

WRM 2025

SATURDAY AFTERNOON

Chemical Biology and Biochemistry Undergraduate Session

Empire Room

Cosponsored by BIOL

L. C. Miller Conrad, M. R. Radlauer, V. Wheaton, *Organizers*
N. Wang, *Presiding*

2:15 006. Synthesis and characterization of *N*-alkylated amino acids for ribosomal translation. **N. Angelisanti**, I. Piper, M. Pressimone, A. Solivan, A. Schepartz

2:30 007. Identification of novel compounds targeting Mycobacterium tuberculosis replicative DNA polymerase using parallel docking and de novo molecule generation. **R. Rajasekar**, K. Singh, A. Eiichi

2:45 008. Bridging carbohydrate chemistry and AI: Calibrated NLP models for glycemic index assignment in nutritional epidemiology. **J. Ebbert**, S. Titensor, D. Della Corte

3:00 009. Synthesis, biological evaluation, and structure-activity relationship of diversified C-4 analogs of podophyllotoxin as tubulin inhibitors. **S. Somanı**, S. Yang, E. Njoo

3:15 010. Deciphering the acidic patch interactions of the human H2A.Z variant nucleosome. **N. Gimranov**, I. Franco, A. Skrajna

Chemical Biology and Biochemistry Undergraduate Session

Regency Ballroom 1

Cosponsored by BIOL

L. C. Miller Conrad, M. R. Radlauer, V. Wheaton, *Organizers*
E. Carroll, *Presiding*

2:15 001. Developing chemical tools to explore how site-specific ubiquitination drives protein destabilization and influences amyloid formation. **J.S. Hopham**, J. Villalpando, N. Dinh, E. Carroll

2:30 002. Education before execution: Rationally constraining AI for effective protein engineering. **W. Heaps**, D. Della Corte, C. Kubalek, M. Argyle, J. Ebbert

2:45 003. Decoding H3.3 variant nucleosome interactome. **E. Krebs**, N. Gimranov, I. Franco, A. Skrajna

3:00 004. Uncovering regulation of bifunctional NAD-kinase/NADP-phosphatase enzymes. **C. Geluz, H. Alkabbani**, V. Jayaraman, E.R. Greene

3:15 005. Investigating cellular metabolites and mutations driving p53 amyloid formation. **A. Bhattacharya**, T. Pham, J. Trinh, K.K. Airen, K. Hoang, E. Carroll

Inorganic and Materials Chemistry Undergraduate Session

Valley Room

Cosponsored by INOR

L. C. Miller Conrad, M. R. Radlauer, V. Wheaton, *Organizers*
A. A. Fuller, *Presiding*

2:15 015. Surface functionalized gold nanospheres in biologically relevant solutions using unique peptoids. **I. Matusich**, A.A. Fuller

2:30 016. Electrochemical oxidation of benzyl alcohol at the interface of gold and nickel electrocatalyst. **E.A. Guzman**, S.T. Spriggs, J. Qiu

2:45 017. Gallium-aluminum-based hydrogen production from water at ambient conditions: The path toward sustainable energy. **R. Waterson**, K. Lofgren, R. Ball, S.R. Oliver

3:00 018. Evaluating metal-organic framework-coated kombucha membranes for removal of wildfire contaminants in water. **E. Reznick**, M.C. So

3:15 019. Baking with salt: Exploring thermal dehydration and decomposition of hydrated cerium chloride. **R.C. Riley**, E.A. Espinoza, A. Chemey, D. McGlamery

3:30 020. Synergistic effect of artificial solid electrolyte interphase with lithophilic seed layers for homogenous lithium plating on lithium metal battery anodes. **R. Lam**, J. Lee, Y. Cui

Inorganic and Materials Chemistry Undergraduate Session

Crystal Room

Cosponsored by INOR

L. C. Miller Conrad, M. R. Radlauer, V. Wheaton, *Organizers*
D. J. Brook, *Presiding*

2:15 011. Design and synthesis of polymer-supported ruthenium-based catalysts for olefin cross metathesis. **D. Balcer, M. Woo, J. Amador Flores, S. Ceja, A. Acosta, M. Omar, S. Velasquez, T. Sapp, K. Huynh, M.R. Radlauer**

2:30 012. Where dendrites begin: Spatial and temporal solid electrolyte interphase evolution as a mechanism for non-uniform lithium plating. **S.D. Liu, J. Lee, C. Serrao, S. Shuchi, A. Cai, W. Zhang, Y. Cui**

2:45 013. Influence of excitation energy on semiconductor nanoparticle photocatalytic performance. **C. Peak, K. Lee, E. Aguilar, T. Harris, R. Lam, G. Vazquez, M. Enright**

3:00 014. Characterizing protein corona formation on functionalized aminofullerenes. **R. Gardner, R. An, C. Alford, S. Billow, M. Serda, K. Wheeler**

Organic Chemistry Undergraduate Session

Gold Room

Cosponsored by ORGN

L. C. Miller Conrad, M. R. Radlauer, V. Wheaton, *Organizers*
R. P. Abrams, *Presiding*

2:15 021. Reactivity-informed pharmacophore editing and biological evaluation of andrographolide and its a-ring analogs: Closing the loop on the oxetane. **R. Raval, G. Liu, A. Chyu, S. Xi, Y. Noh, E. Njoo**

2:30 022. Synthesis of a photoaffinity probe to identify antivirulence target protein in *Pseudomonas aeruginosa*. **K. Maiseyeva, L.C. Miller Conrad**

2:45 023. Structure-activity relationships of dioxo molybdenum(VI) complexes for deoxydehydration reactions. **N. Nickolov, O.M. Ogba**

3:00 024. Synthesis of quaternary arene-containing aldehydes by a zinc-mediated palladium-catalyzed α -arylation of silyl enol ethers. **A.C. Graf, J.E. Rosenow, A.B. Van Lare, L.R. Alleyne, B.J. Stokes**

3:15 025. Investigation into the electronics of para and meta-substituted phenolic esters for selective acylations of amines. **A. Chalasani, N. Sathish, C. Chen, E. Leo, E. Njoo**

3:30 026. Designing adjuvants to improve colistin treatment of *Pseudomonas aeruginosa*. **O. Kaka**

Physical and Computational Chemistry Undergraduate Session

Garden Room

Cosponsored by COMP and PHYS

M. R. Radlauer, V. Wheaton, *Organizers*
L. C. Miller Conrad, *Presiding*

2:15 032. Performance of range-separated local hybrid functionals for metalloenzyme reactions: Importance of the strong-correlation correction. **T.T. Nguyen, A. Kai, R. Grotjahn**

2:30 033. Empowering biomedical research with AI: Development of a drug-target interaction agent. **J. Abdelrazik**

2:45 034. First principles modeling of 2D conductive MOFs for Li-S battery applications. **N. Lopez, K. Kim, L. Wan, M.C. So**

3:00 035. Enhancing interpretability in nutritional epidemiology through Bayesian statistical approaches: Applications to dose-response synthesis and longitudinal modeling. **S. Titensor**

3:15 036. Cracking the carbon cage: Accurate predictions of fullerene isomerization energies with strong-correlation-corrected range-separated local hybrids. **A. Kai, R. Grotjahn**

3:30 554. Using Electrochemical Impedance Spectroscopy to evaluate semitransparent agrivoltaics. **J.C. Salazar, A. Vicini, K. Meehan, M.C. So**

Physical and Computational Chemistry Undergraduate Session

California Room

Cosponsored by COMP and PHYS

L. C. Miller Conrad, M. R. Radlauer, V. Wheaton, *Organizers*

N. E. Esker, *Presiding*

2:15 027. Enhanced biphenyl fluorescence caused by 1,6-Dichlorohexane on Al₂O₃. **A. Lopez**, C. Tobey, B.X. Moses, A.M. Nishimura

2:30 028. Comparative analysis of ground-state energies in pyrethrins and pyrethroids. K.D. Closser, **A.S. Bawa, N. Brockie**

2:45 029. Conformational dynamics and disorder of HPV-16 E6. **L. Kwak**, R. Garza

3:00 030. Interpretability in protein design machine learning programs: Decoding ProteinMPNN. **N. Mukkavilli**, M. McCully, D.A. Beck

3:15 031. Evaluating antimicrobial peptide potency and selectivity using supported lipid bilayers as predictive ex vivo models. **E. Tan**, S. Yang

Polymer Chemistry Undergraduate Session

Crystal Room

Cosponsored by PMSE and POLY

L. C. Miller Conrad, M. R. Radlauer, V. Wheaton, *Organizers*

D. J. Brook, *Presiding*

3:15 037. Multifunctional MOF-polymer composites: From materials design to catalytic detoxification of warfare agents. **A. Rahman**, N.M. Kharji, R. Smaldone

3:30 038. Catalyzing plastic degradation: Novel mechanochemistry treatment for sustainable plastic waste management. **J. Zhang**

Analytical Chemistry Undergraduate Session

Empire Room

Cosponsored by ANYL

L. C. Miller Conrad, M. R. Radlauer, V. Wheaton, *Organizers*

E. Carroll, *Presiding*

3:30 039. Label-free blocking immunoassay to evaluate anti-Adalimumab antibody activity in clinical samples. **J. Abdelrazik**, R.Y. Luo

SUNDAY MORNING

Advances in GPCR Drug Discovery and Therapeutic Applications

Crystal Room

Cosponsored by MEDI

I. S. Darwish, *Organizer*

E. Villemure, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 040. Discovery of small molecule rhodopsin correctors for the treatment of *RHO*-adRP using a high-throughput (HT) drug discovery platform approach. **J.R. Sanzone**, N. Abel, M. Albert, Z. Casey, H. Chan, L.Y. Chan, J. Enquist, E. Jones, S. Kim, S. Kosuri, N. Lubock, M. Mackenzie, N. Mohammed, N. Narasimman, C. Sinz, E. Thompson, R. Warneford-Thomson, T. Zheng

9:30 041. Efficient exploration of vast chemical spaces using a combinatorial docking approach. **A. Kyrylchuk**, I.S. Knight, J. Irwin, B. Shoichet

9:55 042. Discovery of Mu and kappa opioid receptor antagonists from a bespoke virtual library of tangible isoquinuclidines. **S. Vigneron**, S. Ohno, J. Braz, J. Kim, O. Kweon, C. Webb, C. Billesbølle, K. Srinivasan, K. Bhardwaj, J. Irwin, A. Manglik, A. Basbaum, J.A. Ellman, B. Shoichet

10:20 Intermission.

10:30 043. Large library docking identifies positive allosteric modulators of the calcium-sensing receptor. **F. Liu**

10:55 044. Enhanced glucose lowering and weight loss with dual biased agonism of the GLP-1 and GIP receptors. **S. Krishnan**

11:20 Concluding Remarks.

Best Practices to Inspire the Next Generation of Chemistry Students

California Room

Cosponsored by CHED
B. Bekker, *Organizer, Presiding*

9:00 045. Promoting higher-order learning within a flipped classroom: a randomized controlled trial experiment. **M.D. Casselman**

9:30 046. My journey in giving back through the graphical language of organic chemistry. **J.T. Njardarson**

10:00 047. Chemical Technology at Sacramento City College: Hands-on training for career and transfer success. **T.M. Atkins**

10:30 048. Progress towards establishing a useful undergraduate research group. **W.J. Miller**

11:00 049. Overcoming obstacles in course-based undergraduate research. **M. Sommerhalter**

11:30 050. Introducing team-based mentorship: a culture-building approach for research groups in STEMM (science, technology, engineering, math, and medicine). **M.T. Dulay, J.M. DeSimone**

Building Bridges through Alliances and Advances in Technology

Gold Room

Cosponsored by MPPG
A. M. Madonik, *Organizer*
H. Luo, M. P. Wu, *Organizers, Presiding*

9:00 Introductory Remarks.

9:05 051. Advancement of renewable energy in South Texas: Engineering nanostructured catalysts for sustainable solutions. **J.L. Liu**, S. Bashir

9:25 052. Criminal investigations at the U.S.-Mexico border: Nanoforensics advancing accuracy and efficiency with fingerprinting and blood-spatter analysis. **S. Bashir**, j. Lawrence, **J.L. Liu**

9:45 053. Regenerative manufacturing of high-performance pDCPD thermosets. **Y. Xia**, X. Luo, Y.M. Kim

10:05 054. Shape-memory-assisted self-healing of macroscopic punctures via high-energy-density periodic dynamic polymers with tunable actuation temperature. **Y. Shi**, Z. Bao

10:25 Intermission.

10:35 055. New class of dual Ion-electron polymer conductors for electrochemical energy storage. **G. Liu**

10:55 056. Trash to Treasure: upgrading of organic and plastic waste streams through chemical catalysis and biological conversion. **N. Sun**

11:15 057. Enhancing water and oxygen transport through electrode engineering for AEM water electrolyzers. **x. peng**

11:35 058. Converting CO₂ into valuable chemicals by artificial photosynthesis. **Y. Shan**, P. Yang

11:55 Concluding Remarks.

Chemical Biology Approaches in Drug Discovery

Empire Room

Cosponsored by BIOL
E. Villemure, *Organizer*
D. Nomura, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 059. Chemical strategies to rewire immune signaling. **Z. Zhang**

9:45 060. Chemical tools to modulate the “undruggable” human proteome. **L. Dassama**

10:25 Intermission.

10:35 061. Engineering modular biologics for selective rewiring of inflammatory signals. **R. Saxton**

11:15 062. Reimagining druggability using chemoproteomic platforms. **D. Nomura**

11:55 Concluding Remarks.

Empowering Women in Organic Chemistry (EWOC) Research Symposium

Regency Ballroom 1

Cosponsored by MEDI and ORGN

J. Gustafson, E. Villemure, *Organizers*

R. P. Abrams, L. C. Miller Conrad, *Organizers, Presiding*

9:00 Introductory Remarks.

9:05 063. Selective C-F, S-F, and C-S activation of aryl fluorides and aryl sulfonyl fluorides using nickel catalysts. **S.E. Stieber**

9:30 064. Photoredox properties of tetra-alkyl core substituted phenazine photoredox catalysts and their performance in organocatalyzed atom transfer radical polymerization. **A.M. Wolff**, G. Miyake, R.S. Paton, S.A. Lopez, A. Sau, T. Clark, L. Gomes, K. Puffer, N.H. Damrauer, Y. Lamb, B. Portela

9:55 065. Identification of novel coronavirus main protease inhibitors targeting broad spectrum coverage for pandemic preparedness. **K. Garland**

10:20 066. Exploring the unique properties and reactivities of the pentafluorosulfanyl group, its congeners, and reagents. **A. Ragan**

10:45 Intermission.

10:55 067. The evolution of drug discovery for breast cancer. **X. Wang**

11:55 Concluding Remarks.

Memorial Symposium in Honor of John I. Brauman

Garden Room

Cosponsored by PHYS

A. M. Madonik, N. L. McClure, *Organizers, Presiding*

9:00 Introductory Remarks.

9:25 068. Pseudo-Elementary steps: A key concept in elucidating the kinetics and mechanisms of complex systems such as nanoparticle synthesis and assembly. **R.G. Finke**

10:10 Intermission.

10:20 069. Optoelectronic nose: An adventure in molecular recognition. **K.S. Suslick**

11:05 070. Energy transfer and the oxygen-17 anomaly in ozone. **K.A. Boering**

11:50 Concluding Remarks.

Memorial Symposium in Honor of Robert H. Grubbs (Sponsored by Craig Hawker / BioPACIFIC MIP)

Club Regent

Cosponsored by MPPG

J. S. Cannon, K. M. Engle, V. M. Marx, G. Miyake, H. Nelson, D. O'Leary, V. A. Piunova, F. Toste, R. Weitekamp, *Organizers*
C. M. Bates, R. B. Grubbs, *Organizers, Presiding*

9:00 Introductory Remarks.

9:15 071. Electrocatalysis for energy storage. **R.M. Waymouth**, J. Dressel, K.H. Lui, T.W. Funk

9:40 072. Nucleophilic substitution reactions: A radical alternative to S_N1 and S_N2 reactions.
G.C. Fu

10:05 073. Cooperative reactions at late-metal silyl and silylene complexes. **M.T. Whited**

10:30 Intermission.

10:45 074. Au(III) oxidative addition complexes for complex protein-polymer conjugate synthesis. **H.D. Maynard**

11:10 075. Living the Grubbs' entrepreneurial spirit. **J.M. Berlin**

11:35 076. Atom swap in sp³-rich scaffolds. **G. Dong**

Precision Chemistry at all Length-Scales and Dimensions

Valley Room

Cosponsored by INOR

A. M. Spokoyny, *Organizer, Presiding*

9:00 077. Metal-mediated ring fusions in scalable syntheses of conjugated nanocarbons. **T. Tilley**

9:30 078. Precision control of supramolecular glycan architectures for biomolecular recognition. **J. Stauber**

10:00 079. Amphidynamic crystals with ultrafast molecular rotors. **M.A. Garcia-Garibay**, J. Shan

10:30 080. Precise synthesis of open shell transition metal nanoclusters. **T.W. Hayton**

11:00 081. Cluster chemistry one metal atom at a time. M. Osei, H. Xu, N. La, A. Valles, V. Espinoza Castro, **R. Hernandez Sanchez**

11:30 082. Organometallic strategies for precise modification of biomolecules. **A.M. Spokoyny**

Bridging Chemistry and Biology: Covalent Inhibition in Drug Discovery

Crystal Room

Cosponsored by MEDI

E. Villemure, *Organizer*

J. Blair, D. Lapointe, *Organizers, Presiding*

11:30 Introductory Remarks.

11:35 083. Discovery of a picolinamide series of covalent inhibitors of Trypanosoma cruzi protein kinase CLK1 for the treatment of Chagas Disease. **O. Rene**

SUNDAY AFTERNOON

Building Bridges Undergraduate Posters

Regency Ballroom 2

Cosponsored by MPPG

L. C. Miller Conrad, M. R. Radlauer, V. Wheaton, *Organizers*

12:00 - 1:30

084. Compositional Study of Leaves of Toyon, a Native plant to California, Oregon, and the Baja California Peninsula. **Z.R. Jensen**, B.A. Rayson, L.J. Naaktgeboren, Y. Hu

085. Antioxidant Activity and Heavy Metal Uptake Capability Study of White Sage. K.M. Rasmussen, R. Solorio, A.J. Benson, A. Minium, K. Duran, J. Obligar, M. Nunley, **A.G. DeHaro**, B. Koo, Y. Hu

086. Hydrogen Atom Transfer (HAT) or Electron Transfer (ET)? An Undergraduate Mechanism Investigation of the Reduction Reaction of 2,2-Diphenyl-1-picrylhydrazyl (DPPH) in n-Butanol and t-Butanol. **L.J. Naaktgeboren**, B.A. Rayson, Z.R. Jensen, E.B. Torres, A.G. Frala, Y. Hu

087. Towards the synthesis of albicidin. **S. Gonzalez**, S. Heller

088. The first total synthesis of Lorneic Acid F and H. **M. Rios**, C. Lucero

089. Mechanistic studies and reactivity in rhodium Bis(phosphinoalkynyl) pincer ligands. **E. Norton**, M. Deegan, G.P. Yap

090. Investigating the effect of post-translational modifications on Cu²⁺ binding on the antimicrobial peptide PG-KI. **A. Batchelor**

091. Synthesis of homotryptamine derivatives as potential serotonergic antidepressants. **S. Verma**, **A. Marks**, A. Chabroux, R. Iyer, D.E. Olson, C. Arpin

092. Enhancing PHA production in *Pseudomonas putida* via targeted genetic modification. **V. Arreola**, K. Lee, F. Zhang

093. Mild elimination of alcohols to alkenes using sulfonylimidazoles and DBU. **A.R. Smith**, S. Heller

094. Determining the pH profile of DesD. **S. Ivanez**

095. Recovery and Analysis of desferrioxamines via HPLC and LC-MS. **L. Larson**

096. Lighting the path to sustainable pest control: fluorescent chalcones for soil parasite studies. **M. Kiernan, G. Hamilton, A. Calderon-Urrea, C. Arpin**

097. Exploring acetaldehyde photodissociation pathways using interpretable AI models. J.H. Kim, **H. Dang, H. Joshi, D.H. Vyas, A. Wong, S. Sridharan, J.D. Spitzer, E. Bojeh, D. Andreasyan, G. Grazioli**

098. Simulated mechanical testing of amyloid fibrils via large-scale explicit solvent molecular dynamics. **J. Gadingan, A. Ingwerson, B. Rusconi, H. Dang, A. Youngquist, A. Pham, J. Vinod, B. Wong, D. Andreasyan, A. Iyer, G. Grazioli**

099. The efficiency of antibiotic adjuvants on *Pseudomonas aeruginosa*. L.C. Miller Conrad, **R. Shamoon**

100. Evaluating colistin adjuvants in *Pseudomonas aeruginosa*. **R. Rajesh**

101. Molecular mechanisms and energetic characterization of peptide-mediated reversible nanoparticle aggregation via atomistic molecular dynamics. **M. Mullooly, R. Ramji, K.D. Closser, T. Pascal, J.V. Jokerst**

102. Quantification of oligosaccharides from bovine Alpha-Acid Glycoprotein. **N. Diep, A. Franz**

103. Binding study of FslA. **U. Ganbaatar**

104. Applications of electron microscopy in immunotherapy: Visualizing nanoparticle delivery and immune responses. **Z. Seedat**

105. Structural studies of NIS synthetase FslA. **S. Ojha**

106. Establishing a catalytic residue in the *R351Q* variant of FslA, an NIS synthetase. **H. Seyedebrahimnazad**

107. Engineering hybrid surfactants derived from an intrinsically disordered protein sequence. **R. Koparde, P. Whitworth, P. Pratakshya, M.B. Francis**

108. Water oxidation by a Cobalt(II) compound with redox active ligands. **S. Almutairi, M. Escudero, T. Mann, D.J. Brook**

109. Design and synthesis of calamitic promesogenic amine capping ligands for CdSe/ZnS quantum dots. **A.B. Van Lare, J.Q. Vu, P.S. Morihara, N.J. Licauco, B.J. Stokes**

110. Synthesis and reactivity of a bis-bidentate N-heterocyclic carbene nickel complex with a phenyl-substituted backbone. **A. Bryant, A. Alvarez, C. Stieber**

111. Investigating how endogenous human metabolites affect p53 thermodynamic stability. **T. Pham, J. Trinh**, A. Bhattacharya, K.K. Airen, K. Hoang, N. Nguyen, E. Carroll

112. Chiral quaternary aldehyde synthesis by the palladium-catalyzed α -arylation of unsymmetrical silyl enol ethers. **J.E. Rosenow**, A.C. Graf, A.B. Van Lare, B.J. Stokes

113. Synthesis of α -substituted β -nitroalkene scaffolds for use in organocatalyzed reactions. **L.B. Garman**, F.K. Kekessie, J.A. Pigza

114. Determining how chemical analogs of pyruvic acid modulate p53 conformation function. **K.K. Airen**, A. Alagtash, A. Bhattacharya, T. Pham, J. Trinh, K. Hoang, L. Cobb, S. Crudo, V. Ta, T. Vaddiraj, A. Rios, E. Carroll

115. How's it binding? Investigating the binding specificity of DesD in the presence of multiple different cofactors. **A. Bacconi**

116. Understanding the effects of phosphorylation on the binding properties between motif A and SIRT1. **S. Bennett**, C. Tannous, **Q. Nguyen Minh Luu**, N. Wang

117. Heteroatomic and substituent effects on [3,3] sigmatropic rearrangements: Theoretical mechanistic and reactivity study. **K. Share**, J.S. Cannon

118. Synthesis of N-heterocyclic carbene nickel(0) complexes for C-F bond activation of octafluoronaphthalene. **E. Pham**, M. Bravo, C. Stieber

119. Methods for PLA surface smoothing: A comparison between vapor and immersion smoothing with organic solvents. **R. Sidhu**, N. Fanopoulos, J. Hout

120. Recovery and identification of desferrioxamine intermediates. **D. Olsson**

121. Non-polar bond activation via bimetallic Salen-rhenium complexes containing appended nitrogen groups. **D.A. Seymour**, M. Deegan, L. Miller, G.P. Yap

122. Development of kinetic assay for the FSLA enzyme involved in siderophore biosynthesis in *Francisella tularensis*. **D.C. Pat-Onuoha**

123. Insights into the mechanism of the copper chaperone for copper-zinc superoxide dismutase. **M. Lafon**, L. Kane-Barnese

124. Chemical preparation and reactivity of acyl phosphates under prebiotic conditions. **V. Ta, S. Crudo, T. Vaddiraj**, A. Rios

125. Sustained linalool releasing polyvinyl alcohol/Gellam gum hydrogel for infectious burn wounds: Characterized *in-vitro*. **F. Rashid, Q. Faheem**, M. Ikram

126. Understanding drug-induced and hormone-mediated cardiac risks through computational analysis of hERG and CaV1.2-ligand interactions. **S. Brunkow**

127. Characterizing the sequence determinants of a novel interaction between the *E. coli* molecular chaperones DnaK and CbpA. **S. Virgen Ordaz**, Q. Nguyen, S. Chin, V. Chau, D. Quach, A. Mateo, S. Ramirez, T.P. Nguyen, T. Arhar

128. Characterizing the stimulation of DnaK ATPase activity by CbpA: Insights into CbpA's interactions with DnaK in *E.coli*. **A. Mateo, D. Quach, S. Ramirez, T.P. Nguyen**, S. Virgen Ordaz, Q. Nguyen, S. Chin, V. Chau, T. Arhar

129. Optimizing the mono-mesylation of polyethylene glycol. **E. Jaminet**, S. Swartz, B. Grosscup, P. Reist, S. Ward

130. Reactive molecular dynamics study of water droplet boiling on nanoparticle-functionalized surfaces. **M. Vazquez**, L. Hong

131. Carbodicarbenes as hydride donor catalysts in heteroallene reductions. **M.W. Schernikau**, O.M. Ogbu

132. Reusable oxidizing agent, polymer-supported IBX. **L. Andersen**, R. Mouawad, B. Pelletier

133. Understanding oligomeric states of decoration (Dec) protein via integration of computational modeling and experimental analysis. **A. Vergara, I. Lopez**, R. Fukazawa, I. Heu, P. Tare, M. Zepeda-Esquivel, M. Buendia, M. Zhao, K. Khakh, G. Terashi, D. Kihara, M. Uchida

134. Optimizing polydopamine coating on cellulose nanocrystals in biopolymer composites for increased biocompatibility. **I.Z. Dumitriu**, Z. Wang, M.B. Foston

135. Toward clinically viable HyperCEST MRI agents: trisresorcinarene derivatives for targeted bioconjugation. **C. Hasselbrink**, E. Pourshah, E. Flishwick, K. Morris

136. Mutational analyses of nucleotide-binding domains of a bacterial methionine ABC importer. **E. Uohara**, M. Gardner, B. Quinn, C. Foster, J. Yang

137. Role of ligand rotation in ISC rates of two coordinate complexes. **R. Orozco**, T. Nattikallungal, S.E. Bradforth, M. Di Nero, M.E. Thompson

138. Antiviral & bactericidal activity of silver lipoate clusters. **C. Shabani, L. Astoyan, R. Ohanyan, R. Yakubov**, E. Apelian, S. Iskandaryan, E. Avedian

139. Enhanced naphthalene fluorescence via 1,6-dichlorohexane induced morphological reordering. **C. Tobey**, A. Lopez, B. Moses, A.M. Nishimura

140. Beam energy calibrations for FN tandem accelerator using nuclear monitor reactions. **J.C. Wilkes**, J. Shusterman, M. Anastasiou, J. Wilkinson, N.E. Esker

141. Synthesis of selective HDAC6 inhibitors: HPOB. **Z. Cervantes, E. Oliva, C. Wilcox, L.C. Bradford**

142. Targeting bacterial biofilm formation: Investigating novel small molecule inhibitors of curli and phosphoethanolamine cellulose. **A. Zhou**

143. Determining n and k values for biphenyl and naphthalene using Avrami program. **B.X. Moses**

144. Assessing feasibility of tape casting for nuclear targetry. **S. Malmhall, K.J. Maxwell, A.M. Hastings, J. Shusterman**

145. Empowering undergraduate students in chemistry through inquiry-driven molecular simulations. **R. Garcia, I. Patil, O. Sanchez, L. Hwang, T. Meyerott, J. Santner, L. Hong**

146. Simulating structure and diffusivity in the inorganic components of the cathode electrolyte interface. **E. Liu, W. Jeong, L. Wan, N. Adelstein**

147. Cobalt 2,5-diaminobenzene 1,4-dithiolate (CoDABDT) electrocatalysts in the hydrogen evolution reaction (HER). A.T. Nguyen, **V. Chan, M. Kawakami, S. Marinescu**

148. Calibrating beam energy of FN tandem accelerator using monitor reactions across multi-foil stacks. J. Ngo, **S.J. Tumey, M. Anastasiou, J. Shusterman, J. Wilkinson, N.E. Esker**

149. Synthesizing three unique amino acid linkers to incorporate into anti-viral glycodendrimers. **L. Lawrence, D. Zamudio, K.D. McReynolds**

150. Development of nickel-catalyzed cross-coupling reactions of oxetanes. **M. Polino**

Best Practices to Inspire the Next Generation of Chemistry Students

California Room

Cosponsored by CHED
B. Bekker, *Organizer, Presiding*

2:30 151. Specifications grading in introductory and general chemistry. **B.K. Tenn**

3:00 152. Chemistry self-efficacy (4-Yr combined data 2021 to 2024) and ACS placement exam means and DFWI rates (2014 to 2024) in general chemistry I at Fresno Pacific University, a small private Hispanic serving institution in Central Valley of California. **M. Cheung**

3:30 153. Creative conversion to atoms-first approach in general chemistry curriculum: Engaging lecture and engaging laboratory. **T.M. Owen, R. Edwards**

4:00 154. Critical raw materials as a socio-scientific issue in chemistry education. **O. Gulacar, I. Eilks, J. Butow**

4:30 155. REAL chem: A data-driven catalyst for improving learning. **M. Blaser**

5:00 156. OER AI tools in chemistry education. **T.J. Lund**

Bridging Chemistry and Biology: Covalent Inhibition in Drug Discovery

Crystal Room

Cosponsored by MEDI
E. Villemure, *Organizer*
J. Blair, D. Lapointe, *Organizers, Presiding*

2:30 157. Bridging distal binding sites on the same target with bitopic inhibitors. **K. Lou, J.W. Stevenson, K.M. Shokat**

3:00 158. Discovery of a brain-penetrant covalent inhibitor of KRAS G12C. **M. Landry**

3:30 159. Harnessing chemical reactivity to target driver oncogenes. **Z. Zhang**

4:00 Concluding Remarks.

Charting a New Course Through Project SEED

Empire Room

Cosponsored by CPS
A. M. Madonik, *Organizer*
A. Merg, E. S. Yamaguchi, *Organizers, Presiding*

2:30 Introductory Remarks (Part One).

2:35 160. Organizing the CA section SEED program. **E.S. Yamaguchi**

2:45 161. Project SEED, a win-win-win situation. **M.T. Cheng**

2:55 162. Enhancing student lab experience through Project SEED. **J. Brewer**

3:05 163. Cultivating STEM communication through Project SEED. **E. Li**

3:15 164. The roles of the chemistry department at UOP in serving locals. **Q. Zhao**

3:25 165. Teaching high school students about biochemistry in the ACS SEED program at the University of Merced, in California's Central Valley. **P.J. Liwang**

3:35 166. ACS Project SEED at UC Merced: Transforming the lives of students in merced county. **A. Merg**

3:45 Intermission.

4:00 Introductory Remarks (Part Two).

4:05 167. Understanding carbon transformation from whole orchard recycling. **J. Ergo**

4:17 168. Application of matrix-assisted laser desorption/ionization time-of-flight mass spectrometry for hair identification of various species. **Z. Anwar, M. Lin, A. Franz**

4:29 169. Investigating the health effects of agricultural chemicals in a mouse model. **I.C. Sánchez, J. Manilay**

4:41 170. Project SEED research - two case studies: (I) the role the nBAF complex plays in transcription of rapid immediate early genes (rIEGs) and (II) the effects of pyraclostrobin on hematopoietic cells. **L. Valenzuela, J. Manilay, R. Saha**

4:53 171. Analyzing high-dimensional vibrational quantum wavefunctions of the Zundel ion. **E. Aguilar, W. Kern, H.R. Larsson**

5:05 172. The role of IDR's, in nBAF activity-induced neuronal gene transcription. **M. Rivera-Reyes, C. Karen, R. Saha**

5:17 Concluding Remarks.

Chemistry of Agriculture

Gold Room

Cosponsored by AGFD and AGRO

J. M. Van Emon, S. Walse, *Organizers, Presiding*

2:30 Introductory Remarks.

2:35 173. Considerations and progress in developing Multiresidue analysis methods for the residues of postharvest and preplant fumigants. **W.A. Hall**, S. Walse, S.M. Corbett, K. Stiglmeier

2:58 174. Key chemical considerations for commercial-scale wet scrubbing of sulfuryl fluoride. **J. Ramirez-Hernandez**, S.S. Walse

3:21 175. Elimination of sulfuryl fluoride fumigant emissions by electrochemically generated reagents. **C. Napier**, H. Badr, T.F. Jaramillo, S.S. Walse, W. Mitch

3:44 176. Super Q alternatives for trapping plant and insect semiochemicals. **B.A. Pinney**, S.S. Walse

4:07 Intermission.

4:21 177. Abiotic release of mealybug sex pheromones. **K.E. Thiesen**, S.S. Walse

4:44 178. Cold storage phosphine applications for control of Tephritid fruit flies. **G. Gidiglo**, S.S. Walse

5:07 179. High-dose gaseous ozone for pest control in table grapes. **E.R. Rivera**, S.S. Walse

Expanding Best Practices in Laboratory Safety

Valley Room

Cosponsored by CHAS, CWD and ORGN

D. R. Kuespert, *Organizer*

D. Decker, *Organizer, Presiding*

2:30 Introductory Remarks.

2:35 180. Psychological safety is lab safety: Using RAMP to assess DEIR hazards. **D. Decker**

3:00 181. Chemical safety information resources to help you RAMP up before working in the lab. **G. Baysinger**

3:25 182. How risk assessment mitigated an explosion. **J. Reidy**

3:50 183. Can the disabled pursue, preach and practice STEM: An SCC member's response and efforts to propagate the ACS vision/mission. **K.M. Kallury**

4:15 184. Making chemistry accessible to individuals with disabilities. **K. Vasquez**

4:40 185. Making chemistry accessible to all: Recognizing and advancing the contributions of scientists with disabilities through the work of the ACS Committee on chemists with disabilities. **M.T. Dulay**

5:05 186. Strategies for accessibility. **B. Blaser**

Innovative Approaches in Bioanalytical Chemistry

Garden Room

Cosponsored by ANYL

E. Hecht, E. Jamalzade, *Organizers, Presiding*

2:30 Introductory Remarks.

2:35 187. Methods for high throughput discovery of fluoroprobes that recognize amyloid fibril polymorphs. **E. Carroll**, J.E. Gestwicki

3:01 188. SYMPHONY: Accelerating a cellular-level understanding of coral-symbiosis breakdown using AI. **I. Rossi**, E. Meier, D.N. Safarti, F.G. Zamora, s. fung, P. Cleves, A.E. Herr

3:18 189. Comparison of H-ELISA and stem loop RT-qPCR for siRNA quantification. **S. Miao**

3:44 190. Quantitative phosphorus-31 (^{31}P) NMR spectroscopy for quality assessment of RNA-based therapeutics: Applications, advantages, and limitations. **J.G. Napolitano**

4:10 Intermission.

4:20 191. Analytical strategies for impurity detection and quantification in therapeutic bispecific antibodies. **X. Niu**

4:46 192. ProteoParcel: Multimodal single-cell proteomics via microfluidically integrated immunoblotting and LC-MS. **M. Overton**, C. DeRoy, E. Wang, a. lennon, N. Goldhammer, j. rosenbluth, r. mcclure, A.E. Herr

5:03 193. Towards cracking the glycan code: Elucidating glycosylation pathways using mass spectrometry. **M. Alvarez**, S. Chen, Y. Xie, Q. Zhou, y. sheng, S.J. Grijaldo-Alvarez, A. Oloumi, R. Schindler, R. Gogte, A. Adeyemi, K. Pakulski, Y. Bouchibti, C.B. Lebrilla

5:29 Concluding Remarks.

Memorial Symposium in Honor of Robert H. Grubbs (Sponsored by Craig Hawker / BioPACIFIC MIP)

Club Regent

Cosponsored by MPPG

C. M. Bates, J. S. Cannon, R. B. Grubbs, V. M. Marx, G. Miyake, H. Nelson, D. O'Leary, V. A. Piunova, R. Weitekamp, *Organizers*
K. M. Engle, F. Toste, *Organizers, Presiding*

2:30 Introductory Remarks.

2:45 194. From catalyst to commerce: Commercializing specialty materials produced via ring opening metathesis polymerization. **M. Ryan**

3:10 195. Mechanisms for organometallic reactions with large isotope effects. **M. Bowring**, S. Ellis, M. Nguyen, T. Denton, E. Feldman, M. Surbeck

3:35 196. Electrification and decarbonization of chemical synthesis. **K. Manthiram**

4:00 Intermission.

4:15 197. Overturning E2 stereoselectivity: A new route to Z-selective C–H functionalization via paired electrolysis. **Z.K. Wickens**

4:40 198. Ring expansion metathesis polymerization (REMP): Catalysts, polymers, and applications. **A.S. Veige**

5:05 199. Reactivity of carbone as metal-free catalysts in hydroboration reactions. **O.M. Ogba**

Synthetically Modified Nucleosides and Nucleic Acids

Regency Ballroom 1

Cosponsored by ORGN

J. Gustafson, *Organizer*

B. W. Purse, *Organizer, Presiding*

2:30 200. Discovery of GS-7682, a novel 4'-cyano-modified C-nucleoside prodrug with broad activity against pneumo- and picornaviruses and efficacy in RSV-infected African green monkeys. **M.O. Clarke**, D.S. Siegel, J. Pitts, M.S. Vermillion, K. Ishida, B. Chun, G. Chin, B. Goyal, H. Yang, C. Palmiotti, A. Vijjapurapu, T. Wang, X. Zhao, Y. Xu, G. Lee, B. Marchand, M. Seung, A. Nayak, A. Tomkinson, N. Kadrichu, J.K. Perry, J.P. Bilello, P. Kuehl, R. Subramanian, T. Cihlar, R.L. Mackman, D. Byun, G. Birkus, K. Karki, M. Perron, E.M. Doerffler, O. Barauskas, J. Feng, H. Irshad

3:10 201. Discovery and mechanistic study of highly specific steroid aptamers using a high-throughput array platform. **H. Fujita**, Y. Gidi, L. Wan, L. Hein, T. Soh

3:30 202. Design and synthesis of fluorescent nucleoside analogues for metabolic labeling of RNA in live cells. **A. Shalamberidze**, H. Pearce, A.L. Cooksy, R. Kleiner, B.W. Purse

3:50 Intermission.

4:05 204. In vitro selection of an RNA analog bearing unnatural phosphoramidate linkages. **L. Zhou**

4:25 205. The unprecedented reactivity of RNA in water. **E.T. Kool**

The Art and Science of Brewing Beer

Crystal Room

Cosponsored by AGFD

G. Fox, A. M. Madonik, *Organizers, Presiding*

4:15 Introductory Remarks.

4:20 206. The chemistry of beer. **G. Fox**

5:00 207. Assessing method viability for providing insight into the overall “health” of hoppy beverages: Future directions for optimizing antioxidant stability. **E. Weintraut**, G. Fox

5:25 Concluding Remarks.

SUNDAY EVENING

Building Bridges Undergraduate Posters

Regency Ballroom 2

Cosponsored by MPPG

L. C. Miller Conrad, M. R. Radlauer, V. Wheaton, *Organizers*

5:30 - 7:00

208. Chemistry of the Mexican fruit fly. **T. Issaian**, S.S. Walse

209. Methyl bromide sorption by bulk cut peony stems. **S.M. Corbett**, S.S. Walse

210. Hooked! - Molecular Dynamics of Type IV Pili and ecDNA. E. Amponsah, **A. Robinson**, L. Rakesh

211. Mixed-valence thiophene/verdazyl systems. **Y. Pham**, J. Vo, S. Crudo, Y. Mufti, D.J. Brook

212. Investigation of an iron-verdazyl coordination compound. **E. Schweizer**, **D. Hoang**, **W. Lee**, **L. Rehman**, D.J. Brook

213. Minisici coupling approach to (-)-Ardeemin analogs. **R.R. Frink-Sobierajski**

214. Amphiphilic molecules to membrane filtration: Harnessing controlled self-assembly of lyotropic liquid crystals for next-generation water purification. R. Abate, **M. Murai**, S. Zhang

215. Synthesizing star polymer supports for copper catalysts via RAFT. **S. Omar**, **H. Pell**, **N. Oluseyi-Oke**, M.R. Radlauer

216. CRISPRi knockdown of J-domain proteins in *pseudomonas putida*. **J. Do**, T. Arhar, M. Ramos, J. Raab

217. Synthesis of polymer-supported iridium alkane dehydrogenation catalysts. **B. Mai**, **V. Nguyen**, R. Srinivasan, T. Sapp, J. Rojas, N. Roubineau, A. Bargstadt, J.C. Hickey, T. Myint, M.R. Radlauer

- 218.** Organic synthesis for conductive metal organic frameworks. **L. Garcia Martinez**, D. Miranda, J. Lee, S. Marquez, P.T. Dirlam
- 219.** Mitigating hydrophobic recovery in polyurethane via Ar/O₂ plasma surface modification. **D. Malik**, M.J. Hawker
- 220.** Harnessing bioelectricity from organic waste: A microbial fuel cell-enhanced compost system for renewable energy generation. **P. Aquino**, S. Chen
- 221.** Tethered molecular catalyst on CdS nanorods for 1,4 NADH generation: A model subsystem for photosynthetic biohybrids. **J. Wei**
- 222.** Development of a PCET-enabled radical cyclization for oxetane and azetidine synthesis. **T. Tran**, **J. Montes**, T. Thane
- 223.** Electrocatalytic ability of metal-organic frameworks in lithium-sulfur batteries. **L. Kovacevic**, P.T. Dirlam
- 224.** Synthesis & spectral characterization of odorants for database construction. **A.E. Leonard**, **M. Espinoza**
- 225.** Small molecule studies on imine bond formation equilibria relevant to the formation of colloidal COF-300 covalent organic frameworks. **S. Valencia**, H. Negri, L. Hamachi
- 226.** Organic acid catalysts' effects on imine formation and condensation kinetics relevant to COF synthesis. **M. Nelson**, J. Johnson, W. Untung, M. Velasquez, E. Wang, C. Nakamoto, A. Mojica, Z. Jackson Delos Angeles, L. Hamachi
- 227.** Synthesis of verdazyl radical substituted carboranes and approaches to verdazyl substituted metallocarboranes. **T. Jackson**, K. Ong, N. Adams, N. Palomares, D.J. Brook
- 228.** Verdazyl free radical coordination compounds with f-block metal ions. D.J. Brook, **J. Lu**, **A. Buryachenko**, **J. Tamayo**, **K. Liu**
- 229.** Impact of nitrogen plasma treatment on polylactic acid degradation. **I.S. Bual**, M.J. Hawker
- 230.** Examining cellular iron homeostasis of highly glycolytic T cells utilizing sorting by interfacial tension (SIFT). **A. Trivedi**, P. Abbyad
- 231.** Temperature-dependent fluorescence spectroscopy and molecular dynamics of single tryptophan rubredoxins: Comparison of psychrophilic and hyperthermophilic proteins. **M.C. Cole**, I. Leontyev, F.E. Jenney, K. Drumright, S.P. Cramer
- 232.** Using photoactive rhenium sites to investigate proton coupled transfer reactions. **L. Miller**, M. Deegan, O. Sargent, D. Seymour, G.P. Yap

233. Dynamics of extremophile rubredoxins under physiological conditions: Comparisons using synchrotron radiation circular dichroism (SRCD), temperature dependent crystallography, and molecular dynamics. **K. Drumright**, C. Cole, T. Doukov, I. Leontyev, F.E. Jenney, D. George, N. Jones, S.P. Cramer

234. Micellar catalysis of a click reaction. **S. Fulton**, D.B. Ball

235. Thiol nucleophile induced fragmentation kinetics of mono ester carboxylate ylidene norbornadienes derivatives. **D.J. Alamillo**, J. Landa, M.N. Cunningham, D.A. Bercovici

236. Sulphonic acid extraction from Murchison meteorite: Application of ion chromatography. **R. Boucher**

237. Investigation of kinetics of ester amide ylidene norbornadiene fragmentation and stereoelectronic effects of amide substrates. **H. Gamsaragan**, S. Patil, A. Schulte, S. Larson, J. Bellamah, D.A. Bercovici

238. Undergraduate research on water quality in the high sierras in and around yosemite national park, California. **L.N. Anaya, A. Braga, T. King, A. Leeland, P. Stockdale, C. Yee, D. Dormedy**

239. Lipid extraction from sedimentary rock. **S. Pingree, S. Hayes**

240. Spectrochemical characterization of Electrode during CO₂ reduction. **E. Madrid**

241. Synthesis of zero-valent group 10 complexes featuring tert-butyl and phenyl PCCP pincer ligands. **A. Smith**, G.P. Yap, M. Deegan

242. Exploring functional consequences of posttranslational modifications to Argininosuccinate synthetase. **L. Gurung**, M. Von Merta Sustarich, E.R. Greene

243. Photoelectrochemical response of CdSe quantum dot photoelectrodes under illumination. **S. Tanabe**, Z. Lambert, J. Qiu, M. Enright

244. Analyzing the effect of excitation energy on quantum dot and nanorod photocatalysis. **K. Lee**, C. Peak, E. Aguilar, M. Enright

245. Enhancing colistin efficacy through adjuvant compounds. **B. Rodriguez**

246. *In-silico* investigation of small-molecule inhibitors for the treatment of Alzheimer's disease. **A. Chung**, I.W. Tam, G. Ancajas, R. Garza

247. Temperature-dependent dynamics using NMR and MD simulations: Application to the Kalata B1 protein. **E. Kahn**, S.L. Gerlach, K.V. Krishnan

248. Medium-throughput vessel for hydrothermal synthesis reactions: TiO₂ synthesis case study. **M. Sack**, B. Le, J.A. Coronado Sarmiento, A.S. Ichimura

249. CRISPRi knockdown of J-domain proteins in *Pseudomonas putida*. **M. Martinez**, G. Libozada, T. Arhar

250. Stepwise isolation of diverse metabolic cell populations using sorting by interfacial tension (SIFT). **T.J. Mathew**

251. Investigation of colistin adjuvants in Gram-negative pathogens. **A. Lim**, **L.C. Miller Conrad**

252. Investigating the metal binding site on Holothurodin 2 and its implications for antimicrobial activity. **I. Wang**, C. Molina-Rodriguez, K. Davis, M.J. Stevenson

253. Comparing the effects of small molecule modulators on SIRT1. **T. Jagannathan**, **K. Castro**, **I. Perez**, C. Garcia, J. Trieu Dang, N. Wang

254. PEG-Thiol hydrogel coatings for sustained Gentamicin delivery on Polydimethylsiloxane (PDMS) surfaces. **Y.A. Polischuk**, P. Contos, S. Ward

255. Peptoid capping ligands for gold nanospheres in aqueous solutions. **N. Raman**, **E. Filner-Hutchison**, I. Matusich, M. Batek, A.A. Fuller

256. Furthering progress on the synthesis of (−)-ardeemin utilizing convergent one-electron Minisci-type cyclization. **E. Awad**, **E. Boldbaatar**

257. In silico screening of small-molecule inhibitors for multiple sclerosis. **C. King**, R. Garza

258. Carbon monoxide poisoning antidote accessed prophylactically by a bis-pocket Fe(II) porphyrin complex. **L.H. Boretto**, L. Parker, T.C. Johnstone

259. Transforming the gut microbiome through diet: Exploring connections to mental health. **A. Tieu**

260. Exploring switch-like and related regions in sirtuins via ensemble modeling. **B. Nguyen**, **L. Alvarez**, R. Pearson, S. Trikannad, B. Bellinghausen, B. Lustig

261. Evaluation of pyridyl thioesters as carbonyl activator in intramolecular Friedel-Crafts acylation reaction. **A. Leggett**, **A. Cano**, A. Ayala, H. Muchalski

262. Post-translational modification integration on clock protein PER2 regulates CK1 kinase activity within circadian clock. **N. Lee**, M. Torgrimson, C. Partch

263. Data-Driven approach to the optimization of a palladium-catalyzed decarboxylative coupling reaction. **K. Amsden**, M. Alvarado, E. Custo, M. Carrano, R. Navarro

- 264.** Organometallic macromolecule complexes for improving performance of redox flow batteries. **K. Hertz**, E. Despagnet-Ayoub
- 265.** Total synthesis of 4-methyl aziridine carboxylic acid. **A. Mercado**, S. Heller
- 266.** Synthesis of bidentate benzimidazole ligand precursors for nickel complexation. **K.P. Gindratt**
- 267.** Optimization of Fe₃O₄@MIL-100(Fe) magnetic core-shells. **E. Lam**, J. Houston
- 268.** In-silico investigations of flavonoid inhibitors of human tyrosinase. **I.W. Tam**, L. Kwak, R. Garza
- 269.** Influence of solvent polarity and hydrogen bonding ability on the rate of Hünig's base catalyzed acylation. **I. Garcia Ascencio**, S. Heller
- 270.** Toward the synthesis of psychrophilin F using fluorine labeling. **M. Ghanavat**, S. Heller
- 271.** Variability of PM 2.5 at UC Merced: Hand-held particle counter vs. PurpleAir monitor. **A. Biswas**, M. Kibria, A. Adebiyi, A. Adebiyi
- 272.** Synthesis of a biomaterial LEGO block: LA-sNHS-ester silver cluster model. **V. Carrion**, J. Gallardo, J. Lee, C. Linsao, S. Rodas
- 273.** Odorless nosyl deprotection by in-situ formation of a thiolate. **I.T. May**, S. Heller
- 274.** Spin-optotronic properties of Europium (II) doped CsPbBr₃ perovskite quantum dots. **E. Finn**, M. Khvichia, D. Zeitz, K. Chou, J.Z. Zhang
- 275.** Characterization of molybdenum disulfide nanoparticles and carbon quantum dots for use in nanocomposites with PLLA. **X. Duan**, T. Di Luccio, A. Sheng
- 276.** Quantifying the thermodynamics of metal ions binding to the antimicrobial peptide Holothuriodin-2. **C. Molina**, I. Wang, K. Davis, T. Nguyen, M.J. Stevenson
- 277.** Establishing the design rules for aryl-amide atropisomerism in macrocyclic peptides. **E. Lawler**, A. Solivan, A. Schepartz
- 278.** Chemical aging of organic films on sulfuric acid aerosols under upper troposphere/lower stratosphere (UT/LS) conditions. **K. Nguyen**, S. Colina, A. Deepak, M. Elango, O. Lozano, S. Wadhwa, A.K. Chahal, E. Guidicotti, R. Farahani, A.L. Van Wyngarden
- 279.** Flavonoid-tyrosinase interactions: Binding affinities and inhibition mechanisms revealed by microscale thermophoresis and QSAR. **J. Lee**, T. Overdeck

MONDAY MORNING

Bridging Materials, Devices and Simulation: Advances in Polymers for Electronics

California Room

Cosponsored by PMSE and POLY

K. V. Dikshit, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 280. Chemical identification of polymers at nanoscale by nano-IR methods. **A. Danilov**, L. Mester, F. Weston

9:28 281. Liquid crystal enabled anisotropic mixed-conduction of electrons and ions in supramolecular complexes of polythiophene and ionic liquids. **S. Zhang**, N. Bondar

9:51 282. Studying-polymers-on a-chip: High-throughput screening of polymer electrolytes for energy applications. **M.K. McBride**, J.J. Schwartz

10:14 283. Stretchable and biodegradable piezoelectric composite films. **Z. Zhang**, Z. Xu, H. Cai, V. Feig

10:37 Intermission.

10:47 284. Submicron IR microscopy combined with simultaneous Raman and co-located fluorescence for polymer characterization and other applications. **T. Yan**, E. Dillon, M. Kansiz

11:10 285. Magnetic spin pair fluid mechanics. **J.L. Acrivos**

11:33 286. Utilizing mesoporous metal oxide matrices as a platform for studies of polymer nanoconfinement to improve mechanical and dielectric performance. **S. Bindon**, R.H. Dauskardt

11:56 Concluding remarks.

Emerging Leaders in Organic Chemistry

Valley Room

Cosponsored by ORGN
J. Gustafson, *Organizer, Presiding*

9:00 Introductory Remarks .

9:05 287. Synthetic methods to generate and transform benzylic quaternary carbon-containing organic compounds. **B.J. Stokes**, A.C. Graf, J.E. Rosenow, A.B. Van Lare, L.R. Alleyne, R.V. Amsbaugh, X. Cai, A. Tothi, V. Lerda, C. Ramirez

9:30 288. Chemoenzymatic clickable kainoids for chemical neuroscience applications. **S. McKinnie**

9:55 289. Property-based lead optimization of orally bioavailable HPK1 inhibitors. **T. Brewer**

10:20 Intermission.

10:40 290. Voltage-controlled strategies towards selective late-stage functionalization. **J. Derosa**

11:05 291. Regiodivergent Pd-catalyzed decarboxylative coupling reactions. **R. Navarro**

11:30 292. Beginning to understand light-mediated Ni catalysis using physical organic techniques. **A. Bahamonde**

11:55 Concluding Remarks.

Induced Proximity: Unlocking New Therapeutic Avenues (Sponsored by Nurix Therapeutics)

Crystal Room

Cosponsored by MEDI
E. Villemure, *Organizer*
D. Koester, C. Peukert, L. Thai-Savard, *Organizers, Presiding*

9:00 Introductory Remarks.

9:05 293. Death by Design. **S. Malhotra**

9:30 294. Bivalent molecular glues linking lysine acetyltransferases to oncogene-induced cell death. **M. Nix**, S.P. Gourisankar, R. Sarott, B. Dwyer, S. Nettles, H. Abuzaid, M. Martinez, H. Yang, M. Green, S. Hinshaw, N. Gray, G. Crabtree

9:55 295. Exploring two proximity-inducing strategies: From KRAS degradation to KRAS relocation. **A.T. Tran**

10:20 Intermission.

10:35 296. Discovery of NX-5948, an oral targeted degrader of Bruton's Tyrosine Kinase (BTK) for the treatment of B-cell malignancies. **M. Zak**

11:00 297. Molecular glue discovery enabled by targeted degron display. **Z. Zhuang**

11:25 298. Turning up the gain on native protein-protein interactions with molecular glues. **M. Arkin**

Materials and Processes for Energy Storage and Conversion

Garden Room

Cosponsored by INOR

M. J. Greaney, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 299. Investigating the effect of the Nafion ionomer on cobalt electrocatalysts in the oxygen evolution reaction. **T. Lin, J. Qiu**

9:32 300. Effect of electronic substituents on the electrochemical oxidation of benzyl alcohol. **S.T. Spriggs, J. Qiu**

9:59 301. Development of a polymeric-sulfur/MOF composite for viable lithium-sulfur battery chemistries. **D. Miranda, P.T. Dirlam**

10:26 Intermission.

10:39 302. Cobalt and nickel naphthaleneoctathiol-based metal-organic frameworks for electrochemical hydrogen evolution. **A.T. Nguyen, S. Mörsel, S. Marinescu**

11:06 303. $\text{WO}_3\text{-BiVO}_4$ core-shell nanoporous film photoanodes for photoelectrochemical water oxidation. **L. Brennan, M. Law**

11:33 304. Effect of secondary coordination sphere amines on electrocatalytic hydride transfer reactions. **R. Siegel, S. Pattanayak, Y. Liu, J.C. Fettinger, L.A. Berben**

Memorial Symposium in Honor of Attila E. Pavlath

Regency Ballroom 1

Cosponsored by AGFD and PROF
F. Frausto Arellano, *Organizer, Presiding*

9:00 305. Quantifying methionine oxidation as a means of sequencing a prion's conformation.
C.J. Silva, M.L. Erickson-Beltran

9:25 306. Honoring contributions of Attila Pavlath: Scientist, role model, mentor, and leader for ACS.
N. Davis, M.P. Wu

Memorial Symposium in Honor of Robert H. Grubbs (Sponsored by Craig Hawker / BioPACIFIC MIP)

Club Regent

Cosponsored by MPPG
C. M. Bates, K. M. Engle, R. B. Grubbs, V. M. Marx, G. Miyake, H. Nelson, V. A. Piunova, F. Toste, R. Weitekamp, *Organizers*
J. S. Cannon, D. O'Leary, *Organizers, Presiding*

9:00 Introductory Remarks.

9:15 307. ROMPing around: Indispensable metathesis chemistry using Grubbs catalysts for the development of novel polymers. **Y. Xia**

9:40 308. Silver and serendipity: Adventures in chemical catalysis. **A.G. Wenzel**

10:05 309. Medicinal chemistry approaches for developing a clinical pipeline for global health. **A.K. Chatterjee**

10:30 Intermission.

10:45 310. New catalytic reactions and methods for structural elucidation. **H. Nelson**

11:10 311. Synthetic innovations with Grubbs catalysts: From alkene protection to Silicon heterocycles. **G.W. O'Neil**

11:35 312. Necessity is the mother of invention: Natural products and the chemistry they inspire.
S.E. Reisman

Monetizing Molecules: Using Machine Learning and Artificial Intelligence to Bridge the Gap between Computation and Informatics (Sponsored by CAS, a division of the American Chemical Society)

Gold Room

Cosponsored by CINF and COMP
S. Boyer, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 313. What's a prediction worth? The economics of small molecule machine learning. **T.I. Oprea**

9:33 314. From computational chemistry to commercial value: Strategic AI implementation in molecular discovery. **A. Heifets**

10:01 315. Augmenting and accelerating hit finding with Generative AI. J. Fang, S. Cook, L. Shen, P. Kutchukian, **W. Godinez**

10:29 Intermission.

10:36 316. PFACTS: Faster solutions for forever chemicals. **B. Ransom**, D.P. Sanders, J.W. Pitera, C. Ng, D.E. Helbling

11:04 317. Accelerating drug target screening using ML and Gen-AI. **N.N. Vaidya**

11:32 318. Specialized text search of physical properties, tables and molecular formulas using custom parsers and Apache Solr subdocument search. **T. Griffin**, K. Schmidt

Potion to Production: The API Manufacturing Adventure (Sponsored by Gilead Sciences)

Empire Room

Cosponsored by ORGN

J. Gustafson, *Organizer*

J. R. Dunetz, R. Yousefi, *Organizers, Presiding*

9:00 Introductory Remarks .

9:05 319. Developing remdesivir to meet the needs of a global pandemic. **T. Wenderski**

9:33 320. Development of a chemo- and biocatalytic process to the HPK1 Inhibitor GNE-6893.

D. Xu, A. Stumpf, R. Angelaud, F. Gosselin

10:01 321. Process development of an HIV protease inhibitor. **M. Ischay**

10:26 Intermission .

10:36 322. Navigating polymorphic transformation to obtain drug substance with desired powder properties. **E. Horstman**, C. Lai, O. Lapina, D. Bykowski, V. Dhand

11:04 323. Process development for the first GMP synthesis of a novel drug-linker, SGD-9501-TFA. **A.M. Whittaker**

11:32 324. Process optimization of Zamzetoclax: Addressing RCM challenges for manufacturing readiness. **R. Yousefi**

Analytical Frontiers in Energy and Fuels - Symposium In Honor of Neal Byington

Regency Ballroom 1

Cosponsored by ANYL and ENFL

I. Ferrer-Lassala, A. Taheri, *Organizers, Presiding*

10:00 Introductory Remarks.

10:05 325. Neal Byington and the 200 meter gas chromatograph column. **M.T. Cheng**

10:30 Intermission.

10:40 326. Analytical chemistry for the energy transition: Some thoughts. **F.A. Lopez-Linares**, E. Rogel

11:05 327. Automating pipeline joint identification for free-floating pipeline inspection tools to enhance feature localization using neural networks. **M. Byington**, A. van Pol, J. van Pol

11:30 328. Wireless potentiometry of thermochemical heterogeneous catalysis. **N.K. Razdan**, K. Westendorff, Y. Surendranath

11:55 Concluding Remarks.

MONDAY AFTERNOON

Building Bridges General Posters

Regency Ballroom 2

Cosponsored by MPPG

V. M. Marx, N. L. McClure, *Organizers*

12:00 - 1:30

329. Integrating sequence-based modeling and multiscale simulations to probe and engineer haloalkane dehalogenases. **N. Gelfand**, V. Orel, W. Cui, J. Damborsky, C. Li, Z. Prokop, W. Xie, A. Warshel

330. Anomalous ionic current in charged boron-nitride nanotubes. **P. Rehak**, P. Kral

331. Temperature dependence of photoinduced carrier spin relaxation dynamics in CsPbBr₃ and MAPbBr₃ perovskite quantum dots. **M. Khvichia**, D. Zeitz, K. Chou, Y. Ping, J.Z. Zhang

332. In-depth literature review focused on PFAS (per- and poly-fluoroalkyl substances) chemicals and PCB's (polychlorinated biphenyls). **S. Begum**

333. Temperature dependent exciton dynamics of Cs₄CuSb₂Cl₁₂ layered double perovskite nanocrystal thin films. **K. Chou**, R. Wu, O. Chen, J.Z. Zhang

334. Selective reduction and oxidation of aromatic compounds by hot electrons and hot holes. **P. Poorjafari Jafroodi**

335. Investigation of the fluorescent properties of ^{DEA}tC^O and its SNP Discrimination. **M.K. Nguyen**, D. Rosansky, B.W. Purse

336. Oxidative treatment of tetracycline via persulfate activation using cross-linked MnFe₂O₄@green mussel shell chitosan hybrid catalyst in a fixed-bed column reactor. H.D. Villanueva, M.V. Tampos, R.E. Mina III, M.M. Baldivino, **L.E. Borromeo**

337. Real-time enzyme kinetics by ¹⁹F NMR: Hydrolysis of N-trifluoroacetylglycine (TFAG) by Acylase I. **S. Amer**

338. Discovery of Epoxysuccinates as Potent, Covalent Inhibitors of SARS-CoV-2 Papain-Like Protease (PLpro). **F. Soleymani**, G.R. Velma, Z. Shen, C. Holdberg, J. Fu, D. Indukuri, S.R. Musku, E. Lazarova, S. Slilaty, Z. Li, K. Ratia, R. Xiong, G. Thatcher

339. Sulfinyl aziridines as stereoselective covalent destabilizing degraders of the oncogenic transcription factor MYC. **K. Li**, H.T. Rosen, E. Li, T.J. Maimone, D. Nomura

340. Effect of structural variations between Surrogate Reference Standards and Target Analyte on assay values in isocratic HPLC-UV quantitation. **J.O. Ofosu**, S. Asare-Nkansah, J.S. Ayim, W.A. Asamoah

341. Alkyl sulfonyl fluorides as ambiphiles in the stereoselective, palladium(II)-catalyzed cyclopropanation of unactivated alkenes. **Y. Cao**, W. Rodphon, T. Alturaifi, A. Lisboa, Z. Ren, J. Struijs, H. Ni, T. Savchuk, R. Loach, S. Yang, I. McAlpine, D. Blackmond, P. Mykhailiuk, P. Liu, K.B. Sharpless, K.M. Engle

342. Investigating the role of lipoxygenases in mediation platelet function through the endocannabinoid anandamide. **G. Magalang**, K. Goerger, M. Holinstat, T.R. Holman

343. Back to the fungamentals: Antimycotic activity of glycogen synthase kinase inhibitors. **N. Lach**, A. Yokomizo, B.A. Haubrich

344. Inhibition of ERK kinase from an ERKsome parasite. **J. Dolendo**, S.H. Naqvi, A. Yokomizo, D.C. Swinney, B.A. Haubrich

345. A novel pump-probe IR spectroscopy system to investigate the catalytic cycle of hydrogenase. **C. Robertson, M. Hassan**, S.J. George, S. Cramer

346. Repurposing protease inhibitors to target *Acanthamoeba castellanii*: A phenotypic approach. **A. Ghotra**, A. Yang, Q. Ha, A. Yokomizo, B.A. Haubrich

347. PKIqued my interest: Repurposing protein kinase inhibitors for Acanthamoeba keratitis. **A. Yang**, A. Ghotra, Q. Ha, A. Yokomizo, B.A. Haubrich

348. Chemical profiling and anti-proliferative effects of central California-grown hairy fleabane on prostate cancer cells. **D. Hidalgo**, E.Y. Chen, d. Sumrein, K.V. Krishnan, A. Shrestha, Q. Chen

349. Photovoltage of BiVO₄ photoelectrode junctions from applied bias vibrating kelvin probe measurements. **S. Jain**, F.E. Osterloh

350. Synthesis of colistin adjuvants. **S. Vinjamuri**

351. Screening with a quick, qualitative assessment of inhibition kinetics using a parasitic glycogen synthase kinase. **J.A. Solorzano**, J.A. Ma, A. Yokomizo, D.C. Swinney, B.A. Haubrich

352. Studies towards the development of an off-switchable DNA intercalator. **K. McIntyre**, H. Nikolayevskiy

353. Calibration of beam energy for a tandem accelerator. **S. Ahmed**, J. Wilkinson, M. Anastasiou, N.E. Esker

354. Synthesis and exploration of shapeshifting phosphines. **V. Gonzalez**, K. Tomota, D. Berger, T.J. Maimone

355. Biophysical analysis of cyclic substituted flavones. **T. Jiang**, N. Tran, C. Brown, A. Franz, B. Ruvalcaba, B. Bushaw, L. Xue

356. Fungal aficioNADo: Reversible reaction and chemical inhibition of an NAD homeostatic enzyme from *Candida*. **N. Deng**, T. Tran, S.H. Naqvi, A. Yokomizo, B.A. Haubrich

357. Developing a differential scanning fluorimetry (DSF) platform for ubiquitin proteoform detection. **A. Trinh**, J. Ho, E. Carroll

358. Optimizing fluorine enhanced TiO₂ thin films for energy and environmental applications. **B. Le**, A.S. Ichimura

359. Development of highly selective NUAK1 inhibitors with improved potency for cancer treatment. **s. jang**, D. Kim, Y. Kwon, K. Lee, J. Kim, K. Jung

360. Bioassay guided fractionation of aquatic fungal extracts for antimicrobial activity. **P.L. Lee**, **S. Carlson**

361. Exploring how destabilization by site-specific ubiquitination influences amyloid formation. **E. Lopez Ruiz**

362. Ultrafast spin relaxation of charge carriers in strongly quantum confined methylammonium lead bromide perovskite magic-sized clusters. **D. Zeitz**, J.Z. Zhang

363. Optimizing TiO₂ anatase thin film growth for photocatalysis. **G.B. Chavez**

364. Investigating the effect of disease-associated mutations on glutamine synthetase stability. **K. Martinez**, E. Mejia, H. Yamamura, M. Tecson, E. Carroll, E.R. Greene

- 365.** Adsorption and catalytic degradation for clean water solutions. **J.C. Buckley**, C. Lew
- 366.** Ensemble simulations: Folding dynamics of the high-efficiency transfer-messenger RNA PK1 pseudoknot. **D. Chavez-Bonilla**, N. Nguyen, V.X. Ngo, M. Bakhom, T. Gerdes, E.J. Sorin
- 367.** Enhanced ligand exchange in polypyridine ruthenium complexes: New inner-sphere transfer hydrogenation catalysts. **R.J. Engeseth**, E.P. Kelson
- 368.** Mechanism of inhibition underlying glutamine synthetase inhibition by adenylation. **A. Bautista**, E.R. Greene
- 369.** Chiroptical activity of CdSe quantum dots with enantiopure mandelic acid ligands. **J. Etchingham**, M. Enright
- 370.** Phase transitions kinetics study in potassium-intercalated manganese mioxide for energy storage applications. **Z. Erdyneev**
- 371.** Conformational landscape alteration by covalent modification of pesticide to argininosuccinate synthetase revealed by cryoEM. **M. Von Merta Sustarich**, E.R. Greene
- 372.** CryoEM structures of in vitro induced full-length tau amyloids. **E. Hernandez**, J.E. Gestwicki, E.R. Greene
- 373.** Synthesis and characterization of a W-substituted Chevrel phase: Cu₂Mo₅WS₈. **C.A. Nagasaka**, J. Velazquez
- 374.** Carbohydrate composition and structural characterization of *Plantago major* Mucilage: Implications for functional food applications. **B. Tobar**, D. Barile, h. peng
- 375.** Synthesis of small molecule and star polymer supported iron complexes as electrocatalysts for nitrate and nitrite reduction. **R. Chiang**, A. Lykins, D. Lin, T. Nguyen, M.R. Radlauer
- 376.** Exploring regioselectivity of pincer–iridium catalyzed transfer dehydrogenation. **R. Srinivasan**, B. Mai, V. Nguyen, J.C. Hickey, M.R. Radlauer
- 377.** Deaminative ring contraction for the modular synthesis of phenanthrenes and efforts toward (–)-artapilosine A & santiagonamine. **C. Valiton**, A.G. Roberts, W. Dalton
- 378.** Fast-track vasculature engineering for tissue constructs: Light-based 3D printing of synthetic angiosomes. **A. Kwan**, I.A. Coates, Y. Tan, C.A. Kohnke, D.I. Alnasir, A.N. Nguyen, E.E. Heng, M.T. Dulay, S.C. Heilshorn, A. Thakor, E.S. Shaqfeh, J.W. MacArthur, J.M. DeSimone
- 379.** TRAINs: An adsorption-based polymeric gene delivery platform for targeted vaccines and therapeutic applications. **A. Laturski**, V. Duran, M.T. Dulay, B. Schaar, S. Einav, J.M. DeSimone

380. Optimizing an adapter for transferring air- and moisture-sensitive chemicals. **A. Jones**, K. Hekker, G.W. O'Neil

381. Varying selectivity in C-F activation of aryl fluorides as a result of catalyst modifications in bis-bidentate N-heterocyclic carbene nickel complexes. **A.C. Garcia Alvarez**, A. Bryant, D. Huerta, Z. Marr, C. Stieber

382. Ag(I)/K₂S₂O₈-mediated selective oxidation of ynamide-Yne *via* structural reshuffling and consecutive *N*-desulfonylation. **M. Mutra**, C. T. L., T. Wang, J. Wang

383. Sustainable delivery of a bioactive agent via environmentally degradable poly(anhydride-ester)s for agricultural applications. **M. Hasan**, B. Truong, K. Uhrich

384. Predictive correlation between ground-state orbitals and photophysical properties in organic crystals. **A. Abou Taka**, L. McCaslin, H.P. Hratchian

Carbon Capture and Conversion for a Sustainable Future

Garden Room

Cosponsored by ENFL

R. Kowalski, A. Taheri, J. Velazquez, *Organizers*
H. Kaur, B. O. Okoye, R. Siegel, *Organizers, Presiding*

2:30 Introductory Remarks.

2:35 385. Advancing carbon management with cost-effective porous materials: Breakthroughs from simulation and experimental research. **J.L. Liu**, j. Lawrence, J. Choi, **S. Bashir**

3:02 386. Technology landscape in accelerated mineralization technology for carbon capture, utilization, and storage. **C.F. Ovalles**, F.A. Lopez-Linares, B. Fayyaz

3:29 387. Electrochemical CO₂ reduction to C₂+ products with remarkably high Faradaic efficiency in the presence of a proton permeable membrane. **H. Pan**, C. Barile

3:56 Intermission.

4:09 388. Design of a computational framework for circular carbon chemistry. **R.D. Cormia**

4:36 389. Performance analysis of CO₂ absorption in flat-plate gas/liquid membrane contactors enhanced with S-ribbed carbon-fiber slots. **C. Ho**, P. Hsieh, J. Chen

5:03 390. Withdrawn

Chemistry at the Cutting Edge of Catalysis

Regency Ballroom 1

Cosponsored by ORGN

J. Gustafson, *Organizer*

J. Derosa, *Organizer, Presiding*

2:30 Introductory Remarks.

2:35 391. Combining synthetic chemistry and biology for streamlining access to complex molecules. **H. Renata**

3:00 392. Identification of novel *plasmodium* phosphatidylinositol 4-kinase (PI4K) inhibitors for the treatment of malaria. **V.M. Marx**

3:25 393. *De novo* approaches to the synthesis of heteroarene building blocks. **A.C. Sather**

3:50 394. Metallocene mediators for tandem electrocatalytic redox reactions. **J. Derosa**

4:15 Intermission.

4:25 395. Selective olefin functionalization: Strategies, mechanisms, and catalysts. **K.M. Engle**

5:25 Concluding Remarks.

Emerging Leaders in Inorganic and Materials Chemistry

Valley Room

Cosponsored by INOR

A. M. Spokoyny, *Organizer, Presiding*

2:30 396. Understanding nonlinear mechanics of associative polymer networks. **Y. Yang**

3:00 397. Nanoparticle-based bonds to design dynamic polymer networks. **S. Seo**

3:30 398. Reversible room temperature heterolytic activation of vinylic sp² C–H bonds at a gallium center. **M. Nava**, K. Liu, M.Y. Riu, J. Shan, L. Zarnitsa, K.N. Houk

4:00 399. Design of dilute alloy catalysts for efficient oxidation and hydrogenation reactions. **J.D. Lee**

4:30 400. Manganese-dependent Monooxygenases. **J. Rittle**

5:00 401. Macroscopic 2D moiré structures for exploring ultrafast dynamics and thermal properties. **F. Liu**

Extrahepatic-targeted Delivery of xRNA Therapeutics (Sponsored by Novartis)

Empire Room

Cosponsored by MEDI

J. Cao, E. Villemure, *Organizers*
L. Ofori, *Presiding*

2:30 Introductory Remarks.

2:35 402. Advancing extrahepatic delivery of oligonucleotides: The promise of antibody oligonucleotide conjugates. V.R. Doppalapudi, **M. Bird**

3:15 403. Directed evolution reversion analysis produces minimally evolved adenine base editor variants with improved efficiency and precision. **A. Komor**, M. Evanoff, S. Korpal, Z. Krill, Q. Cowan

3:55 Intermission.

4:10 404. In vivo delivery of mRNA with lipid nanoparticles that non-immunogenic. **N. Murthy**

4:50 405. RNA revolution: New delivery systems enable new organ- and cell-selective therapies. **Z. LI, J.L. Hamad**, L. Amaya, A. Ee, S. Wang, P. Yadav, R. Pi, C. Blish, R. Levy, H. Chang, R.M. Waymouth, P.A. Wender

Induced Proximity: Unlocking New Therapeutic Avenues (Sponsored by Nurix Therapeutics)

Crystal Room

Cosponsored by MEDI

E. Villemure, *Organizer*
D. Koester, C. Peukert, L. Thai-Savard, *Organizers, Presiding*

2:30 406. Accelerating molecular glue discovery through computational approaches. **S. Ou**

2:55 407. TrogoTACs for targeted protein transfer between cells. **N. Till**, M. Ramanathan, K. Loh, C.R. Bertozzi

3:20 408. ByeTAC: Bypassing E-ligase-targeting chimeras for direct proteasome degradation. **D.J. Trader**, C. Loy, T. Harris Jr.

3:45 Concluding Remarks.

Memorial Symposium in Honor of Robert H. Grubbs (Sponsored by Umicore)

Club Regent

Cosponsored by MPPG

C. M. Bates, J. S. Cannon, K. M. Engle, R. B. Grubbs, V. M. Marx, G. Miyake, H. Nelson, D. O'Leary, F. Toste, *Organizers*
V. A. Piunova, R. Weitekamp, *Organizers, Presiding*

2:30 Introductory Remarks.

2:45 409. Cyclic polymers accessed through ring-expansion metathesis polymerization. **M.R. Golder**

3:10 410. Beyond the benchtop: Commercializing ruthenium metathesis catalysts. **A. Johns**

3:35 411. Chemically recyclable multiblock plastics. **G. Miyake**

4:00 Intermission.

4:15 412. Mentoring focus: From research with undergraduates to grant management. **A.L. Liberman-Martin**

4:40 413. Organometallic complexes for non-aqueous flow batteries. **E. Despagnet-Ayoub**

5:05 414. Complex natural products as a driving force for discovery in organic chemistry. **B.M. Stoltz**

Monetizing Molecules: Using Machine Learning and Artificial Intelligence to Bridge the Gap between Computation and Informatics (Sponsored by CAS, a division of the American Chemical Society)

Gold Room

Cosponsored by CINF and COMP

S. Boyer, *Organizer, Presiding*

2:30 415. Monetizing molecules through digital disruption of the drug discovery pipeline. **A. Tropsha, A. Cherkasov**

2:58 416. An open-access web service to classify compounds. **L. Weber**

3:26 417. PubChem: a wealth of information to advance science. **E. Bolton**

3:54 Intermission.

4:01 418. 3D, structure-based, deep learning approach for predicting the regioselectivity of transition-metal catalysis. **N. Hadler, I. Rinehart, M. Elkin, J. Nicolai, G. Gheibi, J. Chen, M. Avaylon, R. Maciejewski, M.W. Mahoney, T. Perciano, J.F. Hartwig**

4:29 419. IBM ChemChat - An agentic conversational assistant and platform for material science. **T. Erdmann, R. Le Metayer, S. Zecevic, K. Lionti, B. Ransom, H. Bui, N. Park, J. Hedrick, K. Schmidt**

4:57 420. Natural language searches of authoritative data using a Large Language Model (LLM). **M. Moser, S.K. Boyer**

5:25 Concluding remarks.

True Stories of Entrepreneurs

California Room

Cosponsored by SCHB

B. A. Charpentier, *Organizer, Presiding*

N. L. McClure, *Presiding*

2:30 Introductory Remarks.

2:35 421. True stories of entrepreneurs: Challenges and successes of a serial agbio entrepreneur. **P.G. Marrone**

2:55 422. Sugar, surfactants, and a splash of innovation. **C. Boxley**

3:10 423. Where is the AI in drug discovery, and where should it be instead?. **A. Heifets**

3:25 424. From bench to breakthrough: Why chemists should found biotech startups and how we're helping them succeed. **D. Crawford**

3:50 Intermission.

4:00 425. Entrepreneurship: Is it for me?. **G. Went**

4:20 426. Entrepreneurship journey of Mango Materials: From lab to commercialization. **M. Morse**

4:40 427. How to choose the right incubator to accelerate your startup's growth. **G. Segre**

5:00 Panel Discussion.

Potion to Production: The API Manufacturing Adventure (Sponsored by Gilead Sciences)

Crystal Room

Cosponsored by ORGN

J. Gustafson, *Organizer*

J. R. Dunetz, R. Yousefi, *Organizers, Presiding*

4:00 428. Lenacapavir: Process development of a Suzuki reaction. **A. Wagner**

4:28 429. Adapting new chemistry to Kilo scale: Catalytic nitroarene reductions in pharmaceutical manufacturing. **C.V. Credille**, A. Mohammadlou, M. Dweck, K. Rees, S. Torabi Kohlbouni, J. Kimbrough, C. Farley, J. Graham

4:56 430. Data science and mechanistic tools in process development: Enabling synthesis of NLRP3 modulator building blocks. **J. Jermaks**

5:24 Concluding Remarks .

MONDAY EVENING

Building Bridges General Posters

Regency Ballroom 2

Cosponsored by MPPG

V. M. Marx, N. L. McClure, *Organizers*

5:30 - 7:00

431. Total synthesis of natural products scrophuloside a and scrophuloside B from Neopicrorhiza scrophulariiflora. **Y. Noh, T. Zhang, L. Lam, E. Njoo**

432. Protease-assisted decoding of methacrylation in photo-crosslinkable gelatin methacryloyl (GelMA) with LC/MS. **S. Munjal, I. Adapala, A. Fong, S. Kasibhotla, E. Hui, K. Luong, C. Sofuoglu, A. Yamamoto**

433. Polycation and alkylchain-modified calcium phosphate nanoparticles for non-covalent multiple drug delivery. **A. Fong, R. Bellis, C. Sofuoglu, S. Presswala, S. Kasibhotla, A. Yamamoto**

434. Bridging the broad spectrum of chemistry: Applications of small molecule amino triester lipids as biodegradable surfactants for small molecule drug delivery and for precise control of quantum dot formation. **E. Hsen, A. Gribok, E. Yu, C. Chou, T. Zhang, A. Liu, Y. Noh, A. Chia, E. Njoo**

435. Synthesis, anticancer properties, and *in vivo* profiling of synthetic glycan analogs of proscillarin A. **S. Somani, F. Wang-Johanning, G. Johanning, E. Njoo**

436. Anticancer synthetic arylsulfonamides with Wnt-1 modulating activity. **A. Chalasani, A. Yu, K. Hsu, L. Chen, V. Sharma, L. Kim, D. Boom, K. Huey, A. Wu, E. Njoo**

437. Evaluation of machine learning models for the classification of optimal coupling agents in diverse Amide Coupling Reactions. **A. Chalasani, S. Deb, A. Anand, Y. Li, R. Downing, E. Njoo**

438. Synthesis and evaluation of carmofur analogs as membrane rupture-inducing agents. **C. Chou, E. Yuyama, S. Vaidya, L. Chen, K. Hsu, I. Chepurna, M. Gupta, O. Kwok, J. Zhang, K. Huang, F. Leung, E. Du, A. Zhu, L. Chang, D. Devendiran, K. Fung, M. Chen, J. Pazzi, E. Njoo**

- 439.** Discovery of A4P1W1, a fluorinated atropisomeric Arylisoxazole acrylamide covalent inhibitor for the treatment of solid cancers. **L. Lam, S. Chau, A. Chia, E. Yuyama, I. Chepurna, A. Yu, J. McChesney, S. Vaidya, E. Njoo**
- 440.** Progress towards the asymmetric total synthesis of the sporovexin natural products. **J. McChesney, C. Zhou, A. Gribok, C. Chen, E. Lin, E. Yao, A. Stefan, I. Chepurna, G. Liu, T. Zhang, Y. Noh, E. Njoo**
- 441.** Cathepsin-B responsive hydrogels for the targeted delivery and controlled release of T-cell immunotherapy to tumors. **N. Kaleekal, A. Yamamoto**
- 442.** Blue fluorescent siloxytecans exhibit potent anti-cancer activity and enable direct real time quantification of intracellular uptake. **S. Vaidya, A. Mo, A. Chia, K. Li, J. Parvin, S. Sadagopan, O. Kwok, J. Zhang, J. Pazzi, E. Njoo**
- 443.** Scaleable formal synthesis of (R)-(+)-etomoxir. **R. Raval, E. Lin, E. Njoo**
- 444.** PROTAC-based targeting strategies for the selective degradation of PDE1A and TDP-43 in neurodegenerative disease. **S. Xi, M. Tsui, S. Yang, E. Njoo**
- 445.** Conformational perturbations and functional dynamics of SCN1A sodium channel mutants in Dravet syndrome. **T. Bang**
- 446.** Computational simulations of RNA-based aptamers targeting EpCAM⁺ breast cancer cells. **A. Shivaprasath, G. Sharma**
- 447.** Designing L-RNA-based Spiegelmers against Ecto-GPR37: A novel approach for Parkinson's disease biomarker detection. **A. Kodumuri, G. Sharma**
- 448.** Structure-guided modeling of proteolysis-targeting chimera PROTAC targeting nucleolin protein in glioblastoma. **M. Mishra, G. Sharma**
- 449.** Unlocking medulloblastoma detection: Transketolase (TkT) as a novel biomarker for early diagnosis. **V. Murali, G. Sharma**
- 450.** Therapeutic inhibition of mutant MnSOD using aptamers to attenuate mitochondrial oxidative stress in depression. **N. Arun, G. Sharma**
- 451.** Novel progressive supranuclear palsy detection method utilizing ATP6AP2 protein. **S. Sharma, G. Sharma**
- 452.** Extending the lifespan of *Arundo donax* bassoon and oboe reeds: Evaluating maintenance strategies against enzymatic and microbial degradation. **N. Rao**
- 453.** Chromatographic analysis of lipid-conjugated oligonucleotides. **B. Nguyen**

454. Optimization of permeation agents for transdermal cannabinoid delivery applications. R. Del Sesto, **M.E. Bulloch**, K. Holm, B. Jenkins

455. Biogasoline. **S.R. Vatcha**

456. Early prediction of lithium-ion battery degradation: Using six health indicators to analyze long short-term memory and random forest in battery health prognostics. Y. Zou, **K. Zhao**, I. Lu, E. Liu, M. Hung, R. Song, C. Lin, A. Cha, L. Shi

457. Optimizing Arg detection in lysimeter system: A comparative evaluation of Bactopia and leading genomic pipelines. C. Lee, A. Zhang, C. Zheng, C. Zhang, H. Ming, S. Vadlamudi, **S. Eyunni**, D. Vinegrad, E. Eisenbeis, D. Lam, A. Fang, M. Cho, **R. Poluru**, I. Chin, B. Wu, A. Gowripalli, L. Shi, Y. Men

458. Future of Agriculture: how ABA influences tomato fruit quality under heat stress. **B. Yuan**, B. Stevens, P. Leng

459. Endogenous metabolite activity screening of human glutamine synthetase reveals inflammation link. **R. Jacobs**, **R. Leung**, E.R. Greene

460. Reactive molecular dynamics study of Fe–Ni–Al alloy nanoparticles: Oxidation, aggregation, and energetic behavior. **L. Hong**, **L. Hwang**, P. Luhar, R. Ramirez\

461. Enhancing food and biological science education through molecular dynamics and inquiry-based learning. **L. Hwang**, **L. Hong**

462. Development of Prussian blue-coated 3D-printed electrodes for ammonium removal from water via electro-sorption. **S. Park**

463. GenX degradation by micelle formation using 2-hydroxyphenyl acetic acid and cetyl trimethyl ammonium bromide under UV-LED irradiation. S. Eom, **K. Zoh**

464. Fungi and actinomycete co-culture on solid agar for drug discovery. **A. Parmar**, **G. Merino**, S.N. Carlson

465. Leveraging ACS membership for finding industry contacts, and building and enhancing chemical industry companies' success. **J.L. Bryant**, M. Hurrey

466. Strengthening professional skills education in chemistry for all students through Universal Design. **M.T. Dulay**, S. Podowitz-Thomas, C.B. Monroe, A.C. Mody

467. Release of elements from disposable aluminum cookware during conventional cooking with water. **A. Akhdhar**, M. Binkadem, D. Abd El-Hady, A. Alowaifeer, M. Almutairi, K. Alnabati, K. Elwakeel, F. Zainy, H. Baeissa, S. Alhayyani, H. Albishri, A. AlBogami, J. Feldmann

468. Biocatalytic aza-Michael addition of aromatic amines to enone using α -amylase in water. **S. DUTT**

469. Least square, Theil-Sen and Musgrave models for product yield simulation of oxazoline. **P. Johnson, L. Huang**

470. Spectroscopic study of cyanine dyes behavior in aqueous solutions of metal cations and on surfaces of organic monolayers containing amino silanes. **H. Samha**

471. Ultra-high spatial resolution mass spectrometry techniques for single cell imaging. **W. Hang, X. Yan, Y. Meng**

472. High-throughput single-mitochondrion ATP profiling reveals OXPHOS addiction for precision cancer therapy. **X. Yan, X. Xiao**

473. Explaining the trifecta functions of the dineutron particle and its significance to nuclear energy production. **A. Angus**

474. Colorful connections: Jacaranda flowers as teaching tools in time-limited labs. **A. Kaspi-Kaneti, H. Aranki, B. Morris, D. Zeng, M. Cornejo, A. Rice, H. Ung**

475. Multi-laboratory validation of a robust analytical method for Saxitoxins in aqueous environmental matrices. **J.E. Kelly, M. Chehelamirani, S. Balachandra, T. Bowers**

476. Multi-laboratory validation of a robust analytical method for Trifluoroacetate (TFA) in aqueous environmental matrices. **J.E. Kelly, M. Chehelamirani, S. Balachandra, T. Bowers**

477. *N,N'*-Diarylformamidines in an unusual *E-syn* configuration. **D. Han, Q. Zhao**

478. Characterization and chemical inhibition of glycogen synthase kinase from parasitic and fungal pathogens. **M. Arslanian, C. Hartwell, A. Yokomizo, D.C. Swinney, B.A. Haubrich**

479. Toward a more efficient continuous flow synthesis of tetraphenylporphyrin. **N. Gebhards, A. Wiersma, E. Carlson, M.A. Cranswick**

480. Harnessing novel in-silico techniques: A modern approach for identity testing in large molecule Biologics. **J. Rodriguez**

TUESDAY MORNING

Energy and Fuels General Session

Crystal Room

Cosponsored by ENFL

J. Velazquez, *Organizer*

A. Taheri, *Organizer, Presiding*

8:30 Introductory Remarks.

8:32 481. Discovery of dual ion-electron conductivity of metal-organic frameworks via machine learning-guided experimentation. **M.C. So**, R. Bashiri, P. Lawson, S. He, S. Nanayakkara, K. Kim, V. Stavila, F. El-Gabaly, J. Lee, E. Ayars

8:52 482. Electrochemical reactive conversion of captured CO₂ that are compatible with a Molecular Iron electrocatalyst. **B.O. Okoye**, L.A. Berben

9:12 483. Understanding interfacial phenomena in hydrogen technologies. **A.Z. Weber**

9:32 Intermission.

9:37 484. Fast and selective hydride transfer (electro)catalysis for CO₂ reduction with metal clusters. **L.A. Berben**

9:57 485. Advanced X-ray and electron based techniques for material and cell-level battery analysis. **Z. Wang**

10:17 486. Heterointercalation in chevrel-phase sulfides: A model periodic solid for the investigation of chain electron transfer. **K. Mason**, J. Velazquez

10:37 487. Improved SrNbO₂N photoanodes for solar fuel generation via ammonolysis under mixed NH₃/N₂ atmosphere. **R. Kandel**, F.E. Osterloh, L. Wang, Z. Najaf, M. Salmanion, G. Rao, R.D. Britt, J. Madrigal

10:57 Concluding Remarks .

Extrahepatic-targeted Delivery of xRNA Therapeutics (Sponsored by Novartis)

Regency Ballroom 1

Cosponsored by MEDI

L. Ofori, E. Villemure, *Organizers*

J. Cao, *Presiding*

8:30 488. CARTs: A versatile platform for RNA delivery and therapeutic applications. **Y. Jia**, P.J. Hurst, N. Warlin, S. Zhou, A. Colina, J. Arens, S. Khasnavis, S. Ramsay-Burrough, M. Abdelwakil Abdelrazik, D. Felsher, M. Porteus, R.M. Waymouth

9:05 489. Library screening to discover novel ADAR Guide sequence motifs. **R. Ouye**, K. Campbell, S. Mozumder, C. Tang, P.A. Beal

9:40 490. Modular single component polymeric systems for pulmonary and splenic mRNA Delivery. **S. Khasnavis**, M. AbdElwakil, J. Ni, S. Ramsay-Burrough, P.J. Hurst, Y. Jia, S. Musad, M. Kumar, R.M. Waymouth

10:15 Concluding Remarks.

Inorganic and Materials Chemistry General Session

Valley Room

Cosponsored by INOR

V. M. Marx, *Organizer*

M. Alves, *Presiding*

8:30 Introductory Remarks.

8:35 491. Novel structure formation of hybrid chiral biomolecular crystals and nanosurface systems. **P. Rehak**, P. Kral

8:55 492. Tuning near-infrared luminescence in InAs-based quantum dots for optoelectronic integration. **M. Garbo**, M. Enright

9:15 493. Transition metal complexes supported by an alkyne-based pincer ligand. **M. Deegan**, I. Fejes, D. Gordon, A. Smith, E. Norton, R. Lara Belaunzaran, R. Chafin, G.P. Yap

9:35 Intermission.

9:50 494. Formation of Gold-Cyanide Complexes on Gold Nanoparticles in Aerobic and Anaerobic Conditions: Details and Mechanisms for Complex Formation. **P.W. Jagodzinski**, M.B. Jacobs

10:10 495. Oxidation of emerging contaminants using a metal-organic framework (MIL-100Fe) with an Fe₃O₄ core. **J.R. Houston**, E. Lam, J.A. Watkins

10:30 496. C-S and S-F bond cleavage of aryl sulfonyl fluorides using Bis-Bidentate NHC Nickel(0) complexes. **e. Lopes**, D.S. Galindo, e. Chavarin, C. Stieber

10:50 497. Molten salt synthesis of lanthanide and actinide borides. **E.A. Espinoza**, V. Augustine, D. McGlamery, A. Chemey

11:10 Intermission.

11:25 498. Extending metallocene chemistry to scandium and copper with tri-*tert*-butylcyclopentadienyl ligands. **J. Queen**, W.J. Evans

11:45 499. Trivalent actinide and lanthanide separation by derivatives of Invest species. **G. Odonkor**

12:05 500. Rare-earth terphenylthiolate complexes revisited. **C.R. Stennett**, M.R. Luevano, E. Ma, R. Grotjahn, J.W. Ziller, F.U. Furche, W.J. Evans

12:25 Concluding Remarks.

Intellectual Property Resources and Technology Transfer

Gold Room

Cosponsored by CHAL
H. M. Peters, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 501. Technology transfer at Stanford's Office of Technology Licensing. **E. Elder**

9:00 502. Innovation transfer at UC Santa Cruz. **J. Jackson**

9:25 503. Where the rubber meets the road: Charles Goodyear, vulcanization, and the struggle to protect innovation. **J.L. Krieger**

9:50 504. The ACS Division of Chemistry and the Law. **H.M. Peters**

10:05 Panel Discussion.

Organic Chemistry General Session

California Room

Cosponsored by ORGN
J. Gustafson, *Organizer, Presiding*
N. L. McClure, *Presiding*

8:30 Introductory Remarks.

8:35 505. Impact of oxygen and sulfur heteroatom core substitution on catalyst properties of phenoxazines and their performance in organocatalyzed atom transfer radical polymerization (O-ATRP). **J. Lathrop**, B. Portela

8:55 506. Sustainable synthesis of E-alkenylboronate esters and alkyl gem-diboronate esters catalyzed by triethoxysilane through sequential regioselective hydroboration of terminal alkynes. **H. Kaur**, h. ahuja, R. Arevalo

9:15 507. Total synthesis of analgesic diterpenoid alkaloids: Aconicarmisulfonine a and analogs. **S. Ning**, T.J. Maimone

9:35 Concluding Remarks.

Polymer Chemistry General Session

Empire Room

Cosponsored by PMSE and POLY
K. V. Dikshit, *Presiding*

8:30 Introductory Remarks.

8:35 508. Controlled single bond functionalities incorporation in CANAL ladder polymers: Their properties and gas separation performance. **R. Yin**, A. Robinson, Y. Xia

8:55 509. Low-force, reversible, non-scissile mechanophore enables efficient solid and solution state mechanoactivation. **V. Bhat**, M. Horst, Y. Xia

9:15 Concluding remarks.

Analytical Chemistry General Session

Garden Room

Cosponsored by ANYL

E. Jamalzade, *Organizer*

E. Hecht, *Presiding*

9:00 Introductory Remarks.

9:05 510. Non-chemistry processes needed for a functioning chemistry lab: A case study of the role of staff development and organizational structure. **B. Moradi**

9:25 511. Multi-laboratory validation of a robust analytical method for benzotriazole in environmental matrices. **D. Cordova**

9:45 512. Compositional profiling and prebiotic potential of oligosaccharides in plant-based beverages: comparative insights from oat, soy, coconut, and almond beverages. **H. Peng, Y. Gu, D. Barile**

10:05 Concluding Remarks.

Chemical Biology, Biochemistry, and Medicinal Chemistry General Session

Regency Ballroom 2

Cosponsored by BIOL and MEDI

E. Villemure, *Organizer*

I. S. Darwish, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 513. *De Novo* design and evolution of a generalist binding protein. **S. Bhattacharya, Y. Chen, A.N. Volkov, I.V. Korendovych, W.F. Degrado**

9:25 514. Rapid antibiotic susceptibility determination by fluorescence lifetime tracking of bacterial metabolism. **M.D. Rojas-Andrade, K. Perinbam, Q.T. Nguyen, J.S. Kim, F. Palomba, K. Whiteson, M. Digman, A. Siryaporn, A. Hochbaum**

9:45 515. CyclicCAE: An autoencoder for heterochiral macrocycle sampling. **P. Hosseinzadeh**

10:05 516. Harnessing protein backbone modification to engineer functional biomaterials. **P. Pratakshya, M.B. Francis**

10:25 Intermission.

10:35 517. Machine learning approach to identify determinants of WNT family protein-protein interactions. **S. Capponi**

10:55 518. Finding druggable transcription factors: A data-driven journey from identification to small-molecule synthesis. **S. Newman**

11:15 519. Role of the identical nucleotide binding domains in the Escherichia coli ABC transporter MetNI-Q. **M. Gardner, J. Yang**

11:35 520. Oligomeric state-dependent activity changes and conferred allostery in human glutamine synthetase. **M. Tecson, H. Yamamura, C. Geluz, M. Hales, D. Fournier, E.R. Greene**

11:55 Concluding Remarks.

Memorial Symposium in Honor of Robert H. Grubbs (Sponsored by Umicore)

Club Regent

Cosponsored by MPPG

C. M. Bates, J. S. Cannon, K. M. Engle, R. B. Grubbs, V. M. Marx, D. O'Leary, V. A. Piunova,

F. Toste, R. Weitekamp, *Organizers*

G. Miyake, H. Nelson, *Organizers, Presiding*

9:00 Introductory Remarks.

9:15 521. Carbon pronucleophiles as a new tool in sulfur fluoride exchange (SuFEx). **N.D. Ball**

9:40 522. Catalyst initiation and its effects on Pd-catalyzed couplings. **W. Wolf, D.T. George, S.R. Wisniewski, K.M. Engle, D.G. Blackmond, R. Daley, s. ma, S. Yang, A. Daru, M. Deng, B. Werley**

10:05 523. Megasupramolecules and fluoride-ion batteries: a tale of a couple of Grubbs chemistry startups. **S. Jones**

10:30 Intermission.

10:45 524. Photocatalytic crosslinking-activated sorting (PhoCAS): Library-scale parallel sorting of single cells and biomolecules. **L. Luo**

11:10 525. Supporting (Grubbs) catalysts in structured polymers. D. Balcer, M. Woo, J. Amador Flores, S. Ceja, A. Acosta, M. Omar, S. Velasquez, T. Sapp, M.S. Griffin, K. Huynh, J. Bryant, Y. Mo, J.J. Ramirez, **M.R. Radlauer**

11:35 526. An enantioselective synthesis of indolizidine alkaloids. **J.S. Cannon**

12:00 Concluding Remarks.

Sustainable Materials from Biorenewable Sources

Empire Room

Cosponsored by PMSE and POLY
V. A. Piunova, *Organizer, Presiding*

9:30 Introductory Remarks.

9:35 527. How customer collaboration drives breakthrough discovery. **K. Ingalls**

9:58 528. Machine learning-guided discovery of sustainable biomaterials: A Bayesian optimization framework with embedded domain expertise. **I. Kaur**

10:21 529. Replacing single-use plastics with regenerative materials. **M. Rolandi**

10:44 Intermission.

10:58 530. Engineered Silk Proteins as Bio-Derived Alternatives in Skin and Hair Care. **C. Rasmussen**

11:21 531. Seaweed solutions: Building a new economy beyond single-use plastics. **K. Barker, V.A. Piunova**

11:44 532. Withdrawn

12:07 533. Field evaluation of moisture harvesting biopolymer hydrogels for soil water retention and microclimate enhancement. **S. Li**

Physical and Computational Chemistry General Session

California Room

Cosponsored by COMP and PHYS

V. M. Marx, *Organizer, Presiding*

R. Chakraborty, *Presiding*

9:45 Introductory Remarks.

9:50 534. Solvent effects on cresyl violet: A hybrid QM/MM and spectral simulation study. **G. Carlson**, C. Isborn, L. Shi

10:10 535. The isotopic composition of nitrous oxide formed in a low temperature non-equilibrium plasma. **E. Hazen**, K.A. Boering

10:30 536. Temperature dependence of the oxygen-17 anomaly in ozone. **G. Cazares**, K.A. Boering

10:50 Intermission.

11:05 537. Interplay between stereochemically active lone pair repulsions, Sigma hole interactions, and delocalized redox processes in topochemical fluoride-ion insertion. **A. Pakhira**, S. Hariyani

11:25 538. Rational design and control of mixed ionic-electronic conducting metal organic frameworks for Li-S batteries. **S. Nanayakkara**, N. Lopez, K. Kim, L. Wan, M.C. So

11:45 539. How subtle interactions drive selectivity in intramolecular cyclizations: A computational insight. **P. Bianchi**, K.N. Houk

12:05 540. Crystallization of calcium oxalate in presence of citrate and Ni ions. **P. Rehak**, P. Kral

12:25 Concluding Remarks.

Advances in Natural Products Chemistry - Symposium in Honor of Harry Mosher

Gold Room

Cosponsored by ORGN

N. L. McClure, *Organizer, Presiding*

10:30 Introductory Remarks.

10:35 541. Harry and Carol Mosher: Lifetimes of the advancement of chemistry and service for ACS. **N.L. McClure**

10:55 542. Inspired by nature, informed by design: Exploring the bounties and redefining the boundaries of natural product synthesis in a non-canonical academic setting. **E. Njoo**

11:15 Intermission.

11:25 543. Natural Products Magnetic Resonance Database (NP-MRD): Comprehensive database and repository for NMR data of natural products. **J.R. Cort**

11:45 544. Metabolomic profiling of Taraxacum kok-saghyz reveals tissue-specific bioactive compounds with therapeutic potential. **M. Tan**, D. Swiger, C.S. Jeffrey

12:05 545. Breeding healthier blueberries: Genomic and analytical insights into Monotropine production. **I. Kaur**, C.P. Leisner, D.P. Cladis

12:25 Concluding Remarks.

Analytical Chemistry in Drug Development and Manufacturing

Garden Room

Cosponsored by ANYL

T. Chen, *Organizer*

E. Jamalzade, B. Wei, *Organizers, Presiding*

10:30 Introductory Remarks.

10:35 546. Derivatization strategy to enable quantitation of trace-level boronic acids and boronic esters by LC-MS: Application in pharmaceutical PMI control. **P. ZHANG**

11:15 547. Quality by Design approach for efficient development of robust and discriminatory dissolution methods. **L. Meng**, L. Zhang

11:55 Concluding Remarks.

Carbon Capture and Conversion for a Sustainable Future

Regency Ballroom 1

Cosponsored by ENFL

R. Kowalski, A. Taheri, J. Velazquez, *Organizers*
H. Kaur, B. O. Okoye, R. Siegel, *Organizers, Presiding*

10:30 548. Improving performance and cost of direct air capture in dynamic conditions through modeling and system design. **N. Cross**, A. Aui, W. Li, S.H. Pang

10:50 549. Understanding the unique reactivity of Cu for electrochemical CO₂ reduction through atomistic simulations. **J. Varley**

11:20 Intermission.

11:35 550. Direct air reactive capture and conversion for utility-scale energy storage. **S.H. Pang**, A. Aui, N.C. Ellebracht, H.M. Goldstein, S. Halingstad, M.L. Jue, W. Li, M.J. Rasmussen, M. Yung

12:05 551. Probing corrosion in the electrochemical reduction of captured CO₂ sources using in-situ UV-vis and EPR spectroelectrochemistry. **S.E. Stieber**

12:25 Concluding Remarks .

Materials and Processes for Energy Storage and Conversion

Crystal Room

Cosponsored by INOR

M. J. Greaney, *Organizer, Presiding*

11:05 552. Additive manufacturing of polymer-derived ceramics for Sustainable Systems. **J. Dobson**, P. Onffroy, M.A. Saccone, M.T. Dulay, J.M. DeSimone

11:32 553. Design and fabrication of micro-architected 3D printed carbon structures for Sustainable Systems. **P. Onffroy**, J. Dobson, M. Lagat, S. Chiovoloni, M.T. Dulay, J. Lu, M.A. Saccone, J.M. DeSimone

11:59 Concluding Remarks.