ANYL
DIVISION OF ANALYTICAL CHEMISTRY
K. Agnew-Heard and M. Bush, Program Chairs

SUNDAY MORNING

Placeholder

Nanotechnology & Single Cell Analysis in Biology & Medicine
Nanoscience & Biology & Medicine
Cosponsored by BIOL, COLL, MPPG and PHYS
X. Xu, Organizer, Presiding

8:00 . Subcellular Control Over Focal Adhesion Anisotropy, Independent of Cell Morphology, Dictates Stem Cell Fate. C.A. Mirkin

8:30 . Nanoscale structures modulates protein signaling at the cell membrane. B. Cui

9:00 . Metallic Nanoislands on Graphene as Multimodal Biomechanical Sensors. D.J. Lipomi


10:00 Intermission.

10:10 . Endocytosis and exocytosis of nanoparticles by cells. Y. Xia


11:40 . Cellular adaptability to nanoparticle stress. C.J. Murphy

12:10 . Study of cytotoxic and therapeutic effects of silver nanoparticles against colon tumor cells. R.M. Richardson, K. Raut, T. Zvonare, P. Songkiasai, P. Cherukuri, X. Xu
Placeholder

**Zarefest: Symposium in honor of Richard Zare’s Love for Science**

Cosponsored by PHYS
M. Dulay, A. Orr-Ewing, H. Park, *Organizers*

**8:00** Introductory Remarks.

**8:05**. Applying analytical tools to ovarian cancer detection: Proteomics and aptamers. **R.J. Whelan**

**8:35**. Adventures with Plasmons: Molecular Sensing, Chemical Reactions, and Energy Transfer Processes. **J.P. Camden**


**9:35** Intermission.

**10:00**. New eyes for nanocatalysis: Molecular-scale investigations of nanocatalyst chemistry. **M.A. Hines**

**10:30**. Ultrabright probes for highly multiplexed cellular analysis. **D.T. Chiu**

**11:00**. From chiral cavity polarimetry, to ultrahigh-density spin-polarized hydrogen. **T. Rakitzis**

Section C

Placeholder

**The Origins and Future of Metabolite and Small Molecule Identification**

Cosponsored by BIOL, BIOT and MEDI
Financially supported by Waters
R. S. Plumb, *Organizer*
G. Siuzdak, *Organizer, Presiding*
8:00 . Metabolism’s Future and its Inextricable link to Identifying New Metabolites. G. Siuzdak

8:30 . In-silico Characterization of Metabolites Using Artificial Intelligence. L. Pirhaji

9:00 . Identifying metabolites using mass spectrometry and stable isotopes. C. Guijas, J. Montenegro-Burke, A. Palermo, G. Siuzdak


10:00 . Molecular composition of alcoholic beverages: The good, the bad, and the unnecessary. L. Silva, T. Shulman, M. Chua, A. Lee, J. Jastrzembski

10:30 . The alkynes we eat: where do they come from and how do we identify them?. C. Fischer, J. Jeon, K. Smith, E. Sattely

11:00 . Identifying metabolites from scratch. J. Montenegro-Burke, C. Guijas, A. Palermo, G. Siuzdak

Section D

Placeholder

Measuring Protein Conformations & Folding Inside the Cell

Measuring Protein Conformations & Folding Inside the Cell

Cosponsored by BIOL, BIOT and MEDI
J. Genereux, Organizer, Presiding

8:00 Introductory Remarks.

8:05 . Global analysis of methionine oxidation provides a census of folding stabilities for the human proteome. S. Ghaemmaghami

8:30 . In-Cell Footprinting Coupled with Mass Spectrometry to Study Protein Folding. L.M. Jones


9:45 . Molecular Code for Intracellular Collagen Assembly. M. Shoulders
10:10 Intermission.


10:45 . Structural biology in cellular environments using sensitivity enhanced NMR. K.K. Frederick

11:10 . Probing thiol-reactivity to monitor proteome foldedness and conformational change under proteostasis stress. D. Hatters

11:35 . Detecting the Multi-Step Protein Aggregation Process in Live Cells Using the AggTag Method. X. Zhang

Section E

Placeholder

Chemical Forensics

Chemical Forensics

C. Fraga, Organizer
C. Timperley, Presiding

8:00 Introductory Remarks.

8:05 . The Changing Nature of Analytical and Investigate Chemistry for Chemical Disarmament and Non-Proliferation. J.E. Forman

8:20 . Chemical Forensics Capability Expansion. R. Bull

8:40 . Standardization of impurity profiling for chemical forensics international collaborative research. C. Fraga, A.S. Breton-Vega, K. Höjer Holmgren, L. de Reuver, H. Lignell

9:05 . Score Based Likelihood Ratio Approaches to Chemical Profiling of Methylphosphonic Dichloride (DC) and Derived Products. M.E. Sigman, D. Ramos, K. Jarman, C. Fraga

9:30 Intermission.


10:15 . Reaction Pathways in the Synthesis of Levinstein Mustard. g.n. hondrogiannis
10:40 . Chemical attribution of ricin by profiling of fatty acids using gas chromatography mass spectrometry. R. Webster, S. Ovenden

11:05 . Highly accurate classification of biological spores by culture medium for forensic attribution using multiple chemical signature types and machine learning. P. Ippoliti, M.D. Crenshaw, F. Nargi, T. Boettcher, M. Walsh, A. Casale, J. Han, J. Dettman

Section F

Placeholder

Advances in Wearable & Implantable Sensors

Advances in Wearable & Implantable Sensors

M. A. Daniele, L. Deravi, M. Yokus, Organizers, Presiding

8:00 Introductory Remarks.

8:00 . Ultra-flexible and Stretchable Electronic Systems for Monitoring Brain Activities. T. Sekitani


8:00 . Eavesdropping on neurochemical signaling in vivo. A.M. Andrews


8:00 Intermission.

8:00 . Wearable Biomarker Analysis for Health and Wellness Monitoring at the Point of Person. S. Emaminejad

8:00 . Implantable optoelectronic devices based on CMOS LSI technology. T. Tokuda, M. Haruta, K. Sasagawa, J. Ohta

8:00 . Lysozyme sensing in tear using a contact lens. Z. Ballard, S. Bazargan, D. Jung, S. Sathianathan, A. Clemens, D. Shir, S. Al-Hashimi, A. Ozcan

Characterization of Plastics in Aquatic Environments
Sponsored by POLY, Cosponsored by ANYL, BIOL, CEI, ENVR, I&EC, PMSE‡ and PRES

Getting to the Bottom: Optical & Electron Imaging of Reactive Chemical Systems

Imaging Plasmon-Coupled Processes

Sponsored by PHYS, Cosponsored by ANYL‡

Getting to the Bottom: Optical & Electron Imaging of Reactive Chemical Systems

Imaging Plasmon-Coupled Processes

Sponsored by PHYS, Cosponsored by ANYL‡

SUNDAY AFTERNOON

Section A

Placeholder

Nanotechnology & Single Cell Analysis in Biology & Medicine

Nanoscience

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


1:30 . Nanopore Induced Phase-Shift Sequencing (NIPSS) for universal biomolecule sequencing. S. Huang

2:00 . Imaging Membrane Viscosity of Single Cells through Second Harmonic Light Scattering. H. Dai

2:30 . Endogenous second harmonic and two photon coherence imaging of substructures in neurons in 3D. S. Roke

3:00 Intermission.
3:10 . Sensing the Biological Membranes. **W. Cho**

3:40 . Photoluminescent Cellular Probes based on Mesoporous Silicon Nanoparticles. **M.J. Sailor**


Section B

Placeholder

**Zarefest: Symposium in honor of Richard Zare’s Love for Science**

**Zarefest: Symposium in honor of Richard Zare’s Love for Science**

Cosponsored by PHYS‡
M. Dulay, A. Orr-Ewing, H. Park, *Organizers*

1:00 . Microdroplet Chemistry for Catalysis, Material Synthesis, and Biology. **J. Lee**

1:30 . Reaction dynamics is really interesting, but is it useful?. **K.G. McKendrick**

2:00 . Ambient Ionization Mass Spectrometry and Machine Learning to Guide Clinical Decisions and Improve Patient Outcome. **L. Schiavinato Eberlin**

2:30 Intermission.


3:55 . From Halley's comet to metabolomics: How the Zarelab conquered the spectroscopy of the masses. **M.A. Johnson**

4:25 Concluding Remarks.
The Origins and Future of Metabolite and Small Molecule Identification

Cosponsored by BIOL, BIOT and MEDI
Financially supported by Waters
G. Siuzdak, Organizer
R. S. Plumb, Organizer, Presiding

1:00 . Identification of Putitive BioMarkers of Breast, Liver and Bladder Cancer With IOn Mobility Enabled LC/MS Based Metabolomics. R.S. Plumb


3:00 . Applying a Comprehensive Reference Tandem Mass Spectral Library to Accurate Identification of Human Metabolites. X. Yang, P. Neta, S.E. Stein


4:00 . Axcend Focus LC - Portable Liquid Chromatography Technology for In-Process Monitoring. S. Sharma, L.E. Blue
1:00 Introductory Remarks.

1:05. Optical biosensors for illuminating the biochemical activity architecture of the cell. J. Zhang

1:25. Coordinated Histone Modifications and Chromatin Reorganization in A Single Cell Revealed by FRET Biosensors. Y. Wang, q. peng


2:05. AgHalo: A HaloTag-based multi-color fluorogenic sensor that visualizes and quantifies proteome stress in live cells using solvatochromic and molecular rotor-based fluorophores. X. Zhang

2:25. Fluorescence imaging of Fe(II) flux in ischemic stroke. Y. Wei, L. Wan, R. Pan, K. Liu, W. Wang

2:45 Intermission.

3:00. Genetically encoded fluorescent indicators for 2-photon imaging. A. Aggarwal, K. Podgorski


3:40. Development of mNG-GECO1. L.C. Zarowny

4:00. Fluorescent protein based biosensors for metabolism and neurotransmission. S. Zhang

4:20. In situ Two-photon Fluorescence Imaging of Depression Related Active Molecules. P. Li, b. tang

Chemical Forensics

C. Fraga, Organizer, Presiding

1:00 Introductory Remarks.

1:05. A tool box for forensic investigations in the environment. S.M. Mudge

1:30. Tracing Soman precursors through site specific isotope ratio NMR spectroscopy. S. Lindberg, M. Engqvist, K. Höjer Holmgren, C. Åstot, R. Norlin

1:55. Analysis of chlorohydrins of phospholipids as chlorine biomarkers in biomedical samples of exposed animal models. P. Lindén, P. Hemstrom, L. Elfmark, S. Jonasson, A. Larsson, C. Åstot


2:45 Intermission.

3:05. Source Attribution of Calcium Ammonium Nitrate (CAN) by Handheld Raman Spectroscopy. O.M. Primera, C. Fraga, A.S. Breton-Vega, M. Philip, N.S. Mirjankar


3:55. THz/Far-Infrared spectroscopy at the Australian Synchrotron for the detection and identification of energetic materials and discrimination between energetic materials and precursors. G.S. Walker, R. Lehmann, B.M. Fischer, D. Appadoo

Section F

Placeholder

Advances in Wearable & Implantable Sensors

Advances in Wearable & Implantable Sensors

M. A. Daniele, L. Deravi, M. Yokus, Organizers, Presiding
1:00 . Soft, Skin-interfaced, Wireless, Battery-free, Microfluidic Devices for Chronometric Sweat Capture and Analysis. **A.J. Bandodkar**

1:00 . Flexible lab on the skin for personalized molecular monitoring. **W. Gao**

1:00 . Wearable Sweat Sensors - Towards big data for human health. **A. Javey**

1:00 Intermission.

1:00 . Materials Challenges and Opportunities for Carbon Nanotubes-based Flexible Electronics and Wearable Sensors. **Y. Wang**

1:00 . In Vivo Biosensing of Steroid Hormones Using Corona Phase Molecular Recognition (CoPhMoRe) and nIR Fluorescent Single Walled Carbon Nanotubes for Health Monitoring and Biologging. **M. Strano**

1:00 . Wearable multimodal patches: Concurrent monitoring of human physiology and biochemistry. **M. Yokus**, T. Songkakul, V. Pozdin, A. Bozkurt, M.A. Daniele

**Characterization of Plastics in Aquatic Environments**

Sponsored by POLY, Cosponsored by ANYL, BIOL, CEI, ENVR, I&EC, PMSE‡ and PRES

**Getting to the Bottom: Optical & Electron Imaging of Reactive Chemical Systems**

**Visualizing biology in living cells and in vitro**

Sponsored by PHYS, Cosponsored by ANYL

**SUNDAY EVENING**

Section G

Placeholder

**Analytical Division Poster Session**

Analytical Division Poster Session

K. Agnew-Heard, *Organizer*
8:00 - 10:00

. Diurnal cycle effects on ocean biochemistry during a mesocosmic algal bloom. **M.M. Rogers**, S. Baumler, H.C. Allen


. Tuning carbon nanodots and antioxidant studies. **Z. Ji**


. In Situ Characterization of Protein Corona Formation within Ordered Porous Nanostructures. **W. Qian**, Q. Su

. Electric field assisted electrode modification. **h. wang**, C. Ma


. Microfluidic thread-based electrode system to detect glucose and acetylthiocholine. K. Uchida, L. Duenas, M. Gaines, M. Gonzalez-Guerrero, **F.A. Gomez**

. 3D Microfluidic paper-based analytical devices for colorimetric bioassays. N. Neris, A. Wong, A. Fernandez, **F.A. Gomez**

. Effects of short chain fatty acids on fatty acid and glycogen synthesis in HepG2 cells. **L. Ma**, **J.K. Yee**, S. Lim, W. Lee


. Sensitive Analysis of Breast Cancer Biomarkers Using Laser Wave-Mixing Detector Interfaced to Microfluidics. **J. Liang**

. Evaluation of Statistical Techniques to Normalize Mass Spectrometry-Based Urinary Metabolomics Data. **S. Gamagedara**, T. Cook

Investigation of the adulteration of essential oils by GC-MS. M. Dubnicka, B. Cromwell, M. Levine

Deep ultraviolet resonance Raman spectroscopy of hydrogen bonding along transmembrane α-helices. X. Wei, R.D. Jiji, C. Greenlief

Enzyme-specific imaging achieved by labeling with enzyme activatable probes. A. Owen, R.L. McCarley

Analysis of commercially available mineral supplements: A microwave plasma atomic emission spectroscopy (MP-AES) and X-ray fluorescence (XRF) spectroscopy study. K.J. Kolonko, J. Pulvidente

Gradient chromatofocusing of proteins: Comparison of weak/strong anion/cation exchange HPLC columns. S. Rayaprolu, D.J. Anderson

Isorhamnetin-cyclodextrin inclusion: sensitive fluorescent probe for copper (II). S. Yang, L. Xu, X. Sun, H. Xue, J. Chen

Preliminary study on impurities and by-products formed in the synthesis of CWC-related chemicals. H. Kiljunen, H. Lignell, T. Kauppila, P. Vanninen

Comparison study of the Phytochemicals and Antioxidant activity of Fully Matured and Averagely Matured Crinum jagus bulbs. D.L. Abiona, O.O. Onawumi, S.O. Oladoye

A Microfluidic Device for Oxygen Quantitation in Anoxic Environments. M. Clayson, M.J. Evans, L. Miller, S. Mckay, C.F. Monson

Rapid detection of Bisphenol A in a microfluidic device through the use of hydrogels and aptamers. B. Phelps, N. Perera, M. Piyasena

Development of an analytical method to detect microplastics in the wastewater treatment plant. M. KIM, K. Zoh

Molecular insights into ultrasmall nanoparticle-protein interactions through measurement of binding kinetics. R.S. Ferreira, A.L. Lira, R.J. Torquato, S. Hassan, A.A. Sousa

Rapid screening and semi-quantification of zilpaterol in incurred sheep tissue samples using ambient and semi-ambient mass spectrometry. S. Chakrabarty, W.L. Shelves, D.J. Smith

Probing the rheology of model sea spray aerosol particles using a dual-balance linear quadrupole trap as a micro-analytical tool. D.S. Richards, K. Trobaugh, R.D. Davis

Automated Low Density Solvent Based Demulsification Dispersive Liquid-Liquid Microextraction Followed by Gas Chromatography-Mass Spectrometry for the Determination of Pharmaceutically Active Compounds in Water. L. Guo, H. Lee
Comparative quantitative analysis of cetirizine dihydrochloride by HPLC (high performance liquid chromatography) and q-NMR (quantitative nuclear magnetic resonance) techniques. S. Kumar, M. Villanueva

Development of a simple extraction method for tetracycline analogues from milk with UV detection. O. Cordova, T. Le, K. Ng

Mass Spectrometry Analysis and Theoretical Study of the Enrichment of Phosphopeptides by Different Crystal Forms of TiO₂. y. qi, x. yang, w. zhang, r. jiang, j. zhang, H. Zhong


Rapid and Accurate Determination of the pH of Environmental Water Samples using Smartphone Colorimetry. Z. Naing, H. Liang, D. Sarmiento, J. Brannon, Y. Liu


Indium phosphide quantum dots as benign fluorescent probes for enzymatic assays. D. Bwambok, A. Acoba, S. Uriosttigue

Screening for fungal infections using LC/MS. C. Allison, M.M. Reynolds

Early Diagnosis of Colon Caner with Rapid Hybridization of DNA Biomarkers. S. Lee


Preparation of magnetic molecularly imprinted polymer for the electrochemical analysis of melamine. W. Ho, M. Tse, S. Cheng

Improvement of a sensor for urine creatinine using a copper electrodeposited gold electrode. N. Sato, K. Takeda, H. Ohno, N. Nakamura

Cost-effective and easy-to-use biosensor capable of early diagnosing human cancers with the quantification of carcinoembryonic antigen in a sample. I. Hwang, J. Lee

Silicone membrane modified with chitooligosaccharide in situ purification and detection of Salmonella. C. Yan, C. Ma

New isothermal amplification technique for POCT of foodborne pathogenic bacterium Listeria monocytogenes. J. Chen, Y. Shi
. Loop-Mediated Isothermal Amplification based on naked visualization dye for Salmonella POCT testing. J. Chen, Y. Shi


. Forensic analysis of disposable nitrile gloves utilizing FTIR, XRF, TGA/DSC/Pyrolysis-MS:. J. Angst, D.J. Lecaptain

. Rapid colorimetric detection of Salmonella typhimurium based on Polyamide film and Strand Exchange Amplification. S. Liu, S. Kuang


. Internal Calibration Potentiometric Aptasensors for Simultaneous Detection of Hg^{2+}, Cd^{2+}, and As^{3+} Based on a Screen-Printed Carbon Electrodes Array. W. Tang, P. He

. Multi-organelle concurrent imaging in single cells by 3D superlocalization of dual-code enhanced dark-field microscopy. S. Lee, S.H. Kang


. Development of N,N,N-Trimethyl-2-oxo-2-(2-((7-sulfinobenzo [c][1,2,5]oxadiazol 4-yl)sulfonyl)hydrazinyl)ethan-1-aminium (TOSBA) as a Thiol Specific Fluorogenic Agent for Cell Surface Thiol Imaging in Live Cells. S. Wang, Y. Huang, Y. Alqahtani, A. Najmi, T.M. Seefeldt, X. Guan

. 2D HPLC with coupled with MS to examine Cold medicines using compendial methods as the first dimension. W. Long, K.W. Whitaker


. Development of substitutable interface on dandelion-like SiO\textsubscript{2} / Au thin film and application to sensitive and selective VOCs gas detection. J. Kim, H. Son, Y. Choi, S. Hong
Forensic applications of analytical chemistry: Funding programs at the National Institute of Justice. **G.J. Dutton**

State-of-the-art technologies for relative response normalization of metabolites in mass spectrometry. **S. Dell’Aiera, E. Isin, C. Delatour**

Analysis of Total Mercury in Radioactive Waste using a Direct Mercury Analyzer Instrument. **T.L. White, B. Looney, L. Brown**

An improved method for the measurement of tobacco-specific carcinogen biomarker Urinary 4-(Methylnitrosamino)-1-(3-pyridyl)-1-butanol (NNAL) in tobacco users. **J. Brown, B. Xia, J. Lee, B. Blount, L. Wang**

Polycyclic aromatic hydrocarbons and polyacenes: Analyzing the band structure and elemental composition of organic, heterocyclic crystals. **K. Erlitz, S. Brady, B. Schatschneider**

Effect of Gold Nanoparticles on MCP-1 guided Monocytic Cell Line (THP-1) Chemotaxis in 3D µ-Slide. **X. Zhang, P. Falagan Lotsch, C.J. Murphy**

Determination of cholesterol concentrations in aqueous solutions using screen-printed carbon electrodes and cyclic voltammetry. **D.E. Martyn, S.K. Buehler**

HPLC-UV method development for baseline resolution of 17 cannabinoids. **M.J. Wilcox, E. Franklin**

Development of Efficient Extraction and Detection Method for the Active Components in Commercial Kratom Products. **F. Ceja, P. Tuitt, K. Ng**


Separating chiral steroid compounds by isocratic C18 reversed phase HPLC: Optimization of the acetonitrile/methanol ratio to maximize separation. **E. Kipruto**

Ultrasensitive fluorescent DNA detection through signal amplification and target regeneration via dual-cycling reactions. **I.A. IWE**


Chemometric Analysis of Multidimensional Fluorescence Data Recorded from Benzo[a]pyrene Metabolites in Frozen Matrixes. **M. Chehelamirani**

Determining the avicide DRC-1339 (3-chloro-4-methylaniline hydrochloride) concentration in boiled egg baits using GC/MS/MS. **R.S. Stahl**

Design hub for early phase drug discovery. A. Stracz

Ultrasensitive, colorimetric, paper-based devices for the detection of ppb levels of nitrate and nitrite. T. Mako, A. Levenson, M. Levine

Silver-chlorosilver(I) reference electrodes of the first and second kind for alkylimidazolium bis(trifluoromethylsulfonyl)imide room temperature ionic liquids from solubility and complexation studies. A. García-Mendoza, J.C. Aguilar


Aptamer-modified microelectrodes for the measurement of Neuropeptide Y using Electrochemical Impedance Spectroscopy. L.F. Lopez, N.G. Hernandez, K. Flores, J. Cruz, L. Cunci

Electrochemical Detection of Viable Bacterial Cells Using a Tetrazolium Salt. K. Ishiki, D. Nguyen, H. Shiigi

Real-time monitoring of α-Synuclein-induced cell membrane disruption in Parkinson’s disease by scanning ion conductance microscopy. J. Parres-Gold, S. Wong Su, A. Chieng, M. Chang, Y. Wang

Cancer DNA detection using Gold Nanoparticle Colorimetry and Three ways Target Switching Catalytic Hairpin Assembly. C. PARK, S. Na

Determination of a quantitative indicator of the lytic strength of cell lysing reagents. a. zhao, M. Brody, X. Zhao

Development of a glycan reference material for therapeutic proteins. M. Lowenthal, G. Boons, B. Lang, K. Phinney

2D IR spectroscopy for the characterization of protein side-chain dynamics. S. Ramos, R. Horness, A. Le Sueur, M.C. Thielges

Investigation of 2-amino-thiazole and 2-amino-benzothiazole salicylidenes as sensitive probes for detection of anions and cations. R.O. Alzu’bi, Y. Hijji

Resorufin derived fluorescent probes for the selective detection of ONOO\textsuperscript{-}. M. Weber, T. James, A. Mackenzie, S. Bull

Hierarchical surfaces with biomimetic polydopamine coatings for efficient capture of circulating tumor cells. X. Zhou

Protein Profiling and pseudo-Parallel Reaction Monitoring to Monitor the Fusion-associated Conformational Switch in Hemagglutinin. K.K. Nguyen

Separation and detection of fentanyl from complex mixtures using gradient elution moving boundary electrophoresis. S. Krauss, T. Forbes, D. Ross

Placeholder

**Biosensing: New Strategies & Latest Development**

**Biosensing: New Strategies & Latest Development (Poster)**

Cosponsored by BIOL, BIOT and MEDI

Q. J. Cheng, Organizer, Presiding

8:00 - 10:00

Bacteria identification using a DNA-nGO based sensing array. L. Wang, Y. Wen, X. Yang, L. Li, Y. Li, L. Xu, W. Liang, F. Gong, G. Liu

Far- and deep-ultraviolet surface plasmon resonance sensors. I. Tanabe, K. Fukui

Competitive and noncompetitive immunoassays for the detection of benzothiostrobin using magnetic nanoparticles and fluorescein isothiocyanate-labeled peptides. c. he, x. Hua

Human photoreceptor protein-graphene hybrid material allowing detection of visible light with human-like spectral sensitivities. H. Song

An Activatable Contrast Agent for Photoacoustic Imaging of Gingipains Associated with Periodontal Disease. C. Moore, J.V. Jokerst

Aptamer-based detection of vaspin by phytoplankton-derived biomineral modified electrode. S. Kim, O. Nam, E. Jin, M. Gu

Sensitive SERS Detection of Small Molecules by Photothermal Convection Based Real-Time and Pin-Point Colloidal Assembly. T. Kang, I. Seo, H. An, I. Choi
Poly(ethylene glycol)-dibromomaleimide as a stabiliser for volatile sulfur compounds. G. Kirby, R. Hand, D.M. Haddleton


Decoration of S, N co-doped graphene quantum dots with p-aminothiophenol functionalized AuNPs for molecular imprinted sensing of sofosbuvir in real samples. M. Mahnashi, A. Mahmoud, S. Alkahtani

Enzyme-based colorimetric biosensor for selective detection of L-DOPA. Y. Chou, I. Wang, C. Shih, Y. Yeh


Sensitive Electrochemical Aptasensor for EpCAM by Mesoporous Silica Nanoparticles and Quantum Dots Signal Amplification. L. Zhu, Y. Liu, B. Yang, L. Qiao, B. Liu

Phosphorylation-mediated single-particle assay of protein kinase activity with dark-field microscopy. T. Tian, K. Zhang, Y. Liu, B. Liu

Electrogenerated chemiluminescence imaging of a single protein based on functional nanopores of Ru@SiO₂ nanoparticles. Y. Liu, T. Tian, H. Zhang, J. Liu, B. Liu


Graphene oxide-based paper sensor for enhanced colorimetric sensing of miRNA. J. Lee

Dual-targeting functionalized graphene films for rapid and highly sensitive fluorescence imaging detection of hepatocellular carcinoma circulating tumor cells. c. wu, P. Li, N. Fan, j. han, W. Zhang, W. Zhang, b. tang

Screen-Printed Mesoporous Carbon Electrodes for Efficient Sensing of Dopamine. Y. Lee, Y. Chang, H. Chang, M. Yeh, Y. Yeh, Y. Liu

Observation of Acetylcholinesterase in Stress-induced Depression Phenotypes by Two-photon Fluorescence Imaging in the Mouse Brain. X. Wang, P. Li, c. wu, D. Su, Q. Ding, W. Zhang, b. tang

Using nitric oxide-releasing metal–organic frameworks on the surface of blood-contacting glucose biosensors to reduce biofouling. **A.C. Melvin**, M.M. Reynolds

Application of Super Resolution Radial Fluctuation (SRRF) Single-Molecule Imaging to measurement of DNA Hybridzation Kinetics. **J. Cooper**

Nanobodies and Phage-display peptides - attractive biosensing materials for analytical applications. **N. Vasylieva**, D. Li, Z. Li, B. Barnych, B.D. Hammock


Graphene Oxide and Enzyme-Assisted Dual-Cycling Amplification Method for Sensitive DNA Detection. **I.A. IWE**


Comparative analysis for PCBS and organochlorine pesticides in plasma samples employing C-18 SPE and functionalized electrospun nanofibers. **D.K. Adeyemi**

Functionalized nanopore biosensor for quick and highly sensitive glucose detection in human saliva. **M. Yang**

Microdialysis – fluorescence analysis system for vancomycin detection in pharmaceuticals and plasma. **f. mu**

Section I

**Nanozymes for Bioanalysis and Beyond**

**Nanozymes for Bioanalysis and Beyond**

Cosponsored by BIOL and BIOT

H. Wei, *Organizer*

8:00 - 10:00
. N and B co-doped Graphene: A Suitable Candidate to Substitute Natural Peroxidase in Sensitive and Selective Bioassays. J. Lee, J. Lee

. Mechanisms of oxidase and peroxidase mimicking activities of nanoceria from first principles calculations. w. zhenzhen, X. Gao, c. chen, Y. Zhao

. Regulating oxidase mimicking activity of platinum by surface modifications. S. Xiaomei, X. Gao

. Molecular mechanisms for the peroxidase-mimicking activities of perovskite nanomaterials. X. Gao, X. Wang, H. Wei, X. Gao

. Novel Silk-Biomaterials-Supported Artificial Enzymes: Synthesis and Applications. Y. Lin

Section J

Placeholder

Zarefest: Symposium in honor of Richard Zare’s Love for Science

Zarefest: Symposium in honor of Richard Zare’s Love for Science (Posters)

Cosponsored by PHYS‡
M. Dulay, A. Orr-Ewing, H. Park, Organizers

8:00 - 10:00

. On-demand drug release from polypyrrole nanoparticulate films. C. Chamberlayne, S. Baltsavias, H. Xu, A. Arbabian, J. Annes, R.N. Zare

. A Novel Antibody Drug Conjugates for Pancreatic Cancer Therapy. J. Huang, P. Guo, M. Moses

. Photon-catalyzed photoisomerization of stilbene. J. Meiser, K. Hilsabeck, J.A. Harrison, R.N. Zare

. Spectroscopic Investigation of semiconductor halide compounds interaction with silicon dioxide. S.D. Fleischman

. Simple algorithms for some unconventional uses of the method of least squares. J.B. Tellinghuisen

Can machine learning be used to learn laws of natural science? An Illustration for Planck’s Blackbody Radiation. **V. Shankar**, S. Shankar

Evanescent-Wave Cavity-Ring-Down Imaging. **M.A. Everest**

Kinetic studies on unimolecular processes in Criegee intermediates. **T.A. Stephenson**, M.I. Lester

Solutions for lightweight construction and CO₂ footprint reduction by analysis of surfaces exposed to laser and plasma treatment. **U. Lommatzsch**, K. Thiel, M. Noeske, J. Ihde, R. Wilken

Phenotyping macrophages involved in the onset of diabetes type 1 with label-free and quantitative proteomics. **F. Sandbaumhüter**, G. Christoffersson, **E.T. Jansson**

*Pulsed triboelectric nanospray ionization for analysis of complex organics*. M. Bouza Areces, A. Li, Z.L. Wang, **F.M. Fernandez**


Detecting Bacteria Using an Artificial Antibody. **M. Dulay**, A.C. Mody, R.N. Zare, C. Da-Silva-Granja

Non-cationic and deformable nanolipogels for *in vivo* genome editing of triple negative breast cancer. **P. Guo**, J. Yang, J. Huang, D. Auguste, M. Moses


Droplet spray ionization mass spectrometry for solution chemistry: Advances & future trends. H. Zhang, K. Yu, J. He, **J. Jiang**

Synchrotron infrared nanospectroscopy at the Advanced Light Source. **H.A. Bechtel**, S.N. Gilbert Corder, M.C. Martin

Electronic Structure of Naturally Occurring Aromatic Carbon. **A.E. Pomerantz**

Changing the nature of electroless etching with a syringe pump: ReEtching, MACE and low load MACE. **K.W. Kolasinski**, B.A. Unger, J.D. Swanson, H. Yu, A.T. Ernst, M. Aindow, E. Mäkilä, J. Salonen, K. Tamarov, J. Riikonen, V. Lehto

The Oncogene MYC Regulates Lipogenesis Essential for Neoplastic Growth. **K. Margulis**, A. Gouw, N. Liu, D. Felsher, R.N. Zare

HPLC column for nanoparticles and nanomedicines. **M. Kato**

. Development of new stationary phases for HPLC. **L.A. Colon, J.R. Ezzo**

. 3-D Mapping of the Chemical Contents of Anthropogenic Soils by the Chemometric Analysis of Infrared and Visible Spectra. **D.S. Perry, A.J. Lopa, A. Cava, T. Matney, L. Barrett, D. Maki**

. Synchronization modulated surface plasmon coupled emission for improving spectral resolution. **Y. Zhao, Y. Liu, S. Cao, Y. Li**

. Soft Ionization and Dissociation Based on Laser Activated Interfacial Photoelectron Transfer for Mass Spectrometry. **H. Zhong**

. Aesthetic Education in Chemistry. **H. Zhong**

. Photoacoustic measurements of single aerosol droplets: Microscopic heat transfer and accelerated photoreactions. **J. Cremer**

**Section K**

**Placeholder**

**Structure at Solid-Liquid Interfaces: Effects of Confinement & Chemical Patterning**

**Structure at Solid-Liquid Interfaces: Effects of Confinement & Chemical Patterning (Posters)**

T. C. Davis, T. R. Hayes, *Organizers*

**8:00 - 10:00**


. Surface-seeded folding of DNA origami. **H. Cao, Q. Gu, G.R. Abel, G.V. Gueorguieva, Y. Zhang, W. Nanney, T. Ye**

. Surface Chemistry and Spectroscopic Study of Tyrosinase enzyme Langmuir Monolayer. **s. paudyal**
Theoretical & Experimental Investigations of Water Interactions with Materials

Posters

Sponsored by COLL, Cosponsored by ANYL

MONDAY MORNING

Section A

Placeholder

Nanotechnology & Single Cell Analysis in Biology & Medicine

Nanoscience

Cosponsored by BIOL, COLL, MPPG and PHYS

X. Xu, Organizer, Presiding

8:00. Nanotechnology Approaches to Cellular Therapies. S.J. Jonas, P.S. Weiss


9:00. Mapping the inner world of cells. B. Huang

9:30. Single nanoparticle plasmonic spectroscopy for biomedical applications: from diagnosis to therapy. X. Xu, P. Songkiatisak, P. Cherukuri, K. Raut, R.M. Richardson

10:00 Intermission.


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T. Huang, A. Filbrun, J. Richardson, Y. Tzeng, R. Dickson

11:40. Diagnostics of primary cancer invasion/metastasis via MASS mapping of metalloproteinase of cancer tissue. X. Gao

Section B

Placeholder

**Structure at Solid-Liquid Interfaces: Effects of Confinement & Chemical Patterning**

Cosponsored by COLL‡
T. C. Davis, T. R. Hayes, *Organizers, Presiding*

**8:00** Introductory Remarks.


**8:25** Surface confinement: friend or foe to complex self-assembled DNA architectures?. **T. Ye**, H. Cao, G.R. Abel

**8:55** Confined defects formed by chemical lift-off lithography to pattern multi-functional substrates. N. Nakatsuka, H. Cao, P.S. Weiss, **A.M. Andrews**

**9:25** Protein Structure at the Bio/Abio Interface. **L.J. Webb**

**9:55** Intermission.

**10:10** Surface-mediated peptide self-assembly to modulate surface energy. **Z. Fakhraai**, Y. Lin, M. Skolnick, E. Petersson

**10:40** Dynamic organization of complex droplets via chemotactic surface-mediated interaction. C. Meredith, Y. Chiu, J. Groenewold, W. Kegel, **L.D. Zarzar**, A. van Blaaderen, P. Moerman

**11:10** Uniform, Large-Area, Highly-Ordered Peptoid Monolayer and Bilayer films for Sensing Applications. D. Murray, J. Kim, E. Grzincic, S. Kim, A. Abate, **R.N. Zuckermann**

Section C

Placeholder

**Identification & Design of Catalytic Sites in Electrochemical Reactions**
Identification & Design of Catalytic Sites in Electrochemical Reactions

Cosponsored by ORGN
Y. Liang, H. Wang, Organizers
C. Liu, Organizer, Presiding

8:00. Understanding the active sites of structurally dynamic nanomaterials for CO₂ electrocatalysis to multicarbon products. Y. Li, D. Kim, P. Yang

8:30. Highly Active and Selective Electrochemical CO₂ Reduction to Formate Enabled by Structural Defects on Converted Bi₂O₃ Nanotubes. Y. Li

9:00. Two-Dimensional Copper Nanosheets for Electrochemical Reduction of Carbon Monoxide to Acetate. F. Jiao

9:30 Intermission.

9:45. One-dimensional Core/Shell Nanocrystals with Favorable Interfacial Synergy for Electrocatalysis. S. Zhang, Z. Zhang, C. Liu

10:15. Synthesizing Intermetallic Nanoparticle Catalysts for enhanced catalytic electro-oxidation. W. Huang, Z. Qi

10:45. Controllable Synthesis of N-doped Hollow Carbon Spheres @ Highly Dispersed Mo₂C and Ultra-low Platinum Nanoparticles Core-Shell Electrocatalysts: Remarkable Active toward PEMFCs Hydrogen Oxidation. C. Deng, Q. Feng, Z. Zhao, Z. Zhang, H. Li, H. Wang

11:05. Strain-Driven Energy Electrocatalysis. S. Guo

Placeholder

Advances in Fluorescence & Bioluminescence Imaging Probes

Advances in Fluorescence & Bioluminescence Imaging Probes

Cosponsored by PHYS
H. Ai, Organizer, Presiding
X. Zhang, Presiding

8:00 Introductory Remarks.


8:45. Multifunctional super-resolution microscopy with solvatochromic and conventional fluorescent probes. **K. Xu**

9:05. Fluorescent probes for imaging enzyme activity. **J. Rao**


10:25 Intermission.

10:40. Imaging drug release from biomedical implants via radioluminescence. **G.B. Schober**, J.N. Anker

Section E

**Chemical Forensics**

Chemical Forensics

C. Fraga, *Organizer*
C. Åstot, *Presiding*

8:00 Introductory Remarks.


9:05. Microcystin analysis in biological fluids: Evaluation of 1D and 2D LC-MS/MS methods. B.J. Renner (Garcia-Barboza), S. Botch-Jones, C. Mallet, M. Lame

9:25 Intermission.


10:05. Characterization of Impurities in Gallium Alloys via Laser-Induced Breakdown Spectroscopy. A. Rao, M. Shattan, J.D. Auxier


10:45. Authentication of edible oils using vibrational spectroscopy and pattern recognition techniques. B.K. Lavine, F. Kwofie, I.S. Uba, M. Bamidele, K.S. Booksh

Section F

Placeholder

Advances in Wearable & Implantable Sensors

Advances in Wearable & Implantable Sensors

M. A. Daniele, L. Deravi, M. Yokus, Organizers, Presiding

8:00. What can Conformable Decoders do?. C. Dagdeviren

8:00. Real-time biosensors for continuous measurements of specific biomolecules in live animals. H.T. Soh

8:00. Light-Activated Open Circuit Potentiometry. J.E. Dick

8:00 Intermission.
8:00 . Flexible and wearable sensors for human motion analysis. E. Thostenson, S. Doshi, A. Chaudhari

8:00 . Soft Wearable Systems with Physiological Monitoring and Biochemical Sensing Capabilities. R. Ghaffari

8:00 . Stretchable Conductive Nanocomposite for Wearable and Implantable Bioelectronics. D. Jung, D. Kim

8:00 . A Wearable Microfluidic Sensing Patch for Dynamic Sweat Secretion Analysis and Regional Sweat Studies. H.Y. Nyein, M. Bariya, A. Javey

Liquid Assets: The Business of Water

Sponsored by SCHB, Cosponsored by ANYL, BMGT and I&EC

Getting to the Bottom: Optical & Electron Imaging of Reactive Chemical Systems

Spectroscopy of reactive chemical systems

Sponsored by PHYS, Cosponsored by ANYL

MONDAY AFTERNOON

Section A

Placeholder

Nanotechnology & Single Cell Analysis in Biology & Medicine

Nanoscience

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

1:00 . Single Cell Analysis of Dynamic Signaling Activities with Fluorescent Biosensors. J. Zhang

1:30 . Molecular Imaging and Cellular Reprogramming in Single Cells. Y. Wang

2:00 . Cellular imaging with genetically encoded RNA-based sensors. M. You
2:30 . Stimulated Raman Imaging with Chemical Probes for Subcellular Bioanalysis. L. Wei

3:00 Intermission.

3:10 . Stimulated Raman scattering: the next frontier of light microscopy. W. Min


4:40 . Augmented fluorescent-free 3D super-resolution microscopy based on wavelength-dependent plasmonic scattering illumination. S.H. Kang

Section B

Placeholder

Structure at Solid-Liquid Interfaces: Effects of Confinement & Chemical Patterning

Cosponsored by COLL‡
T. C. Davis, T. R. Hayes, Organizers, Presiding

1:00 . Impact of passively and actively confining self-assembled molecular networks in 2D corrals. S. De Feyter

1:30 . Standing, Lying, and Sitting: Phospholipid Striped Phases as Templates for Nanomaterials at Interfaces. S.A. Claridge

2:00 . Controlled Molecular Assembly at Solid-Liquid Interfaces. G. Liu, J. Zhang, V.A. Piunova, J. Frommer

2:30 . Correlating structure and molecular transport at wet and semi-wet interfaces. D.K. Schwartz

3:00 . Confined growth and transformation of colloidal nanostructures at solid-liquid interfaces. Y. Yin

3:30 . Impact of fixed chemical patterns on moving surfaces. M.M. Santore

Section C
Identification & Design of Catalytic Sites in Electrochemical Reactions

Cosponsored by ENFL and ORGN
C. Liu, H. Wang, Organizers
Y. Liang, Organizer, Presiding

1:00 . Selective CO₂ Reduction on Isolated Transition Metal Single Atomic Sites: From Identification to Scaling-up. H. Wang

1:30 . Atomic design of metal nano-catalysts toward activation of energy-related molecules. Y. Wu

2:00 . Molecular engineering of nickel single-site electrocatalysts. X. Zhang, Y. Liang

2:20 Intermission.

2:35 . Oxygen Evolution Reaction Electrocatalysis on Mixed-Metal Oxyhydroxides. S.W. Boettcher, M. Burke Stevens


3:25 . Probing Electrochemical Reactions under Operando Condition. B. Liu

3:55 . In situ and operando spectroscopy of oxide electrocatalyst surfaces. K.A. Stoerzinger

Section D

Placeholder

Advances in Fluorescence & Bioluminescence Imaging Probes

Advances in Fluorescence & Bioluminescence Imaging Probes

Cosponsored by PHYS
H. Ai, Organizer. Presiding
X. Zhang, Presiding

1:00 . Multi-component bioluminescence imaging with diverse luciferin architectures. J.A. Prescher

1:40 ATP-Independent Bioluminescent Reporters for in vivo Imaging. H. Ai, H. Yeh

2:00 SAFE method for luminescence quantum yield determination. K. Nawara, J. Waluk


2:40 Intermission.

2:55 Methods for improving the biodetection performances of upconversion nanoprobes. S. Xu


3:35 Near-infrared Fluorescent Probe for Fast and Ultrasensitive Detection of Nitroreductase in Live Cells. S. wan

3:55 Near-infrared Hybrid Rhodol Dyes with Spiropyran Switches for Sensitive Ratiometric Sensing of pH Changes in Mitochondria. S. Xia, H. Liu


4:35 Dual enzyme activated fluorescein based fluorescence probe. M. Odyniec, T. James

Section E

Placeholder

Metabolomics in Forensics: Applications, Technical Barriers & Emerging Approaches for Chemical Identification Using In Silico Reference Libraries

Metabolomics in Forensics: Applications, Technical Barriers & Emerging Approaches for Chemical Identification Using In Silico Reference Libraries

Cosponsored by COMP
T. E. Metz, Organizer
D. Wunschel, Organizer, Presiding
T. O. Metz, Presiding
1:00 Introductory Remarks.

1:05 Metabolomics for Forensic Analysis. R. Bull


1:45 Studying the metabolome of Ricinus communis for attribution. S. Ovenden

2:10 Advancement in gas-phase separations for metabolomics. G. Nagy, A. Li, A.L. Hollerbach, R.D. Smith, Y.M. Ibrahim

2:35 LC-HRMS data and in silico fragmentation for identifying transformation products in environmental matrices. J. Schollee, K. Kiefer, R. Gulde, H. Singer, J. Hollender, C. Mc Ardell

3:00 Intermission.

3:15 Tools and Databases for In Silico Compound Identification. D.S. Wishart


4:00 Identification of unknown compounds using in silico fragmentation algorithms and in silico reference libraries. T. Kind


4:45 Optimal conformer selection for accurate in silico chemical property prediction. F. Nielson, D. Thomas, S.M. Colby, y. yesiltepe, R. Renslow

Section F

Placeholder

Advances in Wearable & Implantable Sensors

Advances in Wearable & Implantable Sensors

M. A. Daniele, L. Deravi, M. Yokus, Organizers, Presiding
1:00 . Minimally- and Non-Invasive Continuous Biosensing: Frontiers for Devices and Sensors. **J. Heikenfeld**

1:00 . Minimally Invasive Microneedle Sensor Arrays: A New Window on the Body. **A.E. Cass**, S. Sharma, D. O'Hare

1:00 . Rethinking On/In-Body Biochemical Sensing Strategies to Achieve Long-Term Functionality. **D. Diamond**

1:00 Intermission.

1:00 . A New Antifouling Electrochemical Aptamer-Based Sensor. **R.J. White**, S. Hendrickson

1:00 . Band-Aid©-like electrochemical and electromechanical sensors for continuous physiological monitoring. M. Chu, L. Lin, E. Chou, J. Zakashansky, A. Hikari Imamura, J. Kim, **M. Khine**


1:00 Concluding Remarks.

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**Getting to the Bottom: Optical & Electron Imaging of Reactive Chemical Systems**

**Observing chemical processes and nanostructures in situ at the atomic level**

Sponsored by PHYS, Cosponsored by ANYL

**TUESDAY MORNING**

Section A

Placeholder

**Nanozymes for Bioanalysis and Beyond**

**Nanozymes for Bioanalysis and Beyond**
Cosponsored by BIOL and BIOT  
H. Wei, Organizer, Presiding

8:00 Introductory Remarks.

8:05. Single Atom Nanozyme for Wound Antibacterial Applications. X. Yan

8:45. Imaging and treatment of multidrug-resistant bacteria and biofilms using bioorthogonal transition metal catalyst nanoparticle ‘nanozymes’. V.M. Rotello

9:25. Applications of inorganic nanoparticle enzyme mimics. W. Tremel

10:05 Intermission.


10:50. Metallic Nanostructures for Medical Diagnostics. X. Xia


Section B

Placeholder

Structure at Solid-Liquid Interfaces: Effects of Confinement & Chemical Patterning

Structure at Solid-Liquid Interfaces: Effects of Confinement & Chemical Patterning

Cosponsored by COLL‡  
T. C. Davis, T. R. Hayes, Organizers, Presiding


8:20. Surface microstructure functionalised by multicomponent femtoliter droplets at liquid-solid interface: fabrication and applications. M. Li, x. zhang

8:40. Broad probe for function of crystal nucleation by engineered nucleation features with proteins and small molecules in batch and continuous flow crystallization. A.H. Bond, K. Nordquist, T.L. Kinnibrugh, K.M. Schaab


9:40 Intermission.

10:25. Surface chemistry of silica particles in aqueous solution. A. Marchioro, **S. Roke**


11:25 Concluding Remarks.

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**Section C**

**Placeholder**

**Identification & Design of Catalytic Sites in Electrochemical Reactions**

Cosponsored by ENFL and ORGN
C. Liu, H. Wang, **Organizers**
Y. Liang, **Organizer, Presiding**

8:00. Identification of Active Phase of Oxide-Derived Cu in Electrochemical CO Reduction Reaction with Operando Surface Enhanced Spectroscopy. **B. Xu**


9:00. Cation-mediated evolution of hydrogen on Cu electrodes. **M. Waegele**

9:30 Intermission.

9:45. Identification of active species and mechanisms in non-precious metal oxygen reduction catalysts by poisoning and magnetic measurements. **A.A. Gewirth**, A. Esposito

10:15. High Performance Electrochemical CO₂ Reduction Cells Based on Non-Noble Metal Catalysts. **H. Wang**

10:35. Atomically Precise Metal Nanoclusters for Electrocatalysis. **D. Jiang**

11:05. Understanding the Electronic Structure and Reactivity of Carbon Monoxide Dehydrogenase Model Systems for Carbon Dioxide Reduction. **J. Panetier**
Mass Spectrometry of Biomolecular Assemblies

Cosponsored by BIOT, BMGT and MEDI
Financially supported by Agilent
J. S. Prell, Organizer
M. T. Marty, Organizer, Presiding

8:00 . Role of Surface Collisions in an MS-Based Structural Biology Approach. V.H. Wysocki

8:30 . Ion Mobility Mass Spectrometry to Characterize Formation and Structure of DNA Assemblies. T.L. Pukala, A. Begbie, J. Li

9:00 . Pinpointing Isomerization Sites in Long-lived Proteins using IMS-MS. R. Julian

9:30 Intermission.

9:45 . Multidimensional Ion Mobility of Proteins and Protein Complexes Enabled by Modular Design. M.F. Bush


10:45 Intermission.

11:00 . Tandem-trapped ion mobility / mass spectrometry measurements relates proteoform identity to their tertiary and quaternary structures. C. Bleiholder, F.C. Liu, T.C. Cropley, M. Chai

8:00 Introductory Remarks.

8:10 Principles to influence culture and establish practices regarding safe operation of research instrumentation and application development. **E. Robinson**

8:30 Computer-assisted separation modeling in analytical space translated into improved preparative chromatography productivity. **I. Haidar Ahmad**, F. Tsay, R.A. Bennett, D. Henderson, R. Hartman, B. Mann, I.K. Mangion, E. Regalado


9:10 Safe Solvent Management for LC/MS and GC/MS. **P.A. Reinhardt**, S. Bain

9:30 Panel Discussion.

10:45 Concluding Remarks.

Section F

Placeholder

**ACS Sensors Young Investigators (Invited)**

**ACS Sensors Young Investigators**

J. Gooding, S. O. Kelley, **Organizers**

8:00 Introductory Remarks.

8:05 Multi-Modal Sensing for Measuring Tissue Development and Function in Microphysiological Systems. **M.A. Daniele**, V. Pozdin, K. Rivera, A. Young, P. Erb

8:35 Expanding the scope of biosensors: RNA- and small molecule-generating sensing systems. **B.C. Dickinson**

9:05 Probing and constructing bio-inorganic interfaces within a nanocavity for adaptive single molecule sensing. **S. Huang**

9:35 Intermission.
9:45. Not Everybody Dyes: Leveraging Quantum Dots and Other Luminescent Nanomaterials for New Opportunities in Bioanalysis. W.R. Algar


Getting to the Bottom: Optical & Electron Imaging of Reactive Chemical Systems

High-resolution optical imaging of chemical processes

Sponsored by PHYS, Cosponsored by ANYL

TUESDAY AFTERNOON

Section A

Placeholder

Nanozymes for Bioanalysis and Beyond

Nanozymes for Bioanalysis and Beyond

Cosponsored by BIOL and BIOT
H. Wei, Organizer, Presiding

1:00. Ceria-based nanomaterials for therapeutic antioxidants. T. Hyeon

1:40. Antioxidant Nanostructures for Theranostics ANT. S. Seal

2:20. Peptide-gold clusters as enzyme-like catalyst for in situ cell analysis and induce tumor-specific cell apoptosis. L. Gao

3:00 Intermission.

3:05. Enzyme-Mimic Metal-Bismuth Oxyhalide for Sensing and Antimicrobial Applications. C. Huang, H. Chang, J. Lai

3:45. Truncated tetrahedral CdTe QDs act as endonucleases for site-selective photoinduced cleavage of DNA. C. Xu, M. Sun, H. Kuang, L. Xu, A. Qu


Section B

Placeholder

Analytical Division Awards (Invited)

Analytical Division Awards

K. Agnew-Heard, Organizer, Presiding

1:00 Introductory Remarks.

1:05. Spectroscopy through the Microscope: Chemical Analysis at Liquid/Solid Interfaces. J.M. Harris


2:15. New nano tools for real-time single molecule imaging of single live cells: From fundamental discoveries to biomedical applications. X. Xu

2:50 Intermission.

3:00. Building Learning & Teaching Communities in Analytical Chemistry: From Campus to Textbook. C.A. Lucy

3:35. In vivo and Intraoperative Chemical Analysis and Tissue Diagnosis using the MasSpec Pen Technology. L. Schiavinato Eberlin


Section C

Placeholder

Identification & Design of Catalytic Sites in Electrochemical Reactions

Identification & Design of Catalytic Sites in Electrochemical Reactions
Cosponsored by ENFL and ORGN
Y. Liang, C. Liu, Organizers
H. Wang, Organizer, Presiding

1:00. Ambient electrochemical activation of small molecules with inorganic and hybrid catalysts. **C. Liu**


2:00. CO₂ Reduction by Immobilized Rhenium Bipyridine Moieties. **S.C. Marinescu**

2:30 Intermission.


Section D

Placeholder

**Mass Spectrometry of Biomolecular Assemblies**

**Mass Spectrometry of Biomolecular Assemblies**

Cosponsored by BIOL, BIOT and MEDI
Financially supported by Agilent
M. T. Marty, Organizer
J. S. Prell, Organizer, Presiding

1:00. Temperature-Programmed Native ESI-MS as a Versatile Biophysical Toolbox to Study Noncovalent Complexes. **R. Zenobi**

1:30. Flying viruses – from biophysical to structural characterisation. **C. Uetrecht**

2:00. Native mass spectrometry: Probing gas-phase or solution-phase protein structures? **J.A. Loo**

2:30 Intermission.
2:45 . Role of macroion-droplet interactions in the charge state of macromolecules. S. Consta

3:05 . Investigation of membrane toxin assemblies with native ion mobility-mass spectrometry and Gábor transform. J.S. Prell

3:25 . Characterizing oligomerization of biomolecular assemblies within intact membranes using native mass spectrometry and lipoprotein nanodiscs. M.T. Marty

3:45 Intermission.

4:00 . Denaturing and native top-down proteomics using capillary electrophoresis-tandem mass spectrometry. L. Sun

4:30 . Identifying Protein Interactions Using In-Cell Protein Footprinting Coupled with Mass Spectrometry. L.M. Jones

Section E

Exploration of the Nano-Bio Interface with Analytical Tools

Cosponsored by BIOL and BIOT
W. Zhong, Organizer, Presiding
R. Coreas, Presiding

1:00 . Nanotoxicity and Nanomedicines. Y. Zhao

1:40 . Toxicological profiling of metal and metal oxide nanomaterials in liver cells. T. Xia

2:10 . Investigation of Immune Cell Responses to Engineered Metal Oxide Nanomaterials by Quantitative Proteomics Tools. T. Zhang, M. Gaffrey, B.D. Thrall, W. QIAN

2:40 Intermission.

2:50 . Single Particle Spatiotemporal Analysis of Transmembrane Process of Functionalized Nanocargos. Y. He


Section F

Placeholder

**Biosensing: New Strategies & Latest Development**

Biosensing: New Strategies & Latest Development

Cosponsored by BIOL, BIOT and MEDI
Q. J. Cheng, Organizer, Presiding

1:00 . Single hydrogel nanoparticle SPR imaging measurements for biosensing and bioaffinity uptake. **R.M. Corn**


2:00 . Mirror-Image Nucleic Acid-Based Sensors for Live-Cell Imaging of RNA. **J. Sczepanski**, B. Young, A. Kabza, W. Zhong


2:40 Intermission.


3:25 . Preparation and integration of specifically functionalized biosensors for liquid biopsy. **R. Heer**

3:55 . New catalytic DNA based biosensors for selective metal ions detection. **J. Liu**

4:15 . Using gold nanoparticles for diagnostics and sensing in low cost devices. **K. Hamad-Schifferli**

WEDNESDAY MORNING

Section A

WEDNESDAY MORNING

Section B

Placeholder

Nanozymes for Bioanalysis and Beyond

Nanozymes for Bioanalysis and Beyond

Cosponsored by BIOL and BIOT
H. Wei, Organizer, Presiding

8:00 Strong Candidate Graphene Based Materials to Replace Natural Peroxidase in Sensitive and Selective Bioassays. J. Lee

8:40 Nanozyme-prodrug therapy. A. Zelikin

9:20 Bifunctional nanozyme based on modified carbon nitride photocatalyst that mimics glucose oxidase-peroxidase. W. Choi, P. Zhang, J. Han, D. Kim

10:00 Intermission.

10:05 Combat resistant bacteria with nanozymes. L. Gao

10:45 Nanocatalysis for enhanced multimodal tumor theranostics. X. Jiang


11:45 Fluorescent C₃N₄-based nanozymes for ratiometric biomedical assays. X. Wang, H. Wei

Section B

Placeholder

From Antibody-Based to Mass Spectrometry-Based Analysis of Emerging Contaminants in Water: Advances & Future Trends

From Antibody-Based to Mass Spectrometry-Based Analysis of Emerging Contaminants in Water: Advances & Future Trends

Cosponsored by ENVR
D. S. Aga, R. J. Schneider, Organizers, Presiding
8:00 Introductory Remarks.

8:10. Antibody-based approaches to respond to the environmental analytical challenges. **M. Marco**

8:45. Using Mass Spectrometry to vet Microcystin Concentrations by Enzyme-Linked Immunosorbent Assay. **J. Westrick**

9:10. VHH antibodies are versatile tools for monitoring of environmental chemical contamination. **N. Vasylieva, Z. Li, D. Li, B. Barnych, B.D. Hammock**

9:35 Intermission.

10:00. Improving small molecule annotation in nontargeted soft-ionization GC/LC high-resolution mass spectrometry. **C. Jaeger, J. Lisec**

10:25. Oriented functionalization of magnetic beads with *in vivo* biotinylated nanobodies for rapid MALDI-TOF ultrasensitive quantitation of toxins in biological samples. **M. Pírez-Schirmer, B.M. Brena, G. Gonzalez**

Section C

Placeholder

**Advances in Electrochemistry**

**Advances in Electrochemistry**

L. A. Baker, *Organizer, Presiding*

8:00. Imaging local electrochemistry with ion conductance microscopy. **L.A. Baker**


8:45. Positive and negative feedback theory and experiments in Hot-Tip scanning electrochemical microscopy. **Z. Zhao, A. Boika**


9:25 Intermission.
9:40 · Critical Nuclei Size and Rate of Nanobubble Nucleation. **M.A. Edwards**, S. German, H. Ren, A. Moreno Soto, H. White

10:05 · Mechanism of Histamine Oxidation and Electropolymerization at Carbon Electrodes. **P. Puthongkham**, B.J. Venton


10:45 · Single drop fabrication of the cholesterol biosensor based on synthesized NiFe$_2$O$_4$NPs dispersed on PDDA–CNTs. **C. Moonla**, T. Tangkuaram, A. Preechaworapun

Section D

Placeholder

**Interface between Experiments & Modeling in Unraveling the Physical And Chemical Properties of Charged Droplets**

**Interface between Experiments & Modeling in Unraveling the Physical And Chemical Properties of Charged Droplets**

Cosponsored by COMP, ORGN and PHYS
S. Consta, S. Xantheas, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 · Understanding molecular aspects of aqueous interfacial chemistry with clusters. **M.A. Johnson**

8:35 · Photoemission from charged droplets. **R. Signorell**

9:05 · Diverse Nature of Ion Speciation at the Nanoscale Hydrophobic/Water Interface. E. Zdrali, M.D. Baer, H. Okur, C.J. Mundy, **S. Roke**

9:35 Intermission.

9:50 · Native Electrospray Ionization: From Solution to Charged Droplets to Final Ions. **M.F. Bush**

10:20 · Spectroscopic Characterization and Computational Investigation of Anionic Clusters Generated from Charged Droplets. **X. Wang**


11:50 Discussion.

Section E

Placeholder

**Exploration of the Nano-Bio Interface with Analytical Tools**

Cosponsored by BIOL and BIOT
W. Zhong, Organizer, Presiding

8:00 . Don’t forget the lipids: Biomolecular coronas on nanoparticles. **C.J. Murphy**

8:40 . Pulmonary surfactant corona and nano-bio interactions in the lung. **Y. Zuo**


9:40 Intermission.


11:00 . Gold nanoparticle-based screening platform to assess protein-carbohydrate interactions. **S. Richards**

Section F

Placeholder
**Biosensing: New Strategies & Latest Development**

Cosponsored by BIOL, BIOT and MEDI
Q. J. Cheng, *Organizer*
R. Heer, M. Liu, *Presiding*

8:00. Development of miniature surface plasmon resonance systems and sensor applications. **A. Baba**, S. Nootchanat, C. Lertvachirapaiboon, K. Shinbo, K. Kato, S. Ekgasit

8:30. Supported Lipid Membranes as Biosensing Interface. **Q.J. Cheng**

9:00. Interference Effect of Silica Colloidal Crystal Films and Their Applications on Biosensing. **W. Qian**, Q. Su, F. Wu, P. Xu, A. Dong, C. Liu, Y. Wan


10:00 Intermission.


**Theoretical & Experimental Investigations of Water Interactions with Materials**

Sponsored by COLL, Cosponsored by ANYL‡

**WEDNESDAY AFTERNOON**

Section A
Nanozymes for Bioanalysis and Beyond

Cosponsored by BIOL and BIOT
H. Wei, Organizer, Presiding

1:00. De Novo Design of Nanomedicine: Large Scale Molecular Simulation of Nanoparticle-Biomolecule Interactions. R. Zhou

1:40. Catalytic model bridging computations and experiments for ceria-based nanozymes. Z. Wang, X. Gao


3:00 Intermission.


3:45. Standardization of nanozyme research. m. liang


Section B

D. S. Aga, R. J. Schneider, Organizers, Presiding

1:00. Analysis and fate of antimicrobials in animal manure: Challenges and solutions. D.S. Aga


2:00 Intermission.


3:15 Concluding Remarks.

Section C

Placeholder

Advances in Electrochemistry

L. A. Baker, Organizer, Presiding

1:00. Electrochemical and electrokinetic route for dialysate regeneration. B. Berzina, R. Anand

1:25. Electrochemical sensors for field detection of explosives. S. Trammell


2:10 Intermission.


3:25. Determination of Betadex (β-Cyclodextrin) according to the USP Betadex Sulfobutyl Ether Sodium Monograph. M. Aggrawal, J.S. Rohrer
Interface between Experiments & Modeling in Unraveling the Physical And Chemical Properties of Charged Droplets

Cosponsored by COMP, ORGN and PHYS
S. Consta, S. Xantheas, Organizers, Presiding

1:00 . Ions from solution to the gas phase: The effects of solvent on the final structure. M.J. Hebert, D.H. Russell

1:30 . Understanding Disordered Protein Conformations in Solution as Viewed from the Gas Phase. P.E. Barran

2:00 . Microsolvation effects on the encapsulation of metal ions by crown ethers. Y. Inokuchi

2:30 Intermission.

2:45 . Charging Proteins by Electrospray Ionization. R.R. Loo, J.A. Loo

3:15 . Infrared laser spectroscopy of solvated cations. M.A. Duncan


4:45 Discussion.

Study of Circulating, Cell-Free Biomarkers with Analytical Tools

Cosponsored by BIOL, BIOT and MEDI
W. Zhong, Organizer, Presiding
G. Adkins, M. P. Trinh, Presiding
1:00. Tracking cell-free, circulating nucleic acids from tumors with electrochemical sensors. S.O. Kelley

1:40. Lipid-based normalization of quantum dot probes bound to membrane markers on extracellular vesicles in complex biological samples. T. Hu


3:00 Intermission.


3:50. Chemical operations on a living single cell by open microfluidics. J. Lin


Section F

Placeholder

**Biosensing: New Strategies & Latest Development**

**Biosensing: New Strategies & Latest Development**

Cosponsored by BIOL, BIOT and MEDI

Q. J. Cheng, Organizer

B. Liu, R. Ragan, Presiding

1:00. Aptamer-functionalized microelectrodes and nanopipettes to sense neurotransmitters in neuronal networks. N. Nakatsuka, S. Weaver, D. Eggemann, T. Schlotter, D. Momotenko, J. Vörös


2:40 . Developing Aptamer-Based Biosensor For Onsite Detection Of Stress Biomarkers In Noninvasive Biofluids. S. Dalirirad

3:00 Intermission.


4:35 . Duplex electrochemical DNA sensor to detect B.anthrasis CAP and PAG DNA targets based on the incorporation of tailed primers and ferrocene labelled dATP. I. Magriñá-Lobato, M. Jauset-Rubio, M. Ortiz, A. Simonova, M. Hocek, C. O'Sullivan

Theoretical & Experimental Investigations of Water Interactions with Materials

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THURSDAY MORNING

Section A

Placeholder

Advances in Spectroscopy

Session I: Advances in XRF, NMR, & SEM Spectroscopy

E. A. Smith, Organizer, Presiding

8:00 Introductory Remarks.

8:05 . Detection of toxic metals contamination in cosmetics using MP-AES and X-Ray fluorescence spectroscopy. S. Alsherari, A.W. Apblett


9:05. Applications of Broadband $^{19}$F-$^1$H Cross-Polarization in NMR Spectroscopy: Hetero-TOCSY and ASAP-HSQC. **A.A. Marchione**, E. Diaz

9:25 Intermission.


10:00. Simultaneous measurement of metal coatings thickness and composition using X-ray fluorescence (XRF) spectroscopy. **H. Ataee-Esfahani**, J. Peters

10:20. How Analytical Chemistry is providing basic advances in climate science. **R.F. Hirsch**

10:40. Calibration transfer between low-field NMR instruments. D. Galvan, E. Danieli, D. Borsato, **M.H. Killner**

Section B

Placeholder

**Advances in Mass Spectrometry**

**Advances in Mass Spectrometry**

M. F. Bush, *Organizer, Presiding*

8:00. Electrochemistry-assisted absolute quantitation by mass spectrometry without the use of standards. **H. Chen**, P. Zhao

8:25. Applications of in-situ mass spectrometry, high resolution mass spectrometry, and theoretical methods to the analysis of e-cigarette thermal degradation chemistry. **Y. Li**, A. Burns, T.B. Nguyen

8:45. Studying Reductive Reaction of Triple Bond in Microdroplet by Extractive Electrospray Ionization Mass Spectrometry and in-situ Raman Spectroscopy. **K. Huang**, W. Chou, Y. Wang, C. Hsu
9:05. Heteroatom-doped graphene quantum dots enable negative ion laser desorption ionization mass spectrometry for probing and imaging of small biomolecules. **Q. Min**, X. Huang, M. Liu, J. Zhu


9:45 Intermission.

10:05. Ion Mobility-Mass Spectrometry Reveals the Effect of Sialylation on Glycoprotein Structures. **G. Li**, L. Li


10:45. Native top-down proteomics for mouse brain proteome with capillary zone electrophoresis-tandem mass spectrometry. **X. Shen**, L. Sun

11:05. Module-based method development and life cycle method improvement: two case studies of complex method development, validation and implementation using automated tandem mass spectrometry to support regulatory science issues. **J. Zhang**, P. Faustino


Section C

**Chemometric Analysis for Aqueous Sample**

**Chemometric Analysis for Aqueous Sample**

Cosponsored by COMP and ENVR

Financially supported by The University of Alabama

X. Liang, T. Mako, Y. Xu, X. Yao, **Organizers, Presiding**

8:00 Introductory Remarks.

8:05. Unraveling sample matrix effects for multivariate calibration. **J.H. Kalivas**, T. Lemos
8:30  Use of chemometrics in optimizing paper microfluidic applications. **F.A. Gomez**


9:45  Intermission.

9:55  Temperature-dependent near-infrared spectroscopy for analyzing aqueous samples. **X. Shao, X. Cui, L. Ma, L. Wang, Y. Sun, M. Wang, W. Cai**

10:20  Calibration-based detection and confidence limits are (almost) exact when the data variance function is known. **J.B. Tellinghuisen**

10:45  Multivariate curve resolution and pattern recognition applied to infrared images of paint chips to facilitate the forensic examination of automotive paints. **B.K. Lavine, F. Kwofie**

11:10  Concluding Remarks.

Section D

Placeholder

**Interface between Experiments & Modeling in Unraveling the Physical And Chemical Properties of Charged Droplets**

Cosponsored by COMP, ORGN and PHYS
S. Consta, S. Xantheas, *Organizers, Presiding*

8:00  Reversed interfacial fractionation of carbonate and bicarbonate evidenced by X-ray photoemission spectroscopy and theory. **R.J. Saykally, t. pascal**

8:30  Quantum mechanical studies of protonated water clusters through their IR spectra. **J.M. Bowman, Q. Yu**

9:00  How can we use machine learning to study droplet catalysis?. **T. Rhone, C. O'Connor, R. Hoyt, M. Montemore, C. Kumar, C.M. Friend, E. Kaxiras**

9:30  Intermission.
9:45. Diffusion Monte Carlo approaches for exploring neutral and protonated water clusters. A.B. McCoy, r. dirisio, v. Lee


11:15. Ionic strength is systems that violate the electric neutrality. S. Consta

11:45 Discussion.

11:55 Concluding Remarks.

Section E

Placeholder

Study of Circulating, Cell-Free Biomarkers with Analytical Tools

Study of Circulating, Cell-Free Biomarkers with Analytical Tools

Cosponsored by BIOL, BIOT and MEDI
W. Zhong, Organizer, Presiding
G. Adkins, M. P. Trinh, Presiding

8:00. Fluorescent Nanomaterials for Detection of Cell Markers and Images. H. Chang

8:40. Chemiluminescent gold nanoluminophore-based immunoassays for biomarkers of acute myocardial infarction. H. Cui


9:40. Photocleavable linker for the release of rare cancer biomarkers after microfluidic affinity selection. T. Pahattuge, J.M. Jackson, S.A. Soper

10:00 Intermission.


10:30. DNA terminal structure-mediated enzymatic reaction for ultra-sensitive detection of EGFR exon 19 deletion. M. Zhao


Placeholder

Biosensing: New Strategies & Latest Development

Biosensing: New Strategies & Latest Development

Cosponsored by BIOL, BIOT and MEDI
Q. J. Cheng, Organizer
A. Lambert, H. Lee, Presiding


8:40 Intermission.

8:55 . Microfluidic synthesis and patterning of silver nanoparticles for biomolecular sensing. Y. Nie, J. Zhang


9:55 . Microfluidic paper-based analytical devices (microPADs) with DVD player: Centrifugally assisted flow acceleration for rapid distance readout assays. K. Maejima, Y. Hiruta, D. Citterio

10:15 . Chimeric phage as scaffold for rapid detection of pathogenic bacteria. H. Peng, I. Chen

10:55 . Fast interrogation of electrochemical, aptamer-based (E-AB) sensors for the characterization of small molecule-aptamer binding kinetics. **M.S. Santos Cancel**, R. Lazenby, R. White


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**THURSDAY AFTERNOON**

Section A

Placeholder

**Advances in Spectroscopy**

**Session II: Advances in Optical Spectroscopy: IR, Fluorescence, Absorption, and Raman Spectroscopy**

E. A. Smith, **Organizer, Presiding**

1:00 . Development of fluorescent molecular probes for the highly sensitive and selective detection of living substances using magnetic beads. **Y. Suzuki**


1:40 . Polymeric microfluidic continuous flow mixer combined with hyperspectral FT-IR imaging for studying rapid biomolecular events. **H. Jang**, A. Pawate, R. Bhargava, P.J. Kenis


2:20 Intermission.
2:35. Adversarial Spectroscopy. G.J. Simpson

3:00. Microgel nanostructures for surface-enhanced Raman spectroscopy. S.R. Emory, A. Silva, J. Lo, S. Olson, D.A. Rider
