsis[2]; [1]FORTH-ICEHT; [2]University of Patras

(535) **Organic Monolayer Vibrational Spectroscopy Using Single Reflection ATR**; Nelson Rowell[1], Li-Lin Tay[1], David Lockwood[1], Rabah Boukherroub[2]; [1]National Resarch Council, Ottawa, Ontario, Canada; [2]Interdisciplinary Research Institute, IE

(536) **On The Photooxidation of a Crude Iranian Petroleum Maltenic Fraction as a Film over Seawater**; Babak Nahriniknafs[1]; [1]A.S.S.C

(537) **Optical Diagnostics for the Iodine Sulfur Cycle**; Denis Doizi[1], Vincent Dauvois[1], Jean Luc Roujou[1], Vincent Delanne[1], Bruno Larousse[1], Olivier Hercher[1], Pierre Fauvet[1], Christophe Moulin[1]; [1]CEA

(538) **Determination of the Absolute Configuration and Dimeric Liquid-State Conformation of a Chiral Acetylenic Carboxylic Acid**; Richard W. Duerst[3], Teresa B. Freedman[1], Rina K. Dukor[2], Kerry Swift[3], Rodger F. Henry[3], Laurence A. Nafie[1,2]; [1]Syracuse University, Department of Chemistry; [2]BioTools, Inc.; [3]Abbott Laboratories

(539) **Metrological Characterizationof Didymium Oxide Wavelength Reference Materials in the Short-Wave Near Infrared Region**; Jerry Messman[1]; [1]Stranaska LLC

IR Microspectroscopy Imaging

(540) **A Faster Approach to Infrared Rheo-Optics using Planar Array Infrared Spectroscopy**; Christian Pellerin[1], Simon Frisk[1], John Rabolt[1], Bruce Chase[2]; [1]University of Delaware; [2]DuPont Inc.

(542) **A Sampling Methodology to Overcome Optical Anomalies and Thickness Dependence in FT-IR Imaging and Combined Automated Polarized Light/Raman Microscopy**; Douglas Elmore[1], Chad Leverette[1], Sean Smith[1], Brian Anderson[1], Allen Muroski[1], Var St. Jeor[1]; [1]Cargill, Inc.

(543) **Real Time Study of the Branching Effect in Phospholipids at the Air/Water Interface Using Planar Array Infrared (PA-IR) Spectroscopy**; Yujuan Liu[1], Isabelle Pelletier[1], Christian Pellerin[1], Bruce Chase[2], John Rabolt[1]; [1]University of Delaware, Department of Materials Science; [2]Central Research and Development, DuPont

(544) **Characterization of Nafion Membrane Conversion Using IR and MXRF Imaging**; George Havrilla[1], Matthew Stanton[1], Richard Ames[1]; [1]Los Alamos National Laboratory

(545) **Hyperspectral Imaging for Endogenous and Exogenous Fluorophore Differentiation in Live Cells**; Jerilyn Timlin[1], David Haaland[1], Michael Sinclair[1], Michael Keenan[1]; [1]Sandia National Laboratories

(546) **Microscopic FT-IR Imaging: Spatial Resolution and the Diffraction Limit**; Jonathan Tarr[1], Koichi Nishikida[1], William J. McCarthy[1], N. Simon Nunn[1]; [1]Thermo Electron Corporation

(547) **Objective Data Cube Comparison Following Near-Infrared Spectroscopic Imaging**; Thomas W. Brueggemeyer[1], Mark R. Witkowski[1], JaCinta S. Batson[1], Jill R. Loeliger[1]; [1]U.S. Food & Drug Administration--Forensic Chemistry

(548) **Spread Spectrum Image Steganography**; Srinivasan Allimuthu[1]; [1]Crescent Engineering College

(549) **Real-Time Detection of Chemical Agents Using Planar Array Infrared Spectroscopy**; Christian Pellerin[1], John F. Rabolt[1], D. Bruce Chase[2]; [1]University of Delaware; [2]DuPont Inc.

MS Front-End Devices and New Methodology for Proteomics

(550) **Electrowetting-on-Dielectric for Analysis of Peptides and Proteins by Matrix Assisted Laser Desorption/Ionization Mass Spectrometry**; Robin L. Garrell[1], Aaron R. Wheeler[1], Hyejin Moon[2], Chang-Jin Kim[2], Joseph A. Loo[1]; [1]UCLA Department of Chemistry; [2]UCLA Department of Mechanical Engineerin

(551) **Statistical Tools for Microorganism Identification Using Matrix-assisted Laser Desorption/Ionization Mass Spectrometry.**; Nathaniel Beagley[1], Kristin H. Jarman[1], Nancy B. Valentine[1], Catherine E. Petersen[1], Karen L. Wahl[1]; [1]Pacific Northwest National Laboratory

(552) **Silica Sol-gels for MALDI-MS Application**; Noemi Nagy[1], Suzanne Ackloo[1], Sanela Martic[2], Vladimir Baranov[1], John D. Brennan[2]; [1]MDS Sciex; [2]McMaster University

(553) **Differential Chemistry as a Function of Droplet m/z using a Variation of the tandem MS Theme (EDB+MALDI-MS)**; George Agnes, Samuel Bakhoum[1], Mike Bogan[1]; [1]Simon Fraser University

(554) **The Use of Gallium and MALDI Matrices to Study Proteins by pulsed Glow Discharge Time-of-Flight Mass Spectrometry**; Na Zhang[1], Megan DeJesus[1], Jennifer Robertson[1], Lei Li[1], Yuchen Lu[1], Fred King[1]; [1]West Virginia University[4]

(555) **Survey of Purification Methods for the Analysis of Albumin to Detect Sulfur Mustard Adducts**; Carrie Young[1], Adrian Woolfitt[1], Hercules Moura[1], Lisa McWilliams[1], Anne Boyer[1], John Barr[1]; [1]Centers for Disease Control and Prevention

(556) **Evaluation of Gallium and MALDI Matrices for Pulsed Glow Discharge**; Na Zhang[1], Megan DeJesus[1], Jennifer Robertson[1], lei li[1], Yuchen Lu[1], Fred King[1]; [1]West Virginia University

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

Nanotubes and Nanowires for Sensing

(557) **Confocal Raman-AFM, a New Tool for Materials research**; Olaf Hollricher[1], Ute Schmidt[1], Wolfram Ibach[1], Sabine Hild[2], Joerg Mueller[1], Joachim Koenen[1], Klaus Weishaupt[1]; [1]WItec GmbH; [2]Department 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 Owen[1], J. Steven Lancaster[2], David Littlejohn[1], Thomas Lynch[2], Robert Wright[3]; [1]Department of Pure and Applied Chemistry/CPACT, Un; [2]Hull Research & Technology Centre, BP Ch; [3]Thermo ONIX, Winsford, Cheshire, UK

(559) **Visualizing Vortex Shedding >From a Square Cylinder using Pressure Sensitive Paint**; Christina McGraw[1], Gamal Khalil[1], James Callis[1]; [1]University of Washington Department of Chemsitry

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

Emerging Technologies for Process Analysis

(561) **Identification and Characterization of Process Impurities and Oxidative Degradate Products in Iveremctin**; Chris Beasley[1], Kyle Fliszar[1], Andreas M. Abend[1], Robert A. Reed[1]; [1]Merck Research Laboratories, Merck & Co., Inc.

(562) **HPLC at High Temperature and High pH with a New, Highly Stable Silica Column**; Dale Felix[1], Stephanie Marin[1], Brian Jones[1]; [1]Selerity Technologies

(562) **Non-Invasive Determination of Porosity in Solids by Diode Laser Oxygen Spectroscopy: Application to Pharmaceutical Tablets**; Tomas Svensson[1], Jonas Johansson[2], Stefan Andersson-Engels[1], Sune Svanberg[1], Staffan Folestad[2]; [1]Department of Physics, Lund Institute of Technology, Lun; [2]Astra Zeneca R&D, Molndal, Sweden

(565) **Development/Validation of a New Reversed-Phase Ion-Pair HPLC Method for Detection/Quantitation of New Insulin Related Substances in Purification Processes in Development**; Warren Rowland[1], Xiangli Zhang[1], Renee Ricke[1]; [1]Eli Lilly

(566) **The Use of Thermal Desorption GC/MS To Monitor the Weight Loss During Thermal Gravimetric Analysis**; Charles Pan[1], Marilyn Alvine[1], Frances Liu[1], Richard Vivilecchia[1]; [1]Novartis Pharmaceuticals Corporation

(567) **Calibration Transfer in Near-infrared Spectroscopy**; Mike Claybourn[2], Mark Smith[1], Anthony Moffat[1], David Rees[1]; [1]School of Pharmacy, University of London; [2]AstraZeneca

(568) **Development of an Automated Protocol for Preparation of Samples for Silicone Functionality Analysis by Gas Chromatography**; Herbert Brothers, Cynthia Gould, Tanya Habitz, Ronda Grosse; [1]Dow Corning Corporation

Raman Microscopy and Imaging

(569) **Raman Analysis of Diamonds and Gemstones**; Amanda Jenkins[1], Richard Larsen[1]; [1]Jasco Inc.

(570) **A New Triple Additive/Subtractve Monochromator Design Provides the Ultimate Flexibility**; Ryan Sullivan[1], Bruce True[1], Ravi Guntupalli[1]; [1]Princeton Instruments (a division of Roper Scientic)

(571) **The Combination of Automated Polarized Light Microscopy and Raman Microscopy for the Analysis of Chemical Systems**; Chad Leverette[1], Sean Smith[1], Douglas Elmore[1]; [1]Cargill, Incorporated

(572) **Elastic Deformation of Bone Probed by Raman Spectroscopy: Apparatus and Results**; Andrew Callender[1], William Finney[1], Michael Morris[1]; [1]University of Michigan

(574) **Micro Raman Spectroscopic Investigation of Solvent and Dye Diffusion in Polymers**; Andreas Gupper[1], Jaap van der Weerd[1], Sergei G. Kazarian[1]; [1]Imperial College London

(575) **High Brightness Lasers in Confocal Raman Spectroscopy**; Kelly Cox; [1]Thermo Electron Corporation

(576) **An Ex Vivo Study of Early Dental Caries by Multi-Modal Optical Methods**; Alex C.-T. Ko[1], Lin-P'ing Choo-Smith[1], Mark Hewko[1], Larry Leonardi[1], Cecilia Dong[2], Peter Williams[2], Blaine Cleghorn[3]; [1]Institute for Biodiagnostics, National Research Council; [2]Department of Restorative Dentistry; [3]Department of Dental Clinic Sciences

(577) **Raman Study of GaAs1-xBix/GaAs Epilayers Grown by Molecular Beam Epitaxy**; Li-Lin Tay[1], David Lockwood[1], Erin Young[2], Tom Tiedje[2]; [1]National Resarch Council, Ottawa, Ontario, Canada; [2]Department of Physics, University of British Columbia

(578) **Effect of Reactant Gas Velocity and Geometry on CARS Monitored Pulsed rf Pulsed PECVD Silicon Nitride Thin Films**; BarJean Phillips[1], Rene Rodriguez[1], Lisa Lau[1], Shane Steidley[2]; [1]Idaho State University; [2]AMI Semiconductor

(579) **Contributions to BioDefense and Pathology Utilizing Molecular Chemical Imaging**; Patrick Treado[1], Steve Vanni[1], John Maier[1], Matthew Nelson[1]; [1]ChemImage Corp.

(580) **Raman Microspectroscopy: an Efficient Technique to Determine Quantitatively the Orientation of Protein Fibers**; Thierry Lefèvre[1], Marie-Eve Rousseau[1], Michel Pézolet[1]; [1]Université laval -CERSIM

(582) **Performance of Raman Mapping and Imaging Systems in the Analysis of Solid Dosage Pharmaceuticals**; Slobodan Sasic[1], Don Clark[1], John Mitchell[2], Martin Snowden[2]; [1]Pfizer, Analytical R & D, Ramsgate Road, Sandwich,; [2]Universiity of Greenwich, Medway Science

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

10:30 (583) **Metallomics - Overview and Analytical Opportunity Prognosis**; David W. Koppenaal[1]; [1]Pacific Northwest National Laboratory

10:50 (584) **Microorganisms and the Chemical Elements**; Lawrence Wackett[1]; [1]University of Minnesota

11:30 (585) **Metal isotopes in metallomics**; Ariel Anbar[1]; [1]Arizona State University

11:50 (586) **High Throughput ICP-MS Analysis of the Arabidopsis Ionome**; David E Salt[1], D.J. Eide[2], J.F. Harper[3], J.I. Schroeder[4], J.M. Ward[5], M.L. Guerinot[6]; [1]Purdue UIniversity; [2]University of Missouri; [3]University of Nevada-Reno; [4]UC-San Diego

Thursday Morning, Ballroom 201
APTAMERS IN ANALYSIS
Organizer and Presider: Mike Bower

10:30 (587) **Aptamer Biosensors**; Andrew D. Ellington; [1]University of Texas, Austin

10:50 (588) **Kinetic CE Methods for Selection, Characterization, and Analytical Utilization of Oligionucleotide Aptamers;** Sergey Krylov[1], Berezovski Maxim[1], Drabovich Andrei[1], Svetlana Krylova[1], Musheev Michael[1], Okhonin Victor[1], Petrov Alexander[1]; [1]Department of Chemistry, York University

11:10 (589) **Progress Towards a High-Throughput, Aptamer-Based Nanoextractor**; Vincent Remcho[1], Angela Doneanu[1], Jack Rundel[1], Yolanda Tennico[1]; [1]Oregon State University

11:30 (590) **Molecular Engineering of Nucleic Acids for Bioanalysis and Bionanotechnology**; Weihong Tan[1]; [1]University of Florida

11:50 (591) **Novel Analytical Aptamer Reagents for Microfluidic Chips**; Nils Walter[1], Robert Kennedy[1], Jens-Christian Meiners[2], Phillip Sekella[1], Jennifer Willard[1], Katherine Korbiak[2], Meredith Lambert[1]; [1]Department of Chemistry, University of Michigan; [2]Department of Physics and Biophysics Research

12:10 (592) **CE-SELEX - In Vitro Selection of Functional DNA using Capillary Electrophoresis;** Michael Bowser[1], Shaun Mendonsa[1], Renee Mosing[1]; [1]University of Minnesota

TECHNICAL PROGRAM – THURSDAY
Orals 10:30 AM – 12:30 PM

Thursday Morning, Room B114
CHEMOMETRICS APPLICATIONS OF CLUSTER ANALYSIS AND PATTERN RECOGNITION
Organizer and Presider: Barry Lavine

10:30 (593) **Genetic Algorithms for Pattern Recognition: Feature Selection, Classification, Clustering, and Prediction in a Single Step**; Barry Lavine, Charles Davidson; [1]Clarkson University

11:10 (594) **Multivariate Curve Resolution as a Chemical Classification Tool**; Thomas Hancewicz[1], Ji-hong Wang[2], David Budac[1]; [1]Unilever R & D; [2]JHW Consulting

11:30 (595) **New Approaches to Classification using Wavelets and Trees**; Steven Brown[1], Anthony Myles[1], Nathaniel Woody[1,2]; [1]University of Delaware; [2]Glaxo-SmithKline, RTP, NC

11:50 (596) **The Development of UV Resonance Raman Spectroscopy for Bacterial Identification**; E. Consuelo Lopez Diez[1], Royston Goodacre[1]; [1]UMIST, Department of Chemistry

12:10 (597) **UV Spectroscopy in Conjunction with Chemometrics Analysis: A Simplified Approach for Differentiation of Functional Foods**; Dave Luthria[1], Sudarsan Mukhopadhyay[1], James Harnly[1], John Finley[2], David Burns[3]; [1]Food Composition Lab, USDA; [2]Grand Forks Human Nutrition Research Center; [3]Department of Chemistry, McGill University

Thursday Morning, Room B113
RESEARCH SUPPORTIVE CURRICULA IN ENVIRONMENTAL CHEMISTRY
Organizer and Presider: Anna Cavinato

10:30 (598) **Outcomes of the Undergraduate Research Summit: Developing Research-Supportive Curricula**; Thomas Wenzel; [1]Bates College

10:50 (600) **Analytical-Environmental Chemistry Research in the Undergraduate Curriculum at the Richard Stockton College of New Jersey**; Kristen Hallock-Waters[1], Louise Sowers[1], Raymond Mueller[1], Tait Chirenje[1], Daniela Zima[1], Jamie Hale[1]; [1]The Richard Stockton College of New Jersey

11:10 (601) **Atomic Absorption Spectroscopy in Undergraduate Teaching and Research**; David Goodney; [1]Willamette University

11:30 (602) **Integrating Environmental Analytical Research Throughout the Curriculum**; Kevin Cantrell; [1]University of Portland

11:50 (603) **Enhancing Research and Service Learning Ppportunities in Environmental Chemistry**; Anna Cavinato[1], Ronald Kelley[1]; [1]Eastern Oregon University

Thursday Morning, Room C124
NEW TECHNIQUES IN SAMPLING FOR IR SPECTROSCOPIC DATA
Organizer and Presider: Peter Griffiths

10:30 (604) **With Diamond, Anything is Possible**; John A. Reffner[1]; [1]SensIR Technologies

11:10 (605) **Direct Analysis of Condensed Samples Using Photoacoustic and Transient Infrared Spectroscopies**; John McClelland[1,2], Roger Jones[1], Anthony Wagner[1]; [1]Ames Laboratory-USDOE; [2]MTEC Photoacoustics, Inc.

11:50 (606) **Attenuated Total Reflection Direct-Deposition Nanosampler**; James de Haseth[1], Shelly Seerley[1]; [1]University of Georgia

12:10 (607) **Mid-Infrared Diffuse Reflection Spectroscopy of Species In and On Absorbing Substrates**; Lacey Averett[1], David Heaps[1], Peter Griffiths[1]; [1]Univ. of Idaho

Thursday Morning, Room A105
MS FONT-END DEVICES AND NEW METHODOLOGY FOR PROTEOMICS
Organizer and Presider: Liang Li

10:30 (608) **Imaging MALDI with an Orthogonal TOF Mass Spectrometer**; Werner Ens[1], Gamini Piyadasa[1], James R McNabb[1], Victor Spicer[1], Kenneth G Standing[1]; [1]Dept. of Physics and Astronomy, University of Manitoba

10:50 (609) **Evaluating Large Proteomics Datasets from HPLC-ESI-MS/MS Experiments**; Daniel Figeys[1]; [1]University of Ottawa

11:10 (610) **Analysis of the Ciliome of the Protozoan Tetrahymena Thermophila Using Translated and Unannotated Genomic Information**; K.W. Michael Siu[1,2,3], Jeffrey C. Smith[1,3], Ronald E. Pearlman[2,3]; [1]Department of Chemistry, York University; [2]Department of Biology, York University; [3]Centre for Research in Mass Spectrometry

11:30 (611) **Alternative Separation Strategies for Shotgun Proteomics**; Ron Orlando[1], James Atwood[1], Cameron Cavola[1], Brent Weatherly[2], Todd Minning[2], Rick Tarleton[2]; [1]Complex Carbohydrate Research Center, University of Georgia; [2]Department of Cellular Biology, University of Georgia

11:50 (612) **Improvement of N-terminal Sulfonation Procedures for MALDI PSD Peptide Sequencing and Its Application in Determining Protein Ubiquitination**; Dongxia Wang, Robert J. Cotter; [1]Johns Hopkins University School of Medicine

12:10 (613) **Electrodynamic Charged Droplet Processing to Couple Low Flow Rate Separations with MALDI-MS**; George Agnes[1], Michael J. Bogan[1]; [1]Simon Fraser Univ.

Thursday Morning, Room B115
NANOTUBES AND NANOWIRES FOR SENSING
Organizers: Peter Pehrsson and Jie Liu • Presider: Jie Liu

10:30 (614) **Modulating the Optical Response of Single Walled Carbon Nanotubes to Specific Molecular Adsorption: Tissue Implantable Biosensors**; Michael Strano[1], Seunghyun Baik[1], Paul Barone[1], Daniel Heller[1]; [1]Department of Chemical and Biomolecular Engineering

10:50 (615) **Chemical and Bio Sensors Based on nanowires and Nanotubes**; Chongwu Zhou[1]; [1]University of Southern California

11:30 (616) **Optical pH Sensing Based on Surface-Modified Single-Walled Carbon Nanotubes**; Wei Zhao[1], Chulho Song[1], Pehr Pehrsson[2], Kristy Kelley[1], Brian Benedict[1]; [1]Department of Chemistry, University of Arkansas; [2]Chemistry Division, Naval Research Labor

11:50 (617) **Carbon nanotubes based nanoelectrode arrays: fabrication, evaluation, and chemical & biosensing applications**; Yuehe Lin[1], Yi Tu[2], Fang Lu[1], Wassana Yantasee[1], Zhifeng Ren[2]; [1]Pacific Northwest National Laboratory; [2]Boston College

12:10 (618) **Tailored Assembly of Carbon Nanotubes by Chemical Vapor Deposition**; Pulickel Ajayan[1], Anyuan Cao[1], Yong Jung[1], Guowen Meng[1]; [1]Rensselaer Polytechnic Institute

Thursday Morning, Room B116
STATE OF THE ART INFRASTRUCTURE FOR PAT SPECTROSCOPY IN INDUSTRY
Organizer and Presider: Terry Todd

10:30 (619) **Process Analysis Technology at Roche Ireland Limited, a Holistic Approach**; John O'Reilly; [1]Roche Ireland Limited

10:50 (620) **Collaborations and Teaming for Successful PAT Projects**; Christian Hassell; [1]Los Alamos National Lab

11:10 (621) **Successful Process Analyzer Implementation.**; Ann M. Brearley[1]; [1]Ann M. Brearley Consulting

11:30 (622) **From Chemical to Pharmaceutical Process Analyses: Will Arbitrary Limits Limit Progress?**; Emil Ciurczak[1]; [1]Integrated Technical Solutions

11:50 (623) **Validation of a Near-Infrared Transmission Spectroscopic Procedure for Measuring Assay in Pharmaceutical Tablets;** Howard Mark[1]; [1]Mark Electronics

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

10:30 (625) **Hot stage-Raman Microscopy as a Hyphenated Technique for Investigation of the Thermodynamics of Samples: a Feasibility Study**; Dirk Cleeren[1], Sigrid Stokbroekx[1], Jef Peeters[1], Marcus E. Brewster[1]; [1]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 Miller[1], Jian Ling[1]; [1]Southwest Research Institute

11:10 (627) **Process Monitoring of Paintable Display Production Using Confocal 3D Raman Spectroscopy and Chemometrics**; Peter de Peinder[1], Inge Vorstenbosch[1], Arjan Mank[1]; [1]Philips Electronics

11:30 (628) **Raman Microscopy and Imaging Applications to Nanostructures and Single Molecule Detection**; Ricardo Aroca; [1]University of Windsor

11:50 (629) **Characterization of Phthalocyanine Printing Inks by Micro Raman Spectroscopy**; Gene Hall; [1]Rutgers University

12:10 (630) **Extending the Capabilities of Drop Coating Deposition Raman (DCDR)**; Dongmao Zhang[1], Yong Xie[1], Corasi Ortiz[1], Dor Ben-Amotz[1]; [1]Purdue University

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 (631) **New Mass-Spectrometric Systems for Metallomics**; Gary Hieftje[1], Steven Ray[1], Duane Rogers[1]; [1]Indiana University

3:50 (632) **Collision/Reaction Cell ICP-MS: Enhancements to Elemental Speciation Studies**; Joseph Caruso; [1]University of Cincinnati

4:10 (633) **Particle Beam/Glow Discharge Mass Spectrometry: Simultaneous Acquisition of Molecular, Fragment, and Atomic Mass Spectra**; R. Kenneth Marcus[1], Jakob L. Venzie[1], W. Clay Davis[2]; [1]Clemson University; [2]National Institute of Standards and Technology

4:30 (634) **LC Sector Field ICP-MS for Simultanous Speciation analysis of P and S in Proteins**; Meike Hamester[1], Torsten Lindemann[1], Lothar Rottmann[1]; [1]Thermo Electron

4:50 (635) **Detection of Heteroelements in Proteins by ICP-MS**; Norbert Jakubowski[1], Wolf D. Lehmann[2], Michael Edler[1], Ingo Feldmann[1]; [1]Institute for Analytical Sciences (ISAS); [2]German Cancer Research Institute

5:10 (636) **Chemical Imaging of Biological Materials by NanoSIMS**; Peter Weber[1], Julie Smith[1], Ian Hutcheon[1]; [1]Lawrence Livermore National Laboratory

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

3:30 (637) **Guidelines to Choose Multiway Data Analysis Methods for Multivariate Resolution of Chemical Data Sets**; Anna de Juan[1]; Romá Tauler[2]; [1]Chemometrics Group, University de Barcelona; [2]Department of Environmental Chemistry, Institute of Chemistry and Environemtnal Research, CSIC

3:50 (638) **Purity Applied to PARAFAC**; Neal Gallagher; [1]Eigenvector Research, Inc

4:10 (639) **Study the Process of Refining Wood Using 3-Way PLS Regression Analysis of Fluorescence Spectra**; Valerie Lengard[1], Dongsheng Bu[1], Charu Mati[1], Zala Vijay[1], Waltraud Kessler[2]; [1]Camo Smart Inc; [2]Institut für Angewandte Forschung

4:30 (640) **Characterization of Drug Metabolism Using Chemometric Methods**; Sarah Rutan[1], Raymundo Sanchez-Ponce[1], Sarah Graham[1], Dennis Thekkudan[1], Shom Paul[1]; [1]Virginia Commonwealth University

4:50 (641) **3-Way and 4-Way PARAFAC Applied to Analysis of Pesticides and PAHs,** Karl S. Booksh[1], Yoon-Chang Kim[1], Michelle L. Nahorniak[1], James A. Jordan[1], and Gary A. Cooper[1]; [1]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 Vogt[1], Karl Booksh[1]; [1]Arizona State University

Thursday Afternoon, Room C124
IR MICROSPECTROSCOPY IMAGING
Organizer and Presider: Christine Wehlburg

3:30 (643) **Applications of Infrared Spectroscopic Imaging Utilizing Different-sized MCT Focal Plane Arrays**; Gloria Story[1], Curtis Marcott[1]; [1]The Procter & Gamble

3:50 (644) **Near-Infrared Imaging in Food Safety**; Janie Dubois[1], Frederick S. Fry[2], Elizabeth M. Calvey[2], E. Neil Lewis[3]; [1]JIFSAN, Food and Drug Administration and Universit; [2]CFSAN, Food and Drug Administration; [3]Spectral Dimensions Inc.

4:10 (645) **Near-Infrared Spectral Imaging of Nonwoven Materials**; Curtis Marcott[1], Anthony Dowrey[1]; [1]The Procter & Gamble Co.

4:30 (646) **Infrared Imaging At Sandia National Laboratories**; Kathleen Alam[1], Dion Rivera[1]; [1]Sandia National Laboratories

4:50 (647) **Detection of Metastatic Lymph Nodes by Infrared Spectral Imaging**; Melissa Romeo[1], Rajyasree Emmadi[2], Max Diem[1]; [1]Department of Chemistry and Biochemistry, Hunter College; [2]Department of Pathology, John Stroger Ho

5:10 (648) **New Developments in Planar Array Infrared (PA-IR) Spectroscopy**; Isabelle Pelletier[1], Pellerin Christian[1], John F. Rabolt[1]; [1]University of Delaware

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; [1]University of Alberta

3:50 (650) **Microfluidic Chip Front-ends for MALDI Mass Spectrometry**; Kermit Murray[1], Steve Soper[1], Harrison Musyimi[1], Damien Narcisse[1], Xia Zhang[1], Mark Little[1], Yichuan Xu[1]; [1]Louisiana State University

4:10 (651) **New Surface Enhanced Neat Desorption SELDI Protein Biochip for Proteomic Analysis**; Scot Weinberger[1]; [1]Ciphergen Biosystems, Fremont, CA, USA

4:30 (652) **Liquid Chromatography Coupled to UV-MALDI Using Off-Line Sample Spotting**; Robert Brown[1], Ron Orlando[2]; [1]Utah State University; [2]University of Georgia[4]

4:50 (653) **Protein and Peptide Analysis By Very High Throughput MALDI-TOF Mass Spectrometry of Liquid Chromatography Effluent**; James Reilly[1], Kirk Boraas[1], Noah Christian[1], Sean Stryker[1], Matthew Thompson[1], Weidong Cui[1]; [1]Indiana University

5:10 (654) **Development and Applications of LC/MALDI MS for Comprehensive Proteome Analysis**; Liang Li; [1]Department of Chemistry, University of Alberta

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

3:30 (655) **Silver Nanowire for SERS applications**; Andrea Tao[1], Peidong Yang[1]; [1]UC Berkeley

4:10 (656) **DNA Sensing Based on Silicon Nanowires**; Zhiyong Li[1], Yong Chen[2], Xuema Li[1], Ted Kamins[1], Stan Williams[1]; [1]HP Labs; [2]UCLA

4:50 (657) **Self-Assembly of Colloidal Nanostructures for Nanoelectronics and Nanoplasmonics**; Yi Cui[1], Alexander Liddle[2], Paul Alivisatos[1,2]; [1]University of California, Berkeley; [2]Lawrence Berkeley Lab

5:10 (658) **Electronn-Transfer Chemistry of Octadecylamine-Functionalized Single-Wall Carbon Nanotubes**; Shaowei Chen[1], Yiyun Yang[1], Wei Zhao[2]; [1]University of California - Santa Cruz; [2]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 Hug[1], Ray Reid[1], Pamela Conrad[2], Arthur Lane[2], Rohit Bhartia[2]; [1]Photon Systems; [2]Jet Propulsion Laboratory, Caltech

3:50 (660) **MicroNMR Systems for Process Control**; Michael McCarthy[1], Jeffrey Walton[1], Jeffrey de Ropp[1], Artem Goloshevsky[1], Scott Collins[2]; [1]University of California Davis; [2]University of Maine

4:10 (661) **Portable Surface Plasmon Resonance Sensors**; Alexei Naimushin; [1]Seattle Sensors Systems, Inc.

4:30 (662) **Vapochromic Detection and Quantification of Relative Humidity and Organic Solvent Vapors**; Kent Mann[1], Brian Marquardt[2], Daron Janzen[1], Stephen Drew[3]; [1]University of Minnesota, Department of Chemistry; [2]Center for Process Analytical Chemistry,; [3]Carlton College

4:50 (663) **The Theory and Application of RF/microwave Dielectric Spectroscopy**; Philip Bartley[1], Shelley Begley[2]; [1]Innovative Measurement Solutions; [2]Agilent Technologies

5:10 (664) **Analytical Applications of Modular Sampling Systems (NeSSI)**; Dave Veltkamp[1], Brian Marquardt[1], [1]University of Washington

Thursday Afternoon, Room A106
RAMAN SPECTROSCOPY IN ART AND ARCHAEOLOGY
Organizer and Presider: Howell Edwards

3:30 (665) **Applications of Raman Spectroscopy to Archaeological Biomaterials**; Howell Edwards; [1]Chemical and Forensic Sciences , University of Bradford

3:50 (666) **NIR-FT-Raman Studies of Amber, Paint Layers from Buildings and Archaeological Wood**; Ole Nielsen[1], Elsebeth Kendix[1], Mikkel Christensen[1], Ydalina Moreno[1], Yvonne Shashoua[2], Mads Christensen[2], Poul Jensen[2], Rikke Nielsen[1,3], Palle Jensen[3],; [1]Department of Chemistry, University of Copenhagen,; [2]Department of Conservation, National Museum of Denmark; [3]Department of Chemistry, University of Sotherin Denmark

4:10 (667) **Raman Investigation of Pigments on Ancient Ceramic Shards**; Danita de Waal[1]; [1]Univ. of Pretoria

4:30 (668) **Mobile Raman Spectroscopy: A New Challenge in Art Analysis**; Peter Vandenabeele[1], Luc Moens[1]; [1]Ghent University, Department of Analytical Chemistry

4:50 (669) **Confocal Raman Microscopic Study of Pigments on Old Master Portraits**; Robert Withnall; [1]University of Greenwich

5:10 (670) **Application of Raman Spectroscopy to the Study of Rock Art in the Altamira Cave (Spain)**; Fernando Rull; [1]University of Valladolid