

2025 Midwest Regional Meeting

K. Brorsen, V. Outlaw, *Program Chairs*

M. Greenlief, *General Chair*

SUNDAY EVENING

Memorial Union
Stotler Lounge

MWRM Sci-Mix

K. Brorsen, V. Outlaw, *Organizers*

6:00 - 8:00

1. Soil health assessment in bottomland ecosystems: Chemical approach using nutrient and metabolomic profiling. **P.T. Salifu**, E. Owusu, S. Mahdi, Q. Yang, N. Tu
2. Metabolomic characterization of *Rudbeckia laciniata* using UHPLC–MS/MS: Nutrient-related phytochemicals and seasonal variation. **N. Tu**, S. Mahdi, A. Adeyeye, N. Navarrete-Tindall, R. Mu, Q. Yang
3. Organic matter removal in microplastic extraction: Challenges and methodological solutions. **H. Nath**, M. Salehi, S. Zolfaghari, M. Salehi
4. Folding-induced secretion blockade in the *Legionella pneumophila* Dot/Icm T4SS. **M. Humayun**, O.A. Neely, W. Lai, C. Durie
5. Conformational analysis of MTHFR threonine 59 and tyrosine 275 mutants via hydrogen deuterium exchange and mass spectrometry. **R. Ponce**, E.M. Marzluff, E.E. Trimmer
6. Get involved with the ACS Division of Chemical Education. **J. Boutte**
7. Effects of N5-formyltetrahydrofolate binding on conformation of wild-type type and H273L mutant *E.coli* Methylenetetrahydrofolate Reductase (MTHFR) through HDX and LC-MS. **S. Lopez Gonzalez**, E.M. Marzluff, E.E. Trimmer
8. Simulation of DNA damage as a function of DNA concentration and radiation dose using Geant4-DNA. **N. Tabassum**, K. Brorsen

9. Coordination chemistry of Copper(II) complexes with Cyclen-based bifunctional chelators: DFT and NBO study. **M. Richardson**, D. Hubin, C.J. Anderson, K. Brorsen
10. Design and reactivity of a redox-active dinickel Bispincer complex featuring a bridging Bispincer Nitrenoid ligand. D. De Los Santos, **K. Gour**, M. Shoshani
11. Mixed metal biogenic manganese oxide materials for catalysis and rare earth element sequestration. **J. Brown**, **C. Runge**, S.E. Shaner, K.L. Stone
12. Synthesis and characterization of heteroleptic transition metal complexes. **G. Uralova**
13. Synthesis of various silicates and measurement of their redox potentials. **L. Powers**, L. Hargrave, R. Van Hoveln
14. Expanding the near-infrared palette: 1,6-diheterophenylene-2,5-dione-based fluorophores. **I. Fuentes**, C. Lin, M. Michie, R. Tang, M.Y. Berezin, V. Birman
15. Ligand-controlled coupling of aryltetrafluorosilicate and aryldiazonium salts. **W. Ross**, C. Stultz, D. Dugger, M. Lange, R. Van Hoveln
16. Microwave-assisted synthesis of functional magneto-plasmonic nanosensor (MPNs) for the sensitive detection of foodborne pathogens. **T. Timalaena**, S. Santra
17. Identifying the redox partners of cytochrome P450s in *Pseudomonas aeruginosa*. **Y. Tai**, R.V. Ooteghem, A. Rusch, J. Miller
18. Doxorubicin prodrug encapsulated activatable MR nanoprobe for the theranostic treatment of cancer. **J. Speake**, B. Dous, T. Banerjee, S. Santra
19. Coiled-coil peptides: A template for studying the correlation between Leu to Val mutations and stability using auto-quenching fluorescence. **M. Blackburn**
20. Plug-and-play peptide enables antibody-directed cell targeting and fluorescent imaging of hematological cancers. **J. Shelton**, A. Kalabak, A. Barcellona, B. Ulery
21. Dunham Analysis of the $b\ ^4\Sigma^- - a\ ^4\Pi$ transition of O_2^+ , dioxygen cation. **J.J. O'Brien**, N. Woods, L.C. O'Brien
22. Conformer distribution of normal propyl cyanide in neat and water-rich ices probed by broadband rotational spectroscopy. **E. Hayden**, Q. Borengasser, B.M. Moore, K. Renshaw, B. Broderick
23. Reactivity revealed: Phase changes in SiO_2 driven by molten LiCl , oxygen, and water. **N. Mlynski**, M. MacInnes

24. Multifunctional zinc hydroxide composites enriched with biotin and gelatin: Dual-action biomedical platform. **N. Freiburger**, I.S. Zegar, C. Ward, A. Ghosh, A. F. Martins, M. Parvinzadeh Gashti
25. Impact of arene group identity, annulation and photolabile protecting group on photodeprotection rates of 1,2,3-triazolium salts. **E. Hanneken**, Z.L. Onyschuk, J.T. Fletcher
26. Making friends with 6-bromobenzothiazoles: A structural study. **I. Ginie**, T. Patel, N. Marasinghe Prins, B. Averkiev, C.B. Aakeroy
27. Multiplexed pulsed current sensors for anion detection. **C.S. Gopaul**, S. Mehregan, H.D. Koenig, W. Murphy, C.T. Veal, D.T. Anderson, K. Brorsen, M. Young
28. Potentiostat-free electrochemiluminescence reporting for microchip electrophoresis based detection of nitrotyrosine containing peptides. **S. Barua**, I.K. Warnakula, S.M. Lunte
29. Attaining true multicolor dSTORM images using phasor analysis. **J. Embree**, B. Dong, E. Pott, M. Yang, J.E. Batey
30. Exploring the unique potential pi-stacking properties within Reniochalistatin E: Synthesis and evaluation of a glycine analog. **R. Kearney**, M. Barnett, R. Pierce, R. Rafferty
31. Efforts towards construction of a new paradigm in chemical screening library assembly from natural products: The story of the Brocazines. **A. Wilkinson**, V. Nadar, W. Hulangamuwa, R. Rafferty
32. Light-mediated synthesis of azepine-linked peptide macrocycles. **H. Heidarzadeh Vazifehkhori**, H. Seyrani, V. Outlaw

MONDAY MORNING

Memorial Union
N201C

Midwest Award Symposium: Discovery and Destiny in Organic Chemistry

Financially supported by Dow, Revvity
M. Harmata, *Organizer*
K. R. Buszek, *Presiding*

7:55 Introductory Remarks.

8:00 33. Exploring the power of boron-based radicals in continuous-flow synthesis. **U.K. Sharma**

8:45 34. A redesigned approach to accessing cationic intermediates. **P. Musacchio**

9:30 Intermission.

10:00 35. Fun with unusual functional groups. **S. Sathyamoorthi**

10:45 36. Natural products synthesis and a radical-triggered functional group translocation strategy. **M. Tomanik**

Memorial Union
Stotler Lounge

Polymers and Materials

P. R. Calvo, A. Teator, *Organizers*

8:00 - 9:45

37. Post-polymerization modification of twisted polyacrylamides. **A. Redwine**, A. Teator

38. Synthesis and investigation of metal-chelating polymers: A bottom-up approach. **G. Moran**, P.R. Calvo

39. Tunable chitosan nanoparticles: Effects of crosslinking parameters on size, surface charge, and encapsulation efficiency. **D.N. Dassanayake Mudiyanse**, D. Afsar, P.R. Calvo

40. Machine learning guided discovery of photoresist polymer dopants. **S. Fernandez**, M. Maschmann, M. Young, D.T. Anderson, S. Kovaleski

41. Amphiphilic block copolymer–retinoid conjugates for tunable micellar drug delivery. **S. Overturf**, D. Afsar, P.R. Calvo

42. Incorporation of metal organic frameworks in polyethersulfone membranes for versatile water filtration. **C. McKellep**, C. Johnson-Edler

43. Monitoring of natural aging processes in biodegradable polyurethane foams. **K. Sklenickova**, A. Mahun, L. Kobera, S. Abbrent, O. Kočková, N. Bala, E. Oga, A. Kubatova, H. Beneš

44. Sweet and stiff: Engineering high-performance coatings from sugars. **W. Teggatz**, D. Dileep, A. Subbiah, A. Remus, M.J. Forrester, E.W. Cochran
45. GeO₂ and GeO₂-SiO₂ nanoparticle growth in the presence of polyols. **M.K. Schaefer**, E. Hicks, Z.B. Alhejaj, J.F. Destino
46. Strain-release approach to rigid-ring polymers. **A. Adhikary**, A. Teator
47. Sintering studies of metal-doped silica nanoparticles for stained glass additive manufacturing. **M.J. Varguez**, A.R. Carr, J.C. Chou, J.F. Destino
48. Synthesis of surface-functionalized silica nanoparticles for use in metal-binding applications. **M.G. Wilson**, M.J. Varguez, A.R. Carr, J.F. Destino
49. Fluorescent microparticle-doped thin films for use in the quenchimetric detection of heavy metal ions. **J.O. Wilson**, J.F. Destino
50. Unleashing the potential of unactivated secondary polyacrylamides. **P. Bonagiri**, A. Teator
51. Solvent exchange in MOFs monitored by proton NMR. **C. Rhoads**, A. Devlin
52. Initial investigations into novel assembly of siloxy amino functionalized balafricon A contact lenses with APTES [(3-aminopropyl)triethoxysilane] methods. B.C. Salm, W.L. Mangwi, A.E. Abdulhafiz, C. Eglund, **J.L. Duffy-Matzner**
53. Addition of hydroxybenzoic acids to epoxidized soybean oil for antibacterial applications. **S. Bandy**, A. Martins, C.J. Neef
54. Further investigations for the synthesis and characterization of carboxymethylene chitosan and carboxymethylcellulose microparticle for the delivery of ocular medication. W.L. Mangwi, B.C. Salm, A.E. Abdulhafiz, C. Eglund, **J.L. Duffy-Matzner**
55. Solvent effects on the unexpected reactivity of a mixed-linker MOF. **T. Campbell**, T. Gadzikwa
56. Chemical conversion of corn biomass into water-soluble methylcellulose. **C. Sudalaimani**
57. Steric Effects of Halogens Tune Framework Topology and Confined Reactivity in Pillared Paddlewheel MOFs. **L. Pothupitiya**, T. Gadzikwa
58. Interplay of non-covalent interactions to investigate photoinduced deformation in azobenzene crystals. **R. Kadiyan**, S. Datta, R. Jagan, J. Xu
59. An optimized electrically-polarized graphitic device manifests shielding against a broad-band microbial invasion. **N. Mazumder**, A.Y. Vargas-Lizarazo, M.J. Atienza-Parcon, F. Anshu, A. Fakhoury, D. Prakash, S. Hamilton-Brehm, P. Kohli

- 60.** Antifungal activity of *Trichoderma* filtrate-loaded nanoliposomes against *Fusarium virguliforme*. **M. Atienza**, H. Polat, A.Y. Vargas-Lizarazo, M. Sinkiewicz, J. Bond, P. Kohli, A. Fakhoury
- 61.** Influence of diamine cross-linker on the curing dynamics of eugenol-based epoxy thermosets. **H. patel**, C. Bodhak, R.K. Gupta
- 62.** Customizable circadian-responsive white LEDs enabled by 3D-printed lead-free perovskite conversion layers. **Y. Yue**, H. Zhu, C. Dzorkpata, Y. Chen, P. Zhu
- 63.** Effects of formulation parameters on direct ink write glass printing. **R. Emerson**, N. Tobin, J. Chou, M. Murthi, J.F. Destino
- 64.** Investigating the effect of polymer composition in antimicrobial polymers. **I. Thakur**, D. Afsar, P.R. Calvo
- 65.** Novel approach for fabrication of lactose fibers derived from milk using melt centrifugal/rotary jet spinning concept. **A. Rahman**, S.I. Shah, I.S. Zegar, C. Ward, W. Shou, M.P. Gashti
- 66.** Fe/Co/Ni-DOPED MOS₂ an electrocatalyst for overall water splitting. **H. Inu**
- 67.** Modified limonene and Geraniol via thiolene processes under UV Curing to obtain polyurethane films. **S.R. Patel**
- 68.** Stainless steel as efficient electrocatalyst for oxygen evolution reaction. **C. Uypuanco**, F. Zuo

Memorial Union
N201B

Analytical Chemistry

K. Brorsen, V. Outlaw, *Organizers*
B. Habarakadage, *Presiding*

- 8:10 69.** Characterization of bismuth coated laser induced graphene versus glass carbon electrode for electrochemical detection of heavy metals. **K. Chen**
- 8:35 70.** Gold nanorod-traction force microscopy in resolving traction force and torque simultaneously in live cell. **M. Yang**, B. Dong

9:00 71. Study the influence of water chemistry conditions on lead (Pb) adsorption by new and photodegraded microplastics. **S. Zolfaghari**, M. Salehi

9:25 72. Bioaccumulation pattern of per- and polyfluoroalkyl substances (PFAS) in fish tissues from two freshwater systems. **M.O. Eze**

9:50 Break.

10:10 73. Comprehensive lipidomic mapping highlights region-specific lipid perturbations in early Alzheimer's pathology. **N. Khanom**, A. Prislovsky, N. Lenchik, N. Mandal, M. Islam

10:35 74. Withdrawn

11:00 75. Compositional analysis of glass beads from a Missouri historic site using laser ablation-inductively coupled plasma-mass spectrometry. **D. Qais**, A. Kuo, C. Sall, B. MacDonald

11:25 76. Monitoring residual chloroform and bromoform in aqueous systems: Headspace analysis by GC-FID. **I.K. Warnakula**, M.J. Hageman, Z.T. Logan

Memorial Union
N204

Inorganic Chemistry

K. Brorsen, V. Outlaw, *Organizers*
M. Muhammad, *Presiding*

8:10 77. Withdrawn

8:35 78. Exploring the reactivity of uranium anilido and imido species. **S.C. Bart**

9:00 79. New unsymmetrical diglycolamide ligands for rare earth metal complexation. **B.G. Tokheim**, E. Hintgen

9:25 80. To build a mock enzyme: synthetic transition metal complexes as models of metalloenzyme active sites. **J. Parham**

9:50 Break.

10:10 81. Single crystal X-ray diffraction in structural science: cutting-edge contributions from a venerable technique. **S.P. Kelley**

10:35 82. Exploring low-valent U and Th complexes supported by terphenyl-based frameworks. **J. Chatterjee, J.R. Walensky**

11:00 83. Cooperative bond activation utilizing a bimetallic Ni-Mg complex. **F. Gonzalez, M. Shoshani**

11:25 84. Characterization and reactivity of iron triazametallacyclohexadi-ene complexes: Toward iron-catalyzed multicomponent reactions. **C. McGhiey**

Memorial Union
N214C

Organic Chemistry

K. Brorsen, V. Outlaw, *Organizers*
K. , *Presiding*

8:10 85. Biocatalytic Aza-Michael addition of aromatic amines to enone using α -amylase in water. **S. Dutt**

8:35 86. Structure-based design of 3,4-dihydroquinazolin-2-yl benzenesulfonamides as carbonic anhydrase-targeted anticancer agents. **H. Okda, L. Maram, D. Kanaa, H. Duggan, L. Hegazy, C.T. Supuran, B. Elgendy**

9:00 87. Synthesis of cinnamic acids and their utilization for open-ring analogs of ipomoeassin F. **R.E. Sammelson, P. Tumfuo, W. Shi**

9:25 88. *N*-heterocyclic carbene photocatalysts for aryl halide phosphorylation, borylation, and cyanation. **a. joshy, A.S. Kelley, S. Vadakke Poikail Sasi, A. Portillo, S. Laulhé**

9:50 Break.

10:10 89. Design and synthesis of novel sulfonamide- and oxamide- based agents for treatment of Mycobacterial pathogens. **A.S. Dumbre, E. North**

10:35 90. NMR assignments of esters formed from saturated linear carboxylic acids and linear alcohols. A. Lamb, **J.B. Friesen**

11:00 91. Analysis of palladium residues from catalytic hydrogenation reactions via inductively coupled plasma atomic emission spectroscopy (ICP-OES). **G.P. Nora**

Memorial Union
N214D

Physical Chemistry

K. Brorsen, V. Outlaw, *Organizers*
H. R. Krueger, *Presiding*

8:10 92. Synthesis and application of novel sodium carboxy methyl cellulose-g-poly acrylic acid carbon dots hydrogel nanocomposite (NaCMC-g-PAAC/ CDs) for adsorptive removal of malachite green dye. H. Majeed, T. Idrees, M. Mahdi, M. Abed, **M. Batool**, S. Yousefi, A. Thumma, L. Jasim

8:35 93. Growth of the All-Inorganic Lead-Free 1D CsCu₂X₃ (X = Cl, Br, I) Perovskites with Exceptional Stability for High-Performance White-Light Emitting Diodes. **Y. Chen**, H. Zhu, P. Zhu

9:00 94. Polarity dependent synchronization of oscillatory nickel electrodisolution with asymmetrical nonlinear cathode-anode coupling. **A. Limbu**

9:25 95. Effects of applied potentials on electrical double layer characteristics at Pt/[Bmpy][NTf₂] ionic liquid interface under inert and hydrogen environment. **K. Arora**, Y. He, W. Lai, X. Zeng

9:50 Break.

10:10 96. Spectral engineering and carrier dynamics in Y, Sb-doped double perovskites for solid-state lighting. **C. Dzorkpata**, Y. Chen, H. Zhu, P. Zhu

10:35 97. Designing white-light emission via europium and terbium co-doping in lead-free Cs₂ZrCl₆ perovskites. **A. Islam**, C. Dzorkpata, Y. Chen, P. Zhu

11:00 98. Nucleation of An(IV) ions in presence of anionic and zwitterionic ligands. **G. Donkor-Gyami**, P. Miro

Memorial Union
N201A

Advanced Optical Imaging with Nanomaterials

A. H. Flood, *Organizer*
T. Ito, *Presiding*

8:30 Opening Remarks.

8:35 99. Hierarchically-organized electrochemical-photonics nanostructures for studies of single entities: Molecules to particles to microbes. **P. Bohn**

9:10 100. Synthesis of electroswitchable fluorophores for redox-based ON-OFF fluorescence switching. **D. Gupta**, A.H. Flood, T. Ito

9:30 101. Opto-electrochemical imaging of the formation of nanoparticles and nanobubbles. **V. Sundaresan**, I. Jayalath, S. Shukla

10:05 Break.

10:15 102. Crystal engineering of fluorescent dyes in SMILES nanoparticles for bioimaging. **A.H. Flood**

10:50 103. Simultaneous detection of surface restructuring and catalytic activity of Cu-nanowires in Alkyl-Azide click reactions using multi-channel microscopy system. **B. Rainwater**, G. Salmanian, J. Chen, B. Dong

11:10 104. Directly monitor the chemical transformation of carbocation intermediates in zeolite catalysis at single-molecule level. **B. Dong**

Memorial Union
N214A

Advances in Peptide Chemistry: Synthesis, Structure, and Function

V. Outlaw, *Organizer, Presiding*

8:30 Introduction.

8:35 105. Strategies to eradicate HIV: Developing dual peptidomimetic agents that simultaneously activate HIV latency and prevent new infection. **M.A. Lipton**, J.A. Chmielewski

9:05 106. Chemoselective sulfonyl-fluoride exchange (SuFEx)-induced macrocyclization of tyrosine-containing peptides. **H. Seyrani**, H. Heidarzadeh Vazifehkhori, V. Outlaw

9:25 107. Remodeling the peptide backbone to unlock new approaches in peptide chemistry and drug design. **B. Vanveller**

9:55 Intermission.

10:10 108. Stalking elusive pathogenic bacteria with cationic amphiphilic polyproline helices: How to dive into cells to treat infections. **J.A. Chmielewski**

10:40 109. Phage-assisted continuous selection of cyclic peptide protein aggregation inhibitors. L. Yang, J. Zhang, J. Andon, L. Li, **T. Wang**

11:10 110. Affinity-driven aryl diazonium labeling to study peptide-receptor interactions. S. Sharma, C. Stebbing, M.J. Naldrett, **J.W. Checco**

11:40 111. Decoding transcription complexes: Mechanisms & molecules. **A.K. Mapp**

12:10 Closing Remarks.

Memorial Union
N214B

From Structure to Function in Solid-State Supramolecular Chemistry

K. M. Hutchins, *Organizer, Presiding*

8:30 Opening Remarks.

8:35 112. Conformational inversion in heterotriangulenes for ferroelectric switching. **R.A. Wiscons**

9:05 113. Exploring cocrystallization and polymorphism with mechanochemistry. **D. Botes**, K.M. Hutchins

9:25 114. Hydrogen-bonding directed synthesis of dynamic organic frameworks and cages. **C. Ke**

9:55 Break.

10:15 115. Powders grain-by-grain: High-throughput structural analyses enabled by automated electron diffraction. **J. Burch**

10:45 116. Synthesis and structural analysis of the iodo analogue of Favipiravir and its cocrystals: Insights into structure-property relationships. **N. Marasinghe Prins**, B. Averkiev, C.B. Aakeroy

11:05 117. Pop-up porous molecular Solids as selective sorbents. **K.T. Holman**

Memorial Union
Stotler Lounge

Polymers and Materials

P. R. Calvo, A. Teator, *Organizers*

10:00 - 11:45

118. Cotton candy machines go biomedical: Novel antimicrobial lactose fiber fabrication. **A. Rahman**, S. Shah, I.S. Zegar, C. Ward, W. Shou, M. Parvinzadeh Gashti

119. Synthesis and characterization of surface functionalized nanoscale Ln^{3+} -based metal-organic frameworks for biological imaging applications. **B. Eide**, R.T. Schulte, Z. Schulte

120. A bifunctional MOF catalyst with simultaneous basicity and dual-hydrogen bond donor activation for the Henry reaction. **L. Udube**

121. Rhodamine dipeptide drug delivery system for 5-Fluorouracil with *in-vito* cellular tracking. S. Taneja, **B. Li**, J.R. Parquette

122. Rearrangement-mediated chain growth polymerization for diversity in microstructure. **A. Lininger**

123. Crosslinking corn proteins: Chemical property enhancement of Zein films via silicone crosslinking agents. **S. Wicks**, I.S. Zegar, J.H. Norton, M. Parvinzadeh Gashti

124. From insect to color indicator: Monitoring cheese freshness with cochineal-derived carminic acid. **A. Freiburger**, M. Abdilla, M. Parvinzadeh Gashti

125. Controlled synthesis of ABA triblock copolymers using RAFT polymerization. **P. Kaur**, P.R. Calvo

- 126.** Mechanistic insights into surface wear dynamics of plastics: The interplay of intrinsic and extrinsic properties and implications for environmental plastic pollution. **A. Gopakumar**, M. Salehi, C. Greiner
- 127.** Thermal neutron irradiation as a potential approach to engineer defects in advanced materials for enhanced ionic conductivity: Case study of LiBO_2 . **H.M. Nguyen**, C. Ziemke, Z. Vogelsmeier, N. Narayanan, D. Stalla, B.C. Saha, J. Gahl, Y. Xing, C. Wexler, T. Heitmann
- 128.** Systematic first-principles study of the formation of substitutional defects at lithium sites in Li_3OCl antiperovskite as a potential solid electrolyte for all-solid Li-ion batteries. **C. Ziemke**, H.M. Nguyen, S. Amaya-Roncanci, J. Gahl, Y. Xing, C. Wexler
- 129.** Switching off opportunistic bacteria and Fungi using electrically-polarized 3D-nanoporous microscale silicon oxide antimicrobial surfaces. **A.Y. Vargas-Lizarazo**, C. Tran, M. Atienza, L.M. Griswold, F. Olubiyo, G. Rodriguez, D. Hedrick, D. Mazumdar, A. Fakhoury, Y. Hou, S. Hamilton-Brehm, P. Kohli
- 130.** Assessing the vertical distribution of pristine and weathered microplastics: insights for improving sampling strategies. **A. Beheshtimaal**, R. Xu, B. Wang, M. Salehi
- 131.** Mechanistic study of micro- and nanoplastic transport within biofilm-laden potable-water plumbing materials. **A. Bashir**
- 132.** Molecular Control of Interfacial Electrochemically-Driven Reactions: Machine Learning Interatomic Potentials, Quantum Dynamics Simulations, and Vibrational Spectroscopy. **Q.O. Adewuyi**, M. Momenitaheri
- 133.** Spacer-dependent design of amino-functional methacrylamide polymers: Synthesis, RAFT polymerization, and antimicrobial evaluation. **D. Afsar**, P.R. Calvo
- 134.** Temperature responsive hyperbranched block-copolymers. **B. McLeland**, P.R. Calvo, D. Afsar
- 135.** Engineered NCA-polymerized lipidated poly(amino acid) nanoparticles for targeted non-Hodgkin lymphoma therapy. **B. Boney**, J. Smith, M. Schulte, A. Hemmerla, X. Wang, F. Rezaei, D. Burke, M. Daniels, B. Ulery
- 136.** Osteoinductive microgels for targeted osteoporosis treatment. **L. Schrader**, A. Hemmerla, B. Boney, R. Emlet, D. McTigue, B. Ulery
- 137.** Thermoresponsive metal-chelating copolymers: Controlling binding and removal via phase changes. **L. Elliott**, G. Moran, P.R. Calvo
- 138.** Assessing the potential of biomass hydrothermal liquefaction hydrochar for soil amendment: Chemical/physical characterization and water holding capacity and retention. **A. Issifu**

139. Withdrawn

140. Modular approach to complex precision macromolecular architectures via ADMET polymerization. **D. Bhandari**

141. Synthesis of highly branched metal chelating polymers via RAFT polymerization. **A.K. Imiya Mudiyansele**

142. Cationic ring-opening polymerization of lactones derived from isoprene, butadiene, and CO₂. **R.T. Schulte**, M. Bhatt, C. Webber, I. Tonks

143. Green synthesis of photosensitive MOFs: Towards sustainable photovoltaic materials. **M. Hasan**, T. Dipti, Z. Yang

144. Liquid Assisted Grinding (LAG): A green and scalable approach for mechanochemical synthesis of enzyme@MOFs. **T. Dipti**, M. Hasan, Z. Yang

145. Heavy biocrude (HBC) coating to protect plant fiber twine against biodegradation and weathering. **M.A. Sumi**, C. Zhang

146. Tuning molecular ionic composite electrolytes for use in solid-state lithium batteries. **A.L. Gibson**, N.F. Pietra, L.A. Madsen

147. Short- and mid-term impacts of Hurricane Debby on microplastic pollution in urban drainage systems of Tallahassee, Florida. **S. Zolfaghari**, A. Mobin Ibna Hafiz, **E. Ahmadisharaf**, M. Salehi

148. Chitosan/heparin and Tanfloc (polyphenolic tannin)/heparin multilayers deposited on superhydrophilic poly(ϵ -caprolactone) fibers to enhance hemocompatibility. **A. Martins**, F.R. Veregue, L. Madruga, K. Popat, M. Kipper

149. Dynamics of photoinduced halide segregation in mixed halide perovskites. **A. Teggatz**, A.M. Shareque, Y. Guo

MONDAY AFTERNOON

Memorial Union
Stotler Lounge

Physical Chemistry

K. Brorsen, V. Outlaw, *Organizers*

1:15 - 3:00

150. Molecular Dynamics Simulations of Osmotic Pressure and Membrane Potentials. **J. Crenshaw**, E.A. Ploetz, P.E. Smith

151. Effects of alanine on the hygroscopic properties of inorganic salt aerosols. **A. Serp**, J.P. Darr, S. Griffin, C. Stebbing

152. Construction and electronic properties of realistic nanocone apex tips. **J.R. Dias**

153. Range of water ordering in hydrophobic solvation of inert gases. **C. Yang**, R. Maharjan

154. Assessing stability of metal-organic frameworks in water for energy-efficient dehumidification using DFT. **L.J. Chudacoff**, B. Vlaisavljevich

155. Computational study of covalency in a Neptunium(III) Borohydride complex. **C.R. O'Leary**, S.R. Daly, B. Vlaisavljevich

156. Crystal structure driven electrical properties in layered battery materials: Na₂Ni₂TeO₆ and Li₂Ni₂TeO₆. **B.C. Saha**, A.K. Bera, S. Kesari, S.M. Yusuf, N. Narayanan, T. Heitmann

157. Probing stability and hydrogen bonding in cyclopentadiene carbaldehyde oximes: Dual AICD & GIMIC approach. **S. Daly**, **A. Mahendran**, **A. Castillo**

158. Computational study of bonding in actinyl complexes with pnictogen oxide ligands. **N. Arsenijevic**, C. O'Leary, B. Vlaisavljevich, H.S. La Pierre, B. Solomon

159. Halogen- vs π - π Stacked Charge-Transfer Bonding between p-Phenylenediamine and Iodobenzene Derivatives. **M. Sarker**, S.V. Rosokha

160. Photophysical Investigation of π -Extended [1,4]Benzodioxino[2,3-b]oxanthrene-6,13-dicarbonitrile. **A. Guillen**, C. Anemone, M. Jimenez, **A. Castillo**, **A.M. Jamhawi**

161. Synthesis and characterization of π -extended [1,4]benzodioxino[2,3-b]oxanthrene-6,13-Dicarbonitrile. **C. Anemone**, A. Guillen, **A.M. Jamhawi**

162. Structures and UV-Vis-NIR spectroscopy of the charge-transfer complexes of aromatic (di-)amines with nitrobenzene acceptors. **I. Sarfo**, S.V. Rosokha

163. Computational Investigation of π -System Extension in [1,4]Benzodioxino[2,3-b]oxanthrene-6,13-dicarbonitrile. **M. Jimenez**, **A.M. Jamhawi**, **A. Castillo**

- 164.** Mechanistic study of propene metathesis on heterogenous catalyst. **S. Brahmachari**, M. Caricato
- 165.** Low temperature molecular spin decoherence dynamics using Lindblad master equation method. **K.E. Coffin**, T.J. Krogmeier, A.W. Schlimgen, K. Head-Marsden
- 166.** Computational characterization of a recently identified disinfection byproduct in drinking water: Chloronitramide anion and its monohydrate complexes. **T.M. Ismail**, G.S. Tschumper
- 167.** Concerted proton transfer in small cyclic hydrogen bonded clusters. **M. Tucker**, G.S. Tschumper
- 168.** 2D solution NMR analysis of DNAs containing ribo modifications and a DNA-RNA hybrid. **A. Loughary**, M. Lewis, G.A. Meints
- 169.** Detecting heart failure before it strikes: In silico analysis of aptamer-mediated perm1 protein detection in systolic heart failure. **S. Boinepally**, G. Sharma
- 170.** Dunham Analysis of the $b\ ^4\Sigma^- - a\ ^4\Pi$ transition of O_2^+ , dioxygen cation. **J.J. O'Brien**, N. Woods, L.C. O'Brien
- 171.** Efficient and accurate quantum vibrational spectroscopy with bead-Fourier centroid molecular dynamics. **M. Faruque**, N. London, M. Momenitaheri
- 172.** Withdrawn
- 173.** Structure of benzyl isothiocyanate self-assembled monolayers on Au(111)/mica surfaces using atomic force microscopy. **D. Moïny**, L.S. Tackett, L.N. Penland, D. Ovchinnikov, R.G. Farber
- 174.** Bead-Fourier path-integrals for approximate quantum dynamics. **N. London**, M. Momenitaheri
- 175.** Kohn-Sham decomposition of excited states of Ag nanowires and nanoclusters. **J.T. Bvunzawabaya**
- 176.** Systematic screening of molecular models using physically validated machine learning. **Y. Wijesiriwardena**, C. Fennell
- 177.** Mechanoluminescence and photoluminescence properties of $(\text{Eu}^{2+}, \text{Eu}^{3+}, \text{tm}^{3+}, \text{Tb}^{3+}, \text{Mn}^{2+})$ -doped $\text{Sr}_2\text{P}_2\text{O}_7$ phosphors synthesized by the solid-state method. **Y. Chen**, H. Zhu, P. Zhu
- 178.** Anti-parkinson's therapeutic discovery: Computational chemistry approach. **N.I. Ihechu**
- 179.** Modeling bonding in a series of dinuclear transition metal complexes with tetradentate ligands. **A. Yaddehige**, J. Cardona, S.R. Daly, B. Vlasisavljevich

Memorial Union
N201B

Analytical Chemistry

K. Brorsen, V. Outlaw, *Organizers*
M. O. Eze, *Presiding*

1:20 180. Synergistic toxicity of engineered nanoparticle mixtures on soil microbial networks and biogeochemical functions. **D. KC**, N. Tu, L. Xu, X. Ma, H. Yang, H. Shi, Q. Yang, J. Yang

1:45 181. Mass spectrometry imaging with *in vivo* isotope labeling for spatio-temporal study of galactolipid biosynthesis in *Lemna minor*. **V.T. Tat**, Y. Lee

2:10 182. Decoding paracrine and contact-mediated chemical signals in stress-induced cell fate modulation. **M. Imranuzzaman**, S. Mahdi, N. Tu, X. Zhang, Z. Yin, Q. Yang

2:35 183. Efficacy of green infrastructure systems in microplastic removal from urban stormwater runoff. **R.A. Day**, A. Henry, A. Snider

3:00 Break.

3:20 184. Toward safe silver-based antimicrobial membranes: Electrospun core-shell fibers with embedded AgCl nanoparticles for space applications. **V. Nathan Somasundaram**, J. Koehne, L. Delzeit, M. Anderson, J. Li

3:45 185. Nested-scale monitoring of nutrients and emerging contaminants in a mixed-use watershed using UHPLC-MS/MS and hydrologic analysis. **A. Dhakal**, Q. Yang, S. Mahdi, N. Thomas

4:10 186. Land use-induced soil biochemical shifts: UHPLC-MS/MS-based metabolomics analysis of forest and agricultural soils. **E. Owusu**, Q. Yang, S. Mahdi, P. Salifu

4:35 187. A dual analytical approach to understanding PAH generation in neat HTPB pyrolysis: Methodological advancements and mechanistic insights. **E.A. Oga**, V. Karpovych, N. Bala, N. Haiduk, A. Kubatova, E.I. Kozliak, M. Sulkes

Memorial Union
N214D

Biochemistry

K. Brorsen, V. Outlaw, *Organizers*
C. Durie, *Presiding*

1:20 188. Mapping the catalytic cycle of an iterative NIS synthetase, DesD, using rationally designed inhibitors. **C. Merrick**, K. Patel, N. Gulati, A. Gulick, T.A. Wencewicz

1:45 189. Designing an efficient biocatalyst for a chemobio hybrid upcycling of waste textile. **L. Dissanayake**, S. Ghosh, D. Madushanka, B. Jayanthaa, S. Jayasekara, I. Hou, L.N. Jayakody

2:10 190. Effect of pegylated gold nanoparticles on alpha-synuclein fibrillation. **B.C. Akano**, R. Kanogo, T. Banerjee

2:35 191. Utilizing spectroelectrochemistry for redox cofactor-binding aptamer characterization. **M. Lingle**, M. Sarkis, T.D. Pentland, D.A. Baum

3:00 Break.

3:20 192. Structural characterization of the yeast CAF-1 PIP motif bound to PCNA reveals interactions with PIP flanking residues. **E. Veltri**, K. Orndorff, N. Hoitsma, G. Jaworski, S. Kallepalli, G. Majeres, L. Dieckman

3:45 193. BE2012: A next-generation REV-ERB antagonist with therapeutic potential in muscle and neurodegenerative disorders. **L. Maram**

4:10 194. Lipidomic profiling of human plasma identifies specific lipid shifts linked to diabetes. **S. Mitu**, F. Stentz, N. Mandal, M. Islam

4:35 195. IL-4 suppresses ADCP through increased steric hinderance blocking IgG-FcγR binding on the macrophage cell surface. **S. Islam**, G. Deakins, M. Hossain, B. Fischer, N. Dorn, B. Scott, A. Hoppe

Memorial Union
N204

Inorganic Chemistry

K. Brorsen, V. Outlaw, *Organizers*
B. G. Tokheim, *Presiding*

1:20 196. Withdrawn

1:45 197. From prediction to synthesis: Large language models for accelerating metal-organic frameworks discovery. **Z. Zheng**

2:10 198. Mechanistic insights into calcium aluminium nitrate layered double hydroxide-enhanced hydration of tricalcium silicate, tricalcium aluminate-gypsum, and ye'elemite-gypsum systems. **G.I. Ogbuehi**, M.U. Okoronkwo

2:35 199. Zirconium-89 labeled PAMAM G5 dendrimer for targeting atherosclerotic plaques. **K. Sikligar**, H. Kou, J. Yan, L. watkinson, T. Carmack, M. Rodgers, T. Cui, H. Yang, C.J. Anderson, L. Ma

3:00 Break.

3:20 200. Synthesis and characterization of *G3* family of organoantimony(V) cyanoximates for antimicrobial and antifungal studies. **T. Phan**, N. Gerasimchuk

3:45 201. Withdrawn

4:10 202. Redox-induced ligand exchange of a hydrogen bond acceptor in a zinc complex. C.N. Gilchrist, M. Zeller, **J.J. Kiernicki**

4:35 203. Withdrawn

Memorial Union
N214C

Organic Chemistry

K. Brorsen, V. Outlaw, *Organizers*
A. Dusunge, *Presiding*

1:20 204. Efforts toward the total synthesis of Balgacyclamide C: optimization of macrocyclization through enhance rigidity. **M.H. Rice**, A. Torres Hernandez, R. Rafferty

1:45 205. Brocazine family of natural products: Efforts towards the first total synthesis of Brocazine G and Phomazine B. **V. Nadar**, W. Hulangamuwa, R. Rafferty

2:10 206. Advancing non-opioid therapies: Structure–activity relationship study of GPR183 antagonists in neuropathic pain. **V. Kalajdzic**, I.I. Olayide, D. Salvemini, C.K. Arnatt

2:35 207. Divergent access to sulfur fluorine group-containing molecules. **T. Gatzenmeier**, Y. Liu

3:00 Break.

3:20 208. Bioconjugation with a Fluorogenic Linker. **J. Himmelberg**, F. Gallazzi, W.B. Edwards, T.E. Glass

3:45 209. Elucidating the mysteries of BI₃ reduction of acenes. **A. Corkovic**, F.J. Williams

4:10 210. Sustainable production of tagatose via CaO-promoted galactose isomerization with CO₂ neutralization under ambient conditions. S. Babaei, **J. Zhao**

4:35 211. Engineering trehalose-conjugated Pks13 inhibitors targeting *Mycobacterium tuberculosis*. **U. Kumbalathara Arachchige Dona**, P. Halicki, B. Swarts, K. Rohde, S. Sucheck

Memorial Union
N201A

Advanced Optical Imaging with Nanomaterials

T. Ito, *Organizer*
A. H. Flood, *Presiding*

1:30 212. Behind closed membranes: Illuminating the chemistry of immune defense. **Y. Yu**

2:05 213. New approaches for characterizing biological nano-environments. **R.J. Vazquez**

2:40 214. Following the diffusive motions of single-particles for a better understanding of the microporous hydrogel structure and properties. **K. Tran Ba**

3:15 Break.

3:25 215. Nanoscale ordering of ionic liquids and deep eutectic solvents used in separation science. **E.A. Smith**, J. Opare-Addo, J.L. Anderson, J.W. Petrich, X. Song

4:00 216. Single-molecule tracking reveals the mechanism of molecular diffusion under nanoconfinement. **A. Nathani**, S. Asadi, D.A. Higgins, T. Ito

4:20 217. Super-resolved single-molecule tracking studies of rhodamine B accumulation on nanostructured polyethylene terephthalate surfaces. **D.A. Higgins**, S. Salehi

4:55 Concluding Remarks.

Memorial Union
N214B

From Structure to Function in Solid-State Supramolecular Chemistry

K. M. Hutchins, *Organizer, Presiding*

1:30 218. From tunable halogen- and chalcogen bonds via supramolecular control to enhanced chemotherapeutic properties. V. Panikkattu, V. De Silva, **C.B. Aakeroy**

2:00 219. Control of site-specific deprotonation through mechanochemical interconversion of two salt polymorphs of resveratrol. **B. Ziebarth**, L. Ma, G. George III, K.M. Hutchins

2:20 220. Utilizing dry-vortex grinding to generate co-crystals that undergo a solid-state [2 + 2] cycloaddition reaction. **R.H. Groeneman**

2:50 Break.

3:10 221. Structural control enables unique thermal and reactivity properties in organic solid-state materials. **K.M. Hutchins**

3:40 222. Design considerations for selective binding to perfluoroalkyl sulfonate anions. **S. Moaven**, A.J. Wise, D.L. Watkins

4:00 223. Organic crystals as synthetic laboratories. **L. MacGillivray**

4:30 Closing Remarks.

Memorial Union
N214A

Improving the Reliability of Methods and Processes in an Industrial Setting

B. Morton, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 224. In-depth literature review focused on PFAS (per- and poly-fluoroalkyl substances) chemicals and PCB's (polychlorinated biphenyls).. **S. Begum**

2:00 Intermission.

2:05 225. Case studies for optimization of analytical methods for routine use in pharmaceutical manufacturing. **M. Zart**

2:30 Intermission.

2:35 226. Use of process analytical tools to improve reliability in crystallization processes. **J.T. Gavin**

3:00 Intermission.

3:05 227. Case studies for improving recovery in a GC-HS method, peak identification in an HPLC-UV method, and accuracy of a laser diffraction method for particle size distribution. **B. Morton**

Memorial Union
N201C

Midwest Award Symposium: Discovery and Destiny in Organic Chemistry

Financially supported by Dow, Revvity
M. Harmata, *Organizer*
K. R. Buszek, *Presiding*

1:30 228. Upgrading azine scaffolds through core-retaining atom swapping. J. Han, E. Jacobsen, Z. Liu, **Y. Zhang**

2:15 229. Beyond nature's blueprint: A new biochemical logic for asymmetric reduction of unactivated olefins. J. Vallapurackal, R. Mandal, J. Bossenbroek, A. Rubio, E. Poladian, J. Collings, C. Torres, J. Morales, M. Lyons, H.S. Shafaat, K.N. Houk, **S.V. Athavale**

3:00 Intermission.

3:30 230. Boron trihalides as versatile reagents in synthetic strategy. **F.J. Williams**

4:15 231. Adventures at the interface of synthetic organic & enzymatic chemistry. **D.B. Berkowitz**

Memorial Union
Stotler Lounge

Biochemistry

K. Brorsen, V. Outlaw, *Organizers*

3:00 - 4:45

232. Identification and inhibition of pathways involved in the cellular uptake of Microplastics with a protein corona.. **J.C. Howard**, R.A. Day

233. Structural analysis of OAZ RNA in *Agaricus bisporus*. **N. Sequeira**, L. Nedungadi, J. Strauss Soukup

234. Peroxisome proliferated-activated receptor (PPAR) delta agonist as promising treatment for non-alcoholic fatty liver disease. **X. Luarasi**

235. Optimization of a high-throughput FRET assay to study *glmS* riboswitch self-cleavage in *Staphylococcus aureus*. **S. Nguyen**, L. Nedungadi, J. Strauss Soukup

236. Investigating a potential eukaryotic riboswitch in OAZ mRNA from *Agaricus bisporus* via in-line probing. **S. Fowler**, N. Sequeira, L. Nedungadi, J. Strauss Soukup

237. Effect of pyrimidine and purine base supplementation on pullulan production by *Aureobasidium pullulans* ATCC 201253. E.O. Brefo, C. Lutz, M. Jeffrey, **T.P. West**

238. Developing screening methods for pyruvate dehydrogenase kinase inhibitor discovery. **N.P. Lilla**, M. Moxley

- 239.** Characterization of two non-template directed RNA ligases. **C. Hoffman**, J. Schelzig, T. Opolka, S. DasGupta
- 240.** Structural and biophysical characterization of effector interactions with the IcmSW coupling complex in *L. pneumophila*. **R. Somarathne**, W. Lai, C. Durie
- 241.** HPLC characterization of bergamot extracts and potential inhibition of HMG-CoA reductase. **A. Worland**, N.M. DeVore
- 242.** Analysis of the *Agaricus bisporus* (mushroom) OAZ RNA using Dual Luciferase Assays (DLA). **S. Ahmed**, T. Burke, L. Nedungadi, J. Strauss Soukup
- 243.** NMR analysis of conformational changes in DNA sequences containing insertion-deletion lesions. **J. Terhark**, T. Osborne, G.A. Meints
- 244.** Cholesterol inhibition alters the production and the molecular profile of microvesicles. **M. Johnson**, D. Studer, J. Yaeger, K. Francis, M. Madeo
- 245.** Withdrawn
- 246.** Kinetics and thermodynamics of BI-BII interconversion in DNA: Effects of T:G and A:G mismatches and flanking bases. **H. Kimberlin-Poore**, G.A. Meints
- 247.** Design and structure-activity relationship study of novel REV-ERB agonists as potent therapeutics for chronic inflammatory pain. **G. Veerakanellore**
- 248.** Biophysical characterization of folding-restricted effectors in *Legionella pneumophila*. **O.A. Neely**, M. Humayun, W. Lai, C. Durie
- 249.** Exploring the structural basis of hnRNP C Protein in RNA recognition utilizing AlphaFold 2. **G. Doubrava**, Z. Todd, I.S. Zegar, J.G. McAfee
- 250.** Destabilizing MALAT1: A novel approach to lung cancer cell migration and invasion. **H. Warner**, M. Johnson, J.G. McAfee, I.S. Zegar
- 251.** Investigating flavin-binding aptamers under non-physiological conditions. **M. Sarkis**, T. Pentland, M. Lingle, D.A. Baum
- 252.** Interaction of tubulin associated unit(TAU) with PEGylated nanoparticles. **R. Kanogo**, T.M. Nyabayo, B. Akano, T. Banerjee
- 253.** Feedback inhibition on polyethylene terephthalate (PET) degradation enzymes, a potent challenge for biological recycling. **I. Hou**, L. Dissanayake, L.N. Jayakody
- 254.** Estrogen depletion effects on demyelination and remyelination. **K. Wilson**, E. Holt, M.C. Zupan, M.D. Hartley

255. Doxorubicin prodrug encapsulated activatable MR nanoprobe for the theranostic treatment of cancer. **J. Speake**, B. Dous, T. Banerjee, S. Santra

256. Coiled-coil peptides: A template for studying the correlation between Leu to Val mutations and stability using auto-quenching fluorescence. **M. Blackburn**

257. Improving fluorescein-based fluorogenic carbonates as chemical tools to study human carboxylesterase 1 (CES1) through structure-activity relationship (SAR) studies. **J. Booth**, L. Villalobos, E. Adusah, M.W. Beck

258. Elucidating conformational dynamics of DNA backbones in A:G mismatches and T-insertions using 2D solution NMR. **T. Osborne**, G.A. Meints

259. Plug-and-play peptide enables antibody-directed cell targeting and fluorescent imaging of hematological cancers. **J. Shelton**, A. Kalabak, A. Barcellona, B. Ulery

260. Analysis of aPDT and PFC nanoemulsions on treating biofilms formed by *C. albicans*. **C. Eckenroth**

261. Structure-activity relationship studies of human carboxylesterases using a fluorogenic ester library. **M. Drozs**, E. Adusah, T. Spidle, G.C. Hoops, R. Johnson, M.W. Beck

262. Optimization of a high-throughput FRET assay for identification of potential antibiotic compounds. **D. Cline**, L. Nedungadi, J. Strauss Soukup

TUESDAY MORNING

Memorial Union
N201A

Emerging Biosensing Techniques for Fundamental and Practical Applications

X. Guan, *Organizer*
L. Gu, *Presiding*

7:55 Introductory Remarks.

8:00 263. DNA nanostructure-guided electrochemical biosensor for sensitive microRNA detection. K. Thapa, H. Shuo, W. Liu, **R. Wang**

8:20 264. Multiplex colorimetric biosensor for ultra-sensitive detection of infectious disease biomarkers. **S. Krishnan**, S. Samaraweera, Z. Syed, P. Rahul, J. Ramsey

8:40 265. Advancing synthesis-free and enzyme-free rewritable DNA memory through bio-inspired frameshift encoding and nanopore duplex unzipping decoding. **L. Gu**, K. Tian, S. Chen

9:00 266. New label-free probes for electrochemical detection of genetic repeat mutation on 2D nanomaterials. **M. Shamsi**, P. Das, M. Noby, W. Almy, A. Casebeer

9:20 267. Unraveling the role of zinc ions on dopamine release and uptake in zebrafish. **M.A. Johnson**

9:40 268. Real-time characterization and ultrasensitive detection of single nanoparticles using plasmon-enhanced scattering at nanopore arrays. **V. Sundaresan**

10:00 Intermission.

10:10 269. Nucleic acid-based functional materials in biosensing. **I.V. Nesterova**

10:30 270. Development of multiplex electrochemical biosensors for quantifying overexpressed proteases in cancer diagnostics. **B. Habarakadage**, S. Rajendran, Z. Ren, M. Anderson, J. Koehne, D.H. Hua, J. Li

10:50 271. Zapping antibiotic-resistant microorganisms with electrically-polarized surfaces with low voltage. **P. Kohli**, A.Y. Vargas-Lizarazo, N. Mazumder, M.A. Ali, G.M. Kohli, i. senanayake, M.J. Atienza-Parcon, B.m. goodson, J. Vargas-Muñiz, P. Jensik, M. Olson, S. Hamilton-Brehm, N. Dogra, J. Bond, A. Fakhoury

11:10 272. Molten-salt synthesized metal oxide nanoparticles with high luminescence quantum yield for salivary protein detection. **Y. Mao**, Y. Zhang

11:30 273. Composite nanoparticle-based time-resolved luminescence biosensor for rapid tuberculosis detection in low-resource settings. **L.W. Miller**

11:50 274. CRISPR-based fluorescent assays for detection of protein and protease biomarkers. **X. Guan**, S. Munusamy

Memorial Union
Stotler Lounge

Biochemistry

K. Brorsen, V. Outlaw, *Organizers*

8:00 - 9:45

275. Toward expression of a peptide-ligating enzyme using T7 expression vector system. J.D. Linhardt, **K. Yoshimatsu**

276. Mechanistic modeling for regulatory dynamics of 11 β -Hydroxysteroid dehydrogenase. **O. Oliver**, K.K. Miller, R. Lampkins

277. Withdrawn

278. Effects of proline 145 deletion on thermostable green protein (TGP-E). **A. Elliott**, N.M. DeVore

279. Withdrawn

280. Structural analysis and binding specificity of the OAZ RNA in mouse. **A. Jayan**, E. Meister, L. Nedungadi, J. Strauss Soukup

281. Lipase-catalyzed esterification reactions with green chemistry applications. **A. Lamb**, **J.B. Friesen**

282. Autorna: Advancing RNA motif structural analysis with a fully automated AI agent. **R. Jasthi**, R. Mosad, B. Khan, V. Shenoy, B.M. Znosko, J. Hou

283. Kinetic characterization of the interaction between CAF-1 and PCNA. **I.M. Davies**, I. Williams, L. Dieckman

284. Evaluating turmeric's impact on cholesterol levels and antioxidant activity using UV- Vis spectrophotometry. **C. Norton**, **J. Titgemeyer**, A.P. Malalasekera

285. Peptide-protein relative binding free energy calculations with LaDyBUGS. **S.E. Stieglitz**, J.Z. Vilseck

286. Characterization of ATPase DotO in Dot/Icm T4SS of *Legionella pneumophila*. **R. Shrestha**, W. Lai, C. Durie

Memorial Union
Stotler Lounge

Organic Chemistry

K. Brorsen, V. Outlaw, *Organizers*

8:00 - 9:45

287. Identifying ligands for undruggable targets via on-DNA peptide synthesis. **F. Afroj**, S. Bloom

288. Cycloadditions and thermal expansion within 9-anthramide. **J.R. Gaffney**, G. George III, K.M. Hutchins

289. Withdrawn

290. Exploring the structural landscape of N-(3,5-dibromopyridin-2-yl) acetamide and N-(3,5-dibromopyridin-2-yl) propionamide. **K. Jewett**, N. Marasinghe Prins, B. Averkiev, C.B. Aakeroy

291. Interconversion between polymorphs of pharmaceutical compounds with mechanochemistry. **M. Foster**, D. Botes, K.M. Hutchins

292. Chlorinated-anilines as molecular templates to achieve a series of [2 + 2] cycloaddition reactions within molecular co-crystals. **G. White**, R.H. Groeneman

293. Synthesis of dipeptides for evaluation of their retention behavior in column chromatography and their self-assembling properties. **K.M. Ramaker**, **R.J. Helton**, K. Yoshimatsu

294. Solid-state forms of halogenated 3-hydroxy-2-pyrazinecarboxamide analogs and co-crystallization studies. **S. Welter**, N. Marasinghe Prins, B. Averkiev, C.B. Aakeroy

295. S_NAr mediated turn-on fluorescence sensing of amino acid neurotransmitters. **A. Ramaratnam**, M. Xu, P. Yadav, X. Liu, K.D. Gillis, T.E. Glass

296. Co-crystals sustained by π -type halogen-bond interactions between 1,4-diiodoperchlorobenzene and a series of aromatic acceptors. **E. Feld**, R.H. Groeneman

297. Utilizing green chemistry and the NASH reaction to synthesize 1-methyl-4- (4-nitrophenyl) piperazine. **J. Thompson**, J. Bashkin, H. Nguyen

298. Strategies for synthesis and functionalization of 14-membered sulfamide macrocycles. D. Vithanage, **A.C. Marstall**, J. Martinez, A. Lininger, P.R. Hanson

299. Design of novel anti-cancer agents targeting COX-2 inhibitors based on computational studies. **M. Er-rajy**

300. Design and synthesis of an anthracene-anhydride bioconjugation reagent. **G. Rudebusch**

301. Decarboxylative transformations facilitated via intermolecular halogen transposition using *gem*-bromonitroalkanes. **D. Brar**, E. Joseph, J.A. Tunge

302. Synthesis, characterization, pass prediction, DfT optimization, molecular docking, and pharmacokinetic profiling of poly(amidoamine) derivatives as potential antimicrobial agents. **M. Hosen**, Y. Li, Z. Peng

. Increasing the hydrophilicity of antimicrobial dicationic diarylacetylene quaternary ammonium compounds (QACs). B. Eichler, **P. Ford**, **B. Infield**

Memorial Union
N201C

Polymers and Materials

A. Teator, *Organizer*
P. R. Calvo, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 303. Recent trends and emerging demands in the polymer and textile industries. **M. Gashti**

8:30 304. Role of the air-polymer interface on crystallization of poly(3-alkylthiophene)s. **J. Kuebler**, L. Fernandez-Ballester, S. Dhapola, T. Santelman

8:45 305. Investigation of dynamics at the metal-organic framework and polymer interface. M. Rasin, **A. Devlin**

9:05 306. Enhancing cohesion via cellulose-derived covalent crosslinking. **J. Qi**, J. Zhao

9:20 307. Viscoelastic fluorescent π -conjugated polymer liquids. **J. Xu**

9:45 Intermission.

10:05 308. Micellar biomaterials: Quest for design rules. **B. Ulery**

10:30 309. Degradation of Poly(Bisphenol A) carbonate via molecularly imprinted nanoparticles. **T. Bui**, Y. Zhao

10:45 310. Using liquid crystals to architect light. S. Akhter, M. Hasan, J. Rebours, Y. Molard, **M. Prévôt**

11:05 311. Crosslinked polyethyleneimine networks for rapid and selective gold recovery from electronic waste: Role of crosslinker size. **S. Tushar**, Y. Li, P. Tao, X. Chen, Z. Peng

11:20 312. Data driven discovery of metal oxides for next generation energetic materials. **S. Akter**, M. Momenitaheri

11:35 313. Nanomaterial feedstocks for glass 3D printing. **J.F. Destino**

Memorial Union
N214A

Biochemistry

K. Brorsen, V. Outlaw, *Organizers*
C. Schenck, H. Seyrani, *Presiding*

8:10 314. Reverse transcriptases from DNA viruses. **L. Voth**, D. Burke-Agüero

8:35 315. Characterization of Ligand and Surface Adsorption of Autolysin Amidase (AmiE) from *Staphylococcus epidermidis*. **R. Yadav**, **N.C. Fitzkee**

9:00 316. Exploring bacterial replication and survival dynamics under different oxidative stress conditions at the single-bacterium level. **O. Ahmed**, A. Durantini

9:25 317. Universal *in vivo* ribozyme platform for non-canonical amino acid incorporation, tRNA charging, and functional rescue of protein enzymes. R. Kazmierczak, L. Kraus, P. Joshi, R.H. Apurba, K. Cole, C. Garfio, V. Outlaw, B.L. Golden, A. Luptak, **D. Burke**, P. Brown

9:50 Break.

10:10 318. Spectroscopic investigations of reduction potential-shifting RNA and DNA aptamers. **T. Pentland**, D.A. Baum

10:35 319. Comparative metabolomics of elderberries: Impact of organic certification and GAP on nutritional chemistry. **X. Jones**, S. Mahdi, R. Mu, N. Navarrete-Tindall, Q. Yang

11:00 320. Substrate selectivity in plant flavin-dependent *S*-monooxygenases. **P. Sobrado**

11:25 321. SARS-CoV-2 Omicron variant spike glycoprotein mutation Q954H enhances fusion core stability. **N. Vithanage**, R.H. Apurba, H.E. Ozomarisi, C. Bair, E. Sugg, V. Outlaw

Memorial Union
N204

Inorganic Chemistry

K. Brorsen, V. Outlaw, *Organizers*
K. Sikligar, *Presiding*

8:10 322. Hydrothermal synthesis and spectral optimization of Bi³⁺ and Te⁴⁺ -doped Cs₂ZrCl₆ for LED applications. **C. Dzorkpata**, Y. Chen, H. Zhu, P. Zhu

8:35 323. One-dimensional fluorescent platinum cyanoximates as novel photothermal agents for anticancer therapy. **M. Dragoi**

9:00 324. Isocyanide-bridged substituted 9-Borafluorene complexes of group 6 transition metals (Cr, Mo, W): Synthesis and characterization. **M. Muhammad**, S.P. Kelley, J.R. Walensky

9:25 325. Anchoring zero-valent metals with heavy carbene congener functionalized oxides for heterogeneous catalysis. **D. Culver**, C. Neill, M. Halder, A. Chartouni, F.A. Perras

9:50 Break.

10:10 326. Reactivity of actinide metallocene aryloxide complexes. **G. Kaumini**

10:35 327. Ni-Al hydride cluster bearing site-differentiated Al centers: Demonstration of olefin insertion and alkyl transfer. **J.R. Gipper**, S. Gonzalez-Eymard, M. Shoshani

11:00 328. Proton-responsive boron ligands for tandem reactions with transition metals. **S.R. Daly**, M. Skaria, B. Bhuniya, M. Yang, D. Martinez

11:25 329. Synthesis of the buckled staircase Kagome Mn₃V₂O₈ and the investigation of the coupling between it's ferroic orders. **N. Narayanan**

Memorial Union
N214C

Organic Chemistry

K. Brorsen, *Organizer*
V. Outlaw, *Organizer, Presiding*

8:10 330. Practical and theoretical insights into sulfonylnitrene and sulfonylcarbene mediated skeletal editing. **D. Herndon**, Y. Shao, I. Sharma

8:35 331. Visible light driven deaminative–decarboxylative $c(sp^3)–c(sp^3)$ cross-coupling. **M. Ansari**, S. Senanayake, S. Laulhé

9:00 332. Oxone, a panacea for Green Chemistry in undergraduate organic laboratory?. **D.W. Jensen**, J.R. Boquin

9:25 Break.

9:45 333. Exploring the structural interplay between hydrogen and halogen bonds in Bromo-benzazole derivatives. **T. Patel**, B. Averkiev, C.B. Aakeroy

10:10 334. Effect of disorder in charge-transfer ferroelectric cocrystals. P. Eccles, **J.D. Loya**, N. Aagaard, A.A. Moravek, R.A. Wiscons

10:35 335. Photocatalytic decarboxylative nitro-Mannich Reaction. **D. Brar**, J.A. Tunge

11:00 336. Computational and experimental structure-function study of pyrene and phenanthrene-based PAHs. **A.M. Cole**, R.G. Clevenger, K.V. Kilway

Memorial Union
N214B

Physical Chemistry

K. Brorsen, V. Outlaw, *Organizers*
G. B. Tucker, *Presiding*

8:10 337. A site-specific ultra-coarse-grained model for multi-scale chromatin simulation. **H. Arabzadeh**, D. Kireev

8:35 338. Competition between hydrogen and halogen bonding in the homogeneous trimers, tetramers and pentamers of HCl, HBr and HI. **G.S. Tschumper**

9:00 339. Constrained multicomponent second-order Møller-Plesset perturbation theory for the treatment of nuclear vibrational quantum effects. **G.B. Tucker**, K. Brorsen

9:25 Break.

9:45 340. Theoretical insights into the excitations of the Au₄₂(SCH₃)₃₂ nanorod in the near-infrared region. **S. Samarasinghe**, C.M. Aikens

10:10 341. Modeling ionic liquids in action. **S. Delwakkada Liyanage**, S.R. Gwaltney

10:35 342. Vibrational spectroscopy through quantum dynamics simulations: Theoretical developments, software implementations, and applications to electrochemical reactions. **M. Momenitaheri**

11:00 343. Large-scale critical assessment of physics-based and AI ligand-protein affinity predictors for early-stage drug discovery. X. Wang, H. Hentabli, A. Mettu, S. Gautham, **D. Kireev**

Memorial Union
N214D

Chemical Education

K. Brorsen, V. Outlaw, *Organizers*
B. Dhital, *Presiding*

8:15 344. New developments at ACS Exams: New exams, new products, and instructional workshops. **S. Nedungadi**, O. Michels, J. Trate, K.L. Murphy

8:45 345. Responsible development of nanotechnology for educating the next generation of scientists and engineers. **R.E. Rogers**

9:15 346. Greening process design: Developing a mini-module and inclusive assessments introducing the green chemistry principles to chemical engineering undergraduates.. **V. Shah**, R. Mullen

9:45 Break.

10:00 347. Design and validation of a survey instrument for measuring self-efficacy in laboratory scientific practices. **M. John**, L. Ronda, A.J. Hewitt, S.A. Reid, J. Mutambuki

10:30 348. Developing and validating a chemistry-specific sense of belonging instrument for STEM students. **A.J. Hewitt**, J. Mutambuki, S.A. Reid

Memorial Union
N201B

New Directions in Spectroscopy and Dynamics

B. Broderick, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 349. Understanding electronic metal-support interactions using scanning tunneling spectroscopy. **R.G. Farber**

9:20 350. Unraveling the relaxation dynamics of electrons and holes within semiconductor nanoparticles. **R.A. Loomis**

10:05 Break 1.

10:25 351. Sublimation dynamics and energetic processing of N-containing ices probed by chirped-pulse millimeter wave detection of thermally desorbed species and in situ FTIR RAIRS. **B.M. Moore**, Q. Borengasser, T. Hager, K. Renshaw, E. Hayden, B. Broderick

11:10 352. Actinide-containing molecular structures: A new direction in rotational spectroscopy. **G.S. Grubbs**

Memorial Union
Stotler Lounge

Analytical Chemistry

K. Brorsen, V. Outlaw, *Organizers*

10:00 - 11:45

353. Advanced analytical techniques for forensic analysis of toxic warfare agent sulfur mustard from biological samples. **Y. Akter**, B.A. Logue

354. Development of a water soluble fluorescence probe for the determination of phosphine. **M. Akter**, B.A. Logue

- 355.** Composite cathode $\text{Gd}_{0.2}\text{Ce}_{0.8}\text{O}_{1.9}\text{-SrFe}_{1-x}\text{Ti}_x\text{O}_{3-\delta}$ for nicotiana tabacum carbon fuel based direct carbon fuel cell. **M. Majeed**
- 356.** Restoring context: Applications of analytical chemistry to registration challenges in rural museums. **J. Karas**
- 357.** Detection of atrazine around the Mississippi river ecosystem using LLE-GCMS analysis. **P. McKenna, S.J. Wuerstl, J.D. Thomas, S. Donovan**
- 358.** Elution and concentration *S. cerevisiae* DNA in large inserts using 3D-printed devices. **S. Bursaw, E. Mendez Ortiz, J. Salgado, K. Kounovsky-Shafer**
- 359.** Improved containment of large DNA molecules in an inverted insert. **M. Taylor, K. Kounovsky-Shafer**
- 360.** Elution and concentration *S. cerevisiae* DNA in small inserts using 3D-printed devices. **J. Salgado, E. Mendez Ortiz, S. Bursaw, K. Kounovsky-Shafer**
- 361.** Shining light on metal toxicity: RNA based fluorescent sensors for mercury. **M. Politte, D. Baranko, A. Biswas, S. DasGupta**
- 362.** Determining the concentration of fluorene in lake water: Fluorescence as a means of detection. **R. Albritton**
- 363.** Multi-omic characterization of a human-derived Triculture neuroinflammation platform. **P. Hupert, J. Sibbitts, A. Graziani, G. Caruso, S.M. Lunte**
- 364.** Use of X-Ray fluorescence for identification of metal composition in Grayson Archery Collection thumb rings. **A. Allen, Y. VanFleet, C. Sall, J. Boldt, B. MacDonald**
- 365.** A facile spectrophotometric method for rapid and sensitive detection of zinc in foods and drinking water. **c. white, R. Hona**
- 366.** Identification of laboratory microplastic contamination and potential mitigation techniques. **A. Henry, R. Day, K. Hull**
- 367.** Electrochemical platinum deposition for assessing electrocatalytic activities of single nanoparticles. **N. Harvey, T. Ito**
- 368.** Heavy metal method development and analysis in fruits and vegetables using flame atomic absorption, and graphite furnace atomic absorption. **S. Mustafa, A. Peverly**
- 369.** Method development and quantitative analysis of pesticides using automatic solvent extraction, column chromatograph, and GC/MS. **A. Huenecke, A. Dial, F. Rangel, A. Peverly**

- 370.** Electrochemical uptake of rare earth ions by graphene oxide films. **S.E. Frenk**, A. Uysal, T. Ito
- 371.** Mysteries at the museum: Elemental and molecular analysis of Mater Dolorosa and St. John the Evangelist by Michele di Matteo. **C. Pallas**, M. Moats, K. Weiss, E. Pull
- 372.** LC-MS analysis of targeted metabolite compositions (amino acids & antioxidants) in lettuce exposed to molybdenum disulfide and sulfur nanoparticles. **M. Fakunle**, R. Pope-Buss, B. Akinwande, J. Churchman, C. Rico
- 373.** Understanding of the structure-property relationships in copper nanoparticles catalyzed heterogeneous click reactions. **J.T. Fetsch**
- 374.** Unraveling PFAS transport in realistic subsurface conditions: Effects of flow dynamics, biochar, and groundwater water fluctuations in a pilot-scale groundwater system. **J. Mai**
- 375.** Using archaeological chemistry to differentiate jade thumb rings from the Grayson Archery Collection. **M. Moats**, E. Hendren, C. Sall, J. Boldt, B. MacDonald
- 376.** Spatiotemporal dynamics of PFAS uptake and accumulation in mung bean sprouts. **A. Dhakal**, Q. Yang, S. Mahdi, R. Mu, X. Jones, P. Martano, A. Adeyeye, E. Owusu
- 377.** Aptamer-mediated CTLA-4+ CAR T-cell targeting of CD80 receptors in Non-Small Cell Lung Cancer (NSCLC). **M. Verma**, G. Sharma
- 378.** Molecular docking simulations to identify biomarker and therapeutic target for aggressive neuroendocrine carcinomas. **M. Gudipati**, G. Sharma
- 379.** Development of hierarchical nanoporous gold for use in electrochemical sensors. T.M. Adeniji, P. Sondhi, **K.J. Stine**
- 380.** Collision energy relationships in HCD MS2 spectra between ammonia chemical ionization and electrospray ionization for natural products. **L.M. Bloebaum**, X. Wang, K.P. Goldstein, M. Wang, R.W. Fitch
- 381.** Spectroscopic and computational analysis of bioactive catechins in natural green tea products. **Z.J. McKinley**, S. Kim, M. Watanabe

TUESDAY AFTERNOON

Memorial Union
N201A

Enhancing Sustainability through Chemical Catalysis

W. H. Bernskoetter, *Organizer, Presiding*

1:15 Introductory Remarks.

1:20 382. Amplification of insertion-based transformations through heterometallic hydride bridges. **M. Shoshani**

1:45 383. Ligand involvement in proton and electron management by half-sandwich rhodium catalysts. **J.D. Blakemore**, D.C. Grills, D.E. Polyansky, V.W. Day

2:10 384. Catalytic conversion of carbon dioxide to long chain esters via formate hydroesterification. **K. Virtue**, W.H. Bernskoetter, F.A. Lopez-Linares, C.F. Ovalles, O.A. Mironov, B. Fayyaz-Najafi

2:30 385. Zirconium-catalyzed hydrocarbons functionalization by CH aluminatation. **A.D. Sadow**

2:55 Intermission.

3:05 386. Recent developments in iron-mediated multicomponent reactions. **J. Neely**

3:30 387. Synthesis, characterization and photoproperties of bimetallic photosensitizers. **M.K. Karunananda**

3:55 388. Sulfur containing pincer ruthenium catalysts for CO₂ hydrogenation. A. Mondragon Diaz, N. Hazari, **W.H. Bernskoetter**

Memorial Union
Stotler Lounge

Organic Chemistry

K. Brorsen, V. Outlaw, *Organizers*

1:15 - 3:00

389. Probing the importance of helix cap motifs on folding and stability of SARS-COV-2 spike fusion core. **R. Apurba**, N. Vithanage, T. Kieffner, V. Outlaw

- 390.** Investigating the effects of ring strain in hydroamination of aryl-alkynes. **G.O. Matuszewski**, E. Cummings, T. Troester, M. Le, E.H. Fort
- 391.** Dual catalytic cobalt/quinone photoredox decarboxylative aromatization. **C. Waller**, J.A. Tunge
- 392.** Synthetic efforts on analogs of the Balgacyclamide family: Determination of active pharmacophore. **I.B. Ciftci**, M.H. Rice, A. Torres Hernandez, R. Rafferty
- 393.** Regioselective bromohydrins from styrene using oxone and potassium bromide. **A. Sell**, **D.W. Jensen**
- 394.** Synthesis of deuterium labeled 2-thiophenemethanamine-D5 hydrochloride. **S. Greenwood**, P.J. Deardorff, W. Sherman, D. Slade
- 395.** Simple oxidation of secondary alcohols to ketones using KBr and Oxone. **T. Gerber**, J.R. Boquin
- 396.** Hydantoin-indolinone inhibitors of serotonin-*N*-acetyltransferase. **S. Gawrych**, **M. Bach**, N. Wandrey, D. Gomez, M. Moxley, A.A. Thomas
- 397.** Comparative study of hydroxy-1,8-naphthalimide-based fluorescent probes for H₂S sensing. H. Hernandez-Sandoval, **H. Cao**
- 398.** Expanding the library of organic structure directing agents accessible by hydroamination. **E. Cummings**, M. Le, T. Troester, G.O. Matuszewski, E.H. Fort
- 399.** Withdrawn
- 400.** Base-promoted photoinduced dehalogenation of alkyl motifs. **A.J. Ummunnah**, S. Laulhe, K. Sachidanandan
- 402.** Design and development of a rapid-response fluorescent probe for hydrogen sulfide detection. L. Borer, **H. Cao**
- 403.** Design, synthesis and *in vitro* evaluation of novel benzo[4,5]thieno[3,2-b]pyran derivatives as topoisomerase I and II inhibiting anti-cancer agents. **M. Abdelaziz**
- 404.** Core-Hopping reveals new leads for the treatment of Cryptosporidiosis. **A. Sarkar**, C. Christ, J. Teixeira, C.D. Huston, M.J. Meyers
- 405.** Effect of ammonium salts on the addition of benzoic acid to glycidyl phenyl ether. K. Baldwin, D. Ross, **C.J. Neef**

- 406.** Design and identification of CNS-active 5-HT₃ antagonists for the treatment of neuropathic pain. **J.T. DeRousse**, B. Elgandy, L. Maram, S. KILLARI, L. Hegazy, B. Tan, W. Cheng, G. Akk, A. Germann
- 407.** Ammonium salts as catalysts for the addition of phthalimide to glycidyl phenyl ether. **M. Johnson**, G. Graham, C.J. Neef
- 408.** Thiotritylation as a platform for diverse sulfur functional groups. **Y. Liu**, O. Takashi, T. Gatzenmeier, K. Nozaki
- 409.** Chemoselective transfer hydrogenation of nitroolefins catalyzed by imidazolium ion tethered TsDPENs ligands with iridium (III) in water. **O. Oladapo**, **M. DeMoss**, B. Ni
- 410.** Chemoselective and enantioselective transfer hydrogenation of α,β -unsaturated ketones catalyzed by imidazolium ion tethered TsDPENs ligands with iridium (III) in water. **B. Grinstead**, U. Mohsin, C. Lemus, B. Ni
- 411.** Development of protected benzoxaborole reagent for late-stage Suzuki coupling. **A. Giardina**
- 412.** The development of an amide series targeting the Rel_{mtb} hydrolase enzyme. **K. Richter**
- 413.** Design and Asymmetric synthesis of atropisomeric isoxazoles as isoform selective small molecule Na_v1.7 inhibitors towards treatment for chronic pain. **D. Biscardi**, D.E. Frantz
- 414.** Synthetic strategies toward the development of taccalonolide analogs for the treatment of women's cancers. **I. Hernandez**, D.E. Frantz
- 415.** Light-mediated synthesis of aryl silanes. **C. Roembke**, D. Vire, R. Van Hoveln
- 416.** Understanding steric and electronic effects for nickel catalyzed carboxylation reactions. **S. Kucher**, C. Gallin, M. Delferro
- 417.** Regioisomer distributions in annulation reactions of 1,5-diaryl-1,2,3-triazoles with quinoline and isoquinoline subunits. **K. Lathrum**, J.T. Fletcher
- 418.** Biobinder from hydrothermal co-liquefaction of swine manure and algae. **C.P. Leuning**, C. Zhang
- 419.** Synthesis of novel imidazoles using microwave technology and molecular modeling applications. **B. Barr**, E.A. Nalley

Memorial Union
N201B

Analytical Chemistry

K. Brorsen, V. Outlaw, *Organizers*
K. Chen, *Presiding*

1:20 420. Au-IDE-based biosensor platform for rapid detection of sepsis based on MMP-9 and IL-6. **N.k. Alekhmimi**

1:45 421. Thermal decomposition of PTFE, PVDF, and PCTFE: Insights into fluoropolymer degradation and PFAS byproduct formation. **A. Arhami Dolatabad**, J. Cao, A. Kubatova, F. Xiao

2:10 422. Infrared quantification of siloxanes in biogas at parts-per-billion levels in the presence of spectral interferents. **K. McCreary**, D.A. Higgins, M.L. Spartz

2:35 423. *In vivo* ¹⁵N labeling and mass spectrometry imaging reveal spatial metabolomics of nitrogenous metabolites in *Arabidopsis thaliana* leaves. **P. Hapuarachchige**, Y. Lee

3:00 Break.

3:20 424. Attaining true multicolor dSTORM images using phasor analysis. **E. Pott**, M. Yang, B. Dong

3:45 425. Characterization of metal alloys in crossbow bolts from the Grayson Archery Collection: Quantitative compositional analysis by hXRF. **S.J. Mahan**, C. Sall, J. Boldt, B. MacDonald

4:10 426. Advancing Li-S battery performance with tuned MoS_x/rGO electrocatalysts: insights from cathode hosts and interlayer designs. **Z. Saddam**, J. Li, k. Muthukumar, B. Liu, S. Rajendran

4:35 427. XPS analysis of DNA damage induced by low-energy electrons (1–25 eV): site and energy dependence. **H. Yu**, J. Pereira-da-Silva, J. King, S. Ptasinska

Memorial Union
N214A

Biochemistry

K. Brorsen, V. Outlaw, *Organizers*
N. Vithanage, *Presiding*

1:20 428. Activity-based fluorogenic chemical tools to annotate variability in carboxylesterase-mediated drug metabolism. **M.W. Beck**

1:45 429. Production, characterization, and formulation of membrane associated protoporphyrinogen IX oxidase for safety studies. **C. Wang**, m. Zheng, K. Mathis, S. Saracco

2:10 430. Functional characterization of a diiron protein: Unraveling its role in methanogen oxidative stress response. A. Rai, J. Xiong, W. Leite, J. Byrnes, Y. Guo, **D. Prakash**

2:35 431. Unraveling nonradiative decay in DsRed via molecular dynamics, QM/MM, and machine learning. **J. Subasinghe**, S. Hebert, M. Grougan, A. Walker

3:00 Break.

3:20 432. Alpha-synuclein interaction with Gedunin. **T.M. Nyabayo**, R. Kanogo, k. baffour, I.S. Zegar, S. Santra, T. Banerjee

3:45 433. RNAMotifDB: A hierarchical database of RNA secondary structure motifs for template-based tertiary structure prediction. **D. Liu**, D. Pancholi, B.M. Znosko, J. Hou

4:10 434. Targeting *Staphylococcus aureus* resistance with novel treatment strategies. **P.M. Magdum**, J.N. Grissom, E. North, L. Dieckman, A. Sarkar

4:35 435. Implementing methyl-lysine analog chemical reactions to investigate functional consequences of lysine methylation on non-histone proteins. **T. Evans**, L. Quilliam, E. Doud, E. Cornett

Memorial Union
N214C

Organic Chemistry

K. Brorsen, *Organizer*
V. Outlaw, *Organizer, Presiding*

1:20 436. Enhancement of solid-state properties of famotidine through cocrystallization. **J. Eilers**, P. Seo, L. Ma, S.P. Kelley, K.M. Hutchins

1:45 437. Expanding the scope of a new hydroamination reaction of aryl-alkynes. **E.H. Fort**, E. Cummings, G.O. Matuszewski, M. Le, T. Troester

2:10 438. Synthetic and structural investigations of the cahuitamycin natural products. **M. Barnett**, W. Hulangamuwa, R. Rafferty

2:35 439. Scalable, high-yield synthesis and characterization of THJ-018 pentanoic acid for forensic reference standards. **A. Irianni**, E.C. Young, R.A. Willand-Charnley

3:00 Break.

3:20 440. Regenerative triaryl borates for regioselective C–O bond cleavage. **T. Leventis**, N.G. Veatch, F.J. Williams

3:45 441. Programmable functionalization of dienes directed via controlled self-assembly and wavelength selective [2 + 2] photocycloadditions. **L. Ma**, K.M. Hutchins

4:10 442. Mechanistic studies of iron(III)-catalyzed carbon-carbon bond forming and rearrangement reactions via near-IR spectroscopy. **E. Bauer**

4:35 443. Development of a ketoreductase-mediated kinetic dynamic resolution for the generation of a key intermediate in the synthesis of ABBV-576. **R. Phelan**, J. Brown, N. Rosano

Memorial Union
N214D

Physical Chemistry

K. Brorsen, V. Outlaw, *Organizers*
A. Limbu, *Presiding*

1:20 444. A new method to synthesize ordered microporous carbons with tunable pore size and its application in pollutant removal. **P. Ni**, x. He, F. Xiao, B. Deng

1:45 445. Electron transfer behavior of electroactive species tethered to phosphonate SAMs on ITO. **A. D.G Karunarathna**, S. Kayal, A.H. Flood, T. Ito

2:10 446. Molybdenum chalcogenide cluster supports for lanthanides. **D. Paudel**, P. Miro

2:35 447. Sequence optimization of peptides that fold and self-assemble at water–solid interfaces. **J.R. Comer**

3:00 Break.

3:20 448. Correlating infrared absorption with crystal structure in LiSCN H₂O: An experimental and computational study. **H.R. Krueger**

3:45 449. Layered double hydroxides for recovery and potential reuse of plant nutrients. **N.F. Materer**, P. Kitzel, C. Kelley

4:10 450. Repeat instability of noncanonical nucleic acid structures in disease pathogenesis of neurodegenerative disorders and Huntington's Disease. **N. Saikia**

4:35 451. Structural and electronic properties of benzyl isothiocyanate self-assembled monolayers. **H. Hetti Arachchige**, L.N. Penland, N. Dissanayake, D. Moyn, L.S. Tackett, A. Sadanandan, D. Ovchinnikov, Q. Zhou, R.G. Farber

Memorial Union
N204

Unlocking the Potential of Deep Eutectic Solvents

G. A. Baker, *Organizer, Presiding*
A. Roy, *Presiding*

1:20 Opening Remarks.

1:25 452. The role of hydrogen bonds in the dynamic heterogeneity of deep eutectic solvents. A. Stettler, G.A. Baker, **G. Blanchard**

2:05 453. Quantification and extraction optimization of polyphenols from purple corn pericarp using deep eutectic solvents and ultrasound-assisted extraction. **R. Kumar**, C. Wan, S. Flint-Garcia, B. Vardhanabhuti, **P. Somavat**

2:25 454. Sustainable solvent strategies for halide perovskite nanocrystal synthesis. **A. Roy**, G.A. Baker

2:45 455. Computational investigation of the dynamics of dissolved species in molten salt mixtures. **H. Nguyen**, L.D. Gibson, M.S. Emerson, B. Borah, S. Roy, V. Bryantsev, C.J. Margulis

3:05 Intermission.

3:35 456. Computational insight into the morphological evolution of gold nanoclusters in deep eutectic solvents. **D. Wagle**

4:15 457. Reversible macrocycle-mediated fluorescent thermosensing in a deep eutectic solvent. **M.E. Taylor**, A.C. Kanaherarachchi, G.A. Baker

4:35 458. Design ionic liquid/copper interface for electrocatalytic CO₂ conversion to ethylene. **Y. Yao**, Y. Chen, S. Prakash, Y. Li, X. Zeng

4:55 459. Withdrawn

Memorial Union
N214B

New Directions in Spectroscopy and Dynamics

B. Broderick, *Organizer, Presiding*

1:30 460. *In situ* characterization of rhenium CO₂ reduction catalyst intermediates via 2DIR-SEC. **L.M. Kiefer**

2:15 461. Photoacoustic spectroscopy in a supersonic flow. **Y. Liu**, N. Suas-David, A.G. Suits

2:45 Break.

3:05 462. Multi-messenger spectroscopic approach for polaron formation in emerging semiconductors. **H. Liu**

3:50 463. The role of photoexcitation wavelength and coherent acoustic phonons towards quantum control of photochemical reactions in solution. **A. Bhattacharjee**

Memorial Union
N201C

Polymers and Materials

A. Teator, *Organizer*
P. R. Calvo, *Organizer, Presiding*

1:30 464. Molecularly operated supramolecular 3D-printing polymers. **C. Ke**

1:55 465. Comparative study of microwave and thermal RAFT polymerization of pentafluorophenyl acrylate (PFPA). **D. Afsar**, G. Moran, P.R. Calvo

2:10 466. No time to waste: Rapid, selective, and mild depolymerization of poly(ethylene terephthalate). **D. Dileep**, J. Kaczor, A. Subbiah, W. Teggatz, M.J. Forrester, E.W. Cochran

2:25 467. Conversion of waste biomass and plastic into platform chemicals via microbial biocatalysts for the synthesis of advanced nylon analogs. **L.N. Jayakody**, L. Dissanayake, B. Jayanthaa, C. Beard

2:45 468. Experimental and computational studies on functionalized cellulose as a sustainable adsorbent for PFAS in aqueous systems. **G. Diaz Bukvic**, L. Liu, A. Dwikarina, S. Qasim, E. Rossi, M. Errea, C. Lin, C. Wan, M. Fidalgo

3:00 469. Activated ester polymers as a platform for studying structure-property relationships in functional polymers. **P.R. Calvo**, D. Afsar, A. Imiya, G. Moran

3:25 Intermission.

3:40 470. Fused ring monomers as a route to cyclopolymer materials. **A. Teator**

4:05 471. Synthesis of molecularly imprinted photonic polymer for the rapid detection of 11-keto testosterone hormone. **T. Biswas**, F. Fookes, S. Qasim, C. Lin, M. Fidalgo

4:20 472. 3D-printable polylactic acid composites with hydrochar-stabilized silver nanoparticles for antimicrobial photodynamic therapy. **J. Gomez**, M. Oluwagbemiga, S. Bhattarai, O. Ahmed, B. Zechmann, N. Adegboyega, A. Durantini

4:35 473. Phosphorylcholine polymer conjugation to improve the pharmaceutical performance of protein therapeutics. **M. Zhao**, A. Haghighat, N. Kumar

5:00 474. Corn waste derived to water-soluble cellulosic beads for encapsulating N₂-fixing bacteria. **S. Rijal**

5:15 475. Modifying Material Properties of Polyolefins through Oxazolidinone Incorporation via Frontal Ring Opening Metathesis Polymerization. **E. Rogan**, J. Aguilar-Romero

Memorial Union
Stotler Lounge

Chemical Education

K. Brorsen, V. Outlaw, *Organizers*

3:15 - 5:00

476. Molecular Dynamics studies to Evaluate Binding and Interaction of Organochlorine Pesticides with Human Serum Albumin.. **A. Mishra**, D. Sanford, R. Yadav

477. Empowering undergraduate research through interfacial chemistry at a small liberal arts college. **B. Dhital**

478. The impact of instructor feedback and interpersonal attributes on student success in STEM courses. **L. Applegate**, S. Kispert

479. An experimental approach to building a better STEM summer academy. **M. Aguilar**, **T. Johnson**, E.A. Nalley

480. Withdrawn

Memorial Union
Stotler Lounge

Improving the Reliability of Methods and Processes in an Industrial Setting

B. Morton, *Organizer*

3:15 - 5:00

481. PFAS removal from reverse osmosis and nanofiltration brine by granular activated carbon: Thermodynamic insights into salinity effects. **J. Cao**

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Inorganic Chemistry

K. Brorsen, V. Outlaw, *Organizers*

3:15 - 5:00

482. Synthesis and characterization of anunsymmetrical diglycolamide ligand for rare earth metal complexation. **E. Hintgen**, B.G. Tokheim

483. Evaluating distance dependence for redox active hydrogen bonding interactions. **T.N. Brumley**, P. Fouts, M. Zeller, J.J. Kiernicki

484. Decoupling substituent effects in redox active hydrogen bonding systems. **L.S. Schumaker**, M. Zeller, J.J. Kiernicki

485. Investigation of varied alkoxide catalysts for thionolactone ring-opening polymerization. **E.C. Connelly**, A.G. Justin, K. Frendt, A.M. Luke

486. Electrochemistry-induced direct deposition of mixed-metal zeolitic imidazolate framework thin films. **E. Skinner**, T. Ito

487. Micelle and Pt-Complexes Interaction under NIR. **C.M. Lindner**, M. Dragoi

488. Designing self-quenching thiourea complexes. **P.A. Dotson**, A.G. Davis, M. Zeller, J.J. Kiernicki

489. New advancements in antimony molybdate polyoxometalate chemistry. **S. Basak**, E.M. Villa

490. Periodic trends in heavy metal and lanthanide chalcogenophenecarboxylates. **N. Liao**, E.M. Villa

491. Exploring bonding preferences of hydrogen bond donor ligands and their isomeric counterparts with ferrous halides. **P.M. Fouts**, R.J. Huebner, M. Zeller, J.J. Kiernicki

492. Assessing enthalpic changes in redox-active hydrogen bond donor/acceptor interactions. **R.K. Umran**, P.A. Dotson, A.M. Workman, M. Zeller, J.J. Kiernicki

493. Directing reactivity of Iron-based β -diketiminato complexes towards multicomponent applications: Focusing on Isocyanide substrates. **L. Adams**, J. Neely

494. Host-guest interactions in metal-organic framework composite materials via Raman and UV-vis spectroscopy. **K. Ellis**, A. Devlin

495. Investigating the reactivity potential by modulating the steric effects of earth-abundant transition-metal β -diketiminates (BDE) complexes. **I.J. Akpan**

496. Functionalizing metal-organic Super containers for engineering solid-state porosity. **M. King**, R. Cook, K. Chitrakar, Z. Wang

497. Withdrawn