Joint Midwest & Great Lakes Regional Meeting 2023

St. Louis, MO

October 18 – 21, 2023

Program Co-Chairs

Leah O'Brien

Jim O'Brien

Alex Mironenko

Marvin Meyers

WEDNESDAY EVENING

St. Charles Convention Center
North Hall

Analytical Poster Session

J. J. O'Brien, *Organizer*

7:15 - 9:00

1. Method development for the detection and comparison of trace level compounds in sources of the herbal supplement *Morus alba* using HPLC-UV and AAS. **S. Foote**, E. Price

2. Electrochemical detection of hormones using hierarchical bimodal nanoporous gold electrodes. **N. Haroon**, K.J. Stine

3. Antioxidant capacity of hot-brew and cold-brew tea (Prussian blue method). **M. Combs**

4. Functionalization of humic acid for pollutant extraction using Fe_3O_4 nanoparticles. **B. Hilsabeck**, B. Christensen, A. LaPage, J.J. Determan

5. Transforming separation science for better resolution in residue analysis using Monodisperse Fully Porous Particles (MFPP) columns. **C. Zhang**, L. Riter, E. Faden, G. Faden

6. HPLC determination of cortisol concentrations in hair samples of college chemistry majors. **M. Mistler**

7. Identification of bacteria using low-cost sample preparation and portable surface-enhanced Raman spectroscopy. **F. Alhalabi**, **M. Lingle**, **C. Flores Kaled**, **D. Orlando**, T. Spudich

8. Insert-based microfluidic system for endothelial cell culture with integrated analysis. **S. Azibere**

9. Assessment of Vinyl Chloride contamination in St. Louis water systems using GCMS/SPME analysis. **B. Karki**, **C. Flores Kaled**, **L. Mendoza**, T. Spudich

10. Determination of chromium (VI) and lead (II) in various apple juice brands. **A. Mason**

11. Method development for the detection and comparison of trace level compounds in sources of the herbal supplement *Silybum marianum* using HPLC-UV. **L. Beattie**, E. Price

12. A method on acrylamide elimination: Comparing and tracing reaction pathways of acrylamide and catechin (catechin quinone) using UHPLC-Q-exactive orbitrap mass spectrometry. **X. Liu**, J. Su, Y. Geng, F. Chen, B. Huang, H. Yang, X. Ma, X. Hu, J. Ji, L. Ma

13. Using 3D printed devices to elute and concentrate *S. cerevisiae* DNA. **E. Mendez-Ortiz**, C. Harbison, **J. Boley**, T. Huynh, **K. Kounovsky-Shafer**

14. Determining how the fluorescence changes for the TOTO-1 family of dyes when bound to DNA at different temperatures. **B. Menke**, **K. Kounovsky-Shafer**

15. Analyzing the variability in cannabinoid and terpene content of Cherry Wine hemp cultivars. **A. Tandukar**, M.G. Kinsel

16. Evaluation of content versus label claims of Δ^8-THC consumer products. M.G. Kinsel, **K. Elliott**, A. Tandukar

17. Electrochemical reduction of CO_2 into different useful products by using MXene-based catalysts: Advances, challenges, and future prospects. **s. arain**

18. To end all doubts: Oil and water phases imaged simultaneously using food-safe dyes. **Y. Loethen**

St. Charles Convention Center
North Hall

Biochemistry Poster Session

M. J. Meyers, *Organizer*

7:15 - 9:00

19. Molecular regulation of prenylated Gβγ trafficking between membranes. **s. piyawardana**, k. Olupothage, D. Wijayaratna, A. Karunarathne

20. Mass spectrometry-based structural investions of creatine kinase brain type. **N.K. McLaughlin**, R. Dastvan, M.L. Gross

21. Liquid-liquid phase separation in *Pseudomonas aeruginosa* biofilm matrices. **R. Abarbanel**, N. Fazio, C. Reichhardt

22. Lipopolysaccharide antagonist activity by curcumin derivatives. **R. Domalewski**, C. Sinobas Pereira, M.R. Nichols

23. Investigation of the molecular basis of ligand binding to ERRalpha. **P. Mittal**, L. Hegazy

24. Group 14 metallafluorenes as solvatochromic biological probes. **C.M. Dupureur**, W. McConnell, S. Jarrett-Noland

25. Examining the effects medium and long chain fatty acids on simple coumarin fluorescent lifetime probes bound to HSA. G.W. Bjornstad, S.J. Brekken, **T.P. Gonnella**

26. Matrix composition of anaerobically-grown *Pseudomonas aeruginosa* biofilms. **K. Duong**, A. Zheng, M. Barrington, N. Fazio, C. Reichhardt

27. Engineering an opsin to control Endoplasmic Reticulum exclusive G protein signaling optically. **C. Rajarathna**, S. Ubeysinghe, A. Karunarathne

28. Efficacy modulation by targeting the sodium binding allosteric site in the delta opioid receptor. **B.R. Varga**, S.M. Bernhard, A. El Daibani, S. Zaidi, J. Aquilar, K. Appourchaux, A. Nazarova, J.H. Lam, A. Kouvelis, S.O. Eans, E. Margolis, J.F. Fay, A. Pradhan, V. Katritch, J.P. McLaughlin, S. Majumdar, T. Che

29. Our body's chemical response to stress: Enzymatic oxidation of 11-deoxycorticosterone by cytochrome P450 CYP11B2. K. Knobbe, J. Schell, K.K. Glaser, **R. Glaser**

30. Structure-based design of bisubstrate tetracycline destructase inhibitors that block flavin redox cycling. **E.E. Williford**, C.M. DeAngelo, K. Blake, H. Kumar, K.K. Lam, K.V. Jones, N.H. Tolia, G. Dantas, T.A. Wencewicz

31. Identification of DNA aptamers for treatment of psoriasis and diabetic wound healing. **A. Parvez**

32. Experimental determination of thermodynamic parameters for pseudouridine-guanine pairs in duplexed RNA: Terminal mismatches, tandem pairs, and bulge loops. **J. Stone**, S. Arteaga, B. Znosko

33. Investigating the impact of aptamer binding on flavin cofactors. **T. Pentland**, R. Orr, S. Patel, B. Recupido, D.A. Baum

34. Identification and characterization of RNA triloop sequence families. **M. Hertel**, J. Hou, B. Znosko

35. Development of a high-throughput scale-down model in Ambr®250HT for plasmid DNA fermentation process. S. Fang, **D. SInanan**, M. Perez, **R.G. Cruz-Quintero**, S.R. Jadhav

36. Flash versus conventional ionizing radiation dose rate effects on DNA single and double strand breaks. D. Mulrow, N.E. Gutierrez-Bayona, E. Cacchillo, A. Demeris, S. Lyou, S. Scruggs, Y. Hao, A. Darafsheh, L.G. Sobotka, **J.S. Taylor**

St. Charles Convention Center
North Hall

Organic Poster Session

M. J. Meyers, *Organizer*

7:15 - 9:00

37. Synthesis of phenothiazine-coumarin analogs with large red Stokes' shift. **F.F. Olubiyo**

38. 4,2'pyridine-2-mercaptopyrimidine glycosides. **M. Duffield**, S. Hasty

39. Investigation of carbohydrate leaving group hydrogen bonding. **A. Meyer**, S. Hasty

40. Synthesis and application of macrocyclic aromatic tellurides. **S. Zhang**, C. Yen, J. Jin

41. Structural elucidation of functionalized dibenzalacetone compounds. J. Gitua, **K. Larson**, **B. Hinz**, **B. Dice**, **J. Vins**

42. Comparative study on different Fmoc solid-phase peptide synthesis protocols towards reduced solvent consumption and improved efficiency. **A. Babel**

43. Synthesis of ditriazoleacetylenes and ditetrazoleacetylenes for antimicrobial use. B. Eichler, **E. Dierks**, **X. Gabel**

44. Applications of *N*-vinyltrialkylammonium and *N*-vinylpyridinium tetrafluoroborate salts in the total synthesis of alkaloid natural products. **T. Domingos**, C. Brown, A. Nguyen, K.R. Buszek

45. New unsymmetrically terminated 6,6'-biazulenes. **C. Weghorn**, S. Kelsey, X. Ortiz-Medina, M.V. Barybin

46. Self-complementary semicarbazone-based arrays. **S. Olsen**, V. Birman

47. Preparation of 2-tellurophenecarboxylic acid and 2-tellurophenethiocarboxylic acid. **A.S. Brown**, M.R. Hulce

48. Synthesis of dihalocyclopropane fatty esters. **D. Saakov**, C. Clinger

49. Towards NIR-II activatable two-photon absorbing BODIPY photocages. **A. Egyed**, A. Winter, Y. Aydogan, J. Wachtveitl, A. Heckel

50. Stereoselective hydroacylation of cyclobutenes. **S. Powell**

51. Chemosensing properties of aminopyridine click chelators. **C.A. Price**, J.T. Fletcher

52. HPLC-based automated synthesis of glycans in solution. **G.A. Kashiwagi**, L. Petrosilli, S. Escopy, K.J. Stine, A. Demchenko

THURSDAY MORNING

St. Charles Convention Center
Ballroom B

Analytical

J. J. O'Brien, *Organizer*
C. M. Greenlief, *Presiding*

8:15 Introductory Remarks.

8:20 53. Analysis of human milk for environmental toxins by LC-MS/MS, GC-MS/MS, and LC-HRMS. **E. Bakota**, K. Richards, R. Smith

8:45 54. Lipid droplet composition evaluation in gynecological cancers using MALDI-MSI and LC-MS/MS. **A. Chirchirillo**, S.L. Shan, A. Braundmeier-Fleming, C. Rawlins, K.R. Tucker

9:10 55. Prostaglandin E2 quantitation in porcine plasma via UPLC-MS/MS instrumentation: An approach in animal welfare evaluation. **K.P. Kompalage**, R.J. Tucker, J. Coetzee, C.T. Culbertson

9:35 56. Quantitative UPLC-MS/MS method for aquatic and plasma tryptophan to monitor kynurenine pathway-associated animal behavior. **R.J. Tucker**, K.P. Kompalage, J. Coetzee, C.T. Culbertson

10:00 Intermission.

10:20 57. Quantification of Levodopa in human serum by UPLC-MS/MS: A potential method for the evaluation of Parkinson's therapeutics. **K.P. Kompalage**, R.J. Tucker, C.T. Culbertson

10:45 58. Identifying the antimicrobial composition of honeys from Washington state. **K. Nyarko**, C.M. Greenlief

11:10 59. 14-factor model for catalytic depolymerization product distributions between lignin species. **A. Ponukumati**, Y. Gao, H. Li, M.J. Walker, X. Zou, S. Jeon, J. Barrett, O. Hosseinaei, D.P. Harper, P.C. Ford, B.J. Williams, M.B. Foston

11:35 60. Synthesis and characterization of cellulose acetate /titanium (iv) tungstomolybdate nanocomposite cation exchanger for the removal of selected heavy metals from aqueous solution. **B.M. minase**

St. Charles Convention Center
Meeting Room 103

Bioprocess Chemistry

J. Dong, *Organizer, Presiding*

8:15 Introductory Remarks.

8:20 61. Low-cost low energy pathway to make cellulosic sugars and ethanol from corn stover. **M. Ma**, Y. Zhang, J. Dong

8:55 62. Upcycling corn-ethanol co-products as high value monogastric animal feed via fungal based bioprocessing. X. Sun, **B. Hu**

9:30 63. Lignin-based hydrophobic deep eutectic solvents as sustainable extractants. **Y. Zhang**, C. Liu, Q. Qiao, U. Abbas, Q. Shao, **J. Shi**

10:05 Intermission.

10:25 64. Cellulose solvents for efficient agave biomass conversion. P. Sereerattanakorn, P. Chuangpusri, n. Lertthanaphol, S. Tulaphol, J. Wittayakun, S. Prayoonpokarach, J. Dong, **N. Sathitsuksanoh**

11:00 65. Chemicals production from CO_2 via acetate as an intermediary metabolite in an integrated fermentation process. **J. Dong**

St. Charles Convention Center
Ballroom D2

Inorganic

L. C. O'Brien, *Organizer*
E. J. Voss, *Presiding*

8:15 Introductory Remarks.

8:20 66. Manual Tafel analysis: Pitfalls and alternatives. **J. Coduto**, J. Leddy

8:45 67. Iron-pyrophosphate rectifying urea-rich wastewater pollution for sustainable hydrogen production and electronic coupling to improve charge storage. **R. Srivastava**, H. Chaudhary, F. M. de Souza, **R.K. Gupta**

9:10 68. Defining 18-*n*+*m* isomerism in transition metal-main group intermetallics. **A. Lim**, D. Fredrickson

9:35 . Chemical pressure-based theory for predicting modular intermetallic structures: Discovery of $Pr_{1.1}Mg_4Zn_{10}$. **D. Gressel**, R.T. Fredrickson, D. Fredrickson

10:00 Intermission.

10:20 69. Structural effects on the surface behavior of uranyl complexes. **C.J. Paranjothi**

10:45 70. There and back again: Journey with molecular metal oxides. G. Duggan, S. Rabbani, **P. Miro**

11:10 71. Tandem electrocatalysis between Cu-Zn nanostructures for the selective reduction of CO_2 to C_2 and C_{2+} compounds. **P.P. Jofré**, Z.D. Schultz, M.A. Isaacs

11:35 72. Single molecule imaging of heterogenous charge transfer: Role of surface species on nanoscale photocatalysts. **W. Rackers**, B. Sadtler

St. Charles Convention Center
Jr Ballroom D

Med Pharma Chem

M. J. Meyers, *Organizer*
N. Jentsch, *Presiding*

8:15 Introductory Remarks.

8:20 73. Directly targeting antibiotic resistance and key virulence factors of ESKAPE pathogens. **C.V. Rice**

8:40 74. Functional magneto-plasmonic nanozyme for ultra-sensitive detection of foodborne pathogens. **S. Santra**

9:00 75. Design of new N-salicylidene alanine transition metal Schiff-base complexes with Zn(II), Mn(II), Fe(II), and Fe(III): Synthesis, characterization, toxicity, and computational studies of the potential metal-ligand binding sites. **J. Titah**

9:20 76. Structure-based discovery of novel ERRα modulators. **L. Hegazy**

9:40 77. The hunt for antimicrobial enhancers against resistant *Staphylococcus aureus*. **A. Sarkar**

10:00 Intermission.

10:20 78. Membrane disrupting dual action dihydrofolate reductase inhibitors. **J.D. Georgiades**, A.R. Smith, B.A. Hathaway, T.A. Wencewicz

10:40 79. Discovery, synthesis and characterization of acetamide ether series as novel GIRK1/2 potassium channel activators. **S. Nahid**, Y. Du, B. Spitznagel, C. Weaver, C.R. Hopkins

11:00 80. Synthesis and optimization of Phosphoinositol-4-kinase (PI4K) inhibitors for *Cryptosporidiosis*. **S. Brosend**, E. Oboh, N. Jentsch, J.E. Teixeira, C.D. Huston, M.J. Meyers

11:20 81. Glyoxal-caged nucleoside reverse transcriptase inhibitors as extended-release prodrugs. **D. Karloff**, R.T. Stubbs, S. Knutson, J.M. Heemstra

St. Charles Convention Center
Jr Ballroom C

Novel Approaches to Traditional Challenges in Glycoscience

C. De Meo, *Organizer, Presiding*

8:15 Introductory Remarks.

8:20 82. Nanogels for selective hydrolyses of glycosidic bonds. **S. Striegler**

8:50 83. Microwave-based glycosylation methodology leads to novel immunotherapies. **P.R. Andreana**

9:20 84. Toward better characterized glycoconjugate vaccines: Oligosaccharide models to study regioselectivity of chemical activation and protein conjugation. **J. Xie**

9:50 Intermission.

10:05 85. How important is the nature of the protecting groups at C-4 in sialylations?. **C. De Meo**

10:30 86. Tools to study carbohydrate-protein interactions. **M.P. Farrell**

11:00 87. From batch to flow and manual to automated reactions: The case of glycan synthesis. **N.L. Pohl**

11:30 88. From stereocontrolled glycosylation to automated chemical synthesis of glycans. **A. Demchenko**

St. Charles Convention Center
Jr Ballroom B

Nucleic Acids

J. S. Taylor, *Organizer, Presiding*

8:15 Introductory Remarks.

8:15 89. Thermoreversible control of nucleic acid structure and function with glyoxal caging. **J.M. Heemstra**

8:45 90. Transcriptome-wide profiling and quantification of N^6-Methyladenosine by enzyme-assisted adenosine deamination. **W. Tang**

9:15 91. Interstrand DNA cross-links derived from abasic sites in DNA and initiation of their repair by components of the base excision repair pathway. **K.S. Gates**

9:45 92. DNA G-quadruplex: Structures, functions, and drug targeting. **D. Yang**

10:15 Intermission.

10:30 93. DNAzymes for modifying DNA and RNA nucleobases. **S.K. Silverman**

11:00 94. Evolutionary conservation of ornithine decarboxylase antizyme pseudoknot RNA binding to spermine. **J. Strauss Soukup**, R. McCracken, S. Thompson, G. Soukup

11:30 95. Visualizing a two-state conformational ensemble in stem-loop 3 of the transcriptional regulator 7SK RNA. **C.D. Eichhorn**

St. Charles Convention Center
Ballroom C

Organic

M. J. Meyers, *Organizer*
R. J. Perkins, *Presiding*

8:15 Introductory Remarks.

8:20 96. Rubisco-mimetic CO_2 capture systems: Theoretical and experimental studies of carbamylation using fluorinated tetrapeptides. **B.M. Jameson**, R. Glaser

8:45 97. Transfer hydrodeuteration of unactivated 1,1-disubstituted alkenes. **O. Smetana**, E. Rivera Torres, J. Clark

9:10 98. Insights into $O(^3P)$-mediated oxidation of alkenes: Kinetic isotope effects and computational approaches reveal a stepwise addition mechanism. **P.F. Maness**, R.D. McCulla

9:35 99. Solid-state [4+4] cycloaddition and cycloreversion with use of unpaired hydrogen-bond donors to achieve solvatomorphism and stabilization. **G. George**, K.M. Hutchins

10:00 Intermission.

10:15 100. Characterizing benzamide-based intermediates that are preparatory to ebselen derivatives. **J. Eilers**, B. Averkiev, C.B. Aakeroy

10:40 101. From solution to solid: Multidimensional study of radical materials and dynamic covalent chemistry. **Q. Kashif**, R. Zhang, A. Winter

11:05 102. Perfect dipole parallel alignment in ferroelectric crystals of methoxyphenyl substituted acetophenone azines, (MeO-Ph, Y)-azines: Improved design strategy for highly nonlinear optical (NLO) materials. **H. Bhoday**, N. Knotts, R. Glaser

11:30 103. How to modulate some photophysical properties of cocrystals?. **N. Marasinghe Prins**, B. Averkiev, C.B. Aakeroy

St. Charles Convention Center
Meeting Room 102

Organometallic Catalysis Research at PUIs

J. P. Lanorio, *Organizer, Presiding*

8:15 Introductory Remarks.

8:20 104. Towards earth-abundant photoredox catalysts: Complexes of Mn with asymmetric polyimines. **D. Arias-Rotondo**

9:00 105. Homogeneous catalysis using organometallic complexes as undergraduate research topics. **J.P. Lanorio**

9:40 Intermission.

10:00 106. C-N bond formation from C1 feedstocks. **M. Zhou**, D. Xiao, Y. Wang, X. Zhou, D. Hanson, E. Washburn, M. Ekmekci, D. Dennis, A. Paripati, E. Lee, J. Clore, H. Catania

10:40 107. Computational studies of organometallic catalysis - bond formation and oxidation by first row transition metals. **K.A. Grice**

11:20 Concluding Remarks.

St. Charles Convention Center
Meeting Room 104

Physical

L. C. O'Brien, *Organizer*
D. Ghosh, *Presiding*

8:15 Introductory Remarks.

8:20 108. Photochemistry of O_2 complexed with Aza-zaromatics. **B.F. Parsons**

8:45 109. Electronic structure and dynamics of bisphosphonate polyoxovanadates in noble metal surfaces. **M. Mahama**, B. Vlaisavljevich, P. Miro

9:10 110. Reexamination and reassignment of the low lying electronic states of CuO, copper oxide. A. Herrling, **L.C. O'Brien**, J.C. Harms, J.J. O'Brien, W. Zhou

9:35 Intermission.

10:05 111. Ultraviolet radiation may be prolonging the atmospheric lifetime of primary brown carbon aerosol. **H. Al-Mashala**, K.L. Betz, C. Calvert, J. Barton, E. Bruce, E. Schnitzler

10:30 112. Time-dependent density functional theory predictions of light absorption by biomass burning organic aerosol. **C. Calvert**, E. Schnitzler

10:55 113. Hygroscopicity of secondary brown carbon aerosol from aqueous photo-oxidation of phenolic precursors. **K.L. Betz**, C. Calvert, H. Al-Mashala, E. Schnitzler

11:20 114. Analysis of the $b\ ^4\Sigma^- - a\ ^4\Pi$ transition of O_2^+, dioxygen cation. **N.S. Woods**, L.C. O'Brien, J.J. O'Brien

St. Charles Convention Center
Ballroom D3

Theor/Comp Chem A: New Methods and Approaches

A. V. Mironenko, *Organizer*
M. K. Karunananda, *Presiding*

8:15 115. Cluster-based methods for strongly-correlated spin systems. **A. Papastathopoulos-Katsaros**, T.M. Henderson, G.E. Scuseria

8:35 116. Lanthanide chemistry in quantum computers. **A. Garcia Alejo**, W. Dejong, T.L. Windus

8:55 117. Development of a non-empirical tight binding theory for efficient quantum chemical calculations. **A. Leung**, A.V. Mironenko

9:15 118. Correlation consistent basis sets redesigned for utlization with density functional approximations. **J.J. Determan**

9:35 . Using instantaneous shape ratio and radius of gyration to map conformational landscapes of disordered proteins. **H. Shadman**, J.D. Ziebarth, Y. Wang

9:55 Intermission.

10:15 119. A semiempirical tight-binding-based approach for the simulation of platinum clusters on graphene. **S.L. Pellizzeri**, R. Wang, L. Hendershot, M. Boyd

10:35 120. Path of least resistance: Predictive thermochemical cycles for bulk and surface catalysis. **R.B. Wexler**

10:55 121. Surface phase diagrams from nested sampling. **M. Yang**, L. Bartók-Pártay, R.B. Wexler

11:15 122. Implementing a unified object-oriented framework for benchmarking chemical reaction optimization algorithms. **D. Kulathunga**, Z. Crandall, L. Qi, T.L. Windus

11:35 123. Computational techniques for ligand dissociation rates from protein kinases. **J.M. Spiriti**, C.F. Wong

St. Charles Convention Center
Meeting Room 101

To Flip or Not to Flip? How to Maintain Students' Attention Post-Pandemic

J. G. Andino, *Organizer*
S. A. Sheeley, *Presiding*

8:15 Introductory Remarks.

8:20 124. Building a path to success: Improving learning experiences through constructive alignment of course components. **R.S. Cole**, H.T. Nennig, A. Kreps

8:40 125. Breaking down and comparing student actions in the Open-Response Chemistry Cognitive Assistant Tutor. **E. King**, T. Holme, D. Yaron, S. Raysor, M. Benson, J. Sewall, K. Koedinger

9:00 126. Extending chatbot use cases across chemistry education spaces. **A. Lolinco**, **E. King**, M.J. Clark, T. Holme

9:20 127. The Chemistry Learning Center: A Wicked Solution to A Wicked Problem. **S.A. Sheeley**

9:40 Intermission.

10:00 128. Scaling chemistry writing soundboard sessions for large lecture classrooms using curated chatbots. **A. Lolinco**, T. Holme

10:20 129. The quest for the perfect LMS: A balance between control and ease of use. **J. Andino Martinez**

10:40 Discussion.

St. Charles Convention Center
North Hall

Analytical Poster Session

J. J. O'Brien, *Organizer*

8:30 - 10:15

130. Developing an insert to protect large DNA molecules during cell lysis. C. Polen, **E. Mendez-Ortiz**, C. Harbison, T. Huynh, **K. Kounovsky-Shafer**

131. Single molecule diffusion in nanostructured lyotropic liquid crystals: A closer look. **P. Kaur**, O. Shafiee, D.A. Higgins

132. The quest for quantifying residues of a complex herbicide in soil and sediment using microflow LC-MS/MS technology. **C.M. Allen**

133. Carbon dot biosensing of illicit drugs. **K. Hammer**, T. Raspante, M. White, S. Roach, M. Soendergaard, J.J. Determan

134. Herbicide presence in water tributaries originating from golf courses in the St. Louis region. **B. Karki**, C. Bean Chevez, T. Spudich

135. Antioxidants in hot-brewed and cold-brewed teas. **O. Brinker**, B.J. Bellott

136. Nanoporous gold (NPG) and hierarchical bimodal nanoporous gold (hb-NPG): chronoamperometric detection and detection limit comparison for Acetaminophen and Bisphenol A. **T.M. Adeniji**, P. Sondhi, K.J. Stine

137. Adsorption of perfluorooctanesulfonic acid on nanoparticles. **I. Shakoor**, C. Rico, F. Wang, R.N. Biagioni

138. Performance of scallions (*Allium fistulosum*) after exposure to cerium oxide nanoparticles and perfluorooctanesulfonic acid. **R. Pope**, P. Clubb, C. Rico, M. Reyes

139. Characterization of Adeno-associated viruses. **J. Surtan**, H. Nguyen, S.A. Soper

140. Nanoporous gold nanoparticles synthesis. **D. Lingden**, J. Bhattarai, K.J. Stine

141. Dual-mode colorimetric and fluorometric sensing of toxic metal ions. **H. Subbaiahgari**, J. Munyon, D. Ghosh

142. Measuring antibiotics in Shoal Creek using liquid chromatography mass spectrometry during the COVID pandemic. **C.D. Copling**, K. Maloof, J. Smith, M. Davis, C. Pancake, J. Pierson, L. Kupferle, A. Sullivan, K.R. Tucker

143. Quantitation and localization of beta-blockers and SSRIs accumulation in fathead minnows by complementary mass spectrometry analyses. **K. Selby**, R. Davis, J. Hoang, S. Rizzo, D. Hassan, B. Potter, K.R. Tucker

144. Quantifying insoluble ferulic acid and p-Coumaric acid in *Zea mays* using LC-MS. **V. Zerda Pinto**, A. Stephens, C. Copling, M. Benware, T. Lobb, D. Buckley, P. Carney, H. Labby, F. Romo, C. Butts-Wilmsmeyer, K.R. Tucker, O. Ayegbidun, I. Osikoya, L. Stenger, J. Juvik, L. Chatham, T. Jamann, A. Studer, M. Bohn, L. Roberts

145. Comparison of antioxidant and antibacterial properties in differently plant-sourced honeys. **S. Grana**, G.S. Fernando

146. Synthesis of triazole capped nanoparticles for a prospect towards chemosensing. **M. Castillo Vega**, D. Ghosh

St. Charles Convention Center
Jr Ballroom A

Innovative Analytical Measurements at the Micro and Nano Scale

R. S. Martin, *Organizer, Presiding*

8:30 Introductory remarks.

8:35 147. Chemical tagging and capillary LC-MS for single islet metabolomics. **J. Edwards**

9:00 148. Strategies for improving analysis of cancer-relevant proteins using capillary electrophoresis. **R.J. Whelan**

9:25 149. 3D-printed modular and scalable microfluidics to study ECM's roles in modulating cell metabolism. **C. Chen**

9:50 150. Nanoelectrochemistry for interrogating neurotransmitter dynamics with high spatiotemporal resolution. **M. Shen**

10:15 Intermission.

10:30 151. Nanoelectrochemical imaging with analyte switching. G. Jeffcoat, K.L. Anderson, **M.A. Edwards**

10:55 152. Dynamic interrogation and visualization of signaling and behaviors of cells trapped in 3D. **A. Karunarathne**, W. Thotamune, T. Mohan, S. Ubeysinghe, K. Cenhrang, S. Martin

11:20 153. Automated feeding of stored red blood cells for improved transfusion outcomes. L.D. Soule, S. Branch, **D. Spence**

St. Charles Convention Center
North Hall

Organic Poster Session

M. J. Meyers, *Organizer*

8:30 - 10:15

154. Halogen-bonding interactions template a [2 + 2] cycloaddition reactions within a series of symmetrical olefin-based reactants. M. Andren, E. Bosch, **R.H. Groeneman**

155. Influencing thermal expansion properties within mixed co-crystals utilizing isosteric molecular components. R. Brooks, G. George, K.M. Hutchins, **R.H. Groeneman**

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

157. Preparation and characterization of non-isocyanate polyurethane wood adhesives. **V. Chaudhari**, P. Patel, F. M. de Souza, **R.K. Gupta**

158. Bio-based non-isocyanide polyurethane films: Effect of amine and curing time. **P. Patel**, **R.K. Gupta**

159. Synthesis and study of novel macrocycles containing sulfur, selenium and silicon. **J. Jin**, S. Zhang, B. Gullapelly

160. Synthesis of an anticancer drug targeting the APOBEC3 protein. **E. Thompson**, **A. Regina**, A. Stricklin, J. Olson

161. Structural landscape of 3-amino-1H-1,2,4-triazoles. **M. Raynesford**, B. Averkiev, C.B. Aakeroy

162. Pyridinium-substituted 1,2,3-triazoles: Synthesis and antiseptic evaluation. **A.J. Burr**, J.T. Fletcher

163. Synthesis of cephalosporin antibiotic derivatives and evaluation of antimicrobial properties: New experiment for the undergraduate organic chemistry laboratory. **C. Flores Kaled**, D. Orlando

164. Unlocking supramolecular mysteries: Steric forces and hydrogen bonding in amide-modified heterocyclic compounds. **T. Patel**, B. Averkiev, C.B. Aakeroy

165. Optimizing the preparation of the decapeptide immunostimulant CPDI-02. **D.D. Smith**, J.P. Stewart, J.E. Parriott, S.M. Curran, J. Vetro

166. Design and synthesis of a potential anti-fungal agent. **H. Wolf**, K. Jantzi, J. Pruet

Theor/Comp Chem Poster Session

A. V. Mironenko, *Organizer*

8:30 - 10:15

167. Autodocking studies of oxygenated fullerenes as HIV protease inhibitors. **S. Kumar**, M. Kaminiski

168. Analyzing the nature of chemical bonding in lanthanide-containing solid-state structures. **N. Rehberg**, M. Polinski, B. Vlaisavljevich

169. Reparametrizing platinum-carbon interactions for GFN2-XTB calculations. **L. Hendershot**, R. Wang, M. Boyd, S.L. Pellizzeri

170. Vibrationally averaged dipole moments computed with multicomponent methods. **D. Fowler**, K. Brorsen

171. Calculation of vibrationally averaged molecular properties with constrained multicomponent MP2. **G.B. Tucker**, K. Brorsen

172. Understanding the binding mechanism of the SR8278 antagonist to REV-ERB-α using Gaussian accelerated molecular dynamics (GaMD) simulations. **M. Rahman**, L. Hegazy

173. Toward chemical structure determination from infrared spectra using deep learning. J. Ellis, R. Iqbal, **K. Yoshimatsu**

174. Understanding the nucleation and ESI-MS of lanthanide clusters. **P. Akubuiro**, P. Miro

175. On the choice of coordinate origin in length gauge optical rotation calculations. **T.J. Parsons**, T.C. Balduf, M. Caricato

176. Isotope effect in optical rotation. **B. Faintich**, T.C. Balduf, T.J. Parsons, M. Caricato

177. Comparison of the Gibbs free energy of complexation and hydration of hydrogen peroxide in water by density functional theory calculations. **B. Miller**, J.N. Woodford

178. Computational analysis of peptoid conformers in regards to the amino-ethyl (Nae) side chains. **A. Khan**, B. Tresca

179. Computational investigation of the hexazine anion. **D.M. Palomo**, K. Head-Marsden, A.W. Schlimgen

St. Charles Convention Center
North Hall

Biochemistry Poster Session

M. J. Meyers, *Organizer*

10:15 - 12:00

180. Utilizing simple coumarins as fluorescent lifetime reporters for HSA drug binding sites. **K.R. Ensign**, T.N. Peterick, T.P. Gonnella

181. The role of post-translational modifications in modulating MATR3 aggregation and toxicity. **K. Soe**, M. Sprunger, M. Jackrel

182. The *Pseudomonas aeruginosa* exopolysaccharide Psl as a phage target. **K. Amyx-Sherer**, A. Johannesman, S. Manikandan, K. Kurti, J. Chang, M. LeRoux, C. Reichhardt

183. Development of stable NLRP3 inflammasome protein-expressing ExpiCHO-S cells. **N. Zeller**, M.R. Nichols

184. Development of cell permeable peroxisome import moieties. **C.N. Okolie**, M.W. Beck

185. Structure and interactions of the fibrillar adhesin CdrA. **N. Fazio**, A. Jaysingh, M. Barrington, R. Abarbanel, E. Moss, M. BoClair, C. Reichhardt

186. Design of new N-salicylidene alanine transition metal Schiff-base complexes with Zn(II), Mn(II), Fe(II), and Fe(III): Synthesis, characterization, toxicity, and computational studies of the potential metal-ligand binding sites. **J. Titah**

187. Cross-priming as an approach to build stress and cross-stress tolerance against drought and salinity. **M. Erickson**, **E. McNally**, **E. Horton**, R. Pugh

188. Covalent mechanism-based inhibitors of tetracycline destructases. **R. Li**, T.A. Wencewicz

189. Comparing common biophysical methods to evaluate MS-based footprinting-induced perturbation of protein high order structure. **W. Wagner**, A. Moyle, N.D. Wagner, D.L. Rempel, M.L. Gross

190. Characterizing protein amyloidogenesis in *Staphylococcus aureus* biofilms and countering biofilms with engineered protein disaggregases. **C. Chang**, M. Howard, K. Miller, B. Sohn, J. Ryan, A. Xu, M. Jackrel

191. Characterizing amyloid beta 1-42 using mass spectrometry-based covalent labeling footprinting. **X. Kuang**, M.L. Gross

192. Canine KRAS and canine mutant KRAS G12R purification and crystallization. T. Criblez, **N.M. DeVore**

193. Application of HEK293T cells to study NLRP3 inflammasome-amyloid-β interactions. **C. Sinobas pereira**, M.R. Nichols

194. Alpha glucosidase inhibitory activity of Ailanthus altissima bark. **P. Curry**, **A.S. Wong**, A. Vummenthala

195. Quantification and biological implications of eco-coronated microplastics in urban stormwater run-off. **L. Cash**, S. Davis, R.A. Day

196. Protein characterization and crystal structure of yellow thermostable protein (YTP) Q66E E148D. **V. Ogbeifun**, C. Padgett, N.M. DeVore

St. Charles Convention Center
North Hall

Macro/Polymer Chem Poster Session

A. V. Mironenko, *Organizer*

10:15 - 12:00

197. Effects of magnetic field exposure on cellulose nanocrystal-reinforced soy protein isolate nanocomposite properties. **D. Kobayashi**, Z. Wang, H. Li, M. Foston

198. Development of photocaged amino acid sidechain peptide nucleic acid (PNA) monomers to enable rapid modulation of assembly state. **K.J. Skowron**

199. Metal free reassociating preformed particle gels. **Y.Y. Eriyagama**, T.P. Schuman, B. Bai

200. Effect of electron donating and electron withdrawing group substitutions on phenylalanine during the self-assembly of amphipathic pentapeptides. **A. Das**, U. Pramanik, M. Jackrel, J. Rudra

201. Effects of phenyl side chain length on the self-assembly of amphipathic peptides. **U. Pramanik**, A. DAS, M. Jackrel, J. Rudra

202. Fluorescence and gas sorption studies of thiourea carbon dot-incorporated metal-organic frameworks. **I. Bolzenius**, Z. Giamis, S. Roach, J.J. Determan, M. McConnell

203. Synthesis of biocompatible, renewable protein nanocomposites reinforced by surface-modified cellulose nanocrystals. **Z. Wang**, H. Li, W. Goldberg, M.B. Foston, G. Genin

204. Critical material uptake with novel functionalized electrospun nanofiber mats. **N. Shapiro**, S. Kim, T. Forbes, D.M. Cwiertny

205. Role of diamines on the properties of soybean-based bio-adhesives. **U. Panchal**, J. Patel, P. Patel, **R.K. Gupta**

206. Exploring soybean-based polyol and novel nitrogen-phosphorous additives for enhanced flame resistance in polyurethane foam. **S. Kondaveeti**, P. Patel, **R.K. Gupta**

207. Triethyl phosphate as an effective flame retardant in hemp seed oil-based rigid polyurethane foams. **S. Jariwala**, Y. Desai, T. Dawsey, **R.K. Gupta**

208. Highly flame-retardant bio-based polyurethane foams prepared using melamine-based intumescent flame retardants. **N. Chaudhary**, P. Patel, **R.K. Gupta**

209. Biobased polyester from 2,5-furan dicarboxylic acid: An alternative to poly (ethylene terephthalate). **L. Sharma**, P. Sahu, **R.K. Gupta**

210. Effects of nitrogen, phosphorous, and nitrogen-phosphorous based flame retardants on the properties of bio-based polyurethane foams. **J. Chaudhari**, P. Patel, **R.K. Gupta**

211. Structural and thermomechanical properties of rigid polyurethane foams prepared using fresh and recycled canola oil. **J. Patel**, P. Patel, **R.K. Gupta**

212. Preparation and characterization of soybean oil-based resin for adhesive applications. **J. Patel**, U. Panchal, P. Patel, **R.K. Gupta**

St. Charles Convention Center
North Hall

Med Pharma Chem Poster Session

M. J. Meyers, *Organizer*

10:15 - 12:00

213. Investigation of bromoacetyltryptamine and related analogs as inhibitors of serotonin N-acetyltransferase. **N. Wandrey**, M. Hill, L. Hamilton, M. Moxley, A.A. Thomas

214. Rational design on subtype selective CB_1R covalent ligands. **S.T. Le**, P. Bhattacharjee, M.R. Iyer

215. Development of GPR183 antagonists for the treatment of neuropathic pain. **V. Kalajdzic**, I. Olayide, K. Braden, D. Salvemini, C.K. Arnatt

216. Inhibitory effects of sulfur derivatives on *Leishmania tarentolae c*ell viability and secreted acid phosphatase *in vitro*. **H. Shang**, Z. Zelaya, C.G. Hamaker, M.A. Jones

217. Siderophore-based PET imaging agents of bacterial infection: A synthetic platform. **C. Merrick**, D. Thorek, D. Veis, T.A. Wencewicz

218. Characterization of novel solvents for use in topical emulsions. **T.T. Phan**, D.W. Osborne, G.A. Schick

219. Developing serine protease inhibitors as anti-viral and anti-cancer treatments. **M. Fath**, V.S. Banas, Z. Han, J.W. Janetka

220. Encapsulation of active pharmaceutical ingredients into polymeric micelles. **T. Nguyen**

221. 6-Azaindole derivatives for tau aggregate detection in Alzheimer's disease brain tissues. **M. Gholampour**, C. Brown, T. Domingos, M. Rayhart, A. Nguyen, K.R. Buszek, M. Haeri

222. Structure activity and property relationship studies on pyrazolopyrimidine TgCDPK1 inhibitors for the oral treatment of Toxoplasmosis. **A. Kooner**, C.L. Meena, I. Vilza, M. Medcalf, M.P. Mannino, Z. Huang, L.D. Sibley, J.W. Janetka

223. Lanthanide exposure *in vitro* differentially diminishes MTT cell viability in neuronal and glial cancer cell model systems. D.C. Platt, L. Ferrence, K.M. Terry, F. Breausche, G.M. Ferrence, **M.A. Jones**

224. Identification of BE5112[EB1] as estrogen-related receptors alpha selective agonist: synthesis, design, and structure-activity relationships. **H. Okda**, B. Elgendy

THURSDAY AFTERNOON

St. Charles Convention Center
Ballroom B

Analytical

J. J. O'Brien, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 225. Effects of ion symmetry on molecular ordering transitions in ionic liquid films. **S.K. Shaw**, C.B. Lasar, F. Filippi, A. Horvath, S. Koutsoukos, D. Rauber, M.B. Van Den Top, T. Welton

2:00 226. PolyJet 3D printed microfluidic devices for microchip electrophoresis. **M.A. Selemani**, R.S. Martin

2:25 227. Substrate hydrophobicity affects environmental films' physical and chemical properties. **U.G. AKPORERE**, J. Deyoung, S.K. Shaw

2:50 228. Probing solute nanoconfinement in nanoporous anodic aluminum oxide membranes: Fluorescence correlation spectroscopy investigation of ethanol/water mixtures. **H. Rashidi**, T. Ito, D.A. Higgins

St. Charles Convention Center
Ballroom D1

Biochemistry

M. J. Meyers, *Organizer*
M. Sumita, *Presiding*

1:30 Introductory Remarks.

1:35 229. Mechanism and thermochemistry of rubisco activation by lysine carbamylation reactions: An ONIOM study. K. Knobbe, J. Schell, K. Yang, **R. Glaser**

2:00 230. Novel interaction between two proteins involved in nucleosome assembly. **G. Jaworski**

2:25 231. Stable aptamer-functionalized microelectrode array platform for point-of-care detection of microbial metabolites. **Y. Chang**, K.D. Moeller

2:50 232. Catalytic enhancement of an artificial RNA ligase through engineered domain addition. **D. Morrone**

3:15 Intermission.

3:35 233. Shifty behavior of redox cofactor-binding aptamers. **D.A. Baum**

4:00 234. Progress predicting RNA secondary and tertiary structure from sequence. **B. Znosko**

4:25 235. Immunostaining adenosine-to-inosine editing in cells using endonuclease V. **A. Quillin**

St. Charles Convention Center
Meeting Room 101

Chem Ed

J. J. O'Brien, *Organizer*
S. B. Luesse, *Presiding*

1:30 Introductory Remarks.

1:33 236. Bridging the gap between general chemistry and organic chemistry through a pre-semester review module. **R.J. Perkins**, B. Woods

1:56 237. Student experiences with flipped learning in organic and engineering chemistry. **S.B. Luesse**

2:19 238. Design and development of items for a resonance concept inventory. G.C. Tetschner, **S. Nedungadi**

2:42 239. Use of a hybrid specifications grading system in general and inorganic chemistry courses. **M.J. Drummond**

3:05 Intermission.

3:20 240. Impact of cognitive profiles on organic chemistry performance. **S. Nedungadi**, S. Shenoy

3:43 241. Anti-schistosomiasis compound synthesis in the undergraduate organic chemistry laboratory. **S.L. Debbert**, T.J. Quincy

4:06 242. Methods for modeling norms, integrating real scores, and building custom exams in organic chemistry. D. Schreurs, O. Michels, J.R. Raker, **S. Nedungadi**, K.L. Murphy

4:29 243. Simple 3D-printed spectrophotometer for use in high school and undergraduate chemical education. **J.F. Destino**, E.M. Gross, T. Nguyen, A. Madsen

4:52 244. Bioplastics in the general chemistry lab: Widening the range of possible experiments. **G.R. Wyllie**, T. Eggen, F. Rasulova, H. Olson, J. Weber, D. Traffie, L. Hinckley

St. Charles Convention Center
Jr Ballroom C

Dynamic Properties of Crystals

R. H. Groeneman, *Organizer, Presiding*

1:30 245. From molecular to supramolecular to functional materials. V. De Silva, V. Panikkattu, **C.B. Aakeroy**

2:00 246. Investigation into crystallization and porous systems of metal organic materials. **L. Applegate**, N. Plein

2:30 247. Determination of a rate constant and energy of activation for pedal motion disorder using single crystal X-ray diffraction data. **G.M. Ferrence**, C.E. Fuhlhage, R.H. Groeneman, E. Bosch

3:00 248. Use of motion, temperature, and light to achieve dynamic solid-state materials. **K.M. Hutchins**

3:30 Intermission.

3:45 249. Dimethoxypillar[5]arene as a versatile, pseudo-porous sorbent. **K.T. Holman**

4:15 250. Beautifying your benchtop: Crystal landscaping of photoactive crystalline materials. **J.B. Benedict**

4:45 251. Reactions in organic crystals for the preparation of small molecules. **L. MacGillivray**

St. Charles Convention Center
Meeting Room 102

Electrochemistry

M. J. Shaw, *Organizer, Presiding*

1:30 252. Bioelectrocatalysis for electrosynthesis. **S.D. Minteer**

2:00 253. From molecules to molecular surfaces and back again: Exploiting the synergy between electrochemistry and synthesis. **K.D. Moeller**

2:20 254. Stable and nonflammable gel electrolytes for enhanced performance and safety in lithium-metal batteries. n. Lertthanaphol, M. hossain, S. Tulaphol, T. Maihom, V. Jeager, **N. Sathitsuksanoh**

2:40 255. Electrochemical behavior of electrode/graphene nanoribbon hybrid materials. **K. Glusac**

3:00 Coffee Break.

3:15 256. Network electrochemistry: How to make more synchronized reactions from more heterogenous units. **I.Z. Kiss**

3:35 257. Electrochemistry for the development of selective organic reactions. **C.A. Malapit**

3:55 258. Single CuN_4 sites enable atomic Fe clusters with high-performance oxygen reduction reaction. **S. Wu**, k. Cadien, Z. Li

4:15 259. Synthetic and redox studies of Ru(saloph)(NO)(OMe) (saloph = N,N-bis(salicylidene)-1,2-diaminobenzene). **J.M. Smalling**, M.J. Shaw

4:35 260. Electrochemical investigations of methylimidazole derivatives of ruthenium nitrosyl complexes. **M.J. Shaw**, S.R. Redpath, B.A. Cuppett

4:55 261. Nanotube arrays with cupper substrate for lithium battery performance.. **B.M. minase**

St. Charles Convention Center
Jr Ballroom A

Environmental Chemistry in Agriculture

L. Riter, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 262. Bridging bio-based materials and agro-food systems for environmental sustainability. **D. Kim**, Y. Cao, B. Marelli

1:55 263. Assessment of environmental fate and metabolism of agrochemicals: An industry prospective. **M.F. Bedair**

2:15 264. Analyzing the environmental impact of a commercial aquaponic system in Taiwan using LCA. **S.T. RIKITU**

2:35 265. Promotion of the catalytic polymerization of hydroquinone towards humic-like substances by graphitic carbon nitride. **M.M. Mahmoud Ahmed**, Y. Liu, **S. Desikan**, **D. Tzou**, **H. Nail**, M. Wu, **M. Lin**, **Y. Tzou**

2:55 266. Studying the effect of plastic mulch photodegradation on its biodegradation process. **M. Salehi**, G. Bonyadinejad

3:15 Intermission.

3:30 267. Simplified fatty acid preparation via single pot hydrolysis and methylation. **J. McKenney**, C. Hagerty

3:50 268. 9-1-1 what's your soil emergency?: Delivering a modernized, high-throughput method through cross-functional collaboration. **H. Henderson**, P. Jensen, P. Karunanithi, S. Cao, W. Li, M. Kurtzweil, E. Tesfu

4:10 269. Elucidating factors contributing to dicamba volatilization by characterizing chemical speciation in dried dicamba-amine residues. **K. Parker**

4:30 270. The rebound effect of circular economy and the solution for Sustainable Development Goal 12: Case study of e-waste management. **S.T. RIKITU**

4:50 271. Circular economy models for smart phones: A case of Taiwan. **S.T. RIKITU**

5:10 Discussion.

St. Charles Convention Center
Ballroom D2

Inorganic

L. C. O'Brien, *Organizer, Presiding*

1:30 272. Calcium-containing nanoparticles for sunscreen formulation, gene transfer and drug delivery. **M. Hasan**

2:00 273. Understanding structure-function relationships in the nucleation of polyoxovanadate-alkoxide clusters. **G. Duggan**, S.N. Corsi, P. Miro

2:30 274. Organometallic *f* element complexes with yldiide ligands. **A. Gremillion**, M. Jörges, V.H. Gessner, J.R. Walensky

3:00 Intermission.

3:15 275. Structural divergence of heavy metal complexes with isomeric chalcogenophenecarboxylates: A single crystal investigation. **E.M. Villa**, D.T. Newman, A. Lang

3:45 276. Computational study of glaserites for non-linear optical and lasing properties. **S.L. Pellizzeri**, D. Craig

4:15 277. Unsymmetric metalation of a redox non-innocent, centrosymmetric 2,2'-diisocyano-6,6'-biazulenic π-linker. **M.V. Barybin**

St. Charles Convention Center
Jr Ballroom D

Medicinal Chemistry & Chemical Biology: Discovering New Biology and New Drugs Through Chemistry

A. M. Crider, *Organizer*
M. J. Meyers, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 278. Targeting the sodium binding allosteric site in GPCRs to design novel analgesics. **S. Majumdar**

2:00 279. Identification of 2,5-disubstituted thiophenes as potent estrogen-related receptor agonists. **J.K. Walker**

2:25 280. Development of Rev-Erb agonists as potent non-opioid analgesics for chronic inflammatory pain. **B. El-Gendy**

2:50 Intermission.

3:10 281. Targeting nicotinic acetylcholine receptors for pain and addiction. **A.P. Riley**

3:35 282. Studies of the role of the immunoproteasome under inflammatory conditions. **D.J. Trader**

4:00 283. Uncovering the roles of oxysterols in neuropathic pain. **C.K. Arnatt**

4:25 284. Development of 3,4,5-trisubstituted-1,2,4-triazoles as somatostatin subtype-4 receptor agonists. **A.M. Crider**, K. Witt, K. Sandoval, M. Kontoyianni

St. Charles Convention Center
Ballroom C

Organic

M. J. Meyers, *Organizer*
E. Bauer, *Presiding*

1:30 Introductory Remarks.

1:35 285. Endophytes, caves and insects: Searching for fungi that produce antimicrobial metabolites. **K.P. Manfredi**, J. Nuerhing, B. Guevara, J.P. Peters

2:00 286. Synthesis and characterization of oxaliplatin analogs for their localized controlled release. **K. Cisneros**, T. Fujiwara, T. Brewster, T. Ferdous, A. Akinwole

2:25 287. Efforts to expand diversity in supramolecular synthons: Binary cocrystals of pyridine 2,4-dicarboxylic acid and N-heterocyclic coformers. **C.I. Ezekiel**, L. MacGillivray

2:50 288. Selective photocatalytic functionalization of diamantane and higher-order diamondoids. **M.M. Wymore**, D. Martin

3:15 Intermission.

3:35 289. Detection of glycolipids using multi-component fluorescent sensor system. **F. Aynekulu**, A. Bade, T.E. Glass

4:00 290. Ferroelectric crystals of conjugated donor-acceptor para-substituted 1,4-diphenyl-1,3-butadienes: New dipole-parallel aligned NLO active materials. **J.D. Nulsen**, H. Bhoday, R. Glaser

4:25 291. Efficient chemical decontamination of organophosphate pesticides and nerve agents. **E. Darkwah**, P. Aryal, P. Reddy

4:50 292. Effects of cascade Förster resonance energy transfer fluorophores on carbon dot and N719 sensitized heterojunction TiO_2/NiO solar cells. **T.F. Yadeta**

St. Charles Convention Center
Meeting Room 104

Physical

L. C. O'Brien, *Organizer*
K. J. Stine, *Presiding*

1:30 Introductory Remarks.

1:30 293. Plasma-activated water-mediated destruction of fenitrothion. **M.R. Winburn**, E. DeLeon, K. Schuelke, W. Mei, H. Li, C.L. Cheung

2:00 294. Importance of dispersion in the molecular geometries of Mn(III) spin crossover complexes. S. Roy Chowdhury, **N. Nguyen**, B. Vlaisavljevich

2:30 295. Migration current coupling induced synchronization patterns of complex electrochemical reactions in 3D printed microfluidic flow devices. **J. Tetteh**, I.Z. Kiss

3:00 Intermission.

3:30 296. Surface reaction pathways of monochloramine on iron interfaces for uncovering effects of water disinfection. **K.A. Perrine**, S. Pandey, R. Mackie

4:00 297. Synergistic brønsted and lewis acid sites in amorphous silica-alumina catalysts for efficient isosorbide production from aqueous sorbitol. n. Lertthanaphol, P. Chuangpusri, S. Tulaphol, M. Rahaman, **N. Sathitsuksanoh**

4:30 298. Cooperative Lewis and Brønsted acidities of amorphous silica-alumina catalysts for efficient dihydroxyacetone isomerization to lactic acid in liquid water. P. Chuangpusri, n. Lertthanaphol, S. Tulaphol, T. Maihom, P. Sereerattanakorn, J. Pranpranod, S. Jantasee, P. Weerachawanasak, **N. Sathitsuksanoh**

St. Charles Convention Center
Meeting Room 103

Process Development in Industry: Solving Problems

M. R. Tracey, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 299. Challenges with antibody drug conjugate (ADC) linker reactivity. **T. Ni**, T.J. Hunter

2:00 300. The development of an RP-HPLC method with a mixed-mode column for the determination of process impurities in CPD 1 product. **T.J. McNabb**, S. Kovur, M. Zart

2:25 301. Practical processes in a crunch: CDMO approach to process chemistry in a demand-driven world. **C.J. Kassl**

2:50 302. Novel synthesis of an eco-friendly $MgO●Al_2O_3●SiO_2$ - engineered rice husk biochar for nickel sorption in wastewater. **D.O. Oguntuyi**, P.M. Rodrigo, O. Olabode, A.F. Abdulraheem, C.U. Pittman, T.E. Mlsna

3:15 Intermission.

3:35 303. What do you do when the last company to make your critical reagent stops making it?. **W. Boulanger**

4:05 304. Design of an effective and safe cyanide waste treatment process. **M. Schiesher**, C. Keyes, G.S. Buenger, D.R. Adams, J.R. Durrwachter

St. Charles Convention Center
Jr Ballroom B

Proteins and Lipids

J. K. Bashkin, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 305. Lipids as molecular switches: connecting stress cues to metabolic and growth alterations. **X. Wang**

2:00 306. Alternative mechanisms for DNA engagement by BET bromodomain-containing proteins. **W.C. Pomerantz**

2:25 307. Structure-function relationship of heme oxygenases from *Mycobacterium tuberculosis*. **P. Mak**

2:50 308. Engineering non-heme iron halogenases into promiscuous and selective biocatalysts. **A. Bhagi-Damodaran**

3:15 Coffee Break.

3:35 309. Predicting substitutions outside the active site that make enzymes faster. C. Pierce, G. Casadevall, B. Guan, J. Iglesias-Fernandez, H. Lim, L. Greenberg, M. Walsh, K. Shi, H. Aihara, R. Evans, S. Osuna, **R. Kazlauskas**

4:00 310. Key interactions of the Alzheimer's disease amyloid-beta protein. **M.R. Nichols**

4:25 311. Calcium-induced interactions in NADPH oxidases. **C. Wei**

4:50 312. Ribosome-free peptide biosynthesis. **T.A. Wencewicz**

St. Charles Convention Center
Ballroom D3

Theor/Comp Chem B: Applications in Chemistry and Catalysis

A. V. Mironenko, *Organizer*
M. Momenitaheri, *Presiding*

1:30 313. Dynamic axial ligand exchange in oxygen reduction catalysis. **A. Raeber**, Y. Hu, J. Spencer, J. Tan, T.A. Van Voorhis

1:50 314. Streamlining the exploration of the chemical space of low valent actinide oxide nanoclusters. **P. Miro**

2:10 315. Using computational nanoreactors to provide mechanistic insight into pyrolysis of PFOA. **S.L. Pellizzeri**, E. Serna-Sanchez

2:30 316. Investigating state-ordering in isoquinoline using complete active space methods. **T.J. Krogmeier**, A.W. Schlimgen, B.F. Parsons, K. Head-Marsden

2:50 317. Machine learning as an efficient tool for simulating potential energy and HOMO-LUMO band gap of 2D hybrid perovskite materials. **A. Thomas**

3:10 Intermission.

3:30 318. Phase-dependent promoting effect of surface oxygen on molybdenum carbide catalysts during formic acid electrooxidation. **A. Gautam**, A.V. Mironenko

3:50 319. Mixed quantum-classical studies of unimolecular reaction path dynamics. **L. Bladow**

4:10 320. Exploring the reaction mechanism of THF to butadiene using sulfur-containing zeolite catalysts: A QM/MM study. **J. Barroso**, R.A. Ela, P.J. Dauenhauer, B. Vlaisavljevich

4:30 321. Reaction mechanism and kinetics of methanol carbonylation on atomically dispersed ReO_x/SiO_2 from first principles. **N. Tran**, A.V. Mironenko

4:50 322. Exploring the effect of external acceptors moiety on photovoltaic performances in phenothiazine-based dyes for dye-sensitized solar cells: Computational study. **B. Hachlaf**, T. Saffaj, O. Britel

St. Charles Convention Center
North Hall

Analytical Poster Session

J. J. O'Brien, *Organizer*

1:45 - 3:30

323. Germania nanoparticle growth under various reaction conditions. **S. Cayo**, S. Eltouny, A. Fernandes, J.F. Destino

324. Tin oxide nanosensors distinguish volatile organic compound biomarkers spiked into simulated healthy breath mixtures. **M. Mane**, **S.S. Heranjal**, S. Sherzai, I. Ramrakhiani, E. Schulz, M. Woollam, M. Agarwal

325. Predictive analytics applied to nutrient concentrations and chlorophyll in Otter Lake. **R. Guerra**, K.R. Tucker

326. Fabrication and characterization of fully 3D-printed electrodes for electrochemiluminescence detection. **D.J. Mee**, E.M. Gross

327. Optimization of Au-plating and modification of carbon ink stencil-printed electrodes. **E. Gomez**, M. Johnson-Schmidt, E.M. Gross

328. Analysis of sunscreens and antibiotics in groundwater during the Covid-19 pandemic in the Riviera Maya, Mexico. J. Cooney, M. Lenczewski, R.M. Leal-Bautista, M. Davis, J. Rodriguez, **N. Hanratty**, K.R. Tucker

329. Quantitative MALDI: Improved precision through control of ion signal resolution. **J. Harzan**, M.G. Kinsel, G.R. Kinsel

330. Protein thiolation as a strategy to enhance immobilization and activity upon adsorption to gold nanoparticle. **F. Breausche**, A. Somerlot, J. Walder, J.D. Driskell

331. A non-enzymatic sensor platform fabricated by a consumable inkjet printer. **J. Truong**, M. Prado, A. Wanekaya

332. investigation of synergistic effect in bismuth ferrite by introducing La and Sn ($BiFe_{1-x+y}La_x Sn_x O_3$) for environmental remediation studies. **K. Hameed**

333. Benzoyl fluoride footprinting characterizes the high-order structure of membrane proteins. **M. Chai**, S. Mierxiati, A. Moyle, w. li, M.L. Gross

334. Charge transfer through trinucleotide repeat DNA/MoS2 interface. **P.K. Das**, O. Adil, W. Almy, T. Castillo, M. Shamsi

335. Raman and FTIR spectroscopy as complementary analytical techniques to X-ray diffraction for microscale crystallite characterization. **M. Strait**, B.G. Ooi, O. Hietsoi, N.S. Chong

336. Effect of environmentally relevant concentrations of atorvastatin, lovastatin, and simvastatin on *Eisenia hortensis*. **C. Korte**, K.G. Selby, G.A. Bressendorf, L. Phan, C. Butts-Wilmsmeyer, H.A. Konschak, N. Hanratty, S.R. Worth, T. Lobb, K.R. Tucker

337. Characterization of poly(ether-sulfone) ultrafiltration membranes modified by UV-assisted grafting using fractionated natural organic matter. **I. Ventura**, C. Johnson-Edler

338. Pseudouridine-modified RNA probe for label-free electrochemical biosensing. **P.K. Das**, A. Degregorio, O. Adil, M. Sumita, M. Shamsi

339. Raman spectroscopy as a non-invasive method for detecting cervical changes in early pregnancy. **K. Belcher**, E. Spurlin, J. Etaungo Esteves, P. Jimenez, C. O'Brien

340. Electrografted laser induced graphene biosensor for sensitive detection of neurodegenerative disease biomarker in cerebrospinal fluid. **O. Adil**, C. Adeyeye, M. Shamsi

St. Charles Convention Center
North Hall

Biochemistry Poster Session

M. J. Meyers, *Organizer*

1:45 - 3:30

341. Characterization and annotation of uridine derivatives in previously solved RNA structures. **S. Arteaga**, B. Znosko

342. Identification and characterization of RNA 1 x 2 nucleotide internal loops in previously solved 3D structures. **D. Liu**, J. Hou, C. Kirkpatrick, B. Znosko

343. Characterization of human Endonuclease V substrate preferences via in vitro RNA hairpin library screening. **M. Leffler**, E. Grandi, J.M. Heemstra

344. Functions of nucleolin in its interactions with the MYC promoter G-quadruplex. G. Wu, **L. Chen**, D. Yang

345. Dual targeting MYC G-quadruplex and topoisomerase I by indenoisoquinolines for cancer therapy. K. Wang, G. Wu, M.S. Elsayed, **A. Buric**, N. Deng, M.S. Cushman, D. Yang

346. DDX5 helicase resolves G-quadruplex and transactivates *MYC* expression. **S. Dagher**, G. Wu, X. Zheng, E. Tran, D. Yang

347. Berberine recognition of the dGMP-bound PDGFR-β promoter G-quadruplex: Structural insight into specific drug targeting. K. Wang, **Y. Han**, J. Dickerhoff, D. Yang

348. Synthesis of fluorescent C-nucleoside: 2-aminopyridine. N. Burbach, A. Degregorio, A. Winkler, **M. Sumita**

349. Analysis of bacterial viability in the presence of *glmS* riboswitch ligand analogs. **A. Kakish**, G. Fong, K. Timboe, A. Van Cleave, C. Weber, J. Strauss Soukup

350. Development and optimization of a high-throughput FRET assay to study *glmS* riboswitch self-cleavage. **L. Nedungadi**, J. Strauss Soukup

351. Large-scale synthesis of pseudouridine using an immobilized enzyme. K. Raasch, T. Sanford, A. Riley, M. Clawson, **M. Sumita**

352. Distinguishing photo crosslinked and non-photo crosslinked human telomeres by ion mobility mass spectrometry. **H. Yang**, M. Chai, J.S. Taylor, M.L. Gross

353. Identification and characterization of RNA dinucleotide bulge sequence families. **E. Dani**, J. Hou, B. Znosko

354. DNAzymes for N-acylation of DNA nucleobases with small-molecule acyl donors. **M. Bishka**, P.K. Das, S.K. Silverman

355. Molecular docking and database screening in search of novel selective androgen receptor modulators. **Z. Ruotsala**

356. Fatty acid composition of *Spodoptera frugiperda* to investigate CPT II deficiency. **M. Soyer**

357. Homology modeling and redox parter identification of *Pseudomonas aeruginosa* CYP168A1. **P. Herbert**, J.C. Miller

358. Investigation of *Coxiella burnetiid* phosphatidylglycerol metabolism. **A. Babcock**, A. Wells, **C. Stead**

St. Charles Convention Center
North Hall

Chem Ed Poster Session

J. J. O'Brien, *Organizer*

1:45 - 3:30

359. ETHX: ACS Committee on Ethics and you. **G.M. Larkin**, P.A. Mabrouk, P.R. Deshong, W.W. Leong

360. Bioplastics in the general chemistry lab: Expanding commercial food dye release and uptake studies. **T. Eggen**, G.R. Wyllie

361. Introducing high school students to research: ICP-MS analysis of heavy metals in fish from Lake Springfield, Missouri. **G. Adams**, A. Cooper, E. Graves, T. Norman, T. Osborne, V. Stevens, A. Yates, K. Coates, P. Clubb, M. Reyes, C. Rico

362. Studying the impact of institutional reform on success for all students in STEM. **R. Kattoum**

363. Dropwise EDTA titration of hard water metal ions in tap water for General Chemistry II laboratory. **W. Henning**, S.L. Hiley

364. Development of a non-major chemistry class into a Hy Flex format. **G.P. Nora**

365. Fostering sustainable waste management education: Novel pedagogical approach for undergraduate stem students. **N. Sathitsuksanoh**, Z. Sun, J. Immekus, V. Clay

St. Charles Convention Center
North Hall

Biochemistry Poster Session

M. J. Meyers, *Organizer*

3:30 - 5:15

366. Post-labeling assay for photo-induced non-adjacent cyclobutane pyrimidine dimers that are biomarkers for G-quadruplexes and other non-B DNA structures. N.E. Gutierrez-Bayona, S. Scruggs, H. Yang, M. Chai, M.L. Gross, **J.S. Taylor**

367. Repurposing and enhancing *E. coli* Endonuclease V as a tool for studying and tracking A-to-I RNA editing. **E. Grandi**, J.M. Heemstra

368. Structural studies of a eukaryotic OAZ1-PK RNA. **A. Kakish**

369. Distinguishing photo crosslinked and non-photo crosslinked human telomeres by ion mobility mass spectrometry. **H. Yang**, S. Scruggs, M. Chai, J.S. Taylor, M.L. Gross

370. DNAzymes for site-specific N-alkylation of DNA and RNA oligonucleotide nucleobases. **R.D. Boyd**, M.M. Kennebeck, A.A. Miranda, Z. Liu, S.K. Silverman

371. Structural analysis of OAZ RNA in *Neurospora crassa*. **C.J. Sousley**, J. Strauss Soukup

372. Analysis of the structural characteristics of 1x1 nucleotide internal loops in RNA. **K. Lampe**, C.C. Kirkpatrick, J. Hou, B. Znosko

373. DNAzymes for site-specific N-acylation of DNA and RNA oligonucleotide nucleobases. **M.A. Massa**, M.M. Kennebeck, C.K. Kaminsky, P.K. Das, R.D. Boyd, M. Bishka, S.K. Silverman

374. Custom G4 DNA microarray can determine large-scale binding selectivity of small molecules and proteins to oncogene G-quadruplexes. G. Wu, L. Chen, **K.H. Huseman**, D. Tillo, S. Ray, T. Chang, J. Schneekloth, C. Vinson, D. Yang

375. Can small molecule binding to G-quadruplex DNA be correctly predicted with current molecular docking software?. **J. Dickerhoff**, K.R. Warnecke, K. Wang, N. Deng, D. Yang

376. Minor groove drug binding effects on the BI-BII DNA backbone conformational dynamics in T:T mismatches. **C. Johnson**, G.A. Meints

377. DNAzymes for acylation of peptide lysine residues. **P.K. Das**, J.J. Przybyla, S.K. Silverman

378. Backbone conformational equilibrium correlates with enzyme activity in mismatched DNA. **G.A. Meints**

379. Nearest neighbor parameter prediction with A-modified U residue base pairs. **A. Biju Pillai**, B. Znosko, M. Hopfinger

380. Physiological recognition of the MYC G-quadruplex by berberine. **J. Jang**, J. Dickerhoff, N. Brundridge, S.A. Mcluckey, D. Yang

381. Mechanistic understanding of eco-friendly zwitterionic and non-ionic detergents for XMuLV inactivation. **V. Sharma**, L. Manchester, M. Holstein, X. XU, C. Heldt

382. Enhancing Tissue Regeneration through Electrospun SF-CNT Fibers and Electrical Stimulation. **S. Yoon**, **R.A. Rathnayake**, M. Damaser, M. Kuang, R. Wang

St. Charles Convention Center
North Hall

Organic Poster Session

M. J. Meyers, *Organizer*

3:30 - 5:15

383. Lanthanide complexes of tridentate click chelators: Structure-property relationship study. **M.N. Meyer**, J.T. Fletcher

384. Correlation of temperature dependence of KIEs with donor-acceptor distances for an NADH/NAD model reaction in solvents containing viscogens. P. Rijal, S. Salarvand, B. Mingxuan, **G. Singh**, Y. Lu, E. Akcad

385. Cationic and non-cationic N-heterocyclic carbene-silver complexes with antibacterial activity. H. Palencia, **T. Kraft**, A. Nuxoll, K. Dittmer

386. Selective electrochemical generation of aryl radicals from boronic acids via alternating polarity. **R. Aldhufari**, I. Vanswearingen, M. Boudjelel, C.A. Malapit

387. Preparation and use of a β-methoxy substituted aldehyde for Ugi-Smiles reactions. **S.H. Bickford**, S.B. Luesse

388. Photomediated hexafluoroisopropoxylation of unactivated aryl halides. B. Steeno, A. Metz, N. Haen, **S. Tobin**, T. Taylor, N. Soehner, I. MacKenzie

389. Synthesis and characterization of modular pyrylium photocatalysts for applications in new reaction development. **C. Franklin**, I. MacKenzie

390. Synthesis of a propargylic diol for an intramolecular propargylic substitution reaction to be catalyzed by ferrocenium cations. **K. Fnu**

391. A new class of near-infrared fluorophores. **I. Fuentes**, R. Tang, M. Michie, C. Lin, M.Y. Berezin, V. Birman

392. Synthesis of heterocyclic sulfondiimines. **P. Danyi**

393. Examining the role of conjugated aldehydes in Oxa-Michael Ugi-Smiles reactions. **Z. Campbell**, S.B. Luesse

394. Ferrocenium cation catalyzed cyclopropane ring opening-spectroelectrochemistry studies. **S. Bezawada**, E. Bauer

395. Solvent variation in Ugi-Smiles intramolecular Diels-Alder reactions. **H. Bradley**, S.B. Luesse

396. Reduction of tertiary amides to aldehydes with aluminum hydrides catalyzed by N-vinylpyridinium tetrafluoroborate salts. **A. Nguyen**, T. Domingos, K.R. Buszek

397. Catalyst cooperativity within confined single-chain polymer nanoparticles for [4+2] cycloadditions. **S. Baldwin**, S. Gaikwad, E. Elacqua

St. Charles Convention Center
North Hall

Theor/Comp Chem Poster Session

A. V. Mironenko, *Organizer*

3:30 - 5:15

398. Quantum biological applications for the singular value decomposition algorithm. **E. Oh**, A.W. Schlimgen, K. Head-Marsden

399. Designing kinetic model of $2e^-$ ORR on transition metal chalcogenides: Comparative analysis between c-$NiSe_2$ (100) and c-$CoSe_2$ (100). **I. Mondal**, D. Ross, J.R. Schmidt, S. Jin

400. Additivity of diene substituent Gibbs free energy contributions for Diels−Alder reactions between $Me_2C{=}CMe_2$ and substituted cyclopentadienes. A.S. Flemming, **B.C. Dutmer**, T.M. Gilbert

401. Characterizing excited states of a copper-based molecular qubit candidate with correlated electronic structure methods. A.W. Schlimgen, **Y. Guo**, K. Head-Marsden

402. Binding selectivity studies of AKT inhibitors by covalent bond docking approach. **D.T. Goodwin**, H.A. Zhong

403. Vinyl Chloride contamination following a train derailment in East Palestine, Ohio: A mathematical modeling approach. **B. Karki**, C. Bean Chevez, C. Chambers Colbeck

404. Behavior of silver nanowire dimers within a static electric field. **S. Samarasinghe**, C.M. Aikens

405. Density matrix renormalization group studies on bond dissociation energies of transition metal oxides. **J.S. Lampert**

406. Correlating electronic structure and magnetic anisotropy for small actinide complexes. **N.R. Loutsch**, S. Roy Chowdhury, B. Vlaisavljevich

407. Mechanisms for oxirane formation in interstellar molecular clouds. **D.M. Hiatt**, E.D. Glendening

408. Understanding hydrolysis energy on amorphous silica surface. **S. Brahmachari**, M. Caricato

409. Determining the optical rotation of molecular crystals using periodic boundary conditions. **E. Forson**

410. Nonlinear dynamics model for corrosion wave propagation
. **M. Emmanuel**, D. Jaiswal, B.C. Batista, E. Romanovskaia, V. Romanovski, J.R. Scully, O. Steinbock, I.Z. Kiss

St. Charles Convention Center
Ballroom B

Midwest Award Symposium

S. E. Hayes, *Organizer*
J. M. Heemstra, *Organizer, Presiding*

3:40 Introductory Remarks.

3:45 411. Mimicking the Kreb's cycle electrochemically for fuel cell applications. **S.D. Minteer**

4:25 412. Mapping metabolic interactions between gut bacteria and host tissues. **M. Jackstadt**, G. Patti

5:05 Intermission.

5:10 Plenary Lecture - Introduction to Midwest Award Address.

5:15 413. Enhancing biochemical discovery through the use of stable isotopes. **G. Patti**

FRIDAY MORNING

St. Charles Convention Center
Ballroom B

Analytical

J. J. O'Brien, *Organizer*
D. M. Osbourn, *Presiding*

8:15 Introductory Remarks.

8:20 414. Integration of 3 d printed microfludic devices with electrospun scaffolds and teer measurements for cell culture studies. **K. Cenhrang**

8:45 415. Wearable short-wave infrared photoplethysmography sensor for real-time detection and monitoring of hemodilution during post-partum hemorrhage. **H. Gruensfelder**, K. Branan, F. Bonetta-Misteli, M. Carlgren, J. McMurray, K. Liang, X. Li, G. Cote, L. Shmuylovich, C. O'Brien

9:10 416. Microprobes for label-free detection of short tandem repeats: an insight on alleviating secondary structure effects. **M. Shamsi**

9:35 417. Surface and sub-surface spatial distribution analysis of native glycosaminoglycans in electrospun gelatin-based composites. **H. Li**, L.L. Osorno, N. Domingo, A. Ievlev, M.B. Foston, A. Limaye, T. Arinzeh

10:00 Intermission.

10:20 418. Crispr-based electrochemical biosensor and prediction of CRISPR/Cas12 guide RNA activity using deep learning models. **M. Ozsoz**

10:45 419. Hierarchical bimodal nanoporous gold (hb-NPG) electrode for the sensitive and specific detection of glycoprotein biomarkers. **P. Sondhi**, T. Adeniji, A. Demchenko, K.J. Stine

11:10 420. Detection of periodontal pathogens via SERS associated with deep learning and analysis of saliva complexity. **R.A. Rathnayake**, Z. Zhao, N. McLaughlin, L. Chen, Y. Yan, Q. Xie, W. Li, M. Mathew, R. Wang

11:35 421. An enzyme-coupled istotope dilution mass spectrometry assay for non-adjacent DNA photoproducts as intrinsic probes for G-quadruplexes *in vivo*. **S. Scruggs**, H. Yang, J.S. Taylor, M.L. Gross

St. Charles Convention Center
Jr Ballroom A

Analytical Techniques in Environmental Chemistry

C. S. Bagwill, *Organizer*
K. R. Tucker, *Organizer, Presiding*

8:15 Introductory Remarks.

8:20 422. Developing bioelectrocatalytic techniques for water quality sensing. **S.D. Minteer**

8:50 423. Complementary mass spectrometry analysis for environmental toxicology datasets. K.G. Selby, S.L. Shan, R.B. Davis, R. AminiTabrizi, S.A. Melzer, N.J. Grunloh, **K.R. Tucker**

9:20 424. Enhanced decolorization of Orange II in waste water with modified g-C_3N_4 photocatalyst. **B. GUO**, S. Kaneco, H. Katsumata, I. Tateishi, M. Furukawa

9:50 Intermission.

10:20 425. Use of Pyrolysis gas chromatography-mass spectrometry (py-GCMS) for the analysis of nano-plastics and its application to drinking water samples. **J. Scott**

10:50 426. Addressing emerging water quality crises from an analytical chemistry perspective: Harmful algae blooms. **R. Marfil-Vega**

11:20 427. Pivoting from GC/MS to ELISA in atrazine quantitation by drink water providers: An overview of the burdens of good stewardship. **I. McBride**

St. Charles Convention Center
Ballroom D3

Beyond the Boundaries of Computational Chemistry and Catalysis

Cosponsored by CATL and COMP
A. V. Mironenko, *Organizer, Presiding*

8:15 Introductory Remarks.

8:20 428. The catalytic science of nitrogen. **W.F. Schneider**

9:00 429. Metal-metal bonds in photosensitizers. **M.K. Karunananda**

9:30 430. Interfacial active sites catalyzed efficient thermal and electrochemical CO_2 conversion. **Q. Ge**

10:10 Intermission.

10:25 431. Direct computation of vibrationally averaged properties with multicomponent methods. **K. Brorsen**

10:55 432. Pushing the boundaries of classical dynamics: Phonons and cavity quantum electrodynamics. **R. Tempelaar**, A. Krotz, M. Hsieh

11:25 433. Dynamical studies of ion transport in non-aqueous electrolyte solutions using classical and quantum path integral simulations. **M. Momenitaheri**

St. Charles Convention Center
Ballroom D1

Biochemistry

M. J. Meyers, *Organizer*
A. Durantini, *Presiding*

8:15 Introductory Remarks.

8:20 434. Synthesis and characterization of chemical tools to study human carboxylesterase (CESs). **M.R. Walk**, C.J. Karns, A. Singh, M.W. Beck

8:45 435. Development of fluorogenic chemical tools for studying drug metabolic esterases in live cells. **C.J. Karns**, M.R. Walk, A. Singh, M. Gao, M.W. Beck

9:10 436. Identifying and engineering substrate specific Hsp104:NBD1 variants. **K. Miller** , S. Bhandarkar, A. Wang, K. Jones, J. Ryan, J. Fritsche, M. Jackrel

9:35 437. Engineering and evolving substrate-specific Hsp104 variants. **J. Ryan**, S. Chen, A. Bao, C. Ling, B. Bell, A. Xu, K. Miller, B. Sohn, L. Li, C. Chang, K. Mohammed, M. Staller, M. Jackrel

10:00 Intermission.

10:20 438. Application of solvent paramagnetic relaxation enhancement (sPRE) for probing intermolecular and electrostatic interactions on protein surfaces. **y. okuno**, C.D. Schwieters, G.M. Clore

10:45 439. Computational study of protein-protein interactions in a tetramer of STING proteins. H. Gates, S. Crivelli, **M. Watanabe**

11:10 440. Spectrally blue shifted melanopsins for subcellular optogenetics. **D. Wijayaratna**, F. Sacchetta, L.P. Gonzalez, M. Koyanagi, S. Piyawardana, M. Olivucci, A. Karunarathne

11:35 441. HTRA1 prevents and reverses α-synuclein aggregation, rendering it non-toxic and seeding incompetent. **S. Chen**, A. Puri, B. Bell, J. Fritsche, H. Palacios

St. Charles Convention Center
Jr Ballroom B

Biotherapeutic Process Development and Manufacture in the Midwest

A. Berrill, S. A. Kolodziej, *Organizers, Presiding*

8:15 Introductory Remarks.

8:20 442. Large scale production of plant biotech trait protein to support global regulatory product submissions. **C. Wang**, S. Saracco, B. Li

8:45 443. Comparative analysis of ATF scaling methods for perfusion cell culture in the AMBR250 system. **N. Kasparie**

9:10 444. Protein aggregation: *In-vitro* and *in silico* studies. **D. Forciniti**

9:35 445. Applications of PAT for bioconjugation processes. **J. Spies**, L. Mcdermott

10:00 Intermission.

10:20 446. Utilization of small scale models for mRNA development. **J. Williamson**

10:45 447. Pathogen mimicking nanovaccine platform technology: New paradigm. **B. Narasimhan**

11:10 448. Purifying tagless recombinant proteins with a disruptive self-removing affinity tag platform. **D.W. Wood**

11:35 449. Continuous processing of viral products using aqueous two-phase extraction. **C. Heldt**, N. Nold, S. Waldack, G. James, T. Sarvari, A. Bekkala, L. Manchester, T. Colling, E. Agustin-Mazariegos

St. Charles Convention Center
Meeting Room 101

Chem Ed

J. J. O'Brien, *Organizer*
J. Monahan, *Presiding*

8:15 Introductory Remarks.

8:18 450. Integration of computer-aided drug design in graduate medicinal chemistry courses. **L. Hegazy**

8:41 451. Analysis of CURE survey data during online instruction. **M. Kubacki**, T.J. Bixby

9:04 452. Improving student formal laboratory report outcomes and perceptions through the development and implementation of an anonymous, holistic peer review process. **B. Spencer**

9:27 453. A molecular biochemistry lab education tool that allows for full-color experiments to assist learning. **D. Morrone**

9:50 Intermission.

10:05 454. Characterizing laboratory experiments used in undergraduate analytical chemistry courses for opportunities of engagement in science practices and inquiry. **A. Van Wyk**, A. Bhinu, K. Frederick, M. Lieberman, R.S. Cole

10:28 455. 3D scanning for density measurements. **J.D. Van Horn**, M. Hudson

10:51 456. Targeting persistence: Case studies reveal strengths and challenges in developing mindset and STEM identity. **A.J. Werner**, T.J. Bixby

11:14 457. Visualizing 3D objects in analytical chemistry. **J. Coduto**, A.P. Lazicki, J. Leddy

11:37 458. Creating interactive chemistry models by combining 3D printing and augmented reality. **J.D. Mendez**

St. Charles Convention Center
Ballroom D2

Macro/Polymer Chem

A. V. Mironenko, *Organizer*
A. Kuenstler, *Presiding*

8:15 Introductory Remarks.

8:20 459. Carbon aerogels derived from polybenzoxazine and polybenzodiazine aerogels as high-capacity desiccants. **S. Owusu**, V.A. Edlabadkar, C. Sotiriou-Leventis

8:50 460. Direct air capture via metal-organic supercontainers. **h. li**, Z. Wang

9:20 461. Photo-printed hydrogels loaded with curcumin-zinc complex for controlled drug delivery. **T. Ferdous**, A. Akinwole, K. Cisneros, T. Brewster, T. Fujiwara

9:50 Intermission.

10:05 462. Synthesis and applications of chelating polymers. **P.R. Calvo**

10:35 463. Development of advanced nanofibrous media for simultaneous removal of microplastics and lead (Pb) from water. **A. Gopakumar**, A. Ccanccapa-Cartagena, M. Salehi

11:05 . Sonochemical assisted modulation of Cu doped SnO_2/g-C_3N_4 nanocomposite heterojunction by using green synthesis and degradation of organic dye malachite green. **S. Dwivedi**, G. Pandey

St. Charles Convention Center
Meeting Room 103

Magnetic resonance & NMR meet Industry, Medicine, & Academe

B. Hammann, S. E. Hayes, *Organizers, Presiding*

8:15 Introductory Remarks.

8:20 464. Solid-state NMR insights into alpha-synuclein fibril structure. **C. Rienstra**

8:50 465. *In-situ* solid-state NMR spectroscopy of lignin model polymer disassembly. **J. Zhang**, Y. Gao, M.B. Foston, A. Lipton, L. Qi, S.L. Scott

9:05 466. Quantitative solid state NMR for characterization of kerogen. **A.M. Allgeier**, M. Suekuni

9:20 467. NMR technology and application in Bayer. **B. Xiang**

9:50 Intermission.

10:10 468. Towards new applications for parahydrogen- and xenon-based hyperpolarization: Neutron beams, MOFs, and point-of-care MRI. **B.M. Goodson**

10:40 469. Mechanistic insights into processive polyethylene hydrogenolysis: An *in situ* NMR study. **Y. Zhao**, M. Meirow, A. Tennakoon, X. Wu, A. Paterson, L. Qi, A.M. LaPointe, J. Lamb, T. Kobayashi, M. Delferro, A.D. Sadow, W. Huang, E. Luijten, F.A. Perras

10:55 470. The enhanced electron-deficiency, dynamics, and activity of zeolite-bound organometallic species. **S.A. Southern**, Y. Li, A.D. Sadow, L. Qi, F.A. Perras

11:10 471. *In-situ* study of multiple-phase analytes at high temperatures and pressures with a uniquely designed solid-state NMR spectrometer. **P.T. Judge**, J. Zhang, M.B. Foston

11:25 472. The structure of boron monoxide. **F.A. Perras**, H. Thomas, P. Heintz, R. Behera, J. Yu, G. Viswanathan, D. Jing, L.M. Stanley, W. Huang

St. Charles Convention Center
Ballroom C

Organic

M. J. Meyers, *Organizer*
B. C. Hamper, *Presiding*

8:15 Introductory Remarks.

8:20 473. Fused heteroarenes resulting from an iodine-promoted C–N bond formation. **J.L. Bolliger**

8:45 474. *N*-heterocyclic carbene pincer complex Re: synthesis, structure, and catalytic activities for C-C cross-coupling of ketones, alcohols and one-pot synthesis of quinolines. **H. Pham**, B. Donnadieu, T. Hollis

9:10 475. C-H functionalization of bis(azolium) salts: Direct access to symmetrical and unsymmetrical bis-abnormal CCC-NHC pincer complex precursors. **A. Cecil**, E. Fosu, T. Hollis

9:35 476. Photomediated hexafluoroisopropoxylation of unactivated aryl halides. **I. MacKenzie**

10:00 Intermission.

10:20 477. Carbon-centered radicals as novel building blocks to synthesize dynamic covalent ring assemblies. **L. THALAPALAGE**, A. Winter

10:45 478. Lagunamide C: Total synthesis synthetic efforts, structural revision, and biological studies. **R. Rafferty**, S. Perera, A. Fatino, K. Wildeman

11:10 479. Practical route to highly substituted aminonaphthalenes from benzaldehydes. **H. Ozomarisi**, K. Sharpe, V. Outlaw

11:35 480. Preparing multicomponent solids of beta blockers via mechanochemistry. **D.S. Botes**, J.D. Loya, M. Ghahremani, B. Newham, M. Aleman, D. Unruh, G. George, K.M. Hutchins

St. Charles Convention Center
Jr Ballroom C

Organic Reaction Mechanisms

Y. Lu, *Organizer, Presiding*

8:15 Introductory Remarks.

8:20 481. New strategies for the photocatalytic activation of strong bonds. **D. Martin**

8:50 482. Artificial enzymes through molecular imprinting of micelles: Synthesis and mechanistic studies. **Y. Zhao**

9:20 483. Rare dual-release photochemistry of sulfoximines. **R.D. McCulla**

9:50 Intermission.

10:10 484. Oligomer formation initiated by the one electron reduction of isocyanates and isothiocyanates. **S.J. Peters**, Z. Becerra, M.A. Servos

10:40 485. Solvent polarity and viscosity effects on the temperature dependence of kinetic isotope effects in hydride tunneling reactions of NADH/NAD^+ models. **Y. Lu**

11:10 486. Viscoelastic fluorescent π-conjugated polymer liquids. **J. XU**

St. Charles Convention Center
Jr Ballroom D

Radiochemistry: From Radioactivity to Drug Product

M. Nickels, *Organizer, Presiding*

8:15 Introductory Remarks.

8:20 487. Production of PET radiopharmaceuticals for both IND and FDA approved uses. **S.W. Schwarz**

8:45 488. Improved radiochemistry systems for rapid development of radiopharmaceuticals. K. Malloy, **M.L. Schulte**

9:10 489. Development and translational clinical investigation of a promising PET agent for neuroinflammation in the brain. **Z. Tu**, L. Qiu, M. Brier, R. Gropler, J. Perlmutter, T. Benzinger

9:35 490. Copper-mediated radiolabeling to synthesize PET drugs for personalized medicine and drug hunting. **P.J. Scott**

10:00 Intermission.

10:25 491. Production, isolation, and radiochemistry of [$^{76/77}$Br]bromide for small molecule theranostic radiopharmaceuticals. **P. Ellison**

10:50 492. Lumi804, a chelator for ^{177}Lu(III), ^{161}Tb(III), and ^{89}Zr(IV) theranostic agents for imaging and therapy of cancer. E. Iweha, K. Ho, C. Fong, F. Gallazzi, D. Tatum, P. Bokolo, M. Serasinghe, H. Hennkens, D. Magda, **C.J. Anderson**

11:15 493. Preclinical efficacy of a PARP-1 targeted Meitner-Auger-emitting radionuclide in prostate cancer models. S. Sreekumar, D. Zhou, J. Xu, **B.E. Rogers**

St. Charles Convention Center
Meeting Room 102

Sustainable Transition Metal Catalysis

J. Neely, *Organizer, Presiding*

8:15 Introductory Remarks.

8:20 494. From fundamentals to function: Manipulating the secondary coordination sphere with calixpyrrole ligand architectures to control small molecule activation. **P.E. Sues**, L. Trowbridge, S. Somachandra, T. Ahmed, D. Mazumder

8:50 495. Precision labeling of small molecules. **J. Clark**, B. Pate, R. Sonstrom, J.L. Neill

9:20 496. Multicomponent coupling strategies enabled by unique reactivity in iron complexes. **J. Neely**

9:50 Intermission.

10:00 497. One and two-electron redox catalysis with d0 metals. **C. Roberts**

10:30 498. Iron and ruthenium promotors of carbon dioxide-ethylene coupling reactions. **W.H. Bernskoetter**

11:00 499. Properties and reactivity of Mn-oxygen intermediates and their roles in catalysis. **T.A. Jackson**, S. Brunclik, P. Singh

11:30 500. Toward catalytic C-O functionalization with earth's most abundant heterobimetallic pair. **N.P. Mankad**, S. Sinhababu, R. Singh, M. Radzhabov, S. Subasinghe

St. Charles Convention Center
North Hall

Inorganic Poster Session

L. C. O'Brien, *Organizer*

8:30 - 10:15

501. Electron-rich dinuclear Cr(0) complexes of diisocyano-terminated linear terazulenic π-linkers. **J. Mandigo**, N.R. Erickson, M.V. Barybin

502. Designing hydrogen bond donor catalysts with an element of tunability. **A. Davis**, M. Zeller, J.J. Kiernicki

503. Lead (II) carbonate-alginate nanocomposite materials as contrast agents for fine vascular microCT imaging. **K. Ho**, M.S. Kader, S.W. Buckner, S. McBride-Gagyi, P.A. Jelliss, C. Kirkpatrick

504. Coal ash pollution and trace metals in St. Louis's ground water: A look into Ameren's infamous Sioux Power Plant. **D. Wright**, N.C. Ulrich

505. Charge delocalization in electron-rich complexes of redox non-innocent, isocyanide-terminated 2,2'-biazulenic ligands. **S. Pham**, M.D. Hart, P.T. Connelly, M.V. Barybin

506. Hollow Mn3O4 nanoparticles as a catalyst for the selective pxidation of alkenes to epoxides. **S. Schulz**

507. Iron catalyzed linear trimerization of terminal alkynes. **C. McGhiey**, M. Stockell, J. Wright-Keely

508. Two-step catalyzed sol-gel preparation of hydrophobic silica xerogels containing perfluorinated alkyl groups: Effects of base catalyst addition timing on product formation. **F. Cantillo Villalba**, A.M. Law, S.A. Darveau, C.L. Exstrom

509. One-step syntheses of Co, Ni, and Fe-Based metal-organic frameworks for energy applications. **A. Robinson**, W. Lin, **R.K. Gupta**

510. Synthesis of tridentate ligands and their iron complexes for use in redox flow batteries. **B. Donovan**, M.J. Drummond

511. Tuning of visible silica alcogel gelation time using a two-step catalysis in the preparation of a silica sol for embedding into femtosecond laser processed surfaces. **A.M. Law**, F. Cantillo Villalba, N. Igusa, S.A. Darveau, C.L. Exstrom, G. Kaufman, D. Egbebunmi, J.E. Shield, G. Gogos, C.A. Zuhlke

512. Optimizing the synthesis of Tetra-2-pyridinylpyrazine (tppz) and its iron complexes for use in redox flow batteries. **D. Mislenkov**, M.J. Drummond

513. New structural insights into heavy metal complexes with thiosalicylate. **D.G. Nill**, E.M. Villa

514. Support of pincer complexes on oxides for heterogeneous catalysis and oxide surfaces functionalized with L-type ligands for the support of zero valent metals. M. Halder, **D. Culver**

St. Charles Convention Center
North Hall

Med Pharma Chem Poster Session

M. J. Meyers, *Organizer*

8:30 - 10:15

515. Structure-based discovery of novel non-isoxazole Farnesoid x receptor agonist for the potential treatment of non-alcoholic fatty liver disease. **A.B. Morrison**, M. Elagawany, Y. Fang, L. Hegazy, B. Elgendy

516. Synthesis of 9-hetero 7OH mitragynine analogs. **E. Wells**, B. Paul, R. Ople, S. Majumdar

517. Evaluating the *Leishmania tarentolae* response to inorganic strontium-based oxyfluorides. **K. Terry**, M.A. Jones, E. Sullivan, J. Drinkwater

518. Design and synthesis of novel Mitochondrial Pyruvate Carrier (MPC) inhibitors for the treatment of metabolic disorders. **H. Politte**

519. Developing efflux pump inhibitors against *acinetobacter baumannii*. **H. Alkhateeb**, H. Zhou, R. Tambat, M. Udin, H. Zgurskaya, **J.K. Walker**

520. Development of chitosan/hyalaronic acid microcapsules for incorporation into modified contact lenses. **E.C. Theobald**, J.L. Duffy-Matzner

521. Multidrug delivery in metal-organic frameworks with backbone-coordinated medications. N. Kessler, **R.T. Schulte**, Z. Schulte

522. Design, synthesis and biological evaluation of novel REV-ERB antagonists for muscle regeneration. **g. veerakanellore**, C. Kaiho, J. Lee, A. Valfort, T. P. Burris, L. Hegazy, B. Elgendy

523. Design and synthesis of 2-cyano-3-(3-aryl-1*H*-pyrazol-4-yl) acrylic acid derivatives as mitochondrial pyruvate carrier inhibitors for the treatment of type 2 diabetes and NASH. **L. MARAM**, L. Hegazy, B. Elgendy

524. Rhodanine-indolinones as inhibitors of serotonin N-acetyltransferase for treating circadian rhythm disorders. **M. Hill**, K. Lytle, N. Wandrey, M. Redinger, J. Boley, L. Hamilton, N. Fancher, M. Moxley, A.A. Thomas

525. Synthesis and enzymatic activity of indolyl vinyl sulfonamides and propiolamides as pro-inhibitors of serotonin N-acetyltransferase. **J. Boley**, M. Redinger, A. Haynes, L. Hamilton, N. Wandrey, M. Moxley, A.A. Thomas

526. Synthesis and enzymatic activity of serotonin N-acetyltransferase inhibitors with coenzyme A-targeted warheads. **M. Redinger**, M. Hill, L. Hamilton, N. Wandrey, M. Moxley, A.A. Thomas

527. Optimization of anti-psychotic phenothiazines as novel antifungal agents with reduced affinity towards neuroreceptors. **S. Guin**, K.M. Alden, D.J. Krysan, M.J. Meyers

St. Charles Convention Center
North Hall

Physical Poster Session

L. C. O'Brien, *Organizer*

8:30 - 10:15

528. Cyanide ligands as an active site probe of IsdG and IsdI heme degrading enzymes. **R. Matarise**

529. Emergent pattern formation of four electrochemical cells arranged in a [2x2] configuration. **L. Bordoh**, I.Z. Kiss

530. Structures and 3c-4e N-I-X (X = Cl, Br, I, N) halogen bonding in neutral, cationic, and anionic complexes. **F. ODUBO**, E. Adeniyi, S.V. Rosokha

531. Structural characterization of surface immobilized platinum hydrides by sensitivity-enhanced ^{195}Pt solid-state NMR spectroscopy and DFT calculations. **B.A. Atterberry**, E. Wimmer, S. Klostermann, W. Frey, J. Kästner, D.P. Estes, A.J. Rossini

532. Detection of hydrogen peroxide from commercial aerosol generators using colorimetric analysis. **S.M. Liyanage**, E. Schnitzler

533. Defining the relative stability of the ferric superoxo intermediate of human heme oxygenase. **D.A. Ruhwaya**, P. Mak

534. Synthesis and characterization of carbon quantum dots from amino acids. **H. Branch**, A.M. Keller

535. Solute-solvent interactions in aqueous solution studied via infrared spectroscopic measurements and electronic structure calculations. **H.R. Krueger**

536. Quantifying the influence of relative humidity on aerosol pH utilizing RGB colorimetry. **B.J. Winters**, W.K. Mitts, J.P. Darr

537. Sequestration of pollutants from wastewater using sulfonated graphene oxide: Experimental and computational studies. **O. Oluwasina**, A. Adelodun, O. Oluwasina, S. Olusegun

538. Mapping molecular orientations and surface coupling of porphyrins with Tip-enhanced Raman imaging. **B. Dhital**, P. Valencia Acuna, P.Z. El-Khoury

St. Charles Convention Center
North Hall

Inorganic Poster Session

L. C. O'Brien, *Organizer*

10:15 - 12:00

539. Morphological modification of iron phosphide for green energy production and storage. **A. Gupta**, C. Allison, R. Srivastava, W. Lin, **R.K. Gupta**, T. Dawsey

540. Synthesis of mixed metal aerogels for effective water splitting applications. **N. Maley**, P. Patel, **R.K. Gupta**

541. One-step hydrothermal synthesis of cobalt-MOFs for energy storage applications. **P. Neely**, **M. Andrews**, W. Lin, **R.K. Gupta**

542. Electrochemically-assisted synthesis of vanadium oxide-doped cobalt pyrophosphate as a high-performance electrocatalyst. **D. Hedrick**, **R. Hedges**, W. Lin, **R.K. Gupta**

543. Reactivity of actinide metallocene aryloxide complexes. **G.M. Kaumini**, P. Rungthanaphatsophon, J.R. Walensky

544. The detection of gamma-butyrolactone with the use of metal nanoparticles capped with polyvinylpyrrolidone. **R. Scarpaci**, L. Barnard, J.J. Determan

545. Analyzing illicit drugs utilizing silver nanoparticles. **L. Purcell**, **B. Finley**, **D. Pfeiferling**, M. Soendergaard, J.J. Determan

546. The use of silica nanoparticles as biosensors for illicit drug detection. **M. Pearson**, **A. Webb**, M. Soendergaard, J.J. Determan

547. The inclusion of metallic compounds to resorcinol-formaldehyde aerogel synthesis for electrochemical analysis and water splitting. **A. Davis**, **R.K. Gupta**

548. ^{17}O-NMR studies of the $IMo_6O_{24}^{5-}$ ion in aqueous solution. **A.M. Payne**, E.M. Villa

549. Guanidinium functionalized metal-organic supercontainer for selective anion binding. **A. Tillquist**, K. Chitrakar, R. Cook, S. Dc, Z. Wang

550. Reactivity of manganese complexes with hydrogen peroxide. **Z. Aghaei**, T.A. Jackson

551. Synthesis and structures of novel lanthanide mixed phosphite-sulfate structures formed via *in-situ* ligand reactions. **K.I. Huisman**, E.M. Villa

552. Powder X-ray diffraction analysis of corn stover ash from three central states: Effects of post-burning treatment temperature, grinding and cooling rate on potential pozzolanic reactions. **J. Montañez**, **J. Tovar-Batres**, S.R. Yarnell, C.L. Exstrom, I. Orynbassarov, J. Hu

St. Charles Convention Center
North Hall

Physical Poster Session

L. C. O'Brien, *Organizer*

10:15 - 12:00

553. Reexamination of the $B1 - X0^+$ and $A1 - X0^+$ electronic transitions in tungsten oxide, WO: Evidence of an avoided crossing. K.N. Bales, J.J. O'Brien, **L.C. O'Brien**

554. Electron screening constants: Determination from ionization energy fittings. **J.A. Carroll**

555. Substrate binding by CYP51 from *Mycobacterium tuberculosis*. **A. Mitchell**, P. Mak

556. Emergent hypernetworks in nonlinear coupled oscillatory electrochemical reactions. **J. OCAMPO ESPINDOLA**, E. Nijholt, D. Eroglu, T. Pereira, I.Z. Kiss

557. Heat capacity of PtC using virial coefficients. **L. Biolsi**

558. Application of nanosecond excitation in light-induced cellular processes. **J. Leone**

559. Synthesis of 2,7-dihydroxy-1,8-naphthyridine and determination of the dimerization binding constant by NMR. **S. Kempf**, S.P. Lorimor, J.N. Woodford

560. Origin and evolution of the light absorption of biomass burning aerosol. H. Al-Mashala, K.L. Betz, C. Calvert, S.M. Liyanage, J. Barton, E. Bruce, N. Huskins, **E. Schnitzler**

561. Revolutionizing plastics production: Biodegradable polyhydroxyalkanoates from renewable biomass sources. n. Lertthanaphol, P. Sereerattanakorn, P. Chuangpusri, M. hossain, S. Tulaphol, J. Wittayakun, S. Prayoonpokarach, J. Pranpranod, S. Jantasee, P. Weerachawanasak, J. Dong, **N. Sathitsuksanoh**

562. Enhancing Per- and poly-fluoroalkyl substances removal from water using porous solid metal-organic framework sorbents. P. Sereerattanakorn, n. Lertthanaphol, P. Chuangpusri, S. Prayoonpokarach, J. Wittayakun, S. Tulaphol, **N. Sathitsuksanoh**

563. Harnessing cooperative acidities in alumina-silica catalysts for selective biomass conversion to valuable chemical products. P. Chuangpusri, S. Jantasee, P. Weerachawanasak, J. Pranpranod, **N. Sathitsuksanoh**

FRIDAY AFTERNOON

St. Charles Convention Center
Ballroom B

Analytical

J. J. O'Brien, *Organizer*
E. Navarre, *Presiding*

1:30 Introductory Remarks.

1:35 564. Hydrodynamic wall effect on trapped probes for optical rheological measurements in water. **R. Ghosh**, S.A. Bentil, J. Juarez

2:00 565. Site study of inorganic water species removed by tabletop pitcher water filters. **E. Navarre**, M. Walker, O. Daube

2:25 566. Potable water: Basic essential for life survival. **M. Omorogie**

2:50 567. Studying the kinetics of lead (Pb) deposition onto and release from plastic potable water pipes. **D. Datta**, N. Mirza, S.P. Brown, D. Ladner, M. Salehi

3:15 Intermission.

3:35 568. Single-molecule fluorescence investigation of dye adsorption onto the surface of anodic aluminum oxide nanopores. **A. Nathani**, D.A. Higgins, T. Ito

4:00 569. Solute nanoconfinement in nanoporous anodic aluminum oxide membranes: Study of butanol/water mixtures by fluorescence correlation spectroscopy. **S. Asadi**, H. Rashidi, T. Ito, D.A. Higgins

4:25 570. Photovoltaic performance of perovskite solar cells by TiO_2-carbon dot electron transport film layers. **T.F. Yadeta**, I. Toyoko

4:50 571. Effect of artificial weathering on dye diffusion over polyethylene terephthalate microplastics surface using fluorescence correlation spectroscopy. **O. Shafiee**, H. Rashidi, D.A. Higgins

St. Charles Convention Center
Ballroom D3

Chemical Theory Across Scales

K. Head-Marsden, R. B. Wexler, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 572. Pursuit of strongly correlated electrons on classical and quantum devices. **D.A. Mazziotti**

2:05 573. Tensor trains and quantum computing for highly multidimensional molecular simulations. **M.B. Soley**

2:35 574. Electronic structure of uranium-arene complexes. S. Roy Chowdhury, **B. Vlaisavljevich**

3:05 Intermission.

3:30 575. Finite temperature electronic structure calculations of the nitrogen dimer and the warm dense electron gas. **J.J. Shepherd**

4:00 576. Ab initio thermodynamics and inorganic materials synthesis prediction. **C. Bartel**

4:30 577. The Phase Diagram of All Inorganic Materials. **C. Wolverton**

St. Charles Convention Center
Ballroom D1

Flow Chemistry

T. M. Stark, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 578. Design and application of reactors for continuous flow synthesis. **B.C. Hamper**, T. Smith

2:20 579. Tools and technologies for flow chemistry: How equipment impacts process development. **A. Adamo**

3:05 Intermission.

3:20 580. Development and applications of high-throughput experimentation methods to guide scalable flow synthesis. **D.H. Thompson**

4:05 Flow Chemistry: Reagents, Reactors and Regulation Anecdotes.

St. Charles Convention Center
Jr Ballroom A

From Clear Flasks to Green Fields: Utilizing a Sustainability Mindset in Agrochemical Active Ingredient Development

J. Struble, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 581. Development of a cost effective process to prepare a key raw material in NemaStrike. **D.P. Walker**, K. Koeller, W.H. Miller

2:20 582. Large-scale preparation of chiral pyridyl-backbone for Crabtree/Pfaltz-Type iridium complex. **M.J. Hayes**

3:05 Intermission.

3:25 583. Digital enablement of sample preparation through automation: Innovation that drives efficiency, safety and quality. **C. Zhang**, J. Johnson, S. Kumar Laik, D. Krewer, J. Fisher, E. Tesfu, R.S. Woerndle

4:10 584. Planter box application of plant beneficial methylotrophic microbes. **J.T. Whitteck**, M.E. Frodyma

4:55 Concluding Remarks.

St. Charles Convention Center
Jr Ballroom D

Medicinal Chemistry & Chemical Biology: Discovering New Biology and New Drugs Through Chemistry

M. J. Meyers, *Organizer*
A. M. Crider, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 585. Modulating DNA methylation and demethylation with bifunctional ten-eleven translocation dioxygenases inhibitors. **N.Y. Tretyakova**, A.K. Hurben, T. Karow, S. Le, N.A. Weirath, H.V. Kumar, C. Chao, A. Rahim

2:00 586. Discovery and development of cyclic peptides for the modulation of challenging targets. **E.I. Parkinson**

2:25 587. New synthetic tools for peptide medicinal chemistry. **S. Bloom**

2:50 588. Optimization of the peptide natural product apidaecin, a translation termination inhibitor. **T.W. Moore**, K.J. Skowron, A.C. Allen, K. Long, T. Dean

3:15 Intermission.

3:35 589. Discovery and hit-to-lead optimization of a series of biphenyl thienopyrimidine QcrB inhibitors for the treatment of tuberculosis. **L. McGrane**

4:00 590. Novel targets and small molecule inhibitors for the treatment of parasitic worm infections. V.S. Banas, Z. Han, M. Mahoney, V.C. Damalanka, R. Chugani, A. Maddirala, J. Helander, A. Cruz, M. Elfawal, E. Goetz, B. Rosa, A. Arun, K. Singh, S. Uzoechi, H. Jung, R.

Tyagi, N. Tricoche, R. Peguero, C. Bulman, S.A. Wildman, A. O'Donoghue, J. Sakanari, S. Lustigman, R.V. Aroian, M. Mitreva, **J.W. Janetka**

4:25 591. Drug discovery platform towards a new therapeutic for cryptosporidiosis. **M.J. Meyers**, J.E. Teixeira, E. Oboh, M. Gasonoo, N. Jentsch, C.D. Huston

4:50 592. Selectivity studies of Phosphatidylinositol 3-Kinase (PI3K) inhibitors. **H.A. Zhong**

St. Charles Convention Center
Ballroom C

Organic

M. J. Meyers, *Organizer*
J. Heemstra, *Presiding*

1:30 Introductory Remarks.

1:35 593. Copper catalyzed hydrosilylation of internal aryl alkynes. **K. Smith**, S. Sloane, S. Hintzsche, J. Clark

2:00 594. Cooperatively-catalyzed activation of thioglycosides that bypasses intermediacy of glycosyl halides. **A. Dent**, S. Escopy, A. Demchenko

2:25 595. Electrochemical and spectroelectrochemical investigations of ferrocenium and ferrocenophanium cations related to their application in propargylic substitution reactions. **E. Bauer**, S. Bezawada

2:50 596. Aryl nitriles as post-modifiable handles in metal-mediated [2+2] photodimerizations performed in the solid state. **N.A. Samararathne Muhandiramge**, L. MacGillivray

3:15 Intermission.

3:35 597. Acylative kinetic resolution of alkenyl-substituted hydroxamic acids. **J.D. Liao**, V. Birman

4:00 598. Preparation of chalcogenophenecarboxylic acids, thiocarboxylic aicds, and dithiocarboxylic acifs for metal-organic framework synthesis. **M.R. Hulce**, A.S. Brown

4:25 599. Pulsed electrosynthesis enables the generation of aryl radicals from boronic acids. **I. Vanswearingen**, R. Aldhufari, M. Boudjelel, C.A. Malapit

4:50 600. Inducing regioselectivity in metal-catalyzed aryne reactions via ligand control. **B. Denman**, E. Plasek, A. Umanzor, C. Roberts

St. Charles Convention Center
Jr Ballroom B

Probing Biological Chemistry

M. W. Beck, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 601. Design, construction, and applications of an expansive library of fluorogenic esterase substrates. **R. Johnson**

2:00 602. Chemical probes to investigate the proteome of the mycobacterial outer membrane. **N. Banahene**, K. Biegas, B.M. Swarts

2:25 603. A chemical biology toolbox for probing A-to-I RNA editing. **J.M. Heemstra**

2:50 604. Synthetic biology approaches to target RNA capping enzymes from emerging viruses. **A. Mehta**

3:15 Intermission.

3:35 605. Engineered opsins and photochemical tools to explore subcellular signaling. D. Wijayaratna, S. Ubeysinghe, W. Thotamune, M. Olivucci, M. Young, **A. Karunarathne**

4:00 606. Using phage display for biomarker targeting and identification. J. Newton-Northup, **M. Soendergaard**

4:25 607. Staphylococcal peroxidase inhibitor: Progress toward understanding residue-level contributions of its inhibition of human myeloperoxidase. **S. Fatehi**, T.J. Herdendorf, B.V. Geisbrecht

4:50 608. Probing variations in drug metabolism with chemical tools. **M.W. Beck**

St. Charles Convention Center
Jr Ballroom C

Synthesis and Characterization for Functional Polymeric Materials

A. Kuenstler, W. Loo, *Organizers, Presiding*

1:30 609. Advancing polyoxazolidinone synthesis and characterization for high temperature applications. A. Wong, A. Pal, M. Barrera, **J.R. Lamb**

2:00 610. Using photoredox catalysis to control the structure, properties, and performance of covalent and non-covalent polymer networks. **J.C. Barnes**

2:30 611. Leveraging advanced characterization methods to precisely engineer polymeric hydrogels for non-invasive therapeutic delivery. **M.A. Calabrese**

3:00 612. Effect of polymer gel elasticity on coacervate phase behavior. **S. Morozova**

3:30 Intermission.

3:45 613. Innovative engineering and synthetic routes to improve ion transport at confined electrode interfaces of electrochemical devices. **S.K. Dishari**

4:15 614. Functional polymers in energy storage devices. **J. Lopez**

4:45 615. Mapping the morphological evolution of complexed block copolymer thin films using the solvent vapor absorption-desorption isotherms. **B. Chang**