The 67th Southeastern and 71st Southwest Regional Meeting of the American Chemical Society

November 4-7, 2015

Abby Parrill-Baker, *Program Chair*

WEDNESDAY MORNING

Cook Convention Center
L-2

General Biological Chemistry

S. Pedigo, *Organizer, Presiding*

8:00 1. Hydroxychalcones as inhibitors of *Streptococcus mutans* biofilms. **B. Nijampatnam**, H. Wu, S.E. Velu

8:20 2. F_{420} cofactor dependent glucose-6-phosphate dehydrogenase from *Mycobacterium tuberculosis*: Kinetic and biophysical characterization of wild-type enzyme and a His40 mutant. **M. Oyugi**, G. Bashiri, E. Baker, K.L. Johnson-Winters

8:40 3. A small molecule screen identifies a natural product that disrupts the fungal cell wall integrity pathway by targeting Hsp90. **S. Tripathi**, Q. Feng, M. Jacob, X. Li, A. Clark, A. Agarwal

9:00 4. Development of high-throughput screening of WecA for identification of novel antibacterial agents. **S. Siricilla**, K. Mitachi, M. Kurosu

9:20 5. Investigating enzymatic resistance to fosfomycin by FosB in Gram-positive bacteria. **M.E. Keithly**, M.K. Thompson, D.F. Stec, J. Harp, M.V. Voehler, W.J. Chazin, R.N. Armstrong

9:40 6. Metabolomic analysis of volatile organic compounds emitted from decomposing human cadavers. **D.C. Haines**, T. Deyne

10:00 7. Analysis of site directed mutants of diacylglycerol kinase-β by LC-MS/MS and bi-substrate kinetics. **T.T. Pham**, D.L. Baker

10:20 Intermission.

10:40 8. nNav1.5 blockers for breast cancer metastasis therapy. **S. Dutta**, S. Roger, K. Selander, S.E. Velu, W. Brouillette

11:00 9. Analysis of the bi-substrate kinetics of sphingosine kinase-1 inhibitors. **T.T. Pham**, S.B. Gacasan, D.L. Baker

11:20 10. Kinetic studies of n–heterocyclic carbene–ruthenium complex in catalytic radical reduction. **Y. Htet**

11:40 11. Expanded structure-activity relationship analysis of small molecule autotaxin inhibitors. **L. Ragle**, D.L. Baker, A.L. Parrill-Baker

12:00 12. Design and synthesis of platinum-containing quinazoline-based tyrosine kinase inhibitors as anticancer treatments. **M. Yang**, T.K. West, G.L. Kucera, U. Bierbach

Cook Convention Center
L-6

General Computational Chemistry

H. Kurtz, *Organizer, Presiding*

8:00 13. Combining metabolite-based pharmacophores with Bayesian machine learning models for *Mycobacterium tuberculosis* drug discovery. **S. Ekins**, P. Madrid, M. Sarker, S. Li, N. Mittal, X. Wang, T. Stratton, M. Zimmerman, C. Talcott, P. Bourbon, M. Travers, M. Yadav, J.S. Freundlich

8:20 14. Electronic structure of light-harvesting antennas in purple bacteria. **K. Shrestha**, E. Jakubikova

8:40 15. Computational studies of spin trapping of biologically relevant radicals by new heteroaryl nitrones. **E. Asempa**, S.J. Kirkby

9:00 16. Designing neutralizing antibodies for Marburg and Ebola viruses. **A. Sangha**, J. Meiler, J.E. Crowe

9:20 17. Theoretical aspects of the molecular imprinting of penicillin. **J.M. Saloni**

9:40 18. Opportunities for computational prediction of contaminant toxicity, fate, and transport properties to support disaster response. **W.A. Alexander**, N.J. Deyonker

10:00 19. Phosphoramidate hydrolysis catalyzed by hHINT1: A cluster-model DFT computational study. **G. Liang**, C.E. Webster

10:20 Intermission.

10:40 20. Characterization of C-X...π interactions using state-of-the-art computational techniques. **K. Riley**

11:00 21. Prediction of pKa via a QM/QM approach. **P. Patel**, J. Wang, A.K. Wilson

11:20 22. Structures, relative energies, and ligand dissociation energies of $Ir_x(CO)_y(NHC)_z$ clusters. **S. Zhang**, S. Foyle, B.C. Gates, A.S. Katz, D.A. Dixon

11:40 23. The pivotal role of di-copper catalysis in 1,3-dipolar cycloadditions: A reaction valley study. **T.M. Sexton**, D.H. Cremer

12:00 24. Computational investigations of structural, electronic, and wavefunction effects on molecular hyperpolarizability. **D.A. Clabo**, M. McDaniel, P. Snowden, M. Miles

Cook Convention Center
L-4

General Physical Chemistry

W. A. Alexander, *Organizer, Presiding*
D. J. Bellert, *Presiding*

8:00 25. Nature of metal ion mediated second shell hydrogen bonds. **D. Chakravorty**

8:20 26. Ionic liquid binary mixtures with organic solvent as an electrolyte for wide temperature and high performance supercapacitor applications. **R. Jayawickramage**, J.S. Bonso, J.P. Ferraris

8:40 27. Study of the effect of anion on the x-ray crystal structures and thermal properties of 1,3-dibenylimidazolium based ionic liquids. **E. Gurung**, R. Tao, D. Unruh, M. Cetin, G. Tamas, M.F. Mayer, S.L. Simon, E.L. Quitevis

9:00 28. A novel technique for energy resolved measurements of gas phase ion molecule rearrangement and decomposition reaction kinetics. **Z. Theis**, A. Mansell, D.J. Bellert

9:15 29. Energy resolved transition metal assisted decomposition of simple organic molecules. **A. Mansell**

9:30 30. Single photon initiated dissociative rearrangement reactions (SPIDRR) of transition metal ion/molecule systems. **D.J. Bellert**, A. Mansell, Z. Theis

9:45 Panel Discussion.

10:00 Intermission.

10:40 31. On the importance of conformational analysis for accurate prediction of molecular properties. **W.A. Alexander**, K. Charbonnet, T. Brown, N.J. Deyonker

11:00 32. Diffusion of benzene and alkylbenzenes in *n*-alkanes. **B.A. Kowert**, P.M. Register

11:20 33. Synchrotron based infrared vibrational-rotational spectroscopic study of isobutylene. **S.W. Reeve**, T.N. Clasp, B. Billinghurst

11:40 34. Chemical kinetics in the processing of nuclear materials. **J. McFarlane**, L.H. Delmau, D.W. DePaoli, C.H. Mattus

12:00 35. Adsorption studies of water and methanol on a metal phosphide surface. **H.L. Abbott-Lyon**

Cook Convention Center
L-3

General Analytical Chemistry

J. Russ, *Organizer, Presiding*

8:15 Introductory Remarks.

8:20 36. Real-time measurements of oxidative stress during chronic L-DOPA treatment for Parkinson's disease. **L.R. Wilson**, C.A. Lee, C.F. Mason, L.A. Sombers

8:40 37. Voltammetric method for the determination of diffusion and partition coefficients in plasticized polymer membranes. **J. Sheppard**, E. Lindner

9:00 38. The Stokes-Einstein equation and the diffusion of ferrocene in room temperature ionic liquids (RTILs) studied by cyclic voltammetry. **M. Thakurathi**, E.L. Quitevis, M.F. Mayer, m. cetin, E. Gurung

9:20 39. Quantification of some heavy metals levels in samples of edible nuts. **J. Mierzwa**

9:40 40. Detection of natural product off-rates within complex matrices
. **A. Singh**, J.J. Bowling, R.E. Lee

10:00 Intermission.

10:20 41. Quantification of thiol Raman activity and pK_a values using Raman-based pH titration. **N.S. Suwandaratne**, D. Zhang

10:40 42. Using water Raman intensities to determine the effective excitation and emission pathlengths of fluorophotometers for correcting fluorescence inner filter effect. **C.B. Nettles**, D. Zhang

11:00 43. Raman spectroscopy and liquid-liquid microextractions. **A.F. Callender**, U. Sharma Phuyal

Cook Convention Center
Mississippi Room

General Chemical Education

F. J. Creegan, M. B. Freilich, *Organizers*
G. Bhattacharyya, R. Glazener, *Presiding*

8:20 44. Incorporation of benchtop NMR spectroscopy into undergraduate laboratories: An active-learning approach. **S. Riegel**

8:40 45. A multi-year analysis of commercial bleach solution. **S.K. Hutchison**, C.E. Dahm

9:00 46. Analysis of food dyes in powdered drinks. **S.K. Hutchison**, K.R. Wilson, J.W. Hall

9:20 47. Salicylic acid and 4-nitroaniline removal from water using magnetic bio-char: An environmental and analytical experiment for the undergraduate laboratory. **A.G. Karunanayake**, O.A. Todd, N.B. Dewage, M. Essandoh, T. Mlsna, D. Mlsna

10:00 Intermission.

10:20 48. Making sense of the endless: Information seeking behaviors of organic chemistry graduate students. L. Cain, **G. Bhattacharyya**

10:40 49. Introducing metal catalysis in the introductory organic chemistry laboratory. **C.E. Ballard**

11:00 50. Instructional technology to increase student engagement and participation in chemistry. **R. Glazener**

11:20 51. Monitoring gains in visualization skills. **M. Oliver-Hoyo**

11:40 52. Coupling DFT calculations with experiment in the physical chemistry laboratory. **T.C. Devore**, A. Bagley, J. Yin

Cook Convention Center
L-7

General Organic Chemistry

Synthesis

T. J. Burkey, *Organizer*
K. H. Pannell, *Presiding*

8:20 53. Synthesis of carbocyclic ring systems from donor-acceptor cyclopropanes. **R. Nareddy**, K.T. Mead

8:40 54. Syntheses, structures, and chemistry of a small series of isoindederivatives. **M. Etzkorn**, V.L. Wait, A. Smith, J.L. Franklin, C. Strickland

9:00 55. Synthesis of substituted pyridines from dihydropyridones. **S. Kiren**

9:20 56. Siloxymethylamines: Methylamine transfer reagents leading to new organic chemistry. **K.H. Pannell**, H. Sharma, P.E. Gonzalez, S. Chakrabarty

9:40 57. Palladium-catalyzed direct arylation of C(sp^3)-H bonds of α-cyano aliphatic amides. E. Watkins, **M.D. Reddy**

10:00 Intermission.

10:20 58. Synthesis and isolation of CCC-NHC pincer Rh complexes and catalytic β-boration of α, β-unsaturated carbonyl compounds. **G. Akurathi**, S. Reilly, T.K. Hollis

10:40 59. Highly stereoselective synthesis of terminal chloro-substituted propargylamines and further functionalization. **M.L. Turlington**, S. Jordan, S.A. Starks, M.F. Whatley

11:00 60. Organotellurium chemistry: novel Te, N-containing heterocycles. **T. Junk**, G. Sanford, K. Walker, F. Fronczek

11:20 61. Friedel–Crafts hydroxyalkylation of N-alkylindoles with aryl aldehydes: Isolation of 1:1 adduct through a silyl triflate-mediated reaction. **C.W. Downey**

11:40 62. Regioselective transition metal-free 1,4-conjugate addition of Grignard reagents to dienones and thiodienoates. **E. Amoah**

Cook Convention Center
Sultana Room

Bio-Related Polymers: Synthesis and Applications

T. Fujiwara, *Organizer, Presiding*
E. P. Kharlampieva, *Presiding*

8:30 Introductory Remarks.

8:40 63. Polysaccharide-based biomaterials for regenerative medicine. **T.L. Lowe**

9:20 64. Stimuli-responsive multilayer nanobiomaterials for controlled delivery and transplantation. **E.P. Kharlampieva**

10:00 65. Photo-induced release of retinoic acid from polymer micelles for cardiomyogenic stem cell differentiation. **M.K. Gupta**, D. Balikov, H. Sung

10:20 Intermission.

10:40 66. Polymeric carriers for on-demand therapies and conquering the undruggable . **C. Duvall**

11:20 67. Pattern-based sensing applications of hyperbranched poly(amidoamines). **M. Bonizzoni**

11:40 68. Preparation of lipoate-related branched polymers by two different chemistries: Utilizing radical ring-opening reaction of cyclic disulfide and thiol-ene reaction. **H. Tang**, N.V. Tsarevsky

Cook Convention Center
L-5

General Inorganic Chemistry

N. J. Deyonker, *Organizer, Presiding*

8:40 69. Oxovanadium(IV) carboxylates. **J.W. Hall**, S.K. Hutchison, V.R. Griffin, M.T. Griffin, J.R. Wasson

9:00 70. Facile activation of red phosphorus through solution- and flow-chemistry methods. **A. Dragulescu-Andrasi**, L. Miller, D.T. Mc Quade, M. Shatruk

9:20 71. Ligand-to-ligand and host-to-guest energy transfer in hybrid crystalline scaffolds. **E. Dolgopolova**, D.E. Williams, A.M. Rice, N.B. Shustova

9:40 72. Photoswitch-directed photoluminescence of metal-porphyrin frameworks. **D.E. Williams**, E. Dolgopolova, N.B. Shustova

10:00 73. Metal-organic frameworks with bowl-shaped ligands. **A.M. Rice**

10:20 Intermission.

10:40 74. Visible light active semiconductor composites for enhanced photocatalytic activity. **S.P. Adhikari**, A. Lachgar

11:00 75. Codeposition and potential pulse atomic layer deposition (PP-ALD) of CdTe thin films. **X. Zhang**, J.L. Stickney

11:20 76. Amperometric detection of hydrogen peroxide and uric acid using a zinc oxide carbon nanotube composite. **C.C. Chusuei**, M.B. Wayu

11:40 77. Combinatorial/computational approach to the discovery of new intermetallics. **K. Ryan**, M. Mustyakimov, M. Shatruk

Cook Convention Center
West Mezzanine

General Inorganic Chemistry

N. J. Deyonker, *Organizer*

9:00 - 11:00

78. Metallocene dichlorides intercalation into the inorganic layered nanomaterial zirconium phosphate for potential cancer therapy. **B. Casañas-Montes**, A. Diaz, C.M. Barbosa Nunez, C. Ramos Gonzalez, C. Collazo, E. Melendez, F. Fayon, C. Queffelec, A. Clearfield, B. Bujoli, J.L. Colon

79. Dynamic nanospheres for individualized, localized drug delivery of chemotherapeutics and antibiotics. **P. Cole**, S. Thornburgh, B. Burnett, A. Ozkizilcik, Z. Tian, F. Carbonero

80. Quantifying the thermodynamics that define calcium selectivity: A comparison to cadmium. **R.A. Johnson**, A.M. Spuches

81. Applications of luminogenic iridium azide complexes. **F. Vohidov**, J. Ohata, A. Aliyan, K. Huang, A.A. Marti, Z.T. Ball

82. Incorporation of Zn^{2+} in PbS quantum dots via cation exchange. **W.R. Tilluck**, C. Mings, A.L. Morris, P.G. Van Patten

83. Withdrawn.

84. Exploring new physics in photon-photoelectron interactions on micropatterned, zinc oxide hyper-branched nanorods. **T. Chism**, **G. Torix**, Z. Tian

85. Optical and surface studies of $Pb_{0.95}La_{0.05}Zr_{0.54}Ti_{0.46}O_3$ films deposited by chemical solution deposition method for solar cells applications. **V. Batra**, S. Kotru, C. Ramana

86. Mesoporous materials containing heteropolyacids. **O. Adetola**, A. Vasiliev

87. Copper(I) sulfide nanorods: Utilizing crystal-bound ligands and oriented attachment to create a desirable nanoparticle morphology. **E.H. Robinson**

88. Synthesis, characterization, and antimicrobial studies of manganese (III) and europium (III) metal-doped ZnO nanoparticles. **N. Dragan**, N.D. Darsanasiri, J.M. Lee, I. Bose, C.R. De Silva

89. Using metal coordination complexes in mechanically responsive systems. **K. Hall**, K.J. Franz

90. Low temperature synthesis of amorphous vanadium pentoxide nanofibers and their transformation to crystalline material. **M. Wunch**, W. Perera, D. Yang

91. An aqueous phase synthesis of metal nanoparticles with controlled geometries. **A. Penn**, T. Abeywickrama, H.P. Rathnayake

92. Polyborafluorenes and borafluorene copolymers. **I.A. Adams**, P. Rupar

93. Bactericidal heavy metal nanocomposites for industrial and biomedical platforms. **P. Cole**, S. Thornburgh, B. Burnett, Z. Tian, F. Carbonero

94. New chemistry in making the nonflammable graphene oxide membranes for rechargeable batteries and fuel-cells. **H. Turgut**, R. Rogers, C. White, Z. Tian

95. Dispersion study of exfoliated graphene nanoparticles. **K. Kim**, Y. Kim, C. Kim, S. Lee, J. Park, D. Yang

96. Effects of ionic liquids on stability, structure and reactivity on biological macromolecules. **H.U. Valle**, T.A. Rogers, T. Al-Mohanna, P.C. Hillesheim, J.P. Emerson

97. The effectiveness of methods to functionalize glass-based substrates. **A. Maharanwar**

98. Photochemical synthesis of silver and gold-silver alloy nanoparticles with tunable plasmonic absorption via aqueous and biocompatible media. **D. Korir**, **A. Hilgemier**, **M. Omary**

99. Sustainable green nanotechnology: Remediation of drinking water to industrial effluent treatment strategy. A.L. Daniels, M.M. Simmons, A.M. Barr, **S. Kuriyavar**

100. Plotting the limits of core/shell magnetic exchange. **D. Carnevale**, M. Shatruk, G.F. Strouse

101. Synthesis and characterization of polyphosphonates derived from polyethylene glycols and their use as ligands in styrene hydroformylation catalysts. **T.R. Totsch**, B. Yancey, G.M. Gray

Cook Convention Center
West Mezzanine

General Physical Chemistry

W. A. Alexander, *Organizer*

9:00 - 11:00

102. SCHB is your link to success. **J.E. Sabol**

103. On use of graphene to make supercapacitors with higher ampacity. **K.R. Sharma**

104. Exploring the reactions and transition states of tungsten-pyrrole complexes. **C. Shepard**

105. Anomalous gel-fluid phase transition of solid-supported lipid membranes. **A. Poursoroush**, E.J. Spangler, M. Laradji

106. On complex fluids and diffusion law: *A capite ad calcem* in concentration. **K.R. Sharma**

107. Raman spectroscopic and computational analysis of the effects of noncovalent interactions on DMSO. **H.K. Trent**, A.T. Nicholson, G.S. Tschumper, D.H. Magers, N. Hammer

108. Membrane-mediated aggregation of anistropically curved nanoparticles. **A.D. Olinger**, E.J. Spangler, P. Sunil Kumar, M. Laradji

109. Evaluation of defoamer chemistries for brown stock washing. **R. Hamm**

110. The accuracy of quartic force field computations: Comparison between semi-experimental and computational results. **Z. Lee**, R.C. Fortenberry

111. Investigation of the binding affinity of malachite green on magnetic colloids using surface selective spectroscopy. **T.A. Williams**, J. Lee, C.A. Diemler, M. Subir

112. Reinvestigation of the resonance Raman spectrum of the blue ruthenium dimer. **K.E. Allen**, H.A. Dulaney, J.W. Jurss, N. Hammer

113. Investigating the effects of solvent on the surface-enhanced Raman scattering (SERS) of nitrogen containing molecules: Azabenzenes and 1H-1,2,3 triazole. **V.T. Tran**, L.E. McNamara, J.T. Kelly, N. Hammer

114. Mucin penetrating magentic nanoparticles for therapeutic application. **V.N. Boya**, R. Lovett, V. Gandhi, S. Setua, M. Yallapu, M. Jaggi, S.C. Chauhan

115. High-resolution electronic spectroscopy of the ultraviolet bands of CaO. **M.N. Sullivan**, J. Stewart, M. Heaven

116. An efficient Pd-Cu single atom alloy catalyst prepared by galvanic replacement for acetylene selective hydrogenation. **A. Mirjalili**

117. Investigation of optical properties of gold/near IR emitting quantum dot hybrid nanoparticles. **K.M. Dipple**, M. Jones

118. Assembly of nanobattery array using ion beam deposition. **J.W. Ostrander**, D.C. Teeters

119. Synthesis and spectroscopic characterization of a novel Ru(II)tris(2,2'-bipyridine) templated metal organic framework derived from Zn(II) and 1,4 benzene dicarboxylate. **C. McKeithan**, R.W. Larsen

WEDNESDAY AFTERNOON

Cook Convention Center
L-3

General Analytical Chemistry

J. Russ, *Organizer*
D. L. Baker, *Presiding*

12:55 Introductory Remarks.

1:00 120. Investigating the chemical kinetics of the reaction between haloacetic acids and nicotinamide used in post-column reaction ion chromatography. **N. Harris**, G.L. Emmert, P. Simone

1:20 121. Using automated on-site and hourly trihalomethane concentration data to calibrate empirical models to be site-specific. **R. Snow**, T. Watts III, G.L. Emmert, P. Simone

1:40 122. Stabilization kinetics of melt processable poly(acrylonitrile-co-n-vinylimidazole) carbon fiber precursors. **B.L. Batchelor**, S. Mahmood, M. Jung, H. Shin, D. Yang

2:00 123. Discrimination of the leaf level emissions of volatile organic compounds from chestnut tree species by gas chromatography-mass spectrometry and chemometrics. **J. She**

2:20 124. Analysis of xylitol in sugar-free gum by GC/MS with direct aqueous injection. **S.M. Rajapaksha**, J.C. Brown, K.K. Gerken, T. Mlnsa

2:40 125. Sulfonamides and analogs in extraction-based sensing applications: Combining coordination chemistry and solvent extraction principles for selective sensing of toxic metals and other ionic targets. **K. Kavallieratos**

3:00 Intermission.

3:20 126. Electrochemical investigations into the formation of germanene. **M. Ledina**, J. Jung, J.L. Stickney

3:40 127. Anion sensors. **A. Hossain**

4:00 128. Effect of exfoliated graphene nanoparticle based coatings on corrosion-resistance, and UV spectral study of chemically modified graphene nanoparticles. S. Lee, **K. Kim**, Y. Kim, C. Kim, S. Lee, J. Park, D. Yang

4:20 129. Rebuilding and use on rusty iron surfaces and weathered galvanized steel surfaces with a powdered zinc dust in an EPA sustainable (low carbon footprint), water-thinned acrylic emulsion paint containing barium metaborate. **L.A. Wienert**

4:40 130. Catalytic efficiency of hard Lewis acid metal ions on cadmium vapor generation. **Z. Arslan**, A. Celik

5:00 Concluding Remarks.

Cook Convention Center
Chickasaw Room

DNA Modifying Enzymes

E. Enemark, *Organizer, Presiding*

1:00 131. A structural framework for how homologous recombination is stimulated by the phage T4 recombination mediator protein UvsY. **S.W. White**, S. Gajewski, S. Vaithiyalingam, B. Waddell, A. Nourse, J. Meiler

1:40 132. DNA glycosylase catalysis without base flipping enables base excision repair of bulky lesions. E.A. Mullins, R. Shi, Z.D. Parsons, P. Yuen, S.S. David, Y. Igarashi, **B.F. Eichman**

2:20 133. Structural insights into the NuRD-like SHREC complex and its mechanism of heterochromatin silencing. C. Brugger, G. Job, T. Xu, S. Shanker, Y. Pfister, B. Lowe, J. Banos Sanz, T. Schalch, **J. Partridge**

3:00 Intermission.

3:40 134. Crystal structure of a bacteriophage T7 primase-helicase DNA polymerase complex provides a molecular snapshot of replisome assembly. **J. Wallen**, B.M. Foster, J.L. Collins, T. Ellenberger

4:20 135. Substrate specificity of MutT pyrophosphohydrolase using nucleotide analogues. **M. Hamm**

4:40 136. Insights from the crystal structure of an MCM hexamer. **J.M. Miller**, **E. Enemark**

5:00 137. Mapping the residues of human WRN helicase involved in unwinding G-quadruplex DNA. **A. Ketkar**, M.V. Voehler, T. Mukiza, R.L. Eoff

Cook Convention Center
West Mezzanine

General Analytical Chemistry

J. Russ, *Organizer*

1:00 - 3:00

138. GC-MS measurement of xenon in fluids for neuroprotective applications. **J.R. Hurling**, M.R. Moody, T. Peng, S. Huang, D.D. McPherson, M.E. Klegerman

139. Biocompatible, biodegradable metal-binding cyclic peptides for heavy metal toxicity removal. **Y. Beni**, A. Yadav, A. Banerjee, P. Bhai Patel, A. Shirazi, K. Parang

140. An electrochemical platform for real-time metabolic profiling in liver-on-chip systems. **E.A. Gizzie**, D.E. Cliffel

141. Fabrication and characterization of the micro-impedance detector for enumeration of circulating tumor cell. **J. Watters**

142. Imaging of lipids in the ocular vitreous humor using matrix-assisted laser desorption ionization-mass spectrometry. **A. Schnepf**, M.C. Yappert, D. Borchman

143. ^{31}P NMR characterization of chitosan phosphorylation. **D.J. Suchyta**, M. Schoenfisch

144. Effect of blood and an oxidation agent on a novel cyanide antidote. **X. Dong**, **T. Barcza**, **L. Kiss**, **R.J. Roy**, **I. Petrikovics**, **D. Thompson**

145. Surface enhanced Raman spectroscopy of cyanide metabolite 2-aminothiazolene-4-carboxylic acid (ATCA) on immersed and dried substrates. **M. Kaur**, D. Thompson

146. Electrochemical detection of acetaminophen, H_2O_2, and dopamine using tapered silicon nanowires. **R.R. Pandey**, H.S. Alshahrani, E.H. Williams, S. Krylyuk, A. Dayvydov, C.C. Chusuei

147. Get involved with the ACS Division of Chemical Education. **M.D. Perry**, F.J. Creegan

148. Chromium (III) supercharging in electrospray ionization mass spectrometry of biological peptides. C.J. Cassady, **R. Hacherl**

149. Solid-phase extraction-77K laser excited time resolved fluorescence spectroscopy for the analysis of benzo[a]pyrene metabolites in urine samples. **B.F. Alfarhani**

150. Selective nano-sensing approach for the quantitative analysis of phosphate ions in biological matrixes. **A.A. Fadhel**

151. Polysaccharide-mediated formation of pigments from catecholamines. **M. Alhumaidi**, K. Vercruysse

152. Polysaccharide-mediated formation of pigments from serotonin. **N.A. Alattas**, K. Vercruysse

153. Optimization of a measurement system for pH measurement in tear fluid samples. **B.P. Hambly**, E. Lindner, E. Pinkhassik, S. Dergunov

154. Using fluorescent probes to study the location and interaction of disaccharides with lipid bilayers. **M. Barker**, A.M. Kennedy

155. Thermal stability of gelatin gels confined to silica gel nanopores. **J.R. Prado**, S.V. Vyazovkin

156. Coronene diimide containing polymer films via electropolymerization of diphenylamine end groups. **S.C. Paul**, V. Cammarata

157. Fluorescent assay for beta-galactosidase activity in probiotic gram-positive bacterial cells. **A. Watson**, N. Chiu

Cook Convention Center
West Mezzanine

General Inorganic Chemistry

N. J. Deyonker, *Organizer*

1:00 - 3:00

158. Ternary metal-hydroxo complexes of Fe^{3+} and Cr^{3+} with clofibric acid (CA): A peroxisome proliferator-activated receptors-alpha (PPARα) ligand. **Y.Z. Hamada**

159. Design of mesoporous silica nanoparticles for the delivery of platinum-acridine anti-cancer drugs. **Y. Zheng**, S. Ding, B.W. Bernish, .D. Fahrenholtz, R. Singh, C.S. Day, M.D. Gross, U. Bierbach

160. Investigation of relationship between the γ-ray absorber and polymer matrix in plastic scintillators. **R. Gray**, M. Shatruk

161. Pnictide mixed-aromatics. **J.W. Hall**, M.T. Griffin, J.R. Wasson

162. Seven-coordinate 18 e- complexes of tungsten (II) bearing "N_2S_2" ligands: Synthesis and reactivity. **A. Greene**, S.J. Ferrara, E. Haas, J.T. Mague, J.P. Donahue

163. Synthesis and optical properties of phosphonate-substituted free and locked bithiophenes. **D. French**, J.L. Freeman, Q. Zhao

164. Synthesis, characterization, and biological studies of Ru-Pt bimetallic complexes. **K. Wyland**, E. Hoffman, A. Hagelgans, D. Davis, A. Jain

165. Chiral α,ω-Bis(phosphite) polyether ligands for use in the asymmetric hydroformylation of styrene: Synthesis and characterization. **E. Cagle**, G.M. Gray

166. Long-term, stable, and highly efficient alternatives of Z-907: Amphiphilic Ru(II) sensitizers for dye-sensitized solar cells (DSSC). **H. Cheema**, A. El-Shafei

167. Nitrene transfer to half-sandwich iridium(Cp*) complexes. **C. Turlington**, M. Brookhart, J.L. Templeton

168. Photocatalytic hydrogen evolution by homogeneous molybdenum sulfide complexes. **P.R. Fontenot**

169. Electronic tuning of H_2 production catalyzed by Co complexes with pentadentate ligands. **S.R. Powers**

170. Metathesis reactivity of bis(phosphinite) pincer ligated nickel chloride, isothiocyanate, and azide complexes. **J. Zhang**

171. Nickel-catalyzed CO_2 reduction supported by biaryl-bridged pyridyl-*N*-heterocyclic carbenes. **H.A. Dulaney**, L. Bell, R. Higgins, J.W. Jurss

172. Synthesis of a pentadentate, polypyrazine ligand and its application in cobalt-catalyzed hydrogen production. **A. Khadivi**, M. Singh, J.W. Jurss

173. Robust iron-oxo catalysts for water oxidation. **L. Chen**, H.A. Dulaney, Y. Zhang, S. Farmer, J.W. Jurss

174. Synthesis and characterization of carboxylate complexes of lanthanide (III) ions. **Z. Gebeyehu**, C. Milliron III

175. Synthesis, characterization, and luminescent studies of europium doped $NaYbF_4$ nanoparticles. **J.M. Lee**, G. Attanayake, C.R. De Silva

176. Reliable potential energy surfaces for the reactions of H_2O with ThO_2, PaO_2^+, UO_2^{2+}, and UO_2^+. **M. Vasiliu**, D.A. Dixon, K.A. Peterson, J.K. Gibson

177. Investigating computational, structural, physiochemical and biological properties of a family of pyridoxine-lanthanide metal complexes. **A. Saha**, C.E. Stouder, K. Warren, C.W. Padgett, A.L. Stewart, K.S. Aiken, S.M. Landge, A. Amonette

178. Nanofiber based metal oxide photocatalysts for hydrogen generation through water splitting, pollution remediation, and chemical conversion. K. Latimer, I. Thompson, K. Cook, D. Daniels, P. Elam, **K. Senevirathne**

179. Solventless synthesis and characterization of novel Ag(I) and Cu(I) metal-azolate complexes upon vapor-phase reaction with different substituted cyanopyridines. **A.R. Hinkle**, K. Reyes, S. Hutcheson, K. Maxwell, V. Nesterov, M. Omary

180. Synthesis, characterization, and luminescence of CCC-NHC pincer platinum complexes. **M. Zhang**, X. Zhang, L. McNamara, N. Hammer, N. Kaneza, S. Pan, C.E. Webster, T.K. Hollis

181. Metal–tetrazolate trinuclear complexes and functional non-porous coordination polymers. **R.M. Almotawa**, A. Cimino, V. Nesterov, S. Galli, A. Maspero, M. Omary

182. Utilizing hydrophobic coatings in corrosion protection and anti-icing. **W.K. Yaseen**, M. Rawshdeh, M.A. Omary, T. Golden, S. Nasrazadani

183. Ligand control in the photochemical generation of high-valent porphyrin-iron-oxo derivatives. T. Chen, K. Kwong, **J. Malone**, R. Zhang

Cook Convention Center
L-4

Recent Advances in Chemical Physics

Recent Advances in Chemical Physics

N. Hammer, *Organizer*
D. J. Goebbert, S. Pan, *Presiding*

1:00 184. Local redox events at individual plasmonic nanoparticle electrodes using electrogenerated chemiluminescence microscopy. **S. Pan**

1:20 185. Time resolved IR of Rhenium diimine tricarbonyl donor-acceptor complexes: Tracking events in intramolecular energy and electron transfer reactions. Y. Yue, T.A. Grusenmeyer, I.V. Rubtsov, **R.H. Schmehl**

1:40 186. Characterizing the effects of noncovalent interactions on the photophysics of newly developed near infrared emissive materials. **L.E. McNamara**, T. Rill, E.A. Sharpe, A.J. Huckaba, J.H. Delcamp, N. Hammer

2:00 187. Electrochemical and spectroscopy studies of bodipy-thiophene-triphenylamine based dyes for dye-sensitized solar cells. **N. Kaneza**, S. Pan, Z. Shan, A.S. Panikar, J. Zhang, A. Gupta, H. Liu

2:20 188. Correlation of atomic structure and photoluminescence of single InP/ZnX(X=S,Se) quantum dots. **K. Reid**, N. Orfield, J. McBride, S.J. Rosenthal

2:40 189. Evolution and dynamics of GaN-based blue laser diode emission spectra. **W. Al-Basheer**

3:00 Intermission.

3:20 190. Elucidating quantum dot structure-function relationships one dot at a time. **N. Orfield**, J. McBride, K. Reid, S.J. Rosenthal

3:40 191. Infrared photodissociation spectroscopy of early and late transition metal-acetylene complexes. **A.D. Brathwaite**, T.B. Ward, M.A. Duncan

4:00 192. Unraveling proton transfer in stepwise hydrated N-heterocyclic anions. **J.T. Kelly**, Y. Wang, K.H. Bowen, G.S. Tschumper, N. Hammer

4:20 193. X-ray spectroscopy as a probe of the magnetism in cobalt benzene cluster cations. **S. Akin**, V. Zamudio-Bayer, T. Lau, M.A. Duncan

4:40 194. Mass spectrometric studies of aluminum nitrate anion complexes. **D.J. Goebbert**

5:00 195. Mid-infrared signatures of hydroxyl containing water clusters: Infrared laser stark spectroscopy of $OH\text{-}H_2O$ and $OH(D_2O)_n$ (n=1-3). **J. Brice**, G.E. Douberly

Cook Convention Center
Sultana Room

Bio-Related Polymers: Synthesis and Applications

T. Fujiwara, *Organizer*
C. Duvall, D. L. Watkins, *Presiding*

1:20 196. Injectable and degradable polymeric biomaterials for regenerative medicine. **S. Wang**

2:00 197. Exploring the promise of nanomedicine: Highly specific nano-scaled polymeric biomaterials for imaging and treatment of cancer. **T. Betancourt**, T. Cantu, T. Ozel, C. Munoz, J. Irvin, S. Weigum, E. McIvor, K. Walsh, V. Pattani, J. Tunnell

2:40 198. Design and synthesis of supramolecular Janus-type dendrimers as efficient therapeutic carriers. J. Williams, L. Ezell, N. Le, **D.L. Watkins**

3:00 Intermission.

3:20 199. Multifunctional polyelectrolyte complexes with embedded metal ions. **L. Zhai**, A. Malhotra

4:00 200. Stimuli responsive drug delivery system for curcumin to counteract radiation injuries. **R. Chauhan**, A. Akalkotkar, B. Nunn, P. Soucy, R. Keynton, M. O'Toole

4:20 201. Synthesis and characterization of PXS based polymers for improved nanoparticle drug delivery. **I.B. Kelly**, N. Arnett

Cook Convention Center
Mississippi Room

Cancer Nanotechnology

X. Huang, *Organizer, Presiding*

1:20 202. Highly efficient capture and accurate identification of multiple types circulating tumor cells using multifunctional biocompatible graphene oxide quantum dots decorated magnetic nanoplatform. **P.C. Ray**

2:00 203. Cancer nanotheranostics. **X. Chen**

2:40 204. Plasmon-resonant nanorods and gyromagnetic nanostars: Multifunctional agents for nanomedicine. **A. Wei**

3:20 Intermission.

3:40 205. RNA as a stable anionic polymer for theranostic nanoparticle construction in cancer nanotechnology. **H. Li**, P. Guo

4:00 206. A new interleukin-13 amino-coated gadolinium metallofullerene nanoparticle for targeted MRI detection of glioblastoma tumor cells. **T. Li**, S. Murphy, S. LaConte, Z. Sheng, H.C. Dorn

4:20 207. Nanoparticles for imaging cargo delivery and cellular environments *in-vivo*. **G.F. Strouse**

4:40 208. Controlling nucleic acid delivery from gold nanoparticles in mammalian cells, studied via live-cell fluorescence microscopy. **K.J. Carnevale**, G.F. Strouse

5:00 209. Magnetic-optical hybrid nanoparticles for the capture and detection of cancer cells. **S. Bhana**, R.T. O'Connor, X. Huang

Cook Convention Center
L-6

General Computational Chemistry

H. Kurtz, *Organizer*
M. L. Cafiero, *Presiding*

1:20 210. Evaluation of a perturbative treatment of three-body interactions in HCP ^{4}He. **A.L. Barnes**, R.J. Hinde

1:40 211. Three-body interactions of solid helium calculated within the Einstein model. **D. D'Andrea**, R.J. Hinde

2:00 212. Electrostatics, relativistic effects, and the bonding in group 12 dihalide clusters. **K. Donald**

2:20 213. Theoretical study of metal monoalkylidines. **S. Dickerson**, N.J. Deyonker

2:40 214. Acquiring accurate absorption intensities for HNO from *ab initio* calculations. **H. Dhah**, R.J. Hinde

3:00 215. Withdrawn.

3:20 Intermission.

3:40 216. Transition metals in astrochemistry: Which roads lead to a better understanding of astrobiology? **N.J. Deyonker**, S. Dickerson, T. Brown

4:00 217. Quantifying electron delocalization in stretched bonds. **A. Mehmood**, B.G. Janesko

4:20 218. Comparison of two potential energy functions for predicting fit-for-purpose fuel properties using molecular dynamics. **M.T. Knippenberg**, B.L. Mooney, J.A. Harrison

4:40 219. Computational quantum chemistry studies of proposed reaction mechanisms for direct oxidation of melatonin. **C.E. Warden**, S.J. Kirkby

5:00 220. Computational investigation of linkage isomerization in sulfoxide-containing ruthenium complexes. **R.W. Lamb**, E.V. Dornshuld, C.E. Webster

Cook Convention Center
L-5

General Inorganic Chemistry

N. J. Deyonker, *Organizer, Presiding*

1:20 221. Carbene-stabilized disilicon-based transition metal compounds. **H. Hickox**, Y. Wang, M. Chen, P. Wei, G.H. Robinson

1:40 222. Hexacoordinate polypyridylsilicon(IV) compounds for electronic and catalytic applications. **T.A. Schmedake**, D.M. Peloquin, C. Waters, B.T. Donovan-Merkert, J.W. Merkert

2:00 223. Metallathiacrown ethers: Synthesis and characterization of transition metal complexes containing α,ω-bis(phosphite)-polythioether ligands and an evaluation of their soft metal binding capabilities. **J.R. Martin**, A.L. Lucius, G.M. Gray

2:20 224. Velocity map imaging study of the photoinitiated charge transfer – dissociation of Ag^+(benzene). **J. Maner**, D. Mauney, M.A. Duncan

2:40 225. Studying the reactions between group 5 transition metal atoms and CX_4 molecules (X = H, F, and Cl). **J.T. Lyon**, H. Cho, L. Andrews

3:00 Intermission.

3:20 226. Microwave-assisted synthesis and luminescence rigidochromism for ambipolar polyimines and rhenium (I) complexes thereof. **G.A. Salazar-Garza**, C.M. Williams, V. Nesterov, C. Yang, M.A. Omary

3:40 227. Organomanganese photochromic systems: Linkage isomerization and cage effects of bifunctional pyridine ligands substituted in the 2-position: A time-resolved infrared spectroscopic study. **T.C. McFadden**, T.J. Burkey

4:00 228. Metal-to-metal charge transfer in alkynyl bridged bimetallic complexes. **M. Turlington**, J. Pienkos, P.S. Wagenknecht

4:20 229. Oxido bridged heterobimetallic molecules containing first-row transition metals with long-lived excited states. **A.J. Falzone**, W. Weare

Cook Convention Center
L-7

General Organic Chemistry

Synthetic Methods

T. J. Burkey, *Organizer*
K. R. Wilson, *Presiding*

1:20 230. Debromination of vicinal dibromides in perfluorobenzene sulfonimide (PFSI) compounds. **R. McCloud**, C. Nworie, H. Mei

1:40 231. Developing methods for the synthesis of α-alkenyl- and α-alkynyl-phosphonates. **D. Kercher**, C.W. Alexander

2:00 232. Highly selective oxidation of sulfides to sulfoxides catalyzed by iron (III) corroles with iodobenzene diacetate. **K. Kwong**, T. Chen, W. Luo, J. Malone, R. Zhang

2:20 233. The synthesis of functionalized [*n*](3,3")*p*-terphenylophanes: Precursors to funtionalized cycloparaphenylenes. **R. Meudom**, B.L. Merner

2:40 234. Microwave-assisted cleavage of –alloc and –oallyl protecting groups in solid phase peptide synthesis. **K.R. Wilson**, S.A. Sedberry, R. Pescatore, S. Ballard, B. Love, D. Vinton, E. Williamson

3:00 235. New photochemical reactions and their applications. **P. Wang**, Z. Ding, D. Devalankar, L. Schwartz

3:20 Intermission.

3:40 236. A non-cross-coupling strategy for the synthesis of biaryl bonds: Towards the synthesis of [4] cycloparaphenylene. **C.P. Merryman**, B.L. Merner

4:00 237. Iridium(III)-bis(imidazolinyl)phenyl catalysts for intermolecular enantioselective C–H functionalization with acceptor-only diazoacetates. N.M. Weldy, **A. Schafer**, C. Owens, C. Herting, A. Varela-Alvarez, S. Chen, Z. Niemeyer, J. Musaev, M.S. Sigman, H.M. Davies, S. Blakey

4:20 238. Investigation of the Tsuji-Trost variant of the Winstein-Masamune spirocyclization as a unified approach to select lycopodium alkaloids. **N. Jentsch**, M. Donahue

4:40 239. Synthesis of bis-1,4-electrophiles as linchpins in the Tsuji-Trost variant of the Winstein-Masamune spirocyclization reaction. **R. Wehrle**, M. Donahue

5:00 240. Hydrolytic catalyst selection by affinity chromatography. **A.T. Tran**, J.T. Rapp, K.M. Nicholas

Cook Convention Center
L-2

General Biological Chemistry

S. Pedigo, *Organizer*
S. Davila, *Presiding*

1:40 241. The DNA adduct N-(2'-deoxyguanosin-8-yl)-3-aminobenzanthrone gives rise to a base-displaced intercalated structure. **D.A. Politica**, C. Malik, A.K. Basu, M.P. Stone

2:00 242. Drought effects on seed composition and minerals in soybean genotypes differing in slow-wilting trait. **N. Bellaloui**, A.M. Gillen, A. Mengistu, H. Kebede, D.K. Fisher, J.R. Smith, K.N. Reddy

2:20 243. Characterization of the 2,6-diamino-4-hydroxy-N^5-(methyl)-formamidopyrimidine DNA lesion. **S. Bamberger**, R. Bowen, C. Malik, T. Johnson Salyard, R. Dempster, C.J. Rizzo, M.P. Stone

2:40 244. Parsing the structure of the 8-(deoxyguanosin-N^2-*yl)*-1-aminopyrene adduct. **R. Bowen**, D.A. Politica, C. Malik, A.K. Basu, M.P. Stone

3:00 Intermission.

3:20 245. Deltaretroviral nucleocapsid proteins display non-equivalent levels of nucleic acid chaperone activity. **D.F. Qualley**

3:40 246. HOXB9 is transcriptionally regulated by endocrine disrupting chemical, bisphenol-A. **P. Deb**, **A. Bhan**, **I. Hussain**, K. Ansari, **S. Bobzean**, **L. Perrotti**, S.S. Mandal

4:00 247. Conformational and configurational equilibria of a 2′-deoxyribosylurea DNA adduct. **A.H. Kellum**, M.P. Stone, A.K. Basu, V. Jasti

4:20 248. A potentially vicious carcinogen: Profile of a cyclical reaction involving peroxochromium(IV) and glutathione. **R.A. Marin**, Y. Ahuja, R.N. Bose

4:40 249. Development of an amyloid-beta protofibril-selective antibody. **M.R. Nichols**, B. Colvin, V. Rogers, E. Ridgway

5:00 250. Effects of olive metabolites on DNA cleavage mediated by human topoisomerase II. **K. Vann**, C.A. Sedgeman, J. Gopas, A. Golan-Goldhirsh, N. Osheroff

Cook Convention Center
West Mezzanine

General Biological Chemistry

S. Pedigo, *Organizer*

3:20 - 5:20

251. Effect of glass color on IBU perception and IBU measured value on beer exposed to UV light. **N.O. Flynn**, P. Baumgardner

252. Promiscuity of CDO with alternative metals. **D.L. Forbes**, H.R. Ellis

253. Investigation into the potential dual role of SirC in the biosynthesis of tetrapyrroles in *Methanosarcina acetivorans* C2A. **V.L. Owens**, K. Zhen, S. Mansoorabadi

254. Synthesis and antimicrobial studies of pyrazole derivatives as potent antibacterial agents. **R. Trent**, **D. Gibler**, **J. Brider**, A.C. Ontko, D. Gilmore, M.A. Alam

255. Anti-metastatic effects of thiopurine prodrugs on prostate cancer by targeting Rac1. **H. Umutesi**, J. Heo

256. Chemical analysis of chicken bone during diagenesis in soil. **M.J. Danker**, J. Bytheway, D.C. Haines

257. Assay development for the screening of antimicrobial peptoids. **K. Fisher**, A. Corson, K. Bicker

258. Oxysterol-binding protein family (OSBP/ORP) ligand binding and natural product drug development. **J.I. Nunez**, N.R. Kothapalli, A.W. Burgett

259. Characterizing the canonical macrodomain of the bat coronavirus HKU4 nonstructural protein 3 (nsp3). **R. Hammond**, M. Chan, X. Tan, C. Tian, M.A. Johnson

260. Novel exogenous agonist design for caseinolytic protease. **J.W. McDonald**, S.E. Velu

261. Association between volatile organic compounds and microbes present during the decomposition of a cadaver. **T. Deyne**, D.C. Haines, A. Lynne, S. Bucheli

262. Isothermal titration calorimetry of *Ceriporiopsis subvermispora* bicupin oxalate oxidase. **H. Rana**, L.S. Rocha, E.W. Moomaw

263. Liposomal encapsulation of UV filters. **R.J. Roy**, L. Kiss, I. Petrikovics, L. Budai, M. Budai

264. P450BM-3 enzyme activity on acyl homoserine lactone (AHL) and thiolactone (AHTL) quorum sensing signals. **U.V. Ariyaratne**, D.C. Haines

265. Application of golden gate assembly method to combine the catalytic core of luciferase enzyme and fluorescent protein in pETDuet-1 cloning vector to detect protein-protein interactions. **T.R. Ratnayake**, D.C. Haines

266. Extraction of antibacterial compounds produced by *Pseudomonas* and *Serratia* species, and induction of antibiotic production by bacterial competition. **K. Blair**, S.C. Seaton, A.L. Wolfe

267. Investigating post-translational modifications in cysteine dioxygenase. **C.J. Graham**, H.R. Ellis

268. Isolation and characterization of natural product antibiotics produced by *Sarracenia purpurea* pitcher plant bacteria, and induction of antibiotic production during co-culture with *Streptomyces griseus* and other inducer strains. **J. Tweed**, S.C. Seaton, A.L. Wolfe

269. Phosphorylation of serine, threonine, and tyrosine residues of the CXCR3 receptor establish a barcode that regulates distinct downstream pathways. **N. Desai**, J. Smith, S. Rajagopal, P. Alagesan

270. Investigating metabolic mechanisms of bacterial CDO. **L.K. Stanford**, H.R. Ellis

271. Rh(II)-catalyzed protein modification as a method for determining ligand affinity. **S.E. Knudsen**, F. Vohidov, Z.T. Ball

272. Towards a new class of inhibitors of cysteine proteases: Cruzain and falcipain-2. **B.C. Chenna**, X. Zhai, S.A. Perez, T.D. Meek

273. Chemical composition of *Blumea lacera* essential oil from Nepal: Biological activities of the essential oil and (Z)-lachnophyllum ester. **P. Satyal**, W.N. Setzer

274. Proteins interacting with protein kinase C highlight roles in filamentous fungal cell wall synthesis. **Z. Atiq**, **E. Olsen**, C. Matthew, L. Myers, T. Hill, L. Jackson-Hayes

275. Optimizing expression of *Pf*PK9. **J. He**, R. Raphemot

276. Analysis of amino acid residues predicted to be essential for loading of T7 DNA polymerase on to a primase-helicase ring. **B.M. Foster**, J.L. Collins, M. Carver, T. Ellenberger, M. Gainey, J. Wallen

277. Synthesis and molecular docking of pyrollobenzodiazepine derivatives as potential non-β-lactam β-lactamase inhibitors. **J.O. Osazee**, **A. Shilabin**

Cook Convention Center
West Mezzanine

General Organic Chemistry

Synthetic Methods

T. J. Burkey, *Organizer*

3:20 - 5:20

278. Synthesis of tethered aromatic compounds for use with fluorescence studies. **H.V. Clontz**, A. Manzewitsch, J.M. Gibson, S. Daniel

279. Efficient masking of carbonyl groups in the presence of nucleophiles using transient aluminum-aminals. **F.J. Barrios**, D.A. Colby

280. TMSOTf-mediated additions of acetonitrile to aldehydes, acetals, and nitrones. J. Santa, W.M. Stith, A. Lee, C.J. Botelho, **C.W. Downey**

281. Trimethylsilyl trifluoromethanesulfonate-mediated additions of indoles to aldehydes and nitrones. C.D. Poff, A.N. Nizinski, **C.W. Downey**

282. One-pot enol silane-formation-aldol condensation and Mannich addition reactions mediated by trimethylsilyl trifluoromethanesulfonate and amine base. H.M. Glist, J.A. Ingersoll, **C.W. Downey**

283. Acyl group activation of a 4-bromopyrrole ester in Suzuki cross-coupling reactions: Application to the synthesis of rigidin E and polycitones A and B. **J.T. Gupton**, A. Harrison, S. Yeudall, J. Wen, A. Shimozono, J. Ortolani, V. Moore-Stoll, E. Huff, E. Crawford, W. Curry, J. Patteson, M. Hoerrner, K. Lounsbury

284. Nitro and cyano group activation of a 4-bromopyrrole ester in Suzuki cross-coupling reactions: Application to the synthesis of KL-3-95, a pyrrole-containing, colchicine site inhibitor. **J.T. Gupton**, S. Yeudall, E. Huff, E. Crawford, M. Hoerrner, K. Lounsbury, K. Lescalleet

285. Enantioselective carbon dioxide fixation in small molecules using a bifunctional Brønsted acid/base organocatalyst. **T.J. Struble**, B.A. Vara, J.N. Johnston

286. A divergent/convergent epoxide approach towards the synthesis of (-)-dolabriferol. **K. Morales**, J.A. Prieto

287. Metal mediated reactions of hydrocarbons with carbon dioxide: An approach to study the mitigation of greenhouse gases. **A. Rahman**, K.M. Nicholas

288. Synthesis and characterization of *N*-alkylbenzoxazaboroles. **S. George**, D.E. Gross

289. Adsorption of immunoglobulin on cellulose and chitin films using surface plasmon resonance. **D. Sutton**, V. Popik

290. Cationic palladium catalyzed acetylation of alcohols and carbohydrate derived polyols. **E.A. Mensah**, F.R. Reyes, E.S. Standiford

291. Synthesis of 4,4-dialkoxy-BODIPYs via nucleophilic substitution. **A. Nguyen**, P.N. Bobadova-Parvanova, F. Fronczek, K.M. Smith, G. Vicente

292. The isolation and identification of phytochemicals from the leaf extract of *Tabernaemontana longipeas*. **S.D. Carothers**, M. Williams, H. Zhang, I.V. Ogungbe

293. Library of aurone derivatives synthesized through coupling reactions. **Z. Taylor**

294. Ni(II)-diamine complexes catalyzed asymmetric sequential Michael reactions of phenylketoesters and nitroalkenes: Synthesis of multifunctionalized cyclohexene derivatives. **S. Huang**, K. Scherer, B. Ni

295. A highly enantioselective [4+2] cycloaddtion of aldehydes and *β,γ*-unsaturated-*α*-keto ester using enamine catalysis. **N. Katakam**

296. Ceric ammonium nitrate oxidations of 2-alkyl-1,4-dialkoxybenzenes. **A.L. Simmons**, B.E. Love

297. Effective Cu-Pd dual catalyst system for direct amidation reaction from potassium organotrifluoroborates and amides. M. Al-Masum, **M. Islam**, W. Shaban

298. Imidazolium ion tethered TsDPENs as efficient ligands for iridium catalyzed asymmetric transfer hydrogenation of ketophosphonates in water. **M. Sun**, J. Campbell, B. Ni

299. Development of new glycosylation method and synthesis of complex carbohydrates. **P. Wang**, D. Devalankar, C. Christian

300. Synthesis of alpha, beta unsaturated carboxylic acids and their transformation to cyclobutane derivatives using solid state reactions. **K. Banerjee**, **A. Hanna**

301. Calcium catalyzed Mukaiyama-Mannich reaction. **E. Congdon**, K.A. Nolin

302. Controlling the stereochemistry of new C1 substituted carbapenems. **T. Nguyen**, M. Bennett, S. Casco, P. Nguyen, M. Alqurafi, C. Edwards, P. Gupta, C. Chiang, M. Lohry, M. Cox, E. Kim, M. Chepuru, R. Chepuru, D. Le, S. Smriti, P. Oelschlaeger, **J.D. Buynak**

303. Reactivity of bi(pyrazol-1-yl)acetic acid ligands with diiodo(η^6-*p*-cymene)ruthenium(II). B.P. Quillian, **A.E. Fields**

304. A new process of synthesizing anandamide derivatives from arachidonic acid in the presence of boron catalyst. M. Al-Masum, **L.S. Quinones**

305. Fe-catalyzed synthesis of 3-aryl-4-propenyl oxazolidines. **S. Murru**, C.S. Lott, **R. Srivastava**

THURSDAY MORNING

Cook Convention Center
West Mezzanine

General Biological Chemistry

S. Pedigo, *Organizer*

8:00 - 10:00

306. Volume change of the random coil to folded conformational transition of *Thermomyces lanuginosus* xylanase at 24^{o}C and pH = 7.0 via application of the Clausius-Clapeyron equation. **B. Britt**

307. Ensemble compactness is independent of charge and ionic strength in a multi-site phosphorylateable protein. **E. Martin**, A. Holehouse, R.V. Pappu, T. Mittag

308. Novel reductive pathways for hydroxywarfarin metabolism. **J. Burrell**, D. Pouncey, J. Hartman, G.P. Miller

309. Investigation of the catalytic mechanism of *Mycoplasma pneumoniae* L-alpha-glycerophosphate oxidase: Mutation of the proposed catalytic base. **C. Crowley**, A. Butler, A. Plaza-Rodriguez, D. Parsonage, A. Claiborne, J. Wallen

310. Preliminary studies of the proton induced folding of $(CCCTAA)_4$ using isothermal titration calorimetry. **T. Sutorius**, M.L. McKim, R.D. Sheardy

311. SPOP cancer mutations reduce protein assembly size, resulting in loss of function. **M.R. Marzahn**, S. Marada, J. Lee, A. Nourse, S. Kenrick, S.K. Ogden, T. Mittag

312. Determination of the cellular levels of the oxysterol-binding proteins OSBP and ORP4 upon treatment with the anti-cancer natural product OSW-1. **B. Roberts**, N.R. Kothapalli, A.W. Burgett

313. A novel-designed heterocyclic diamidine that recognizes mixed base pair DNA sequences: NMR characterization. **N.K. Harika**, M.W. Germann, A. Paul, Y. Chai, E. Stroeva, D.W. Boykin, W. Wilson

314. Exploring molecular driving forces of hnRNPA1 liquid-liquid phase separation. **N. Milkovic**, A. Palud, M. Frenkel, E. Martin, J. Taylor, T. Mittag

315. Design, synthesis, and microbiological evaluation of ampicillin-tetramic acid hybrid antibiotics. **P.T. Cherian**, A. Deshpande, M. Cheramie, D. Bruhn, H. Julian, R.E. Lee

316. Investigating function of water-soluble β2 adrenoreceptor mimics using circular dichroism. **S.B. Gacasan**, V.I. Godwin, L. Wink, B. Nguyen, P. Kurtzweil, L. Church, S. Iqbal, A. Kikonyogo, A.L. Parrill-Baker

317. Cyano-nilutamide conjugates with a DNA minor groove methylating agent for selective destruction of prostate cancer cells. M. Powell, E.A. Elliott, N.E. Neill, A. Bourdelais, **S. Varadarajan**

318. Novel fluorinated 9-amino acridones as covalent topoisomerase IIα poisons. **L. Infante**, A. Sledge, C.O. Okoro, N. Osheroff

319. Inhibition of carboxylesterases by *Salvia miltiorrhiza* "Danshen" root. **M.J. Hatfield**, R.J. Binder, L.G. Tsurkan, C. Jeffries, T.J. Smillie, R.M. Wadkins, P. Potter

320. Determination of the breakdown rate of pentobarbital in various soil types. **A. Saha**, G.M. Goodin, M. Abdallah, S. Siddiqi, P.C. Kline

321. Chemical footprinting of secondary DNA structures within the KRAS promoter. **R. Morgan**, T.A. Brooks

322. The location and number of the amidine groups on the classic duplex minor groove binder diminazene necessary for the low nanomolar dissociation constants associated with g-quadruplex binding. **C. Mikek**, J. Zhou, C. Wang, X. Ma, E.A. Lewis, H.O. Sintim

323. Biophysical investigations of c-MYC NHE-III_1 complementary strand forming i-Motif capped with flanking duplex ends. **A.M. Metz**, J.I. DuPont, E.A. Lewis

324. The effect of synthetic and natural compounds on tumor cell lines. **K. Alhaidari**, D. Myles, Jr, M.R. Karim

325. Effect of diallyl sulfide (DAS) and its commercially available analogues on *in vitro* cellular toxicity and inhibition of CYP2E1 enzyme. **M.A. Rahman**, P. Rao, N.M. Midde, S. Kumar

326. Ligand binding properties of the diheme protein in MauG. **N. Grace**, **A. Brown**, J. Brown, J. Cotton, M. Feng

327. Mechanistic studies of the tyrosinase-catalyzed oxidative cyclocondensation of 2-aminophenol to 2-aminophenoxazin-3-one. **N.R. McIntyre**

328. Effect of HPV-infected cervical cancer cells on HIV-infected monocytic cells: Clinical significance of HPV/cervical cancer and HIV/AIDS comorbidity. **B. Patters**, N. Sinha, S.C. Chauhan, S. Kumar

329. Expression and characterization of straight α-helix concatemers for nanosheet formation. **R.A. Bartlett**, V.P. Conticello

330. Structure of an MCM double-hexamer. **M. Meagher**, L. Epling, E. Enemark

331. Exploring the dynamics of polymerase switching among different DNA replication complexes. **M. Cranford**, A. Chu, M.A. Trakselis

332. Soft interactions between model molecular crowders and the ligands of dihydrofolate reductase. **M.R. Duff**, E.E. Howell

333. Physical and dynamics studies of the AlgH protein from *Pseudomonas aeruginosa* and the AlgH protein family. **J.L. Urbauer**, R. Bieber Urbauer

Cook Convention Center
West Mezzanine

General Computational Chemistry

H. Kurtz, *Organizer*

8:00 - 10:00

334. Probing the energetics of proton transfer in hydrated sulfuric acid clusters: $H_2SO_4(H_2O)_{n=1-6}$, with CCSD(T) computations. **T.L. Ellington**, G.S. Tschumper

335. Dependence of electrostatic potential critical point values on basis set size. K. Tran, **K. Riley**, P.A. Politzer, J.S. Murray, P.M. Lane

336. Computational investigations of isoform selectivity in liver X receptor. M. Ndukwe, **K. Riley**, J. Sridhar

337. DFT investigation of C-F bond activation by a low coordinate cobalt(I) complex. **Q. Jiang**, T.R. Cundari

338. Analysis of residue mutations on the enantiospecificity of CYP2C9. L. Bond, T. Meece, G.P. Miller, **M.D. Perry**

339. Intrinsic energetics of proton transfer from a weak acid to water in binary $(HF)_m(H_2O)_n$ clusters. **S.N. Johnson**, G.S. Tschumper

340. CDD Vision: A new reactive web platform for multidimensional drug discovery data mining and visualization. A. McNutt, **S. Ekins**, K. Gregory

341. A density functional theory study of novel catalysts for the "green" synthesis of aziridines. **C. Guan**, S. Karbalaei Khani, T.R. Cundari

342. Balancing inter- and intra-molecular forces: The challenging case of dihydrogen bonding and coordinate covalent bonding in ammonia borane clusters. **K.M. Dreux**, G.S. Tschumper

343. MP2 and CCSD(T) energetics for proton transfer in $(HCl)_m(H_2O)_n$ clusters, where $m+n \leq 6$. **A. Baumann**, G.S. Tschumper

344. Structural identification of fibroin and cellulose: Test of monotonically decreasing local minima optimization program. **R. Noumbissi**, B. Steckling, E. Koizumi, H. Koizumi

345. Transparent density functional code for quantum chemistry class. K. Saito, **N. Tanaka**, H. Jiang, E. Koizumi, **H. Koizumi**

346. Homology modeling of alpha viruses drug targets and virtual screening to identify their potential inhibitors. **J.T. Collins**

347. Water clusters in proton cancer therapy: Electron nuclear dynamics of $H^+ + (H_2O)_n$ at 100 keV. **A. Privett**, J. Yoo, E. Teixeira, C. Stopera, J.A. Morales

348. Withdrawn.

349. Calculating enthalpies of formation for amino derivatives of trinitrotoluene. S.L. Raines, E.Q. Chong, A. Sood, G.A. Hill, **D.H. Magers**

350. The conventional strain energies of cyclopropylborane, borirane, boretane, and the diboretanes. S. Nookala, J. Sims, S.A. Smith, **D.H. Magers**

351. Conventional strain energies of aziridine, oxirane, phosphirane, and thiirane. N. Alanazi, N. Alzaidi, S.A. Smith, **D.H. Magers**

352. Applying comparative modeling strategies and virtual docking toward deorphanization of GPR26. **L. Wink**, A. Kikonyogo, A.L. Parrill-Baker

353. Role of the substituent effects on the luminescent efficiency of phenazine-based europium β-diketonate complexes: A density functional theory study. **C.P. Jensen**, M. Pearce, J. Beasley, A.M. Lillie, S. Sedberry, B. Dinkelmeyer, C.R. De Silva

354. Application of surface enhanced Raman spectroscopy for distinguishing among isomeric structures of nitroanilines. **J. Fosten**, W.H. Ilsley, B. Ooi

355. Investigating physical properties of fuel components using molecular dynamics. **M.V. Sayger**, T. Knippenberg

356. Mechanism and kinetics of antioxidant activity of two recently synthesized antioxidants. **L. Pandey**

357. Computational investigation of substituent effects on guanine binding of 1-, 2-, and 1,2-substituted naphthalenes. **J.C. Horn**, S. Hayes, J. Korba, A.M. Priddy, A.Y. Lewis, J. Turner, M.A. Lewis

358. Hydrogen, ammonia borane, and carbon dioxide activation by phosphinoboranes. **M. Mendez**, D.A. Dixon

359. Automated design of small molecules with Rosetta. **R. Moretti**, S. Combs, J. Meiler

360. Predicting ^{195}Pt NMR chemical shifts in small Pt(II) and Pt(IV) organometallic compounds with density functional approaches. **E.V. Dornshuld**, M. Zhang, X. Zhang, T.K. Hollis, C.E. Webster

361. Density functional theory investigation of uranyl (VI) complexes with nitrogen donor terpyridine-type ligand derivatives. **C.R. De Silva**, P. Yang, J. Li

Cook Convention Center
L-4

Recent Advances in Chemical Physics

N. Hammer, *Organizer*
M. A. Duncan, C. S. Feigerle, *Presiding*

8:00 362. Revealing the pressure-induced breakdown pathway in WS_2 nanotubes. **J. Musfeldt**

8:40 363. Enhancements and applications of C_{60} in energy storage materials. **P.A. Ward**, B. Compton, R. Zidan, J.A. Teprovich, P. Jena, H. Colon-Mercado, V. Schwartz, G. Veith

9:00 364. Developing spectroscopy techniques to study interaction of anticancer drugs with DNA. **N. Mirsaleh-Kohan**

9:20 365. Adventures in anion photoelectron spectroscopy: CO_2 activation, water splitting, and rare earth mimics. **K.H. Bowen**

10:00 Intermission.

10:20 366. What is so positive about negative ions? **P. Jena**

11:00 367. Spectroscopy and decomposition dynamics of nitrophenoxide anions. **J.D. Steill**

11:20 368. Photoelectron spectroscopy and photochemistry of ozonide cluster anions, $O_3^-(H_2O)_n$ and $O_3^-(Ar)_n$,. **W.C. Lineberger**, A.M. deOliveira, J.H. Lehman

12:00 Concluding Remarks.

Cook Convention Center
Sultana Room

Bio-Related Polymers: Synthesis and Applications

T. Fujiwara, *Organizer, Presiding*
M. C. Stefan, *Presiding*

8:20 369. Functional polycaprolactones for delivery of anticancer drugs. **M.C. Stefan**, K. Washington, R. Kularatne

9:00 370. Biodegradable three-layered micelles for efficient non-viral gene delivery systems. **D.G. Abebe**, R. Kandil, T. Kraus, M. Elsayed, O. Merkel, T. Fujiwara

9:40 371. Design of hydrogels containing alginate and modified cellulose as superabsorbent materials. **P. Jimenez-Bonilla**, H. Haber, M.L. Auad

10:00 Intermission.

10:20 372. Mechanochemistry for soft, active materials and devices. **G.R. Gossweiler**, T. Kouznetsova, X. Zhao, S. Craig

10:40 373. Using multi-step synthesis for the production of hydrogels with adhesive properties. **J. Deardorff**, C.H. Lisse

11:00 374. Fast pyrolysis bio-oils as precursors of thermosetting epoxy resins. **B. Sibaja**, M.L. Auad

11:20 375. Mechanical analysis of chemically treated coir fibre polyester composites. **S. Bhagat**

11:40 Concluding Remarks.

Cook Convention Center
Mississippi Room

Cancer Nanotechnology

X. Huang, *Organizer, Presiding*

8:20 376. Protein corona on magnetic nanoparticle. **M. Yallapu**

9:00 377. Interdisciplinary approaches to evaluation the toxic potential of engineered nanomaterials: A regulatory perspective. **Y. Zhang**

9:40 378. Understanding the interactions of theranostic gold-based nanostructures with complex biological environment. **J. Chen**

10:20 Intermission.

10:40 379. Tuning the optical-plasmonic properties of Ag/Au hybrid nanoparticles for SERS detection. **E. Chaffin**, X. Huang, Y. Wang

11:00 380. Size- and shape-controlled synthesis and properties of magnetic-plasmonic core-shell nanoparticles. **E. Kwizera**, S. Bhana , X. Huang

11:20 381. Novel self-patented gold nanoparticles for augmented antineoplastic activity. **J. Payne**, R. Dakshinamurthy

11:40 382. Multifunctional NIR light-inducible plasmonic liposomes for combination anti-cancer therapy. **R.A. Crouch**, B.L. Hallmark, S.J. Jones, A. Pramanik, S.S. Sinha, P.C. Ray

12:00 383. Photosensitizer-loaded gold nanorods for combined photodynamic and photothermal cancer therapy. **R.T. O'Connor**, S. Bhana , X. Huang

Cook Convention Center
L-5

General Inorganic Chemistry

N. J. Deyonker, *Organizer, Presiding*

8:20 384. Screening racemic catalysts in Pt-catalyzed asymmetric synthesis of P-stereogenic bis(phosphines). **M.D. Sanderson**, Z. Xu, V. Farkas, D.S. Glueck, A.L. Rheingold

8:40 385. An N-heterocyclic carbene–ruthenium complex that catalyzes the reduction of radicals in aqueous solutions. **A.G. Tennyson**, Y. Htet

9:00 386. Controlling dimerisation of metallo-aminoalcohol complexes for supramolecular mixed metal structures. **A. De Sousa**

9:20 387. Coordination chemistry of versatile N-heterocyclic thione (NHT) and related ligands. **D. Rabinovich**

9:40 388. The role of steric factors in hydrogen activation: Incorporation of bulky N-heterocyclic carbene ligands into the coordination sphere of Bu^t_3Sn-Pt complexes leads to novel reactivity and catalysis. **B. Captain**, A. Koppaka, V. Yempally, M. Temprado, C.D. Hoff

10:00 Intermission.

10:20 389. The next experiment: Some successful applications of computational chemistry. **B.G. Janesko**

10:40 390. Carbene-stabilization of elusive main group oxide. **G.H. Robinson**, Y. Wang, P. Wei, H.F. Schaefer

11:20 391. The activation and functionalization of strong carbon-hydrogen bonds: A computational perspective. **T.R. Cundari**

Cook Convention Center
L-7

General Organic Chemistry

Natural Products/Medicinal

T. J. Burkey, *Organizer*
B. C. Goess, *Presiding*

8:20 392. Synthesis of functionalized purine analogs for antibody conjugation. **B. Akinbobuyi**, J. Quintana, C. Chang, J. Horton, H. Chen, W. Yin, K.C. Upchurch, S. Oh, R.R. Kane

8:40 393. Synthesis of ascarylose diphosphate nucleotides. **R.A. Jones**, A. Schubert, R.A. Butcher

9:00 394. Unsymmetrical ketone synthesis using a heterocyclic tosyl hydrazone and aromatic aldehydes for synthesis of STAT3 inhibitors. **S.D. Wood**, W.R. Roush

9:20 395. Chemoselective conversion of biologically sourced polyols into chiral synthons. **J.A. Dabrowski**, T. Bender, L.L. Adduci, M.R. Gagne

9:40 396. Total synthesis of hibiscone B. **B.C. Goess**

10:20 Intermission.

10:00 397. Progress of the total asymmetric synthesis of antascomicin B. **B. Walker**, M.C. McIntosh

10:40 398. Combretastatin and chalcone B-ring analogues via indole aldehydes. B.J. Shields, C.M. Bridges, **H. Holt**

11:00 399. Synthetic studies on muraymycin antibiotics for Gram-negative bacterial infections. **K. Mitachi**, M. Kurosu

11:20 400. Practical synthesis of novel polymyxin analogs for *in vivo* studies. **Y.E. Kurosu**, M. Kurosu

11:40 401. Synthesis of human milk trisaccharides en route to functionalized galacto-oligosaccharides. **D.L. Ackerman**, S.D. Townsend

12:00 402. Method for the synthesis of difluoroglucosides for incorporation into anti-oxidant natural products. **R. Hazlitt**, J.P. John, Q. Tran, D.A. Colby

Cook Convention Center
L-3

Materials for Alternative Energy Applications

X. Zhao, *Organizer, Presiding*

8:20 403. Hydrogen generation using single component Pt(II) NCN system. **A.D. Kulkarni**, R.H. Schmehl

8:40 404. Increased efficiency and oxygen resistance of Ru,Rh,Ru water reduction photocatalysts in air-saturated aqueous solutions containing polyelectrolytes. **T. Canterbury**, S.M. Arachchige, R.B. Moore

9:00 405. H_2 production catalyzed by Co complexes with pentadentate ligands. **X. Zhao**, R. Mittapalli, S. Powers, K. Knight , K. Driskill, T. Rice , C. Lyons, Y. Gueye

9:20 406. Tracking catalyst intermediates in photoinduced generation of hydrogen with transient spectroscopic and mass spectral methods. B. Shan, P.R. Fontenot, J.P. Donahue, **R.H. Schmehl**

9:40 407. Using theory to guide design: Development of hydrogenase inspired Ni and Fe H_2 oxidation catalysts. **M. Helm**, S. Raugei, J. Darmon, N. Kumar, R. Stolley

10:20 Intermission.

10:40 408. Micellar effects on photoinduced electron transfer in aqueous solutions: Dramatic enhancement of cage escape yields in surfactant Ru (II) diimine complex / $[Ru(NH_3)_6]^{2+}$ systems. **R.E. Adams**, R.H. Schmehl

11:00 409. Structure-property relationships: Ancillary ligand molecular design for Ru (II) complexes and how it leads from 5% to 10% efficiency in dye-sensitized solar cells. **H. Cheema**, A. El-Shafei

11:20 410. Designing a family of long lifetime copper(I) phenanthroline complexes. **C. McCusker**, F.N. Castellano

Cook Convention Center
L-6

Computational Studies of Protein Function

D. Bashford, *Organizer, Presiding*

8:40 411. The mechanism of dinoflagellate bioluminescence: A computational approach to elucidating the structure of the luminophore of dinoflagellate luciferase. **P. Ngo**, S. Mansoorabadi

9:00 412. Comprehensive prediction of drug-protein interactions and side effects for the human proteome. **J. Skolnick**

9:40 413. Predicting and characterizing protein functions in the "big data" era. **N. Kannan**

10:20 Intermission.

10:40 414. Concepts of protein dynamics in drug design. **J.C. Smith**

11:20 415. Molecular dynamics simulations of the NF-κB inducing kinase. **M.R. Jones**, J. Yue, A.K. Wilson

Cook Convention Center
River Bluff Room

Biomolecular NMR

J. Young, *Organizer*
R. Kriwacki, A. Viacava Follis, *Presiding*

9:00 416. The dynamics of GCN4 facilitate DNA interaction: A model-free analysis of an intrinsically disordered region. **A.G. Palmer**

9:40 417. Functional activation of the pro-apoptotic BAX by the intrinsically disordered N-terminus of p53. **A. Viacava Follis**, F. Llambi, P. Merritt, J. Chipuk, D. Green, R. Kriwacki

10:00 Intermission.

10:40 418. Non-Fourier methods for improving multidimensional NMR. **J.C. Hoch**

11:20 419. Exploring the thermodynamics of the Pin1-histone interaction. **D.S. Jinasesna**, H. Gyamfi, N. Fitzkee

11:40 420. Molecular recognition by disordered protein regions. D. Ban, A. Viacava Follis, J. Hunter, L. Iconaru, D. Mitrea, A. Phillips, **R. Kriwacki**

Cook Convention Center
West Mezzanine

General Analytical Chemistry

J. Russ, *Organizer*

10:20 - 12:20

421. Profiling chemical fingerprints of lead-free gunshot residue analogs. **L. Fambro**, E. Miller, W. Abdul Khalek, D. VanDenbos, C.R. Dockery

422. Analysis of biogenic amines as quality indicators of three fish species commonly consumed in Kuwait. **A. Anderson**

423. Investigating pyrene levels in water and sediment samples in presence of bioturbators. **F. Louka**, A.M. Cazan, S. Osman, P. Morandi, M. Hoag , P. Klerks

424. Construction of a semiconduction-biological interface for solar energy conversion: P-doped silicon/photosystem i/zinc oxide. **J. Beam**, G. LeBlanc, E.A. Gizzie, B.L. Ivanov, G. Jennings, C.M. Lukehart, D.E. Cliffel

425. The simple approach to measuring calcium via ICP-MS. **N. Scott**, F. Meadows

426. Digital imaging and fluorescence characterization of Langmuir films of quantum dots. **Z. Whitfield**, J.J. Weimer, H. Jani

427. Using thermogravimetric analysis to differentiate between ethylene bis-stearamide and polyamides in paper machine deposits where FTIR results are inconclusive. **T. Cotter**

428. The determination of inorganic and organic compounds in kombucha. **M.A. Harris**, A.L. Salido

429. Amperometric determination of aurocyanide for hydrometallurgical gold processing. **W. Dickinson**

430. Method development for portable HPLC as a tool for onsite accurate analysis of THC in oral fluid. **L. Howard**

431. Forensic identification and differentiation of visually indistinguishable fiber pairs using excitation-emission fluorescence microscopy paired with multi-way chemometric analysis. **N. Mujumdar**, H. Goicoechea, A. Munoz de la Pena, A. Campiglia

432. Humic acid's influence on surfactant toxicity as measured by *Artemia franciscana*. **R.D. Deese**, M.R. LeBlanc, R.L. Cook

433. Studies of electronic cigarette emissions for assessing human exposure to harmful chemicals. **K. Kazipeta**, N.S. Chong, B. Ooi

434. Entropic and enthalpic correlations in S_N2 reactions between dianions and alkyl halides by mass spectrometric techniques. **N. Le**, S.V. Gronert, K.T. Jackson, D. Eseonu

435. Investigation of speciation of Cu^{2+} in the synthesis of HKUST-1 using UV-visible spectrophotometry. **C. Williams**, K.T. Jackson, D. Eseonu, N. Le

436. Magnetic enhancement in powerchip LIBS microplasmas. **J.A. Merten**, M. Northcutt

437. Radiocarbon dating rock paintings at Eagle Cave, TX. **P. Samuel**, **D. Jessica**, A. Trinidy, K.L. Steelman

438. Rapid LC-MS/MS analysis of chlorogenic acid, phlorizin, epicatechin, and catechin in apple juice. **M.J. Vergne**, L. Shade, S. Islam, A. Patras

439. Comparison of two analytical methods for the measurement of nitrate concentrations across different concentration ranges of standard solutions and environmental samples. **M.S. Morton**, G. Prusky

440. Analysis of ambient air pollution at natural gas production facilities by GC/MS and FTIR. **P. Sripathi**, S. Wylie, V. Lourdes, S. Wilson, B. Baziel, D. Thomas, N.S. Chong

441. Developing a reliable approach for surface-enhanced Raman headspace sampling and kinetic studies within a cuvette. **M. Alam**, **M. Hossain**, **X. Dong**, **K. Jackson**, **K. Karlovitz**, **D. Thompson**

442. Immobilized redox active substrates on indium tin oxide surface modeled as immunosorbent assay device. **R. Chauhan**, J. Ghitan, E. Chaudhary, S. Mendes, M. O'Toole

443. Solid phase extraction Cd(II) from environmental samples using a novel ion imprinted polymer and determination by ICP-MS. **Z. Arslan**, V. Yilmaz, H. Yilmaz, J.R. Leszczynski

444. Chemical vapor generation for determination of transition metals: Preliminary studies on manganese and cobalt. **A. Celik**, V. Yilmaz, Z. Arslan

Cook Convention Center
West Mezzanine

General Biological Chemistry

S. Pedigo, *Organizer*

10:20 - 12:20

445. Biophysical characterization of pathological tau oligomers. **B. Colvin**, M.R. Nichols

446. Structural studies of HIV-1 and HTLV-II long terminal repeat substrates. **Q. Li**, C.N. Johnson, C. Jonsson, M.W. Germann

447. Chronic exposure of benzo(a)pyrene and benzo(b)fluoranthene, tobacco constituents, induces oxidative stress, apoptosis, and cellular toxicity in U937 monocytic cells, perhaps through CYP pathway: Implications with HIV pathogenesis. **S. Ranjit**, M.A. Rahman, B. Patters, N.M. Midde, N. Sinha, P. Rao, S. Kumar

448. Uncovering the forces driving higher-order SPOP self-association. **J.J. Bouchard**, M.R. Marzahn, A. Nourse, S. Vaithiyalingam, H. Zhao, G. Ben-Nissan, S. Kenrick, M. Sharon, P. Schuck, T. Mittag

449. Structure and activity relationship studies of a highly endosomolytic fluorescently labeled dimer of the cell penetrating peptide TAT (dfTAT): Effects on cytosolic cellular penetration. **K. Najjar**, A. Erazo-Oliveras, J. Pellois

450. Pursuit of an inhibitor for MAGE-B2, a novel oncogene restricted in expression to the testis and cancers. **J. Weon**, S. Ramanathan, K. Fon Tacer, H. Niederstrasser, S. Perkins, B. Posner, P.R. Potts

451. Examination of creatine kinase-B's role in triple negative metastatic breast cancer. **H.C. Barch**

452. Wet-laid soyfiber reinforced scaffold: Fabrication, mechano-morphological, and cell proliferation studies. **A.T. Wood**

453. Nanofiber bioscaffold sensor for cancer cell detection. **H. Alismail**, Y. Du, J. Zhou, A. Manoharan, Z. Tian

454. Late endosomes and its unique anionic lipid bis(monoacylglycero)phosphate act as doorways for the endosomal escape and cytosolic entry of the fluorescently-labeled dimeric cell-penetrating peptide dfTAT. **A. Erazo-Oliveras**, K. Najjar, T. Wang, D.J. Brock, J. Pellois

455. Engineering CRISPR/Cas9 system for diagnostic application. **A. Kini**, M. Kim

456. Synthetic studies of colletoic acid, a selective 11β-hydroxysteroid dehydrogenase inhibitor. **A. Putnam**, T. Ling, F. Rivas

457. Synthesis and anti-melanoma activity of the marine alkaloid calothrixins. **S. Xu**, T. Singh, S. Katiyar, S.E. Velu

458. Characterizing protein adsorption to gold nanoparticles. **M. Davidson**, C. Wilks, K. Woods, N. Fitzkee

459. Analysis of site-directed mutants of sphingosine kinase-1 by LC-MS/MS and bi-substrate kinetics. **T.T. Pham**, D.L. Baker

460. Identification and characterization of a novel chlorophyll catabolite from the bioluminescent dinoflagellate *Pyrocystis fusiformis*. **P. Ngo**, S. Mansoorabadi

461. Examples of alternate antibody conjugation strategies. **J. Quintana**, R.R. Kane, B. Akinbobuyi, J. Horton, C. Chang, M. Cepeda, A. Alaniz, S. Oh, K.C. Upchurch, W. Yin

462. Excess sodium ion concentrations: The plight of the peptide chemist. R.L. Lewis, E. Seal, R.C. Fortenberry, **A.L. Stewart**

463. Charge distribution influences conformational properties and signaling efficiency of the intrinsically disordered cell cycle inhibitor p27. **A. Phillips**, R. Das, Y. Huang, R.V. Pappu, R. Kriwacki

464. On electrophoretic methods used in gene mapping and finite speed diffusion. **K.R. Sharma**

465. Design and optimization of simple sensing ensembles using multivariate analysis. **A. Mallet**, M. Bonizzoni

466. Repeated and folded DNA sequence optically switch silver cluster adducts. **M. Ganguly**, J.T. Petty, C. Bradsher, P. Goodwin

467. Understanding the structural properties of the C-terminal domain of Alb-3 from *Pisum sativum*. **C.J. Timmermann**

THURSDAY AFTERNOON

Cook Convention Center
L-2

Tomorrow's Therapeutics: Natural Products

R. E. Lee, *Organizer*
R. K. Guy, F. Rivas, *Organizers, Presiding*

12:50 Introductory Remarks.

1:00 468. Mode of action and biomarker discovery for anti-cancer natural products. **M. Potts**, E. McMillan, Y. Hu, J. MacMillan, M. White

1:40 469. Development of adjuvant therapeutics for leukemia: Potent and selective AKR1C3 inhibitors based on a natural product scaffold. K. Verma, T. Zang, T.M. Penning, **P.C. Trippier**

2:20 470. Marine alkaloid synthesis as a platform for chemical and biological discovery. **J.G. Pierce**

3:00 Intermission.

3:20 471. Development of spectinamides as new anti-tuberculosis drug candidates. **J. Liu**, D. Bruhn, T. Matt, M. Scherman, D. Madhura, Z. Zheng, S.L. Waidyarachchi, E. Bottger, A. Lenaerts, B. Meibohm, R.E. Lee

4:00 472. Marine natural products as powerful molecular tools for the control of cancer and infectious disease. **M.T. Hamann**

4:40 473. Natural products inspired synthesis. **M.C. McIntosh**

Cook Convention Center
L-5

Biomolecular Crystallography

S. W. White, *Organizer, Presiding*

1:00 474. Identification and characterization of an allosteric inhibitory site on dihydropteroate synthase. **D. Hammoudeh**

1:40 475. Glucosamine analogue inhibitors of *Trypanosoma cruzi* glucokinase. **E.L. D'Antonio**, M.S. Deinema, S.P. Kearns, T.A. Frey, S. Tanghe, K. Perry, T.A. Roy, H. Gracz, A. Rodriguez, J. D'Antonio

2:20 Intermission.

2:40 476. Development of chemical biology probes of the pro-apoptotic Bcl-2 effector protein BAK. **G. Singh**, C. Guibao, W. Shadrick, W. Lin, G. Royappa, T. Chen, T. Moldoveanu, R.E. Lee

3:20 477. Structure and function studies of conserved residues in the bacterial fatty acid binding protein family. **T.C. Broussard**, D.J. Miller, P. Jackson, A. Nourse, C. Rock

4:00 Intermission.

4:20 478. The crystal structure and mechanism of a bacterial phospholipid remodeling acyltransferase. **S.W. White**, J. Yao, C. Rock, R. Robertson

Cook Convention Center
Chickasaw Room

DNA Modifying Enzymes

E. Enemark, *Organizer, Presiding*

1:00 479. Targeting translesion DNA polymerases for inhibition in cancer. **R.L. Eoff**, M.K. Zafar, L. Maddukuri, S. Eddy, A. Ketkar, N. Penthala, P.A. Crooks

1:40 480. Influence of electrostatic interactions at the sliding clamp interface on clamp loading and stability. L.G. Douma, K. Yu, F. Tondnevis, J. Binder, A. Purohit, M. Levitus, **L. Bloom**

2:20 Intermission.

2:40 481. HDX-MS used to validate interactions with the excluded DNA strand during hexameric helicase unwinding. **M.A. Trakselis**, B. Graham, K. Dodge, C. Thaxton, D. Olaso

3:20 482. Medulloblastoma-associated mutations in DDX3X drive stress granule assembly and impair protein translation. **Y.A. Valentin-Vega**, Y. Wang , D.M. Patmore, N. Kim, A. Kanagaraj, J. Moore, B.J. Winborn, M. Rusch, D. Finkelstein, D. Ellison, R. Gilbertson, J. Zhang , H. Kim, J. Taylor

4:00 Intermission.

4:20 483. Structural basis for RNA-mediated regulation of lysine specific demethylase-1. Z. Luka, A. Hirschi, B. Martin, L. Loukachevitch, C. Wagner, **N. Reiter**

5:00 484. MCM ring hexamerization is a prerequisite for DNA-binding. **E. Enemark**, C.A. Froelich, A. Nourse

Cook Convention Center
L-11

Frontiers in Nucleic Acids Chemistry

G-Quadruplex and Other Structures

D. E. Graves, *Organizer*
E. A. Lewis, *Organizer, Presiding*

1:00 485. Capped G-quadruplexes flanked by duplex DNA photochemically cross-linked using psoralen: A model for human c-MYC NHE-III1. K.D. McConnell, V.H. Le, **E.A. Lewis**

1:40 486. Development and therapeutic potential of clamp-mediated stabilization of G-quadruplex DNA3. T. Hao, **T.A. Brooks**

2:20 487. Linking pH, temperature, and conformation for the DNA i-motif. **R.D. Sheardy**, M.L. McKim, T. Sutorius, C. Johnson, A. Metz, A. Buxton

3:00 Intermission.

3:20 488. On the road to controlling gene expression with DNA minor groove binders. **W. Wilson**, A. Paul, S. Laughlin, A. Kumar, P. Guo, A.A. Farahat, R.A. Abou-Elkhair, N.K. Harika, Y. Chai, M.W. Germann, D.W. Boykin

4:00 489. DNA damage by one-electron oxidants: Implication of charge transfer in DNA. **M. Roginskaya**, D. Ampadu-Boateng, D. Seneviratne, Y. Razskazovskiy

4:40 490. Nuclease biodegradable poly(ethylene glycol) hydrogels prepared by copper-free click chemistry. **T. Betancourt**, K. Barker, S. Rastogi, J. Dominguez, T. Cantu, W.J. Brittain

5:00 491. Ionic strength-specific, photo-oxidative DNA cleavage by a 9-aminomethylanthracene dye. **M.S. Safiarian**, M.S. Pearson, K.B. Grant

Cook Convention Center
West Mezzanine

General Organic Chemistry

Medicinal/Synthesis

T. J. Burkey, *Organizer*

1:00 - 3:00

492. A potent new class of drugs for treating human African trypanosomiasis revealed by phenotypic screening. **P.T. Weiser**, D.A. Patrick, J.R. Gillespie, F.S. Buckner, R.R. Tidwell

493. Synthesis and antibiotic activity of azabicycle compounds. **E. Lanier**, A.L. Wolfe

494. Discovery and characterization of the choline transporter inhibitor: N-((3-isopropylisoxazol-5-yl)methyl)-4-Chloro-3-((1-methylpiperidin-4-yl)oxy)benzamide, VU6001221. **J. Bertron**, J.C. Tarr, C.R. Hopkins, E.A. Ennis, J. Wright, C. Locuson, R. Blakely, C.W. Lindsley

495. Comprehensive access to apoptolidin-derived chemical probes to study cancer cell metabolism. **K.M. Chong**, R.W. Davis, N. Leelatian, D.C. Earl, Y. Du, J.M. Irish, B.O. Bachmann, G.A. Sulikowski

496. Determining the most effective peptoid submonomer mimic of arginine and aspartic acid. **S.S. Almadhhi**, K. Bicker

497. A greener coupling of silicon and boron compounds. C. McNamara, C. Lindsey, J. Carter, **J. Hershberger**

498. Synthesis and biological evaluation of novel HER2 inhibitors for the treatment of trastuzumab-resistant breast cancer. **R. Schroeder**, M. Sfondouris, N. Goyal, P. Tram, T. Stone, K. Nguyen, F. Joseph, V.C. Miles, F. Jones, J. Sridhar

499. Identification and development of novel casein kinase 1 inhibitors. **R. Schroeder**, N. Goyal, P. Tram, T. Stone, K. Nguyen, F. Joseph, V.C. Miles, E. Skripnikova, M. Bratton, J. Sridhar

500. Synthesis of clinical tools for detecting G-proteins in cancer cells. **S. Sedberry**, C.R. De Silva, K.R. Wilson, B. Dinkelmeyer

501. Screening and identification of inhibitors of *T. brucei* cathepsin L with antitrypanosomal activity. **T. Jefferson**

502. Synthesis and characterization of a novel series of pyrrolo[2,1-c][1,4]benzodiazepine derivatives with potential biological activity. **J.K. Annor-Gyamfi**, **A. Shilabin**

503. Extraction and characterization of an antibiotic- like molecule produced by *Rhodococcus* sp. MTM3W5.2. **P. Reddyvari Manikindi**, A.L. Ward, B.C. Lampson, A. Shilabin

504. Design and synthesis of ORP4-selective compounds. **A.T. Le**

505. Synthesis and characterization of new 5,7-dibromo-3-phenyl-3,4-dihydroacridin-1 (2H)-one derivatives: Potential anticancer compounds. **A. Almushayti**, **C.O. Okoro**, A. Sledge

506. Bis-naphthylcycloprea metal free source of carbon monoxide. **C.D. McNitt**, V. Popik

507. Conjugation of bicyclol-polymer conjugates for protecting liver from injury. L. Wang, L. Wu, **D.R. Janagam**, K. Li, N.L. Li, T.L. Lowe

508. Synthesis of novel, anti-inflammatory *N*-arylpyrazolo[3,2-*c*]-based molecules and applications in treating type 1 diabetes mellitus. **C. Prevatte**, S. Collier, R. Smith, A. May, L. Dunlap, J. Collier, S.R. Campagna

509. Preparation and antitubercular properties of novel *p*-aminosalicylic ester thioureides. **M. Hearn**, M. Cynamon

510. Synthesis of phthalimides and indazolones as selective CDK inhibitiors. **F. Joseph**, V.C. Miles, P. Tram, R. Schroeder, T. Stone, K. Nguyen, H. McFerrin, J. Sridhar

511. Synthesis and evaluation of electronic and steric depsidone analogs for use as antibiotics. **J. Terrell**, A.L. Wolfe

512. Synthesis and antibiotic evaluation of heterocyclic a and c ring depsidone analogs. **J. Katz**, A.L. Wolfe

513. Synthetic studies toward metabolically stable puromycin analogs. **G. Gumina**, A.R. Messersmith, D.H. Eagerton, B.D. Feske

514. Isolation and characterization of phytochemicals from the leaf extract of *Tapirira mexicana*. **H. Zhang**, W.N. Setzer, I.V. Ogungbe

515. 2,6-bis-hydrazinopyridine hydrazones: Potential metal ligands. **M. Jones**, K.A. Brien

516. Synthesis of novel norcantharimide derivatives. **A. Kose**, N. Kishali, G. Sanli-Mohamed, Y. Kara

517. Stereoselective bora-Wittig olefination of ketones with a diazaborolane -acetonitrile enolate. **S. Nguyen**, Y. Takahashi, T. Tomioka, D.L. Mattern

518. Synthesis of the azabicyclo[3.1.0]hexane ring core of ficellomycin. **M. McMechen**, A.L. Wolfe

519. Tris(3,5-dimethylpyrazol-1-yl)methane and 1,1,1-tris-(3,5-dimethylpyrazol-1-yl)-2-(trimethylsiloxy)ethane platinum compounds: Synthesis, reactivity and structure. **A. Lorbecki**, B.P. Quillian, T. Gunnoe

Cook Convention Center
West Mezzanine

General Physical Chemistry

W. A. Alexander, *Organizer*

1:00 - 3:00

520. A surface science study on the reaction of carbon monoxide and methanol with a meteoritic mineral analogue. **D. Qasim**, A. Pital, T.J. Beckman, H. Abbott-Lyon

521. On use of graphene oxide dispersions in electrorheological fluid applications. **K.R. Sharma**

522. Aggregation of spherical nanoparticles on lipid membranes. E.J. Spangler, **M. Laradji**

523. Non-covalent interactions between trimethylamine N-oxide (TMAO) and urea in water. **K. Warren**, J.C. Prather, J. Cauley, D.H. Magers, N. Hammer

524. Quantum chemical rovibronic data for *c*-C_3H with application to the interstellar medium. **M. Bassett**, R.C. Fortenberry

525. Withdrawn.

526. Equilibrium and photo-kinetic properties of *p*-nitrophenolate at the air-water interface. **D. Headley**, M. Schmits, J. Vogel, J. Lee, **M. Subir**

527. Using spectroscopy to engage students in STEM and physical chemistry. **A.E. Steen**, K.D. Scott, N. Hammer

528. Complete basis set limits for the Hartree-Fock and second-order Møller Plesset energies for DMPO, EMPO and their hydroxy-radical adducts. H.B. Short, **S.J. Kirkby**

529. Comparison of laboratory evaluation methods for defoaming chemistries. **C. Kirwan**, R. Hamm, L. Bava

530. Investigating the chemical reactions with naphthalenium in the interstellar medium. **J. Velazquez**

531. Spectroscopic and computational study of chlorine dioxide/water interactions. **S.C. Sutton**, W.E. Cleland, N. Hammer

532. Synthesis and characterization of carbon quantum dots with varying amounts of nitrogen. **S.J. Jones**, P.C. Ray

533. Deep ultraviolet stimulated Raman scattering crystal calcium borate. **Y. Liu**, **Z. Wang**, **X. Sun**, **X. Xu**

534. Effects of nanoscale surface curvature on the adsorption and desorption of thiolated ligands on gold nanoparticles. **E. Villarreal**, H. Wang

535. The thermodynamic properties of recyclable plastics with exposure to UVB light. **A. Bosio**, C. Fowler, T. Knippenberg

536. Determination of rate constant, binding constant, and binding number by fluorescence measurements of $Gd_3N@C_{80}(OH)_{20}$ in D_2O. **A. Rodriguez**

Cook Convention Center
L-3

Materials for Alternative Energy Applications

X. Zhao, *Organizer*
Y. Sun, *Presiding*

1:00 537. Investigation of hydrothermal conversion of methylosinus trichosporium to bio-oil. **J.D. Wheeler**, J. Saravia, R. Bhatti, W. Jang

1:20 538. Hematite coated gold thin films for enhanced photocatalytic water splitting. **A.S. Panikar**, Z. Shan, S. Pan, A. Gupta

1:40 539. Surface enhanced titanium based electrode for efficient oxygen evolution reaction. **Z. Shan**, A. Gupta, S. Pan

2:00 540. Platinum based binary electrocatalysts supported on carbon for a single compartment direct ethanol fuel cell. **J. Kuo**

2:20 541. Catalytic bio-oil upgrading using a Mo/Co/K catalyst with addition of water gas shift active metals with bio-syngas. **G.A. Burk**, W.R. Moore, R.T. Wijayapala, T. Mlnsa

2:40 542. Earth-abundant materials for renewable energy catalysis. **Y. Sun**

3:20 Intermission.

3:40 543. Microwave assisted nanocarbonization of conducting polymers for battery applications. **S. Poyraz**

4:00 544. Hydrated titanium phosphates as promising materials for rechargeable batteries. **G. Lee**, C. Varanasi, J. Liu

4:20 545. Synthesis of diazonium (perfluoroalkyl) benzenesulfonimide (PFSI) monomer from perfluoro (3-oxapent-4-ene) sulfonyl fluoride for proton exchange membrane fuel cells. **F. Ibrahim**, H. Mei

4:40 546. The enhanced physical properties of a nanostructured $LiCoO_2$ cathode utilized in a nanoengineered all-solid-state lithium ion battery. **M.A. Poyner**, I.U. Jayasekara, D.C. Teeters

Cook Convention Center
L-6

Computational Studies of Protein Function

D. Bashford, *Organizer, Presiding*

1:20 547. Exploring the insertion mechanism of SVS-1 β-hairpin peptide into an anionic lipid bilayer. **K. Reid**

1:40 548. Conceptually simple approaches to complex structural problems: Ligand migration in myoglobin. **A.V. Onufriev**

2:20 549. Proteins under pressure. **T. Ichiye**

3:00 550. Hydrogen-bonding networks dictate conformational sampling of a *Pneumococcal* fibronectin-binding adhesive protein. **D. Chakravorty**

3:20 Intermission.

3:40 551. Protein solubility to aggregation and structure. D. Karandur, R. Harris, **B.M. Pettitt**

4:20 552. Protein-protein docking and molecular dynamics simulations suggest potential mechanisms of electron transfer between ferredoxin and cyanobacterial photosystem I. **D.J. Cashman**, L. Nientimp, K. Kapoor, J.Y. Baudry

Cook Convention Center
Mississippi Room

Intrinsically Disordered Proteins: From Physical Chemistry to Biology

R. Kriwacki, A. Viacava Follis, *Organizers*
F. Laukien, T. Mittag, *Presiding*

1:20 553. Role of intrinsically disordered proteins in cellular signaling and regulation. **P.E. Wright**

2:00 554. NPM1 facilitates assembly of nucleolar components through phase separation. **D.M. Mitrea**, J. Hunter, C.S. Guy, D. Ban, P. Bannerjee, C.B. Stanley, A.A. Deniz, R. Kriwacki

2:20 555. The role of IDPs in aggregation associated with Parkinson's disease. **J. Baum**

3:00 Intermission.

3:40 556. The role of protein disorder and self-association in the formation of membrane-less organelles. M.R. Marzahn, A. Palud, S. Marada, J. Lee, A. Nourse, P. Taylor, S.K. Ogden, **T. Mittag**

4:40 557. Decoding functions and phase behavior of IDPs using sequence design. **R.V. Pappu**

Cook Convention Center
L-4

Recent Advances in Chemical Physics

N. Hammer, *Organizer, Presiding*
K. H. Bowen, *Presiding*

1:20 558. Ion issues in physical chemistry. **J.V. Coe**

1:40 559. Photofragment imaging studies of metal-ligand charge transfer. J. Maner, **M.A. Duncan**

2:20 560. Laser experiments for chemistry and physics. **R.N. Compton**, M.A. Duncan

3:00 Intermission.

3:20 561. Chiroptical spectroscopy: An emerging tool for chiral molecular structural determination. **P.L. Polavarapu**

4:00 562. Detecting the surface sum frequency generation signal from noncentrosymmetric crystal. **E.W. Plummer**, Z. Zhang, J. Kim, R. Khoury, L.H. Haber

4:40 563. The Compton effect. **C.S. Feigerle**

Cook Convention Center
River Bluff Room

Entrepreneur's Tool Kit: Resources and True Stories

Cosponsored by SCHB
J. E. Sabol, *Organizer, Presiding*

1:40 564. Member benefits and business resources from the ACS Division of Small Chemical Businesses (SCHB). **J.E. Sabol**

2:20 565. From academic laboratory to commercial plant: The ThruPore story. **M.G. Bakker**, F. Sayler

3:00 Intermission.

3:40 566. Findings on blending hemp with thermal coal for power generation or gasification. **R.D. Ford**

4:20 567. Out of the frying pan, into the fire, and swimming upstream. **J.E. Sabol**

Cook Convention Center
Sultana Room

Mass Spectrometry

D. L. Baker, *Organizer, Presiding*

1:40 568. Dissociation pathways, rearrangement reactions, and relative stabilities of O-sulfated amino acids and small peptide. **A.L. Patrick**, N.C. Polfer

2:00 569. Effects of acidic peptide sequence on metal attachment and electron transfer dissociation tandem mass spectrometry. **J.J. Commodore**, C.J. Cassady

2:20 570. Structural analysis of 9cUAB30 methyl derivatives and coactivator peptide GRIP1 on rexinoid X receptor by hydrogen deuterium mass spectrometry. **E.J. Cowart**, A. Proper, D.D. Muccio, M. Renfrow

2:40 571. Gas-phase acidities of the phosphorylated amino acid and their amides. **C.E. Plummer**, M.L. Stover, D.A. Dixon, C.J. Cassady

3:00 Intermission.

3:20 572. Competitive binding of copper(I) and zinc(II) by methanobactin from *Methylosinus trichosporium* OB3b and analog methanobactin peptide. **J.W. McCabe**, R. Vangala, L.A. Angel

3:40 573. Fragmentation of lanthanide-adducted oligosaccharides by collision-induced dissociation and electron transfer dissociation. **R.M. Schaller-Duke**, C.J. Cassady

4:00 574. Desorption by impulsive vibrational excitation (DIVE): Ultrafast/ultrasoft laser ablation for mass spectrometry and biodiagnostics. **W.D. Robertson**, Y. Lu, C. Louwrens, R. Miller

4:20 575. Negative electron transfer dissociation mass spectrometry of acidic peptides. **C. McMillen**, C.J. Cassady

Cook Convention Center
West Mezzanine

General Organic Chemistry

T. J. Burkey, *Organizer*

3:20 - 5:20

576. Determination of the structure of steroid and saccharide molecules in solution using residual dipolar couplings (RDCs). **F. Mahmoudi**

577. Determining the structure of metal ligand complexes in solution by nuclear magnetic resonance (NMR) spectroscopy using residual dipolar couplings (RDCs). **S. Gukathasan**, W. Carroll

578. It's easy being green: Budget-friendly, safety-conscious chemistry labs for the science classroom of today. **M.D. Garrett**

579. Progress towards solutions to diseases: Developing new materials and alternative energy with heterocyclic amines. **J.M. Hahn**

580. Poly-functional porous-organic polymers: Structure-function relationships in CO_2 sorption. **M.H. Alkordi**

581. Fabrication of alginate nanoparticles using microfluidics, effect of flow rate on dispersity of particle diameters. **S.P. Jamkhindikar**, H.A. Stretz, J. Massingill

582. An improved synthesis of fulgenic acid and its use in constructing metal organic frameworks and coordination polymers. **A. Stutesman**, B. Dinkelmeyer, R.D. Pike

583. Synthesis of novel graft-interpenetrating polymer networks. **R.A. Ballestero**, B.M. Sundaram, H.V. Tipuur, M.L. Auad

584. Synthesis of two candidate donor-sigma-acceptor molecular rectifiers with anionic donors and a quinolinium acceptor. **T. Vaughan**, D.L. Mattern

585. The dynamic nature of benzodiazaborole formation and the synthesis of benzodiazaborole based oligomers. **C.P. Manankandayalage**, S.D. Lokugama, D.E. Gross

586. Beta-sitosterol/polyethylene glycol water soluble complexes as drug delivery vehicles for cancer therapeutics. **A.O. Alqarni**, A. Alzharani, E. Allehyani, G. Zhou, I.M. Khan

587. 1,2,3- triazoles as controlled molecular switches. **A. Atkinson**, D. Ghosh, W. Ming, C.W. Padgett, K.S. Aiken, S.M. Landge

588. Synthesis and application of novel initiators in atom transfer radical polymerization techniques. **M. Shetty**, C.E. Hobbs

589. The development of porphyrin-thiazolothiazole donor-acceptor materials for solar energy conversion. **K. Ren**, D.M. Marin, N.G. Grubich, J.M. Kolesar, S.J. Hall, M.G. Walter

590. Harnessing solar energy using poly(3-hexylthiophene) and a buckyball. **P.R. Pulley**, D.J. Patterson

591. Understanding thermal behavior and morphology of long chain alkylated porphyrins in excitonic solar devices. **M. Kaushal**, A. Ortiz, G. Singh , D. Lee, M.G. Walter

592. Preparation and characterization of polylactic acid (PLA) nano-cellulose composites. **W. Simmons**, E.A. Mintz

593. Structure-property relationship of ancillary benzyl containing ionic compounds: Insight for development of low melting organic salts. **W. Clark**, H.U. Valle, J.E. Castillo, C. Cain, H. Khani, J.P. Emerson, P. Hillesheim

594. Structure and properties of a highly strained [2.2]naphthalenophane. **M.B. Houck**, D.T. Glatzhofer, D.R. Powell

595. Photocatalytic reduction of CO_2 to CO with Re-NHC complexes. A. Huckaba, **E.A. Sharpe**, J.H. Delcamp

596. The reactivity of propargyl alcohols and propargyl acetates in the presence of trimethylsilyl trifluoromethanesulfonate. D.N. Confair, **C.W. Downey**

597. SAR studies directed at optimizing the anti-tumor activity of NT-7-16: Functional group changes at the 5-position of the pyrrole scaffold. **J.T. Gupton**, A. Harrison, S. Yeudall, J. Wen, N. Telang, M. Wormald, K. Lescalleet, S. Mooberry, G.E. Kellogg, C. Rohena

Cook Convention Center
West Mezzanine

Undergraduate Posters

General Topics

A. L. Parrill-Baker, *Organizer*

3:20 - 5:20

598. Effect of cooking methods on polyphenol content and antioxidant activity of kale. **B. Hill**

599. Synthesis and characterization of thermochromic pyridinium salts. **E. Larrabee**, D. Olivier, L.V. Koplitz

600. A prebiotic source of glyoxylic acid. **L. Francis**, G.G. Springsteen

601. Development of an active learning: General chemistry laboratory experiment on the identification of unknown halide salts for use as a recruiting tool during the first UNC Asheville NSF S-STEM "Chemistry First Prospective Scholars and Teacher Day". **M. Snyder** , A.L. Wolfe

602. Involving high school students in summer chemistry research. **D.R. Zuidema**, L.B. Herndon

603. Biosorption of cadmium from aqueous solutions using highly characterized peats. A. Rizzuti, L. Whitley Cosme, **K. Mouzone**

604. Incorporation of titania into porous PMMA for photocatalytic applications. **J.D. Glover**, J.E. Boyd

605. Synthesis and antimicrobial evaluation of an α-methylalanine analog of puromycin. **C. Moracho**, A.R. Messersmith, B. Weaver, B.D. Feske, G. Gumina

606. Effectiveness of various visual cues included in video instruction on pre-laboratory preparation in the general chemistry laboratory. M.A. Erdmann, **A.A. Helton**, J. March, C.F. Black

607. A comparison of interaction energies in 2-cyano-1-methylpyridinium salts. **F. Vaccaro**, D. Olivier, M. Kramer, K. Riley, J.T. Mague, L.V. Koplitz

608. GPR88 modeling and antagonist discovery. **E. Jackson**, A.L. Parrill-Baker

609. Analysis of telomere fragments from various apoptotic cancer cell lines. **M. Habash**, **P. Patel**

610. Heat-reflecting window coatings: Improved design with novel materials. **J. Zou**

611. Protein modeling using 3D printing. **S. Cuellar**, D. Oliver, T. Neumann

612. Synthesis and characterization of novel polyamide thin film composite reverse osmosis water desalination membranes. **S. Jackson**, O. Wadsworth, N. Arnett

613. Synthesis of phosphonated biphenol precursors for polymer composite membranes for fuel cell applications. **J.A. Smith**, T.N. Thompson, N. Arnett

614. Synthesis and characterization of novel polyamide thin film composite reverse osmosis water desalination membranes. **R. Williams**, O. Wadsworth, N. Arnett

615. Synthesis and characterization of biphenol based monochloro-1,3,5-triazine (BP-TT) monomer precursors for disulfonated poly(arylene ether sulfone) hybrid copolymer preparation. **J. Wallace**, N. Arnett

616. Synthesis of hydroquibased poly(arylene ether sulfone)-2,4,6-monochloro-1,3,5-triazine hybrid coploymers. **J. Ewers**, N. Arnett

617. pH and salinity dependence of copper leaching from anti-fouling marine paints. **D.W. Carpenetti**, A.C. Martin, C. Rust

618. Investigating the effects of disaccharides on bacteria. **A. Pinkham**, A.M. Kennedy, E. Anderson

619. Creation of an ELN for quantitative analysis. R. Montgomery, **A.G. Taylor**, **J. Van Dyke**

620. ASU ACS chapter community outreach: Educating local students. **C. Anderson**, H. Koizumi

621. Toxic chemical emissions in smoke produced via burning of scrap tires, firewood, and liquefied petroleum gasoline as fuel sources for singeing meat. **R. Barham**, E. Afriyie-Gyawu

622. Flipping pre-labs for organic chemistry. **T. Edwards**, T.R. Hayden

623. Investigating the effect of the dispersant Corexit 9500A on the movement of an oil-in-water emulsion through an Alabama beach sand. **A.B. Brasher**, K.K. Manley, A.C. Nichols, D.A. Steffy

624. The development of 3D printed materials for selective growth of ZnO nanorods with applications in photovoltaics. **R.A. Kuntz**, E. Adcock Smith, K. Roberts

625. Nature of metal ion mediated second shell hydrogen bonds. **N. Bhattacharyya**, J. Xiang, T.T. Tran, D.K. Chakravorty

FRIDAY MORNING

Cook Convention Center
L-11

Frontiers in Nucleic Acids Chemistry

DNA Structures and Perturbations

D. E. Graves, E. A. Lewis, *Organizers*
R. D. Sheardy, *Presiding*

8:00 626. Structural perturbations induced by aflatoxin adducts in DNA. **M.P. Stone**, K.L. Brown, L. Li

8:40 627. Structure and dynamics of DNA containing single ribonucleotide damage. **M. Evich**, A.M. Spring-Connell, K.D. Koh, F. Storici, M.W. Germann

9:20 628. H NMR solution structure and biophysical characterization of aminoglycoside interaction with Sp1 transcription factor consensus sequence 5'-d[(G/T)GGGCGG(G/A)(G/A)]. **E. Davis**, M. Hennig, M. Spano, D.P. Arya

9:40 629. A repeated and folded DNA sequence and its fluorescent silver cluster adduct. J.T. Petty, **M. Ganguly**

10:00 Intermission.

10:20 630. Construction of diverse synthetic antibody library for therapeutic antibody optimization. **X. Gao**

11:00 631. Using NMR combined with molecular dynamics to link structural and dynamic effects of the universal base 8-aza 7-deaza N8-linked adenine analog. **A.M. Spring-Connell**, M. Evich, H. Debelak, F. Seela, M.W. Germann

11:20 632. Site-specific DNA methylation targeted to androgen receptor-positive cells. **S. Varadarajan**, M. Powell, E.A. Elliott, N.E. Neill, A. Bourdelais

Cook Convention Center
L-3

Materials for Alternative Energy Applications

X. Zhao, *Organizer*
J. H. Delcamp, *Presiding*

8:00 633. A proaromatic thienothiophene building-block for dye-sensitized solar cells. **P. Brogdon**, F. Giordano, G. Puneky, A. Antonysamy, S. Zakeeruddin, M. Nazeeruddin, M. Graetzel, J.H. Delcamp

8:20 634. Thieopyrazine as a proaromatic building block for NIR organic dyes and their use in DSCs. **N.P. Liyanage**, A. Yella, M. Nazeeruddin, M. Graetzel, J.H. Delcamp

8:40 635. Design, discovery, thin-film preparation, and characterization of lead-free perovskites. **B. Saparov**, F. Hong, J. Sun, H. Duan, W. Meng, S. Cameron, I. Hill, Y. Yan, D. Mitzi

9:00 636. Growth of ZnS nanofilm by pulse potential atomic layer deposition. **N. Bui**, J.L. Stickney

9:20 637. Doping Ge quantum dots for solar applications. **B.L. Oliva-Chatelain**, A.R. Barron

9:40 638. Photocatalytic conversion of CO_2 to fuels and electricity generation with solar energy. **J.H. Delcamp**, A. Huckaba, E.A. Sharpe, L. McNamara, A. Yella, N. Hammer, M. Nazeeruddin, M. Graetzel

10:00 Intermission.

10:20 639. Routes to improving polymer solar cells: Improving crystalline polymer diffusion and reducing spontaneous charge transfer to TiO_2 nanostructures. **A. Haring**, A.J. Morris, E. Sadler

10:40 640. Withdrawn.

11:00 641. Electrochemical atomic layer deposition of CdS on Au and tin-doped indium oxide. **S. Shen**, X. Zhang, J.L. Stickney

11:20 642. Coatings with improved eco-profile enabled by EVOQUE™ pre-composite polymer technology. **A.M. Maurice**

11:40 643. Studying the melt processibility of carbon fiber precursors towards high strength fibers. **S. Mahmood**, B.L. Batchelor, M. Jung, H. Shin, W. Voit, B.M. Novak, D. Yang

Cook Convention Center
L-5, L-6, L-7

Plenary Lecture

Financially supported by Eastman Chemical Company
A. L. Parrill-Baker, *Organizer, Presiding*

8:55 Introductory Remarks.

9:00 644. Production of soluble, homogeneous protein for structural studies. **L.J. DeLucas**, W.W. Wilson, S. Aller, C. Deivanayagam, D. Chattopadhyay, T. Green, N. Schorman, D. Johnson

Cook Convention Center
Chickasaw Room

Biomedical Materials and Sensors

J. D. Bumgardner, *Organizer*
E. Lindner, *Organizer, Presiding*

10:20 645. Clinically important parameters that influence sensor design and utility. **B.D. Pendley**

10:40 646. Nitric oxide-releasing mesoporous silica nanoparticle dopants for polyurethane-based glucose sensor coatings. **R.J. Soto**, M. Schoenfisch

11:00 647. Monitoring urine carbon dioxide in septic shock. **J. Atherton**, B.D. Pendley, M. Guzinski, A. Jasinski, W. King, E. Lindner

11:20 648. Ion-selective electrodes with PEDOT(PSS) on platinum, gold and glassy carbon – equilibration time. **M. Guzinski**, J.M. Jarvis, B.D. Pendley, E. Lindner

11:40 649. Immobilization of biomolecules on multiple-branched DNA structures. **E.K. TeSelle**, D.A. Baum

12:00 650. The development of a microfluidic conductivity sensor to detect evaporation from gas permeable PDMS organ-on-a-chip devices. **A.N. Davis**, J.P. Wikswo, D.E. Cliffel

Cook Convention Center
River Bluff Room

Ion-Conducting Polymers

J. E. Ritchie, *Organizer, Presiding*

10:20 651. Nanoporous polysulfone fabrication and performance in redox flow batteries. **B. Gindt**, D.G. Abebe, Z. Tang, L. Melanie, T. Zawodzinski, T. Fujiwara

10:40 652. Ionic liquid and polymer blends for solid state battery electrolytes. **I.U. Jayasekara**, D.C. Teeters

11:00 653. Synthesis and characterization of comb polysiloxane polyelectrolyte containing polyethers and sulfonate-terminated side chain. **B. Liyanage**, J.E. Ritchie

11:20 654. Optimizing the properties and performance of polystyrene based anion exchange membranes via structural modification of the polymer. **S. Tuli**, R. Elgammal, A. Roy, t. Zawodzinski, T. Fujiwara

11:40 655. Evolving electrical conductivity in the matrix of cross-linked PDMS. **J. Bertram**, M.J. Nee, H.P. Rathnayake

Cook Convention Center
L-10

Multiscale Modeling of Macromolecular Systems

J. Ma, V. Rangachari, Y. Wang, *Organizers*
F. Wang, *Organizer, Presiding*

10:20 656. Exploring enzymatic reaction pathways using QM/MM methods. **P. Tao**

11:00 657. Numerical studies of the electron polarization effects in QM and QM/MM calculations. **Y. Shao**

Cook Convention Center
L-12

Nanomaterials: Synthesis, Characterization, and Applications

Synthesis

A. Antonysamy, A. L. Parrill-Baker, *Organizers*
E. Chaffin, *Presiding*

10:20 658. Hybrid nanoparticles: Synthesis and applications. **D.S. Koktysh**

10:40 659. On-surface redox chemistry to control well-defined oxidation states of transition metal single-site centers. D. Skomski, C. Tempas, B.J. Cook, A.V. Polezhaev, K. Smith, K.G. Caulton, **S.L. Tait**

11:00 660. Activation of the molecular nanocluster FeMoC-EtOH in growth of carbon nanotubes. **G. Esquenazi**, A.R. Barron

11:20 661. The effects of colloidal C_{60} particle size on zeta potential. **K. Fujimoto**, S. Cates, K.D. Ausman

11:40 662. Epoxidation of cyclohexene on Ag catalysts supported on hierarchically porous SiO_2 and Co_3O_4 monoliths. **Y. Hakat**

Cook Convention Center
L-4

Recent Advances in Chemical Physics

Recent Advances in Chemical Physics

N. Hammer, *Organizer*
R. C. Fortenberry, *Presiding*

10:20 663. Mitigation of ionospheric scintillation by chemi-ionization: Benefits of fundamental chemical physics. **S.G. Ard**

10:40 664. Visualizing and quantifying the nonvalence character of excess electrons: Multipole-bound states and clusters. **T. Sommerfeld**

11:20 665. On the role of anharmonic effects on the vibrational spectra of $X^{\pm}$ $(H_2O)_n$ clusters. **K.D. Jordan**

12:00 Concluding Remarks.

Cook Convention Center
L-2

Tomorrow's Therapeutics: Natural Products

R. K. Guy, *Organizer*
R. E. Lee, F. Rivas, *Organizers, Presiding*

10:20 666. The development of a comprehensive platform for the on-demand synthesis of peptide natural products containing unusual α-amino amides. **J.N. Johnston**

11:00 667. High throughput plant phenotyping at the plant imaging consortium. **A. Lorence**

11:40 668. Which chamomile is which? Taxonomy, chemistry, biology, and safety implications: Exploring all directions. **I. Khan**

12:20 Concluding Remarks.

Cook Convention Center
West Mezzanine

Undergraduate Posters

Analytical Chemistry

A. L. Parrill-Baker, *Organizer*

10:20 - 12:20

669. Residue analysis of archaeological smoking pipes from the southeastern US. **R.K. Hunt**, J. Lima Hooven, S.B. Carmody, J. Russ

670. Analysis of organic residues from Native American noded vessels using GC-MS and GC-FID. **J. Lima Hooven**, R.K. Hunt, D.H. Dye, J. Russ

671. Neurotransmitter quantification to understand alcohol tolerance in non-mammalian organisms. **M.H. Stodghill**, C.D. Hallman, N.J. Kuklinski

672. Preliminary analysis of the molecular distribution of polyhexamethylene biguanide using equilibrium dialysis and gel filtration chromatography. **H.C. Davis**, **R.J. Pandya**, F.D. David, S. Wheeler, J. Wheeler

673. Synthesis and characterization of *cis*-[Cr(TMP)(DPPZ)(1-MeImid)]$^{3+}$. **I.Y. McCraw**, S.R. Goudy, J.A. Wheeler, C.D. Stachurski, K.W. Sun, M.E. Davis, S. Wheeler, J. Wheeler, N.A. Kane-Maguire

674. Optimization of an analytical method to determine the KCN antidote (SDX) in blood by HPLC. **B.A. Mendenhall**, S. Holmes, J. Ross, R.J. Roy, J. Lowry, S. Crews, E. Stephens, C. Chou, L. Kiss, D.E. Thompson, I. Petrikovics

675. Determining purity of ginkgo biloba extract in the presence of non-native flavonol aglycones and isoflavone glycosides using HPLC and mass spectral analysis. **J.J. Cordoba**, K.A. Young, S. Wheeler, J. Wheeler

676. Analysis of a potassium ferrocyanide based pyrotechnic material as forensic evidence. **E. Miller**, L. Fambro, C.R. Dockery

677. Reaction kinetics of low molecular weight carboxylic acids with carbonate aerosols. **K. Watson** , B. Fong, H.M. Ali

678. Manufacturing of anticancer drug fluorouracil loaded polycaprolactone nanoparticles using emulsion solvent evaporation. **A.L. Timberlake**, M. Khan, S. Iqbal, M. Friel

679. HPLC UV-Vis and MS analysis of endocrine-active compounds in the symbiotic relationship between algae and sea anemones. **K.N. Rule**, A.M. Roark, M.B. Drewry, **N.J. Kuklinski**

680. Method development for the determination of isoflavones in *Aiptasia pallida* using SPE and GC-MS. **M.B. Drewry**, K.N. Rule, A.M. Roark, **N.J. Kuklinski**

681. Characterization of citrate-acetate mobile phases for high performance liquid chromatography with electrochemical detection. **J.R. Obermeier**, C.D. Hallman, **N.J. Kuklinski**

682. Identifying fertilizer origin using portable FT-IR and handheld Raman spectroscopy. **M.A. Philip**, C. Fraga

683. Voltammetric detection of silver ions using carbon paste electrodes for nanosilver oxidation studies. **O.M. Pearce**, K.M. Mullaugh

684. Synthesis and characterization of surface-enhanced Raman scattering gold nanoparticle probes for detection and capture of circulating tumor cells. **A.R. Jones**, R.T. O'Connor, X. Huang

685. Crystallization kinetics of salts from aqueous solutions. **C.M. McCulley**, V. Stanford, J.R. Prado, S.V. Vyazovkin

686. Identifying the polyphenols present in green, black, and herbal teas. **K. Jones**, **G. Sarabia**, **A.C. Suroviec**

687. Kinetics of phenolphthalein color fading experiment via a small footprint diode array spectrometer. **Z. Popovic**, **P. Lott**, R. Fietkau

Cook Convention Center
West Mezzanine

Undergraduate Posters

Inorganic Chemistry

A. L. Parrill-Baker, *Organizer*

10:20 - 12:20

688. Equatorial and axial ligation of Ru2(dpf)3(O2CCH3)Cl where dpf = N,N'-diphenylformamidinate anion. **D.C. Patterson**

689. Reactions of some hydroxy carboxylic acids with Cu^{2+} and Cr^{3+} in aqueous solutions. **Y.Z. Hamada**

690. Copper and iron glycine complexes in aqueous solutions. **Y.Z. Hamada**

691. Investigating metal-to-metal charge transfer in bimetallic Fe-Ti complexes through spectroelectrochemistry. **E. Carlton**, K. Wroblewski, J. Pienkos, P.S. Wagenknecht

692. Redox potentials of ruthenium complexes to understand catalytic ability in water. **A.A. Lopez**, R. Adams, S. Bellows, T.R. Cundari

693. Steps toward a mechanically active gadolinium chelate. **P. Johnson**, C. Brown, S. Craig

694. Photochemical and oxidative degradation of Fe-Ti complexes. **K. Wroblewski**, A. Myers, E. Carlton, J. Pienkos, **P.S. Wagenknecht**

695. Synthesis, characterization, and reactivity of tris(2,2,2-trifluorethyl)phosphite complexes of ruthenium(II) with electron-rich arene ligands. **P. Zdunek**, J.P. Lee

696. Building a nanothermometer for localized magnetic induction heating. **R.N. Kress**, R.R. Shah, A.L. Paulson, D. Pladers, C.S. Brazel, D.E. Nikles

697. Rhodium and iridium complexes of a fused N-heterocyclic carbene as catalysts in hydrosylation reactions. **C. Boudreaux**, **B. Norvell**, O.J. Buckner, D. Tapu

698. Investigate the interface of amino acid on graphene surface. **F. Beltran**, **M. Sheikh**, M. Aun, H. Fan

699. Stabilizing ligands for highly active water oxidation catalysts used in renewable energy conversion. **C.M. McCulley**, E. Sackville, U. Hintermair

700. N-heterocyclic carbenes based on a triazine backbones: Synthesis and complexation to transition metals. A. Adnan, **D. Tapu**

701. Synthesis and chemical analysis of KP1019–(poly)lactic acid nanoparticle. **D. Patel**, L.K. Stultz

702. Synthesis and toxicity studies of C_{12}EDMAB coated gold nanorods: A comparison to CTAB. J.W. Stone, **J. Allen**, J. Xu

703. Amyloid beta (Aβ) peptides and the exposure of their hydrophobic residues upon copper(II) complex formation: Probing mechanisms of amyloid plaque formation in human and rat peptide with fluorescence spectroscopy. **S. Sipe**, A.M. Spuches

704. Synthesis of chromium(III) nutritional supplement. **A.G. Morales**, J.B. Vincent

705. Iron-catalyzed hydrophosphination. **J.N. Izaguirre**, R.L. Webster, T.A. Nile, A.G. Glenn

706. Fate of dietary copper: Is the form of copper in the diet key to prevent it from becoming toxic? **M.K. Kuykendall**, R.E. Honan, J.B. Vincent

707. Luminescent enhancement of europium (III)-doped GaF_3 nanoparticles by surface modification. **L.K. Browder**, C.R. De Silva

708. Synthesis of phosphorus containing ligands for cobalt complexes for hydrogen production. **K. Knight**

709. Ligand exchange or polymerization of an enzyme-mimic Schiff-base copper(II) complex? A kinetic study. **B. Rose**, S. Williams, J. Krause, **J.J. Stace**

FRIDAY AFTERNOON

Cook Convention Center
Chickasaw Room

Biomolecular Crystallography

S. W. White, *Organizer, Presiding*

1:00 710. Structural and chemical biology of fosfomycin resistance in Gram-positive pathogens. **M.K. Thompson**, M.E. Keithly, N.D. Hammer, E.P. Skaar, R.N. Armstrong

1:40 711. Pathogen selective antibiotic minimizes disturbances to the microbiome. **J. Yao**, C. Rock

2:20 Intermission.

2:40 712. Chemical control of cullin neddylation. **J.T. Hammill**, D. Scott, J. Min, M. Connelly, D. Bhasin, G. Huang, R. Barrios, V. Sviderskiy, K. Bharatham, R. Attia, G. Holbrook, F. Zhu, A. Matheny, Y. Chen, B. Evison, T. Chen, A. Shelat, B. Singh, B. Schulman, R.K. Guy

3:20 713. Evaluation of colletoic acid: from structure to function. **F. Rivas**

4:00 Intermission.

4:20 714. Identification and characterization of influenza variants resistant to a viral endonuclease inhibitor. **G. Kumar**, M. Song, W. Shadrick, W. Zhou, T. Jeevan, P. Slavish, T. Fabrizio, S. Yoon, T. Webb, R.J. Webby, S.W. White

Cook Convention Center
River Bluff Room

Biomolecular NMR

J. Young, *Organizer, Presiding*

1:00 715. Using NMR spectroscopy to understand the thermodynamics of gold nanoparticle-protein interactions. A. Wang, K. Woods, R. Perera, **N. Fitzkee**

1:40 716. Measuring the kinetics of ground-state motion in disordered proteins and how it is influenced by small-molecule binding. **D. Ban**, L.I. Iconaru, A. Ramanathan, R. Kriwacki

2:00 717. Structure and binding studies of the bi-functional *Chlamydia trachomatis* protein, Scc4. **M. Macnaughtan**, O. Goodwin, A. Songok

2:40 718. Solution NMR refinement of a metal ion bound protein using metal ion restrained molecular dynamics methods. **D. Chakravorty**

3:00 Intermission.

3:40 719. Computational and experimental studies of mono- and poly-ADP-ribosylation of peptides. **M.A. Johnson**, A. Goel, M. Chan, X. Tan, R. Hammond

4:20 720. Discovery of small molecules that inhibit the disordered protein, $p27^{Kip1}$. **L.I. Iconaru**, D. Ban, K. Bharatham, A. Ramanathan, A. Shelat, J. Zuo, R. Kriwacki

Cook Convention Center
L-8

Environmental Analysis

G. L. Emmert, P. Simone, *Organizers, Presiding*

1:00 721. Using neutrons to study fluid-rock interactions. **V.H. DiStefano**, J. McFarlane, L. Anovitz, A.D. Gordon, R.E. Hale, R.D. Hunt, S.A. Lewis, K.C. Littrell, A.G. Stack, S.J. Chipera, E. Perfect, H.Z. Bilheux, L.M. Kolbus

1:20 722. *In-situ* soil carbon analysis using inelastic neutron scattering. **G. Yakubova**, A. Kavetskiy, S. Prior, H. Torbert

1:40 723. Spectroscopic monitoring of atmospheric methane near the Craighead County landfill. **S.W. Reeve**, T. Johnson

2:00 724. Sorptive removal of Pb^{2+} and mechanisms of adsorption on chitosan-modified biochar. **N.W. Bombuwala Dewage**, T. Mlnsa

2:20 725. Assessment of down-hole membrane-diffused hydrogen for stimulating uranium reduction and immobilization. **L. Haynes**, L.W. Clapp

2:40 726. Fabrication and characterization of nanoscale pillar arrays for planar chromatography. **M.J. Sepaniak**

3:00 Intermission.

3:20 727. Ion transfer stripping voltammetry for the detection drugs in real samples. **A. Izadyar**

3:40 728. Electrochemical detection of TNT using vanadium dioxide particle films. **A.W. Daniel**, M. Casey, D.E. Cliffel

4:00 729. Predictive models of aqueous organic contaminant binding properties on carbon surfaces: QSPR and QM computations applied to emerging contaminants of concern. **W.A. Alexander**, J. Bach, D. Knappe

4:20 730. Comparison of teratogenic and toxic effects of ortho-phthalate esters in xenopus embryos. S. Gardner, R. Lester, A.T. Wood, P. Onkst, N. Burnham, **D.H. Perygin**, R. James

Cook Convention Center
L-11

Frontiers in Nucleic Acids Chemistry

Protein-DNA Interactions

D. E. Graves, E. A. Lewis, *Organizers*
L. D. Williams, *Presiding*

1:00 731. Interactions of fluoroquinolones and MGIs with *Mycobacterium tuberculosis* gyrase: Enhancing drug activity against wild-type gyrase and resistant mutants. K.J. Aldred, T.R. Blower, R.E. Ashley, E.G. Gibson, R.J. Kerns, J.M. Berger, **N. Osheroff**

1:40 732. Iron mediates catalytic function of nucleic acid processing enzymes. **L.D. Williams**

2:20 733. Elucidating the mechanism of charge transport in human DNA primase. **M.K. Thompson**, L.E. Salay, M.E. Holt, E. O'Brien, A.C. Ehlinger, J.K. Barton, W.J. Chazin

2:40 734. Using restriction endonuclease activity assays to examine cooperativity and competition in the binding of small molecules to DNA. **S.A. Winkle**

3:00 Intermission.

3:20 735. Bypass and misincorporation of DNA polymerases at DNA-peptide crosslinks. **C.A. Sedgeman**, K.M. Johnson, F. Guengerich

4:00 736. Investigating different metal ion concentrations for *in vitro* selection of DNA aptamers for pesticide targets. E.K. TeSelle, **D.A. Baum**

4:20 737. Exploring the origins of RNA: Spontaneous formation and assembly of plausible proto-nucleotides. **N.V. Hud**

Cook Convention Center
L-2

General Biological Chemistry

S. Pedigo, *Organizer*
C. Fox, *Presiding*

1:00 738. Mechanism of action of N-hydroxylating flavin-dependent monooxygenases. **P. Sobrado**

1:20 739. Methods for the identification of potential therapeutics from combinatorial peptoid libraries. **K. Bicker**, K. Fisher, A. Corson

1:40 740. E-4-Hydroxy-3-methylbut-2-enyl diphosphate reductase (IspH): An isoprenoid synthesis enzyme. **S.M. Ghebreamlak**, E.C. Duin

2:00 741. Novel approaches for the biosynthesis and diversification of polyketides. **S.A. Meiser**, G.J. Williams

2:20 742. The role of the S-loop of human glutathione synthetase. **M.E. Anderson**, T.R. Cundari, B. Shrestha, H. Conrad Webb, B.L. Ingle

2:40 743. Molecular structure and oxidation of methionyl dipeptide. **S. Babu**, F. Fronczek, R.M. Uppu, M.O. Claville

3:00 Intermission.

3:20 744. Global metabolomic profiling of cuprizone-induced demyelination in the central nervous system. **A. Taraboletti**, L. Shriver

3:40 745. Principles of transition metal selectivity and transport in transmembrane ion pumps. **G. Meloni**, D. Mattle, O. Sitsel, F. Tadini Buoninsegni, M.R. Moncelli, L. Zhang, P. Gourdon, P. Nissen, D.C. Rees

4:00 746. Synthesis and pharmacology of a radioiodinated δ-opioid selective agonist based on the [$_{D}$Ala^{2}]deltorphin II template. **K.R. Wilson**, R. Pescatore, G.F. Marrone, S.A. Sedberry, D. Vinton, N. Finkelstein, Y.E. Katlowitz, G.W. Pasternaka, J.D. McSwain, S. Majumdar

4:20 747. Investigation of polymethine cyanine dyes: Oxidation and thermal DNA cleavage. **Z. Li**, C. Holder, E. Soriano, M. Henary, K.B. Grant

4:40 748. Uptake of fluorescently-labeled amyloid-β42 by primary murine microglia. **L.K. Gouwens**, M.R. Nichols

5:00 749. Study membrane protein structure by neutron scattering. **S. Qian**

Cook Convention Center
L-12

Nanomaterials: Synthesis, Characterization, and Applications

Synthesis

A. Antonysamy, A. L. Parrill-Baker, *Organizers*
R. T. O'Connor, *Presiding*

1:00 750. Preparation of Au_2S—$Cu_{2-x}S$ hybrid nanoparticles via cation exchange. **S.L. Arrowood**, J. Macdonald

1:20 751. Simple synthesis of luminescent graphene quantum dots using acetone and their facile incorporation into polymer matrices. **J. Fosdick**, G. Gyanwali

1:40 752. Electron transport in nanocomposites of silver telluride and naphthalene-diimide–bithiophene co-polymer films.**T. Sutch**, L. Presson, G. Szulczewski

2:00 753. Area specific atomic layer deposition enabled by microcontact printing. **B. Patel**, S. Chopra, H. Nallan, J.G. Ekerdt

2:20 754. Chemical methylation of lysine residues can severely weaken gold nanoparticle-protein interactions. **Y.R. Perera**, K. Woods, C. Wilks, A. Wang, N. Fitzkee

2:40 755. Exploring composites of high work function 2D materials with semi-metal and semiconducting 2D materials. **C. Herrera**, S. Warren

3:00 Intermission.

3:20 756. Synthesis and characterization of organo-soluble $Au_{102}(SPh)_{44}$ nanomolecules. **M. Rambukwella**

3:40 757. Dextran-iron oxide nanoplates and nanoflowers showing excellent aqueous phase stability. **S. Palchoudhury**, R. Orr, H. Alkushiban, J. Limas Chavez, M. Downs

4:00 758. Triblock copolymers for thermally triggered drug delivery. **J.A. Nikles**, D.E. Nikles

4:20 759. Colloidal self-assembly of multifluorescent silsesquioxane microparticles. **N. Neerudu Sreeramulu**, H.P. Rathnayake

4:40 760. Hybrid nanoparticles: Progress towards photocatalytic water splitting. **A.D. LaCroix**, J. Macdonald

5:00 761. Bottom-up fabrication of porous gold with large surface area. **H.S. Perera**, D. Zhang

Cook Convention Center
L-3

Student-Centered Learning in the Chemistry Classroom and Laboratory

Cosponsored by CHED
M. B. Freilich, *Organizer*
F. J. Creegan, *Organizer, Presiding*

1:00 762. The best of both worlds: Incorporating peer instruction with POGIL activities. **M.D. Perry**

1:20 763. Balancing chemical equation in middle school classrooms. **A.L. Curry**, E. Andrews, T. Robinson, M.L. Curry

1:40 764. Chemical enrichment Fridays at San Jacinto College using ACS Webinars and other internet resources to motivate student engagement with science courses. **R.H. Whitmarsh**

2:00 765. Using Skype as a mentoring tool for chemistry majors: An online field trip. **J. Emily**

2:20 766. Interdisciplinary application of thermodynamics for a mechanism of binding of ions to a cell membrane. U.C. Panse, **V.C. Waghulde**

2:40 767. Cheminformatics OLCC: An evolving ontological framework based intercollegiate course management system. **R.E. Belford**

3:00 Intermission.

3:20 768. Science attitudes in an introductory chemistry course: Examining group differences and its relationship with achievement. **S. Villafane-Garcia**, J.E. Lewis

3:40 769. Developing and implementing an assessment technique to measure linked concepts. **L. Ye**, S.E. Lewis, R. Oueini

4:00 770. Academic motivation scale-chemistry: A theory-based instrument to investigate student motivation toward chemistry. **Y. Liu**, B. Ferrell, J. Barbera, J.E. Lewis

4:20 771. Exploring the role of students' study habits in general chemistry. **S.E. Lewis**, L. Ye, R. Oueini, A.P. Dickerson

4:40 772. Examining student conceptual understanding using automated lexical analysis of open-ended responses. **X. Xu**, J.A. Loertscher, V.M. Thorsell, J.E. Lewis

5:00 773. Characterizing postsecondary chemistry instructional practices: A pilot test of survey items and a stratified sampling strategy. **J.R. Raker**, M.N. Stains, E. Laga

Cook Convention Center
West Mezzanine

Undergraduate Posters

Biological Chemistry

A. L. Parrill-Baker, *Organizer*

1:00 - 3:00

774. Measurement of NADH production by lipid bodies in *Brassica napus*. **K. Nguyen**, G.A. Giles

775. Ladybirds: Detection and determination of alkaloid compounds. **W. Perry**, Y. Kajita, M.F. Santiago

776. Synthesis of chalcones that mimic resveratrol and curcumin and inhibit amyloid-beta (1-40) aggregation. **C.S. Bray**, D. Higgins, J. Reed, P.A. Martino

777. The structural analysis of aspartame using a 60 MHz NMR. **J. Beale**, W.A. Tallon, C. Clinger

778. Biosynthesis of the recently discovered peptide hormone preptin. **A. Stallone**, T. Pritchett, J.M. Meyers

779. Characterization and biochemical analysis of noncanonical coronavirus macrodomains. **M. Chan**, R. Hammond, C. Tian, X. Tan, A. Goel, M.A. Johnson

780. Identification of factors stabilizing the 3D structure of the goodpasture autoantigen of glomerular basement membrane. **T. Mikhailova**

781. Loss of extracellular matrix Protein X causes altered function of sensory neurons in *Drosophila*. **C. Formby**, H. Cathcart, E. LeMosy

782. Development of a neuronal viability assay using SH-SY5Y cells. **R. Bujol**, D.E. Oseid, A.S. Robinson

783. Biogenesis of cytochrome oxidase: Mechanism of heme *a* synthase. **N.G. Taylor**, N.J. Harris, J.L. Fox

784. SdsA1 sulfohydrolase and homologous proteins. **G.L. Waddell**, C. Smith, N. Denman, M. Forconi, J.L. Fox

785. Synthesis and screening of antimicrobial peptoid combinatorial libraries against the fungi *Aspergillus*, *Candida*, and *Cryptococcus*. **A. Corson**, K. Fisher, K. Bicker

786. Kemp eliminase activity of ketosteroid isomerase: Kinetic behavior of active site mutants. **L.R. Fanning**, E. Sanchez, M. Forconi

787. Synthesis of resveratrol analog to block Aβ-peptide (1-40) aggregation. **J.P. Reed**, P.A. Martino

788. Computational modeling for understanding the activation of the receptor for advanced glycation end products. **D. Martin**, I. Christopher, D. Graham, K. Amoah, S. Damo

789. Pegylation of bacterioferritin, a protein scaffold for delivery of toxic iron to cancer cells. **C. Kennedy**, E. Boice, D.M. Kurtz

790. A routine ESI-MS method to screen drug effectiveness in inhibition of amyloid-beta peptide aggregation rate. **M. Herbert**, P.A. Martino

791. SdsA1: A bioinformatics and kinetic study. **N. Denman**

792. Role of gag domains in bovine leukemia virus RNA packaging. **H. King**, D.F. Qualley

793. Purification and RNA-binding properties of the West Nile virus core protein. **K. Hambrick**, D.F. Qualley

794. Integrin subunits α3 and α6 mediate FGF10-dependent signaling events in collecting duct cells bound to LM511. **S. Toe**

795. Bioconversion of curcumin and its analog. **G.D. Martin**

Cook Convention Center
West Mezzanine

Undergraduate Posters

Organic Chemistry

A. L. Parrill-Baker, *Organizer*

1:00 - 3:00

796. Statistical analysis of tobacco for country of origin via ^{1}H-NMR and multivariate component analysis. **D.L. Paredes**, C. McCleave, J.A. Bjorklund, N.L. Peterson

797. Silver(I)-promoted regioselective oxidative aryl−aryl cross-coupling resulting in a direct C-H activation. **S.C. Berkessa**, **K.A. Jeansonne** , J. Fotie

798. Model studies of the synthesis of the 2-(5*H*)-furamoiety of myrtoidine. **J. Liu**, E. Andreansky, S. Blakey

799. Indolizine-squaraine NIR fluorescent materials. **T. Rill**, L.E. McNamara, A. Huckaba, E.A. Sharpe, N. Hammer, J.H. Delcamp

800. Divergent synthesis of novel 3-α- and 3-β-*C*-functionalized ribose derivatives. **J. Carter**, B. Weaver, M. Chiacchio, W.E. Lynch, B.D. Feske, G. Gumina

801. Lewis acid-catalyzed Minisci reactions. **J.L. Biaco**, S.L. Jones, T.J. Barker

802. Exploring amino acid-derived scaffolds to construct “smart” therapeutics. **S.F. Grady**, H.M. Khan, A.J. Lampkins

803. Advances in the development of druggable β-secretase inhibitor prodrugs. **A.C. Feagans**, A.J. Lampkins

804. Novel aromatic bridging ligands as nanoparticle colloid stabilizing agents. **T. Gravolet**, R. KOMATI, G. Goloverda, V.L. Kolesnichenko

805. Design and synthesis of a cyclic citryl-ornithine analog as a novel inhibitor for Staphyloferrin A biosynthesis. **A. West**, K. Craft, S. Gore, W. Kittleman, D.J. Schedler

806. Multifunctional polyurethane hydrogels for biomedical applications. **C. Seitz**, M. Nguyen-Kim, J. Borghs, J. Wallenborn, A. Böker

807. One-pot sequential conversion of aldehydes to N-tert-butyl amides. **R. Cecil**, R.C. Mebane

808. Identification and development of novel CDK inhibitors. **V.C. Miles**, F. Joseph, P. Tram, R. Schroeder, T. Stone, K. Nguyen, H. McFerrin, J. Sridhar

809. An alkyne strategy for the stereoselective synthesis of piperidines. **N. Robinson**, D. Penk, M.L. Turlington

810. Synthesis of ginkgotoxin and related ether analogs. **J. Yazarians**, G.R. Boyce

811. Withdrawn.

812. Preliminary syntheses of tricyclic furan-bridged ring systems. P. Wiget, **A. MacLean**

813. Design, synthesis, and antimicrobial evaluation of a novel 3’-*C*-acetohydrazide puromycin analog. **J. Carter**, B. Weaver, M. Chiacchio, A.R. Messersmith, B.D. Feske, G. Gumina

814. Synthesis of isoxazolopyridines via cyclization of 3-acylpyridine *N*-oxide oximes. **B.J. Hicks**, J.M. Hanna

815. Synthesis and evaluation of unsymmetrical biphenyltetrols as aggregation inhibitors for Alzheimer’s amyloid-β peptide. **J.A. Roberts**, A.L. Taylor, M.J. Hurtt, B.P. Hernandez, S. Wicks, J.M. Hanna, R.K. Lammi

816. Palladium-catalyzed synthesis of ureas. **L. Jay**, T.J. Barker

817. Mosquitocidal and antibacterial activity of the essential oil of *Solidago gigantea* (Giant Goldenrod). **C. Ardizzone**, N. DeVito, T.A. Estrada, J. Woolman, M. Cochran, W. Dees, C. Struchtemeyer, O.E. Christian

818. Concentration-dependent antibacterial evaluation of the essential oil of *Pycnanthemum tenuifolium* against *Staphylococcus aureus*. **N. DeVito**, T.A. Estrada, C. Ardizzone, J. Woolman, C. Struchtemeyer, W. Dees, O.E. Christian

819. Effect of botanical metabolites from 21 plant species on the yellow fever mosquito, *Aedes aegypti*. **C. Ardizzone**, **W. Dees**, O.E. Christian, J. Theriot, K. Leonards, A. Fusilier, C. Richmond, J. Hightower, A.D. Richard, J. Dupre, M. Cochran, J. Byrne, T.A. Estrada, A. Daugereaux, S. Mopper, J. Woolman

Cook Convention Center
L-10

Multiscale Modeling of Macromolecular Systems

J. Ma, F. Wang, Y. Wang, *Organizers*
V. Rangachari, *Organizer, Presiding*

1:20 820. Milestoning. **R. Elber**

2:00 821. Dynamic potential surfaces for sodium diffusion in type II silicon clathrates. J.G. Slingsby, N.A. Rorrer, L. Krishna, E. Toberer, C.A. Koh, **C.M. Maupin**

2:40 822. Mp2 solvation free energy of simple ions obtained through force matching to simple pairwise potentials. J. Li, **F. Wang**

3:20 Intermission.

3:40 823. Modeling of protein systems with complex landscapes. **U. Hansmann**

4:20 824. Using simulations to link molecular design to macromolecular morphology and function in polymer composites. **A. Jayaraman**

5:00 825. Density functional model for nondynamic and strong correlation. **J. Kong**, E. Proynov

Cook Convention Center
L-4

Recent Advances in Chemical Physics

N. Hammer, *Organizer*
T. Sommerfeld, G. S. Tschumper, *Presiding*

1:20 826. Newly developed methods for describing excited states. **R. Bartlett**

2:00 827. Large-scale variational 2-RDM-driven CASSCF methods. **A.E. DePrince**

2:20 828. Methodologies and development towards quantitative accuracy for the heavy elements: Structural, energetic, and spectroscopic properties. **A.K. Wilson**, G. Schoendorff

3:00 Intermission.

3:20 829. Getting down to the fundamentals of hydrogen bonding. **G.S. Tschumper**

4:00 830. Advances and challenges in the calculations of intermolecular potentials with spectroscopic accuracy. **K. Patkowski**

4:20 831. Rovibronic quantum chemistry. **R.C. Fortenberry**, W. Morgan

4:40 832. Amino derivatives of 6-methylpentacene and 6-methylene-6,13-dihydropentacene. **D.H. Magers**

5:00 833. Applying kinematics models to obtain insights into surface structure from gas/surface collisions. **W.A. Alexander**

Cook Convention Center
West Mezzanine

Undergraduate Posters

Analytical Chemistry

A. L. Parrill-Baker, *Organizer*

3:20 - 5:20

834. Determination of fluoride levels in name and generic brand mouthwashes. **E. Henshaw**, R. Fietkau

835. Application of Cr(III) as a protonating enhancement agent in MALDI/TOF mass spectrometry: Studies of small peptides. **R.R. Persaud**

836. Transformation of $Au_{144}(SCH_2CH_2Ph)_{60}$ to $Au_{133}(SPh\text{-}t Bu)_{52}$ nanomolecules: X-ray crystallography, optical, electrochemical, experimental, and theoretical analysis. **S. Theivendran**, A. Antonysamy, P. Nimmala, C. Kumara, V.S. Reddy, A. Fortunelli, L. Sementa , G. Barcaro, E. Apra, X. Zuo, B. C. Noll

837. Monitoring surface water of Lake Sinclair in Georgia. **J. Olmstead**, C.H. Lisse

838. Qualitative identification of volatile organic compounds present in electronic-cigarette vapor via GC/MS detection. **E. Smith**, C.H. Lisse

839. Determination of protein binding constants of epigallocatechin-3-gallate (EGCG) with rapid equilibrium dialysis and LC/MS/MS analysis. **L. Shade**, M.J. Vergne

840. Method development and optimization for detection of cyanide antidote sulfur donor X (SDX) by use of gas chromatography-mass spectrometry. **J. Ross**, C. Chou, X. Dong, V. Coronado, D. Brown, B.A. Mendenhall, R.J. Roy, L. Kiss, D.E. Thompson, I. Petrikovics

841. The surveillance of anions in natural water determined by ion chromatography. **C. Naylor**, S.W. Huffman

842. Automated spectrophotometric titrations: Seeing the unseen. **M.B. Acuff**, J.A. Lynch

843. Analysis of aspartame in Diet Coke using solid phase extraction and HPLC. **M.S. Lersch**, C.R. Simmons

844. Investigation of novel hydrogen bond donors and halogens in deep eutectic solvents. **S. Schmitz**, S. Asare, D.E. Raynie

845. Uptake and release studies of the biocides polyhexamethylene biguanide and alexidine on contact lenses utilizing ultra performance liquid chromatography and mass spectrometry. **M. Syed**, J.M. Wheeler, S. Wheeler, J. Wheeler

846. Determination of Appalachian stream health in the Maryville College woods. **B. Evans**, N. Duncan

847. Size characterization and alternative synthesis of monolayer-protected quantum dots. W.L. Wright, S.C. Francone, L.R. Tinoco, F.E. Acosta, **E.A. Shriner**, **D.T. Miles**

848. Correlation between different extraction methods and the ratio of neral to geranial in the essential oils of lemongrass. **S.G. Mize**

849. Evaluating the use of dicationic pairing reagents for detecting alkylsulfonates by paired-ion electrospray ionization mass spectrometry. **R. Travis**, B.W. Gregory

850. Validation of separated hemoglobin variants A, F, S, C. R. Montgomery, **A. Afshari**

851. Automation of dynamic isoelectric focusing. R. Montgomery, **D. Williams**

Cook Convention Center
West Mezzanine

Undergraduate Posters

Organic Chemistry

A. L. Parrill-Baker, *Organizer*

3:20 - 5:20

852. Synthesis and characterization of 3,4-dialkoxybenzyl substituted bis-urea organogelators. **D. Loya**, A.J. Carr

853. Examining the effects of cis double bond incorporation in the alkyl tail region of bis-urea organogelators. **H. Bader**, A.J. Carr

854. Analysis of the terpene and sesquiterpene hydrocarbons of lemon and lime oils. **M. Anderson**

855. Elucidating the exciton transport in tetracarboalkoxyphenyl porphyrin thin films for enhanced organic optoelectronics. **D. Lee**, M. Kaushal, G. Singh, A. Ortiz, J. Kassel, M.G. Walter

856. Development of lipid probe for labeling and discovering lipid-binding proteins. **J.M. O'Leary**, M. Best

857. Synthesis of polycyclic compounds using NHC-borenium ions. **K. Heitmeier**, R.J. Felix

858. Synthesis of *N*-acetyl oligopeptides and their methyl ester derivatives. **J. Ndungu**, J.N. Haseltine

859. Synthesis of oligopeptides to be subjected to HIV-1 protease cleavage. **T. Law**, J.N. Haseltine

860. The multi-step synthesis of the tripeptides Ac-Sar-Sar-Sar-OEt and Ac-Sar-Sar-Pro-OEt. **K. Patel**, **C. Taylor**, J.N. Haseltine

861. Kinetics of tripeptide ester methanolysis. **C.L. Padgett**, S. Knapp, J.N. Haseltine

862. Synthesis and activation of N-heterocyclic carbene boranes. **R. Rahman**, R.J. Felix

863. Synthesis, design, and computational analysis of a novel multifunctional porphyrin-thiazolothiazole framework. **D. Lee**

864. Synthesis of novel benzoisothiazolone organocatalysts for dehydrative condensation reactions. **M. Morimoto**, L.S. Liebeskind, P. Gangireddy Reddy

865. Novel deoxygenation dimerization of benzoisothiazolones. **J.D. Cisneros**, L.S. Liebeskind, P.R. Gangireddy

866. Optimization of direct arylation of 1,2,3-triazoles. **A. Kosiak**, A. Neuman

867. Selective mono-reduction of conjugated ester functional groups using lithium borohydride. **W.P. Rice**, **L. Miller**, **W. Kwochka**

868. Functionalized nanoporous polysulfone membranes via silane chemistry. **L. Dunlap**, P. Koenig, B.P. Gindt, T. Fujiwara

869. Synthesis of novel 1,2,3-triazoles using click chemistry. **M. Tohidi**

870. One-pot Suzuki coupling synthesis of substituted isoxazoles under green, microwave conditions. **M. Stofberg**, B. Harmon, **N.L. Powell**

871. Synthesis and catalytic activity of (R)-3-methylpyrrolidine-3-carboxylic acid. **S. Dickerson**, D.S. Masterson

872. Design and synthesis of small molecule HDAC inhibitors for selective targeting of breast cancer. **M. Dennis**

873. Sugar-coated PDA liposomes for pathogen detection. **R. Holmes**, T.W. Hanks

874. Solution ATRP reaction of oligo(ethylene glycol) methacrylate and sulfobetaine methacrylate for the preparation of antifouling surfaces. **D. Pottle**, T.W. Hanks

SATURDAY MORNING

Cook Convention Center
Chickasaw Room

Biomedical Materials and Sensors

E. Lindner, *Organizer*
J. D. Bumgardner, *Organizer, Presiding*

8:00 875. Temperature-responsive polymersomes for controlled delivery of anticancer drugs. **F. Liu**, V.A. Kozlovskaya, E.P. Kharlampieva

8:20 876. Live tissue as a drug-delivery vehicle - surface modification of pancreatic islets. **R.R. Kane**, B. Naziruddin, B. Akinbobuyi, C. Chang, J. Horton

8:40 877. Electrospun chitosan nanofiber membranes for guided bone regeneration. **J.D. Bumgardner**, C. Wu, H. Su, T. Fujiwara, N. Ghadri, A. Karydis, K. Anderson , W. Haggard, F. Garcia-Gody, P. Adatrow

9:00 878. Tetracycline loaded chitosan microspheres utilized for local drug delivery. **G. McGraw**, J.D. Bumgardner, W. Haggard, J.A. Jennings

9:20 879. Development of injectable *in situ* forming depot systems for long-acting contraception. **D.R. Janagam**, L. Wu, K. Chaudhry, S. Ananthula, T.D. Mandrell, J.R. Johnson, T.L. Lowe

9:40 880. Tuning cell/surface interactions on microporous materials for neuronal scaffolds using organic surface coating strategies: Surface properties of emerging aerogel biomaterials and planar substrates. **W.A. Alexander**, D.C. Grigsby, F. Sabri

10:00 Intermission.

10:20 881. High protein loading efficiency by kinetic doping for biosensor applications. **M. Crosley**, W.T. Yip

10:40 882. Poly octylthiophene-based solid contact electrodes with improved potential reproducibility. **J.M. Jarvis**, M. Guzinski, B.D. Pendley, E. Lindner

11:00 883. Sugar sensing using boronic acid-modified poly(amidoamine) dendrimers. **X. Liang**, M. Bonizzoni

11:20 884. Intracellular degradable hydrogel cubes and spheres for anti-cancer drug delivery. **B. XUE**, V.A. Kozlovskaya, E.P. Kharlampieva

11:40 885. Developing a copper responsive MRI contrast agent. **N.N. Paranawithana**, A.F. Martins, P. Zhao, G. Kiefer, A.D. Sherry

Cook Convention Center
River Bluff Room

Drug Discovery Technologies

T. Chen, F. Fan, *Organizers, Presiding*

8:00 886. CDD Vault, CDD Vision, and CDD Models for drug discovery collaborations. **S. Ekins**, A. Coulon-Spektor, K. Gregory, C. Weatherall, K. Dole, A. McNutt, P. Nyberg, T. Gilligan, X. Ba, B. Holtz, S. Ernst, F. Cole, M. Navre, A. Clark, B. Bunin

8:40 887. Discovery of ClpP allosteric activators using ^{19}F fragment screening. **J.J. Bowling**, E. Griffith, A. Singh, R. Tangallapally, R.E. Lee

9:00 888. Investigation of possible suicide inhibition of cytochrome P450BM-3 by *N*-fatty acyl amino acids with terminal carbon-carbon triple bonds in their acyl chain. **S. Yavari**, D.C. Haines

9:20 889. A directed high-throughput screening approach for the identification of a novel small molecule inhibitor of Constitutive Androstane Receptor (CAR). **M.T. Cherian**, W. Lin, L. Yang, T. Chen

9:40 890. *Streptococcus mutans* glucosyl transferase inhibitors for the prevention of dental caries. **S.E. Velu**, B. Nijampatnam, T. Nguyen, Q. Zhang, H. Wu

10:20 Intermission.

10:40 891. Photoligation mechanism of DNA bases to the cis bis-aqua Ru(II)bis(2,2'-bipyridine) complex. **R.W. Larsen**

11:20 892. Use of ferrocenylated N-heterocyclic carbenes to alter the metabolism of reactive oxygen species in human cancer cells. J.F. Arambula, K. Arumugam, **R.E. McCall**, D.J. Magda, C. Bielawski, V. Lynch, J.L. Sessler

11:40 893. Dynamic injection surface plasmon resonance enables one pass fragment kinetics and affinity in addition to aggregation assessment through determination of diffusion coefficients. **R. Cope**

Cook Convention Center
L-11

Frontiers in Nucleic Acids Chemistry

DNA Targeting and Capture

E. A. Lewis, *Organizer*
D. E. Graves, *Organizer, Presiding*

8:00 894. Nucleic acid detection and multivalent display on synthetic PNA backbones. **D.H. Appella**

8:40 895. Sequence-targeted invasion of DNA and RNA G quadruplexes by peptide nucleic acid. **B.A. Armitage**

9:20 896. Gamma peptide nucleic acids: As orthogonal nucleic acid recognition codes for organizing molecular self-assembly. **D.H. Ly**

10:00 897. Micro-RNA-21 responsive DNA nanostructures for sensing and therapeutics. **C.H. Battle**, X. Chu, J. Jayawickramarajah

10:20 Intermission.

10:40 898. Nucleic acids: The target or the ligand. **D.E. Graves**, K. Harris, K. Selander, K. Hayden, B. Tucker

11:00 899. Effects of 5-hydroxymethylcytosine epigenetic modifications within the VEGF promoter region on G-quadraplex and i-motif DNA structure and stability. **M.M. Molnar**, R. Morgan, B. Summerford, T.A. Brooks, R.M. Wadkins

11:20 900. DNA in tight spaces: Linking structure, stability, and protection in packaged DNA. **J.E. Derouchey**

Cook Convention Center
L-10

Multiscale Modeling of Macromolecular Systems

J. Ma, V. Rangachari, F. Wang, *Organizers*
Y. Wang, *Organizer, Presiding*

8:00 901. Effective Riemannian diffusion model for conformational dynamics of membrane transporters. **M. Moradi**

8:40 902. Membrane-protein interactions: Analysis using particle and continuum models. **Q. Cui**

9:20 903. Wrapping, aggregation and spontaneous endocytosis of nanoparticles by tensionless lipid membranes. **M. Laradji**

10:00 Intermission.

10:20 904. Transformer proteins: Friends and foes. **B. Gerstman**

11:00 905. Multiscale modeling of peptide folding and self-assembly. **J. Li**

11:40 906. The role of the mucus layer in the human tear film. **A. Vaidya**

Cook Convention Center
L-12

Nanomaterials: Synthesis, Characterization, and Applications

Characterization

A. Antonysamy, A. L. Parrill-Baker, *Organizers*
E. Kwizera, *Presiding*

8:00 907. *In situ* spectroscopic characterization of an organic dye at the surface of TiO_2 and ZnO nanoparticles dispersed in a liquid medium. J. Vogel, A.A. Al-Nossiff, L. Dreier, K. Shane, C. Nelson, **M. Subir**

8:20 908. Functionalization of single wall carbon nanotubes with group 6 metals. **K.D. Wright**, A.R. Barron

8:40 909. One pot synthesis of hierarchically porous carbon/Ni nanoparticle monolithic composites by nanocasting and their catalytic activity for 4-Nitrophenol reduction. **C. Thambiliyagodage**

9:00 910. Designed emergent behavior in molecular magnets. **C. Lampropoulos**

9:20 911. Study on the effect of ligand incorporated metal on the graphitization and electrical conductivity of hierarchically porous monolithic carbon. **T. Kotbagi**, C. LeDoux, H. Cho, J. Van Zee, K.H. Shaughnessy, M.G. Bakker

9:40 912. Investigation of the stability of silver bromide films on the atomic scale. **J.A. Phillips**, H. Morgan, L. Jackson, G.H. Jones, S. Wang, E.V. Iski

10:00 Intermission.

10:20 913. Modulation of the electron transfer rate of gold nanoparticles by changes in pH and ligand composition. **D. Crisostomo**, D.E. Cliffel

10:40 914. Photoelectrochemical studies of TiO_2 and Fe_2O_3 nanoparticulate surface-modified films. **L. De La Garza**, H. Kim

11:00 915. Coupling and plasmonic enhancement of chromophores with hybrid gold nanoparticles. **A.K. Tobias**, M. Jones

11:20 916. Defect luminescence from wurtzite $CuInS_2$ nanocrystals. **A. Leach**, X. Shen, A. Faust, M. Cleveland, A.D. LaCroix, U. Banin, S.T. Pantelides, J. Macdonald

11:40 917. Synthesis and characterization of bulky-thiolated nanomolecules. **T.C. Jones**

12:00 918. Contradictory dual effects: Organothiols can induce both silver nanoparticle disintegration and formation under ambient conditions. **W.D. Siriwardana**, D. Zhang

Cook Convention Center
West Mezzanine

Undergraduate Posters

Biological Chemistry

A. L. Parrill-Baker, *Organizer*

8:00 - 10:00

919. Molecular inhibition of oligomer formation and Aβ peptide (1-40) aggregation in Alzheimer's disease. **D.W. Higgins**, P.A. Martino

920. Cellular uptake of polyphenols in a bacterial protein expression system. **B.K. Griffin**, **E. Fairchild**, J. Meyers

921. The fight against Alzheimer's disease: Combatting Aβ aggregates synthesized on latex beads. **S. Woidill**, K.M. Matera

922. Introduction of fluoroaromatics in proteins via S_NAr. **J. Derryberry**, J.F. Mansure, B. Norton-Baker, M. Forconi

923. Effects of dextran on the stabilization of i-motif DNA. **K.D. Abston**, R.M. Wadkins

924. Development of a sensing system for the measurement of the hydrolysis of β-lactam antibiotics. **N. McGuire**, L.G. Puckett

925. Biosynthesis of mitochondrial derived peptide MOTS-c for biological characterization. **J. Smith**, J. Meyers

926. Oxidation of endocrine disrupting chemicals by *Trametes versicolor* laccase. **H.E. Patterson**, C.M. Johnson

927. Synthesis of MTSL-labeled elastin-like proteins for paramagnetic NMR. **C.J. Price**, Y. Zhang, N. Fitzkee

928. GPR31 modeling and pharmacophore-guided antagonist discovery. **N.A. Galindo**, A.L. Parrill-Baker

929. Modeling GPR6: A potential therapeutic target in the treatment of Parkinson's disease. **R. Coleman**, A.L. Parrill-Baker

930. LKE as a potential therapeutic for neurodegeneration in a mouse model of neuronal ceroid-lipofuscinosis. **C. Willis**, K. White, H. Magee, R. Laufmann, D. Timm, J.M. Weimer

931. Heat shock response in lung fibroblasts to changes in environmental calcium. C. Oculam, O. Creech, **B. Sharma**

932. Characterization of transcription factors from the extremophile *Thermus thermophilus*. **K. Hiam**

933. Characterization of a potential allosteric site in tetrahydrodipicilonate-N-succinyltransferase (DapD) using the effector molecule 2-aminoterephthalic acid. **A. McMurry**, **N.A. Clanton**, C.M. Johnson

934. Cloning, expression, and purification of two pyridoxal 5'phosphate-dependent enzymes to be used in the development of novel activity-based probes. M. Smith, **C.M. Johnson**

935. Synthesis and characterization of modified poly (xylitol sebacate) (PXS) copolymers for improved nanoparticle formation. **J.A. Morris**, N. Arnett

936. Functional analysis of NMDAR *GRIN1* mutations associated with infantile-onset epilepsy and encephalopathy. **J. Pecha**, C. Hu, H. Kusumoto, W. Chen, H. Yuan, S. Traynelis

937. Geochemistry before biochemistry: Plausible prebiotic reaction spaces involving mineral surfaces. **A. Pital**

938. Engineering a mutation in the heparin binding pocket of the human fibroblast growth factor. **R. Patel**

Cook Convention Center
West Mezzanine

Undergraduate Posters

Inorganic Chemistry

A. L. Parrill-Baker, *Organizer*

8:00 - 10:00

939. Synthesis, characterization, and activity of graphene oxide (GO) modified bismuth niobium oxide (BNO). **E.N. Mahmood**, S.P. Adhikari

940. Synthesis, characterization, and catalytic oxidation studies of first-row copper and cobalt complexes supported by redox-active ligands. **S. Cemaj**

941. Synthesis of $Cu_2(Zn_{1-x}Co_x)SnS_4$ solid solutions and kinetics of methylene blue adsorption. **A. Sharma**, A.H. Pinto, R. Penn

942. Synthesis of isoquinoline derived pentadentate ligands. **C. Lyons**, R. Mattapalli, K. Driskill, K. Knight, X. Zhao

943. Photocatalytic TiO_2 coatings for reduction of ammonia and methane livestock emission concentration. **K. Oziminski**, **D. Batchelor**, J. Zitnyar, A.H. Shelton

944. Toward the synthesis of small silver clusters. **A.D. Royappa**, B. Tate, J.P. Sadighi

945. Development of new iminophosphorane-based catalysts for the ring-opening polymerization of renewable lactones. **E. Rees**, A. Buchard, T.A. Nile, A.G. Glenn

946. Effect of particle size on the magnetic induction heating efficiency for magnetite nanoparticles. **A.L. Paulson**, R.R. Shah, T. Davis, C.S. Brazel, D.E. Nikles

947. Initial investigation on structural mimicking of the photosynthetic catalysts. A. Saha, **B.K. Long**

948. Spectroscopic investigation of amyloid beta(1-28) in the absence and presence of Cu(II): Comparing and contrasting human, R5G, H13R, and rat peptides. **A. Pinkham**, S. Sipe, J. Kenney, A.M. Spuches

949. Solid-state anticancer drug synthesis using Merrifield resin. **A. Emig**, S. Flower, T.A. Nile, A.G. Glenn

950. Developing iron triazene and formamidine catalysts. **A.N. Kozak**, R.L. Webster, T.A. Nile, A.G. Glenn

951. New catalysts for ethanol conversion to biofuels. **T.L. Strider**, K. Pellow, D. Wass, A. Glenn, T.A. Nile

952. A stimuli-responsive, site-specific nano-drug delivery ideal for oral administration. **A. Ozkizilcik**, S. Murphy, Z. Tian

953. Titanium-mediated reduction of imine substrates. **L.A. Freeman**, T. Varner, R. Himes

954. Towards multinuclear spin crossover Fe(II) complexes in {N4S2} coordination environments. **V. Stubbs**, A. Dragulescu-Andrasi, M. Shatruk

955. Synthesis of iron(II) chloride alkyl and aryl complexes. **A. Hairston**, D. Elorriaga, R. Bedford, A. Glenn, T.A. Nile

956. Ligand photorelease from Ru(II)bis(2,2'-bipyridine)L_2 complexes encapsulated within a Zn(II)-trimesic acid based metal organic framework. **J.M. Lee**, T.A. Word, R.W. Larsen

957. Importance of phosphine ligand design in the elucidation of homogeneous gold (I) mechanisms. **F. Liu**, C. Griebel , A.C. Jones

958. Serotonin gold nanocorals for trace level detection of nitroexplosives. **J.R. White**, J. Evans, S.I. Hughes, H. Yu, S.S. Dasary

959. Synthesis of nitrogen-rich ligands and cobalt complexes for hydrogen production. **T. Rice**, S.R. Powers, Y. Gueye, X. Zhao

960. A pedagogic green chemistry demonstration using dye-sensitized solar cells. **L. Gargus**, H. Streckert, K.A. Harris, J. Alexander, S.K. Airee

Cook Convention Center
L-3

General Organic Chemistry

Analytical & Materials

T. J. Burkey, *Organizer*
C. E. Hobbs, *Presiding*

8:20 961. Benchtop NMR spectroscopy for at-line and on-line reaction monitoring. **S. Riegel**

8:40 962. Exploring the potential and limits of two-channel benchtop NMR with indirect detection capabilities for undergraduate research. **P. Wiget**, A. MacLean, C. Plourde, T. Clark

9:00 963. Small-molecule models of poly(amidoamine) dendrimers. **N. White**

9:20 964. Routes toward greener, polymer-supported catalysts and polymer functionalization. **C.E. Hobbs**

9:40 965. Synthesis of a 3-diazonium-4-(trifluorovinyloxy) - perfluorobutanesulfonylfluoride zwitterionic monomer for polymer electrolyte membrane fuel cell. **I.D. Addo**

10:00 Intermission.

10:20 966. Artificial membrane fusion driven by click chemistry. **S. Whitehead**, S. Alam, M.D. Best

10:40 967. A dehydrative aromatization protocol for the synthesis of highly distorted para-phenylenes: A new tool for the synthesis of carbon nanostructures. **N. Mitra**, B.L. Merner

11:00 968. Azulene-modified polysiloxane for use as a gas chromatography stationary phase. **M. Jackson**, J. Schaffer, C.M. Garner

11:20 969. Synthesis, supramolecular chemistry and solid-state reactivity of 2,3-substituted dienes: 3,4-Bis(methylene)hexanedioic acid and fulgenic acid. **B. Dinkelmeyer**, S.W. Huffman, C. Steddum, A. Stutesman, C. Jones, R.D. Pike

11:40 970. Functionalized polyanilines as novel curing agents for epoxy resins. **J. Cook**

Cook Convention Center
L-4

Student-Centered Learning in the Chemistry Classroom and Laboratory

Cosponsored by CHED‡
F. J. Creegan, *Organizer*
M. B. Freilich, *Organizer, Presiding*

8:20 971. Student-centered learning in the chemistry laboratory: The POGIL approach. **F.J. Creegan**

8:40 972. Incorporating gas chromatography-mass spectrometry into one-year general chemistry courses. **B. Liburd**

9:20 973. Teaching nucleophilic substitution reactions of alkyl/aryl halides using inquisitive approach. **V.C. Waghulde**, U.C. Panse

9:40 974. Revisiting course design to address higher level learning outcomes in a general chemistry laboratory. **C.M. Taylor**, A. Hines, A. Jordan

10:00 Intermission.

10:20 975. Spatial reasoning for the 21st century student: Computer vs. handheld models. **J.E. Barker Paredes**

10:40 976. Increasing student engagement using cross-disciplinary course-based research experiences. **L.K. Stultz**, P.K. Hanson

11:00 977. The first-year research experience (FYRE) program: Introducing research to first year students at the University of Oklahoma. **N. Kothapalli**, R. Halterman, A.W. Burgett

11:20 978. Student engagement strategies and small-scale research in a community college setting. **G. Gyanwali**

11:40 979. How we teach; what students learn. **A.L. Jeffery**

Cook Convention Center
203

Undergraduate Papers

Analytical Chemistry

A. L. Parrill-Baker, *Organizer*
A. R. Jones, *Presiding*

8:20 980. Examining the effects of urbanization on Boone Creek. **C. Macemore**, C.M. Babyak

8:40 981. Sulfide induced dispacement of gold nanoparticle ligands. **A. LaCour**, H.S. Perera, D. Zhang

9:00 982. Acute toxicity of FA-GLU, surfactin, and surfactin isomers, microbial based biosurfactants, on larval gulf killifish *Fundulus grandis*. **H. Olivier**, **R. Nuss**

9:20 983. Withdrawn.

9:40 Intermission.

10:20 984. Extraction and analysis of xylitol in sugar free gum: A "green" laboratory experiment for chemistry students. **J.C. Brown**

10:40 985. Quantitative HPLC analysis of n-(n-butyl) thiophosphoric triamide (NBPT) using UV detection. J.K. Dogbe, **B. Skinner**, G. Whitehurst

11:00 986. Determination of mVOCs for distinguishing virulent from hypo-virulent *Cryphonectria parasitica* via headspace-SPME-GC-MS. **M. King**, J. She

11:20 987. Development and validation of HPLC-MS methods for the quantification of eumelanin and pheomelanin pigments in tissue samples. **L.M. Nikont**, K. Glass

11:40 988. Characterizing structure-function relationships in bisurea organogelators using infrared spectroscopy. H. Gao, A.J. Carr, **K.S. McCain**

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Undergraduate Papers

Physical Chemistry

A. L. Parrill-Baker, *Organizer*
J. M. Yarbro, *Presiding*

8:20 989. Deviations of the glass transition temperature (T_g) of polystyrene nanospheres under hard and soft confinement. **N.M. Sikes**, R. Torres Guzman, D.W. Holley

8:40 990. Spectroscopic and theoretical investigation of solvent and temperature effects on optical activity of (*R*)-3-methylcyclohexadominant conformers. **A. Alenaizan**, W. Al-Basheer, M.M. Musa

9:00 991. Synthesis of metal-impregnated xero- and aero-gel catalysts for carbon dioxide reduction. **C. Jackson**

9:20 992. Longitudinal alignment and optical characterization of gold nanostars in electrospun polymer fibers. **V. Varanasi**, B. Chapman, G. Firestone, L. Clarke, J. Bochinski, J.B. Tracy

9:40 993. Thermal, mechanical, and optical characterization of luminescence-doped PDMS thin film sensors. **K. Mitchell**, S. Allison, F. Sabri

10:00 Intermission.

10:20 994. Why does the acetaldehyde enolate favor reaction at the O atom during gas-phase nucleophilic substitution? Contributions by resonance and inductive effects. **C. Seitz**, J.M. Karty

10:40 995. Assigning acetol: Simulated IR spectra using high-level ab initio methods. **N. Tipton**

11:00 996. Characterization of P3HT/graphene composites synthesized via *in-situ* GRIM methods. **D. Presto**, V. Song, D.S. Boucher

11:20 997. Adsorption of immunoglobulin on cellulose and chitin films using surface plasmon resonance. **N.T. Anderson**, A. Esker

11:40 998. Green synthesis: Characterization of saccharide coated gold nanoparticles for catalytic applications. **H. Moolani**, J. Payne, R. Dakshinamurthy

Cook Convention Center
L-2

General Inorganic Chemistry

N. J. Deyonker, *Organizer, Presiding*

8:40 999. Selected *f*-element coordination polymers incorporating glutarate and terephthalate derivatives. **R.A. Zehnder**, M. Zeller

9:00 1000. Structural and magnetic characterization of Mn/Ln (Ln = Gd, Tb, Dy, Ho) single-molecule magnet clusters from the use of 2-(hydroxymethyl)pyridine and its bulkier derivatives. **L. Pham**, K. Abboud, W. Wernsdorfer, G. Christou

9:20 1001. Predicted properties of LnF_4 and LnF_4^- complexes: The role of the Ln oxidation state. **Z. Lee**, D.A. Dixon, V.E. Jackson, Z. Fang

9:40 1002. Synthesis of red, green, and blue phosphors for solid state lighting. **M. Foley**, G.F. Strouse

10:00 1003. Computational study of metallo-bis(dithiolene) complexes. Effect of d-electron count on the central twist angle between two MS_2 planes; a surprising discovery for d^9 systems. **C.C. Kirkpatrick**, B.A. Kowert, J.N. Truong

10:20 Intermission.

10:40 1004. New annulated N-heterocyclic carbenes and their transition metal complexes. **O.J. Buckner**, C. Boudreaux, B. Norvell, D. Tapu

11:00 1005. Synthetic analogs of the nickel superoxide dismutase catalytic site. **V.G. Snider**, A. Mukherjee

11:20 1006. Biomimetic models of ni-superoxide dismutase: Exploring the impact of N rich primary coordination sphere. **N. Singh**, A. Mukherjee

11:40 1007. Pincer-type N-heterocyclic carbene complexes of late transition metals: Synthesis, characterization, and reactivity studies. **L. Tahsini**, R. Latifi

Cook Convention Center
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Undergraduate Posters

Analytical Chemistry

A. L. Parrill-Baker, *Organizer*

10:20 - 12:20

1008. Development of a turkey DNA allele frequency database. M. Stockdale, **D. Faught**

1009. Analysis of e-liquids. **T. Turner**, A. Frantzen

1010. Analysis of flathead catfish for mercury content in Lake Columbia, AR. **B.K. Hedstrom**, G. Geme

1011. Carbon 13NMR studies of saturated fatty acids bound to bovine serum albumin. **R. Montgomery**, H. McAlexander

1012. Determination of effect of chewing rate on releasing xylitol from gum sticks. S.M. Rajapaksha, **G. St Louis**, T. Mlnsa

1013. Purification and clean-up of glycans. R. Montgomery, K. Stumpo, **R. Wolters**

1014. Stability-indicating UPLC-MS/MS assay for 1960's Eli Lilly and Company pharmaceuticals in dosage forms. **C. Quinn**, T.R. Rybolt, S. Symes

1015. Analysis of urine organic acids via GC/MS-based metabolomics to determine the effect of diet on urine composition. **J.L. Minnick**, C.H. Lisse

1016. Discrimination of carbohydrate isomers as transition metal adducts using ion mobility spectrometry and tandem mass spectrometry. **L. Petrosh**, Y. Huang, E.D. Dodds

1017. Analysis of electrolyte changes in athletes using ICP. **C.C. O'Hara**, G. Geme, G. White

1018. Analysis of pen inks using a portable Raman spectrometer. A. Boone, **K. Johnson**, **C. Hudson**, U.P. Kalapathy

1019. Plant uptake of commonly prescribed pharmaceuticals and Splenda® in reclaimed water by water lettuce (*Pistia stratiotes*). **T.D. Strickland**, M.R. Pruyn, P.R. Gardinali

1020. Spectrophotometric determination of concentration of phosphates and nitration in vegetables, soils, fertilizer, and water samples by molybdenum blue method. **S. Wilson**

1021. Monitoring click reactions on titanium dioxide using ATR infrared spectroscopy. D. Medford, S.D. Prinslow, **K.S. McCain**

1022. Mineralized springs of Lampasas, Texas. **M. Jenkins**, A. Frantzen

1023. Detection of microbial volatile organic compounds from *Cryphonectria parasitica* species by gas chromatography, mass spectrometry, and pattern recognition. **M. Mlsna**, J. She, M. King

1024. The relation of synthesis time and calcination temperature to resultant size of TiO_2 nanoparticles. **C. Roberts**, O. Love

1025. Improving NOE methods in obtaining inter-proton distances for 3-methylpiperidine. **N. Oragwam**, C. Butts, J. Bame, C. Dickson, T.A. Nile, A.G. Glenn

1026. The effects of vegetated mats on nutrient levels of storm water retention ponds. **J. Clark**, **H. Goad**, M. Howard

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Undergraduate Posters

Physical Chemistry

A. L. Parrill-Baker, *Organizer*

10:20 - 12:20

1027. Photoacoustic spectroscopy with SF_6, an optically thick greenhouse gas. **W. Murphy**, H. Park

1028. A kinetic study of the dependence of ascorbic acid concentration on temperature and time. **I. Ilieva**, M. Richardson, D. Garrett

1029. Wettability of mercaptoundecanoic acid and dodecanethiol on gold. **J. Watkins**, M.R. Martin

1030. Convex solubility parameters for polymers. D.S. Boucher, **B. Stephens**, J. Howell

1031. Experimental and theoretical gas-phase studies of $Fe(NO_3)_4^-$ and $Co(NO_3)_3^-$ anion clusters. **C. Martinez-Martinez**, D.J. Goebbert

1032. Convergent quantum chemistry for challenging dispersion-dominated non-covalent dimers. **M. Clement**, G.S. Tschumper

1033. Practical methodologies towards analytical analysis of iron nickel phosphides. **T.J. Beckman**

1034. Reactivity of aqueous thorium(IV) and plutonium(IV) clusters. **S. Polansky**, M. Vasiliu, D.A. Dixon

1035. Molecular dynamic simulations to study the self assembly of fullerene molecules on graphene. **F.J. Claire**, K.D. Krantzman, Y.G. Yingling

1036. A microcalorimetry study of cations adsorption at the goethite solution interface: Effect of valence and hydration energy. **N. Allen**, **L. Le**, N. Kabengi

1037. Infrared, Raman, NMR, and conformational stability of 1,1,3,3,5,5-hexafluoro-1,3,5-trisilacyclohexane. G.A. Guirgis, **D.V. Hickman**

1038. DNA-conjugated silver clusters with near-infrared spectra. **C. Bradsher**, J.T. Petty

1039. Circular dichroism studies of Ag+-DNA complexes. **M. Gillan**, M. Ganguly, J.T. Petty

1040. Electronic spectroscopy and mass spectrometry studies of DNA-conjugated silver clusters. **I. Rankine**, M. Ganguly, J.T. Petty

1041. Conventional strain energies and relative stabilities of the isomers of dimethylcyclobutadiene. **B.G. Peyton**, Q. Cheng, B. Cao, S.A. Smith, D.H. Magers

1042. Relative stabilities of derivatives of 9-methylanthracene and 9-methylene-9,10-dihydroanthracene. **A.G. Morales**, B. Cao, S.A. Smith, D.H. Magers

1043. Conventional strain energies of the oxaphosphetanes and the oxadiphosphetanes. **M. Westrope**, D.H. Magers, S.A. Smith

1044. Enthalpies of formation of cyano and methyl derivatives of furan and pyrrole by homodesmotic reactions. **C.D. Lewis**, E.Q. Chong, S.A. Smith, D.H. Magers

1045. Characterization of historical lime mortar using single-sided nuclear magnetic resonance. **B. Fortman**, V. Lee, T.K. Meldrum

1046. Ultrafast two-dimensional relaxometry with single-sided NMR. **J. King**, V. Lee, V. Telkki, T.K. Meldrum

1047. Rovibrational analysis of third row atom hydroxides and isomers. **M. Kitchens**, R.C. Fortenberry

1048. Withdrawn.

SATURDAY AFTERNOON

Cook Convention Center
L-3

Undergraduate Papers

Bio-Organic and Biological

A. L. Parrill-Baker, *Organizer*
R. Coleman, *Presiding*

1:00 1049. The predicted ensemble of 3D structures for OR1A1-4. **C. Seitz**, W.A. Goddard, S. Kim

1:20 1050. Ketosteroid isomerase catalyzed Kemp elimination. **E. Sanchez**, **L. Fanning**, K. Howe, M. Forconi

1:40 1051. The effects of mercury (II) ion on secondary DNA structures formed by T-rich DNA. **H. Wang**

2:00 1052. Single-cell mass spectrometry: A tool for rapid biochemical analysis. **C. Townsend**, N.R. Kothapalli, N. Pan, Z. Yang, A.W. Burgett

2:20 1053. Developing a PiggyBac gene delivery system to generate autonomously bioluminescent stem cells. **W. Handagama**, T. Xu, S.A. Ripp

2:40 1054. Carbapenem functionalized gold nanoparticle synthesis, characterization and antibacterial susceptibility testing. **F. Chavda**, J. Payne, R. Dakshinamurthy

3:00 Intermission.

3:20 1055. "Click" approach to HMGA disruption. **D. Mesa Sanchez**, H. Stubbs, L. Rabenold, K.L. Buchmueller

3:40 1056. Metalloregulation by Nur from *Streptomyces coelicolor*. **O. Manley**, N.E. Grossoehme

4:00 1057. Utilization of biologically derived polyester polyols in surfactants for polyurethane foams. **B. Stephens**, N. Tonks

4:20 1058. Solid-phase peptide synthesis and antimicrobial assessment of a plant-derived cyclic peptide. **C.L. Telzrow**, A.J. Wommack

4:40 1059. Encapsulation of calcein within polymerizable diacetylene vesicles. **B. Mitchell**, T.W. Hanks

5:00 1060. Using rational drug design to identify novel flavonoid derivatives as acetylcholinesterase inhibitors for the treatment of Alzheimer's disease. **J. Minnick**, A. Kranzlein, C.J. Mills

Cook Convention Center
L-4

Undergraduate Papers

Organic Chemistry

A. L. Parrill-Baker, *Organizer*
E. Jackson, *Presiding*

1:00 1061. Time-resolving unimer exchange in block copolymer micelles. **K.M. Miller**, B. Kidd, X. Li, T. Cooksey, M.L. Robertson, L.A. Madsen

1:20 1062. Optimization of the transfer-to approach for bottlebrush polymer synthesis. **M. Corley**, S. Radzinski, J. Foster, J. Matson

1:40 1063. Synthesis of heteroditopic AB monomer for host-guest supramolecular polymer system. **F. Mazzini**, H. Wessels, T. Price, H.W. Gibson

2:00 1064. Development, synthesis, and degradation studies of drug-infused biologically compatible polymers. **A. Violette**

2:20 1065. Expedient access to 1,2-oxazadecalin core and studies towards 1,2-oxazadecalin secondary metabolites. **J.E. Burch**, A.M. Mfuh, A. Vo, O. Larionov

2:40 1066. Zinc triflate catalyzed Minisci reactions. **S. Jones**, J.L. Biaco, T.J. Barker

3:00 Intermission.

3:20 1067. Synthesis of new gold carbene complexes with potential catalytic ability. **A. Romano**

3:40 1068. Total synthesis of the natural products hibiscone C and hibiscone B. **H. Rudd**, B.C. Goess

4:00 1069. Synthesis, substitution, and attempted metalation of a rigid, fused bis-indenyl “batwing” ligand. **T. Varner**, C. Reed, J.K. Wyatt, R. Himes

4:20 1070. Synthesis and isolation of 5,6,7-trimethoxy indoles for the creation of novel combretastatin derivatives linked at the 3-position. **T. Rocha**, H. Holt

4:40 1071. Scope expansion of the Winstein-Masamune reaction: Tsuji-Trost variant. **L. Spencer**, M. Donahue

5:00 1072. Cationic gemini surfactants used for enhanced oil recovery. **A.X. Woods**, K.A. Daus

Cook Convention Center
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Undergraduate Posters

Organic Chemistry

A. L. Parrill-Baker, *Organizer*

1:00 - 3:00

1073. Synthesis of 1,3-*S*,*O*-esters from α-oxoketene dithioacetals. **J. Law**, D. Kercher, C.W. Alexander

1074. Asymmetric reduction of single geometric isomers of diaryl oxime ethers. **B. Sharma Poudel**, I. Bonck, S.K. Ayer, C. Dugan, Z. Li, T.S. Snowden, D.D. Dolliver

1075. Synthesis of single geometric isomers of *N*-benzyloxydiarylimines. **I. Bonck**, B. Sharma Poudel, S.K. Ayer, C. Dugan, Z. Li, T.S. Snowden, D.D. Dolliver

1076. Fluorescent amphiphile exchange in polydiacetylene liposomes. **I. Miller**, M. Evans, T.W. Hanks

1077. Zwitterion polymer brush growth in a quartz crystal microbalance. **E. Bundy**, T.W. Hanks

1078. Synthesis of polypyrrole-alginate ionomeric composites. **M. Kuester**, T.W. Hanks

1079. Synthesis and kinetic studies of a manganese(V)-oxo corrole. **H. Jeddi**, W. Luo, R. Zhang

1080. Synthesis, characterization, and luminescent properties of lanthanide dipyridophenazine functionalized complexes for potential bio-imaging applications. **A.M. Lillie**, J. Beasley, B. Dinkelmeyer, C.R. De Silva

1081. 5-isopropyl 1,3-cyclohexanedione synthesis. **C. Schiavone**, B.C. Goess

1082. Abstract of synthesis and characterization of Co complex with isoquinoline group for H_2 production. **K. Driskill**

1083. A process for the production of a stain-resistant polymer application. **J. Holland**, A. Shupert

1084. Determining the mechanism of oxidation of β-estradiol by lactoperoxidase. **T. Glenn**, K.M. Matera

1085. Modification of fabric surfaces to prevent biofouling. T.W. Hanks, **S. Douglas**, G. Mbah

1086. Biological activity of hibiscone C. **J.L. Craig**, B.C. Goess

1087. (7-oxa)norborene derivatives containing TEMPO and PEG for the production of copolymeric materials via ROMP with potential vasodilating properties. **C.A. Jones**, H. Saenz, H.J. Schanz

1088. Functionalizing (7-oxa)norbornene derivatives with TEMPO and PEG via click reaction. **C. Bohannon**, S.E. Roessler, H.J. Schanz

1089. Design and synthesis of tetrahydro-β-carbolines. **D. Cain**, **B. Egbudin**, **M. Reynolds**, **B. Schumann**, P.G. Sheridan

1090. Synthesis of polyphenylethynylarenes as antitumor agents. **C. Fisher**, T.D. Selby

1091. Characterization of halogen bond interactions in thiophene-based building blocks. **J.L. Wilson**, C. Petkovsek, P.L. Reves, J. Williams, J.W. Jurss, N. Hammer, G.S. Tschumper, D.L. Watkins

1092. Design and synthesis of hybrid furan-based oligomers for application in optoelectronic devices. **N. Le**, J. Williams, D.L. Watkins

1093. Synthesis of flat dendrimers. **A. Zylstra**, T.D. Selby

1094. Synthesis of 2-dimensional aminopolyphenylethynylarenes. **E. Taylor**, B. Hasan, T.D. Selby

1095. Synthesis of conjugated macrocyclic polyphenylethynylarenes. **L. Bicker**, T.D. Selby

1096. The Wittig reaction: Analysis of product yield, purity, and greenness. **J. Whitmire**, E.L. Bailey

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West Mezzanine

Undergraduate Posters

Physical Chemistry

A. L. Parrill-Baker, *Organizer*

1:00 - 3:00

1097. Vapor liquid coexistence properties of hydrofluoromethanes using first principles Monte Carlo simulations. **C. Butler**, H. Goel, N. Rai

1098. Preparation and characterization of a palladium catalyst on ceria support. **J. Hovey**, **K. Fitch**, A.C. Banerjee

1099. Construction of p-type heterojunction CuO|CuBi2O4 nanowires for photochemical reduction of aqueous protons as sustainable source of energy. **K. Bhattacharya**, Q. Tejani

1100. Molecular electronics: Using computational chemistry to design devices. **S. King**, B. Topham

1101. Molecular rotors: An investigation of planar boron clusters as Wankel motors. **S.S. Kourdov**, K.J. Donald

1102. Conventional strain energies of thiaziridine and the thiazetidines. J. Gramm, S.A. Smith, **D.H. Magers**

1103. The influence of organic substituents on the stability of dative bonding. **E. Befekadu**, K.J. Donald

1104. Conventional strain energy in ketene acetals and ketene aminals. S.G. Travis, S.A. Smith, **D.H. Magers**

1105. Monitoring the development of intermolecular networks during the curing of coatings using single-sided NMR. **F. Morin**, T.K. Meldrum

1106. Polarizing substituents dictate the relative energies of weak (halogen-bonding) interactions. **J. Jaini**, K.J. Donald

1107. Mixed self-assembled monolayers of alkanethiols and their formation on gold substrates. **S. Graham**, M.R. Martin

1108. Characterizing mixed self-assembled monolayers of dodecanethiol and 11-mercapto-undecanol. **A. Glover**, M.R. Martin

1109. Computational studies of the binding of quinoline-based ligands to plasmepsin IV. **A. Ewurum**, V.F. Waingeh

1110. The impact of soot morphology and mixing state on particle optical properties. **E.N. Eckl**, C. Qiu, A. Khalizov

1111. Quenching of cyanoaromatics fluorescence and aromatic carbonyl triplets by model sulfur compounds. **H. Wurtz**, P.K. Das

1112. Effect of pretreatment procedure on Cu-Pd/Al_2O_3 catalysts for selective hydrogenation of acetylene. **A. Bradicich**, G. Malin

1113. Bonding in group 12 dihalides and limitations on accuracy in optimizations with certain counterpoise correction strategies. **R. Sjovold**, K. Donald

1114. Computational investigation of O-H bond cleavage reactions of primary alcohols and water on stepped rhodium (211) and planar rhodium (111) surfaces using density functional theory. **G. Nagzibekova**, K. Panichakornkul, D. Lingerfelt, S.A. Wasileski

1115. Computational investigations of molecular electronic properties and hyperpolarizability of organic molecules. **M. Miles**, D.A. Clabo

1116. Gas-phase decomposition studies of Ni^+-aldehyde systems. **A. Africa**, A. Mansell, Z. Theis, D.J. Bellert

Cook Convention Center
L-2

General Physical Chemistry

W. A. Alexander, *Organizer, Presiding*
T. C. Devore, *Presiding*

1:20 1117. Why doesn't thermal analysis give consistent Arrhenius parameters for simple systems? **T.C. Devore**, N. Cooper

1:40 1118. Method for determining the enthalpy of reaction for metal oxalates using DSC. **T.C. Devore**, R. Snell-Feikema

2:00 1119. Reaction paths and path profiles: A new perspective for understanding reaction mechanism. **B.K. Dey**

2:20 1120. Reactions of solvated electrons initiated by sodium atom collisions at the vacuum-liquid interface: Insights into solvation and ionization. **W.A. Alexander**

2:40 1121. Photochemical reduction of $CHCl_3$ in SPEEK/HCO_2- aqueous medium via a free radical mechanism. **M.S. Islam**

3:00 1122. Developing spectroscopy techniques to study interaction of anticancer drugs with DNA. **N. Mirsaleh-Kohan**

Cook Convention Center
L-10

Undergraduate Papers

Analytical and Inorganic

A. L. Parrill-Baker, *Organizer*
E. A. Kurfman, S. Stanley, *Presiding*

1:20 1123. Hydrodeoxygenation (HDO) of guaiacol and furfural using a Cu based water gas shift and Mo/Ni/K catalyst system. **M. Crowley**, A.G. Karunanayake, R.T. Wijayapala, T.E. Mlsna

1:40 1124. Direct aminoglycoside coated gold nanoparticles synthesis, characterization, and antibacterial susceptibility testing. **S. Tockstein**, J. Payne, R. Dakshinamurthy

2:00 1125. Optimizing the ionization suppression effects of Cs on accurate ICP-OES determination of Li. **K. Jimenez**, **J.K. Dogbe**

2:20 1126. Heavy metal removal from wastewater using magnetic rinsed ultra biochar. **O.A. Todd**, A.G. Karunanayake, T. Mlnsa

2:40 1127. Investigating the antioxidant activity of sulfur/selenium compounds utilizing mass spectrometry, gel electrophoresis, and polymerase chain reaction. **E.A. Kurfman**, B.S. Stadelman, J.L. Brumaghim, S. Wheeler, J. Wheeler

3:00 Intermission.

3:40 1128. Preventing nosocomial infections: Antimicrobial photodynamic textiles. **S. Stanley**

4:00 1129. Metal-organic frameworks with embedded basic sites for heavy metal capture from aquatic environments. **C. Fast**, T.A. Makal

4:20 1130. Characterization of mixed diacetylene self-assembled monolayers. **N.A. Rivers**, M. Milkovska, L.L. Wright

4:40 1131. Designing a unique therapeutic agent involving gold nanoparticles conjugated with cephalosporins for potent antibacterial applications. **W.R. Hamilton**, J. Payne, R. Dakshinamurthy

Cook Convention Center
L-11

Undergraduate Papers

Physical Chemistry

A. L. Parrill-Baker, *Organizer*
A. E. Bullington, M. McDaniel, *Presiding*

1:20 1132. Solid surface free energy determination via contact angle measurement: An inexpensive undergraduate physical chemistry laboratory experiment. **A.E. Bullington**, E.B. Henry, A.A. Mahmood, T.B. Cavitt

1:40 1133. Binding of novel earth abundant metal coordination complexes as molecular spacers to single-walled carbon nanotubes. **C.X. McNeill**, J. Mitchell, I.N. Shcherbakov, J.C. Poler

2:00 1134. Liquid structure of hydrofluoromethanes using first principles Monte Carlo simulations. **Z. Windom**, H. Goel, N. Rai

2:20 1135. Surface energy: A combinatorial experimental design for novel UV-curable coatings. **A.A. Mahmood**, E.B. Henry, T.B. Cavitt

2:40 1136. Determination of the surface energy for UV-curable easy release coatings. **E.B. Henry**, A.A. Mahmood, T.B. Cavitt

3:00 Intermission.

3:40 1137. A physical approach for the determination of nanoparticle toxicity. **N. Wolfe**, A. Nath

4:00 1138. Supraparamagnetic Fe_3O_4 nanoparticles for magnetic isolation of anion exchange resin during water purification. **E. Schmidt**, B.R. Johnson, T. Eldred, J.C. Poler

4:20 1139. Withdrawn.

Cook Convention Center
L-12

Nanomaterials: Synthesis, Characterization, and Applications

Applications

A. Antonysamy, A. L. Parrill-Baker, *Organizers*
E. Kwizera, *Presiding*

1:40 1140. Gate-free electrical breakdown of metallic pathways in single-walled carbon nanotube crossbar networks. **J. Li**, A. Franklin, J. Liu

2:00 1141. Dual-mode organic-inorganic passivation of quantum dots. M. Turo, X. Shen, N.K. Brandon, S. Castillo, A. Fall, S.T. Pantelides, **J. Macdonald**

2:20 1142. The preparation of biofouling-resistant films of surface-modified polyaniline nanofibers. **B. DiTullio**, P. Molino, T.W. Hanks

2:40 1143. Silver cluster encapsulated by DNA strands. **J.T. Petty**, M. Ganguly, I. Rankine, M. Gillan, C. Bradsher, Y. Wang

3:00 Intermission.

3:40 1144. *In-situ* synthesis of vanadium pentoxide nanofibre/exfoliated graphene nanohybrid and its supercapacitor applications. C. Arup, J.S. Bonso, M. Wunch, K.S. Yang, J.P. Ferraris, **D. Yang**

4:00 1145. Thermally activated release from polymer micelles. **D.E. Nikles**, L.N. Cobb, J.A. Gettinger, B.J. McCormick, S.M. Nikles, M. Painter, A.L. Glover, J.A. Nikles, C.S. Brazel

4:20 1146. Subconjunctivally injectable nanogels for enhancing drug permeability across ocular barriers. **D.R. Janagam**, J. Zhang, T.L. Lowe

4:40 1147. Synthesis and characterization of anion exchange resin nanotubes for water purification. T. Eldred, B.R. Johnson, **J.C. Poler**

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Undergraduate Posters

Biological Chemistry

A. L. Parrill-Baker, *Organizer*

3:20 - 5:20

1148. Antimicrobial properties of gallium against *Bacillus subtilis*. **K. Albanese**, Z. Fang, P.C. Dos Santos, G.L. Donati

1149. Understanding the role of glycine134 in heparin binding of FGF-1. **A.W. Burroughs**

1150. Modulating the mitogenic activity of the fibroblast growth factor. **J.L. Anderson**, S. Jayanthi, S.K. Thallapuranam

1151. Post-translational modifications of FUN30 and its role in chromatin remodeling. **J.T. Alewine**

1152. Synthesis of dendrimer-encapsulated mono- and bimetallic Cu and Ni nanoparticles and investigation of their antimicrobial activity. **D. Finley**, M. Ashan, A. Ethridge, W.E. Collier, M.L. Curry

1153. The importance of Ile716 in BF polymerase toward the mutagenic potential of 8-Oxo-2'-deoxyguaosine. **R. Gilbert**

1154. Production of phenolic compounds by *Brettanomyces*. **D.M. McMahan**, N. Duncan, J. Brigati

1155. DLS characterization of netropsin aggregates. **R. Alexander**, C. Blake, K.L. Buchmueller

1156. Interaction of a novel mitochondrial protein, 4-nitrophenylphosphatase domain and non-neuronal SNAP25-like protein homolog 1 (NIPSNAP1) with NAD and NADH. **J.M. Yarbro**, S.B. Gacasan, J. Ziebarth, Y. Wang, A.L. Parrill-Baker, R. Homayouni

1157. Antimicrobial properties of extracts from *Hedera helix*. **C. Jennings**, N. Duncan, A.D. Gibson

1158. Thermodynamic contributions of the inhibition of AT hooks by netropsin. **R. White**, J. Schoen, C. Quandt, A.H. Gorensek, K.L. Buchmueller

1159. Development of a PCR-based system to study HMGA disruption. **H. Stubbs**, D. Mesa Sanchez, L. Rabenold, **K.L. Buchmueller**

1160. Probing the stability and ligand binding of heme proteins 'mineralized' within the ZIF-8 metal organic framework. **D. Grassie**, C. McKeithan, R.W. Larsen

1161. Can native enzyme conformation act as a template for refolding of RNase A. **H.K. Bogy**, S. Jayanthi, S.K. Thallapuranam

1162. The partial purification of a polyphenol oxidase from *Scorzonera hispanica*. **A. Allison**, C. Clinger

1163. Electrochemical investigations of FAD-binding RNA aptamers. **J.S. Samuelian**, I. Emahi, R. Poudyal, S.A. Staller, D.H. Burke, D.A. Baum

1164. PtSIT1: Protein function in silicic acid transport for biomimetic silica synthesis. **B. Kirk**, L. Senior, P. Curnow, **T.A. Nile**, A. Glenn

1165. Natural product isolation and activity-based fractionation of bioactive compounds found in English ivy, *Hedera helix*. **B.B. Denney**, A.D. Gibson, N. Duncan

1166. Novel labeling strategy of nucleic acids: Less is more. **S. Nguyen**, E. Strovea, M.W. Germann

1167. PCBP2 knockdown leads to iron overload in mouse liver tissue. **A. Rivas**, C. Philpott, F. Li

1168. The role of histone acetyltransferase 1 in DNA double-strand break repair. **N. Boyle**, P.Z. Ferreira, M.R. Parthun

1169. Characterization of the pattern and properties of fluorescence in Opiliones (harvestmen) captured in Cusuco National Park, Honduras. **S.R. Hagans**, A.D. Gibson, M. Lock

1170. An attempt to enhance the cell proliferation activity of the human fibroblast growth factor. **E.G. Fields**

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Undergraduate Posters

Organic Chemistry

A. L. Parrill-Baker, *Organizer*

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1171. The optimization of catalytic loading in benzoxaborole synthesis. **C.P. Macintosh**, A.G. Glenn, T.A. Nile, S. Flower, K. Murlock

1172. Synthesis of a fluorescent universal DNA nucleoside. **T. Kaelin**, J.N. Izaguirre, L. Davis

1173. Synthesis of a sulfate binding ligand. **D. Parker**, N. Duncan

1174. Investigation of the shape of atropisomers using dipolar couplings. **E.E. Schiller**, W. Carroll

1175. Decarboxylative protein functionalization via photoredox catalysis. **M. Daemo**

1176. Synthesis of a BIPY-urea ligand for the extraction of sulfate anions from a competitive aqueous environment. **C. Kidd**, N. Duncan

1177. The metal-free hydration of terminal alkynes. P.A. Shelton, H.W. Robison, **J. Thompson**, **S. Sulcer**

1178. Synthesis of organic compounds with biological properties. **N. Wells**, M. Teel, C. Tirla, B. Bahr

1179. Synthesis of the disaccharide moiety of the natural product OSW-1. **M. Barron**

1180. Novel N-benzylbenzamide- ased tyrosinase inhibitors. **D. Monteith**, G.G. Springsteen

1181. Selective reduction of carbonyl and nitro groups by fruits and vegetables. **J. Davis**, A.A. Gallo

1182. Progress toward the total synthesis of lauroside B. S. Genessa, **C. Haynes**, **D. Johnson**

1183. Synthesis of new dihydropyrimidiscaffolds. **J. Hershberger**, S. Gonzalez

1184. Using microwaves for organic syntheses in undergraduate organic labs. **A. Rivas**, E.A. Nalley

1185. Formation of asymmetric rhodamine derivatives for chiral sensing. **D. Rich**, **N. Kam**, **N. Aleman**, M. Maher, J. Romaire, C. Stephenson

1186. Microwave synthesis of phenyl salicylate and phenyl salicylate derivatives. **S. Rupakheti**, E.A. Nalley

1187. Microwave synthesis of tetraphenylporphyrins and tetraphenylporphyrin derivatives. **P. Hyolmo**, E.A. Nalley

1188. Incorporation of dyes in polymers as a means of producing faux stained glass windows. **P. Worthen**, E.A. Nalley

1189. Studies on the synthesis and biological activity of hibiscone C. **H. Tan**, B.C. Goess

1190. Diels-Alder reactions of 2-cycloalkenylthiophenes and 2-cycloalkenylbenzo[*b*]thiophenes. W.E. Noland, V. Kumar, V.S. Narina, **A. Uprety**, D. Aschbacher, G. Flick, H. Kim, J. Xie

1191. Efforts towards the direct γ-functionalization of cyclopentenones. **B. Jimenez**, A. Bracken, G.R. Boyce

1192. Overcoming aromaticity: Progress towards the cyclization of cyclopropenones. **S. Coury**, **S. Tokamov**, G.R. Boyce

1193. Halogen effects on the enantiomeric excess (EE) of an S_N 1 reaction. **C. Lockridge**, E.L. Bailey