64th Annual Pentasectional Meeting of the American Chemical Society

100 YEARS OF CHEMISTRY

Program and Abstracts
13 April 2019
NCED Hotel & Conference Center
Norman, OK

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13 April 2019
The NCED Hotel and Conference Center
2801 East State Hwy 9
Norman, Oklahoma 73071

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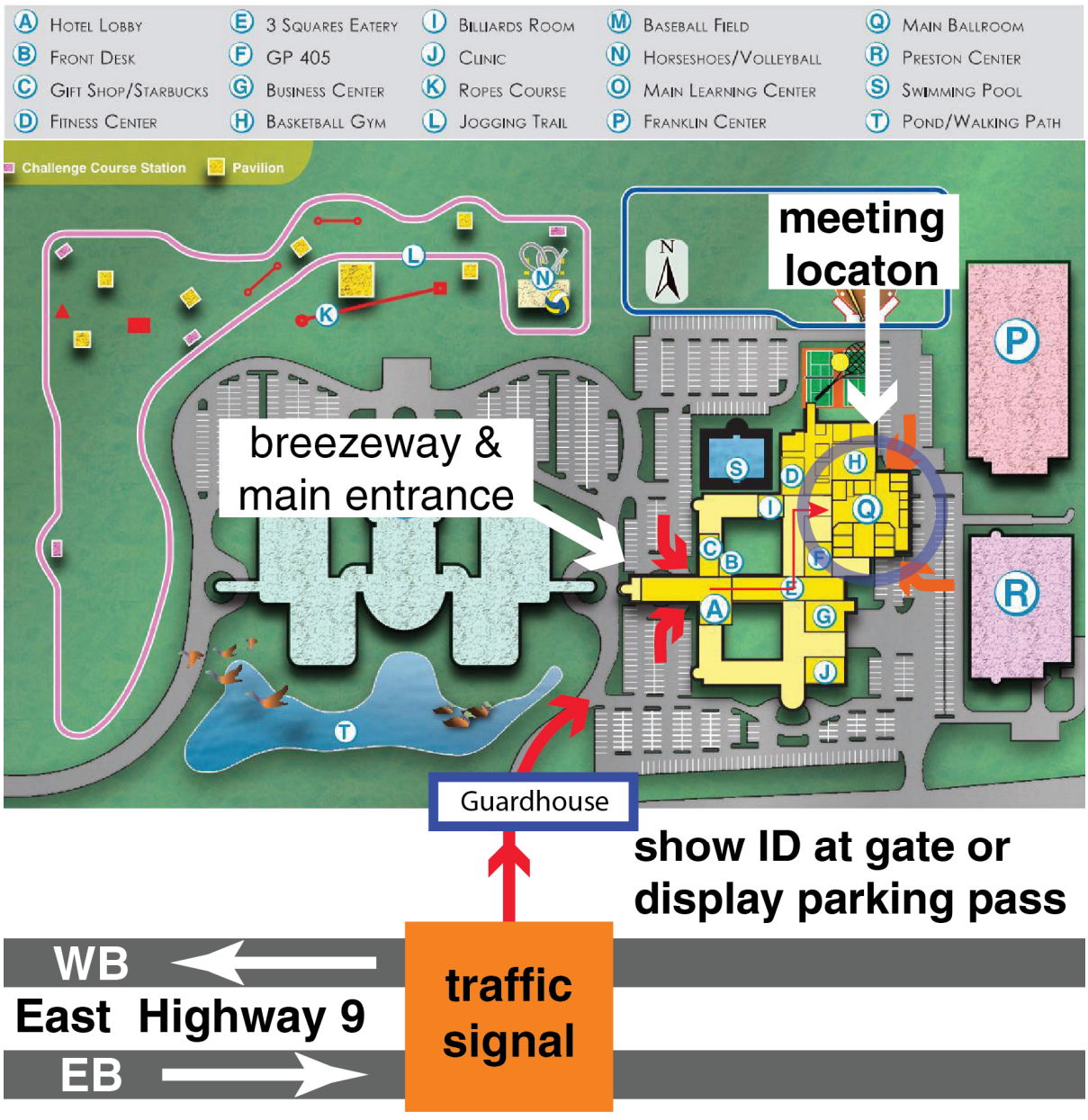
Technical Program

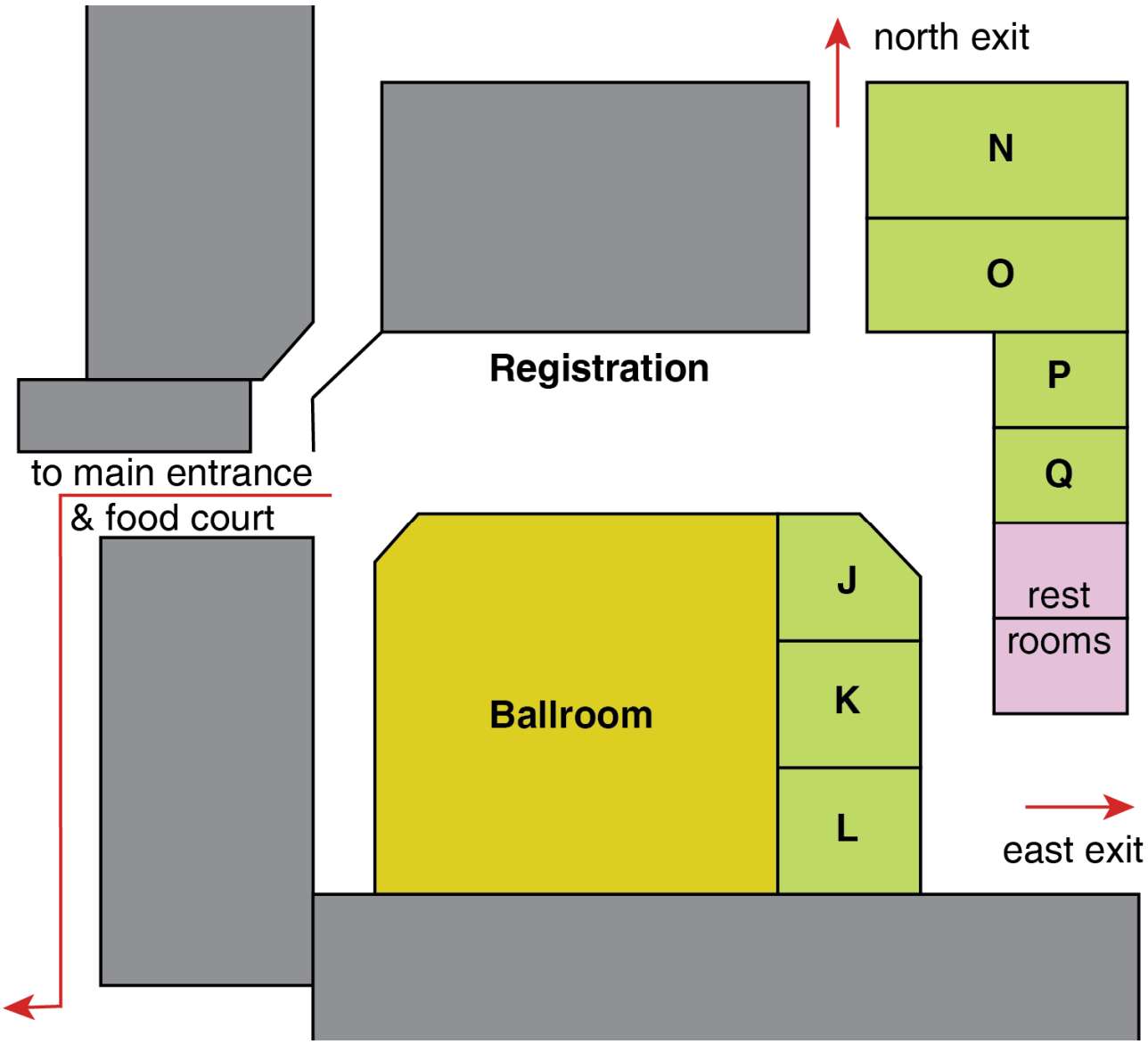
2019 Pentasectional Organizing Committee
Lloyd A. Bumm (Physics and Astronomy, The University of Oklahoma) — General Chair
Naga Rama Kothapalli (Chemistry and Biochemistry, The University of Oklahoma) — Program Chair
Nicholas F. Materer (Chemistry, Oklahoma State University) — Web Operations

Getting to the Conference

Getting Around the NCED



Conference Venue Floor Plan



Conference Program Overview

Time	Ballroom	J	K	L	N	O	P
7:30 - 8:30 am	poster set up						
8:30 - 10:20 am	Poster Session, Vendors, and Continental Breakfast *Students should be with posters during this time*						
10: 20 - 10:30 am	Break						
10:30 am - 12:10 pm	Poster Viewing and Vendors	Chemical Education	Analytical Chemistry	Nano Materials	Biochemistry	Organic Chemstry	Physical Chemistry
12:10 - 12:40 pm	LUNCH						
12:40 - 1:00 pm	Awards						
1:00 - 1:45 pm	Oklahoma Chemist Talk						
1:45 - 2:00 pm	15 min Break						
2:00 - 3:30 pm	Poster Viewing and Vendors	History of Chemistry in Oklahoma	Computational Chemistry	Inorganic Chemistry	Biochemistry and Structural Biology	Medicinal Chemistry and Organic Chemistry	Materials Chemistry
3:00 - 3:30 pm		Break -- refreshments Visit the Vendors and Posters					
3:30 - 4:50 pm		History of Chemistry in Oklahoma	Computational Chemistry	Inorganic Chemistry	Biochemistry and Structural Biology	Medicinal Chemistry and Organic Chemistry	Materials Chemistry
4:50 - 6:00 pm	take down posters						

2019 Oklahoma Chemist

Kenneth M. Nicholas of the University of Oklahoma's Department of Chemistry and Biochemistry has been selected as the 2019 recipient of the Oklahoma Chemist Award for his outstanding contributions to the discovery, fundamental understanding and applications of chemical reactions promoted by transition metal compounds. His research group's studies have centered on: 1) the stability and reactivity of metal-coordinated organic species; 2) carbon dioxide activation/conversion promoted by transition metals; 3) the metal-promoted nitrogenation of hydrocarbons; 4) bio-inspired transition metal catalysis; and 4) the catalytic deoxygenation and refunctionalization of renewable chemical resources. The results of these studies have been presented at numerous regional, national and international scientific conferences and published in approximately 200 peer-reviewed journal articles and book chapters and 3 U.S. Patents. These projects have been financially supported with approximately five million dollars from federal and state agencies and foundations including: the Research Corporation, the Oklahoma Center for the Advancement of Science and Technology, the Petroleum Research Fund of the American Chemical Society, the Office of Naval Research, the National Institutes of Health, the U. S. Department of Energy, and the National Science Foundation. Prof. Nicholas' research team is probably most well known for the invention and development of a chemical reaction (often referred to as the Nicholas reaction) which is facilitated by cobalt-coordination to alkynes, that enables their efficient conversion to diverse and useful products.

Dr. Nicholas has supervised and mentored approximately 60 undergraduate research assistants, 16 M.S. degree recipients, 26 Ph. Ds. and 38 postdoctoral research fellows, almost all of whom have enjoyed careers in industry, medicine, government or academia. Professor Nicholas has organized a number of scientific conferences and workshops, served on the editorial board of the journal *Organometallics*, and he helped to establish the O.U.-Blaise Pascal U. (Fr) joint M.S. degree program. Prof. Nicholas was a popular, yet challenging instructor of organic chemistry to a few thousand undergraduates and of organic and organometallic chemistry to hundreds of graduate students, many of whom are engaged in successful careers in medicine, the corporate world, teaching and government. Dr. Nicholas has been recognized for his teaching and research accomplishments by the A.P. Sloan Foundation, the University of Oklahoma Regents, by the American Chemical Society's A. C. Cope Scholar Award (for research excellence in organic chemistry), and as a George Lynn Cross Research Professor, the highest research award at O.U. Dr. Nicholas earned a B.S. in Chemistry from Stony Brook University (NY), his Ph. D. from the U. Texas (Austin), did postdoctoral research at Brandeis University, and was on the faculty at Boston College (1973-1984) before joining the Department of Chemistry and Biochemistry at the University of Oklahoma in 1984.

Oklahoma Chemist History

The Oklahoma Chemist Award was initiated in the early 1970s and was primarily started by Dr. George R. Waller who was a faculty member in the Biochemistry Department at Oklahoma State University. Oklahoma is divided into five sections of the American Chemical Society, and each Section agreed to support this award on an annual basis. The concept for the award was to honor truly outstanding contributions made to the science and to the state by a chemist in recent years within the state of Oklahoma. Although originally designed to honor research chemists, an amendment was introduced in the 1980s to allow candidates to be nominated who had made extraordinary contributions to the area of chemical education whether it be to youth or to the public in general. Three such awards have been made to chemical educators over the years since the inception of the award in 1971. One award was to be given each year if a suitable candidate was identified from the research community of from education. The original award consisted of $500 and a handsome plaque formed in the shape of the state of Oklahoma.

One member from each of the five Sections was appointed to compose a reviewing committee to accept nominations which were to be received around February 1 of each new year. The date was to permit sufficient time for the winner to be selected and to receive the cash award and plaque at the next annual Pentasectional Meeting in the spring. The Pentasectional Meeting brings together chemists from academia and from industry within the state one time each year to present research results. It is the largest meeting of chemists in Oklahoma.

The OKLAHOMA CHEMIST AWARD is the most prestigious award given to a chemist within Oklahoma. The award now consists of $1000 as well as the plaque described above. A brief description of the accomplishments by the recipient are engraved on the plaque and are submitted, along with a photo of the winner, to Chemical and Engineering News for official publication in a forthcoming issue. Chemical and Engineering News is a major publication of the American Chemical Society and has world-wide distribution.

Past Recipients of the Oklahoma Chemist Award

The Oklahoma Chemist Award is sponsored by the five Oklahoma Sections of the American Chemical Society with the additional support of the chemical industries of the state of Oklahoma. We are grateful for the support. The recipient is the automatic nominee for the Southwest Chemist Award of the Southwest Region. Nominations for next year should be submitted to the local section representative of the Oklahoma Chemist Committee. The permanent committee chair is K. Darrell Berlin, 107 Physical Sciences I, Chemistry Department, Oklahoma State University, Stillwater, OK 74078.

OKLAHOMA CHEMIST AWARD WINNERS

1971 **Wayne White**, *Ozark-Mahoning Company*, for developing commercial processes for stannous fluoride and sodium monofluorophosphate, the two fluorides most widely used as dentifrice additives.

1972 No award

1973 **Otis C. Dermer**, *Oklahoma State University*, for his outstanding service to the people of Oklahoma in building a first-rate Chemistry Department at Oklahoma State

University and for his nationally recognized contribution to the chemical nomenclature and chemical education.

1974 **Robert L. Banks**, *Phillips Petroleum Company*, in recognition of his outstanding contributions to the field of chemistry in the olefin disproportionation reaction and in catalysis.

1975 **Charles M. Starks**, *Conoco, Inc.*, in recognition of and publications on phase transfer catalysis.

1976 **Kang Yang**, *Conoco, Inc.*, in recognition of his scientifically sound and innovative theoretical concepts in radiation chemistry, photochemistry, rate theory, electrochemistry and catalysis, and application of chemical kinetics to these concepts.

1977 **Kenneth Darrell Berlin**, *Oklahoma State University*, in recognition of his many, and significant contributions to heterocyclic phosphorus chemistry.

1978 **Gerard Kraus**, *Phillips Petroleum Company*, for his outstanding contributions to the physical chemistry of industrial polymers.

1979 **Lionel M. Raff**, *Oklahoma State University*, for pioneering work in the use of theoretical chemical physics as a practical tool for electrical structures, reaction rates, and energy transfer processes.

1980 **Wayne F. Hower**, *Halliburton Services*, for invaluable contributions to the science and practice of well completions and well stimulation methods in the petroleum and related industries.

1981 **Alfred Clark**, retired from *University* of *Oklahoma* after retirement from *Phillips Petroleum Company*, in recognition of outstanding contributions to theory and applications of adsorption and catalysis.

1982 **Marvin M. Johnson**, *Phillips Petroleum Company*, in recognition of his many innovative contributions in the areas of metal passivation on cracking catalysts and reclamation of used motor oil.

1983 **Simon Wender**, *University of Oklahoma*, for his contributions to the understanding of the chemistry and biochemistry of plant phenolics.

1984 **E. J. Eisenbraun**, *Oklahoma State University*, in recognition of his many contributions in the field of natural products and high purity organic chemicals.

1985 **Dick van der Helm**, *University of Oklahoma*, in recognition of his contributions in the field of structural analyses by x-ray crystallography.

1986 **Sherril D. Christian**, *University of Oklahoma*, in recognition of his contributions to the field of colloid chemistry.

1987 **Francis J. Schmitz**, *University of Oklahoma*, for his achievements in the isolation, characterization, and pharmacological applications of marine natural products.

1988 **Marvin K. Kemp**, *Amoco Production Company*, for his contributions in developing and expanding the science enrichment program for fourth and fifth grade students, education, and practical geochemistry research applications.

1989 **Glenn Dryhurst**, *University of Oklahoma*, in recognition of outstanding achievements in the field of chemical research and education in the state of Oklahoma.

1990 **Horace A. Mottola**, *Oklahoma State University*, in recognition of his contributions in the areas of continuous flow kinetics and immobilized enzymes.

1991 No award

1992 **Elizabeth Anne Nalley**, *Cameron University*, in recognition of her contributions to the teaching of chemistry to grade school, high school, and college students.

1993 **Bing M. Fung**, *University of Oklahoma*, in recognition of his contributions in the fields of liquid crystals and nuclear magnetic resonance spectroscopy.

1994 No award.

1995 **Gilbert J. Mains**, *Oklahoma State University*, in recognition of his contributions in the fields of photochemistry and computational chemistry and as an educator.

1996 **Max P. McDaniel**, *Phillips Petroleum Company*, in recognition of his contributions to olefin polymerization catalysis and the polyethylene industry.

1997 **Donald L. Thompson**, *Oklahoma State University*, for pioneering work in molecular dynamics and contributions to chemistry in Oklahoma.

1998 **Roger E. Frech**, *University of Oklahoma*, for his contributions in the research of solid-state ionic materials, teaching and mentoring students, and establishing cooperative research centers with other Oklahoma scientists.

1999 **Warren T. Ford**, *Oklahoma State University*, for his outstanding contributions in polymer chemistry.

2000 **Robert E. Howard**, *University of Tulsa*, for outstanding contributions to chemical education at the elementary, secondary, and college levels.

2001 **George R. Waller**, *Oklahoma State University*, for outstanding contributions to biochemistry, mass spectrometry, and natural product chemistry.

2002 **P. K. Das**, *Phillips Petroleum Company*, for outstanding contributions to computational methods for catalyst design with emphasis on the development and characterization of metallocene- based polyolefin catalysts.

2003 **James Weaver**, *Halliburton Research Services*, for contributions in chemistry for improving petroleum production efficiency and worker safety with minimum environmental impact.

2004 **Daniel E. Resasco**, *University of Oklahoma*, for outstanding contributions in nanotechnology and in petroleum refining.

2005 **Neil Purdie**, *Oklahoma State University*, for outstanding contributions in chemical education at the university level and for the development of a computer program for assisted analysis of lipid profiles.

2006 **Donald D. Knudsen**, *ChevronPhillips Company*, for outstanding contributions to the field of polyolefin catalysis and outstanding leadership and technical expertise in the development and commercialization of selective 1-hexene technology.

2007 **Ziad El Rassi**, *Oklahoma State University*, for outstanding contributions to chemistry in the state of Oklahoma in the field of chromatography, especially in the area of liquid phase separation techniques.

2008 **Joe Allison**, *Conoco Company*, for outstanding contributions to chemistry over broad areas spanning the oil, gas, and chemical industries and his significant service to the ACS on both the local and national levels.

2009 **Richard A. Bunce**, *Oklahoma State University*, for outstanding contributions to synthetic organic chemistry and the development of tandem reactions for the synthesis of carbocyclic and heterocylic systems.

2010 **Jiten Chatterji**, *Halliburton Energy Services*, for outstanding contributions in the areas of cementing and fracturing in the industry of oil recovery.

2011 **Dale Teeters**, *University of Tulsa*, for outstanding contributions in fabrication and characterization of electrolyte systems in nanoporous membranes.

2012 **Donna Nelson**, *University of Oklahoma*, for outstanding contributions in unifying additions to alkenes via physical organic chemistry, determining SWCNT functional group molecular level interactions, quantifying research university STEM faculty demographics, and chemical advising to congress, television, and professional organizations.

2013 **Tushar Choudhary**, *Phillips 66 Research Center*, for outstanding work in clean fuels optimization, diesel hydrotreating catalysis, catalyst development for gasoline desulfurization, clean hydrogen production for fuel cell applications, and oxidation catalysis.

2014 **Allen W. Apblett**, *Oklahoma State University*, for outstanding contributions in chemical research, education, leadership, and entrepreneurship in the state of Oklahoma.

2015 **A. K. Fazlur Rahman**, *Oklahoma School of Science and Mathematics*, for outstanding contributions in chemical education and leadership at the secondary level and the college level.

2016 **Frankie Wood-Black**, Director of Process Technology at *Northern Oklahoma College* and Principal of *Sophic Pursuits, Inc.*, for outstanding contributions in the oil and gas industry and in chemical education from the elementary to college level in the State of Oklahoma.

2017 **Dwight L. Myers**, *East Central State University*, for outstanding contributions in chemical education at the college level.

2018 **Robert E. Anderson**, *University of Oklahoma Health Sciences Center*, for outstanding contributions to the understanding of the role of lipids in visual function, the discovery of the importance of docosahaenoic acid in retina function, and for mentoring students.

2019 **Kenneth M. Nicholas**, *University of Oklahoma*, for outstanding contributions to the discovery, fundamental understanding and applications of chemical reactions promoted by transition metal compounds.

Schedule of Events

Registration (Prefunction area outside ballroom)

On-Site Registration and Badge Pickup from 7:30 am – 10:30 am

Poster Session (Main Ballroom: 8:30 am – 10:20 am)

Morning Continental Breakfast (8:30 – 10:20)

Posters should be set up by 8:30 am.

Presenters are encouraged to be by their posters from 8:30 am – 10:20 am.

The poster session will run through the day until 4:50 pm.

Posters should be removed by 6:00 pm.

Morning Technical Sessions (10:30 am – 12:10 pm)

Chemical Education	Room J
Analytical Chemistry	Room K
Nanoscience and Nanomaterials	Room L
Biochemistry	Room N
Medicinal and Organic Chemistry I	Room O
Physical Chemistry	Room P

Luncheon Program (12:00 pm – 1:45 pm in the Main Ballroom)

Lunch Fajita Buffet 12:00 – 1:30

Poster Awards & Oklahoma Chemist Award 12:45 – 1:00

2019 Oklahoma Chemist Talk 1:00 – 1:45

Afternoon Technical Sessions (2:00 pm – 4:50 pm)

Afternoon Snack Break within the afternoon technical session (3:00-3:30)

Note: Pentasectional Planning Meeting (Room Q at 3:00 pm – 3:30 pm)

For past, present, and future organizers of Pentasectional meetings.

History of Chemistry in Oklahoma	Room J
Computational Chemistry	Room K
Inorganic Chemistry	Room L
Biochemistry & Structural Biology	Room N
Medicinal and Organic Chemistry II	Room O
Materials Chemistry	Room P

Social Hour & poster take down (Main Ballroom 4:50 pm – 6:00 pm)

Oklahoma Section Governance

2019 Oklahoma ACS Section Officers and Standing Committee Chairs

Naga Rama Kothapalli	Chair
Stephanie L. Skiles	Chair Elect
Allen Apblett	Immediate Past Chair
Lloyd A. Bumm	Secretary
Jason Wickman	Treasurer
Allen Apblett	Councilor + Nominations Committee
Nicholas Materer	Alternate Councilor
Charles V. Rice	Awards Committee
Lloyd A. Bumm	Newsletter and Publications Committee
Reza Latifi	Chemistry Olympiad Committee
Michael Ferguson	National Chemistry Week Committee
Cheryl Frech	Public Relations
Nicholas F. Materer	Web Master

The Oklahoma Section communicates with its membership through several channels, including email, a printed newsletter, and our web page. If you haven't been getting notifications of upcoming meetings and other section activities by email, perhaps we do not have your current email address. We use the email address list obtained from and maintained by the ACS.

There are 3 different ways you can update your information.
1) Log in to the ACS website (www.acs.org) and edit your profile —via the Edit My Profile link located under the welcome banner after you login.
2) Phone the ACS Customer Service team (1-800-333-9511).
3) Send an email to the ACS Customer Service team (service@acs.org).

Help us keep in touch!
—The Oklahoma Section of the ACS Executive Committee

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Lecture Sessions at the 64th Annual Pentasectional Meeting of the American Chemical Society

Saturday, April 13, 10:30 AM. S1: Analytical Chemistry
Session Chair: Stephanie Skiles (University of Central Oklahoma)
Location: Room K

10:30 T1: **Assessment of Metal Impurities in Cosmetics**
Presenter: Sahr A. Alsherari
Authorship: Sahr A. Alsherari and Allen Apblett - *Department of Chemistry, Oklahoma State University*

10:50 T2: **Simultaneous Determination of Renal Cell Carcinoma Biomarkers in Urine using Water-Rich Mobile Phases**
Presenter: Kaushalya Sharma Dahal
Authorship: Kaushalya Sharma Dahal and Barry K. Lavine - *Department of Chemistry, Oklahoma State University*

11:10 T3: **Library Search Prefilters for Manufacturer's Automotive Paints using Simulated Attenuated Total Reflection (ATR) Spectra**
Presenter: Francis Kwofie
Authorship: Francis Kwofie, Barry K. Lavine and Nuwan D. Perera - *Department of Chemistry, Oklahoma State University*

11:30 T4: **Hexadecyl Imidazolium Ionic Liquid Stationary Phase Bonded to Silica Microparticles**
Presenter: Nilushi Paranamana
Authorship: Nilushi Paranamana and Ziad El Rassi - *Department of Chemistry, Oklahoma State University*

Saturday, April 13, 10:30 AM. S2: Biochemistry
Session Chair: Laura-Isobel McCall (University of Oklahoma)
Location: Room N

10:30 T5: **Chemical Cartography: Resolving Small Molecule Spatial Organization by LC-MS/MS and 3D Mapping during Parasitic Infection**
Presenter: Laura-Isobel McCall
Authorship: Laura-Isobel McCall[1], Ekram Hossain[1], Chaoyi Wu[1], Sharon Lostracco-Johnson[2], Diane Thomas[2], Danyang Li[3], Mitchelle Katemauswa[1] and Camil Gosmanov[1] - *[1]University of Oklahoma, [2]University of California San Diego and [3]Beijing Normal University*

10:50 T6: **Non-Invasive Testing of Bladder Cancer Patient Cells at the Single-Cell Level**

Presenter: Ryan C. Bensen
Authorship: Ryan C. Bensen, Shawna J. Standke, Devon H. Colby, Naga Rama Kothapalli, Anh T. Le, Anthony W. G. Burgett and Zhibo Yang - *Chemistry and Biochemistry, University of Oklahoma*

11:10 T7: **Spacer Integration Occurs Differently between Sub-groups of Type II-A CRISPR Systems**

Presenter: Mason J. Van Orden
Authorship: Mason J. Van Orden, Sydney Newsom and Rakhi Rajan - *Chemistry and Biochemistry, University of Oklahoma*

11:30 T8: **Oxysterol-Binding Protein as a Prophylactic Antiviral Target of the Natural Product Small Molecule, OSW-1**

Presenter: Zachary C. Severance
Authorship: Zachary C. Severance, Brett Roberts, Ryan C. Bensen, N. R. Kothapalli, Anh Le, Cori Malinky, Hongyan Ma, Si Wu, William J. Reddig, Earl L. Blewett and Anthony W.G. Burgett - *Chemistry and Biochemistry, University of Oklahoma*

11:50 T9: **Synthesis of Doxorubicin-Based Prodrug and Activatable MR Nanoprobe for the Imaging and Treatment of Cancer**

Presenter: Arth Patel
Authorship: Arth Patel, Bayan Ahmad Dous and Santimukul Santra - *Department of Chemistry, Pittsburg State University*

Saturday, April 13, 10:30 AM. S3: Chemical Education
Session Chair: Jacinta Mutambuki (Oklahoma State University-Stillwater)
Location: Room J

10:30 T10: **Priestley Medal Addresses: Tools for Teaching About the Recent History of Chemistry**

Presenter: Luis D. Montes
Authorship: Luis D. Montes - *University of Central Oklahoma*

10:50 T11: **We Don't Learn Anything: The Impact of Contextualized Authentic Research-Based Experiences Modules on STEM Majors' Perceptions of a Chemistry Laboratory Course**

Presenter: Jacinta Mutambuki
Authorship: Jacinta M. Mutambuki[1], Herb Fynewever[2], Kevin Douglass[3], William Cobern[4], and Sherine Obare[5] - *[1]Department of Chemistry, Oklahoma State University, [2]Department of Chemistry and Biochemistry, Calvin College, [3]MPI Research, a Charles River Company, [4]Department of Biology and Biological Sciences, Western Michigan University and [5]Joint School of Nanoscience and Nanoengineering, University of North Carolina at Greensboro*

11:10 T12: **Using Fluency Quizzes to Talk Chemistry**
Presenter: Christopher T. Jones
Authorship: Christopher T. Jones - *Oklahoma Baptist University*

11:10 T13: **Chemistry, Data and Undergraduates: Fitting Data Literacy into Chemical Education**
Presenter: Kay K. Bjornen
Authorship: Kay K. Bjornen - *Edmon Low Library, Oklahoma State University*

11:50 T14: **Self-Starting Functions for Nonlinear Fitting of Enzyme Inhibition**
Presenter: Nathan J. Malmberg
Authorship: Nathan J. Malmberg - *Department of Chemistry, Oklahoma Baptist University*

Saturday, April 13, 10:30 AM. S4: Nanomaterial
Session Chair: Allen Apblett (Oklahoma State University)
Location: Room L

10:30 T15: **Highly Ordered Bionanofibrous Films Fabricated by a Simple Self-Assembly Approach**
Presenter: Ningyun Zhou
Authorship: Ningyun Zhou and Chuanbin Mao - *University of Oklahoma*

10:50 T16: **Functionalizing the Surface of Gold Nanorods with Single-Stranded DNA**
Presenter: Stephen Kane
Authorship: Stephen Kane and Bailey Spears and Nathan Green - *Northeastern State University*

11:10 T17: **Reactivity of Chromium Anchored Al-MCM-41 Nanomaterial: An FT-IR Study of Detoxification of Organic Compounds**
Presenter: Dilip K. Paul
Authorship: Dilip K. Paul - *Department of Chemistry, Pittsburg State University*

11:30 T18: **Nanoconfinement of Organics in Mesoporous Silica: Applications in Explosive Stabilization, Chemical Dosimeters, and Water Treatment**
Presenter: Allen Apblett
Authorship: Allen Apblett, Nicholas Materer, Evgueni, Kaddosov, Randy Butt - *Oklahoma State University and XploSafe, LLC*

11:50 T19: **Poly(Vinyl Pyrrolidone) has Reduced Mobility in Graphene Oxide Nanocomposites**
Presenter: Ishan N. Jayalath
Authorship: Ishan N. Jayalath and Frank D. Blum - *Oklahoma State University*

Saturday, April 13, 10:30 AM. S5: Organic and Medicinal Chemistry I
Session Chair: Shanteri Singh (University of Oklahoma)
Location: Room O

10:30 T20: **Metal Carbenoid Initiated Cascade Reactions for the Synthesis of Diverse Medium-sized Heterocycles**

Presenter: Nicholas P. Massaro
Authorship: Nicholas P. Massaro, Kiran Chinthapally, Joseph C. Stevens, Aayushi Chatterji and Indrajeet Sharma - *Department of Chemistry and Biochemistry, and Institute of Natural Products Applications and Research Technologies, University of Oklahoma*

10:50 T21: **Targeting Tumor Metabolism for Cancer Therapy**

Presenter: Toby Nix
Authorship: Horrick Sharma and Toby Nix - *Department of Pharmaceutical Sciences, College of Pharmacy, Southwestern Oklahoma State University*

11:10 T22: **Sulfabenzamide Diversification using Alkyl Pyrophosphate Analogues by NphB Reveals N-Prenylation Catalytic Functions**

Presenter: Andrea Batchev
Authorship: Andrea Batchev, Erin Scull, Eric Gardner, Chandrasekhar Bandari, Tejaswi Bavineni, Johanna Masterson, Rachel Tran, Abigail Lange and Shanteri Singh - *Chemistry and Biochemistry, University of Oklahoma*

11:30 T23: **Copper-Catalyzed Synthesis of Enamino Carbonyl Compounds**

Presenter: Syed R Hussaini
Authorship: Syed R Hussaini and Arpan Pal - *Department of Chemistry and Biochemistry, The University of Tulsa*

11:50 T24: **Chemoenzymatic Synthesis of Novel Tryprostatin Analogs using Prenyltransferases**

Presenter: Eric Gardner
Authorship: Eric Gardner, Andrea Batchev, Abigail Lange, Johanna Masterson, Chandrasekhar Bandari and Shanteri Singh - *Chemistry and Biochemistry, University of Oklahoma*

Saturday, April 13, 10:30 AM. S6: Physical Chemistry
Session Chair: Bin Wang (University of Oklahoma)
Location: Room P

10:30 T25: **Kinetic Doping of Branched Polyethylenimine: A Novel Approach to Amine Functionalization of Silica Thin Films**

Presenter: Jessica Jensen
Authorship: Jessica Jensen and Wai Tak Yip - *Chemistry and Biochemistry, University of Oklahoma*

10:50 T26: **Aldol Condensation of Cyclopentanone and Acetone on MgO: A Mechanism Study by DFT**

Presenter: Yu Yan
Authorship: Yu Yan, Duong T. Ngo, Daniel E. Resasco and Bin Wang - *School of Chemical, Biological and Materials Engineering, University of Oklahoma*

11:10 T27: **Modeling Infrared Spectra of Ordered Monolayers**

Presenter: Nafisa Amin
Authorship: Nafisa Amin, Soumya Bhattacharya and Lloyd A. Bumm - *Homer L. Dodge Department of Physics and Astronomy, University of Oklahoma*

11:30 T28: **Probing Internal Structure of Alkanethiol Self-Assembled Monolayers with STM**

Presenter: Mitchell P. Yothers
Authorship: Mitchell P. Yothers, Soumya Bhattacharya and Lloyd A. Bumm - *Homer L. Dodge Department of Physics and Astronomy, University of Oklahoma*

11:50 T29: **Thermally Stable Nano-Thin Film of Ag on Au(111)**

Presenter: Kennedy Boyd
Authorship: Kennedy Boyd, Jesse A. Phillips, Lauren K. Harville, Gabriel LeBlanc and Erin V. Iski - *Department of Chemistry and Biochemistry, University of Tulsa*

Saturday, April 13, 2:00 PM. S2: Biochemistry/Structural Biology
Session Chair: Rakhi Rajan (University of Oklahoma)
Location: Room N

2:00 T30: **Differential HDX-MS for Characterizing Protein-protein Interaction**

Presenter: Jiwon Kang
Authorship: Jiwon Kang, Zhe Wang, Mulin Fang, Kellye A Cupp-Sutton and Si Wu - *Department of Chemistry and Biochemistry, University of Oklahoma*

2:20 T31: **Subhemolytic Shear Environment and Conformational Changes in Transmembrane Protein**

Presenter: James Buerck
Authorship: James Buerck and Edgar A. O'Rear - *School of Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK*

2:40 T32: **Bridge Helix of CAS9 Contributes to Target DNA Cleavage Selectivity**

Presenter: Kesavan Babu
Authorship: Kesavan Babu[1], Nadia Amrani[2], Wei Jiang[3], Peter Z. Qin[3] and Rakhi Rajan[1] - *[1]Department of Chemistry and Biochemistry, University of Oklahoma[2], RNA Therapeutics Institute, University of Massachusetts Medical School[3], Department of Chemistry, University of Southern California*

3:00 **Coffee Break**

3:30 T33: **NMR and Molecular Dynamics Simulation Reveal the Impact of V23D Mutation on the Function of Yeast Oligosaccharyltransferase Subunit OST4P**

Presenter: Bharat Chaudhary
Authorship: Bharat Chaudhary, David Z. Zoetewey and Smita Mohanty - *Oklahoma State University*

3:50 T34: **Structure and Function Studies of Asian Corn Borer Ostrinia Furnacalis Pheromone Binding Protein2**

Presenter: Salik Ram Dahal
Authorship: Salik Ram Dahal - *Oklahoma State University*

4:10 T35: **Combination Therapy of Prostate Cancer: PARP Inhibitor Synergizes the Therapeutic Efficacy of Doxorubicin**

Presenter: Himanshu Polara
Authorship: Himanshu Polara, Momin Ansare, Saloni Darji, Tuhina Banerjee and Santimukul Santra - *Department of Chemistry, Pittsburg State University*

Saturday, April 13, 2:00 PM. S7: Computational Chemistry
Session Chair: Yihan Shao (University of Oklahoma)
Location: Room K

2:00 T36: **Efficient and Accurate Estimation of Free Energy Profiles for Enzymatic Reactions**

Presenter: Xiaoliang Pan
Authorship: Xiaoliang Pan[1], Ye Mei[2] and Yihan Shao[1] - *[1]Department of Chemistry and Biochemistry, University of Oklahoma and [2]State Key Laboratory of Precision Spectrosc., East China Normal University*

2:20 T37: **New Insights on the Au/S Interface of the Alkanethiol Self-Assembled Monolayers on Au(111): A DFT Study**

Presenter: S. Bhattacharya
Authorship: S. Bhattacharya[1], G. Speyer[4], D. K. Ferry[3], G. Zhou[2], L. Huang[2] and Lloyd A. Bumm[1] - *[1]Physics and Astronomy and [2]Chemical Biological and Materials Engineering at the University of Oklahoma, and [3]Electrical, Computer and Energy Engineering and [4]Research Computing at Arizona State University*

2:40 T38: **Effects of Solvents on Hydrogen Adsorption on a Palladium Surface**

Presenter: Jacob Crouch
Authorship: Jacob Crouch and Bin Wang - *School of Chemical, Biological and Materials Engineering, University of Oklahoma*

3:00 **Coffee Break**

3:30 T39: **Atomistic Force Field Model Development for the Thiolate/Defective Au(111) Interface**

Presenter: Guobing Zhou
Authorship: Guobing Zhou, Lloyd A. Bumm and Liangliang Huang - *School of Chemical, Biological and Materials Engineering and Department of Physics and Astronomy, University of Oklahoma*

3:50 T40: **Computational Vibrational Analysis of Large Systems - Lomustine Matrix Isolated in 20 K Argon**

Presenter: William B. Collier
Authorship: William B. Collier, Zackory D. Boisselle, Jonathan W. Davis, Mathew S. Faso, Austin D. Ryden and Gary Ritzhaupt - *Department of Chemistry, Oral Roberts University*

4:10 T41: **Molecular Dynamics Study of Protein Mortalin and Anti-Cancer Compounds Flex-Hets**

Presenter: Dipendra Bhandari
Authorship: Dipendra Bhandari, Maryam Mashayekhi, Gil Repa and Donghua Zhou - *Department of Physics, Oklahoma State University*

Saturday, April 13, 2:00 PM. S8: Inorganic Chemistry
Session Chair: Laleh Tahsini (Oklahoma State University)
Location: Room L

2:00 T42: **Metalloheme-NO_x Intermediates in the Global N-Cycle**

Presenter: Erwin G. Abucayon
Authorship: Erwin G. Abucayon, Douglas R. Powell and George B. Richter-Addo - *Department of Chemistry and Biochemistry, University of Oklahoma*

2:20 T43: **N-Heterocyclic Carbene Copper Complexes as Attractive Targets in Strong Bonds Activation and Catalysis**

Presenter: Laleh Tahsini
Authorship: Laleh Tahsini, Jennifer Minnick, Doaa Domyati and Reza Latifi - *Department of Chemistry, Oklahoma State University*

2:40 T44: **Synthesis and Thermal Decomposition of Iron 2-Oximinocarboxylate Complexes**

Presenter: Waleed Alamier
Authorship: Waleed Alamier and Allen Apblett - *Oklahoma State University*

3:00 **Coffee Break**

3:30 T45: **The Amazing World of Nitrogen Oxides: Relevance to the Global Nitrogen Cycle**

Presenter: George B. Richter-Addo
Authorship: George B. Richter-Addo - *Price Family Foundation of Structural Biology, Department of Chemistry and Biochemistry, University of Oklahoma*

3:50 T46: **Role of Water in Aldol Condensation Reactions Catalyzed by MCM-41 Functionalized with Sulfonic Groups**

Presenter: Gengnan Li
Authorship: Gengnan Li, Duong T. Ngo, Tuong V. Bui, Bin Wang and Daniel E. Resasco - *School of Chemical, Biological and Materials Engineering and Center for Interfacial Reaction Engineering (CIRE), University of Oklahoma*

4:10 T47: **Photovoltaic Response of Germanium(II) Sulfide Synthesized by Sublimation**

Presenter: Brandon K Durant
Authorship: Brandon Durant[1, 2] and Bruce A. Parkinson[2] - *[2] Homer L. Dodge Dept. of Physics and Astronomy, University of Oklahoma, [2]Department of Chemistry, University of Wyoming*

Saturday, April 13, 2:00 PM. S9: Materials Chemistry
Session Chair: Sanjeewa Gamagedara (University of Central Oklahoma)
Location: Room P

2:00 T48: **A Novel Method for Fabricating Ni, Cu and Zn Oxide Thin Films by Hydrolysis of Their Acetates**

Presenter: Dewan Russel Rahman
Authorship: Dewan Russel Rahman and Allen Apblett - *Oklahoma State University*

2:20 T49: **Reactive Molecular Dynamics Simulation of Cellulose and its Property Evolution under Pyrolysis Conditions**

Presenter: Qi Qiao
Authorship: Qi Qiao and Liangliang Huang - *School of Chemical, Biological and Materials Engineering, University of Oklahoma*

2:40 T50: **Observation of Amino Acid-assisted Island Formation on Au(111) using EC-STM**

Presenter: Jesse Phillips
Authorship: Jesse Phillips, I. Baljak, K. Boyd, L. Harville and E.V. Iski - *University of Tulsa*

3:00 **Coffee Break**

3:30 T51: **Microstructured Hydrogel Surfaces for Stem Cell Differentiation**

Presenter: Y. Vasquez
Authorship: Y. Vasquez[1], Hasani J. Jayasinghe[1] and Sundar Madihally[2] - *[1]Department of Chemistry, and [2]Department of Chemical Engineering, Oklahoma State University*

3:50 T52: **Characterization of Solid Composite Electrolytes for use in Solid State Batteries, the Effect of Grain Boundaries**

Presenter: John W. Ostrander
Authorship: John Ostrander and Dale C. Teeters - *University of Tulsa, Department of Chemistry and Biochemistry*

4:10 T53: **XPS Characterization of Dilute Nitride GaInAs Materials**

Presenter: Samantha Scudder
Authorship: Samantha Scudder and Nicholas Materer - *Department of Chemistry, Oklahoma State University*

Saturday, April 13, 2:00 PM. S10: Oklahoma History of Chemistry
Session Chair: Cheryl Frech (University of Central Oklahoma)
Location: Room J

2:00 T54: **100 Years and Counting: History of the Oklahoma Section of the ACS**

Presenter: Cheryl B. Frech
Authorship: Cheryl B. Frech - *University of Central Oklahoma*

2:20 T55: **A Salute to Excellence: 60 Years of Successful Programing: Wichita Falls-Duncan Section**

Presenter: E. Ann Nalley
Authorship: E. Ann Nalley - *Department of Chemistry, Physics & Engineering, Cameron University*

2:40 T56: **Twenty-Six Years of Chemistry at the Oklahoma School of Science and Mathematics: An History of Students Academic Excellence**

Presenter: A. K. Fazlur Rahman
Authorship: A. K. Fazlur Rahman - *Chemistry Department, Oklahoma School of Science and Mathematics*

3:00 **Coffee Break**

3:30 T57: **Chemistry at East Central University: 1909 to Present**

Presenter: Dwight L. Myers
Authorship: Dwight L. Myers - *Department of Chemistry and Physics, East Central University*

3:50 T58: **The Tulsa Section of American Chemical Society: From Oil and Fluorine to Fluorine and Nanotechnology**

Presenter: Dale Teeters
Authorship: Dale Teeters - *Department of Chemistry and Biochemistry, University of Tulsa*

4:10 T59: **Chemistry in Southeast Oklahoma**

Presenter: Tim Smith
Authorship: Dr. Tim Smith - *Department of Chemistry, Computer and Physical Sciences, Southeastern Oklahoma State University*

4:30 T60: **The History of Chemistry at OU**

Presenter: George B. Richter-Addo
Authorship: George B. Richter-Addo - *Price Family Foundation of Structural Biology, Department of Chemistry and Biochemistry, University of Oklahoma*

Saturday, April 13, 2:00 PM. S5: Organic and Medicinal Chemistry II
Session Chair: Anthony Burgett (University of Oklahoma)
Location: Room O

2:00 T61: **Chemoenzymatic Diversification of Daptomycin**

Presenter: Johanna Masterson
Authorship: Johanna Masterson, Erin Scull, Eric Gardner and Shanteri Singh - *University of Oklahoma*

2:20 T62: **Virtual Screening-Guided Identification of Novel LDHA Inhibitor Against Cancer**

Presenter: Horrick Sharma
Authorship: Horrick Sharma and Toby Nix - *Department of Pharmaceutical Sciences, College of Pharmacy, Southwestern Oklahoma State University*

2:40 T63: **Rhenium(IV) Catalyzed Addition of Radicals Generated from Activated Alcohols to Olefins**

Presenter: Chandrasekhar Bandari
Authorship: Chandrasekhar Bandari and Kenneth M. Nicholas - *Department of Chemistry and Biochemistry, University of Oklahoma*

3:00 **Coffee Break**

3:30 T64: **Antibiofilm Synergy of β-Lactams and Branched Polyethylenimine Against Methicillin-Resistant Staphylococcus Epidermidis**

Presenter: Anh K. Lam
Authorship: Anh K. Lam, Cassandra L. Wouters, Erika L. Moen, Jennifer Pusavat, and Charles V. Rice - *Department of Chemistry and Biochemistry, University of Oklahoma*

3:50 T65: **Transition Metal Catalyzed Synthesis of Unsymmetrically Substituted Triazolium Salts**

Presenter: Scott M. Hutchinson
Authorship: Scott M. Hutchinson and Jeanne L. Bolliger - *Oklahoma State University*

4:10 T66: **Photoredox 1,4-Skip Dienes: A Simultaneous Birch-Like Dearomatization and C-C Bond Formation**

Presenter: Jon I. Day
Authorship: Jon I. Day, Mohammed Bani Khaled and Jimmie D. Weaver III - *Oklahoma State University*

Poster Session at the 64th Annual Pentasectional Meeting of the American Chemical Society

Poster Session

8:30 AM - 10:30 AM Ballroom

Ref.	Presenter	Title and Authorship
P1	Quentin Avila	A Multi-Approach Strategy to Improve the Spectrum of CLPP Activators - Quentin Avila - *Department of Chemistry and Biochemistry, Stephenson Life Sciences Research Center, University of Oklahoma*
P2	Matthew Hamilton and Alyssa Noel	A Single Step Selective Polyfluoroarylation of Amides - Matthew Hamilton, Alyssa Noel, Jimmie Weaver, Jon Day, Brock Keen and Daniel Jespersen - *Oklahoma State University*
P3	Kimberly L. Bennett	Adapting a Thin-Layer Chromatography Method to an At-Home Kit for Lichenology - Kimberly L. Bennett and Stephanie L. Skiles - *Department of Chemistry, University of Central Oklahoma*
P4	Hongyan Ma	Bioactive Natural Products Analysis in Complex Microbial Environment by Metabolomics Study - Hongyan Ma, Michaela Murphy and Robert Cichewicz - *Department of Chemistry and Biochemistry, Natural Products Discovery Group and Institute for Natural Products Applications and Research Technologies, University of Oklahoma*
P5	Matt Swann	Catalyst Design for Small Molecule Splitting - Matt Swann and Ken Nicholas - *University of Oklahoma*
P6	Shermali Ratnasinghe and Shevon Alexander	Characterization of Diethyl-2-(4-Hydroxy-3-Nitrobenzilidene) Malonate and Diethyl-2-(5-Hydroxy-2-Nitrobenzylidene) Malonate with Electrochemistry and UV-VIS Spectroscopy - Shermali Ratnasinghe, Shevon Alexander, Christopher A. Hansen and Jianguo Shao - *Midwestern State University*
P7	Michael Harris	Characterization of Gamma-Sarcoglycan by NMR - Michael Harris, Michael Jamaleddine and Gabriel A. Cook - *Oklahoma State University*
P8	David A. Rogers	Chlorination of Deactivated Arenes and Heteroarenes with Trichloroisocyanuric Acid under Visible-Light Photoredox Catalytic Conditions - David A. Rogers and Angus A. Lamar - *University of Tulsa*

P9	Shelby Smoot, Dorothy Walton and Sonia Nsenga	Classification of 4DIU - Shelby Smoot,[1] Dorothy Walton[1] and Sonia Nsenga[1] - *[1]Department of Biology, Oklahoma Christian University and [2]Rochester Institute of Technology*
P10	Matthew Finneran	Cloning ORP Protein Family Members for Novel Therapeutic Drug Development - Matthew Finneran, Juan Nunez, Naga Rama Kothapalli and Anthony Burgett - *University of Oklahoma*
P11	Nelson McEwen	Comparing and Contrasting Undergraduate Organic Chemistry Textbooks - Nelson McEwen, Donna J Nelson, Mason Brown, Ndry Konakou, Rachel Blanche, Paula Rueda Paz, Erin Haastrup and Jaclyn Miller - *Department of Chemistry and Biochemistry, University of Oklahoma*
P12	Uendi Pustina	Computational Study of Volatile Aluminum Hydroxide $Al(OH)_3$ - Uendi Pustina and Dwight L. Myers - *East Central University, Department of Chemistry and Physics*
P13	Jonathan W. Davis, Mathew S. Faso and Austin D. Ryden	Computational Vibrational Analysis of Large Systems - Lomustine Matrix Isolated in 20 K Argon - William B. Collier, Zackory D. Boisselle, Jonathan W. Davis, Mathew S. Faso, Austin D. Ryden and Gary Ritzhaupt - *Department of Chemistry, Oral Roberts University*
P14	Ishaq Alalq	Controlling the Acidity of Phosphonate Ligands over Amorphous Silica - Ishaq Alalq and Bin Wang - *School of Chemical, Biological, and Material Engineering University of Oklahoma*
P15	Austin Curnutt	Correlation of Microstructural and Viscoelastic Properties of Mucin Biopolymer in Response to pH and $[Ca^{2+}]$ - Austin Curnutt, Kaylee Smith, Emily Darrow and Keisha B. Walters - *School of Chemical, Biological and Materials Engineering, University of Oklahoma*
P16	Tanner Martin	Design and Development of Surveys Distributed Through QR Codes to Assist the Pencil-Paper Problem Solving Process in Organic Chemistry - Tanner Martin and Robyn Biggs - *Chemistry and Biochemistry, University of Oklahoma*
P17	Austin R. Anderson	Detection of Shed Syndecan-1 - Austin R. Anderson and Gabriel Cook - *Oklahoma State University*
P18	Garret Morton	Development of an in Vivo Assay for Directed Evolution of Type II-A CRISPR Adaptation - Garret Morton, Mason Van Orden and Rakhi Rajan - *University of Oklahoma*
P19	L. Chooback, L. Thomas, W. E. Karsten and C. Schartz	DHDPS and Antibiotic Drug Design: Kinetics and Structural Studies of Dihydrodipicolinate Synthase and 2-Bromopropionic Acid - L. Chooback, L. Thomas, W. E. Karsten and C. Schartz - *University of Central Oklahoma*

P20	Sarah Hobson	Dissolution of Mackinawite (FES) Facilitated by Dioic Acids under Oxic Conditions - Sarah Hobson,[1] Alejandra Hernandez[1] and Mark A. Nanny[1,2] - *[1]School of Civil Engineering and Environmental Science, Gallogly College of Engineering and [2]Institute for Energy and the Environment, Mewbourne College of Earth and Energy, University of Oklahoma*
P21	Richard Van	Drug Design: Small Molecule Inhibitor for Pro-Apoptotic BAX Protein in Cells - Richard Van, Nicholas Massaro,[1] Xiaoliang Pan,[1] Indrajeet Sharma,[1] Jialing Li° and Yihan Shao[1] - *[1]Univeristy of Oklahoma and [2]University of Oklahoma Health Science Center*
P22	Collin Britten	Effects of Ligand Structure on the Kinetics of ATRP for Monomers Containing Tertiary Amines - Collin Britten, Jorge Carvalho, Kristen Lason, Yokly Leng and Keisha B. Walters - *University of Oklahoma*
P23	Jordan Flower	Epoxide Functionalization and Characterization of Dye-Doped Silica Nanoparticles - Jordan Flower and Nathan Green - *Northeastern State University*
P24	Madison R. Tytanic	Experiential Learning and Observational Learning Applied to Ethics and Diversity - Madison R. Tytanic and Donna J. Nelson - *Department of Chemistry, University of Oklahoma*
P25	Megan Hays	Fabrication and Characterization of Conductive Organic Fibers as Non-Metallic Electrodes for Clinical Applications - Megan Hays,[1] Santosh Adhikari,[1] Bertram Richter,[2] Saadyah Averick[2] and Toby L. Nelson[1] - *[1]Department of Chemistry, Oklahoma State University and [2]System Department of Neurosurgery, Allegheny Health Network*
P26	Jessi J. Gardner	First-Generation Structure-Activity Relationship Studies of 2,3,4,9-Tetrahydro-1H-Carbazol-1-Amines as CpxRA Modulators - Jessi J. Gardner,[1] Yangxiong Li,[1] Katherine R. Fortney,[2] Stanley Spinola,[2] and Adam S. Duerfeldt[1] - *[1]Department of Chemistry and Biochemistry, University of Oklahoma and [2]Department of Microbiology and Immunology, Indiana University School of Medicine*
P27	Nagendra Sastri Yarla	Fragment Based Drug Design and Synthesis of Microsomal Prostaglandin E Synthase-1 and 5-lipoxygenase Dual Inhibitors for Their Preventive and Therapeutic Applications in Inflammatory and Oncologic Diseases - Nagendra Sastri Yarla,[1] Gopal Pathuri,[1] Hariprasad Gali,[2] Anil Singh,[1] Janani Pannerselvam,[1] Venkateshwar Madka[1] and Chinthalapally V. Rao[1] - *[1]Center for Cancer Prevention and Drug Development, Department of Medicine, Hematology-Oncology Section,*

		Stephenson Cancer Center and [2]College of Pharmacy, University of Oklahoma
P28	Dilip Paul	FT-IR Investigation of C-C Bond Formation on TiO_2-based Nanomaterials - Dilip Paul and Jennifer Moffat - *Department of Chemistry, Pittsburg State University*
P29	Rashmi Vadivelu Amarender	Functional Insect Protein Extracts for Food Applications - Rashmi Vadivelu Amarender,[1] Kanika Bhargava,[1] Aaron Dossey[2] and Sanjeewa Gamagedara[3] - *[1]Department of Human Environmental Sciences, University of Central Oklahoma, [2]All Things Bugs LLC, and [3]Department of Chemistry, University of Central Oklahoma*
P30	Megan D. Hopkins	Heteroaryl Aldehyde Substrates for use in a Non-Traditional Method of N-Sulfonyl Imine Formation - Megan D. Hopkins, Felagot Abebe, Robert J. Sheaff and Angus A. Lamar - *University of Tulsa*
P31	Lizbeth Robles-Fernandez	High Temperature Solid State Reactions of Silicon, Titanium and Yttrium Oxides - Lizbeth Robles-Fern, Fernando Salazar-Salas and Dwight L. Myers - *East Central University, Department of Chemistry and Physics*
P32	Stewart Bragg Younger-Mertz	High-symmetry Low-coordinate Complexes of Cerium(III) and Uranium(III): Tris[bis(trimethylsilyl)amido] Phosphine Oxide Compounds for Empirical f-Element Electronic Structure Investigations - Stewart Bragg Younger-Mertz, Doug J. Powell, Donna J. Nelson and Robert K. Thomson - *University of Oklahoma*
P33	Stewart Bragg Younger-Mertz	Synthesis of Tris(silylamido) Phosphinimide Complexes of Uranium(IV) and Cerium(IV) via Protonolysis and Fluorotrimethylsilane Elimination - Stewart Bragg Younger-Mertz, Donna J. Nelson and Robert K. Thomson - *University of Oklahoma*
P34	Vy Thao Nguyen	Identification of Different Protonic Species in H-ZSM5 - Vy Thao Nguyen,[1] Jeffey White[2]and Bin Wang[1] - *[1]School of Chemical, Biological, Materials Engineering, University of Oklahoma and [2]School of Chemical Engineering, Oklahoma State University*
P35	Morgan Thurman and Jerrik Burson	Instrumental Hardware-Software Interfacing - Morgan Thurman, Jerrik Burson and Shawna York - *Southern Nazarene University*

P36	Fatoumata Ide Seyni	Interfacial Toughness of Diblock Carbon Nanotubes Reinforced Immiscible Polymer Blends - Fatoumata Ide Seyni, Lawrence Barrett, Brian P. Grady and Steven Crossley - *School of Chemical, Biological and Materials Engineering, University of Oklahoma*
P37	Megan Shelton and Morgan Freeman	Investigation of Enzyme 3CBW Function - Megan Shelton ,[1] Morgan Freeman,[1] Lindsey Long[1] and Biochemistry Authentic Scientific Inquiry Lab group (BASIL)[2] - *[1]Department of Biology, Oklahoma Christian University and [2]Rochester Institute of Technology*
P38	Restituto Paris and Stephen Myers	Investigation of Microwave and Ultrasonic Energy in the Synthesis of Heterocycles Related to Medicinal Chemistry - Restituto Paris, Stephen Myers and E. Ann Nalley - *Department of Chemistry, Physics and Engineering, Cameron University*
P39	Lindsay Maez	Investigation of Microwave Energy in the Synthesis of Heterocycles Related to Medicinal Chemistry - Lindsay Maez, Victoria Brown and E. Ann Nalley - *Department of Chemistry, Physics and Engineering, Cameron University*
P40	Theo A Rusmore	Kinetic Resolution of Chiral Phosphines via Metal-Catalyzed OAT - Theo A Rusmore, Daniel T Glatzhofer and Kenneth M Nicholas - *University of Oklahoma*
P41	Xavier Martinez	Lanthanum Iron Sulfide as an Electrocatalyst for Water Splitting Application - Xavier Martinez, K. Siam, P.K. Kahol and Ram K. Gupta - *Pittsburg State University*
P42	Karina Flores	Metabolomic Screening of the Effects of Carnitine Treatment during in Vitro T Cruzi Parasite Infection - Karina Flores,[1] Ekram Hossain[2] and Laura-Isobel McCall[2] - *[1]Department of Biology and [2]Department of Chemistry and Biochemistry, University of Oklahoma*
P43	Abdulmajeed Alayyaf	Metal Oxides Nanoparticles Catalysts for Carbon-Carbon Bond Formation and Intermolecular Rearrangement Reactions - Abdulmajeed Alayyaf and Allen Apblett - *Oklahoma State University*
P44	Theresa Hinkle	Microwave Synthesis of Novel Esters using Sulfuric Acid and Imidazole as Catalysts - Theresa Hinkle and E. Ann Nalley - *Department of Chemistry, Physics & Engineering, Cameron University*
P45	Addy J. Evans	Modeling Water using Spherical Harmonic Interactions - Addy J. Evans and Christopher J. Fennell - *Department of Physics and Department of Chemistry, Oklahoma State University*

P46	Camila Zequine	Molybdenum-Based Metal Oxides for Overall Water Splitting and Supercapacitors - Camila Zequine, Khamis Siam, Pawan K. Kahol and Ram K. Gupta - *Pittsburg State University*
P47	Jinesh Niroula	New Bioassays for Diabetes Autoantibodies with Binding Kinetics - Jinesh Niroula, Gayan Premaratne and Sadagopan Krishnan - *Department of Chemistry, Oklahoma State University*
P48	Jeremy R. Zink	Nitroxyl (HNO) Complexes of Ruthenium Porphyrins - Jeremy R. Zink, Erwin G. Abucayon and George B. Richter-Addo - *Department of Chemistry and Biochemistry, University of Oklahoma*
P49	Michael R. Jordan	Oxidation-Reduction Potential as a Method for Determining Water Quality - Michael R. Jordan, Isaac Gray, Stephanie Hayes, Fernando Morillas and Devika Wilson - *Oklahoma Baptist University*
P50	Kwame Glinton	Phosphorescent Three-Coordinate Copper(I)-NHC Complexes: Synthesis, Characterization and Photoluminescent Studies - Kwame Glinton, Reza Latifi, Shepard Cockrell and Laleh Tahsini - *Oklahoma State University*
P51	Stephen J. McBride	Photocatalytic Degradation of Acesulfame Potassium using TiO_2/UVA, $S_2O_8^{2-}/Fe^{2+}$/UVA, and H_2O_2/Fe^{2+}/UVA Processes - Stephen J. McBride and Clinton D. Bryan - *Cameron University, Department of Chemistry, Physics, and Engineering*
P52	Nick Meaux	Photophysical Dynamics of Probemolecules Inside Reverse Micelles - Nick Meaux and Rajesh Nayak - *Cameron University*
P53	Jennifer L. Minnick	Pincer-Type N-Heterocyclic Carbene Copper (I) Complexes and Their Utilization in Transfer Hydrogenation Reaction - Jennifer L. Minnick, and Laleh Tahsini - *Oklahoma State University*
P54	Chaoyi Wu	Principal Coordinate Analysis of Gastrointestinal Tissue Sections from Infected and Uninfected Animals in Chagas Disease - Chaoyi Wu, Ekram Hossain and Laura-Isobel McCall - *Department of Chemistry and Biochemistry, University of Oklahoma*
P55	Aaron Zahn	Protein YXIM_BACsu Putative Function Through Computational and Kinetic Analysis - Aaron Zahn - *Oklahoma Christian University*
P56	Joel K. Annor-Gyamfi	Quinazolin-4(3H)-Ones and 5,6-Dihydropyrimidin-4(3H)-Ones from Beta-Aminoamides and Orthoesters - Joel K. Annor-Gyamfi,[1] Joshua T. Gavin[2] and Richard A. Bunce[1] - *[1]Oklahoma State University, [2]REU Student (Summer 2018)*

P57	Rajendra Maharjan	Seeding Ice Crystallization in Molecular Simulations - Rajendra Maharjan and Christopher J. Fennell - *Department of Chemistry, Oklahoma State University*
P58	Alejandra Hernandez-Santana	Shewanella Oneidensis MR-1, an Iron Reducing Bacterium, Catalyzes the Oxidation of Metallic Iron - Alejandra Hernandez-Santana and Mark Nanny - *The University of Oklahoma*
P59	Daniel Jespersen and Brockton Keen	Solubility of Iridium and Ruthenium Organometallic Photoredox Catalysts - Daniel Jespersen,[1] Brockton Keen,[1] Jon I. Day,[1] Anuradha Singh,[2] Justin Briles,[1] Duncan Mullins,[1] Jimmie D. Weaver[1,2] - *[1]Oklahoma State University and [2]Weaver Labs LLC*
P60	Menuka Adhikari	Solution Phase Conversion of β-FeOOH to FeP and FeS_2 Nanoparticles - Menuka Adhikari and Y. Vasquez - *Department of Chemistry, Oklahoma State University*
P61	Viridiana E. Herrera	Structural and Functional Changes Induced by Alkyl RNO Binding to Myoglobin and Hemoglobin - Viridiana E. Herrera, Samantha M. Powell, Kiana Prather, Nancy T. Nguyen, Bing Wang, Jun Yi and George B. Richter-Addo - *Price Family Foundation Institute of Structural Biology, Department of Chemistry and Biochemistry, University of Oklahoma, Norman, OK*
P62	Jared Haymore	Structural Characterization of Clostridioides Difficile Response Regulator (RR_1586) Protein - Jared Haymore, Smita Menon, Skyler Hebdon and Ann H. West - *University of Oklahoma Department of Chemistry and Biochemistry*
P63	Samantha M. Powell	Structural Characterization of Hemoglobin Adducts with Hydroxylamines - Samantha M. Powell, Viridiana E. Herrera, Kiana Prather, Nancy Nguyen and George B. Richter-Addo - *Price Family Foundation Institute of Structural Biology and Department of Chemistry and Biochemistry, University of Oklahoma*
P64	Ganga R. Neupane	Structural, Optical and Electrical Properties of Co- and Fe-doped ZnO Nanoparticles Synthesized by Microwave Method - Ganga R. Neupane, Amrit Kaphle, Rusiri Rathnasekara and Parameswar Harikumar - *University of Tulsa*
P65	Katrina Betz and Maxwell Archer	Study of Iodine Distribution and Stability in Western Oklahoma Brine Waters - Katrina Betz,[1] Maxwell Archer,[1] Jason R. Wickham[1] and David Edlin[2] - *[1]Department of Natural Science, Northwestern Oklahoma State University and [2]Iofina, Alva, OK*

P66	Tyler Souza	Survey of Lake Water Quality Across Oklahoma - Tyler Souza and Shawna York - *Southern Nazarene University Department of Chemistry*
P67	Mha Albqmi	Synthesis and Characterization of Different Lanthanum Phosphate Phases - Mha Albqmi and Allen Apblett - *Oklahoma State University*
P68	Michael Smith	Synthesis and Characterization of Oligonucleotide Conjugated Gold Nanorods - Michael Smith and Nathan Green - *Northeastern State University*
P69	Brandon S. Abbott	Synthesis and Surface Modification of Silica Nanoparticles - Brandon S. Abbott, Jorge Carvalho, Luis Trevisi and Keisha B. Walters - *School of Chemical, Biological and Materials Engineering, University of Oklahoma*
P70	Oladayo Seweje	Synthesis of Cyclic Imides using Microwave Radiation - Oladayo Seweje and E. Ann Nalley - *Department of Chemistry, Physics and Engineering, Cameron University*
P71	Khalid Alrashidi	Synthesis of Lanthanide Molybdates via Reaction of Molybdenum(VI) Oxide with Aqueous Acetate Salts - Khalid Alrashidi and Allen Apblett - *Oklahoma State University*
P72	Mengmeng Zhai	Highly Efficient Non-Viral VEGF Gene Delivery to STEM Cells by Lipid Based Nanoparticles - Mengmeng Zhai and Chuanbin Mao - *Department of Chemistry and Biochemistry, University of Oklahoma*
P73	Tyler Gore	Synthesis, Functionalization, and Thermal Characterization of Monodispersed Dye-Doped Silica Nanoparticles - Tyler Gore, Marukh Zia and Nathaniel Green - *Northeastern State University*
P74	Lauren Haygood	Testing an Ion Chromatography Technique to Separate Rare Earth Elements from Major Cations in Carbonate Minerals - Lauren Haygood and Bethany Theiling - *Department of Geosciences, University of Tulsa*
P75	Susan J. Schroeder	The Challenges of Predicting Viral RNA with Multiple Functional Structures - Susan J. Schroeder - *University of Oklahoma*
P76	Victoria Anderson	The Chemical, Genetic, and Geographical Diversity of the Genus Alternaria in North America - Victoria Anderson,[1,2] Robert Cichewicz,[1,2] Laura-Isobel McCall,[2] Karen Wendt[1,2] - *[1]Natural Product Discovery Group, Institute for Natural Products Applications and Research Technologies and [2]Department of Chemistry and Biochemistry, Stephenson Life Science Research Center, University of Oklahoma*

P77	Alexander Chandler	The Synthesis of Aluminum Clusters using Naphthalene Based Crystallization Agents - Alexander Chandler, Maggie Ward, Emily Cowen, Cha'Lita Thomppson and Eric S. Eitrheim - *University of Central Oklahoma, Department of Chemistry*
P78	Paidaishe F. Mangwiro	The Synthesis of Ethyl 4-(4-Hydroxyphenyl)-6-Methyl-2-Oxo-1,2,3,4-Tetrahydropyrimidine-5-Carboxylate: Comparison of Two Methods - Lois Ablin and Paidaishe F. Mangwiro - *Department of Biology and Chemistry, Oral Roberts University*
P79	Patrice Lewis	The Synthesis of Ethyl-4-(4-dimethylaminophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate and an Investigation of its Cytotoxic Effect on MDA-MB-468 Tumorigenic Versus Mcf-10a Non-tumorigenic Mammary Epithelia - Lois A. Ablin, Patrice Lewis and William P. Ranahan - *Department of Biology and Chemistry, Oral Roberts University*
P80	Bailey Smoot	Thermodynamic Analysis of the RAS Q61 Moiety via Non-Equilibrium Entropic Changes in GTP Hydrolysis - Bailey Smoot, Salvatore Capotosto, Preet Sharma, Randal Hallford - *Midwestern State University*
P81	Gautham	Using Biomarkers to Predict Treatment Efficacy for Chagas' Disease Through Metabolite Profile - Gautham,[1] Laura-Isobel McCall,[1] Ekram Hossain,[1] Igor C. Almeida[2] and Joaquim Gascón[3] - *[1]University of Oklahoma, [2]University of Texas, El Paso and [3]Institute of Global Health, Barcelona, Spain.*
P82	Rachel Ann Hoffmeister	Using Bridged Nucleic Acids for Detection of Phosphatidyl 3-Kinase Catalytic Subunit Alpha Mutation - Rachel Ann Hoffmeister and Sung-Kun (Sean) Kim - *Northeastern State University*
P83	Elham Fazelpour	Using Residue Interactions to Predict Biomolecular Diffusion - Elham Fazelpour,[1] Jennifer M. Haseleu[1, 2] and Christopher J. Fennell[1] - *[1]Department of Chemistry, Oklahoma State University and [2]Department of Chemistry, Saint Vincent College*

Lecture Abstracts

T1: Assessment of Metal Impurities in Cosmetics
Presenter: Sahr A. Alsherari
Authors and Affiliation: Sahr A. Alsherari and Allen Apblett - *Department of Chemistry, Oklahoma State University*

Millions of people use cosmetics daily worldwide; therefore, it is very important that they are safely regulated to minimize the health hazards people may encounter when using them. An investigation was performed on more than one hundred cosmetic samples from countries all over the world, checking them for toxic metals such as lead. (USA, Spain, Germany, Italy, Saudi Arabia, Jordan, Lebanon, Turkey, Korea, China, Taiwan, Thailand, Indonesia, Czech Republic, Hong Kong, France and India). The investigation found that some of the cosmetics did contain toxic metals like such as lead, it also revealed that a couple of the samples had a very high concentration of rubidium. The cosmetic samples were acid digested and then analyzed using Agilent's Microwave Plasma-Atomic Emission Spectrometer (MP-AES). Some of the samples, exceeded The US Food and Drug Administration (FDA) maximum recommended levels for lead in cosmetics. Furthermore, there are no regulatory or guidance standards existing for rubidium set by the FDA. The samples in the study were also investigated using an EDAX Orbis Vision X-Ray fluorescence spectrometer to measure the impurities in cosmetics, which is considered a non-destructive method for analyzing samples rather than using the acid digestion method. This part of the investigation consisted of making lead XRF standards using silica gel. This allowed the cosmetic samples to be quantitatively analyzed for lead without destroying the samples. The results of this study were compared to the concentrations of lead determined using MPAES, to validate each method.

T2: Simultaneous Determination of Renal Cell Carcinoma Biomarkers in Urine using Water-Rich Mobile Phases
Presenter: Kaushalya Sharma Dahal
Authors and Affiliation: Kaushalya Sharma Dahal and Barry K. Lavine - *Department of Chemistry, Oklahoma State University*

Renal Cell Carcinoma (RCC) is the third most common form of kidney cancer. Current methods to diagnose RCC in patients are based on magnetic resonance imaging and computerized tomography scans. Unfortunately, these methods are not suited for routine population screening. Previous work performed in our laboratory has shown that reverse phase liquid chromatography (RPLC) is an accurate and effective method to characterize RCC biomarkers (e.g., creatinine, quinolinic acid, gentisic acid and 4- hydroxybenzoic acid) in urine. Using water-rich mobile phases (e.g., 0.1% butanol in water with 0.6% acetic acid), separation of these four biomarkers in synthetic urine is obtained with a Zorbax C_{18} column, which is not the case with traditional RPLC mobile phases. Calibration curves for each biomarker are linear over a thousand parts per million range. Recovery tests at low (20 ppm), middle (100 ppm) and high (700 ppm) concentrations revealed that the proposed RPLC

method is effective at high biomarker concentrations but detection at low and mid-range concentrations is limited due to the background of the urine matrix.

T3: Library Search Prefilters for Manufacturer's Automotive Paints using Simulated Attenuated Total Reflection (ATR) Spectra
Presenter: Francis Kwofie
Authors and Affiliation: Francis Kwofie, Barry K. Lavine and Nuwan D. Perera - *Department of Chemistry, Oklahoma State University*

Pattern recognition techniques have been applied to the transmission infrared (IR) spectral libraries of the Paint Data Query (PDQ) database to differentiate between nonidentical but similar IR spectra of automotive paints. To tackle the problem of library searching, search prefilters were developed to identify the vehicle make from IR spectra of the clear coat, surfacer–primer, and e-coat layers. To develop these search prefilters with the appropriate degree of accuracy, IR spectra from the PDQ database were transformed into attenuated total reflection (ATR) data to minimize the effect of peak shifting that occurs due to the use of high-pressure diamond anvil cells to collect IR spectra for inclusion in PDQ. The transformed spectral data were then preprocessed using the discrete wavelet transform to enhance subtle but significant features in the IR spectra. Wavelet coefficients characteristic of vehicle make were identified using a genetic algorithm for pattern recognition and feature selection. Search prefilters to identify automotive manufacturers through IR spectra obtained from a paint chip recovered at a crime scene were developed using 1652 original manufacturer's paint systems spanning six manufacturers (General Motors, Chrysler, Ford, Honda, Nissan, and Toyota) within a limited production year range (2000–2006). Search prefilters for vehicle manufacturer developed as part of this study were successfully validated using transformed IR spectral data obtained directly from the PDQ database. Information obtained from these search prefilters can serve to quantify the discrimination power of original automotive paint encountered in casework and further efforts to succinctly communicate trace evidential significance to the courts.

T4: Hexadecyl Imidazolium Ionic Liquid Stationary Phase Bonded to Silica Microparticles
Presenter: Nilushi Paranamana
Authors and Affiliation: Nilushi Paranamana and Ziad El Rassi - *Department of Chemistry, Oklahoma State University*

Hexadecyl imidazolium functionalized silica stationary phase was obtained by first bonding the surface of 5 μm silica particles with 3-chloropropyl trimethoxysilane forming the so-called a primary sublayer followed by attaching a top layer of hexadecyl imidazole. This resulted in the formation of ionic liquid based reversed phase column, which was evaluated in the separation of a variety of small molecules and proteins with high separation efficiencies under a wide range of elution conditions. Concurrently, the retention behaviors of these molecules were investigated in detail. The hexadecyl imidazolium column thus obtained exhibited relatively symmetrical peak shapes and high separation efficiencies for the studied analytes with a wide array of functional groups including ionizable analytes. An advantage of the ionic liquid stationary phases is their ability to handle aqueous-rich mobile

phases without undergoing significant hydrolytic degradation and in turn maintaining stable solute retention over an extended period of use. In addition, the observed unique retention characteristics can be attributed to the multi interactions of these phases with solutes including hydrophobic, electrostatic, π–π and hydrogen bonding interactions.

T5: Chemical Cartography: Resolving Small Molecule Spatial Organization by LC-MS/MS and 3D Mapping during Parasitic Infection
Presenter: Laura-Isobel McCall
Authors and Affiliation: Laura-Isobel McCall,[1] Ekram Hossain,[1] Chaoyi Wu,[1] Sharon Lostracco-Johnson,[2] Diane Thomas,[2] Danyang Li,[3] Mitchelle Katemauswa[1] and Camil Gosmanov[1] - *[1]University of Oklahoma, [2]University of California San Diego and [3]Beijing Normal University*

Spatial context is essential in understanding host-microbe-environment interactions and linking chemical structure to biological function. Here, we leveraged a novel integration of analytical chemistry, microbiology and "big data" analytics termed "chemical cartography", to map the spatial distribution of biological small molecules (50-1,500 Dalton) in the gastrointestinal tract of parasite-infected animals. Using a mouse model of infection with the parasite Trypanosoma cruzi, we systematically determined small molecule profiles throughout the gastrointestinal tract of infected and uninfected animals by liquid chromatography tandem mass spectrometry (LC-MS/MS). 3D data reconstruction enabled us to differentiate between sites where infection strongly altered tissue chemical profiles and sites where the effect of the parasite was minor. These results can help determine locations where the parasite is able to hide from the host and persist in the body. Random forest machine learning identified several molecules with altered spatial distribution and abundance in infected animals compared to controls. In particular, acylcarnitine family members showed differential abundance in the esophagus depending on infection status (e.g. elevation of 3-hydroxydodecanoyl carnitine in infected animals), while peak short-chain acylcarnitine levels were more distal in infected animals compared to uninfected controls. Building on these results, treatment of infected mice with 1.3% carnitine in drinking water induced disease tolerance. Overall, these results indicate that chemical cartography is a powerful approach to study host-pathogen interactions and mechanisms of disease. Our results are also helping identify new ways to treat parasitic infections.

T6: Non-Invasive Testing of Bladder Cancer Patient Cells at the Single-Cell Level
Presenter: Ryan C. Bensen
Authors and Affiliation: Ryan C. Bensen, Shawna J. Standke, Devon H. Colby, Naga Rama Kothapalli, Anh T. Le, Anthony W. G. Burgett and Zhibo Yang - *Chemistry and Biochemistry, University of Oklahoma*

Personalized chemotherapeutic drug monitoring development through advanced analytical techniques can increase the success of cancer treatment and produce a greater safety margin. Ideally, a personalized drug regiment would be implemented on an individual bases with specifically prescribed drugs and dosages. To determine optimal dosages, new bioanalytical tools must be established to quantify the amount of drug compound inside of a single cancer cell, ideally, in a non-invasive manner. Here, we provide a novel methodology for quantifying

anti-cancer small molecules inside single suspended cells. This methodology was applied to a suspension leukemia cell line model by incorporating the Single-probe quantitative single cell mass spectrometry method with the integrated cell manipulation platform previously developed in our lab. Importantly, this method was applied for the first-time quantification of the anti-cancer compound, Gemcitabine, from cells isolated from the urine of bladder cancer patients.

T7: Spacer Integration Occurs Differently between Sub-groups of Type II-A CRISPR Systems

Presenter: Mason J. Van Orden
Authors and Affiliation: Mason J. Van Orden, Sydney Newsom and Rakhi Rajan - *Chemistry and Biochemistry, University of Oklahoma*

CRISPR-Cas systems are adaptive immune systems found in bacteria and archaea that provide protection against foreign nucleic acid. Organisms gain immunity by acquiring and inserting short pieces of the invading nucleic acid, termed spacers, into their CRISPR array. The CRISPR array consists of alternating repeats and spacers which, when transcribed, form CRISPR RNA that guide CRISPR-associated (Cas) nucleases to the invading nucleic acid. Preceding the CRISPR array is the leader, which contains the promoter for transcribing the CRISPR array. New spacers are always inserted where the leader region meets the first repeat of the CRISPR array, the leader-repeat junction. In type II-A systems, Cas1 and Cas2 form a complex (Cas1-Cas2) that integrates new spacers by producing two separate cuts at the leader-repeat junction. Our previous bioinformatic studies showed that when comparing leader-repeat junctions amongst type II-A systems from different bacterial genera, three distinct groups of leader ends are present. In the present work, we performed in vitro biochemical analysis using Cas1-Cas2 from different bacteria representing each distinct leader-repeat end. Cas1-Cas2 complexes originating from different groups have different requirements for the first (half-site) and second (full-site) cuts during integration. Group 1 Cas1-Cas2 requires only 12 nucleotides of the leader-repeat junction for half-site integration and is deficient in full-site integration under in vitro conditions. Full-site integration occurred readily with Group 2 Cas1-Cas2 but showed a requirement of upstream leader elements for successful integration. Our results expand the understanding of adaptation and demonstrate the prevalence of multiple mechanisms to integrate spacer sequences.

T8: Oxysterol-Binding Protein as a Prophylactic Antiviral Target of the Natural Product Small Molecule, OSW-1

Presenter: Zachary C. Severance
Authors and Affiliation: Zachary C. Severance, Brett Roberts, Ryan C. Bensen, N. R. Kothapalli, Anh Le, Cori Malinky, Hongyan Ma, Si Wu, William J. Reddig, Earl L. Blewett and Anthony W.G. Burgett - *Chemistry and Biochemistry, University of Oklahoma*

Oxysterol-binding protein (OSBP) and the OSBP-Related Proteins (ORPs) comprise a conserved protein superfamily found in all eukaryotic organisms. The functions of the 12 human OSBP/ORPs are not fully understood; however, these proteins have been implicated in lipid transport, signaling, and regulation activities. OSBP and the ORPs share a ~50kDa C Terminal ligand binding domain which can bind a variety of oxysterols and cholesterol. The

founding member of this protein family, OSBP, a ubiquitously expressed protein, has been shown to act as a scaffold protein in lipid related signaling events, as well as mediating cholesterol trafficking from the ER to the Golgi. Various members of this protein family have been implicated in a variety of human diseases. OSBP has been shown to be vital for the replication of a number of viral human pathogens including Enterovirus genus, Hepatitis C virus (HCV), Dengue, and Zika virus. OSBP is exploited by infected cells to transport cholesterol from the ER into the viral replication organelle (RO) for fortification in virally infected cells. The RO protects the virus from host elements and helps promote viral replication. The natural product compound, OSW-1, is a high affinity ligand for OSBP (K_i 16 +/- 4 nM). Our lab has discovered that OSBP cellular protein levels can be regulated by treatment of the OSW-1-compound. Low dose (1 nM), short term treatment (6 hr) of the OSW-1 compound induces ~90% multigenerational decrease in cellular OSBP levels, and the protein levels remain repressed for over 72 hours after the OSW-1 compound is removed in certain cell lines, with no cytotoxicity or decrease in cellular proliferation. We have been able to exploit this unique, long-term OSBP repression after the OSW-1 compound has been removed to induce a significant prophylactic antiviral response. We have also compared the OSW-1 compound's antiviral efficacy to that of other antiviral compounds that target OSBP (itraconazole, TTP, THEV) and were able to show that OSW-1 causes the most significant antiviral response at ten thousand-fold less concentration compared to the other OSBP targeting antiviral compounds. Further, OSW-1 was the only compound that caused OSBP degradation or repression, and the only compound that was able to generate a prophylactic antiviral response. Additionally, through iTRAQ LC/MS/MS analysis we have determined that the OSW-1-compound does not broadly alter the cellular proteome; suggesting an endogenous OSBP specific regulation system may be triggered upon the binding of specific ligands (i.e. OSW-1). Here we discuss the prophylactic antiviral activity of OSW-1 and potential mechanisms that contribute to the long-term repression of OSBP that confer this prophylactic antiviral response.

T9: Synthesis of Doxorubicin-Based Prodrug and Activatable MR Nanoprobe for the Imaging and Treatment of Cancer

Presenter: Arth Patel
Authors and Affiliation: Arth Patel, Bayan Ahmad Dous and Santimukul Santra - *Department of Chemistry, Pittsburg State University*

In this work, we report a novel gadolinium-DTPA and Doxorubicin-based molecular probe-encapsulating iron oxide nanoparticle for the construction of activatable MRI nanoprobe. In our design, the Gd-DTPA-SS-Doxo is synthesized and is encapsulated within the poly (acrylic acid) (PAA) coating of iron oxide nanoparticle (IONP), producing a nanoprobe (IO-Gd-DTPA-SS-Doxo) with quenched longitudinal spin lattice magnetic relaxation (T1). When the folate-conjugated activatable nanoprobe was incubated in LNCaP cells, which has overexpression of folate receptors, an increase in the 1/T1 signal was observed. After receptor mediated internalization, Gd-DTPA-SS-Doxo was liberated from the nanoprobe's polymeric coating due to the acidic microenvironment of the tumor. Thus, resulting in an intracellular release of Gd-DTPA complex and Doxo with subsequent T1 activation and cytotoxic effect, respectively. Therefore, the proposed activatable nanoprobe would provide dual mode MR imaging of cancer and targeted target treatment of the disease.

T10: Priestley Medal Addresses: Tools for Teaching About the Recent History of Chemistry
Presenter: Luis D. Montes
Authors and Affiliation: Luis D. Montes - *University of Central Oklahoma*

The past 100 years have witnessed a significant increase in chemical knowledge. This has led to greater roles for chemistry in education, government, and industry, and advancements in chemistry play important roles in our daily lives. Despite this increased role, we as chemical educators often find little time to teach about the history of our discipline, much less the recent past. Our chemistry majors learn plenty about chemical principles, but what do they know about the many roles recent chemists played in promoting chemistry through their research, teaching, and service? To remedy this, I have used Priestley Medal Addresses to provide students with an introduction to the recent history of chemistry, as well as exposure to the many role's chemists play in society apart from their work in the lab. In this talk I will present a brief history of the Priestley Medal and a summary of the range of topics covered by the various awardees. I will conclude with some thoughts on how Priestley Medal Addresses can be incorporated into the curriculum for a chemistry major.

T11: We Don't Learn Anything: The Impact of Contextualized Authentic Research-Based Experiences Modules on STEM Majors' Perceptions of a Chemistry Laboratory Course
Presenter: Jacinta Mutambuki
Authors and Affiliation: Jacinta M. Mutambuki,[1] Herb Fynewever,[2] Kevin Douglass,[3] William Cobern,[4] and Sherine Obare[5] - *[1]Department of Chemistry, Oklahoma State University, [2]Department of Chemistry and Biochemistry, Calvin College, [3]MPI Research, a Charles River Company, [4]Department of Biology and Biological Sciences, Western Michigan University and [5]Joint School of Nanoscience and Nanoengineering, University of North Carolina at Greensboro*

Training STEM students on authentic research experiences in chemistry laboratory courses is pivotal for preparing a competent STEM workforce, and can make abstract chemistry concepts more palatable to students. Some institutions have adopted a course-based research experiences (CUREs) model to scale up the preparation of STEM workforce by immersing students into real-world scientific practices. Most CUREs have been reported in the General Chemistry courses; however, they tend to lack relevance to student personal life. The current study investigated the impact of "relevant" CURE modules integrated into a cookbook conventional Quantitative Analysis Chemistry laboratory course on student affective outcomes. Findings and implications for future practice will be discussed.

T12: Using Fluency Quizzes to Talk Chemistry
Presenter: Christopher T. Jones
Authors and Affiliation: Christopher T. Jones - *Oklahoma Baptist University*

Since chemistry seems to be a different language for some students, this is a method to increase chemical literacy in the areas of basic definitions, calculations, nomenclature,

relationships, and more. The objective is to allow more time for complex concepts by providing online drill and practice time for some basic skills. The model utilizes quizzing features available in most learning management systems. Quizzes are developed from large pools of comparable questions. A typical fluency quiz is 20 multiple choice or true/false questions randomly selected from a pool of 100 questions with a 2-minute time limit. Each quiz can be taken an unlimited number of times with the highest score kept as the grade. Fluency quizzes have been developed for significant figures, naming anions and cations, naming ionic and binary covalent compounds, pH of solutions, Le Chatelier's Principle, identifying reaction types, VSEPR theory, identifying functional groups, and naming organic compounds with common names.

T13: Chemistry, Data and Undergraduates: Fitting Data Literacy into Chemical Education
Presenter: Kay K. Bjornen
Authors and Affiliation: Kay K. Bjornen - *Edmon Low Library, Oklahoma State University*

Data literacy is a concept that research professionals have historically learned through trial-and-error, often at great pain. The age of big data and digital scholarship has expanded the scope of skills needed for thinking critically with data, managing data effectively and using tools for data discovery, cleaning and analysis. Learning these skills as early as possible allows chemistry undergraduates to reinforce them in their advanced labs and classes and to be prepared for research experience at either the undergraduate or graduate level. Surveys have found that most undergraduate teaching faculty feel that they cannot reasonably add data literacy concepts to their already full syllabi. This presentation will make a case for the importance of data literacy and data management best practices and introduce some ways to slip them into existing lab and classroom curricula.

T14: Self-Starting Functions for Nonlinear Fitting of Enzyme Inhibition
Presenter: Nathan J. Malmberg
Authors and Affiliation: Nathan J. Malmberg - *Department of Chemistry, Oklahoma Baptist University*

Traditional undergraduate analysis of enzyme kinetics data involves linearization of the data, which avoids some of the complexities of nonlinear fitting but makes the data heteroscedastic, complicates the calculation of the kinetic parameters and makes a quantitative comparison of different models of inhibition impractical. This work presents an R package with functions for nonlinear fitting of enzyme kinetics data to different reversible inhibition models. The fitting process directly calculates the kinetic parameters, and the input is flexible with regard to substrate and inhibitor concentrations. The models can be analyzed with built-in R functions to compare inhibition models for the data.

T15: Highly Ordered Bionanofibrous Films Fabricated by a Simple Self-Assembly Approach
Presenter: Ningyun Zhou
Authors and Affiliation: Ningyun Zhou and Chuanbin Mao - *University of Oklahoma*

Nanofibers is a type of nanomaterial with a large surface area to volume ratio. They are very useful tools in nanocatalysis, tissue scaffolds, and nano-electronics. There are many different methods to fabricate nanofibers, such as electrospinning, phase separation, template synthesis, etc. Here, we use a simple method to control the assembly of semi-flexible biological nanofibers into various structures, which have potential biological applications. We found that the negatively charged nanofibers can self-assemble into highly ordered thin films on a positively charged substrate. Microscopy study showed that the nanofibers exist as sematic phase liquid crystals in the film. We attribute the driving force of such self-assembly behavior to the flow-induced crystallization (FIC) process.

T16: Functionalizing the Surface of Gold Nanorods with Single-Stranded DNA
Presenter: Stephen Kane
Authors and Affiliation: Stephen Kane and Bailey Spears and Nathan Green - *Northeastern State University*

Gold nanorods exhibit unique optical properties that have applications in sensing, light harvesting, and novel photonic materials. The most common syntheses of gold nanorods (AuNRs) rely on the use of the surfactant, hexdecyltrimethylammonium bromide (CTAB) which suffers from temperature sensitivity, bioincompatibility, and other material challenges. TheCTAB coating must thus be replaced in order to realize the full material applications of AuNRs.In this report, AuNRs were synthesized via a seed-mediated method, which are capped with abilayer of CTAB. In order to conjugate AuNRs to other materials we aim to load single-strandedDNA (ssDNA) molecules onto AuNRs; however, direct displacement of CTAB by ssDNA is notpermissible as the CTAB bilayer obstructs the formation of the sulfur−Au bond between thethiolated DNA and AuNR surface. Therefore, to avoid these electrostatic interactions, theexchange of CTAB surfactant for an intermediate stabilizing layer of sodium dodecylsulfate(SDS) and polyvinylpyrrolidone (PVP) is necessary. We demonstrate a reproducible approach ofdisplacing CTAB with ssDNA. The recoating process was followed by UV-Visible (UV-VIS)spectroscopy as AuNR absorbance is sensitive to surface chemistry changes. AuNR morphologywas confirmed via transmission electron microscopy (TEM) imaging. In future experiments, we aim to explore long-range radiationless energy transfer by conjugating ssDNA-AuNRs with dye-dopes silica nanoparticles along a DNA-based nanostructure.

T17: Reactivity of Chromium Anchored Al-MCM-41 Nanomaterial: An FT-IR Study of Detoxification of Organic Compounds
Presenter: Dilip K. Paul
Authors and Affiliation: Dilip K. Paul - *Department of Chemistry, Pittsburg State University*

The acidity of Cr-incorporated Al-MCM-41 nanomaterials was investigated by adsorbing pyridine using transmission infrared spectroscopy. Both Lewis and Bronsted acid sites were found to be present as determined by corresponding IR modes on surfaces. Adsorption of acetaldehyde was used a model compound to understand the reactivity of the nanoparticles towards catalytic degradation. During adsorption at low temperature, the acetaldehyde molecule binds through H-bonding with surface –OH groups. In addition, a fraction of acetaldehyde adsorbed through Lewis acid sites- Cr (IV) and Al (III). The combination of both H-bonded and Lewis acid sites bound acetaldehyde underwent condensation reaction forming aldol which then dehydrated at elevated temperature forming 2-butenal. Acetaldehyde underwent photodecomposition to CO_2 during photooxidation at 273 K and 173 K This oxidation involves photoactive acetyl radical and Cr ion. A variety of condensation products also identified using TPD during photochemical reaction.

T18: Nanoconfinement of Organics in Mesoporous Silica: Applications in Explosive Stabilization, Chemical Dosimeters, and Water Treatment
Presenter: Allen Apblett
Authors and Affiliation: Allen Apblett, Nicholas Materer, Evgueni, Kaddosov, Randy Butt - *Oklahoma State University and XploSafe, LLC*

Nanoconfinement in the pores of mesoporous silica has remarkable effects on the sorption and stability of organic and inorganic compounds. For example, the notoriously sensitive peroxide-based explosives TATP and HMTD are so stable when sorbed in mesoporous silica that the resulting materials do not explode by impact, friction or even when a flame is applied. As such the materials are ideal for the manufacture of training aids for explosive-sensing dogs or vapor sources for safely developing and testing explosive sensors. Similar principles of high adsorption capacity and the ability to stabilize reactive compounds also make mesoporous silica highly effective for the manufacture of chemical dosimeters. Finally, mesoporous silica has also proven useful for sorption of organic compounds such as dyes and trichloroethylene. For example, the sorption capacity for methylene blue is greater than 100% be weight.

T19: Poly(Vinyl Pyrrolidone) has Reduced Mobility in Graphene Oxide Nanocomposites
Presenter: Ishan N. Jayalath
Authors and Affiliation: Ishan N. Jayalath and Frank D. Blum - *Oklahoma State University*

Poly(vinyl pyrrolidone) (PVP) is a water-soluble linear polymer, which has hydrophilic and lipophilic groups. We are interested in the interphase of PVP and graphene oxide (GO). Here, we report the effect of the GO surface on the thermal behavior of PVP/GO nanocomposites using temperature-modulated differential scanning calorimetry (TMDSC) and

thermogravimetric analysis (TGA). Glass transition behavior and the specific heat capacities of PVP-GO nanocomposites with small adsorbed amounts of polymer were measured, and we find that the polar, perhaps hydrogen bonding interactions between PVP and GO significantly change of glass transition behavior of the polymer composites compared to the bulk polymer. Therefore, we will make an attempt to model and understand the behavior of PVP on graphene oxide surface using thermal measurements

T20: Metal Carbenoid Initiated Cascade Reactions for the Synthesis of Diverse Medium-sized Heterocycles
Presenter: Nicholas P. Massaro
Authors and Affiliation: Nicholas P. Massaro, Kiran Chinthapally, Joseph C. Stevens, Aayushi Chatterji and Indrajeet Sharma - *Department of Chemistry and Biochemistry, and Institute of Natural Products Applications and Research Technologies, University of Oklahoma*

Current drug scaffolds have provided significant therapeutic advances in a wide array of human ailments. Unfortunately, the efficacy of these scaffolds is beginning to plateau leaning focus towards more modern molecular targets encompassing three-dimensional architecture. Medium sized rings (8-12 membered) encompass an array of complex natural products and relevant scaffolds with a wide range of biological applications, often due to their constrained ring conformations which provide enhanced binding affinity, bioavailability and cell permeability over their linear alternatives. Nonetheless, medium sized rings are completely absent in the current top 200 brand name and generic drugs on the market due to the numerous challenges associated with their syntheses. To address this challenge, we have developed a simultaneous ring formation/ring expansion approach, which utilizes ambiphilic metal carbenes derived from diazo synthons to access highly functionalized medium sized heterocycle of varying ring sizes.

T21: Targeting Tumor Metabolism for Cancer Therapy
Presenter: Toby Nix
Authors and Affiliation: Horrick Sharma and Toby Nix - *Department of Pharmaceutical Sciences, College of Pharmacy, Southwestern Oklahoma State University*

Cancer is the second-leading cause of deaths in the United States. Despite recent advances in chemotherapy, metastasized cancer is still incurable. Further, current chemotherapeutic drugs are associated with systemic toxicity and significant side effects. Thus, exploration of novel targets and development of new treatment options is desperately required. Dysregulated metabolism is one of the hallmarks of cancer cells. Although heterogeneous, all tumor cells show profound metabolic adaptations to meet their growing energy and biosynthetic demands. Oncogenic signaling upregulates metabolic enzymes and nutrient transporters to sustain tumor cell growth and proliferation. Elevated aerobic glycolysis, also known as the Warburg effect, and increased dependency on glutamine are key metabolic adaptations of tumor cells. Targeting altered tumor metabolism has emerged as a promising therapeutic strategy against cancer.

T22: Sulfabenzamide Diversification using Alkyl Pyrophosphate Analogues by NphB Reveals N-Prenylation Catalytic Functions
Presenter: Andrea Batchev
Authors and Affiliation: Andrea Batchev, Erin Scull, Eric Gardner, Chandrasekhar Bandari, Tejaswi Bavineni, Johanna Masterson, Rachel Tran, Abigail Lange and Shanteri Singh - *Chemistry and Biochemistry, University of Oklahoma*

NphB from Streptomyces sp. strain CL190 is an aromatic prenyltransferase, a class of enzymes that catalyzes the attachment of isoprenoid pyrophosphates onto electron-rich acceptor molecules. Many prenyltransferases have demonstrated relaxed substrate specificities, making them good candidates for drug diversification. NphB is a prenyltransferase that demonstrates such promiscuity. It is responsible for the geranylation of a variety of phenolic or hydroxyl-containing aromatic molecules by performing C-C or C-O prenylations in nature. Prenylations are often the target for natural product modification because many prenylated compounds express enhanced bioactivity compared to their unprenylated precursors. The broad substrate scope of NphB was probed using 45 unique alkyl pyrophosphate analogues. NphB catalyzed the transfer of 15 alkyl pyrophosphate analogues onto sulfabenzamide, a sulfonamide that exhibits antibiotic and some anticancer properties. Through NMR characterization of the products, a previously unreported N-prenylation capability for NphB was revealed. The findings in this study reveal a new catalytic function of NphB, providing a better understanding for the promiscuity and regiospecificity of the enzyme, and we generated numerous sulfabenzamide derivatives, which may have improved biological applications.

T23: Copper-Catalyzed Synthesis of Enamino Carbonyl Compounds
Presenter: Syed R Hussaini
Authors and Affiliation: Syed R Hussaini and Arpan Pal - *Department of Chemistry and Biochemistry, The University of Tulsa*

Enamino carbonyl compounds can react as both nucleophiles and electrophiles, and because of that, they are important synthetic intermediates. There are two major methods for the synthesis of exocyclic enamino carbonyl compounds. The first is the Eschenmoser sulfide contraction (ESC) and the second is the imino ester (imidate) approach. Both of these methods are sensitive to steric hindrance and neither of these methods have any examples of N-Boc protected thioamides or amides as the coupling partners. The metal-catalyzed coupling of thioamides and carbenoids overcomes steric issues associated with these reactions and provides enamino carbonyl compounds. We will share our progress towards the intermolecular copper-catalyzed coupling of thioamides and diazo compounds for the synthesis of enamino carbonyl compounds. The reaction gives excellent yields of enamino carbonyl compounds. The reaction has the potential to become the most economical, sustainable and practical method for the formation of exocyclic enamino carbonyl compounds.

T24: Chemoenzymatic Synthesis of Novel Tryprostatin Analogs using Prenyltransferases
Presenter: Eric Gardner
Authors and Affiliation: Eric Gardner, Andrea Batchev, Abigail Lange, Johanna Masterson, Chandrasekhar Bandari and Shanteri Singh - *Chemistry and Biochemistry, University of Oklahoma*

Prenyltransferases (PTs) are versatile alkylating enzymes which are critical in the production of a vast spectrum of bioactive secondary metabolites. Many PTs have been shown to have a broad substrate scope, accepting many unnatural donor and acceptor substrates. PTs are useful biocatalysts capable of regio- and chemoselectively functionalizing aromatic rings using alkyl pyrophosphate donors. Prenylation has been shown to increase the lipophilicity and activity of many small molecules. Tryprostatin A is a remarkable prenylated cyclic dipeptide capable of inhibiting cancer by inhibiting both tubulin polymerization, and topoisomerase II. Breast cancer resistance protein (BCRP), a drug efflux pump commonly overexpressed in drug resistant tumors, is also inhibited by Tryprostatin A. We have chemoenzymatically synthesized several novel Tryprostatin analogs using our library of unnatural donors. This work demonstrates how the biocatalytic late stage modification of bioactive natural products unlocks a new spectrum of drug analogs previously inaccessible by purely synthetic methods.

T25: Kinetic Doping of Branched Polyethylenimine: A Novel Approach to Amine Functionalization of Silica Thin Films
Presenter: Jessica Jensen
Authors and Affiliation: Jessica Jensen and Wai Tak Yip - *Chemistry and Biochemistry, University of Oklahoma*

Amine-functionalized thin films are highly desirable technologies for analytical, materials, and biochemistry applications. Current functionalization procedures can be costly, environmentally unfriendly, and require many synthetic steps. Here, we present an inexpensive and facile way to functionalize a silica thin film with 25000 MW branched polyethylenimine (BPEI), consistent with green chemistry principles. To our knowledge, this is the first time that BPEI has been doped into silica thin films. Using UV-Vis spectroscopy and scanning electron microscopy, BPEI was determined to be loaded into the film at millimolar concentration levels. The films were also tested for copper (II) sequestration and were determined to load copper (II) ions with a capacity of 10 mmol/g of film, an approximately five-fold increase over commercially available resins. Films proved to be usable three times, using EDTA to chelate copper and regenerate the films, with only a 6% reduction in the amount of copper (II) ions sequestered by the third use. The films also proved stable over the course of one week in solution, with less than 1% of the original BPEI lost under various storage conditions (i.e. storage in DI water, storage in dilute BPEI solution, storage in DI water after annealing). These films show promise for multiple applications, from heavy metal sequestration to anti-fouling applications.

T26: Aldol Condensation of Cyclopentanone and Acetone on MgO: A Mechanism Study by DFT
Presenter: Yu Yan
Authors and Affiliation: Yu Yan, Duong T. Ngo, Daniel E. Resasco and Bin Wang - *School of Chemical, Biological and Materials Engineering, University of Oklahoma*

Aldol condensation is of great importance to form C-C bonds in organic synthesis and has a wide range of potential applications in fine chemicals. In this study, we report density functional theory (DFT) calculations, though which we interpret the experimental finding of aldol condensation of cyclopentanone (C) and acetone (A) catalyzed by solid base catalyst MgO nanocrystal. Experimental results suggest that the [C]-activated products play a dominant role, as indicated by the initial rates with various A-to-C feed ratios at 200°C. Further adsorption experiments and DFT calculations confirm the preferential chemisorption and α-H abstraction of cyclopentanone on MgO surface with respect to acetone. For each ketone reactant, α-H abstraction is the rate-determining step as the formation rate of [C]-activated products remains constant, while that of [A]-activated products increases proportionally to the A-to-C feed ratio. This rate-limiting step is further supported by DFT calculations.

T27: Modeling Infrared Spectra of Ordered Monolayers
Presenter: Nafisa Amin
Authors and Affiliation: Nafisa Amin, Soumya Bhattacharya and Lloyd A. Bumm - *Homer L. Dodge Department of Physics and Astronomy, University of Oklahoma*

Infrared (IR) vibrational spectroscopy has been very successful for structural characterization of thin films. We are proposing refractive index tensor for different structures in an anisotropic medium. Unlike Isotropic medium, there will be transition dipole moment and orientations in different direction for each mode. This makes this system more interesting as we must approach in a different way to calculate various structural information for our proposed system. To calculate the reflectivity of the system, structural information like number of layers, thickness and refractive index of each layer is required. We can construct the refractive index tensor either by adjusting various structural parameters or by using parameters from Molecular Dynamics. All this information will be used in a 4x4 transfer matrix method to obtain reflectivity for various proposed structures. To test the obtained result, we will compare them with experimental IR spectra data. In particular, we want to establish refractive index tensor for different structures using the model which will be compared with experimental IR spectra and lastly, obtain the best proposed structure.

T28: Probing Internal Structure of Alkanethiol Self-Assembled Monolayers with STM
Presenter: Mitchell P. Yothers
Authors and Affiliation: Mitchell P. Yothers, Soumya Bhattacharya and Lloyd A. Bumm - *Homer L. Dodge Department of Physics and Astronomy, University of Oklahoma*

Accurate measurements of structures at the nanoscale are of fundamental importance for developing nanofabrication techniques. Using alkanethiol self-assembled monolayers (SAMs) as a model system, we demonstrate a way to make high-precision measurements of

crystalline structures imaged with a scanning tunneling microscope (STM). These measurements are made using real-space lattice averaging on distortion-corrected STM images. Using this technique to measure guest-host bicomponent SAMs with two different alkanethiol chain lengths, we determine the alkanethiol chain tilt direction and resolve chain twist differences between lattice sites.

T29: Thermally Stable Nano-Thin Film of Ag on Au(111)
Presenter: Kennedy Boyd
Authors and Affiliation: Kennedy Boyd, Jesse A. Phillips, Lauren K. Harville, Gabriel LeBlanc and Erin V. Iski - *Department of Chemistry and Biochemistry, University of Tulsa*

In previous studies conducted by Iski et al. and Itaya et al., it was discovered that a silver (Ag) monolayer could be formed on an Au(111) surface in a chloride-rich and a chloride-free environment. The Ag monolayer was applied to the surface through an electrochemical method called underpotential deposition (UPD). Two Ag sources were investigated, AgCl and $AgClO_4$. In the previous studies, a single deposition potential was investigated. Through our own electrochemical study, we found that there are two different potentials in which UPD can be used to apply a Ag monolayer to a Au(111) surface. The two different potentials also correspond to two different mechanisms, one resulting in the reduction of Ag^+ to the surface and the other resulting in the reduction of a solvated silver halide unit (AgX) to the surface. Dependent upon the potential of the system, the monolayer formed on the surface can be thermally stable up to 1,000 K. The atomic structure of the thin films formed on the surface can be studied via electrochemical scanning tunneling microscopy (EC-STM). EC-STM not only allows for atomically resolved images of the surface, but it also facilitates the taking of cyclic voltammograms (CVs), which can be used to examine the redox behavior of the system and energetic changes of the surface. Through this electrochemical manipulation of the system, the thermal stability can be investigated as well as the reduction of Ag^+ to the surface in various silver halide systems. Although many studies have been conducted on these types of thin films, very few studies have directly investigated the thermal stability of the UPD of Ag on Au(111) using varied silver halide sources. EC-STM allows for the imaging of the atomically modified surface and the investigation of the Ag monolayer within a fluid cell while maintaining a constant potential. Evidence shows that regardless of the Ag source, the quantity of Ag applied to the surface does not change. However, the applied potential directly effects the Ag coverage. Furthermore, the deposition potential can be directly correlated to thermal stability. Electrochemical studies have proven extremely useful in better understanding the unique properties associated with these surfaces as well as the exact nature of the redox chemistry occurring at different potentials. Through our own EC-STM investigation of the two underpotential regions, valuable information was gathered on the effects of different AgX sources on the thermal stability of the adsorbed monolayer and the enhanced physical properties of the system.

T30: Differential HDX-MS for Characterizing Protein-protein Interaction
Presenter: Jiwon Kang
Authors and Affiliation: Jiwon Kang, Zhe Wang, Mulin Fang, Kellye A Cupp-Sutton and Si Wu - *Department of Chemistry and Biochemistry, University of Oklahoma*

Understanding protein-protein interaction has vital importance in the biological systems. The antibody-antigen reaction is the most fundamental reaction of the immune system among others. The distinct characterization of the binding site of an immune complex is required to understand the immune response and mechanisms of related disease. Hydrogen-deuterium exchange mass spectrometry (HDX-MS) has become a promising technique for determining protein structures. HDX-MS often includes three steps. The first step is the hydrogen/deuterium exchange, the second step is protein digestion, and the third step is peptide separation and detection. In this study, we optimized each step by the following experiments: In the first step, samples are exposed to deuterium water (D_2O). For the protein complexes, HDX highly occurs in the surface regions and the regions which are not involved in hydrogen bonding. Binding sites of free proteins are not protected, and therefore the HDX rate is comparatively faster. In the second step, the protein complex is digested by the enzyme such as pepsin or protease VIII into smaller peptide pieces so that the rate of deuteration for each peptide can be determined in the next step. The ultimate goal is to get high sequence coverage to identify the exact binding site from the HDX sample. In the third step, the HDX sample is rapidly back exchanged into hydrogen since it is no longer in D_2O. Therefore, we applied a low-temperature liquid chromatography/mass spectroscopy (LC-MS) to minimize the back-exchange rate, and to have good separation for better sequence coverage. The enzymatic digestion step has to be conducted under properly optimized conditions for maximizing the sequence coverage to identify HDX sample. The conditions can be differentiated by incubation time, temperature, the enzyme to protein ratio and so on. The results show that the sequence coverage percentage was 39.2% for BSA (60 minutes, RT), 77.0% for Beta-lactoglobulin (10 minutes, 0 °C), and 82.6% for Beta-lactoglobulin (120 minutes, 0°C). BSA shows low sequence coverage percentage, but Beta-lactoglobulin showed relatively high sequence coverage percentage in short incubation time and even much higher percentage in longer incubation time. Additionally, since two Beta-lactoglobulin samples showed high sequence coverage percentage at 0 °C, the optimal digestion temperature is 0 °C for small size protein. In conclusion, different protein sizes lead to different digestion efficiency. The large size protein requires longer incubation time for high sequence coverage, and small size protein doesn't require long incubation time at the same time.

T31: Subhemolytic Shear Environment and Conformational Changes in Transmembrane Protein
Presenter: James Buerck
Authors and Affiliation: James Buerck and Edgar A. O'Rear - *School of Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK*

Introduction: Medical devices can impose supra-physiological flow on the cellular components of blood as it passes through the unit. Ventricular assist devices (VADs), only one such implantable device, are commonly prescribed to patients with heart failure as a

means for bridge to transplant or destination therapy. The therapeutic intervention with VADs alters physiologic blood flow and puts high stresses on blood cells. The increased shear stresses and pressures may modify blood cell biology that is detrimental to their routine function and circulatory lifespan. We hypothesized that membrane alterations and other changes after exposure in some medical devices might be similar to that seen in senescent cells. Materials and Methods: Venous blood was collected from a pool of healthy, human donors and then RBCs separated, washed and re-suspended with a final hematocrit of ~37%. Microfluidic channels were created using poly-dimethyl siloxane (PDMS) at a 1:10 ratio of curing agent to base poured over a mold made through use of negative photolithography. A set of microfluidic channels were designed with constrictions to control shear rate, with exposure times of 0, 5, 10 and 15 ms in a high shear region. The 0 ms exposure time was used as a control where the micro channel had no constriction. After washed RBCs were flowed through the channel, they were analyzed using a BD C6 flow cytometer and fluorescent markers. Results and Discussion: Using a gating scheme to ensure positive selection with two fluorescent markers, one aimed at a senescent marker and another towards RBCs, we observed a positive trend with exposure time and shear for the conformational change within the RBC membrane. At the same time, annexin V with a fluorescent tag failed to show a significant increase of exposed phosphatidylserine (PS), a marker for eryptosis, on RBCs after exposure. The data collected from the flow cytometer did indicate a trend in erythrocyte microparticle (EMP) formation in the size range from 0.5 to 1.0 μm ($p<0.05$). The increase in EMP formation from the control to the longest exposure time showed over a ten-fold increase. In addition, we have found a higher percentage of red cells exhibiting the fluorescent tag known against the structural change in protein on RBC membranes ($p<0.05$) from collected flow cytometry. The extent of binding increased with exposure time to the high shear stresses. Conclusions: Increased high shear of 10 ms duration occurs with a resulting increase in membrane alterations. The number of EMPs observed also rose with exposure time. EMPs shed during shear show an increase in the same protein conformational changes seen on cells. Unlike the RBCs from which the EMPs are shed, a majority of EMPs show externalized PS as well. The results collected through flow cytometry lines up with results collected from senescent RBCs.

T32: Bridge Helix of CAS9 Contributes to Target DNA Cleavage Selectivity
Presenter: Kesavan Babu
Authors and Affiliation: Kesavan Babu,[1] Nadia Amrani,[2] Wei Jiang,[3] Peter Z. Qin[3] and Rakhi Rajan[1] - *[1]Department of Chemistry and Biochemistry, University of Oklahoma,[2] RNA Therapeutics Institute, University of Massachusetts Medical School,[3] Department of Chemistry, University of Southern California*

CRISPR-Cas systems are adaptive immune systems found in bacteria and archaea to confer immunity against foreign genetic elements. Cas9, a type II CRISPR effector protein, is widely used for gene editing applications since a single guide RNA (sgRNA) can direct Cas9 to cleave DNA targets of interest. A short nucleotide found in target DNA known as protospacer adjacent motif (PAM) and the complementarity between the guide region of sgRNA and target DNA is essential for cleaving the target DNA. In addition, binding of RNA and DNA induces protein conformational changes that include positioning of nuclease domains to produce double-stranded breaks. The relationship between RNA-mediated

conformational changes in Cas9 and DNA targeting is being pursued actively for developing Cas9 variants with minimal off-targeting effects. The structure of Cas9 is organized into two lobes. The two lobes are connected by an arginine-rich motif called bridge helix (BH), which is highly essential for protein function. In the present study, we show that substitutions within the BH of Streptococcus pyogenes (Spy) Cas9 impair its DNA cleavage activity. The DNA cleavage deficiency is more pronounced in DNA targets that are mismatched with the guide region of sgRNA at the PAM proximal side. BH substitutions cause an accumulation of nicked products, leading to a reduction of target DNA linearization. Gene editing experiments performed on human cells (HEK293T) showed that even though the BH-variant is not as efficient as the wild-type protein in editing all the tested sites, the off-target effect on edited sites is considerably reduced compared to the wild-type protein. Mechanistic analyses show that the BH-substitution does not reduce sgRNA-binding affinity, but substantially reduces the stability of the protein-RNA complex. We propose BH-substitution as a mechanism to fine-tune CRISPR-based gene editing applications since BH is conserved in several CRISPR systems.

T33: NMR and Molecular Dynamics Simulation Reveal the Impact of V23D Mutation on the Function of Yeast Oligosaccharyltransferase Subunit OST4P
Presenter: Bharat Chaudhary
Authors and Affiliation: Bharat Chaudhary, David Z. Zoetewey and Smita Mohanty - *Oklahoma State University*

Oligosaccharyltransferase (OST), a multi-subunit enzyme localized in the endoplasmic reticulum, catalyzes N-glycosylation of proteins. This process is an essential, highly conserved modification reaction that occurs in all eukaryotes and some prokaryotes. Complete loss of function of this enzyme is lethal for all organisms. In Saccharomyces cerevisiae, OST is composed of nine non-identical membrane proteins. Among them, Ost4p is a very small subunit containing only 36 residues and a single transmembrane domain. This subunit is critical for the OST activity and the stability of the OST complex. Mutation of any hydrophobic residue from position 18-24 to ionizable residue results in the destabilization of the complex leading to impaired cell growth and in vitro OST activity. To determine the atomic resolution structure of Ost4p, we have initiated the structural studies of both Ost4p and Ost4V23D mutant proteins in DPC micelles using high-resolution solution-state NMR. Ost4V23D mutant is functionally important. This mutation is lethal for yeast. We have determined the 3D structure of Ost4p and Ost4pV23D in DPC micelle. What is important to note that the 3D structure of Ost4p in DPC micelles is quite different than the previously determined 3D structures of yeast and human Ost4p proteins in the chloroform-methanol-water system as a membrane mimetic. However, our 3D structure in DPC micelle is similar to the 3D structure of Ost4p determined through cryo-EM of yeast OST complex. The 3D structure determined in DPC micelles will be presented and structural comparison with other methods (mixed organic solvent and cryo-EM) will be discussed.

T34: Structure and Function Studies of Asian Corn Borer Ostrinia Furnacalis Pheromone Binding Protein2
Presenter: Salik Ram Dahal
Authors and Affiliation: Salik Ram Dahal - *Oklahoma State University*

Lepidopteran male moths have an extraordinarily sensitive olfactory system that is capable of detecting and responding to minute amounts of female-secreted pheromones over great distances. Pheromone-binding proteins (PBPs) in male antennae ferry the hydrophobic ligand across the aqueous lymph to the olfactory receptor neuron triggering the response. PBPs bind ligands at physiological pH of the lymph and release them at acidic pH near the receptor while undergoing a conformational change. In Anthereae polyphemus PBP1, ligand binding to the hydrophobic pocket and its release is regulated by two biological gates: His70 and His95 at one end of the pocket and C-terminus tail at the other end. Interestingly, in Asian corn borer Ostrinia furnacalis PBP2 (OfurPBP2), critical residues for ligand binding and release are substituted in both biological gates. The impact of these substitutions on the ligand binding and release mechanism in OfurPBP2 is not known. We report here overexpression of soluble OfurPBP2 and structural characterization at high and low pH by circular dichroism (CD) and NMR. Ligand binding and ab initio model development were carried out with fluorescence and small-angle X-ray scattering (SAXS) respectively. OfurPBP2 in solution at pH 6.5 is homogeneous, well-folded and has a compact globular shape.

T35: Combination Therapy of Prostate Cancer: PARP Inhibitor Synergizes the Therapeutic Efficacy of Doxorubicin
Presenter: Himanshu Polara
Authors and Affiliation: Himanshu Polara, Momin Ansare, Saloni Darji, Tuhina Banerjee and Santimukul Santra - *Department of Chemistry, Pittsburg State University*

Iron oxide nanoparticles were synthesized, conjugated with folic acid and therapeutic drugs were encapsulated for treating prostate cancer. IONPs coated with polyacrylic acid were synthesized with water-based solvent precipitation method, then functionalized with folate to target prostate cancer cells (LNCaP), which have been found to overexpress folate receptors. The IONPs were conjugated with folic acid by propargylation using EDC/NHS reaction and followed by click chemistry. Doxorubicin and olaparib were encapsulated in the IONPs together using the solvent diffusion method. The nanoparticles were characterized by their size, zeta potential, and UV/fluorescence emission and absorbance. The two drugs were used together to explore the possible synergistic effects of the drugs for the effective combination therapy. The cytotoxicity was explored through MTT assay, and cell uptake studies. The cell death was observed through apoptosis, ROS, and comet assay studies. Finally, the anti-metastatic potential of the therapeutic nanoparticles was studied via migration assay.

T36: Efficient and Accurate Estimation of Free Energy Profiles for Enzymatic Reactions

Presenter: Xiaoliang Pan
Authors and Affiliation: Xiaoliang Pan[1], Ye Mei[2] and Yihan Shao[1] - *[1]Department of Chemistry and Biochemistry, University of Oklahoma and [2]State Key Laboratory of Precision Spectrosc., East China Normal University*

In the computational modeling of an enzymatic reaction, the central task is to assess the free energy profile along a one-dimensional reaction coordinate. Molecular dynamics (MD) simulations employing an ab initio quantum mechanical molecular mechanical (AI-QM/MM) Hamiltonian, combined with enhanced sampling techniques such as umbrella sampling, can be a valuable tool for studying such condensed-phase reactions. However, such computations are still not routinely practiced, due to their high computational cost. In this work, we report a reference potential simulation protocol, for producing AI-QM/MM quality free energy profiles for chemical reactions in a solvent or macromolecular environment. This protocol involves three stages: (a) using force matching to recalibrate a semi-empirical quantum mechanical (SE-QM) Hamiltonian for the specific reaction under study; (b) employing the recalibrated SE-QM Hamiltonian (in combination with molecular mechanical force fields) as the reference potential to drive umbrella samplings along the reaction pathway; and (c) computing AI-QM/MM energy values for collected configurations from the sampling and performing weighted thermodynamic perturbation to acquire AI-QM/MM corrected reaction free energy profile. For three model reactions (identity SN_2 reaction, Menschutkin reaction, and glycine proton transfer reaction) in aqueous solution and one enzyme reaction (Claisen arrangement in chorismate mutase), our simulations based on recalibrated PM3 SE-QM Hamiltonians well reproduced AI-QM/MM free energy profiles (at the B3LYP/6-31G* level of theory) all within 1 kcal/mol with a 20 to 50 fold reduction in the computer time.

T37: New Insights on the Au/S Interface of the Alkanethiol Self-Assembled Monolayers on Au(111): A DFT Study

Presenter: S. Bhattacharya
Authors and Affiliation: S. Bhattacharya,[1] G. Speyer,[4] D. K. Ferry,[3] G. Zhou,[2] L. Huang[2] and Lloyd A. Bumm[1] - *[1]Physics and Astronomy and [2]Chemical Biological and Materials Engineering at the University of Oklahoma, and [3]Electrical, Computer and Energy Engineering and [4]Research Computing at Arizona State University*

Self-assembled monolayers (SAMs) of alkanethiols on Au(111) has been extensively studied for more than 35 years for their potential applications in organic electronics, nanotechnology, lithography, surface coating for corrosion prevention, chemical sensing, among others. Although the basic structure of the SAMs at the molecule/air interface and the orientations of the molecular backbone are now well-established, there is no consensus on the atomic structure at the Au/S interface. Molecular modeling could be used to differentiate between proposed models of the Au/S interface if the interfacial force field (FF) parameters were known. Here, we report potential energy surfaces calculated from the density functional theory (DFT) for different adsorption sites. We have studied three common bonding scenarios (atop, bridge, and staple) to examine the symmetry of the potential for each. Our study concludes that the Au/S interface can significantly influence the structure of the

monolayer. We are currently working on developing the molecular dynamics (MD) FF from the DFT potential.

T38: Effects of Solvents on Hydrogen Adsorption on a Palladium Surface
Presenter: Jacob Crouch
Authors and Affiliation: Jacob Crouch and Bin Wang - *School of Chemical, Biological and Materials Engineering, University of Oklahoma*

Hydrogen adsorption on metal surfaces has been used as a descriptor to predict the catalytic activity of the metal for the electrochemical hydrogen evolution and oxidation reactions as well as hydrotreating reactions in refinery operations. Previous kinetic studies suggested that the hydrogenation adsorption energy could vary depending on the solvents in the liquid-phase hydrogenation reactions, but the mechanism is not clear. Here, density functional theory (DFT) calculations were reported which suggest how the hydrogenation adsorption energy correlates with the polarity of the solvents. Furthermore, the data shows that the adsorption energy also depends on the coverage of the solvents on the catalyst surface. Understanding the effects of solvents will help researchers find an economically viable replacement for expensive platinum catalysts which are widely used in electrochemical reactions and design a better catalytic process for liquid-phase reactions.

T39: Atomistic Force Field Model Development for the Thiolate/Defective Au(111) Interface
Presenter: Guobing Zhou
Authors and Affiliation: Guobing Zhou, Lloyd A. Bumm and Liangliang Huang - *School of Chemical, Biological and Materials Engineering and Department of Physics and Astronomy, University of Oklahoma*

A molecular-level understanding of the interplay between self-assembled monolayers (SAMs) of thiolates and gold is of great importance to a wide range of potential applications in surface science and nanotechnology. The surface properties of SAMs are largely determined by the structure and chemistry of the thiolate-gold interface. Despite theoretical research progress of the past decade, an atomistic model, capable of describing key features of SAMS at defective gold surfaces, is still missing. In this work, by means of periodic ab initio density functional theory (DFT) calculations, we have developed a new atomistic force field model for ethylthiolate SAMs on the defective Au (111) surface. In particular, new force field parameters were carefully trained to reproduce characteristic ethylthiolate configurations of the bridge and staple motifs: the non-bonded interactions were derived following the Optimized Potential for Liquid Simulations (OPLS) force field and the paper by Rai et al.;[1] the bonded force field parameters were extensively fitted via a comparison between DFT and molecular dynamics calculations, until a good match has been achieved, for vibration spectra for bonds and angles, for torsional energy profile for dihedral angles. Such atomistic force field model development will provide a new fundamental understanding of SAM/gold models and add advancement to existing interface research knowledge.
Reference [1]Rai, B.; Sathish, P.; Malhotra, C. P.; Pradip; Ayappa, K. G., Langmuir, 2004, 20, 3138.

T40: Computational Vibrational Analysis of Large Systems - Lomustine Matrix Isolated in 20 K Argon
Presenter: William B. Collier
Authors and Affiliation: William B. Collier, Zackory D. Boisselle, Jonathan W. Davis, Mathew S. Faso, Austin D. Ryden, Gary Ritzhaupt and William B. Collier - *Department of Chemistry, Oral Roberts University*

Vibrational analysis, normal coordinate analysis, is a common computational method of identifying key molecular probe vibrations for molecules. It can be extended to large systems quickly, easily and accurately with the use of super-computers and appropriate software. Here we examine the pharmaceutical lomustine isolated in a frozen matrix of argon gas. Initially one would think that a simple ideal gas computation of the vibrational modes would adequately describe the system. This is partially true, and partially not. Our results present the matrix isolated monomer spectrum of lomustine and vibrational shifts seen when the argon matrix is heated to 35 K to soften the matrix to promote complexation. SQM scaled LCAO-MO computational Hessian studies at the B3LYP/6-311G(d,p)++ and higher theoretical levels are in progress to understand this system. The structural models of this pharmaceutical and its hydrogen bonded complexes were studied using GAMESS to find the harmonic frequencies and SQM scale them with FCART 7.0. Results reveal that lomustine was successfully isolated with few water or lomustine hydrogen bonded dimers except when the argon matrix is heated to 35 K after deposition. Acquisition of a new 1200 core parallel supercomputer ("Titan") coupled with a parallelized GAMESS installation is allowing us to investigate these structures at high density functional theoretical levels and expand our theoretical modelling to inclusive structures that include the argon cage matrix within which the lomustine molecule is isolated. The results look very promising.

T41: Molecular Dynamics Study of Protein Mortalin and Anti-Cancer Compounds Flex-Hets
Presenter: Dipendra Bhandari
Authors and Affiliation: Dipendra Bhandari, Maryam Mashayekhi, Gil Repa and Donghua Zhou - *Department of Physics, Oklahoma State University*

SHetA2 is a non-toxic, flexible heteroarotionoid (Flex-Hets) compound developed for anticancer activities. It has been shown that SHetA2 and its analogues significantly inhibit the growth of ovarian cancer cells A2780. In this work, we study the binding of SHetA2 with a mitochondrial heat shock protein mortalin, which was "fished" out by magnetic-bead-attached SHetA2 from cancer cell extracts. The selective induction of apoptosis of cancer cells but not healthy cells might be attributed to the fact that mortalin is upregulated in cancer cells. We determined the binding site of SHetA2 with mortalin using molecular docking and Molecular Dynamics (MD) simulation methods. Molecular modeling study indicated that increasing the hydrophobicity of the chroman ring unit in the compound could potentially increase the binding affinity. Therefore, several series of SHetA2 compounds were synthesized with strategically varying degrees of hydrophobicity. Cancer cell growth inhibition data of these compounds proved that increasing the hydrophobicity significantly improve the anti-cancer capacity, in terms of both efficacy (maximum inhibition) and potency (drug concentration needed to be effective). We further performed MD simulations

on several mortalin mutants, showing that the S473A mutant binds to SHetA2 much stronger than the wild-type mortalin. SHetA2 inhibited growth of cancer cells transfected with S473A mortalin better than cells transfected with wild-type mortalin. This agreement between simulation and biological experiments in the cells supports that mortalin is indeed the receptor of Flex-Hets.

T42: Metalloheme-NO_x Intermediates in the Global N-Cycle
Presenter: Erwin G. Abucayon
Authors and Affiliation: Erwin G. Abucayon, Douglas R. Powell and George B. Richter-Addo - *Department of Chemistry and Biochemistry, University of Oklahoma*

The conversion of nitric oxide (NO) to the greenhouse gas nitrous oxide (N_2O) is an integral component of the denitrification process. Such transformation is important not only being part of the global N-cycle, but also relevant to climate change as N_2O is a more potent greenhouse gas than the known carbon dioxide (CO_2). N_2O is generated in biology via fungal and bacterial denitrification, where NO is reduced to N_2O by monoheme and diFe-active sites of nitric oxide reductase (NOR), respectively. Fundamental concepts in inorganic chemistry applied in metalloheme model reactions were employed to provide mechanistic insights into the NO-to-N_2O reduction by bacteria and fungi. This presentation will be highlighting some of our research efforts in probing NO to N_2O reduction, as part of the on-going research program on heme-mediated NO_x chemistry in Richter-Addo lab at the University of Oklahoma.

T43: N-Heterocyclic Carbene Copper Complexes as Attractive Targets in Strong Bonds Activation and Catalysis
Presenter: Laleh Tahsini
Authors and Affiliation: Laleh Tahsini, Jennifer Minnick, Doaa Domyati and Reza Latifi - *Department of Chemistry, Oklahoma State University*

Since the first application of copper-NHC complexes in catalysis reported by Woodward, they have become increasingly popular over the last decade. Despite the diversity of copper complexes bearing mono-, bis- and poly-NHC ligands, only neutral Cu(NHC)X complexes with mono-NHC ligands (X = halide, hydroxide, etc.) have been intensely examined in catalysis. Recently, we have developed and fully characterized pyridyl- and pyridylmethyl-linked copper(I)-bis(NHC) complexes bearing electron-donating alkyl wingtips and their analogs with electron-withdrawing substituents. The complexes served as catalysts in Sonogashira-type coupling of aryl iodides with phenylacetylene derivatives and Ullmann-type coupling of aryl halides with azole and phenol substrates. Unlike other copper catalysts that require an inert atmosphere to prevent side reactions and/or conduct the best catalytic activity, the Cu-pincer bis(NHC) complexes provide good to excellent cross-coupling yields in air. Mechanistic studies reveal the reactivity of pyridylmethyl-linked Cu(I) complexes towards O_2 leading to Cu-O_2 adducts, and towards KO^tBu forming the dearomatized complex. Furthermore, electrochemical studies of pyridyl-linked Cu(I)-NHC complexes indicate a quasi-reversible ligand-based reduction event at $E > -2.0V$ (vs Fc/Fc+). The presented data support the potential applicability of Cu-pincer NHC complexes as bifunctional catalysts in challenging bond activation reactions.

T44: Synthesis and Thermal Decomposition of Iron 2-Oximinocarboxylate Complexes
Presenter: Waleed Alamier
Authors and Affiliation: Waleed Alamier and Allen Apblett - *Oklahoma State University*

The low temperature deposition of metal oxides can be critical to the formation of nanocrystalline materials with unusual and useful chemical and physical properties. In this respect, 2-oximinocarboxylates, $M(O_2C{=}NOH)R)_n$, are promising precursors that are designed to decompose to small, volatile organic frameworks and their constituent metal oxides. The chemical and physical properties of iron (II) 2-oximinocarboxylate complexes with R= H, CH_3CH_2, and $C_6H_5CH_2$have been investigated. The iron-complexes were characterized using Fourier transform infrared spectroscopy, thermal gravimetric analysis (TGA), and single-crystal X-ray structure determination. The magnetic moment values of the complexes showed that the Fe 2-oximinocarboxylates are high-spin paramagnetic compounds. Thermal decomposition of these materials at low temperatures produces high surface area nanocrystalline or amorphous materials

T45: The Amazing World of Nitrogen Oxides: Relevance to the Global Nitrogen Cycle
Presenter: George B. Richter-Addo
Authors and Affiliation: George B. Richter-Addo - *Price Family Foundation of Structural Biology, Department of Chemistry and Biochemistry, University of Oklahoma*

The simple nitrogen oxides (NO_x) are employed in biology to serve many functions in human health, and some of these functions are enabled by heme proteins. Heme proteins have evolved to select combinations of (i) distal pocket amino acids, (ii) metal, and (iii) macrocycle (e.g., porphyrin vs chlorin) to help achieve specific interactions with incoming NO_x ligands that promote their metabolic activation. NO is a known vasodilator that requires a heme protein for its function, and the small molecule HNO is biologically relevant in its interactions with heme proteins. Similarly, the alkyl/aryl nitroso compounds (RNO) are biologically relevant species that interact with heme to inhibit protein function. Our recent findings on the role of the heme proteins such as Mb and Hb in directing their interactions with various NOx species will be presented. In addition, our findings on the generation and reactivity of heme model–HNO/RNO compounds, as well as their roles in N–N bond forming reactions to generate N_2O of relevance to the global N cycle will be presented for discussion.

T46: Role of Water in Aldol Condensation Reactions Catalyzed by MCM-41 Functionalized with Sulfonic Groups
Presenter: Gengnan Li
Authors and Affiliation: Gengnan Li, Duong T. Ngo, Tuong V. Bui, Bin Wang and Daniel E. Resasco - *School of Chemical, Biological and Materials Engineering and Center for Interfacial Reaction Engineering (CIRE), University of Oklahoma*

Cyclopentanone aldol condensation is an important carbon-carbon bond formation reaction with potential applications in biomass conversion. For this reaction that can be catalyzed by acids or bases, the presence of water is typically undesirable since it competes for active

sites, inhibiting the intrinsic activity. However, water is often unavoidable, particularly in the biomass upgrading process. Therefore, quantifying and controlling the influence of water in activity, selectivity, and catalyst deactivation is essential for advancing this technology. We have recently investigated functionalized MgO and MCM-41 catalysts, which not only are tolerant to water, but they show an enhancement in activity in the presence of water. The kinetic analysis shows that C-C coupling is the rate limiting step for both functionalized base and acid catalysts. On hydrophobic MgO, the grafted octadecyltrichlorosilane (OTS) molecules interfere between active sites, making adsorbate-adsorbate interaction on the surface less likely and reducing the rate of C-C coupling. The promotional role of water assists the C-C bond-forming step. This step can follow either a bimolecular Langmuir-Hinshelwood (LH) model between two surface species or an Eley-Rideal (ER) model between an adsorbed intermediate and an electrophile in the bulk. We have conducted our kinetics analysis allowing both contributions to occur simultaneously on the MCM-41 catalyst functionalized with sulfonic groups. For high-acid-density catalyst, the best fitting of the data is obtained with only the LH contribution to LH+ER fit due to the close proximity of sites on the surface. By contrast, when a low-acid-density catalyst was used, reaction pathway is dominated by ER model. With the addition of water, not only the activity greatly increased, but the best fit on this catalyst switched from ER to LH model. Water may help the second molecule be polarized from a remote acid sites via bridging by a chain of H-bonded molecules.

T47: Photovoltaic Response of Germanium(II) Sulfide Synthesized by Sublimation
Presenter: Brandon K Durant
Authors and Affiliation: Brandon Durant[1, 2] and Bruce A. Parkinson[2] - *[2] Homer L. Dodge Dept. of Physics and Astronomy, University of Oklahoma, [2]Department of Chemistry, University of Wyoming*

Germanium (II) sulfide (GeS) was synthesized by sublimation technique by limiting the sulfur content of the ampules to produce macroscopic crystals with dimensions of several millimeters. The photoelectrochemical properties were investigated for the first time and showed low carrier collection efficiencies below 1%, but a band gap of Eg = 1.59-1.60 eV was estimated based on photocurrent spectra that agrees well with previous optical measurements. As synthesized p-type GeS crystals showed very low doping densities on the order of 10^{14} cm^{-3}.

T48: A Novel Method for Fabricating Ni, Cu and Zn Oxide Thin Films by Hydrolysis of Their Acetates
Presenter: Dewan Russel Rahman
Authors and Affiliation: Dewan Russel Rahman and Allen Apblett - *Oklahoma State University*

Later 3d transition metal oxides are excellent candidates to be employed as thin films in various applications such as sensors, photovoltaics and other optoelectronic devices and in such processes as photo- and electro- catalysis etc. This presentation will discuss a novel hydrothermal method for fabricating uniform thin films of nickel, copper or zinc oxide from their acetates. Mild heating of aqueous Ni and Zn acetate aqueous solution at surprisingly

low temperatures between 90 ˚C and 95 ˚C produces thin films of the corresponding hydroxide acetate salts, $Ni(OAc)_{2-x}(OH)_x$ and $Zn(OAc)_{2-x}(OH)_x$. These films upon further heating at elevated temperature can be converted to Ni and Zn oxide. Cu acetate solutions at 90˚C directly deposit CuO on films. Particle size distribution analysis indicates that the hydrolysis process involves an initial incubation period and then nucleation and rapid growth of $M(OAc)_{2-x}(OH)_x$ particles from $[M(H_2O)]^{2+}$, (where M is metal). The FT-IR spectra of the deposited Ni and Zn materials showed peaks for acetate and hydroxyl groups. ^{13}C solid state NMR spectroscopy of Zn-hydroxy acetate also confirmed the presence of acetate. SEM images revealed a network structure of the films of Ni-hydroxy acetate and NiO, uniformly distributed nano-spheres of Zn-hydroxy acetate films and aggregated nano-spheres of CuO.

T49: Reactive Molecular Dynamics Simulation of Cellulose and its Property Evolution under Pyrolysis Conditions
Presenter: Qi Qiao
Authors and Affiliation: Qi Qiao and Liangliang Huang - *School of Chemical, Biological and Materials Engineering, University of Oklahoma*

An increasing attention has been paid to environment friendly materials to address natural resource shortage and global climate change. Cellulose, known as a primary component of cell walls of plants, algae, bacteria and other natural biomaterials, has attracted research attentions and is the key to effective conversion of natural biomaterial into processable advanced functional materials. From the chemistry point of view, cellulose consists of a linear chain of hundreds of b 1-4 linker glucose units. Despite a study of more than 170 years, an atomic model of supramolecular cellulose and the fundamental mechanism of how structure and chemical properties of cellulose transform under pyrolysis processes are still missing. In this work, a series of reactive molecular dynamics calculations have been designed to reveal the structural evolution of crystalline cellulose under thermal treatments. Through a detailed analysis of cellulose configuration change, hydrogen bonding network variation, reaction and redistribution of carbon, oxygen and hydrogen elements, we construct a molecule level understanding of the structure-property-treatment relationship for crystalline cellulose. We anticipate those theoretical results effectively promote the design, the manufacture and the optimization of cellulose based materials and relevant emerging applications.

T50: Observation of Amino Acid-assisted Island Formation on Au(111) using EC-STM
Presenter: Jesse Phillips
Authors and Affiliation: Jesse Phillips, I. Baljak, K. Boyd, L. Harville and E.V. Iski - *University of Tulsa*

With the increasing interest into the origin of life as well as the advancement of medical research using nanostructured architecture, investigations into amino acid interactions have increased heavily in the field of surface science. The growth of amino acids on surfaces is important to many fields ranging from biochemistry to early life studies. Amino acid self/assisted-assembly on metallic surfaces is typically investigated with Scanning Tunneling Microscopy (STM) at low temperatures (LT) and under ultra-high vacuum (UHV) in order to understand how amino acids interact and form various surface structures. However, in only

studying these systems at LT and UHV, results often tend to be questionable when moving to more relevant temperatures and pressures. This investigation focuses on the study of five simple amino acids (L-Valine, L-threonine, L-Isoleucine, L-Phenylalanine, and L-Tyrosine) as well as two modifications of a single amino acid (L-Isoleucine Ethyl Ester and N-Boc-L-Isoleucine), and the means by which they interact with a Au(111) crystal surface. Results indicate that an increase in molecular weight will have a subsequent increase in the area of the islands formed. Furthermore, by shifting from a nonpolar to polar side chain, island area will also increase. By analyzing the results gathered via in situ EC-STM at ambient conditions, fundamental insight can be gained into not only the behavior of these amino acids with varied side chains, but also into the relevance of LT-UHV STM data as it compares to the EC-STM data for biological studies.

T51: Microstructured Hydrogel Surfaces for Stem Cell Differentiation
Presenter: Y. Vasquez
Authors and Affiliation: Y. Vasquez,[1] Hasani J. Jayasinghe[1] and Sundar Madihally[2] - *[1]Department of Chemistry, and [2]Department of Chemical Engineering, Oklahoma State University*

Materials bearing microscale patterns have important biomedical applications such as scaffolds in tissue engineering, and as drug delivery systems, sensors, and actuators. Research on the interaction of cells with microscale patterns on materials such as silicon, epoxy, and hydrogels will be presented. In particular, we will discuss the patterning of intricate microstructures onto hydrogel surfaces. The patterning process is particularly challenging for hydrogels because of their physical (low mechanical strength) and chemical properties such as crosslinking density, or adhesion that make them incompatible with the templating process. We will report the use of a solvent assisted, soft lithography technique to successfully transfer arrays of micropillars onto a poly(2-hydroxyethyl methacrylate)-based hydrogel. Using two different pillar heights of the hydrogel, we show that some solvents help in the swelling of the hydrogel and facilitate the reproducible replication of the pattern. Furthermore, the micropillar pattern promotes stem cell attachment onto this hydrogel, which is not inherently adhesive when unpatterned. Pillar height dictates spreading and, as a result, differentiation of mesenchymal stem cells.

T52: Characterization of Solid Composite Electrolytes for use in Solid State Batteries, the Effect of Grain Boundaries
Presenter: John W. Ostrander
Authors and Affiliation: John Ostrander and Dale C. Teeters - *University of Tulsa, Department of Chemistry and Biochemistry*

Lithium ion batteries have been in production since 1991 in recent years have become the focus of product safety issues due to battery failure. This is due in part to the power demands of modern electronics. One possible step in making a safer and more durable battery is an all-solid-state battery (SSB) that would address this and other issues. An SSB would include a solid electrolyte such as ceramics, polymers and composites. Lithium conducting ceramic and polymers will be discussed, as well as recent findings of a polymer in ceramic composite (less than 50% polymer) that may address some of the shortcomings of ceramic powders due

to grain boundary resistance. We primarily utilize impedance spectroscopy (IS) and galvanostatic battery cycling in addition to other methods to characterize the grain boundary regions in these materials, and the suspected methods of ion conduction at the grain boundary regions.

T53: XPS Characterization of Dilute Nitride GaInAs Materials
Presenter: Samantha Scudder
Authors and Affiliation: Samantha Scudder and Nicholas Materer - *Department of Chemistry, Oklahoma State University*

GaInNAs materials have been investigated for their application in four-junction multi-junction solar cells. The incorporation of small amounts of nitrogen (few percent) into the lattice created a dilute nitride semiconductor which significantly modify the electrical and physical properties of the GaInAs. However, improvements depend on rapid thermal annealing and the sample. A hydrogenation process was also found to passivate nitrogen-related defects and impurities, extensively through elimination of trap states. To examine chemical changes, X-ray photoelectron spectroscopy (XPS) was used to analyze the composition of these materials that were annealed to different temperatures, and before and after hydrogenation. The indium peak ($3d_{5/2}$) at (447eV) was consistent with all of the samples. The nitrogen associated region of the spectra (385-420 eV) contained three peaks. The lowest binding energy peak (396 eV) was assigned as substitutable nitrogen in the lattice, and in the form of InN. Prior to hydrogenation there is a broad feature located near 406 eV with a shoulder feature at higher binging energy (410.5 eV). Consistent fits for the broad feature were obtained using two G-L peaks. Similar binding energies for the as grown and 300°C were shifted to a higher binding energy (406 and 412eV), and peaks were observed for the 600° and 850° at (406 and 409 eV). After hydrogenation, this region contained more pronounced peaks at these positions and showed consistencies with the 300° sample prior to hydrogenation. Assignments of these high-binding energy peaks is ongoing.

T54: 100 Years and Counting: History of the Oklahoma Section of the ACS
Presenter: Cheryl B. Frech
Authors and Affiliation: Cheryl B. Frech - *University of Central Oklahoma*

The Oklahoma Section celebrates its centennial in 2019. The section's members and officers have always reflected the shifting emphases in chemistry in the state. Early Oklahoma chemists were involved in production and analysis related to local industries and agriculture. Decades of oil and gas production skewed the membership until the 1990s. Many of the section's members are now employed at various academic institutions. In this presentation, glimpses from the section's archives will be presented to illustrate 100 years of chemistry and chemists in Oklahoma.

T55: A Salute to Excellence: 60 Years of Successful Programing: Wichita Falls-Duncan Section
Presenter: E. Ann Nalley
Authors and Affiliation: E. Ann Nalley - *Department of Chemistry, Physics & Engineering, Cameron University*

The Wichita Falls-Duncan Section of the American Chemical Society was chartered on September 15th, 1959, at the 136th National Meeting in Atlantic City, NJ. The section was founded to serve the needs of chemists residing in four counties in Oklahoma and eleven counties in Texas. The majority of these were employed at Halliburton Technical Services in Duncan, Oklahoma and at Midwestern University and small chemical industries located in Wichita Falls, Texas. At that time Cameron was a junior college and not many chemists were located in the Lawton area. This presentation will review the steps required to form a new local ACS Section and will present an overview of the successes and problems associated with keeping a small ACS Section active. The section is celebrating its 70th anniversary this year.

T56: Twenty-Six Years of Chemistry at the Oklahoma School of Science and Mathematics: An History of Students Academic Excellence
Presenter: A. K. Fazlur Rahman
Authors and Affiliation: A.K.Fazlur Rahman - *Chemistry Department, Oklahoma School of Science and Mathematics*

The Oklahoma School of Science and Mathematics is a two-year, public residential high school located in Oklahoma City, Oklahoma. Established by the Oklahoma state legislature in 1983, the school was designed to educate academically gifted high school juniors and seniors in advanced mathematics and science. This presentation will provide a brief narrative of chemistry teaching and research to advanced high school students for the last 26 years. Some aspects of the presentation will include the academic curriculum, student success in STEM competitions such as national science Bowl, Test of Engineering aptitude in Science, and Chemistry Olympiad.

T57: Chemistry at East Central University: 1909 to Present
Presenter: Dwight L. Myers
Authors and Affiliation: Dwight L. Myers - *Department of Chemistry and Physics, East Central University*

East Central University was established by the legislature in 1909 as one of three regional state normal schools in the eastern half of Oklahoma. First known as East Central State Normal School, it later became East Central State College in 1939, and in 1985 was renamed East Central University. The history of chemistry instruction at the college dates from 1913. In 1919, the six normal schools were authorized to offer the bachelor's degree in education and became known as teacher's colleges. In 1939 East Central and the other regional teacher's colleges were authorized to offer degrees in the Arts and Sciences in addition to Education. The history of chemistry instruction at East Central through the years will be presented. Notable changes include increased numbers of faculty, improved and expanded laboratories

and chemical instrumentation, and an increased emphasis on research as an option for the undergraduate degree.

T58: The Tulsa Section of American Chemical Society: From Oil and Fluorine to Fluorine and Nanotechnology
Presenter: Dale Teeters
Authors and Affiliation: Dale Teeters - *Department of Chemistry and Biochemistry, University of Tulsa*

The Bylaws of the Tulsa Section of the American Chemical Society were approved on September 3, 1947. The Tulsa Section was born being very involved in the chemistry of the petroleum industry and fluorine chemistry, both prevalent in the Tulsa area. While the Tulsa Section for many years was dominated by the industrial chemistry and chemist in the area, The University of Tulsa was one of the larger academic presences in the section. As with the community at large, The University of Tulsa was founded by and very concerned with the petroleum industry. It is not surprising the first “chemist” and the founder of the Tulsa Chemistry Department was a petroleum geologist. The Tulsa Section at its beginning and the history leading up to what it is today will be discussed.

T59: Chemistry in Southeast Oklahoma
Presenter: Tim Smith
Authors and Affiliation: Dr. Tim Smith - *Department of Chemistry, Computer and Physical Sciences, Southeastern Oklahoma State University*

In the presentation the history of chemistry of Southeastern Oklahoma with be presented in terms of past and present chemical industries and resources found in the area. The history of the Chemistry Program at Southeastern Oklahoma State University will be summarized.

T60: The History of Chemistry at OU
Presenter: George B. Richter-Addo
Authors and Affiliation: George B. Richter-Addo - *University of Oklahoma*

Chemistry is often referred to as the "central science". This is even more evident when one considers the origin of STEM programs at the University of Oklahoma. One of the first 4 faculty members at OU in 1892, Edwin DeBarr, a trained pharmaceutical chemist, taught the science courses during the first year of OU's existence. Aided by a donation of chemical supplies from a Detroit company, chemistry lecture and laboratory courses were formulated and taught beginning 1893, and a pharmacy course was introduced in that same year. Interestingly, the first two graduates from OU were in the Pharmaceutical Chemistry (Ph.D.) program. New faculty members were hired in pharmacy, allowing DeBarr to focus on the chemistry program. The chemistry and pharmacy laboratories, then located in the basement of Science Hall, were also used as the State Pure Food and Public Health Laboratories. The Chemistry Chair was also the director of the school of engineering, which was at the time considered a division of the department. In 1916, the chemistry department and school of pharmacy moved into the new DeBarr Hall. During the 1920's, much of the research was tied to chemical/petroleum engineering. In 1938, the School of (Chemical) Engineering separated

from the chemistry department, allowing the latter to focus on theoretical chemistry. Safety concerns ultimately to the construction of a major addition to DeBarr Hall in 1952, the Chemistry Annex building. An increased need for physical space was accommodated in part by the occupation of sections of the Physical Sciences Center beginning in 1971. Due largely to persistent student pressure in the 1980s, the name of DeBarr Hall was changed to "Chemistry Building". Dryhurst, who served as department chair for the 25-year period ending 2006 with his retirement, oversaw major advancements in the research enterprise. New faculty hires in the 1981-1990 period brought in expansions of the department's research programs, which resulted in forefront research in areas such as the Human Genome Project (Roe) and the formation of the Interdisciplinary Institute for Applied Surfactant Research (Christian). The research and administrative components of the department moved to the new Stephenson Life Sciences Research Center in 2010, allowing the department to advance strategic initiatives in multidisciplinary programs, updating its graduate program offerings, and substantially increasing participation of undergraduates in forefront research programs.

T61: Chemoenzymatic Diversification of Daptomycin
Presenter: Johanna Masterson
Authors and Affiliation: Johanna Masterson, Erin Scull, Eric Gardner and Shanteri Singh - *University of Oklahoma*

Natural product derivatization provides a means through which novel pharmaceuticals are discovered, as alterations to structure often result in alterations in functionality. However, late stage diversification of natural products remains challenging to accomplish synthetically. One natural product of interest is daptomycin, a thirteen-residue lipoprotein antibiotic of last resort. Late stage diversification of daptomycin would provide a powerful means to alter or improve the native activity of the molecule rapidly. Such diversification was proposed with the use of the prenyltransferase, CdpNPT, in conjunction with a library of allylic pyrophosphate donors. As such, a library of allylic pyrophosphate donors was synthesized using traditional organic methods. This library was screened to determine viable donors for the CdpNPT catalyzed alkylation of the tryptophan moiety in daptomycin. Herein, we report the successful donor molecules as well as the scaled-up chemoenzymatic synthesis of a daptomycin derivative.

T62: Virtual Screening-Guided Identification of Novel LDHA Inhibitor Against Cancer
Presenter: Horrick Sharma
Authors and Affiliation: Horrick Sharma, Horrick Sharma and Toby Nix - *Department of Pharmaceutical Sciences, College of Pharmacy, Southwestern Oklahoma State University*

Metabolic reprogramming is considered as one of the hallmarks of cancer and development of inhibitors targeting tumor metabolism has emerged as a promising approach against cancer. Warburg effect reflects a switch from OXPHOS to aerobic glycolysis and is one of the fundamental changes that occur in many tumor cells. Lactate dehydrogenase-A (LDHA) is a key glycolytic enzyme and a mediator of the Warburg effect. LDHA is overexpressed in many cancers and is shown to promote tumor proliferation, invasion, and survival. With an aim to identify inhibitors of LDHA, we conducted virtual screening of ZINC, a database of

~18 million compounds. We used a combination of 2D atom-based screening, pharmacophore modeling, and ensemble docking and discovered a novel small molecule that demonstrated promising inhibition of LDHA in vitro and caused reduction of viability of MIA PaCa-2 cells. Future studies will involve hit-to-lead optimization using iterative medicinal chemistry and structure-based design to develop an extensive structure-activity relationship (SAR) with an aim to discover lead LDHA inhibitors with potent anticancer potency.

T63: Rhenium(IV) Catalyzed Addition of Radicals Generated from Activated Alcohols to Olefins

Presenter: Chandrasekhar Bandari
Authors and Affiliation: Chandrasekhar Bandari and Kenneth M. Nicholas - *Department of Chemistry and Biochemistry, University of Oklahoma*

Homolytic carbon-heteroatom bond cleavage is a promising strategy to introduce carbon radicals into organic synthesis. The direct use of the alcohols in radical reactions and its practical application to C-C bond formation is less exploited. Recently we discovered reductive self-coupling (RC) of activated alcohols catalyzed by $ReO_2I(PPh_3)_2$ and PPh_3 as reductant. Encouraged by these results here in we report Rhenium catalyzed reductive cross coupling of activated alcohols with olefins. This reaction particular has potential advantages over traditional methods. The generation of radicals directly from the alcohols is rare and valuable, additionally reaction system is catalytic.

T64: Antibiofilm Synergy of β-Lactams and Branched Polyethylenimine Against Methicillin-Resistant Staphylococcus Epidermidis

Presenter: Anh K. Lam
Authors and Affiliation: Anh K. Lam, Cassandra L. Wouters, Erika L. Moen, Jennifer Pusavat, and Charles V. Rice - *Department of Chemistry and Biochemistry, University of Oklahoma*

Microbial biofilms are ubiquitous in nature, and they pose a serious threat to public health. Staphylococcus epidermidis is the most common clinical isolate from healthcare- and medical device-related biofilm infections. No antibiotic currently on the market can defeat pathogenic biofilms, which contain complex defense mechanisms composed of slime-like extracellular polymeric substances (EPS). Understanding the need to develop alternative approaches, we examine 600-Da branched polyethylenimine (BPEI) against methicillin-resistant Staphylococcus epidermidis (MRSE) biofilms. Here, a microtiter biofilm model is used to test the synergistic effects between the two components of our combination treatment: BPEI and β-lactam antibiotics. Electron microscopy was used to confirm the growth of MRSE biofilms from the model. Minimum biofilm eradication concentration (MBEC) assays and biofilm kill curves suggest that BPEI exhibits antibiofilm activity and can potentiate β-lactams to eradicate MRSE biofilms. Our method shows promise as an antibiofilm treatment option.

T65: Transition Metal Catalyzed Synthesis of Unsymmetrically Substituted Triazolium Salts
Presenter: Scott M. Hutchinson
Authors and Affiliation: Scott M. Hutchinson and Jeanne L. Bolliger - *Oklahoma State University*

Unsymmetrically substituted carbenes have become a useful tool in asymmetric catalysis, either as ligands for transition metal catalysts or on their own as organocatalysts. An efficient, generic method to synthesize 1,4-substituted 1,2,4-triazolium salts from inexpensive starting materials would significantly improve the accessibility of modified ligands and catalysts. Here we would like to present an alternative pathway to obtain a wide variety of 1,4-substituted 1,2,4-triazolium salts under mild condition which, upon deprotonation, serve as ligands for transition metal complexes.

T66: Photoredox 1,4-Skip Dienes: A Simultaneous Birch-Like Dearomatization and C-C Bond Formation
Presenter: Jon I. Day
Authors and Affiliation: Jon I. Day, Mohammed Bani Khaled and Jimmie D. Weaver III - *Oklahoma State University*

The remarkable success of the fluorine-containing drugs and agrochemicals provides an enormous motivation for chemists to discover new methods for preparation of organofluorine compounds. As methodology to synthesize partially fluorinated compounds has evolved, allowing deployment in ever increasing and more sophisticated settings, however, the access to multifluorinated building blocks is far from straightforward. C–F functionalization of highly fluorinated arenes is proving to be a powerful synthetic strategy for accessing multifluorinated arenes. We will discuss the photocatalytic C–F functionalization of perfluoroarenes which takes place with dearomatization of an arene coupling partner. This results in a product of both a C-C coupling and a 1,4-cyclohexyldiene Birch-like reduction. In addition, it provides a tractable route toward highly unnatural fluorinated analogs of the natural product tetrahydrocannabinol, the bioactive constituent of cannabis (marijuana).

Poster Abstracts

P1: A Multi-Approach Strategy to Improve the Spectrum of CLPP Activators
Presenter: Quentin Avila
Authors and Affiliation: Quentin Avila - *Department of Chemistry and Biochemistry, Stephenson Life Sciences Research Center, University of Oklahoma*

The persistent and expedient evolution of multi-drug resistance, paired with a dwindling pipeline of therapeutic answers, amplifies the urgency for novel antimicrobials. New generations of current antimicrobials may provide short-lived solutions to resistance but are often susceptible to rapid cross-resistance evolution. However, therapeutics that exploit new targets provide modern challenges to bacteria; and thus, require the development of a completely new resistance regime, potentially lengthening the duration of action. One promising target that deserves further assessment is caseinolytic protease P (ClpP). Chemo-activation of this protease results in uncontrolled protein degradation and subsequent bacterial cell death. While known ClpP activators exhibit impressive potency against Gram-positive pathogens, they fail to cross Gram-negative membranes and/or are recognized by drug efflux pumps; thus, limiting activity to Gram-positive microbes and impeding their utility as broad-spectrum antibiotics. If ClpP activators, however, are administered with polymixin B, a permeabilizing agent, or applied to efflux deficient cell lines, activity against Gram-negatives is observed. This demonstrates that if efflux incompatible and/or cell permeable ClpP activators can be developed, this class may establish itself as a first-in-class antibiotic. This poster will present our efforts towards overcoming the ineffectiveness of ClpP activating chemotypes against Gram-negatives. The results presented will center around two approaches: (1) structural diversification of N-acyl 3,5-difluorophenylalanines and (2) ClpP activator-cephalosporin hybrids. The first approach focuses on understanding the physicochemical and structural properties governing permeation and accumulation to allow the rational design of broader spectrum agents. The second approach leverages the cephalosporin core as a cleavable vehicle to improve the permeability of conjugated ClpP activators. Rationale, synthetic approach, and preliminary biological data will be presented for molecules arising from each strategy.

P2: A Single Step Selective Polyfluoroarylation of Amides
Presenters: Matthew Hamilton and Alyssa Noel
Authors and Affiliation: Matthew Hamilton, Alyssa Noel, Jimmie Weaver, Jon Day, Brock Keen and Daniel Jespersen - *Oklahoma State University*

Per- and polyfluoroarenes are important synthetic chemistry targets because they are bioactive components in many pharmaceuticals, agricultural chemicals, and industrial manufacturing products. Many of the current methods of synthesizing these fluoroarenes involves selectively adding aryl fluorines one at a time through rudimentary and harsh reaction conditions with poor yields. Novel substrates can be reached, however, through selective hydrodefluorination or functionalization, i.e. fluorine sculpting. This research builds on an existing method that produces the desired substrate fluoroarenes for directed hydrodefluorination in two steps, but improves the process by utilizing nucleophilic aromatic substitution to synthesize per- and poly-fluoroaryl amides in a single step.

P3: Adapting a Thin-Layer Chromatography Method to an At-Home Kit for Lichenology
Presenter: Kimberly L. Bennett
Authors and Affiliation: Kimberly L. Bennett and Stephanie L. Skiles - *Department of Chemistry, University of Central Oklahoma*

Lichens are a symbiotic organism that consist of an algae or cyanobacteria in conjunction with fungi in a mutualistic relationship. Lichens come in many sizes, shapes, forms, and colors. They serve such functions as food, biodegradations, dyes, and medicines. They are known to be some of the first organisms to repopulate after events such as fires and landslides, therefore they can be used to track recovery after these traumatic events. There is an established need for greater mapping of the biodiversity of lichens in the central regions of the contiguous United States. Lichen biodiversity mapping tends to fall to amateur lichenologist as crowd sourced citizen science. These citizens have little to no availability of high-grade reagents and supplies afforded to most university research laboratories. Recently I was contacted by OAKTABLE an amateur lichenology study group out of the Oklahoma, Arkansas, Kansas, and Texas region about helping to convert some of the existing methods for identifying lichens to a more readily available protocols. Lichen taxonomy relay on major indicators in environment, morphology, color, and presence of a known chemical. My focus is on the chemical identifiers. While several methods exist for this determination, most are expensive and unavailable outside of the research laboratory. Of these, thin-layer chromatography is one of the most common methods used and likely the easiest to convert to an amateur method. This project entails the process of switching out reagent grade chemicals to consumer available product.

P4: Bioactive Natural Products Analysis in Complex Microbial Environment by Metabolomics Study
Presenter: Hongyan Ma
Authors and Affiliation: Hongyan Ma, Michaela Murphy and Robert Cichewicz - *Department of Chemistry and Biochemistry, Natural Products Discovery Group and Institute for Natural Products Applications and Research Technologies, University of Oklahoma*

Natural products represent an important chemical resource for new drug discovery. The immense chemical diversity and a broad range of biological activities (e.g., antibiotic, anticancer, and antifungal) have made natural products an attractive starting point for drug discovery throughout the last century. Our research group the Natural Products Discovery Group (NPDG)—is focused on the discovery of new therapeutic compounds from fungi, which have the capacity to combat human diseases (e.g., cancer and infectious diseases). Whereas classical natural products drug discovery approaches typically rely on securing bioactive compounds from single source microorganism, we envision that more efficient and exciting opportunities await from the systematic development of mixed culture fermentation strategies. To enhance new metabolite production from the existing microorganism, natural product chemists have resorted to the mixed fermentation systems. These approaches have yielded intriguing results with new molecules identified stemming from the purported competition and stimulation microorganisms received in mixed cultures. Inspired by such

successes, we hypothesized that secondary metabolite production would be positively affected by the competition and interactions afforded by the highly complex microbial environment (e.g., natural soils and co-cultivation involving many dozens of fungal strains.). To test this idea, our group has developed a new method for the co-cultivation of up to 96 fungi on solid phase media. This new culture system triggered additional new challenges including the necessity redevise bioassay strategies that are compatible with immensely complex natural product mixtures. To address this problem, we have developed a DNA binding assay for bioactive natural products analysis using the molecular cutoff-based ultrafiltration approach. Ultrafiltration enables the separation of bioactive compounds from complex metabolite mixtures based on their highly specific affinity interactions to the DNA target on the filter membrane. While the inactive compounds flow through the ultrafiltration membrane, the bound ligands will retain on the filter membrane. The filtrates are analyzed by LC/MS and the MS fingerprints of the active compounds are used to guide their purification. Results of our pertaining to our co-culture system creation and DNA binding assay method development using 5 known DNA binders with different binding modes (i.e. groove binding and intercalation are presented. The major advantage of this combined approach is the ability to detect bioactive chemical components from extremely complex mixtures coupled with the ability to shift compound purification to chemical (LC/MS) based metabolomics techniques.

P5: Catalyst Design for Small Molecule Splitting
Presenter: Matt Swann
Authors and Affiliation: Matt Swann and Ken Nicholas - *University of Oklahoma*

Carbon Dioxide and Nitrous oxide are abundant in the atmosphere and are significant contributors to climate change and greenhouse effects. We are designing transition-metal based catalysts to split these abundant molecules into more benign or useful products, e.g. CO_2 --> $CO + O_2$; N_2O --> $N_2 + O_2$; H_2O --> $H_2 + O_2$. We will present our initial computational energetics and experimental reactivity results relevant to the potential thermal and photochemical splitting reactions promoted by LRu/LRuO complexes.

P6: Characterization of Diethyl-2-(4-Hydroxy-3-Nitrobenzilidene) Malonate and Diethyl-2-(5-Hydroxy-2-Nitrobenzylidene) Malonate with Electrochemistry and UV-VIS Spectroscopy
Presenters: Shermali Ratnasinghe and Shevon Alexander
Authors and Affiliation: Shermali Ratnasinghe, Shevon Alexander, Christopher A. Hansen and Jianguo Shao - *Midwestern State University*

Antimicrobial properties of compounds containing a benzene ring substituted with various functional groups are well known. In this study our group will utilize the Knoevenagel condensation reaction to synthesize Diethyl-2-(4-Hydroxy-3-Nitrobenzilidene) Malonate and Diethyl-2- (5-Hydroxy-2-Nitrobenzylidene) Malonate. The UV-vis spectroscopic and electrochemical data will be discussed and used to help characterized these products. IR, GC-MS, and NMR data will also be utilized to completely characterize these products. The ultimate goal is to determine if these new compounds contain any antimicrobial activity.

P7: Characterization of Gamma-Sarcoglycan by NMR
Presenter: Michael Harris
Authors and Affiliation: Michael Harris, Michael Jamaleddine and Gabriel A. Cook - *Oklahoma State University*

Muscular dystrophy, a human disease in which muscular degeneration occurs, is a result of specific gene mutations. The disease leads to a low quality of life due to loss of muscle functions throughout the body. One form of muscular dystrophy, limb-girdle muscular dystrophy, leads to death, often with a life expectancy of less than twenty years. The membrane glycoprotein gamma-Sarcoglycan has been directly linked to this form of muscular dystrophy. In order to learn more about the role of this protein we are characterizing it using structural techniques. Therefore, recombinant expression of full-length gamma-Sarcoglycan and its subsequent purification has been accomplished and preliminary NMR experiments have been performed on the pure protein in detergent environments. Further studies of gamma–Sarcoglycan will lead to the determination of its secondary structure and possible protein-protein interactions. We hope that this leads to a better understanding of the cause of this deadly disease and that it eventually leads to treatment therapies.

P8: Chlorination of Deactivated Arenes and Heteroarenes with Trichloroisocyanuric Acid under Visible-Light Photoredox Catalytic Conditions
Presenter: David A. Rogers
Authors and Affiliation: David A. Rogers and Angus A. Lamar - *University of Tulsa*

Chlorination of arenes and heteroarenes is a synthetically valuable transformation for the production of end-targets and intermediates in pharmaceuticals, agrochemicals, and advanced materials. Traditional methods of chlorination using trichloroisocyanuric acid (TCCA) require harsh acidic reaction conditions in order to activate the electrophilic chlorinating agent in reactions that use deactivated arenes as substrates. As an alternative, our research group has recently discovered a mild, atom-economical method for chlorinating substrates using a visible-light-promoted photocatalytic approach. In the present study, the reactivity of a variety of deactivated arenes as well as heteroarenes have been investigated. In addition, a comparison of the described method versus other traditional methods of arene chlorination will be included, and our progress towards the scope of reaction will be presented.

P9: Classification of 4DIU
Presenters: Shelby Smoot, Dorothy Walton and Sonia Nsenga
Authors and Affiliation: Shelby Smoot,[1] Dorothy Walton[1] and Sonia Nsenga[1] - *[1]Department of Biology, Oklahoma Christian University and [2]Rochester Institute of Technology*

Enzyme are a special subset of protein. Found within all living organisms, enzymes play an important role in many biological processes. The function of enzymes is to increase the rate of reactions. All reactions have a threshold of energy, called activation energy, that must be reached before the reaction can occur. Some reactions have such a high activation energy that they would never occur during the lifespan of a living cell without the interference of an

enzyme. Enzymes interact with the substrates of a reaction, binding to them in a special part of the enzyme called the active site, and lower the activation energy of the reaction, thus enabling it to proceed more rapidly. However, a single enzyme cannot bind to every substrate it encounters; instead, each enzyme has certain types of molecules it binds to optimally. Enzymes are classified based on the type of molecule they interact with. The purpose of this research project was to determine the classification and function of the previously unclassified enzyme, 4DIU. Because enzymes with similar structure often share similar functions, we used bioinformatic tools to compare the structure of 4DIU with other enzymes that have known functions. From these data, we hypothesized that 4DIU may be a hydrolase, more specifically a carboxylesterase. To examine this hypothesis. we isolated the protein through a series of transformation, expression, and purification procedures. This allowed the activity of the purified enzyme to be tested in vitro using enzyme activity assays. We found that 4DIU reacted with an ester/short lipid substrate; although 4DIU was also tested with lipid and carbohydrate substrates, it showed no activity with either of these two substrates. Therefore, the results obtained with the laboratory experiments supported the hypothesis formed from the bioinformatic work. Determining the classification and function of 4DIU was important because once the function of the enzyme is clearly understood it may have a useful place in medicine or industry.

P10: Cloning ORP Protein Family Members for Novel Therapeutic Drug Development
Presenter: Matthew Finneran
Authors and Affiliation: Matthew Finneran, Juan Nunez, Naga Rama Kothapalli and Anthony Burgett - *University of Oklahoma*

The Oxysterol-Binding Protein (OSBP) and OSBP-Related Proteins (ORPs) are implicated as being important proteins in the transport and regulation of cellular lipids, especially in controlling the composition of organelle membranes. The OSBP/ORPs are an understudied evolutionarily conserved protein family present in all eukaryotes, with twelve OSBP/ORPs present in humans. These OSBP/ORPs share a conserved ~50 kDa ligand binding domain and based on this domain organization the OSBP/ORPs evolved from an initial capability to bind small lipid molecules for a biological purpose. The biological functions of the OSBP/ORPs as a complete family or of the individual protein members have not been fully elucidated, and there are currently no crystal structures of any full-length or mammalian OSBP/ORP proteins. The endogenous ligands of which the OSBP/ORP proteins bind are also not well studied, and therefore the understanding of the OSBP/ORP structure and function is limited. To better understand the OSBP/ORP protein family structure and function in eukaryotic cells, this project aims to clone various ORP proteins so that they may be expressed for further structural and functional analyses. Specifically, ORP5, ORP8, and ORP11 were cloned into the sequencing vector pJET1.2/blunt and the expression vector pcDNA3.1myc-His (-) C for subsequent transfection and overexpression in HEK293T cells. The overexpressed ORP5, ORP8, and ORP11 proteins may now be further characterized through their ligand binding with an established radioactive competitive binding assay, their effects on cellular function in knockout models, and their structure-activity relationship with their ligands through X-ray crystallography.

P11: Comparing and Contrasting Undergraduate Organic Chemistry Textbooks
Presenter: Nelson McEwen
Authors and Affiliation: Nelson McEwen, Donna J Nelson, Mason Brown, Ndry Konakou, Rachel Blanche, Paula Rueda Paz, Erin Haastrup and Jaclyn Miller - *Department of Chemistry and Biochemistry, University of Oklahoma*

Presentation of selected topics in undergraduate organic chemistry textbooks will be compared and contrasted. Comparison will be with each other, as well as with the research literature.

P12: Computational Study of Volatile Aluminum Hydroxide $Al(OH)_3$
Presenter: Uendi Pustina
Authors and Affiliation: Uendi Pustina and Dwight L. Myers - *East Central University, Department of Chemistry and Physics*

Reactivity and compatibility of oxides with other materials and with each other play a significant role in choice of materials for developing Thermal Barrier Coatings (TBCs) or Environmental Barrier Coatings (EBCs) for use in combustion environments. Aluminum oxide is one material with potential for these applications. However, the oxide coating itself can be eroded away by reaction with hot water vapor in a combustion environment, forming volatile hydroxides. Aluminum oxide can react with water vapor to form a volatile aluminum hydroxide. We are performing a computational study of the gas phase molecule aluminum hydroxide. The ultimate goal of this study is to obtain a reliable value of the enthalpy of formation of aluminum hydroxide. The software we are using is the GAMESS ab initio package. The geometry of the molecule has been optimized at the B3LYP/Dunning cc-pVTZ level. Presently, energies of the aluminum hydroxide and fragments are being computed. Results to date will be presented.

P13: Computational Vibrational Analysis of Large Systems - Lomustine Matrix Isolated in 20 K Argon
Presenters: Jonathan W. Davis, Mathew S. Faso and Austin D. Ryden
Authors and Affiliation: William B. Collier, Zackory D. Boisselle, Jonathan W. Davis, Mathew S. Faso, Austin D. Ryden and Gary Ritzhaupt - *Department of Chemistry, Oral Roberts University*

Lomustine is a lipid-soluble, alkylating nitrosourea-based chemotherapy drug often used to treat brain tumors and Hodgkin's Lymphoma. While the general pharmaceutical action of the drug is known, the active site and reactivity of in vitro lomustine is not. This poster presents the 20 K frozen argon matrix isolated FTIR spectrum of lomustine. Our results present the matrix isolated monomer spectrum of lomustine and vibrational shifts seen when the argon matrix is heated to 35 K to soften the matrix to promote dimerization. SQM scaled LCAO-MO computational Hessian studies at the B3LYP/6-31G+(d,p) and higher theoretical levels are underway to understand the structure and possible conformers of this pharmaceutical and its hydrogen bonded dimers using the vibrational assignments calculated with GAMESS and SQM scaled with FCART 7.0. Initial results reveal that lomustine was successfully isolated with few water or lomustine hydrogen bonded dimers except when the argon matrix is heated

to 35 K after deposition. Acquisition of a new 1200 core parallel supercomputer ("Titan") coupled with a parallelized GAMESS installation is allowing us to investigate these structures at high density functional theoretical levels and expand our theoretical modelling to inclusive structures that include the argon cage matrix within which the lomustine molecule is isolated. The initial results look very encouraging.

P14: Controlling the Acidity of Phosphonate Ligands over Amorphous Silica
Presenter: Ishaq Alalq
Authors and Affiliation: Ishaq Alalq and Bin Wang - *School of Chemical, Biological, and Material Engineering University of Oklahoma*

Tuning the acidity of the active sites is valuable for controlling the reaction activity and selectivity in acid-catalyzed reactions. Here, we report a theoretical analysis that involves tuning and modifying different phosphonate ligands over amorphous silica. Using density functional theory calculations (DFT), we calculate different binding configurations of phosphonate ligands on amorphous silica. We further evaluate the effect of different substitutional groups in the phosphonate ligands on the acidity of the proton acidity. The different acidity was further supported by calculated vibrational frequencies. This method will help further improve the catalytic activities of amorphous silica altered by phosphonate ligands, which could be applicable for practical chemical processes such as dehydrogenation and polymerization.

P15: Correlation of Microstructural and Viscoelastic Properties of Mucin Biopolymer in Response to pH and [Ca^{2+}]
Presenter: Austin Curnutt
Authors and Affiliation: Austin Curnutt, Kaylee Smith, Emily Darrow and Keisha B. Walters - *School of Chemical, Biological and Materials Engineering, University of Oklahoma*

Mucus is a viscoelastic biopolymer solution that exhibits complex fluid behavior and plays a crucial physiological role, especially where surfaces and interfaces are in contact with external elements such as the lungs and stomach. The sol-gel transition and viscoelastic behavior found in mucus results from reversible interactions between functional group sites allowing for a complex network to form in native mucus and mucin solutions. These changes in viscoelastic response are critical in the ability of mucus to serve as a protective barrier against foreign substances and for transport/removal of these materials. However, in the case of therapeutics it is crucial a drug be absorbed and transported to epithelial and macrophage cells for uptake when administered via a respiratory, gastrointestinal, or other mucus-protected organ. For both pathological conditions and drug delivery design, it is important to understand how local chemical conditions can affect viscoelastic and structural properties of mucus. In this study, microstructural and viscoelastic properties of aqueous solutions of porcine gastric mucin (PGM)—the biopolymer in mucus—were investigated in response to changes in pH and $CaCl_2$concentration. Mucin solutions were characterized using rheology, dynamic light scattering (DLS), zeta potential, surface tension, and FT-IR spectroscopy to correlate microscale structural changes with macroscopic viscoelastic behavior. Significant property changes were induced in PGM solutions by changing pH, with a transition from solution to

gel-like behavior occurring at and below pH values ca. 4. The addition of 0.01 M $CaCl_2$ resulted in an increase in the sol-gel transition pH value. After gelation, the mucin polymer forms a network structure allowing the material to demonstrate an increase in viscosity and an elastic behavior. The relationships between ionic strength and valency and the sol-gel network transition in mucin can be extended to contribute to a better understanding of other biopolymers, biomimetic polymers and other synthetic polyelectrolytes, as well as other hydrogel materials.

P16: Design and Development of Surveys Distributed Through QR Codes to Assist the Pencil-Paper Problem Solving Process in Organic Chemistry
Presenter: Tanner Martin
Authors and Affiliation: Tanner Martin and Robyn Biggs - *Chemistry and Biochemistry, University of Oklahoma*

Practicing problems is important for student success in organic chemistry. The ability to solve these problems through handwritten answers is thought to increase performance on assessments due to motor memory. A downside to pencil-paper assignments is that it is difficult to lead students through the problem-solving process with hints or tips, which online homework systems can easily do. In order to preserve the hand-written nature of assignments and have the ability to lead students through questions, Quick Response (QR) codes have been used to link problems on the assignments with a survey to provide hints and elaborate on key aspects of the problem solving process. The design of these surveys for organic synthesis problems in a second-semester introductory organic chemistry course will be discussed.

P17: Detection of Shed Syndecan-1
Presenter: Austin R. Anderson
Authors and Affiliation: Austin R. Anderson and Gabriel Cook - *Oklahoma State University*

The cleavage and subsequent shedding of the extracellular portion of syndecan-1(SDC-1) is highly regulated by the human body. In times of cellular stress, the ectodomain of this integral membrane protein is cleaved and lost into the bloodstream. Studies have correlated serum concentrations of SDC-1 ectodomain with the presence and prognosis of various cancers. Matrix metalloproteinases (MMPs) are one of the factors implicated in the shedding of SDC-1 and many of these MMPs are upregulated as cancer overtakes a cell. We extend upon the work by Manon-Jensen [FEBS Journal, (2013) 280(10), pp.2320-2331] showing distinct MMPs can cleave SDC-1 in primarily two locations; producing two different lengths of the soluble ectodomain. Current research on serum levels of SDC-1 has used polyclonal antibodies that are non-specific for binding of different lengths of the ectodomain. The goal of this research is to develop a detection method for specific chain lengths of the shed SDC-1 ectodomain using monoclonal antibodies. We have accomplished the first steps of this project via expression of the different lengths of SDC-1 in E. coli. Purification is done using Ni-NTA affinity chromatography and checked via gel electrophoresis and MALDI mass spec. Results may lead to new methods for the detection and prognosis of cancers.

P18: Development of an in Vivo Assay for Directed Evolution of Type II-A CRISPR Adaptation
Presenter: Garret Morton
Authors and Affiliation: Garret Morton, Mason Van Orden and Rakhi Rajan - *University of Oklahoma*

The Clustered Regularly Interspaced Short Palindromic Repeats and CRISPR associated proteins (CRISPR-Cas) comprise systems of adaptive immunity in bacteria and archaea, allowing prokaryotes to defend against invading nucleic acids. First, in the adaptation stage of CRISPR, the organisms must acquire segments of the foreign DNA, known as spacers, and integrate them into an existing repeat-spacer array. Studies have shown that in type II-A CRISPR-Cas systems, the Cas1 and Cas2 proteins are essential for the adaptation process, and that it depends on sequence-specific interactions between these proteins and the 3' end of the CRISPR leader region. The goal of this project is to establish an assay which can detect spacer integration in vivo. We will first introduce a plasmid encoding a type II-A CRISPR locus into bacteria lacking any Cas proteins. Upon successful transformation and verification of spacer acquisition, we will introduce a second plasmid containing the toxic ccdB gene, which will only be tolerated by bacteria capable of acquiring spacers targeting and inactivating the toxic plasmid. This high-selective pressure in vivo integration assay will be key in future directed evolution studies aimed at developing Cas1-Cas2 variants capable of spacer integration at specific DNA targets for genome tagging applications.

P19: DHDPS and Antibiotic Drug Design: Kinetics and Structural Studies of Dihydrodipicolinate Synthase and 2-Bromopropionic Acid
Presenters: L. Chooback, L. Thomas, W. E. Karsten and C. Schartz
Authors and Affiliation: L. Chooback, L. Thomas, W. E. Karsten and C. Schartz - *University of Central Oklahoma*

Bacterial infections create a serious need for development of new antibacterial drugs. One area of research has been focused on inhibition of the lysine biosynthetic pathway in bacteria. The DAP biosynthetic pathway is an attractive target for the development of antibacterial compounds owing to the presence of the pathway in bacteria, but not in mammals. Inhibitors of enzymes in this pathway are expected to have limited toxicity to humans. 2-bromopropionic acid (pyruvate analogues) was used for kinetic studies showed that the DHDPS loses nearly all activity in the presence of this ligand at low mM concentrations. Crystals of DHDPS co-complexed with 2-bromopropionic acid formed in polyethylene glycol 3350 and 0.2 M sodium tartrate at pH 7.5. The diffraction data was collected at the University of Oklahoma X-ray facility. Crystals diffracted to ~2.15 Å and belong to the P1 space group. The crystal structure confirms the displacement of bromine and formation of a covalent attachment between propionic acid and lysine 161 (K161) at the active site of the enzyme. We have also tested the growth inhibition in liquid media for both JM109 and PS1. Both cultures ceased to grow at 1 mM concentration of the above ligands. We are working on design of a bacterial phenotype rescue experiment.

P20: Dissolution of Mackinawite (FES) Facilitated by Dioic Acids under Oxic Conditions
Presenter: Sarah Hobson
Authors and Affiliation: Sarah Hobson,[1] Alejandra Hernandez[1] and Mark A. Nanny[1,2] - *[1]School of Civil Engineering and Environmental Science, Gallogly College of Engineering and [2]Institute for Energy and the Environment, Mewbourne College of Earth and Energy, University of Oklahoma*

Corrosion of carbon steel pipelines and storage tanks costs the oil and gas (O&G) industry approximately $8.4 billion annually. Microbial influenced corrosion (MIC) is estimated to be responsible for up to 30% of this corrosion. Formation of hydrogen sulfide by sulfate-reducing bacteria, that can utilize hydrocarbons as a carbon source, drives most of the MIC in the O&G industry. Ferrous iron produced during the oxidation of metallic iron reacts with hydrogen sulfide to form ferrous sulfides deposits on the steel surface. During anoxic-oxic fluctuations, e.g. draining and filling of produced water storage tanks, exposure of ferrous sulfide deposits to oxygen results in oxidation to ferric oxides. The ferric oxide layer can form a protective layer over the ferrous sulfide deposits preventing further oxidation. However, adsorption of organic acids to the ferric oxide layer may facilitate dissolution of ferric-organic ligand complexes, thereby exposing the ferrous sulfide deposits to additional oxidation. Cycling of the oxidation-adsorption-dissolution mechanisms under oxic conditions will result in the eventual removal of ferrous sulfide deposits and facilitate continued corrosion of exposed steel. Dioic acids (oxalic, malonic and succinic acids) have been identified in production waters from the Barnett Shale in north Texas and Putumayo, Colombia. These acids have high stability binding constants with ferric iron and form soluble ferric-ligand complexes. To test the hypothesis that dioic acids facilitate the oxidation and dissolution of ferrous sulfide under oxic conditions, mackinawite (FeS) powder was suspended in nanopure water open to the atmosphere for seven days in the presence of dioic acids. It was found that both total dissolved iron and pH increased in proportion to the stability binding constant (oxalic > malonic > succinic). It is concluded that under oxic conditions, dioic acids can facilitate the oxidative removal of ferrous sulfide deposits from steel surfaces, thereby accelerating corrosion of steel.

P21: Drug Design: Small Molecule Inhibitor for Pro-Apoptotic BAX Protein in Cells
Presenter: Richard Van
Authors and Affiliation: Richard Van, Nicholas Massaro,[1] Xiaoliang Pan,[1] Indrajeet Sharma,[1] Jialing Lin[2] and Yihan Shao[1] - *[1]Univeristy of Oklahoma and [2]University of Oklahoma Health Science Center*

The synthesis of small molecule inhibitors for BAX protein induced apoptosis allows for the protection of cells from excitotoxicity, for example, the death of cardiac cells during cerebrovascular accidents. Current drugs available have much room for improvement in areas of binding affinity and selectivity. Using computational tools to screen and optimize small molecule design allows for streamlining experimental procedures. These small molecules, which are preparing for assay trials, were found from screening over 200 compounds, and were optimized to theoretically provide improved binding affinity to BAX.

P22: Effects of Ligand Structure on the Kinetics of ATRP for Monomers Containing Tertiary Amines
Presenter: Collin Britten
Authors and Affiliation: Collin Britten, Jorge Carvalho, Kristen Lason, Yokly Leng and Keisha B. Walters - *University of Oklahoma*

Controlled (or living) radical polymerization (CRP) mechanisms are an important synthesis tool in the production of stimuli-responsive polymers. One of the most studied CRP mechanisms is atom transfer radical polymerization (ATRP). In ATRP, the key parameter to maintaining control of the reaction system is selecting the proper ligand-catalyst pair. Ligands typically contain two to four tertiary amine groups, which complex with the transition metal catalyst to facilitate the controlled polymerization. However, with some stimuli-responsive polymers, the same monomer chemical moieties that impart the responsive behavior in the polymer can interfere with the ligand-catalyst complex and disrupt the expected level of control for certain ligand-catalyst pairs. One system displaying this issue is the ATRP synthesis of poly[(dimethylamino)ethyl methacrylate] (PDMAEMA), a polymer with pendant groups containing tertiary amines. The monomer amine groups can competitively complex with the catalyst in solution, disrupting the intended ligand-catalyst complexation. In this work, PDMAEMA was synthesized by Cu(0) catalyzed ATRP with four different ligands: 2,2'-bipyridine (2bpy); tris(2-pyridylmethyl)amine (TPMA); N,N,N',N",N"-pentamethyldiethylenetriamine (PMDETA); and tris[2-(dimethylamino)ethyl]amine (Me_6TREN). Ligands were selected to examine the effects of (i) alkyl and aromatic amines and (ii) ligand denticity. Synthesized polymers were characterized using gel permeation chromatography (GPC), dynamic light scattering (DLS) and nuclear magnetic resonance (NMR) to examine the impact of ligand on molecular weight and molecular weight distributions (MWDs). Functional groups were verified using Fourier-transform infrared spectroscopy (FT-IR). Results demonstrate that ligands containing aromatic amines offer superior control, yielding final products with narrower MWDs. Increasing denticity was found to generally improve control, especially for shorter reaction times.

P23: Epoxide Functionalization and Characterization of Dye-Doped Silica Nanoparticles
Presenter: Jordan Flower
Authors and Affiliation: Jordan Flower and Nathan Green - *Northeastern State University*

Silica nanoparticles are stable biocompatible materials with low toxicity that can be utilized to carry small molecules, such as dyes and bioactive compounds, to discreet locations due to the relative ease of functionalizing their surface. One such organizational technique employs DNA-based nanostructures to arrange nanoparticles along discreet locations of the DNA surface. To address the issue of attaching the silica to a DNA template and possible ways to bind the silica to other nanomaterials an epoxide surface functionalization process was used. Silica nanoparticle seeds were synthesized using an aqueous organic bilayer method to control the rate of nanopaticle growth. The seeds were then physisorbed to the cationic fluorescent dye rhodamine-B before being encapsulated using a second silica layer. The rhodamine-B could then be proven as encapsulated by observing its bright pink color as well

as its adsorption peak on a taken UV visible (UV-VIS) spectrum. A final functionalization was done to attach epoxides to the surface of the silica. The epoxide functionalized particles were then observed using IR spectroscopy to observe the corresponding peaks for both silica and epoxides. Using the epoxide functional group to react with DNA will allow for the DNA to then become attached to the surface of the silica, moving one step towards the goal product of a nanoscale assembly.

P24: Experiential Learning and Observational Learning Applied to Ethics and Diversity
Presenter: Madison R. Tytanic
Authors and Affiliation: Madison R. Tytanic and Donna J. Nelson - *Department of Chemistry, University of Oklahoma*

Students participated in applying experiential learning and observational learning to lessons in ethics and diversity. As a group, a class of students watched and then discussed the portrayal of real-life examples of ethics violations, racism, sexism, poor judgement, and other behaviors which many people find offensive or dangerous. Then each student selected a similar real-life example to present to the class, for discussion. One student from the class will present her experiences, opinions, and learning.

P25: Fabrication and Characterization of Conductive Organic Fibers as Non-Metallic Electrodes for Clinical Applications
Presenter: Megan Hays
Authors and Affiliation: Megan Hays,[1] Santosh Adhikari,[1] Bertram Richter,[2] Saadyah Averick[2] and Toby L. Nelson[1] - *[1]Department of Chemistry, Oklahoma State University and [2]System Department of Neurosurgery, Allegheny Health Network*

Recently, organic conductive fibers have emerged as promising materials for non-metallic electrodes. These materials can be biocompatible, lightweight, better integrated, easily fabricated, and have low heat transfer compared to the metallic electrodes. Our group has developed a facile, economical, and scalable method for fabricating new organic conductive fibers. The new organic conductive fibers are prepared by staining non-conductive fibers like polyester and cotton threads with a conductive ink composed of two conductive materials, poly(3-hexylthiophene) and single-walled carbon nanotubes. The preparation, characterization and recording properties of organic new organic conductive fibers will be presented.

P26: First-Generation Structure-Activity Relationship Studies of 2,3,4,9-Tetrahydro-1H-Carbazol-1-Amines as CpxRA Modulators
Presenter: Jessi J. Gardner
Authors and Affiliation: Jessi J. Gardner,[1] Yangxiong Li,[1] Katherine R. Fortney,[2] Stanley Spinola,[2] and Adam S. Duerfeldt[1] - *[1]Department of Chemistry and Biochemistry, University of Oklahoma and [2]Department of Microbiology and Immunology, Indiana University School of Medicine*

The urgent need to develop new antibacterials is indisputable, especially for infections resulting from multi- and extensively-drug resistant Gram-negative pathogens. The current arsenal of antibacterials target a limited number of essential enzymes and processes and resistance evolution now outpaces our ability to derivatize known chemotypes and advance the new entities through clinical evaluation. Despite great effort, very few new targets have been identified for Gram-negative bacteria in the last 50 years. In contrast to the dogma that only compounds that completely inhibit cell growth will find clinical utility, one strategy gaining significant traction is to render organisms vulnerable to host immune clearance by targeting virulence determinants or processes that control the expression of pathogenicity. In this context, bacterial two-component signal transduction systems (2CSTS) represent promising targets. Bacterial 2CSTS are conserved across many drug-resistant Gram-negative pathogens and are known to regulate gene transcription involved in cell growth, envelope integrity, quorum sensing, and expression of virulence factors. As such, modulation of these systems represents a promising antibacterial strategy and is expected to exhibit complementarity to existing approaches. CpxRA is a 2CSTS found in many drug-resistant Gram-negative pathogens and genetic activation of CpxRA abolishes the virulence of a number of pathogens in murine models. Recently, small molecule 2,3,4,9-tetrahydro-1H-carbazol-1-amines were shown to activate the CpxRA system by inhibiting the phosphatase activity of CpxA. This poster will present our recent progress towards advancing this chemotype to provide chemical probes poised for utilization in advancing the understanding of the biological significance and therapeutic potential of CpxRA and 2CSTS in general. Results will include a discussion of the stereochemical requirements of this chemotype and the features that drive potency.

P27: Fragment Based Drug Design and Synthesis of Microsomal Prostaglandin E Synthase-1 and 5-lipoxygenase Dual Inhibitors for Their Preventive and Therapeutic Applications in Inflammatory and Oncologic Diseases

Presenter: Nagendra Sastri Yarla

Authors and Affiliation: Nagendra Sastri Yarla,[1] Gopal Pathuri,[1] Hariprasad Gali,[2] Anil Singh,[1] Janani Pannerselvam,[1] Venkateshwar Madka[1] and Chinthalapally V. Rao[1] - *[1]Center for Cancer Prevention and Drug Development, Department of Medicine, Hematology-Oncology Section, Stephenson Cancer Center and [2]College of Pharmacy, University of Oklahoma*

Background: Fragment-based drug discovery (FBDD) is a high-throughput screening approach for the generation of chemical leads and their optimization and is widely used to design drugs, some of which have entered into clinical trials as wells as market (Bian et al., 2018). Licofelone, a cyclooxygenase (COX) and 5-lipoxygenase (5-LOX) dual inhibitor, is under clinical trials for several inflammatory and oncologic diseases. However, its poor water solubility and COX-2-inhibition associated toxicity are limiting its clinical applications. Aim and objective: The main aim of this work is to modify the licofelone pharmacophore to obtain better binding orientation, which led to target microsomal prostaglandin synthase-1 (mPGES-1) (the downstream enzyme of COX-2) and 5-LOX while excluding COX-2 inhibition. Experimental: Molecular modelling methods were used to identify optimized ligand with the addition of a required fragment (licofelone + glycine) that binds to the desired drug target (mPGES-1 and 5-LOX) with required binding mode and further optimized lead

molecule validated the efficacy using in vitro enzyme assays and isothermal calorimetry (ITC) based binding assays (Kim et al. 2008; Gambini et al., 2018). Drug-likeness properties of LFA9 and licofelone was calculated using Molinspiration tool. Results and Discussion: LFA9 was designed using fragment-based drug discovery and synthesized (previously patented procedure Chinthalapally et al. 2019) by conjugating licofelone with glycine at its carboxylic end which leads to inhibiting mPGES-1 and 5-LOX but not COX-2. In molecular docking studies, LFA9 strongly binds to human 5-LOX and mPGES-1 with binding energies of -199.85 Kcal/mol and -245.34 Kcal/mol respectively. Interaction analyses demonstrated that LFA9 binds with amino acids of the active sites of 5-LOX and mPGES-1. Further, the ITC technique was used to validate the binding affinities between LFA9 and 5-LOX (Kd_1 = 255 μM; Kd_2 = 83 mM), mPGES-1 (Kd = 16 μM) and COX-2 (Kd >1mM). LFA9 substantially inhibited human mPGES-1 (IC_{50}=0.87 μM; p>0.0001) and 5-LOX (IC_{50}=2.75 μM) but not COX-2 (IC_{50}>1mM). LFA9 strongly binds to mPGES-1 and 5-LOX, thereby inhibits their enzyme activities. Moreover, LFA9 (cLogP = 4.34) obeys Lipinsky`s rule of 5 for drug likeness and shows better water solubility unlike licofelone (cLogP = 6.15). Conclusions: LFA9 substantially inhibited mPGES-1 and 5-LOX activities but did not inhibit COX-2. Hence, it can be a better drug candidate than its parental compound licofelone for pre-clinical studies related to inflammatory and oncologic diseases.

P28: FT-IR Investigation of C-C Bond Formation on TiO_2-based Nanomaterials
Presenter: Dilip Paul
Authors and Affiliation: Dilip Paul and Jennifer Moffat - *Department of Chemistry, Pittsburg State University*

The role of acid-base sites on Ga-In doped TiO_2-nanomaterials was determined using various probe molecules adsorbed on the surface at different temperatures using a specially designed ultra-high vacuum (UHV) infrared cell. The UHV cell is attached to a vacuum manifold which is continually pumped by a 60 L turbo-molecular pump and a diaphragm roughing pump to obtain a routine pressure of $1x10^{-8}$ Torr. It was found that at 233 K, acetaldehyde adsorbed through hydrogen bonding to surface hydroxyl groups as well as through Lewis acid sites over pretreated TiO_2-based surfaces. The formation of 2-butenal was observed as the product of aldol condensation reaction. This C-C bond formation is found to be due to the presence of Brønsted and Lewis acid sites. Upon blocking these acid sites with NH_3 adsorption, the C-C bond formation can be substantially suppressed, which in turn indicates that acid sites indeed are responsible for C-C bond formation. Various TiO_2-based nanomaterials were compared in order to elucidate the contribution of local surface structures.

P29: Functional Insect Protein Extracts for Food Applications
Presenter: Rashmi Vadivelu Amarender
Authors and Affiliation: Rashmi Vadivelu Amarender,[1] Kanika Bhargava,[1] Aaron Dossey[2] and Sanjeewa Gamagedara[3] - *[1]Department of Human Environmental Sciences, University of Central Oklahoma, [2]All Things Bugs LLC, and [3]Department of Chemistry, University of Central Oklahoma*

The world population has been increasing rapidly which results in high demand for a nutrient dense food supply. Conventional animal protein sources may be insufficient to meet this need, subsequently opening a door to alternative sources. Edible Insects are, in general, rich in protein, Vitamins, Minerals and can provide all the essential amino acids, unsaturated fatty acids, and micronutrients. This study suggests Cricket (Gryllidae), is a potential source of protein for human consumption. In this study protocol, Ethanol (99.5%) and Hexane (100%) was used for defatting cricket powder at a solvent to the material ratio of 5 mL/g. The solution was centrifuged at 4800 rpm for 10 minutes. The filtrate was then passed through nitrogen gas. The fat and the solvent were separated using a rotary evaporator and the fat percentage was calculated. The proteins were then extracted using 0.5M NaOH and ammonium sulfate from the ethanol and hexane de-fatted cricket powder. The protein extract was then freeze-dried to a moisture content less than 5%. The proximate analysis was carried out on the cricket powder and the Protein content was 74.42%, ash 5.09%, Calories 407 kcal/100 g, Carbohydrates 7.14%, Moisture 4.70% and fat 9.27%. The original cricket powder had a fat content of 20.86% and using Ethanol we were able to reduce the fat content from 20.86 to 9.27% by evaporating 11.59% of ethanol using rotary evaporation. Protein extraction using ascorbic acid gave the highest yield in comparison to NaOH. The efficiency of the extraction rate was about 70%. The Protein solubility reached its highest value at pH 9 (74%). The consumption of insects, therefore, contributes positively to the environment, food and nutritional security, and healthy life for present and future generations. The afore-stated method shows that insects can be used as an alternate source of protein. The future investigation of this research will be to incorporate the protein powder in low nutrient-dense foods, study its properties, and analyze the use of insect-based protein powders on an industrial scale.

P30: Heteroaryl Aldehyde Substrates for use in a Non-Traditional Method of N-Sulfonyl Imine Formation
Presenter: Megan D. Hopkins
Authors and Affiliation: Megan D. Hopkins, Felagot Abebe, Robert J. Sheaff and Angus A. Lamar - *University of Tulsa*

Our research group has developed a mild synthetic method to install N-sulfonyl units, which are employed within the drug discovery field as bioisosteres in a variety of pharmaceuticals and bioactive compounds, directly into aldehyde functionality under non-traditional conditions. The resulting N-sulfonylimines can be employed as valuable intermediates in a wide range of synthetic applications. Our recent progress towards the exploration of the substrate scope of the heteroaryl aldehydes and the resulting bioactivity of the products will be presented.

P31: High Temperature Solid State Reactions of Silicon, Titanium and Yttrium Oxides
Presenter: Lizbeth Robles-Fernandez
Authors and Affiliation: Lizbeth Robles-Fern, Fernando Salazar-Salas and Dwight L. Myers - *East Central University, Department of Chemistry and Physics*

Reactions of titanium oxide and silicon dioxide are of importance in materials used in high temperature environments. There are questions concerning the reaction of titanium dioxide

(rutile) with silica. Both are important as potential materials or reaction products in thermal barrier coatings or environmental barrier coatings in combustion environments, as for example in gas turbine technologies. The extent of reaction and temperature range are important questions to answer for this chemical system. Experimental evidence would suggest that a third cation is necessary to have compound formation. Presently we are exploring the reaction of titanium dioxide with silicon dioxide with small amounts of yttrium oxide being added as substitution for titanium with a 1:1 (Y,Ti):Si ratio. Mixtures of the three oxides are being subjected to heatings at various temperatures from ca. 1200-1500 °C. Compositions studied to date are 10 and 30 mol % yttrium substituted for titanium. Samples are characterized before and after heating by means of X-ray diffractometry and diffuse reflectance infrared spectroscopy, transmission infrared spectroscopy, and/or diffuse reflectance UV/Vis spectroscopy as appropriate. Results to date will be presented.

P32: High-symmetry Low-coordinate Complexes of Cerium(III) and Uranium(III): Tris[bis(trimethylsilyl)amido] Phosphine Oxide Compounds for Empirical f-Element Electronic Structure Investigations

Presenter: Stewart Bragg Younger-Mertz
Authors and Affiliation: Stewart Bragg Younger-Mertz, Doug J. Powell, Donna J. Nelson and Robert K. Thomson - *University of Oklahoma*

This work reports the synthesis and characterization of trivalent four-coordinate tris(silylamide) phosphine oxide complexes of Uranium and Cerium with approximate C3 symmetry. To our knowledge, f-element tris(silylamido) phosphine oxide complexes with substituted-aryl phosphine oxide ligands have not been characterized via XRD or NMR. Substituted aryl-derivatives exhibit different reactivities and spectroscopic properties than the simple triphenylphosphine oxide framework, because the relative electron densities on the phosphorus and oxygen atoms are highly influenced by the electronic character of the organic substituents bound to the phosphorus. The nature of the organic substituents on phosphorus therefore highly influences the nature of the metal-oxygen bond in phosphine oxide coordination complexes. These axially symmetric four-coordinate silylamide phosphine oxide complexes are suitable models for studying the relative differences in f-block metal-ligand covalency using ^{31}P NMR spectroscopy and X-ray emission spectroscopy. Expanding this structural framework to other lanthanide and actinide metals, and fully characterizing a series of pseudo-isostructural complexes featuring various organic substituents on the phosphine oxide (beyond simple triphenylphosphine oxide system), would provide considerable insight concerning phosphine oxide bonding interactions with f-block metals. In addition to being convenient ligands for spectroscopic studies of f-element electronic structure, phosphine oxides (and the details of their interactions with f-block metals) are directly relevant to the nuclear fuel cycle. The fundamental nature of f-block metal-phosphine oxide bonds is not well understood, and deeper empirical insight into the nature of these interactions is needed in order to facilitate large-scale computational screening of potential extractants for trivalent Ln/An separations. Herein we report the synthesis, X-ray crystallography, and paramagnetic NMR spectroscopy of a series of trivalent Cerium and Uranium tris(silylamido) phosphine oxide complexes; $M[N(SiMe_3)_2]_3[OPR_3]$, M = Ce, U.

P33: Synthesis of Tris(silylamido) Phosphinimide Complexes of Uranium(IV) and Cerium(IV) via Protonolysis and Fluorotrimethylsilane Elimination
Presenter: Stewart Bragg Younger-Mertz
Authors and Affiliation: Stewart Bragg Younger-Mertz, Donna J. Nelson and Robert K. Thomson - *University of Oklahoma*

Herein we report the synthesis of tris[bis(trimethylsilyl)amido] phosphinimide complexes of Uranium(IV) and Cerium(IV). The Uranium complexes were synthesized via protonolysis of the well known metallacycle, and the Cerium complexes were synthesized via fluorotrimethylsilane elimination of the tetravalent tris(silylamido) fluoride precursor. The NMR spectra for the Uranium derivatives feature extremely large paramagnetic shifts, suggesting an elevated degree of orbital mixing in these mostly ionic (polarized covalent) metal-ligand bonds. The tetravalent Cerium complexes, despite having formally closed-shell configurations (f^0) and being diamagnetic, also feature large ^{31}P NMR chemical shifts relative to the free phosphinime ligands. This work provides another set of empirical evidence for what some researchers have labeled the "Uranium-like covalency" of tetravalent Cerium compounds.

P34: Identification of Different Protonic Species in H-ZSM5
Presenter: Vy Thao Nguyen
Authors and Affiliation: Vy Thao Nguyen,[1] Jeffey White[2]and Bin Wang[1] - *[1]School of Chemical, Biological, Materials Engineering, University of Oklahoma and [2]School of Chemical Engineering, Oklahoma State University*

The nature of the protonic species may be critical for controlling activity and selectivity of various zeolite-catalyzed reactions. Here, H1 NMR of H-SZM-5 zeolite has been calculated using Density Functional Theory (DFT), through with we show that computed data are consistent with experimental signals for the protonic species in dealuminated H-ZSM-5 zeolite. These different species include the silanol group (Si-OH), the isolated Bronsted acid site (BAS), extra-framework aluminum (EFAl), and EFAl/BAS in the proximity. We further show that the chemical shift of isolated BAS depends on the location of the framework Al and the hydrogen position. The BAS that have more surrounding oxygen atoms has larger chemical shift. The results from DFT calculation suggest that the EFAl/BAS synergy may significantly enhance the Bronsted acid activity of dealuminated H-ZSM-5 zeolite. In addition, the chemical shift of BAS with EFAl nearby at different position was calculated, and these results affirm the proposed structure of EFAl species. These findings are valuable for predicting the activity of dealuminated zeolite in acid catalysis.

P35: Instrumental Hardware-Software Interfacing
Presenters: Morgan Thurman and Jerrik Burson
Authors and Affiliation: Morgan Thurman, Jerrik Burson and Shawna York - *Southern Nazarene University*

This project sought to overcome the “black box” mindset by exploring the intricate workings of various laboratory equipment. Many universities pay massive amounts of money to specialized hardware and software companies to keep their laboratory testing equipment

functioning and interfacing with computers. Certain equipment requires a specific computer program and data collection mechanism to output readings in a readable format on a computer where it can then be analyzed, and when a computer crashes or a program is lost, repairing the compatible interface can cost almost as much as the original instrument if no one knows how to fix it. During this research, LabVIEW 2009 Education Edition and a Vernier SensorDAQ interface were used to create a Virtual Instrument (VI) program that could read and interpret the electrical signal output from an instrument to then display and analyze it accordingly. The instruments interfaced with were a gas chromatograph, solution calorimeter and various smaller probes.

P36: Interfacial Toughness of Diblock Carbon Nanotubes Reinforced Immiscible Polymer Blends
Presenter: Fatoumata Ide Seyni
Authors and Affiliation: Fatoumata Ide Seyni, Lawrence Barrett, Brian P. Grady and Steven Crossley - *School of Chemical, Biological and Materials Engineering, University of Oklahoma*

We have synthesized diblock nanotubes in our laboratory; morphologically these are identical to block copolymers. We are investigating the effectiveness of block nanotubes as interfacial strengthening agents by measuring the fracture toughness of the interface between two immiscible polymers, polystyrene and poly (methyl methacrylate). We are measuring the fracture toughness using the asymmetric double cantilever beam (ADCB) method which has been previously used to determine the fracture toughness of PS/PMMA and PS/PVP interfaces reinforced with block and random copolymers. The aim of this work being to establish the effectiveness of our block nanotubes as interfacial strengthening agents, results of this work will be compared to the results obtained previously with copolymers as well as results with single-chemistry nanotubes.

P37: Investigation of Enzyme 3CBW Function
Presenters: Megan Shelton and Morgan Freeman
Authors and Affiliation: Megan Shelton ,[1] Morgan Freeman,[1] Lindsey Long[1] and Biochemistry Authentic Scientific Inquiry Lab group (BASIL)[2] - *[1]Department of Biology, Oklahoma Christian University and [2]Rochester Institute of Technology*

Proteins are vital to living organisms and their functions are critical within the cells that make organisms thrive. These proteins have specific functions that lead to specialized works within cells and throughout the living organism. Some commonly recognized categories of proteins are hormones, enzymes, and antibodies. Specifically, enzymes speed up the rate of chemical reactions within cells and help support life. Examples of well-known enzymes are maltase, which breaks down sugar to form glucose, and amylase, which converts starch into sugar. Enzymes operate by temporarily binding a chemical molecule, a substrate, to a specific location on the enzyme known as the active site. This binding allows the substrate to proceed through the chemical process in a rapid manner. The absence of enzymes would cause chemical reaction to proceed too slowly and necessary products would be exhausted. Knowing the function of enzymes can help improve the understanding of chemical reactions that occur within living organisms. This project focused on identifying the function of a

specific enzyme, 3CBW. The structure of 3CBW is known, but the function of the enzyme has not been elucidated. Because enzymes with similar structures also have similar functions, we used bioinformatic tools to compare the structure of 3CBW to structures of enzymes with known functions. These data suggested that 3CBW is a putative Mannan-Endo-1-4-Beta-Mannosidase, which is a type of hydrolase. 3CBW was purified and enzymatic assays were performed to measure the activity of 3CBW with three different substrates. The enzyme displayed the highest activity with 4-nitrophenyl butyrate, an ester/lipid substrate. This data was not supported by the original hypothesis that 3CBW would react best with a carbohydrate substrate. Future directions would be to test the activity of 3CBW with a specific mannosidase substrate.

P38: Investigation of Microwave and Ultrasonic Energy in the Synthesis of Heterocycles Related to Medicinal Chemistry
Presenters: Restituto Paris and Stephen Myers
Authors and Affiliation: Restituto Paris, Stephen Myers and E. Ann Nalley - *Department of Chemistry, Physics and Engineering, Cameron University*

Allowing many chemical reactions to be completed within minutes, microwave heating and ultrasonic energy have revolutionized preparative chemistry. Both are green technologies and as a result, are becoming widely adopted in both academic and industrial laboratories. This is especially true for microwave synthesis but not many applications of ultrasonic energy in organic synthesis have been reported. Heterocycles are very important functional groups especially in medicinal chemistry. Not only are they pivotal in the synthesis of drugs but also form part of the structure of a diversity of drugs, vitamins, natural products and biomolecules. In this poster we will present the results of syntheses of imidazoles and azolines by both microwave and ultrasonic energy. Derivatives of these two classes of compounds are known for analgesic, antifungal, antihypertensive, anti-obesity, anticancer and other biological activity.

P39: Investigation of Microwave Energy in the Synthesis of Heterocycles Related to Medicinal Chemistry
Presenter: Lindsay Maez
Authors and Affiliation: Lindsay Maez, Victoria Brown and E. Ann Nalley - *Department of Chemistry, Physics and Engineering, Cameron University*

Allowing many chemical reactions to be completed within minutes, microwave technology has revolutionized preparative chemistry. Since it is a green technology, it is becoming widely adopted in both academic and industrial laboratories. Heterocycles are very important functional groups especially in medicinal chemistry. In this research, heterocyclic precursors of pharmaceuticals are synthesized using microwave radiation. An important class of heterocyclics, derivatives of isatin (indole-2,3-dione), as well as its Schiff and Mannich bases, have already been reported to show a variety of biological activities, such as antibacterial, antifungal and anti-HIV activities. The wide spectrum of isatin derivatives and their various chemical properties has led to their increasingly expanded use as precursors for the preparation of many biologically active compounds. Hydrazine derivatives of isatin have

been found to be active against Walker carcinosarcoma. In this research, isatin derivatives were synthesized using microwave technology. Their antimicrobial activity will be tested.

P40: Kinetic Resolution of Chiral Phosphines via Metal-Catalyzed OAT
Presenter: Theo A Rusmore
Authors and Affiliation: Theo A Rusmore, Daniel T Glatzhofer and Kenneth M Nicholas - *University of Oklahoma*

Chiral phosphines are important as ligands for chiral catalysis but are generally hard to isolate by separation techniques. In order to avoid the necessity of chiral column separations, this project aimed to use the family of dioxomolybdenum (VI) (N,N′-(±)-trans-1,2-cyclohexylenebis(5-nitrosalicylideneamine) [MoO_2L] catalysts, which have been shown to catalyze oxygen atom transfer for epoxidation chemistry, to quickly and efficiently separate a racemic mixture of chiral phosphines by oxidizing one enantiomer while leaving the other untouched. The mixture resulting from this kinetic resolution can then be separated using non-chiral chromatography. The ligand structure has been varied in order to introduce steric bulk around the active site of the catalyst as a means of increasing the $\Delta\Delta G‡$ for the kinetic resolution process, and thus improving the enantiomeric excess of the reaction. Effectiveness of the kinetic resolution was characterized by chiral HPLC, and the resultant selectivity (s) compared to that obtained by DFT calculations.

P41: Lanthanum Iron Sulfide as an Electrocatalyst for Water Splitting Application
Presenter: Xavier Martinez
Authors and Affiliation: Xavier Martinez, K. Siam, P.K. Kahol and Ram K. Gupta - *Pittsburg State University*

Recent initiatives to mitigate the damaging effects climate change have pressed the urgency to move away from fossil fuels to more environmentally friendly energy sources. Overall water splitting, with the aid of an electrocatalyst, produce hydrogen and oxygen for use as a clean, carbon-free fuel. The electrocatalytic properties of lanthanum-based perovskite metal oxides have been studied and found to be effective in reducing the overall energy (overpotential) needed for the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). In contrast, little research into any of the properties, let alone electrocatalytic properties of these metal sulfides have been published. Herein, $LaFeS_3$ (LFS) was formed by hydrothermal sulfurization of the intermediate compound in the synthesis of $LaFeO_3$ (LFO). LFS was characterized by X-ray diffraction and then dip coated onto nickel foam as an electrode in a standard three electrode system. The electrochemical properties of LFS were analyzed with electrochemical impedance spectroscopy, line scan voltammetry, and cyclic voltammetry for its electrocatalytic activity towards both the HER and OER. It was shown that toward the HER, LFS reduced the overpotential to 203 mV at 10 mA/cm^2 compared to 217 mV of LFO. With respect to the OER, LFS showed an overpotential of 290 mV at 10 mA/cm^2 where the overpotential of LFO was 310 mV. Investigation of LFS for use in energy storage devices is expected and forthcoming.

P42: Metabolomic Screening of the Effects of Carnitine Treatment during in Vitro T Cruzi Parasite Infection

Presenter: Karina Flores
Authors and Affiliation: Karina Flores,[1] Ekram Hossain[2] and Laura-Isobel McCall[2] - *[1]Department of Biology and [2]Department of Chemistry and Biochemistry, University of Oklahoma*

Chagas disease is an infectious disease caused by the protozoan T. cruzi. Commonly found in Central and South America, about 5 million people are known to be infected. Transmission can happen through fecal matter of the kissing bug, congenitally, or through blood transfusion. Chagas disease can cause heart disease and gastrointestinal problems associated with mega syndromes of the colon and esophagus. Recently, 3D mapping of small molecules in the heart of infected animals revealed differences in acylcarnitine levels in fatal and non-fatal outcomes in mouse models. Subsequent work indicated that carnitine treatment can protect against acute-stage Chagas disease. In this study we wanted to investigate whether carnitine can cause changes in the metabolism of T. cruzi-infected or uninfected cells through an in vitro study. Changes in metabolites can give us insight into the mechanism of carnitine protection, including metabolism-associated disruptions that can affect parasite growth and/or mechanism for infection. We grew T. cruzi strain CL+luc parasites to infect host cells, administered water or carnitine (80 μM), collected whole cells, and extracted metabolites using dichloromethane:methanol:H2O. Using liquid chromatography-tandem mass spectrometry, we analyzed our samples and conducted statistical analysis to identify changes in metabolites caused by carnitine treatment. A molecular network of chemical families was constructed to aid in the analysis. We found a significant upregulation of 63 molecules and downregulation of 77 molecules in cells treated with carnitine. Propionyl carnitine was observed at high levels in the infected-carnitine treatment group while oleamide, an amide of oleic acid, was downregulated. Long chain acylcarnitines were elevated in carnitine-treated infected samples, while some specific phosphatidylcholine family members were decreased. Insight into chemical changes during carnitine treatment can provide addition information to further drug development for Chagas disease and help infected individuals combat this disease.

P43: Metal Oxides Nanoparticles Catalysts for Carbon-Carbon Bond Formation and Intermolecular Rearrangement Reactions

Presenter: Abdulmajeed Alayyaf
Authors and Affiliation: Abdulmajeed Alayyaf and Allen Apblett - *Oklahoma State University*

Nanocrystalline metal oxides are very promising catalysts for numerous organic conversions that are useful for medical and industrial applications. It is extremely important that methods for the preparation of such catalysts allow for the tuning of their surface properties for particular catalytic reactions. For this reason, this investigation focused on the comparison of nanocrystalline oxides produced from two different type precursors: one which produced an oxide surface and the other a hydroxylated one. The latter materials were produced using metal complexes of pyruvic acid oxime complexes while oxalate complexes were used to directly produce oxide surfaces. The two types of catalysts were used in Claisen-Schmidt

condensation, intermolecular cyclization, and Beckmann rearrangement reactions and their activities and selectivities were correlated with their surface acidity/basicity properties, their composition, and their surface areas. Notably, it was possible to perform these reactions with neat reactants without solvent, an important parameter for green chemistry.

P44: Microwave Synthesis of Novel Esters using Sulfuric Acid and Imidazole as Catalysts
Presenter: Theresa Hinkle
Authors and Affiliation: Theresa Hinkle and E. Ann Nalley - *Department of Chemistry, Physics & Engineering, Cameron University*

As recent literature indicates that microwaves are quickly becoming an accepted tool for investigators in the organic laboratory. Microwave synthesis enables reactions to proceed more rapidly with greater yields than many conventional techniques. In this research we have investigated the synthesis of several esters using both a conventional microwave oven and a CEM Explorer Microwave Synthesizer. We have also compared these syntheses using both sulfuric acid and Imidazole as catalysts.

P45: Modeling Water using Spherical Harmonic Interactions
Presenter: Addy J. Evans
Authors and Affiliation: Addy J. Evans and Christopher J. Fennell - *Department of Physics and Department of Chemistry, Oklahoma State University*

Modeling of water is essential for accurate simulations of biological systems. Improvements in the efficiency of water modeling allows for the study of larger systems for longer times. To address this need for efficiency, we built a simple water model that depends only on short-range, tetrahedral hydrogen bond potentials. In this model, we treat hydrogen bonding using spherical harmonic functions, which reduces the number of interaction calculations between water molecule pairs. Within our simulations, we varied the particle size (σ), the dispersion interaction strength (ε), and the hydrogen bond interaction potential (v_0) between pairs of water molecules. To arrive at optimal sets of σ, ε, and v_0 parameters, we performed over 700,00 simulations of pure aqueous solutions. We sorted these models based on their abilities to reproduce experimental properties of water, such as the density and the diffusion coefficient. We have tested this model and found that it reproduces many of the unique properties of water, such as the temperature of maximum density and high liquid heat capacity.

P46: Molybdenum-Based Metal Oxides for Overall Water Splitting and Supercapacitors
Presenter: Camila Zequine
Authors and Affiliation: Camila Zequine, Khamis Siam, Pawan K. Kahol and Ram K. Gupta - *Pittsburg State University*

Today's clean energy scenario emphases on sustainable energy conversion and storage devices. The idea is to develop new materials that can generate and store energy efficiently without damaging the environment. Transition metal oxides are very attractive for these

applications due to their low-cost and rich electrochemical properties. In this study, nickel, cobalt, and iron molybdates were synthesized via a hydrothermal method in order to fabricate electrodes for oxygen evolution reaction (OER) and a supercapacitor. $FeMoO_4$ showed the lowest overpotential (294 mV at 10 mA/cm^2) for OER among all the studied samples, serving as a key material for oxygen generation. For the charge storage applications, the specific capacitance of $FeMoO_4$was observed to be 11.5 F/cm^2 at a current density of 1 mA/cm^2, which is the highest among the studied samples ($FeMoO_4$, $NiMoO_4$, and $CoMoO_4$). In addition to high charge storage capacity, these electrodes exhibited excellent cyclic stability in the galvanostatic charge-discharge study. They retained almost 100% of charge and Coulombic efficiency over 5,000 cycles. From the overall study, it can be concluded that the electrochemical properties of the molybdates depend on the transition metal in the molybdates. These transition metal based molybdates could be promising materials for high-performance energy generation and storage devices.

P47: New Bioassays for Diabetes Autoantibodies with Binding Kinetics
Presenter: Jinesh Niroula
Authors and Affiliation: Jinesh Niroula, Gayan Premaratne and Sadagopan Krishnan - *Department of Chemistry, Oklahoma State University*

Autoantibodies against β-cell antigens namely, glutamic acid decarboxylase-65 (GAD-65), islet antigen-2 (IA-2), and insulin, are reported to appear years before the clinical onset of type 1 diabetes. In a study, according to American Association for Clinical Chemistry, 43.5% of patients who tested positive for two or more autoantibodies developed T1D within 5 years, 69.7% of them within 10 years, and 84.2% within 15 years. This emphasizes the importance of detection of autoantibodies in biological matrices as it assists in developing a prediction model to identify patients with higher susceptibility to diabetes. We developed our biosensor using GAD-65 antigen as the biorecognition element, which was immobilized on carboxylated graphene. This sensor surface was incubated with autoantibody against GAD-65 captured from 10% serum samples with the help of magnetic beads, and charge-transfer resistance (Rct) was measured as signal output. The sensor displayed a wider dynamic range of 0.02 – 2.00 ng ml^{-1} and a limit of detection of 48 pg ml^{-1} for autoantibody detection. Surface plasmon resonance imager (SPRi) was employed to monitor the real-time binding kinetics of the antigen-antibody complex. The binding constant for autoantibody to its antigen on a graphenyl surface was calculated to be 5.6 ± 1.0 pM. Furthermore, the graphenyl sensor surface was compared against the conventional self-assembled monolayer based immunosensor to obtain quantitative insights in the analytical performance of the graphenyl assay. We concluded that graphene-based sensor provided a wider dynamic range and lower limits of detection along with lower non-specific bindings than the conventional monolayer surface.

P48: Nitroxyl (HNO) Complexes of Ruthenium Porphyrins
Presenter: Jeremy R. Zink
Authors and Affiliation: Jeremy R. Zink, Erwin G. Abucayon and George B. Richter-Addo - *Department of Chemistry and Biochemistry, University of Oklahoma*

The simple molecule nitroxyl (HNO) is known to elicit important biological responses including vasodilation and muscle constriction, in addition to serving as a key intermediate in several heme-mediated biological processes such as NO detoxification by fungal cytochrome P450 and nitrite reduction by cytochrome c nitrite reductase. Few examples of well-characterized heme-HNO model compounds have been reported previously, and the observed instability of these compounds has made it difficult to perform more in-depth studies on the chemical reactivity of heme-bound HNO. To more effectively correlate the chemical properties of HNO to the observed biological effects and reactivities, several (por)Ru(HNO)(MeIm) (por = TPP, TTP and TAP) compounds have been prepared in high purity via hydride attack at the nitrosyl precursor. These compounds have been well-characterized by low-temperature ^{1}H NMR and FTIR spectroscopy displaying expected spectral signals for the Ru-HNO groups at ca. 13.60 ppm and 1380 cm^{-1}, respectively. The preparation, characterization, and reactivity of the (por)Ru(HNO)(MeIm) compounds will be presented and discussed.

P49: Oxidation-Reduction Potential as a Method for Determining Water Quality
Presenter: Michael R. Jordan
Authors and Affiliation: Michael R. Jordan, Isaac Gray, Stephanie Hayes, Fernando Morillas and Devika Wilson - *Oklahoma Baptist University*

A platinum electrode from Vernier Software and Technology was used to test the potential of numerous water samples. Treated city water, well water, and natural waters were the three types of water samples tested. As expected, natural waters had the lowest potentials and city water samples the highest potentials. By determining a normal range of potentials for different types of waters, it may be possible to detect oxidizing impurities using a simple and inexpensive electrochemical sensor.

P50: Phosphorescent Three-Coordinate Copper(I)-NHC Complexes: Synthesis, Characterization and Photoluminescent Studies
Presenter: Kwame Glinton
Authors and Affiliation: Kwame Glinton, Reza Latifi, Shepard Cockrell and Laleh Tahsini - *Oklahoma State University*

Phosphorescent metal complexes have been used in various fields including organic light-emitting device (OLED) screens, imaging, lasers and photocatalysis.[1] However, most of these complexes contain precious metals such as Ru, Au and Pt which are rather costly and of high toxicity. With the rising demand for light-emitting molecules in different areas, the need for alternative metal complexes at a reduced cost and minimal environmental issues have also increased. Photoluminescent Cu(I) complexes have attracted a great deal of attention as inexpensive alternatives to the heavy metal-based light emitters.[2] These recently developed Cu-based complexes have shown comparable results to other third-row photoluminescent metals and are better candidates in green chemistry application. Recently, mononuclear Cu(I) complexes bearing monodentate N-heterocyclic carbene (NHC) and nitrogen-based bidentate ligands were examined for their light emitting properties.[3] The light-emitting efficiency and the stability of the Cu luminophores was attributed to the presence of antihydrogen bonding interactions between α hydrogen of Hdpa and the center of the NHC wingtip substituents.

Further investigation of these luminophores is needed to clarify the role of the α-hydrogen and the extent of its contribution to the stability and luminescence of these complexes. Herein, we report the synthesis of three-coordinate Cu(I) complexes bearing saturated and unsaturated NHC ligands as well as different bidentate N-donor ligands, e.g. mesBIAN, Hdpa, asymmetrically substituted Hdpa, and phenanthroline. The complexes have been fully characterized by ^{1}H NMR, ^{13}C NMR, elemental analysis, X-ray crystallography, electrochemistry, UV-vis, and fluorescence spectroscopy for absorption and emissions of these complexes. References: Ford, P. C.; Cariati, E.; Bourassa, J. Chem. Rev., 1999, 99, 3625–3627. Evans, R. C.; Douglas, P.; Winscom, C. J. Coord. Chem. Rev., 2006, 250, 2093−2126. ACS Applied Materials & Interfaces, 2016, 8, 14678-14691.

P51: Photocatalytic Degradation of Acesulfame Potassium using TiO_2/UVA, $S_2O_8^{2-}$/Fe^{2+}/UVA, and H_2O_2/Fe^{2+}/UVA Processes
Presenter: Stephen J. McBride
Authors and Affiliation: Stephen J. McBride and Clinton D. Bryan - *Cameron University, Department of Chemistry, Physics, and Engineering*

Acesulfame potassium (ACE) is a ubiquitous artificial sweetener that has recently been shown to be toxic to the environment and damaging to DNA in both mice and humans. Photocatalytic degradation of ACE using TiO_2/UVA, $S_2O_8^{2-}$/ Fe^{2+}/UVA, and H_2O_2/Fe^{2+}/UVA processes show promising results with complete degradation and 57-80% mineralization of ACE and their resulting products have been shown to be non-toxic to the environment. The reaction kinetics of these two processes are examined.

P52: Photophysical Dynamics of Probemolecules Inside Reverse Micelles
Presenter: Nick Meaux
Authors and Affiliation: Nick Meaux and Rajesh Nayak - *Cameron University*

Reverse micelles (RMs) are thermodynamically stable nanometer sized water droplets surrounded by surfactant molecules in a non-polar organic solvent. We investigated the photo physical properties of fluorescent probe molecules inside reverse micelles using steady-state UV/vis and fluorescence spectroscopy. We observed that the probe molecules behave differently in a compartmentalized reverse micellar environment as compared to free aqueous environment. Furthermore, our observation gives us a protocol to use RM as a simple model system to understand the dynamic properties of biomolecules.

P53: Pincer-Type N-Heterocyclic Carbene Copper (I) Complexes and Their Utilization in Transfer Hydrogenation Reaction
Presenter: Jennifer L. Minnick
Authors and Affiliation: Jennifer L. Minnick, and Laleh Tahsini - *Oklahoma State University*

Transfer hydrogenation (TH) has become a popular, alternative route to classical hydrogenation in the past few years. The method allows for the reduction of various polar bonds under relatively mild conditions, especially in the reduction of ketones. In this context, transition metal complexes of precious metals, e.g. rhodium, ruthenium, and palladium have

shown promising reactivities towards TH reactions. Given the high cost and environmental concerns associated with precious metals, efforts are undertaken to develop more cost-effective catalysts using 3d metals. However, the stability of the 3d metal complexes is often compromised due to their propensity to single electron transfer events leading to decomposition. An efficient strategy to overcome the stability problem of these metal complexes is to utilize ligands that can associate the metal in bond activation of multi-electron transfer processes. Recently, we have developed pyridine-based pincer N-heterocyclic carbene copper (I) complexes that can catalyze such processes including Sonogashira- and Ullmann-type cross-coupling reactions.[1-3] Herein, we present the application of these bifunctional catalysts in transfer hydrogenation as a relatively unexplored area for homogenous copper catalysts. Properties of the pincer Cu-NHC complexes and their potential influence on the reduction of various functional groups is examined via the reduction of acetophenone to its corresponding alcohol, 2-phenylethanol, using 2-propanol as the hydrogen source. GC and ^{1}H NMR analyses are employed to determine rates of conversion and overall efficiency of the system. References: [1] Domyati, D. et al. Inorg. Chem., 2016, 55, 11685-11693 [2] Domyati, D. et al. Organomet. Chem., 2018, 860, 98-105. [3] Minnick, J. et al. Front. Chem. 2019, 7:12, 1-9.

P54: Principal Coordinate Analysis of Gastrointestinal Tissue Sections from Infected and Uninfected Animals in Chagas Disease

Presenter: Chaoyi Wu
Authors and Affiliation: Chaoyi Wu, Ekram Hossain and Laura-Isobel McCall - *Department of Chemistry and Biochemistry, University of Oklahoma*

The protozoan parasite Trypanosoma cruzi infects 7 million people worldwide. 30-40% of those infected will develop cardiac damage, megacolon and megaesophagus (Chagas disease). Recently, we found that the fecal microbiome and metabolome are significantly altered by T. cruzi infection. We are now investigating the local gastrointestinal tissue pathways affected by T. cruzi. Each infected and uninfected gastrointestinal organ was systematically sectioned, small molecules (50-1,500 Da) extracted, and analyzed by liquid chromatography-tandem mass spectrometry. Principal Coordinate Analysis (PCoA) plots were generated for each organ and organ sub-region, comparing infected and uninfected samples. Statistical testing was performed using PERMANOVA to obtain p values and R^2. The impact of infection on the stomach was very minor, with significant differences in the stomach small molecule profile only in the lowest part of the organ 89 days post-infection. In the small intestine, we only observed significant changes in the distal regions; these changes were more spread out during acute infection and became restricted to the most distal part of the small intestine by day 89. In the large intestine, we observed a major shift between early and late infection: in early infection, the proximal large intestine was most affected, while the distal large intestine was most affected in chronic infection. Overall, these results are assisting in understanding which organs and organ sites are most affected at the different infection timepoints during T. cruzi infection. These results will help inform drug development approaches.

P55: Protein YXIM_BACsu Putative Function Through Computational and Kinetic Analysis
Presenter: Aaron Zahn
Authors and Affiliation: Aaron Zahn - *Oklahoma Christian University*

Enzymes are proteins that reduce the activation energy for metabolic reactions. They play an integral role in all organisms and are necessary to be alive. Scientists have worked hard to identify the structure and function of different enzymes, though many enzymes remain uncharacterized despite having a known structure. YXIM_BACsu, better known by its PDB ID, 2O14, is one of such enzymes, found in Bacillus subtilis. The purpose of this research was to provide a hypothetical characterization of 2O14 based on enzyme kinetic data and in silico data. To acquire this data, 2O14 was expressed in E. coli cells and isolated. The activity of the isolated enzyme was measured for substrates 4-nitrophenyl acetate and 1-nitrophenyl butyrate. These results were analyzed to determine the kinetics of 2O14. The sequence of 2O14 was compared on databases such as BLAST, Pfam, and DALI in order to determine similarities with characterized enzymes and enzyme classes. These results allowed for a deeper understanding of the function of 2O14.

P56: Quinazolin-4(3H)-Ones and 5,6-Dihydropyrimidin-4(3H)-Ones from Beta-Aminoamides and Orthoesters
Presenter: Joel K. Annor-Gyamfi
Authors and Affiliation: Joel K. Annor-Gyamfi,[1] Joshua T. Gavin[2] and Richard A. Bunce[1] - *[1]Oklahoma State University, [2]REU Student (Summer 2018)*

Quinazolin-4(3H)-ones have been prepared in one step from 2-aminobenzamides and orthoesters in the presence of acetic acid. Simple 2-aminobenzamides were easily converted to the heterocycles by refluxing in absolute ethanol with 1.5 equivalents of the orthoester and 2 equivalents of acetic acid for 12-24 h. Ring-substituted and hindered 2-aminobenzamides as well as cases incorporating an additional basic nitrogen required pressure tube conditions with 3 equivalents each of the orthoester and acetic acid in ethanol at 110 °C for 12-72 h. The reaction was tolerant towards functionality on the benzamide and a range of structures was accessible. Workup involved removal of the solvent under vacuum and either recrystallization from ethanol or trituration with ether-pentane. Several 5,6-dihydropyrimidin-4(3H)-ones were also prepared from 3-amino-2,2-dimethylpropionamide. All products were characterized by melting point, FT-IR, ^{1}H-NMR, ^{13}C-NMR and HRMS.

P57: Seeding Ice Crystallization in Molecular Simulations
Presenter: Rajendra Maharjan
Authors and Affiliation: Rajendra Maharjan and Christopher J. Fennell - *Department of Chemistry, Oklahoma State University*

Because of its propensity for supercooling, water typically crystallizes by means of heterogeneous ice nucleation, where a defect or impurity acts as a site for initiation of crystal growth. Despite the general acceptance of this process, little is known about the size, shape, and molecular-level makeup of effective nucleating seeds. In this study, we explore ice crystallization and growth using molecular dynamics of supercooled liquid (SCL) water

using the TIP4P/Ice model simulations at different temperatures, densities, and system sizes. We find that the optimal crystal growth rate occurs near 240 K and the standard SCL density for the TIP4P/Ice model at this temperature. Varying the seed size and shape resulted in successful crystal growth from seeds as small as 24 water molecules in size. Additionally, when seeded under the optimal growth conditions, we could readily grow metastable ice polymorphs, like cubic ice, by providing a polymorph specific seed. This work provides a foundation for investigation into the kinetics and molecular-level mechanism of ice crystal and clathrate growth and inhibition.

P58: Shewanella Oneidensis MR-1, an Iron Reducing Bacterium, Catalyzes the Oxidation of Metallic Iron

Presenter: Alejandra Hernandez-Santana
Authors and Affiliation: Alejandra Hernandez-Santana and Mark Nanny - *The University of Oklahoma*

Given that iron is the second most abundant redox-active element in the Earth, there are many life forms that rely on it as either a terminal electron acceptor or an electron donor. Microbial ferric iron reduction is crucial for carbon cycling in anaerobic environments, and it sustains primary production in the oceans since ferrous iron is essential for phytoplankton. Less is known about microbial metabolism of metallic iron. In our research, we evaluate the metallic iron oxidation capabilities of Shewanella oneidensis MR-1, a facultative bacterium widely distributed in the environment. S. oneidensis has been a model organism for dissimilatory iron reduction. However, few years ago, the ability of S. oneidensis to take electrons from electrodes was discovered, suggesting that it could also take electrons from metallic iron. We have conducted microcosm anaerobic experiments with steel coupon as electron donor and fumarate as electron acceptor. By monitoring iron species concentration, pH, and organic acids concentration we have demonstrated that S. oneidensis MR-1 catalyzes the oxidation of metallic iron, releasing ferrous iron. Furthermore, when oxalate, a dicarboxylic acid that can complex iron, is also present in the system, the reaction proceeds at a greater extent. By using Linear Polarization Resistance, we have demonstrated that oxalate lowers the corrosion potential of steel, making it easier to oxidize the steel surface. The ability of iron reducing bacteria to engage in oxidation of metallic iron is not well understood and it is not known how widespread this is in the environment, and more importantly, how it interconnects with the ferrous and ferric iron cycling. Nonetheless, we anticipate this recently discovered metabolic mode can have important consequences in environments such as the ocean, where iron limitation significantly impacts primary production and where there is increasing steel infrastructure from wind farms, oil rigs, and ships.

P59: Solubility of Iridium and Ruthenium Organometallic Photoredox Catalysts
Presenters: Daniel Jespersen and Brockton Keen
Authors and Affiliation: Daniel Jespersen,[1] Brockton Keen,[1] Jon I. Day,[1] Anuradha Singh,[2] Justin Briles,[1] Duncan Mullins,[1] Jimmie D. Weaver[1,2] - *[1]Oklahoma State University and [2]Weaver Labs LLC*

Despite the exponential growth of the field of photocatalysis, for reasons that are not entirely clear, these precious photocatalysts are often used in the literature at loadings that exceed their maximum solubility. On an industrial scale, the quantity of any precious metal catalyst can be a substantial financial burden or a sourcing issue, not to mention concerns as to the ecological and earth abundance of these catalysts. We believe that inattention to solubility has made these reactions appear less efficient than they actually are, because much of the photocatalyst remains undissolved. Therefore, the maximum solubilities of iridium and ruthenium centered photocatalysts have been systematically identified in industrially relevant solvents. Further, a literature photocatalytic reaction which our results suggested was beyond the maximum solubility has been revisited, with interesting results.

P60: Solution Phase Conversion of β-FeOOH to FeP and FeS_2 Nanoparticles
Presenter: Menuka Adhikari
Authors and Affiliation: Menuka Adhikari and Y. Vasquez - *Department of Chemistry, Oklahoma State University*

Iron phosphide (FeP) and iron sulfide (FeS_2) nanoparticles are an emerging category of electrocatalysts for water splitting. Conversion of iron oxide (Fe_3O_4) and β-FeOOH into FeP nanoparticles have been reported in the literature. The most common route for the transformation of β-FeOOH into FeP nanoparticles is the high-temperature solid phase phosphorization treatment with sodium hypophosphate (NaH_2PO_2). Phosphine (PH_3) gas generated during the process acts as a phosphorus source, however, the gas is toxic and not eco-friendly. Herein, we report a facile solution-phase conversion of β-FeOOH to FeP and FeS_2 at 320 using trioctylphosphine (TOP) as a phosphorus source and sulfur powder as a sulfur source. The resulting nanoparticles have been characterized by TEM, XRD, and XPS. Interestingly, from the TEM analysis, FeP nanoparticles were found to exhibit bundle shape morphology. References 1 Muthuswamy, E.; Brock, S. L., Journal of the American Chemical Society 2010, 132 (45), 15849-15851. 2 Xiong, D.; Wang, X.; Li, W.; Liu, L., Chemical Communications 2016, 52 (56), 8711-8714.

P61: Structural and Functional Changes Induced by Alkyl RNO Binding to Myoglobin and Hemoglobin
Presenter: Viridiana E. Herrera
Authors and Affiliation: Viridiana E. Herrera, Samantha M. Powell, Kiana Prather, Nancy T. Nguyen, Bing Wang, Jun Yi and George B. Richter-Addo - *Price Family Foundation Institute of Structural Biology, Department of Chemistry and Biochemistry, University of Oklahoma, Norman, OK*

Myoglobin (Mb) and hemoglobin (Hb) are some of the most studied proteins, and their roles in dioxygen (O_2) transport and storage are widely understood. Less understood is their

involvement in the overall global nitrogen cycle, their interactions with biologically relevant organic nitrogen oxides (RNO_x), and the structural and functional changes that these proteins undergo in the process of RNO_xinterconversion, which is the focus of this work. The functions of Mb and Hb reside mainly in their heme cofactor, as O_2 binds directly to the Fe atom embedded within it. Organic nitrosoalkanes (RNO) are valence isoelectronic with O_2, and as a result, RNOs often compete with $O_2$for binding and may form "inhibitory" Fe(II)-RNO complexes. Organic nitrosoalkanes are made physiologically from the oxidation of amines (RNH_2) and hydroxylamines (RNHOH) or by the reduction of nitro (RNO_2) containing compounds. Once RNOs are created, they can bind hemoproteins which may lead to harmful outcomes. For instance, binding of RNOs to human Hb may lead to methemoglobinemia which can then cause heme loss and successive Fe accumulation in the spleen. Also alarming is the damage caused to liver cytochrome P450s; upon binding, RNOs inhibit P450s, annulling their function in detoxification of xenobiotics. Despite the adverse health implications, there is little structural information regarding the mode of binding of RNOs to hemoproteins, and the effect of such binding on overall protein structure and function. We will present high-resolution X-ray crystal structures that illustrate the interactions of Mb with nitrosoalkanes. Furthermore, we will show the step-by-step mechanism that leads to Hb degradation upon RNO binding to the protein. Altogether, our results illustrate how RNOs, which are naturally occurring metabolites, bind to Mb and Hb disturbing the vital roles that these proteins have on O_2 utilization.

P62: Structural Characterization of Clostridioides Difficile Response Regulator (RR_1586) Protein

Presenter: Jared Haymore
Authors and Affiliation: Jared Haymore, Smita Menon, Skyler Hebdon and Ann H. West - *University of Oklahoma Department of Chemistry and Biochemistry*

The recent emergence of hypervirulent strain 20291, the intractability of treatment, and increasing concerns about antibiotic resistance have led to a need to develop novel methods of treatment for Clostridioides difficile. Two-component systems (TCS) are a well-defined means of signal transduction common in prokaryotes and some lower eukaryotes. TCS are primarily composed of a sensory histidine kinase (HK) that transfers a phosphoryl group to a cognate response regulator (RR), but they are also characterized by a diverse field of functions, such as osmotic and sporulation regulation. The hypervirulent strain of C. difficile has 54 HKs and 57 RRs, many of which remain uncharacterized. In a previous study from the West lab, one of the C. difficile response regulators of interest, RR_1586, was identified as a potential regulator of phosphate transport and sporulation using a bacterial one-hybrid assay. We continued our efforts to further characterize RR_1586 and here present the unphosphorylated (apo) RR_1586 structure obtained through x-ray crystallography using molecular replacement. Further efforts are being made to obtain crystals for the phosphorylated form of this protein. Elucidating a model for RR_1586 structure in both forms may help characterize the mechanism for affecting cell response and key residues for RR function.

P63: Structural Characterization of Hemoglobin Adducts with Hydroxylamines
Presenter: Samantha M. Powell
Authors and Affiliation: Samantha M. Powell, Viridiana E. Herrera, Kiana Prather, Nancy Nguyen and George B. Richter-Addo - *Price Family Foundation Institute of Structural Biology and Department of Chemistry and Biochemistry, University of Oklahoma*

The blood protein, hemoglobin (Hb), is responsible for dioxygen (O_2) transport in mammals. Hb is a tetrameric protein made up of two a and two b subunits, each of which possess a heme at which O_2binds to the central Fe atom. Nitroso-compounds (RNOs) can bind to the heme Fe since they are valence isoelectronic with O_2 and once present, can inhibit the function of Hb and other heme proteins. One route to produce RNOs is through the oxidative metabolism of amines and hydroxylamines. Many amines are used commercially to produce a variety of goods such as rubbers, pesticides and prescription drugs. In the body, amines are converted by cytochrome P450s to their hydroxylamine (RNHOH) forms at which point, they can interact with Hb to form nitroso-Hb adducts. Much is still unknown about the RNO-heme interaction formed from RNHOHs. Phenylhydroxylamine (PhNHOH) is a toxic derivative of aniline, an amine used widely in industrial settings. The interaction between PhNHOH and Hb has never been structurally characterized. N-hydroxyamphetamine (AmphNHOH) is an oxidative metabolite of amphetamine, an amine-containing drug used in some commonly prescribed medications. It has been hypothesized by others that Hb cannot accommodate such a large ligand in its active site. Presented here are the UV-vis spectra of the complexes formed between PhNHOH and AmphNHOH with human Hb. We present the X-ray crystal structures of the product of the interaction between Hb and PhNHOH and of the Hb-nitrosoamphetamine adduct. Our results show for the first time how PhNHOH and Hb interact structurally, and more interestingly, our structure displays the early signs of Hb damage. We also show that Hb is capable of accommodating large ligands such as AmphNO in its active site. Furthermore, differences are observed in both structures between the alpha and beta subunits.

P64: Structural, Optical and Electrical Properties of Co- and Fe-doped ZnO Nanoparticles Synthesized by Microwave Method
Presenter: Ganga R. Neupane
Authors and Affiliation: Ganga R. Neupane, Amrit Kaphle, Rusiri Rathnasekara and Parameswar Harikumar - *University of Tulsa*

We have reported structural, optical and electrical properties of Co- and Fe-doped ZnO (0%, 5%, 10%, and 15%) nanoparticles synthesized by a microwave method. Morphology and crystal structure were studied with high resolution transmission electron microscopy (HRTEM). Studies reveal formation of spherical nanoparticles with decreasing diameter with doping concentration. The diameter of particles size decreased from 17 nm to 11 nm for iron doping (0-15%) whereas diameter of particle size decreased from 15 nm to 9 nm for cobalt doping (0-15%). Energy dispersive X-ray spectroscopy (EDS) spectrum showed incorporation of iron and cobalt in ZnO nanoparticles and the intensity of respective peak signal increased with increasing concentration of dopant (iron and cobalt). X-ray diffraction (XRD) showed the existence of wurtzite ZnO structure in Fe-doped ZnO samples whereas some secondary peaks were observed in Co-doped ZnO samples. Optical properties were

studied using UV-vis absorption spectra. UV-vis absorption measurements show a systematic increase in bandgap from 3.21 eV to 3.25 eV for iron and 3.22 eV to 3.27 eV for cobalt nanoparticles with doping concentration from 0 to 15% respectively. Electrical conductivity of both Fe-and Co-doped ZnO nanoparticles were studied using van der Pauw method and the results will be compared.

P65: Study of Iodine Distribution and Stability in Western Oklahoma Brine Waters
Presenters: Katrina Betz and Maxwell Archer
Authors and Affiliation: Katrina Betz,[1] Maxwell Archer,[1] Jason R. Wickham[1] and David Edlin[2] - *[1]Department of Natural Science, Northwestern Oklahoma State University and [2]Iofina, Alva, OK*

In the late 1970's, it was discovered that the brine waters of NW OK contain significant amounts of Iodine (above 60 ppm). However, the exact amounts and distributions of Iodine throughout this region were unknown. Currently, the majority of the world's supply of Iodine comes from mining Iodate minerals in Chile (≈ 65%), brine water aquifers in NW Oklahoma (≈ 5%) and Japan (≈ 25%), and seaweed extraction. With the growing need for Iodine compounds in various fields the demand for Iodine is higher than ever. Thus, Iofina has recruited the aid of NWOSU to quantify the Iodine concentrations and distribution throughout the brine aquifer, as well as, determine the longevity of these iodine concentrations. Currently, this study has led to the discovery of new sites within the aquifer that may be of commercial interest and has taken an in-depth look at five of these as possible new plant sites, with one of these sites being built and beginning operation during February 2018. Fluctuations in iodine concentrations of up to 100 ppm have been observed throughout this study which is a much larger fluctuation than the expected 10 ppm. Currently, we are investigating rather these fluctuations are due to the changed from vertical to horizontal wells as a function of the inhomogeneity within the brine aquifer.

P66: Survey of Lake Water Quality Across Oklahoma
Presenter: Tyler Souza
Authors and Affiliation: Tyler Souza and Shawna York - *Southern Nazarene University Department of Chemistry*

With the ongoing threat of environmental degradation and climate change altering the chemistry of the world’s environment, it is becoming more necessary to determine the current health of valuable natural resources like water, soil, and air. This project involves testing the quality of surface waters of Oklahoma lakes spanning across a wide range of the state. Testing methods include on-site and in-lab testing for nitrate and phosphate concentrations, alkalinity, conductivity, and overall water hardness as determined by the concentration of calcium and magnesium. These results will be compared to the data given by federal agencies like the USGS. This testing procedure begins with gathering water samples from Lake Texoma, Lake Hefner, Lake Overholser, Lake Eufaula, and Canton Lake. These lakes will provide a geographical representation of Oklahoma water ranging from across the state. The on-site testing involves Vernier technologies ISE as well as Hach testing kits for testing for phosphate levels in the water. The in-lab testing methods will include wet-

lab titrations of EDTA to chelate any metals found in the water samples to determine overall water hardness.

P67: Synthesis and Characterization of Different Lanthanum Phosphate Phases
Presenter: Mha Albqmi
Authors and Affiliation: Mha Albqmi and Allen Apblett - *Oklahoma State University*

Metal phosphates have important applications as oxide conductor, catalysts, and optical materials including glasses, phosphors, nonlinear optical materials, and laser host materials. Single-sources precursors for lanthanum phosphate phases were synthesized by the stoichiometric reactions of mono-alkyl and di-alkyl phosphate esters with lanthanum nitrate. The alkyl groups were varied and included isopropyl, butyl and 2-ethyl hexyl. These precursors thermally decompose at low temperatures (250-300 °C) producing lanthanum phosphate phases. The characterization of the products obtained from thermal pyrolysis of the precursors will be discussed in light of possible structures. Methods of characterization included thermogravimetric analysis, solid-state ^{31}P NMR spectroscopy, X-ray powder diffraction, and Infrared spectroscopy

P68: Synthesis and Characterization of Oligonucleotide Conjugated Gold Nanorods
Presenter: Michael Smith
Authors and Affiliation: Michael Smith and Nathan Green - *Northeastern State University*

Gold nanorods (AuNRs) have unique optical properties with strong potential in novel theranostic applications such as photothermal therapy, biological imaging, and optical sensing. Furthermore, AuNRs may have potential as waveguides for the nonradiative transfer of energy across nanoscale distances. However, AuNRs are necessarily stabilized, during and post synthesis, by surfactants like cetyltrimethylammonium bromide (CTAB), which makes AuNRs incompatible with biological and energy transfer applications. Here we demonstrate a technique to recoat AuNRs with short single-stranded oligonucleotides to produce AuNRs stable in media sufficiently complex to be biologically relevant without compromising unique optical properties. Furthermore, this coating of single-stranded DNA may allow for organization of AuNRs with other nanomaterials, particularly DNA-based nanostructures, to develop hierarchical nanomaterials that further leverage unique optical properties. AuNRs were synthesized utilizing a seed mediated method while a low pH recoating technique was employed to rapidly conjugate synthetic, thiolated oligonucleotides to AuNR surfaces. Nanorods were characterized with UV-visible (UV-vis) spectroscopy and transmission electron microscopy (TEM) before and after conjugation to ensure nanoparticle fidelity during processing. AuNR DNA conjugation was confirmed via gel electrophoresis. Synthesized AuNRs strongly absorbed visible light dependent on particle morphology, which allows for stability confirmation between treatments. The low pH conjugation of oligonucleotides to AuNRs quickly produced stable rods. Gel electrophoresis indicated successful recoating of AuNRs with DNA and demonstrated increased stability. DNA coatings grant AuNRs a robustness that significantly increases the viability of these nanomaterials in diluted environments as well as previously incompatible solutions. Furthermore, the oligonucleotide coating can be conjugated with DNA-based nanostructures,

which facilitates organization of materials that may further leverage the unique photo-optical properties of AuNRs.

P69: Synthesis and Surface Modification of Silica Nanoparticles
Presenter: Brandon S. Abbott
Authors and Affiliation: Brandon S. Abbott, Jorge Carvalho, Luis Trevisi and Keisha B. Walters - *School of Chemical, Biological and Materials Engineering, University of Oklahoma*

Silica nanoparticles are used in a wide range of applications including advanced separations, anti-friction devices, biomaterials, and drug-delivery vehicles. Control over size, size distribution, and surface chemistries of these particles allows for them to be tailored for better performance, expanded uses, and improved manipulation. Silica nanoparticles were synthesized through a sodium hydroxide base-catalyzed Stöber process, and commercially available silica nanoparticles (LUDOX TM-50 and LUDOX CL-P) were also examined. Self-assembled organosilane monolayers were used to change the surface functional groups and allow for subsequent surface modification. Monolayer deposition was obtained through the self-assembly of (3-aminopropyl)triethoxysilane (APTES). These amine-functionalized particles were then used to examine the grafting of polymers from the silica nanoparticles in a controlled manner. Attenuated total reflectance Fourier transform infrared spectroscopy (ATR-FTIR) was used to determine chemical moieties present throughout the various stages of surface modification. Both electron microscopy (EM) and dynamic light scattering (DLS) were used to determine silica particle size. Electrostatic surface effects were analyzed using zeta potential. Results from this study provide a reproducible synthesis route for surface-confined graft polymerization of hydroxylated surfaces.

P70: Synthesis of Cyclic Imides using Microwave Radiation
Presenter: Oladayo Seweje
Authors and Affiliation: Oladayo Seweje and E. Ann Nalley - *Department of Chemistry, Physics and Engineering, Cameron University*

Allowing many chemical reactions to be completed within minutes, microwave heating has revolutionized preparative chemistry. This is a green technology and is becoming widely adopted in both academic and industrial laboratories. Heterocycles are very important functional groups especially in medicinal chemistry. Not only are they pivotal in the synthesis of drugs but also form part of the structure of a diversity of drugs, vitamins, natural products and biomolecules. In this research a clean green method was implemented for the preparation of different cyclic imides from acid anhydrides using aniline or N-substituted anilines with microwave radiation as the energy source. The unsubstituted imides were synthesized by reacting the acid anhydrides with urea using imidazole as a catalyst. These compounds will be evaluated against antibacterial and antifungal species.

P71: Synthesis of Lanthanide Molybdates via Reaction of Molybdenum(VI) Oxide with Aqueous Acetate Salts
Presenter: Khalid Alrashidi
Authors and Affiliation: Khalid Alrashidi and Allen Apblett - *Oklahoma State University*

Reaction of aqueous solutions of either lanthanum or cerium acetate with molybdenum(VI) oxide (MoO_3) produces a mixed lanthanide molybdate acetate, $Ln(O_2CCH_3(MoO_4)•XH_2O$ (Ln= La, Ce) that is an excellent single source precursor for stoichiometric $Ln_2Mo_2O_9$. The reaction is very sensitive to the radius of the lanthanide metal used: metals with smaller radii (e.g. yttrium, praseodymium or neodymium) produce a hydroxyl molybdate product, $M(OH)_x(MoO_4)_{1-x}$, instead of an acetate molybdate. The products were fired at high temperatures for further investigation. The products were characterized by thermal gravimetric analysis (TGA) and infrared and NMR spectroscopy. The conversion of the products to lanthanide molybdenum oxides was used to study the possibility of producing phosphors, $La_2Mo_2O_9:Ln^{3+}$ by doping lanthanum molybdenum oxides with other lanthanide metals such as praseodymium acetate. Also, fluorescence spectroscopy was run to study the doping material.

P72: Highly Efficient Non-Viral VEGF Gene Delivery to STEM Cells by Lipid Based Nanoparticles
Presenter: Mengmeng Zhai
Authors and Affiliation: Mengmeng Zhai and Chuanbin Mao - *Department of Chemistry and Biochemistry, University of Oklahoma*

Vascular endothelial growth factor (VEGF) is a protein that can trigger blood vessel formation and thus is used for healing cardiovascular diseases, such as myocardial ischemia and bone diseases, such as bone defects. Stem cell-based non-viral VEGF gene therapy is now considered more effective that the direct injection of VEGF protein into diseased sites. In this approach, the VEGF gene carried by a vector such as nanoparticles is transferred into stem cells, followed by transplantation of the transfected stem cells. The stem cells will produce fresh VEGF protein through gene expression and also differentiate into functional cells such as bone forming cells. However, this method is limited by the low transfection efficiency. The newly formed blood vessels induced by VEGF gene delivery are unstable and require continued VEGF stimulation for about 4 weeks. If VEGF gene expression is lost before this time point, the new blood vessels will regress and disappear. Thus, the sustained expression of VEGF is critical to the success of VEGF gene therapy. To solve these problems, we developed a new stem cell-based non-viral VEGF gene therapy to achieve highly efficient VEGF gene transfer into hMSC with sustained expression. In our study, we identified a stem cell-targeting peptide using a stem cell screen technique. we also integrated the stem cell-targeting peptide and VEGF-SB into lipid-based nanoparticles to develop a novel non-viral vector for the delivery of the VEGF gene into stem cells with high transfection efficiency and sustained expression. The high transfection efficiency and sustained expression with the lipid-based nanoparticles were also verified by flow cytometry and confocal microscopy.

P73: Synthesis, Functionalization, and Thermal Characterization of Monodispersed Dye-Doped Silica Nanoparticles
Presenter: Tyler Gore
Authors and Affiliation: Tyler Gore, Marukh Zia and Nathaniel Green - *Northeastern State University*

Silica nanoparticles are a highly versatile material due to their simple preparation, readily available precursors, and capabilities for internal and surface functional modifications. Previous applications of these particles were limited because of the inefficient control of particle size and shape. The protocol utilized in our research provides more precise control over particle diameter and monodispersity, enabling the synthesis of highly uniform silica nanoparticles. This is accomplished through an aqueous organic bi-layer approach to limit the rate of hydrolysis of a siloxane precursor thus controlling the growth rate of the silica nanoparticles. This approach provides a viable source of silica nanoparticles adept for functionalization and potential applications in high-temperature plastic extrusion, cancer drug delivery, biomedical imaging, and nano-photonic cell systems.

P74: Testing an Ion Chromatography Technique to Separate Rare Earth Elements from Major Cations in Carbonate Minerals
Presenter: Lauren Haygood
Authors and Affiliation: Lauren Haygood and Bethany Theiling - *Department of Geosciences, University of Tulsa*

It is not yet understood how rare earth elements (REEs) are associated with carbonate-bearing minerals and rocks, the most common of which is the mineral calcite and limestone rock ($CaCO_3$). There are two common hypotheses for how REEs are associated with carbonate minerals: (1) REEs substitute for the major cation, Ca^{2+}, in $CaCO_3$ or (2) REEs are adsorbed on the surface of commonly associated clay minerals. If we can understand how REEs are incorporated into carbonate mineral assemblages, we will be able to more accurately use REE analyses of geologic materials to evaluate carbonate mineral alteration (diagenesis) and trends and fluctuations in ocean and river chemistry over spatial and temporal scales, all of which facilitate a more accurate understanding of feedbacks in the earth-system. Our first step towards answering this question is to develop an ion chromatography technique that effectively extracts and separates REEs from major cations such as Ca^{2+} and Mg^{2+} in solution. High concentrations of Ca^{2+} from bulk sample analysis run the risk of saturating instrument detectors, and therefore bulk sample solutions are significantly diluted. However, diluting bulk carbonate samples to safe levels of Ca^{2+} can make REE undetectable or subject to large error, due to the low (<ppm) concentrations of REE in carbonate minerals. Our experimental extractions used an REE standard for inductively coupled plasma (ICP) spectrometers of 10 mg/L for all REE. Seven methods were compared, using various lengths and volumes of cation exchange columns loaded with TRU-SP resin. Each extraction was analyzed using an inductively coupled plasma optical emission spectrometer (ICP-OES). Our results demonstrate that the 1.5mL columns with a length of 5.3cm most efficiently eluted all REEs. Our results also illustrate that heavy REEs (HREEs) need a longer elution time than light REEs (LREEs).

P75: The Challenges of Predicting Viral RNA with Multiple Functional Structures
Presenter: Susan J. Schroeder
Authors and Affiliation: Susan J. Schroeder - *University of Oklahoma*

The revolution in sequencing technology demands new tools to interpret the genetic code. As in vivo transcriptome-wide chemical probing techniques advance, new challenges emerge in the RNA folding problem. The emphasis on one sequence folding into a single minimum free energy structure is fading as a new focus develops on generating RNA structural ensembles and identifying functional structural features in ensembles. Swellix is a new combinatorially complete approach to determining all possible non-pseudoknotted structures for an RNA sequence. Swellix can provide a profile of the frequency of motifs that bind proteins or small molecule therapeutics for an ensemble of RNA structures. Swellix can incorporate unique experimental constraints, such as the minimum number and lengths of helices from crystallography or cryoelectron microscopy. The applications of Swellix and other RNA folding tools to Human Endogenous Retroviral RNA, prohead RNA, and Satellite Tobacco Mosaic Virus RNA will be discussed.

P76: The Chemical, Genetic, and Geographical Diversity of the Genus Alternaria in North America
Presenter: Victoria Anderson
Authors and Affiliation: Victoria Anderson,[1,2] Robert Cichewicz,[1,2] Laura-Isobel McCall,[2] Karen Wendt[1,2] - *[1]Natural Product Discovery Group, Institute for Natural Products Applications and Research Technologies and [2]Department of Chemistry and Biochemistry, Stephenson Life Science Research Center, University of Oklahoma*

The Natural Products Discovery Group has amassed over 200 isolates of Alternaria from 35 states through its Citizen Science Soil Collection Program. Alternaria is a ubiquitous and common agricultural pathogen with host plants ranging from grains to cauliflower to cherries. Alternaria has the ability to produce a diverse range of secondary metabolites, which can cause issues with food safety, but can also be a treasure trove for natural products. For instance, altertoxin-II was previously isolated from an Alternaria tenuissima isolate from a soil sample from South Carolina and has been shown to have potent and selective activity against Ewing sarcoma cell lines (unpublished data). This project will examine both the chemical and genetic diversity of the genus Alternaria across the United States. There has been some indication that the metabolite profiles of some Alternaria species are sufficient to distinguish between species-groups. Chemical diversity of isolate extracts will be examined using LCMS metabolomics, while genetic diversity will be probed using the ITS region. ITS is the “universal DNA barcode marker” for fungi because it is a non-coding region so shows higher levels of evolution making it suitable to distinguish fungi at the genus level but includes the 5.8S gene which tends to be more conserved. We hope to expand the current understanding of this genus by examining chemical diversity through the lens of genetic and geographical diversity

P77: The Synthesis of Aluminum Clusters using Naphthalene Based Crystallization Agents
Presenter: Alexander Chandler
Authors and Affiliation: Alexander Chandler, Maggie Ward, Emily Cowen, Cha'Lita Thomppson and Eric S. Eitrheim - *University of Central Oklahoma, Department of Chemistry*

Oxy-Hydroxy-Aluminum clusters have various industrial uses, including waste water treatment and materials science. There may also be used for these clusters to remove contaminants from aqueous environmental systems. It is important to synthesize, then isolate these clusters to observe how they will behave and bind in environmental systems to contaminants or surfaces. Using basic starting materials, we are attempting to synthesize these clusters in aqueous systems for study. An aluminum hydroxide solution was created from $Al(OH)_3$ dried gel with the addition of selenic acid. Then we attempted to isolate the clusters by slow evaporation or by using different naphthalene-based crystallization agents from previous work. Once the clusters were crystallized and observed under a microscope, we plan to characterize them using single crystal x-ray diffraction. Our goal was to synthesize the Al8 selenate cluster, based on a previously synthesized Al8 sulfate cluster, using this dissolution method with selenic acid. It is unclear if this cluster is naturally occurring, though the conditions of synthesis are similar to acidic environmental systems including acid mine drainage or acid rain systems.

P78: The Synthesis of Ethyl 4-(4-Hydroxyphenyl)-6-Methyl-2-Oxo-1,2,3,4-Tetrahydropyrimidine-5-Carboxylate: Comparison of Two Methods
Presenter: Paidaishe F. Mangwiro
Authors and Affiliation: Lois Ablin and Paidaishe F. Mangwiro - *Department of Biology and Chemistry, Oral Roberts University*

In a multi-component Biginelli reaction, the compound ethyl 4-(4-hydroxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate was synthesized from 4-hydroxybenzaldehyde, ethyl acetoacetate and urea. Two methods, microwave irradiation and the grindstone reaction, were used to synthesize the compound with citric acid and p-toluenesulfonic acid as catalysts. The microwave reaction using citric acid as the catalyst produced more favorable results than the grindstone reaction. Products were determined and characterized by thin layer chromatography, purification and spectroscopic techniques.

P79: The Synthesis of Ethyl-4-(4-dimethylaminophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate and an Investigation of its Cytotoxic Effect on MDA-MB-468 Tumorigenic Versus Mcf-10a Non-tumorigenic Mammary Epithelia
Presenter: Patrice Lewis
Authors and Affiliation: Lois A. Ablin, Patrice Lewis and William P. Ranahan - *Department of Biology and Chemistry, Oral Roberts University*

In a three-component, microwave Biginelli reaction, ethyl-4-(4-dimethylaminophenyl)-6-methyl-2-oxo-1,2,3,4-tetra-hydropyrimidine-5-carboxylate was synthesized from 4-dimethylaminobenzaldehyde, ethyl acetoacetate, and urea with a citric acid catalyst. The

compound's dose dependent cytotoxic effect was tested on MDA-MB-468 breast cancer cells versus MCF-10A normal cells using DMSO as the solvent. Results obtained through spectrophotometric analysis depicted a significantly higher mortality rate for cancer cells compared to normal cells.

P80: Thermodynamic Analysis of the RAS Q61 Moiety via Non-Equilibrium Entropic Changes in GTP Hydrolysis
Presenter: Bailey Smoot
Authors and Affiliation: Bailey Smoot, Salvatore Capotosto, Preet Sharma, Randal Hallford - *Midwestern State University*

The ab-initio determination from crystal structures of the thermodynamic properties of the hydrolysis of the GTP gamma-phosphate in normal and abnormal cell functions of the RAS protein mutant Q61 lead to a description of energy cycle deviations in the abnormal mitogen activated protein kinase cascade. A predictive algorithm describing the non-linear changes for these open and finite-lifetime systems follows from reasonable enthalpy and entropy values between the normal and mutated forms based on structures including GTP, GDP and a possible hydrolysis state at the allosteric site.

P81: Using Biomarkers to Predict Treatment Efficacy for Chagas' Disease Through Metabolite Profile
Presenter: Gautham
Authors and Affiliation: Gautham,[1] Laura-Isobel McCall,[1] Ekram Hossain,[1] Igor C. Almeida[2] and Joaquim Gascón[3] - *[1]University of Oklahoma, [2]University of Texas, El Paso and [3]Institute of Global Health, Barcelona, Spain.*

Chagas disease (CD) is one of the 17 neglected tropical diseases. It affects about 7-8 million people all over the world but is endemic to Latin America. CD results in cardiomegaly, arrhythmias, apical aneurysm, megacolon, and megaesophagus. The two existing therapeutic drugs (benznidazole and nifurtimox) are accompanied by severe side-effects and variable efficacy. Our hypothesis is that chronic CD continuously promotes inflammatory immune responses and these changes at the biochemical and metabolic level can be used to predict treatment response. Our study examined these changes using small molecule-focused liquid chromatography mass-spectrometry (LC-MS) of serum samples from CD patients, collected before and after treatment with benznidazole. Principal coordinate analysis (PCoA), random forest machine learning and molecular networking were employed to determine metabolomic differences between treatment-responsive and non-responsive patients. Statistically significant (PERMANOVA $p<0.05$) clustering on PCoA plots based on responsive vs. non-responsive status was only observed at timepoint 0. Random forest models were also able to predict with moderate accuracy the responsiveness to the treatment at timepoint 0, using the total serum metabolite profile. Furthermore, when only the top 15 metabolites were used to perform random forest, the prediction ability was improved. Therefore, analyzing the patient's metabolite profile before drug administration and detecting a few selected metabolites that play a vital role in promoting treatment response may represent a new way to predict treatment efficacy.

P82: Using Bridged Nucleic Acids for Detection of Phosphatidyl 3-Kinase Catalytic Subunit Alpha Mutation
Presenter: Rachel Ann Hoffmeister
Authors and Affiliation: Rachel Ann Hoffmeister and Sung-Kun (Sean) Kim - *Northeastern State University*

PIK3CA is responsible for producing the catalytic subunit (p110) of the lipid kinase heterodimer phosphoinositide 3-kinase (PIK3 or PI3K). The E545Q mutation, which is due to single nucleotide mutation (c.1633G>C) and found in the highly conserved helical domain of PIK3CA, has been linked to cases of non-small-cell lung carcinoma (NSCLC). Bridged nucleic acids (BNAs) are modified nucleic acid analogs that have the ability to bind DNA with high affinity so that the resulting T_m values are altered. Moreover, the BNA's resistance to nucleases leads to increased stability in vitro and in vivo. We designed several BNA probes to bind more tightly to wild-type DNA than to mutant DNA. Thus, using BNA we observed lower resulting T_m values of samples of DNA containing the mutant sequence than that of the wild-type DNA. The T_m values of the mutant were significantly lower than that of the wild-type. Using BNAs, a greater difference between T_m values was observed than that of the control, (e.g., solely DNA used, with no BNAs involved). This method of using BNAs for the detection of PIK3CA mutations was successful and could be utilized for earlier and more accurate diagnosis of NSCLC.

P83: Using Residue Interactions to Predict Biomolecular Diffusion
Presenter: Elham Fazelpour
Authors and Affiliation: Elham Fazelpour,[1] Jennifer M. Haseleu[1, 2] and Christopher J. Fennell[1] - *[1]Department of Chemistry, Oklahoma State University and [2]Department of Chemistry, Saint Vincent College*

Diffusion coefficients of biomolecules are reasonably well-correlated to their molecular weights; however, predictions of diffusion coefficients using only mass information can have errors greater than 30%. In order to address this concern, we decided to see if detailed information on surface residue exposure could be used to form more accurate predictions of protein diffusion. We first determined the diffusion coefficients for all the monomeric amino acids to build a scale for assembling a macromolecular diffusion coefficient from the surface exposure of the individual residues. In principle, estimating the hydrophobicity and hydrophilicity of a protein along its amino acids sequence allows us to map relative diffusivity to protein surface. We performed detailed molecular dynamics calculations of protein structures to determine "gold standard" diffusion coefficients, and we tested the accuracy of this approach alongside simple mass relations for predicting these diffusion coefficients. We find that using solvent exposed residue information leads to significantly more accurate predictions, and even leads to accurate predictions of experimental diffusion coefficients directly from knowledge of a protein's structure.

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