ANYL

DIVISION OF ANALYTICAL CHEMISTRY

K. Agnew-Heard and M. Bush, *Program Chairs*

SUNDAY MORNING

Section A

Marriott Marquis San Diego Marina
San Diego Ballroom Salon C

Nanotechnology & Single Cell Analysis in Biology & Medicine

Nanoscience, Biology & Medicine

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

8:00 1. Cellular adaptability to nanoparticle stress. **C.J. Murphy**

8:30 2. Study of cytotoxic and therapeutic effects of silver nanoparticles against colon tumor cells. **R.M. Richardson**, K. Raut, T. Zvonare, P. Songkiatisak, P. Cherukuri, X. Xu

8:45 3. Biophysical and bio-nano-mechanical insights from tracking single gold nanoparticles in live cells. **N. Fang**

9:15 4. Profiling cells inside and out using magnetic nanoparticles. **S.O. Kelley**

9:45 5. Endocytosis and exocytosis of nanoparticles by cells. **Y. Xia**

10:15 Intermission.

10:25 6. Nanoscale structures modulates protein signaling at the cell membrane. **B. Cui**

10:55 7. Photonic modification of cell-culture landscapes. **J. Shear**, K. Michelson, J. Connell, D. Hernandez, E. Ritschdorff

11:25 8. Metallic nanoislands on graphene as multimodal biomechanical sensors. **D.J. Lipomi**

11:55 9. Subcellular control over focal adhesion anisotropy, independent of cell morphology, dictates stem cell fate. **C.A. Mirkin**

Section B

Marriott Marquis San Diego Marina
Torrey Pines 3

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

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

8:00 Introductory Remarks.

8:05 10. Applying analytical tools to ovarian cancer detection: Proteomics and aptamers. **R.J. Whelan**

8:35 11. Adventures with plasmons: Molecular sensing, chemical reactions, and energy transfer processes. **J.P. Camden**

9:05 12. Nanoscale chemical analysis and imaging using tip-enhanced Raman spectroscopy. **R. Zenobi**

9:35 Intermission.

10:00 13. New eyes for nanocatalysis: Molecular-scale investigations of nanocatalyst chemistry. **M.A. Hines**

10:30 14. Ultrabright probes for highly multiplexed cellular analysis. **D.T. Chiu**

11:00 15. From chiral cavity polarimetry, to ultrahigh-density spin-polarized hydrogen. **T. Rakitzis**

Section C

Marriott Marquis San Diego Marina
Presidio 1

Origins & Future of Metabolite & Small Molecule Identification

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

8:00 16. Metabolism's future and its inextricable link to identifying new metabolites. **G. Siuzdak**

8:30 17. *In-silico* characterization of metabolites using artificial intelligence. **L. Pirhaji**

9:00 18. Identifying metabolites using mass spectrometry and stable isotopes. **C. Guijas**, J. Montenegro-Burke, A. Palermo, G. Siuzdak

9:30 19. Using stable isotope labeling to facilitate unknown metabolite identification. **W. Lu**, L. Wang, X. Xing, Y. Xu, J. Rabinowitz

10:00 20. Molecular composition of alcoholic beverages: The good, the bad, and the unnecessary. **L. Silva**, T. Shulman, M. Chua, A. Lee, J. Jastrzembski

10:30 21. 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 22. Identifying metabolites from scratch. **J. Montenegro-Burke**, C. Guijas, A. Palermo, G. Siuzdak

Section D

Marriott Marquis San Diego Marina
Presidio 2

Measuring Protein Conformations & Folding Inside the Cell

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

8:00 Introductory Remarks.

8:05 23. Global analysis of methionine oxidation provides a census of folding stabilities for the human proteome. **S. Ghaemmaghami**

8:30 24. In-cell footprinting coupled with mass spectrometry to study protein folding. **L.M. Jones**

8:55 25. Covalent protein painting reveals aberrant protein folding in cells *in vivo*. **C.C. Bamberger**, S. Pankow, S. Martínez-Bartolomé, J.R. Yates

9:20 26. Measuring cellular protein stability through Hsp40 affinity purification coupled with mass spectrometry. **J. Genereux**

9:45 27. Molecular code for intracellular collagen assembly. **M. Shoulders**

10:10 Intermission.

10:20 28. Quantifying a protein-protein interaction in living cells. S.L. Speer, A.J. Guseman, **G.J. Pielak**

10:45 29. Structural biology in cellular environments using sensitivity enhanced NMR. **K.K. Frederick**

11:10 30. Probing thiol-reactivity to monitor proteome foldedness and conformational change under proteostasis stress. **D. Hatters**

11:35 31. Detecting the multi-step protein aggregation process in live cells using the AggTag method. **X. Zhang**

Section E

Marriott Marquis San Diego Marina
Torrey Pines 2

Chemical Forensics

C. Fraga, *Organizer*
C. Timperley, *Presiding*

8:00 Introductory Remarks.

8:05 32. The changing nature of analytical and investigate chemistry for chemical disarmament and non-proliferation. **J.E. Forman**

8:20 33. Chemical forensics capability expansion. **R. Bull**

8:40 34. 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 35. 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.

9:50 36. Source attribution of sulfur mustard in complex matrices. **K. Höjer Holmgren**, L. Mörén, L. Ahlinder, D. Wiktelius, R. Norlin, C. Åstot

10:15 37. Reaction pathways in the synthesis of Levinstein mustard. **G.n. Hondrogiannis**

10:40 38. Chemical attribution of ricin by profiling of fatty acids using gas chromatography mass spectrometry. **R. Webster**, S. Ovenden

11:05 39. 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

Marriott Marquis San Diego Marina
Leucadia

Advances in Wearable & Implantable Sensors

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

8:00 Introductory Remarks.

8:05 40. Ultra-flexible and stretchable electronic systems for monitoring brain activities. **T. Sekitani**

8:35 41. Mechanically-softening intracortical implants for sensing and drug delivery. **A. Dunning**, G. Maguire, E. Szabo, S.J. Rowan, D. Tyler, J. Capadona

9:05 42. Eavesdropping on neurochemical signaling *in vivo*. **A.M. Andrews**

9:35 43. Micro-invasive biochemical sampling of brain interstitial fluid for investigating neural pathology. **R. Raman**, E. Rousseau, M. Wade, R. Langer, M. Cima

10:05 Intermission.

10:20 44. Wearable biomarker analysis for health and wellness monitoring at the point of person. **S. Emaminejad**

10:50 45. Implantable optoelectronic devices based on CMOS LSI technology. **T. Tokuda**, M. Haruta, K. Sasagawa, J. Ohta

11:20 46. 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

High-Resolution Optical Imaging of Chemical Processes

Sponsored by PHYS, Cosponsored by ANYL

SUNDAY AFTERNOON

Section A

Marriott Marquis San Diego Marina
San Diego Ballroom Salon C

Nanotechnology & Single Cell Analysis in Biology & Medicine

Nanoscience

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

1:00 47. Electrochemical zero-mode waveguide nanovials for capture and bimodal interrogation of single entities. J. Kim, S. Baek, S. Kwon, G. Crouch, H. Do, **P.W. Bohn**

1:30 48. Nanopore induced phase-shift sequencing (NIPSS) for universal biomolecule sequencing. **S. Huang**

2:00 49. Imaging membrane viscosity of single cells through second harmonic light scattering. **H. Dai**

2:30 50. Endogenous second harmonic and two photon coherence imaging of substructures in neurons in 3D. **S. Roke**

3:00 Intermission.

3:10 51. Sensing the biological membranes. **W. Cho**

3:40 52. Photoluminescent cellular probes based on mesoporous silicon nanoparticles. **M.J. Sailor**

4:10 53. Nanoscale-manipulation of the force field fluctuation and energy landscape entanglement in protein non-covalent recognition dynamics. **H. Lu**

4:40 54. Nanoplasmonics for characterizing EGFR heterogeneity. **S. Zhang** , B.M. Reinhard

4:55 55. Generation of a compact quantum dot conjugate for imaging dopamine transporter membrane dynamics in acute brain slices. **L.B. Thal**, V.R. Mann, I.D. Tomlinson, D. Sprinzen, J.R. McBride, K.R. Reid, D.G. McMahon, B.E. Cohen, S.J. Rosenthal

Section B

Marriott Marquis San Diego Marina
Torrey Pines 3

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

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

1:00 56. Microdroplet chemistry for catalysis, material synthesis, and biology. **J. Lee**

1:30 57. Reaction dynamics is really interesting, but is it useful?. **K.G. McKendrick**

2:00 58. Ambient ionization mass spectrometry and machine learning to guide clinical decisions and improve patient outcome. **L. Schiavinato Eberlin**

2:30 Intermission.

2:55 59. Finding the smoking gun: Solving the mystery of soot formation. **H.A. Michelsen**, K.O. Johansson, J. Hendrix, D. Hait, M.P. Head-Gordon, P.E. Schrader, K.R. Wilson

3:25 60. To see a world in a grain of sand: CAESAR comet sample return mission. **S.J. Clemett**

3:55 61. From Halley's comet to metabolomics: How the Zarelab conquered the spectroscopy of the masses. **M.A. Johnson**

4:25 Concluding Remarks.

Section C

Marriott Marquis San Diego Marina
Presidio 1

Origins & Future of Metabolite & Small Molecule Identification

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

1:00 62. Identification of putitive bio markers of breast, liver, and bladder cancer with IOn mobility enabled LC/MS based metabolomics. **R.S. Plumb**

1:30 63. Metabolite identification and unknown characterization for metabolomics activity screening. **A. Palermo**, J. Montenegro-Burke, C. Guijas, G. Siuzdak

2:00 64. Development of a shark health matrix using metabolomics coupled with metagenomics. **E.M. Forsberg**, A.Z. Goodman, Z. Walters, R.A. Edwards, E. Dinsdale

2:30 65. Advanced metabolomics and chemical biology approaches for selective analysis of microbiota and human co-host metabolism. **M. Povoa Correia**, C. Ballet, L. Conway, N. Garg, D. Globisch

3:00 66. Applying a comprehensive reference tandem mass spectral library to accurate identification of human metabolites. **X. Yang**, P. Neta, S.E. Stein

3:30 67. Investigation of host-microbiota co-metabolism as a new strategy for biomarker discovery: New chemical biology tools for metabolomics analysis. M. Povoa Correia, L. Conway, W. Lin, C. Ballet, N. Garg, **D. Globisch**

4:00 68. Withdrawn

Section D

Marriott Marquis San Diego Marina
Presidio 2

Advances in Fluorescence & Bioluminescence Imaging Probes

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

1:00 Introductory Remarks.

1:05 69. Optical biosensors for illuminating the biochemical activity architecture of the cell. **J. Zhang**

1:25 70. Coordinated histone modifications and chromatin reorganization in a single cell revealed by FRET biosensors. **Y. Wang**, Q. Peng

1:45 71. Role of local electric field in controlling fluorescence quantum yield of red fluorescent proteins. **M. Drobizhev**, J. Scott, P.R. Callis, R. Molina, G. Lambert, N.C. Shaner, A. Salih, T.E. Hughes

2:05 72. AgHalo: 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 73. Fluorescence imaging of Fe(II) flux in ischemic stroke. Y. Wei, L. Wan, R. Pan, K. Liu, **W. Wang**

2:45 Intermission.

3:00 74. Genetically encoded fluorescent indicators for 2-photon imaging. **A. Aggarwal**, K. Podgorski

3:20 75. Development of a genetically encoded intensiometric lactate indicator iLACCO1. **Y. Nasu**, Y. Wen, J. Lemieux, S. Zhang, R.E. Campbell

3:40 76. Development of mNG-GECO1. **L.C. Zarowny**

4:00 77. Fluorescent protein based biosensors for metabolism and neurotransmission. **S. Zhang**

4:20 78. *In situ* two-photon fluorescence imaging of depression related active molecules. **P. Li**, B. Tang

4:40 79. Mycophenolic acid core intermediates as a new chemosensing fluorophore class: Selenium-based ROS biological probes. **J. Choi**, D.G. Churchill

Section E

Marriott Marquis San Diego Marina
Torrey Pines 2

Chemical Forensics

C. Fraga, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 80. Tool box for forensic investigations in the environment. **S.M. Mudge**

1:30 81. Tracing Soman precursors through site specific isotope ratio NMR spectroscopy. **S. Lindberg**, M. Engqvist, K. Höjer Holmgren, C. Åstot, R. Norlin

1:55 82. Analysis of chlorohydrins of phospholipids as chlorine biomarkers in biomedical samples of exposed animal models. P. Lindén, P. Hemstrom, L. Elfsmark, S. Jonasson, A. Larsson, **C. Astot**

2:20 83. Investigation of the use of deuterium and oxygen in illicit fentanyl analysis. J. Casale, M. Lott, **J. Mallette**

2:45 Intermission.

3:05 84. 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

3:30 85. Chemometric analysis of spectroscopic and spectrometric data from energetic materials. **R. Lehmann**, S. Walker, D. Armitt

3:55 86. 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

Marriott Marquis San Diego Marina
Leucadia

Advances in Wearable & Implantable Sensors

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

1:00 87. Soft, skin-interfaced, wireless, battery-free, microfluidic devices for chronometric sweat capture and analysis. **A.J. Bandodkar**

1:30 88. Flexible lab on the skin for personalized molecular monitoring. **W. Gao**

2:00 89. Wearable sweat sensors: Towards big data for human health. **A. Javey**

2:30 Intermission.

2:45 90. Materials challenges and opportunities for carbon nanotubes-based flexible electronics and wearable sensors. **Y. Wang**

3:15 91. *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**

3:45 92. 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

San Diego Convention Center
TBD

Analytical Division Poster Session

K. Agnew-Heard, *Organizer*

8:00 - 10:00

93. Rapid vertical flow assay on AuNP plasmonic paper for SERS-based point of need diagnostics . **R. Frimpong**, W. Jang, J. Kim, J.D. Driskell

94. Quantification of hydrophilic layer on bioresolve SCX mAb particles. **B. Niu**, M. Xu, X. Song, Y. Xu

95. Effect of cultivation elevation of tea leaves on the formation and size control of silver nanoparticles for mercury ion sensing. **B. Giri**, A. Bhattarai, A. Chandra, J. Adhikari, N. Sharma, A. Yadav, M. Singh

96. Quantitative analysis of organic nitrogen in the atmosphere. **X. Huang**

97. Design hub for early phase drug discovery. **A. Stracz**

98. Simulation of fluid catalytic riser and regenerator used for monitoring catalyst retention: Case study of Kaduna refining and petrochemical company FCC reactor. **J. Olujinmi**

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

100. Mesoporous $CaCO_3$ -based alkaline stable reversed-phase HPLC packing material. **M. Mochida**, Y. Nagai, H. Kumagai, H. Imai, D. Citterio, Y. Hiruta

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

102. Use of ATR FT-IR spectroscopy in identification of immature fiber (*im*) mutant and Texas Marker-1 (TM-1) cotton fibers. **Y. Liu**, H. Kim

103. Attaining quantitative speciation by leveraging varying strengths of amalgamation by mercury species in gold-bead traps. **A.J. Boggess**, B. Looney, M. Jones, T. White

104. *In situ* characterization of protein corona formation within ordered porous nanostructures. **W. Qian**, Q. Su

105. Electric field assisted electrode modification. **H. Wang**, C. Ma

106. Potential role of halogen bonding in the gas phase: Ambient ionization mass spectrometry utilizing iodine. **J. Ganske**, L.M. Wingen, V. Perraud, B.J. Finlayson Pitts

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

108. 3D microfluidic paper-based analytical devices for colorimetric bioassays. N. Neris, A. Wong, A. Fernandez, **F.A. Gomez**

109. Effects of short chain fatty acids on fatty acid and glycogen synthesis in Hep G2 cells. **L. Ma**, **J.K. Yee**, S. Lim, W. Lee

110. Colorimetric detection of carcinogenic alkylating fumigants on nylon 6 nanofibrous membrane with self-catalytic function. **P. Tang**, G. Sun

111. Detection of steroids and human growth hormone using color-changing cyclodextrin systems. **A. Haynes**, J. Racicot, D. Jones, M. Levine, A. Yonchak, B. Point

112. Sensitive analysis of breast cancer biomarkers using laser wave-mixing detector interfaced to microfluidics. **J. Liang**

113. Evaluation of statistical techniques to normalize mass spectrometry-based urinary metabolomics data. **S. Gamagedara**, T. Cook

114. Colorimetric detection of aliphatic alcohols in β-cyclodextrin solutions. **A. Haynes**, M. Levine, P. Halpert

115. Withdrawn

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

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

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

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

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

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

122. Comparison study of the phytochemicals and antioxidant activity of fully matured and averagely natured *Crinum jagus* bulbs. **D.L. Abiona**, O.O. Onawumi, S.O. Oladoye

123. Microfluidic device for oxygen quantitation in anoxic environments. **M. Clayson**, **M.J. Evans**, L. Miller, S. Mckay, **C.F. Monson**

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

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

126. 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

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

128. 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

129. 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

130. Comparative quantitative analysis of cetirizine dihydrochloride by HPLC (high performance liquid chromatography) and q-NMR (quantitative nuclear magnetic resonance) techniques. **S. Kumar**, M. Villanueva

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

132. Mass spectrometry analysis and theoretical study of the enrichment of phosphopeptides by different crystal forms of TiO_2. **Y. Qi**, **X. Yang**, **W. Zhang**, **R. Jiang**, **J. Zhang**, **H. Zhong**

133. Efficiency study of pH sensitive drug release of carbon dots-doxorubicin conjugation in glioblastoma brain tumor cells. **S.D. Hettiarachchi**, R.M. Graham, S. Paudyal, E. Seven, R.M. Leblanc

134. Rapid and accurate determination of the pH of environmental water samples using smartphone colorimetry. **Z. Naing**, H. Liang, D. Sarmiento, J. Brannon, Y. Liu

135. Evaluation of human serum albumin nanoparticles for drug delivery and biomedical imaging. D. Bwambok, **L.A. Arrioja**, **A. Bituin**

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

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

138. Early diagnosis of colon cancer with rapid hybridization of DNA biomarkers. **S. Lee**

139. Super-resolution stimulated Raman scattering microscopy. **D. Kim**, Y. Lee, D. Choi, J. Kwon, H. Lee, M. Cho, S. Shim

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

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

142. Withdrawn

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

144. New isothermal amplification technique for POCT of foodborne pathogenic bacterium *Listeria monocytogenes* . **J. Chen**, **Y. Shi**

145. Loop-mediated isothermal amplification based on naked visualization dye for *Salmonella* POCT testing. J. Chen, **Y. Shi**

146. Evidence of direct reaction between ozone and oleanolic acid in plant cuticular waxes under laboratory and ambient conditions. **T.L. Longin**, V. Huerta Navarro, B. Romero, C. Smith, T. Rogoff, T. Kochar, D.P. Soulsby

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

148. Rapid colorimetric detection of *Salmonella typhimurium* based on polyamide film and strand exchange amplification. **S. Liu**, S. Kuang

149. Practical derivatization protocol for phosphonic acid markers of G-agents at low levels in various soils. **C.A. Valdez**, R.N. Leif, S. Hok, E.P. Salazar, A.K. Vu, A. Alcaraz

150. 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

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

152. Colorimetric breath analyzer using photonic gel in hydrophobic ionic liquid. **H. Choi**, W. Lee

153. Fabrication of inverse opal hydrogel sensors on flexible substrate by transfer process. **S. Yoon**, W. Lee, H. Lee

154. 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

155. 2D HPLC coupled with MS to examine cold medicines using compendial methods as the first dimension. **W. Long**, K.W. Whitaker

156. Sensitive detection of heart failure biomarkers using multiphoton laser wave-mixing spectroscopy. **J. Suprapto**, I. Chavez, M. Mohamed, W.G. Tong

157. Analysis of chemicals generated from plastic decomposition in the ocean. H. Kimukai, **K. Koizumi**, B. Kwon, K. Kim, K. Metori, M. Okada, T. Hiaki, T. Kusui, K. Takatama, **K. Saido**

158. Accelerated charge separation and stabilization in a fused bis zinc porphyrin-quinone conjugate via cation-quinone interactions. **M. Thomas**, Y. Hu, H. Wang, F. D'Souza

159. Development of substitutable interface on dandelion-like SiO_2 / Au thin film and application to sensitive and selective VOCs gas detection. J. Kim, H. Son, Y. Choi, **S. Hong**

160. Forensic applications of analytical chemistry: Funding programs at the National Institute of Justice. **G.J. Dutton**

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

162. Analysis of total mercury in radioactive waste using a direct mercury analyzer instrument. **T.L. White**, B. Looney, L. Brown

163. 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

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

165. 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

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

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

168. Development of efficient extraction and detection method for the active components in commercial kratom products. **F. Ceja**, P. Tuitt, K. Ng

169. Development of a peptide mapping protocol to minimize oxidation and deamidation for biotherapeutic characterization. **K. Chanthamontri**, P. Jalili, K. Ray

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

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

172. Microfluidic trapping and observation of size-sorted liposomes prepared by water-in-oil emulsion transfer method. **H. Sugiyama**, T. Osaki, S. Takeuchi, T. Toyota

173. Chemometric analysis of multidimensional fluorescence data recorded from benzo[a]pyrene metabolites in frozen matrixes. **M. Chehelamirani**

174. Thermal desorption coupled gas chromatography-mass spectrometry analysis of low emission polyurethane foam for automobile applications. **Y. Tan**, A.L. Grzesiak, Y. Zhang, E. Pearce, G. Marr, K. Kiszka

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

176. 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**

177. Fungal degradation of defense materials and assets. **T.T. Brown**, J.S. Lee

178. 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

179. Electrochemical detection of viable bacterial cells using a tetrazolium salt. **K. Ishiki**, D. Nguyen, H. Shiigi

180. 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

181. Cancer DNA detection using gold nanoparticle colorimetry and three ways target switching catalytic hairpin assembly. **C. Park**, S. Na

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

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

184. 2D IR spectroscopy for the characterization of protein side-chain dynamics. **S. Ramos**, R. Horness, A. Le Sueur, M.C. Thielges

185. 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

186. Co-release of dopamine and serotonin upon optogenetic stimulation of dopaminergic neurons. **K. Perrotta**, H. Yang, A. Hachisuka, M. Dagher, S. Erwin, S. Masmanidis, A.M. Andrews

187. Resorufin derived fluorescent probes for the selective detection of $ONOO^-$. **M. Weber**, T. James, A. Mackenzie, S. Bull

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

189. Protein profiling and pseudo-parallel reaction monitoring to monitor the fusion-associated conformational switch in hemagglutinin. **K.K. Nguyen**

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

191. Enhancing the disposal wells permeability monitoring by applying ASTMD7678 for the measurement of oil in water in GOSPs disposal lines. **A.M. AlSubaie**

192. Electrochemical biosensor using *p*-AP oxidation reaction on the mixed SAM Au electrode. **Y. Song**

193. Study on mechanism of single silver nanoparticle collided upon copper ultramicroelectrode in alkaline solution. **K. Kim**

194. Multifunctional, aramid-wrapped, multiwalled carbon nanotubes as an analytical microextraction sorbent. **A. Alhendal**, S. Sharaif, R. AbdulMoaen, Z. Ahmad

195. Conductometric titration as a method for measurement of elevated sulfate levels in groundwater. **R. Srinivasan**, M.B. Mudd, H.C. Stephen, B.R. Rothrock, **L.D. Schultz**

196. Organosilica-based adsorbents for treatment PFAS impacted groundwater. H.A. Hartmann, **P. Edmiston**

197. A single molecule examination of salting out in protein-polymer membrane interactions. **N. Moringo**, L.D. Bishop, N.C. Carrejo, H. Shen, W. Wang, A. Misiura, R. Baiyasi, F. Ye, J.T. Robinson, C.F. Landes

Section H

San Diego Convention Center
TBD

Biosensing: New Strategies & Latest Development

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

8:00 - 10:00

198. 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

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

200. Competitive and noncompetitive immunoassays for the detection of benzothiostrobin using magnetic nanoparticles and fluorescein isothiocyanate-labeled peptides. **C. He**, X. Hua

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

202. An activatable contrast agent for photoacoustic imaging of gingipains associated with periodontal disease. **C. Moore**, J.V. Jokerst

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

204. Sensitive SERS detection of small molecules by photothermal convection based real-time and pin-point colloidal assembly. **K. TaeHo**, I. Seo, H. An, I. Choi

205. Poly(ethylene glycol)-dibromomaleimide as a stabiliser for volatile sulfur compounds. **G. Kirby**, R. Hand, D.M. Haddleton

206. Mirror image fluorogenic aptamer sensor for live-cell imaging of microRNAs. **W. Zhong**, J. Sczepanski

207. Iodide-doped gold/silver hybrid nanorods report reactive oxygen species concentrations via photoacoustic imaging. **Y. Mantri**, J.V. Jokerst

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

209. Enzyme-based colorimetric biosensor for selective detection of L-DOPA. Y. Chou, I. Wang, C. Shih, **Y. 葉怡均**

210. Novel nanobody-based-electrochemical immunosensor on nylon nanofibrous membranes for detection of 3-phenoxybenzoic acid in human urine. **A. El-Moghazy**, J. Huo, **N. Amaly**, N. Vasylieva, B. Hammock, G. Sun

211. Sensitive electrochemical aptasensor for EpCAM by mesoporous silica nanoparticles and quantum dots signal amplification. L. Zhu, **Y. Liu**, B. Yang, L. Qiao, B. Liu

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

213. Electrogenerated chemiluminescence imaging of a single protein based on functional nanoprobes of Ru@SiO_2 nanoparticles. **Y. Liu**, T. Tian, H. Zhang, J. Liu, B. Liu

214. Basic roles of lysophospholipid receptor signaling studied by compensated interferometric reader (CIR). **M. Ray**, A. Kussrow, K. Nagai, M. Kammer, D. Bornhop, J. Chun

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

216. 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

217. Screen printed mesoporous carbon electrodes for efficient sensing of dopamine. **Y. Lee**, Y. Chang, H. Chang, M. Yeh, Y. Yeh, Y. Liu

218. 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

219. Specific, *in vivo* two-photon fluorescence imaging of malondialdehyde in mice brains using an easily-prepared nanolight. **D. Su**, P. Li, X. Wang, W. Zhang, Y. Zhang, C. Wu, W. Zhang, Y. Li, W. Tai, B. Tang

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

221. Application of super resolution radial fluctuation (SRRF) single-molecule imaging to measurement of DNA hybridzation kinetics. **J. Cooper**

222. Nanobodies and phage-display peptides: Attractive biosensing materials for analytical applications. **N. Vasylieva**, D. Li, Z. Li, B. Barnych, B.D. Hammock

223. Novel aptamer candidates for serotonin and dopamine field-effect transistor neurosensing. **S.T. Mensah**, O. Lukoyanova, K. Yang, K.M. Cheung, W. Dai, P.S. Weiss, M.N. Stojanovic, A.M. Andrews

224. Novel microfluidic-chemiluminescence detection coupled with microscale separation: Toward highly sensitive analytical technique. **S.M. Al Kindy**, A. Kadavilpparampu, H. Al Lawati

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

226. Functionalized nanopore biosensor for quick and highly sensitive glucose detection in human saliva. **y. miao**

227. Microdialysis: Fluorescence analysis system for vancomycin detection in pharmaceuticals and plasma. **f. mu**

San Diego Convention Center
TBD

Nanozymes for Bioanalysis & Beyond

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

8:00 - 10:00

228. N and B co-doped graphene: Suitable candidate to substitute natural peroxidase in sensitive and selective bioassays. **J. Lee**, J. Lee

229. Mechanisms of oxidase and peroxidase mimicking activities of nanoceria from first principles calculations. **W. Zhenzhen**, X. Gao, C. Chen, Y. Zhao

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

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

232. Novel silk-biomaterials-supported artificial enzymes: Synthesis and applications. **Y. Lin**

Section J

San Diego Convention Center
TBD

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

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

8:00 - 10:00

233. Teaching through research: Freshman research initiative at the University of Texas at Austin. **R.I. Shear**, K.H. Rogers, S.E. Eichhorn

234. Ultra-narrow linewidth lasers for atom-based devices. **A. Matsko**, A. Savchenkov, D. Eliyahu, S. Williams

235. High sensitivity differential temperature detection. **G.J. Diebold**

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

237. Novel antibody drug conjugates for pancreatic cancer therapy. **J. Huang**, P. Guo, M. Moses

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

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

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

241. Using DESI-MSI to identify the genetic basis and tumorigenic mechanism of pheochromocytomas. **S.E. Noll**, N. Armstrong, K. Margulis, V. Shankar, C. Storey, P. Kunz, L. Fishbein, R.N. Zare, J. Annes

242. Can machine learning be used to learn laws of natural science? Illustration for Planck's blackbody radiation. **V. Shankar**, S. Shankar

243. Evanescent-wave cavity-ring-down imaging. **M.A. Everest**

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

245. Solutions for lightweight construction and CO_2 footprint reduction by analysis of surfaces exposed to laser and plasma treatment. **U. Lommatzsch**, K. Thiel, M. Noeske, J. Ihde, R. Wilken

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

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

248. Mathematical Knowledge for Teaching to support student learning in chemistry. **L.A. Posey**, K.N. Bieda, P.L. Mosley, C.J. Fessler, V.A. Kuechle, E.N. Thomas

249. Detecting bacteria using an artificial antibody. **M. Dulay**, A.C. Mody, R.N. Zare, C. Da-Silva-Granja

250. 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

251. Multiplexed quantitative MALDI MS approach for assessing activity and inhibition of protein kinases based on post-enrichment dephosphorylation of phosphopeptides by MOF-templated porous CeO_2. **Q. Min**, H. Xu, M. Liu, X. Huang, J. Zhu

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

253. Synchrotron infrared nanospectroscopy at the advanced light source. **H.A. Bechtel**, S.N. Gilbert Corder, M.C. Martin

254. Electronic structure of naturally occurring aromatic carbon. **A.E. Pomerantz**

255. 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

256. Oncogene MYC regulates lipogenesis essential for neoplastic growth. **K. Margulis**, A. Gouw, N. Liu, D. Felsher, R.N. Zare

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

258. Solar-driven biohybrid N_2 and CO_2 fixation. **S. Cestellos-Blanco**, Y. Shen, P. Yang

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

260. 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

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

262. Soft ionization and dissociation based on laser activated interfacial photoelectron transfer for mass spectrometry. **H. Zhong**

263. Aesthetic education in chemistry. **H. Zhong**

264. Photoacoustic measurements of single aerosol droplets: Microscopic heat transfer and accelerated photoreactions. **J. Cremer**, P. Covert, E. Parmentier, M. Diveky, S. Roy, R. Signorell

Section K

San Diego Convention Center
TBD

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

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

8:00 - 10:00

265. Large-scale noncovalent functionalization of 2D materials through heated roller Langmuir-Schaefer conversion. **T.R. Hayes**, A.G. Porter, E.N. Lang, S.A. Claridge

266. Effective loading of plasmonic silver nanoparticles into mesopores for SERS applications. **S. Chen**, Y. Chang, H. Hou, W. Chiang, Y. Liu

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

268. 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

Marriott Marquis San Diego Marina
San Diego Ballroom Salon C

Nanotechnology & Single Cell Analysis in Biology & Medicine

Nanoscience

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

8:00 269. Nanotechnology approaches to cellular therapies. S.J. Jonas, **P.S. Weiss**

8:30 270. New tools for single-cell genotyping and analysis. **D.T. Chiu**

9:00 271. Mapping the inner world of cells. **B. Huang**

9:30 272. 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.

10:10 273. Beyond biomarkers: Array-based profiling for diagnostics and geno-/phenotypic screening for precision medicine. **V.M. Rotello**

10:40 274. Nanoengineered materials and devices to detect DNA hybridization and single nucleotide polymorphisms. K.M. Cheung, H. Cao, N. Nakatsuka, J. Abendroth, P.S. Weiss, **A.M. Andrews**

11:10 275. Rapid determinations of antibiotic susceptibility phenotypes using label-free cytometry and new adaptive statistic. T. Huang, A. Filbrun, J. Richardson, Y. Tzeng, **R. Dickson**

11:40 276. Nanostructure imaging mass spectrometry (NIMS) for metabolomics and systems biology. **A. Palermo**, E.M. Forsberg, B. Warth, A.E. Aisporna, E. Billings, E. Kuang, P.H. Benton, D. Berry, G. Siuzdak

Section B

Marriott Marquis San Diego Marina
Torrey Pines 3

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.

8:05 277. Advances in chemical lift-off lithography. **K.M. Cheung**, D.P. Goronzy, D.M. Stemer, C. Zhao, T.D. Young, J.N. Belling, T. Base, A.M. Andrews, P.S. Weiss

8:25 278. Surface confinement: Friend or foe to complex self-assembled DNA architectures?. **T. Ye**, H. Cao, G.R. Abel

8:55 279. Confined defects formed by chemical lift-off lithography to pattern multi-functional substrates. N. Nakatsuka, H. Cao, P.S. Weiss, **A.M. Andrews**

9:25 280. Protein structure at the bio/abio interface. **L.J. Webb**

9:55 Intermission.

10:10 281. Surface-mediated peptide self-assembly to modulate surface energy. **Z. Fakhraai**, Y. Lin, M. Skolnick, E. Petersson

10:40 282. 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

11:10 283. 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

Marriott Marquis San Diego Marina
Presidio 1

Identification & Design of Catalytic Sites in Electrochemical Reactions

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

8:00 284. Understanding the active sites of structurally dynamic nanomaterials for CO_2 electrocatalysis to multicarbon products. Y. Li, D. Kim, **P. Yang**

8:30 285. Highly active and selective electrochemical CO_2 reduction to formate enabled by structural defects on converted Bi_2O_3 nanotubes. **Y. Li**

9:00 286. Two-dimensional copper nanosheets for electrochemical reduction of carbon monoxide to acetate. **F. Jiao**

9:30 Intermission.

9:45 287. One-dimensional core/shell nanocrystals with favorable interfacial synergy for electrocatalysis. **S. Zhang**, Z. Zhang, C. Liu

10:15 288. Synthesizing intermetallic nanoparticle catalysts for enhanced catalytic electro-oxidation. **W. Huang**, Z. Qi

10:45 289. Controllable synthesis of N-doped hollow carbon spheres @ highly dispersed Mo_2C 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

11:05 290. Strain-driven energy electrocatalysis. **S. Guo**

Section D

Marriott Marquis San Diego Marina
Presidio 2

Advances in Fluorescence & Bioluminescence Imaging Probes

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

8:00 Introductory Remarks.

8:05 291. Rational design of fluorogenic and spontaneously blinking fluorophores for live-cell, super-resolution imaging. **Q. Zheng**, I. Chung, A. Weigel, A. Ranjan, A.X. Ayala, J. Grimm, C. Wu, J. Lippincott-Schwartz, R.H. Singer, L.D. Lavis

8:25 292. Optical sensors for detecting signaling phospholipids. **A. Chandra**, S. Mondal, R. Venkatramani, A. Datta

8:45 293. Multifunctional super-resolution microscopy with solvatochromic and conventional fluorescent probes. **K. Xu**

9:05 294. Fluorescent probes for imaging enzyme activity. **J. Rao**

9:25 295. Imaging of disease targets in cells via stimulus-responsive molecular probes. **R.L. McCarley**

9:45 296. Benzoxanthene probes with inherent pancreatic ductal adenocarcinoma selectivity. **I.R. Munhenzva**, **L. Wang**, **M. Sibrian-Vazquez**, **J. Escobedo**, **R.M. Strongin**

10:25 Intermission.

10:40 297. Imaging drug release from biomedical implants via radioluminescence. **G.B. Schober**, J.N. Anker

Section E

Marriott Marquis San Diego Marina
Torrey Pines 2

Chemical Forensics

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

8:00 Introductory Remarks.

8:05 298. Applications of the US EPA's CompTox Chemistry Dashboard to support structure identification and chemical forensics using mass spectrometry. **A.J. Williams**, A. Chao, T. Cathey, T. Transue, E.M. Ulrich, J. Sobus

8:25 299. New evaluation methods for building a seized-drug electron ionization mass spectral library. **W. Ji**, W.E. Wallace, D.V. Tchekhovskoi, S.E. Stein

8:45 300. Towards standardless identification of trichothecene-based mycotoxins. **B.P. Mayer**, M.C. Prieto-Conaway, M. Dreyer, K.E. Mason, T. Corzett, A.M. Williams

9:05 301. Microcystin analysis in biological fuids: Evaluation of 1D and 2D LC-MS/MS methods. **B.J. Garcia-Barboza**, S. Botch-Jones, C. Mallet, M. Lame

9:25 Intermission.

9:45 302. Identification of organophosphorus chemical warfare agents (CWAs), precursors, and decomposition products with a fieldable NMR spectrometer using earth's magnetic field. **R.F. Williams**, D. Kaseman, S. Widgeon Paisner, J.L. Yoder, P.E. Magnelind, M.T. Janicke, R. Michalczyk, A.V. Urbaitis, M.A. Espy

10:05 303. Characterization of impurities in gallium alloys via laser-induced breakdown spectroscopy. **A. Rao**, M. Shattan, J.D. Auxier

10:25 304. Enhanced peroxidase-like catalytic assay for the colorimetric aptamer-based biosensing of amphetamine-type stimulants using multi-shaped gold nanoparticle-graphene oxide-hemin hybrid nanozyme. **O. Adegoke**

10:45 305. 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

Marriott Marquis San Diego Marina
San Diego Ballroom Salon A

Advances in Wearable & Implantable Sensors

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

8:00 306. What can conformable decoders do?. **C. Dagdeviren**

8:30 307. Real-time biosensors for continuous measurements of specific biomolecules in live animals. **H.T. Soh**

9:00 308. Light-activated open circuit potentiometry. **J.E. Dick**

9:30 Intermission.

9:45 309. Flexible and wearable sensors for human motion analysis. **E. Thostenson**, S. Doshi, A. Chaudhari

10:15 310. Soft wearable systems with physiological monitoring and biochemical sensing capabilities. **R. Ghaffari**

10:45 311. Stretchable conductive nanocomposite for wearable and implantable bioelectronics. **D. Jung**, **D. Kim**

11:00 312. 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

Imaging Plasmon-Coupled Processes

Sponsored by PHYS, Cosponsored by ANYL

MONDAY AFTERNOON

Section A

Marriott Marquis San Diego Marina
San Diego Ballroom Salon C

Nanotechnology & Single Cell Analysis in Biology & Medicine

Nanoscience

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

1:00 313. Single cell analysis of dynamic signaling activities with fluorescent biosensors. **J. Zhang**

1:30 314. Molecular imaging and cellular reprogramming in single cells. **Y. Wang**

2:00 315. Cellular imaging with genetically encoded RNA-based sensors. **M. You**

2:30 316. Stimulated Raman imaging with chemical probes for subcellular bioanalysis. **L. Wei**

3:00 Intermission.

3:10 317. Stimulated Raman scattering: Next frontier of light microscopy. **W. Min**

3:40 318. Quantitative super-resolution microscopy of the mammalian glycocalyx. L. Möckl, K. Pedram, **A. Roy**, V. Krishnan, A. Gustavsson, O. Dorigo, C.R. Bertozzi, W.E. Moerner

4:10 319. Variable-angle plasmonic fluorescence microscopy for tracking the endocytic pathway. M. Chen, X. Pan, Q. Liu, **Y. Li**

4:40 320. Augmented fluorescent-free 3D super-resolution microscopy based on wavelength-dependent plasmonic scattering illumination. **S.H. Kang**

Section B

Marriott Marquis San Diego Marina
Torrey Pines 3

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

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

1:00 321. Impact of passively and actively confining self-assembled molecular networks in 2D corrals. **S. De Feyter**

1:30 322. Standing, lying, and sitting: Phospholipid striped phases as templates for nanomaterials at interfaces. **S.A. Claridge**

2:00 323. Controlled molecular assembly at solid-liquid interfaces. **G. Liu**, J. Zhang, V.A. Piunova, J. Frommer

2:30 324. Correlating structure and molecular transport at wet and semi-wet interfaces. **D.K. Schwartz**

3:00 325. Confined growth and transformation of colloidal nanostructures at solid-liquid interfaces. **Y. Yin**

3:30 326. Impact of fixed chemical patterns on moving surfaces. **M.M. Santore**

Section C

Marriott Marquis San Diego Marina
Presidio 1

Identification & Design of Catalytic Sites in Electrochemical Reactions

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

1:00 327. Selective CO_2 reduction on isolated transition metal single atomic sites: From identification to scaling-up. **H. Wang**

1:30 328. Atomic design of metal nano-catalysts toward activation of energy-related molecules. **Y. Wu**

2:00 329. Molecular engineering of nickel single-site electrocatalysts. **X. Zhang**, Y. Liang

2:20 Intermission.

2:35 330. Oxygen evolution reaction electrocatalysis on mixed-metal oxyhydroxides. **S.W. Boettcher**, M. Burke Stevens

3:05 331. *In situ* stimulated Raman spectroscopy shows phosphate assited cobalt oxide formation. **C.J. Eom**, G. Brunin, G. Hautier, J. Suntivich

3:25 332. Probing electrochemical reactions under *operando* conditions. **B. Liu**

3:55 333. *In situ* and *operando* spectroscopy of oxide electrocatalyst surfaces. **K.A. Stoerzinger**

Section D

Marriott Marquis San Diego Marina
Presidio 2

Advances in Fluorescence & Bioluminescence Imaging Probes

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

1:00 334. Multi-component bioluminescence imaging with diverse luciferin architectures. **J.A. Prescher**

1:20 335. Structure-luminescence relationship of near-infrared firefly luciferin analogues. **Y. Ikeda**, Y. Hiruta, D. Citterio

1:40 336. ATP-independent bioluminescent reporters for *in vivo* imaging. **H. Ai**, H. Yeh

2:00 337. SAFE method for luminescence quantum yield determination. **K. Nawara**, J. Waluk

2:20 338. Novel NanoLuc substrates enable bright and sustained bioluminescence imaging in animals. J.R. Walker, Y. Park, T.P. Smith, D.C. Wang, M.P. Hall, L.X. Liu, R. Hurst, Y. Su, l.P. encell, N. Kim, K. Casey, T.A. Kirkland, **M. Lin**

2:40 Intermission.

2:55 339. Methods for improving the biodetection performances of upconversion nanoprobes. **S. Xu**

3:15 340. Short-wavelength infrared nanosensors for imaging dopamine neuromodulation in the brain. **J.T. Del Bonis-O'Donnell**, A. Beyene, K. Delevich, I. McFarlane, D. Piekarski, R. Page, L. Wilbrecht, M. Landry

3:35 341. Near-infrared fluorescent probe for fast and ultrasensitive detection of nitroreductase in live cells. **S. Wan**

3:55 342. Near-infrared hybrid rhodol dyes with spiropyran switches for sensitive ratiometric sensing of pH changes in mitochondria. **S. Xia**, H. Liu

4:15 343. Ratiometric near-infrared fluorescent probes for sensitive detection of intracellular pH changes. **H. Liu**

4:35 344. Withdrawn

Section E

Marriott Marquis San Diego Marina
Torrey Pines 2

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.

1:05 345. Metabolomics for forensic analysis. **R. Bull**

1:20 346. Identification of emerging opioids in clinical samples using high-resolution tandem mass spectrometry. **K.D. Swanson**, L. Krajewski, W. Bragg, R. Shaner, E. Hamelin, M. Carter, R. Johnson

1:45 347. Studying the metabolome of *Ricinus communis* for attribution. **S. Ovenden**

2:10 348. Advancement in gas-phase separations for metabolomics. G. Nagy, A. Li, A.L. Hollerbach, R.D. Smith, **Y.M. Ibrahim**

2:35 349. 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. McArdell

3:00 Intermission.

3:15 350. Tools and databases for *in silico* compound identification. **D.S. Wishart**

3:40 351. *In silico* metabolite property libraries and quantitative chemical space analysis: Path toward novel molecule identification and false discovery assessment. **R. Renslow**, S.M. Colby, J. Nunez, Y. Yesiltepe, N. Govind, D. Thomas, J.R. Cort, J.G. Teeguarden, K. Wahl, D. Wunschel, T.O. Metz

4:00 352. Identification of unknown compounds using *in silico* fragmentation algorithms and *in silico* reference libraries. **T. Kind**

4:25 353. Evaluation of molecular ionization propensities in different ionization modes: Providing evidence for the presence of small molecules in synthetic blinded samples. **J. Nunez**, S.M. Colby, T.O. Metz, J.G. Teeguarden, R. Renslow

4:45 354. Optimal conformer selection for accurate *in silico* chemical property prediction. **F. Nielson**, D. Thomas, S.M. Colby, Y. Yesiltepe, R. Renslow

Section F

Marriott Marquis San Diego Marina
San Diego Ballroom Salon A

Advances in Wearable & Implantable Sensors

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

1:00 355. Minimimally- and non-invasive continuous biosensing: Frontiers for devices and sensors. **J. Heikenfeld**

1:30 356. Minimally invasive microneedle sensor arrays: New window on the body. **A.E. Cass**, S. Sharma, D. O'Hare

2:00 357. Rethinking on/in-body biochemical sensing strategies to achieve long-term functionality. **D. Diamond**

2:30 358. Facilitating collaboration to advanced nanotechnology-enabled wearable and implantable sensors: NNI sensors signature initiative. **S.D. Standridge**

3:00 Intermission.

3:15 359. New antifouling electrochemical aptamer-based sensor. **R.J. White**, S. Hendrickson

3:45 360. 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**

4:15 361. Implantable aptamer field-effect transistor neuroprobes: Towards *in vivo* neurotransmitter detection. **C. Zhao**, I. Huang, K.M. Cheung, N. Nakatsuka, H. Yang, L. Scarabelli, L. Heidenreich, J. Belling, P.S. Weiss, H.G. Monbouquette, A.M. Andrews

4:30 362. Inkjet printing electronic materials on textile platforms and processing strategies for wearable electronics. **I. Kim**, Y. Zhou, B. Li, J. Jur

4:45 Concluding Remarks.

Eminent Scientist Lecture with Dr. Marya Lieberman

Sponsored by SOCED, Cosponsored by ANYL

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

MONDAY EVENING

Section A

San Diego Convention Center
TBD

Sci-Mix

K. Agnew-Heard, M. F. Bush, *Organizers*

8:00 - 10:00

55, **74**, **99**, **111**, **127**, **128**, **180**, **207**, **236**, **241**, **263**, **289**, **291**, **296**, **312**, **329**, **349**. See Previous Listings.

368, **369**, **416**, **458**, **477**, **537**, **538**, **557**. See Subsequent Listings.

TUESDAY MORNING

Section A

Marriott Marquis San Diego Marina
Rancho Santa Fe 2

Nanozymes for Bioanalysis & Beyond

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

8:00 Introductory Remarks.

8:05 363. Single atom nanozyme for wound antibacterial applications. **X. Yan**

8:45 364. Platinum-nickel nanozyme and branched ruthenium nanoparticle catalysts. **R. Tilley**

9:25 365. Applications of inorganic nanoparticle enzyme mimics. **W. Tremel**

10:05 Intermission.

10:10 366. New strategies for nanozyme-based bioanalysis. **J. Liu**

10:50 367. Ceria-based nanomaterials for therapeutic antioxidants. **T. Hyeon**

11:30 368. Nanozyme based tumor catalytic theranostics. **K. Fan**, X. Yan

Section B

Marriott Marquis San Diego Marina
Torrey Pines 3

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

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

8:00 369. Stabilizing noncovalent monolayers on MoS_2 through edge-on adsorption of multi-chain functional alkanes. **T.C. Davis**, S.R. Russell, S.A. Claridge

8:20 370. Surface microstructure functionalised by multicomponent femtoliter droplets at liquid-solid interface: Fabrication and applications. **M. Li**, x. zhang

8:40 371. 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

9:10 372. Functional chemical patterns as useful analytical devices. **W. Liao**, C. Chen, C. Wang

9:40 Intermission.

9:55 373. Relative permittivity in the electrical double layer from nonlinear optics. **F. Geiger**, M. Boamah

10:25 374. Surface chemistry of silica particles in aqueous solution. A. Marchioro, **S. Roke**

10:55 375. Experimental and theoretical study of hydration and dehydration of zeolites. **T. Guo**, D. Donadio

11:25 Concluding Remarks.

Section C

Marriott Marquis San Diego Marina
Presidio 1

Identification & Design of Catalytic Sites in Electrochemical Reactions

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

8:00 376. Probing structure-performance relation for electrocatalysis using multimodal characterization techniques. **D. Su**

8:30 377. Atomically precise metal nanoclusters for electrocataysis. **D. Jiang**

9:00 378. Identification of active species and mechanisms in non-precious metal oxygen reduction catalysts by poisoning and magnetic measurements. **A.A. Gewirth**, A. Esposito

9:30 Intermission.

9:45 379. Understanding the electronic structure and reactivity of carbon monoxide dehydrogenase model systems for carbon dioxide reduction. **J. Panetier**

10:15 380. Cation-mediated evolution of hydrogen on Cu electrodes. **M. Waegele**

10:45 381. High performance electrochemical CO_2 reduction cells based on non-noble metal catalysts. **H. Wang**

11:05 382. Identification of active phase of oxide-derived Cu in electrochemical CO reduction reaction with *operando* surface enhanced spectroscopy. **B. Xu**

Section D

Marriott Marquis San Diego Marina
Presidio 2

Mass Spectrometry of Biomolecular Assemblies

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

8:00 383. Role of surface collisions in an MS-based structural biology approach. **V.H. Wysocki**

8:30 384. Ion mobility mass spectrometry to characterize formation and structure of DNA assemblies. **T.L. Pukala**, A. Begbie, J. Li

9:00 385. Pinpointing isomerization sites in long-lived proteins using IMS-MS. **R. Julian**

9:30 Intermission.

9:45 386. Multidimensional ion mobility of proteins and protein complexes enabled by modular design. **M.F. Bush**

10:15 387. Fourier transform ion mobility-Orbitrap spectrometer for native mass spectrometry. J. McCabe, M. Shirzadeh, **D.H. Russell**

10:45 Intermission.

11:00 388. 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

11:30 389. Nanoscale ion emitters in native mass spectrometry for measuring ligand–protein and ligand-DNA binding affinities. **W.A. Donald**

Section E

Marriott Marquis San Diego Marina
Torrey Pines 2

Connecting Safety, Education, Training & Productivity in Analytical Laboratories

Cosponsored by CCS, CHAS‡, CINF and PRES
C. D. Incarvito, J. L. Maclachlan, *Organizers, Presiding*

8:00 Introductory Remarks.

8:10 390. Principles to influence culture and establish practices regarding safe operation of research instrumentation and application development. **E. Robinson**

8:30 391. Computer-assisted separation modeling in analytical space translated into improved preparative chromatography productivity. **I. Haidar Ahmad**, F. Tsay, R.\. Bennett, D. Henderson, R. Hartman, B. Mann, I.K. Mangion, E. Regalado

8:50 392. Generic GC-FID method for high-throughput analysis of residual solvents in pharmaceutical substances. **T. Nowak**, F. Bernardoni, H. Halsey, A.A. Makarov, E. Regalado

9:10 393. Safe solvent management for LC/MS and GC/MS. **P.A. Reinhardt**, S. Bain

9:30 Panel Discussion.

10:45 Concluding Remarks.

Section F

Marriott Marquis San Diego Marina
San Diego Ballroom Salon A

ACS Sensors Young Investigators

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

8:00 Introductory Remarks.

8:05 394. Multi-modal sensing for measuring tissue development and function in microphysiological systems. **M.A. Daniele**, V. Pozdin, K. Rivera, A. Young, P. Erb

8:35 395. Expanding the scope of biosensors: RNA- and small molecule-generating sensing systems. **B.C. Dickinson**

9:05 396. Probing and constructing bio-inorganic interfaces within a nanocavity for adaptive single molecule sensing. **S. Huang**

9:35 Intermission.

9:45 397. Not everybody dyes: Leveraging quantum dots and other luminescent nanomaterials for new opportunities in bioanalysis. **W.R. Algar**

10:15 398. Integration of dielectrophoretic selective single-cell capture at a wireless electrode array with on-chip analysis. M. Li, D. Pagariya, **R.K. Anand**

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

Spectroscopy of Reactive Chemical Systems

Sponsored by PHYS, Cosponsored by ANYL

TUESDAY AFTERNOON

Section A

Marriott Marquis San Diego Marina
Rancho Santa Fe 2

Nanozymes for Bioanalysis & Beyond

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

1:00 399. Imaging and treatment of multidrug-resistant bacteria and biofilms using bioorthogonal transition metal catalyst nanoparticle "nanozymes". **V.M. Rotello**

1:40 400. Peptide-gold clusters as enzyme-like catalyst for *in situ* cell analysis and induce tumor-specific cell apoptosis. **L. Gao**

2:20 401. e_g occupancy as an activity descriptor for guiding the design of transitional oxide-based peroxidase mimics. X. Wang, X. Gao, L. Qin, C. Wang, L. Song, Y. Zhou, G. Zhu, W. Cao, S. Lin, Q. Zhou, K. Wang, H. Zhang, Z. Jin, P. Wang, X. Gao, **H. Wei**

3:00 Intermission.

3:05 402. Enzyme-mimic metal-bismuth oxyhalide for sensing and antimicrobial applications. **C. Huang**, H. Chang, J. Lai

3:45 403. Truncated tetrahedral CdTe QDs act as endonucleases for site-selective photoinduced cleavage of DNA. **C. Xu**, M. Sun, H. Kuang, L. Xu, A. Qu

4:25 404. Withdrawn

Section B

Marriott Marquis San Diego Marina
Torrey Pines 3

Analytical Division Awards

K. Agnew-Heard, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 405. Spectroscopy through the microscope: Chemical analysis at liquid/solid interfaces. **J.M. Harris**

1:40 406. Structure-activity relationships at complex electrodes from correlative electrochemical multi-microscopy. **P.R. Unwin**

2:15 407. New nano tools for real-time single molecule imaging of single live cells: From fundamental discoveries to biomedical applications. **X. Xu**

2:50 Intermission.

3:00 408. Building learning & teaching communities in analytical chemistry: From campus to textbook. **C.A. Lucy**

3:35 409. *In vivo* and intraoperative chemical analysis and tissue diagnosis using the MasSpec Pen technology. **L. Schiavinato Eberlin**

4:10 410. Atomic ions to intact protein complexes: 25-year quest for structure, dynamics, and thermodynamics. **D.H. Russell**

Section C

Marriott Marquis San Diego Marina
Presidio 1

Identification & Design of Catalytic Sites in Electrochemical Reactions

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

1:00 411. Ambient electrochemical activation of small molecules with inorganic and hybrid catalysts. **C. Liu**

1:30 412. Designing functional sites in framework materials for energy storage devices. **V. Thoi**

2:00 413. CO_2 reduction by immobilized rhenium bipyridine moieties. **S.C. Marinescu**

2:30 Intermission.

2:45 414. Hydricity as an activity descriptor for molecular hydrogen evolution electrocatalyst design. **J.Y. Yang**, D.W. Cunningham, B. Ceballos

3:15 415. Phthalocyanine precursors to construct atomically dispersed metal electrocatalysts. **Y. Liang**, Y. Wang, Z. Jiang

3:45 416. Electrocatalytic oxidation of d^0-oxo for ambient methane functionalization. **j. deng**, J. Iñiguez, D. Yang, D. Xiang, G. Chan, C. Liu

Section D

Marriott Marquis San Diego Marina
Presidio 2

Mass Spectrometry of Biomolecular Assemblies

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

1:00 417. Temperature-programmed native ESI-MS as a versatile biophysical toolbox to study noncovalent complexes. **R. Zenobi**

1:30 418. Flying viruses: From biophysical to structural characterisation. **C. Uetrecht**

2:00 419. Native mass spectrometry: Probing gas-phase or solution-phase protein structures?. **J.A. Loo**

2:30 Intermission.

2:45 420. Role of macroion-droplet interactions in the charge state of macromolecules. **S. Consta**

3:05 421. Investigation of membrane toxin assemblies with native ion mobility-mass spectrometry and Gábor transform. **J.S. Prell**

3:25 422. Characterizing oligomerization of biomolecular assemblies within intact membranes using native mass spectrometry and lipoprotein nanodiscs. **M.T. Marty**

3:45 Intermission.

4:00 423. Denaturing and native top-down proteomics using capillary electrophoresis-tandem mass spectrometry. **L. Sun**

4:30 424. Identifying protein interactions using in-cell protein footprinting coupled with mass spectrometry. **L.M. Jones**

Section E

Marriott Marquis San Diego Marina
Torrey Pines 2

Exploration of the Nano-Bio Interface with Analytical Tools

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

1:00 425. Nanotoxicity and nanomedicines. **Y. Zhao**

1:40 426. Toxicological profiling of metal and metal oxide nanomaterials in liver cells. **T. Xia**

2:10 427. 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.

2:50 428. Single particle spatiotemporal analysis of transmembrane process of functionalized nanocargos. **Y. He**

3:20 429. Membrane-protein-hydration interaction of α-synuclein with anionic vesicles in solution probed via angle-resolved second harmonic scattering. J. Dedic, S. Rocha, P. Wittung Stafshede, **S. Roke**

3:50 430. Toxicological risk assessment of cellulose nanofibrils by using a fluorescent molecular probe. **I. Patel**, J.W. Woodcock, J. Shatkin, S. Stranick, G. DeLoid, P. Demokritou, S. Harper, J.W. Gilman, D. Fox

Section F

Marriott Marquis San Diego Marina
San Diego Ballroom Salon A

Biosensing: New Strategies & Latest Development

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

1:00 431. Single hydrogel nanoparticle SPR imaging measurements for biosensing and bioaffinity uptake. **R.M. Corn**

1:30 432. Supramolecular assemblies for chiral molecular sensing. **M. Liu**, L. Zhang

2:00 433. Mirror-image nucleic acid-based sensors for live-cell imaging of RNA. **J. Sczepanski**, B. Young, A. Kabza, W. Zhong

2:20 434. Microfluidic biochip platform incorporating hydrogel-based differential Coulter counting technology for rapid, multiplexed quantification of proteins. T. Cowell, E. Valera, A. Jackelow, J. Park, R. Ding, R. Bashir, **H. Han**

2:40 Intermission.

2:55 435. Microscale interfaces for sensitive biosensing and comprehensive identification of biomolecules. **B. Liu**, Y. Wang, H. Zhang, K. Zhang, L. Qiao, J. Liu

3:25 436. Preparation and integration of specifically functionalized biosensors for liquid biopsy. **R. Heer**

3:55 437. New catalytic DNA based biosensors for selective metal ions detection. **J. Liu**

4:15 438. Using gold nanoparticles for diagnostics and sensing in low cost devices. K. Hamad-Schifferli, **C. Rodriguez-Quijada**

4:35 439. Switchable chemical reactivity to multiplex aptamer-field-effect transistor sensing. **O. Lukoyanova**, S.T. Mensah, J. Stauber, W. Dai, C. Zhao, K. Cheung, P. Weiss, M.N. Stojanovic, A.M. Spokoyny, A.M. Andrews

WEDNESDAY MORNING

Section A

Marriott Marquis San Diego Marina
Rancho Santa Fe 2

Nanozymes for Bioanalysis & Beyond

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

8:00 440. Strong candidate graphene based materials to replace natural peroxidase in sensitive and selective bioassays. **J. Lee**

8:40 441. Nanozyme-prodrug therapy. **A. Zelikin**

9:20 442. Bifunctional nanozyme based on modified carbon nitride photocatalyst that mimics glucose oxidase-peroxidase. **W. Choi**, P. Zhang, J. Han, D. Kim

10:00 Intermission.

10:05 443. Combat resistant bacteria with nanozymes. **L. Gao**

10:45 444. Biological applications by nucleobase analogues capped gold nanoclusters with peroxidase-like activity. **H. Jiang**, Y. Zheng, L. Liu, X. Wang

11:15 445. Fluorescent C_3N_4-based nanozymes for ratiometric biomedical assays. **X. Wang**, H. Wei

Section B

Marriott Marquis San Diego Marina
Torrey Pines 3

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.

8:10 446. Antibody-based approaches to respond to the environmental analytical challenges. **M. Marco**

8:45 447. Using mass spectrometry to vet microcystin concentrations by enzyme-linked immunosorbent assay. **J. Westrick**

9:10 448. 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.

10:00 449. Improving small molecule annotation in nontargeted soft-ionization GC/LC high-resolution mass spectrometry. **C. Jaeger**, J. Lisec

10:25 450. Ultrasensitive MALDI-TOF quantitation of microcystins in complex matrices by direct on-target analysis of nanobody-captured toxins. M. Pírez-Schirmer, B.M. Brena, **G. Gonzalez**

Section C

Marriott Marquis San Diego Marina
Presidio 1

Advances in Electrochemistry

L. A. Baker, *Organizer, Presiding*

8:00 451. Imaging local electrochemistry with ion conductance microscopy. **L.A. Baker**

8:25 452. Using image processing algorithms to treat electrochemical images. **L. Stephens**, N. Payne, S. Skaanvik, D. Polcari, M. Geissler, J. Mauzeroll

8:45 453. Positive and negative feedback theory and experiments in hot-tip scanning electrochemical microscopy. **Z. Zhao**, A. Boika

9:05 454. Bubble nucleation-based electrochemical detection method for perfluorinated surfactants. **R. Ranaweera**, L. Luo

9:25 Intermission.

9:40 455. Critical nuclei size and rate of nanobubble nucleation. **M.A. Edwards**, S. German, H. Ren, A. Moreno Soto, H. White

10:05 456. Mechanism of histamine oxidation and electropolymerization at carbon electrodes. **P. Puthongkham**, B.J. Venton

10:25 457. Neurotransmitter detection at near the theoretical performance limit of electroenzymatic sensors. **I. Huang**, M. Clay, H.G. Monbouquette

10:45 458. Single drop fabrication of the cholesterol biosensor based on synthesized $NiFe_2O_4$NPs dispersed on PDDA–CNTs. **C. Moonla**, T. Tangkuaram, A. Preechaworapun

Section D

Marriott Marquis San Diego Marina
Presidio 2

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

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

8:00 Introductory Remarks.

8:05 459. Understanding molecular aspects of aqueous interfacial chemistry with clusters. **M.A. Johnson**

8:35 460. Photoemission from charged droplets. **R. Signorell**

9:05 461. 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.

9:50 462. Native electrospray ionization: From solution to charged droplets to final ions. **M.F. Bush**

10:20 463. Spectroscopic characterization and computational investigation of anionic clusters generated from charged droplets. **X. Wang**

10:50 464. Vibrating sharp-edge spray ionization (VSSI) for in-droplet hydrogen/deuterium exchange reactions. **S.J. Valentine**, N. Ranganathan, C. Li, X. Li, K. Attanayake, S. Majuta, A. Kiani Karanji, P. Li

11:20 465. Adventures in anion photoelectron spectroscopy. **K.H. Bowen**

11:50 Discussion.

Section E

Marriott Marquis San Diego Marina
Torrey Pines 2

Exploration of the Nano-Bio Interface with Analytical Tools

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

8:00 466. Don’t forget the lipids: Biomolecular coronas on nanoparticles. **C.J. Murphy**

8:40 467. Pulmonary surfactant corona and nano-bio interactions in the lung. **Y. Zuo**

9:10 468. Protein conformational change induced by nanomaterials elucidated with limited proteolysis. **W. Zhong**, Y. Duan, R. Coreas

9:40 Intermission.

9:50 469. Optimized carbon dots: Green imaging agents at the nano-bio interface. **C.L. Haynes**

10:20 470. Fluorescent black carbon surrogates: Probing biological impacts of black carbon while relating form and function in creating fluorescent carbon dots. **C. Sumner**, R.L. McCarley

10:40 471. Characterizing protein coronas with limited proteolysis and lipid coronas with liquid-liquid extractions coupled to liquid chromatography-mass spectrometry. **R. Coreas**, J. Lee, Y. Duan, W. Zhong

11:00 472. Gold nanoparticle-based screening platform to assess protein-carbohydrate interactions. **S. Richards**

Section F

Marriott Marquis San Diego Marina
San Diego Ballroom Salon A

Biosensing: New Strategies & Latest Development

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

8:00 473. Development of miniature surface plasmon resonance systems and sensor applications. **A. Baba**, S. Nootchanat, C. Lertvachirapaiboon, K. Shinbo, K. Kato, S. Ekgasit

8:30 474. Supported lipid membranes as biosensing interface. **Q.J. Cheng**

9:00 475. 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

9:20 476. Electrochemical quantification of bladder cancer biomarkers with a phage-based bioresistor. **E.C. Sanders**, A. Attar, A. Santos, S. Majumdar, R.M. Penner, G.A. Weiss

9:40 477. Polymeric nanofilter biointerface for potentiometric small-biomolecule recognition. **S. Nishitani**, S. Himori, F. Nishimori, T. Sakata

10:00 Intermission.

10:15 478. Better analysis for proteins with metallic and non-metallic nanoparticle-integrated biosensing platforms. **H. Lee**

10:45 479. Towards development of fluorescence quenching-based biosensors for drought stress in plants. **T. Guo**, S. Brady

11:05 480. Oxidative stress imaging using LED-based photoacoustic imaging system. **A. Hariri**, E. Zhao, J.V. Jokerst

11:25 481. Massively parallel single-molecule detection platform using nano-electronics. **Y. lee**, K.L. Shepard

Theoretical & Experimental Investigations of Water Interactions with Materials

Sponsored by COLL, Cosponsored by ANYL‡

WEDNESDAY AFTERNOON

Section A

Marriott Marquis San Diego Marina
Rancho Santa Fe 2

Nanozymes for Bioanalysis & Beyond

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

1:00 482. *De novo* design of nanomedicine: Large scale molecular simulation of nanoparticle-biomolecule interactions. **R. Zhou**

1:40 483. Catalytic model bridging computations and experiments for ceria-based nanozymes. Z. Wang, **X. Gao**

2:20 484. Metallic nanostructures for medical diagnostics. **X. Xia**

3:00 Intermission.

3:05 485. Portable sensors incorporating nanomaterials with enzyme-mimetic properties for bioanalysis. A. Othman, F. Mustafa, M. Hassan, **E. Andreescu**

3:45 486. Standardization of nanozyme research. **M. Liang**

4:25 487. NanoZymes for colorimetric sensing and beyond. **R. Ramanathan**, V. Bansal, P. Weerathunge, N. Karim, M. Singh, P. Mariathomas, S. Hashmi, S. Prasad

Section B

Marriott Marquis San Diego Marina
Torrey Pines 3

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

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

1:00 488. Analysis and fate of antimicrobials in animal manure: Challenges and solutions. **D.S. Aga**

1:35 489. Immobilization of multivalent nanobodies onto bacteria magnetic particles for the rapid detection of tetrabromobisphenol A in the environment. J. He, J. Xu, J. Tian, J. Li, S. Gee, B.D. Hammock, Q.X. Li, **T. Xu**

2:00 Intermission.

2:25 490. Analysis of bisphenol A, octyl and nonyl phenol, estrogens, and other selected pharmaceuticals in surface and wastewater by liquid chromatography-negative ion electrospray-tandem mass spectrometry. g. aborkhees, **R. Raina-Fulton**, O. Thirunavukkarasu

2:50 491. Determination of emerging micropollutants in urban waters and wastewater by portable immunoanalytical methods. P. Carl, I.I. Ramos, M.A. Segundo, **R.J. Schneider**

3:15 Concluding Remarks.

Section C

Marriott Marquis San Diego Marina
Presidio 1

Advances in Electrochemistry

L. A. Baker, *Organizer, Presiding*

1:00 492. Electrochemical and electrokinetic route for dialysate regeneration. **B. Berzina**, R. Anand

1:25 493. Electrochemical sensors for field detection of explosives. **S. Trammell**

1:50 494. Electrochemical reduction of carbon dioxide to formate and carbon monoxide on lead−tin alloys. **A. Hailu**, S.K. Shaw

2:10 Intermission.

2:25 495. Proton transfer regulation across soft interfaces of water. **H. Tavassol**, L. Nguyen, C. Mao, K. Asham

2:45 496. Coherent X-ray diffraction/absorption microscopy for analyzing organic and inorganic materials. **J. Park**

3:05 497. Influence of electrochemical polymerization protocols on composite conducting polymer films for supercapacitor electrode materials. **A. Al-Betar**

3:25 498. Determination of betadex (β-cyclodextrin) according to the USP betadex sulfobutyl ether sodium monograph. **M. Aggrawal**, J.S. Rohrer

Section D

Marriott Marquis San Diego Marina
Presidio 2

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

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

1:00 499. Ions from solution to the gas phase: Effects of solvent on the final structure. M.J. Hebert, **D.H. Russell**

1:30 500. Understanding disordered protein conformations in solution as viewed from the gas phase. **P.E. Barran**

2:00 501. Microsolvation effects on the encapsulation of metal ions by crown ethers. **Y. Inokuchi**

2:30 Intermission.

2:45 502. Charging proteins by electrospray ionization. **R.R. Loo**, J.A. Loo

3:15 503. Infrared laser spectroscopy of solvated cations. **M.A. Duncan**

3:45 504. Chemistry driven by electrons: Metastable electronic states and spin-forbidden processes. **K.B. Bravaya**

4:15 505. Many-body expansion for ion-water clusters: Convergence, size and basis set effects, and solvation structure. **J.P. Heindel**, S.S. Xantheas

4:45 Discussion.

Section E

Marriott Marquis San Diego Marina
Torrey Pines 2

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*

1:00 506. Tracking cell-free, circulating nucleic acids from tumors with electrochemical sensors. **S.O. Kelley**

1:40 507. Lipid-based normalization of quantum dot probes bound to membrane markers on extracellular vesicles in complex biological samples. **T. Hu**

2:20 508. High-resolution single-vesicle flow cytometry. **J. Nolan**

3:00 Intermission.

3:10 509. Analyzing maternal blood serum preterm birth risk biomarkers in 3D printed microfluidic devices. **A. Woolley**, M. Beauchamp, A.V. Nielson, E.K. Parker, J.B. Nielsen, H.M. Almughamsi, G.P. Nordin

3:50 510. Chemical operations on a living single cell by open microfluidics. **J. Lin**

4:30 511. Analysis of extracellular vesicle (EV) enabled by nanostructures. **W. Zhong**, K. Guo, Q. Jiang

Section F

Marriott Marquis San Diego Marina
San Diego Ballroom Salon A

Biosensing: New Strategies & Latest Development

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

1:00 512. Aptamer-functionalized microelectrodes and nanopipettes to sense neurotransmitters in neuronal networks. **N. Nakatsuka**, S. Weaver, D. Eggemann, T. Schlotter, D. Momotenko, J. Vörös

1:30 513. Stimulus-responsive nanomaterial for highly efficient intracellular sensing and gene therapy. **Y. Liu**, K. Kw Ren, H. Ju

2:00 514. Illuminating bacterial communities with plasmonic nanoantennas. **R. Ragan**, W.J. Thrift, A.S. Cabuslay, A. Hochbaum

2:20 515. Single molecule fluorescence counting assay to measure biomolecules. H. Zhang, Y. Liu, K. Zhang, X. Huang, B. Li, B. Liu, **J. Liu**

2:40 516. Developing aptamer-based biosensor for onsite detection of stress biomarkers in noninvasive biofluids. **S. Daliririad**

3:00 Intermission.

3:15 517. Detection of antibiotic-resistant bacteria using nanoparticle-mediated microfluidic capture. **C. Nemr**, S.J. Smith, P. Aldridge, W. Liu, A. Mepham, R. Mohamadi, M. Labib, S.O. Kelley

3:35 518. Paper-based lateral flow immunoassay for detection of traumatic brain injury biomarkers. **K. Curtin**, X. Gao, N. Wu

3:55 519. Fabrication of wafer-scale metal oxide nanoribbon field-effect transistor biosensors using chemical lift-off lithography. **C. Zhao**, Q. Liu, K.M. Cheung, W. Liu, Q. Yang, X. Xu, A.M. Andrews, C. Zhou, P.S. Weiss

4:15 520. Thermally carbonized porous silicon for robust label-free DNA optical sensing. **R. Layouni**, M. Choudhury, P.E. Laibinis, S.M. Weiss

4:35 521. Duplex electrochemical DNA sensor to detect B.anthracis 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

Sponsored by COLL, Cosponsored by ANYL‡

THURSDAY MORNING

Section A

Marriott Marquis San Diego Marina
Rancho Santa Fe 2

Advances in Spectroscopy

XRF, NMR, & SEM Spectroscopy

E. A. Smith, *Organizer*
R. F. Hirsch, *Presiding*

8:00 Introductory Remarks.

8:05 522. Detection of toxic metals contamination in cosmetics using MP-AES and X-Ray fluorescence spectroscopy. **S. Alsherari**, A.W. Apblett

8:25 523. Low resolution size chromatographs? The potential applications of diffusion ordered spectroscopy NMR in analysis of polymer size distributions. **T.A. Swift**, S. Rimmer

8:45 524. Imaging and analysis of ancient decorative metal threads using scanning electron microscope-based X-ray spectroscopies. **A. Popowich**, E. Vicenzi, T. Lam

9:05 525. 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.

9:40 526. Advancing innovation and the adoption of emerging technology in pharmaceutical freeze-drying through laboratory research at FDA's office of testing and research. **M. Korang-Yeboah**, L. Hengst, A. Ako-Adounvo, C. Srinivasan, M. Ashraf, C.N. Cruz

10:00 527. Simultaneous measurement of metal coatings thickness and composition using x-ray fluorescence (XRF) spectroscopy. **H. Ataee-Esfahani**, J. Peters

10:20 528. How analytical chemistry is providing basic advances in climate science. **R.F. Hirsch**

10:40 529. Calibration transfer between low-field NMR instruments. D. Galvan, E. Danieli, D. Borsato, **M.H. Killner**

Section B

Marriott Marquis San Diego Marina
Torrey Pines 3

Advances in Mass Spectrometry

M. F. Bush, *Organizer, Presiding*

8:00 530. Electrochemistry-assisted absolute quantitation by mass spectrometry without the use of standards. **H. Chen**, P. Zhao

8:25 531. 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

8:45 532. 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

9:05 533. 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

9:25 534. Multilayered gold-nanoparticle thin film as a sample substrate in SALDI-MS for osteoporosis risk assessment. **Y. Chang**, T. Kuo

9:45 Intermission.

10:05 535. Ion mobility-mass spectrometry reveals the effect of sialylation on glycoprotein structures. **G. Li**, L. Li

10:25 536. Improved profiling of sialylated *N*-linked glycans by ion chromatography-mass spectrometry. **S. Patil**, J.S. Rohrer

10:45 537. Native top-down proteomics for mouse brain proteome with capillary zone electrophoresis-tandem mass spectrometry. **X. Shen**, L. Sun

11:05 538. 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

11:25 539. Trace metals in LPG (liquified petroleum gas) by ICP-MS (inductively coupled plasma mass spectrometry). **S.S. Chudasama**, K. Lehuta

11:45 540. Multidimensional fractionation and molecular characterization of lingering oil compounds in coastal sediments: A nine year evolution. **A.M. McKenna**, H. Chen, C.C. Davis, S.F. Niles, C.R. Weisbrod, A. Hou, M.L. Chacon-Patino, Q. Lin, R.P. Rodgers

Section C

Marriott Marquis San Diego Marina
Presidio 1

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.

8:05 541. Unraveling sample matrix effects for multivariate calibration. **J.H. Kalivas**, T. Lemos

8:30 542. Differential sensing of multiplex MAPK isoforms using expanded SOX-peptide library. **L. Zeng**, D. Zamora-Olivares, T.S. Kaoud, K. Dalby, E.V. Anslyn

8:55 543. Chemometrics to guide the design of a lignin electrocatalytic reactor. **P.D. Harrington**, Z. Chen, M. Naderinasrabadi, J. Staser

9:20 Intermission.

9:30 544. Temperature-dependent near-infrared spectroscopy for analyzing aqueous samples. **X. Shao**, X. Cui, L. Ma, L. Wang, Y. Sun, M. Wang, W. Cai

9:55 545. Calibration-based detection and confidence limits are (almost) exact when the data variance function is known. **J.B. Tellinghuisen**

10:20 546. 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

10:45 Concluding Remarks.

Section D

Marriott Marquis San Diego Marina
Presidio 2

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

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

8:00 547. Reversed interfacial fractionation of carbonate and bicarbonate evidenced by X-ray photoemission spectroscopy and theory. **R.J. Saykally**, t. pascal

8:30 548. Quantum mechanical studies of protonated water clusters through their IR spectra. **J.M. Bowman**, Q. Yu

9:00 549. 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.

9:45 550. Diffusion Monte Carlo approaches for exploring neutral and protonated water clusters. **A.B. McCoy**, R. Dirisio, V. Lee

10:15 551. Reaction acceleration in charged microdroplets: Scratching the surface. **B.M. Marsh**, K. Iyer, R.G. Cooks

10:45 552. Highly charged droplets of superfluid helium. **M. Gatchell**, F. Laimer, P. Martini, L. Tiefenthaler, S. Albertini, F. Zappa, P. Scheier

11:15 553. Ionic strength is systems that violate the electric neutrality. **S. Consta**

11:45 Discussion.

11:55 Concluding Remarks.

Section E

Marriott Marquis San Diego Marina
Torrey Pines 2

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*

8:00 554. Fluorescent nanomaterials for detection of cell markers and images. **H. Chang**

8:40 555. Chemiluminescent gold nanoluminophore-based immunoassays for biomarkers of acute myocardial infarction. **H. Cui**

9:20 556. Ultrasensitive quantification strategy of extracellular vesicles using CuS microgel and filter membrane. **Q. Jiang**, Y. Liu, W. Zhong

9:40 557. Photocleavable linker for the release of rare cancer biomarkers after microfluidic affinity selection. **T. Pahattuge**, J.M. Jackson, S.A. Soper

10:00 Intermission.

10:10 558. Nanomaterial-assisted extraction and quantification of circulating non-coding RNAs in serum. **M.P. Trinh**, Y. Zheng, W. Zhong

10:30 559. DNA terminal structure-mediated enzymatic reaction for ultra-sensitive detection of EGFR exon 19 deletion. **M. Zhao**

10:50 560. Single exosome analysis based on exosomal proteins using flow cytometry. **K. Guo**, W. Zhong

11:10 561. Characterizing extracellular vesicles using asymmetrical flow field-flow fractionation: Combining traditional nanoparticle characterization techniques with biomolecular probing. **G.B. Adkins**, E. Sun, W. Zhong

Section F

Marriott Marquis San Diego Marina
San Diego Ballroom Salon A

Biosensing: New Strategies & Latest Development

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

8:00 562. Nucleic-acid-functionalized field-effect transistors for biomedical applications. **K.M. Cheung**, N. Nakatsuka, K. Yang, C. Zhao, H. Yang, J.M. Abendroth, P.S. Weiss, M.N. Stojanovic, A.M. Andrews

8:20 563. SPR-MALDI Biosensing via carbohydrate small molecule probes. **A. Lambert**, C. Chen, Q.J. Cheng

8:40 564. Microfluidic synthesis and patterning of silver nanoparticles for biomolecular sensing. **Y. Nie**, J. Zhang

9:00 565. Supported lipid bilayer-based biosensor to detect phospholipase A2 -lipid membrane interaction. **S. Hossain**, K. Pai, M. Piyasena

9:20 566. Nanobody-based binding assay for the discovery of potent inhibitors in drug development. **N. Vasylieva**, S. Kitamura, J. Dong, B. Barnych, K. Hvorecny, D. Madden, S. Gee, D.W. Wolan, C. Morisseau, B.D. Hammock

9:40 Intermission.

9:55 567. Microfluidic paper-based analytical devices (microPADs) with DVD player: Centrifugally assisted flow acceleration for rapid distance readout assays. **K. Maejima**, Y. Hiruta, D. Citterio

10:15 568. Chimeric phage as scaffold for rapid detection of pathogenic bacteria. **H. Peng**, I. Chen

10:35 569. Fully integrated paper microfluidic single-walled carbon nanotubes chemiresistive biosensor arrays for point-of-care diagnostics. **Y. Shen**, A.K. Mulchandani

10:55 570. 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

11:15 571. Advantages of gallium indium eutectic contacts for In2O3 field-effect transistors. **s. Rahimnejad**, L. Stewart, C. Zhao, A. Andrews, P. Weiss

11:35 572. Using single-molecule RNA: DNA electrical conductance measurements for ultra-sensitive pathogen detection. Y. Li, **J.M. Artes Vivancos**, B. Demir, S. Gokce, H.M. Mohammad, M. Alangari, A. Anantram, E.E. Oren, J. Hihath

Theoretical & Experimental Investigations of Water Interactions with Materials

Sponsored by COLL, Cosponsored by ANYL‡

THURSDAY AFTERNOON

Section A

Marriott Marquis San Diego Marina
Rancho Santa Fe 2

Advances in Spectroscopy

Optical Spectroscopy: IR, Fluorescence, Absorption, and Raman Spectroscopy

E. A. Smith, *Organizer*
R. F. Hirsch, *Presiding*

1:00 573. Development of fluorescent molecular probes for the highly sensitive and selective detection of living substances using magnetic beads. **Y. Suzuki**

1:20 574. Pump-probe UV resonance Raman spectroscopic analysis of the redox cofactors in photosystem II. **J. Chen**, J. Chen, Y. Liu

1:40 575. 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

2:00 576. Cyano-derivatized tryptophans, as a novel 2D IR probe-pair for protein dynamics. **F. Chalyavi**, J. Mauro, A. Schmitz, M.W. Fennie, M.J. Tucker

2:20 Intermission.

2:35 577. Adversarial spectroscopy. **G.J. Simpson**

3:00 578. Microgel nanostructures for surface-enhanced Raman spectroscopy. **S.R. Emory**, A. Silva, J. Lo, S. Olson, **D.A. Rider**

3:20 579. Investigating the anion-cation intermolecular interactions in imidazolium acetate ionic liquids by Raman spectroscopy and multiple regression analysis. **J. Li**, J.W. Petrich, E.A. Smith

3:40 580. All-dielectric, mid-infrared metasurfaces for vibrational circular dichroism enhancement. **J. Abendroth**, J. Hu, L. Poulikakos, M. Solomon, M. Lawrence, J. Dionne