

44th ACS Western Regional Meeting
October 3-6, 2013
Hyatt Regency Santa Clara

B. Charpentier and J. Gunzner-Toste, *Program Chairs*

THURSDAY MORNING

Napa I

Chemistry and the Law: Where Chemistry Meets the Law
The America Invents Act

Sponsored by the ACS Division of Chemistry and the Law

S. Thompson, *Organizer, Presiding*

- 8:30** 1. An Introduction to the America Invents Act. **S. Thompson**
- 9:15** 2. Practical Implications of the Leahy-Smith America Invents Act: Avoiding Prior Art Pitfalls and Other Traps for the Unwary. **R. M. Thiessen**
- 10:00** Intermission.
- 10:30** 3. The AIA 1 Year on: the New Landscape for Challenging Patents. **R. G. Bone**
- 11:15** 4. How does the new patent law impact the research of biotech scientists and managers. **A. Y. Nie**

Camino Real

Ethnobotanical Drugs
Ethnobotany as Inspiration for Drug Discovery and Development
Sponsored by the ACS Division of Medicinal Chemistry

M. Tempesta, *Organizer, Presiding*

- 8:30** 5. Traditional medicine inspired drug discovery for some modern day diseases. **A. Gunatilaka**
- 9:00** 6. Scientific and regulatory challenges in the US Botanical Marketplace. **J. M. Betz**
- 9:30** 7. The Discovery of SP-303 (Crofelemer/Fulyzaq), a Novel Polyphenol Isolated from *Croton lechleri*.
M. S. Tempesta
- 10:00** Intermission.
- 10:30** 8. The development of the first oral botanical drug Fulyzaq™: connecting ethnobotany, conservation, biocultural diversity, global public health and indigenous knowledge. **S. R. King**, P. Chaturvedi, F. C. Ayala Flores, C. G. Lozano Diaz, E. K. Tsajamen, G. C. Mashian, M. F. Pariona, E. N. Meza, E. L. Soto
- 11:00** 9. Crofelemer: a Novel Antidiarrheal Medicine from the Amazon Rainforest-Mechanism of Action and Clinical Applications. **T. J. Carlson**

Sonoma

Nuclear Chemistry

Symposium in Honor of Prof. Darleane Hoffman

*Sponsored by Lawrence Livermore National Labs and the
ACS Division of Nuclear Chemistry and Technology*

D. Shaughnessy, *Organizer, Presiding*

M. Neu, *Presiding*

8:30 Introductory Remarks.

8:40 **10.** 65 years as a nuclear chemist - a retrospective view. **D. C. Hoffman**

9:30 **11.** Darleane C. Hoffman: An element of success. **K. Thomas**

10:00 Intermission.

10:30 **12.** Tribute to Prof. Darleane Hoffman: Pioneering nuclear chemist and architect of the next generation.
D. E. Hobart

11:00 **13.** The many elements of Darleane Hoffman: A grateful student comments on her accomplishments and influences. **M. P. Neu**

11:30 **14.** Success of the Glenn T. Seaborg Institute at Lawrence Livermore National Laboratory is due in large part to the pivotal vision and leadership of its first director, Dr. Darleane Hoffman. **A. B. Kersting**

Ballroom A

Inorganic/Organometallic Chemistry

General Session on Inorganic/Organometallic Chemistry

Sponsored by the ACS Division of Inorganic Chemistry

L. Cheruzel, *Presiding*

9:00 **15.** Insights in enzyme modification for renewable solar hydrogen. **I. T. Yonemoto**, P. D. Weyman, H. O. Smith

9:30 **16.** Visible light photoredox catalysis: Selective reduction of carbon dioxide to carbon monoxide by a nickel N-heterocyclic carbene-isoquinoline complex. **N. Kornienko**, S. V. Thoi, C. Margarit, P. Yang, C. Chang

10:00 Intermission.

10:30 **17.** Synthesis, crystal structure, and transport properties of a new Li-containing layered material, $\text{Li}_x\text{Sn}_{3-x}\text{As}_2$. **K. Lee**, K. Kovnir

11:00 **18.** Selective light-driven aerobic hydroxylation of C-H bonds using hybrid P450 biocatalysts.
L. E. Cheruzel

Ballroom E

Medicinal Chemistry

Recent Advances in Medicinal Chemistry

Sponsored by the ACS Division of Medicinal Chemistry, Genentech and Senn Chemicals

Y. Xu, A. Garofalo, *Organizers, Presiding*

- 9:00** 19. Discovery of the First Small Molecule Activators of Cardiac Myosin for the Treatment of Heart Failure. **A. R. Muci**
- 9:30** 20. Hit-to-Lead Optimization of a Pan-Genotypic Tetrahydroquinoline scaffold for the Treatment of HCV. **E. Canales**, K. Babaoglu, R. Beran, C. Bush, M. Clarke, S. Eng, R. Higgins, T. Kobayashi, R. Martinez, P. Morganelli, B. Murray, R. Saito, H. Trinh, M. Paulson, S. Lazerwith
- 10:00** Intermission.
- 10:30** 21. Small Molecule BTK Inhibitors: an Update from Pharmacocyclics. **Z. J. Jia**
- 11:00** 22. Identification of Potent, Selective and Orally Bioavailable TYK2 Inhibitors for Psoriasis and Inflammatory Bowel Diseases (IBD). **J. Liang**
- 11:30** 23. Discovery of potent and bioavailable Pim inhibitors for multiple myeloma. **X. Wang**

Napa III

Renewables: Biofuels

Value-added Commodity Chemicals from Biofuel Platforms

M. Mulvihill, *Organizer, Presiding*

- 9:00** 24. Using the Tools of Green Chemistry and Biomimicry to Identify new Functional BioBased Chemicals for Industrial Applications. **M. J. Mulvihill**
- 9:30** 25. Biobased chemicals and fuels in historical and economic perspective. **A. Ringer**
- 10:00** Intermission.
- 10:30** 26. Cost effective production of cellulosic two and three carbon molecules using the ZeaChem process. **B. Yeh**
- 11:00** 27. Small molecule modulators of lipid production in microalgae and NMR spectroscopic analysis of lipids for biofuel applications. **L. A. Anderson**, D. M. Wong, M. A. Danielewicz, J. R. Boothe, A. K. Franz

POSTER SESSIONS
Posters will remain up throughout the day.
Presenters should attend their posters during breaks.

Ballroom C

N. McClure, *Organizer*

9:00 - 5:00

Biochemistry Posters

28. Selective Oxidation of 8-oxoguanine by Os(phen)₂dppz³⁺. **K. R. Miller**, Z. A. Perez, E. D. Stemp
29. Metal dependence of the Mre11 DNA repair nuclease. **O. D. Rivera**, T. Barfoot, Y. Gao, S. W. Nelson
30. New wide pore C18 phase for fast and efficient purification of peptides by flash chromatography.
M. Wilcox, J. Bystron, M. Jacyno, C. Sundararajan, N.K. Bopanna, **R. Nguyen**

Biological Chemistry Posters

31. Biosynthetic, stimulus-sensitive protein brushes inspired by neurofilament sidearm domain. **N. Srinivasan**,
M. Bhagawati, B. Ananthanarayanan, S. Kumar

Environmental Chemistry Posters

32. Analysis of chemical changes in soil composition due to the effects of plant growth. P. Johnson,
L. Huang
33. Phytotoxicity and reduced translocation during root uptake of organic contaminants by wheat
seedlings. **A. He**, Y. Chen, D. Sheng
34. Trace determinations of hexavalent chromium in soil using automated solvent extractions and ion
chromatography. **T. T. Christison**, R. Jack, L. Basumallick, L. Lopez
35. Detection and Quantification of Inorganic Arsenic in Fruit Juices Using Capillary Ion
Chromatography. **H. Yang**
36. Kinetics investigation of OH reaction with Styrene at 240 – 340 K and 1 – 3 Torr using the Relative
Rate/Discharge Flow/ Mass Spectrometry Method. **J. Cho**, Z. Li
37. Kinetics investigation of OH reaction with naphthalene at 240-340 K and 1-3 Torr using the Relative
Rate/Discharge Flow/Mass spectrometry technique. **M. M. Roueintan**, Z. Li
38. Withdrawn

Inorganic Chemistry Posters

39. Unusual Zn Clusters Supported by Formamidinates. **Y. Tsai**, Q. Zhao
40. Monometallic Complexes Supported by Ligands with Excessive Basic Centers. **Y. Tsai**, Q. Zhao
41. Characterization of Derivatized Cyclams and Their Applications in Metalation. **A. Cao Minh**, Q. Zhao
42. Effects of Hydrogen Bonding Self-Assembly on the Spin Crossover Behavior of Mononuclear Complexes of 6-
(3,5-Diamino-2,4,6-triazinyl)2,2'-bipyridine. **M. C. Young**, E. Liew, R. J. Hooley
44. Seeking the single molecule magnet: Investigating magnetic characteristics of low coordinate transition metal

- compounds. **A. M. Bryan**, P. P. Power
45. Mild route to novel Ga–N and In–N compounds. **R. J. Wilson**, M. V. Bennett
46. Late transition metal complexes of a 1,3-dipyridylverdazyl: Studies of metal and ligand redox processes. **D. Chung**, S. Ponce, D. Brook
47. Synthesis of rare earth pre-catalysts for the transformation of organic molecules. **S. D. Bunge**
48. Synthesis and characterization of polytopic verdazyl ligands capable of self assembly. **E. Johnson**, D. J. Brook
49. Exploring Metal-Containing Monomers for Material Development. **C. Tran-Math**, Q. Zhao

Organic Chemistry Posters

50. Computational and experimental study of the thermal cyclization of enediynes and dieneynes. **C. Q. Li**, B. F. Gherman, J. D. Spence
51. Photoexcitation of enediyne compounds and implications for their Bergman cyclization reactivity. **P. J. Marzouk**, B. F. Gherman, J. D. Spence
52. Withdrawn
53. Pseudorotaxane formation targeting on nucleic acids. **K. Onizuka**, Y. Ito, H. Abe
54. Adjuvant-free MUC1 glycopeptide antitumor vaccines containing Neu5Gc. **T. J. Lanoue**, H. Malekan, H. Yu, Y. Li, X. Chen
55. Continuous flow synthesis of valuable triols in a tube-in-tube microreactor. **C. Park**, C. Park
56. A Microchemical Synthesis of Chiral Epoxy Alcohols. **H. Lim**, C. Park
57. Novel Chemoenzymatic Approach towards Synthesizing Chondroitin Sulfate Analogs. **N. Tasnima**, H. Yu, M. Xue, J. Qu, Y. Li, X. Chen
58. Water soluble verdazyls with polyhydroxy groups in the 1 and 5 positions. **D. A. Matteo**, T. Truong, V. Gaoiran, D. J. Brook
59. Heterocycle to Heterocycle Strategies: Isoxazoles and Oxadiazoles as Branch Points towards Skeletally Diverse Fluorescent Small Molecules. **T. A. Palazzo**, K. C. Coffman, J. S. Yang, D. J. Tantillo, M. J. Kurth
60. A general and high yield method for the synthesis of 6-vinylfulvenes. I. Erden, **J. Ma**
61. Probing the scope of the chemical synthesis of S-ribosyl-L-homocysteine (SRH) from various homocysteine and ribose moieties. **E. I. Showell-Rouse**, B. J. Corcoran, E. S. Murzinski, D. L. Cudia, M. E. Bolitho
62. Concise Synthesis of Highly Substituted Adamantanones from Bicyclo[3.3.1]nonan-9-ones. **G. S. Lee**, M. E. Jung
63. Organocatalytic enantioselective synthesis of polysubstituted spirooxindole derivatives via a Michael-Michael tandem sequence. **N. Ramireddy**, S. Abbaraju, N. K. Rana, J. Zhao
64. Phosphine/Palladium Sequential Catalysis Syntheses of Alkylidene Phthalans, Indanes, and Indanones. **Y. Fan**, O. Kwon
65. Synthesis and bioactivity of thiazolo-, thiazino- and thiazepino-2*H*-indazoles synthesized via the Davis-Beirut reaction. **K. M. Gottlieb**, M. J. Haddadin, M. J. Kurth
66. Synthesis and Biological Activity of Fluorinated N-Methanocarbothymidine Analogs. **T. A. Dwight**, M. E. Jung, F. Vigant

Organometallic Chemistry Posters

67. Platinum-Catalyzed C–H Arylation of Simple Arenes. **A. M. Wagner**, A. J. Hickman, M. S. Sanford
68. An efficient and stereoselective method for constructing seven-membered carbo- and heterocycles. G. G. Melikyan, **K. Duncan**
69. Synthesis and spectroscopic characterization of structurally unique trialkylboranes: Evidence of unusual geometries stabilized by dispersion effects. **M. A. Faust**, P. P. Power

Renewables and Biofuels Posters

70. How to get the most out of your analytical laboratory: Cutting costs and maintaining quality in a high throughput lab. **A. Morgenthaler**, T. Treynor, H. Fuller, B. Van Deren, D. McAdam, M. Leavell
71. Finding 80 needles in a hydrocarbon haystack: Measuring oxygenate impurities in farnesene by GC. **L. Perelman, D. Diola**, S. Afaghani, L. McDougald, B. Van Deren, S. Gaucher, M. Leavell
72. Engineering yeast for the expression and secretion of cellulase cocktails. **S. Batt Throne**, D. Wong, D. Wan, S. Xie, E. Truong, R. Doi
73. Enzyme nanoassemblies for biomass conversion. **C. C. Lee**, R. E. Kibblewhite, K. Wagschal, C. D. Paavola

THURSDAY AFTERNOON

Bayshore West

Analytical Chemistry: General

Sponsored by the ACS Analytical Chemistry Division

J. M. Van Emon, *Presiding*

- 1:30 74. Characterization of the composition and thermal decomposition profile of recycled carpet samples by TG-FTIR, TG-MS, and TG-GC-MS. **P. J. Shapiro**, C. Fischer
- 1:55 75. Capillary IC – A New Platform for High Throughput or High Resolution Separations of Ionic Compounds. **P. Bodsky**
- 2:20 76. Analytical scheme for determining cytotoxicity and biomarkers of exposure for chlorpyrifos and 3,5,6-trichloro-2-pyridinol. **J. M. Van Emon**, P. Pan

Bayshore East

Analytical Chemistry: NMR Spectroscopy

Recent Advances and Applications in NMR Spectroscopy

Sponsored by Agilent Technologies

L. Cegelski, *Organizer, Presiding*

- 1:30 77. High-Resolution Structural Basis of G-protein Coupled Receptor Signaling Complexity. **R. Nygaard**
- 2:00 78. Redefining high-throughput - CRAFT: A tool for automated deconvolution of NMR spectra. **K. Krishnamurthy**
- 2:30 79. Sum of the Parts: Composition and Architecture of the Bacterial Extracellular Matrix. **L. Cegelski**, O. McCrate, X. Zhou, C. Reichhardt, J. Lim

- 3:00** Intermission.
- 3:30** **80.** NMR investigation of protein-protein interactions of the cataract-related variant G18V of human YS-crystallin. C. N. Kingsley, W. D. Brubaker, S. Markovic, A. Diehl, H. Oschkinat, **R. W. Martin**
- 4:00** **81.** Low Field Solid state NMR Investigations of Network Formation and Motional Dynamics in Well-Defined Model Poly(dimethylsiloxane) Elastomers. **J. P. Lewicki**, S. J. Harley, R. S. Maxwell
- 4:30** **82.** Using NMR spectroscopy to identify how a slow conformational switch regulates the 24-hour circadian clock. **C. L. Partch**, P. J. Sammons, C. L. Gustafson

Camino Real

Biochemical Technology

Advances in Biochemical Technology

J. Coffman, *Organizer*

C. Komives, *Organizer, Presiding*

- 1:30** **83.** Function, structure, and stability of enzymes confined in hydrogels. J. Kunkel, S. Long, **P. Asuri**
- 2:00** **84.** Automated Algorithm-Based Oxygen Transfer Rate Characterization in Production Bioreactors. **B. Dahlin**, E. Cervantes, C. Chun
- 2:30** **85.** Expression of recombinant protein in *B. methanolicus*; a thermotolerant methylotroph. **C. Komives**, D. Nilasari, B. Wong
- 3:00** Intermission.
- 3:30** **86.** *Trans*-acting acyltransferase domains: Tools for engineering polyketide biosynthesis. **B. Dunn**, K. Watts, C. Khosla
- 4:00** **87.** Non-invasive acoustical sensing and acoustic microfluidics: Applications in upstream bioprocessing. **S. S. Datwani**
- 4:30** **88.** Development of Enzyme Systems for the Production of Cellulosic Ethanol. **T. Kaper**

Mendocino

Chemical Health and Safety

Changes in Laboratory Safety Management: The Revised Lab Standard and GHS

Sponsored by the ACS Division of Chemical Health and Safety

D. M. Decker, R. Phifer, *Organizers, Presiding*

- 1:30** Introductory Remarks.
- 1:35** **89.** GHS and what it means to laboratories. **R. W. Phifer**
- 1:55** **90.** Laboratory hazardous waste management: Best practices and the impact of the GHS. **D. J. Keenan**
- 2:15** **91.** Hazard assessment opportunities under the new Laboratory Standard. **D. M. Decker**
- 2:35** **92.** Safety in the academic environment - a 30 year retrospective look forward. **J. G. Palmer**
- 2:55** Intermission.
- 3:10** **93.** University System-wide Actions to Improve Laboratory Safety Culture. **K. Smith**
- 3:30** **94.** UC and Cal-OSHA lab settlement agreement: One year later. **K. L. Smith**

3:50 95. Quo Vadis: Laboratory safety after UCLA. **N. Langerman**

4:10 Concluding Remarks.

Napa I

Chemistry and the Law: Where Chemistry Meets the Law Alternative Careers for Chemists

Sponsored by the ACS Division of Chemistry and the Law

S. Thompson, *Organizer, Presiding*

1:30 96. From The Control Room to the Courtroom. **C. Lippenberger**

2:00 97. Food and Drug Administration laws and regulations - Food Safety - How chemists are involved.
E. S. Furukawa

2:30 98. Beyond the bench: Careers in patent law for chemists. **K. Bolin**

3:00 Intermission.

3:15 99. Pathways to Intellectual Property: Options for Scientists. **J. A. Lefstin**

3:45 100. A Day in the Life: Patent Attorney. **S. Thompson**

Ballroom A

Inorganic/Organometallic Chemistry Small-Molecule Activation and Redox Catalysis with Metal Complexes and Surfaces

Sponsored by the ACS Division of Inorganic Chemistry

M. Kanan, *Organizer, Presiding*

1:30 101. Electrocatalytic Reduction of H⁺ and CO₂ by a Series of Iron Carbonyl Clusters. **L. A. Berben**

2:15 102. Using redox-active ligands to promote multi-electron reactivity at electrophilic metal centers.
A. F. Heyduk, A. Hollas, R. Munha, J. Lora

3:00 Intermission.

3:30 103. Group 10 Metal-Mediated N-O Bond Activation. **J. S. Figueroa**

4:15 104. Two-Step Electroreduction of CO₂ to Ethanol Catalyzed by Oxide-Derived Metal Nanoparticles.
M. Kanan

Ballroom E

Medicinal Chemistry Recent Advances in Medicinal Chemistry

Sponsored by the ACS Division of Medicinal Chemistry, Genentech and Senn Chemicals

Y. Xu, A. Garofalo, *Organizers, Presiding*

1:30 105. Discovery of Muscarinic Acetylcholine receptor antagonist and Beta 2 adrenoceptor agonist (MABA) dual pharmacology molecules. **A. D. Hughes**, E. K. Bradley, Y. Chen, S. S. Hegde, J. R. Jasper, T. Lee, A. McNamara, M. Mammen, M. Pulido-Rios, T. Steinfeld

- 2:00** 106. Discovery of NAMPT inhibitors with favorable physicochemical properties as potential treatments for cancer. **M. Zak**, N. Skelton, T. O'Brien, B. M. Liederer, J. Ly, L. Wang, D. Sampath, J. Oeh, W. Wang, K. W. Bair, X. Zeng, Y. Ho, T. Baumeister, P. Yuen, P. S. Dragovich
- 2:30** 107. Increasing target residence time in drug discovery; Optimization via covalent reversible interactions. **T. D. Owens**
- 3:00** Intermission.
- 3:30** 108. The potential of boron-containing small molecules in medicinal chemistry. **Y. Liu**
- 4:00** 109. Targeting the Immunoproteasome. **D. L. McMinn**
- 4:30** 110. Inhibiting protein-protein interactions. **J. C. Medina**, S. H. Olson, Y. Rew, F. Gonzalez Lopez De Turiso, M. D. Bartberger, H. P. Beck, J. Canon, A. Chen, J. Deignan, B. Fox, A. Z. Gonzalez, D. Gustin, X. Huang, X. Jiao, L. Jin, F. Kayser, D. Kopecky, Y. Li, J. D. Oliner, T. Osgood, X. Yan, Q. Ye, D. Yu, D. Sun

Sonoma

Nuclear Chemistry

Symposium in Honor of Prof. Darleane Hoffman

Sponsored by Lawrence Livermore National Labs and the ACS Division of Nuclear Chemistry and Technology

D. Shaughnessy, *Organizer, Presiding*

M. Neu, *Presiding*

- 1:30** 111. NNSA Radiochemistry Center of Excellence at the University of Tennessee. **H. L. Hall**
- 2:00** 112. Real-world application of nuclear chemistry in a time of crisis: A summary of analytical support to the DOE Fukushima response by the Lawrence Livermore National Laboratory. **S. A. Kreek**, N. G. Wimer, B. B. Bandong
- 2:30** 113. Experimental nuclear and radiochemistry at Lawrence Livermore National Laboratory: A radiochemistry renaissance. **D. A. Shaughnessy**, K. J. Moody, R. Henderson, N. Gharibyan, P. Grant, J. Despotopulos
- 3:00** Intermission.
- 3:30** 114. Target fabrication & characterization for nuclear experiments at LLNL. **R. A. Henderson**
- 4:00** 115. Radioanalytical Method Development for Nuclear Forensics and Safeguards: New Challenges and Old Familiars. **R. Sudowe**
- 4:30** 116. Heavy element research at Texas A&M University. **C. M. Folden**

Ballroom F

Organic Chemistry: General

General Session on Organic Chemistry

M. Duncton, *Presiding*

- 1:30** 117. Effect of ionic liquid cosolvent on the methanolysis of pivaloyl triflate. **B. D. Kochly**, S. Citrak, N. Gathondu, G. Amberchan
- 2:00** 118. Water soluble Verdazyl Radicals synthesized from Aldoses. **T. T. Le**, D. J. Brook

- 2:15** 119. Multiplying the catalytic output of reactions through bifunctional substrates. **M. Kaviani-Joupari**, M. P. Schramm
- 2:30** 120. An efficient approach to the total synthesis of acylfulvenes, a class of potent antitumor agents. **I. Erden**, J. Ma
- 3:00** Intermission.
- 3:30** 121. Asymmetric synthesis of 2,3-dihydrobenzofurans via Rh(II) catalyzed C-H insertions. **K. N. Lamb**, C. Soldi, R. Squitieri, J. T. Shaw
- 4:00** 122. Cation Stabilizing Strategies for Sc-catalyzed Enantioselective [3+2] Carbocycle Annulations with Allylsilanes. **N. Ball-Jones**, J. J. Badillo, B. M. Anderson, A. K. Franz
- 4:30** 123. Synthesis of *trans*-2-(trifluoromethyl)cyclopropanes *via* Suzuki cross-coupling reactions with a MIDA boronate. **M. A. Duncton**, R. Singh

Napa III

Renewables: Chemicals and Polymers *Chemicals and Polymers*

W. Orts, M. Foster, *Organizers, Presiding*

- 1:30** 124. Towards a PLA for durable goods. **A. Flynn**, L. Torres
- 2:00** 125. Extended donor-acceptor alternating narrow band-gap molecules for organic photovoltaics: Bridging between polymers and small molecules. **X. Liu**, G. C. Bazan
- 2:30** 126. Novel amphiphilic and super absorbent cellulose nanofibril aerogels. **F. Jiang**, Y. Hsieh
- 3:00** Intermission.
- 3:30** 127. Biodegradable Plastic Produced by Bacteria. **A. J. Pieja**
- 4:00** 128. Torrefaction of agricultural by-products: Effects of temperature and time. **B. Chiou**, C. Bilbao-Sainz, D. Valenzuela-Medina, A. Klaczynski, R. Milczarek, R. Avena-Bustillos, W. Du, S. Imam, G. Glenn, W. Orts
- 4:30** 129. Optimizing the value of agriculturally-derived fibers based on their source & properties. **W. J. Orts**, G. M. Glenn, E. S. Medeiros, E. d. Teixeira, A. de Campos, M. F. Rosa, L. H. Mattoso

FRIDAY MORNING

Bayshore West

Analytical Chemistry *Applications in Electronic Manufacturing* *Sponsored by Air Liquide Electronics – Balazs NanoAnalysis*

L. Milstein, *Organizer, Presiding*

- 8:30** 130. Survey of Analytical Techniques Useful for Thin Film Material Evaluation in High Technology Applications. **H. E. Gotts**
- 9:00** 131. Characterization of Precursors used in Semiconductor Manufacturing using a diverse set of Analytical

Techniques. **C. Mckenna**, V. Thirumala

9:30 132. Analytical Characterization of Thin Films for ALD. **L. S. Milstein**, P. L. Clancy, H. E. Gotts

10:00 Intermission.

10:30 133. Photovoltaic Materials Defect Characterization Techniques. **S. A. Myers**, H. E. Gotts

11:00 134. Trace Degradation Analysis in Li-ion Battery Electrolytes. **P. Voelker**

Sonoma

Computational Chemistry

Modern Computational Chemistry

Sponsored by Genentech and the ACS Division of Computers in Chemistry

J. Pitera, S. Boyer, *Organizers, Presiding*

8:30 135. Gas permeability and Klinkenberg effects in carbon micro and mesopores. **M. Firouzi**, J. Wilcox

9:00 136. International chemical identifier for reactions (RInChI). **G. Grethe**, J. M. Goodman, C. Allen

9:30 137. Improved Ligand Binding Energies Derived from Molecular Dynamics: Replicate Sampling Enhances the Search of Conformational Space. **M. Adler**, P. Beroza

10:00 Intermission 1.

10:30 138. Improving the Prediction of Drug Disposition in the Brain with Mechanistic Models of Brain Penetration Characteristics. K. Lanevskij, P. Japertas, R. Didziapetris, **G. A. McGibbon**

11:00 139. Organic Acid-Catalyzed Polyurethane Formation via a Dual-Activated Mechanism: Unexpected Preference of N-activation over O-activation of Isocyanate. **H. W. Horn**, H. Sardon, A. C. Engler, J. M. Chan, J. M. Garcia, D. J. Coady, A. Pascual, D. Mecerreyes, G. O. Jones, J. E. Rice, J. L. Hedrick

11:30 140. Computer-aided design of permeable cyclic peptides. **S. S. Leung**, R. Lokey, M. P. Jacobson

Alameda

Education in Chemistry: Two-Year Colleges

A Legitimate Pathway for Underrepresented Minorities

Pursuing Careers in STEM Areas

Sponsored by the ACS Committee on Minority Affairs

A. Rivera Figueroa, *Organizer*

O. Gaglione, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 141. Undergraduate research with community college students and how it supports student transfer. **T. B. Higgins**, H. Ungar

9:05 142. ChemEd Bridges: Bridging community college chemistry faculty into the national educational community. **H. Ungar**, T. B. Higgins, M. Boyd, D. Brown

9:35 Brainstorming.

10:00 Intermission.

10:30 143. Strategies for successfully transitioning underrepresented minority students from two-year to

four-year colleges. **M. A. Scharberg**

11:00 144. Accessibility versus success: Challenges and benefits of teaching an evening hybrid general, organic, biochemistry course at a community college. **J. C. Medina**

11:30 145. Affirming the two-year college as a legitimate pathway to the baccalaureate and beyond and to careers in the chemical sciences, engineering and education. **O. G. Gaglione**

Napa I

Entrepreneurship in Chemistry Business Considerations for Science Entrepreneurs

B. Charpentier, *Organizer*

N. McClure, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 146. Aligning capital, scientific, and drug development interests: Lessons learned from Edison Pharmaceuticals. **G. Miller**

9:05 147. How to Protect Your New Chemical Business. **S. Thompson**

9:35 148. ACS Entrepreneur Founders: Choice of Entity, Funding and Founding Your Own Enterprise. **G. Sato**

10:05 Intermission.

10:35 149. Entrepreneurial programs and services from ACS. **D. E. Harwell**, K. J. Polk, R. E. Brown, E. I. Fraser

11:05 150. Finding and executing a business model for science based companies. **A. Tajonar**

Camino Real

Environmental Chemistry Hydraulic Fracturing in California: Environmental Issues with the Largest Shale Oil Formation in the US

Sponsored by the ACS Division of Environmental Chemistry and the ACS Division of Geochemistry

E. Warren, D. Drogos, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 151. Air dispersion modeling of volatile organic emissions from multiple natural gas wells in Decatur, Texas. **A. Sutherland, P. Rosenfeld**, R. Hesse, A. Zapata

9:00 152. Isotopic forensic techniques for methane source discrimination. **J. K. Sueker**, G. Cramer, B. Clark, E. Nichols

9:20 153. Hydraulic fracturing and the impacts to groundwater and water quality: the importance of a monitoring program. **M. Zeko**, E. Vavricka

9:40 154. Protection of groundwater resources in the vicinity of hydraulic fracturing operations: Lessons from New York State and the Marcellus Shale. **M. Becker**, R. D. Jacobi

10:00 Intermission.

10:30 155. Analysis, treatment and tracing of frac and produced water. **A. R. Barron**

10:50 156. Analysis by ion chromatography of fracking flowback water from the Marcellus Shale using in-line

conductivity and automated dilution. **C. Fisher**, L. Lopez

11:10 157. Optimized Geochemical Modeling of Produced Fluids Provides Important Insight into NORM-Related Issues. **D. Carpenter**, E. Nichols

11:30 158. Hydraulic Fracturing, Wastewater Injection and Unintended Earthquakes. **W. L. Ellsworth**

Bayshore East

Food Chemistry

The Many Flavors of Food Chemistry

Sponsored by the ACS Division of Agriculture and Food Chemistry

S. Risch, *Organizer, Presiding*

8:30 159. Many flavors of food chemistry. **S. J. Risch**

9:00 160. Culinary science: Deliciousness facilitated by scientific insight. **A. Bouzari**

9:30 161. Wine flavor chemistry: From the vineyard to the bottle. **S. E. Ebeler**

10:00 Intermission.

10:30 162. Eucalyptol and the "Eucalyptus" aroma in red wines. **E. Herve**

11:00 163. Determinations of inorganic anions and organic acids in beverages using suppressed conductivity and charge detection. **T. T. Christison**, A. Zhang, C. Tanner, L. Lopez

11:30 164. Targeted unknown UHPLC-(ESI+)-Q/TOF MS approaches for understanding flavonoid bioavailability and metabolism. **A. E. Mitchell**

Napa III

Nanomaterials (organic)

Functional Carbon-Based Nanomaterials

F. Fischer, *Organizer, Presiding*

8:30 165. Withdrawn

9:00 166. Decacyclene-Based Materials: A New Frontier of Renewable Energy and Optoelectronic Research. **F. Toma**, T. V. Pho, F. Wudl

9:30 167. Conclusion to the 22 year mystery of the fullerene (C₆₀) pentane solvate structure. **E. A. Sarina**, M. A. Rivera, M. M. Olmstead, A. L. Balch

10:00 Intermission.

10:30 168. Indenofluorenes - a new class of electron-accepting materials. **M. M. Haley**

11:20 169. Investigation on inhibition of polysulfides dissolved into electrolyte using porous carbon in rechargeable lithium-sulfur batteries. **M. Gao**, C. Li, Y. Chen, Y. Huang

11:40 170. Heat-induced coarsening of gold nanoparticles on graphene. **H. Pan**, Y. Abate, Y. Shon

Ballroom F

Organic Chemistry

Recent Advances in Organic Chemistry

Sponsored by the ACS Division of Organic Chemistry

T. Maimone, *Organizer, Presiding*

- 8:30** 171. New advances in the construction of C–N and C–O bonds for organic synthesis. **J. Read de Alaniz**
- 9:15** 172. Asymmetric Catalysis with Cations and Anions. **F. Toste**
- 10:00** Intermission.
- 10:30** 173. Engineering Cytochrome P450 for Cyclopropanation. **Z. Wang**, P. Coelho, F. Arnold
- 11:15** 174. Total Synthesis and Glucokinase Activating Properties of Tatanans A-C. J. Jackson, **A. Zakarian**, Q. Xiao

Ballroom E

Medicinal Chemistry

Recent Advances in Medicinal Chemistry

Sponsored by the ACS Division of Medicinal Chemistry, Genentech and Senn Chemicals

A. Garofalo, Y. Xu, *Presiding*

- 9:00** 175. Hydrazino-iso-Pictet-Spengler Ligation: A new method for the generation of stable ADCs. **A. W. Garofalo**
- 9:30** 176. Rational design of inhibitors targeting the drug resistant influenza A virus M2 (A/M2) proton channel. **J. Wang**, Y. Wu, C. Ma, L. H. Pinto, R. A. Lamb, W. F. DeGrado
- 10:00** Intermission.
- 10:30** 177. Liquid handling and dilutions profoundly affect biological assays. **J. Olechno**, S. Ekins, A. J. Williams, R. Ellson
- 11:00** 178. Optimizing synthetic access to the quorum sensing substrate *S*-ribosylhomocysteine (SRH). **M. E. Bolitho**, B. J. Corcoran, E. I. Showell-Rouse, K. Wang
- 11:30** 179. Adventures with AKT: Small molecule inhibition and mechanism of activation. N. J. Skelton

POSTER SESSIONS

Posters will remain up throughout the day.
Presenters are expected to attend their posters during breaks.

Ballroom C

N. McClure, Organizers

9:10 - 5:10

Polymer Chemistry Posters

180. Viscoelastic characterization of a thin film biopolymer of phenylalanine glycine repeat domains using the Quartz Crystal Microbalance with Dissipation Monitoring. **E. Schneider**, N. B. Eisele, F. I. Andersson, S. Frey, R. P. Richter
181. Hybrid Elastin-like Polypeptide-Polyethylene Glycol (ELP-PEG) Hydrogels with Improved Transparency for Three-dimensional Cell Culture. **H. Wang**, L. Cai, A. Paul, A. Enejder, S. Heilshorn
182. One-step conjugation of bioactive peptides to elastin-like hydrogels to form tunable tissue engineering scaffolds. **C. Dinh**, L. Cai, S. Heilshorn
183. Synthesis and characterization of functionalized gold nanoparticle-cored dendrimers (NCDs) with average core sizes of 3, 10, and 17 nm as a theragnosis device for cancer treatment. **S. S. Deol**, **N. Weerasuriya**, Y. Shon
184. Thermoreversible fluorescence switching of hydrogel patterns generated by e-beam lithography. **E. Lin**, E. Bat, H. D. Maynard
185. Formulation of soluble chemically reduced graphene oxide through noncovalent approach with various aliphatic polymers. **I. In**
186. A Journey to Metal-Containing Polymers. **C. Tran-Math**, Q. Zhao
187. Characterization of light-controlled graphene-elastin composite actuators. **M. S. Desai**, E. Wang, S. Lee

Analytical Chemistry Posters

188. Comparative study of the loading capacity of preparative 5 m Gemini NX-C18 and Kinetex XB-C18 columns. **A. N. Guillen**
189. Counter ion analysis with Ion Chromatography in small molecule drug candidates. **D. D. Wang**
190. Temperature independent free energy relationships for three ionic liquids based on the trifluorotris(perfluoroethyl)phosphate anion. **T. W. Stephens**, W. E. Acree, Jr., M. H. Abraham
191. Trace analysis of hydrazine in pharmaceuticals by reversed phase HPLC. **J. Wang**, L. Wigman, K. Zhang

Catalysis Posters

192. Application of DFT methods for three way catalyst modelling. **I. Onal**, D. Gerceker
193. DFT study: Direct methanol oxidation to formaldehyde by N₂O on [VO]¹⁺-ZSM-5 cluster. **I. Onal**, M. F. Fellah
194. Controlling activity of ligand-capped Pd nanoparticle catalysts: effects of thiolate ligand structure and functionality. **M. S. Maung**
195. Expanding the scope of light-driven P450 biocatalysts: from non-natural substrates to other members of the

P450 superfamily. **S. Mahadevan, M. Bhandarkar, T. Dao, S. Mullen**, C. White, A. U, M. Kato, A. Cortez, E. Nunez, A. Colbert, A. Nguyen, T. Nguyen, L. Cheruzel

Computational Chemistry Posters

- 196.** Understanding the Electron Reorganization along the Thermal Isomerization Reactions of Cyclobutenes. Origins of Inward Pseudodiradical Torquoselectivity. **A. Morales-Bayuelo**
- 197.** In-Silico Combination of Docking, QM/MM analysis and MD Simulations for Tetrahydrobiopterin Analogous: Binding Towards Non-Heme Active Site of Phenylalanine Hydroxylase and A313T Mutant Type for Neurological Cascades. **N. Chadha**, A. K. Tiwari, S. Chaturvedi, M. D. Milton, A. K. Mishra
- 198.** Theoretical study of formation routes and dimerization of methanimine: implications for the aerosols formation in the upper atmosphere of Titan. **M. Rosi**, S. Falcinelli, N. Balucani, P. Casavecchia, D. Skouteris
- 199.** Withdrawn
- 200.** Charge transfer and ionic hydration. **M. Soniat**, S. W. Rick
- 201.** Theoretical investigation of OH reaction with Styrene. **J. Cho**, Z. Li
- 202.** Efficient and precise techniques for parallelization of kinetic Monte Carlo techniques. **J. Nilmeier**

Food Chemistry Posters

- 203.** Stability of oxidative products in Quinoa (*Chenopodium quinoa*) during accelerated aging. **A. Anderson**
- 204.** Phytonutrient analysis of fresh and cooked Yucca (*Yucca whipplei*) fruit pods and blossoms. G. Gihana, **J. Mattice**, J. Dsouza, M. Barth, Y. Hu, D. McCarthy
- 205.** Compositional analysis of stinging nettle (*Urtica dioica*) leaves. H. Zhuang, **C. L. Carson**, J. Mattice, **F. Nduwayo, J. Dsouza, M. DeVore**, Y. Hu, M. Barth, D. McCarthy
- 206.** Esculeoside A content of commercial tomato varieties. **A. Vilches**, A. P. Breksa
- 207.** Nutrient and organoleptic properties of 10 vintage tomato varieties. **D. E. King**, A. P. Breksa, J. A. Labate, L. D. Robertson, B. A. King

Fuel Chemistry Poster

- 208.** Mesoporous materials for adsorptive desulfurization of JP-8 fuel. **J. M. St. John**, D. T. Tran, S. R. Oliver

Medicinal Chemistry Posters

- 209.** Importance of tetrahydrobiopterin mediated interactions in aromatic amino acid hydroxylases enzymes family: Assessing effect on biosynthesis due to effect of single site mutation on thermodynamic stability of hydroxylases. **N. Chadha**, A. K. Tiwari, S. Chaturvedi, M. D. Milton, A. K. Mishra
- 210.** Inhibition of stearoyl-CoA desaturase drives uptake of exogenous fatty acids and sensitizes glioblastoma cells to lipoapoptosis. **T. Thompson**, S. Heinemann, **J. H. Jones**
- 211.** Development of Benzotriazine Oxides targeting replicating and non-replicating *M. tuberculosis*. **A. A. Tambo-ong, P. B. Madrid**, S. Chopra, G. A. Koolpe, K. N. Matsuyama, K. J. Ryan
- 212.** Synthesis of Azagenisteins for the cytotoxic evaluation towards Prostate Cancer Cell Lines. **P. Xiong**, Q. Chen

213. Hit to lead discovery of novel N-methylated imidazo-, pyrrolo-, and pyrazolo-pyrimidines as potent and selective mTOR inhibitors. **K. D. Robarge**
214. Synthesis and neuronal cells protection of third generation quinoline compounds. **J. Nguyen**, J. Lu, S. Weerasekara, I. Maezawa, L. Jin, D. H. Hua
215. Comparative evaluation of automated flash chromatography and preparative HPLC for bench-scale purification of a broad range of sample types. **M. Jacyno, J. Bystron, M. Wilcox**, C. Sundararajan, B. NK, **R. Nguyen**
216. Discovery and optimization of small molecule AMPK activators. **I. S. Darwish**, J. Yu, H. Hong, S. Thota, R. Singh, X. Xu, S. Issakani, T. Sun, W. Li, S. Holland, V. Markovtsov, Y. Jenkins, Y. Li, A. Pan, G. Uy, Y. Hitoshi, D. Sweeny, G. Park, R. Mandell, M. Standlee, L. Ste. Marie, P. Pine, D. Payan
217. Novel quinolone inhibitors of NS5B Polymerase. **B. P. Hart**, D. L. Wyles, K. Skuster
218. Synthesis and characterization of an anti-tubercular Benzothiazinone derivative. **W. Sweis, M. Bond**, A. Richter, P. Imming, N. Osei-Agyekum

Natural Products Posters

219. Evaluation of Aloe and Cactus for burn treatment by comparison of anti-oxidant properties and free radical inhibition. **A. Jones**
220. Improved isolation and purification of natural products by automated flash chromatography. **M. Wilcox, J. Bystron, R. Nguyen, M. Jacyno**

Physical Chemistry Posters

221. Combustion Products of Ethyl Tert-Butyl Ether using Synchrotron Photoionization. **R. Yao**, M. Ng, D. L. Osborn, C. A. Taatjes, G. Meloni
222. Investigation of methyl & ethyl formate combustion reactions by photoionization mass spectrometry. **B. Bryan**, D. L. Osborn, C. A. Taatjes, G. Meloni
223. Photocatalytic Properties of Oriented, {001} Faceted Anatase TiO₂ Films. **S. Y. Kabak**
224. Studies of non-Kekule heterocycles. **Z. Li**, D. J. Brook

Solar Chemistry Posters

225. Controlling photochemical electron transfer in rhodium-doped strontium titanate nanoparticles through surface modification. **B. A. Nail**

FRIDAY AFTERNOON

Bayshore West

Analytical Chemistry

Best Practices of HPLC in Pharmaceutical Analysis

Sponsored by the ACS Division of Analytical Chemistry

M. Dong, C. Venkatramani, *Organizers, Presiding*

- 1:30** 226. Best practice of ultra-high pressure liquid chromatography (UHPLC) in pharmaceutical analysis. **M. W. Dong**
- 2:00** 227. Utilizing Design of Experiments (DOE) for Method Robustness Optimization. **D. Prudhomme**
- 2:30** 228. Adaption of Retention Models to Allow Optimization of Peptide and Protein Separations. P. Petersson, J. Munch, M. Euerby, A. Vazhentsev, K. Kassam, **G. A. McGibbon**
- 3:00** Intermission.
- 3:30** 229. Genotoxic impurities analysis and control in pharmaceutical development. **A. Kumar**, K. Zhang, L. Wigman
- 4:00** 230. Mixed-Mode Chromatography and Its Uses in Pharmaceutical Analysis. **X. Liu**, C. Pohl
- 4:30** 231. Applications of two-dimensional liquid chromatography mass spectrometry in pharmaceutical analysis. **C. Venkatramani**

Sonoma

Computational Chemistry

Modern Computational Chemistry

Sponsored by Genentech and the ACS Division of Computers in Chemistry

J. Pitera, S. Boyer, *Organizers, Presiding*

- 1:30** 232. Interactive shape and pharmacophore similarity search enabled by GPUs. **J. Feng**
- 2:00** 233. Understanding the Electronic Structure of Cobalt-Dithiolene H₂ Evolution Catalysts. **J. A. Panetier**, C. S. Letko, T. D. Tilley, M. Head-Gordon
- 2:30** 234. Interactive *ab initio* molecular dynamics. **N. Luehr**, A. Jin, T. J. Martinez
- 3:00** Intermission.
- 3:30** 235. Predicting drug secondary pharmacology and mechanistic targets. **M. J. Keiser**, J. J. Irwin, B. L. Roth, B. K. Shoichet
- 4:00** 236. Proteus among proteins: A collection of short stories about conformational changes in GPCRs and Kinases. **D. Shukla**, V. S. Pande
- 4:30** 237. Automated Catalytic Site Detection. **J. P. Nilmeier**

Napa I

Entrepreneurship in Chemistry Models and Roles of Incubators

N. McClure, *Organizer*

B. Charpentier, *Organizer, Presiding*

- 1:30 238. Innovation, Innovation Ecosystems, and Incubators: Bridging the Innovation Gap. **M. Hudes**
- 2:00 239. Creating an Innovation Ecosystem. **K. Bortone**
- 2:30 240. Enabling Awesome-QB3's Life Science Incubators. **D. Crawford**
- 3:00 Intermission.
- 3:30 241. Bayer's new approaches to building connections for partnered research. **C. Haskell**
- 4:00 242. Creating a multidimensional, laboratory intensive, support system. **E. Amento**
- 4:30 Panel Discussion.

Camino Real

Environmental Chemistry

Hydraulic Fracturing in California: Environmental Issues with the Largest Shale Oil Formation in the in the United States

Sponsored by the ACS Division of Environmental Chemistry and the ACS Division of Geochemistry

E. Warren, D. Drogos, *Organizers, Presiding*

- 1:30 243. The Science and Politics of Hydraulic Fracturing in California. **M. Nechodom**
- 2:00 244. Advocating for safe oil and natural gas extraction policies; an overview of FracTracker as a mechanism for overcoming the barriers to scientific advocacy and community engagement. **K. J. Ferrar**, S. L. Malone, M. T. Kelso, B. Lenker
- 2:20 245. Hydraulic Fracking and The Battle Over Beneficial Water Use in California, The Next Phase of Fracking Litigation in California. **E. Hagström**, M. Brooks
- 2:40 246. How API's Shale Gas Standards and Best Practices support Sustainable Shale Gas Development. **D. Miller**
- 3:00 Intermission.
- 3:20 Panel Discussion.

Bayshore East

Food Chemistry

The Many Flavors of Food Chemistry

Sponsored by the ACS Division of Agricultural and Food Chemistry

S. Risch, *Organizer, Presiding*

- 1:30 247. How environmental research can lead to more sustainable food production systems. **J. N. Seiber**
- 2:00 248. Determination of Volatile Carbonyls in Olive Oil using Ultra Performance Liquid Chromatography

- and Gas Chromatography-Electron Ionization Mass Spectrometry. **H. Zhu**, S. Wang, C. O. Shoemaker
- 2:30 249.** Tissue concentrations of β -cryptoxanthin in Mongolian gerbils increase in parallel with its dietary concentration. M. R. La Frano, C. Zhu, **B. J. Burri**
- 3:00** Intermission.
- 3:30 250.** Meaningful Food Chemistry Innovation through Partnering. **T. McHugh**
- 4:00 251.** The physicochemical stability and in vitro bioaccessibility of beta-carotene in oil-in- water sodium caseinate emulsions. **J. Yi**, W. Yokoyama, F. Zhong
- 4:30** Concluding Remarks.

Napa III

Fuels Chemistry

Petroleum and Bio-Fuel Analysis

M. Cheng, D. Crider, *Organizers, Presiding*

- 1:30** Introductory Remarks.
- 1:35 252.** Hydrocarbon Renewable and Synthetic Diesel Fuel Blendstocks: Composition and Properties. **T. G. Smagala**, E. Christensen, **K. M. Christison**, R. E. Mohler, E. Gjersing, R. L. McCormick
- 2:00 253.** Rapid and Sensitive Determination of Biofuel Sugars by Ion Chromatography. **P. Bodsky**
- 2:25 254.** Cold Flow and Phase Transition of Transparent and Opaque Oils and Fuels. **G. Chui**
- 2:50** Discussion.
- 3:00** Intermission.
- 3:30 255.** Quantitation of Low Levels of FAME, Fatty Acid Methyl Esters, in Fuel and Waste Water. **T. Miao**, M. T. Cheng, J. D. Hudson, T. Smagala
- 3:55 256.** Elemental Analysis of Fuels Using Monochromatic X-Ray. **B. Bearner**
- 4:20 257.** Solid Phase Microextraction GCMS of Organics in Water. **J. D. Hudson**, M. T. Cheng
- 4:45 258.** Increased Use of Spectrographic Methods for Fuels Analysis. **D. Crider**

Ballroom F

Organic Chemistry

Cope Scholar Symposium in Honor of Professor Sarah Reisman: Advances in Total Synthesis

Sponsored by the ACS Division of Organic Chemistry

T. Maimone, *Organizer, Presiding*

- 1:30 259.** Chemical synthesis of secondary metabolites. **R. A. Shenvi**
- 2:15 260.** Synthesis of natural products with conformational chirality. **C. Beaudry**
- 3:00** Intermission.
- 3:30 261.** Recent progress in the synthesis of complex natural products. **J. Wood**
- 4:15 262.** Natural Product Synthesis: A Platform for Chemical Discovery. **S. E. Reisman**

Ballroom A

Pharmaceutical Science

Solid State Properties in Drug Development: Challenges for Drug Substances and Dosage Forms

Sponsored by Pion, Inc.

M. Brandl, *Organizer, Presiding*

- 1:30** 263. Understanding the Interplay of Physicochemical Properties in the Drug Development Process. K. Tsinman
- 2:15** 264. Pharmaceutical API properties modulation using co-crystals. **P. Andres**
- 3:00** Intermission.
- 3:30** 265. Solid-state challenges during drug development: Processing induced phase transformations and their impact on pharmaceutical product quality. **P. Chakravarty**
- 4:15** 266. Solubility & Dissolution Enhancement of Weakly Basic Compounds – Understanding Precipitation & Supersaturation. **J. Mole**

SATURDAY MORNING

Bayshore West

Analytical Chemistry: Mass Spectrometry

Qualitative Applications

Sponsored by the ACS Division of Analytical Chemistry

B. Fitch, *Organizer, Presiding*

- 8:30** 267. High resolution MS proves that the developmental cancer drug, RRx-001, alkylates the hemoglobin beta chain. **W. L. Fitch**, T. McLaughlin, M. Fens, J. Scicinski
- 9:00** 268. Application of High Resolution Mass Spectrometry in Structural Determination of Natural Products Present in Withania Somnifera Fruits. **J. Bolleddula**, B. Fitch, S. K. Vareed, M. Nair
- 9:30** 269. Spectral Accuracy on High Resolution Mass Spectrometers and Application to Elemental Composition Determination. **J. C. Erve**
- 10:00** Intermission.
- 10:30** 270. MS proteomic characterization of the protein interface of nanoparticles. R. Eigenheer, E. Castellanos-Jimenez, M. Nakamoto, A. Lampe, **K. Wheeler**
- 11:00** 271. Desorption electrospray ionization mass spectrometry imaging in biomedical research. **L. S. Eberlin**, R. N. Zare
- 11:30** 272. Using desorption electrospray ionization mass spectrometry to monitor ruthenium-catalyzed C-H functionalization. **C. Flender**, J. Roizen, E. McNeill, J. Du Bois, R. Zare

Napa I

Entrepreneurship in Chemistry

Sources of Funding for Entrepreneurs

Sponsored by the ACS Division of Business Development and Management

N. McClure, B. Charpentier, *Organizers*

S. Risch, *Presiding*

- 8:30** 273. Introduction to Funding Mechanisms. **D. Mosby**
- 9:00** 274. The Science of Crowdfunding. **E. Perlstein**
- 9:30** 275. How to find angel investors. **D. Mosby**
- 10:00** Intermission.
- 10:30** 276. SBIR Grants: What, Why, When and How. **A. Boggs**
- 11:00** 277. Securing venture capital funding for your company. **T. Saxton**
- 11:30** 278. Key to Unlock: Getting your Newco Venture Funded. **M. Powell**

Bayshore East

High School and Undergraduate Education

Sponsored by the ACS Division of Chemical Education

J. Medina, *Organizer*

H. Ungar, *Organizer, Presiding*

- 8:30** Introductory Remarks.
- 8:40** 279. Poeticizing Chemistry: Getting the general public interested in chemistry in a world of dirty power plants, pesticides, and chemical super-funds. **K. A. Eister**
- 9:00** 280. Peer-led Team learning: A method for narrowing students' achievement gap in chemistry courses at San Jose City College. **J. Parsons**, M. Adamczeski
- 9:20** 281. Peer-led team learning: study on positive impacts that peer leaders provide toward student success, retention and faculty professional development in STEM courses at a Two-Year Hispanic-Serving-Institution. **T. Zand**, **N. K. Hong**, M. Adamczeski
- 9:40** 282. Designing a comprehensive program management system to monitor the implementation of San Jose City College's peer-led team learning program. **R. R. Abd Latif**, **A. Zand**, M. Adamczeski
- 10:00** Intermission.
- 10:30** 283. Teaching first and second semester general chemistry in the hybrid environment at a community college. **T. Higgins**, R. Tse
- 10:50** 284. Organic chemistry in high school: A project in collaboration with a local community college. **F. Gandara-Guzman**, **J. C. Medina**
- 11:10** 285. ChemEx² at Stanford. **J. Lythcott**, G. Benz, K. Doyle
- 11:30** 286. Visualizing the Chemistry of Climate Change (VC3Chem): Interactive resources for teaching and learning chemistry through the rich context of climate science. **L. C. McKenzie**, M. Towns, A. N. Versprille, P. Mahaffy, M. M. Kirchhoff

Ballroom E

Natural Products Chemistry

New Technologies in Natural Products Discovery and Organic Chemistry Approaches to Natural Products Development

Sponsored by the ACS Division of Medicinal Chemistry

R. Linington, T. Amagata, *Organizers, Presiding*

- 8:30** 287. Strategies to investigate microbial natural products from deep-sea hydrothermal vents. **K. L. McPhail**, O. B. Vining, E. A. Mitchell, C. C. Thornburg, I. Wierzbicki, A. E. Sikora
- 9:05** 288. New analogs of 6-deoxyerythronolide B and erythromycin A produced by precursor directed biosynthesis and in vitro reconstitution of the 6-deoxyerythronolide synthase. **R. V. O'Brien**, M. Capece, B. Lowry, T. Robbins, C. Weng, D. E. Cane, V. S. Pande, J. D. Puglisi, C. Khosla
- 9:30** 289. Use of high content molecular networks to profile and quantitate marine cyanobacterial metabolomes. **J. R. Winnikoff**, E. Glukhov, J. Watrous, P. C. Dorrestein, W. H. Gerwick
- 9:45** 290. Application of overlapping techniques to profile a well-studied cyanobacterial strain affords a richer understanding of its metabolome. **P. D. Boudreau**, W. H. Gerwick, P. C. Dorrestein, L. Gerwick, E. A. Monroe, S. Desfor
- 10:00** Intermission.
- 10:30** 291. Walking in the woods with quantum chemistry - Studying natural product biosynthesis with computational chemistry. **D. J. Tantillo**
- 11:05** 292. Thiol-based probes for the discovery of electrophilic natural products from marine bacteria of the genus *Salinispora*. **C. C. Hughes**, D. Hahn
- 11:30** 293. Inhibitory mechanisms of tannins on the enzyme Tyrosinase. **A. Murray**, I. Kubo
- 11:45** 294. Mass Spectrometry Based Investigations of Cheese-Derived Natural Products. **L. M. Sanchez**, J. Button, B. Wolfe, R. Dutton, P. C. Dorrestein

Napa III

Organic Chemistry: Process Chemistry

Innovation in Process Chemistry

Sponsored by Biogen Idec, Infa, Inc, DavosPharma, Austin Chemical, Hovione and the Almac Group

M. Humora, *Organizer, Presiding*

- 8:30** 295. Process development of PI3K inhibitor GDC-0980. **T. Humphries**
- 9:00** 296. A novel, versatile, and scalable general short synthesis for most of prostanoids has been achieved in our labs. **G. Yiannikouros**
- 9:30** 297. Process optimization and scale up activities for preparation of an HCV NS5B polymerase inhibitor. **M. Masjedizadeh**
- 10:00** Intermission.
- 10:30** 298. ELND006: Process Chemistry Improvements to the Key Enantioselective Step. **M. S. Dappen**, J. J. Jagodzinski, D. A. Quincy, J. Wu, L. H. Latimer
- 11:00** 299. Early process research strategies: evaluating multiple routes with multiple suppliers for addressing a key feature of a target molecule. **M. Humora**
- 11:30** 300. From few grams to multi Tons. Some tips. **G. Bertolini**

Ballroom A

Physical Chemistry

Physical Chemistry for a Sustainable Future

Sponsored by the ACS Division of Physical Chemistry

O. Gessner, M. Ahmed, H. Bluhm, *Organizers, Presiding*

- 8:30** 301. Autoignition chemistry of oxygenated molecules: Linking biofuel development with advanced engine combustion. **C. A. Taatjes**
- 9:05** 302. Secondary organic aerosol phase and impacts on heterogeneous oxidation. **C. D. Cappa**, K. Kolesar, C. Ruehl, G. Buffaloe, K. R. Wilson
- 9:40** 303. Molecular Understanding of Self-Cleaning and Depolluting Photocatalytic Processes on Urban Surfaces. **H. Destailats**, M. Sleiman, O. Rosseler, N. Montesinos, D. Bikiel, M. Litter, H. Bluhm, M. Ahmed, M. Salmeron
- 10:15** Intermission.
- 10:45** 304. Dynamic perspective on optimizing charge transfer and transport in quantum dot sensitized metal oxide nanostructures for light energy conversion. **J. Z. Zhang**
- 11:20** 305. Sub-50 fs electron delocalization dynamics via resonant auger spectroscopy: The case of oriented organic semiconductor interfaces. **A. L. Ayzner**, D. Nordlund, D. L. Kim, Z. Bao, M. F. Toney
- 11:40** 306. Femtosecond x-ray spectroscopy studies of electronic excited states in coordination chemistry. **W. Zhang**, K. Gaffney

POSTER SESSIONS

Sponsored by an ACS Office of Undergraduate Affairs Grant

Ballroom C

N. McClure, *Organizers*

9:00 – 11:00 AM

Chemical Education Posters

307. Peer-Led Team Learning at San Jose City College: A student-faculty partnership to transform the learning environment and promote student success, retention, leadership, teamwork, creativity, and critical thinking in STEM courses. **N. K. Hong, J. Parsons, T. Zand**
308. San Jose City College student ACS chapter: Community outreach and promoting interest and involvement in chemistry. **S. Ngo, L. Trac**, M. Adamczeski
309. Chemistry Club: A place to learn, share, and grow. C. ACS Student Chapter, **J. J. Magpayo**, A. V. Carrazco, A. Kester, D. Marcks, A. Rummerfield, **B. F. Gherman**, C. Kellen-Yuen
310. An Undergraduate Research Program for Deaf and Hard-of-Hearing Students. **A. D. Ross**, S. B. Smith
311. Get involved with the ACS Division of Chemical Education. **C. Muzzi**
312. Anti-Science Legislation in California. **I. J. Wilk**

Undergraduate Research Posters

G. Muller, *Organizer*

9:00 - 11:00 AM

43. Synthesis, characterization and kinetics study of Mo₃ clusters with a μ_3 -O and μ_3 -CR trinuclear core. **A. J. Burton**, J. R. Houston
313. Is Conformational Flexibility Indicative of Compound Promiscuity?: A PDB Survey. **M. W. He**, Z. K. Sweeney, P. S. Lee
314. Characterization and Determination of Inhibitor Interaction with Streptomyces griseus Aminopeptidase. **L. Vang**, J. Moses, L. Ming
315. Using computational chemistry to design an optimal biomimetic ligand for the active site of the peptide deformylase enzyme. **K. Minnick**, B. F. Gherman
316. Investigating the folding dynamics of the RNA pseudoknot structural motif via massively parallel molecular dynamics. **A. Radcliffe**, S. Cao, B. Pham, P. La, M. Bakhom, R. Wang, E. Sorin
317. Synthesis of Lysyl Oxidase Inhibitors. **N. C. Oragwam, J. J. Spaeth, J. M. Thornton**, D. M. Solano
318. Nontargeted profiling of the metabolome of a clockless mutant of Arabidopsis thaliana overexpressing a master regulator in the circadian clock, CCA1, reveals the holistic metabolic impact of locking plants in morning mode. **Y. Leung**, K. Kaiser, B. Thines
319. Potential anti-tuberculosis components from an extract of a cellulose degrading marine bacterium. **S. Beasley**, J. Elkins, J. A. Trischman

320. Effects of Al-doping on the synthesis and performance of orthorhombic LiMnO₂. **Q. Zou**, X. Wu, S. Zhang, Y. He, X. Yang
321. Photochemical degradation of fluoranthene in aqueous solution. **O. Barashy**
322. Solvolyses in ionic liquid dual-solvent systems. **G. A. Amberchan**, S. Citrak, N. Gathondu, B. D. Kochly
323. Utilizing Diffuse Reflectance Infrared Fourier Transform (DRIFT) spectroscopy to probe the solid state diffusion of cations through zeolite materials. **E. Gorrie**, **K. Hernandez**, S. M. Crawford
324. Synthesis and characterization of zeolite beta (BEA) and titanosilicate beta (Ti-BEA) using titanium(IV) tetrafluoride. **H. E. Lacy**, A. S. Ichimura
325. Analysis of peptoid tertiary-like structure through fluorescence spectroscopy utilizing the environmentally sensitive 4-DMN fluorophore. **C. A. Holmes**, S. Hiew, A. A. Fuller
326. Understanding the cytotoxicity of transition-metal permalloy microdisks. **A. Karapetrova**, E. Rozhkova, V. Novosad, S. Ciocys, B. Flores, P. Gach
327. Synthesis of frustrated Lewis pairs based on ferrocenyl phosphines. **E. Askounis**, R. Kirss
328. New methodology toward the formation of highly substituted tetrahydropyranones. G. C. Tay, **C. Y. Huang**, S. D. Rychnovsky
329. Enhanced photo-Bergman cyclization of an electron rich mono-substituted arenediyne. **K. Velazquez**, J. D. Spence
330. Design and synthetic approach towards novel quinoxalenediynes. **S. A. Toscano**, J. D. Spence
331. Structural studies of water-soluble peptoids incorporating (*S*)-*N*-1-naphthylethyl side chains. **B. Yurash**, E. N. Schaumann, F. J. Seidl, A. A. Fuller
332. Montmorillonite for the synthesis of substituted oxindoles. **K. J. Darnell**, J. P. MacDonald, A. K. Franz
333. Isolating anti-tuberculosis metabolites produced by a unicellular marine bacterium. **Z. Cruz**, J. A. Trischman
334. Novel oxime ether surfactants: Physicochemical characterization. **R. Rowe**, K. Matasci, A. Rickelmann, H. Palandoken, J. Hagen
335. The hydroxyl effect on the fate of fulvene endoperoxide decompositions. **J. Basada**, I. Erden, F. Xu
336. Analysis of Conformational Influences Within (2*R*,3*R*)-butanediol. **Z. M. Estrada**, M. D. Drake
337. Synthesis of novel oxime ether surfactants. **A. T. Bellinghiere**, C. S. Muli, S. Touba, H. S. Ewan, A. M. Veitschegger, T. B. Smith, W. L. Pistel, J. Hagen, H. Palandoken
338. Identification and quantification of essential oils contained in hops (*Humulus lupulus*). **M. Fazio**, J. A. Trischman
339. Optical properties of chromophoric dissolved organic matter (CDOM) in Southern California salt marsh pore waters. **J. Bowen**
340. Mixed metal oxides for the desulfurization of jet fuel. **L. Y. Chong**, J. M. St. John, D. T. Tran, S. R. Oliver
341. Electrochemical characterization of first-row transition metal corroles for use as oxygen reduction catalysts. **B. McNicholas**, L. Rubin, H. Buckley, D. Gryko, J. Chlistunoff, J. Arnold
342. NMR spectroscopic monitoring of transesterification catalyzed by triazabicycloguanidine. **K. A. Gibson**, L. A. Anderson, A. K. Franz
343. Zinc-salophens as catalysts in electrohydrocyclization: Mechanism and stereoselectivity studies. **L. M. Littell**, J. A. Miranda
344. Green Catalytic Activation of H₂O₂ by Organochalcogenide Compounds. **K. M. Villines**, M. D. Drake
345. Hypervalence in Monoxides and Dioxides of Superalkali Clusters. **E. Cochran**, G. Meloni

- 346.** Imaging photoelectron photoion coincidence (i-PEPICO) investigation of furfural. **G. L. Laguisma**, M. Wooten, A. Bodi, G. Meloni
- 347.** Computational investigation of Stone-Wales isomerization in polycyclic aromatic hydrocarbons. **E. Brayfindley**, E. Irace, W. Karney, C. Castro
- 348.** Characterization of Isobutanol + OH Reaction at Room Temperature via Multiplexed Photoionization Mass Spectrometry. **J. Nelson**, Q. He, C. A. Taatjes, D. L. Osborn, G. Meloni

SATURDAY AFTERNOON

Bayshore West

Analytical Chemistry: Mass Spectrometry

Quantitative Applications

Sponsored by the ACS Division of Analytical Chemistry

B. Fitch, *Organizer, Presiding*

- 1:30** **349.** Nanodiamonds and taxon-specific biomarkers for mapping tight-shale sweet spots to optimize hydrocarbon production from fracking and for delineating mixed-source oil production. **J. M. Moldowan**, J. E. Dahl
- 2:15** **350.** Mass spectrometric methods for studies of nicotine metabolism and tobacco carcinogen exposure: Applications in clinical research. **P. Jacob**
- 3:00** Intermission.
- 3:30** **351.** New methods for solving fundamental challenges in Mass Spectrometry using DMS - Ion Mobility. **E. B. Jones**
- 4:00** **352.** Analysis of polar compounds using HPLC-MS. **J. J. Pesek**, M. T. Matyska
- 4:30** **353.** Automated Sample Prep, Ultra Fast Mass Spectrometry and Cloud Based Informatics Accelerate Modern Assay Development. **K. Krock**, J. Russel, C. Gillies, S. Kuzdzal

Napa I

Entrepreneurship in Chemistry

True Stories of Entrepreneurs

Sponsored by the ACS Division of Small Chemical Business

B. Charpentier, N. McClure, *Organizers*

J. Sabol, *Organizer, Presiding*

- 1:30** **354.** The Story of ETS Laboratories. **G. Burns**
- 2:00** **355.** Stories from a Chemist/Chemical Engineer of several Life Science startups. **G. T. Went**
- 2:30** **356.** Apexigen - a spin-out story. **M. Nevins**
- 3:00** Intermission.
- 3:30** **357.** Start-up challenges: The Story of Mango Materials. **M. Morse**

- 4:00 358. Is it worth starting your own company? **K. Paulvannan**
4:30 359. From Full Time Employment to Consulting - Strategies for Successful Transition. **D. E. Levy**

Bayshore East

High School and Undergraduate Education

Sponsored by the ACS Division of Chemical Education

J. Medina, *Organizer*

H. Ungar, *Organizer, Presiding*

- 1:30 Panel Discussion.
2:20 360. Anyone can do it...the democratization of the distribution of educational tools. **M. A. Bishop**
2:40 361. Drawing every electron and considering orbitals in chemical structures using Formalarrows, a stepping stone language to Lewis structures. **J. Newdoll**
3:00 Intermission.
3:30 362. Implementing a free online homework system for first semester general chemistry. **W. J. Miller**
3:50 363. Online Homework with Targeted Instructional Feedback Leads to Improved Student Learning Outcomes. **S. Cowley**

Ballroom E

Natural Products Chemistry

New Technologies in Natural Products Discovery and Organic Chemistry Approaches to Natural Products Development

Sponsored by the ACS Division of Medicinal Chemistry

R. Linington, T. Amagata, *Organizers, Presiding*

- 1:30 364. New chemical methods for the selective, on-resin N-methylation of cyclic peptides to generate compounds with improved membrane permeability. **S. A. Lokey**
2:05 365. Natural products from the human microbiota. **M. Donia**
2:30 366. Lead Diversification through a Prins-Driven Macrocyclization Strategy: Application to Functionalized B-Ring Bryostatins Analogues. **K. L. Billingsley**, P. A. Wender
2:45 367. Enantioselective synthesis of (*R*)-homocitric acid lactone-1,2-¹³C₂. **J. T. Moore**, N. V. Hanhan, M. E. Mahoney, S. P. Cramer, J. T. Shaw
3:00 Intermission.
3:30 368. Exploring Class III HDAC Inhibitors from Marine Sediment-Derived Actinomycetes Using an HDAC-Based Yeast Screening Method. **T. Amagata**
4:05 369. Alkaloids from *Microcos paniculata* L. with cytotoxic and non-competitive nicotinic receptor antagonistic activities: The transition from terrestrial plants to marine organisms. **P. C. Still**, B. Yi, T. F. González-Cestari, L. Pan, H. Chai, J. R. Fuchs, T. N. Ninh, D. D. Soejarto, B. J. Henderson, D. B. McKay, A. D. Kinghorn, P. Crews
4:30 370. Probing terpene enzymatic functionality and the inherent dynamical preferences in carbocation rearrangements. **R. P. Pemberton**, D. J. Tantillo

Ballroom A

Physical Chemistry

Physical Chemistry for a Sustainable Future

Sponsored by the ACS Division of Physical Chemistry

O. Gessner, M. Ahmed, H. Bluhm, *Organizers, Presiding*

- 1:30** 371. Probing energy transfer and structural evolution during ultrafast charge transfer processes. **M. Khalil**
- 2:05** 372. Revealing the electronic structure governing energy transfer through simulated spectroscopy. **D. Prendergast**, I. Zegkinoglou, M. Ragoussi, C. Pemmaraju, P. Johnson, D. Pickup, J. E. Ortega, G. de la Torre, F. Himspel
- 2:40** Intermission
- 3:30** 373. The Role of Fast Charge Carrier Dynamics at the Catalyst/Reactant Interface: Water Oxidation on Transition Metal Oxide Surfaces. **T. Cuk**
- 4:05** 374. Nonstoichiometric Oxides Surfaces Far from Equilibrium. **W. C. Chueh**

Ballroom F

Polymer Chemistry

Polymers at the Interface with Biology

J. Linhardt, J. Mabry, S. Heilshorn, *Organizers*

- 1:30** Introductory Remarks.
- 1:35** 375. Silicone elastomer modification using symmetric silicone macromers containing surface active pendants. **J. Goff**, B. Arkles, S. Sulaiman
- 2:00** 376. Elastin-like Polypeptide Hydrogels with Grafted VEGF-Mimetic Peptides for Enhanced Endothelial Cell Function. **L. Cai**, C. Dinh, S. Heilshorn
- 2:20** 377. Engineering 3D microenvironments for pancreatic islets. **C. Nyitray**, G. Faleo, R. Chang, Q. Tang, T. Desai
- 2:40** 378. Nanoscale control of endothelial cell-matrix interactions on electrospun Elastin-like protein scaffolds. **S. Mascharak**, P. Benitez, H. Heilshorn
- 3:00** 379. Sorting bacterium cells using cell-imprinted polymer thin films: from concept to applications. **K. Ren**, N. Banaei, R. N. Zare
- 3:20** Intermission.
- 3:40** 380. Tailored Polymers for Surface Coating of Silicone Devices. **J. G. Linhardt**, J. F. Kunzler, D. Shipp
- 4:05** 381. High-resolution imaging of dendrimers used in drug delivery via scanning probe microscopy. **S. L. Riechers**, L. Shi, C. J. Fleming, N. Yin, J. Luo, K. S. Lam, G. Liu
- 4:25** 382. Nanofibrous polypropylene films reduce myofibroblast differentiation through the TGF β pathway. **J. L. Allen**, J. Ryu, T. A. Desai
- 4:45** 383. 3-helix Micelles as a Drug Nanocarrier Platform: Cargo Loading and Biological Evaluation. **N. Dube**, T. Xu
- 5:05** 384. Dynamics of conformational transitions of a water-soluble poly(3-hexylthiophene) derivative by surfactant complexation. **S. Zhang**

Mendocino

Solar Chemistry

Lowcost Materials for Photovoltaics and Nanomaterials for Solar Energy

Sponsored by the ACS Division of Physical Chemistry

E. Menke, *Organizer, Presiding*

- 1:30 385.** Nanowire Solar Cells. **S. Brittman**, A. Wong, Y. Yoo, N. Dasgupta, D. Zhang, P. Yang
- 2:15 386.** Hybrid organic-inorganic core-shell nanowires toward high efficiency photovoltaics. **S. Zhang**
- 2:40 387.** Solution phase growth of Indium Phosphide nanowires and their application for photoelectrochemical energy conversion. **N. Kornienko**, P. Yang
- 3:00** Intermission.
- 3:30 388.** A direct thin-film path towards low-cost large-area III-V photovoltaics. **R. Kapadia**, Z. Yu, A. Javey
- 4:15 389.** Atomic layer deposited tunnel oxides stabilize silicon photoanodes for catalytic water splitting. **A. G. Scheuermann**, C. E. Chidsey, P. C. McIntyre
- 4:40 390.** Relationships between structure and alkaline stability of imidazolium cations for fuel cell membrane applications. **S. C. Price**, F. L. Beyer

Napa III

Women Chemists

Women Chemists at Various Stages of Their Careers

Sponsored by Chevron and the California Section Women Chemists Committee

E. Yamaguchi, *Organizer, Presiding*

- 1:30** Panel Introduction.
- 1:35 391.** Women chemists at various stages of their careers-A graduate student perspective. **L. Paw U**
- 1:50 392.** Learn how to learn. **Y. A. Zhu**
- 2:05 393.** Community colleges offer something beyond education to students. **I. Lazik**
- 2:20 394.** Advice from a non-traditional chemist. **J. Schunk**
- 2:35 395.** Women Chemists Panelist. **T. Lionel**
- 2:50** Panel Discussion.
- 3:00** Intermission.
- 3:30** Panel Discussion.
- 3:50** Assessment.