

**The 71st Southeastern Regional
Meeting of the American Chemical Society
October 20-23, 2019
Savannah, GA**

Brent Feske, *Program Chair*

SUNDAY MORNING

Savannah Marriott Riverfront
Ballroom C

Chemistry Education in the Technical College System of Georgia

J. Kiser, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 1. Community outreach and its impact on science students. **C. Letson**

8:25 2. Employability skills through critical thinking. **J. Kiser**

8:45 3. Why is chemistry so hard (to teach)? Exploring strategies for the chemistry courses at Gwinnett Technical College. **S. Johnson**, K. Francois

9:05 4. Teaching STEM classes at the technical college level. **A.A. Anderson**

Savannah Marriott Riverfront
Chatham

Inorganic Chemistry

General

Financially supported by Division of Inorganic Chemistry

W. E. Lynch, *Organizer*

B. Wicker, *Presiding*

8:00 Introductory Remarks.

8:05 5. Shaken, not stirred: Exploration into the synthesis of group 2 amide compounds. **I.R. Speight**, T.P. Hanusa

8:25 6. Catalytic application of cobalt complex bearing a tetradentate tripodal ligand for the homo-coupling of secondary alcohols. **L. Bryant**, D. Taylor, K. Ding

8:45 7. Synthesis and reactivity of expanded-ring heterocyclic selones. **K. Dowling**, D. Rabinovich

9:05 8. Synthesis, structure and anticancer activity of organometallic gold(III) complexes bearing dach ligands. **S. Gukathasan**, S. Parkin, S.G. Awuah

9:25 9. Activation of terminal alkynes by trimethylamine: Synthesis and reactivity of zwitterionic aminoalkyne ligands in pentaruthenium carbonyl cluster complexes. **H. Akter**, R.D. Adams

9:45 10. Modelling the H-cluster subsite of [FeFe]-hydrogenases: Catalysts for hydrogen production. **C.A. Mebi**

10:05 Intermission.

10:20 11. Synthesis of the first heterocyclic telone complexes of silver and mercury. **K.V. Arcena**, D. Rabinovich

10:40 12. Phosphonium ionic liquids: Versatile platform for future applications. **B.F. Wicker**, S.C. Jones, J.H. Davis, R. Sykora

11:00 13. Harnessing light and proton-coupled electron transfer to drive dinitrogen reduction at rhenium. **Q.J. Bruch**, G. Connor, C. Chen, P.L. Holland, J.M. Mayer, F. Hasanayn, A.J. Miller

11:20 14. Electrochemical analysis of nickel dithiocarbamate complexes for redox flow battery applications. **M.R. Mazumder**, C. Richburg, S. Saha, B.H. Farnum

11:40 15. New molecular and ionic actinide fluorides: Simple systems, complex chemistry. **G. Gotthelf**

Savannah Marriott Riverfront

Oglethorpe B

Organic Chemistry in Fluorescence Microscopy

L. Zhu, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 16. Click, fluoresce, and release: Tracking drug delivery through the concomitant generation of a fluorophore. **B. Wang**

8:32 17. Assessment of liposome triggered release and lipid metabolic labeling using fluorescence techniques. **M. Best**, J. Lou, X. Zhang, T. Ricks, D. Alves, C. Cassilly, F. Barrera, T. Reynolds

8:59 18. Aurones as a scaffold for fluorescent probes and sensors. **S.T. Handy**

9:26 19. Metal ion-responsive ratiometric fluorescent probes for two-photon microscopy. **C.J. Fahrni**

9:53 Intermission.

10:08 20. Lessons from super-resolution microscopy: Choosing the right method and sample preparation considerations. **J. Allen**

10:35 21. Photoswitchable fluorophores for bioimaging applications. **F.M. Raymo**

11:02 22. Conjugated oligomers for fluorescent live cell imaging. **J. Moon**, H. Torabi, A. Barrios, A. Halim, S. Sarker

11:29 23. Photo-click strategies for selective substrate labelling with 4D resolution. **V. Popik**

11:56 Concluding Remarks.

Savannah Marriott Riverfront
Franklin

Biobased & Bio Inspired Polymers & Composites

R. L. Quirino, *Organizer, Presiding*

8:10 Introductory Remarks.

8:15 24. Beneficial effect of deionized collagen in the properties of biocomposites prepared from the reinforcement of a tung oil-based thermosetting resin. **R.L. Quirino**, A. Lorts, A. Scholz, M. Bachan, C. Morris, H. Hartman, A.L. Stewart

8:35 25. Monomer from abietic acid and tung oil. **K.A. Monroe**, A. Hulleter, R.L. Quirino

8:55 26. Synthesis and characterization of UV resistant castor wax-based polyurethane coatings. **T.F. Garrison**

9:15 27. Non-isocyanate polyurethanes (NIPUs) obtained from fatty acids. J.D. Rodrigues, F.H. Kobiraki, L.G. Paterno, **M.A. Sales**

9:35 28. Controlling macromolecular topologies towards sustainable bioplastics. **C. Tang**

9:55 Intermission.

10:15 29. Enzymatic ring-opening polymerization of ϵ -caprolactone: Effect of organic solvents and ionic liquids. **H. Zhao**, N. Kanpadee, C. Jindarat, G. Nathaniel, P.C. Merenini

10:35 30. Polymeric memory resistive devices from poly(*N*-alkyl methacrylate)s as an artificial synapse. **B. Grant**, S.H. Foulger, I. Bandera

10:55 31. Thermo-mechanical, rheological, physical and chemical characterization of poly(lactic acid)/poly(hydroxybutyrate)/lignin coated cellulose nanocrystals nanocomposites prepared by high torque melt mixing. **A. Tucker**, D. Jackson, E.A. Mintz

11:15 32. Sonochemically functionalized boron nitride nanomaterials as reinforcement for aerogels. **H. Harrison**, J.R. Alston, S. Twiddy, S.H. Huneycutt

11:35 33. Phase transferable polymer encapsulated metallic nanoparticles. **M.P. Confer**, J.P. Harris, S. Street

Savannah Marriott Riverfront
Reynolds

Biochemistry

SAR, Drug Discovery, & Methods

T. Leeper, *Organizer, Presiding*

8:10 Introductory Remarks.

8:15 34. Hydrophobic ligands influence the structure, stability, and processing of the major cockroach allergen Bla G 1. **A.C. Foo**, P.M. Thompson, L. Perera, S. Arora, E.F. Derose, J.G. Williams, G. Mueller

8:35 35. Deciphering the biophysical effects of glycosylation on membrane proteins. **G. Cook**

8:55 36. Novel peptide protects mitochondrial structure-function: Implications for cationic, lipophilic peptides as endogenous assembly factor mimetics. **R.J. Grams**, M. Allen, E. Pennington, A.B. Bandara, A. Thomson, J. Perry, T. Green, T. Ryan, A. Gates, W. Santos, J. McClung, S.R. Shaikh, D.A. Brown

9:15 37. VGSC blockers with cell invasion inhibitory activity in breast cancer cells. **S.E. Velu**

9:35 38. Peripheral protein unfolding drives membrane bending. **H. Siaw**, G. Raghunath, R.B. Dyer

9:55 Intermission.

10:15 39. Uncovering the many roles of Stk1 in MRSA virulence and resistance gene regulation. **M.S. Blackledge**

10:35 40. Concept for a cell-based biosensor for early Alzheimer's disease detection. **B. Watson**, F. Gonzalez, M. Moss

10:55 41. Crystallographic and analytical characterization of an enzyme catalyzed transformation of a conjugated polymer. **H. Spivey**, T. Leeper

11:15 42. Micro-technique isolation of insect binding proteins as an antibody assay source. **M. Lassiter**, B. Welborn

11:35 43. Photodynamic inactivation of antibiotic-resistant bacterial strains using lignin-photosensitizer conjugates. **P. Sadrpour**, R.A. Ghiladi

Savannah Marriott Riverfront
Oglethorpe A

f-Element Chemistry & Separations

Financially supported by Division of Inorganic Chemistry and Auburn University - Department of Chemistry and Biochemistry

A. E. Gorden, E. J. Werner, *Organizers, Presiding*

8:10 Introductory Remarks.

8:15 44. Molecular tetravalent lanthanide complexes. **H.S. La Pierre**

8:35 45. Thermodynamics and stability studies of actinide-based metal-organic frameworks. **O.A. Ejegbavwo**, M.D. Smith, N.B. Shustova

8:55 46. Catch-and-release trivalent americium oxidation electrocatalysis using a ligand-modified electrode. M.V. Sheridan, J.R. McLachlan, A. Hernandez, J.R. Gonzalez-Moya, T.S. Grimes, **C. Dares**

9:15 47. Preparation of novel complex uranium oxides via exploratory crystal growth methods. **K. Pace**, H. Zur Loye

9:35 48. Tailoring redox active ligands for probing the reactivity of actinides. **A.E. Gorden**, J. Niklas, J.T. Mayhugh, J.D. Gorden

9:55 49. “Soft spot” for uranyl: Derivatization of a soft-donor hexadentate ligand for UO_2^{2+} recognition. **J. Niklas**, J.T. Mayhugh, M.G. Forbes, J.D. Gorden, A.E. Gorden

10:15 Intermission.

10:35 50. Tripodal CMPO ligands for selective f-element extraction. **E.J. Werner**, S.M. Biros, W.B. Larrinaga, A. Martinez, M. Glander

10:55 51. Incorporation of new secondary building units into uranium framework materials by flux crystal growth. **C.A. Juillerat**

11:15 52. Tridentate and tetradentate N-donor extractants for minor actinide separations. **C.A. Hawkins**, M.L. Brown, K. Lawson, B.T. Kilgore, J.D. Carrick

11:35 53. Large area airborne contamination monitoring. **T. Whiteside**, K.M. Fenker, A. Judy, D.P. Diprete

11:55 Concluding Remarks.

Savannah Marriott Riverfront
Pulaski

Organic Chemistry

Drug Discovery

X. Chen, *Organizer*

D. A. Colby, *Presiding*

8:10 Introductory Remarks.

8:15 54. Complexation thermodynamics between cyclodextrins and fatty acids. **X. Yao**, M. Bonizzoni, L. Kong

8:35 55. Synthesis and antimicrobial activity of *n,n'*-bis-substituted triazolium salts with lipophilic substituents on 1,2,3- and 1,2,4-triazole rings. Z. Lin, J. Wilson, T. Ta, D. Fico, S.S. Johnson, J.D. Gorden, M. Frazier, L. King, **K.S. Taylor**

8:55 56. Identification and development of antifungal peptoids. **K. Bicker**

9:15 57. Evaluation of peptoid derivatives of ultra short antifungal peptides. **R.M. Green**

9:35 58. Design, synthesis and biological evaluation of some novel oxazolidinone derivatives as potential anti-mycobacterial and antibacterial agents. **R.M. Bokhtia**, T. Ibrahim, A. Al-Mahmoudy, E.H. Abdel-Aal, S.S. Panda

9:55 Intermission.

10:15 59. Synthesis approaches 4,6-diaryl- and 4,8-diarylquinoline-methylcarboxylate scaffolds as inhibitors of the HIV-1 integrase in enzyme. **L.P. Dinh**, C.D. Glenn, L. Yet

10:35 60. Uncouplers of oxidative phosphorylation as obesity therapeutics. **J.A. Santiago-Rivera**

10:55 61. Mitochondrial uncouplers as disease therapeutics. **C.J. Garcia, J. Salamoun, W. Santos**

11:15 62. Total synthesis and biological investigation of metal-binding natural products as bacterial inhibitors. **K.R. Morrison**, J.A. Shapiro, R.A. Allen, S.S. Chodisetty, W. Wuest

11:35 63. Design, synthesis and antimicrobial evaluation of new fluoroquinolone-dichloroacetic acid conjugates as a potential DNA gyrase inhibitors. **I.A. Seliem**, T. Ibrahim, A. Al-Mahmoudy, Z.K. Abdel-samii, S.S. Panda

Savannah Marriott Riverfront
Ballroom B

Synthesis & Application of Novel Nanocatalysts

J. Wu, *Organizer, Presiding*

8:10 Introductory Remarks.

8:15 64. pH responsive colloidal gold nanoparticle catalysts for recovery and reuse. **C. Joshi**, S. Chakraborty, **C.L. Kitchens**

8:35 65. Magnesium oxychloride formation kinetics and enhanced water stability for sustainable building materials applications. **R.F. Gochez**, C.L. Kitchens

8:55 66. Photoswitchable nanoparticle ligands to modulate and control catalytic reactivity. **M.R. Knecht**

9:15 67. Nickel nanoparticles supported on multi-walled carbon nanotubes as an effective catalyst in Suzuki cross coupling reactions. **A. Siamaki**

9:35 68. Molecular/heterogeneous catalyst for the selective hydrodeoxygenation of oxygenated aromatics related to lignin biomass. **A.K. Vannucci**

9:55 69. Continuous flow system for the heterogeneous catalytic production of advanced biofuels. **N.E. Fraley**, A. Lachgar, M. Wright

10:15 70. Plasmon drag effect pinning and molecule adsorption. **M. Durach**

Savannah Marriott Riverfront
Ballroom E

Undergraduate Research Experiences: The Power of Quality Mentorship & Programming

Financially supported by Sorbtech
K. S. Aiken, *Organizer, Presiding*

8:10 Introductory Remarks.

8:15 71. High-impact undergraduate research experiences through the eyes of the undergraduate scholar. **S.T. Mensah**

8:35 72. MAP (mentorship advancing to Ph.D.): Role mentorship played in a McNair program scholar's life. **F. Minter**

8:55 73. Mentors matter for all students from high school to graduate school and beyond. **J.M. Iriarte-Gross**

9:15 74. Mentoring high school students in nanoscience research at Hampton University. **P.N. Njoki**

9:35 75. SciWrite: Workshop development and mentorship in scientific writing for summer undergraduate researchers. **R.R. Ramoutar**

9:55 Intermission.

10:15 76. Integrating scientific research to create meaningful undergraduate experiences. **K.S. Marriott**

10:35 77. REU Site that recruits faculty-student teams. **K.L. Buchmueller**

10:55 78. Mentoring and support for the REU-INFEWS: Food, energy, water security program at Mississippi State University. **D. Mlsna**

11:15 79. Assessing the quality of undergraduate research experiences: Perspectives of in-lab mentors. **D.A. Canelas**, E.W. Hunsaker

11:35 80. Kennesaw State University chemistry and biochemistry summer undergraduate research experience. **K.J. Linenberger Cortes**

Savannah Marriott Riverfront
Academy

Analytical Chemistry

Materials & Nanomaterials

C. McKenas, *Organizer, Presiding*

8:15 Introductory Remarks.

8:20 81. Novel ionic rectification based on functionalized silica nanoparticle and track-etched nanopores for switchable drug delivery. **C. Pintro**, M. Davenport-Munoz, K. Spitzer

8:40 82. Evaluation of metal-organic framework as sorbents for the BTEX family of compounds. **J.E. Shankwitz**, D. Speed, D. Sinanan, G. Szulczewski

9:00 83. Electrochemical monitoring of the thermal sintering behavior of electrode-attached 1.6 nm diameter gold nanospheres. **B.P. Mainali**, D.K. Pattadar, J.N. Sharma, F.P. Zamborini

9:20 84. Synthesis and characterization of radioluminescent NaGdF₄: EU nanoparticles as a potential light source for optogenetics studies. **M. Ranasinghe**, M. Arifuzzaman, S. Battacharya, J.N. Anker

9:40 85. Polyaniline modified biochar to remove nitrate from aqueous system. **A. Herath**, T.E. Mlsna, C. Reid

10:00 Intermission.

10:20 86. Tuning the surface plasmon resonance by patterning plasmonic nanoparticles using metal grid/stamp, glucose crystal deposition and mechanical deformation. **M. Ranasinghe**, F. Ameer, T. Estrada-Mendoza, L. Hu, A. Rao, G. Chumanov, J.N. Anker

10:40 87. Aminoxy-functionalized metal monolayer-protected custers (MPCS) for catalysis applications. **T.R. Sibakoti**, M.H. Nantz, F.P. Zamborini

11:00 88. Nitrogen-Doped Screen-Printed Carbon Electrodes (N-SPCEs) and Carbon Ultramicroelectrodes (N-CUMEs) as platforms for electrocatalysis and immobilization of metal nanoparticles. **G.W. Bishop**, C. Ogbu, E. Amoah, D. Mawudoku, E. Adeniji

11:20 89. Corrosion resistance of a tetrafunctional epoxy-amine resin coating. **E. Caldon**, D. Wipf, D.W. Smith

11:40 90. High-temperature fast-flow reactor for the study of radical-radical reactions. **Y. Lee**

Savannah Marriott Riverfront
Ballroom D

Project SEED

Financially supported by Project SEED
A. Mallia, D. Masterson, *Organizers, Presiding*

8:20 Introductory Remarks.

8:25 91. Using the society for science & the public advocate grant to encourage Project SEED students to enter science competitions. **D.S. Masterson**

8:55 92. Growing a Project SEED site at Boise State University. **D.L. Warner**

9:25 93. ACS Project SEED at Clark Atlanta University. **I.M. Khan**

9:55 Intermission.

10:15 94. ACS Project SEED student participation in molecular materials research at UNC Charlotte. **M.G. Walter**

10:45 95. Polymer-protein biomaterial scaffolds for wound healing and cancer research. **M. Gaines**, G. Brim, D. Ingabire, A. Mancia, K. Smith, K.M. Jackson

11:15 96. Project SEED program at Georgia Gwinnett College: Successfully organizing Project SEED at a primarily undergraduate institution. **A. Mallia**

11:45 Concluding Remarks.

Savannah Marriott Riverfront
Plaza

Undergraduate Papers

General

Financially supported by American Chemical Society and the Coastal Georgia Local Section of the ACS

M. Weiland, *Organizer*

N. Davis, *Presiding*

8:30 Introductory Remarks.

8:35 97. Janus micromotors improve the catalytic efficiency of immobilized enzymes. **A. Pan**

8:50 98. Development of a fluorescence sensor for tracking heme insertion into proteins. **A. Whitten**, L. Plate

9:05 99. Investigating Tat-SF1 interactions with HIV RNA. **J. Trautman**, S. Roszczenko, K.H. Fogarty, H.B. Miller

9:20 100. Kinetic isotope effect in the Kemp elimination catalyzed by heme systems. **B. Taormina**, E.A. Smolenski, A. Callaway, M. Forconi

9:35 101. Glyoxylate-based protometabolism serves as an analog of the citric acid cycle. **R.T. Stubbs**, G.G. Springsteen

9:50 102. Vitamin K2 analogs as anti-epilepsy therapeutics. **L. Prosser**, E. Watt, R. Himes, C. Chou, S. Chan, C. Christie, T. Williamson

10:05 Intermission.

10:25 103. Study of 5-HT_{1D} and 5-HT_{1F} receptor interactions with mini G proteins via BRET analysis. **A. Trang**, N. Okashah, A.C. Spencer, N. Lambert

10:40 104. 2-ethynylpyridine polymerization using His-tagged T4L, a variant of bacteriophage T4 lysozyme. **W. Turner**, S. Thomas, T. Leeper

10:55 105. Toward an understanding of the relationship between sequence, acylation, and solution behavior in human ghrelin. **E.E. McGee**, M.W. Giuliano

11:10 106. Bilayer interactions of the endogenous opioids. **D.W. Jay**, M.W. Giuliano

11:25 107. Molecular modeling of histone deacetylase complexes. **J.T. Sivak**

11:40 108. Effects of cholesterol on amyloid beta aggregation in Alzheimer's disease. **B. Gilmore**, K.M. Matera

Savannah Marriott Riverfront
Mercer

Undergraduate Papers

General

Financially supported by American Chemical Society and the Coastal Georgia Local Section of the ACS

M. Weiland, *Organizer*

A. Saha, *Presiding*

8:40 Introductory Remarks.

8:45 109. Synthesis, structural characterization, and reactions of a new penta-coordinated cadmium(II) ion. M. Raja, **K. Barnes**, G. Raja, S. Dixon, M.D. Smith

9:00 110. Synthesis and structural characterization of a new coordination polymer with nine-coordinated La(III) ions. M. Raja, **S. Dixon**, K. Barnes, G. Raja, M.D. Smith

9:15 111. Transformation of metal oxide nanoparticles in surface coatings: Hazards of inhalation and ingestion during application. **A. Hatch**, J.G. Clar

9:30 112. Lewis acid catalyzed formation of ligand-stabilized highly crystalline Cu₂O nanoparticles via a hot injection esterification method. **N. Gibson**, A.R. Combs Bredar, B.H. Farnum

9:45 113. ¹H-NMR investigation of displacement of oleate at PbS quantum dot surfaces using carboxylic acids, thiols, amines, and halides. **P. Wasdin**, M.R. McPhail

10:00 Intermission.

10:20 114. New synthetic route to heteroaromatic *N*-oxides bound to boron trifluoride: Synthesis, characterization and X-ray structural studies. **D. Boatright**, S. Lynch, W.E. Lynch, C.W. Padgett, B.P. Quillian

10:35 115. X-ray study of the chemistry of haloaurates with heteroaromatic *N*-oxides. **S. Lynch**, C.W. Padgett, W.E. Lynch

10:50 116. Property and structure relationship of lanthanide paramagnetic ionic liquids. **T.D. Jones**, J.E. Knoop, J.R. Alston

11:05 117. Reductive removal of pertechnetate and chromium by zero valent iron under variable ionic strength conditions. **A. Maria**, Y. Katsenovich, J. Williams, H. Emerson, D. Boglalienko, T. Levitskaia

11:20 118. Mechanism and kinetics studies for the ruthenium-catalyzed oxidation of silyl ethers to silyl esters. **A.M. Weinhofer**, C.L. Brown, J.M. Walker, B.C. Goess, S.K. Goforth

Savannah Marriott Riverfront
Atrium

Undergraduate Posters

Financially supported by American Chemical Society - Undergraduate Programs; Coastal Georgia Local Section of the American Chemical Society
M. Weiland, *Organizer*

9:30 - 11:00

119. Synthesis and characterization of thiosemicarbazones and its inhibition of topoisomerase II?
A. Spent, P.J. Rosado, E.C. Lisic, X. Jiang, W. Medawala

120. Computational studies of bis-phosphinimine NCN-pincer nickel(II) complexes. **M. Kauz**,
C. Mendez-Childers, G. Guillet, w. turner

121. Formation and further application of silyl esters in one-pot reactions. **J.M. Walker**, A.M.
Weinhofer, B.C. Goess, S.K. Goforth

122. Detection of TNT and other nitroaromatic explosives using porphyrin-doped silica sol-gels.
D. Collins, C.H. Lisse

123. HPLC for separation and detection of organic gunshot residues extracted from silicone
personal passive sampling devices. **S.O. Sweck**, C.R. Dockery, G.E. Potts

124. Substrate scope of ruthenium-catalyzed oxidations of primary and secondary silyl ethers.
C.L. Brown, A.M. Weinhofer, J.M. Walker, B.C. Goess, S.K. Goforth

125. Efforts towards the total synthesis of synoxazolidinone C. **B. Stemen**, J. Pierce

126. Chemical determination of the efficacy of new and worn self-cleaning materials. **L.B.**
Galopin, **M. Williams**, J. Kern

127. Conformational flexibility in linear amino alcohols investigated by high-resolution Fourier-
transform microwave spectroscopy and *ab initio* calculations. **S. Spann**, R. Lavrich

128. Purification and characterization of wild-type and modified small laccase from
Streptomyces coelicolor in preparation for attachment to a surface. **M. Sullivan**, B.W. Gregory,
P.A. Baker, C.M. Johnson

129. Bioinspired polymers for sequestration of doxorubicin during chemotherapy treatment. **W.**
Vaughn, M. Bardot, O. Wadsworth, M.D. Schulz

- 130.** Quantifying the connection between polymer architecture and metal chelation. **A. Fiorito, S. Winn, P. MacNicol, W.R. Archer, M.D. Schulz**
- 131.** Isolation of calcium oxalate from fresh spinach. J.T. Cooper, **S. Falk**
- 132.** Chemoselective synthesis of α,α' -homodifunctional polymeric systems. R.A. Olson, C. Figg, **J.S. Levi, B.S. Sumerlin**
- 133.** Calorimetric study of the adsorption of oxalate on hematite nanoparticle. **N.C. Clarke, D.H. Bui, M. Oganga Cooper, E. Stroeva, H.A. Al-Abadleh, N. Kabengi**
- 134.** Antiproliferative structure-activity relationships of 5-substituted indoles and indole-based chalcones. **F. Kidd, D.W. Crick**
- 135.** Using multi-step synthesis for the production of hydrogels with adhesive properties. **C. Seudieu, S. Bonser, C.H. Lisse**
- 136.** Molecular docking binding activity of quinoline derivatives on Zika virus RNA-dependent RNA polymerase. **E.H. Chaisson, A. Smaltz, B. Duffy, J.J. Pajski**
- 137.** Sphingosine kinase inhibition using modified variants of a sphingosine kinase inhibitor. T.C. Grattan, **K.J. Butler**
- 138.** Sulfamation of tethered aminoalkenes with *in situ* generated hypervalent iodine. **S. Safford, C. Beveridge, J.M. Carney, D.V. Liskin**
- 139.** Characterization of the 3' untranslated region of *SAGA* mRNA from group A *Streptococcus*. **K.J. Calderon, S.G. Nibar, R.A. Finn, C.R. Carroll, A.S. Brown, B.M. Lee, G.C. Perez Alvarado**
- 140.** Use of zinc-specific DNazymes on nucleic acid functionalized nanocapsules for sensing applications. **B. Tate, J.L. Rouge**
- 141.** Computational studies of the structures and electron-density topology of the group 14-substituted butatrienes $x=C=C=CH_2$ ($x=CH_2, Cf_2, SiH_2, SiF_2, GeH_2, SnH_2, PbH_2$). **A. Gonzales, D.A. Clabo**
- 142.** Design and application of green, solid-supported palladium catalysts for synthesis of important chemical targets in water. **J. Burrell, D. Paull**
- 143.** Investigation of the weathering of automotive clear-coat formulations using Fourier-transform infrared spectroscopy (FTIR) for forensic purposes. **H. Elaskalani, N.T. Perera**
- 144.** Amino acids in soy sauces and alternatives: How do they affect the taste? **X. Sillie, M. Fujita**

- 145.** Identification of volatiles in tobacco products via thermogravimetric analysis. **K. Conner**, N. Grinalds, M. Thomas, E.M. McCorquodale, K. Fogarty
- 146.** Design and synthesis of solid-supported palladium catalysts using N-heterocyclic carbenes for greener coupling reactions. **A.T. Cagle**, D. Paull
- 147.** Systematic study of the dependence of the quantum theory of atoms-in-molecules analysis of chemical bonding in first- and second-row chlorides (XCl, X-H, Li-F, Na-Cl). **J. Cyrus-Green**, D.A. Clabo
- 148.** Synthesis and characterization of l-asparaginase (l-asnase) encapsulated poly-l-lysine-graft-poly(ethylene) glycol (pll-g-peg) polymer nanoparticles for the efficient delivery of therapeutics. **K. Goff**, R.S. Hikkaduwa Koralege
- 149.** Analysis of cannabinoid-infused consumer products. **T. Griffin**, L. Billotto, H.J. Murdock
- 150.** Analysis of the 5' untranslated region of *saga/pel* in *Streptococcus pyogenes*. **A.S. Brown**, C.R. Carroll, R.A. Finn, L.R. Angello, S.G. Nibar, K.J. Calderon, B.M. Lee, G.C. Perez Alvarado
- 151.** Analysis of cannabidiolic acid (CBDA) and cannabidiol (CBD) ratios in consumer products. K. Focke, S. Jones, V.R. Griffin, **T. Griffin**
- 152.** Finding functionality of enzyme 3H04 through computational analysis. **S.E. Jennings**, A.A. Carter, P.A. Craig
- 153.** Development and validation of a differential FTIR method for the analysis of model prebiotic peptides. **K. Rezaeerood**, J.G. Forsythe
- 154.** Vitamin K2 analogs in toxin-induced and genetic models of Parkinson's disease. **E. Watt**, L. Prosser, R. Himes, C. Chou, S. Chan, C. Christie, T. Williamson
- 155.** Molybdenum-catalyzed cycloisomerization of alkynyl anilines to indoles. L. Broome, **M.S. Hobbs**, C. Mejia, T.L. Scott
- 156.** GC-MS measurement of the intermediates of beta oxidation in the lipid bodies of *Brassica napus*. A. Davidson, **G.A. Giles**
- 157.** Investigating the role of chirality in the formation and hydrolysis of model prebiotic peptides. **M.B. McDonald**, R. Peter, J.G. Forsythe
- 158.** Microwave synthesis for materials chemistry labs. **J. Sanchez**, M. Foley
- 159.** Synthesis and testing of selective pyrrophen systems for visual uranyl (UO₂²⁺) detection. **M. Forbes**, J. Niklas, J. Mayhugh, J.D. Gorden, A.E. Gorden

160. Enzymatic dynamic kinetic resolution for the stereoselective synthesis of α -hydroxy ketones. **K.G. Darrigrand**, P.W. Robbins, E. Reynolds

161. Design and synthesis of self-complexing multi-substituted boronic acid derivatives as potential selective glucose sensors. **A. Gordon**

162. Oxidative copper(II) catalyzed alcoholysis of 3-hydroxyflavone: Synthesis, characterization and structure of 3-hydroxy-2,3-dialkoxy-2-phenylchroman-4-ones and 3-dihydroxy-2-alkoxy-2-phenylchroman-4-ones. **E.M. Beasley, B.P. Quillian**

163. Cellulose based edible film from soy hull. **H. Cobbs**, J. Tolbert, U.P. Kalapathy

164. Preparation and preliminary catalysis of a viable ruthenium-based olefin hydroarylation catalysis supported by bis(pyrazolyl)acetate. **J.G. Bazemore**, W. Zhu, **T. Gunnoe**, B.P. Quillian

165. Synthesis of seedless latex emulsions for use in waterborne coatings. **E. Moscoso**

Savannah Marriott Riverfront
Ballroom C

Advances in Polymer Science & Engineering

P. Kalelkar, *Organizer, Presiding*

9:35 Introductory Remarks.

9:40 166. Fluorescent responsive behavior of a soluble adenine-functionalized polythiophene synthesized via direct arylation polymerization. **S. Sabury**, G.S. Collier, S. Kilbey

10:00 167. Exploring multi-tiered conjugated oligomers as models for conjugated materials. **A.E. Johns**, D.M. Collard

10:20 Intermission.

10:35 168. Crystallization-driven self-assembly of cationic cobaltocenium-containing block copolymers. **Y. Cha**, C. Tang

10:55 169. Systematic exploration of structure-property relationship and thermotropic liquid crystallinity of branched side chain poly(3-alkylthiophene)s. **B. Cox**, D.M. Collard

11:15 170. Biomaterial-assisted delivery of lysostaphin to eliminate *Staphylococcus aureus* infection in non-union bone defects. **P. Kalelkar**, C.T. Johnson, A. Garcia

11:35 171. Mechanistic and kinetic studies of a sustainable catalysis of a conjugated polymer by an enzyme. **T. Leeper**

Savannah Marriott Riverfront
Forsyth

Smart Polymer Materials & Coatings

W. Ming, *Organizer, Presiding*

10:00 Introductory Remarks.

10:05 172. Intimate and permanent ligating of photoresponsive and thermoresponsive polymers on plasmonic nanoparticles with switchable self-assemblies, optical properties, and catalytic activities. **Z. Lin**

10:35 173. RF plasma treatment of cellulose materials to fabricate paper-based analytical devices. **D.W. Hess**

11:05 174. Electrospun polyelectrolyte fibers as nanoreactors. **L. Zhai**

SUNDAY AFTERNOON

Savannah Marriott Riverfront
Chatham

Advances in Phosphorous-Based Ligands

Financially supported by Southeastern Louisiana University - College of Science & Technology and Department of Chemistry & Physics
G. G. Stanley, B. Wicker, *Organizers*

1:00 Introductory Remarks.

1:05 175. Synthesis of phosphonium salts and their potential as cationic ligands. **B. Wicker**, B.A. Atwater, F.R. Fronczek

1:25 176. Chemistry of phosphoethynolato with early transition metals. **D.J. Mindiola**

1:50 177. Bond activation reactions by boryl pincer complexes. **O. Ozerov**, W. Shih, Y. Cao, N. Bhuvanesh

2:15 178. Benzoxaphospholes as ligands for transition metals. **J.D. Protasiewicz**

2:40 179. Lessons in phosphine ligand design: Best laid plans often go astray. **G.G. Stanley**

3:05 Intermission.

3:20 180. New catalysts and strategies for the enantioselective coupling of nucleophiles and unsaturated hydrocarbons. **S. Malcolmson**, N. Adamson, S. Park, H. Jeddi

3:45 181. Suzuki-Miyaura and Buchwald-Hartwig reactions utilizing a set of complementary imidazopyridine phosphine ligands. **L. Yet**

4:10 182. Mechanistic studies and catalytic applications of conformationally flexible phosphine ligands. **K.H. Shaughnessy**

4:35 183. Phosphine center stage: Profile of a leading and supporting actor in organometallic catalysis. **B.V. Popp**

Savannah Marriott Riverfront
Academy

Analytical Chemistry

Bioanalytical

C. McKenas, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 184. Measuring pH in tumors with plain radiography by a hydrogel-based biosensor. **S.D. Kiridena**, U. Wijayaratna, M. Arifuzzaman, J.N. Anker

1:25 185. What's really in your e-cigarette? Analysis of psychoactive drugs found in over-the-counter vape products. **D.C. Josey**, S. Zingales

1:45 186. Application of low-cost embedded computers and 3D-printing for automated titrimetric analysis. **N. Boppana**, R.A. Snow, W.T. Mcloed, A. Kim, M.A. Brown, P.S. Simone, G.L. Emmert

2:05 187. Redox-based fingerprinting method to sense antioxidants. **F. Lozada**, M. Bonizzoni

2:25 188. Novel aptamers for serotonin and dopamine sensing on field-effect transistors. **S.T. Mensah**, K. Yang, K. Cheung, M.N. Stojanović, P.S. Weiss, A.M. Andrews

2:45 189. Analysis of heavy metals and antioxidant capacity in Slippery Elm bark samples. **J. Mierzwa**

3:05 Intermission.

3:20 190. Implantable hydrogel-based synovial fluid pH sensor to detect hip infections using X-ray imaging readout. **U. Wijayaratna**, S.D. Kiridena, M. Arifuzzaman, J.N. Anker

3:40 191. Development of a low-cost liquid delivery system using Raspberry Pi and 3D-printing. **N. Boppana**, R.A. Snow, M.A. Brown, P.S. Simone, G.L. Emmert

4:00 192. X-ray Excited Luminescence Chemical Imaging (XELCI) of implant associated bacterial infection by a chromoionophore based pH sensor. **A.C. Rajamanthrilage**, P. Millhouse, U. Uzair, S. Beladi-Behbahani, T.J. Tzeng, J.N. Anker

4:20 193. Sensing of penicillins and cephalosporins using a pamam-calcein complex in neutral buffered water. **Y. Xu**, M. Bonizzoni

4:40 194. Implantable fluidic sensor for non-invasive measurement of tibial plate strain with plain radiography. **A.C. Rajamanthrilage**, M. Arifuzzaman, P. Millhouse, C.J. Behrend, J. DesJardins, J.N. Anker

Savannah Marriott Riverfront
Pulaski

Organic Chemistry

Drug Discovery & Others

X. Chen, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 195. Development of allosteric modulators of MC4R for the treatment of obesity. M.M. Naguib, W.S. Hedges, G.E. McCartney, A.G. Leaver, B.A. Abdelmessih, Z.D. Fasig, L.E. Gimenez, R.D. Cone, **R.N. Daniels**

1:25 196. Design of agonists of the GABAB receptor from α -amino difluoromethyl ketones. **D.A. Colby**

1:45 197. Vial organic: Safer, cheaper pedagogy for organic chemistry labs. **T.J. Russo**

2:05 198. Spectroscopic analysis of medium-sized constrained rings for potential long-range hyperconjugation: Steric or donor-acceptor effects? **P. Wiget**

2:25 199. Photosensitizers for molecular switching of single- and dual-component photo-electro flexors. **K.S. Keane**, S.C. Blackstock

2:45 Intermission.

3:05 200. Aurone as a fluorescent probe for the selective detection of H₂S in environmental and biological systems. **A. Kafle**, S. Bhattarai, J.M. Miller, S.T. Handy

3:25 201. Method for photocatalytic synthesis of diazo compounds. **J. Sitter**, A.K. Vannucci

3:45 202. Theranostic nanoparticles for simultaneous detection and treatment of cancer cells. **S. Dada**, M. Hua

4:05 203. Synthesis of non-nucleoside SAM-competitive protein methyltransferase inhibitors. **A. Chakraborty**, A.C. Umeano, Z. Nikolovska Coleska, S.C. Schürer, R.C. Reynolds, T.S. Snowden

4:25 204. Catalysis of the aza-Diels-Alder reaction by hydrogen and halogen bonds. **V. Nzuwah Nziko**, S. Scheiner

Savannah Marriott Riverfront
Atrium

Project SEED

Cosponsored by SEED
Financially supported by Committee on Project SEED
A. Mallia, D. Masterson, *Organizers*

1:00 - 2:00

205. Silver nitrate complexes as a potential cancer therapeutic. **S. Eisen**, M. Chandler, K. Dowling, K. Afonin, D. Rabinovich

206. Qualitative identification of volatile organic compounds found in electronic-cigarette vapor and e-juice via GC/MS detection. **T. Vargas-Miguel**, C.H. Lisse

207. Synthesis and characterization of porphyrin entrapped silica sol-gels for heavy metal detection. **A. Rose**, C.H. Lisse

208. Utilizing sol-gel technology to create a portable detector of DNA. **G. Allred**, W. Medawala, C.H. Lisse

209. Synthesis and characterization of a reusable pH sensor using silica sol-gels and ormosils. **H. Mitchell**, C.H. Lisse

210. Identification of volatile organic compounds on strawberries using gas chromatography/mass spectroscopy. **C. Smith**, C.H. Lisse

211. Release of liquid hydrogen using perhydro dibenzyltoluene. **L. Zachary**

- 212.** Development and characterization of azaleu-enkephalin analogs. **S. Cornish**
- 213.** Hard and soft particle detection using machine learning. **T.N. Saleh**
- 214.** Leucine-based copolymers for drug delivery vesicles: Effect of solvent and inclusion of a single valine on their self-assembly behavior. **M. Wicaksana**
- 215.** Design and synthesis of novel iridium N-heterocyclic carbene based complexes for application in magnetic resonance imaging. **J. Flores**
- 216.** Investigating the carrier protein CRM197 to shuttle molecules across the blood-brain barrier. **S. Kanduri**, J. Travis, N.J. Wymer
- 217.** Anti-inflammatory activity of *Hypericum brachyphyllum* . **D. Teklay**, C.L. Gerald, **O.E. Christian**
- 218.** Lowering poly(vinyl chloride)'s glass transition temperature with urea and its derivatives. **J. White**
- 219.** Preparing for additive manufacturing using semi-conductive polymers. **Q. Cornish**
- 220.** Comprehending the molecular chemistry and chemical processing of high performance fibers. **D.A. Davis**
- 221.** Water quality chemical and microbial analysis of select water resources in Gwinnett County, GA. **J. Sheikh**, T. Gluick, R. Simmons
- 222.** Synthesis and studies of N-(phenylalkyl)octadecanamides as low molecular mass gelators. **J. Kim**, A. Mallia
- 223.** Preparation and characterization of deep eutectic solvents based on amino acids. **J. Suazo**, A. Mallia
- 224.** Molecular docking of the interactions of fluorinated heterocyclic sulfonamides with human and plasmodium DHFR. **M. Nguyen**, N.Y. Forlemu
- 225.** Investigating the performance and stability of an enzyme inspired catalyst. **R. Smith**, J. Nguyen, B. Huffman, T. Rodriguez, J.L. Dempsey
- 226.** Preparation of biodiesel using a DES. **I. Tirmizi**, A. Mallia, D.P. Pursell
- 227.** Magnetic drug delivery of xanthohumol to adipocytes using ultrasmall superparamagnetic iron oxide nanoparticles (USPIO). M. Drammeh, N. Naren, T. Fields, S. Rayalam, A. Singh, **V.V. Mody**

Savannah Marriott Riverfront
Forsyth

Smart Polymer Materials & Coatings

W. Ming, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 228. Preprogrammed dynamic microstructured polymers. **S. Minko**

1:35 229. Development of enzymosomes: Core-shell polymer particles with functional protein corona. **Q. Wang**, L. Zhang, D. Ma

2:05 230. Insights into intra-chain cross-linking. **E.B. Berda**

2:35 231. Development of smart polymer nanofiber mats for selective removal of PFAS from landfill leachate. **M. Feng**

2:50 232. Preparation and characterization of nanocomposites prepared from poly-3-hydroxybutyrate (PHB), lignin and cellulose nanocrystals by high torque melt mixing. **K. Blue**, S. McNeil, G. Schueneman, U. Agarwal, E.A. Mintz

3:05 Intermission.

3:20 233. Biobased polymer coating and antimicrobials. **C. Tang**

3:50 234. Modification and characterization of polyol based polymers for ice recrystallization inhibition and thermal hysteresis activity. M. Mousazadeh, **J. Tsavalas**, P.W. Baures, K. Varga, E. Asenath Smith

4:20 235. Reversible thermochromic alkali metal polydiacetylene microcrystals. **J.B. Parker**, T.W. Hanks

4:35 236. Effects of paraffinic oil on the mechanical behavior of the thermoplastic elastomer styrene-ethylene-butylene-styrene. **E.G. Bury**, A. Koh

4:50 237. Free radical polymerization of alkyl-substituted stilbenes with maleic anhydride. **C.J. Brown**, R.D. Gandour, S.R. Turner

Savannah Marriott Riverfront
Ballroom C

Advances in Polymer Science & Engineering

P. Kalelkar, *Organizer, Presiding*

1:05 Introductory Remarks.

1:10 238. Increasing the functionality of electrospun polymer fibers through large particle inclusion. **B. Brettmann**

1:35 239. Development of nitric oxide releasing polymers to improve biocompatibility of medical devices. **E.J. Brisbois**

2:00 240. Polydiacetylene nanostructures as sensor platforms. **T.W. Hanks**

2:25 241. Crawford group: At the interface of sensors and soft materials. **K. Crawford**

2:50 242. Structural transitions and encapsulation selectivity of thermoresponsive polyelectrolyte complex micelles. S. Shah, **L.F. Leon Gibbons**

3:15 Intermission.

3:35 243. Charge photogeneration in water-soluble conjugated polymer solar cells. **B.R. Gautam**, A. Davita, T. Wright

4:00 244. Robust metallo-polyelectrolyte membranes towards energy storage applications. **T. Zhu**, C. Tang

4:20 245. Soft material based analyte sensing device to noninvasively identify implant infection. **M. Arifuzzaman**, P. Millhouse, S. Behbahani, T.J. Tzeng, J.N. Anker

4:40 246. Effects of hybrid additives on the thermomechanical properties of PMMA parts printed by fused filament fabrication. **W. Ledford**, D.P. Street, S. Sabury, M. Kilbey

Savannah Marriott Riverfront
Ballroom D

Catalysis in Aqueous & Alternative Media

H. J. Schanz, *Organizer*

K. H. Shaughnessy, *Organizer, Presiding*

1:10 Introductory Remarks.

1:15 247. Aqueous romp and RCM, fast and furious. A.M. Ashcraft, G.T. Watson, C.A. Jones, **H.J. Schanz**

1:35 248. Polyoxometalate oxidation catalysts in solar fuels and anticancer chemotherapy. **C.L. Hill**

1:55 249. Electrochemical water oxidation by a large pore, catalyst loaded, metal-organic framework. **B.J. Gibbons**, A.J. Morris

2:15 250. Determination of optimal mild organic solvents for synthesis of PdNPs for carbon-carbon coupling reactions. **B.B. Penland**, T. Biswas

2:35 251. Study of photo-induced electron transfer from CdTe quantum dots to nickel molecular complexes in water. **N. Botcha**, R. Gutha, S. Sadeghi, A. Mukherjee

2:55 252. Visible light driven photocatalytic reduction of CO₂ to CO and CH₄ with transition metal complexes. H. Shirley, X. Su, J.W. Jurss, **J.H. Delcamp**

3:15 Intermission.

3:35 253. Aqueous CO₂ reduction catalyzed by Earth-abundant complexes bearing redox-active ligands. **J.W. Jurss**, X. Su, L. Chen, K. McCardle, J. Panetier

3:55 254. Carbon dioxide reduction catalysis with protic metal pincer complexes. **E.T. Papish**, S. Das, C.M. Boudreaux, W. Yao, D.B. Burks, J.H. Delcamp, C.E. Webster, A.K. Vannucci

4:15 255. Understanding cobalt oxide-promoted catalytic reduction of para-nitrophenol. **L. Shultz**, T. Jurca

4:35 256. Conversion of methane, ethane and propane to form alkyl esters: Oxy-esterification as a strategy for selective partial oxidation. **T. Gunnoe**, J.T. Groves, W.A. Goddard, N. Schwartz, N. Boaz, S.E. Kalman, J. Goldberg, R. Fu, R.J. Nielsen

Savannah Marriott Riverfront
Reynolds

Recent Advances in Bioinorganic Chemistry

Financially supported by Rotunda Scientific Technologies
J. D. Caranto, *Organizer*
T. Stich, *Presiding*

1:10 Introductory Remarks.

1:15 257. Heme sensor and inter-domain control of o₂-dependent globin coupled sensor signaling. **E.E. Weinert**

1:40 258. Modeling nitric oxide reductase utilizing Cu(II) centers and secondary sphere H-bonding functionalities: Intramolecular proton transfer facilitates $N_2O_{(g)}$ release. **G.B. Wijeratne**, M. Bhadra, M. Seigler, K.D. Karlin

2:05 259. HNO trapping mechanisms with ferric heme proteins. Y. Shi, **Y. Zhang**

2:30 260. Maturation and assembly of the key enzyme of methanogenesis. **S.O. Mansoorabadi**

2:55 Intermission.

3:15 261. Biological implications of amino acid coordination to Cu(II) and Fe(II). J.M. Murphy, **J.L. Brumaghim**

3:40 262. Non-native redox processes by synthetic cytochrome *C* oxidase mimics. **S. Hematian**

4:05 263. Substrate tuning traps intermediates in radical SAM enzyme reactions. **T. Stich**

4:30 264. Demystify the chemical logic of mononuclear iron enzyme catalyzed olefin and nitrile groups installation. **W. Chang**, Y. Guo, M. Davidson, Y. Tang, C. Yu, R. Fan

Savannah Marriott Riverfront
Mercer

Undergraduate Papers

Financially supported by American Chemical Society and the Coastal Georgia Local Section of the ACS

M. Weiland, *Organizer*

S. R. Carpenter, *Presiding*

1:10 Introductory Remarks.

1:15 265. Synthesis of coumarin-derived hydrogen sulfide chemosensors. R.E. Lee, **E.J. Haasbroek**, **S.M. Kang**, J.B. Kramer, P.E. Heiple

1:30 266. Asymmetric synthesis of nitrogen heterocycles by electrophilic cyclization reactions. **S.L. Boyd**, G.J. Rustin, M.G. Donahue

1:45 267. Towards a greener multidentate NacNac ligand. **P.M. Jimenez Antenucci**, H. Marcello, B. Wicker

2:00 268. Synthesis and analysis of primary amine functionalized silica sol-gels for catalyst extraction. **J. Fortwengler**, C.H. Lisse, R. Okoth

2:15 269. Synthesis, characterization, analysis, and use of biofuel from campus dining operations waste oil and grease. **C. Bourdeau, E. Calina, L. Kadima,** D.P. Pursell

2:30 270. Microwave-assisted oxidation of silyl ethers into silyl esters. **K.G. Darrigrand,** A.J. Ritz, A.M. Weinhofer, B.C. Goess, S.K. Goforth

2:45 271. Investigating novel nanocrystals as catalysts for heterogeneous cross-coupling reactions. **K. Storo,** S. Geyer, P. Lundin

3:00 Intermission.

3:20 272. Mechanical properties of boron nitride nanoparticle reinforced aerogels. **S. Twiddy,** S.H. Huneycutt, H. Harrison, J.R. Alston

3:35 273. Sonochemical generated radical detection in fluorinated solvents. **S.H. Huneycutt,** S. Twiddy, H. Harrison, J.R. Alston

3:50 274. Investigation of acid catalyzed Pictet-Spengler cyclization with sulfonamides. **K. Birkhoff,** M.G. Donahue

4:05 275. Synthesis and application of a trifunctional small-molecule probe to study time-resolved protein-protein interactions. **R.M. Clark,** A.M. Metts, L. Plate

4:20 276. Modification of thiols via nucleophilic aromatic substitution. **J. Dunne,** M.W. Giuliano, M. Forconi

4:35 277. Thermal shift assay development for finding novel antibiotics targeting a cystic fibrosis pathogen. **K. Meyberg,** T. Leeper

Savannah Marriott Riverfront
Ballroom E

Understanding Coastal Environments through Toxicological Applications & Tools

W. E. Gato, *Organizer, Presiding*

1:10 Introductory Remarks.

1:15 278. Utilization of organic contaminants as chemical tracers of elasmobranch ecology and physiology. **K. Lyons,** D. Kacev, D. Gillett, A. Preti, H. Dewar, S. Kohin, C. Bedore

1:45 279. Controlled-PCO₂ aquaculture for long-term investigation of ocean acidification. **C. Hintz,** H. Schroeder

2:15 280. Experimental determination of flame retardant effects on aquatic communities of the Southeastern Coastal Plain. **R. Cohen**

2:45 281. Drivers and dynamics of change in Altamaha, Doboy, and Sapelo Sounds along the Georgia coast. **K.K. Takagi**, K.S. Hunter, J.B. Deemy, W. Cai, S. Joye

3:15 Intermission.

3:30 282. Research framework for coupled hydrologic and biogeochemical systems in freshwater wetlands on Georgia coast barrier islands. **J.B. Deemy**, K. Takagi

4:00 283. Detection and risk analysis of UV filter and paraben micropollutants in the tidal freshwater Potomac River. **T. Haji**, G.D. Foster, T.B. Huff

4:30 284. Detoxification of waste water of Pb^{2+} and Cd^{2+} using agricultural waste of boiled groundnut (*Arachis hypogaea*) shells. **T.A. Abii**

Savannah Marriott Riverfront
Franklin

Advances in Connecting Structure, Dynamics & Functions of Macromolecules using Computational Methods

V. F. Waingeh, *Organizer*

N. Y. Forlemu, *Organizer, Presiding*

1:15 Introductory Remarks.

1:20 285. Molecular dynamics simulations of micelle formation by surfactants and peptides. **J. Kindt**

1:40 286. Electrostatic tuning maps and average protein configurations: Strategies to aid in studying flavoproteins. Y. Orozco-Gonzalez, M. Kabir, **S. Gozem**

2:00 287. Design of asymmetric catalysts through virtual screening. **S.E. Wheeler**

2:20 288. Computational studies of 3-hydroxy-3-methyl-glutaryl-CoA (HMG-CoA) reductase complexes with steroid-based statin analogs. **V.F. Waingeh**, M. Hackbarth

2:40 289. Benchmarking G-protein coupled receptor homology model template selection in tandem with *de novo* loop generation. **G. Szwabowski**, P.N. Castleman, C.K. Sears, L.H. Wink, A.L. Parrill-Baker, D.L. Baker, J.A. Cole

Savannah Marriott Riverfront
Oglethorpe A

X-Ray in the Southeast: Single Crystal

Financially supported by Division of Inorganic Chemistry and Rigaku Americas Corporation
W. E. Lynch, *Organizer*
R. A. Groom, *Organizer, Presiding*

1:15 Introductory Remarks.

1:20 290. Polymorphism and low-temperature data collection: Cautionary tale. **W.T. Pennington**, K. Kobra, C. McMillen, R. Sachdeva

1:40 291. Polymorphs, enantiomers, and intra/intermolecular interactions of D⁸ transition metal complexes. **D.E. Janzen**

2:00 292. Organic sulfate crystallography: Versatile tool for chiral identification. **C. McMillen**, B. Brummel, K. Lee, D.C. Whitehead, J.W. Kolis

2:20 293. Similarities and dissimilarities between transition metal silicates and germanates. **M. Smart**, T. Smith-Pellizzeri, C. McMillen, L.D. Sanjeeva, J.W. Kolis

2:40 294. Computational and crystallographic studies of aromatic N-oxide oxygen-iodine halogen bonding. **C.W. Padgett**, S.N. Bailey, k. hillis, M. Tran, D. Adams, A. Goetz, G. Guillet, W.E. Lynch

3:00 Intermission.

3:20 295. Multinuclear Cu^I bis(amidates) as highly luminescent molecular strings. **M. Stollenz**, J. Arras, A. Calderon, E.T. Miller, N. Bhuvanesh, C. McMillen

3:40 296. Structure and reactivity relationship of mononuclear Cu(II) complexes with peroxides. **A. Mukherjee**

4:00 297. Polydentate bis(amidines) as versatile ligand platforms for multinuclear coinage metal assemblies. **J. Arras**, M. Stollenz, O. Ugarte Trejo, C. O'Dea, N. Bhuvanesh, C. McMillen

4:20 298. Exploring the continuum of halogen bonding and higher polyhalide anions. **C. McMillen**, K. Kobra, B. Hicks, Y. Li, W.T. Pennington

4:40 299. The Rigaku Oxford Diffraction *XtaLAB Synergy*: from powder analysis to electron density study and protein structure solution.. **J.D. Ferrara**, P. Le Magueres, M. DelCampo, K. Saito, J. Wojciechowski, M. Meyer

Savannah Marriott Riverfront
Plaza

Undergraduate Papers

General

Financially supported by American Chemical Society and the Coastal Georgia Local Section of the ACS

M. Weiland, *Organizer*

C. R. Dockery, *Presiding*

1:20 Introductory Remarks.

1:25 300. Broadening the understanding of selective microwave heating on the 1,2-meisenheimer rearrangement. **A. Ziegelmeier**, G.B. Dudley, M. Frasso

1:40 301. Analysis of organic gunshot residues on activated charcoal passive sampling devices. **R. Cronin**, C.R. Dockery

1:55 302. Water purification efficiency using low-temperature atmospheric plasma jet under varying conditions. **M. Thompson**, R. Gott, K. Xu

2:10 303. Inhibition of oxidation of cosmetic foundation. **A. Hartman**

2:25 304. Aggregation patterns of insulin and amyloid-beta peptides. **S. Brown**

2:40 305. HPLC analysis and evaluation of cephalexin for DPAL (Distributed Pharmaceutical Analysis Laboratory). **C. Fegan**, M. Davila-Banrey, M. Howard

2:55 Intermission.

3:15 306. Photocatalytic degradation of glutaraldehyde in simulated fracking wastewater. **C. Cross**, L. Souza, J.E. Boyd

3:30 307. Removal of organophosphorus compounds from water. **J.T. Mathew**

3:45 308. Systematic study of the effects of functionalization on the interaction between CO₂ and calixarenes. **J. Hymel**, J. Townsend, K.D. Vogiatzis

4:00 309. Photophysical characterization of novel rhodamine B dimers. **N.J. Grinalds**, K.H. Fogarty, P.M. Lundin

4:15 310. Complex synchronization patterns in small networks of chemical oscillators. **T. Hung**, S. Nkomo

Savannah Marriott Riverfront
Oglethorpe B

Cope Scholar Symposium in honor of Seth Marder: Development of Organic Semiconductor Materials

Financially supported by Division of Organic Chemistry

S. M. Landge, *Organizer, Presiding*

M. A. Lnu, *Presiding*

1:30 Introductory Remarks.

1:35 311. Development of redox dopants for organic semiconductors and interface modification.

S.R. Marder

2:25 312. Synthesis of degradable polyacetals using enyne metathesis polymerization. **W.R.**

Gutekunst

2:55 Intermission.

3:15 313. Silole-containing polymers for organic semiconducting materials. **C.N. Scott, M.**

Bisen, D. Stemer, S. McKinnin, C. Luscombe

3:45 314. Development of C-H functionalization reactions for the incorporation of electron deficient building blocks in organic semiconducting materials. **S. Blakey**

4:15 315. Advances in 3D printing functional nano-photonic devices by multi-photon lithography. **S.M. Kuebler**

Savannah Marriott Riverfront

Atrium

Biochemistry

T. Leeper, *Organizer*

2:15 - 3:45

316. Development of heterocyclic molecules for recognition of mixed DNA sequences with two G•C base pairs. **P. Guo, A. Paul, A. Farahat, A. Kumar, D.W. Boykin, W. Wilson**

317. Leveraging a FapR biosensor for malonyl-CoA and non-natural extender units. **M.M. Mitchler, A.A. Malico, R.E. Kalkreuter, G.J. Williams**

318. Impact of acid insertions on packaging and damage of reconstituted arginine peptide-condensed DNA. **E. Oikeh, J.E. Derouchey**

- 319.** Protein-RNA complex characterization using biolayer interferometry and isothermal titration calorimetry. **M. Seemann, F. Abaza,** T. Leeper
- 320.** Elucidate possible reaction mechanism of cyclopropanation found in cycloclavine. **X. Li,** W. Chang
- 321.** Elucidate the mechanism of key cyclization in the fumiquinazolines biosynthesis. **L. Cha,** W. Chang
- 322.** Change in expression of host selenoproteins SePP1 and TR1 in cell lines due to Zika infection. **G. Dailey, E. Taylor, J. Ruzicka**
- 323.** Using choline kinase as a drug target leads to inhibition of *Streptococcus pneumoniae* growth via dysregulation of lipoteichoic acid production. **T. Zimmerman,** V. Chasten, J. Lacal, S.A. Ibrahim
- 324.** Identification of staphylococcal autoinducing peptides with ultrahigh performance liquid chromatography: High resolution mass spectrometry. **L. Mejia Cruz,** D. Todd, N.B. Cech
- 325.** Characterization of early steps from the biosynthetic pathway of the exomethylene β -branch in the polyketide difficidin from *Bacillus velezensis* FZB42. **R. Tikkanen,** J.J. Reddick
- 326.** Synthesis & mitochondrial analysis of sigma-1 selective ligands. **E.L. Martin,** B. Byrne, M. Prasad, K.S. Marriott
- 327.** Exploring allosterically induced enzyme dynamics in pyruvate kinase M2. **B.A. Andrews,** E.M. Guettler, R.B. Dyer
- 328.** Investigating 2-methylcitrate dehydratase (*mmgE*) in *Bacillus subtilis*: Victoria G. Meadows, Don A. Mora, and Jason J. Reddick. **V.G. Meadows**
- 329.** Determination of mitochondrial metabolism using western blot protein analysis. **A.D. Brantley,** K.S. Marriott, M. Prasad
- 330.** Analysis of mitochondrial protein regulatory function in presence of synthetic compounds. **J.W. Cox,** K.S. Marriott, M. Prasad
- 331.** Kinetic characterization of the rate-limiting C-H activation step of *M. oryzae* lipoxygenase and the effects of *N*-linked glycosylation. **C. Whittington,** A. Kostenko, K. Ray, A.R. Offenbacher
- 332.** Inclusion complex formation of synthetic AHL receptor antagonists and related compounds with β -cyclodextrin, a quorum sensing sequestration inhibitor. **E. Ziegler,** A.G. Palmer, A.B. Brown, N. Nesnas

- 333.** Assessing the ability to predict drug-induced mitochondrial toxicity in mammals. **N. Mitchell, M. Prasad**
- 334.** Effects of chaperones on protein-protein interactions. **D. Tinsley, A. Chowdhury, M. Prasad**
- 335.** Regulation of G-protein signaling: Interaction of RGS10 proteins with calmodulin and the G-alpha subunit. **C.A. Tope, J.L. Urbauer, R. Urbauer, S. Hooks, K. Rojas**
- 336.** Biochemical characterization of phosphoethanolamine methyltransferase from *Eimeria tenella*. **D. Etoroma, B. Cox, S. Lee**
- 337.** Salivary hormonal study on individuals of African ancestry living in different socio-economic environments, in order to understand etiology of prostate cancer. **M. Andrews, R. Cundey, E. Kaninjing, C. Mills, S. Rotimi, W. Medawala**
- 338.** Detecting prostate cancer associated glycosylation patterns from human serum using a boronic acid functionalized synthetic lectin array. **M.G. Hollenbeck**
- 339.** Identification of a novel transcriptional repressor gene in Kumao, a novel temperate bacteriophage. **L. Neri, M. Gainey**
- 340.** Isolation, whole-genome sequencing, and antimicrobial activity of the slow-growing aquatic *Pseudomonas* sp. RIT623. **K. Steiner, A. Parthasarathy, N. Wong, N.T. Cavanaugh, A.O. Hudson**
- 341.** Isolation, sequencing, and antibacterial properties of *Exiguobacterium* sp. RIT452. **N.T. Cavanaugh, K. Steiner, A. Parthasarathy, N. Wong, M. Hallenbeck, A.O. Hudson**
- 342.** Directed evolution of a natural product prenyltransferase towards alkyl-diversification of isoprenoids. **M. Calzini, G.J. Williams**
- 343.** Prey-associated quorum signals impact specialized metabolism and predatory features of predatory myxobacterium *Cystobacter ferrugineus* Cbfe23. **S. Akbar**
- 344.** Simplifying molecular probes for interrogating bacterial surface polysaccharide bioassembly. **A. Reid, B. Scarbrough, T. Williams, C. Gates, J.M. Troutman**
- 345.** Structure-based design of INGAP peptide analogs to promote viability and function of pancreatic islet beta cells. **J. Su, K. Gonzales, S. Mungre**
- 346.** Characterization of lipid binding by full-length NoxO1. R. Gallaher, **N. Davis**
- 347.** Isolation, sequencing, and antibacterial properties of *Paraclostridium* sp. MH636. **M. Hallenbeck, J. Chu, N.T. Cavanaugh, A. Parthasarathy, N. Wong, A.O. Hudson**

348. Decoding the machinery behind the thermodynamically unstable disubstituted β -branch formed in difficidin. **B. Kiel**, J.J. Reddick

349. Design of mimic peptides for inhibition of methyl-binding proteins. **A. Vanotteren**, A.L. Stewart

350. Biological evaluation of botanical extracts against *Staphylococcus aureus* and methicillin resistant *Staphylococcus aureus*. **C. Pelzer**, D. Jones Jr., N.B. Cech

351. Peptides as model systems for sequence specific transcriptional regulation. **A. Vanotteren**, **A.L. Stewart**

352. Analysis of enzymes involved in polymyxin resistance in *Escherichia coli* using fluorescent bactoprenyl phosphate. **B. Scarbrough**, C. Eade, A. Reid, J. Troutman

353. Characterization of novel protein domains in the DNA polymerase gamma from the human pathogenic yeast *Cryptococcus neoformans*. **C.A. Baumgardner**, S. Walter, I. Bose, J. Wallen

Savannah Marriott Riverfront
Ballroom B

Chemical Education

Teaching in the Laboratory

S. R. Mooring, *Organizer, Presiding*

2:35 Introductory Remarks.

2:40 354. How sweet it is: Using table sugar to teach single crystal X-ray crystallography at all levels of the undergraduate laboratory curriculum. **A.M. Beauparlant**, C.T. Eagle

3:00 355. Cross curricular themes of water quality in introductory general biology and chemistry courses. **R. Mohseni**

3:20 356. 3D printed models of atomic, hybrid, and molecular orbitals. **K.H. Fogarty**, R. De Cataldo, K. Griffith

3:40 357. Teaching essential QA/QC in the undergraduate analytical laboratory through pharmaceutical analysis: Cephalexin (DPAL project). **M. Howard**, C. Fegan, M. Davila-Banrey

4:00 358. Evaluation of virtual reality resources for an Organic Chemistry laboratory. **M.T. Gallardo-Williams**

4:20 359. Making a case for hands on activities in spectroscopy. **L. Strange de Soria**

4:40 360. Determining the quantity of acetic acid in household vinegar: Undergraduate laboratory titration experiment using three independent monitoring techniques. **R. Dabke**, S. Melaku, Z. Gebeyehu, S. Harris, J. Gonzales

Savannah Marriott Riverfront
Franklin

Advancements in Fermentation Chemistry

Z. S. Davis, *Organizer, Presiding*

3:25 Introductory Remarks.

3:30 361. NGS profiling of a mother culture used in the production of sour beer. **C. Cornelison**, M. Griffin, H. Den Bakker

3:50 362. Bypassing the malting process with Koji. **B.F. Taubman**, T. Williams

4:10 363. Investigation of volatile and semi-volatile aroma compounds in beer originating from either sorghum or barley malt. **D. Budner**

4:30 364. Effect of yeast strain on distilled spirit aroma and flavor: Sensory perception. W.N. Lory, **Z.S. Davis**

Savannah Marriott Riverfront
Atrium

Undergraduate Posters

Financially supported by American Chemical Society and the Coastal Georgia Local Section of the ACS

M. Weiland, *Organizer*

4:00 - 5:30

365. Testing and characterizing a novel bioactive glass containing nanocerium. **D.D. Paige**, A. Coke, N. Maya, K. Ranasinghe, D. Day, R. Singh

366. Design and synthesis of new aminoflavonol benzyl quinolone carboxylic acid (BQCA) analogs as potential Alzheimer's disease drugs. **S. Jarrell**, S. Zingales

367. Small molecule inhibitors of MEMO1: Biochemical and biological evaluation. **C.N. Hilton**, **L. Zhou**, C.L. Labrecque, K.J. Rubenstein, H.D. Evans, C.A. Taylor, C.A. Parish, J.A. Pollock

- 368.** Expression, purification, and characterization of the *Staphylococcus aureus* pasta kinase STK1. **M. Callender**, N. Labban, M.S. Blackledge, J.A. Pollock
- 369.** Regulation of pyrimidine degradation in *Pseudomonas chlororaphis*. **A.E. Chew**, M.F. Santiago
- 370.** Pro-ligands of estrogen receptor beta and implications in neurodegenerative diseases. **J.D. McEachon**, H. Park, J.A. Pollock
- 371.** Encapsulation of small molecules in the virus-like particle q β . **P. Chijioke Nyeche**, C. Moynihan, C. Bayas, K.A. Nolin, J.A. Pollock
- 372.** Expression and characterization of mutant virus-like particles. **C. Bayas**, **C. Moynihan**, P. Chijioke Nyeche, R. Bose, S. Laughlin, S. Bala, K.A. Nolin, J.A. Pollock
- 373.** Autoinhibitory loop of endothelial nitric oxide synthase: Structural characterization and kinetics with MAPKs. **E. Henry**, J.L. McMurry, C.A. Chrestensen, T. Leeper, S. Hill
- 374.** Synthesis of multi-metallic acetylide compounds of D¹⁰ transition metals. **S.L. McDarmont**, L.D. Jaques, J.A. Pienkos
- 375.** Synthesis of ^tbpyPt(C₂2Py)₂ and its interactions with Cu(I) and Pd(II) metals. **L.D. Jaques**, S.L. McDarmont, C. McMillen, S. Neglia, J.P. Lee, J.A. Pienkos
- 376.** Synthetic strategies for generating 4-ethynyl-2,3,5,6-tetrafluoropyridine. **T.T. Truong**, A.M. McConkey, Z.D. Moser, S.L. McDarmont, J.P. Lee, W. Yang, J.A. Pienkos
- 377.** Third-row molecules in space. **C.Z. Palmer**, M. Davis, A.R. Chard, R.C. Fortenberry
- 378.** Investigating sulfur and selenium antioxidants and the role plasmid DNA conformation has on data collection using PCR, CGE, and gel electrophoresis. **A. Adrian**, B. Ward, E.A. Kurfman, S.K. Wheeler, J.F. Wheeler, L. Kurfman, J.L. Brumagim
- 379.** Competitive reduction of ferrihydrite and nontronite and implications for lacustrine sediments. **D.M. Davis**, J. Chidzugwe, D. Deocampo
- 380.** Predicting reactivity of homologous sulfohydrolases via bioinformatics. **A.E. Reeves**, J.L. Fox, M. Forconi
- 381.** Assessing the release and transformation of metal additives from consumer plastics. **M. Hughes**, J.G. Clar
- 382.** Mycoremediation of atrazine and its metabolites from soil utilizing high-performance liquid chromatography. **S. Gowen**, R. Pandya, N. Kuklinski, L. Olson, S.K. Wheeler, J.F. Wheeler

- 383.** Hydrothermal syntheses and crystal structures of molybdenum tellurites. **D. Burgess**, H. Zhang, J. Ling
- 384.** Development of an oxidative [3+2] photocycloaddition reaction for the synthesis of huaspenone D. **H.E. Johnson**, M.E. Daub
- 385.** Oxidative [3+2] photocycloaddition reactions of 4-hydroxy-2-pyrones. **G.A. Elmore**, M.E. Daub
- 386.** Measuring heat related to the dissociation and reformation of ferritin using isothermal titration calorimetry. **B.W. Ellison**, **A.T. Perez**, F.W. Outten, N.E. Grosseohme
- 387.** Capillary electrophoresis as a screening technique for atrazine and atrazine metabolites. **C. Bailey**, J.F. Wheeler, S.K. Wheeler
- 388.** Thermostability characterization of tetrahedrite nanoparticles synthesized by a modified polyol process. **C.D. Fasana**, G.E. Garcia Ponte, M.E. Anderson
- 389.** Electrophoretic investigation of the inhibition of ROS-induced DNA damage using n,n'-dimethylimidazole selone. **L. Kurfman**, A. Adrian, E.A. Kurfman, B. Ward, J.L. Brumaghim, S.K. Wheeler, J.F. Wheeler
- 390.** Investigating the mechanism of eukaryotic heme A synthase. **M.L. Huebsch**, N.G. Taylor, N.J. Harris, O. Khalimonchuk, J.L. Fox
- 391.** Interactions between heme biosynthetic proteins in mitochondria. **H.G. Addis**, N.G. Taylor, N.J. Harris, O. Khalimonchuk, J.L. Fox
- 392.** Novel tris-indolyl compound possesses anti-cancer properties. **A. McNamee**, A. Wallace, T. Tolentino, C.R. Whitlock
- 393.** Quantum mechanics study of QSAR in synthetic cathinones. **J. Airas**
- 394.** Introduction of fluoroaromatic probes into peptides and proteins via nucleophilic aromatic substitution. **J. Linzel**, J. Dunne, M.W. Giuliano, M. Forconi
- 395.** Photoredox-mediated alkylation of imines with potassium organotrifluoroborates in the presence of an organic photocatalyst. **E.H. Thibodeaux**, B.E. Ciesa, J.M. Hanna
- 396.** Discovery and evaluation of small molecules that potentiate antibiotics in methicillin-resistant *Staphylococcus aureus* (MRSA). **R. Berndsen**, G. Norris, H.B. Miller, M.S. Blackledge
- 397.** Syntheses and structures of manganese tellurite chloride. **M.S. Davis**, H. Zhang, J. Ling
- 398.** Temperature dependent stabilities of various isomers of C₃₂ and C₃₆ endohedral metallofullerenes. **S. Church**, T.J. Fuhrer

- 399.** Recipe for a great scientist: Geometry, music, and mechanical drawing. **S. Powell**, T.J. Fuhrer
- 400.** Synthesis and reactivity of bioinspired mononuclear copper(II) complexes. **A.G. Sentell**, T. Jones, A. Mukherjee
- 401.** Kinetic isotope effect on the Kemp elimination. **E.A. Smolenski**, B. Taormina, F.J. Heldrich, M. Forconi
- 402.** Surface tension and critical micelle concentration measurements of seawater and estuarine water. **A. Deegan**, R. Bramblett, T. Burdette, A.A. Frossard
- 403.** Employing a binol based ligand for the design of chiral metal-organic frameworks. **I.A. Riha**, G.J. McManus
- 404.** Synthesis of metal-organic frameworks using four-connected imide containing linkers. **J. Jeffries**, G.J. McManus
- 405.** Constructing metal-organic frameworks from unique tetracarboxylic acid ligands. **K. Gusty**, G.J. McManus
- 406.** Metal phosphites: Synthesis, characterization, and susceptibility to oxidation. **K.M. Greene**, E. Reece, S.J. McElhenney, K. Slavicinska, M.A. Pasek, H.L. Abbott-Lyon
- 407.** Development of an active learning, organic chemistry laboratory experiment on extraction and LCMS identification of fragrant esters from fruits for use as a recruiting tool during UNC Asheville's NSF S-STEM "Chemistry First Day". **D.O. Jackson**, A.L. Wolfe
- 408.** Synthesis of polypeptides via emulsion polymerization of N-carboxyanhydrides. **M.P. Hale**, D.W. Holley
- 409.** Synthesis, characterization, and reactivity of a heterobimetallic organometallic complex with a *trans* bidentate ligand for catalytic carbon-hydrogen bond activation. **S. Neglia**, J.P. Lee, J.A. Pienkos
- 410.** Acetate: Assisted C-H bond activation: Attempts to prepare and isolate a key Co(III)-cyclometallated intermediate. **T. Paratore**, J.P. Lee
- 411.** Modification of head-groups on 10,12-pentacosadiynoic acid using click chemistry. **C.T. Stueber**, T.W. Hanks

SUNDAY EVENING

Savannah Marriott Riverfront
Atrium

Undergraduate Posters

Financially supported by American Chemical Society and the Coastal Georgia Local Section of the ACS

M. Weiland, *Organizer*

6:00 - 7:30

412. Preparation, thermal properties and gelation studies of 3 β -cholesteryl N-(9-acridinyl) carbamate as low molecular mass gelator and aggregation studies with DNA. T. Sawyer, **J. Lainez**, N.Y. Forlemu, T. Gluick, A. Mallia

413. Preparation, self-assembly and gelation studies of *N*-(4-hydroxyphenyl)alkanamides as low molecular mass gelators. **C. Landaverde**, S. Farre, A. Mallia

414. Surface modified polydopamine-polypyrrole coatings. **Z. Wang**, T.W. Hanks

415. Isolation methods for cannabinoids from hemp. **R. Harbit**, G. Hanna, K.M. Mullaugh

416. Synthetic progress towards asymmetrical pyridine-based CXCR4 modulators. **C.N. Tran**

417. Control of encapsulation and embed magnetic nanoparticles within the aqueous interior bilayer of liposomes prepared from 10,12-pentacosadiynoic acid. T.W. Hanks, **M. Fuller**

418. Siloxy functionalized nanoclays and nanosilica towards automotive crashworthiness applications. **Z. Murphy**, E. Koricho, S.M. Landge

419. Exposure of hepatocellular carcinoma cells (Hep-G2) to CDSTE quantum dots. **A.L. Ponton**, L. Alamo-Nole

420. Cytochrome P450 activity of Hep-G2 cells after the exposition of quantum dots. **I.J. Ortiz**, L. Alamo-Nole

421. Determination of fluorescence quenching constants. **J. Ellenburg**, **J. Bachmann**, **E. Storck**, P.B. Nolibos

422. Electrochemical synthesis of polyoxometalate based organic-inorganic hybrids. **J. Ondus**, **Q. Zhang**, S. Hwu

423. Synthesis of boronate ester derivatives of triphenylphosphine. **S. Shen**, M.W. Johnson

- 424.** Analysis of lanthipeptides produced by *Salinispora* and characterization of the cyclase. **S. Shah**, C.G. Kittrell, E. Limbrick
- 425.** Synthesis of bidentate bis(phosphino) pyrrole ligands and their complexes for nickel catalysis. **J. Vidlak**, M.W. Johnson
- 426.** Expression of electron transport chain complexes following exposure to tumor-suppressant α -TOS. **A. Palos-Jasso**
- 427.** Synthesis of bis-(2-phosphinopyrrole) pincer ligands and their respective metal complexes. **N.K. Sriramaneni**, M.W. Johnson
- 428.** Structure activity relationship (SAR) studies of neurotoxin quinoline-derivatives. **D. Smeyne**, V. Sittaramane, M.A. Lnu
- 429.** Readily accessible microfluidic devices using conventional 3D-printers. **B.T. Persaud**, R. Saleb, C. Miller, J. Sharma, S. Ambre
- 430.** Determination of trace amounts of pesticides in green tea. **A.M. Le**, J.M. Plummer
- 431.** Exploration of controlled release properties of polypyrrole films. **A. Knepper**, R. Wetherill, P. Molino, T.W. Hanks
- 432.** Bio-based materials to synthesize a novel surfactant used in the production of polyurethane foams. **C. Crull**
- 433.** Purification and characterization of Notch TM by NMR. **M. Zhuang**, C. Wang, J. Zhao, Y. Xiao, J. Gibson
- 434.** New pathway for CO₂ reduction: Amine-CO₂ activation followed by traditional hydride reduction. **Z. Yang**, M.R. Norris, C.A. Parish
- 435.** Ligand exchange of PbS quantum dot thin films: Mechanism and kinetics. **A. Milam**, M.R. McPhail
- 436.** Study of the lysine deprotonation mechanism in UBC13. **K. Elliott**, N. Seward, H. Hampton, I. Sumner
- 437.** Construction of an oligo(ethylene glycol)-based self-assembled scaffold using N-hydroxysuccinimide conjugation chemistry for the chemical attachment of enzymes to gold surfaces. **A. Nelson**, C.M. Johnson, P.A. Baker, B.W. Gregory
- 438.** Synthesis and characterization of copper proazaphosphatrane complexes as potential pre-catalysts for cross-coupling reactions. **J. Thomas**, M. Johnson

- 439.** Compositional analyses of potsherds from an ancient Jewish pottery industrial site by inductively coupled plasma optical emission spectrometry. **J.M. Trail, A.C. Rodgers, J.R. Strange, B.W. Gregory**
- 440.** Data-guided permeability estimations for polymeric membranes. **R. Duke, J. Townsend, K.D. Vogiatzis**
- 441.** Investigating the oxidative mechanism leading to atherosclerotic lesions. **J.P. Post, K.M. Matera**
- 442.** Evaluating the binding of a novel carbon POSs-based HIV protease inhibitor drug. **Y.C. Solis, J. Airas**
- 443.** Theoretical study of variable gas adsorption by the robust metal-organic framework NKMOF-1-Ni'. **G. Beemer, T. Pham**
- 444.** Photocatalytic oxidation of aqueous ethylene glycol using solar illumination. **L. Souza, C. Cross, T.R. Hayden, J.E. Boyd**
- 445.** Using chalcones to re-sensitize methicillin-resistant *Staphylococcus aureus* (MRSA) to antibiotics. **A. LeBeau, J. Brigati, N. Duncan**
- 446.** Photochemistry of silver cluster: DNA conjugates. **S. Carnahan, J.T. Petty**
- 447.** Silver cluster conjugates with a DNA template. **D. Lewis, J.T. Petty**
- 448.** Identification of toxic metabolites produced by *Batrachochytrium dendrobatidis* fungus. **L.E. Moore**
- 449.** Cracking the theobromine dimer through co-crystal formation with salicylic acid derivatives. **A.N. Kerr, G.J. McManus**
- 450.** Studies toward functionalization of tenulin and isotenulin via Diels-Alder reactions. **J. Wilson, K.S. Knight**
- 451.** Calculation of critical and incident angles of complex reflection-absorption infrared systems. **S.J. McElhenney, K. Slavicinska, H.L. Abbott-Lyon**
- 452.** Interaction of hydroxyapatite thin films with prebiotic solutions. **A.J. Nastase, E. Garcia, K. Slavicinska, C.J. Luda, A. Poyraz, H.L. Abbott-Lyon**
- 453.** Electrodeposition and characterization of hydroxyapatite thin films on metal substrates. **C.J. Luda, E. Garcia, K. Slavicinska, A.J. Nastase, A. Poyraz, H.L. Abbott-Lyon**
- 454.** Exploration of unexpected Ph-dependent acidic aromatic hydrogen in 1,8-diamino-2,7-naphthyridine-4-carbonitriles. **J. Ewald, M. Pfanner, T.T. Truong, W. Yang**

455. Phosphonates as a precursor to phosphonylated biomolecules. **S.A. Khweis**, K. Slavicinska, M.A. Pasek, H.L. Abbott-Lyon

456. Developing small molecules selectively targeting the sequence-based secondary structure of SSDNA, CCG repeats. **M. Pfanner**, S. Erwin, M. Linkous, W. Yang

457. Tetrahedrite and Cu-Sb-S intermediates synthesized by a modified polyol process. **M.S. Jensen**, T.R. MacAlister, M.E. Anderson

458. Modification of polysiloxane surface coatings with zwitterionic thiols using thiol-ene click. T.W. Hanks, **J.M. Owen**

459. Investigating MOF ultra-thin film thickness by ellipsometry and atomic force microscopy. **A.M. Weeks**, F.G. Gonzalez, M.E. Anderson

460. 3D printed laboratory accessories as a vital component of the undergraduate research experience. **E.S. Quinn**, N.T. Green, R.M. Hughes

461. Screening and characterization of a commercially available lipase library for catalysis of a Morita-Baylis-Hillman reaction. **K.D. Hernandez Gomora**, R.M. Hughes

MONDAY MORNING

Savannah Marriott Riverfront
Ballroom C

Advancements in Biocatalysis

A. S. Bommarius, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 462. Catalytic promiscuity versus stereochemical fidelity in enzymatic dynamic reductive kinetic resolution (DYRKR): Insights from biocatalytic studies and structural biology. G.P. Kudalkar, V.K. Tiwari, G.A. Applegate, K. Panigrahi, P. Madzellan, M.A. Wilson, **D.B. Berkowitz**

8:33 463. Exploring sequence-function space in the old yellow enzyme superfamily. **S. Lutz**

9:01 464. Understanding the limited stereo-complementary nature of old yellow enzymes 1 & 3: Loop movement dictated by a single amino acid. **R.R. Watkins**, S. Lenka, M. Buteler, J.D. Stewart

9:21 465. Bubble column enables higher reaction rate for deracemization of (*R,S*)-1-phenylethanol with coupled alcohol dehydrogenase/NADH oxidase system. **B. Bommarius**

9:49 466. Data-Rich Development of a Novel Biocatalytic Aerobic Oxidation Across Scales. **S. Grosser**

10:17 Intermission.

10:32 467. Development of a commercial biocatalytic process to produce dextroamphetamine salts. **D. Hallow**, W. Zhang, G. Mkrtchyan

11:00 468. Recent advances in commercial scale biocatalytic processing. **M. Abrahamson**

11:28 469. Directed evolution of an amide bond-forming enzyme in organic solvent. **B. Dorr**

Savannah Marriott Riverfront
Forsyth

Applications of Mass Spectrometry for Drug Discovery & Precision Medicine

Financially supported by Division of Analytical Chemistry
J. D. Tipton, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 470. Quick discussion on multiomics with mass spectrometry and standardization in metabolomics. **J.D. Tipton**

8:30 471. Mass spec applications to natural products drug discovery. **B. Baker**

8:55 472. Mass spectrometry metabolomics in clinical research. **T.J. Garrett**, C. Chamberlain, V. Rubio

9:20 473. Plant health, performance and metabolome perturbation measured by high throughput mass spectrometry and automated greenhouse technology. **B. Ruddy**, T.K. Harp, E.R. Schultz, J. Wu, J.E. Habben, T.R. Wright, C.N. Yerkes, J.P. Hazebroek

9:45 474. Pharmacoproteomics: Mass spectrometry-based approach to determine drug targets and their effects in an unbiased manner. **L. Herring**, J. Beri, A. Prevatte, T. Gilbert, L. Graves

10:10 Intermission.

10:30 475. PepSAVI-MS for the identification of novel bioactive cyclotides. **N.C. Parsley**, L.M. Hicks

10:55 476. High-throughput screening by adaptation of IR-MALDESI-MS. **D.C. Muddiman**, M. Ekelof, J. Dodds, E.S. Baker, J. Williams, N. Elsen

11:20 477. Effects of buffers on the conformation and aggregation of an adalimumab biosimilar studied with hydroxyl radical protein footprinting. **R.C. Orlando**, S. Mirsa, S. Weinberger, J. Sharp

11:45 Concluding Remarks.

Savannah Marriott Riverfront
Chatham

Chemistry Education from Research to Practice

Financially supported by Wilson Dam Local Section of the American Chemical Society
M. Anzovino, S. L. Johnson, *Organizers, Presiding*

8:00 478. Assessment in postsecondary chemistry courses: Results from a national survey. **J.R. Raker**, K.L. Murphy

8:20 479. Longitudinal investigation of changes in teaching beliefs of chemistry faculty at research-intensive institutions. **M. Popova**, J. Harshman, M.N. Stains

8:40 480. Characterizing observation feedback provided to trainee graduate teaching assistants. **C.A. Randles**, F.K. Lang, K.A. Jeffery

9:00 481. Improving the training of teaching assistants at Purdue chemistry: Incorporating what they really need and want. **F.K. Lang**, C.A. Randles, K.A. Jeffery

9:20 Intermission.

9:30 482. Specifications grading: Method to improve student retention and progression? **M. Anzovino**, **T. Gluick**, **M.S. Morton**, D. Behmke, M. Tsoi, O. Villanueva, C. Woodbridge

9:50 483. Utilizing evidence-based pedagogies to make general chemistry more individualized and accessible to under-prepared students. **J.H. Broome**

10:10 484. What student know and say about acid-base equilibrium. **S. Mooring**, N.A. Kilpatrick

Savannah Marriott Riverfront
Reynolds

Diversity: Minority Serving Organizations

Financially supported by ACS Local Section Activities Committee, Coastal Georgia Local Section of the American Chemical Society, NOGLSTP.

R. A. Groom, B. P. Quillian, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 Panel Discussion.

8:45 485. Diversity and inclusion: Perspective from a quarter of a century in a minority serving institution. **S.Y. Ablordeppey**

9:15 486. ACS PROF and NOGLSTP: Making history for LGBTQ+ chemical professionals. **C.J. Bannochie**

9:45 Intermission.

10:10 487. American Chemical Society Committee on Chemists with Disabilities: Empowering ability. **R.I. San Miguel**

10:40 488. SACNAS: Achieving true diversity in STEM. **P. Silveyra**

11:10 489. Faculty research mentoring strategy at a PWI versus an HBCU. **P.I. Binda**

11:40 Discussion.

Savannah Marriott Riverfront
Franklin

Advancements in Chemical Biology

Financially supported by Division of Analytical Chemistry; North Carolina State University and the University of Georgia

G. J. Williams, *Organizer*

Y. Zheng, *Presiding*

8:05 Introductory Remarks.

8:10 490. Synthetic glycomics: Chemo-enzymatic synthesis of oligosaccharides, polysaccharides, glycolipids, glycopeptides and glycoproteins. P.G. Wang, J. Song, **J. Zhang**

8:35 491. Molecular basis for the evolution of methylthioalkylmalate synthase and chain elongation of methionine-derived glucosinolates. **S. Lee**

9:00 492. Fragment-based drug discovery targeting *P. aeruginosa* inhibitor of vertebrate lysozyme: Approach to active site-directed irreversible inhibition. **A.B. Schultz**, T. Leeper

9:15 493. More QACS, more questions: Investigation of next-generation quaternary ammonium compounds. **K. Morrison**, M.C. Jennings, R.A. Allen, A. Kaplan, K.P. Minbiole, W. Wuest

9:30 494. Human milk and the art of (microbial) war. **S.D. Townsend**

9:55 Intermission.

10:15 495. Exploiting an NQO1 bioactivatable quinone for the selective treatment of *BRCA1/2*-mutant human breast cancers. L. Palmquist, H. Dixon, **M.C. Srougi**

10:40 496. Expanded genetic code to study protein post-translational modifications. **T.A. Cropp**

11:05 497. Unravelling the druggability of E3 ubiquitin ligase Nedd4 as a target for the alleviation of α -synuclein toxicity in Parkinson's disease. **A. Hatstat**, D.G. McCafferty

11:20 498. Metabolomics-based differentiation of gram-positive bacterial strains. **A. Shahbandi**, D. Todd, D. Jones Jr., N.B. Cech

11:35 499. Tunable chemistry for global discovery of protein function and ligands. **K. Hsu**

Savannah Marriott Riverfront
Mercer

Polymers at Interfaces

B. Brettmann, *Organizer*

L. F. Leon Gibbons, *Organizer, Presiding*

8:10 Introductory Remarks.

8:15 500. Dynamic polymer biointerfaces. **S. Minko**

8:45 501. Interfacial behavior of soft thermoreversible microgel particles on flat surfaces. **M. Gaines**, N. Anderson, G. Brim, D. Ingabire, P. Kamuche, L. Oliver, J. Weatherington, E. Westbrook, L. Williams

9:15 502. Polymer interpenetration and chain connectivity on the local glass transition and dynamical gradients near and across polymer interfaces. **C.B. Roth**

9:45 503. Study of kinetics and functionalization efficiency of sonochemical assisted nanoscale anion exchange resins for water purification. **A. Sahu**, R. Sheikh, J.C. Poler

10:00 Intermission.

10:25 504. Polymer coatings for aerospace applications. **D. Priftis**

10:55 505. Counterion condensation in polymer electrolytes and its role on ionic conductivity in electrochemical processes. **C.G. Arges**

11:25 506. Pattern-based metal cation sensing at trace levels in water using fluorescent polymeric receptors. **M. Ihde**, J. Tropp, J.D. Azoulay, M. Bonizzoni

11:40 507. Ultra-stretchable conductive polymer complex with repeatable autonomous self-healing ability. **J. Horne**, D. Hong, A. Faunce, L. McLoughlin, R. Ploeger, D. Sanchez, S.G. Yim, Y. Lu, J. Jeon, **E.K. Wujcik**

Savannah Marriott Riverfront
Ballroom D

Strategy & Methods for Complex Molecule Synthesis

Financially supported by Division of Organic Chemistry
E. M. Ferreira, A. J. Grenning, *Organizers, Presiding*

8:10 Introductory Remarks.

8:15 508. Beyond CP*: Mechanism guided design of a new rhodium complex for enantioselective C-H functionalization. **S. Blakey**

8:45 509. Understanding catalyst substrate interactions and reaction selectivity. **S. Wiskur**

9:15 510. Photochemical cyclization techniques: Synthesis of carbetocin. J.N. O'Brien, W.A. LeFever, E. Barksdale, M. Srougi, **A.J. Wommack**

9:35 511. Pericyclic reactions in the total synthesis of natural products. **J. Leahy**

10:05 Intermission.

10:25 512. Synthesis of α - and β -carbolines via tandem catalysis. **S.P. Mulcahy**

10:45 513. Development of alkyne metathesis catalysts for organic materials synthesis. **S. Lee**, R.R. Thompson

11:15 514. Benzimidazolyl-metal complexes as simple bifunctional templates in sustainable catalysis. **V. Lindsay**

Savannah Marriott Riverfront
Oglethorpe A

Structure-Based Drug Design

Financially supported by Cresset
R. J. Bienstock, *Organizer, Presiding*

8:10 Introductory Remarks.

8:15 515. Activating silent biosynthetic gene clusters in fungi via co-cultivation. **S.L. Knowles**, H.A. Raja, A.J. Wright, A.L. Lee, L.K. Caesar, N.B. Cech, M.E. Mead, J.L. Steenwyk, A. Rokas, N.H. Oberlies

8:40 516. Bacterial and fungal ribosome RNA targeted antimicrobials. **D.P. Arya**

9:05 517. Antibiotic resistance: Protons, promiscuity and polymerases. **M.J. Cuneo**

9:30 518. Computer-aided design and synthesis of potential pharmacophores. **S.S. Panda**

9:55 Intermission.

10:15 519. Structure-based design of panthothenate kinase modulators for the treatment of COA deficiencies. **R.E. Lee**

10:40 520. Type IV inhibitors of B-Raf kinase that block dimerization and overcome paradoxical MEK/ERK activation. **C. McInnes**

11:05 521. Data-driven construction of innate immune checkpoint inhibitors with controlled polypharmacology. **D. Kireev**

Savannah Marriott Riverfront
Oglethorpe B

WCC: Modern Issues for Women in Chemistry

S. Zingales, *Organizer*
C. Knight, D. E. Williams, *Presiding*

8:10 Introductory Remarks.

8:15 522. Navigating teaching, research, service and motherhood at a primarily undergraduate institution. **P. Riggs-Gelasco**

8:30 523. Barriers in the laboratory and perceptions of femininity. **C. Knight**

8:45 524. Pregnancy and parenting in academia. **M.S. Blackledge**

9:00 525. Succeeding in academia: Keep calm and say "no". **S.L. Johnson**

9:15 Panel Discussion.

10:00 Intermission.

10:30 526. My experience as an inexperienced negotiator. **D.E. Williams**

10:45 527. Encouraging success and access to opportunities for women and people of color at a primarily white undergraduate institution. **J.H. Ferguson**, A. Maxwell, J.R. Ward

11:00 528. Finding your voice and taking up space. **C. Theodore**

11:15 529. Empowering undergraduate students through chemical biology research. **J.A. Pollock**

11:30 Panel Discussion.

Savannah Marriott Riverfront
Ballroom E

New Forms of Carbon: Fullerenes, Metallofullerenes, Nanotubes & Graphene

Financially supported by President-Elect of the American Chemical Society
H. C. Dorn, *Organizer, Presiding*

8:15 Introductory Remarks.

8:20 530. Recent crystallographic studies of fullerenes and endohedral fullerenes. **A.L. Balch**,
M.M. Olmstead, M. Roy

8:50 531. Actinide endohedral metallofullerenes: From cage selection to actinide-actinide interactions. **J.M. Poblet**

9:20 532. Actinide-based buckyball maracas: Fullerene cages as nanocontainers that stabilize monometallic and actinide clusters inside. **L. Echegoyen**, W. Cai, J.M. Poblet

10:10 Intermission.

10:30 533. Single-electron lanthanide-lanthanide bonds inside a carbon cage: Towards robust metallofullerene molecular magnets. **A. Popov**

10:50 534. Isolation of tubular carbon ("fullertubes"): Fullerenes, nanotubes, or neither? **S. Stevenson**

11:20 535. Nanocarbon reactions for formation of cluster-encapsulated fullerenes. **P.W. Dunk**, M. Mulet-Gas, C. Hendrickson, M.R. Ceron, L. Echeгойen, A. Moreno-Vicente, A. Rodriguez-Fortea, J.M. Poblet

Savannah Marriott Riverfront
Ballroom B

Plastics & Microplastics in the Environment

J. A. Brandes, *Organizer, Presiding*

8:15 Introductory Remarks.

8:20 536. Availability of plastic-associated chemicals to northern fulmar seabirds. **E. Crater**, K. Huncik, J. Hoguet, J. Kucklick

8:45 537. Mapping microplastics in Georgia's coastal waters: Engaging the citizen scientist. **D. Sanders**, J.A. Brandes

9:10 538. Patterns of microplastic abundances in Georgia estuarine waters. **J.A. Brandes**, D. Sanders

9:35 539. Photochemical degradation of microplastics under aquatic conditions. **K. Ma**, J.A. Brandes

Savannah Marriott Riverfront
Plaza

Recent Advances in Cellulose, Lignin or Hemicellulose Derived Materials & Chemicals

S. Chatterjee, *Organizer, Presiding*

8:15 Introductory Remarks.

8:20 540. Robust route to multi-functional cellulose-based polymeric bottle-brush cocoons. **Z. Wang**, Z. Lin

8:40 541. Low cost production of xylose from biomass hydrolyzates. **J. Satyavolu**

9:00 542. Interaction of lignin dimers and derivatives with β -cyclodextrin. **X. Tong**, M. Moradipour, B. Novak, B. Knutson, S. Rankin, B. Lynn, D. Moldovan

9:20 543. Effectiveness of mercury sorbents derived from biomass precursors. **A. Johs**, D.P. Harper, J.M. Chalker, M.A. Mayes, S. Brooks, E.M. Pierce, M.J. Peterson

9:40 544. Cellulose and lignin based biocomposites for thermal energy management in buildings. **Y. Kim**, X. Zhang, G. Bahsi Kaya, B. Vega, B. Via

10:00 Intermission.

10:20 545. Carbon fibers derived from fractionated solvated lignin: Graphitic layers in amorphous matrix? **V. Bermudez**, J. Jin, M.C. Thies, A.A. Ogale

10:40 546. Cellulose-derived bottlebrush-like block copolymers enable the crafting of one-dimensional functional nanorods with unprecedented control over dimensions, compositions, architectures and surface chemistry. **Z. Lin**

11:00 547. Biohybrid aerogel from self-assembled nanocellulose and nanochitin as a high-efficiency absorbent for water purification. **X. Zhang**, I. Elsayed, C. Navarathna, G. Schueneman, E.M. Hassan

11:20 548. Nanocellulose based functional textile coatings. A. Liyanapathiranage Dona, S. Dilliwar, R. Melnyk, V. Tokarev, S. Sharma, **S. Minko**

11:40 Concluding Remarks.

Savannah Marriott Riverfront
Pulaski

Polymeric Materials for the Next Generation Sensing, Diagnostics, & Therapy

Financially supported by Division of Polymer Chemistry
D. L. Watkins, *Organizer*
C. N. Scott, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 549. Facial amphiphilic antimicrobial polymers against gram-negative bacteria. **C. Tang**

9:35 550. Multifunctional polysilsesquioxane nanoparticles for the treatment of cancer. **J.L. Vivero**

10:05 Intermission.

10:20 551. Polymer-tetrodotoxin conjugates to induce prolonged duration local anesthesia with minimal toxicity. **C. Zhao**

10:35 552. Temperature-responsive polymersomes of poly(n-vinyl-2-methylcaprolactam)-*block*-poly(n-vinylpyrrolidone) to dampen drug-induced cardiotoxicity. **V.A. Kozlovskaya**, E.P. Kharlampieva

10:50 553. Promising screening platform to identify oligonucleotide ligands. **V.T. Milam**, M. Tapp, J. Slocik, P. Dennis, **R.R. Naik**

11:20 554. Fundamental studies and biomaterials application of peptoid polymers. **D. Zhang**

Savannah Marriott Riverfront
Atrium

Undergraduate Posters

Financially supported by American Chemical Society and the Coastal Georgia Local Section of the ACS

M. Weiland, *Organizer*

9:30 - 11:00

555. Determination of optimal mild organic solvents for synthesis of PdNPs for carbon-carbon coupling reactions. **T. Biswas**, B.B. Penland

556. Synthesis of indolenine and quinoline derived water-soluble squaraine dyes. **B. Marx**

557. A single-entity method to actively control the nucleation-crystal growth process (I) - basics in lysozyme crystallization. **R. Lee**, R. Yang, G. Wang

558. A quantum chemical study of enolate, enol, and alkene structures as predictive models for the site of alkylation. **A. Kumar**, J.P. Bowen

559. Biosynthesis of iron oxide nanoparticles by ammonia diffusion. **S.O. Ekiyor Katimi**

560. Reaction pathway for tetrahedrite synthesized by a modified polyol process. **T.R. MacAlister**, M.S. Jensen, M.E. Anderson

561. Towards the synthesis and complexation of a new Janus-type N-heterocyclic carbene. E. Swalles, **J.M. Ralston**, **J. Scott**, D. Tapu

562. Influence of ligands and pH on the dissolution of metal oxide nanoparticles. **E.R. Ramsayer**, K.M. Mullaugh

563. *In vivo* UGT isoenzyme glucuronidation of daidzein. **S.A. DeFiglia**, J.W. Brock

- 564.** Ring functionalized D- π -a titanocenes for use in dye-sensitized solar cells. **J.S. McCarthy**, P.S. Wagenknecht
- 565.** Sulfidation of silver nanoparticles by zinc sulfide. **B. Nguyen**, H. Lieb, K.M. Mullaugh
- 566.** Handheld near-infrared Raman spectrometer. S.C. Pasley, **T. Griffin**, J.W. Hall
- 567.** Effects of CUBR or AGCL coordination on the photochemistry of arylalkynyltitanocenes. **H. London**, D.Y. Pritchett, P.S. Wagenknecht
- 568.** Synthesis of amines by nucleophilic ring opening of aziridines. **A.M. Bogatkevich**, T.J. Barker
- 569.** Affordable determination of the elemental composition of quantum dots with portable X-ray fluorescence spectroscopy. **J. Land**, A. Landin, J.D. Keene
- 570.** Detecting endocrine disrupting compounds: Development of a differential sensing array for use in aqueous media. **T.C. Meeks**, M. Meadows
- 571.** Optimization of reversible-deactivation radical polymerization procedure. **S. Welch**, N. Shank, K.J. Noonan
- 572.** Computational study of FXBN spin trap derivatives with hydroxyl radicals. **A.K. Harvey**, S.J. Kirkby
- 573.** Reaction of alkylboronic esters with epoxides. **S.G. Gierszal**, T.J. Barker
- 574.** Application of evolved tryptophan synthases to encode unnatural tryptophan amino acids into designer peptides. **A. Ohler**, C. Whittington, D. Murray, W.E. Allen, A.R. Offenbacher
- 575.** Photoacoustic thermometer: Shift in the photoacoustic signal frequency of ethene due to temperature variation. **J. Taylor**, H. Park
- 576.** Reaction between benzylboronic esters and alkyl halides. **R.W. Russell**, T.J. Barker
- 577.** Patterning conjugated polymer growth by microcontact printing. **I. Postle**, P.M. Lundin, B. Augustine
- 578.** Mechanistic investigation of the platinum-catalyzed acylation of 2-phenoxy pyridines. **J. Neu**, S. Huo
- 579.** *In vitro* glucuronidation of monobenzyl phthalate glucuronidation with UDP-glucuronosyltransferase 2B7. **T.D. Pentland**, J.W. Brock
- 580.** Studies into the mutagenic potential of 8-oxo-2'-deoxyguanosine with human polymerase kappa. **S. Zielinski**, M. Hamm

- 581.** Synthesis of a novel perfluoroalkyl(aryl) sulfonylimide (PFSI) monomer as a precursor for PEM fuel cells. **S.E. Garland**
- 582.** Modular synthesis of fluorescent probes for metal ion detection. **A.M. Hay**, T. Dowell, P.H. Mueller, N. Deifel
- 583.** Effects of replacing CP with indenyl on metal-to-metal charge-transfer in $CP_2Ti(C_2FC)_2$ complexes. **K.T. Nguyen**, E.E. Lane, J.A. Pienkos, P.S. Wagenknecht
- 584.** Multi-step electrodeposition of p-type metal chalcogenides as components of water splitting tandems. **B. McCloskey**, C. Harris
- 585.** Coordination chemistry, luminescence, and f-element extraction selectivity of a tripodal carbamoylmethylphosphine oxide-based ligand. **W.B. Larrinaga**, A. Martinez, E.J. Werner
- 586.** Incorporation of lignin-coated cellulose nanocrystals (L-CNCS) in poly(hydroxybutyrate) (phb)/poly(lactic acid) (PLA) blends and characterization by DSC and TGA. **D. Jackson**, A. Tucker, E.A. Mintz
- 587.** Synthesis, characterization, and fluorescence spectroscopy of new ligands and complexes. **B.M. Vaught**, T. Dowell, N. Deifel, P.H. Mueller
- 588.** Forensic application in determining the age estimation of documents using infrared spectroscopy. **P. Mickel**, J. McCutcheon
- 589.** Direct allylation of ketones with trimethylsilyl trifluoromethanesulfonate and triethylamine. **I. Zhong**, E. Heafner, A. Lin, C.W. Downey
- 590.** Synthesis of new cinnamaldehyde derivatives as anti-diabetic agents. **E. Reed**, P.I. Binda
- 591.** Nitrile aldol reactions mediated by trimethylsilyl trifluoromethanesulfonate. **S.R. Bottum**, K.M. Britt, C.W. Downey
- 592.** Binding of cucurbit[5]uril with alkali metal ions via ESI-MS. **J. Davison**, **J. Adebajo**, **A. Webb**, F.A. Khan
- 593.** Crossed Aldol reactions of aldehydes and subsequent styrene formation promoted by trimethylsilyl trifluoromethanesulfonate. **G. Dixon**, C.W. Downey
- 594.** Synthesis of chiral carboxylic acids from hydrocarboxylation of alkenes. **T. Smalls**, P.I. Binda
- 595.** One-pot furan synthesis from ketones and propargyl acetates. **D. Sklar**, C.W. Downey
- 596.** Binding studies of cucurbit[6]uril with alkali metal ions via ESI-MS. **M. Zhang-Smith**, **O. Basant**, **F. Ghiathi**, **B. Lonse**, **N. Scafidi**, **F.A. Khan**

597. Effect of the trifluoropropynyl ligand on emissive platinum complexes. **M.J. McCormick**, R. Hambrick, P.S. Wagenknecht

598. Identification of the function of protein 3L1W. **A. Nelson**, A.A. Carter, P.A. Craig

599. Synthesis of 5'-triphosphate-8-thio-2'-deoxyinosine, an analogue of 5'-triphosphate-8-oxo-2'-deoxyguanosine. **G.A. Leconte**, M. Hamm

600. Wound healing in space: Final frontier and the role of biomimetic polymers. **A. Walker**, S.K. Hamilton

601. Synthesis of colloidal gold aggregates for speckle patterning of mouse aorta. **S. Alford**, L. Du, S. Lessner

602. Crystal structure of phosphoethanolamine methyltransferase from *Eimeria tenella*. **B. Cox**, D. Etoroma, S. Lee

603. Synthesis of 1,2-diketones through platinum-catalyzed C-H functionalization. **J. Neu**, A. Hatch, S. Huo

604. Investigating the structures and properties of mixed silicon-copper, germanium-copper and germanium-gold clusters. **N.S. McKenney**, **A. Quang**, **J. Kobe**, J.T. Lyon

Savannah Marriott Riverfront
Chatham

Chemistry Education: Active Learning Methods

S. Verberne-Sutton, *Organizer. Presiding*

10:35 Introductory Remarks.

10:40 605. Gas chromatography relay: passing the baton from one laboratory student group to the next. **S. Verberne-Sutton**

11:00 606. Escaping from quant lab: Using competition and teamwork to build critical lab skills. **L.A. Hiatt**, H.B. Musgrove, W.M. Ward

11:20 607. Study for STARS (self-tracking, assessment and reflection study) in organic chemistry course: Time management project. **S.M. Landge**, I. Graves, K. Greer, J.N. Orvis

11:40 608. POGIL in the physical chemistry lecture and lab. **A.A. Carter**

MONDAY AFTERNOON

Savannah Marriott Riverfront
Chatham

Computational Chemistry Applied to Interesting Problems

Financially supported by Division of Computers in Chemistry (COMP), Journal of Chemical Information and Modelling (JCIM) and Furman University

G. C. Shields, *Organizer, Presiding*

12:45 609. Computational chemistry applied to interesting problems. **G.C. Shields**, T. Ball, A. Gale, T.T. Odbadrakh

1:15 610. Molecular studies of halogen bonding, protein dynamics and combustion. **C.A. Parish**

1:45 611. Noncovalent interactions in solution and crystals. **C.D. Sherrill**

2:15 612. New insights into the mechanisms of ubiquitin conjugating and ubiquitin ligase enzymes. **I. Sumner**

2:45 613. Adventures in DFT designing of organic electronic materials. **A.L. Tomlinson**

3:15 Intermission.

3:30 614. Toward a comprehensive predictive model of stacking interactions. **S.E. Wheeler**

4:00 615. Applications of computational chemistry to engineering problems. A. Miraz, C.D. Wick, **B. Ramachandran**

4:20 616. Unraveling the mechanism of polyethylene microstructure modulation using a redox-active Ni-based olefin polymerization catalyst. **R.C. Chapleski**, J. Kern, B.K. Long, S. Roy

4:40 617. Reproducible, rational, and rigorous QM-cluster enzyme models. **N.J. Deyonker**, Q. Cheng, T.J. Summers, M. Palma

Savannah Marriott Riverfront
Franklin

Advancements in Chemical Biology

Financially supported by Division of Analytical Chemistry; North Carolina State University and the University of Georgia

G. J. Williams, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 618. Biochemical mechanistic investigations to enable the synthetic biology of type I polyketide synthases. **C.B. Bailey**, E.E. Drufva, E.G. Hix, M. Curry

1:30 619. Harnessing actinomycete biosynthetic pathways to expand diketopiperazine chemical diversity. **A.L. Lane**

1:55 620. Investigating the transcript dependence of improved recombinant protein expression in *E. coli* with dynamic metabolic control. **J. Hennigan**, M. Lynch

2:10 621. Analysis and characterization of lanthipeptide gene clusters in *Salinispora*. **E. Limbrick**, S. Shah, C.G. Kittrell, D. Scott, M. Halbert

2:25 622. Dihydroxyacid dehydratases containing the [2Fe-2S] cluster are a promising antimicrobial target. **Y. Ding**

2:50 Intermission.

3:10 623. Engineered biosynthesis of non-natural polyketides and isoprenoids. **G.J. Williams**

3:35 624. Genetically encoded fluorescent sensors to illuminate cellular chloride signaling. **S. Dodani**

4:00 625. Small-molecule poly (ADP-ribose) polymerase (PARP) and PD-L1 inhibitor conjugates as dual-action anticancer agents. **S. Ofori**, S.G. Awuah

4:15 626. Pharmacologic modulation of ER protein folding to identify host/flavivirus interactions and inhibit viral propagation. **K. Almasy**, J. Davies, S. Lisy, R. Tirgar, S. Tran, L. Plate

4:30 627. Bioorthogonal probes of protein acetylation. **Y. Zheng**

Savannah Marriott Riverfront
Plaza

Advancements in Environmental Chemistry

Financially supported by Division of Environmental Chemistry
V. Anagnostopoulos, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 628. Sequestration of gadolinium in sediments of a constructed wetland. **M.J. Beazley**, A. Altomare

1:25 629. Environmental occurrence and fate of emerging contaminants from *Lyngbya wollei* blooms. **J.L. Ferry**, S. Putnam, M. Smith, T. Metz, M. Bodine, D. Westerman, G. Scott, T.J. Shaw, S.D. Richardson

1:45 630. Uranium immobilization in wetlands varies spatially and temporally in response to hydrogeochemical conditions. **D. Kaplan**, J.C. Seaman, C.J. Parker, B.A. Powell, E.J. O'Loughlin, P.B. Weisenhorn, K.M. Kemner, M. Boyanov

2:05 631. Role of proton-coupled electron transfers in energy efficient environmental restoration of oxyanion-contaminated waters: Example of chromate reduction. C.M. Stern, D.W. Hayes, L.O. Kgoadi, **N. Elgrishi**

2:25 632. Manganese oxide geochemical controls over Tc-99 fate in the environment: TcO₂ oxidative dissolution. J. Stanberry, I. Szlamkowicz, A. Grabe, **V. Anagnostopoulos**

2:45 633. Properties of surfactants in atmospheric aerosol and estuarine waters in coastal Georgia. **A.A. Frossard**, T. Burdette, R. Bramblett, A. Deegan, W.C. Hudson, K. Zimmermann

3:05 Intermission.

3:20 634. Mechanistic understanding of ozone-assisted oxidation reaction of trans-2-butene in a jet stirred reactor. **D.M. Popolan-Vaida**

3:40 635. Post-detonation fate and transport of radioactive debris. **A. Ladshaw**, Y. Kim, S. Yiacoumi, C. Tsouris

4:00 636. Influence of aging on the iodine adsorption capacity of reduced silver adsorbents. **A. Wiechert**, A. Ladshaw, Y. Nan, S. Choi, L.L. Tavlarides, J. Moon, C. Tsouris, S. Yiacoumi

4:20 637. Encapsulation of heavy metals from coal-fired generated wastewater. **M. Bansal**, G. Gupta, A. Kearns, T. Kalbfleisch, M. Ghorbanian

4:40 638. Peracetic acid fate and decomposition in poultry processing wastewater streams. J. Chen, **S.G. Pavlostathis**

Savannah Marriott Riverfront
Atrium

Inorganic Chemistry

Financially supported by Division of Inorganic Chemistry
W. E. Lynch, *Organizer*

1:00 - 2:30

- 639.** A study on the effect of steric hindrance on the reactivity of phosphinimine NCN-pincer complexes of nickel(II) with dibromomethane. **A. Eaton**, S. Pitts, G. Guillet
- 640.** Functionalization of porphyrinic metal organic-framework nanoparticle additives for enhanced reverse osmosis membrane performance. **B. Bonnett**, E. Smith, M. de la Garza, M. Cai, B.J. Gibbons, S. Martin, A.J. Morris
- 641.** Synthesis and utilization of polyoxometalate compounds as antimicrobial agents. **C.P. Hodges**
- 642.** Mapping the electronic structure of an iron(II) polypyridine complex with ligand-centered frontier orbitals. **H. Kwon**, E. Jakubikova
- 643.** Tailoring the electronic structure of corannulene-integrated crystalline materials. **G. Leith**, A.M. Rice, B. Yarbrough, N.B. Shustova
- 644.** Versatility and structural functionality of heterometallic metal-organic frameworks (MOFs). **O.A. Ejegbavwo**, M.D. Smith, D.A. Chen, N.B. Shustova
- 645.** Gallium(III) complexes with redox-active quinol-containing ligands as mimics of superoxide dismutase. **J.L. Moore**, J. McElroy, D.D. Schwartz, C.R. Goldsmith
- 646.** Electrochemical crystal growth of POM-based complex oxides. S. Hwu, **Q. Zhang**, **J. Ondus**
- 647.** Zirconium-based metal-organic frameworks as a platform for nuclear waste remediation. **V.A. Galitskiy**, **A. Berseneva**, N.B. Shustova
- 648.** Photophysics and electronic properties of photoswitchable frameworks. **C.R. Martin**, N.B. Shustova
- 649.** Comparative study of the ABTS redox indicator in various solvents. **K.J. Doheny**, S. Hematian
- 650.** Mitochondrial targeting cyclometallated Au(III) complexes bearing dithiocarbamate ligands: Synthesis, biological evaluation, and mechanistic insights. **R.T. Mertens**, S. Parkin, S.G. Awuah
- 651.** Porphyrin modified polyhedral oligomeric silsesquioxane molecules for the photodynamic therapy of cancer cells. **A. Johnston**, P. Loman-Cortes, P. Siano, J.L. Vivero-Escoto
- 652.** Extending the ³MICt state of osmium(II) tris-(2,2'-bipyridine) through encapsulation within zinc(II) trimesic acid metal-organic frameworks. **J.M. Mayers**, R.W. Larsen
- 653.** Heme/copper model complexes: Oxidative chemistry and mechanistic studies. **M.C. Carrasco**, H. Pourhadi, K. Dezarn, S. Hematian

- 654.** Guest to framework photoinduced electron transfer in a cobalt substituted Kullek type metal-organic framework. **C. McKeithan**, R.W. Larsen
- 655.** Pore modulation of guest photophysics in metal-organic framework: Photophysical studies of meso-tetra (n-methyl-4-pyridyl) porphine encapsulated within MOM-11 and MOM-12. A. Alanzi, L. Wojtas, **R.W. Larsen**
- 656.** Synthesizing and investigating the catalytic properties of (Cu(II)I)2Mn(II) complexes. **C. Wolfe**, N. Deifel
- 657.** Computational study of iron(II)-polypyridines as chromophores for dye sensitized solar cells. **G.M. Curtin**, E. Jakubikova
- 658.** Using salphenazine-type imidazoles in chemosensing for detection of [UO₂]²⁺ and other metal ions. **E.A. Hiti**, C.D. Tutson, E.E. Hardy, B.A. Maynard, A.E. Gorden
- 659.** Synthesis of novel bismuth containing oxides. **A.T. Hines**
- 660.** Photocatalytic hydrogen production via dual photon absorption pathway. **P. Ayare**, A.K. Vannucci
- 661.** Thermodynamic and structural characterization of Cd(II) and Ca(II) binding to EF-hand peptides by isothermal titration calorimetry and circular dichroism spectroscopy. **C. Taylor**, K. Byers, E. Karnik, A.M. Spuches
- 662.** Linear Cu^I₄ bis(amidates) as flexible molecular strings. **A. Calderon**, N. Maya, **C. O'Dea**, N. Bhuvanesh, C. McMillen, M. Stollenz
- 663.** New hexadentate bis(amidines) as flexible ligands for dichloro-dicopper(I) and -digold(I) complexes. **C. O'Dea**, O. Ugarte Trejo, **J. Arras**, N. Bhuvanesh, M. Stollenz
- 664.** Determination of the binding affinity of Cd(II) to Ca(II) bound human cardiac troponin C using isothermal titration calorimetry: Competition study. **A. Cunningham**, C. Palmer, K. Vang, A.M. Spuches, R. Johnson
- 665.** Developing new optical and magnetic materials. **A. Kaczmarek**, A.A. Dickey, M. Smart, C. McMillan, J.W. Kolis
- 666.** Redox inactive catalysts for aldehyde deformylation. **A.C. Saunders**, C. Burch, A. Scott, C.R. Goldsmith
- 667.** Characterizing the binding of Pb(II), Ca(II), and Cd(II) to EF-hand peptides III and IV of human cardiac troponin C and EF-hand peptide V of calbindin D_{28k} using circular dichroism spectroscopy. **A. Wilson**, C. Taylor, L. Bauza-Davila, K. Byers, A.M. Spuches

668. Study of electrocatalytic CO₂ reduction by nickel and copper complexes. **S. Saha**, A. Stephens, C. Richburg, M.R. Mazumder, B.H. Farnum

669. Synthesis and characterization of tri-iron, tri-cobalt, and nickel di-lithio complexes with 2,6-bis(trimethylsilylamino)pyridine. **K.Y. Arpin**, D.M. Elwell, G.L. Guillet

670. Hydrodeoxygenation of vanillyl alcohol by ruthenium pincer complexes. **W. Yao**, S. Das, A.K. Vannucci, E.T. Papish

671. Isolation of two novel polynuclear Mn₃ and Mn₇ clusters incorporating the anion of 4,5-bis(hydroxymethyl)-2-methylpyridin-3-ol. **K. Moncur**, A. Saha

672. Towards the synthesis of a metal sensor: Varying reaction conditions in the synthesis of silver nanoparticles with 8-hydroxy-5-quinolinesulfonic acid hydrate. **K.E. Ragland**

673. Existence of pnictide analogs of small nitrogen and phosphorus compounds: Review. **J.W. Hall**, T. Griffin, S. Hutchison

Savannah Marriott Riverfront
Ballroom E

New Forms of Carbon: Fullerenes, Metallofullerenes, Nanotubes & Graphene

Financially supported by President-Elect of the American Chemical Society
H. C. Dorn, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 674. New covalent reactions to tune the optical properties of single-wall carbon nanotubes. **R.B. Weisman**

1:35 675. Many faces of carbon. **P. Jena**

2:05 676. Molecular self-assembly on 2D materials studied by STM. **C. Tao**

2:35 677. Scrolling behavior of nanosheet materials. **T.T. Salguero**

3:05 Intermission.

3:25 678. Integration of fullerenes as electron-acceptors in 3D graphene networks. **M.R. Ceron**, C. Zhan, T.A. Pham, P.G. Campbell, L. Echegoyen, J. Biener, M.M. Biener

3:55 679. Fullerene-based triboelectric nanogenerators. **A. Rao**, P. Parajuli, H. Behlow

4:25 680. Interfacing with nano: Nanoengineering with interfacial chemistry. **J.R. Alston**, R. Goodwin, H. Harrison, J.E. Knoop, B. Sadiku, S.H. Huneycutt, S. Twiddy, T.D. Jones

Savannah Marriott Riverfront
Atrium

X-Ray in the Southeast

Financially supported by Division of Inorganic Chemistry and Rigaku Americas Corporation
W. E. Lynch, *Organizer*

1:00 - 2:30

681. X-ray study of the chemistry of lanthanide complexes with heteroaromatic N-oxides. C. Miller, K. Sheriff, m. Raymundo, W.E. Lynch, **C.W. Padgett**

682. A single-entity method to actively control the nucleation-crystal growth process (II) – electrical and optical signatures during lysozyme crystallization. **R. Yang**, G. Wang

683. Halogen bonding (XB) consortium in several iodide vs. triiodide cocrystals. **K. Kobra**, C. McMillan, W.T. Pennington

684. Halogen bonding as a route to new cocrystals and potential green solvents. **W. Gardner**, K. Kobra, R. Sachdeva, C. McMillen, W.T. Pennington

Savannah Marriott Riverfront
Forsyth

Ion Mobility-Mass Spectrometry: Adding a New Dimension to Omics Analysis

Financially supported by Agilent
C. D. Chouinard, *Organizer, Presiding*
L. Fenn, *Presiding*

1:10 Introductory Remarks.

1:15 685. Advanced structural mass spectrometry strategies in systems, synthetic, and chemical biology. **J.A. McLean**

1:40 686. Mapping structural diversity with TIMS-MS: From small molecules to protein complexes. **F. Fernandez-Lima**

2:05 687. Simplified sampling and characterization of THC and CBD using differential mobility spectrometry-mass spectrometry (DMS-MS). **I. Ayodeji**, T.G. Nguyen, L. Song, K. Evans-Nguyen, B. Musselman

2:30 688. Understanding circadian dysfunction in Alzheimer's disease: Cylindrins trigger peptide release in living suprachiasmatic nucleus brain slices. **T. Do**

2:55 Intermission.

3:15 689. Ozone-based methods for improved differentiation of steroid stereoisomers. S. Maddox, R.H. Fraser Caris, K. Baker, A. Burkus-Matesevac, **C.D. Chouinard**

3:40 690. Tandem-trapped ion mobility / mass spectrometry: Analysis of protein systems. **C. Bleiholder**

4:05 691. Mechanisms of sequential ion-molecule reactions in protonated methanol using mass spectrometry, *ab initio* methods, and statistical modeling. **J. Melko**

4:30 692. Exposomic applications of ion mobility-mass spectrometry: Development of analytical methods for emerging perfluoroalkyl substances (PFAS). **J. Dodds**, E.S. Baker

Savannah Marriott Riverfront
Mercer

Recent Advances in Green Metal Nanoparticle Synthesis & Applications

Financially supported by Division of Colloid and Surface Chemistry
B. B. Penland, *Organizer, Presiding*

1:10 Introductory Remarks.

1:15 693. Determining the role of intact proteins on green nanoparticle synthesis using *Verbascum thapsus*. **K.A. Trausch**, E.A. Waddell, J.J. Weimer, C.V. Nguyen, M. Thompson, A.M. Holmes

1:35 694. DNA conjugates with molecular silver clusters. **J.T. Petty**, J. Bush, S. Carnahan, D. Kim, D. Lewis

1:55 695. Chalcogenide nanocrystals for energy applications. **A. Gupta**

2:15 696. Morphologically controlled SiO₂ overcoating of Au nanorods and functionalization with Fe₃O₄ nanoparticles. W. Wu, B.S. Chapman, L.R. Rowe, **J.B. Tracy**

2:35 697. Out of the furnace: Synthesis and application of cellulose-derived carbon materials containing metallic nanoparticles. **C.D. Garcia**

2:55 Intermission.

3:15 **698.** Assembling nanoparticles with peptides: From static to dynamic nanoparticle superstructures. **N.L. Rosi**, Y. Zhou

3:35 **699.** Rationally-designed iron oxide nanoparticles for biomedical applications. **Y. Bao**

3:55 **700.** Designing amphiphilic peptoids for bio-inspired synthesis of hybrid materials. **C. Chen**

4:15 **701.** Sustainable fabrication of metal oxide nanomaterials for environmental remediation. **M.R. Knecht**

4:35 **702.** Nanotechnology enables hot gold nanorods to kill cancer cells and to stop alive sick cells from migrating to other places in the body. **M.A. El-Sayed**

Savannah Marriott Riverfront
Oglethorpe A

Structure-Based Drug Design

Financially supported by Cresset
R. J. Bienstock, *Organizer, Presiding*

1:15 Introductory Remarks.

1:20 **703.** Electrostatic complementarity, a powerful tool for drug design: Optimizing binding and selectivity of protein-ligand complexes. **R.J. Bienstock**, T. Cheeseright, M.R. Bauer, M.D. Mackey

1:45 **704.** Structural selection of immunomodulatory HLA binding small molecules. **D. Ostrov**

2:10 **705.** Allosteric modulation of the NMDA receptor: Identifying and exploring novel binding pockets. **P. Burger**, T. Kaiser, S. Kell, H. Kusumoto, G. Shaulsky, S. Bhattacharya, M. Epplin, K. Strong, E.J. Miller, B. Cox, D. Menaldino, S. Traynelis, D. Liotta

2:35 **706.** Identification of allosteric exosites on the cannabinoid CB1 receptor using grand canonical Monte Carlo simulated annealing and validation via mutation and SAR. **P. Reggio**

3:00 Intermission.

3:20 **707.** Structure-based drug design: When 3D-docking meets machine learning and dynamic protein-ligand interactions. **D. Fourches**

3:45 708. Integrating computational and experimental approaches for neglected disease drug discovery. **T. Lane**, V. Makarov, J. Nelson, J.S. Freundlich, S. Ekins

4:10 709. Effective way to apply AI to the design of new drug lead compounds. **S. Keinan**, W.J. Shipman, E. Addison

4:35 Concluding Remarks.

Savannah Marriott Riverfront
Oglethorpe B

WCC: Modern Issues for Women in Chemistry

S. Zingales, *Organizer*

D. W. Dixon, S. K. Hamilton, *Presiding*

1:15 710. Establishing a career mentoring network to support women in chemistry. **M.C. Srougi**

1:30 711. Influential and courageous mentorship in STEM. **K.S. Aiken**

1:45 712. Non-traditional careers and mentorship. **A. Weisbruch**

2:00 713. Mind the gap: Underrepresentation of women in chemistry and the impact of networking and mentorship in a woman's career. **S.K. Hamilton**

2:15 Panel Discussion.

3:00 Intermission.

3:30 714. Supporting female graduate students in STEM: Role of doctoral career training programs. **C.E. MacBeth**

3:45 715. Strategies for dealing with gender bias in STEM fields. **J.L. Brumaghim**

4:00 716. Raising the profile of women in chemistry. **D. Reeser**, A.T. Yarnell

4:15 717. Women in chemistry in the United States: From the past to the future. **D.W. Dixon**

4:30 Panel Discussion.

5:15 Concluding Remarks.

Savannah Marriott Riverfront
Reynolds

Diversity: Opportunities, Scholarships, Fellowships, & Internships

Financially supported by ACS Local Section Activities Committee, Coastal Georgia Local Section of the American Chemical Society, NOGLSTP.

R. A. Groom, B. P. Quillian, *Organizers, Presiding*

1:20 Introductory Remarks.

1:25 Panel Discussion.

2:00 718. National science foundation programs that support undergraduate chemistry education. **J.E. Lewis**

2:30 719. Opportunities as a Florida Georgia Louis Stokes Alliance for Minority Participation (FGLSAMP) fellow. **G. Rocabado**

3:00 Intermission.

3:25 720. NOGLSTP scholarship funds: Advancing LGBTQ+ students in STEM careers. **C.J. Bannochie**, R. Diamond, B. Belmont

3:55 721. Joining forces: McNair Scholars Program and National Science Foundation research experiences for undergraduates. **I. Taylor**

4:25 Discussion.

Savannah Marriott Riverfront
Ballroom C

Frontiers in Nucleic Acid Chemistry

D. P. Arya, N. Shank, *Organizers*

F. Leng, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 722. Peptide nucleic acids with backbone modifications to control binding and applications. **D.H. Appella**

2:05 723. Smart-responsive nucleic acid nanoparticles designed to modulate immune behavior. **K. Afonin**

2:35 724. Fluorescence imaging reagents based on RNA aptamers, synthetic polymers and fluorogenic cyanine dyes. **B.A. Armitage**

3:05 Intermission.

3:25 725. Investigating a disulfide linkage in the backbone of peptide nucleic acid. **N. Shank**

3:55 726. Enhanced nucleic acid recognition by small molecule-oligonucleotide conjugates. **D.P. Arya**

4:25 727. Examination of RNA-privileged small molecule chemical space and elucidation of important recognition properties. **S. Wicks**, B. Morgan, A.E. Hargrove

4:40 728. G-Quadruplexes in both subunits of the human ribosome. **S. Mestre-fos**, P. Penev, L.D. Williams

Savannah Marriott Riverfront
Pulaski

Polymeric Materials for the Next Generation Sensing, Diagnostics, & Therapy

Financially supported by Division of Polymer Chemistry
C. N. Scott, *Organizer*
D. L. Watkins, *Organizer, Presiding*

1:30 729. Theranostic microcapsules for imaging and ultrasound-triggered drug delivery. **E.P. Kharlampieva**

2:00 730. Polymer-functionalized optical nanosensors for diagnostics. **J. Budhathoki-Uprety**

2:15 731. Electrosynthesis and characterization of isoindigo based copolymers for use as NIR-II imaging agents. **N. Sparks**

2:30 732. Polymer modified magnetic colloids: Surface binding, colloidal stability, and added functionality. **O.T. Mefford**

3:00 Intermission.

3:15 733. Coating orthopedic implants with a polymer based pH sensitive layer to noninvasively image pH changes on the implant surface using X-ray excited luminescence chemical imaging. **U. Uzair**, P. Millhouse, M. Arifuzzaman, S. Beladi-Behbahani, T.J. Tzeng, J.N. Anker

3:30 734. Development of a high-temperature multi-composite reactor: Monodisperse nanoscintillators for noninvasive optogenetics. **E. Zhang**, A.A. Dickey, I. Bandera, I. Foulger, J.N. Anker, J. Ballato, J.W. Kolis, S.H. Foulger

3:45 735. Discrimination of seawater contaminants using conjugated polymers. **J. Tropp**, M. Ihde, M. Bonizzoni, J.D. Azoulay

4:00 Concluding Remarks.

Savannah Marriott Riverfront
Ballroom D

Strategy & Methods for Complex Molecule Synthesis

Financially supported by Division of Organic Chemistry
E. M. Ferreira, A. J. Grenning, *Organizers, Presiding*

1:40 736. New strategies for the C-H functionalization of amines. **D. Seidel**

2:10 737. Search for narrow-spectrum antibacterials & ways to access fluorinated molecules. **S. Roy**

2:40 738. Azetidine functionalization by transition metal and electrochemical methods. **J.B. Morgan**, K. Martin, D. Hill, E. Bostic, S. Scribner

3:00 Intermission.

3:20 739. Synthetic methodologies inspired by complex dimeric natural products. **S.M. Wilkerson-Hill**, A. Zahara, A. Nguyen

3:50 740. Photoredox catalysis in the undergraduate research laboratory: Synthesis, characterization, and application of carbazoles as single-electron reductants. **A.R. Longstreet**, M. Keller, T.D. Weinhold

4:10 741. Make allylation great again. **M. Chen**

4:40 742. Semisynthesis: Unexpected pathway to novel methodology development. **M.P. Croatt**

Savannah Marriott Riverfront
Ballroom B

Analytical Chemistry

Mass Spectrometry

C. McKenas, *Organizer, Presiding*

2:50 Introductory Remarks.

2:55 743. Quantification of 11 amino acids in human plasma using LC-MS/MS: Applications in the prediction of prediabetes. **A. Taylor**, D.E. Davis, G.S. Codreanu, J.M. Colby, C.C. Marasco, S.D. Sherrod, J.A. McLean

3:15 744. Enhanced protonation upon addition of chromium(III) during matrix-assisted laser desorption ionization mass spectrometry. **N. Dieke**, C.J. Cassady

3:35 745. Glucuronidation of Bisphenol A by UGT2B15 and possible inhibition by over-the-counter drugs. **H. Middlesworth**, J.W. Brock

3:55 746. Enhanced protonation due to chromium(III) during liquid chromatography-electrospray ionization mass spectrometry. **M. Mireles**

4:15 747. Temporal monitoring of MVOCs from *Macrophomina phaseolina* using HS-SPME GC/MS. **C. Gamlath Mohottige**, T.E. Mlsna, R. Baird

4:35 748. Determination of pesticide residues in vegetable samples. **D. Cook**, C.H. Lisse

4:55 Concluding Remarks.

Savannah Marriott Riverfront
Atrium

Organic Chemistry

X. Chen, *Organizer*

3:00 - 4:30

749. Synthesis of immune modulating benzofuran-2-carboxylic acid derivatives. **D. Still**, S. Lidge, A. McAdory, K.S. Marriott

750. Utilizing α -aminocycloalkylcopper reagents to synthesize 1,2,3,4-tetrahydroquinoline alkaloids and derivatives. **Z. Bertoli**, A. Ahmed, C.W. Alexander

751. Enantioselective rhodium-catalyzed dearomative addition of boronic acids to aromatic nitrogen heterocycles. **D.J. Robinson**, R. Karimov

752. Identification and characterization of biocatalysts for synthesis of the Wieland-Miescher ketone. **M.P. Patel**, R.M. Hughes

753. Synthesis of novel diazonium N-(perfluoroalkyl) benzenesulfonimide polymer for use in proton exchange membrane fuel cells. **J. Marshall**

- 754.** Exploration of silicon phthalocyanines as viable photocatalysts for organic transformations. **S. Dickerson**, S. Wiskur
- 755.** Synthesis and conformational analysis of aza-peptide β -hairpin analogs. **P. Gourville**, E. Willis, M. McMechen, C. Proulx
- 756.** Investigation of the reaction of monochloramine and 2,6-dichlorophenol as a model for the purification process of drinking water. **N.M. Bauer**, S. Smith, D. Zoetewey
- 757.** Extensive alignments of atomic orbitals in the substrate-binding strands of HIV-1 protease mutant ASP25ASN. P. Little, **J.N. Haseltine**
- 758.** Repurposing nTZDpa: Antimicrobial effective against growing and persistent *Staphylococcus aureus*. A. Steele, E.E. Csatory, **M. Dekarske**, W.M. Wuest
- 759.** C-H functionalization of five-membered heteroarenes with aryl halides using carbazole as photocatalysts. **T.D. Weinhold**, A.R. Longstreet
- 760.** Substituted [3]-radialene dianions as catholytes for energy storage. **N.A. Turner**, C. Bejger, M. Freeman
- 761.** Synthesis and complexation of boronic acid derivatives with N-oxides. **H. Kline**, **K.S. Thomas**, W.R. Kwochka
- 762.** Synthesis and characterization of new albuterol double salt ionic compounds. **J. Thorn**, O.A. Cojocar
- 763.** Epoxy isonitriles, a unique class of antibiotics: Synthesis of their metabolites and biological investigations. **I. Wilt**, G. Ernouf, S. Zahim, W. Wuest
- 764.** Increased organoid nutrition using TPG as a dynamic natural collagen analogue. **M. Nayak**
- 765.** Improving student knowledge of GC-MS through analysis of electronic cigarettes in organic chemistry. **P. Patel**, K. Conrad, A. Pathirana, L.A. Hiatt
- 766.** Adsorption of juglone free acid and its tetrabutylammonium derivative on hydrophilic mesoporous silica. **R. Paris**, T.W. Majors, O.A. Cojocar
- 767.** Drug delivery of naringenin to adipocytes using ultrasmall superparamagnetic iron oxide nanoparticles (USPIO). **N. Naren**, M. Drammeh, T. Fields, S. Rayalam, A. Singh, V.V. Mody
- 768.** Dual red and near infrared emitting charge transfer probe for detection of serum albumin. **R. Choudhury**
- 769.** Enantioselective ring opening of epoxides with anilines. **D. Jefferson**, J.B. Morgan

770. Developing biocompatible thiol-ene coupling conditions. **W.A. LeFever**, A.J. Wommack
771. Oxidation reaction screening of tricyclic ketones towards the synthesis of furan-bridged medium-sized rings. **E. Prester**, **N. Brandau**, P. Wiget
772. Application of a visible light-catalyzed [2+2] photocycloaddition to the synthesis of natural products containing medium-sized rings. **J.A. Rein**, M.E. Daub
773. Quantitative study of Van der Waals interactions in organic solvents using N-arylimide molecular balance. **S.M. Strickland**, E.C. Vik, P. Li, K.D. Shimizu
774. Metal catalyzed coupling in the synthesis of bis-*para*-anisyl alkanes. **A. Pampu**
775. Mild & efficient solid phase synthesis using cesium carbonate. **L. Kline**
776. D- γ -tocotrienol: Promising radioprotective agent isolated from palm oil. **K. Fobi**, R. Mohseni, J.A. Hyatt, A.G. Shilabin
777. Synthesis and virtual screening of novel acridone derivatives as potential topoisomerase II α catalytic inhibitors. **A.S. Oyedele**, C.O. Okoro
778. Search for highly selective and potent CB1 and CB2 inhibitors: Synthesis and characterization of (s,e)-11-[2-(thionylmethylene)hydrazono]-pbd. **K. Kankam**, A.G. Shilabin
779. Investigating the importance of binding pocket size for nerve gas binding to rhodamine-b derivatives. **Z. Reynolds**, A. Rich, Y. Cai, D.E. Wheeler, J. Bates, A.J. Weerasinghe
780. Synthesis of ionic liquids. **B. Cork**, J. Hamlin, M. Montilus, C. Tirla
781. Synthesis of cyclopropane aminoisoquinolines as highly selective kinase inhibitors. **H.M. Gordhan**, C. Lichorowic, J.M. Sturdivant, M.A. DeLong, D. Ellis, C. Daphne, S. Miller, K. Vick
782. Design, synthesis and biological evaluation of imidazo[2,1-*b*]oxazole derivatives as ^{V600E} BRAF kinase inhibitors acting as melanoma therapy. **E.M. Ali**, M.S. Abdel-Maksoud, U.M. Ammar, K.I. Mersal, C. Oh
783. Aryl ring modifications of sphingosine kinase 2 selective inhibitors. **C. Sibley**, Y. Kharel, A. Brown, D.R. Bevan, K.R. Lynch, W.L. Santos
784. Development and characterization of organic photoredox catalysts. **M. Bobo**, A.K. Vannucci
785. Carolacton-inspired analogs for CH functionalization and biological exploration. **E. Shaw**, A. Diaz, T. Hari, A. Scharnow
786. Using enyne metathesis to reterminate ROMP. **A. Irvin**

787. Tetraarylphosphonium/tetrakis(pentafluorophenyl)borate (TAP^R/TFAB) salts as non-aqueous electrolytes for organic redox flow batteries. **J. Bibbs**, G. Mandouma

788. Transmission μ -FTIR of unconventional source rocks using improved thin section preparation methods for monitoring changes in kerogen chemistry. **J.L. Brothers**, D. Jacobi, S. Althaus, S. Eichmann

789. Purifying complex reaction mixtures via high-performance flash chromatography. **J.R. Bickler**

790. Elucidation of greener chemistry methods on the synthesis of O-methyl resveratrol derivatives. **W.K. Myers**, D. Abramovitch

791. Design and synthesis of EF-24 analogs as anti-cancer agents. **R. Smith**

792. Modeling reactive intermediate analogues of gold(I)-catalyzed reactions by Lewis acid mediated gamma-ionization. **N. Kim**, R. Widenhoefer

Savannah Marriott Riverfront
Ballroom C

Plenary: John Laurence Busch

B. D. Feske, *Organizer, Presiding*

5:10 793. Corrosion Presentation: Building the First "Steamship" in History. **J. Busch**

TUESDAY MORNING

Savannah Marriott Riverfront
Oglethorpe B

Advancements in Mechanistic Enzymology

J. M. Miller, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 794. Temperature dependent kinetic isotope effects reveal the origins of lipoxygenase C-H activation efficiency. **A.R. Offenbacher**, J. Klinman, B.M. Hoffman

8:25 795. Combined solution and crystal methods reveal the electrostatic tethers that provide a flexible platform for replication activities in the bacteriophage T7 replisome. **J. Wallen, B. Foster, D. Rosenberg, H. Salvo, K.L. Stephens, B.J. Bintz, M. Hammel, T. Ellenberger, M. Gainey**

8:45 796. Conformational dynamics of G protein-coupled receptors: One receptor at a time. **R. Lamichhane**

9:05 797. Molecular mechanisms of enzyme catalyzed protein unfolding and translocation by class 1 AAA+ motors. **A.L. Lucius**

9:25 798. Temperature dependence of conformational heterogeneity of enzyme thermolysin. **M. Dong, B.J. Bahnson**

9:45 799. Hydrogen peroxide activated estrogen receptor beta ligands. **J.A. Pollock**

10:05 Intermission.

10:20 800. Insights to a structure-based catalytic mechanism from neutron and X-ray crystallographic structures of the *Thermococcus thioreducens* inorganic pyrophosphatase. **J.D. Ng**

10:40 801. Radicals, switches, and a protein-based cofactor: Expanding the catalytic abilities of an old active site. **D.C. Goodwin**

11:00 802. Oxidative stress promotes altered YME1L conformational dynamics. C. Brambley, **J.M. Miller**

11:20 803. AAA ATPase AFG1 helps maintain protein homeostasis in the mitochondrial matrix. **J.L. Fox, E.M. Germany, N. Zahayko, M.L. Huebsch, V. Prahlad, O. Khalimonchuk**

11:40 804. Sequestered imine intermediate and interplay of nucleophilic catalysis with proton transfer during reduction of nitrile to amine by the nitrile reductase QueF from *Escherichia coli*. **J. Jung, B. Nidetzky**

Savannah Marriott Riverfront
Forsyth

Biodegradable Polymers: Recent Innovations & Applications

Financially supported by Division of Polymer Chemistry and Malvern
P. I. Binda, H. Zhao, *Organizers*
P. Binda, *Presiding*

8:00 Introductory Remarks.

8:05 805. Synthesis of functionalized biodegradable poly(α -methylene- γ -butyrolactone). **P.I. Binda**

8:25 806. Bio-based composites with enhanced matrix-reinforcement interactions from the polymerization of α -eleostearic acid. A. Murawski, **R.L. Quirino**

8:50 807. Hydrogel stabilized, fully organic, X-ray radioluminescent crystalline colloidal arrays. **H.W. Jones**, I. Bandera, S.H. Foulger

9:10 808. Synergistic effects of potassium dimethyl 5-sulphonatoisophthalate (LAK-301) and lignin coated cellulose nanocrystals (L-CNCS) on the nucleation and crystallization of poly(lactic acid) (PLA). **R. Ford**, W. Simmons, R. Lumpkin, E.A. Mintz

9:30 809. Preparation and characterization of poly(lactic acid) (PLA) and poly-3-hydroxybutyrate (PHB) polymer matrix nanocomposites prepared with bio-based, biodegradable cellulose/lignin nanofillers. **E.A. Mintz**

9:55 Intermission.

10:10 810. Bio-based antimicrobial coating. **W. Ming**

10:35 811. Enzymatic synthesis of polylactide in ether-functionalized ionic liquids. **H. Zhao**, L. Afriyie, N. Larm, G.A. Baker

10:55 812. Multifunctional polyacrylates with reducing properties in biomedical applications. K. Thomas, A.K. McMahan, M.E. Michaud, A. Diaz, N.Z. Singleton, O. Alomainy, **H.J. Schanz**

11:20 813. Physical insights on mechanism of photoinduced charge transfer & charge recombination transfer via internal acceptors in n,n'-dialkylaniline organic dyes: Computational approach. **J.K. Roy**, J.R. Leszczynski

11:40 814. Preparation and characterization of poly(lactic acid) nanocomposites incorporating lignin-cellulose nanocrystals (SL-CNCS) prepared by sulfuric acid hydrolysis. **Z. Barnes**, G. Schueneman, U. Agarwal, E.A. Mintz

Savannah Marriott Riverfront
Reynolds

Diversity: Experiences & Initiatives

Financially supported by ACS Local Section Activities Committee, Coastal Georgia Local Section of the American Chemical Society, NOGLSTP.

R. A. Groom, B. P. Quillian, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 Panel Discussion.

8:35 815. The ARC network: Driving change through an empowered virtual community. **R.L. Williams**

9:05 816. Starting a SACNAS chapter at the University of South Florida. **G. Rocabado**

9:35 817. Transgender and gender non-binary STEM students: Academic climate and persistence. **M. Mayberry**, M. Hughes Miller, C.A. Smith, R. Campbell, H. Wao

10:05 Intermission.

10:30 818. Out of the closet and into the chemistry classroom: Importance of visibility. **J.R. Raker**

11:00 819. Increasing diversity in chemistry and physics graduate programs by focusing on best practices in inclusion and recruitment. **S.E. York**, E. Tanebaum, L. Ritzow

11:30 Concluding Remarks.

Savannah Marriott Riverfront
Plaza

Incorporating Research into the Analytical Curriculum

Financially supported by Division of Analytical Chemistry
C. R. Dockery, G. E. Potts, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 820. Student projects in the quantitative analysis laboratory. **L. De La Garza**

8:25 821. Project-based integrated lecture and laboratory upper division analytical chemistry curriculum. **D. Budner**, B.K. Simpson

8:45 822. Bioanalytical chemistry: Classroom undergraduate research experience. **J.G. Forsythe**, **M.W. Giuliano**

9:05 823. Incorporating current events in the undergraduate analytical chemistry laboratory. **C.R. Dockery**

9:25 824. How clean is the water: Student designed analytical lab project. **J.J. Weaver**

9:45 825. Measuring mass percent calcium in *E. carinifera* and *E. modesta* gastropod shells: Pilot course-embedded undergraduate research experience for analytical chemistry laboratory. **K.**

Zimmermann, X. Li, W. Huang, R. Simmons, M. Kirberger, H. Guan, S. Mwangela, C. Brown, R. Fiorillo

10:05 826. Using nanoparticles in undergraduate research to teach analytical techniques. **B.B. Penland**

Savannah Marriott Riverfront
Mercer

Inorganic Chemistry

General

Financially supported by Division of Inorganic Chemistry
W. E. Lynch, *Organizer*
M. Lufaso, *Presiding*

8:00 Introductory Remarks.

8:05 827. Flux crystal growth and characterization of new oxides containing early transition metals. **D. Carone**, H. Zur Loye

8:25 828. CsFeGeO₄: Non-centrosymmetric ABW-zeotype iron germanate grown from molten alkali halide flux. **M. Usman**

8:45 829. Design and electronic exploration of crystalline corannulene-integrated materials. **G. Leith**, N.B. Shustova

9:05 830. Photophysics control by confinement environment: Cage, MOF, and COF. **A. Berseneva**, N.B. Shustova

9:25 831. Crystal growth, structures and properties of inorganic fluorides and oxyfluorides. **G.B. Ayer**

9:45 832. Single source precursor route to isolate controlled metal carbide and metal nanocrystals. **E.T. Nguyen**, D.A. Hardy, G.F. Strouse

10:05 Intermission.

10:20 833. Chemical substitutions and structure-property relationships of bismuth mixed-metal oxides. **M. Lufaso**

10:40 834. Oxygen, carbon dioxide and carbon monoxide sensing properties of oxygen-deficient perovskites, aa'bb'o_{6-δ} (a = Ca, Sr; b = Fe; b' = Fe, Mn). **S.B. Karki**, F. Ramezanipour, R.K. Hona

11:00 835. Experimental and theoretical studies on lithium-ion conductivity of novel layered perovskites $\text{Li}_2\text{LaMTiO}_7$ ($m = \text{Ta}$ and Nb). **S.J. Fanah**, F. Ramezanipour, M. Yu, A. Huq

11:20 836. X-ray excited luminescence studies of rare earth oxide nanospheres as a potential light source for optogenetics. **A.A. Dickey**, E. Zhang, S.H. Foulger, J.W. Kolis

11:40 837. Synthesis and characterization of rare earth uranium sulfides. **L. Breton**, H. Zur Loye

Savannah Marriott Riverfront
Ballroom E

New Forms of Carbon: Fullerenes, Metallofullerenes, Nanotubes & Graphene

Financially supported by President-Elect of the American Chemical Society
H. C. Dorn, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 838. Nanoparticle fullerene is a stellar candidate for treatment of back pain. **L. Jin**

8:35 839. Functionalization and polymerization of fullerenes. **H.W. Gibson**, H. Wang, D. Schoonover

9:05 840. Fullerene-based nanomaterials for cancer diagnosis and therapy. Y. Peng, **T. Cai**

9:35 841. Regioselective multi-addition reactions for endohedral metallofullerenes. **J. Zhang**, Y. Li

10:05 Intermission.

10:20 842. Density functional theory investigation of fulvene derivatized fullerenes as candidates for organic solar cells. **T.J. Fuhrer**, J. Snelgrove, G.J. Balaich, S.T. Iacono

10:50 843. Synthesis and characterization of terbium containing endohedral metallofullerenes. **J.C. Duchamp**, X. Lui, M. Roy, M.M. Olmstead, A.L. Balch, H.C. Dorn

11:20 844. Study of dual modality anti-oxidant and fluorescent properties for terbium endohedral metallofullerenes derivatives. **R. Huang**, L. Xiao, C. Li, L. Jin, X. Li, H.C. Dorn

11:50 845. Preparation of red emissive carbon dots for biomedical applications. **K.J. Mintz**, R.M. Leblanc

Savannah Marriott Riverfront
Academy

Physical Chemistry

Computational

C. W. Padgett, *Organizer, Presiding*

8:00 846. RPA renormalized perturbation theory applied to the asymmetric Hubbard dimer. **J.E. Bates**, J.A. Derteano

8:20 847. Classical-wave based simulation of chemical reaction dynamics: Avoiding the curse of multi-scale time problems in MD simulation. **B.K. Dey**

8:40 848. Thermodynamic and modeling study of cyclopropane adsorbed on graphite. **C.A. Crain**, J.Z. Larese

9:00 849. QM level investigation into binding of aromatic and non-aromatic ionic liquid cations to active site of cytochrome P450 employing DFT calculations. **A. Banerjee**, J. Shah

9:20 850. Computational investigations of the structure and bonding of group IV allenylidenes $CP_2M=C=C=CH_2$. **D.A. Clabo**, H.F. Schaefer

9:40 851. Molecular structures and energetics of small copper, silver, and gold nanoclusters. **R. Persaud**, Z. Fang, M. Chen, D.A. Dixon

10:00 Intermission.

10:20 852. Understanding the complex adsorption equilibria of small alkanols on $SrTiO_3(001)$ using density functional theory. **R.C. Chapleski**, S. Roy, B. Doughty

10:40 853. Structures and properties of mixed metal / metalloid clusters. **J.T. Lyon**

11:00 854. ^{13}C fractionation during aqueous alanine transamination. **A.S. McNeill**, B. Dallas, J. Eiler, D.A. Dixon

11:20 855. Thermochemistry of phase-changing borane containing hydrogen storage materials. **M.P. Confer**, H. Burnham, S. Street, D.A. Dixon

11:40 856. Heterogeneous oxidation of aqueous organic aerosols by OH radical. **T.w. Masaya**

Savannah Marriott Riverfront
Oglethorpe A

Spectroscopic Imaging: Bridging the Gap between Chemical & Spatial Heterogeneity

A. Ghosh, *Organizer, Presiding*

8:00 Introductory Remarks.

8:10 857. Nanoscale spectroscopy and chemical imaging with conventional and with nanophotonic AFM probes. **A. Centrone**

8:40 858. Monitoring charge transfer in thin films and single crystals with femtosecond stimulated raman microscopy. **R.R. Frontiera**

9:10 859. Near-field optical spectroscopy for the study of electronic properties in semiconducting nanostructures. **J. Atkin**

9:40 860. Applications of nanoscale functional imaging to reveal the role of heterogeneities in complex systems for sustainable energy applications. **L. Tetard**

10:10 Intermission.

10:30 861. Hyperbolicity and polaritonic strong coupling: Towards enhancing IR sensing and imaging platforms. **J.D. Caldwell**, T. Folland

11:00 862. Infrared spectroscopic imaging of microplastic contamination <20u. **C.A. Marcott**, J. Anderson, F. Weston, M. Kansiz, R.C. Hale

11:30 863. Investigating chemical heterogeneities in organohalide perovskites with multiscale infrared imaging. **A. Ghosh**

Savannah Marriott Riverfront
Pulaski

Advancing Infrared Spectroscopic Techniques & Vibrational Sensing

Infrared Polaritons

Financially supported by Piketec GMBH; Neaspec GMBH; MKS Spectra Physics
J. D. Caldwell, *Organizer*
L. E. Buchanan, *Organizer, Presiding*

8:10 Introductory Remarks.

8:15 864. Nonlinear phonon polariton spectroscopy and microscopy. **A. Paarmann**

8:45 865. Doped semiconductors as components in infrared plasmonic systems. **S. Law**

9:15 866. Exploring and exploiting the properties of highly anisotropic media with infrared spectroscopy. **T.G. Folland**, J.D. Caldwell

9:45 867. Active tuning of phonons and surface-phonon polariton resonances. **A.D. Dunkelberger**, C. Ellis, D. Ratchford, A. Giles, S. Katzer, V. Breslin, A. Grafton, M. Kim, C.S. Kim, I. Vurgaftman, J. Tischler, J. Owrutsky, J.D. Caldwell

Savannah Marriott Riverfront
Ballroom D

Astrochemistry in the Southeast & Beyond

Laboratory/Theoretical Astrochemistry & Beyond

R. C. Fortenberry, *Organizer, Presiding*

8:10 Introductory Remarks.

8:15 868. Far-infrared synchrotron spectroscopy of some important interstellar molecules. **P. Raston**

8:45 869. Tools to rapidly assign the rotational spectra of molecules in vibrationally excited states. **S.T. Shipman**

9:15 870. Rovibrational Spectroscopy of magnesium acetylide (MGCCH) and its detection in the interstellar medium. **N.J. Deyonker**, J.E. Burns, Q. Cheng, R.C. Fortenberry, L.M. Ziurys

9:45 871. Interstellar inheritance of primitive bodies in the solar system. **S.N. Milam**

10:15 Intermission.

10:35 872. Infrared spectroscopy of hydrogen molecular ions and their clusters. **M.A. Duncan**

11:05 873. Challenges and opportunities in the investigation of astrochemical surface chemistry. **H.L. Abbott-Lyon**

11:35 874. *Ab initio* predictions for the formation of SO_x and NO_x based Brønsted acids with atmospheric and astrochemical implications. **Z. Lee**, S. Zhang, L.A. Flores, D.A. Dixon

Savannah Marriott Riverfront
Chatham

Environmental Chemistry

General

W. E. Lynch, *Organizer*
R. C. Wingfield, *Presiding*

8:10 Introductory Remarks.

8:15 875. Effects of nutrient overload and environmental conditions on algal bloom formation: Case study of private ponds in Madison County, Kentucky. **L.N. Sutton**, C.J. Tran

8:35 876. Strategies toward industrial paints with improved safety- and eco-profiles: Design of high-performance polymers for imetal coating applications. **D.N. Haase**

8:55 877. Rapid removal of emerging pharmaceutical contaminants from aqueous solution by adsorption on magnetized Douglas fir biochar. **A. Liyanage**, S. Canaday, T.E. Mlsna

9:15 878. Multi-pronged strategy for treatment of emerging and conventional persistent organic contaminants in real wastewater by electroperoxone. **R. Srinivasan**, I. Nambi

9:35 879. Pattern-based recognition of environmental pollutants using simple optical spectroscopic measurements. **M. Bonizzoni**, M. Ihde, Y. Xu, X. Liang

9:55 Intermission.

10:15 880. Preparing vulnerable populations for the impacts of climate change: Family/community emergency preparedness and resiliency. **R.C. Wingfield**, V. Watson

10:35 881. Removal of molybdenum from water using Douglas fir biochar/iron oxide nanocomposites. **N. Das**, C. Navarathna, K. Lee, C.U. Pittman, T.E. Mlsna

10:55 882. Periodic table-based descriptors for chemometric modeling of toxicity of metal oxide nanoparticles: Exploration of toxicity mechanisms to multiple species. **S. Kar**, P. De, K. Roy, J.R. Leszczynski

11:15 883. Assessing Latin American *Guadua chacoensis* bamboo biochar and activated magnetite analogues for aqueous arsenic(V) remediation. **C. Navarathna**, J. Alchouron, C.U. Pittman, T.E. Mlsna

11:35 884. Liquid crystal electrode-assisted hybrid bio-electrochemical treatment technology: Sustainable approach towards biofilm enhancement and wastewater treatment. **R. Srinivasan**, I. Nambi, J. Senthilnathan

Savannah Marriott Riverfront
Ballroom C

Frontiers in Nucleic Acid Chemistry

D. P. Arya, F. Leng, *Organizers*
N. Shank, *Organizer, Presiding*

8:15 885. Base pair sequence and minor groove shape in the design of mixed sequence DNA-binding agents. **W. Wilson**, A. Paul, P. Guo, A. Farahat, N. Harika, A. Kumar, D.W. Boykin

8:45 886. Targeting the mammalian high mobility group protein AT-hook 2 for drug discovery. **F. Leng**

9:15 887. Sequence-dependent DNA minor groove recognition by an extended heterocyclic dication. V.L. Ha, N. Erlitzki, A.A. Farahat, A. Kumar, D.W. Boykin, **G. Poon**

9:45 888. Mechanisms and specificity of Cas10 mediated interference. M. Nasef, F.C. Walker, S.J. Rowe, A. Hatoum-Aslan, **J.A. Dunkle**

10:15 Intermission.

10:35 889. Design and use of oligonucleotide substrates to probe the mechanism and inhibition of type IA topoisomerases. **Y. Tse-Dinh**

11:05 890. Targeting breast and prostate cancer cells with DNA-methylating molecules bearing nuclear receptor targeting ligands. **S. Varadarajan**

11:35 891. Mixed DNA sequence binding compounds: Promising approach to convert “undruggable” DNA targets to “druggable” receptors. **A. Paul**, P. Guo, A. Kumar, A. Farahat, D.W. Boykin, G. Poon, W. Wilson

Savannah Marriott Riverfront
Ballroom B

Relating Research to Community

K. Marriott, *Organizer, Presiding*

8:15 Introductory Remarks.

8:20 892. Structure-antioxidant correlations of heterocyclic thioether derivatives of carvacrol and thymol. **G.E. Henry**

8:40 893. Protein-protein networking: Discovering mitochondrial metabolic disease pathways. **M. Prasad**

9:00 894. Sigma-1 receptors in mitochondrial steroid synthesis: Potential new therapeutic target. **V. Thapliyal**

9:20 895. Chemistry research: Making bonds in your community. **K.S. Marriott**

9:40 896. Communicating chemistry through the local cuisine and beyond. **K.M. Jackson**

10:00 897. Challenges, methodologies, and benefits associated with community-based participatory research. **B. Lian**

Savannah Marriott Riverfront
Franklin

Heterocyclic Chemistry in the Southeast & Beyond

Financially supported by ViiV Healthcare

Q. Wang, *Organizer*

C. E. Stephens, *Organizer, Presiding*

8:20 Introductory Remarks.

8:25 898. Decarboxylative amination of redox-active esters using diazirines. **J.M. Lopchuk**

8:45 899. Access to and derivitization of heterocycle-rich sulfamate esters and sulfamides. **J.L. Roizen**, A. Kanegusuku, J.M. Blackburn, R.T. Simons, G. Scott

9:05 Intermission.

9:15 900. Functionalized benzo-fused heteroaromatics via metal-catalyzed cascade benzannulations. **S.A. France**

9:35 901. Native chemical ligation: Potential synthetic strategy for drug development. **S.S. Panda**

9:55 Intermission.

10:15 902. Cabotegravir: Playing the long game to combat HIV. B.A. Johns, **E. Velthuisen**

10:35 903. Cycloadditions using photocatalysis based on earth-abundant metals with heterocyclic ligands. **E.M. Ferreira**

10:55 Intermission.

11:05 904. Photoassisted synthesis of structurally complex natural products. **J. Frederich**

11:25 905. Copper-catalyzed amino difunctionalization of alkenes using nitrogen-heteroatom bonds. **Q. Wang**

Savannah Marriott Riverfront
Atrium

Undergraduate Posters

Financially supported by American Chemical Society and the Coastal Georgia Local Section of the ACS

M. Weiland, *Organizer*

8:30 - 10:00

906. Functional dynamics of human cyclophilin. **F. Ahmed**

907. Synthesis of hydroxyl polyester for medical and pharmaceutical applications. **S. Buteaux**, P.I. Binda

908. Expression and purification of the R367H mutant of bovine nitric oxide synthase III oxygenase domain.. **S. Jacobson**, A. Lesmes Ortega, C. Lloyd, M.L. Huebsch, H.G. Addis, J.L. Fox, A. Rogers

909. Using M062X/aug-cc-pVTZ model chemistry to study the lowest energy isomers of sulfuric acid-water clusters. **S. Smith**

910. Synthesis of diphenyl oxalates used for testing the chemiluminescence characteristics of multiple fluorophore dyes. **R. Aldaghir**

911. Progress towards a micro-structured Stark quadrupole guide. **J. Bracewell**, L. Duffy

912. Synthesis, characterization, and biological analysis of opioid peptides and cyclic derivatives containing a Sonogashira linkage. **T.L. McGomery**, **A.L. Williams**, J.C. Ouellette, M. Goertzen, S. Majumdar, K.R. Wilson

913. Serum stability of opioid peptides incorporating a Sonogashira cyclization. **A.L. Williams**, **T.L. McGomery**, J.C. Ouellette, M. Goertzen, S. Majumdar, K.R. Wilson

914. Molecular modeling of the opioid peptide DPDPE and a derivative of this peptide containing a unique sonogashira cyclization. **J.C. Ouellette**, A.L. Williams, T.L. McGomery, S. Majumdar, K.R. Wilson

915. Squalene hopene cyclase from *Alicyclobacillus acidocaldarius* as a biocatalyst. **J. Carter**, D. Weber, J. Perry Cecile

916. Multimer networks for recyclable materials. **M. Bardot**, B.R. Elling, W.R. Dichtel

917. Solubility of select azolium compounds. **C.A. Rose**, J.M. Meyers

- 918.** Synthesis of transition metal-based catalyst using functionalized nanoclay for oxidation reactions. **M. Kent**, C. Freeman, S.M. Landge
- 919.** Investigation of amine substituted 4-oxazolidinones and their biological activity. **C. MacAllister**, B. Frohock, K. Robinson, J.G. Pierce
- 920.** Quantitative analysis of the components of gun shot residue (GSR) deposited at various distances using different caliber firearms. **A. Wilcox**, S.E. Hooper
- 921.** Immobilized metal affinity chromatography polymeric high internal-phase emulsion foams for protein purification. **S. McDonald**, J. Pribyl, K.B. Wagener
- 922.** Achieving chemiluminescence with dyes isolated from natural products. **A.H. Horchar**, A. Barrientos Solis, E. Sarver, S. Komma, N. Park, A.G. Glenn
- 923.** Utilizing chemiluminescence for metal detection in tap water. **T. Jones**, M. Ali, K. Weatherspoon, K. Soma, C. Mesa, A.G. Glenn, D.W. Millican
- 924.** Second-generation kappa opioid agonist as a peripherally-restricted analgesic in the ProNeura platform. **E. Schneider**, T. Beck, T. Dix
- 925.** Microwave-assisted synthesis of zinc oxide nanoparticles using diethylene glycol as the surface capping ligand. **L. LaPlant**, C.R. De Silva
- 926.** Microwave-assisted synthesis of europium-doped calcium fluoride nanoparticles for potential biomedical applications. **W. Garabedian**, C.R. De Silva
- 927.** Synthesis and characterization of Si(bzimpy)₂ analogs for application within organic light emitting diodes. **K.E. Norman**, M. Kocherga, T.A. Schmedake
- 928.** Toward the stereoselective synthesis of olefins. **T. Ramsey**, N.N. Shaw
- 929.** Detailed investigation of the nitroxide-mediated oxidation of primary alcohols. **M.S. Ward**, H.J. Schanz
- 930.** Photopolymer suitability for a 3D printed model of the bile ducts. **N. Faist**, L. Troop, R. Guru, J. Thomas
- 931.** Incorporation of hybrid gold nanoparticles to investigate differences in plasma protein biomarkers of chronic obstructive pulmonary disease (COPD) in a population of smokers. **D.J. Swinton**, T. McClary, B. Yarbrough, K. Tyree
- 932.** Secondary metabolites in *Abies fraseri*: Protective and regenerative properties. **T. Darnell**, L. Grochowski, T. Durham

- 933.** Expedited microwave assisted synthesis of 1,2,3-triazoles for ion sensing. **I. Graves**, S.M. Landge, A. Ugboya, K.S. Aiken
- 934.** Hydroamination of difunctional maleimides: Access to polyaminoamides. **A.J. Caroland**, S. Schrickel, A.K. McMahan, H.J. Schanz
- 935.** Effect of dimerization and interaction with nanoparticles on the absorption and emission spectra of 2,7-dichlorofluorescein. **T. McPherson**, **O. Mojek**, U.P. Kalapathy
- 936.** Monosaccharide lithium affinities and how they relate to water adduction to the lithium cationized molecule. **C. Rumley**, P. Soma, G.L. Glish
- 937.** Preliminary crystallization results for poly(aspartic acid) hydrolase-2 (paaH-2). **T.J. Yared**, H. Salvo, J. Wallen, M. Weiland
- 938.** Multifunctional polyacrylates containing TEMPO, PEG and a hemoglobin binding group. **K. Thomas**, A.K. McMahan, H.J. Schanz
- 939.** Synthesis of multifunctional polyacrylates via reversible addition fragmentation chain transfer (RAFT) polymerization. **A. Diaz**, N.Z. Singleton, H.J. Schanz
- 940.** Mitotropic liposome for targeted delivery of antifibrotics in IPF. **C. Nigg**, S. Bui
- 941.** Forensic application of GC/MS for identification of drugs in human hair. **A. Reynolds**, C.H. Lisse
- 942.** Design, synthesis and anticancer evaluations of piplartine analogues bearing 1,3,4-oxadiazoles as potential anticancer agents. **J. Noel**, C. Okwo, K. Latimer, L. Thomas, K.K. Redda, R. Reams, E. Mazzio, B. Mochona
- 943.** Photophysics of two-dimensional organic inorganic perovskites. **W.R. Ware**, B.R. Gautam
- 944.** Investigation of aroma and flavor compounds generated by various yeast strains. **W.N. Lory**, Z.S. Davis
- 945.** Designing a zwitterionic conjugation-extended viologen for robust aqueous organic redox flow batteries. **J. Palmer**, N. Sayresmith, N. Herr, M. Walter
- 946.** Impact of solvent and fluorination on aggregation of conjugated polymers. **T. Wright**, **M.C. Rose**, B.R. Gautam
- 947.** Structural analysis of RNA elements spanning the ribosome binding site in mRNA transcripts of the streptolysin A associated gene from group A *Streptococcus*. **C.R. Carroll**, A.S. Brown, R.A. Finn, K.J. Calderon, S.G. Nibar, G.C. Perez Alvarado, B.M. Lee

948. Synthesis of chiral indanone precursors: Short formal syntheses of indatraline and SB-209670 and SB-217242. **T. Carney**, A.T. Morehead, B. Hill

949. Regulatory RNA structure in *Streptococcus pyogenes*: Terminator of the streptolysin S-associated gene A. **S.G. Nibar**, K.J. Calderon, R.A. Finn, C.R. Carroll, A.S. Brown, G.C. Perez Alvarado, B.M. Lee

950. Access to borylated trifluoromethylalkenes via a Boryl-Wittig process. **T. Jones**, C. Kelly

951. Role of solvent when forming palladium nanoparticles on gold nanorods for plasmonic catalysis. **M. Sumner**, **B.B. Penland**

952. Raman spectroscopy for the investigation of molecules associated with human decomposition. **B.M. Oberlander**, B. Sharma, G. Sarabia, A. Daniel, A. Wood

953. Regulating redox and spin state behavior of bis-terpy Fe(II) via steric and inductive influence of ligand substituents. **J. Harris**, **N. Blackburn**, P.S. Ray, S. Slattery

954. Synthesis, characterization and gelation studies of N-(acridin-9-yl)alkanamides based low molecular mass gelators. **S. Ndiaye**, A. Mallia

955. Design and synthesis of Fe(II) complexes composed of a novel tridentate ligand for studying spin state transition coupled to proton transfer. **A. Denny**, P.S. Ray, S.J. Slattery

Savannah Marriott Riverfront
Atrium

Undergraduate Posters

Financially supported by American Chemical Society and Coastal Georgia Local Section of the American Chemical Society
M. Weiland, *Organizer*

10:15 - 11:45

956. Substituted pyrazolines as microtubulin inhibitors under hypoxic conditions. **C. Anderson**, J.H. Ferguson, H. Holt

957. Synthesis of pyrrole molecules as anticancer drug targets. **M. Wolfe**, J.H. Ferguson, H. Holt

958. Synthesis, thermal properties and gelation studies of anthraquinonylalkanamides as low molecular mass gelators. **E. Lee**, T. Dairo, A. Mallia

959. Chemistry in the arts: Identification and documentation of 1920s physicians' kits. **S. Ramos**, A. Brooks, R. Bush, R. Lynch, K.S. Taylor

- 960.** Synthesis and anti-proliferative activity of ATP-inspired compounds as cancer killing agents. **D.A. Fico**, J. Spires, S.S. Johnson, J.D. Gorden, M. Frazier, J.M. Meyers, K.S. Taylor
- 961.** Embedding multiwalled carbon nanotubes in natural polymer nanofibrous mats. **W. Neal**, K. Penton, S.K. Hamilton
- 962.** Progression in the development of an alternative energy synthetic pathway to nylon 6,6 through the use of solar irradiation as the sole heat source. **C.B. Hammond**, B. Agee
- 963.** Quantification of Rosmarinic acid in dried rosemary. **C. Mathis**, H.V. Clontz
- 964.** Investigation and analytical characterization of *Lavandula angustifolia* essential oils. **J. Viera**, B. Quarles, N. Hollabaugh
- 965.** Progress toward the synthesis of paramagnetic luminophores: Mn(II) dipyrinato complexes. **M. Gunter**, **S.M. Thodupunoori**, A.B. Scharf
- 966.** Facile fabrication of pristine nickel hexaminobenzene ($\text{Ni}_3(\text{HIB})_2$) metal-organic framework supercapacitor electrodes via electrophoretic deposition. **S. Wechsler**, F. Amir
- 967.** Removing copper from aqueous solutions utilizing cotton plant waste. A. Rizzuti, **R. Winston**
- 968.** Extraction and analysis of the essential oils of fruit rinds and other materials using liquid carbon dioxide. **J.A. Estevez Nolasco**, **E. Call**, B. Tutkowski
- 969.** RTILS as a greener extraction solvent for carbamazepine. **A.L. Coker**, T.R. Hayden
- 970.** What is the chemistry behind medicinal plants? **S.E. Taylor**, J. Haldeman, T.R. Hayden
- 971.** Comparison of the stereochemical effects on the cyclization of sorbitol and allitol sugars and non-sugar model 1,4-pentanediol utilizing $\text{B}(\text{C}_6\text{F}_5)_3$ and allylsilane CO-catalysis. **E.B. Armstrong**
- 972.** Electrolysis of base hydrolyzed cellulose to oxalate. **M. Wheeler**, D.W. Scott
- 973.** Renewable polymers: Towards the ADMET polymerization of plant, animal and fungus alkenes. **H. Cole**, **E. Thompson**, J.T. Cooper, N.E. Huddleston, J. Konzelman
- 974.** Formation constants for Cr(III)-DNA binary adducts. **C.S. Thomas**, S. Brown, J.B. Vincent
- 975.** Redox mediator synthesis for dye sensitized solar cells. **C. Dale**, C.M. Boudreaux, J.H. Delcamp, E.T. Papish
- 976.** Development of a rapid presumptive test that differentiates between hemp and marijuana. **C.E. Lapointe**, J.O. Boles

- 977.** Targeted antibacterial therapeutics for multi drug resistant *Pseudomonas aeruginosa*. **T. Massengill**
- 978.** Effect of guest molecules on the hydrogen bonding of water to resorcin[4]arene in supramolecular assemblies. **P. Landry**, A. Katiyar, W.H. Thompson
- 979.** Studies of the small regulatory RNAs, FASX, and PEL from *Streptococcus pyogenes*. **R.A. Finn**, S.G. Nibar, L.R. Angello, C.R. Carroll, A.S. Brown, K.J. Calderon, B.M. Lee, G.C. Perez Alvarado
- 980.** Development of Pd nanoparticle catalysts supported on carbonaceous ZrO₂ for Suzuki cross coupling reactions. **D. McTaggart**, J. Bobb, M.S. El-Shall
- 981.** Measurement of chlorophyll in green vegetables by fluorescence. **E. Call**, C.E. Dahm
- 982.** Comparison of the rates of decay from glow in the dark paints. **E.D. Fluman**, C.E. Dahm
- 983.** Changes in enamel surface roughness and *S. mutans* growth after vital bleaching. **S. Carreno**
- 984.** Computational investigation of the importance of tryptophan to the Myo19 ATPase cycle. **J. Airas**, E. Modeste, Y. Ali, C.A. Parish, O. Quintero
- 985.** Investigating the *in silico* binding energetics of novel aromatic-substituted POSs and “POCs” HIV-1 protease inhibitors. **E.K. Acosta**, J. Airas, C.A. Parish
- 986.** Forced degradation of acetaminophen under high heat, humidity, and radiation. **F. Najjar**, W. Cory, V. James, E.L. Lawson, N. Cahill
- 987.** Investigating aged and irradiated meclizine tablets for NASA space mission planning. **N. Cahill**, E.L. Lawson, F. Najjar, V. James, W. Cory
- 988.** DFT study of the Bergman cyclization of several enediyne. **C. Ancajas**, C.A. Parish
- 989.** Total phosphorus monitoring in Georgia’s Lake Lanier watershed. **M. Dennis**, L.J. Wilson
- 990.** Spin-flip characterization of the Bergman cyclization of the HEPTA-1, 6-diyne system. **S.G. Wairegi**, A. Luxon, C.A. Parish
- 991.** Analyzing conformational changes of steroid response activator RNA (SRA-RNA) bound to sharp suppressor protein using circular dichroism. **B.O. Okosun**
- 992.** Synthesis and characterization of new phosphonium ionic liquids. **S.C. Jones**, G.K. Coleman, J.H. Davis, B.F. Wicker

- 993.** NacNac: New synthetic routes to a well-known ligand. **P.M. Jimenez Antenucci, H. Marcello, B.F. Wicker**
- 994.** Synthesis and analysis of biologically compatible drug-infused polymers. **K.N. Weeks**
- 995.** Analysis of adonitol as a resource for future sustainable consumer products. **P. Vanna, J.A. Dabrowski**
- 996.** Catalytic cyclization of 1-amino-1-deoxy-d-galactitol towards a renewable alternative to petroleum-based medicines. **E. Scimone, J.A. Dabrowski**
- 997.** Comparing the efficacy of commercial water filters with homemade water filters using atomic emission spectroscopy. V.A. Mativo, **E. Browne, A. Green**
- 998.** Nickel-catalyzed hydroarylation of alkynes under reductive conditions with aryl bromides and water. **H.M. Hynds, C.P. Stephens, H.E. Lemons, M.T. Fredrickson, D. Wilger**
- 999.** Ni-catalyzed Larock annulation with *ortho*-bromobenzoates. H.M. Hynds, **H.E. Lemons, C. Phillips, M.T. Fredrickson, C.P. Stephens, D. Wilger**
- 1000.** Anomalous redox behavior of bis(serinato)copper(II) complex and comparison to closely related bis(homoserinato)copper(II) complex: Update. **Q. Nguyen, T.L. Venable**
- 1001.** Characterization of truncated peptides from the novel peptide preptin. T.N. Anguilm, **A. Scott, J.M. Meyers**
- 1002.** Stabilization of a β oligomers using serotonin, indole, and catechol and their effects on DNA. **E.A. Chapman, K.M. Matera**
- 1003.** Quantitative and colorimetric evaluation of hemoglobin in bloodstains over various time intervals using UV/VIS spectroscopy and chemical enhancements. **S. Knox, S.E. Hooper**
- 1004.** Accessing novel metal organic frameworks using reticular chemistry. **E.D. Shrewsbury, L.Z. Miller**

Savannah Marriott Riverfront
Pulaski

Advancing Infrared Spectroscopic Techniques & Vibrational Sensing

Novel Infrared Techniques & Materials

Financially supported by Picketec GMBH; Neaspec GMBH; MKS Spectra Physics
J. D. Caldwell, *Organizer*
L. E. Buchanan, *Organizer, Presiding*

10:35 1005. Designer phonons to sculpt infrared properties. **T. Beechem**, A. Jarzembki, E. Paisley, S. Smith, C. Saltonstall, J.D. Caldwell, J. Valentine, P. Hopkins, E. Hoglund, J. Howe, R. Engel-Herbert

11:05 1006. Nano-FTIR correlation nanoscopy for organic and inorganic material analysis. **S. Mastel**, T. Gokus, N. Hartmann

11:35 1007. Time resolved infrared spectroscopy studies of proton coupled electron transfer. **R.B. Dyer**

Savannah Marriott Riverfront
Plaza

Incorporating Primary Literature into the Curriculum

Financially supported by Division of Analytical Chemistry
L. Strausberg, *Organizer, Presiding*

10:45 Introductory Remarks.

10:50 1008. Incorporating primary literature and writing instruction in an upper-level capstone chemistry laboratory course. **J.D. Keene**, A.M. Kiefer, C.S. Seney

11:10 1009. Addressing scientific literacy through scaffolded literature review in inorganic chemistry. **M.R. McPhail**

11:30 1010. Guiding students to recognize chemical concepts in primary literature. **L. Strausberg**

TUESDAY AFTERNOON

Savannah Marriott Riverfront
Ballroom B

Diversity Luncheon: Connecting Diversity to Humanity

Financially supported by ACS Local Section Activities Committee, Coastal Georgia Local Section of the American Chemical Society, NOGLSTP.

B. P. Quillian, *Organizer*

R. A. Groom, *Organizer, Presiding*

12:00 1011. Connecting diversity to humanity. **R.L. Williams**

Savannah Marriott Riverfront
Atrium

Materials Chemistry

W. E. Lynch, *Organizer*

1:00 - 2:30

1012. Characterization of SURMOFs and exploration of patterning techniques. **F.G. Gonzalez**, A.M. Weeks, M.E. Anderson

1013. Solar-blind ultraviolet-C persistent luminescence phosphors for self-sustained tagging in all lighting conditions. **X. Wang**

1014. Zirconium and hafnium tritellurides for next generation electronic applications. **M. Seivert**, T.T. Salguero

1015. Electrodeposition of Photosensitive Metals across Micron-gap Gold Electrodes. **S. Taylor**, R. Dasari

1016. *In situ* formation of calcium copper tetrasilicate in Egyptian faience. **E. Abdelrahman**, T. Salguero

1017. Properties and nanostructuring of Cr(II) and Cr(II)/Fe(II) containing tetrasilicates. **H. Rathnaweera**, T. Salguero

1018. Mixed transition metal trichalcogenide materials. **Y. Ghafouri**, T. Salguero

1019. Exfoliation of metal hexaborides via metal ion incorporation techniques. **M. Milkovska**, R. Ramachandran, T. Salguero

1020. Efficient removal of toxic metal ions from aqueous solutions using micro-porous nitrogen-doped carboxylated activated carbon. **A.M. Bakry**, S. El-Shall

1021. Sulfur host based on cobalt phosphides-graphitic nanocages for advanced lithium-sulfur batteries. **A.A. Abdelkader**, A. Alzharani, H.M. Elkaderi

1022. Initial studies of biolubricants obtained from the epoxidation of macaúba (*Acrocomia aculeata* (jacq.) Lood. Ex mart) kernel oil. R.A. Breves, T.A. Serafim, R.V. Lopes, **M.A. Sales**

1023. Novel semiconductors for dye-sensitized solar cells. **W.M. Ward**, D. Miller

1024. TiO₂ nanotubes electrode decorated with NiS nanoparticles applied as a photoanode for photoelectrocatalytic degradation of penicillin G. **F. Sayao**, M. Boldrin Zanoni

1025. Synthesis, characterization, and antimicrobial studies of silver nanoparticles synthesized using *Annona glabra* plant extract. **C.R. De Silva**, S. Wickramarachchi, L. Amarasinghe, S. Sithara, A. Aberathna

1026. Carbon dioxide adsorption on a stilbene-based manganese metal-organic framework. **T.J. Ferguson**, S.T. Golafale, C.W. Ingram

1027. Hexacoordinate silicon complexes for OPV and OLED applications. **M. Kocherga**, M.G. Walter, T.A. Schmedake

Savannah Marriott Riverfront
Atrium

Organic Chemistry

X. Chen, *Organizer*

1:00 - 2:30

1028. Synthesis and biological investigation of aeruginosic acid and derivatives. **A. Kaplan**

1029. One-pot allylsilane synthesis from enolizable aryl ketones. **M.L. Kwan**, P. Challen, Y. Zhou, Q. Tran

1030. Synthesis of divalent and tetravalent carbohydrates to improve sensitivity of glycosidases synthesis of divalent and tetravalent carbohydrates to improve sensitivity of glycosidases. **L. Pham**, **L. Orduno**, T. Jai, Y. Lou, J. Fang, S.S. Iyer

1031. Effects of enzymatic treatment on vitamin E and mineral contents of raw peanuts. **R. Bonku**, N. Mikiashvili, B. Holmes, J. Yu

1032. Primary amine synthesis of functionalized ketones by reductive amination. **D. Harper**, **R. Francis**, B.D. Feske

1033. Effects of enzymatic treatment on sucrose content and sensory quality of peanuts. **N. Idris**, B. Holmes, J. Yu

1034. Biologically active tri-substituted pyridazine compounds as anti-cancer agents. **C. Wallace**, A. Williams, J. Wilson, L. Demby, V. Sittaramane, S.M. Landge

1035. 3-step synthesis of fluoroflavones as potential neuroprotective agents. **M. Alshammari**, N.M. Ashpole, D.A. Colby

1036. Oxidation kinetic studies on porphyrin-manganese(IV)-oxo intermediates via chemical and photochemical generation. **S. Klaine**, W. Ning, R. Zhang

- 1037.** Quinidine and quinine based double salt ionic liquids for liver injury prevention. **T.D. Robertson**, O.A. Cojocar
- 1038.** Synthetic and catalytic studies of metalloporphyrin complexes for biomimetic oxidations. **F. Bratcher**, C. Alcantar, R. Zhang
- 1039.** Characterization of unmodified and bleached peanut hulls for use as an inexpensive biosorbent for waste water treatment. **M.J. Sands**, **C.L. Huffman**
- 1040.** Activity of resveratrol analogues against triple-negative breast cancer (TNBC) cells and LCMS monitoring of molecular isomerization. **H.S. Benmerabet**, D. Paull
- 1041.** Synthetic simplification enables the discovery of a unique biofilm target in *Streptococcus mutans*. **A. Scharnow**, A.E. Solinski, W. Wuest
- 1042.** Electrochemical behavior and stability of juglone in buffers of varying pH. **C.H. Rogers**, O.A. Cojocar, J. Moldenhauer, T.W. Majors
- 1043.** Synthesis of a biochemically important aldehyde, 3,4-dihydroxyphenylacetaldehyde (DOPAL). **J.C. Donnelly**, **M.L. Smith**, D.D. Huber, T.E. Gavin, R.N. Salvatore
- 1044.** Two-step synthesis of flavonol-derived ligands for metal-flavonol complexes and CO release. **R. Dean**, S. Zingales
- 1045.** Development of a 1,2,3-triazole chemosensor for the detection of organophosphate nerve agents. **O. Akinsoji**
- 1046.** Structure-activity relationship and anticancer profile of second-generation anti-MRSA synthetic retinoids. **A. Cheng**
- 1047.** Spectroscopic characterization of new phenothiazine double salt ionic liquids. **E.E. Etheridge**, L.G. Pipkin, O.A. Cojocar
- 1048.** Synthesis of biased κ -opioid agonist collybolide-A. **S. Spurlin**, K. Schaefer, R. Karimov
- 1049.** Synthesis and characterization of new silica immobilized juglone materials. **I.L. Crouch**, O.A. Cojocar, T.W. Majors
- 1050.** Swellable organically modified silica facilitated synthesis of biodiesel fuel: Complete story. **A. Lowry**, N.N. Shaw
- 1051.** Anthelmintic activity of prenylated benzophenones from *Vismia guianensis*. **R. Adesina**, C. Valentine, C.L. Gerald, **O.E. Christian**

Savannah Marriott Riverfront
Atrium

Polymer Chemistry

W. E. Lynch, *Organizer*

1:00 - 2:30

1052. Ultra-stretchable polymer wearable strain sensor with excellent linearity and repeatable autonomous self-healing ability. **J. Horne**, D. Hong, A. Faunce, L. McLoughlin, R. Ploeger, D. Sanchez, S.G. Yim, Y. Lu, J. Jeon, **E.K. Wujcik**

1053. Charge effects and their role on particle transport in polyampholyte gels. **K. Nuti**

1054. Investigations of succinylated polyethylenimine derivatives for enhanced transfections in serum. **M. Uddin**, L. Warriner, D. Pack, J.E. Derouchey

1055. Surface modification of titanium surfaces for improved tendon adhesion. **H. Feinberg**, **T.W. Hanks**

1056. Cationic tricyclic natural product-derived polymers as antimicrobial agents. **L. Kurnaz**, M. Lamm, C. Tang

1057. Modification of polymeric carbon nitride films for increased photoelectric density. **A. Turturici**

1058. Preparation of metallopolymer hydrogels. **J. Hwang**, T. Zhu, Y. Cha, C. Tang

1059. Controlling topologies of biobased copolymers from renewable rosin and soybean oil. **Y. Ma**, Y. Sha, T. Zhu, M. Rahman, C. Tang

1060. Optical and electronic properties of benzodithiophene-based conjugated polymers with nucleobase side chain functionality. **T.J. Adams**, S. Sabury, M. Kocherga, M.G. Walter, M. Kilbey

1061. Polymer from pine rosin and tung oil. **A. Hulette**

Savannah Marriott Riverfront
Mercer

The Past, Present, & Future of the Periodic Table

Financially supported by Division of the History of Chemistry
D. Rabinovich, R. H. Wallace, *Organizers*
C. W. Padgett, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 1062. Elements of alchemy. **C.W. Padgett**

1:30 1063. Elemental name game. **C.E. MacGowan**

1:55 1064. Law & order: Periodic table. **D. Rabinovich**

2:20 1065. Musical tables: Two early periodic arrangements of the elements. **C.J. Giunta**

2:45 1066. South Carolina: Wonderful iodine state. **W.T. Pennington**

3:10 Intermission.

3:25 1067. History of the valence electronic structure of the actinides. **H.S. La Pierre**

3:50 1068. History Pu-238 production at the Savannah River Site. **E.B. Fox**

4:15 1069. Future of new superheavy element discoveries. **C.M. Folden**

4:40 Concluding Remarks.

Savannah Marriott Riverfront
Ballroom E

Coordination Chemistry: Synthesis, Characterization & Application

Financially supported by Division of Inorganic Chemistry
A. Saha, *Organizer, Presiding*

1:10 Introductory Remarks.

1:15 1070. Dinitrogen coordination and activation by weak-field ligated multimetallic complexes. **L.J. Murray**

1:40 1071. Naphthylsalophen lanthanide(III) complexes with tunable emissions. E.E. Hardy, E.A. Hiti, J.D. Gorden, **A.E. Gorden**

2:05 1072. Sustainable synthesis of organometallics through mechanochemistry. **T. Jurca**

2:30 1073. Metal-organic frameworks: Perspectives and applications. **N.B. Shustova**

2:55 1074. Metal organic-frameworks for noble gas adsorption. **P.K. Thallapally**

3:20 Intermission.

3:35 1075. Investigating bonding and catalytic activity of TpCu(Co) complexes. **A. Ison**, E.A. Ison

3:55 1076. Catalytic two-electron oxidation of a cobalt(II) complex supported by a redox-active ligand scaffold: Synthesis, characterization, and catalytic activity. **E.E. Liu**, O. Villanueva, M.R. Leidy, J. Bacsá, C.E. MacBeth

4:15 1077. Mechanism of frataxin “bypass” in human iron-sulfur cluster biosynthesis with implications for Friedreich’s ataxia. **D. Das**, S. Patra, D.P. Barondeau, J. Bridwell-Rabb

4:35 1078. Flux crystal growth and magnetic properties of new f-element chalcogenides. **V. Klepov**, H. Zur Loye

4:55 1079. Nature-inspired molecular sensors for the selective detection of metal ions. **A.D. Johnson**

Savannah Marriott Riverfront
Plaza

Cure Chemistry Research in Lab

A. Sikora, *Organizer, Presiding*

1:10 Introductory Remarks.

1:15 1080. Bio-molecule course-based research experience for sophomores. **N.L. Powell, B. Harmon, D. Das**

1:35 1081. Cures beyond the classroom: Student’s perspective. **M. Khoja, A. Sikora**

1:55 1082. Using spectroscopy to identify a forgery: Inquiry-based, hands-on experience for non-majors. **C. Theodore**

2:15 1083. Incorporating an unexpected procedural flaw in a traditional undergraduate organic laboratory into a discovery-based laboratory experience. **S. Bridges**, A.M. Kiefer

2:35 1084. Assessing meaningful learning through thematic analysis of creative exercises in inorganic chemistry. **J. Shaw**

2:55 Intermission.

3:15 1085. Teaching proteomics without instrumentation: Novel undergraduate curriculum. **S. Robertson**

3:35 1086. TIME 4 Real Science: Unique high school CURE. **J.S. Williams**

3:55 1087. Crossing floors: Developing an interdisciplinary cure between an environmental toxicology and analytical chemistry course. **K.R. Roth**, J. Lau

4:15 1088. Undergraduate research at scale: What if the treatment is a cure? **E.L. Dolan**

4:35 1089. How do middle grade students interpret particulate level animations? **T. Kinner**, K. Linenberger-Cortes

4:55 Concluding Remarks.

Savannah Marriott Riverfront
Ballroom C

Frontiers in Nucleic Acid Chemistry

F. Leng, N. Shank, *Organizers*
D. P. Arya, *Organizer, Presiding*

1:10 1090. Transcription through roadblocks. **L. Finzi**

1:40 1091. Probing chemical biology of DNA damage using NMR. **M.P. Stone**, S.N. Bamberger, A.H. Kellum, C.K. Malik, T.L. Johnson-Salyard, M.W. Voehler, C.J. Rizzo, R.S. Lloyd

2:10 1092. Structural micro-heterogeneity of DNA and DNA bound peptide and protein complexes. **F. Fernandez-Lima**

2:40 1093. DNA in tight spaces: Linking structure, stability and protection in sperm chromatin. **J.E. Derouchey**

3:10 Intermission.

3:25 1094. Replication of an RNA duplex containing an active ribozyme: Exploring the possible role of viscous solvents in the emergence of functional nucleic acids. A. Lozoya-Colinas, C. He, I. Gallego, M. Grover, **N.V. Hud**

3:55 1095. Transcription factor discovery in the extreme thermophile *Thermus thermophilus* HB8. **M. Van Dyke**

4:25 1096. Elucidation of the dynamics of transcription-coupled DNA repair initiation by RNA polymerase II and CSB using kinetic network models. **C. Yan**, T. Dodd, D. Wang, I.N. Ivanov

4:40 1097. Evaluation of the binding contribution and cooperativity of TIAR/TIA-1 RRM modules for RNA. **J.L. Siemer**, T. Le, J. Zhang, M.A. Brinton, M.W. Germann

4:55 Concluding Remarks.

Savannah Marriott Riverfront
Chatham

Teaching, Creating & Sustaining a Safety Culture

M. B. Koza, *Organizer, Presiding*

1:10 Introductory Remarks.

1:20 1098. Nurturing a safety culture through student engagement. **R. House**, O. Williams, A.J. Miller, D.S. Lawrence, J.S. Johnson

1:45 1099. Supporting a culture of safety with teachable moments. **M.C. Box**, M.T. Gallardo-Williams

2:10 1100. Successful execution of top-down safety culture at UNC-Chapel Hill. **J. Potts**

2:35 1101. Collaborative safety training and integrative program development. **M. Lassiter**

3:00 Intermission.

3:20 1102. Cultivating a culture of safety in undergraduate chemistry labs at UNC Chapel Hill. **K. Nevins**

3:45 1103. From rules to ramp: Embracing safety culture's expanding frontier as a recent graduate. **R. Bocwinski**

4:10 1104. SOPs, SOCs, and docs: Developing peer-to-peer safety to fight complacency in synthetic inorganic chemistry. **Q.J. Bruch**, A.J. Miller

4:35 1105. Laboratory safety culture at UNC-CH. **M.B. Koza**

Savannah Marriott Riverfront
Pulaski

Advancing Infrared Spectroscopic Techniques & Vibrational Sensing

Ultrafast & Raman Characterization

Financially supported by Piketec GMBH; Neaspec GMBH; MKS Spectra Physics
L. E. Buchanan, *Organizer*
J. D. Caldwell, *Organizer, Presiding*

1:15 Introductory Remarks.

1:20 1106. Measuring protein structure at the protein-nanoparticle interface via 2D infrared spectroscopy. **L.E. Buchanan**, K.R. Webb

1:50 1107. Probing plasmon-mediated processes with ultrafast surface-enhanced Raman spectroscopy. **R.R. Frontiera**

2:20 1108. Raman spectroscopy for *in vivo* and *in vitro* neurochemical sensing. **B. Sharma**

2:50 1109. Using Raman spectroscopy to probe the vibrational and structural properties of quantum dots. A. Beecher, R. Dziatko, N. Saenz, A. Oza, L. Hamachi, M.L. Steigerwald, J.S. Owen, **A. Crowther**

Savannah Marriott Riverfront
Reynolds

Aquatic Biogeochemistry

S. E. Gray, *Organizer*

C. E. MacGowan, D. Mullenax, *Presiding*

1:15 Introductory Remarks.

1:20 1110. Implications of ice sheet retreat for nutrient export from periglacial landscapes in Greenland. **A.J. Pain**, S. Rahman, J.B. Martin, E.E. Martin

1:40 1111. Is dissolved organic carbon the key to understanding the fate of Arctic permafrost soil carbon? **L. Ziolkowski**

2:00 1112. In a sea of microbes and organic matter: Identifying the organisms and metabolisms that power the ocean's carbon cycle through genomics and transcriptomics. **S. Gifford**

2:20 1113. What controls dissolved organic matter composition in marsh-dominated estuaries? **P.M. Medeiros**

2:40 1114. Elucidating tidally-driven factors influencing dissolved inorganic carbon export to the coastal ocean. **C. Hintz**

3:00 1115. Cation exchange reactions between silver nanoparticles and metal sulfides. **K.M. Mullaugh**, H. Lieb, B. Nguyen, E.R. Ramsayer

3:20 Concluding Remarks.

Savannah Marriott Riverfront
Forsyth

Frontier Research in Polymer Science

E. B. Berda, *Organizer, Presiding*

1:20 Introductory Remarks.

1:25 1116. Multi-mechanophore stress-relieving polymers synthesized via raft polymerization. **B. Bowser**, S. Craig

1:45 1117. Antifogging/frost-resisting polymer coating. **W. Ming**

2:05 1118. Precision synthesis of degradable acrylate and acrylamide copolymers with thionolactones. **W.R. Gutekunst**

2:25 1119. Rethinking single-chain nanoparticles. **E.B. Berda**

2:45 Intermission.

3:05 1120. Bulk ADMET polymerization of aliphatic polysulfones. **J. Pribyl**, S. McDonald, S. Wheeler, M.H. Bell, H.G. Hester, K.B. Wagener

3:25 1121. Hierarchical molecular design of benzothiadiazole, diketopyrrolo-pyrrole and thienothiadiazole containing polymeric materials via electro-polymerization. **T.A. Ranathunge**, N. Sparks, N.H. Aththanayake, D. Karunathilake, D.R. Strongin, J.H. Delcamp, G. Rajapakse, D.L. Watkins

3:45 1122. Simplifying the design of anti-icing polymers. Y. Lin, H. Gomez, **J. Tsavalas**, P.W. Baures, K. Varga, E. Asenath Smith

4:05 1123. Non-conjugated polymers as memristors in neuromorphic applications. **S.H. Foulger**

Savannah Marriott Riverfront
Oglethorpe B

Frontiers in Mechanistic Enzymology

M. K. Thompson, *Organizer, Presiding*

1:20 Introductory Remarks.

1:25 1124. New insights into the chemical reactivity of dehaloperoxidase: Multifunctional catalytic hemoglobin. **R.A. Ghiladi**

1:55 1125. Neurodegenerative diseases and the mitochondrial unfolded protein response. **R. Silvers**

2:25 1126. Characterization of the genomically encoded fosfomycin resistance enzyme from *Mycobacterium abscessus*. S. Travis, M. Shay, S. Manabe, N. Gilbert, P.A. Frantom, **M.K. Thompson**

2:55 Intermission.

3:15 1127. Redox-modulator or metal buffer? Exploring the role of glutathione in cellular copper homeostasis. **C.J. Fahrni**

3:45 1128. Exploring the heterogeneity of insect arylalkylamine *N*-acyltransferase. **B. O'Flynn**, D.J. Merkler

4:15 1129. On the mechanism of ANGPTL3 and ANGPTL4 inhibition of LPL. **S. Neher**

4:45 Concluding Remarks.

Savannah Marriott Riverfront
Franklin

Heterocyclic Chemistry in the Southeast & Beyond

Financially supported by ViiV Healthcare

C. E. Stephens, *Organizer*

Q. Wang, *Organizer, Presiding*

1:20 Introductory Remarks.

1:25 1130. Strategies and tactics inspired by biologically active alkaloids. **J.M. Smith**

1:45 1131. Marine natural products synthesis: Platform for chemical and biological discovery. **J.G. Pierce**

2:05 Intermission.

2:15 1132. Umpolung approaches to the synthesis and application of heterocycles enabled by hypervalent iodine reagents. **S. Wengryniuk**

2:35 1133. Synthesis and study of polyfunctional and fused-ring heterocycles: Research progress at Georgia Gwinnett College. **J. Sloop**, A. Mallia

2:55 1134. Synthesis and characterization of high-performing explosive and propellant heterocyclic materials. **J.J. Sabatini**, E. Johnson, E. Bukowski

3:15 Intermission.

3:35 1135. Catalytic, enantioselective synthesis of indole derivatives by epoxide opening. **M. Healey**, M. Montgomery, J.B. Morgan

3:55 1136. Synthesis of azepinoindoles via ring expansion of 1-methyl-tetrahydro- β -carbolines. **S. Ding**, M. Ghavami, P.R. Carlier

4:15 1137. Chemoselective aerobic 5-hydroxylation of a 2-aminopyrrole derivative. A.C. Bean, S. Mondal, **C.E. Stephens**

4:35 Concluding Remarks.

Savannah Marriott Riverfront
Ballroom D

Astrochemistry in the Southeast & Beyond

Solar System Astrochemistry & Beyond

R. C. Fortenberry, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 1138. Millimeter/submillimeter spectroscopic detection of desorbed ices: New technique in laboratory astrochemistry. K.M. Yocum, E. Todd, A. Jones, S.N. Milam, P.A. Gerakines, **S.L. Widicus Weaver**

2:05 1139. Fragment species in the comae of comets: Observations and challenges. **D. Pierce**

2:35 1140. Molecular water ice formation and processing in solar systems. **T.M. Orlando**, B.M. Jones, A. Alexandrov, K. Fiege

3:05 Intermission.

3:25 1141. Laboratory studies of thermally processed ice mixtures relevant to outer-planetary surfaces. **D. White**

3:55 1142. High impact chemistry: Design and testing an icy moon penetrator organic analyzer. **A.M. Stockton**, M. Cato, N. Speller, J. Kim, S. Foreman, P. Putman, J. Epperson, E. Spiers, B. Schmidt

4:25 1143. Potential pathway to O₂ observed in comets 67P/Churyumov-Gerasimenko and 9P/Tempel: Dissociation of radiolytically produced parent carbon oxide species. **C.J. Bennett**, B. Ferrari, R.C. Fortenberry

4:55 Concluding Remarks.

Savannah Marriott Riverfront
Oglethorpe A

Spectroscopic Imaging: Bridging the Gap between Chemical & Spatial Heterogeneity

A. Ghosh, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 1144. Discovering complex microscopic interactions with broadband coherent Raman microscopy. **M.T. Cicerone**

2:05 1145. Characterization of extracellular vesicles derived from red blood cells using Raman spectroscopy and machine learning. **R.A. Dluhy**, A. Konutham, S. Nazeer, J. Oh, A. Gaggar, R. Patel

2:35 1146. High-resolution label-free biochemical imaging of histology tissue sections can improve cancer detection and staging. **F.E. Robles**

3:05 Intermission.

3:25 1147. Imaging mass spectrometry of lipid isomers using gas phase ion/ion reactions. **B.M. Prentice**

3:55 1148. Metabolomics approaches to decipher response of pathogens in disease. **N. Garg**

4:25 1149. Spatial mapping with portable X-ray fluorescence spectroscopy to identify corrosion on ferrous metal alloy substrates on U.S. Air Force assets. **J.D. Keene**, K.M. Bucholtz

Savannah Marriott Riverfront
Atrium

Biochemistry

T. Leeper, *Organizer*

3:00 - 4:30

1150. Small molecule modulators of chaperone Hsp70 for amyloid remodeling. M. Weber, S. Le, **C. Haney**

1151. Allergenicity of different fractions of protein extract from enzymatically hydrolyzed peanut flour. **N. Mikiashvili**, J. Yu

1152. Enzymatic biodegradation of polymers: Undergraduate study using poly(aspartic) acid. **A.J. Burke**, A.L. Bolay, M. Weiland

1153. Predicted functions of FtrA and FtrB protein from the four-component uptake system, FtrABCD, in *Brucella* spp. **M.N. Chanakira**, S. Banerjee, R. Roop, D. Martin

1154. Trojan horse approach: Novel drug delivery mechanism. **R.C. Eakes**, S. Banerjee, S. Stamey, D. Martin

1155. Characterization of a pH-responsive nanocage based on the ferritin iron storage protein. S. Singh, N.E. Grosseohme, **F. Outten**

1156. Bactericidal activity of copper-ascorbic acid mixture against *Staphylococcus aureus* spp.. **T. Zimmerman**, R. Gyawali, S. Aljaloud, S.A. Ibrahim

1157. QM/MM simulations of flavin electronic spectra in different electrostatic environments. **M. Kabir**, Y. Orozco-Gonzalez, S. Gozem

1158. Pharmacophore benchmarking: Role of ligand function in model development. **P. Castleman**, G. Szwabowski, D.L. Baker, A.L. Parrill-Baker

1159. Hemagglutinin mediated membrane fusion: Dynamics of fusion peptide insertion and interaction with transmembrane domain. **A. Prokopik**, R.B. Dyer

1160. Characterization of CdSe based nanoparticles for integration into photocatalytic systems. **S. Narehood**, M. Sanchez, R.B. Dyer

1161. Bioinformatic and *in vitro* characterization of primase-polymerase enzymes from viruses that infect Actinobacterial hosts. **N.B. Folse**, S.R. Watson, J. Wallen

1162. Altering zinc oxide metal-based nanoparticles and the potential changes in the antimicrobial properties. **K. Brasecker**

1163. Interaction of Grx4 with the SUF machinery for iron-sulfur cluster biogenesis in *E. coli*. **E. Sanchez**, F. Outten

Savannah Marriott Riverfront
Ballroom B

Environmental Chemistry

W. E. Lynch, *Organizer*
C. McKenas, *Presiding*

3:00 Introductory Remarks.

3:05 1164. Heterogeneous oxidation of phenolic aldehydes. **M. Rana**, M.I. Guzman

3:25 1165. Mesoporous adsorbents for perfluorinated compounds. **B. Lotsi**, A.A. Kuvayskaya, R. Mohseni, A. Vasiliev

3:45 1166. Computational predictions of polarizabilities and refractive indices of guanine complexes. **H. McAlexander**, M.K. Shukla

4:05 1167. Potassium doped iron oxide catalyst on photocatalytic CO₂ reduction. **M. Hoque**, M. Gnanamani, Z. Liang, K. Graham, J.P. Selegue, M.I. Guzman

4:25 1168. Photochemical study on terrestrial dissolved organic matter using fluorescence spectroscopy. **A. Goranov**, A.C. Bryan, H. Chen, P.G. Hatcher

4:45 1169. Polymer fiber-based visible colorimetric sensor for selective and sensitive on-site determination of polycyclic aromatics hydrocarbons in aquatic ecosystems. **J. Horne**, D. Sanchez, J. Perch, C. Cook, Y. Lu, M. Elliott, **E.K. Wujcik**

Savannah Marriott Riverfront
Atrium

Physical Chemistry

C. W. Padgett, *Organizer*

3:00 - 4:30

1170. Molecular dynamics simulations of the interactions between triose phosphate isomerase and sulfonamides. **N.Y. Forlemu**, J. Sloop

1171. Nanoscale infrared spectroscopy of beta amyloid fibrils and prefibrillar aggregates. **L. Zhang**, A. Phadkule, A. Ghosh

1172. Decomposition of organophosphorus compounds on zirconium-based metal organic frameworks at the gas-MOF interface. **H. Siegal**, N.S. Sapienza, J.R. Morris

1173. Inverse temperature dependent conductivity of heme bacterial nanowires. **X. Ru**, P. Zhang, D.N. Beratan

1174. Force constants and bond strength of functional groups in organic molecules: Fourier transform infrared spectroscopic analysis. **K. Marsack**, M. Daniel, R. Gunasinghe, P.B. Nolibos

1175. Exploring the evaporative properties of acoustically levitated solvent droplets. **H. McCardle**, E.R. Duranty

1176. Molecular structure of 1-isocyano-1-silacyclopent-2-ene: Combined microwave spectral and theoretical study. **T. McFadden**, R. Sonstrom, B.H. Pate, G.A. Guirgis

1177. Preparation, characterization, conformational stability and theoretical calculations of 4-methyl-1,1-dichloro-1-silacyclohexane. G.A. Guirgis, **B. Shumberger**, R. Sonstrom, B.H. Pate

1178. Computational study of the spin trapping behavior of melatonin and selected derivatives. **O.S. Oladiran**, S.J. Kirkby

1179. Effect of graphene oxidation rate and residue substitution on the adsorption of polyalanine peptides. **K.D. Krantzman**, H. Kim, Y.G. Yingling

1180. Elucidation of prominent features in the spectra of N_4H^+ and N_4D^+ clusters: Driven molecular dynamics study. D. Boutwell, **M. Kaledin**

1181. Preparation and activity of palladium catalyst on fumed silica support. **D. Fertal**, M. Billor, A.C. Banerjee

1182. Molecular dynamics of $O(^1D) + CCl_4 \rightarrow ClO + CCl_3$ probed by cavity enhanced sub-THz spectroscopy. **R. O'Neal**, L. Duffy

1183. Formation mechanisms of interstellar C_3H_2O isomers from quantum mechanical calculations. **R. Johnson**, S. Gozem

1184. Photophysical modulation of a triazole molecule in a cationic micelle. **E. Dobson**, C. Freeman, K.S. Aiken, S.M. Landge, D. Ghosh

1185. Endocannabinoid entry into TRPV1, the ionotropic cannabinoid receptor. **C. Muller**, D. Lynch, D. Hurst, P. Reggio

1186. Laboratory submillimeter spectroscopic detection of desorbed CO ices. **K.M. Yocum**, E. Todd, S.N. Milam, P.A. Gerakines, S.L. Widicus Weaver

1187. Spectral analysis of the reaction between $O(^1D)$ and methylamine. **H.A. Bunn**, C. Schultz, J.A. Kroll, S.L. Widicus Weaver

1188. Effective determination of the theoretical infrared spectra of formic acid dimer $(HCOOH)_2$. **D.R. Boutwell**, M. Kaledin

1189. Solid phase extraction of heavy metal ions from aqueous solutions using amorphous melamine zirconium phosphate. **A.M. Bakry**, S. El-Shall

1190. Nanoscale infrared spectroscopic imaging of chemical heterogeneities in hybrid organic-inorganic perovskites. **A. Phadkule**, L. Zhang, M. Hasan Ul Iqbal, A. Ghosh

1191. Excited state dynamics of photo-ODIBO using transient absorption and stimulated Raman spectroscopies. **W. Thompson**

1192. Examining biomarker survivability in Enceladus plume capture conditions using laser-induced projectile impact testing. **K.M. Seaton**, B.L. Henderson, I. Kanik, T.M. Orlando, A.M. Stockton

1193. Treatment of the free electron wave function in photoelectron spectroscopy: Systematic benchmark study. **M. Mahbub**, S. Gozem

1194. Investigation of the low-energy isomers of $\text{SO}_4^{2-}(\text{H}_2\text{O})_N$ ($n=1-5$) clusters. **K. Pokorny**

1195. Structure based drug design and synthesis of novel GPR6 modulator. **I. Isawi**, P. Morales, D. Hurst, A. Herraiz, N. Jagerovic, P. Reggio

1196. Recent investigations of pure and Cu decorated ZnO nanoparticles. **L.J. Langston**, J.Z. Laresé

Savannah Marriott Riverfront
Pulaski

Advancing Infrared Spectroscopic Techniques & Vibrational Sensing

Financially supported by Piketec GMBH; Neaspec GMBH; MKS Spectra Physics
L. E. Buchanan, *Organizer*
J. D. Caldwell, *Organizer, Presiding*

3:40 Introductory Remarks.

3:45 1197. Investigating the effects of α -acetylation on amphiphilic peptide self-assembly with 2DIR spectroscopy. **W.B. Weeks**, M. Pan, L. Buchanan

4:05 1198. Nondispersive infrared (NDIR) sensing of CO_2 using CdO films. **A.K. Livingood**, J.R. Nolen, T.G. Folland, J.D. Caldwell

4:25 1199. Enhancing chemical sensing through SEIRA and silicon carbide gratings. **A.R. Bruncz**, T.G. Folland, J.D. Caldwell

4:45 1200. Mapping polarity and hydrogen-bonding environments in live cells by hyperspectral stimulated Raman scattering microscopy. **X. Lang**, K. Welsher

Savannah Marriott Riverfront
Reynolds

Geochemistry

C. E. MacGowan, D. Mullenax, *Organizers, Presiding*

3:45 Introductory Remarks.

3:50 1201. Investigation into the effect of aging and aluminum-substitution in ferrihydrite under aerobic conditions using flow microcalorimetry, XRD, and XAS. **S. Zigah**, **B. Martin**, C.I. Pearce, K. Rosso, N. Kabengi

4:15 1202. Development, characterization and reactivity of phosphate mineral thin films. **E. Garcia**, K. Slavicinska, A.J. Nastase, C. Luda, A. Poyraz, H.L. Abbott-Lyon

4:40 1203. Developing a hybrid surface complexation model for aluminum-substituted ferrihydrite. **F. Adams**, M.L. Machesky, J.D. Kubicki, N. Kabengi

Savannah Marriott Riverfront
Mercer

History of Chemistry

Past, Present & Future of the Periodic Table

Financially supported by Division of the History of Chemistry
R. H. Wallace, *Organizer, Presiding*

4:45 Introductory Remarks.

4:50 1204. Galantamine: History of an Alzheimer's drug. **D.W. Dixon**

5:10 1205. Look back at two important chemurgy projects. **R.H. Wallace**

TUESDAY EVENING

Savannah Marriott Riverfront
Atrium

Frontiers in Nucleic Acid Chemistry

D. P. Arya, F. Leng, N. Shank, *Organizers*

5:00 - 6:00

1206. Gallic acid-based bacterial DNA gyrase inhibitors. **E. Alfonso Maqueira**, R. Troche, **A. Caceres**, Z. Deng, F. Leng

1207. New fluorescence-based method to identify DNA topoisomerase inhibitors. **Z. Deng**, F. Leng

1208. Electrostatics dominate the interactions between the tethered intrinsically disordered regions and the DNA-binding domain of PU.1, a model eukaryotic transcription factor. **S. Khani**, S. Esaki, M. Khanezarrin, M.W. Germann, G. Poon

1209. Long-lived intermediates in oxidation of guanine by one-electron oxidants: Kinetics of formation and lifetime under biologically relevant conditions. **E. Campbell**, Y. Razskazovskiy, M. Roginskaya

1210. Recognition of single ribonucleotides in duplex DNA by RNase HII. **S.T. Brenden**, S.V. Nguyen, M.W. Germann

1211. Identification and characterization of preferred DNA-binding sites for the *Thermus thermophilus* HB8 transcriptional regulator TTHB099. **K. Moncja**, **M. Van Dyke**

1212. Oxidative damage to guanine bases in DNA: Reaction pathways leading to the formation of 2,5-diaminoimidazolone lesion and their relative contribution. **C.S. Thomas**, Y. Razskazovskiy, M. Roginskaya

1213. Tunable immunostimulation through chemically modified nucleic acid nanoparticles. **J. Halman**, B. Johnson, I. Marriott, E.F. Khisamutdinov, K. Afonin

1214. Immune stimulation by functionalized RNA nanorings. **M. Chandler**, Y. Avila, E. Stassenko, M. Dobrovoskaia, K. Afonin

1215. Exploring stability and steric effects of disulfide bonds incorporated into the backbone of peptide nucleic acid (PNA). **T.C. Hood**, N. Shank

1216. Role of flanking amino acids in DNA binding by AT-Hook peptides. **S. Wright**, K.L. Buchmueller

1217. Dynamic RNA and DNA nanoassemblies with controlled immunological properties. **W. Ke**

1218. Design and synthesis of cyano-nitlutamide conjugated DNA bis-methylating molecules that can target androgen receptor positive cancer cells. **C.H. Murphy**, J. King, C. McNeely, C. Cribb, A. Frampton, S. Varadarajan

1219. Design and investigation of DNA bis-alkylating agents for increased toxicity towards cancer cells. **A.M. Williams**, L. Lowder, C. Mills, C.H. Houston, C. Crib, S. Batts, T. Banh, A. Frampton, S. Varadarajan

1220. Potent inhibition of the mammalian high mobility group protein AT-Hook 2 binding to DNA by natural polyphenols. **L. Su**, J.W. Chambers, F. Leng

1221. Role of hydration in DNA recognition by structurally homologous transcription factors. **A.V. Albrecht**, K. Huang, G. Poon

1222. Suboptimal binding drives DNA site recognition in the transcription factor ETS-1. **K. Huang**, S. Xhani, A.V. Albrecht, G. Poon

1223. Identification of a DNA-binding consensus sequence for TTHA1359, a *Thermus thermophilus* HB8 transcriptional regulator. **J. Teague**, M. Van Dyke

WEDNESDAY MORNING

Savannah Marriott Riverfront
Academy

Physical Chemistry

Experimental

C. W. Padgett, *Organizer*
T. Whiteside, *Presiding*

8:00 Introductory Remarks.

8:05 1224. Magnetic characterization of chromium intermediates in the reduction of chromium(VI) by glutathione in acidic solutions. **R.A. Marin**, R. Bose, **B. Dabrowski**, **S. Kolesnik**

8:25 1225. Infrared spectroscopic studies of the CO oxidation reaction mechanism on Cu/TiO₂ and the role of strong metal-support interactions. **A. Maynes**, J.R. Morris, D.M. Driscoll

8:45 1226. Hydrogen atom abstractions from carboxylic acids: Experimental mechanistic interpretation. **M. Paradzinsky**, J. Tanko

9:05 1227. Transient absorption microscopy in the total internal reflection geometry. **B. Colon**

9:25 1228. Acoustic levitation and infrared thermography: Sound approach for studying processes occurring in isolated droplets. **E.R. Duranty**, H. McCardle, A. Hotaling, K. Abbuhl, W.M. Reichert, J.H. Davis

9:45 1229. Laser spectroscopy of OCS dimers in helium nanodroplets. **I. Miller**, T. Faulkner, J. Saunier, P. Raston

10:05 Intermission.

10:20 1230. Particle-by-particle *in situ* characterization of the protein corona via real-time 3D single particle tracking microscopy. **X. Tan**, K. Welsher

10:40 1231. Covalently-linked rhodamine B dimers: Stereochemistry and photophysical interplay. N. Grinalds, L. Pferdmenges, B. Hunter, P. Lundin, **K.H. Fogarty**

11:00 1232. Thermodynamic, modeling, and neutron scattering investigation of acetylene adsorption of graphite. **A. Pedersen**, J.Z. Larese

11:20 1233. Design and development of a quartz microbalance based ethylene detector. **Z. Stroupe**, J.Z. Larese, N. Marshall, W. James

11:40 1234. Speeding up 3D fluorescent laser scanning microscopy for live cell imaging. **C. Johnson**, K. Welsher

12:00 1235. Analysis of the Calcination of Plutonium(IV) Oxalate to Plutonium(III) Oxalate. **C. South**, L. Roy

Savannah Marriott Riverfront
Oglethorpe B

Biochemistry

Bioinorganic

T. Leeper, *Organizer*
G. Meloni, *Presiding*

8:10 Introductory Remarks.

8:15 1236. Reactivity studies of dehaloperoxidase B with biphenol substrates: Spectroscopic and mechanistic studies. **D. Yun**, R.A. Ghiladi, A. McGuire, T. Malewschik

8:35 1237. Investigation into the catalytic cycle of cytochrome P-450 involving imidazolium-based ionic liquid cations as substrate in a QM-based framework. **A. Banerjee**, J. Shah

8:55 1238. Enzymatic degradation of 4-cyanophenol pesticides with the multifunctional hemoglobin dehaloperoxidase. **P. Staton**, T. Malewschik, A. McGuire, R.A. Ghiladi

9:15 1239. Antimicrobial properties of cotton treated with altered zinc-metal based nanoparticles. **K. Brasecker**

9:35 1240. Enhanced protonation of amino acids and dipeptides using Cr(III): Developing the basis for proteomics studies. **R. Persaud**, C.J. Cassady, D.A. Dixon

9:55 Intermission.

10:15 1241. *Corynebacterium diphtheriae* heme uptake: Roles of HTaB, CHtA and ChtB. **D.W. Dixon**, C. Odhiambo, R. Uluisik, B. Ferrell, S. Adrian, M. Schmitt, G. Lukat-Rodgers, K.R. Rodgers

10:35 1242. Copper-thiolate cluster selectivity and assembly in human metallothionein-3. J.S. Calvo, N. York, B.S. Pierce, **G. Meloni**

10:55 1243. Investigation of the catalytic cycle of [FeFe] hydrogenase using time-resolved infrared spectroscopy. **M. Sanchez**, J. Birrell, E. Reijerse, W. Lubitz, R.B. Dyer

11:15 1244. Development of a genetically-encoded methyltransferase biosensor. **J. Garcia**, G.J. Williams

11:35 1245. Observations, hypothesis, and consequence in the role of selenium and selenocysteine into HIV *Nef* protein expression and Zika viral RNA interactions with host cell mRNA and protein expression. **G. Dailey**, J. Ruzicka, E. Taylor

Savannah Marriott Riverfront
Ballroom D

Chemical Education

S. R. Mooring, *Organizer, Presiding*

8:10 Introductory Remarks.

8:15 1246. General chemistry lab practical exams at Augusta University. **A.C. Spencer**, S.A. Myers, C. Eidell

8:35 1247. Teaching organic chemistry concepts to non-science majors. **J.E. Barker Paredes**, J. Sloop

8:55 1248. CalLevIR: Modern alternative to coffee cup calorimetry. **K. Abbuhl**, E.R. Duranty

9:15 1249. Culinary transformations: Translating chemistry for non-majors. **J.A. Dabrowski**

9:35 1250. Redesign of general chemistry with digital and adaptive learning courseware/technology supported high-touch student services. **E.A. Mintz**, C.W. Ingram, D. Teodorescu

9:55 Intermission.

10:15 1251. Impact of group quizzes in undergraduate organic chemistry. **M.E. Leake**, X. Xu, C.B. Nettles, D. Mlsna

10:35 1252. Development of an instrument to comprehensively assess core concepts in general chemistry. **D. Inman**, M. Balabanoff, A.C. Moon

10:55 1253. Increasing the yield in general chemistry: How students think about stoichiometry. **K. Patel**, E. Gallagher

11:15 1254. Developing and maintaining a multi-year, multi-disciplinary faculty learning community focused on the implementation of a specifications grading assessment protocol in courses at Georgia Gwinnett College. **M.S. Morton**, **M. Anzovino**, D. Behmke, T. Gluick, M. Tsoi, O. Villanueva, C. Woodbridge

11:35 1255. Only time will tell: Imagining the future of the scientific poster. **R. Bocwinski**

11:55 1256. Chemical Facility Anti-Terrorism Standards (CFATS). **N. Owens**

Savannah Marriott Riverfront
Chatham

Inorganic Chemistry

General

Financially supported by Division of Inorganic Chemistry
W. E. Lynch, *Organizer*
M. Johnson, *Presiding*

8:10 Introductory Remarks.

8:15 1257. Novel coordination and catalytic properties of Pd(II)-compounds of di-2-pyridyl ketone hydrazone compounds. **M.A. Bakir**

8:35 1258. Synthesis, characterization, and reactivity of bis(phosphino) pyrrole ligands and their complexes. **H. Fokwa**, M. Johnson

8:55 1259. Synthesis, characterization, and reactivity of palladium proazaphosphatrane complexes. **A. Matthews**, M.W. Johnson

9:15 1260. Understanding the photophysics of Ln(III) doped nanoparticles. **R.E. Ortega**, G.F. Strouse

9:35 1261. Synthesis and reactivity of benzyl-silyl phosphines for transition metal complexation. **N.S. Abeynayake**, V. Montiel-Palma

9:55 1262. Sterically encumbered dianionic dicarboranyl pincer ligand $(C_5H_3N)(C_2B_{10}H_{11})_2$ and its nickel(II) complex. **M. Islam**, D.V. Peryshkov

10:15 Intermission.

10:30 1263. Nickel catalysts supported by redox active ligand scaffold for aziridination. **D. Liu**, J. Bacsa, C.E. MacBeth

10:50 1264. Development of modular bis(phosphino) pyrrole ligands for late metal-catalyzed cross-coupling. **M. Johnson**

11:10 1265. Thermodynamic characterization of Ca(II) and Cd(II) binding to wild type and mutant C35A, C84A, and C35A/C84A HcTnC using isothermal titration calorimetry and inductively coupled plasma optical emission spectroscopy. **C. Palmer**, A. Cunningham, A.M. Spuches

11:30 1266. Modulation of proton movement at the active site of a [NiFe]-hydrogenase: Cooperativity between the first and second coordination spheres. **G. Vansuch**, B. Greene, C. Wu, D.K. Haja, B. Chica, S.A. Blair, M.K. Johnson, M.W. Adams, R.B. Dyer

11:50 1267. Selective imine and amine synthesis catalyzed by a well-defined cobalt complex and a base. **K. Paudel**

12:10 1268. Early transition metal complexes for C-N bond formation: New insights towards DNA hybrid catalysis. **J. Cope**, B. Donnadieu, D. Wolgemuth, S. Elmore, H.U. Valle, J.P. Emerson

Savannah Marriott Riverfront
Reynolds

Materials Chemistry

W. E. Lynch, *Organizer*
G. Morrison, *Presiding*

8:10 Introductory Remarks.

8:15 1269. Tuning the frequency of localized surface plasmon resonances. **C.R. Conti**, G.F. Strouse

8:35 1270. Understanding ORR/OER catalysis in alkaline media using MnFe_2O_4 and LaNiO_3 : Towards epitaxially grown bifunctional catalysts. **A.R. Combs Bredar**, M.D. Blanchet, R.B. Comes, B.H. Farnum

8:55 1271. Exceptionally high C_2H_2 adsorption affinity in robust ultramicroporous metal-organic frameworks. **T. Pham**, K. Forrest, Y. Peng, Z. Zhang, B. Space

9:15 1272. Physical and electrochemical properties of copper deficient CuCrO_2 for application in Li-ion batteries. **A. Chown**, B.H. Farnum

9:35 1273. Using thiazolothiazoles as highly stable and highly fluorescent bridges for electrochromic and membrane voltage sensing applications. **N. Sayresmith**, J. Sailer, S. Patberg, A. Saminathan, K. Sandor, Y. Krishnan, M.G. Walter

9:55 1274. Materials discovery via family expansion: Structure prediction in the wadeites and superwadeites. **G. Morrison**, V. Kocevski, S. Misture, N.R. Spagnuolo, A.T. Hines, T. Besmann, B.O. Wilkins, M.D. Smith, H. Zur Loye

10:15 Intermission.

10:35 1275. Design strategies to enhance amidoxime chelators for uranium recovery. **B. Aguila**, S. Ma

10:55 1276. Monodisperse perovskite oxide nanocrystals with tunable size and composition for enhanced oxygen reduction reaction. **Y. Harn**, Z. Lin

11:15 1277. PbTiO_3 nanosheets from a layered titanate precursor. **M.A. Pedraza**, M. Davidson, T. Salguero

11:35 1278. Fluorinated imidazolium paramagnetic ionic liquids. **J.E. Knoop**, T.D. Jones, J.R. Alston

11:55 1279. Synthesis, structural, and photophysical properties of series of closo-decaborates with 1-pyridinium-10-x substituents. **M.B. Abdulmojeed**, T. Schafer, A.C. Friedli, P. Kaszynski, A. Pietrzak

Savannah Marriott Riverfront
Ballroom E

Well-Defined Supramolecular Materials

Financially supported by Division of Inorganic Chemistry
N. B. Shustova, *Organizer, Presiding*

8:10 Introductory Remarks.

8:15 1280. Designing MOFs for trace CO₂ capture. **C.R. Wade**, C. Bien, Z. Cai, Q. Liu

8:45 1281. Conformal, ultra-thin MOF-based films: Characterization of growth, porosity, and electronic transport. **M.E. Anderson**

9:00 1282. Gas-phase synthesis of hierarchically structured and responsive metal-organic frameworks. **T. Kempa**

9:30 1283. Light harvesting and energy transfer in a porphyrin-based metal-organic framework. **S.M. Shaikh**, A. Chakraborty, J. Alatis, M. Cai, E.O. Danilov, A.J. Morris

9:45 1284. Modulating guest based photophysics in metal organic frameworks. **R.W. Larsen**

10:00 Intermission.

10:15 1285. Self-assembled reversed bilayer vesicles through pnictogen bonding: Step one in the design of a truly artificial cell. S. Moaven, **A.F. Cozzolino**

10:45 1286. Electronic properties and photophysics of photochromic frameworks. **C.R. Martin**, N.B. Shustova

11:00 1287. Syntheses of copper tetrachalcogenide metallate (Mo/W) nanoparticles and their applications towards energy storage. **M.M. Li**, S. Ivanov

11:30 1288. Ruthenium(II)-polypyridyl doped zirconium(IV) metal-organic framework UiO-67-Ru films for solid-state electrochemiluminescence. **M. Cai**, Q. Loague, J. Zhu, S. Lin, A.J. Morris

11:45 1289. Redox reactivity of soft and porous materials. **C.K. Brozek**

Savannah Marriott Riverfront
Mercer

Forensic DNA Analysis & Beyond: Enabled by Biological Chemistry

O. Venderpuye, *Organizer, Presiding*

8:15 Introductory Remarks.

8:20 1290. History and introduction to forensic DNA testing. **O. Venderpuye**

9:00 1291. The comparison of MtDNA control region haplotypes between individuals of known maternal lineage and ancient skeletal remains from the flevaeis plot archaeological Site in rhodes. **P. Marshall, M. Lohr**

9:40 1292. Case study analysis of DNA evidence: An examination of criminal defense and prosecution systems in south georgia. **M. Gilbert**

10:20 Intermission.

10:40 1293. Development of cannabis sativa autosomal and organelle genotyping methods for forensic and intelligence purposes. **R. Houston, D. Gangitano, M. Roman**

11:20 1294. Forensic epigenetics, a powerful technique to determine body fluids and phenotype. **B. Mccord**

Savannah Marriott Riverfront
Pulaski

Advancement in Microwave Chemistry

Financially supported by CEM
S. M. Landge, *Organizer, Presiding*

8:30 1295. Interactive experience with microwave technology in teaching and research labs. **S. Ly, L. Robinson**

9:10 1296. Selective microwave heating of organic reaction mixtures. **G.B. Dudley**

9:30 1297. Microwave initiated nanomanufacturing towards energy applications. **X. Zhang, S. Sarwar**

9:50 Intermission.

10:05 1298. One-pot microwave assisted Suzuki coupling synthesis of substituted isoxazoles: Efforts to minimize self-coupling byproducts. **N.L. Powell, B. Harmon**

10:25 1299. Green synthesis of five and six membered nitrogen containing heterocycles. **S.M. Landge**

10:45 1300. Microwave induced solution-combustion synthesis of complex metal oxides. **A.L. Washington**, C. Dandeneau

11:05 CEM Workshop Demonstration.

Savannah Marriott Riverfront
Atrium

Chemical Education

S. R. Mooring, *Organizer*

8:30 - 9:45

1301. What I did for summer vacation: Experiences of a high school student in a college research lab. **G.K. Coleman**, B. Wicker

1302. How yogurt can be used to teach biochemistry. **T. Zimmerman**, S.A. Ibrahim

1303. Investigating the effects of laboratory learning environment on students' learning outcomes in a general chemistry course. **D.M. Samarasekara**, D. Mlsna

1304. Hands-on electrospray ionization-mass spectrometry for undergraduate biochemistry students: Peptide identification by ladder sequencing. **V.L. Perera**, B. Acharya, A.L. Patrick, D. Mlsna

1305. NSF Noyce program: REMAST (recruit and engage math and science teachers) at Newberry College, phase I (2009-2015) and phase II (2015-2020) through year 5. **C.P. McCartha**, C. Horn, R. Stubbs, S. Peters, N. Simmons, C. Aulbach, K. Simmons, G. Rushton

1306. Food chemistry applications through baking and sensory analysis in a summer research apprentice program. **H. Colleran**, R.C. Silva, S. Ibrahim

1307. Pt(0) nano-dispersed in a range of organically modified silicates as catalysts for the hydrosilylation of imines and oximes. **S. Giglio IV**, **M. Agbo**, B. Bernard, J. Fotie

1308. Consumer considerations of local value-added dairy products in North Carolina's original research triangle cities. **G.A. Agyekum**, S.A. Ibrahim, K. Jefferson-Moore

1309. Optimized growth medium for the selective enumeration and differentiation of *Lactobacillus* ssp. *bulgaricus*. **S.A. Ibrahim**, S.O. Aljaloud, A. Oyeniran, A. Krastanov

1310. Preliminary assessment of food safety knowledge and practices at a university food service establishment in Bulgaria. **H. Fidan**, S.A. Ibrahim

1311. Peer mentoring: Analysis of success and web resources for STEM tutoring centers. **D.W. Dixon**, J. Boone, K. Wellborn, A. Craig

1312. Green oxidations using oxoammonium salt for the undergraduate laboratory and student research. **A.L. Bartelson**

1313. Get involved with the ACS division of chemical education. **S.L. Johnson**

1314. Wheetrometer project: Low cost, lab built instruments for UV / VIS / near-IR spectrophotometry. **J.S. Summers**

1315. Determination of the density of eggs as they age to improve a general chemistry laboratory experiment. **S. Hutchison**, K.R. Wilson

1316. Teaching GOB organic chemistry as a general science core class for non-science majors. **D.R. Zuidema**, J. Jian

1317. Tandem reduction and cyclization of 2-nitrophenylacetylenes as a preparation of indoles. **C. Ballard**, **L. Repke**

Savannah Marriott Riverfront
Franklin

Entrepreneurs Tool Kit

J. E. Sabol, *Organizer*

J. Skinner, *Presiding*

8:30 1318. Small business development center assistance for existing and prospective small business owners. **B. Brownlee**

9:00 1319. Intellectual property and contract considerations for start-ups. **M.D. DeMott**

9:30 1320. Managing your online presence. **C. Cowart**

10:00 Intermission.

10:30 1321. Sales as a career alternative in the chemical industry. **J.P. Stoner**

11:00 1322. Board of directors and scientific advisory board: Know the needs for your start-up company. **J. Skinner**

11:30 Panel Discussion.

Savannah Marriott Riverfront
Atrium

Environmental Chemistry

W. E. Lynch, *Organizer*

8:30 - 9:45

1323. Functionalized shell-shell-core (SSC) nanopesticide for mosquito control. **A. White**, L.R. Pokhrel

1324. Analysis of factors affecting the removal of polyacrylamide from water by UV persulfate method. **J. Huang**, D. Yang, W. Pang

1325. Electrospinning of nanofiber polystyrene and silica layered mats for the visible colorimetric detection of polycyclic aromatic hydrocarbons in water. **J. Horne**, D. Sanchez, C. Cook, J. Perch, Y. Lu, M. Elliott, **E.K. Wujcik**

1326. Hygroscopic properties of marine aerosol particles and their role in cloud droplet formation. **R. Bramblett**, A.A. Frossard

1327. Seasonal measurements of atmospheric PAHs in the Atlanta metropolitan region via passive air sampling. K. Del Risco, D. Patel, **K. Zimmermann**

1328. Encapsulated oxygen releasing compounds in biodegradable micromaterials for environmental remediation. **K.R. McCormac**, M.J. Beazley

1329. Investigation of hygroscopic properties of giant cloud-condensation nuclei with an aerosol optical trap and humidified tandem differential mobility analyzer. **B.E. Swanson**, R. Bramblett, A.A. Frossard

1330. Impacts of the mountain valley pipeline: Longitudinal changes in the baseline assessment of Mill Creek, Bent Mt., Virginia. **M. Bennington**, K. Bishop, K.R. Roth

1331. Heavy metal pollution and loss of metal metabolism in eastern oysters (*Crassostrea virginica*) from the Elizabeth River, Virginia. **B.F. Lasseter**, R.P. Burke, B.W. Auchmoody, A. Russotti

1332. Change in wax profiles for CCD colonies. **B.F. Lasseter**, D.V. Liskin, R. Schopp, C. Reed

1333. Development of an extraction technique for surfactants in ambient aerosols and estuarine water from Skidaway Island, GA. **T. Burdette**, R. Bramblett, W.C. Hudson, D. Phillips, K. Zimmermann, A.A. Frossard

1334. Biosorption of copper(II) to ground peanut hulls: pH dependence and regeneration capacity. **S. Adom**, C.L. Huffman

1335. Assessment of environmental adversity of chemicals in traditional laboratory experiments: Best practices and benefits. **K. Banerjee**

1336. Chemostratigraphy of the Big Harris River system using trace metal and particle size analyses. **S.N. Sullivan**, **G. Carney**, C.L. Huffman, J.R. Miller

1337. Hydrogen molybdenum tungstate bronze films for reduction of carbon dioxide to formate. D.W. Scott, **M. Basjunaid**

1338. Preparation and characterization study of modified multi-walled carbon nanotubes using iron oxide. **T. Tran**, D. Deocampo, N. Kabengi

1339. Sonochemical degradation of metribuzin in aqueous solutions. N. Mayon, **D. Wayment**

1340. Synthesis, isolation, and evaluation of oxidative behavior of aqueous fullerene oxide (C₆₀O) suspensions. **J. Ingham**, R.S. Hikkaduwa Koralege

1341. Vermicompost from stormwater pond phycoremediation: Multidisciplinary (EPA-P3) STEM project. **M. Howard**, E. Malcolm, P. Rock, K. Henry, W. McConnell, A. Marosi, N. Craft, G. Steel, E. Hipple, P. Venanzi, W. Canady, M. Class

1342. Sink or swim: Biotic influences on carbon cycling in a vegetated barrier island ecosystem. **E. Long**, S.L. McCallister, J.C. Zinnert

1343. Geochemical fingerprinting reveals effects of urbanization and geology on natural water across Middle Tennessee. **B. Davis**, A.F. Callender

1344. Concentrations and sources of trace metals in water and sediments of the South Fork New River, Ashe County, North Carolina, and their potential effects on aquatic biota. **X. Watkins**

Savannah Marriott Riverfront
Johnson

K-12 Teachers

L. W. Padgett, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 1345. Chemical ecology made easy: Teaching students about the link between toxin chemistry and HABs. **M.C. Curran**, A. Robertson, M. Richlen

9:35 1346. Leveraging engineering for student success in chemistry. **T. Kinner**

10:35 1347. Classroom demonstration on ocean acidification. **C. Hintz**

11:35 1348. Implementing culturally responsive curriculum in the chemistry classroom. **S. Oxley**

Savannah Marriott Riverfront

Oglethorpe A

Organic Chemistry

Method Development

X. Chen, *Organizer*

W. Lei, *Presiding*

8:30 Introductory Remarks.

8:35 1349. One spot synthesis of highly regioselective 2,3-dihydrobenzofurans acetate through palladium catalyzed annulation of acrylic ester as synthons. M. Khan, **A. Nath**

8:55 1350. Brønsted base mediated *trans* hydroboration of alkynamides. **R. Fritzemeier**, R.J. Grams, W.L. Santos

9:15 1351. Low-waste synthesis of long-chain alkylbenzenes on superacidic mesoporous catalysts. **A.A. Kuvayskaya**, A. Vasiliev

9:35 1352. Novel chromium(III) photocatalysts for radical cation cycloadditions. **B.K. Gall**, E.M. Ferreira

9:55 1353. Transition metal catalyzed asymmetric dearomatization of heteroarenes. **R. Karimov**

10:15 Intermission.

10:35 1354. Stereoselective synthesis of olefins using swellable organically modified silica nano-reactors. **A. Azieva**, N.N. Shaw

10:55 1355. One-pot enol silane formation-Mukaiyama aldol reactions promoted by trimethylsilyl trifluoromethanesulfonate. **C.W. Downey**

11:15 1356. Swellable organically modified silica facilitated organic synthesis. **N.N. Shaw**

11:35 1357. Selected synthetic transformations of a polycyclic diene toward novel oxa-bowls. **M. Etzkorn**, M.J. Faussett

Savannah Marriott Riverfront
Ballroom C

Organic Chemistry

Method Development: Functionalization

X. Chen, *Organizer*
G. Gumina, *Presiding*

8:30 Introductory Remarks.

8:35 1358. Palladium-catalyzed synthesis of α -trifluoromethyl benzylic amines via fluoroarylation of *gem*-difluoro-2-azadienes enabled by phosphine-catalyzed formation of an azaallyl-silver intermediate. **C.I. Onyeagusi**

8:55 1359. Synthesis, isolation, and characterization of alpha-oxo gold carbenoids. **C.P. Stow**, R. Widenhoefer

9:15 1360. Regioselectivity influences in platinum-catalyzed enol ether formation. **J.P. Costello**, K. Huynh, E.M. Ferreira

9:35 1361. Trifluoromethyl fragmentation approach to accessing β -fluoro Michael acceptors. **A.T. Adam**, F.R. Fronczek, D.A. Colby

9:55 1362. Deoxyhalogenation of alcohols to alkyl halides using a silatrane moiety and acetyl chloride. **S.E. Varjosaari**

10:15 Intermission (C-H functionalization).

10:35 1363. Intermolecular allylic C-H etherification of internal olefins. **T. Farmer Nelson**, S. Blakey

10:55 1364. C-H functionalization of aromatic alcohols utilizing readily attachable and cleavable molecular scaffolds. **S.L. Jackson**, B.J. Knight, J. Rothbaum, Q. Li, E.M. Ferreira

11:15 1365. Regioselective CP*Ir(III)-catalyzed allylic C-H sulfamidation of terminal olefins. **A. Kazerouni**, S.W. Chen, K.R. Sharp, T. Farmer Nelson, S. Blakey

11:35 1366. Convergent synthesis to access an enantiopure indenyl ligand scaffold. **C. Poff**, S. Blakey

Savannah Marriott Riverfront
Forsyth

Patent Law for Chemists: What You Need to Know

A. Weisbruch, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 1367. Patent law for chemists: What you need to know. **A. Weisbruch**, T. Carr

9:35 Intermission.

9:45 1368. Patent law for chemists: what you need to know. **T. Carr**

10:45 Intermission.

10:55 Panel Discussion.

11:25 Concluding Remarks.

Savannah Marriott Riverfront
Atrium

Analytical Chemistry

C. McKenas, *Organizer*

10:00 - 11:30

1369. Characterization and analysis of binding interactions between photactive Cr(III) diimine complexes and DNA. **H. Burney**, N.A. Kane-Maguire, J.F. Wheeler, S.K. Wheeler

1370. Determination of deoxynivalenol and ochratoxin A in North Carolina grown organic wheat grains. **J. Yu**, N. Mikiashvili, C. Liang

1371. Investigating antioxidant activity of sulfur and selenium-containing complexes. **B. Ward**, A. Adrian, L. Kurfman, C. Edmunds, J.L. Brumaghim, S.K. Wheeler, J.F. Wheeler

1372. Bacterial exometabolomics by high-resolution mass spectrometry. **C.A. Chamberlain**, M. Hatch, T.J. Garrett

1373. Characterization of red blood cell derived extracellular vesicles using Raman spectroscopy. **A. Konutham**, J. Oh, R. Patel, A. Gaggar, R.A. Dluhy

1374. Feasibility study of using ion mobility-mass spectrometry to detect RNA modifications. **H. Wang**, J. Simpson, D. Todd, N. Chiu

- 1375.** Profiling the epitranscriptome in glioblastoma. **J.H. Simpson**, D. Todd, J. Teng, B. Tannous, N. Chiu
- 1376.** Applying standard additions to chronoamperometric reactive oxygen species measurements in cancer cells. **R.R. Pandey**, Y. Guo, Y. Gao, C.C. Chusuei
- 1377.** Evaluating self-segregation of semen components via SERS. **M. Bond**, D.D. Evanoff
- 1378.** Iron bioavailability in a novel soy-based cookie. **A. McBride**, K.R. Roth
- 1379.** Wax oleogel: Prospect of a healthy saturated fat substitute. **R.C. Silva**, B.D. Johnson, H. Collieran, S. Ibrahim
- 1380.** Quantifying the atrazine degradation ability of mycelium utilizing high performance liquid chromatography (HPLC) and quadrupole time of flight mass spectrometry (QTOF-MS). **R. Pandya**, L. Olson, S. Gowen, S. Wheeler, J.F. Wheeler
- 1381.** Development of an analytical method to detect commonly used herbicides, glyphosate and AMPA. **A.C. Staiano**, E.N. Graves, T. Griffin, S. West
- 1382.** Identification of microplastics in green sea turtle (*Chelonia mydas*) gastrointestinal contents. **M.I. Smith**, R.E. Bachman, N. Richárd, R. Hazelkorn, G. Lovewell
- 1383.** Secondary metabolite profiling and natural product discovery from cyanobacterial blooms of North Carolina. **M. Recchia**, K. Wright, A. Grogan, K. Clement, C. de Souza, R. Williamson, W.K. Strangman
- 1384.** Exploring a multi-spectral analytical scheme for color dye identification. N. Chong, **D. Taylor**
- 1385.** Investigation of toxic heavy metals in coffee samples by graphite furnace atomic absorption spectroscopy. **J. Lyons**, **S.M. Abegaz**
- 1386.** Valorization of lignin through a mild organosolv treatment of biomass. **M. Dorrani**, B. Lynn
- 1387.** Is goldenseal stable under different storage conditions? Targeted and untargeted approaches to study the effects of storage conditions on stability of *Hydrastis canadensis* (Goldenseal). **M. Khin**
- 1388.** Electrochemical detection of dopamine with doped and undoped silicon nanowires. **N. Karki**, S. Krylyuk, A. Davydov, C.C. Chusuei
- 1389.** Comparison of the observed size-dependent melting point of CdSe nanocrystals to theoretical predictions. **A.D. Dukes**, C.D. Pitts, A.B. Kapingidza, D.E. Gardner, R.C. Layland

- 1390.** Surface-enhanced resonance Raman scattering of rhodamine B in thin films of multilayer $\text{Ti}_3\text{C}_2\text{T}_x$ MXene nanosheets. **K. Allen-Perry**, R. Lascola, D.E. Autrey
- 1391.** Size-dependent electrochemical deposition of Au on Au nanoparticles. **H. Nambiathan Nambiar**, F.P. Zamborini
- 1392.** Combination of a Prussian blue modified electrode with a glucose oxidase encapsulated xerogel for the detection of glucose. **O. Butbul**, D. Budner
- 1393.** Glucose oxidase and Prussian blue nanoparticles encapsulated within a xerogel for the detection of glucose. **D. Baker**, D. Budner
- 1394.** Electrochemical characterization of potassium chromate in buffered acidic solutions for water purification. **C.M. Stern**, D.W. Hayes, L.O. Kgoadi, N. Elgrishi
- 1395.** Initial investigation of Prussian blue electrode applications with cholesterol and galactose. **E. Zhang**, D. Budner
- 1396.** Statistical modeling for identifying dyes on fibers found at crime scenes. **D. Rich**, A. Abraham, N. Ratnasena, K. Livingston, S.L. Morgan
- 1397.** Use of DRIFTS in the identification of accelerants in fire debris. **R. Kerr**, J. McCutcheon
- 1398.** Comparative study between feed forward neural networks and least absolute shrinkage and selection operator for the degradation detection of polyester-urethane audio magnetic tapes. **N. Ratnasena**, A. Abraham, D. Rich, L. Cunha, S.L. Morgan
- 1399.** N-donor heterocycles for trivalent actinide and lanthanide separations. **B. Kilgore**, J.D. Carrick, C.A. Hawkins
- 1400.** Prediction of diesel fuel physicochemical parameters using partial least squares regression and mid-infrared spectroscopy data. **H.Z. Msimanga**, C.R. Dockery, D. VanDenbos