

SERMACS PROGRAM

C. D. Sherrill, *Program Chair*

WEDNESDAY MORNING

Electronic Structure in Complex Environments

Large Systems and Molecular Properties

Loews Atlanta Hotel
Salon G

T. Crawford, *Organizer*
L. Slipchenko, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 1. Strategies for accurate calculations on large systems. **M. Gordon**

8:45 2. Beyond 'biologically relevant': Applying computationally tractable standards for noncovalent interactions to develop next-generation chemical databases. **L. A. Burns**, J. C. Faver, M. S. Marshall, Z. Zheng, C. D. Sherrill, K. M. Merz

9:05 Intermission.

9:25 3. XSAPT: A fast and accurate method for incorporating explicit solvent molecules. **J. M. Herbert**, K. Lao

10:05 4. Magnetic resonance parameter calculations: Gas phase vs solution vs solid state. **J. Autschbach**

Inorganic Chemistry General Session

Loews Atlanta Hotel
Pittman

J. Shaw, *Organizer, Presiding*

8:00 5. Acid-Base and aggregation behavior of water soluble N-confused porphyrin. **J. L. Shaw**, J. L. McMurry, E. H. Bennett, P. Salehi, A. Stovall

8:15 6. Cyclometallated gold(III) complexes containing a trithiacrown ligand. **G. J. Grant**, D. E. Janzen, S. R. Doherty, D. A. Benefield, H. M. Vashi

8:30 7. Photoacoustic calorimetry studies of the photoaquation of Ru(II)bis(2,2' bipyridine)(acetonitrile)₂ and Ru(II)bis(2,2' bipyridine)(6,6' dimethyl 2,2' bipyridine) complexes. **R. W. Larsen**, A. Karolak, T. Word, M. T. Kemp, C. L. Whittington, A. van der Vaart

8:45 8. Building blocks for organosilver catalysis: Applications in renewable energy. **B. K. Tate**, C. M. Wyss, J. Bacsá, K. Kluge, L. Gelbaum, J. P. Sadighi

9:00 9. Long-lived excited state lifetime of a titanium(IV) oxo chromophore and the extension of its lifetime by use of new heterobimetallic charge transfer mechanisms. **E. M. Goggins**, T. T. Lekich, W. W. Weare

- 9:15 10.** Synthesis, characterization of hetero tri/bimetallic oxo-bridged titanium(IV)-chromium(III) complexes for application of solar conversion. **T. Huang**, X. Wu, W. Weare, R. Sommer
- 9:30 11.** Synthesis and characterization of heterobimetallic systems containing d^0 titanium and d^1 vanadium acceptors for applications in solar energy conversion. **X. Wu**, T. Huang, T. Lekich, W. W. Weare
- 9:45 12.** Influence of heterometal location on charge transfer lifetimes in Keggin polyoxometalate chromophores. **E. N. Glass**, J. Fielden, A. L. Kaledin, D. G. Musaev, T. Lian, C. L. Hill
- 10:00 13.** Bis(mercaptoimidazolyl)alkane complexes of zinc, cadmium and mercury. **S. S. Zwayyer**, D. Rabinovich
- 10:15 14.** Syntheses and structures of bis(pyridyl)selone complexes. **L. Hernandez**, D. Rabinovich

Medicinal Chemistry General Session

Loews Atlanta Hotel
Centennial

J. Arceneaux, *Organizer, Presiding*

- 8:00 15.** Parthenolide promotes histone deacetylase I depletion and HDM2 hyperubiquitination independent of glutathione depletion and reactive oxygen species enrichment. E. Chanchorn, T. Lee, M. Clarke, **M. W. Van Dyke**
- 8:20 16.** Design and synthesis of dual action antimetabolic chemotherapeutic drugs: Tubulin and aurora-A kinase inhibitors. **K. Augustyn**, B. Norton-Baker, B. Hoover, K. Klas, Y. Peterson, C. Beeson, J. Wyatt
- 8:40 17.** Effects of intercalator substituent and nucleotide sequence on intercalator-DNA binding strength. **M. Lewis**, L. K. Hardebeck, C. A. Johnson, G. A. Hudson, Y. Ren, B. M. Znosko
- 9:00 18.** Triggered liposomal release via a synthetic phosphatidylcholine analog bearing a photocleavable moiety embedded within the sn-2 acyl chain. **A. M. Bayer**, S. Alam, S. Matthern-Schain, M. D. Best
- 9:20 19.** Synthesis of fluorescent NIR dyes for bioimaging applications. **M. Henary**, C. N. Njiojob, N. Lakshminarayana, H. Choi, Y. Ashitate, J. Frangioni
- 9:40 20.** Mitochondrial Targeted Photodynamic Therapy as a Potent Immune Boosting Treatment for Breast Cancer. **S. Marrache**, S. Tundup, D. A. Harn, S. Dhar
- 10:00 21.** Time-Dependent Regulation of Apoptosis by Aen and Bax in Response to 2-Aminoanthracene Dietary Consumption. **W. E. Gato**, D. B. Hales, J. C. Means, S. McGee
- 10:20 22.** Lidocaine-Ibuprofen Ionic Liquid for Dermal Anesthesia. **H. Park**, M. R. Prausnitz

Novel Bonding Types in Inorganic Chemistry

Main-Group Chemistry

Loews Atlanta Hotel
Chastain

J. Thrasher, *Organizer*
A. Arduengo, *Presiding*

8:00 Introductory Remarks.

8:05 23. One Electron Oxidations. **K. Seppelt**

8:45 24. Tipping the balance: Steric mimicry of electronic effects in the structures of main-group complexes. **T. P. Hanusa**, N. C. Boyde, E. J. Bierschenk, L. K. Engerer

9:25 Break.

9:40 25. Synthesis and applications of pentafluorosulfanyldifluoroacetic acid. A. V. Matsnev, M. A. Stanton, S. Qing, X. Wang, G. Haufe, **J. S. Thrasher**

10:10 26. Investigation of tetrahedral pnictides. **J. W. Hall**, M. T. Griffin, J. R. Wasson

Physical Chemistry General Session

Loews Atlanta Hotel
Inman

R. Fortenberry, A. Schrand, *Organizers, Presiding*

8:00 27. Integrating Concepts from Bio-Nano-Energetic Materials Research. **A. M. Schrand**

8:20 28. Electron spin resonance investigation of matrix isolated CH_6^+ . **J. Felmly**, J. J. Banisaukas, III, L. B. Knight, Jr

8:40 29. Stochastic potentials for coarse-grained solvents with varying softness. **G. T. Craven**, A. V. Popov, R. Hernandez

9:00 30. Thermal decomposition of metal oxalates. **T. C. DeVore**, N. Cooper

9:20 Break.

9:40 31. Novel microfluidic mixer utilizing infrared imaging spectroscopy with a submillisecond mixing time. **D. Kise**, D. Magana, M. Reddish, B. Dyer

10:00 32. Dynamics of an ultrafast folding beta-hairpin in the context of WW-domain formation. **C. Davis**, B. Dyer

10:20 33. Zinc(II) 1,3,5,-tris(4-carboxyphenyl)benzene metal organic frameworks templated by Ruthenium(II)tris(2,2'-bipyridine): Photophysical properties. **C. L. Whittington**, L. Wojtas, R. W. Larsen

Recent Advances in Ion Mobility Mass Spectrometry

Loews Atlanta Hotel
Salon I

J. McLean, F. Fernandez, *Organizers, Presiding*

8:00 34. Increasing molecular coverage in complex biological and environmental samples by using IMS-MS. **E. S. Baker**, K. E. Burnum-Johnson, J. M. Jacobs, Y. M. Ibrahim, D. J. Orton, W. F. Danielson III, K. L. Crowell, Y. Kim, T. O. Metz, G. A. Anderson, R. D. Smith

8:30 35. Multiplexed Ion Mobility Pulsing Schemes: What can Hadamard do for you? **B. Clowers**, X. Zhang, W. Siems

9:00 36. Advances in comprehensive metabolomic strategies using structural mass spectrometry. **J. G. Forsythe**, C. R.

Goodwin, J. C. May, K. M. Hines, N. M. Lareau, J. A. McLean

9:30 37. Coupling Ambient MS Ion Sources with IMS. **J. D. Keelor**, P. Dwivedi, F. M. Fernandez

10:00 38. Structural mass spectrometry of protein modification by lipid electrophiles. **L. Xu**, J. G. Forsythe, N. A. Porter, J. A. McLean

Supramolecular Chemistry: From Little Things, Big Things Grow

Loews Atlanta Hotel
Dunwoody

K. Shimizu, *Organizer*
J. Lavigne, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 39. Sulfur- and selenium-containing MOFs in the search for electrical conductivity. **T. P. Vaid**, D. L. Turner, M. Singh, K. H. Stone, P. W. Stephens

8:30 40. Fabrication of Superamphiphiles: From Micro-Sheets into Nano-Fibers by Charge Transfer Interaction. **P. Wang**, J. Hu, Q. Wang

8:45 41. Polymeric semiconductors: the impact of molecular ordering. **E. Reichmanis**, B. Fu, N. Kleinhenz, K. Nayani, J. Park, M. Srinivasarao

9:10 Intermission.

9:25 42. Multilayer thin films from renewable and/or environmentally-benign polyelectrolytes for flame retardant protection of polymeric substrates. **J. C. Grunlan**

10:05 43. Functional supramolecular materials and interactions: Sensors, solar cells, and stimuli-responsive vesicles. **S. Saha**

The Chemistry of Star and Planet Formation

Loews Atlanta Hotel
Ravinia

S. Widicus Weaver, *Organizer, Presiding*

8:00 44. Spectroscopy and astrochemistry with *Herschel*. **D. C. Lis**

8:30 45. Chemistry at the dawn of star formation. **P. Caselli**

9:00 Intermission.

9:30 46. Multiwavelength Observations of Comets: Constraining the Molecular Evolution of the Solar System. **S. N. Milam**, A. Gicquel, M. Cordiner, G. Villanueva, I. Coulson, A. Remijan, N. Biver, D. Bockelee-Morvan, S. Charnley, Y. Kuan, Y. Chuang

10:00 47. Origins of chemical complexity in the early stages of star formation. **K. Oberg**

The RNA World

Loews Atlanta Hotel
Piedmont

L. Williams, *Organizer*

8:00 Introductory Remarks.

8:05 48. RNA World yes. RNA first maybe. **S. A. Benner**, H. Kim

8:30 49. RNA and protein - a match made in the Hadean. **L. D. Williams**

8:55 50. Evolutionary Landscapes of RNA. **I. A. Chen**

9:20 Break.

9:30 51. Embracing the mess: Consequences of product mixtures in model prebiotic reactions. **A. Engelhart**, M. W. Powner, J. W. Szostak

9:55 52. Evolution of the Ribosome and the Origin of Biology. A. S. Petrov, **C. R. Bernier**, C. C. Waterbury, C. Hsiao, L. D. Williams

10:05 53. Ribozyme ligation of RNA in Ice. **L. Lie**, R. M. Wartell

10:15 Panel Discussion.

10:35 Concluding Remarks.

Posters: Biological Chemistry

Loews Atlanta Hotel
Over Look/Exhibit Hall

D. Sherrill, *Organizer*

9:00 - 11:00

54. Correlation of local effects of DNA sequence and position of β -alanine inserts with polyamide-DNA interaction. **S. Wang**, R. Nanjunda, K. Aston, J. K. Bashkin, W. D. Wilson

55. Axial ligation of the HmuT heme binding protein in *Corynebacterium diphtheriae*. **E. H. Bennett**, N. P. Akbas, J. Burgos, M. Schmitt, D. Collins, J. Dawson, D. W. Dixon

56. Design, synthesis and biophysical evaluation of novel DNA mixed base pair sequence specific heterocyclic diamidines. **Y. Chai**, A. Paul, D. W. Boykin, W. D. Wilson

57. Molecular paleontology: A biochemical model of the ancestral ribosome. **T. K. Lenz**, C. Hsiao, J. K. Peters, P. Fang, D. M. Schneider, E. J. Anderson, T. Preeprem, J. C. Bowman, E. B. O'Neill, L. Lie, S. S. Athavale, J. Gossett, C. Trippe, J. Murray, A. S. Petrov, R. M. Wartell, S. C. Harvey, N. V. Hud, L. D. Williams

58. HtaA-CR2: A novel protein in the heme uptake mechanism in *Corynebacterium diphtheriae*. **R. Uluisik**, N. P. Akbas, D. Collins, J. Dowson, C. Allen, M. Schmitt, D. W. Dixon

59. Design, Synthesis and Evaluation of Novel Diamidines for Selective Recognition of Mixed Base Pair Sequences of DNA. **A. Paul**, R. Nanjunda, A. Kumar, D. W. Boykin, W. D. Wilson

60. Examination of the thermodynamic mechanism for *E. coli* ClpAP. **E. C. Duran**, A. L. Lucius
61. Kinetic mechanism of *Escherichia coli* ClpA catalyzed ATP hydrolysis and thermodynamic linkage to macromolecular assembly. **C. L. Weaver**, A. L. Lucius
62. Crystal structure of choline oxidase from *Arthrobacter globiformis* in complex with glycine betaine suggests the importance of the dimer interface for substrate access to the active site. **F. Salvi**, Y. Wang, I. Weber, G. Gadda
63. JNK binds to and regulates the activity of endothelial nitric oxide synthase. **K. E. Rhoades**, C. A. Chrestensen, J. C. Salerno, J. L. McMurry
64. Impact of single rNMP damage on DNA structure. **M. Evich**, A. M. Spring, K. D. Koh, F. Storici, M. W. Germann
65. Chemical modification and site-directed mutagenesis of His48 in D-Arginine Dehydrogenase. **J. Ball**, D. Su, G. Gadda
66. Understanding minor groove recognition by small molecules using mixed DNA sequences and electrospray ionization mass spectrometry. **S. R. Laughlin**, S. Wang, A. Kumar, D. W. Boykin, W. D. Wilson
67. Physical basis for defects in calmodulin: Mutations associated with life threatening heart arrhythmias in young children. **C. N. Johnson**, M. D. Feldkamp, S. G. Rathi, A. L. George Jr., W. J. Chazin
68. Nonproteolytic roles of the 26S proteasome in transcription elongation. **A. M. Spring**, N. Maganti, A. D. Truax, T. D. Moody, E. Cacan, N. Boyd, M. W. Germann, S. F. Greer
69. Evidence for hydride tunneling in the human glycolate oxidase reaction: A stopped-flow study at various temperatures. **E. Romero**, G. Gadda
70. Targeting the Core of a Holliday Junction. **C. J. Hamilton**, M. W. Germann
71. Denaturation studies of heme-binding proteins using guanidine agents. **K. Bartlett**, D. Dixon
72. Selective G-quadruplex DNA recognition by a new class of designed cyanines. **H. T. Huynh**, R. Nanjunda, K. Zybrev, A. Levitz, M. M. Henary, W. Wilson
73. Multiple TIAR Proteins Bind to the 3' Terminal Stem- loop of the West Nile Virus Minus-strand RNA. **J. Zhang**, **H. Liu**, M. A. Brinton, M. W. Germann
74. A novel assay to identify antibacterial compounds targeting bacterial topoisomerase I. **T. Annamalai**, C. Parra, Y. Tse-Dinh
75. Mapkap kinase 2 regulation by oxidation. **A. D. Duc**, E. Rye, C. A. Chrestensen
76. Design, Syntheses and GC Base-pair Binding Evaluation of Heterocyclic Benzamidazole Diamidines containing variable linkers. **A. S. Chaudhary**
77. Structural and binding studies on an Aspartic Proteinase Inhibitor from human lymphatic filarial nematode, *Brugia Malayi*. **R. Nagampalli**, K. Gunasekaran, R. Narayanan, A. Peters, R. Bhaskaran
78. Dynamic interactions in regulation of flagellar biogenesis in *H. pylori*. **L. M. Beasley**, J. L. McMurry
79. Generation of electrochemical gradient from peptide self-assembly. **S. Li**, A. Sidorov, A. K. Mehta, D. Das, N. R. Anthony, K. M. Berland, Z. Jiang, T. M. Orlando, D. G. Lynn
80. Novel modes of eNOS regulation. **V. Ngwa**, **M. Mickanen**, J. McMurry, J. Salerno, C. Chrestensen

81. Engineering peptide materials with reversible linkages. **C. Chen**, J. Tan, M. Hsieh, M. Zhou, J. Goodwin, A. Mehta, M. Grover, F. Fernandez, D. Lynn
82. Circular dichroism studies of Mg(II) and Fe(II) binding to folded and unfolded RNA. **C. D. Okafor**, N. V. Hud, L. D. Williams
83. Characterization of an alcohol dehydrogenase deoxyribozyme. **N. McCourry**, M. Novak, K. M. Bhatt, V. Samant, S. Igwe, M. Fresia, J. Speaks, K. Buchmueller
84. Diatoms and their silicon transporters. **D. Paudel**, P. Curnow, T. A. Nile
85. Post-Translational modifications:Regulating the regulator. **J. E. Morgan**, S. F. Greer
86. Intercalation-mediated assembly of non-natural nucleic acids. **C. Musetti**, B. J. Cafferty, K. Kim, R. Krishnamurthy, N. V. Hud
87. Rescue of catalase-inactive intermediates of KatG by peroxidatic electron donors. **O. J. Njuma**, E. N. Ndontsa
88. Analysis of structural changes of Retinoid X Receptor alpha ligand binding domain complexed with GRIP1 and UAB derivatives by Hydrogen Deuterium Exchange Mass Spectrometry. **E. J. Cowart**, M. B. Renfrow, D. M. Muccio, B. Moore
89. Selective G-quadruplex DNA recognition by a new class of designed cyanines. **E. M. Stroeva**, R. Nanjunda, E. A. Owens, L. Mickelson, T. L. Dost, M. M. Henary, W. D. Wilson, M. W. Germann
90. Chimeric Biomolecule Self-Assemblies. **J. E. Smith**, J. T. Goodwin, D. G. Lynn
91. Synthetic receptors for post-translational modifications of proteins discovered using iterative redesign in dynamic combinatorial chemistry. **J. E. Beaver**, L. I. James, M. L. Waters
92. Biosynthetic studies of F430, the key coenzyme of methanogenesis. **B. R. Mueller**, X. Yang, S. O. Mansoorabadi
93. Isolation and characterization of Syndecan-1 mutants involved in cell wound migration. **L. V. Greene**, L. Chase, J. Koblinski
94. Amyloid peptides as self-assembling supramolecular catalysts for chemical evolution. **T. O. Omosun**, S. W. Childers, D. Das, A. K. Mehta, N. R. Anthony, K. M. Berland, D. G. Lynn
95. Optimization of the Extraction Procedures of Indigo from Selected Plants. **L. Misigaro**, B. Ooi
96. High specificity of RNA base pairing with 2-Se-Uridine. **H. Sun**, S. Jiang, J. Sheng, Z. Huang
97. Selenium-derivatized nucleic acids (SeNA) for structure and function studies. **S. Jiang**, H. Sun, J. Sheng, J. Gan, Z. Huang
98. The influence of solution conditions on *E. coli* Hfq binding to RNA. **S. Y. Goo**, R. M. Wartell
99. Understanding Binding-Induced Conformational Change in Pin1. **H. Gyamfi**, N. C. Fitzkee, A. Bax, A. Grishaev
100. Hydrophobic drug binding by calmodulin is eliminated by methionine oxidation. **H. T. Niedermaier**, R. J. Bieber Urbauer, J. L. Urbauer
101. Methionine oxidation in calmodulin alters the dynamics of bound proteins. **H. P. Broussard**, R. B. Urbauer, J. L. Urbauer
102. Investigations into the mutagenic potential of 8-oxo-2'-deoxyguanosine using Klenow Fragment and Human DNA

Polymerase β . **E. J. McFadden**

- 103.** Clear cell renal cell carcinoma and SETD2: Effects of loss on cell migration and invasion. **Z. R. Husk**, K. Rathmell, K. E. Hacker, Z. Debebe, A. B. Sender
- 104.** Identification of the calmodulin binding domains in Cx43 gap junction via protein and peptide engineering. **M. Salarian**, J. Zou, Y. Chen, X. Liu, J. J. Yang
- 105.** Role of C-terminus tail in the ligand binding and release mechanisms of *Antheraea polyphemus* pheromone binding protein1 (ApolPBP1). **S. Mazumder**, U. V. Katre, S. Mohanty
- 106.** Inhibiting Drosha-catalyzed microRNA biogenesis. **D. Ishimaru**, E. Davis, T. S. Mack, D. P. Arya, M. Hennig
- 107.** Single-molecule studies on loop-loop kissing interactions in guanine-sensing riboswitch. **V. Chandra**, H. Xu, M. Mandal
- 108.** Interrogating potential interactions of macrolide - stall peptide hybrids and the ribosomal exit tunnel. **A. Z. Washington**, S. Tapadar, Y. Oyelere
- 109.** Synthesis and incorporation of S-(3-(acetylthio)propyl)-5-(mercaptomethyl)-2'-deoxyuridine triphosphate into DNA by DNA polymerase. **R. Esmaeili**, M. Kaur, Z. Huang
- 110.** Oxidative DNA cleavage by pentamethine cyanine dyes using visible light. **C. T. Mapp**, E. A. Owens, M. Henary, K. B. Grant
- 111.** Structural and biochemical characterization of DEMETER, a multidomain 5mC glycosylase. **S. C. Brooks**, M. Szulik, J. H. Huh, R. L. Fischer, M. P. Stone, B. Eichman
- 112.** Discovery and identification of Hfq-binding nanoRNAs in *Escherichia coli*. **J. Patterson**, S. Cao, J. Clardy, C. Mura
- 113.** Fe²⁺ as the ancient predecessor of Mg²⁺ in RNA and protein folding and catalysis. **S. S. Athavale**, C. Hsiao, A. S. Petrov, C. D. Okafor, J. J. Gossett, L. Lie, N. V. Hud, R. M. Wartell, S. C. Harvey, L. D. Williams
- 114.** Characterization of the Dickerson-Drew Dodecamer containing 5-Hydroxymethylcytosine. **M. W. Szulik**, M. Voehler, I. Khutsishvili, B. Nocek, A. Joachimiak, L. A. Marky, M. P. Stone
- 115.** Cationic porphyrin-ruthenium(II) conjugates as potential selective stabilizers of G-quadruplex. C. Musettia, T. Gianferrara, **C. Sissia**
- 116.** Dinoflagellate bioluminescence: An investigation into the mechanism, cooperativity and pH regulation of luciferase from *Pyrocystis fusiformis*. **C. E. Scull**, P. D. Ngo, S. O. Mansoorabadi

Plenary Session

Loews Atlanta Hotel
Salon D/E/F

11:00 117. DRIVE: An innovative, non-profit drug discovery company. **D. Liotta**

WEDNESDAY AFTERNOON

Analytical Chemistry General Session

Loews Atlanta Hotel
Ardmore

R. Wu, *Organizer, Presiding*

- 1:00 118.** Electrochemical Analysis of Parathion-ethyl Pesticide by Zirconium Oxide-Laponite Composite Modified Glassy Carbon Electrode. **M. N. Bui**, S. S. Seo
- 1:20 119.** An *In Situ* Electrode Calibration Strategy for Voltammetric Measurements *In Vivo*. **J. G. Roberts**, J. V. Toups, E. Eyuaem, G. S. McCarty, L. A. Sombers
- 1:40 120.** Desulfurization and Desorption of Organothiols on Gold Nanoparticles using Sodium Borohydride in Water. **S. M. Ansar**, S. Zou, C. U. Pittman Jr, D. Zhang
- 2:00 121.** Surface Enhanced Photoelectrochemical Performance Using Surface Plasmon Towards Solar Water Splitting. **Z. Shan**, S. Pan, D. Clayton, P. S. Archana, A. Gupta
- 2:20 122.** Silver Nanoparticle Damping the R6G Resonance Raman Enhancement. **F. S. Ameer**, C. U. Pittman, Jr., D. Zhang
- 2:40 123.** Single-molecule spectroelectrochemistry (SMS-EC) of (4, 4'-difluoro-4-bora-3a, 4a-diaza-s-indacene) BODIPY dyes. **J. Liu**, S. Pan
- 3:00 124.** High-resolution scanning electrochemical microscopy pH imaging using carbon-fiber ultramicroelectrodes modified by iridium-oxide-nanoparticles. **H. Khani**, D. O. Wipf
- 3:20** Intermission.
- 3:35 125.** IR Monitoring and electronic calibration transfer for chemical process understanding and control. **C. A. Goss**, S. E. Condon, B. E. Cooley, H. W. Graddy, K. Amponsah-Manager, S. J. Sisk
- 3:55 126.** Using temperature programmed analytical techniques to understand and optimize Fischer-Tropsch catalyst thermal treatments. **K. Cook**, W. Hecker, K. Keyvanloo
- 4:15 127.** Highly ordered pillar arrays as platforms for planar chromatography. **T. B. Kirchner**, N. A. Hatab, N. A. Crane, D. R. Lincoln, N. V. Lavrik, M. J. Sepaniak
- 4:35 128.** Electron transfer dissociation mass spectrometry of neutral peptides with alkyl side chains. **C. Feng**, C. J. Cassady
- 4:55 129.** A novel, direct coupling of Simultaneous DSC/DTA-TGA (STA) and FTIR called Perseus™. **T. Doll**, R. Fidler
- 5:15 130.** Comprehensive analysis of protein N-glycosylation by a MS-based novel chemical method. W. Chen, J. Smeekens, **R. Wu**

Biological Chemistry General Session

Enzymology, Protein Engineering, and Metabolism

Loews Atlanta Hotel
Inman

A. Reddi, *Organizer, Presiding*

- 1:00 131.** Peroxygenase activity of dehaloperoxidase from *Amphitrite ornata*. **N. Lucas**
- 1:15 132.** Temperature and pH dependence on the catalytic activity of histidine ammonia lyase. **J. T. Reilly**, T. J. Paul, R. H. Gumper
- 1:30 133.** Dinoflagellate bioluminescence: Elucidation of the biosynthetic pathway of luciferin in *Pyrocystis fusiformis*. **P. D. Ngo**, S. O. Mansoorabadi
- 1:45 134.** Solving the puzzle of a green flavin isolated from D-arginine dehydrogenase. **S. Gannavaram**, A. M. Spring, M. W. Germann, G. Gadda
- 2:00 135.** Mechanistic study of D-arginine dehydrogenase I335H with pH profiles and rapid kinetics. **D. Ouedraogo**, G. Gadda
- 2:15 136.** Thermodynamic analysis of the bacterial loop of E. coli β -glucuronidase. **S. E. Hickling**, S. Hengeli, K. Lane
- 2:30 137.** Characterization of bacterial propionate 3-nitronate monooxygenase from Pseudomonas sp. Strain JS189. **D. Su**, K. Francis, G. Gadda
- 2:45 138.** Reevaluation of the role of H466 in the active site of choline oxidase. **C. Smitherman**, K. Rungsriruriyachai, M. W. Germann, G. Gadda
- 3:00 139.** Transforming *in vitro* enzymatic reactions from flask into microbial cell: Production of polyhydroxylated molecules via engineered *E. coli*. **M. Wei**, Z. Li, L. Cai, B. Wu, P. Wang
- 3:15 140.** Rescuing activity of an glycosyltransferase by glycosylation. **G. Zhao**, L. Li, T. Li, P. G. Wang
- 3:30 141.** Bioorthogonal profiling of lysine acetylation with an engineered enzyme and derivatives of coenzyme A. **J. Mi**
- 3:45 142.** A new role for an old copper enzyme in glucose and oxygen sensing. **A. Reddi**
- 4:00 143.** Analysis of BCL-2 proteins during heart development. **T. A. Davis**, V. Del Gaizo Moore
- 4:15 144.** Identification of powdery mildew resistance related metabolites in rootstocks of watermelon using NMR. **I. Mahmud**, R. Hassell, C. Kousik, K. Chowdhury, A. Boroujerdi
- 4:30 145.** NMR-based metabolomics differences between nutrient uptake of embryogenic and non-embryogenic sugarcane calli from growth medium. I. Mahmud, **M. Thapaliya**, A. Boroujerdi, K. Chowdhury
- 4:45 146.** Sugarcane (*Saccharum officinarum* L.) tissues have distinct NMR-based metabolomics profiles. I. Mahmud, **J. Pleasant**, A. Boroujerdi, K. Chowdhury

Frontiers in Nucleic Acid Chemistry

Nucleic Acids 1

Loews Atlanta Hotel
Piedmont

M. Germann, *Organizer*

- 1:00 147.** Investigations of DNA with choline and TMA as counter ions: Origins of altered folding and stability of nucleic acids in aqueous and in water-free solvents. **N. V. Hud**, M. W. Germann, F. M. Lannan, I. Mamajanov, G. Portella, M. Orozco

- 1:30 148.** Thermodynamic Signature to DNA Damage. **B. Gold**, M. Ganguly, M. W. Szulik, M. P. Stone
- 2:00 149.** Excision of 5-methylcytosine and its oxidized derivatives by the DEMETER family of DNA glycosylases. S. C. Brooks, M. Szulik, J. H. Huh, R. L. Fischer, M. P. Stone, **B. F. Eichman**
- 2:30 150.** Structural Studies of the 2-Amino-3-methylimidazo[4,5-f]quinolone N²-dG DNA Adduct. **M. P. Stone**
- 3:00** Intermission.
- 3:15 151.** Unfolding and Targeting Thermodynamics of DNA Stem-Loop Motifs. **L. A. Marky**, I. Khutsishvili, I. Prislán
- 3:45 152.** Monomeric HIV-1 Rev is an intrinsically disordered protein and folds upon self-association and RNA binding. **M. Hennig**, F. Casu, M. Marenchino, S. P. Edgcomb, B. M. Duggan
- 4:15 153.** Structure and function of RNA processing and silencing enzymes in the CRISPR immunity. **H. Li**
- 4:45 154.** Information Content in RNAs from the "Prebiotic Ribosome" to Modern Viruses. **S. C. Harvey**

Inorganic Chemistry General Session

Loews Atlanta Hotel
Pittman

J. Shaw, *Organizer*
C. Scarborough, *Presiding*

- 1:00 155.** Carbene-stabilized unusual main group molecules: Synthesis, structure, and reactivity. **R. J. Gilliard**, Y. Wang, G. H. Robinson
- 1:15 156.** Emerging chemistry of N-heterocyclic dicarbenes. Y. Wang, **D. R. Sexton**, G. H. Robinson
- 1:30 157.** Pt-heteroatom complexes for 1,2-CH-addition. **J. Webb**, T. Gunnoe, T. R. Cundari, M. Sabat
- 1:45 158.** Mechanistic investigations in the hydroamination/cyclization of unactivated amino-alkenes with a CCC-NHC Zr pincer complex. W. D. Clark, J. Cho, H. U. Valle, T. R. Helgert, **T. K. Hollis**, E. J. Valente, K. N. Leigh, C. E. Webster
- 2:00 159.** Synthesis and characterization of transition-metal-substituted polyoxometalates as water oxidation catalysts. **G. Zhu**, C. L. Hill
- 2:15 160.** Phosphate ester hydrolysis of phosphatidylcholine in aqueous solutions of cerium(IV) and bis-tris propane. **D. E. Williams**, K. B. Grant
- 2:30 161.** Bandgap engineering of germanium nanoparticles through tin alloying and quantum confinement effects. **R. J. Esteves**, I. Arachchige
- 2:45 162.** Sol-Gel assembly of silver nanoshells into aerogel frameworks. **X. Gao**, I. U. Arachchige
- 3:00 163.** Quinoxolinol salen ligands for spectrophotometric molecular recognition. **M. DeVore II**, A. Gorden, S. Kerns
- 3:15 164.** Quinoxalinol salens: Ligands for actinide sensors and sensing polymers. **A. E. Gorden**
- 3:30 165.** Structural and functional models of quercetin 2,3-dioxygenase using trisimidazolylphosphine complexes. **W.**

E. Lynch, D. Nivens, N. Peek, J. Stone

3:45 166. Development of new mixed-donor ligands for the preparation of synthetic analogues of methanobactin. **D. Rabinovich**

4:00 167. Sterically-demanding N-heterocyclic thiones (NHTs): Synthesis and reactivity. **M. S. Styron**, D. Rabinovich

4:15 168. Synthesis and coordination chemistry of new bis(pyridyl)- and bis(picoyl)thione ligands. **N. K. Spencer**, D. Rabinovich

Mass Spectrometry Applications in Clinical Chemistry and Environmental Health

Loews Atlanta Hotel
Salon I

V. De Jesus, *Organizer, Presiding*

1:00 169. Screening dried blood spots from newborns for inherited metabolic diseases using tandem mass spectrometry. **D. H. Chace**

1:30 170. Expansion of bio-monitoring of tobacco exposure through automated sample preparation and improved LC/MS/MS methods. **L. Wang**, E. McGahee, C. Sosnoff, Y. Xia, J. Feng, B. Blount

2:00 171. LC-MS determination of molecular markers of water pollution from animal production. **J. J. Harwood**, S. L. Narayanan

2:30 172. Analysis of hemoglobin adducts for exposure assessment and disease diagnostics. **M. P. Ospina**, S. Toth, H. W. Vesper

3:00 173. Mass spectrometric identification of microRNA biomarkers with ultra-high accuracy. **N. H. Chiu**

3:30 174. Toward a better biomarker of exposure to carcinogens: Addressing sample preparation steps. **J. L. Powers**, M. Yang, H. Vesper

4:00 175. Semi-automated solid phase extraction method for the mass spectrometric quantification of 12 specific metabolites of organophosphorus pesticides, synthetic pyrethroids, and select herbicides in human urine. **M. D. Davis**, L. Valentin-Blasini, E. Wade, W. Roman-Esteva, A. Calafat

Organic Chemistry General Session

Loews Atlanta Hotel
Candler

B. Feske, *Organizer*
L. Davis, *Presiding*

1:00 176. Phosphoric acid mediated tautomerism of imines: Addition of imines to aldehydes. **L. O. Davis**, M. Putri

1:20 177. Solvent-Free Per-O-acetylation of Carbohydrates. L. Cai, **C. Rufty**, M. Liqueois

1:40 178. Regio- and Diastereoselective Halofunctionalization Reactions of Functionalized and Non-functionalized Olefins. **R. C. Dhakal**, R. K. Dieter

2:00 179. Long-Range intramolecular S to N acyl migration: a study of the formation of native peptide. **K. Ha**, A. Katritzky

- 2:20 180.** One-pot procedure for the generation of cyanocarbenes. **I. Hyatt**, M. P. Croatt, M. Maxwell
- 2:40 181.** Ion-exchange chromatography to measure relative anion- π binding of substituted benzenes. **M. Lewis**, C. Bagwill, S. Wireduaah
- 3:00 182.** Synthesis of novel 2-[2-acylamidoethyl]-6(phenyl)pyridine analogues. **J. G. Draper**, T. Wenzler, R. Brun, D. W. Boykin
- 3:20 183.** Synthesis of heterocyclic combretastatin analogues via indole aldehydes and ethynyl indoles. **B. J. Shields**, H. L. Holt, Jr.
- 3:40 184.** The glyoxoin reaction: A catalytic route to an abiotic citric acid cycle. **C. J. Butch**, E. D. Cope, P. Pollet, L. Gelbaum, R. Krishnamurthy, C. Liotta
- 4:00 185.** Correlating *N*-alkyl group electronegativity with DFT-computed Parr global electrophilicity values of imidate ester analogs. **J. M. Carr**, A. P. Lathem, G. S. Tschumper
- 4:20 186.** Revisit of a popular fluorophore: skeletal characterization and structural modification. **H. Li**, Q. Wang
- 4:40 187.** Synthesis of symmetrical and unsymmetrical Bis-2,5-Diketopiperazines utilizing benzotriazole-mediated lactamization reactions. **K. Martin**
- 5:00 188.** Addition of enol silanes, silyl ketene acetals, and zinc acetylides to nitrones under silylative conditions. **C. Downey**
- 5:20 189.** Further study of structure dependence in the solvolysis kinetics of oligopeptide esters. J. M. Wunderle, J. S. Baugh, M. A. Missinne, **J. Haseltine**

Posters: Agricultural Chemistry

Loews Atlanta Hotel
Over Look/Exhibit Hall

D. Sherrill, *Organizer*

1:00 - 3:00

- 190.** Reducing the allergenicity of wheat flour by proteases. **Y. Li**, J. Yu
- 191.** In vitro Digestibility of macronutrients in the presence of grape pomace polyphenols. **J. Yu**, S. Ji, Y. Mi
- 192.** Effects of Alcalase from *Bacillus licheniformis* on peanut allergenicity. **J. Yu**, H. Li, M. Hernandez, M. Ahmedna, I. Goktepe

Posters: Environmental Chemistry

Loews Atlanta Hotel
Over Look/Exhibit Hall

D. Sherrill, *Organizer*

1:00 - 3:00

- 193.** Development of a protein-based system for the detection of organophosphates using the pH dependence of

enhanced green fluorescent protein. **A. Henson**, J. Harris, L. G. Puckett

194. Urinary diamines as biomarkers of exposure to diisocyanates. **Y. Qiu**, R. Newton, A. Udeni, B. Blount

195. Propagated Uncertainty in Scattering in Humidified Nephelometers. **H. A. Morrow**, A. Jefferson, J. Ogren, J. Sherman, B. Taubman

196. Biosorption of Hexavalent Chromium from Aqueous Solutions Utilizing Agricultural Waste Products. A. M. Rizzuti, **K. A. Wilson**, L. W. Cosme

197. Investigation eutrophication of Lake Sinclair. **J. Olmstead**

198. Aqueous Cu(II) adsorption by modified and unmodified peanut hulls. **K. O. Davis**, C. L. Huffman

199. H₂Oconee & Beyond: Assessing the Water Quality in the Oconee River. **H. A. Pekarek**, C. H. Lisse

200. Development of a GC-MS Method for the Analysis of Ambient Air Toxics from Industries and Biogenic Terpenes. **A. Tirumala**, B. Ooi, C. Jia, Z. Xue, J. Holt, N. Chong

201. Assessing soil feasibility for edible university landscapes and campus gardens. **J. K. Williams**, R. A. Richards, S. Mutiti

202. Dispersive liquid-liquid microextraction combined with gas chromatography-mass spectrometry for determination of estrogens in water. **J. Kwon**, J. Rodriguez

203. Ingested plastics as a transport medium for marine toxicants to the gastrointestinal tract of loggerhead sea turtles, *Caretta caretta*. **M. D. Wilbanks**, P. J. Seaton

Posters: Medicinal Chemistry

Loews Atlanta Hotel
Over Look/Exhibit Hall

D. Sherrill, *Organizer*

1:00 - 3:00

204. Synthesis and thermal stability evaluation of six-membered cyclic triphosphates containing three nucleotides. **Y. A. Beni**, K. Parang

205. Design and synthesis of potential CXCR4 antagonists. **T. Gaines**, S. Mooring

206. Microwave Synthesis and Characterization of δ -Opioid Peptide Agonists Containing Bulky Aromatic Amino Acids. D. Collins, E. Williamson, **K. R. Wilson**

207. Investigation of microgel mediated taxel based drugs for the treatment of breast cancer cell. **A. Khanal**, **S. S. Seo**

208. Epigenetic Manipulation of a Filamentous Fungus by the Proteasome-Inhibitor Bortezomib Induces the Production of a New Secondary Metabolite. **K. M. VanderMolen**, B. A. Darveaux, C. J. Pearce, N. H. Oberlies

209. Applying desorption electrospray ionization to streamline the discovery of bioactive compounds from fungi. **V. Sica**, N. Oberlies, B. Ehrmann, H. Raja, T. El-Elimat

210. Polyamine-anthracene conjugates: the effects of high ionic strength on DNA interactions and photocleavage. **K. Nguyen**, J. J. Archer, O. Phanstiel IV, K. B. Grant

- 211.** Synthesis of Heterocyclic N-Oxides: Development of Myxin-Glycoside Analogs. **J. D. Joyner**, T. D. Li, W. D. Wang, B. Dun, P. G. Wang
- 212.** Sustainable production of flavonolignans from a fungal endophyte of *Silybum marianum*. **T. El-Elimat**, H. A. Raja, T. N. Graf, N. B. Cech, N. H. Oberlies
- 213.** Design and synthesis of *trans*-cyclooctene modified thymidine triphosphate for post-synthesis DNA modification. **K. Wang**, C. Dai, W. Chen, Y. Zheng, V. Chittavong, B. Wang
- 214.** Design, synthesis and evaluation of conformationally-constrained primidine-triazole analogues of SecA Inhibitor. **C. Dai**, J. Jin, J. Cui, A. S. Chaudhary, K. Demera, W. Chen, P. Tai, B. Wang
- 215.** Novel Antibacterial Agents Targeting the SecA Machinery: Evaluation of the Physical Properties of Potential Drug Candidates. **A. B. Draganov**, W. Chen, N. Ni, A. Sagwal, J. Cui, J. Jin, P. C. Tai, B. Wang
- 216.** Small molecule SecA inhibitors against methicillin-resistant *Staphylococcus aureus*. **J. Jin**, J. Cui, Y. Hsieh, H. Zhang, K. Damera, H. Yang, B. Wang, P. Tai
- 217.** SAR Studies of pyrimidine SecA inhibitors as potential antimicrobial agents. **A. S. Chaudhary**
- 218.** Rose Bengal Analogs as Probes to Study Bacterial SecA Inhibition. **K. Damera**, J. Jin, J. Cui, C. Dai, B. Wang, Y. Hsieh, H. Zhang, H. Yang, P. Tai
- 219.** High resolution MS, MS/MS database using LTQ-Orbitrap XL mass spectrometer interfaced with HESI for dereplication of fungal secondary metabolites. **N. D. Paguigan**, T. El-Elimat, C. J. Pearce, N. H. Oberlies
- 220.** Optimization of endocrine-specific NIR imaging agents: Synthesis of carbocyanine fluorophores. **E. A. Owens**, T. L. Dost, H. Hyun, H. Choi, M. Henary
- 221.** Cancer imaging using a fluorescent conjugate of a boronolactin selective for sialyl Lewis X. **D. Wang**, Y. Chu, K. Wang, Z. Liu, B. Weston, B. Wang
- 222.** Design and synthesis of conjugates of a trityl tag with carbohydrate for imaging mass spectrometric applications. **Y. Zheng**, C. Dai, L. Wang, B. Wang
- 223.** Design and synthesis of a series of analogs based on the Motualevic acids: Application of a novel, convergent synthesis. **F. A. Diaz**, **K. Black**, A. Aycock
- 224.** Synthesis and evaluation of carbocyanine dyes as PRMT inhibitors and imaging agents. **A. Levitz**, L. Yan, Y. G. Zheng, M. Henary
- 225.** Evaluation of functionally selective kappa opioid receptor (KOR) ligands. **K. M. Lovell**, L. Zhou, K. J. Frankowski, S. S. Slauson, A. M. Phillips, J. M. Streicher, E. Stahl, C. L. Schmid, P. Hodder, F. Madoux, M. D. Cameron, T. E. Prisinzano, J. Aubé, L. M. Bohn
- 226.** Potent chiral Inhibitor of histone deacetylase. **J. hou**
- 227.** Design and synthesis of inhibitors of the HIF pathway. **J. N. Holmes**, K. Damera, S. K. Burroughs, N. S. Devi, E. G. Van Meir, B. Wang
- 228.** N3-methyladenine formation by estradiol conjugates with a DNA minor groove methylating agent: Effect of structure on DNA methylation and cell toxicity. S. Miller, R. Kishton, K. Mastro, C. Kelly, **M. Powell**, A. Linares, M. Chelvanambi, V. K. Gore, G. R. Akkaraju, **S. Varadarajan**
- 229.** Glucosamine conjugates of a minor-groove methylating agent: DNA-reactivity and cell toxicity. T. Goodwin, M.

Buchanan, S. Welniak, L. Chauvigne-Hines, **J. Turman**, M. White, A. Frampton, **S. Varadarajan**

230. Evaluation and synthesis of combilexin-like amidines anchored by a minor groove binder. **J. Green**, S. Wang, W. Wilson, D. W. Boykin

231. Design, synthesis and biological evaluation of novel limonin derivatives. **Y. Yang**, Q. Zhu, Y. Xu

232. Polyethylene Glycol containing ROMP Polymers for the modification of neuro-protective Hemoglobin. **A. L. McCollum**, H. J. Schanz

233. Study of antioxidant activity of acai extracts (euterpe oleracea). **S. Kandagatla**, G. M. Raner, R. T. Uhl, T. N. Graf, N. H. Oberlies

234. Microgel encapsulated methylene blue for the treatment of breast cancer cell by photodynamic therapy. **A. Khanal**, S. S. Seo

Supramolecular Chemistry: From Little Things, Big Things Grow

Loews Atlanta Hotel
Dunwoody

J. Lavigne, K. Shimizu, *Organizers*

1:00 235. Polydiacetylenes for sensor applications. **W. T. Pennington**, S. C. Hill, P. L. Dawson, T. W. Hanks

1:25 236. FRET-based indicators for zinc ions. **L. Zhu**

1:50 237. Iterative redesign in DCC: Identification of a new synthetic receptor that recognizes trimethyllysine with nanomolar affinity. **N. K. Pinkin**, M. L. Waters

2:05 238. Sensing anions with fluorescent ureas. **W. E. Allen**

2:30 239. Molecular probes for Zinc(II) and Iron(III) ions. **K. J. Wallace**, E. Manandhar

2:55 Intermission.

3:10 240. Supramolecular approaches to developing sensors for modified amino acids in proteins. **M. L. Waters**

3:50 241. Molecular probes based on the supramolecular interactions of rhodamine B derivatives with organic analytes. **C. Stephenson**

4:05 242. Binding and selectivity of oxoanions with synthetic receptors. **M. Hossain**, A. Pramanik, M. Rhaman, S. A. Haque, M. Emami Khansari

4:30 243. Experimental studies of the effect of polarizability on the π - π interaction. **J. Hwang**, B. Dial, M. Kozik, K. D. Shimizu

4:45 244. From “little” boronate ester sensors grow “big” supramolecular boronate sensors (with tiny pores). **J. J. Lavigne**

5:10 Concluding Remarks.

The Chemistry of Star and Planet Formation

Loews Atlanta Hotel

Ravinia

S. Widicus Weaver, *Organizer, Presiding*

1:00 245. The formation of complex interstellar molecules. **E. Herbst**

1:30 246. Excitation of carbon monoxide: Full-dimensional structure and dynamics for inelastic scattering. **P. Stancil**

2:00 247. Ab initio ro-vibrational IR spectra of H_5^+ D_5^+ and HOCO. **J. Bowman**, S. Carter, Y. Wang

2:30 248. Computational prediction of $I-C_3H^-$ in the Horsehead Nebula PDR. **R. C. Fortenberry**, X. Huang, D. Crawford, T. J. Lee

3:00 Intermission.

3:30 249. Vacuum Ultraviolet photon-stimulated formation of CO_2 at buried ice: graphite grain interfaces. **T. M. Orlando**, J. Shi, G. Grieves

4:00 250. Phosphorus in planet formation. **M. A. Pasek**

4:30 251. Chirped-pulse spectroscopy from 110 - 170 GHz with real-time digitizers. L. Bernier, **S. Shipman**

Novel Bonding Types in Inorganic Chemistry

New Materials and Catalysts for Energy Conversion and Storage

Loews Atlanta Hotel
Chastain

J. Thrasher, *Organizer*
T. Gunnoe, *Presiding*

1:10 252. Mechanism-based design of precursors for the deposition of inorganic films and nanoparticles. **L. McElwee-White**

1:50 253. Dihydroxybipyridine Complexes of Ruthenium and Iridium show that Ligand Deprotonation Can Dramatically Enhance Rates of Catalytic Water Oxidation and Hydrogenation in Some Cases. **E. T. Papish**, J. DePasquale, S. Bhagan, I. Nieto, D. C. Marelius, D. J. Charboneau, J. M. Kamdar, A. R. McGettigan, B. J. Freeman, C. E. Moore, A. L. Rheingold, M. Zeller, J. J. Paul, D. B. Grotjahn

2:30 254. Synthesis of mono-oxo bridged first row transition metal heterobimetallic molecules as long-lived, redox-tunable chromophores. **W. W. Weare**

3:10 Break.

3:30 255. Ionic and metallic carbides grown in metal fluxes. **S. Latturner**

4:10 256. Oxyfunctionalization with Cp^*Ir complexes. **E. A. Ison**

4:50 257. Harnessing redox-active ligands for low-barrier radical coupling reactions at oxidizing oxo complexes. **J. D. Soper**

Chemical Patent and Trademark Law

Loews Atlanta Hotel
Salon H

M. Katz, *Organizer, Presiding*

1:20 Introductory Remarks.

1:30 258. Chemical inventorship. **D. B. Shortell**

2:00 259. Claiming a genus: US patent issues and strategies. **M. Terapane, R. Monheit**

2:30 260. Patents: Obviousness in chemical inventions. **K. W. Hathcock**

3:00 Intermission.

3:20 261. Intellectual Property Pitfalls and Pratfalls in Collaborative Research and Development Arrangements. **P. G. Pappas**

3:50 262. All you need to know about trademarks. **W. H. Needle**

Electronic Structure in Complex Environments

Biological Environments and Energy Conversion

Loews Atlanta Hotel
Salon G

L. Slipchenko, T. Crawford, *Organizers*
L. Burns, *Presiding*

1:20 263. A flickering resonance mechanism for biological charge transfer. **D. N. Beratan**

2:00 264. Using quantum mechanics in biological structure refinement. **K. M. Merz**

2:40 265. Electron transport and transfer through molecular-resolved interfaces: Insight by *ab-initio* modeling. **B. D. Dunietz**

3:20 Intermission.

3:40 266. On the electron-donating abilities of fluorescent proteins: the case of phototoxic KillerRed protein. **K. Bravaya, A. I. Krylov**

4:20 267. The on-the-path random walk sampling to enable multi-step-multi-coordinate enzymatic reaction simulations. L. Cao, **W. Yang**

5:00 268. How does catalase release nitric oxide? Elucidating the reaction mechanism with QM/MM. **F. L. Kearns, S. Vankayala, H. Woodcock**

Neuropeptergic Targets for CNS Disorders

Loews Atlanta Hotel
Centennial

F. Carroll, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 269. Neoclerodane diterpenes as novel treatments for drug abuse. **T. E. Prisinzano**

2:05 270. Identification of Neuropeptide S antagonists for CNS disorders. **S. Runyon**, C. Schmoutz, N. Goeders, C. Garau, S. Negus, J. Bonano, C. Hassler

2:35 271. Evaluation of ligand bias at the kappa opioid receptor: Spanning compound development to effects in neurons. **L. M. Bohn**

3:05 272. Nociceptin/orphanin FQ opioid receptor functional selectivity, signaling and behavior. **M. R. Bruchas**

3:35 Concluding Remarks.

Posters: Organic Chemistry

Loews Atlanta Hotel
Over Look/Exhibit Hall

D. Sherrill, *Organizer*

4:00 - 6:00

273. Brønsted Acid Catalyzed Intramolecular Friedel-Crafts Addition of Indoles to Tertiary Allylic Alcohols. R. Barnes, T. Chisolm, **A. Klarich**, **V. A. Knotts**, B. Wakefield

274. Formyl Group Activation for Suzuki Cross-Coupling Reactions of Bromopyrroles. **A. Harrison**, **M. Wormald**, J. Gupton

275. New Approaches to the Synthesis of the Marine Alkaloid Lycogarubin C. **A. Harrison**, **M. Wormald**, J. Gupton

276. Total synthesis of (\pm)-2-methoxy-6-octadecenoic acid, identified in the Caribbean sponge *Sphaciospongia cuspidifera*, as possible therapeutic agent against neuroblastoma cells. **N. Montano**, W. O. Marrero, N. M. Carballeira

277. Identification of OTC and Prescription Drug Mixtures Using Chemistry Spot Tests in Forensic Analysis. **D. M. Santiago**, D. Barbour, S. Coticone

278. Synthesis of cyclic peptides by intra-molecular lactamization and cyclo-oligomerization of dipeptidyl benzotriazolides. **S. Hamedzadeh**, K. Ha

279. Pyrimidine based potential liquid crystals. **T. A. Bradshaw**, **Z. A. Ratka**, B. S. Clark, S. Q. Smith

280. Total synthesis of Hibiscone C. **A. G. Boyd**

281. Efficient benzotriazole-mediated route to C₂ symmetric cyclo-tetrapeptides containing β -amino acids. **R. E. Quinones**, K. Ha

282. Hypervalent-iodine mediated substitution of aromatic compounds with sodium periodate. **P. A. Shelton**, H. Kim, K. Kim, W. Crosby

283. Solvent-free synthesis of oxindole derivatives through C-H activation in air. **S. Son**, J. Lee, W. Lee

284. Withdrawn.

285. Development of alternative synthetic routes for the production of resveratrol. **M. B. Cuthbert**, B. Goess

- 286.** Synthesis of cysteine ester macrocyclic peptoids by benzotriazole methodology. **L. Nhon**
- 287.** Gold(I) Catalyzed Racemization of 1,3 disubstituted Allenes. **R. J. Harris**, R. A. Widenhoefer
- 288.** Syntheses of 2-Silyl-1,3-Dienes. **P. P. Choudhury**, C. S. Junker, R. R. Pidaparathi, M. E. Welker
- 289.** Simple One Step Oxidation of Steroidal Olefins. **W. Grainger**, E. Parish
- 290.** Progress toward the Synthesis of Callophycolide A, an Antimalarial Benzene Diterpenoid. **R. E. Key**, S. France
- 291.** Synthesis of cyclic tetra-peptides by an intra-molecular imine-induced ring-closing/contraction strategy. **G. G. Simpson**, K. Ha
- 292.** Photo-Dibenzocyclooctadiyne (hv-DIBOD): A linchpin for efficient crosslinking of azide-tagged substrates. **D. V. Sutton**, V. V. Popik
- 293.** Synthesis and study of hydrolase models and intramolecular catalysis. **I. O. Kady**, C. N. Ndi
- 294.** Lewis acid-catalyzed interrupted formal homo-Nazarov cyclization. **R. Shenje**
- 295.** Dimerization of Cinnamic acid derivatives using green photochemistry. **K. Banerjee**, **T. Schmit**, **P. Hao**, **B. Bill**
- 296.** Chemo enzymatic preparation of α -methyl- β -proline analogues: Efficient template based development of organocatalysts for asymmetric *anti*-Mannich reactions. **H. Kotapati**, J. Robinson, G. Keen, S. Banerjee, D. S. Masterson
- 297.** Lewis acid-catalyzed ring opening annulations of polarized strained rings in the presence of amines. **M. C. Martin**
- 298.** Novel homodinuclear *exo*-ruthenium complex containing a *bis*-urea bipyridine macrocycle. **S. R. Salpage**, L. S. Shimizu
- 299.** Chemoenzymatic synthesis of homogenous activity-reversible biotinylated ultralow molecular weight (ULMW) heparin. **B. Wu**, V. Thon, T. Li, P. G. Wang
- 300.** Oxidation of Hibiscone C towards synthesis of recently discovered Natural Products. **J. H. Tryon**
- 301.** Oxa-dibenzocyclooctyne (ODIBO): The most reactive cyclooctyne for uncatalyzed alkyne azide reactions. **C. D. McNitt**, V. V. Popik
- 302.** Novel applications of the Prins reaction. **L. C. Peace**, T. A. Nile, C. Willis
- 303.** Further Insight into the Generation of Cyanocarbenes. **M. A. Maxwell**, M. Croatt, I. F. Hyatt
- 304.** Chemo-enzymatic Synthesis of Polysaccharides. **T. Li**
- 305.** Lactonization of 5-hydroxy α -substituted ester using chiral Bronsted acid : A kinetic resolution strategy for synthesis of chiral α -Substituted δ -lactone. **G. qabaja**, K. Petersen
- 306.** Towards the synthesis of a tripyrromethane derivative mimicking the active site of coenzyme F430. **C. Crooks**, A. Gorden
- 307.** Efficient Synthesis of Dicarboxylic Acid Tetracene Derivatives. **P. B. Honeycutt**, B. R. Wiener, K. S. Petersen
- 308.** New General and Practical Method for the Deprotection of Aryl/Alkyl Allyl Ethers and Allyl Esters. **R. A. Taylor**, **J. A. Campbell**, M. T. Coolbaugh

- 309.** Synthesis of (+)-Bakuchiol using the desymmetrization of a prochiral hydroxy diester with a bulky Brønsted acid. **A. T. Stacy**, K. S. Petersen
- 310.** Probing the Binding Properties of Dendrimers as Supramolecular Hosts . **A. Jolly**
- 311.** Intramolecular Photochemical Cyclizations of Dihydropyridones. **S. Kiren**, D. Butler
- 312.** Atom-modified fluorescent labels for nucleic acid based detection. **M. Kaur**, J. Caton-Williams, Z. Huang
- 313.** Synthesis, characterization, and biological applications of Nile red derivatives. **V. Martinez**, E. Alsolmy, M. Henary
- 314.** Total synthesis of Calothrixins A and B. **S. Xu**, I. Pomilio, M. C. Vitale, T. Nguyen, S. E. Velu

THURSDAY MORNING

Plenary Session

Loews Atlanta Hotel
Salon D/E/F

- 8:00 315.** Academia-Industry-Government Relations in Practice. **D. P. Duncan**

Organic Chemistry General Session

Loews Atlanta Hotel
Candler

B. Feske, *Organizer, Presiding*

- 9:00 316.** Synthesis of complex alkaloids as a driving force for discovery. **J. G. Pierce**
- 9:20 317.** Brønsted Acid Promoted Friedel-Crafts Additions of Indole. **B. Wakefield**
- 9:40 318.** Calcium catalyzed addition reactions. **K. Nolin**
- 10:00 319.** Total Synthesis and Biological Activity of Hibiscone C. **B. C. Goess**
- 10:20 320.** Facile synthesis of enantioenriched hydroxy esters through Brønsted acid catalyzed kinetic resolution. **A. Benavides**, G. Qabaja, K. Petersen
- 10:40 321.** Highly selective Lactonization of racemic Diesters to yield enantioenriched γ -Lactones. **J. E. Wilent**, K. Petersen
- 11:00 322.** Lewis Acid/Brønsted Acid-Catalyzed Csp^3 -H Bond Functionalization of 2-Methyl Azaarenes. **A. Shaikh**
- 11:20 323.** Chemo-enzymatic Synthesis of Structurally Defined N-glycan Library. **Y. Liu**, L. Li, P. G. Wang
- 11:40 324.** Silver-promoted [2,3]-rearrangement reactions of *O*-allylhydroxylamines. **J. B. Vu**

Synthesis, Structure, and Properties of f-element materials

f-element intermetallics

Loews Atlanta Hotel
Inman

T. Albrecht-Schmitt, *Organizer*
S. Lattuner, *Organizer, Presiding*

9:15 Introductory Remarks.

9:20 325. Structural preferences and stability of rare earth intermetallics in pursuit of growth of novel magnetic materials. **J. Chan**

10:00 326. Nd₂Co₂SiC and other intermetallics grown from rare earth / transition metal melts. **S. Zhou**, T. Mishra, S. E. Lattuner

10:25 Intermission.

10:35 327. Magnetism in giant unit cells: does cobalt participate in magnetic ordering in R₁₁₇Co_{52+δ}Sn_{112+γ} structures? **M. Shatruk**, P. Chai, K. Kovnir

11:15 328. Synthesis of rare-earth cobalt arsenides from Bi flux. **X. Tan**, C. M. Thompson, K. Kovnir, M. Shatruk

11:40 329. Magnetic properties of R₂₁Fe₈M₇C₁₂ (R = La, Ce; M = Si, Ge, Sn) intermetallic phases. **S. E. Lattuner**, T. Mishra

Approaches to Organic Synthesis Across Disciplines

Loews Atlanta Hotel
Salon H

D. Whitehead, S. Wiskur, *Organizers*

9:20 Introductory Remarks.

9:25 330. Towards the synthesis of the malagashanine alkaloids – Molecules with a stereochemically unique framework that have the potential to impact malaria chemotherapy. **S. B. Blakey**

10:10 331. Taking advantage of the chemistry of heterocycles in advanced catalyst ligand supports. **A. E. Gorden**

10:30 Intermission.

10:45 332. Chelation-assisted, copper(II) acetate-catalyzed azide-alkyne cycloaddition and amine dehydrogenation. **L. Zhu**

11:05 333. Gold(I)-catalyzed functionalization of C=C bonds. **R. A. Widenhoefer**

Biological Chemistry General Session

Chemical Biology, Metabolism, and Nucleic Acids

Loews Atlanta Hotel
Ravinia

A. Reddi, *Organizer, Presiding*

9:20 334. Fate of chromium nutritional supplements. **K. L. Russell**, J. B. Vincent

9:35 335. NMR-based metabolomics approach for the biochemical characterization of embryogenic and non-embryogenic calli of *Saccharum officinarum* L. I. Mahmud, **B. Shrestha**, A. Boroujerdi, K. Chowdhury

9:50 336. Copper(I)-catalyzed azide-alkyne cycloadditions for functionalization of enzyme packaged viral nanoparticles. **R. Hincapie**, C. McKay, M. Finn

10:05 337. Chemical approaches to the investigation of protein-membrane binding interactions using synthetic lipid probes. **M. D. Best**, M. M. Rowland, M. D. Smith, H. E. Bostic

10:20 338. Synthesis of analogs of myo-inositol to enable chemical biology studies. **T. J. Ricks**, M. D. Best

10:35 339. Designing a novel class of protein-based MRI contrast agents (ProCAs) for metastatic tumors in liver and molecular imaging of disease biomarkers. J. Qiao, S. Xue, F. Pu, **J. Yang**

10:50 340. Effect of molecular crowding on the stability of human c-MYC promoter sequence I-Motif at neutral pH. E. A. Lewis, **V. H. Le**, J. Cui

11:05 341. *In vitro* study of assembly events during bovine leukemia virus replication. **D. F. Qualley**

11:20 342. Site-specific DNA methylating agent targeted to estrogen receptor-positive cells. R. Kishton, S. Miller, C. Kelly, K. Mastro, A. Linares, M. Chelvanambi, V. K. Gore, G. R. Akkaraju, **S. Varadarajan**

11:35 343. DNA ligase-mediated translation of DNA into densely functionalized nucleic acid polymers. **R. Hili**, J. Niu, D. R. Liu

Electronic Structure in Complex Environments

Potential Surfaces and Excited States

Loews Atlanta Hotel
Salon G

L. Slipchenko, T. Crawford, *Organizers*
G. Tschumper, *Presiding*

9:20 344. Automatic search of reaction pathways in complex environments. **K. Morokuma**

10:00 345. Spatial partitioning of symmetry adapted perturbation theory: the A-SAPT heuristic. **R. M. Parrish**, C. D. Sherrill

10:20 Intermission.

10:40 346. Energy transfer in dendrimeric systems: Non-adiabatic molecular dynamics in large conjugated molecules. **A. E. Roitberg**

11:20 347. Orthogonality Constrained Density Functional Theory for Electronic Excited States. **F. A. Evangelista**

Frontiers in Nucleic Acid Chemistry

Nucleic Acids 2

Loews Atlanta Hotel
Piedmont

M. Germann, *Organizer*

9:20 348. Drugging RNA: Targeting structured HIV-1 RNA with branched peptide boronic acids. **W. L. Santos**, W. Zhang, J. Wynn

9:50 349. Investigations of the Structure, Stability, and Ligand Binding Properties of G-Quadruplex and I-Motif DNAs. **E. A. Lewis**, V. R. Machha, V. H. Le

10:20 Intermission.

10:35 350. Recognition and binding of human telomeric G-quadruplex DNA by unfolding protein (UP1). J. S. Hudson, L. Ding, V. Le, E. Lewis, **D. Graves**

11:05 351. Folding pathway of the human telomere G-quadruplex. R. D. Gray, **J. B. Chaires**

NanoElectrochemistry in Biomedical Research and Energy Technology

General Topics

Loews Atlanta Hotel
Centennial

L. Bottomley, J. Stickney, G. Wang, *Organizers, Presiding*

9:20 Introductory Remarks.

9:25 352. Mechanistic Electrochemistry with Cyclic Square Wave Voltammetry. **L. A. Bottomley**, M. A. Mann

9:55 353. Recessed carbon-fiber microelectrodes for use with FSCV in living tissue. **A. C. Schmidt**, L. Dunaway, J. G. Roberts, T. J. Shogren, M. P. Zach, L. A. Sombers

10:15 354. Surface enhanced light Absorption and Photoelectrochemical Performance of photoanodes towards Solar Water Splitting. **S. Pan**, J. Wang, Z. Shan

10:45 355. Electrodeposition of non-dendritic lithium by addition of alkaline earth metals. **J. K. Stark**, P. A. Kohl

11:05 356. Transport and Nanosize Nucleation of Lithium Chloride at Charged Solid-electrolyte Interfaces. **W. D. Brown**, Y. Li, D. Wang, M. Kvetny, G. Wang

11:25 357. Imaging and measuring single molecular specific interactions by single molecule recognition and force spectroscopy. **B. Xu**, B. Wang, C. Guo

New Opportunities for Chemical Businesses

Loews Atlanta Hotel
Pittman

M. Beug-Deeb, *Organizer, Presiding*

9:20 Introductory Remarks.

9:30 358. An Overview of 3D Printing and an Introduction to Some Emerging Additive Manufacturing Technologies with Disruptive Potential. **S. Das**

10:10 359. International Trade Services and Chemical Exports from Georgia; and The Benefits of Georgia. **T. Ponce, W. R. Harrison**

10:50 360. Accelerating Medical Device Commercialization in the Southeast. **T. W. Karp**

11:30 361. Local Content --- Opportunities for Business Expansion – A New Way to Market. **P. Dismer**, M. Beug-Deeb

Novel Bonding Types in Inorganic Chemistry

NHC Chemistry

Loews Atlanta Hotel
Chastain

J. Thrasher, *Organizer*
K. Seppelt, *Presiding*

9:20 362. Tricks with Polydentate Carbenes and Iminium Salts. J. W. Runyon, G. Gurau, Y. Uchiyama, J. S. Dolphin, J. C. Nelson, **A. J. Arduengo, III**

10:00 363. Electron-deficient bonding in oligonuclear group 11 metal complexes. **J. P. Sadighi**, B. K. Tate, C. M. Wyss, T. J. Robilotto, J. Bacsa, K. Kluge, M. Wieliczko

10:40 Break.

11:00 364. Evolving Main Group Chemistry of N-Heterocyclic Carbenes. **G. H. Robinson**

11:40 365. Development of novel N-heterocyclic carbenes for a linearly opposed coordination. **D. Tapu**, Z. McCarty, C. McMillen

Physical Chemistry General Session

Loews Atlanta Hotel
Ardmore

A. Schrand, R. Fortenberry, *Organizers*

9:20 366. Achievement of near-reversible cyclic voltammograms of carotenoids. **A. Focsan**, L. D. Kispert

9:40 367. Energetic and Kinetic Profile for CO Binding to Chloramine-T Modified Horse Heart Cytochrome-c. **T. A. Word**, R. W. Larsen

10:00 368. Photoreactivity and singlet oxygen generation of select mononitrofluoranthenes. **S. Gavalda**, R. Arce

10:20 369. DNA equilibrium in chromophoric silver nanocluster-based sensors. **O. O. Sergev**, B. Giri, D. A. Nicholson, D. R. McMullan, P. M. Goodwin, J. T. Petty

10:40 Break.

11:00 370. Kinematics and dynamics of atomic-beam scattering from liquid and self-assembled monolayer surfaces. **W. A. Alexander**, T. K. Minton

11:20 371. Controlling Silver Clusters using DNA Hybridization. **D. A. Nicholson**, O. O. Sergev, J. T. Petty

11:40 372. Widely accessible fast mixer to study biophysical reactions. **M. J. Reddish**, B. Dyer

Supramolecular Chemistry: From Little Things, Big Things Grow

Loews Atlanta Hotel
Dunwoody

J. Lavigne, K. Shimizu, *Organizers*

9:20 Introductory Remarks.

9:25 373. Biomolecular synthesis of the conducting polymer PEDOT:PSS. **C. Payne**

9:50 374. Noncovalent polymerization in water by monomers that were inspired by the nucleobases. **B. J. Cafferty**, M. C. Chen, I. Gállego, N. V. Hud

10:05 375. Controlling the structure and dynamics of supramolecular G-quadruplexes from the nano- to the micro-scale. **J. M. Rivera**

10:30 Intermission.

10:45 376. Post-synthesis DNA modifications with the boronic acid moiety for sensing applications. **B. Wang**

11:25 377. Water-Soluble Polyelectrolytes as Supramolecular Hosts. **M. Bonizzoni**

Posters: Nanochemistry and Spectroscopy: Symposium Honoring Mostafa El-Sayed

Loews Atlanta Hotel
Over Look/Exhibit Hall

P. Wine, Z. Zhang, *Organizers*

10:00 - 12:00

378. Spectroscopy, kinetics, and thermochemistry of the $(\text{CH}_3)_2\text{SeCl}$ radical. **J. M. Nicovich**, Z. Zhao, P. L. Laine, M. L. McKee, P. H. Wine

379. Proton coupled electron transfer in biomimetic beta hairpin peptides. **C. V. Pagba**, J. Yohannan, T. McCaslin, M. McDaniels, B. A. Barry

380. The role of surface diffusion in determining the shape of noble-metal nanocrystals. **X. Xia**, S. Xie, M. Liu, Y. Xia

381. Synthesis of Cationic Polyamine and Polyguanidine Type Polymer-Capped Gold Nanoparticles: Heterogeneous Catalysis. **C. Padgett**, N. A. Green, G. J. Gabriel, B. Baruah*

382. Quantitative analysis of the coverage density of Br^- ions on Pd{100} facets and its role in controlling the shape of Pd nanocrystals. **H. Peng**, Y. Xia

383. Kinetically controlled synthesis of palladium icosahedra and their catalytic properties. **T. Lv**, Y. Wang, S. Choi, Y. Xia

384. Surfactant-Coated Nanoparticles as Substrates for Surface Enhanced Raman Spectroscopy. **B. S. Thompson**, **K.**

Wulkowicz, B. Baruah

- 385.** Development of highly luminescent europium-based silica nanomaterials for biomedical applications. **A. N. Darsanasiri, I. Bose, C. R. De Silva**
- 386.** Complete water splitting with hybrid nanoparticles and hole-extracting ligands. **A. D. La Croix, J. Macdonald**
- 387.** Progress towards synthesis of Au@SiO₂-Cu_{2-x}Se hybrid nanoparticles for surface plasmon interaction studies. **S. L. Arrowood, J. Macdonald**
- 388.** Size- and shape-controlled synthesis of wurtzite CuInS₂ nanoparticles for photocatalytic reduction of water. **B. C. Howard, E. Hernández-Pagan, J. Macdonald**
- 389.** Optically modulatable fluorescent proteins. **A. E. Jablonski, I. Issaeva, Y. Chen, R. B. Vegh, J. Hsiang, P. Bagchi, C. J. Fahrni, L. M. Tolbert, R. M. Dickson**
- 390.** Electrochemical formation of tungsten nanosharp tips. **M. Nave, B. Rubin, V. Maximov, S. Creager, K. Kornev**
- 391.** Determination of the maximum dopant threshold of cobalt ferrite spinels with gadolinium as the dopant. **P. A. Edmonds, Z. J. Zhang**
- 392.** Change of magnetic properties in nanoparticles for surface detection. **J. Robbins, Z. J. Zhang**
- 393.** Using self-assembled DNA nanostructures to stimulate cell surface receptors. **R. Pedersen, T. H. Labean, E. G. Lobo**
- 394.** Hollow gold nanorectangles: The roles of polarization, substrate and orientation. **R. Near, M. El-Sayed**
- 395.** Determining Drug Efficacy Using Targeted Plasmonically Enhanced Single Cell Imaging Spectroscopy. **L. A. Austin, B. Kang, M. A. El-Sayed**
- 396.** Plasmonic Coupling Of Three Pairs Of Sharp Corners Of Solid Cubes, Two Pairs Are Homogeneous (Au or Ag) And The Third Pair Is Of Silver And Gold. **N. Hooshmand, D. O'Neil, M. El-Sayed**
- 397.** Construction of 3D Porous All-inorganic Polyoxometalate Frameworks. **C. Zhao, E. N. Glass, D. G. Musaev, D. T. Kim, J. Bacsá, G. Zhu, C. L. Hill**
- 398.** Most Effective Gold Nanorod Size for Plasmonic Photothermal Therapy: Theory and Experiment. **M. A. Mackey, M. Ali, L. A. Austin, R. D. Near, M. A. El-Sayed**
- 399.** Determining the mechanism of solution metallic nanocatalysis with solid and hollow nanoparticles: homogeneous or heterogeneous. **B. Garlyyev, M. Mahmoud, M. El-Sayed**
- 400.** Bulky organic D-A- π -A dye on sensitized TiO₂ film: A possible strategy to suppress charge recombination in DSSC. **X. Kang, J. Zhang, A. J. Rojas, D. O'Neil, P. Szymanski, S. Marder, M. A. El-Sayed**
- 401.** Spectroscopic investigations of electron transfer in di-nuclear ruthenium-osmium complexes. **J. Tate, S. Yamazaki, A. Cadranel, B. M. Trosel, P. Albores, L. M. Baraldo, V. D. Kleiman**
- 402.** Study on Faraday Rotation Spectra for Cobalt Ferrite Thin Films. **H. i. Doo, Z. J. Zhang**
- 403.** Platinum-silver alloy nanocage catalysts exhibit low activation energies with minimal platinum content. **J. A. Bordley, M. A. El-Sayed**
- 404.** Synthesis of Lipid-Capped Nanoparticles as SERS Substrates. **J. A. Law, C. Megedyuk, B. Baruah**

- 405.** Synthesis of Polyoxometalate-Capped Nanoparticles: SERS substrates. **T. Miller**, B. Baruah
- 406.** Water soluble ultra small gold nanomolecules. **N. Kothalawala**, J. L. West, A. Dass
- 407.** Capture and detection of cancer cells in whole blood with magnetic–optical nanoovals. **S. Bhana**, E. Chaffin, Y. Wang, X. Huang
- 408.** Kinetic control: a versatile and powerful route to controlling the shape of metal nanocrystals. **X. Xia**, Y. Xia
- 409.** Particle size effect on the photocatalytic activity of BiNbO₄. **S. P. Adhikari**, K. Senevirathne, A. Lachgar
- 410.** Probing of local photoelectrochemical events on single crystal TiO₂ with nanometer scale resolution. **D. A. Clayton**, G. J. Szulczewski, S. Pan

Posters: Computational Chemistry

Loews Atlanta Hotel
Over Look/Exhibit Hall

D. Sherrill, *Organizer*

10:00 - 12:00

- 411.** Computational ecology: Elucidating novel chemical defense mechanisms of Antarctic sea sponges. **F. L. Kearns**, S. Vankayala, H. Woodcock
- 412.** An Aerobic Oxidative C-C Bond Formation from Novel Pd complexes: a theoretical study. **Q. Peng**, M. B. Hall
- 413.** Discovery of potent inhibitors targeting protein arginine methyltransferases using in silico virtual screening. **C. Yan**, L. Yan, Y. G. Zheng, I. Ivanov
- 414.** Towards an accurate description of methane physisorption on carbon nanotubes. **D. G. Smith**, K. Patkowski
- 415.** Infrared spectra of H₅O₂⁺ and H₅O₂⁺Ar: Ab initio classical molecular dynamics calculations. **D. T. Adedeji**, **M. Kaledin**
- 416.** Using Adaptive Steered Molecular Dynamics (ASMD) to determine the energetics of secondary structures in peptides. **H. Bureau**, E. Hershokvitz, R. Hernandez, D. Merz, S. Quirk
- 417.** Atomistic modeling of connexin 26 using molecular dynamics flexible fitting. **E. K. Carter**, C. Yan, I. N. Ivanov
- 418.** Understanding room temperature ionic liquid effects upon organic reactions from QM/MM/MC/FEP simulations.. **C. R. Allen**, B. W. McCann, O. Acevedo
- 419.** Docking studies of Modafinil to neurological receptors. **K. Huang**, P. G. Wang, N. W. Allen
- 420.** Free energy dependence of lipid bilayer systems on buckle angle using atomistic simulations. **K. V. Uppulury**, **J. T. Kindt**
- 421.** Computational modeling of missense mutations in human opioid receptors related to substance dependence. **C. A. Henry**, Z. Zhang, E. Michonova-Alexova
- 422.** Development of new MOF Charge Parameterization Methods. **K. Wang**, C. R. Cioce, H. L. Woodcock, B. Space

- 423.** DFT of RDX fragmentation pathways: Computational evidence for the lack of molecular ion peak in RDX mass spectrum. **K. A. Duncan**, Y. A. Jeilani
- 424.** PRMT1: Exploring the mechanism and product specificity from molecular dynamics simulations. **S. Gathiaka**, J. Hevel, O. Acevedo
- 425.** Highly accurate potential energy surface for the He-H₂ dimer. **B. W. Bakr**, D. G. Smith, K. Patkowski
- 426.** Vesicle phase transition dynamics in a coarse-grained simulation. **L. A. Patel**, J. T. Kindt
- 427.** Molecular mechanism of dynamic recognition of octamer-binding transcription factor (OCT4) to its target DNA. L. Li, L. Luo, C. Luo, **K. K. Li**
- 428.** Structurally distinct complexes of ubiquitin and SUMO-modified PCNA lead to distinct functional outcomes. C. Yan, X. Xu, **I. Ivanov**

Posters: Physical Chemistry

Loews Atlanta Hotel
Over Look/Exhibit Hall

D. Sherrill, *Organizer*

10:00 - 12:00

- 429.** Temperature dependence of the thermodynamics for binding histone H1⁰, its carboxyl domain (H1⁰-C), or its globular domain (H1⁰-G) to calf-thymus DNA. **V. Machha**
- 430.** Electron spin resonance investigation of matrix isolated C₂H₆⁺. **C. Burton**, J. J. Banisaukas, III, L. B. Knight, Jr
- 431.** Synthesis of Silver Cyanide by Pulsed Laser Ablation in N,N-dimethylformamide. **S. Lee**, M. Y. Choi
- 432.** Enhanced dechlorination of m-dichlorobenzene using Fe/Pd/C nanoparticles Produced by Pulsed Laser Ablation in Liquid(PLAL). **Y. Yu**, M. Y. Choi
- 433.** Reductive Dechlorination of Tetrachloroethylene(PCE) using Bimetallic Nickel-Palladium Nanoparticles Produced by Pulsed Laser Ablation in Liquid (PLAL). **H. J. Jung**, M. Y. Choi
- 434.** Photochemical reduction of CO₂ on sphalerite (ZnS) mineral surfaces. **R. Zhou**, **M. I. Guzman**
- 435.** Tuning bipolaron populations in PEDOT:PSS via biological catalysts. **J. Morris**, C. Payne
- 436.** Structural modifications improving optical modulation of cyanine dye fluorescence. **D. P. Mahoney**, C. Fan, E. A. Owens, M. Henary, R. M. Dickson
- 437.** Spectral characterization of intermediate species in the catalytic degradation of hydroxyurea by horse heart myoglobin. **P. Huhta**, R. Larsen
- 438.** Production of biodiesel through the hydrocracking of peanut oil. K. McGill, **J. McPhail**, **M. Youngs**, **V. Belisle**, **S. Beauchamp**
- 439.** Photo-initiating the enzymatic reaction of mushroom Tyrosinase utilizing the Ru(II)bis(2'-Bipyridine)(Tyramine)₂ complex as a substrate photo-releasing agent. **V. Fuillerat**, T. Word, P. Huhta, R. W. Larsen

440. Photosensitized Reduction of Diaziridinylbenzoquinones by the Pheophorbide-a. **Y. Diaz Espinosa**, R. Arce, A. E. Alegria

441. Effect of shape and symmetry of gold and silver nanoparticles on their mechanical properties. **D. O'Neil**, M. Mahmoud, M. El-Sayed

442. Time resolved fluorescence measurements to study electron transfer in DMPD-Pro-Coumarin and two coumarin control compounds. **M. Fekhry**, R. Abdel Malak Rached, E. Castner, J. Wishart

THURSDAY AFTERNOON

Minority Affairs Committee Luncheon

(Ticketed event)

Loews Atlanta Hotel
Salon A

J. Green, K. Jackson, *Organizers*

12:00 443. Considering the chemistry of a crisis. **K. Bobb**

Frontiers in Nucleic Acid Chemistry

Nucleic Acids 3

Loews Atlanta Hotel
Piedmont

M. Germann, *Organizer*

1:00 444. DNA-Encapsulated Silver Clusters. **J. Petty**, D. Nicholson, O. Sergev

1:30 445. Single-Molecule Studies of Guanine Sensing Riboswitch. **M. Mandal**

2:00 446. Development of Benzimidazoles alkynes in Nucleic Acid Recognition. **D. P. Arya**, N. Ranjan

2:30 447. Nucleic Acid NMR, new Tools and Methods. **C. Anklin**

3:00 Intermission.

3:15 448. Identification of new, biologically relevant, G-quadruplexes formed within the critical promoter of kRAS as promising molecular targets. C. A. Hockings, **T. A. Brooks**

3:35 449. Integrative modeling of complex nucleic acids assemblies. C. Yan, X. Xu, **I. Ivanov**

3:55 450. DNA origami: Constructing nanomaterials and nanorobotics from DNA. **R. M. Wadkins**, J. Waller

4:15 451. Supercooled aqueous NMR. **A. M. Spring**

4:30 452. One DNA minor groove - many possibilities: From the basics of AT base pair recognition to more complex binding modes and interactions. **W. Wilson**, A. Paul, S. Wang, R. Nanjunda, A. Kumar, Y. Chai, C. E. Stephens, D. W. Boykin, G. M. Poon

Minority Serving Institutions and their Role in the STEM Pipeline

Loews Atlanta Hotel
Candler

K. Jackson, *Organizer*

1:00 Introductory Remarks.

1:10 453. The contributions of HBCUs to the STEM pipeline: Challenges and opportunities. **W. Pearson**

1:40 454. Role of HBCU's in the education and employment of African American women chemists. **J. E. Brown**

2:10 455. Sustaining the Legacy: The Role of Spelman College in Diversifying the STEM Pipeline. **L. Winfield**

2:40 456. Can a Solid Undergraduate Research Program in STEM Help a Hispanic Serving Institution Become Tier One? **L. E. Echegoyen**

3:10 Intermission.

3:25 457. Diversity: A Competitive Advantage for Global Innovation. **O. N. Petzold**

3:55 458. Diversifying the STEM Enterprise. **D. Barnes**

4:25 459. STEM education praxis: Role performance of MSIs in K12 education. **A. T. Tucker Blackmon**

4:55 Panel Discussion.

Nanochemistry and Spectroscopy: Symposium Honoring Mostafa El-Sayed

Loews Atlanta Hotel
Salon I

P. Wine, *Organizer*

Z. Zhang, *Organizer, Presiding*

G. Schatz, *Presiding*

1:00 460. Reflections on Mostafa's Contributions to Physical and Materials Chemistry. **J. D. Simon**

1:20 461. For Mostafa – with energy and charge. **M. Ratner**

2:00 462. The structure and dynamics of patterned nanospheres. **R. Hernandez**

2:20 463. Tuning the optical properties of iron oxide-gold core-shell nanoparticles for cancer detection and treatment. **E. Chaffin, S. Bhana, X. Huang, Y. Wang**

2:40 464. Energy transfer in collisions of highly excited allyl radical in Argon. **R. Conte, P. L. Houston, J. M. Bowman**

3:00 Intermission.

3:20 465. The Contribution of Femtosecond Laser Spectroscopy to the Development of Optoelectronic Nanomaterials. **C. Burda**

3:40 466. Solar energy conversion using artificial atoms, molecules and solids. **T. Lian**

4:00 467. Reformulation of disulfiram with Au nanoparticles for targeted drug delivery in cancer therapy. **J. Mi, J. Song, X. Peng, S. Nie, D. M. Shin**

4:20 468. Ligand-Conjugated Gold Nanoparticles as Probes for Cell Surface Receptors. **A. Y. Oyelere, B. E. Gryder, E. C. Dreaden, I. O. Raji, L. A. Austin, S. Fathi, M. A. El-Sayed**

4:40 469. A Chemist's Approach to Nanofabrication: Towards a "Desktop Fab". **C. A. Mirkin**

New Opportunities for Chemical Businesses

Loews Atlanta Hotel
Pittman

M. Beug-Deeb, *Organizer, Presiding*

1:00 470. Current Trends in Shale Oil and Gas Exploration Including Hydraulic Fracturing Operations. **C. L. Alfaro**

1:40 471. US Shale Gas – Implications for the Global Chemical Industry. **H. Disteldorf**

2:20 472. New Chemical Business Opportunities in Saudi Arabia and Gulf States. **T. M. Deeb**

3:00 Intermission.

3:10 473. The Business Case for Sustainability. **F. M. Clark**

3:50 474. Crowdfunding Your Way to Success. **A. Cape**

Supramolecular Chemistry: From Little Things, Big Things Grow

Loews Atlanta Hotel
Dunwoody

J. Lavigne, K. Shimizu, *Organizers*

1:00 475. Creating Complex Interfaces Using Orthogonal Click Reactions. **J. Locklin**

1:25 476. Towards Intelligent Materials. **D. G. Lynn, C. Chen, J. Tan, T. Omosun, D. Das, S. Li, A. Mehta, J. Goodwin, N. Anthony, L. Zhang, T. Pan, R. Rengifo, C. Liang, A. Mowles, N. Li, J. Smith, M. Hsieh, M. Grover, K. Berland**

1:50 477. 8-Aryl-2'-deoxyguanosine derivatives as G-quadruplex DNA ligands. **M. d. Rivera-Sánchez, A. V. Morales-de-Echegaray, M. García-Arriaga, G. Hogley, J. M. Rivera**

2:05 478. Self-assembled bis-urea macrocycle hosts as functional molecular containers. **L. S. Shimizu**

2:30 479. Consequences of hydrogen bonding on the molecular organization and performance of one class of organic photovoltaic materials. **B. M. Schulze, N. T. Shewmon, J. Zhang, D. L. Watkins, J. P. Mudrick, W. Cao, R. Bou Zerdan, A. J. Quartararo, I. Ghiviriga, J. Xue, R. K. Castellano**

2:55 Intermission.

3:10 480. How breaking bonds can keep materials whole. **S. L. Craig**

3:50 481. Supramolecular pH-responsive G-quadruplexes. **L. M. Negrón, J. M. Rivera Ortiz**

4:05 482. Preparation, structures and host-guest chemistry of selected fluorinated frameworks. **M. Etzkorn**, J. C. Timmerman, M. D. Brooker, D. T. Nguyen, C. M. Kane, D. S. Jones, M. Gerken

4:30 483. Fascinating Topologies of Metallacycles Derived from the 2,6-Bis(Ferrocenylketoenolyl)-pyridine ($H_2L^{2,6}$) Ligand. **C. Gwengo**, M. Raja, J. Cole, Y. Chen, D. L. Reger, M. L. Smith

4:45 484. Versatile model system for studying non-covalent interactions of aromatic surfaces. **K. D. Shimizu**

5:10 Concluding Remarks.

Novel Bonding Types in Inorganic Chemistry

Halogen Bonding

Loews Atlanta Hotel
Chastain

J. Thrasher, *Organizer, Presiding*

1:10 485. From crystal engineering to function engineering with halogen bonding. **P. Metrangolo**, G. Cavallo, G. Resnati, G. Terraneo

1:50 486. Halogen bonding of bromosubstituted electrophiles with halides, pseudohalides and halometallates: from charge-transfer complexes to electron-transfer reactions. **S. Rosokha**

2:30 487. Halogen Bonding: Charge Saturation in Inorganic Analogues of Halomethanes and the Tuning of Sigma Holes. **K. Donald**, B. Wittmaack, C. Crigger, M. Tawfik

3:10 Break.

3:30 488. Pseudo-polyhalides. **W. T. Pennington**, A. M. Siegfried, S. E. Creager, T. W. Hanks

4:10 489. DFT Calculations Of Multi-Halogen Bonded Systems. **T. Hanks**, R. Giesecking, J. Smith, W. Pennington

4:50 490. Alkane functionalization by iodate: The surprising effect of chloride. **T. Gunnoe**, J. T. Groves, G. C. Fortman, N. C. Boaz, M. M. Konnick, R. A. Periana

Southern Chemistry History Lessons for 21st Century America

Loews Atlanta Hotel
Ardmore

D. Hicks, *Organizer, Presiding*

1:10 Introductory Remarks.

1:15 491. Accidental crusader for the world's largest(USA) chemistry based industry. **D. G. Hicks**

1:50 492. National Historic Chemical Landmarks in the South. **W. R. Oliver**

2:25 493. Evolution of the Herty Advanced Materials Development Center. **A. A. Koukoulas**

3:00 Intermission.

3:20 494. Chemistry-related industries of the southern USA: Then and Now. **M. P. Walls**

3:55 495. Georgia Research Alliance: An economic development model for the South and nation. **C. L. Liotta**

4:30 496. Captain Charlie's keys to 21st Century STEM career success. **E. Reichmanis**

5:05 Concluding Remarks.

Electronic Structure in Complex Environments

Condensed-Phase Environments

Loews Atlanta Hotel
Salon G

L. Slipchenko, *Organizer*
T. Crawford, *Organizer, Presiding*

1:20 497. Modeling condensed-phase effects on electronic structure and spectroscopy. A. V. Marenich, **C. J. Cramer**, D. G. Truhlar

2:00 498. Electronic optical activity: Intrinsic behavior and environmental perturbations. P. Lahiri, K. B. Wiberg, **P. H. Vaccaro**

2:40 499. Solution phase coupled cluster response properties using an n-body approach. **T. J. Mach**, T. D. Crawford

3:00 500. Harmonic vibrational frequencies for hydrogen bonded clusters: Towards the CCSD(T) complete basis set limit for explicit solvation. **G. S. Tschumper**

3:20 Intermission.

3:40 501. Towards the Accurate Simulation of UV/Vis Spectra in Solution. **M. Caricato**

4:20 502. Chemical reactions at aqueous surfaces and in ionic liquids from QM/MM simulations. **O. Acevedo**

5:00 503. Evaluation of implicit solvation models for the prediction of solution-phase intramolecular CH/ π interactions. **T. M. Parker**, N. Pokhrel, S. Janardan, A. E. DePrince, C. D. Sherrill

Synthesis, Structure, and Properties of f-element materials

f-element oxides, arsenides, etc

Loews Atlanta Hotel
Inman

S. Latturner, *Organizer*
T. Albrecht-Schmitt, *Organizer, Presiding*
A. Sefat, *Presiding*

1:20 504. Plutonium and Beyond: Understanding Structure and Bonding in Transuranium Borates. **T. E. Albrecht-Schmitt**

2:00 505. New oxytelluride: Perovskite and CsCl intergrowth in Ba₃Yb₂O₅Te. J. B. Whalen, **T. Besara**, R. Vasquez, F. Herrera, J. Sun, D. Ramirez, R. L. Stillwell, S. W. Tozer, T. D. Tokumoto, S. A. McGill, J. Allen, M. Davidson, T.

Siegrist

2:25 506. Crystal growth, structure determination and physical properties of new uranium containing complex oxides and oxy-chlorides. **H. zur Loye**

3:05 Intermission.

3:20 507. Crystal Growth, Structures, and Magnetic Properties of New Reduced Uranium (IV) Fluorides. **J. Yeon**, M. D. Smith, A. S. Sefat, J. Tapp, T. T. Tran, A. Moeller, P. S. Halasyamani, H. Zur Loye

3:45 508. New Vanadates as Hosts for Lanthanide Ions: A Long and Winding Road. **J. W. Kolis**, M. Kimani, C. McMillen

4:25 509. Single crystal synthesis of europium (II) oxide utilizing an alkaline earth metal flux growth system. **D. Ramirez**, T. Siegrist, J. Whalen, T. Besara

4:50 510. Evidence of filamentary superconductivity in praseodymium-doped CaFe_2As_2 crystals. **A. S. Sefat**

Approaches to Organic Synthesis Across Disciplines

Loews Atlanta Hotel
Salon H

D. Whitehead, S. Wiskur, *Organizers*

1:30 511. New chemo- and stereoselective reactions catalyzed by coinage metals. **J. M. Schomaker**, J. W. Rigoli, R. D. Grigg, C. S. Adams, C. D. Weatherly

2:15 512. Ring-constrained nucleosides and nucleotides as ligands of cell-surface receptors. **K. A. Jacobson**, S. Paoletta, S. Chakraborty, D. K. Tosh

3:00 Intermission.

3:15 513. Lewis acid-catalyzed ring-opening annulation approaches to fused benzene rings. **S. France**

4:00 514. Chemo-, regio-, and stereoselective reactions of Grignard and organozincate reagents for generating small molecular synthons. **R. Dieter**

4:45 515. Vanadium oxide catalysis for organic synthesis. **D. C. Whitehead**

NanoElectrochemistry in Biomedical Research and Energy Technology

Biomedical/Bioanalytical

Loews Atlanta Hotel
Centennial

J. Stickney, *Organizer*
L. Bottomley, G. Wang, *Organizers, Presiding*

1:30 516. Electrochemical Energy Conversion using Photosystem Protein Complexes. **D. E. Cliffel**, G. LeBlanc, E. Gizzie

2:00 517. Visualizing hydrogen oxidation reaction activity of polycrystalline platinum by scanning electrochemical

microscopy (SECM). **Y. Wang**, D. O. Wipf

2:20 518. Carbon nanotube yarn microelectrodes for enhanced detection of neurotransmitter dynamics in live brain tissue. A. C. Schmidt, X. Wang, Y. Zhu, **L. A. Sombers**

2:50 519. Silver nanoparticles-enhanced light absorption and photoelectrochemical performance of hematite ($\alpha\text{-Fe}_2\text{O}_3$) thin-film electrodes for water splitting. **J. Wang**, S. Pan

3:10 520. Characterization of charge storage process of manganese oxide-based pseudocapacitor material using *in-operando* Raman spectroscopy. **D. Chen**, G. Waller, X. Li, M. El-Sayed, M. Liu

3:30 Intermission.

3:45 521. Electrochemical Proximity Assay: a Highly Sensitive and Selective Multiplexed Direct-Readout Method for Quantitative Analysis of Proteins at Femtomolar Levels. **C. Shannon**, L. Zhang, S. Somasundaram, X. Li, C. J. Easley

4:15 522. Enhanced neurotransmitter detection with nanostructured-carbon microelectrodes. **C. B. Jacobs**, A. Zestos, B. Venton

4:45 523. Biomimetic nanomaterials for energy technologies. **M. R. Knecht**

5:15 524. Redox and optical activities in the dithiolate and monothiolate stabilized gold complexes and nanoclusters. **J. Jiang**, C. V. Conroy, T. Ahuja, J. W. Padelford, T. Wang, G. Wang

Posters: Analytical Chemistry

Loews Atlanta Hotel
Over Look/Exhibit Hall

D. Sherrill, *Organizer*

1:30 - 3:30

525. Withdrawn.

526. An automated dual stage solid phase extraction procedure for 15 F2t-isoprostane (8-iso Prostaglandin2a) from BSA and human serum as lipid markers of oxidative stress. J. Bosken, F. Kero, V. Vandell, T. Enzweiler, **M. Cherrier**

527. Sol-gel Thin Film of Zirconium Oxide for Detection of Organophosphate Compounds and Pesticides. **M. N. Bui**, S. S. Seo

528. Gold Nanoparticle Conjugated Polystyrene Particles Thin Film For DNA Hybridization Detection Using ATR-FTIR Spectroscopy. **M. N. Bui**, J. Otano, S. S. Seo

529. Detection of Glutamate, Glycine, Acetylcholine, and GABA using High-Performance Liquid Chromatography for Non-Mammalian Systems. **C. D. Hallman**, C. Dorismond, N. J. Kuklinski

530. Determination of arsenic, cadmium and chromium in commercial wine samples. K. Smith, **S. Melaku Abegaz**

531. Amperometric Detection with a Dendrimer-Encapsulated Platinum Nanoparticle-Carbon Nanotube Composite. **A. K. Deb**, A. Saha, M. Wayu, T. Devkota, C. C. Chusuei

532. Determination of the Conformation of Specific Residues in a Model Peptide by C_{13} Isotope Edited ATR-FTIR in Regular Water. **S. Potana**, C. Wang

- 533.** Interference of Carbon Nanodots to Conventional Toxicity Assay. **P. Wright**, H. Qin, M. M. Choi, Z. Jia, N. H. Chiu
- 534.** Development of a Raman spectroscopic database of artists' pigments. **C. E. Phipps**, S. W. Huffman
- 535.** Real-time voltammetric detection of met-enkephalin in rat adrenal tissue. **L. E. Dunaway**, A. C. Schmidt, G. S. McCarty, L. A. Sombers
- 536.** Creating an ongoing learning environment through experimentation and root cause investigation to understand sources of variation in measurements of Opiate analyte concentrations obtained via LCMS/MS analysis. **J. Supica, J. Hull**
- 537.** Optimizing return on investment for LCMSMS consumable components in a high throughput toxicology laboratory using Six Sigma methodologies. **J. Hull, J. Supica**
- 538.** Higher Order Derivative Voltammetry For Irreversible Processes at Spherical Electrode. T. Hong, I. Rusodimos, **M. Kim**
- 539.** Determination of Avogadro's number using multiple diverse experimental techniques. **M. Lewis**, M. H. Kabir, J. Cramer
- 540.** Water Quality Analysis of the Ocmulgee River. **K. Taylor**, C. Lisse
- 541.** Determination of trace and heavy metals in some herbal teas and spices. **J. Mierzwa**
- 542.** New Gas-Phase Deprotonated Tyrosine Structure. **C. E. Plummer**, S. S. Bokatzian-Johnson, M. L. Stover, D. A. Dixon, C. J. Cassady
- 543.** GC-MS method for the accurate quantitation of trans-fatty acids. **N. Wei**, H. C. Kuiper, H. W. Vesper
- 544.** Negative chemical ionization method for the analysis of trans-fatty acids. **A. R. Smith**, H. C. Kuiper, H. W. Vesper
- 545.** Quantitative and qualitative analysis of fatty acids in human plasma. **C. W. Waters**, H. C. Kuiper, H. W. Vesper
- 546.** Investigation of pharmaceutical pollution of surface water in georgia. **N. Potter**, C. H. Lisse
- 547.** Gold nanoparticle-doped sol-gel amperometric glucose biosensors. **J. R. Hall, N. G. Poulos**, M. H. Freeman, M. C. Leopold
- 548.** Identification of Flavonoid Content in Poplar and Sourwood Honey. M. Martin, S. Mastromarino, **E. Grimley**
- 549.** Analysis of Kentucky bluegrass and rye grass pollen glycans using Mass Spectrometry. **K. Stumpo**
- 550.** Development and implementation of dynamic IEF. **R. Montgomery**
- 551.** Gold coated TiO₂ nanotubes as a visible light surface enhanced photocatalyst for water splitting applications. **A. S. Panikar, Z. Shan**, S. Pan, A. Gupta
- 552.** Separation and characterization of high mannose glycan isomers from bovine Ribonuclease B. **J. Qu**, B. Dun, P. G. Wang
- 553.** Effects of lanthanide metal cationization on electron transfer dissociation mass spectrometry of the acidic peptide Fibrinopeptide B. **J. J. Commodore**, C. J. Cassady
- 554.** Towards pattern-based recognition with self-assembled receptors. **A. Mallet**, M. Bonizzoni

555. In-vitro calibration of microiontophoresis pipets. **P. A. Flowers**

556. Properties of the SPI/HPMC blending films. M. Chen, Q. Huang, **J. Ye**, J. Xiong

557. Electrochemical and Optical Studies of Thiolate Stabilized Bimetallic Ag-Au Nanoclusters. **J. W. Padelford**, J. Jiang, T. Ahuja, C. V. Conroy, G. Wang

558. Removal of molecular adsorbates on silver nanoparticles using sodium borohydride in water. **H. S. Perera**

559. Adsorption, desorption, exchange, and reaction of adenine and 2-mercaptobenzimidazole (MBI) on aggregated gold nanoparticles (AuNPs). **M. Gadogbe**, W. E. Collier, D. Zhang

Posters: Polymer Chemistry

Loews Atlanta Hotel
Over Look/Exhibit Hall

D. Sherrill, *Organizer*

1:30 - 3:30

560. Modulating the temperature responsivity of thermoresponsive microgel thin films. **K. C. Clarke**, L. A. Lyon

561. π -Stacked models for conjugated polymers. **E. M. Henry**, D. M. Collard

562. Fluorescent liposome-based multiplexing biosensor system. **M. Evans**, C. Hansen, D. Ebzery, T. Hanks, C. Wright

563. Synthesis and characterization of microemulsion polymerization of Polymethyl Methacrylate-net-Polyethylene Glycol Dimethacrylate encapsulated linear Polystyrene. **C. J. Scanlon**, D. W. Holley

564. Novel π -conjugated polymers containing fused arenes. **C. R. Kulkarni**, D. M. Collard

565. Functional poly(lactic acid)s: Synthesis and potential applications for bone tissue engineering. **P. P. Kalelkar**, G. R. Alas, D. M. Collard

566. Patterned Surface Modification of Conducting Polymer Films. **B. Toney**, P. Molino, T. Hanks

567. Exploring the liquid crystallinity of poly(3-alkylthiophene)s. **B. E. Cox**, D. M. Collard

568. Molecular weight effects on PBT-6 charge carrier mobility. **A. Ravi Sankar**, E. Reichmanis, B. Fu

569. Polystyrene Coated Silver Nanoparticles with Applications in Optical Data Storage. L. Zhu, G. Zhang, **E. Zlibut**

570. Adsorption of heavy metals by modified agricultural waste materials. **Z. M. Akhtar**, I. N. Urhoghide

571. Binding of As, Ni, and Mn metal ions by grafted carboxyl methyl- containing cellulosic materials. **G. Pacareu**, I. N. Urhoghide

572. Separation of heavy metal ions from solution using modified cellulosic materials. I. N. Urhoghide, G. Pacareu, **J. Vettaparambil**

573. Protein and cell resistant brush polymer on medical grade stainless steel. **G. R. Alas**, D. M. Collard, A. J. Garcia

574. Interfacial Polymerization Synthesis of Polyamide-Polyetheramide (PAPEA) Thin-Film Composite Reverse Osmosis Membranes. **A. F. Olatokunbo**

575. Enhancing Hydrolytic Stability of Covalent Organic Frameworks via Edge and Face Modifications. **M. W. Di Carmine**, J. J. Lavigne

576. Polydiacetylene sensor substrates: Cellulose and cellulose acetate. **S. C. Hill**, P. L. Dawson, T. W. Hanks, W. T. Pennington

577. Ternary nanocomposites based on poly(n-butyl methacrylate), cellulose acetate butyrate and an Algerian bentonite. **S. Djadoun**, K. Ouaad, N. Ziani, Y. Ouchelli

Small Business Innovation Research Seminar

Loews Atlanta Hotel
Ravinia

3:30 578. Understanding how to tap into federal funds through the small business innovation research (SBIR) and small business technology transfer (STTR) programs. **C. G. Casteel**

Posters: Inorganic Chemistry

Loews Atlanta Hotel
Over Look/Exhibit Hall

D. Sherrill, *Organizer*

4:30 - 6:30

579. Detection of volatile organic compounds in enclosed spaces. **K. M. Henline**, C. Wang, R. D. Pike

580. Ergothioneine and methimazole: Investigating antioxidant activity and the effects of structure on activity. **M. T. Zimmerman**, J. L. Brumaghim

581. Synthesis, surface immobilization, and electrochemical characterization of cobalt bis(glyoxime) hydrogen catalysts. **K. J. Hauser**, C. Ester, K. Barnes, D. Wheeler, M. Hambourger

582. Synthesis and electrochemical evaluation of Ru single-site electrocatalysts for solar fuel applications. **D. P. Harrison**, Z. M. Kibler, J. A. Tavanner, Z. S. Wood

583. Structural diversity in the reactions of mixed-donor ligands with bromine and iodine. **J. Velasco**, D. Rabinovich

584. The synthesis and reactivity of a hydride-bridged dicopper cation supported by an N-heterocyclic carbene ligand. **C. M. Wyss**, B. K. Tate, J. Bacsá, T. G. Gray, J. P. Sadighi

585. Characterization of Metal-Organic Frameworks using magnetic susceptibility in the undergraduate Inorganic Chemistry laboratory. **S. Xhani**, G. J. McManus

586. Synthesis and characterization of model square planar platinum group metal complexes with asymmetric α,ω -bis(phosphite)-polyether ligands for use in the Rh catalyzed hydroformylation of styrene. **E. C. Cagle**, G. M. Gray

587. Metal-oxo complexes with redox-active ligands: Toward oxyl reactivity. **A. M. McDaniel**, J. D. Soper

588. Redox-active N-heterocyclic carbene nickel complexes as cross-coupling catalysts. **C. F. Harris**, J. D. Soper

589. Bis(pyridyl)selenone complexes of tin(IV) and lead(II). **A. Fowler**, D. Rabinovich

- 590.** CCC-NHC Pincer Ta (V) Complexes: Synthesis, Ligand Exchange, NHC Rearrangement to a Mixed NHC–MIC (Mesoionic Carbene) Pincer, and Intramolecular Catalytic Oxidative Hydroamination of Alkenes. T. R. Helgert, **T. K. Hollis**, A. G. Oliver, H. U. Valle, Y. Wu, C. E. Webster
- 591.** Use of Ligand Functionalized Resins for Metal Extractions. **C. D. Tutson**, A. E. Gorden
- 592.** Unconventional high temperature synthesis of two water-soluble Keggin-based salt inclusion solids (SISs): $\text{Cs}_6\text{Cl}_2\text{Na}(\text{PMo}^{\text{VI}}_{10}\text{Mo}^{\text{V}}_2\text{O}_{40})$ (**1**) and $\text{Cs}_6\text{IClNa}(\text{PMo}^{\text{VI}}_{10}\text{Mo}^{\text{V}}_2\text{O}_{40})$ (**2**). **D. Sulejmanovic**, S. Hwu
- 593.** Metallathiacrown ethers: Transition metal complexes of α,ω -bis(phosphite)-polythiaether ligands as sensors for environmental pollutants. **J. R. Martin**, G. M. Gray
- 594.** Synthesis and cytotoxicity studies of Eu(III) doped- Fe_3O_4 nanoparticles using YPEN rat endothelial cells. **K. L. Schumann**, M. Clark, W. Polk, K. Dreher, C. R. De Silva
- 595.** Synthesis and x-ray structure determination of transition metal complexes using tris-1-ethyl-4-methylimidazolylphosphine. **N. Peek**, W. Lynch
- 596.** Synthetic approaches to new emissive transition metal alkynyl complexes. **D. Crapps**, P. S. Wagenknecht
- 597.** The Synthesis of New Phosphine Ligands for Use in Asymmetric Catalysis. **F. Chen**, L. Hazeland, T. A. Nile, P. Pringle
- 598.** Synthesis of Zirconocene Amino Alcohol Frustrated Lewis Pairs. B. Boonseng, T. A. Nile, D. F. Wass, **C. M. Alfaro**
- 599.** Mechanochemical synthesis of halogen-bonded cocrystals involving bis(diphenylphosphino) alkane disulfides/selenides and tetraiodoethylene. **A. M. Siegfried**, H. D. Arman, W. T. Pennington
- 600.** Synthesis and coordination chemistry of dipyridosiloles. **D. M. Peloquin**, C. Maguylo, S. K. Moon, J. D. Lee, T. A. Schmedake
- 601.** Synthesis and characterization of of a two-dimensional antiferromagnetic oxyphosphate: $\text{Sr}_{1.25}\text{Na}_{1.5}\text{Fe}_5\text{O}_2(\text{PO}_4)_5$. **L. D. Sanjewa**, C. M. Brown, J. He, D. Hitchcock, S. Hwu, A. Pfirman
- 602.** Electrochemical water oxidation with a heterogeneous polyoxometalate water oxidation catalyst. **J. M. Sumliner**, H. Lv, Y. V. Geletii, C. L. Hill
- 603.** POM-based catalytic gelating nanoarray for the decontamination of mustard agent analogs. **K. Sullivan**, D. Hillesheim, W. Neiwert, H. Zeng, C. L. Hill
- 604.** Withdrawn.
- 605.** Synthesis and characterization of two dirhenium compounds that contain bis(diphenylphosphino)acetonitrile. **D. R. Derringer**, C. M. Ammermann
- 606.** Synthesis of BODIPY-cobaloxime catalysts for photon-driven proton reduction. **A. J. Francis**, W. W. Weare, J. Bartelmess

Posters: Materials Chemistry

Loews Atlanta Hotel
Over Look/Exhibit Hall

D. Sherrill, *Organizer*

4:30 - 6:30

- 607.** Porphyrin-Based Polysilsesquioxane Nanoparticles to Improve Photodynamic Therapy for Cancer Treatment. **L. K. Fritts**, D. Vega, J. Vivero-Escoto
- 608.** MCM-NaTaO₃ composite catalysts for photocatalytic organic molecule conversion. **K. Senevirathne**, L. Zhang, R. T. Williams, A. Lachgar
- 609.** Electrospun Si/TiO₂ composite nanofibers for advanced lithium ion batteries. **K. R. McCormac**, T. Tran, J. Wu
- 610.** SYNTHESIS OF PbS/TiO₂ NANOCOMPOSITES USING THE SOL-GEL PROCESS FROM COVALANTLY INCORPORATED LEAD THIOLATES. **K. Patel**, J. T. Moore
- 611.** Development of redox-responsive silica-based nanoparticles for photodynamic therapy applications. **D. L. Vega**, J. L. Vivero-Escoto
- 612.** Development of sustainable nanotechnology for environmental remediation. **S. I. Kuriyavar**, T. Joell, A. Apblett
- 613.** Processing and Applications of Sol-Gel Materials. **K. Ehret**
- 614.** Peptide seeding reshapes the energy landscape of self assembly. **C. Liang**, N. Li, S. Johnson, A. Metha, D. G. Lynn
- 615.** Assessing the ability of dye conjugated gold nanorods to recognize and bind to cell surface receptors. **K. Mills**, J. Wilson, M. Turnage, K. Walker, J. W. Stone
- 616.** Gold nanorod-drug conjugates toward inhibited amyloid fibril in Alzheimer's disease. **M. Melvin**, P. McGlynn, A. Shaikh, J. W. Stone
- 617.** Rescinnamine as a promising drug therapeutic against advanced, chemotherapy-resistant prostate cancer. **B. Crowe**, A. Diamanduros, J. W. Stone, K. Scarpinato
- 618.** Mesogenic flavones. **A. J. Jordan**, D. J. Timmons
- 619.** Selection and propagation of functional assembly in Dynamic Chemical Networks. **J. Tan**, C. Chen, M. Hsieh, M. Zhou, J. Goodwin, A. Mehta, M. Grover, F. Fernandez, D. Lynn
- 620.** Porphyrin conjugated gold nanorods as targeted therapeutic agents toward breast and prostate cancer cell destruction. **M. Dang**, A. Robinson, M. Melvin, J. LoBue, K. Scarpinato, J. Stone
- 621.** A novel Naphthalene diimide linker on Au and Ag nanoparticles: Synthesis and Characterization. **S. C. Paul**, V. Cammarata
- 622.** Donor-modified asymmetric squaraine sensitizers for dye-sensitized solar cells. **R. B. Hill**, I. Davydenko, X. Kang, D. O'Neil, F. Jradi, P. Szymanski, T. C. Parker, S. Barlow, M. A. El-Sayed, S. R. Marder

FRIDAY MORNING

Biological Simulations using Molecular Dynamics, Monte Carlo, and Multiscale Approaches

Loews Atlanta Hotel
Salon G

O. Acevedo, *Organizer, Presiding*

8:00 623. Probing the Intricate Coupling between Enzyme dynamics and Catalysis. **D. Hamelberg**

8:30 624. Development of HIV inhibitors targeting cyclophilin A guided by free energy perturbation calculations. **O. Acevedo**

9:00 625. "Bicelle" lipid mixtures: Atomistic, coarse-grained, and thermodynamic modeling. **J. T. Kindt**

9:30 626. Molecular dynamics of biomolecules in the times of GPUs and Replica exchange: What dreams are made of... **A. E. Roitberg**

10:00 Intermission.

10:20 627. Determining free energy curves of proteins through adaptive steered molecular dynamics (ASMD). **R. Hernandez**

10:50 628. The orthogonal space sampling scheme to enable quantitative free energy simulations. L. Zheng, **W. Yang**

11:20 629. Bio-inspired catalysts for efficient peptide hydrolysis. **R. Prabhakar**

Chemistry Education General Session

Loews Atlanta Hotel
Ardmore

M. Koether, *Organizer, Presiding*

8:00 630. Implementation of a project-based guided inquiry approach to general chemistry labs. **L. B. Wheeler**, B. Barnhill, C. Lariviere, C. Grisham

8:15 631. Authentic Chemistry Experiments(ACE) in the general chemistry lab curriculum: Design, implementation and the role of teaching assistants in the freshman laboratory. **V. Lykourinou**, A. Villalta-Cerdas, T. Gatlin

8:30 632. Qualitative/Quantitative analysis of artificial food dyes: A UV/VIS course-embedded research experience for Principles of Chemistry at Georgia Gwinnett College. **I. H. Krouse**, S. M. Mwongela, G. Giles, M. S. Morton, S. H. Park, D. G. Sauder, B. C. Shepler

8:45 633. Coupling DFT calculations with experimental measurements in the physical chemistry lab. **T. C. DeVore**, A. C. Bagley

9:00 634. Comparison of student performance on various laboratory assessments following the creation of a self-created technique video. **M. A. Erdmann**, J. L. March

9:15 635. Development and assessment of a hybrid introductory chemistry laboratory course. **J. L. Poteat**

9:30 636. Using electronic laboratory notebooks to improve student learning outcomes. **M. C. Koether**

9:45 637. Contextualizing chemistry with art. **A. Gaquere-Parker**

10:00 638. Using Marzano's taxonomy to assess and improve learning outcomes. **T. D. Shepherd**

10:15 639. Organic chemistry students' knowledge structures of fundamental general chemistry concepts: Lewis structures and bonding. **S. R. Mooring**, N. L. Burrows

10:30 Intermission.

11:00 640. Nomenclature – The “mail man” analogy: Organic chemistry. **S. Landge**

11:15 641. Role of iPads in chemistry curriculum at Anderson University. **D. A. Abramovitch**

11:30 642. Forensic science track at Georgia Regents University. **S. Myers**

11:45 643. Pedagogical view of metrology in analytical forensic science. **J. Messman**

New Pedagogy and Approaches to Improve Student Learning Outcomes in Undergraduate Chemistry Education

Loews Atlanta Hotel
Dunwoody

G. Potts, C. Dockery, *Organizers, Presiding*

8:00 644. Computer animations in chemistry: How chemical education research can help chemistry instructors. **M. J. Sanger**

8:30 645. Engaging students in the inorganic chemistry classroom with well-defined learning objectives: Interactive learning through group activities, literature discussions, and even field trips. **J. P. Lee**

9:00 646. New computational physical chemistry experiments: Using POGIL techniques with ab initio and molecular dynamics calculations. **M. S. Reeves, R. M. Whitnell**

9:20 647. Integrated approach for development of scientific writing skills in undergraduate organic lab. **E. C. Duran, C. L. Weaver, J. A. Nikles**

9:40 648. Use of the enzyme-substrate interactions concept inventory to measure biochemistry students' misconceptions. **K. Linenberger, S. Lowery Bretz**

10:10 Intermission.

10:30 649. Can a PLTL teaching reform targeting General Chemistry improve student progression throughout a Chemistry curriculum? **S. E. Lewis**

11:00 650. Let's give them something to talk about: participation strategies that improve student engagement and learning. **K. D. Kloepper**

11:30 651. Undergraduate Research as Pedagogy: Promoting and Sustaining a Culture of Undergraduate Research among Chemistry Majors. **C. Mills, J. K. Metzker, R. A. Richards**

Polymer Chemistry General Session

Loews Atlanta Hotel
Ravinia

X. Zhang, *Organizer, Presiding*

8:00 652. Direct Visualization of Polyelectrolyte Mobility in Microgel Thin Films. **E. S. Herman, L. A. Lyon**

8:20 653. Highly effective Emulsion ROMP of DCPD and COE using pH-responsive Ru-Alkylidene Complexes. **H. J. Schanz, S. L. Balof**

- 8:40 654.** Synthesis and characterization of Phosphonated-bisphenolA dopants for solid state proton conduction in polyfunctional acid membranes. **K. Reid**
- 9:00 655.** One-step synthesis and characterization of Poly(o-toluidine) nanofiber/metal nanoparticle composite networks as non-enzymatic biosensors. **S. Poyraz**, Y. Liu, N. Lu, Z. Liu, M. Kim, X. Zhang
- 9:20 656.** Liquid Crystal Phase in Poly(3-hexylthiophene) Solutions. **N. Kleinhenz**, K. Nayani, J. Park, M. Srinivasarao, E. Reichmanis
- 9:40 657.** Synthesis of Polyamide-Polyetheramide (PAPEA) Thin-Film Composite Reverse Osmosis Membranes. **O. J. Wadsworth**, A. Olatokunbo, M. Gayle, N. Arnett
- 10:00 658.** Improved methodology for observing the molecular weight distributions of wood components in original and processed wood. **T. Leskinen**, S. Kelley, D. S. Argyropoulos
- 10:20 659.** Synthesis & Characterization of Poly(arylene ether sulfone)Kraft LigninHeat Stable Copolymers. **R. Sun**, D. Argyropoulos, H. Sadeghifar, C. Cui, S. Sen
- 10:40 660.** Synthesis and characterization of bisphenol A tetrachlorocyclotriphosphazene poly(arylene ether sulfone) hybrid copolymers for proton exchange membrane fuel cells. **T. N. Thompson**, N. Arnett
- 11:00 661.** Poly(n-alkyl methacrylates)/Algerian bentonite nanocomposites prepared via in situ polymerization, initiated by a novel complex. **S. Djadoun**, K. Ouad
- 11:20 662.** Nanostructure, ion transport, and mechanical properties of LiTFSI and PVDF based solid polymer electrolyte. **J. Chen**
- 11:40 663.** Optimizing of UV coatings and their curing behavior by means of Thermal Analysis. **T. Doll**

Nanochemistry and Spectroscopy: Symposium Honoring Mostafa El-Sayed

Loews Atlanta Hotel
Salon I

P. Wine, Z. Zhang, *Organizers*
C. Landes, S. Link, *Presiding*

- 8:20 664.** Nanoscale manipulation of light: New physical insights and technological opportunities. **N. Halas**
- 9:00 665.** Elucidating chemical transformations one nanocrystal at a time. **P. K. Jain**
- 9:20 666.** Role of Ligand Coordination Geometry in Controlling Binding of Thiolated Target Molecules to Quantum Dot Surfaces. **C. D. Heyes**
- 9:40 667.** A monolayer graphene;Au surface enhance Raman spectroscopy platform for DNA damage studies. **T. M. Orlando**, A. Sidorov
- 10:00** Intermission.
- 10:20 668.** Mostafa and the golden age. **C. J. Murphy**
- 11:00 669.** Nanoparticle surface charge directs the cellular binding of nanoparticle-protein complexes. **C. C. Fleischer**, C. K. Payne
- 11:20 670.** An NMR-based model for protein-gold nanoparticle interactions. **N. C. Fitzkee**, A. Wang, K. Vangala, D.

Zhang

11:40 671. A Water-Soluble High-Contrast Cu(I)-Selective Fluorescent Probe with Parts-Per-Trillion Sensitivity. **M. T. Morgan, A. M. McCallum, C. J. Fahrni**

NanoElectrochemistry in Biomedical Research and Energy Technology

General Topics

Loews Atlanta Hotel
Centennial

L. Bottomley, J. Stickney, G. Wang, *Organizers, Presiding*

8:30 672. Mixed electronic / ionic conduction in carbon / ionomer composites. **S. Creager**, J. Shetzline, J. Oh, J. Park

9:00 673. Enhanced charge storage capacity of conducting polymer electrodes by the entrapment of p-benzoquinone. **M. R. Arcila-Velez**, M. E. Roberts

9:20 674. Lipid-Assembled Light-Harvesting/Photoconverting Supercomplexes. **W. Zhan**, M. Wang

9:50 675. Single molecule spectroelectrochemistry of MEH-PPV on nanostructured TiO₂ surfaces. **C. M. Hill**, S. Pan

10:10 Intermission.

10:25 676. The Use of Gold Nanoparticles in Dye-Sensitized Solar Cells and Biosensing. **F. P. Zamborini**, T. Luitel, S. Beeram, L. Bao, A. Fang

10:55 677. Ink-jet printing of enzymes to fabricate biosensors for metabolic monitoring of organ-on-chip bioreactors. **J. R. McKenzie**, A. N. Davis, D. E. Cliffl

11:15 678. Quenching and Enhancement of Fluorescence and Electrogenenerated Chemiluminescence When CdSe/ZnS Mixed With CdTe/CdS Quantum Dots. Y. Wusimanjiang, **W. Miao**

11:45 679. High temperature Surface Enhanced Raman Spectroscopy for in situ study of Solid Oxide Fuel Cells. **X. Li**, J. Lee, D. Chen, L. A. Bottomley, M. A. El-Sayed, M. Liu

Posters: Undergraduate Research

Analytical/Inorganic/Environmental Chemistry

Loews Atlanta Hotel
Over Look/Exhibit Hall

V. Singh, *Organizer*

8:30 - 10:00

680. Modification of Polysaccharides with Attachment of Iron Chelating Ligands. **A. Parker**, C. J. Fowler

681. Better nicotine fix? : Analysis of alkaloids in e-cigarette filling solutions by HPLC. **J. Murray**, G. E. Potts

682. Investigating the DNA binding behavior of Cr(III) Diimine systems capable of inducing DNA photooxidation. **M. A. Caulkins**, W. D. Netterville, M. M. Sprinkle, N. A. Kane-Maguire, S. K. Wheeler, J. F. Wheeler

- 683.** Enhancing biomolecular class separation in complex sample analysis using ion mobility-mass spectrometry (IM-MS). **R. M. Reyes**, N. M. Lareau, J. C. May, J. A. McLean
- 684.** Extraction and Separation of Organic Environmental Pollutants by Sol-Gel Capillary Microextraction coupled to Gas Chromatography. **K. J. Meise**, A. Alhendal, A. Husain, A. Malik, K. Bisht
- 685.** Oxygen reduction reactions catalyzed by (nitro)cobalt(III) hexadecafluorophthalocyanine derivatives. **T. H. Aslund**, J. A. Goodwin
- 686.** Isolation and derivatization of pentobarbital. **A. Farooq**, S. F. Hornbuckle
- 687.** The Addition of Thiols to Electron-Deficient Cyclopropanes Catalyzed by a Ca (II) Complex. **C. Braun**, K. Nolin
- 688.** Thiol Additions to Epoxides Catalyzed by a Rhenium(V)-Oxo Complex. **A. Badiceanu**, K. Nolin
- 689.** Heteroleptic palladium(II) and platinum(II) complexes containing a crown thioether and monodentate phosphines. **T. P. Latendresse**, J. P. Lee, C. L. Keller, G. J. Grant
- 690.** Synthesis, characterization, and reactivity of *p*-cymene ruthenium(II) complexes with fluorine-containing phosphite ligands. **M. J. Hankins**, J. P. Lee
- 691.** Hydrogen uptake on palladium catalysts. **C. E. Milliron**
- 692.** Analysis of Cold and Flu Medications Found in DayQuil™ and NyQuil™ Using HPLC and Cyclic Voltammetry. **J. Stewart**, C. E. Dahm, K. R. Wilson
- 693.** Copper and zinc acetylacetonate: How one electron changes everything. **A. Brown**, L. Pinelo, B. S. Ault
- 694.** Detection of Naturally Produced Organohalogen Compounds in Marine Sponges from the Bahamas and Florida Coast. **S. D. Shaw**, N. Rosenfelder, J. R. Pawlik, J. Kucklick
- 695.** Seeded Growth of Pd Nanocrystals: The Influence of Surface Capping Agent. **Z. Li**, H. Peng, Y. Xia
- 696.** Studying imidazole coordination to Mn(III) porphyrins by UV-Vis absorption spectroscopy. **L. L. Cyr**, L. Arnold, G. B. Ray
- 697.** Effect of pH on Cytochrome *c* Voltammetry. **M. R. Chandler**, **R. J. Quarles**, K. R. Hoke
- 698.** Quantification of ethanol in rainwater using solid-phase microextraction (SPME). **C. Andreacchi**, K. M. Mullaugh
- 699.** Synthesis of Organometallic-Based Biologically Active Compounds: In vitro Antibacterial and Spectroscopic of Ferrocene-Derived Penicillin Chelates. **K. Barnes**, A. Kalsum, M. Raja, C. Gwengo, A. Peters
- 700.** Studies of DNA binding interactions with [Rh(9S3)Cl₃], [Rh(9S2O)Cl₃], and [Ir(9S3)Cl₃] using fluorescence spectroscopy. **H. J. Greve**, J. Kim
- 701.** Study of the binding between Fe²⁺/Fe³⁺ and the fluoroquinolones. **M. A. Addo**, **U. Kalapathy**, H. Fan-Hagenstein
- 702.** Characterization of chemical and biological properties of extracts from American Pokeweed. **B. L. Parker**, **G. S. Barrett**, D. Ivankovic, D. A. Abramovitch
- 703.** Optimization of glycan labeling for plant pollen protein analysis by UPLC. **P. Wesner**, K. Stumpo
- 704.** Substrate and metal selectivity of PPM1A phosphatase. **P. J. Pryor**, **D. B. Kelly**, D. F. McCain

- 705.** Developing Separations of Cr(III) Diimine Complexes Using Chiral Capillary Electrophoresis. **C. D. Stachurski**, T. F. Harris, N. A. Kane-Maguire, S. K. Wheeler, J. F. Wheeler
- 706.** Quantification of the uremic toxin p-cresol in serum of ESRD and normal patients. **J. M. Murphy**, M. F. Santiago, S. R. Whitson
- 707.** Rhodium and iridium complexes of NHC as catalysts in hydrosylation reactions. Z. McCarty, **D. Woodruff**, **D. Lee**, **D. Tapu**
- 708.** Analysis of volatile organic compound signatures from wildfire emissions in southeast Texas. **B. S. Morgan**, Y. Zhou, B. C. Sive
- 709.** Analysis of Thiocyanates in *Wasabia Japonica*. **C. R. Dockery**, J. Lu, **M. Giedd**, **B. Patterson**
- 710.** Automated spectrophotometric titrations and the determination of chemical equilibria. **J. C. Hammond**, J. A. Lynch
- 711.** Characterization of silver coated silica nanoparticles. **E. Trapp**, S. Kuriyavar, H. Fan, U. Kalapathy
- 712.** Mutational Analysis of Bovine Leukemia Virus Nucleocapsid Protein. **V. Sokolove**
- 713.** Fluorescence enhancement of coupled metal monolayer-protected clusters. **J. M. Ruddock**, D. Crisostomo, J. C. Tuberqueria, D. E. Cliffl
- 714.** Long-term Variability in the Aerosol Chemistry of the Appalachian Mountains in North Carolina. **M. Link**, Y. Zhou, B. Sive, B. Taubman
- 715.** Mosquito repellent to heavy metals: Chemical impacts on local neighborhoods. **L. M. Bianco**, **M. B. Bowen**, **I. D. Patel**, **C. R. Wilson**, J. L. Look
- 716.** Application of coffee as an electron donor to reduce hexavalent chromium: column test. **S. A. Fatima**, C. Kim, S. Park
- 717.** Relative binding of halide ions with tetrabutylammonium ions: ESI-MS and computational studies. **W. Steward**, **K. P. Swanson**, T. Morris, C. Brown, S. Swamy-Mruthinti, M. Fujita, F. A. Khan
- 718.** Photoactivated hydrazone metal chelation: The HAPI approach. **R. McAtee**
- 719.** Spectroscopic analysis of metal desorption from industrial Georgia clay. **C. L. Quattlebaum**, **E. L. Oliver**, K. A. Knapper, B. Cicerchi, D. Ma, R. Carter, K. D. Kloepper
- 720.** Discovery of robust biosurfactants for agricultural and environmental applications. **J. L. Armstrong**, **A. King**, K. L. Miller, E. Sastoque, J. W. Kloepper, G. L. Crawford, K. D. Kloepper
- 721.** The Sweet Smell of Carolina Jessamine: Evaluating the Floral Scent Profile of *Gelsemium sempervirens*. **A. Blackwell**, **B. O. Johnson**, A. Golonka
- 722.** Method development for metabolomic analysis of *Saccharomyces cerevisiae* by LC-MS. **S. M. Elcik**, W. C. Cory, J. L. Fox
- 723.** Determination of Enzyme Kinetics Using Electrophoretically Mediated Microanalysis. **K. J. Woodard**, L. G. Puckett
- 724.** Investigation of casein kinase II via mass spectrometry. **E. DeVlieger**, J. Hunter, L. Bedard, A. Mosley
- 725.** Solid phase extraction method for the simultaneous determination of an aminoglycoside and a glycopeptide from a

biodegradable medical implant. **P. O'Brien**, C. Quinn, S. Symes

726. Heavy metals remediation using hydrogels. **M. Connor**, A. Fields, T. Hizer, C. E. MacGowan

727. Creating a Pocket-Sized Biosensor for the Detection of Heavy Metals in Drinking Water. **B. R. Tierney, R. A. Whitaker**

728. Quantitative analysis of minerals in vitamins and fortified cereal centered on child nutrition from before birth to preteen years. **T. Brown, B. Cook**, R. Thompson, S. A. Wasileski

729. Multi-technique Quantitative Analysis and Socioeconomic Considerations of Lead, Cadmium, and Arsenic in Children's Toys/Jewelry. M. Leopold, **M. Hillyer, L. Finch**

730. Mass Spectrometry Approach to Identify MRSA Quorum Sensing Inhibitors. **D. B. Zich**, K. A. Ettefagh, D. A. Todd, H. A. Raja, N. H. Oberlies, A. R. Horswill, N. B. Cech

731. Development of an activity-based probe for cystathionine gamma lyase. **S. Bowhay**, C. M. Johnson

732. Analysis of intact proteins from gels using mass spectrometry. **A. Balius**, B. Rollins, R. Montgomery

733. Novel Biosensor for point-of-care medical diagnostics. **A. Wilkes**

734. Can variations in chromatographic peak asymmetry factors and peak retention times give insight into the dependence of DOM–surface interactions on DOM surface coverage in liquid chromatographic studies of DOM adsorption? **S. Z. Sutton**, G. Whitetree, Y. Wu, D. Kreller

735. Comparison of two analytical methods for the measurement of nitrate concentrations in standard solutions and environmental samples. **G. Prusky, M. S. Morton**, D. Carbonell

736. Synthesis and characterization of cis-disubstituted tetracarbonylmolybdenum(0) complexes with binaphthol-based chlorophosphite ligands. **R. D. Davidson**, S. D. Hastings, G. M. Gray

737. Cyclic voltammetry of carotenoids. **W. M. Potter**, A. Focsan

738. Synthesis of a Cationic Metal-Organic Solid Solutions Based on CO(II) and Zn(II) and their applications in Chromate trapping. **G. Hernandez**, H. =. Fei, S. Oliver

739. Neonicotinoids: Chemistry behind the controversy. **W. F. Davis**, J. M. Carr

740. NMR, MALDI-TOF-MS, FT-ICR and cell line studies of copper-antibiotic complexes. **R. Mikula**, A. Calvin, H. Lee, T. Manning, G. Wylie, D. Phillips, B. Bythell

741. NMR, FT-ICR, TOF-MS and Cell Line studies of novel copper-cancer complexes. **A. Calvin**, M. S. Clark, T. Manning, G. Wylie, D. Phillips, B. Bythell, F. Zhang

742. Simultaneous detection of glucose and lactic acid in flowing environments. **A. T. Harding**, A. H. Suroviev

743. Fluorescence and electrophoresis studies on lysozyme modifications induced by pbenzoquinone. **J. W. McDonald**, H. Greeve, J. Kim, T. V. Albu

744. Quantitative analysis of pesticide tank rinses for residues. **K. D. Swanson**, P. P. Osborne, L. Xu, T. Walker

745. Investigations into the preparation of NHC-ligated copper(II) acetate complexes. **K. C. Lambeth**, J. M. Carr

746. Broad survey reveals tolerance of Fe-S clusters to substitution in [NiFe] hydrogenase. **B. R. Clarkson**, I. T. Yonemoto, P. D. Weyman

747. Characterization of a customized thin layer flow cell interfaced to an ion trap mass spectrometer for electrospray ionization mass spectral studies of self-assembled monolayers. **S. K. Hartman**, A. B. Murphy, **B. W. Gregory**

748. One-pot enol silane formation-Mukaiyama aldol and Mukaiyama-Mannich reactions of ketones and thioesters. **C. M. Dombrowski**, **J. A. Ingersoll**, C. Downey

749. TMSOTf-accelerated opening of epoxides with halogens and α -hydroxylation of ketones. **A. T. Barnett**, **N. C. Yeutter**, C. Downey

Advancing Graduate Education in the Chemical Sciences

Loews Atlanta Hotel
Candler

P. Houston, *Organizer*

9:00 750. Advancing graduate education in the chemical sciences. **B. Z. Shakhashiri**

9:15 751. ACS Commission on Advancing Graduate Education in the Chemical Sciences: Overview and responses to big questions. **L. R. Faulkner**

9:40 752. Overview of the symposium and recommendations of the ACS Commission on Graduate Education. **P. L. Houston**

10:05 753. Reformation of Graduate Education in Chemistry: A 40 Years Journey The Best Predictor of Future Behavior is Past Behavior. **G. B. Schuster**

10:30 Intermission.

10:45 754. Comments on the Commission's Report from the Perspective of the National Science Foundation. **J. Ferrini-Mundy**

11:15 Panel Discussion.

Approaches to Organic Synthesis Across Disciplines

Loews Atlanta Hotel
Salon H

D. Whitehead, S. Wiskur, *Organizers*

9:00 755. Brønsted acid catalyzed enantioselective lactonization strategies. **K. S. Petersen**

9:45 756. From molasses to biogasoline: A synthetic approach. **S. Emelife**, M. Raja, C. Gwengo, B. White, L. Ambrosia

10:05 Intermission.

10:20 757. Synthesis, characterization, and photophysical properties of a novel bis(N-heterocyclic thione) (NHT's) SCS-Pd pincer complex. **G. E. Tyson**, K. Tokmic, D. Rabinovich, H. U. Valle, T. K. Hollis, C. E. Webster, J. T. Kelly, N. I. Hammer

10:40 758. Silylation-based kinetic resolutions: Substrate scope and mechanistic investigations. **S. L. Wiskur**

Synthesis, Structure, and Properties of f-element materials

f-element coordination polymers

Loews Atlanta Hotel
Inman

S. Latturmer, T. Albrecht-Schmitt, *Organizers*
C. Cahill, D. de Lill, *Presiding*

9:00 759. Supramolecular assembly of f-element hybrid materials. **C. L. Cahill**, R. G. Surbella

9:40 760. Observing the NC bridge of the actinide tetracyanometallate compounds. **B. A. Maynard**, R. E. Sykora, A. E. Gorden

10:05 Intermission.

10:15 761. Non-aqueous and high-temperature solvent synthesis and crystal growth of rare-earth metal organics and rare-earth double phosphates. **L. A. Boatner**

10:55 762. Postsynthetic rearrangement/metalation: A route to otherwise inaccessible bimetallic uranyl bearing materials. **A. T. Kerr**, C. L. Cahill

11:20 763. Examining the antenna effect within lanthanide coordination polymers. **D. T. de Lill**

Undergraduate Research Symposium

Undergraduate Keynote Speaker and Research Symposium 1

Loews Atlanta Hotel
Piedmont

N. Kirk, *Organizer*

9:00 764. Undergraduate Research Symposium Keynote Talk. Extracting Value From Patents: Lessons Learned From a Six Year Litigation. **D. C. Liotta**

9:45 Intermission.

10:00 765. Separation and detection of 19 neurochemically significant biogenic amines and acids in non-mammalian systems. **E. C. Marder**, S. Steagall, C. Dorismond, C. D. Hallman, N. J. Kuklinski

10:15 766. Synthesis and properties of silver nanoparticles formed in the presence of cationic polymers. **M. E. Booher**, B. Baruah, G. J. Gabriel

10:30 767. Investigation of Photoinduced DNA Damage by Cr(III) Complexes as Assessed by PCR, Capillary Gel Electrophoresis, and UPLC-MS. **A. G. Kantor**, T. F. Harris, J. H. Wade, Y. Álvarez-García, N. A. Kane-Maguire, S. K. Wheeler, J. F. Wheeler

10:45 768. Utilization of metathesis to achieve water solubility of nanoparticles. **L. G. Mast**, J. E. Macdonald, M. J. Turo

11:00 769. Synthesis of Large Polyacenes. **K. D. Gebhard**, S. Miao

11:15 770. Synthesis of a novel dual action cytosporone/triazole antibiotic. **A. Wimbish**, R. Murphy, S. Johnson, J. Wyatt

11:30 771. Pyrene-based organic semiconductors. **J. Ji**, S. Miao

11:45 772. Solution aggregation and polymorphism of platinum(II) bipyridine complexes. **M. H. Hudson**, R. E. Bachman*

Undergraduate Research Symposium

Undergraduate Research Symposium 2

Loews Atlanta Hotel
Chastain

N. Kirk, *Organizer*

10:00 773. Copper(I)-catalyzed azide-alkyne cycloadditions for functionalization of enzyme packaged viral nanoparticles. **R. Hincapie**, C. McKay, M. Finn

10:15 774. Determining the mechanism of periodic precipitation (Liesegang) reactions. **A. W. Bruch**, A. Sowell, J. M. Karty

10:30 775. Synthesis of hydroxy substituted indole chalcones. **C. M. Bridges**, H. L. Holt, Jr.

10:45 776. Synthesis and evaluation of biphenyltetrols as amyloid- β aggregation inhibitors. **S. L. Wicks**, J. M. Hanna, Jr.

11:00 777. Rational design of platinum complexes with enhanced nonlinear optical properties. **D. C. Yost**, K. Martin, S. Kilina, W. Sun

11:15 778. Estrogenic hormones: Their interactions with Lactoperoxidase and potential for DNA mutations. **N. M. Clark**, K. M. Matera

11:30 779. Polymer functionalization of single-wall carbon nanotubes for nano-resin water purification. **W. M. Payne**, J. E. Amburgey, J. C. Poler

11:45 780. Straightforward Synthesis of Monoarylethylenediamines - easy Access to unsymmetric N-Heterocyclic Carbene Ligands. **J. L. Gray**, H. J. Schanz

Posters: Undergraduate Research

Organic/Medicinal Chemistry

Loews Atlanta Hotel
Over Look/Exhibit Hall

V. Singh, *Organizer*

10:30 - 12:00

781. New methods for C-arylglycol construction: Suzuki-Miyaura cross-coupling of dihydropyranylphosphates. **M. Leidy**, J. M. Hoffman, R. Pongdee

782. Construction of N,N-diethylbenzamides employing a non-classical Mitsunobu reaction. **J. M. Hoffman**, J. N. Miller, M. E. Gardner, D. R. LePar, R. Pongdee

- 783.** Inhibition of Copper Thiostrepton's Oxidation of DTBC to DTBQ. **S. Herrera**, J. Moses, L. Li-June Ming
- 784.** Synthesis of glycosaminoglycans and mimics to explore binding affinity to malarial proteins. **C. J. White**, B. G. Trogden, G. Geist, K. Ferrill, J. Hogges
- 785.** Analysis of secondary metabolites in *Carpinus caroliniana* and *Ostraya virginiana*. J. A. Boudell, S. F. Hornbuckle, **J. M. Mikula**
- 786.** Catalytic homologous conjugate additions of heteroaromatic nucleophiles to electron-deficient cyclopropanes. **C. Dulin, K. Murphy**, K. Nolin
- 787.** One-pot deoxygenation of crude Grignard adducts and similar compounds. **A. P. Honeycutt, B. W. Love**, J. M. Gibson, H. V. Clontz
- 788.** Co-crystallization of the *E. coli* membrane protein intimin with engineered single chain antibody fragments. **D. P. Heaner**, S. Kalyoncu, J. Johnson, I. Morales, J. Hyun, K. Etzminger, J. C. Pai, J. A. Maynard, R. L. Lieberman
- 789.** Palladium-Catalyzed Removal of –Alloc and –OAllyl Groups in Solid Phase Peptide Synthesis Using a Microwave Synthesizer. **R. Pescatore**, B. C. Wham, S. Hutchison, E. Williamson, K. R. Wilson
- 790.** Synthesis of 2-amino-7-benzyl-6-hydroxy-7H-purin-8(9H)-one derivatives as potential inhibitors of folate requiring enzymes. **A. Jackson**, E. Brazil, R. Vaden, P. S. Ray
- 791.** Connecting halomethane analogues and Lewis bases: Sigma hole interaction trends. **M. Tawfik**, K. J. Donald
- 792.** Synthesis of small molecules as potential inhibitors of CXCR4. **G. Adodo**, K. Sarpong, S. Mooring, T. Gaines
- 793.** (BPA)RuBr(PPh₃)₂ as a multipurpose reagent: Alcohol dehydration/oxidation and alkene isomerization. **M. Sharma**, D. Chace, **B. Quillian**
- 794.** New ruthenium(II) complexes supported by bis(pyrazolyl)acetate as intermediates to olefin hydroarylation catalysts: Synthesis, characterization and structure. **M. Trivitayakhun**, B. Quillian
- 795.** Effect of Acetaminophen to Cyclodextrin Ratios in the Presence of Polymeric Excipients on Crystal Morphology. **B. Collins**, R. Wilcox
- 796.** Mechanistic investigation of the hydration of 5-oxo-1-alkynes into methyl ketones via a one-pot oxy-iodination/reduction reaction. **B. R. Jones**, W. J. Morgan, J. Trossarello, A. Egunjobi, R. Ahamed, K. S. Aiken
- 797.** Method development for the derivitization of 3-phenoxybenzyl alcohol. **M. M. Lockart**, S. A. Radford
- 798.** Reactions of benzaldehyde in boiling water with both thermal and microwave heating. **M. G. Potter, C. A. Lowder**, B. Belachew, A. Patel, K. R. Wilson, C. E. Dahm
- 799.** Catalytic transfer hydrogenation (CTH) of ketoximes with Raney nickel catalyst and 2-propanol as hydrogen donor. **K. Taylor**, R. Mebane, C. L. Keller, D. R. Zuidema, W. D. Ricketts, J. W. Groenendyk
- 800.** Synthesis of oligo-benzo[c]cinnoline ethynylene as molecular junctions. **B. R. Sands, D. N. Mitchell**, G. R. Mandouma
- 801.** Development of molecular probes for chiral sensing based on atropisomeric rhodamine derivatives. **F. M. Haque**, J. P. Romaine, C. J. Stephenson
- 802.** Polydiacetylene Liposomes Encapsulation of Trifluoroethanol and Fluoride Salts. **I. Miller**, J. Rapley, C. Wright, T. Hanks

- 803.** Ortho-alkoxylation of diaryl ketoxime ethers. **E. A. Kimball**, K. Shaughnessy, T. Snowden, F. Fronczek, J. Moore, D. D. Dolliver
- 804.** Ortho-bromination of diaryl ketoxime ethers. **S. Adhikari**, B. T. Bhattarai, K. Shaughnessy, T. Snowden, D. D. Dolliver
- 805.** Host-guest complexes of coumarin derivatives and organic dyes in a self-assembled bis-urea macrocycle. **B. A. Koscher**, S. R. Salpage, L. S. Shimizu
- 806.** Microwave Deprotection of Boc-Protected Amino Acids Under Mildly Acidic Conditions. **S. Sedberry**, M. I. Moore, K. R. Wilson
- 807.** Structure activity relationship study of phenolic antioxidants. **S. Obeng**, A. Roberts, B. Scruggs, V. J. Geisler
- 808.** Optimization of the Suzuki reaction for thiophene-containing monomers with electron-deficient coupling partners. **E. Hull**, P. Lundin
- 809.** Ring-closing metathesis reactions of novel dienes. **P. Carey**, K. Knight
- 810.** Design and synthesis of novel dual-action phthalazinone chemotherapies. **F. Claire**, B. Norton-Baker, B. Hoover, K. Klas, Y. Peterson, C. Beeson, J. Wyatt
- 811.** Regioselective synthesis of a novel bis-indene “batwing” catalyst. C. Reed, **T. Varner**, R. Himes, H. Palandoken, J. Wyatt
- 812.** Overexpression and characterization of manganese catalase from *L. plantarum*. **R. Murphy**, P. Riggs-Gelasco
- 813.** Synthesis towards IL-supported hypervalent iodine compounds. **W. B. Unthank**, T. R. Hayden
- 814.** Studies toward a convergent total synthesis of Motualevic Acids A-E. **F. A. Diaz**, **K. Black**
- 815.** Green methods for the oxidation of small ring nitrogen heterocycles. **P. L. Colasurd**, J. H. Shugart
- 816.** Development of a Sonogashira Catalyst-Transfer Polycondensation for a *Para*-substituted Monomer. **X. Powers**, P. Lundin
- 817.** Catalyst development for a Sonogashira catalyst transfer polycondensation. **K. Singer**, P. Lundin
- 818.** Benzotriazole-Mediated synthesis of symmetrical and unsymmetrical bis-2,5-diketopiperazines. **A. Nasajpour**
- 819.** Synthesis of Unusual Trifluoromethylated Amino Acids via Electrophilic Addition of 2-Methyl Azaarenes with α -Trifluoromethylimino Esters. **M. Blocker**, A. Shaikh
- 820.** Optimization of the Suzuki Coupling of Haloarenes. **J. D. Houle**, W. Medina-Ramos, C. Senter, P. Pollet, C. L. Liotta, C. A. Eckert, J. Fisk, B. Holden
- 821.** Solvent dependent regioselective hydroxy-trifluoroalkylation of indoles. **R. S. Stocking**, J. Alonzo, M. Christianson, S. Landge, B. Torok
- 822.** Cysteine modification via nucleophilic aromatic substitution. **J. Kapp**, M. Forconi
- 823.** Addition of Metal-mediated Allylic Reagents to α -Acylphosphonates to Synthesize α -Hydroxyphosphonates. **H. Khosrownia**, **M. D. Womack**, D. Kercher, J. Parr, M. Shahzad, C. W. Alexander
- 824.** Role of conserved amino acid residues in heme *a* synthase. **F. D. Esquivel**, **L. R. Penland**, O. Khalimonchuk, J. L. Fox

- 825.** Production of Biodiesel via Hydrocracking. **M. Hilliard, K. Dickens,** K. McGill
- 826.** Microwave-assisted synthesis of 4 and 4'-substituted 3,5-diphenylisoxazoles. **Y. Zhang,** S. Son, N. L. Powell
- 827.** The exploratory synthesis of glutamate lipid-derived naphthalene and perylene organogelators. **R. R. Denham,** R. E. Bachman*
- 828.** Mutagenic analysis of the oligomerization of E. coli β -glucuronidase. **G. Burchett,** K. T. Lane
- 829.** Methods for the Synthesis of α -Hydroxyphosphonates and α -Acylphosphonates. **O. Akinniyi,** J. Parr, C. W. Alexander
- 830.** Indole derivatives and their interaction with cations. **E. Nanje, S. Alexander, J. Denton, A. Arruda,** F. A. Khan, M. Fujita
- 831.** Developing strategies for the preparation of rationally designed analogs of the furanosteroid family of natural products. **D. Vogt,** B. Goess
- 832.** Synthetic strategies towards indole analogues of a Tamoxifen® metabolite. **M. Long,** M. L. Wright, H. L. Holt, Jr.
- 833.** Synthesis of bromo-substituted dipyridosiloles. **P. Hang,** P. Wei, D. M. Peloquin, T. A. Schmedake
- 834.** An approach to synthesize phenstatin analogues from azidochalcones. **J. E. Stanton,** H. L. Holt, Jr.
- 835.** Classic synthetic methods towards cyclohexene and cyclohexadiene analogues of chalcones. **C. A. Olsson,** H. L. Holt, Jr.
- 836.** Investigation of Novel Amine Dehydrogenases for the Asymmetric Synthesis of Amines. **J. Groover,** B. Bommarius, A. Bommarius, B. D. Feske
- 837.** The monofluorination of Diethyl Cyanomethylphosphonate. **D. Singleton,** T. Hizer, B. D. Feske
- 838.** Synthesis of the pharmaceutical Bepreve using biocatalysis as the key asymmetric step. **A. Casas,** B. Weaver, J. Groover, B. D. Feske
- 839.** Synthesis and Characterization of N-Heterocyclic Carbene Pincer Ligands and Their Transition Metal Complexes. **A. Puetz,** M. Callis, R. Meier
- 840.** New bounds in oxycalix[4]arene synthesis: acetylene activated S_NAr . **D. A. Harper,** J. Katz, N. Bizier
- 841.** Synthesis and characterization of doubly functionalized carbon nanotubes for removal of dissolved organics from water. **M. Saeed, A. Nguyen,** W. M. Payne, J. E. Amburgey, J. C. Poler
- 842.** Metalloradical catalyzed N=N bond formation with fluoroaryl azides: A new approach to the synthesis of fluoroazobenzene compounds. **T. N. Arzua,** L. Jin, P. Zhang
- 843.** Synthesis, characterization, and reactivity of p-cymene ruthenium(II) complexes with fluorine-containing phosphine ligands. **A. D. Riner,** J. P. Lee
- 844.** Exploring initial reactions with a chiral N,O,O based ligand in transition metal cluster chemistry. **K. Warren,** B. K. Long, A. Saha
- 845.** Revisiting valinomycin: effect of water on the conformation of valinomycin-cation complex. **A. Kazerouni,** A. Contractor, F. A. Khan, M. Fujita

- 846.** Exploring the Chlorination of Diethyl cyanophosphonate. **A. Dykes**, T. Hizer, B. D. Feske
- 847.** Ditopic N-heterocyclic carbene ligands: 9,10-anthracene linked imidazolylidenes. **A. A. Kellum**, A. Mangalum, **A. G. Tennyson**
- 848.** Trans-chelating N-heterocyclic carbene ligands: Dialkyl-amine linked benzimidazolylidenes. **A. C. Rollings**, A. Mangalum, Y. Htet, **A. G. Tennyson**
- 849.** Development of Brønsted acid catalyzed intramolecular imino-ene reaction. **M. Putri**, L. Davis
- 850.** Reactions of unexpected nucleophiles with aldehydes: acetate-catalyzed additions by α -silyl nitriles and TMSOTf-catalyzed additions by indoles. **C. J. Mueller**, **A. N. Nizinski**, C. Downey
- 851.** Zinc acetylides in the presence of TMSOTf: Addition to nitrones and alkylation with methyl ethers. **E. N. Maxwell**, **D. C. Obenschain**, C. Downey

FRIDAY AFTERNOON

Approaches to Organic Synthesis Across Disciplines

Loews Atlanta Hotel
Salon H

D. Whitehead, S. Wiskur, *Organizers*

1:00 852. Recent progress in alkaloids synthesis. **V. H. Rawal**

1:45 853. New ligand space through novel hydrophosphinations. **C. Busacca**

2:30 Intermission.

2:45 854. New synthetic methods as an entrée to biological discovery. **S. E. Schaus**

3:30 855. Synthesis of chiral allylboron and enolborane reagents via allene and acrylamide hydroboration reactions, and applications to the synthesis of natural products. **W. R. Roush**

4:15 Concluding Remarks.

CHED Chemistry Education General Session

Loews Atlanta Hotel
Ardmore

M. Koether, *Organizer, Presiding*
M. Dean, *Presiding*

1:00 856. Impact of the Chemistry Scholars Program at UNC Asheville on recruitment and retention of majors and department culture. **S. A. Wasileski**, J. M. Schmeltzer, H. Holt

1:15 857. Best practices in undergraduate supplemental instruction in STEM disciplines. **C. H. Lisse**, **R. A. Richards**, J. Haslam, M. H. Gleason, M. H. Chiorescu, L. A. Buttitta

1:30 858. Alternative method to enhance student performance and retention in STEM majors at Georgia Perimeter College. **J. Lee-Joyner**, **A. Steinau**, I. Ricketts

- 1:45 859.** Use of problem solving to elicit self-explaining in General Chemistry. **A. Villalta-Cerdas**, S. Sandi-Urena
- 2:00 860.** Online homework with targeted instructional feedback leads to improved student learning outcomes. **J. E. Bara**
- 2:15 861.** In-class demonstrations by students enhance learning in general chemistry course. **P. M. Todebush**
- 2:30 862.** Approach to flipping the classroom to enhance student participation in large chemistry courses. **M. Lewis**
- 2:45 863.** Enhancing student understanding of intermolecular interactions using surface wetting lecture demonstrations. M. A. Luckey, P. W. Alexander, **W. A. Alexander**
- 3:00** Intermission.
- 3:30 864.** Improving student learning outcomes in general chemistry using a First-Year Chemistry Wizard program: Three years of assessment. **M. Kendrick-Murphy**, D. D. Jackson
- 3:45 865.** Understanding the obstacles to incorporation of graphing and graphing-related mathematics into the general chemistry curriculum. **D. W. Carpenetti II**, A. Woofter, Z. B. Snead, H. N. Tran, M. Weber
- 4:00 866.** Engaging general chemistry students with POGIL and climate change. **G. H. Webster**, D. King, J. E. Lewis, K. Anderson, D. Latch, S. Sutheimer, C. Middlecamp, R. Moog
- 4:15 867.** Tales from the other side of the podium: How to use a flipped classroom model to increase student learning and engagement in organic chemistry. **K. Daus**
- 4:30 868.** Use of RateMyProfessors.com as a supplemental tool for the assessment of General Chemistry instruction. **S. Sandi-Urena**, **P. McKeny**, **A. Villalta-Cerdas**, A. Bergin, K. Sharp, T. Gatlin, A. Gower
- 4:45 869.** Chemistry in Berlin, Germany - a study abroad program experience for majors. **R. Fietkau**

Computational Chemistry General Session

Loews Atlanta Hotel
Salon G

A. DePrince, *Organizer, Presiding*

- 1:00 870.** Calculation of standard enthalpies of formation. 1 Hydrocarbons. **R. Bacaloglu**, L. Cotarca
- 1:20 871.** Explaining the stabilities of fullerene anion isomers: The aromatic pentagon. **T. J. Fuhrer**, H. Dorn
- 1:40 872.** New structural framework for integrating replication protein A into DNA processing machinery. **C. Yan**, C. A. Brosey, I. Ivanov, W. J. Chazin
- 2:00 873.** Anisotropy in the Debye-Waller factor of hcp solid ^4He . **A. L. Barnes**, R. Hinde
- 2:15 874.** Computational insights for the AlkD base extrusion strategy. **B. Kossmann**, I. Ivanov
- 2:30** Intermission.
- 2:40 875.** Spin-orbit transitions of halogen atom dopants in solid parahydrogen matrices. **R. Hinde**
- 3:00 876.** Characterization of a stripe liquid crystal phase in simple binary water solutions. **T. D. Shepherd**, M. Parry, R. Okumu, V. Molinero

3:20 877. Roaming trajectories in a reduced-dimensional model of ketene. **I. S. Ulusoy**, J. F. Stanton, R. Hernandez

3:40 878. Opening pathways of the DNA clamps proliferating cell nuclear antigen and Rad9-Rad1-Hus1. **X. Xu**

3:55 879. Density functional calculations of an inhomogenous ^4He system. **M. Dutra**, R. Hinde

4:10 Intermission.

4:20 880. Computational investigations of the hyperpolarizabilities of saccharin, phthalimide, and related molecules and their fluorinated analogs, anions, and salts. **D. A. Clabo, Jr.**

4:40 881. Computational investigation of substituted benzene-pyrene binding. **S. Wireduaah**, L. K. Hardebeck, J. Coleman, D. Rucker, R. M. Love, M. Lewis

4:55 882. Estimating non-additive three body effects on the lattice energy of crystalline benzene. **M. R. Kennedy**, A. R. McDonald, M. S. Marshall, R. Podeszwa, C. D. Sherrill

5:10 883. Density-fitted singles and doubles coupled cluster theory on graphics processing units. **E. DePrince**, D. Sherrill

Environmental Chemistry General Session

Loews Atlanta Hotel
Candler

A. Suroviec, *Organizer, Presiding*

1:00 884. Neighborhood chemistry: Combining undergraduate research, analytical chemistry and service learning to understand local environmental issues. **J. L. Look**

1:15 885. Thermal Stability and Pyrolysis of Powdered and Powder-Free Laboratory Examination Waste Gloves. **N. Hamidi**, R. Massoudi, S. Shrestha, L. Lalmansingh, T. Pascoe, C. Oriakhi, L. Whitesides

1:30 886. Photochemical Degradation and Environmental Fate of Pharmaceutically Active Compounds in Simulated Natural Water Samples. **W. Cory**

1:45 887. Conversion of iodide to hypoiodous acid and molecular iodine at the air-water interface. **M. I. Guzman**, **E. A. Pillar**

2:00 888. Photolysis of 2-oxopropanoic acid: A study of intermediates and products. **A. J. Eugene**, S. Xia, **M. I. Guzman**

2:15 889. Intermediates and products of the photolysis of 2-oxopropanoic acid. **A. J. Eugene**, S. Xia, **M. I. Guzman**

2:30 890. Insecticides and insecticide degradates present in baby foods: Implications for risk assessment. **S. A. Radford**, P. Panuwet, R. E. Hunter, B. Ryan, D. B. Barr

2:45 891. Soil Quality Analysis Using Qualitative and Quantitative Analytical Methods. **S. C. Miller**

3:00 Intermission.

3:15 892. Molecular dynamics simulation in comparison of efficacy of cationic organic polyelectrolyte and dual polyelectrolyte systems in drinking water coagulation. **S. Park**, Y. Choi, H. Lee, S. Jang

3:30 893. Predicting organic carbon chromatograms and monitoring adsorptive fractionation using dual-wavelength UV

absorbance detection in liquid chromatographic studies of dissolved organic matter adsorption. **D. Kreller**, Y. S. Wu, S. Sutton, G. Whitetree

3:45 894. Does the method of predicting [DOC] from UV absorbance at two wavelengths work in liquid chromatography? **G. Whitetree**, S. Sutton, Y. Wu, D. Kreller

4:00 895. Measuring a UV-VIS absorption spectrum of aerosols and greenhouse gases using a photoacoustic spectrometer. **J. R. Wiegand**

4:15 896. Incoherent broadband cavity enhanced spectroscopy for measuring extinction coefficients of atmospheric species throughout the UV-visible spectrum. **D. A. Fischer**, G. D. Smith

4:30 897. Retrieval of Complex Refractive for an Absorbing Aerosol Binary Mixture Using Cavity Ringdown Spectroscopy at 355nm. **K. Schuldt**

4:45 898. Origin of optical absorptivity in brown carbon aerosols. **S. Phillips**

Materials Chemistry General Session

Chemistry of Materials

Loews Atlanta Hotel
Pittman

B. Baruah, *Organizer*
I. U. Arachchige, *Presiding*

1:00 899. Controlling the Interfacial Junction Properties of Hybrid Organic/Inorganic PEDOT:PSS / n-, p-, and n⁺-Si Devices for Solar Energy Conversion Applications. **M. G. Walter**

1:15 900. Photoinduced Inter-Cavity Electron Transfer between Ru(II)tris(2,2'-bipyridine) and Co(II)tris(2,2'-bipyridine) Co-Encapsulated within a Zn(II)-Trimesic Acid Metal Organic Framework. **R. W. Larsen**, L. Wojtas

1:30 901. Crystal-bound vs. surface-bound thiols on semiconductor nanoparticle surfaces: achieving water solubility and charge transfer properties. **M. J. Turo**, J. E. Macdonald

1:45 902. Small molecule organic dye synthesis and design based on ullazine for Dye Sensitized Solar Cells. **J. Delcamp**, A. Yella, M. Nazeeruddin, M. Grätzel

2:00 903. Introducing New Fully-Integrated TGA-GC-MS and TGA-FTIR Systems for Characterization of Materials Including Polymers, Biomass and More. **T. Doll**

2:15 904. Increased efficiency of gold conversion via a re-seeding approach. **J. W. Stone**, S. Canonico-May, K. Beavers, C. Duvall

2:30 905. Bio-based materials to synthesize a novel surfactant in the production of polyurethane foams. **B. S. Snyder**, N. Tonks

2:45 Intermission.

2:55 906. New Materials Based on Cellulose and Natural Biopolymers. **R. Kotek**, R. Boy

3:10 907. Drug delivery polyurethane materials using bio-based polyols. **N. J. Adamson**, N. Tonks

3:25 908. Self-healing microgel coatings. **M. W. Spears Jr.**, L. Lyon

- 3:40 909.** Non-Ordered Metal Hollow Particle Superstructures: Metal Aerogels. T. H. Luong, X. Gao, K. G. Ranmohotti, **I. U. Arachchige**
- 3:55 910.** Lignin Extracted from Black Liquor for Composite and Pellet Binder Applications. M. Smith, B. McCluskey, **R. L. Quirino**
- 4:10 911.** Flavones with liquid crystal properties. **D. J. Timmons**, A. J. Jordan, A. M. Gernhardt, T. A. Bradshaw
- 4:25 912.** Interfacial phenomena in glass fiber – polymer composites. **N. M. Tambe**, J. P. Rust, R. E. Gorga, J. Willoughby
- 4:40 913.** Microwave approach to ultrafast synthesis of nanomaterials. **X. Zhang**
- 4:55 914.** Cotton-derived fillers as reinforcing agents in thermoplastic films and fibers. **N. Farahbakhsh**, J. Jur, R. Venditti
- 5:10 915.** Anisotropic growth of metallic nanocrystals by high frequency mechanical stirring. **M. Mahmoud**, M. El-Sayed, U. Landman

Nanochemistry and Spectroscopy: Symposium Honoring Mostafa El-Sayed

Loews Atlanta Hotel
Salon I

Z. Zhang, *Organizer*
P. Wine, *Organizer, Presiding*
R. Dickson, *Presiding*

- 1:00 916.** Multifunctional mesoporous inorganic nanoparticles controlled by nanomachines for *in vitro* and *in vivo* drug delivery. **J. I. Zink**
- 1:40 917.** A gold-rich heterogeneous catalyst controlled at the atomic level. **W. Huang**, C. Xiao, L. Wang, R. V. Maligal-Ganesh, V. Smetana, H. Walen, P. A. Thiel, G. J. Miller, D. D. Johnson
- 2:00 918.** Hollow metallic nanoparticles in nanocatalysis: High catalytic efficiency and studying the mechanism of the solution catalysis. **M. Mahmoud**, M. El-Sayed
- 2:20 919.** Protein nanoparticles with catalytic function. J. D. Fiedler, J. Cheng, M. Hovlid, C. Scheibe, S. D. Brown, **M. Finn**
- 2:40 920.** Ionic Rectifier Based on Carbon Nanotube Membranes. B. Patel, M. Patel, M. Bassett, S. Landge, **J. Wu**
- 3:00** Intermission.
- 3:20 921.** New developments in the synthesis of colloidal noble-metal nanocrystals. **Y. Xia**
- 4:00 922.** Silver Atom Doping to Ultra-Small and Plasmonic Gold Nanomolecules. **C. Kumara**, D. Cullen, A. Dass
- 4:20 923.** Transformation of Ag nanocubes into Ag-Au hollow nanostructures with enriched Ag contents to improve SERS activity and chemical stability. **D. Qin**, Y. Yang
- 4:40 924.** Nanoparticles Immobilized on Cellulose Fibers: SERS Substrate and Catalytic Reaction. **B. Baruah**

Perspectives in Undergraduate Forensic Chemistry Education

Loews Atlanta Hotel
Dunwoody

H. Msimanga, C. Dockery, *Organizers, Presiding*

1:00 925. Perspectives in Undergraduate Forensic Chemistry Education. **Z. Oommen**

1:30 926. Multivariate analysis techniques in teaching forensic analytical chemistry at the undergraduate level. **H. Z. Msimanga, C. R. Dockery**

2:00 927. Introductory and advanced forensic chemistry. **W. E. Brewer**

2:30 928. From classroom to laboratory: Creating an effective transition for scientists. **D. Wallace-Duckworth**

3:00 Intermission.

3:15 929. Forensic toxicology education. **O. A. Vanderpuye**

3:45 930. Development of specialty courses on forensic toxicology and forensic microscopy. **L. G. Puckett**

4:15 931. The CSI effect on college curricula: Educational considerations for scientists entering the field of forensics. **R. J. Ollis**

4:45 Panel Discussion.

NanoElectrochemistry in Biomedical Research and Energy Technology

Energy/Materials

Loews Atlanta Hotel
Centennial

L. Bottomley, *Organizer*
J. Stickney, G. Wang, *Organizers, Presiding*

1:30 932. Toward a new generation of solid oxide fuel cells: Recent progress, challenges, and perspectives. **M. Liu**

2:10 933. Polypyrrole/Poly(4-Styrenesulfonic Acid) Supercapacitor Electrodes for Energy Storage Applications. **K. P. Diaz-Orellana, M. E. Roberts**

2:30 934. Transient Ion Transport Against Concentration Gradient through Conical Nanopipettes. **G. Wang, Y. Li, D. Wang, M. Kvetny, W. Brown**

3:00 Intermission.

3:15 935. Evidence for the electrochemical formation of Germanene. **J. L. Stickney, M. Ledina, B. Perdue**

3:45 936. Dimension dependent near-surface phase transitions in Pt and their effect in electrocatalytic properties. **F. M. Alamgir, A. Vitale**

4:15 937. Carbon and Doped Titania Catalyst Supports for Resilient Electrochemical Cells. **W. A. Rigdon**

Synthesis, Structure, and Properties of f-element materials

f-element materials: theory and applications

Loews Atlanta Hotel
Inman

S. Lattuner, *Organizer*

T. Albrecht-Schmitt, *Organizer, Presiding*

1:30 938. New directions in the molecular chemistry of high valent uranium and cerium. **E. J. Schelter**

2:10 939. Synthesis and characterization of holmium and dysprosium containing garnet nanoparticles for radiotherapy. **K. Balkus**, I. Munaweera, A. DePasqua, Y. Shi

2:40 Intermission.

2:55 940. Probing actinide bonding using multiphoton excitation and photoelectron spectroscopy. **M. C. Heaven**

3:35 941. Lanthanide-based nanomaterials with improved luminescence properties for potential biomedical applications. **C. R. De Silva**, G. Attanayake, A. N. Darsanasiri, M. Clark

Undergraduate Research Symposium

Undergraduate Research Symposium 3

Loews Atlanta Hotel
Piedmont

N. Kirk, *Organizer*

1:30 942. Synthesis of benzisoxazolo[2,3-*a*]quinoxalium tetrafluoroborates. **J. R. Murakami**, J. M. Hanna, Jr.

1:45 943. Alpha synuclein aggregation regulation in vitro by DL-norepinephrine in Parkinson's disease. **A. F. Fischer**, K. Matera

2:00 944. Synthesis and biological evaluation of a series of potential anticancer phthalazinone agents designed utilizing a novel 2D-QSAR model. **B. Norton-Baker**, K. Klas, B. Hoover, Y. Peterson, C. Beeson, J. Wyatt

2:15 945. Comparative Study of Gold Nanoparticle Structure Modifications Induced by Aggregation Reagents. **E. Stafford**, S. M. Ansar, D. Zhang

2:30 946. Modeling lactate dehydrogenase enzyme kinetics with temperature jump spectroscopy. **K. Panwar**

2:45 947. Effect of the hydrophobic environment on the retro-aldol reaction: Comparison to a computationally-designed enzyme. **J. Schmidt**, C. Ehasz, M. Epperson, M. Forconi

3:00 Intermission.

3:30 948. Aromatic organothiols interactions with silver nanoparticles in water. **G. E. Salomon**, S. Ansar, D. Zhang

3:45 949. Towards quantum information in a cryogenic ion trap. **K. A. Burkhardt**

4:00 950. Energetic contribution of poly(C) binding protein-2 (PCBP-2) in the formation of the i-Motif. **C. R. Funk**, Y. Bhavsar-Jog, R. M. Wadkins

4:15 951. Computational analysis of water...2-aminopyrimidine hydrogen bonding interactions with protein kinase

GSK-3 β . **L. E. Jobe**, K. M. Elokely, R. J. Doerksen

4:30 952. Synthesis, purification and analysis of novel "zone 4" sphingosine kinase-1 inhibitors. **L. Mount**, T. Grattan

4:45 953. A menthol-derived synthon for preparing homoallylic alcohols bearing three contiguous elements of stereochemistry. **N. A. Ochs**, K. Carroll, F. E. McDonald

5:00 954. Synthesis and morphology of NiO and CoO nanoplate - carbon nanotube materials for energy storage. **D. Brokaw**, J. C. Poler

Undergraduate Research Symposium

Undergraduate Research Symposium 4

Loews Atlanta Hotel
Chastain

N. Kirk, *Organizer*

1:30 955. Spectroscopic characterization of class Ib ribonucleotide reductases. **B. Keenan**, C. Seacrist, J. Cotruvo, J. Stubbe, P. Riggs-Gelasco

1:45 956. Characterization of copper (I) binding thermodynamics to small molecules. **D. Johnson**, N. Grosseohme

2:00 957. Effects of zinc and clioquinol on oligomerization of Alzheimer's amyloid- β peptide. **K. McLaurin**, E. Amenson, A. Bradner, M. Humphrey, R. K. Lammi

2:15 958. Molecular Docking Studies of Novel Flavonoid Derivatives as Acetylcholinesterase Inhibitors. **O. M. Newman**

2:30 959. Effects of aflatoxin B1 on Jurkat T-cell function. **L. E. Sutherland**, T. Laakko Train

2:45 960. Utilizing heat capacity to understand the competition between netropsin and A/T hook for DNA. **C. Quandt**, A. Gorenssek, K. L. Buchmueller

3:00 Intermission.

3:30 961. Circular Histone H4 peptides as novel epigenetic enzyme inhibitors. **J. Truong**, L. Yan, Y. G. Zheng

3:45 962. Insight Into the Hydrophobic Effect by ^1H NMR Analysis of the Hofmeister Series. **R. S. Carnegie**, C. L. Gibb, B. C. Gibb

4:00 963. Synthesis and biological activity of hibiscone C. **D. P. Rhinehart**, B. C. Goess, J. S. Rawlings

4:15 964. Spin crossover in Fe(II) complexes with dicyanometalate bridging ligands. **A. Arroyave**, O. Hietsoi, H. Stout, C. Achim, M. Shatruk

4:30 965. Progress towards "brilliant" materials: Iron core, gold shell nanoparticles with engineered optical, magnetic, and biological functionality. **B. Rittgers**, T. Jewett, D. A. Stuart

4:45 966. ROMP Monomers and Polymers Containing a Primary Amino Functionality. **M. E. Mullens**, H. J. Schanz

5:00 967. ROMP Polymers Containing Organic Radicals for Treatment of Traumatic Brain Injuries. **C. H. Feriante**, H. J. Schanz

Posters: Undergraduate Research

Material/Polymer/Biochemistry

Loews Atlanta Hotel
Over Look/Exhibit Hall

V. Singh, *Organizer*

2:00 - 3:30

- 968.** Synthesis of Alginate/Conducting Polymer Composites for Fabrication of Tissue Scaffolds. **T. Pannell**, C. Yore, C. Wright, B. Zhang, T. Hanks
- 969.** Polymer Impregnation of Graphite Rods for Reducing Interfacial Capacitance. **A. B. Reed**, S. E. Creager
- 970.** Toward new inorganic/organic conjugate dyes for solar harvesting. **S. A. Parks**, R. E. Bachman*
- 971.** Double walled carbon nanotube and graphene bilayer models for a general representation of carbon nanoporosity and molecule-surface binding energies. **H. W. Cho**, J. H. Son, T. R. Rybolt, C. R. Funk, M. J. Rice, H. E. Thomas
- 972.** Synthesis of Boronate Ester-Linked Polymers of Intrinsic Microporosity (PIMs). **A. D. Santilli**, L. M. Lanni
- 973.** Influence of Planar Organic Electrochemical Transistor Device Geometry in the Characterization of Barrier Tissue. **K. Margita**, M. Ramuz, G. Malliaras
- 974.** Measuring thermodynamic properties of recyclable materials. **R. Redmond**, M. T. Knippenberg, C. J. Fowler
- 975.** Studies on Polymer Coated Magnetite for Drug Targeting. **B. N. Louthen**, R. D. Wilcox
- 976.** AB block copolymers via click reactions using an unsymmetrical bisazide linker. **M. E. Booher**, Z. Yuan, Q. J. Meisner, L. Zhu, G. J. Gabriel
- 977.** Phosphonated cationic polymers with flame-resistant properties. **K. B. Nottke**, G. J. Gabriel
- 978.** Synthesis and optimization of multifunctional, upconverting nanoparticles. **A. D. Marsh**, B. Langloss, J. Stecher, M. Therien
- 979.** Progress towards the synthesis of an enhanced donor-acceptor nanotubular assembly. **A. Seal**, A. H. Coffman
- 980.** Synthesis and Characterization of Phosphonated Bisphenol A as a Precursor for Proton Exchange Membranes in Fuel Cells. **M. C. Boyer**, K. Reid, N. Arnett
- 981.** Synthesis of Bisphenol-A Tetrachlorocyclotriphosphazene (BATCCP) from Bisphenol-A and Hexachlorocyclotriphosphazene: The Effect of Reaction Solvent. **S. E. Davies**
- 982.** Cellular binding of anionic gold nanoparticles as a function of surface modification. **C. Thompson**, C. Fleischer, C. Payne
- 983.** Study of the effects of chemical etchants on the quality of silver nanowires grown on periodically poled lithium niobate. **J. C. Snow**, J. M. Schmeltzer, J. R. Perkins
- 984.** Freestanding semi-flexible composite carbon nanofiber oxide films using functionalized carbon nanotubes and polyvalent crosslinking ions. **C. Blanco**, G. Lee, J. Liu

- 985.** Nanoparticle film assemblies as interfaces for electrochemical biosensing: Factors affecting the amperometric signal enhancement of hydrogen peroxide. **A. R. Schmidt**, N. D. Nguyen, M. C. Leopold
- 986.** Interfacial polymerization of bisphenol A tetrachlorocyclotriphosphazene monomers to synthesize poly (arylene ether sulfone) hybrid copolymers. **J. Robertson**, T. Thompson, N. Y. Arnett
- 987.** Attack Move—Attract: Electrostatic Interactions Between Small Molecules and Charged Peptide Self-Assemblies. **R. C. Brooks**, N. Xiang, An Li, A. K. Mehta, D. G. Lynn
- 988.** Tuning Iodine Content in Poly(epsilon-caprolactone): Synthetic Hydroxylamines for Grafting. **L. L. Davis**, S. E. Nicolau, C. C. Duncan, B. A. Van Horn
- 989.** Synthesis and Characterization of Coordination Polymers with Long Nitrogen Donor Ligands. **A. Ransom**, L. Peterson, K. Fullard, J. Kelley
- 990.** Tuning Iodine Content in Poly(epsilon-caprolactone): Optimization of the polymer synthesis. **S. E. Nicolau**, L. L. Davis, C. C. Duncan, B. A. Van Horn
- 991.** Donor-Acceptor Behavior of Benzobisazole Cruciformic Polymers. A. L. Tomlinson, **K. Morgan**, **C. Collins**
- 992.** Quantum yields for one- and two-photon cycloreversion of a photochromic molecular switch. **S. L. Allen**, A. L. Houk, C. G. Elles
- 993.** Investigating cellular death mechanisms in response to targeted gold and silver nanospheres. L. A. Austin, **S. Ahmad**, M. Mahmoud, M. A. El-Sayed
- 994.** Visible-Absorbing Phosphonium Polyelectrolytes: Synthesis, Ion-Exchange, Photophysics and Film Morphology. **C. R. Powell**, C. A. Conrad, A. A. Buel, R. C. Smith
- 995.** Surface Modification with Phosphonium Polyelectrolytes. **K. M. Jolly**, C. A. Conrad, A. A. Buel, R. C. Smith
- 996.** Conjugated Polymers and Small-Molecule Chromophores Featuring the 1,4-fluorenylene Linker. **S. J. El Homsy**, M. K. Burdette, B. J. Laughlin, J. Ma, B. E. Levy, A. G. Tennyson, R. C. Smith
- 997.** Stimulating the imagination: A green tech, deep ocean retrieval system. **C. Moncrief**, E. Haas, E. A. Atkinson, D. F. Law, B. Little, C. D. Northcutt, R. Langford, H. F. Lee, G. A. Jackson, N. Fight, J. L. Lippincott, T. Manning
- 998.** Synthesis of Halogen Bond Donors for Iodine Transport in Iodine-Rich Electrolytes. **A. Kropilak**, S. Creager, W. Pennington, T. Hanks
- 999.** Controlled Zwitterionic Polymer Growth on Conducting Polymer Films. **L. Pendleton**, T. Hanks
- 1000.** Molecular engineering of aquaporin to improve stability. **T. A. Combs**, C. Ye, Y. Wei
- 1001.** Determination of the photoproducts of amphiphilic cyanine dyes in monomeric and aggregated forms. **R. Kozlowski**, J. Womick
- 1002.** Phenylketonuria: An indication of end stage renal disease. **R. E. Dunn**, S. R. Whitson, M. F. Santiago
- 1003.** Preliminary results for the crystallization of the yeast aldo-keto reductase family member YDL-124w. **W. Mojadedi**, Y. Nguyen, M. H. Weiland
- 1004.** Characterization and Determination of Inhibitor Interaction with *Streptomyces griseus* Aminopeptidase. **L. Vang**, J. Moses, L. Ming
- 1005.** Antimicrobial secondary metabolites from endophytic fungal isolates of Goldenseal (*Hydrastis canadensis*). **J. M.**

Egan, A. Kaur, A. R. Brown, H. A. Raja, N. H. Oberlies, N. B. Cech

- 1006.** Progress towards the synthesis of a pyrimidodiazepine-based folate as a potential inhibitor of glycinamide ribonucleotide formyltransferase. **A. Gann, L. Gonzalez, P. S. Ray**
- 1007.** Investigations into the incorporation of 5'-triphosphate-8-oxo-2'-deoxyguanosine (OdGTP) and related analogues with polymerase RB69. **A. M. Weaver, M. Hamm**
- 1008.** Investigation of the incorporation efficiency of OdGTP and its analogues opposite dC and dA with polymerase BF. **K. Alexander, M. Hamm**
- 1009.** Targeted DNA endonucleases promote degradation of Epstein-Barr Virus oriP containing episomes. **A. V. Kornepati, E. M. Kennedy, A. L. Mefferd, H. P. Bogerd, B. R. Cullen**
- 1010.** Synthesis of novel universal fluorescent DNA nucleosides. **A. C. Gaspard, L. O. Davis, A. Hearn**
- 1011.** Examinations of the Incorporation of 8-Oxo-2'-deoxyguanosine with the A-family Polymerase Klenow Fragment. **J. Capalbo, M. Hamm**
- 1012.** Study of the binding thermodynamics between DNA and two quinolone antibiotics using isothermal titration calorimetry. **J. Singh, S. I. Kuriyavar, H. Fan-Hagenstein, U. Kalapathy**
- 1013.** Investigating protein interactions of the enzyme OGA. **K. C. Cotto, R. A. O'Keefe, G. G. Crawford**
- 1014.** Interactions between creatinine and serum albumin: a study of free and bound nitrogenous uremic toxins. **S. A. Harris, S. R. Whitson, M. F. Santiago**
- 1015.** Purple Urine Bag Syndrome: Regulation of Pyrimidine Enzymes by Tryptophan. **A. N. Broadway, M. F. Santiago**
- 1016.** Expression and purification of the bovine leukemia virus (BLV) polyprotein Gag. **B. L. Boleratz, D. F. Qualley**
- 1017.** Towards the synthesis of a tripyrromethane derivative mimicking the active site of coenzyme F430. **C. M. Crooks, N. Klann, A. E. Gorden**
- 1018.** Tat-specific factor 1's role in insulin signaling. **J. Pearson, L. Fritts, M. Zupp, H. Miller**
- 1019.** Mechanistic insights into small-molecule inhibitors of amyloid- β aggregation. **K. Carden, J. M. Hanna, Jr., R. K. Lammi**
- 1020.** Synthesis and characterization of disulfonated Bis[4-(3-aminophenoxy)phenyl] sulfone polyamide copolymers for proton exchange membrane fuel cells. **K. Luitel, J. Poland, A. Aaron, N. Y. Arnett**
- 1021.** SdsA1: A true alkylsulfatase? **K. Morgenstern, C. Shea, N. Adamson, A. Zierk, J. Holt, M. Forconi**
- 1022.** Chemical modification of a computationally-designed enzyme. **K. Diederich, C. Teichman, J. Schmidt, M. Forconi**
- 1023.** Geometric Shifts in the Zn²⁺ Chelating Pocket of the ZN-1 Domain within *E. coli* LeuRS Contribute to the Stabilization of Adenylate. **K. E. Polivka, R. A. Whitaker**
- 1024.** Study of RNA binding to Matrix Domain of *Gag* protein in Bovine Leukemia Virus. **A. Rimer, D. F. Qualley**
- 1025.** OGA, the O-GlcNAc cleaving enzyme, displays concentration dependent specific activity. **K. A. Brown, G. L. Crawford**

- 1026.** Investigating growth conditions for a biosurfactant producing *Bacillus* strain. **M. P. Fanning**, K. D. Kloepper, G. L. Crawford
- 1027.** Tetrahydrodipicolinate N-succinyltransferase (DapD) from *Mycobacterium Bovis*: Overexpression and purification. **D. Osula**, C. M. Johnson
- 1028.** Synthesis and screening of small molecules as Tumor Necrosis Factor α inhibitors. **S. Bentil-Owusu**, **E. Vallery**, **D. McClain**, **C. Needham**, L. McNulty, **N. East**, N. K. Kobritz, M. E. Harris-White, S. P. Gabbita, **S. Varadarajan**
- 1029.** Development of Novel Mitochondrially-Targeted Electrophilic Compounds as Potential Anti-Metastatic Drugs in Breast Cancer Cells. **H. Golzarian**, P. Vayalil, A. Landar, S. E. Velu
- 1030.** Biocatalytic reduction of a non-aromatic nitro group by a nitroreductase from *Salmonella typhimurium*. T. Reams, **R. Oliff**, J. Park, A. Bommarius, B. D. Feske
- 1031.** A Biocatalytic Approach to Synthesizing lactones. **E. Branch**, R. Watkins, S. Franz, B. Weaver, B. D. Feske
- 1032.** Synthesis of citric acid cycle intermediaries from diketopiperazines. **J. Crowetipton**, G. Springsteen
- 1033.** Characterizing Substrate-Specificity in the Aldo-keto Reductases, YHR104w and YOR120w. **C. Poole**, S. C. Mateer
- 1034.** Withdrawn.
- 1035.** Probing the promiscuity of polyketide biosynthesis with non-natural polyketide building blocks. **M. M. Draelos**, I. Koryakina, J. McArthur, S. Randall, E. M. Musiol, D. C. Muddiman, T. Weber, G. J. Williams
- 1036.** Equilibrium binding of the uremic toxin *p*-cresol to serum albumin. **J. A. Kennedy**, M. F. Santiago, S. R. Whitson
- 1037.** Structural and energetic characterization of an ethidium-DNA adduct. **M. K. Longmire**, D. Graves
- 1038.** Future of iron drug therapy: Synthetic vs. protein. **R. M. Majors**, A. M. Laufer, C. M. Davis McGibony

Posters: Chemical Education

Loews Atlanta Hotel
Over Look/Exhibit Hall

D. Sherrill, *Organizer*

4:00 - 5:30

- 1039.** Chemistry anxiety, attitudes, and self-efficacy in high school students. **P. W. Rose**, V. M. Chabalengula, F. Mumba
- 1040.** Adopting ACS exams as assessment tools. **M. R. Nelson Jr.**, P. Roessle
- 1041.** Students as Enzymes: An interactive activity to introduce enzyme kinetics. E. A. Shugart, P. L. Colasurd, **J. H. Shugart**
- 1042.** Organic chemistry students' knowledge structures of fundamental general chemistry topics: Lewis structure and bonding. **N. L. Burrows**, S. Mooring
- 1043.** A model for a sophomore level research class. **H. V. Clontz**, K. R. Wilson, C. E. Dahm

- 1044.** Peer-Led Tutoring for Principles of Chemistry II at Georgia Perimeter College. **A. Cook**
- 1045.** Testing of Stormwater Runoff Water Quality in Baldwin County. **D. D. Norby**, C. Lisse
- 1046.** Using short focused research projects to engage science majors at a two year institution. **M. Trani, V. Mativo**, P. Pedroso
- 1047.** Guided inquiry experiments for physical chemistry: The POGIL-PCL project. **R. M. Whitnell**, S. S. Hunnicutt, A. Grushow
- 1048.** Preliminary Assessment of Changes in Quantitative Chemistry Knowledge and Attitudes Following a Summer STEM Enrichment Program for College Freshman at a Liberal Arts College. **A. D. Gibson**, M. Siopsis
- 1049.** Green Knoevenagel–Doebner reaction using microwave and catalysis: Study of substrate scope and limitations. **K. Banerjee**, P. Hao, **R. Patel**, B. Bill, **K. Olson**, **M. Johnson**, J. B. Gray, H. Madamidola, **D. Hieber**
- 1050.** Sol-gel Encapsulated Horseradish Peroxidase. **B. Ottoson**
- 1051.** Customizing the synthesis of aspirin: An inquiry study into the esterification reaction requirements. **F. M. Burke**, D. Patel
- 1052.** Direct perspective: Undergraduate participation in experiment development. **L. Mandeltort**, J. D. Gorden
- 1053.** Computational investigation of a biomimetic model of acireductone dioxygenase. **M. Ownbey**, K. Smith, J. K. Padden Metzker
- 1054.** Get involved with the ACS Division of Chemical Education. **M. B. McGinnis**
- 1055.** Fundamentals of Chemistry: Course impact and retention. **A. H. Shelton**
- 1056.** Chlorine Dioxide-Phenol Reaction: A Kinetic Laboratory Experiment. A. T. Pratt, **E. Grimley**, D. W. Wright
- 1057.** Analysis of food coloring in introductory chemistry. **S. K. Hutchison**, M. T. Griffin, K. R. Wilson, J. W. Hall
- 1058.** Using innovative middle school science modules to improve student learning. A. B. Bufford, E. J. Andrews, A. A. Arnold, M. B. Reeves, **A. L. Curry**, M. L. Curry
- 1059.** Determination of energy content of some conventional and alternative fuels by calorimetric technique. **H. Baccas**, W. Mayberry, H. Khan, L. Pagnotti, M. Wolf, M. H. Kabir, J. Cramer
- 1060.** Enhancing engagement in undergraduate education. **D. W. Dixon**
- 1061.** Journey through Harry Potter: A demonstration show. **K. A. Jiles**, **K. A. Brown**, J. L. Armstrong, G. L. Crawford, J. L. Look
- 1062.** Z-spectroscopy of a dynamically heterogeneous system: A biomolecular NMR experiment for undergraduate labs with permanent magnet systems. **A. Vazquez**, J. J. Pajski

Posters: Undergraduate Research

Physical/Computational/General Chemistry

Loews Atlanta Hotel
Over Look/Exhibit Hall

V. Singh, *Organizer*

4:00 - 5:30

- 1063.** Microwave spectrum and *ab-initio*- calculations of 2-chloro-3-fluoropyridine. **S. T. Arnold**, J. C. Chewning, G. G. Brown
- 1064.** Computational investigations of the borohydride reduction of ketones: The mechanistic source of the stereoselectivity of the reduction of benzil. **B. Sauls**, D. A. Clabo, Jr.
- 1065.** Fluorescence Determination of Zirconium with Quercetin Using Surfactants. **C. Day**, D. Y. Pharr, R. D. Miccio
- 1066.** Electrochemical analysis of symmetric 1,4-fluorenylenes functionalized with electron donating and electron withdrawing groups. **B. E. Levy**, B. J. Laughlin, Y. Htet, R. C. Smith, **A. G. Tennyson**
- 1067.** Theoretical studies of hydrogen abstraction reactions from hydrofluoroethanes. **T. A. Dray**, T. V. Albu
- 1068.** Comparison of the reaction rates between tetramethyl orthosilicate and various carboxylic acids. **C. R. Garrett**, C. E. Dahm
- 1069.** Theoretical study of the pyridine involved hydrogen bond and the impact to the ring breathing vibration. **A. O. Ejiawoko**, **U. Kalapathy**, H. Fan-Hagenstein
- 1070.** Modeling studies of binding of gingerol to Bcl-2 protein. **L. A. Sharpe**, D. A. Abramovitch, F. A. Norris
- 1071.** Determination of the release rate of two antibiotics embedded in a nanofiber mesh applicable to limb salvage. **C. Quinn**, P. O'Brien, S. Symes
- 1072.** Quinoxalinol salen ligands for spectrophotometric molecular recognition. **S. Kerns**, M. DeVore II, A. Gorden
- 1073.** Microwave spectrum and *ab initio* calculations of 2-chloro-6-fluoropyridine. **J. C. Chewning**, S. T. Arnold, G. G. Brown
- 1074.** Modeling of pulsatile Nonnewtonian blood flow as a Bingham fluid in a branched artery. **A. Vanlandingham**, R. Wilcox
- 1075.** Computational study on the electronic structures of functionalized cyclosilanes. **D. C. Yost**, S. Kilina
- 1076.** Presence of pharmaceuticals and personal care products in treated wastewater from a small college community. **A. Bray**, E. M. White
- 1077.** Approach toward 1,2,3-triazoles sensors for the detection of heavy transition metal cation. **K. V. Hawkins**, N. Ballantyne, K. Afeku, K. S. Aiken, S. M. Landge
- 1078.** Theoretical studies of tautomeric Equilibria of pyridazinol ether. **K. Banerjee**, **H. Madamidola**, J. B. Gray, **B. Bill**
- 1079.** How sweet it is: Developing an undergraduate laboratory experiment on the spectroscopy of sweet tea. **C. C. Rogers**, **B. B. Fenn**, J. L. Armstrong, K. D. Kloepper
- 1080.** Photodegradation of Loratadine in Simulated Natural Water Samples. **A. Jenkins**, W. Cory
- 1081.** Photodegradation Mechanisms of Vardenafil and Sildenafil. **L. Herbert**, W. Cory
- 1082.** Photodegradation of Diphenhydramine in Simulated Natural Water Samples. **A. Dumas**, W. Cory

- 1083.** Photodegradation of Naproxen and its Photodegradants in Simulated Natural Water Samples. **J. Ramirez**, W. Cory
- 1084.** Using DNA Computational Design to Construct and Image Nanostructures. **J. Waller**, R. Wadkins
- 1085.** Protein similarity networks reveal relationships among sequence, structure, and function within the cupin superfamily. **R. Uberto**, E. Moomaw
- 1086.** Ion binding by beauvericin investigated by electrospray ionization mass spectrometry. **J. K. Denton**, **J. B. Kimbrell**, S. English, S. Swamy-Mruthinti, M. Fujita, F. A. Khan
- 1087.** Progress Towards Sideband Cooling of Atomic Ion-Molecular Ion Coulomb Crystals. **J. Gray**
- 1088.** Computational studies of paradifluorobenzene cations with two HCN molecules. **J. C. Rowe**
- 1089.** Engaging rural students in place-based chemistry: Development and implementation of contextualized experiments for agricultural regions. **L. S. Fitts**, **S. R. Fulgham**
- 1090.** Effect of ultrasounds on alpha-amylase. **A. Rizzo**, A. Gaquere-Parker
- 1091.** Iron competition: Protein vs. synthetic drug. **A. Laufer**, R. M. Majors, C. M. Davis McGibony
- 1092.** Can cosmetic surfactants be benignly precipitated from aqueous solutions? **E. D. Keith**, **M. N. Richardson**, **K. A. Sands**, H. S. Leach, J. M. Carr
- 1093.** Solvent effects on the absorption maxima of conjugated dyes: Testing the applicability of the particle-in-the-box model. **A. Brislinger**, **C. Williamson**, **M. Kendrick-Murphy**
- 1094.** Viscosity, conductivity, specific heat, and colligative properties of alcohols. **W. W. Brown**, A. T. Calvin, S. I. Edwards, B. S. Farley, H. A. Franklin, R. E. Graham, J. S. Ingram, T. McGregor, R. T. Mikula, A. J. Mock, A. N. Neloms, C. D. Northcutt, M. P. Patel, R. L. Robertson, F. A. Stackhouse, G. R. Anzalone, P. L. Brown, A. V. DeLong, A. J. Fino, A. B. Garza, A. G. Humphries, B. S. Larcart, J. C. Lord, C. B. Massey, T. L. Peterson, M. J. Reaves, J. M. Roland, K. M. Seville, T. Manning, A. P. Gramatges
- 1095.** Simulating the quantitative effect of glucose on post-mortem ethanol production by *Candida albicans*. **T. Vasiljevic**, **S. E. Hooper Marosek**
- 1096.** Implementing Elaborate Visual Analogies in Organic Chemistry Course - Nomenclature. S. Landge, **S. Rhodes**
- 1097.** Computational simulation of the binding of deltorphin I to the δ -opioid receptor. **M. A. Tapia**, K. S. Kroeger
- 1098.** An investigation of W438 as a route of misguided electron transfer for KatG. **E. McCurdy**, O. Njuma, E. Ndonsta, D. Goodwin
- 1099.** UV damage recognition by UV-DNA damage binding protein. **A. L. Hughes**, G. M. Gray, A. van der Vaart
- 1100.** Revealing the binding affinity of β -glucuronidase/ligand complexes via computational chemistry. **J. D. Mace**, **D. S. McKnight**, T. J. Fuhrer
- 1101.** Degradation of estrogen by lignolytic enzymes from Oak Mountain State Park fungi. **C. Farmer**, **A. Hampton**, C. M. Johnson, D. Gregory
- 1102.** A focus on focusing proteins. **M. Roberson**, R. Montgomery
- 1103.** Synthesis, NMR assignments, mass spec, and NCI cell line studies and a proposal as a treatment for autism, research with byrostatin. **R. Robertson**, T. McGregor, H. Franklin, J. L. Perry, T. Manning, G. Wylie, D. Phillips, B.

Bythell, F. Zhang

1104. Alternative approach to confirming precipitation reactions in aqueous solutions. **S. Brigham**, P. Walters, **M. Han**

1105. Summertime measurements of non-methane hydrocarbons in rural western North Carolina. **R. Cook**, Y. Zhou, B. C. Sive

1106. Reliability of fire debris analysis evidence storage containers. **A. Noble**

1107. Investigation of snake Arenavirus recombination. **K. E. Leon**, M. Stenglein, J. DeRisi

1108. Implementation of a new graphical multiscale modeling interface into the CHARMMing web-portal. **V. Schalk**, F. C. Pickard, Y. Pevzner, B. T. Miller, H. L. Woodcock

1109. *In vitro* selection with stem loop DNA. **M. Harrell**, A. C. Spencer

SATURDAY MORNING

Posters: High-School

Loews Atlanta Hotel
Over Look/Exhibit Hall

N. Kirk, *Organizer*

11:00 - 12:00

1110. Synthesis, characterization and kinetics of the fastest-folding WW domains. **D. Ruiz**, C. Davis, B. Dyer

1111. Synthesis of Silver Nanoparticles using Domestic Microwave. **S. S. Kim**, **L. Kim**, **S. Kang**, **G. Paniconi**

1112. Improved performance in microbial fuel cells. **M. Shin**, **S. Kang**, **S. Woo**, **S. Chung**

Symposium for Undergraduates on Careers in Chemistry

Loews Atlanta Hotel
Salon H

N. Kirk, *Organizer*

11:00 1113. Chemistry in art conservation. **R. Stein**

11:40 1114. Scientific progress: Industry versus Academia. **J. MacDonald**

12:20 1115. Trace residue analysis for the US Army. **K. E. Mooney**

SATURDAY AFTERNOON

Undergrad Awards Luncheon

(Ticketed event)

Loews Atlanta Hotel

Salon A

N. Kirk, *Organizer*

1:00 1116. Science from the International Space Station. **L. J. Delucas**