SUNDAY MORNING

Placeholder

Low-Cost & Open-Source Analytical Chemistry

J. P. Grinias, Organizer, Presiding

8:00. Enabling Real-Time Processing of High-Volume Electrochemical Measurements via Open Source Software. N. Arroyo


8:40. Silicon photomultiplier as a low-cost fluorescence detector for capillary electrophoresis. B. Petersen, N.L. Allbritton


9:40 Intermission.

10:00. Low cost paper-based immunoassays for infectious disease diagnostics. K. Hamad-Schifferli


10:40. Chemical fingerprinting of carboxylate anions on low-cost paper supports. Y. Xu, M. Bonizzoni
11:00. An Analysis of the Quality of Beta-Lactam Antibiotics collected in Nepal. W. Lewis, M. Benjamin

11:20. Open-access resources for the teaching of analytical chemistry. D.T. Harvey

11:40. Open-source analytical chemistry in the laboratory and the classroom. J.P. Grinias, J.A. Naese, J. Emig

Section B

Placeholder

Active Learning in the Undergraduate Analytical Chemistry Curriculum (Invited)

M. L. Kovarik, J. K. Robinson, T. J. Wenzel, Organizers

8:00 Introductory Remarks.

8:05. The role of active learning in inclusive teaching and student belonging. J.K. Robinson

8:25. 3D Printing of Quantitative Chemical Containers (QCCs): An Active Learning Activity for Analytical Chemistry. M.L. Morris

8:45. Active learning in analytical lab lecture. B.J. Venton

9:05. Transforming a traditional quantitative laboratory into a research-focused analytical laboratory. A.M. Gonzalez

9:25 Intermission.

9:40. Testing in the Age of Active Learning. M.F. Tuchler

10:00. Quantitative analysis in context: Introducing analytical chemistry concepts using beer brewing. R.A. Hunter

10:20. Hands-On Laboratory Activities During Lecture for Instrumental Analysis. S.P. Plummer Oxley

10:40. Exploring computer-based simulations through guided-inquiry activities to introduce concepts in instrumental analysis. A. Le

11:00 Panel Discussion.
Third Annual Joint Symposium from the Separations Science Subdivisions
Sponsored by I&EC, Cosponsored by ANYL

2D Materials for Energy, Sensing & Quantum Information Science
Synthesis and Light Harvesting
Sponsored by PHYS, Cosponsored by ANYL and COMP

Molecular Capsules: From Design to Application
Sponsored by CATL, Cosponsored by ANYL, I&EC and PHYS

SUNDAY AFTERNOON

Section A

Placeholder

Low-Cost & Open-Source Analytical Chemistry

J. P. Grinias, Organizer, Presiding

1:00. Rethinking Scientific Data Opens a Door to New Levels of Reproducibility, Interoperability and Access. D. Vanderwall

1:20. Converting High-Throughput Solubility Data into the Alltrope Data Format. K.M. Grinias, E. Wu, K. Wells

1:40. Characterization of Commercial Tattoo Inks. J. Swierk, E. Horoszewski, F. Bateman, D. Wilhelm, V. Kompanijec, B. Stevenson

2:00. Prediction of agricultural pesticide liquid chromatography retention times via ab initio calculations. S. Carbone, S. Simpson


2:40 Intermission.
3:00 . Creating a device to detect substandard omeprazole medicines. **E. Barstis**, T.L. Barstis


4:00 . DNA-Regulated Proximity Assembly Circuit for Molecular Sensing of Biotargets. **J. Fu**


4:40 Concluding Remarks.

**Section B**

Placeholder

**Active Learning in the Undergraduate Analytical Chemistry Curriculum (Invited)**

M. L. Kovarik, J. K. Robinson, T. J. Wenzel, *Organizers*

1:00 Introductory Remarks.


1:25 . Active Learning in the Community College Chemistry Classroom and Laboratory. **D. Barron**

1:45 . A Hybrid Active Learning Approach in the Instrumental Analysis Laboratory: Focusing on Method Development and Validation. **S.J. Ray**

2:05 . Bringing the Laboratory into the Classroom: Developing In-Class Experiments and Teaching Method Development by Deconstructing the Scientific Literature. **K.R. Riley**

2:25 Intermission.

2:40 . Impact of student learning through scenario-based laboratories with a writing intensive component in analytical chemistry. **L. Petry**, R. Pompano, K.J. Shinkle, A. Walkowicz

3:00 . Stepping out of the comfort zone: implementing active learning in the analytical chemistry course. **V. Lopez-Mejias**
3:20. Active learning, at home and abroad. **K.M. Mullaugh**

3:40. The Active Learning Site of the Analytical Sciences Digital Library. **T.J. Wenzel**

4:00 Panel Discussion.

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**2D Materials for Energy, Sensing & Quantum Information Science**

**Synthesis, Light Harvesting and Catalysis**

Sponsored by PHYS, Cosponsored by ANYL and COMP

**Molecular Capsules: From Design to Application**

Sponsored by CATL, Cosponsored by ANYL, I&EC and PHYS

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**SUNDAY EVENING**

**Placeholder**

**Analytical Division Poster Session**

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P. Bohn, *Organizer*

7:00 - 9:00

- Mass spectrometry fragmentation of barium adducted human milk oligosaccharides. **J. Rensner**, A. Diepenbrock, E.D. Dodds

- Temperature-Dependent Near-Infrared Spectroscopy for Analyzing the Water in the Change of Chemical Structure. **X. Shao**, L. Ma, L. Wang, W. Cai

- Enriching analytical chemistry curriculum with service-learning and inquiry-based projects. **Z. Zajickova**

- Redox Properties of Silver Nanoparticles. **B. Tran**, A. Restani, P.G. Tratnyek, P. Hall, A. Pavitt

. CRAFT sour beer: Quantification of metabolites over time in spontaneously fermented beer using quantitative $^1$H NMR spectroscopy and time-domain analysis. **D.P. Soulsby**, B. Doty, A. Cooper


. Role of glutathione disulfide (GSSG) in the metal-mediated oxidative DNA damage. **A. Agarwal**, D. Morris


. Proximate and Mineral Composition of *Cnidoscolus aconitifolius* (Hospital Too Far) Leaf.. **Q.S. Obu**, T.O. Magu

. Determination of urinary sulfate levels in horses and swine by conductometric titration. B.R. Rothrock, S.A. Andrews, J.D. Goode, M.S. McAfee, **L.D. Schultz**


. Evaluation of microchip-CE technology for metabolomics applications. **C. McNaney**, S. Hnatyshyn


. SALDI-MS analysis of real world samples utilizing transition metal oxide nanoparticles as surfaces. **M.P. Lapak**, S. Ward, **T.B. Best**, K.S. Molek

. Got lead? Low-cost analysis of lead in drinking water by preconcentration on a carbon felt filter. M. Tighe, A. Cooper, S. Carpenter, G.F. Peaslee, **M. Lieberman**

. Screening and quantitation of trace metals in food samples by ICP-MS. **S. Antonio**

. Natural cyanogenic compounds in food: Direct and rapid detection of hydrogen cyanide in *Macadamia* using selected ion flow tube-mass spectrometry (SIFT-MS). **H. Castada**, S. Barringer


. Analysis of drug-protein interactions using ultrafast affinity extraction. **S. Iftekhar**, D.S. Hage

. UV-Vis Spectrophotometric Determination of Glyphosate in Foods and Environmental Samples. **F. Albalawi**, M. Medeiros, Y. Zuo


. Structures and Spectroscopic Properties of Mono and Bridged BODIPYs. **S. Shin**, **S. Bae**

. Spatial and temporal trends of melamine and its derivatives in sediment from Lake Shihwa, South Korea. **H. zhu**, K. Kannan

. Optimizing GC-MS and GC-MS/MS analysis of 3-MCPD and glycidyl esters. **J. Rousova**, J. Konschnik, H. Majer, C. English
Numerical Modeling and Simulation of a Microfluidic Platform for Enrichment of Low Abundance Proteins. F. Matthews, M. Hossan, S. Gamagedara

Label-free three-dimensional raman imaging of carbon nanotubes in mammalian cells. M. Huynh, C. Mikoryak, P. Pantano, R. Draper

GC-MS method development for soil and water environmental sampling to determine crude oil presence and possible microbial degradation activity in freshwater lakes. A. Grauherr, D. Learman, J. Mouradian, D. Uzarski, D.J. Lecaptain, A. Vassilakos

HPLC Analyses of glyphosate residues in Zea mays. S. Azibere, C. Awuah, J. Agyei-Ohemeng, I. Emahi

Recognition of methylated cytosine in a DNA polymerase for dGTP: Retrieving association rate constant at the single molecule level. J. Lee, J. Park

Detection of microRNA on the nano-scale controlled surface by using metal-enhanced fluorescence nanoparticles. S. Park, J. Hwang, J.M. Nam, J. Park

Developing LC-MS methods for the quantitative analyses of creatine phosphate in brain samples. S.L. Wang

Analysis of designer benzodiazepine flualprazolam and its in vitro metabolites using GC-MS. J.B. McGill, E. Gardner

The reaction of artemisinin and its derivatives with DNA bases catalyzed by heme proteins: LC/MS characterization of the reaction products. K. Vijayan, A.M. Mugweru


Analytical Division Poster Session

Analytical Division Poster Session

P. Bohn, Organizer

7:00 - 9:00


. Optical Voltammetry / Closed-Cell Bipolar Electrochemistry Based Sensor for Portable, Low-Cost Heavy Metal Water Testing. **J. Monge**, E. Fahrenkrug

. Use of a 3-hydroxyflavone derivative as a fluorescent probe for the indirect determination of aminothiols after separation with ion-pair HPLC. **L. Mikaliunaite**, D.B. Green


. Determination of nicotine in toenails as a biomarker for secondhand smoke by LC-MS. **X. Li**


. Chiral and Achiral HPLC Separation of NSAIDs. **K. Camilo**, J.P. Foley

. Chemoselective and enantioselective recognition of amino acids in water: a micelle approach. **G. Du**


. Understanding the chemistry of mordançage, a historic photographic process. **R.M. Jones**, C. Fudala

. In Field XRF of Mercenaria mercenaria: a Bioindicator of Heavy Metal Legacy Pollution. **M. Mitchell**, S.P. Nugent, S.K. O'Shea


. Parallel Analysis of Tyrosine, Tyramine, L-DOPA, and Dopamine via Enzyme-Based Colorimetric Biosensors. **H. Chen**, L. Hsu, Y. Chou, Y. Yeh
. Analysis of Nepali Antidiabetic Ayurvedic Samples for Chemical Contamination. **M. Lamb**

. Optimizing the stability of an optical bio-sensor for differentiating free silver ions (Ag+) from silver nanoparticles (AgNPs) in biological medium. M.A. Omary, S. Marpu, **N.A. Perera**, D. Garcia


. Atomistic-scale modeling of azobenzene photoisomerization in the confined cavity of molecular cages. **L. Pesce**, A.B. Grommet, R. Klaejn, g. pavan


. Improved separation performance by using tandem-column LC with conventional U/HPLC instrumentation. **Z. Liu**, J.P. Foley


. Robotic Implementation for MTT proliferative and β-glucuronidase assays to determine bio-therapeutic β-glucuronidase enzyme activity from pilot bioreactor CHO cell lines. **A. Masood**, C. Madhavarao, F.J. Patrick

. Theoretical methods of calculating conical intersections. **D. Behrendt**, S. Matsika


. Determination of Arsenic in Desiccated Material from Skeletal Remains. **J.M. Kelly**, J.G. Davis

. High throughput automation for quantitation of amino acid analysis via UPLC of basal and feed bioreactor samples in upstream cell culture bioprocesses. **S.A. Schallenhammer**, B. Ramanathan, Y. Hu, N. Larmore


. In Situ Remediation of *Benzo[a] pyrene*. **A. Kante**
. Identifying microbial populations and pathways central to macromolecule synthesis and degradation in Enhanced Biological Phosphorus Removal (EBPR) systems. **S. Keshani Langroodi**, J.R. Price, Y. Nan, C.M. Sales

. Effect of cyclic diamine isomers on chiral selectivity of amino acid based surfactants. A. Risley, M. Aleksich, **F.H. Billiot**, E. Billiot, K. Morris, Y. Fang


. Total Antioxidant Capacity of Differently Brewed Teas (FRAP Method). **A. Anderson**, B.J. Bellott

. Comparison of Flavonoid Concentration in Differently Brewed Teas. **D. Moss**, B.J. Bellott


. Composition of tattoo inks. **E. Horoszewski**, J. Swierk


. The identification of mixture of compounds from IR spectrum using Artificial intelligence. **D. Yang**, J. Darsey

. Development of New Indicators to Demonstrate the Extremely Low Basicity of Slightly Soluble Arrhenius Bases in Qualitative Analysis. D. Barclay, **M. Arbalidoost**, A. Mousavi

. Sink/float immunodiagnostic tests for proteins and disease specific antibodies. **P. Chorti**, D. Christodouleas


. Removal of Chromium (VI) from aqueous solution using ZnO nanoparticles an investigation into the effect light and dark conditions on the binding. **D. Ramirez**
Analytical Division Poster Session

P. Bohn, Organizer

7:00 - 9:00


. Understanding the decomposition of tattoo pigments and their photoproducts. K. Moseman

. Synthesis of a Fluorescent and Colorimetric Chemosensor for the Detection of Trivalent Cations. C. Quintero, A. Garza, S. Plummer Oxley


. Design and synthesis of sensitive fluorogenic substrates as quantitative reporters for protease activity assays. E.E. Rastede, T.M. Rodriquez


. "Head-to-head comparison of the dipeptide and sugar-based molecular micelles for the chiral separation of a broad range of chiral analytes by MEKC-MS". F. Akter


. Variation of Amino Acid Analysis in Defatted Soybean Meal using U-HPLC & AccQ Tag Technology. V. Spourdalakis, B.J. Bellott, M.A. Berhow


. FT-EDM Measurements of Functionalized Semiconductor Quantum Dots. M.J. Murray, S.L. Neal
Simultaneous Determination of Vitamin C, Uric Acid and Creatinine in Human Fluids and Vitamin C-Induced Uricosuria by HILIC. R. Zuo, S. Zhou, Y. Zuo, Y. Deng


Simultaneous HPLC determination of the antidiabetic drugs metformin and pioglitazone on a cyano column. C. Martín, Y. Zuo


Peptide conjugated multipurpose carbon dots as nano-cargoes for glioblastoma brain tumors. S. Hettiarachchi, R.M. Graham, Y. Zhou, S. Vanni, E. Seven, R.M. Leblanc

Multivariate analysis of the excitation wavelength dependence of frequency-domain PRODAN emission decay matrices. D.B. Sanap, S.L. Neal

Electroanalytical tools and molecular-based assays to measure the impact of noise on dopamine neurotransmission in the central auditory pathway. P. Wilson, A. Apawu

Optimization of Indophenol Blue Reaction for Atmospheric Ammonia Analysis. Z. Naing, Y. Liu

Spectrophotometric Determination of Active Ingredients in Over-the-Counter Pharmaceuticals. S. Brown, K.T. Jackson

Elucidating the neurochemical basis for the effect of chronic toluene inhalation on accumbal dopamine release. K. Reiser, A. Apawu

Tunable optical metamaterial-based sensors enabled by closed bipolar electrochemistry. C. Oh, G. Crouch, K. Fu, P. Bohn

Evaluating changes in reactive oxygen species (ROS) as a plausible mechanism underlying the effect of noise on dopamine release. B.D. Doc, P. Wilson, A. Apawu

Kinetic and Thermodynamic Studies of the Adsorption of Arsenic on Calcined Chemically Modified Oxidic Variable Charged Soils as Substrate for Water Purification. X. Ren, J. Liu, F. Millan, E. Wang

Analytical Division Poster Session

Analytical Division Poster Session

P. Bohn, Organizer

7:00 - 9:00

Assessing Utility of Laser Induced Breakdown Spectroscopy for Dalbergia Speciation. C.P. Celani

Analysis of Cannabinoids in CBD Oil using GC-MS and HPLC techniques. D.A. Patel, S. Kadam, V. Arekar, E. Franco, D.M. Ramanathan

Integrating Clinical Analytical Research Projects into Chemistry Curriculum. Y. Zuo

Semi-Automated Identification of Metabolites to Aid in Drug Discovery and Disease Diagnostics. H. Noel, R. Powers, F. Bhinderwala, A. Parrett, T. Vu

Development of automatic alternate-current electrochemical etching system for the probe of scanning tunneling microscope and the byproducts of metal particles without using strong acids. T. Takami, K. Oya, K. Aoshika, H. Kadoma

Flexible polyurethane sponge-based electrode prepared by convenient and economical method and its application in glucose sensors. G. Shixi, Z. Chunhong, Y. Ming, Z. Yanli, B. Changlong, L. Qingtao


Quantification of Furanocoumarins in Grapefruit Supplements. M.H. Bregman, E. Hondrogianis, B.H. Tran, S. Stokes

MEMS Liquid and Gas Chromatography for Human and Robotic Missions. R.D. Kidd, B. Bae, S. Waller, P. Willis, Y. Tai, S. Madzunkov, M. Darrach

Relationships between chirality and photophysical properties of chiral systems probed by circularly polarized luminescence spectroscopy. G. Muller

Synthesis and chiral recognition of helical poly(phenylacetylene)s bearing 3,5-dimethylphenylcarbamate residue of L-Cyclohexylglycinol. Z. Ruiqi, Z. Chunhong, w. zhongpeng, Z. Yanli, T. Satoh, Y. Okamoto
. Distinguishing intra- and extra-cellular analytes by LIBS using sodium/potassium ratios. N. Denniston, D. Rusak


. Smart Synthesis of Trimethylethoxysilane (TMS) Functionalized Core – Shell Magnetic Nanosorbents Fe3O4@SiO2 for Removal of Pesticides: A Full Factorial Design – Assisted Statistical Approach. s.m. idoudi

. Comparative metabolomics of MCF-7 breast cancer cells using different extraction solvents assessed by mass spectroscopy. M. Semreen, H. Alniss, S. Grgic, R. El-Awady, A. Almehdi, M. Mousa, R. Hamodi


. Determination of silicate in waste and recycled engine coolants using capillary electrophoresis. A.F. Schaum, T. Krizek

. Determination of aniline, *p*-cresidine, and 4-nitro-*p*-cresidine in FD&C Red No. 40 using LC-MS/MS. N. Belai, C. McClure, N. Richardson

. Fluorination and analysis of ethinylestradiol (EE2) by EI-GC-MS and GC-MS-FPD. R.N. Leif, A.K. Vu, E.P. Salazar, A. Alcaraz, C.A. Valdez

. Rapid, sensitive plasmonic sensor of Chlamydia without DNA amplification. R.M. Cary, I. Monroe, J. He, L. Sagle

. Determination of aniline and other unsulfonated aromatic amines in FD&C Blue No. 2 using LC-MS/MS. N. Belai, J.N. Barrows

. Development of a simple, low-cost, field-kit method to determine inorganic arsenic species in rice. Y. Zhang, J.F. Tyson


. Liquid-phase Peak Force Infrared Microscopy. H. Wang, X. Xu

. Effect of solvent characteristics in evaluating targeted leachables in simulated-use extractions. C. Fuller, V. Chandrasekar, K. Nahan, S. Wickramasekara


. Comparative study of fresh and dried *Garcinia kola* using proximate and phytochemical analysis. O.O. Onawumi, T.J. Adegboyega, V. Animasahun, A.I. Atere

. Adsorption Behavior of Chemically/Charged Modified Antibody on Gold Nanoparticles. S. Okyem, O. Awotunde, J.D. Driskell

. Development of Abraham model correlations for an analytically important extraction solvent MIBK. E. Garcia, K. Smart, W.E. Acree


. DNA-modified silver amalgam sensor for electrochemical determination of 1-nitropyrene. J. Swenson, R. Pfeifer, V. Vyskočil

. Thinking outside of the box: Designing a simple solution to quantitate a mutagenic impurity in a complex matrix. L. Pfund, J. Zheng

. Study of Two-Dimensional NMR Data Extraction Methods for Quantitative Analysis. L. Jiang, K. Howlett, K. Patterson, B. Wang


. Unknown nepetalactone isomer elucidated from *Nepeta citriodora* extract. J. Dykstra, L. Nawab, T.L. Walker, I.S. Taschner

. Exploring the temporal dynamics of caspase activity during different pathways of apoptosis. R.D. Reif, C. Zwemer
QUALITATIVE AND QUANTITATIVE ANALYSIS OF ELECTRONIC CIGARETTE LIQUIDS USING GAS CHROMATOGRAPHY- ORBITRAP MASS SPECTROMETRY. A. Ladak, J. Cooper, R. Tapper, C. Cojocariu, C. Allen

Determination of Fluoride content in Dental Varnish via solvent extraction and measurement by Fluoride ISE in Flow Injection Analysis. P.J. Iles, K. Green, J. Cook, R. Kochambilli, S. Moore, R.V. Valcarce, L.D. Giddings


Direct electrochemical evaluation of energy metabolism level of single mitochondrion in Alzheimer's disease. l. qi

Synthesis and Characterization of Fluorescent Graphene Quantum Dots (GQDs) for Cell Imaging. A. Vasquez, S. Reagan

MONDAY MORNING

Section A

Placeholder

ACS Award in Chromatography: Symposium in honor of Lane C. Sander (Invited)

S. A. Wise, Organizer, Presiding

8:00 Introductory Remarks.

8:05 Structure and function of chromatographic surfaces. L. Sander

8:45 Advances in Two-dimensional Liquid Chromatography – From Ultra-fast to Ultra-high Resolution. M. Pursch, A. Wegener, S. Buckenmaier, K. Zhu, S. Eeltink, G. Desmet

9:25 Fundamentals of Chromatography for Dietary Supplement Analysis. C. Rimmer

10:05 Intermission.

11:00. Shape Selectivity in Chromatographic Separations of Polycyclic Aromatic Compounds. S.A. Wise, W.B. Wilson, L. Sander

Section B

Placeholder

Nanotechnology, Single Molecule & Single Cell Imaging in Biology and Medicine (Invited)

Cosponsored by BIOL, BIOT, COLL, MPPG and PHYS
X. Xu, Organizer, Presiding

8:00. A nanomaterial-based system for the controlled generation of free radicals inside cells. Y. Xia

8:30. 'Marker of Self' in biophysics, nanotechnology, & emerging medicines. D.E. Discher

9:00. Interrogating Immune Functions with Engineered BioInterfaces. Y. Yu

9:30. Beyond biomarkers: Array-based profiling for diagnostics and geno-/phenotypic screening for precision medicine. V.M. Rotello

10:00 Intermission.


11:40. DNA probes that store mechanical information reveal transient piconewton forces applied by T cells. R. Ma, K. Saladita


Section C
Broadband Dielectric Spectroscopy as a Modern Analytical Technique

Introduction to Broadband Dielectric Spectroscopy

W. Woodward, Organizer, Presiding

8:00 Introductory Remarks.

8:05. Dielectric approach to viscous materials at high electric fields. R. Richert

8:30. Glassy dynamics of polymers under external and internal nanometric 1- and 2-dimensional constraints. F. Kremer


9:45 Intermission.

10:00. Multiple glassy dynamics in dipole functionalized triphenylene-based discotic liquid crystals revealed by broadband dielectric spectroscopy, advanced calorimetry and neutron scattering. A. Schoenhals

10:25. The interplay of metalloproteins with the dynamic structure of water. P. Ben Ishai

10:50. Application of dielectric spectroscopy for investigation of crystallization kinetics of supercooled liquids at ambient and elevated pressure. M. Paluch

11:15. Application of dielectric spectroscopy to study crystallization behavior of molecular systems under varying thermodynamic conditions. K. Adrjanowicz

2D Materials for Energy, Sensing & Quantum Information Science

Sponsored by PHYS, Cosponsored by ANYL and COMP

MONDAY AFTERNOON

Section A
ACS Award in Analytical Chemistry: Symposium in honor of Mark E. Meyerhoff (Invited)

ACS Award in Analytical Chemistry

M. A. Arnold, Organizer, Presiding

1:00 Introductory Remarks.

1:05 Chemical Sensors for Medicine: 45 years of Fun Investigating New Sensing Chemistries, Designs, and Applications. M.E. Meyerhoff

1:45 Electrochemical Sensors: The Quest for Selectivity. W.R. Heineman

2:25 Polyion Sensors, a Trigger for Conceptual Advances in Electrochemical and Optical Ion Sensing. E. Bakker

3:05 Intermission.

3:20 The Nanoliter Lab: Droplet Microfluidics for Screening and Sensing. R. Kennedy

4:00 Noninvasive Glucose Measurements in People with Type 1 Diabetes with Near Infrared Spectroscopy. M.A. Arnold

Section B

Nanotechnology, Single Molecule & Single Cell Imaging in Biology and Medicine (Invited)

Cosponsored by BIOL, BIOT, COLL, MPPG and PHYS
X. Xu, Organizer, Presiding

1:00 Imaging Single Spheroids, Cells, Blebs, and Integrins: Towards a Mechanistic Understanding of a Novel Migratory Mode. L. Kaufman

1:30 Elucidating the molecular mechanisms of translesion polymerase recruitment. E.S. Thrall, S. Chang, S. Piatt, J.P. Kath, J. Loparo

2:00 Single-molecule FRET imaging of G protein-coupled receptor conformational dynamics and dimerization in living cells. W.B. Asher, P. Geggier, M.D. Holsey, S. Mathiasen, G.

2:30. Photostable nano probes for single molecule sensing and imaging of single live cells. X. Xu, P. Songkiatisak, P. Cherukuri

3:00 Intermission.


3:40. Shaking a brain one molecule at a time: Watching a neuronal protein spontaneously raptures like the burst of a balloon. H. Lu

4:10. Amino acid-based fluorophores for biological spectroscopy and microscopy. F. Gai

4:40. Imaging biological water inside single living cells by stimulated Raman excited fluorescence microscopy. L. Shi, W. Min

5:10. Subcellular magnetic control of phagosome maturation in living cells. Z. Zhang, Y. Yu, Y. Yu

Section C

Placeholder

Broadband Dielectric Spectroscopy as a Modern Analytical Technique

Broadband Dielectric Spectroscopy of Ionic Systems

W. Woodward, Organizer, Presiding

1:00. Dielectric Spectroscopy of associating and ion conducting polymers. A.P. Sokolov

1:25. Conductivity and mechanical behavior of ionic melts. F. Wieland, P. Münzner, V. Bocharova, A.P. Sokolov, R. Böhmer, C. Gainaru

1:50. Mesoscale organization and dynamics in ionic liquids: insights from broadband dielectric spectroscopy. J. Sangoro

2:15 Intermission.

2:30. Understanding ion transport confined in multilayer polymer films using broadband dielectric spectroscopy. X. Chen, E. Allahyarov, L. Zhu
2:55. Broadband Dielectric Spectroscopy for Studies of Amorphous Ionic Pharmaceuticals. Z. Wojnarowska, M. Paluch


3:40 Concluding Remarks.

Molecular Capsules: From Design to Application
Sponsored by CATL, Cosponsored by ANYL, I&EC and PHYS

2D Materials for Energy, Sensing & Quantum Information Science
Sponsored by PHYS, Cosponsored by ANYL and COMP

MONDAY EVENING

Section A

Placeholder

Sc-Mix

P. Bohn, M. F. Bush, Organizers

8:00 - 10:00

TUESDAY MORNING

Section A

Placeholder
To SERS with Love: Symposium in honor of Richard Van Duyne (Invited)

Cosponsored by PHYS
A. J. Haes, C. L. Haynes, J. Zhao, Organizers, Presiding

8:00 Introductory Remarks.

8:10 SERS, TERS, hot electrons and the Van Duyne legacy. G.C. Schatz

9:00 Remembering Dr. Richard P. Van Duyne: Emergence of Two Near-Infrared Windows for In-Vivo and Intraoperative SERS. S. Nie, L. Lin, R. Xue, L. Lane

9:20 Polymer-enabled Plasmonic Sensing. C.L. Haynes

9:40 SERS of non-thiolated molecules. A.J. Haes, W. Xi, S. Kumarage

10:00 Intermission.

10:20 Monitoring electrochemical reactions at plasmonic nanoparticle surfaces. K.A. Willets

10:40 Excitation Wavelength Effect on the Lifetime of Fluorescent Emitters near Plasmonic Nanoparticles. Y. Sun, J. Zhao

11:00 New Strategies for Surface-Enhanced Sensing: N-Heterocyclic Carbenes as a Robust Platform for Nanoparticle Functionalization and In Situ Modification. J.P. Camden


11:40 Portable Localized Surface Plasmon Resonance Sensors. P. Hall

Section B

Placeholder

Nanotechnology, Single Molecule & Single Cell Imaging in Biology and Medicine (Invited)

Cosponsored by BIOL, BIOT, COLL, MPPG and PHYS
X. Xu, Organizer, Presiding

8:00 Single-particle Dynamic Light Scattering: Shapes of Individual Nanoparticles. H. Yang

8:30 Nanoparticle Diffusion Probes Network Heterogeniety in Gels and Cells. R.J. Composto, E. Parrish

9:30 . Spectroscopic tracking of single plasmonic nanoparticles for probing nano-environments of developing embryos. X. Xu, M. Johnson, P. Songkiiatsak, L.M. Browning, P. Nallathamby

10:00 Intermission.


10:40 . Label Free, Second Harmonic Imaging of Molecules at the Membrane of Single Cells. H. Dai


Section C

Placeholder

Broadband Dielectric Spectroscopy as a Modern Analytical Technique

Broadband Dielectric Spectroscopy of Polymers

W. Woodward, Organizer, Presiding

8:00 Introductory Remarks.

8:05 . Using dielectric spectroscopy to investigate the impact of irreversible adsorption on the dynamics of thin polymer melts. S. Napolitano, C. Rodríguez-Tinoco, Z. Song


8:55 . In Situ Monitoring the Imbibition of poly(n-butyl methacrylates) in Nanoporous Alumina by Nanodielectric Spectroscopy. C. Tu, M. Steinhart, H. Butt, G. Floudas

9:25 Intermission.

9:40 Isotopic effects on the dynamics of bio- and non-biological aqueous solutions studied by means of broadband dielectric spectroscopy. **S. Cerveny**

10:05 Polymer dynamics in nano-structured surroundings: Structure-property relations unraveled by broadband dielectric spectroscopy. **M. Tress**, P.J. Lutz, R. Mülhaupt, F. Kremer, K. Xing, S. Ge, P. Cao, T. Saito, A.P. Sokolov

10:30 Vitrification and physical aging in polymer glasses by broadband dielectric spectroscopy. **D. Cangialosi**

10:55 Analyzing the polymer dynamics and the nanoparticle network dynamics of polymer nanocomposites through dielectric spectroscopy and rheology. **S. Cheng**, J. Yang

**2D Materials for Energy, Sensing & Quantum Information Science**

Sponsored by PHYS, Cosponsored by ANYL and COMP

**TUESDAY AFTERNOON**

Section A

Placeholder

**To SERS with Love: Symposium in honor of Richard Van Duyne (Invited)**

Cosponsored by PHYS
A. J. Haes, C. L. Haynes, J. Zhao, *Organizers, Presiding*

1:00 Undergraduate project- and research-based labs using Raman spectroscopy. **J.M. Wiester**

1:20 Dye-Based SERS Studies: Applications to Art Conservation and Biosensing. **K.L. Wustholz**

1:40 Combining single molecule surface enhanced raman spectroscopy with single molecule fluorescence spectroscopy. W. Lum, X. Hu, J. Diao, **L. Sagle**

2:00 Ultrafast and nanoscale Raman spectroscopies. **R.R. Frontiera**

2:40 Intermission.

3:00 SERS and SORS Neurochemical Sensing – A Career Influenced by Rick Van Duyne. B. Sharma


3:40 Panel discussion. P.S. Weiss, M. Moskovits, B. Ren, C.A. Mirkin, C.J. Murphy, G.L. Richmond, P. Bohn

4:50 Concluding Remarks.

Section B

Placeholder

Nanotechnology, Single Molecule & Single Cell Imaging in Biology and Medicine (Invited)

Cosponsored by BIOL, BIOT, COLL, MPPG and PHYS

X. Xu, Organizer, Presiding

1:00 Metaoptics Enabled Multifunctional Imaging of Single Cells of Myxococcus Xanthus. H. Do, V. Sundaresan, C. Madukoma, J. Shrout, P. Bohn

1:30 Single-cell mass spectrometry reveals metabolite gradients in the vertebrate frog embryo (Xenopus laevis). E.P. Portero, L. Pade, P. Nemes

2:00 Imaging Bioactivities with Genetically Encoded Fluorescent and Bioluminescent Biosensors. H. Ai

2:30 Single Cell Analysis….A Billion Cells at a Time. S.O. Kelley, D. Philpott

3:00 Intermission.

3:10 Separating Fullerenes from FullerTubes: Chemical Isolation of FullerTube Molecules that Possess a Carbon Nanotube Belt Region AND Fullerene End Caps. R.M. Koenig, K.R. Tepper, T.L. Seeler, H.M. Franklin, S. Stevenson

3:40 Programmable DNA origami motors that convert chemical energy into linear motion. A. Bazrafshan, K. Salaita

3:55 Simultaneous Imaging of Dynamics and Biochemical Activities of Single Phagosomes. Y. Yu, Z. Zhang, Y. Yu

4:25. Peptide–Cluster Probe Based Single-Cell Quantification of Tumor Cell Membrane Proteins. **X. Ren**

Section C

Placeholder

**Broadband Dielectric Spectroscopy as a Modern Analytical Technique**

**Microwave Dielectric Spectroscopy**

W. Woodward, *Organizer, Presiding*


1:00. Dielectric characterization of polymers and polymer composites in the microwave frequency range. **M. Lanagan**, S. Perini, M. Sarkarat, T. Bonnett, S. Shetty, M. Yuan, R. Rajagopalan

1:00. Microwave microfluidics. **n. orloff**, A. Stelson, M. Liu, N. Stephanopoulos, J. Booth

1:00. Measuring Ion-Pairing and Hydration in Supramolecular Cages with Microwave Microfluidics. **A. Stelson**

1:00 Concluding Remarks.

**WEDNESDAY MORNING**

Section A

Placeholder

**Advances in Spectroscopy**

P. Bohn, *Organizer*
8:00 . Computational Raman study of organic adsorbent on graphene. S. Afroosheh, A. Zayak

8:20 . Thin films for characterization of aging using ATR/FTIR spectroscopy. K. Alam, L. Martin, R. Knepper, M. Marquez

8:40 . Structure elucidation of peroxide adducts in solution and in the solid state. F.F. Arp, J. Bluemel

9:00 . Low-Field$^1$H nuclear magnetic resonance spectroscopy for compositional analysis of multicomponent polymer systems. M. Minkler, B. Beckingham

9:20 Intermission.

9:40 . Controlled chemistry by the contactless merging of two droplets suspended in a single-axis acoustic levitator. S. Brotton, R. Kaiser

10:00 . Magnetic Chemistry and Possible Applications in Analytical Chemistry and Other Fields. M. Burns


10:40 . Direct Detection of Heavy Metal Ions Using Liquid Crystals. S.A. Oladepo

Section B

Placeholder

**Advances in Mass Spectrometry**

M. F. Bush, Organizer


8:20 . Improving routine analysis using inductively coupled plasma mass spectrometry (ICP-MS). S. Antonio

8:40 . Isotope Ratio Analysis of Rainwater Samples by Inductively Coupled Plasma Triple Quadrupole Mass Spectrometry. S.F. Li, O. Woo, S. Watts

9:00 . Practical Considerations for Quantitative Gas Analysis with Quadrupole Mass Spectrometers. G. Thier, L. Kephart
9:20. Using TD-DART-MS to analyze the exterior of drug packaging to predict the contents. E. Sisco, E.L. Robinson, A. Burns, R. Mead

9:40 intermission.


10:10. Identification of impurities in pharmceutical products using advanced analytical tools. G. Singh

10:30. Mapping the Dark Space of Chemical Reactions with Extended Nanomole Synthesis and MALDI-TOF MS. H. Sheng


11:10. Mass spectrometry is essential for research in climate science. R.F. Hirsch

Section C

Placeholder

Advances in Electrochemistry

L. A. Baker, H. Ren, Organizers, Presiding


8:25. A Rapid Response Electrochemical Biosensor for Detecting Thc In Saliva. S. Prasad, H. Stevenson, A. Bhide, V. Dhamu

8:50. Electrochemical textile-based biosensor for long-term noninvasive glucose monitoring in human sweat. r. fan, T.L. Andrew

9:15. Carbohydrate determinations by HPAE-PAD using a PdH reference electrode. M. Aggrawal, J. Rohrer

9:40 Intermission.


11:15 . Chemically Functionalized PET Nanopore for Protein Biomarker Detection. **Y. Zhang**, X. Guan, X. Chen, G. M Roozbahani

**WEDNESDAY AFTERNOON**

Section A

Placeholder

**Advances in Spectroscopy**

P. Bohn, *Organizer*

1:00 . Novel fluorescence method coupled with microdialysis sampling for on-line monitoring of propofol. f. fan

1:20 . Efficiency of colorimetric sensors for reactive oxygen species detection under biorelevant conditions using time-resolved, broadband UV-Vis absorbance measurements. **J. Herman**, S.L. Neal

1:40 . Developing methods for detecting target analytes using UV-Vis transparent membranes. **N. ibnul**, C.P. Tripp

2:00 . Simultaneous chemical and electrical mapping of photoactive materials with ~10 nm spatial resolution through the detection of induced cantilever oscillations. **D. Jakob**

2:20 Intermission.


3:00 . Development of carbon quantum dot-hydrogel material as a spectroscopic and electrochemical sensor for active corrosion. **L.N. Kissell**, T. Lasseter Clare
3:20 . Attenuation length versus packing density – Nitrogen based self-assembled small molecule film on copper with thermal treatment. Z. Lee, P. Hsu, C. Chi, Y. Tai


Section B

Placeholder

Advances in Mass Spectrometry

M. F. Bush, Organizer

1:00 . An Overview of IRMPD Spectroscopy for Isomeric and Isobaric Biomolecule Analysis: Focus on Modified Amino Acids and Peptides. A.L. Patrick


2:00 . Investigation of Atmospheric Pressure Ionization of Alkanes and Fatty Acid Methyl Esters. J. Powers, H.F. Castro, S.R. Campagna


2:40 Intermission.

3:00 . Systematic Quantification of the Dynamics of Newly Synthesized Proteins in Human Cells Unveiling Their Degradation Pathways. M. Tong, R. Wu

3:20 . Towards the development of an integrated automated online LC/MS/MS Multi-Attribute Method (MAM) workflow for the daily monitoring of multiple product quality attributes during cell culture process. Y. Liu

3:40 . Real time monitoring of the suitability of high resolution LC-MS systems by image recognition algorithm using peaks of spiked-in internal standards. S. Hnatyshyn, R. Hnatyshyn, J. Ott

**Section C**

Placeholder

**Advances in Electrochemistry**

L. A. Baker, H. Ren, *Organizers, Presiding*

1:00. Ion Transport in Charged Nanopores, Chemistry Beats Debye?. **C.R. Martin**, S. Walters-Bush


1:50. Adventitious hydrocarbons and the graphite-water interface. **J. Hurst**, L. Li, H. Liu


2:40 Intermission.

3:00. Facile nitrogen doping of graphite and carbon fiber for electrochemical sensing applications and immobilization of metal nanoparticles. **G.W. Bishop**


**THURSDAY MORNING**

**Section A**
**Advances in Spectroscopy**

P. Bohn, *Organizer*

8:00 . Study of radio-luminescence nanoparticles for non-invasive, in vivo optogenetic neuron stimulation. **M. Ranasinghe**, M. Arifuzzaman, S. Bhattacharya, J.N. Anker


8:40 . New portable multi-wavelength fibreoptic Raman analysis with micro-Raman capability. T. Batten, T. Prusnick, **S. Shidler**, R.W. Bormett

9:00 . In-line monitoring of the powder flow behavior and drug content in a Fette 3090 feed frame at different operating conditions using Near Infrared spectroscopy. **N.O. Sierra-Vega**, A. Sanchez-Paternina, N. Maldonado, V. Cárdenas, R.J. Romanach, R. Mendez-Roman

9:20 Intermission.


**Section B**

**Advances in Separations**

M. Hayes, *Organizer*

8:00 . Determination of MB-102 in human plasma by HPLC analysis for measurement of glomerular filtration rate. **J. Shieh**

8:40. Challenges of VOC emission testing for coating materials. M. Gallagher, P. Doll

9:00. Investigating simplified approaches to characterize volatile extractables from polymeric medical devices. K. Nahan, B. Oktem, E. Sussman, S.I. Wickramasekara

9:20 Intermission.

9:35. Laser-assisted dissolution: Dissolving geologic samples faster and with better precision. C. Durrant, R. Mariella, J. Combitsis, D.G. Weisz

9:55. Identification of methyl-substituted isomers of five-ring C_{20}H_{12} PAH products from the supercritical pyrolysis of n-decane and 1-octene. V. Vutukuru, E. Hurst, S. Kalpathy, N. Poddar, M. Wornat

10:15. Application of advanced liquid chromatographic column technologies for regulatory science. J. Wang, H. Qu, X. Feng, P. Faustino

10:35. How much better are the selectivity and resolution provided by two serially-coupled HPLC columns compared to those obtained using any single HPLC column?. J.P. Foley, Z. Liu

THURSDAY AFTERNOON

Section A

Placeholder

Advances in Spectroscopy

P. Bohn, Organizer

1:00. Ionophore-Based Biphasic Chemical Sensing in Droplet Microfluidics. X. Wang


1:40. Fluorescence microscopy of lithium ions in the oxidation of lithium cobalt oxide(LCO) nanoparticles. M. Wu, A. Cavell, M. Mattei, R.H. Goldsmith

2:00. Synthetic and genetically encoded biosensors and contrast agents for ultrasensitive $^{129}$Xe NMR. S. Zemerov, B. Roose, K.L. Farenhem, M.L. Greenberg, Y. Wang, I.J. Dmochowski
2:20 Intermission.

2:40  Self-assembly Au@Ag@β-cyclodextrin nanoparticles at the liquid-solid interface to fabricate SERS array substrate for sensitive detection of phthalate esters based on guest-host system and the coffee ring effect. **J. Zhang**

3:00  Dynamic fluorescence measurements of rose bengal photosensitization in octanol. **Y. Zhang**, S.L. Neal

3:20  Electron-Spin Delocalization along the Stabilizing Ligands in Paramagnetic Atomic-Precise Neutral Au25(SR)18 clusters as Measured by High-Resolution Solution 13C-NMR Spectroscopy. **R. Zheng**, T.C. Allison, Y. Tong

Section B

Placeholder

**Advances in Separations**

M. Hayes, *Organizer*

1:00  Real Time Online Chromatography Monitoring of Product Quality Attributes for Biologics Continuous Manufacturing Process. **G. Xue**

1:20  Improved analytical methods for a follow-on biologic: Method development and strategy to establish equivalency to monograph methods. **D. Watson**, A. Andrew, S. Yadav, B. Kunnel, L. He, M. Peery, J. Clark, J. Myers, J. Wright, D. Wylie, M. Chartrain


2:00  A fast and automated method for determination of oxalate in cromolyn sodium. **S. Patil**, J. Rohrer

2:20 Intermission.


2:55  2D-LC-HRMS/MS for direct structural characterization of small molecule drugs. **A. Crawford**, W. Tang
Development, validation and implementation of a Headspace GC/MS method for screening and quantification of NDMA, NDEA, NDIPA and NEIPA impurities in valsartan drug substances and drug products. D. Shakleya, S.D. Selaya, P. Faustino