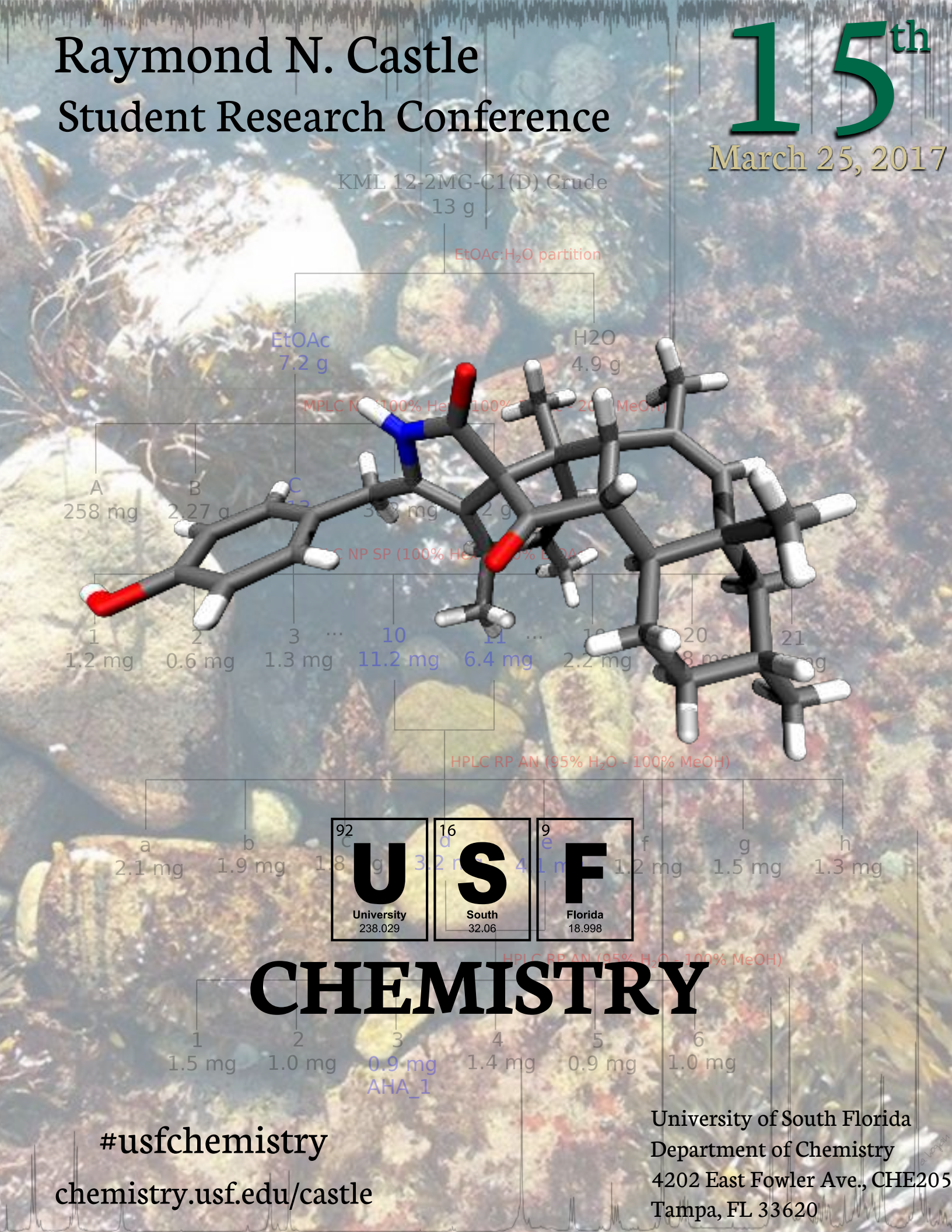
Raymond N. Castle
Student Research Conference

15th
March 25, 2017



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University of South Florida
Department of Chemistry
4202 East Fowler Ave., CHE205
Tampa, FL 33620

15th Raymond N. Castle Student Research Conference

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Welcome from the Castle Conference Committee

Dear Colleagues and Friends,

Welcome to the 15th Raymond N. Castle Student Research Conference hosted by the University of South Florida. In honor of Dr. Raymond N. Castle, this Conference was created to promote his goals of scientific collaboration and science education.

The Raymond N. Castle Student Research Conference continues to be organized by students for students as an excellent opportunity for undergraduate and graduate chemistry students to share scientific ideas and research progress. Students are encouraged to not only gain presentation experience, but to use the conference as a chance to further their research endeavors by gaining valuable feedback from other members of the chemistry community. It is this interaction and the sharing of ideas that makes the Raymond N. Castle Student Research Conference a worthwhile experience and a continued success.

We are especially proud of the research done by all students in the department, both graduate and undergraduate. With the continued success of the Raymond N. Castle Student Research Conference and to more clearly promote scientific collaboration, we have expanded our invitation for presentation to students in other Natural Science Departments as well as Colleges and Universities in Tampa and the surrounding areas. Today, we have an opportunity to hear from students in chemistry related disciplines from around Florida. Chemistry research will be highlighted with our special guest, Dr. Rigoberto Hernandez. We encourage everyone to take advantage of this occasion and attend both the poster and oral presentations, especially the Plenary Lecture. We are honored and greatly appreciative that Dr. Hernandez will be giving a presentation on his exciting research and experience in the field of chemistry.

Lastly, we would like to thank all that chose to volunteer their time and efforts, particularly the judges, Dr. Fields and Dr. Leahy for helping us plan and coordinate this year's conference. In addition, we are grateful for the financial support that allows us to host this conference and owe special thanks to Dean and Barbara Martin, Tampa Bay Local Section of the American Chemical Society, University of South Florida College of Arts and Sciences, and University of South Florida ResearchOne, as well as the multiple other sponsors and affiliates who have generously contributed to this event. Most importantly, this conference would not exist without the efforts of those of you presenting your research today. Therefore, we gratefully acknowledge you and your research advisors, as well as all in attendance. Thank you all and we hope you enjoy and learn from the 15th Raymond N. Castle Student Research Conference.

Sincerely,

The Castle Conference Committee

15th Raymond N. Castle Student Research Conference Committee

Committee Members

Adam Hogan (Chair)
Douglas Franz (Chair)
Alekhya Nimmagadda
Geoffrey Gray
Chavis Stackhouse
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15th Raymond N. Castle Student Research Judges

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H. Lee Woodcock, PhD
Kenyon Daniel, PhD
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Theresa Evans-Nguyen, PhD
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Jason Montgomery, PhD
Deborah Bromfield Lee, PhD

All Saints Academy

Jeanine Yacoub

Bristol-Myers Squibb

Ellen Leahy, PhD

Building Map

Schedule of Events

Saturday, March 25th, 2017

8:00 AM	-	9:00 AM	**Welcome Session** *Registration and Breakfast*	Chemistry Courtyard
9:00 AM	-	10:45 AM	**Morning Talk Session** *Graduate Student Presentations*	CHE 100
10:45 AM	-	11:00 AM	**Castle Conference Welcome** *Dr. James Leahy*	CHE 100
11:00 AM	-	12:00 PM	**Plenary Speaker** *Dr. Rigoberto Hernandez*	CHE 100
12:00 PM	-	1:00 PM	**Lunch** *Sponsored by the ACS Tampa Bay Local Section*	Chemistry Courtyard
12:00 PM	-	1:30 PM	**ACS Tampa Bay Local Section Meeting**	CHE 100
1:00 PM	-	3:00 PM	**Poster Session** *Graduate and Undergraduate Presentations*	CHE 1st Floor Classrooms
3:00 PM	-	3:15 PM	**Break**	
3:15 PM	-	5:00 PM	**Afternoon Talk Session** *Graduate Student Presentations*	CHE 100
5:00 PM	-	5:15 PM	**Break**	
5:15 PM	-	5:30 PM	**Awards Ceremony**	CHE 100
5:30 PM	-	7:00 PM	**Chem Bowl** *Undergraduate Chemistry Society*	CHE 101A

Professor Raymond N. Castle

1916 – 1999

Raymond N. Castle was born on June 24, 1916 in Boise, Idaho where he attended Boise High School and Boise Junior College. A 1938 graduate in Pharmacy from the University of Idaho, Southern Branch in Pocatello, he completed the M.A. degree in Chemistry at the University of Colorado at Boulder in 1941. Shortly thereafter, he became a Chemistry instructor at the University of Idaho and then in 1943, returned to the University of Colorado in Boulder for a Ph.D. in Chemistry with a minor in Microbiology. After two years as a research chemist at the Battelle Memorial Institute in Columbus, Ohio, Dr. Castle accepted a position at the University of New Mexico as an Assistant Professor of Chemistry. He served as Chairman of the Chemistry Department from 1963 until 1970 before moving to Brigham Young University as Professor of Chemistry.

In 1981, Dr. Castle joined the faculty at University of South Florida as a Distinguished Research Professor. He and his wife, Ada, were a vibrant part of the Chemistry Department and for many years sponsored the Castle Lecture Series, which brought in numerous prominent scientists for lectures at USF.

A prolific researcher, Dr. Castle was an internationally recognized father figure in heterocyclic chemistry, both for his research and his involvement in meetings, symposia, and editorial boards. In 1964, he founded the Journal of Heterocyclic Chemistry and served as its editor. He also edited the Lectures in Heterocyclic Chemistry series, a publication of plenary lectures given at the International Congresses of Heterocyclic Chemistry, and was the American advisory editor for the English translation of the Russian Journal of Heterocyclic Compounds. He lectured at hundreds of institutions worldwide. He was General Chairman of the First International Congress of Heterocyclic Chemistry held in Albuquerque (1967), Secretary of the Second International Congress held in Montpellier, France (1969), and Vice-President of subsequent Congresses held in Sendai, Japan, Salt Lake City, Utah, Ljubljana, Yugoslavia, and Tehran, Iran. Dr. Castle was also Chairman and Committee Member for the American Chemical Society. In addition, he was cofounder of the International Society of Heterocyclic Chemistry, which he served as Chairman of the Executive Committee, and President (1973-1975). Professor Castle received numerous awards and honors, including the prestigious International Award in Heterocyclic Chemistry (1983) for outstanding contributions to the field of heterocyclic chemistry, presented in Tokyo, Japan. Dr. Castle was listed in the first edition of Who's Who in Science and in Who's Who in the World.

The Chemistry Department remains deeply indebted to Professor Castle for his many outstanding contributions to the Department, and to science overall. He would have been a strong supporter of this student symposium, and thus, it is fitting that we dedicate this and future symposia to his memory.

Dr. Rigoberto Hernandez

Plenary Speaker

Dr. Rigoberto Hernandez is the Gompf Family Professor in the Department of Chemistry at the Johns Hopkins University as of July 1, 2016, and remains as the Director of the Open Chemistry Collaborative in Diversity Equity (OXIDE) since 2011. Before Hopkins, he was a Professor in the School of Chemistry and Biochemistry at Georgia Tech, and Co-Director of the Center for Computational Molecular Science and Technology he co-founded. He holds a B.S.E. in **Chemical Engineering and Mathematics** from Princeton University (1989), and a Ph.D. in **Chemistry** from the University of California, Berkeley (1993). (Hernandez was born in Güinez, Havana, Cuba but was raised and educated in the United States of America since he was in primary school. He is a U.S. citizen by birthright.)

Dr. Hernandez's research area can be broadly classified as the theoretical and computational chemistry of systems far from equilibrium. This includes a focus on microscopic reaction dynamics and their effects on macroscopic chemical reaction rates in arbitrary solvent environments. His current projects involve questions pertaining to the diffusion of mesogens in colloidal suspensions and liquid crystals, the structure and dynamics of assemblies of Janus and other patchy particles, fundamental advances in transition state theory, the role of molecular reactions in nonequilibrium air and the dynamics of protein folding and rearrangement.

Dr. Hernandez is the recipient of a National Science Foundation (NSF) **CAREER Award** (1997), Research Corporation Cottrell Scholar Award (1999) , the **Alfred P. Sloan Fellow Award** (2000), a Humboldt Research Fellowship (2006-07), the **ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences** (2014), the CCR Diversity Award (2015), and the **RCSA Transformative Research and Exceptional Education (TREE) Award** (2016). He is a **Fellow** of the American Association for the Advancement of Science (AAAS, 2004), the **American Chemical Society** (ACS, 2010), and the **American Physical Society** (APS, 2011). In 2015-2016, he was a Phi Beta Kappa Visiting Scholar. At Georgia Tech, he served as the first Blanchard Assistant Professor of Chemistry (1999-2001), the first Goizueta Foundation Junior Rotating Faculty Chair (2002-07) and a Vasser Woolley Faculty Fellow (2011-13). His recent board memberships include the National Academies Panel within the Army Research Laboratory Technical Assessment Board (2005-2011), the National Academies Board on Chemical Sciences and Technology (2007-2010), the Telluride Summer Research Conference Board of Directors (2007-09), the NIH Study Section on Molecular Structure and Function B (MSFB, 2009-2013), the Research Corporation Cottrell Scholars Advisory Committee (member 2011-15, and chair 2016-17), the DOE Committee of Visitors (Division of Chemical Sciences, Geosciences and Bio-sciences, 2014) and the **American Chemical Society Board of Directors (2014-2019)**.

Dr. Dean and Barbara Martin

Special Thanks

Dr. Dean F. Martin is Distinguished University Professor Emeritus and Director of the Institute for Environmental Studies at the University of South Florida, where he has been a member of the faculty since 1964. Dr. Martin received his B.A., with Honors, from Grinnell College (1955), where he met his future wife Barbara while both were chemistry majors. They were married in 1956 while both attended Pennsylvania State University as graduate students and in 1958 Dr. Martin received his Ph.D. and Mrs. Martin her Master's degree. In 1958-59, he was a National Science Foundation Post-Doctoral Fellow at University College, London after which he returned to the States and accepted a faculty position at the University of Illinois, Urbana-Champaign, as Instructor and Assistant Professor of Inorganic Chemistry (1959-1964). He received (1969-1974) a Career Development Award from the Division of General Medical Sciences, NIH, to study the chemistry and chemical environment of algal toxins. In 1970-71, he was a Visiting Professor of Physiology and Pharmacology at Duke University Medical Center.

Dr. Martin and his wife share research interests concerned with the coordination chemistry of natural water systems, including problems of red tide and aquatic weeds and they have collaborated in research involving the properties of coordination compounds, as well as aspects of environmental chemistry. Currently, they are investigating the removal of metals and organic compounds from water by means of supported chelatings agent. Dean Martin is the author or co-author of over 300 publications, including four books. He was the recipient of the 1975 Florida Award and the 1987 Civic Service Award of the Florida Section, ACS; in 1978, he received the F. J. Zimmermann Award in Environmental Science from the Central Wisconsin Section, sponsored by Zimpro Inc.; and in 1983, he was elected Fellow of the American Association for the Advancement of Science. Dean and Barbara Martin were the co-recipients of the 1994 Medalist Award of the Florida Academy of Sciences, its highest award. Dean Martin has been active in the Florida Section of the American Chemical Society (Chairman, 1986), and he has held several positions in the Aquatic Plant Management Society (President, 1986-87). Both of the Martins have received the Alumni Award of Grinnell College.

The Martins have endowed six chemistry funds, including the George Bursa Award, given annually to a deserving graduate student within the Chemistry Department who has demonstrated notable professional dedication and consideration for others, as well as a Graduate Student Travel Award. Together the Martins have edited Florida Scientist since January 1984 and are now Editors Emeriti. Dr. Martin initiated and continues to edit the departmental newsletter and has written a departmental history to coincide with the 40th Anniversary of the founding of the department.

The Martins have six children; Diane, Bruce, John, Paul, Brian, and Eric, and six grandchildren.

Sponsors

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Graduate Talks Morning Session (CHE 100)

Session Chair: Douglas Franz

9:00- 9:15 AM **Fiona Kearns**
Efficient and Accurate QM/MM Free Energy Simulations using the QM-NEW Method.

9:15- 9:30 AM **Ashleigh Bachman**
Phosphorylation induced global structural destabilization of a small protein domain.

9:30- 9:45 AM **Olapeju Bolarinwa**
Constrained Peptides that inhibit HIV-1 fusion.

9:45- 10:00 AM **Break**

10:00- 10:15 AM **Geoffrey Gray**
Enhanced Sampling Simulations of Repetitive Motifs Found in Spider Dragline Silk.

10:15- 10:30 AM **Benjamin Pollard**
Optimizing Protocols for Computing Carbohydrate NMR Chemical Shifts.

10:30-10:45 AM **Danielle Demers**
The Antarctic Circumnavigation Expedition: Tales from the High Seas.

Graduate Talks Afternoon Session (CHE 100)

Session Chair: Alekhya Nimmagadda

3:15-3:30 PM **Douglas Franz**
Simulations of gas sorption in rht-MOF-9.

3:30- 3:45 PM **Alison Hughes**
High-throughput screening of mangrove-associated fungal extracts against pathogenic C. albicans.

3:45- 4:00 PM **Darrell Cole Cerrato**
"Beeting" Alzheimer's: Inhibition of Cu(II)-β-amyloid mediated oxidation and peroxidation by betanin from sugar beets.

4:00- 4:15 PM **Break**

4:15- 4:30 PM **Zachary Shultz**
Versatile enantioselective synthesis of the cannabinoids - THC, CBD and unnatural analogs.

4:30- 4:45 PM **Philip Hudson**
Accelerating QM/MM Free Energy Computations via Intramolecular Force Matching.

4:45- 5:00 PM **Rainer Metcalf**
Computational Modeling and Drug Discovery for STING-mediated Production of IFN-beta

Graduate Poster Session
CHE 101A

Graduate: Group GP All Disciplines

The Barbara and Dean F. Martin Poster Session
CHE 103

Undergraduate: Analytical (AN), Computational (CO), Chemical Education (CE), Inorganic (IN), Physical (PC), Biophysical (BP)

The ACS Tampa Bay Local Section Poster Session
CHE 101

Undergraduate: Natural Products (NP), Organic (OR), Biochemistry (BC)

GRADUATE TALKS

GT-01 **Fiona Kearns**[1], Phillip S. Hudson[1], Stefan Boresch[2], H. Lee Woodcock[1]
[1]Department of Chemistry, University of South Florida, Tampa, Florida
[2]Department of Computational Biological Chemistry, University of Vienna, Vienna, Austria

Efficient and Accurate QM/MM Free Energy Simulations using the QM-NEW Method

Modeling deprotonation via free energy simulations (FES), which is essential for calculating pKa, is challenging due to the need to accurately represent inter- and intramolecular interactions, which often requires quantum mechanics, while still adequately sampling conformational space, which requires long simulations. We have focused our efforts on improving the estimation of free energy differences along the connecting legs within an indirect scheme, i.e., free energy differences between levels of theory, to thereby improve the reliable prediction of pKas. Towards this aim, we have used the Quantum Mechanical Non-equilibrium Work (QM-NEW) method to predict the pKa of ethylthiol, and we have predicted pKas of 8.0 and 10.4 respectively. Further investigation of QM-NBB results, reveals that a discrepancy between charge definitions at different levels of theory can drastically affect local solvent arrangement and thus overlap in equilibrium FES.

GT-02 **Ashleigh Bachman**[1], Radwan Ebna Noor[1], Dimitra Keramisanou[1], Ioannis Gelis[1]
[1]Department of Chemistry, University of South Florida

Phosphorylation induced global structural destabilization of a small protein domain

Protein phosphorylation at a single or multiple sites is utilized to regulate protein functional outcomes and overall cellular activities through signaling pathways. At a molecular level, the addition of a phosphoryl group may alter the function of a protein through distinct and versatile mechanisms. These include allosteric structural and dynamic changes, direct positive or negative modulation of affinities, masking or unmasking of cofactor binding sites, autoinhibition and local disorder-to-order or order-to-disorder transitions. Here to present evidence from NMR spectroscopy and other biophysical techniques that protein phosphorylation may lead to a global domain destabilization. Upon phosphorylation a small protein domain acquires a molten globule state, where at least two stable folding intermediates exist in equilibrium with a heterogeneous conformational ensemble. This conformational transition modulates in turn the affinity for protein partners but also permits rapid domain refolding upon removal of the phosphoryl group.

GT-03 **Olapeju Bolarinwa**[1], Erin Mulry[1], Jianfeng Cai[1]
[1]Department of Chemistry, University of South Florida

Constrained Peptides that inhibit HIV-1 fusion

The utilization of bioactive peptides in the development of highly selective and potent pharmacologic agents for the disruption of protein-protein interactions has become more appealing for drug discovery. However, this strategy is limited by loss of bioactivity and instability to proteases. HIV-1 entry into host cell is through a fusion process that is mediated by the trimeric viral glycoprotein gp120/41 which are obtained from gp160 through proteolytic processing. Linear peptides derived from the HIV gp41 C-terminus have proven potent in inhibiting the fusion process. These peptides have shown good interaction and significant binding to the hydrophobic pocket on gp-41 N-terminus which was previously identified as a potential inhibitor site. In this study, we introduce a 23-residue C-peptide, OB-XEK22 that was optimized for HIV-1 gp-41 N-terminus binding and proteolytic stability through sulfono-γ-AApeptide substitution and all-hydrocarbon stapling. OB-XEK22 inhibited envelope-mediated membrane fusion in cell-cell fusion assays at nanomolar potency and showed improved protease resistance.

GT-04 **Geoffrey M. Gray**[1], Brittany Thiessen[1], Arjan van der Vaart[1]
[1]Department of Chemistry, University of South Florida

Enhanced Sampling Simulations of Repetitive Motifs Found in Spider Dragline Silk

Spider dragline silk possesses a unique combination of strength and elasticity making it a highly desirable material. Despite this, little is known about the secondary structure adopted by silk. To help elucidate secondary structural characteristics inherent to the sequence, enhanced sampling simulations were performed on several common dragline silk sequence motifs under aqueous and non-aqueous conditions. Results show that these motifs have little secondary structure under aqueous conditions, while having a higher frequency of turns and helices under non-aqueous conditions. Chemical shift calculations were compared to experimental values and will be discussed.

GT-05 **Benjamin C. Pollard**[1], Michael T. Kemp[1], Fiona L. Kearns[1], Phillip S. Hudson[1], Michael F. Crowley[2], H. Lee Woodcock[1]
[1]Department of Chemistry, University of South Florida
[2]National Renewable Energy Laboratory, Lakewood, CO

Optimizing Protocols for Computing Carbohydrate NMR Chemical Shifts

Computing accurate NMR chemical shifts for carbohydrates has been challenging since it requires satisfying three criteria: computing the NMR shifts with an adequate level of theory, incorporating environmental effects, and accounting for the relevant regions of conformational space. Here we address the first by employing QM/MM methods in a NMR benchmark with a selection of levels of theory and basis sets. To account for environmental effects, a set of small, rigid molecules were solvated with explicit waters and the appropriate size of the QM region was determined to obtain converged NMR shifts. Additionally we show that through a mixed basis set approach, computational time can be greatly reduced while retaining the ability to calculate accurate shifts. We find that ωB97x-D/6-31G* gave the best results (13C RMSE = 3.06 ppm), NMR shifts converge at a radius of 5 Å, and basis set projection works best for reducing computational expense.

GT-06 **Danielle H. Demers**[1,2], Bill J. Baker[1,2]
[1]Department of Chemistry, University of South Florida
[2]Center for Drug Discovery and Innovation, University of South Florida

The Antarctic Circumnavigation Expedition: Tales from the High Seas

The Antarctic Circumnavigation Expedition (ACE) departed Capetown, South Africa in December, 2016. By the end of March, 2017, it will return to Capetown, having successfully sailed around the Antarctic continent. Carrying 60 scientists on 22 different projects, hailing from 30 countries, this international research expedition put together by the primarily privately funded Swiss Polar Institute was a truly one of a kind experience. As a part of a team studying the genetic history and chemistry of benthic marine organisms, we joined climatologists, oceanographers, glaciologists, and other biologists on board. With a focus on collaboration and cooperation, the data collected on the ACE is poised to make a large impact in understanding Antarctica, its surrounding waters, and the role of climate change worldwide. A summary of some this work will be presented.

GT-07 **Douglas Franz**[1], Tony Pham[1], Katherine Forrest[1], Zac Dyott[1], Brian Space[1]
[1]Department of Chemistry, University of South Florida

Simulations of gas sorption in rht-MOF-9

Metal-organic frameworks are highly porous crystalline materials well-suited for computer simulation (primarily because of periodicity of structure). Grand-canonical (constant μ,V,T) Monte Carlo (a method mostly known for random perturbations which are accepted or rejected by a Boltzmann probability) simulations of hydrogen (77 and 87K), carbon dioxide, methane, acetylene, ethylene, and ethane gas (298K) sorption in rht-MOF-9 were performed using Massively Parallel Monte Carlo (MPMC), a statistical-mechanical molecular simulation code developed by our lab. Gas uptake (storage) isotherms and Qst (heat of adsorption) were calculated, and efforts were made to discover the primary binding-sites of the gases via radial distribution calculations and simulated annealing. rht-MOF-9 is a copper based MOF with 3 distinct cages. Theoretical results were compared to experimental data.

GT-08 **Alison H. Hughes**[1], Bill J. Baker[1]
[1]Department of Chemistry and Center for Drug Discovery and Innovation, University of South Florida

High-throughput screening of mangrove-associated fungal extracts against pathogenic C. albicans.

Candida spp. are the 4th leading cause of nosocomial bloodstream infections in the U.S., with approximately 46,000 cases per year. As evolution has shown, microorganisms are far more adroit at competing amongst each other than we have ever been. With that in mind, we aim to screen a library of crude extracts obtained from Floridian mangrove-associated fungi. It is believed that cryptic genes within these fungi are responsible for their production of defensive secondary metabolites in response to stressors in the environment. Our lab has developed a method of culturing fungi on media treated with epigenetic modifiers to create three distinct extracts from each fungus. This screening programme aims to test the activity of fungal crude extracts against a panel of 14 drug-resistant C. albicans strains, obtained from the American Type Culture Collection (ATCC). Procurement of the compound(s) responsible for activity will be achieved using both NMR- and bioassay-guided isolation.

GT-09 **Darrell Cole Cerrato**[1], Li-June Ming[1]
[1]Department of Chemistry, University of South Florida

"Beeting" Alzheimer's: Inhibition of Cu(II)-β-amyloid mediated oxidation and peroxidation by betanin from sugar beets

Alzheimer's disease affected up to 5 million Americans in 2013 and is expected to affect up to 14 million by 2050 according the Centers for Disease Control. One of the leading suspected biomolecules behind the disease is the the mis-folded β-amyloid (Aβ) peptide sequence, especially after coming in contact with metals, such as copper(II). It has been previously established that metal-bound Aβ has the ability to also cause oxidative stress in its environment, exacerbating and leading to other biological issues. In this study, a common chemical found in sugar beets (Beta vulgaris), betanin, was chosen to investigate its ability to prevent metal-mediated oxidative stress caused by Cu(II)-Aβ. Paramagnetic NMR and kinetic spectrophotometric techniques show betanin's ability to bind to metals and also prevent Cu(II)-Aβ oxidative and peroxidative chemistry.

GT-10 **Zachary Shultz**[1]
[1]Department of Chemistry, University of South Florida

Versatile enantioselective synthesis of the cannabinoids - THC, CBD and unnatural analogs

Phytocannabinoids, such as Δ9 tetrahydrocannabinol (THC) and cannabidiol (CBD), are known to exhibit a wide range of biological activity. It was once thought that the endogenous cannabinoid receptors (CB1/CB2) were the only biological targets of the cannabinoids. The wide range of biological activity may be contributed to unknown biological targets and mechanisms of action. In this vein, we developed a versatile enantioselective total synthesis of the cannabinoids for analog development and potential molecular tools in order to probe biological function. The synthetic strategies implemented in the construction of the cannabinoids and their analogs will be discussed as well as the utility of our synthesis in analog and molecular probe development.

GT-11 **Phillip S. Hudson**[1], Stefan Boresch[2], David Rogers[1], H. Lee Woodcock[1]
[1]Department of Chemistry, University of South Florida
[2]Department of Computational Biological Chemistry

Accelerating QM/MM Free Energy Computations via Intramolecular Force Matching

Employing the so-called "indirect" approach to free energy simulations (FES) with quantum or hybrid quantum mechanical / molecular mechanical (QM/MM) Hamiltonians can be extremely challenging. This is primarily due to the need of converged FES between levels of theory, which results in numerous problems related to poor overlap between the high and low levels of theory. Herein, we demonstrate that by reparameterizing classical intramolecular potentials to reproduce high level forces (i.e. force matched), significantly improve configurational overlap between, e.g., a low (i.e. classical) and a high (i.e. quantum) level of theory. This ultimately leads to much improved application of the indirect FES approach.

GT-12 **Rainer Metcalf**[1], Wayne Guida[1]
[1]Department of Chemistry, University of South Florida

Computational Modeling and Drug Discovery for STING-mediated Production of IFN-beta

STING is a protein involved in the innate immune system activated by cyclic dinucleotides created when foreign DNA is detected due to viral/bacterial infection or oncogenic processes. STING-mediated production of IFN-β can result in cellular protection from infection or, if within the tumor microenvironment, can result in activation of tumor antigen-specific CD8+ T-cell immunity that can lead to tumor regression. STING activation should result in innate T cell-mediated anti-tumor immunity in the tumor microenvironment and have significant potential as a therapeutic strategy for the treatment of patients with advanced solid tumors. Additionally, STING agonists could be used as general antivirals. On the other hand, inhibition of STING would lead to a decreased production of IFN-β which could have implications in the treatment of autoimmune disease such as lupus erythematosus. Computational models have been developed through crystallography, Molecular Dynamics simulations, and induced fit docking to lead drug discovery efforts.

GRADUATE POSTERS

GP-01 **Tamalia Julien**[1], Julie P. Harmon[1]
[1]Department of Chemistry, University of South Florida

Thermomechanical Behavior of Molded and Electrospun Thermoplastic Biopolymer Nanocomposites

An industrial batch of an ultrasoft thermoplastic polyurethane (TPU) was synthesized and found to have high performance and biocompatible characteristics. This novel type of polyurethane material targets growing markets of biocompatible polymers and has been used for peristaltic pump tubing, balloon catheters and enteral feeding tubes. This material is ideal for replacing materials such as soft plastisols containing diethylhexyl phthalate for use in biomedical and industrial applications. The incorporation of nanoparticles was used to impart enhanced mechanical, thermal and adhesion properties. Additionally, nanofibers were processed by electrospinning and characterized. The fact that polyurethane nanocomposites can be electrospun into nanofibers has allowed its applications to be broadened in the medical and industrial fields to produce sensors, drug delivery systems and scaffolds for tissue engineering. In these studies the utilization of thermal and mechanical testing were completed to obtain the characteristic of the molded and electrospun polymer nanocomposites.

GP-02 **Garrett Craft**[1], Alejandro Rivera[1], Disha Thadhani[1], Jonathan Gomogda[1], Julie Harmon[1]
[1]Department of Chemistry, University of South Florida

Characterization of a Novel Polyimide and the Structure-Property Relationships of its Monomers

Polyimides are a diverse class of polymeric materials containing an imide linkage. The polymers are often fully aromatic and thermosetting, with extreme heat and solvent resistance and high mechanical properties owing to that aromaticity. However, this temperature and solvent resistance makes them intractable in terms of manufacturing and processing. In this work we will synthesize and characterize a novel thermoplastic polyimide and determine how the molecular weight and sterics of aliphatic diamine linkers effect crystallinity, along with the glass and melt transitions.

GP-03 **Alejandro Rivera**[1], Yesenia Perez[1], Garrett Craft[1], Julie Harmon[1]
[1]Department of Chemistry, University of South Florida

Synthesis and Characterization of Novel Melt Processable Aliphatic Polyimide-Polyurea Hybrids

A series of polypropylene oxide diamines (Jeffamines) with the addition of 2-ureido-4[1H]-pyrimidinone (UPy) were used to synthesize flexible polyimides. The aliphatic monomer introduces flexibility giving the polyimides thermal properties that allow them to be melt-processed. The UPy, introduced as a Hydrogen-bond end capper, provides an intermolecular collaboration between the polymer chains improving physical properties. The polyimide-polyurea hybrids were prepared by a two-step polycondensation procedure from pyromellitic dianhydride (PMDA), Jeffamine D series (D230, and D400), 4,4'-Methylenebis(2,6-dimethylaniline) (TMMDA) and a UPy linked with hexamethylene diisocyanate. The glass transition range, from 4ºC to 100ºC, is below the decomposition temperatures.

GP-04 **Stephanie Feola**[1], Vasantha Kumar Machohally Venkateshaiah[1], Dimitra Keramisanou[1], Ioannis Gelis[1]
[1]Department of Chemistry, University of South Florida

Chemical Analysis of Ancient Pottery Sherds

Unglazed pottery sherds unearthed at archaeological sites are analyzed via chemical means as a way to determine the contents of the vessel, such as animal or plant products. This analysis is performed through the extraction of lipids absorbed from the contents by the pottery. Lipids are extracted from the samples of interest using a solvent based extraction and then portions of the extracts are subjected to derivatization (Methylation and Trimethylsilyation) to determine the various components of the lipid extract. Extracted and derivatized samples are then analyzed using NMR and GC-MS. Pottery sherd samples excavated from Castelluccio, Italy have been subjected to solvent extraction and analysis using NMR and methods are currently being refined for further analysis via GC-MS.

GP-05 **S M Anisul Islam**[1], Mildred Acevedo-Duncan[1]
[1]Department of Chemistry, University of South Florida

The role of atypical Protein Kinase C in LoVo Colorectal cancer cell growth, proliferation and metastasis

The exact mechanisms of cell growth, survival, metastasis and inter & intracellular signaling pathways involved in colon cancer are still a major challenge for scientists. Hence, investigating the signaling pathways that lead to colon carcinogenesis may give insight into the therapeutic target. In this study, the role of atypical Protein kinase C (aPKC) on colon cancer was identified by using two inhibitors of aPKC: 1) ζ-Stat, specific inhibitor of PKC-ζ and 2) ICA-I, specific inhibitor of PKC-ι. The cell lines tested were CCD18CO normal and LoVo metastatic colon cancer. Although PKC-ι is an oncogene in many cancers, we found that the PKC-ζ was responsible for the abnormal growth, proliferation and metastasis in LoVo metastatic colon cancer cells. Additionally, the inhibition of aPKCs did not bring any significant toxicity on CCD18CO normal colon cell line. These results suggest the potentiality of utilizing PKC-ζ inhibitors to block colon carcinogenesis.

GP-06 **Fengyu She**[1], Alekhya Nimmagadda[1], Peng Teng[1], Ma Su[1], Xiaobing Zuo[2], Jianfeng Cai[1]
[1]Department of Chemistry, University of South Florida
[2]X-ray Science Division, Argonne National Laboratory

Helical 1:1 α/sulfono-γ-AA heterogeneous peptides with antibacterial activity

Antibiotic resistance is one of the greatest threats facing mankind in 21st century. Host-defense peptides (HDPs) have the potential to combat emerging drug-resistant bacteria through disruption of their membranes, such as the helical magainin 2 and its analogs. They adopt cationic amphipathic conformations upon interaction with bacterial membranes, leading to membrane disruption and bacterial cell death. We have previously reported that amphipathic sulfono-γ-AApeptides exhibit bactericidal activity by mimicking magainin 2. Here we demonstrate for the first time that amphipathic helical 1:1 α/sulfono-γ-AA heterogeneous peptides, in which regular amino acids and sulfono-γ-AApeptide building blocks are alternatively present in a 1:1 pattern, display potent antibacterial activity against both Gram-positive and Gram-negative bacterial pathogens. Small Angle X-ray Scattering (SAXS), fluorescence microscopy and time-kill experiments indicate that the lead sequences adopt defined helical structures and exert antimicrobial activity by mimicking the mechanism of HDPs.

GP-07 **Wishrawana Ratnayake**[1], Raja BommaReddy[1], Mildred Acevedo-Duncan[1]
[1]Department of Chemistry, University of South Florida

A novel atypical protein kinase C inhibitor DNDA can repress epithelial to mesenchymal transition (EMT) in malignant melanoma

Melanoma is one of the fastest increasing cancers in the United States expecting 87,110 new cases and nearly 11,000 deaths in 2017. We believe that aPKCs (PKC-ι and PKC-ζ) play an important role in malignancy of melanoma by involving the signaling pathways which induces EMT. Both PKC-ι and PKC-ζ are over expressed in melanoma cells. In the current study, we have investigated the effects of a novel aPKC inhibitor; 3,4-Diaminonaphthalene-2,7-disulfonic acid (DNDA) on the cell proliferation, apoptosis and invasion of melanoma cell lines compared to normal melanocytes. DNDA decreased the levels of total and phosphorylated PKC-ζ and PKC-ι and also altered the levels of E-cadherin, NF-κB p65, Vimentin, β-catenin and CD44. Melanoma cell proliferation, migration and invasion were significantly reduced and apoptosis was induced by DNDA. Overall, results show that aPKCs are essential for melanoma progression and metastasis, and they could be effective therapeutic targets for melanoma.

GP-08 **Timothy Odom**[1], Fengyu She[1], Peng Teng[1], Jianfeng Cai[1]
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Analysis of γ-AA-peptide secondary structure

Two peptide sequence were design to determine secondary structure based on previously observed helical structure. The peptides were formed through synthesis of a combination of γ-AA-peptides and regular α-amino acids. Modification of peptide sequence was performed in order to test solubility of similar peptides in solution and effects on crystallization. Crystallization of peptide derivatives are currently being attempted through slow evaporation and diffusion techniques.

GP-09 **Ashleigh Bachman**[1], Radwan Ebna Noor[1], Dimitra Keramisanou[1], Ioannis Gelis[1]
[1]USF Department of Chemistry

Phosphorylation induced global structural destabilization of a small protein domain

Protein phosphorylation at a single or multiple sites is utilized to regulate protein functional outcomes and overall cellular activities through signaling pathways. At a molecular level, the addition of a phosphoryl group may alter the function of a protein through distinct and versatile mechanisms. These include allosteric structural and dynamic changes, direct positive or negative modulation of affinities, masking or unmasking of cofactor binding sites, autoinhibition and local disorder-to-order or order-to-disorder transitions. Here to present evidence from NMR spectroscopy and other biophysical techniques that protein phosphorylation may lead to a global domain destabilization. Upon phosphorylation a small protein domain acquires a molten globule state, where at least two stable folding intermediates exist in equilibrium with a heterogeneous conformational ensemble. This conformational transition modulates in turn the affinity for protein partners but also permits rapid domain refolding upon removal of the phosphoryl group.

GP-10 **Adam Aboalroub**[1], Ashleigh Bachman[1], Ioannis Gelis[1]
[1]USF

Arylalkylamine Transferase from Bombyx mori (Bml3 AANAT), Mode of Action and Substrates Binding Mechanism.

Arylalkylamine acetyltransferase AANAT, is the rate limiting and the penultimate enzyme in melatonin biosynthesis pathway, and thereby it controls the biological timing in vertebrate. AANAT using Acetyl-CoA to acetylate wide range of substrates range in size from proteins to small amines, but its acetylation mechanism still ambiguous. Here, we have employed NMR and ITC techniques in order to understand what makes this protein able to catalyze this gamut of substrates, and to reveal its mode of action. The preliminary results have showed that; AANAT has higher affinity for AcCoA compared to un-acetylated form (CoA), and moreover, the binding of AANAT to AcCoA makes it more attractive to Arylalkylamine such as; Tryptamine, Octopamine and more, thus supports the notion that AcCoA binding to AANAT facilitates its acetylation task.

GP-11 **Alekhya Nimagadda**[1], Jianfeng Cai[1]
[1]Department of Chemistry, University of South Florida

Synthesis of Biodegradable Polycarbonate Nanostructures with Selective Lysis against Gram Positive Bacteria

The resistance developed by the bacteria toward antibiotics has become a major concern in public health. There has been a significant interest in the development of antimicrobial cationic polymers due to the ease and low-cost of manufacture compared to host-defense peptides (HDPs). Herein, we report the design and synthesis of amphiphilic polycarbonates containing primary amino groups. These polymers exhibit potent antimicrobial activity and excellent selectivity to Gram-positive bacteria, including multi-drug resistant pathogens. Fluorescence and TEM studies suggest that these polymers are likely to kill bacteria by disrupting bacterial membranes. These polymers also show low tendency to elicit resistance in bacteria. Their further development may lead to new antimicrobial agents combating drug-resistance.

GP-12 **Mussie Gide**[1], Alekhya Nimmagadda[1], Jianfeng Cai[1]
[1]Department of Chemistry, University of South Florida

Lipidated Dendrimers displaying Broad Spectrum Antibacterial Activity

The resistance developed by the bacteria against antibiotics has become in a major concern in the health care department. Therefore, there has been a significant interest in the development of antimicrobial polymers and dendrimers due the ease of manufacture and low manufacture cost compared to small antimicrobial peptides (AMPs). Here in we present the synthesis of lipidated amphiphilic dendrimers that mimic the bacterial mechanism of AMPs by disrupting the cell membrane. These dendrimers had displayed a potent antimicrobial activity against gram –positive and gram –negative bacteria.

GP-13 **Constantine Shuniak**[1], Scott Lewis[1]
[1]Department of Chemistry, University of South Florida

Investigation Into Which Questions Promote Deep Learning in General Chemistry

The distinction between deep and surface approaches to learning has been described in the literature as “appearing to be a powerful form of categorization for differences in learning strategies”. One possible way to encourage deep learning is to design and use questions that require deeper understanding of chemical concepts, and perhaps reduce dependence on questions relying on memory or plugging variables into formulas. In our 3000 student general chemistry cohort we found an interesting distribution in one semester’s grades which seemed to indicate a correlation between certain question types and students’ self-report as a deep or surface learner using Biggs’ r-SPQ-2F. To further investigate the observation we analyzed similar data in general chemistry I and general chemistry II. Although the research cannot recommend specific problem types to promote deep learning, the question classification and data analysis methods presented may inform those seeking to undergo similar work.

GP-14 **Anne-Claire Limon**[1], Bill Baker[1]
[1]Department of Chemistry

Isolation of Alcyopterosin compounds produced by an Antarctic coral of the Gersemia sp.

Drug resistance causing the spread of infectious agents and diseases is a global problem, in need of innovative solutions and novel drugs. Marine organisms from Antarctica have been investigated for their potential natural product chemistry. Antarctic corals produce unique secondary metabolites as a defense mechanism to compensate for their immobility. These adaptations persist throughout evolution, accumulating novel secondary metabolites in subsequent generations. The compounds behind these chemical defense systems could be a significant source of novel chemistry to be further developed into new drugs. The purification of extracts from an Antarctic coral, Gersemia sp. has led to the isolation of several known compounds of the alcyopterosin family. Coral samples were freeze-dried, treated to Soxhlet extraction and liquid-liquid partition. MPLC and HPLC were performed to purify terpenoid compounds. The purification process was guided by NMR. Once characterized, isolates were subjected to assays against infectious agents to assess bioactivity and drug potential.

GP-15 **Imalka Marasinghe Arachchilage**[1], Julianne Harmon[1]
[1]Department of Chemistry, University of South Florida

Cationic polymerization to Synthesize Laccol Polymers and Laccol/Styrene Copolymers for Radiation Hard Applications

Lacquer sap is an ecofriendly natural resource polymer that can be used in electronic and automobile industries as well as in space operations. Its ability to persist under harsh conditions makes laccol polymers ideal for the above applications. A novel methodology is introduced herein to polymerize laccol extracted from Vietnamese lacquer sap (Rhus succedanea) via cationic initiators. Polymerization of laccol was investigated using an aluminium chloride and ethyl acetate (AlCl3.EtOAc) initiator complex and sulphuric (H2SO4) acid initiator. The unsaturated groups present in long side chain of laccol engaged in polymerization. Additionally, a copolymer made up of laccol and styrene was investigated using the above initiators. The thermal and physical properties of the polymers were analyzed using Infrared Spectrophotometry (FTIR), Differential Scanning Calorimetry (DSC) and Thermal Gravimetric Analysis (TGA).

GP-16 **Abhijeet Iyer**[1], Venkat Bhethanabotla[1]
[1]Department of Chemical Engineering, University of South Florida

Sorption of Benzene, Dichloroethane, Dichloromethane and Chloroform by PEG, PCL and Their Copolymers at 298.15 K Using a Quartz Crystal Microbalance

Solubilities of benzene, dichloroethane, chloroform and dichloromethane in polyethylene glycol (PEG), polycaprolactone (PCL), and several di-block PEG/PCL copolymers at 298.15 K are reported. Activity vs. weight fraction data were collected using a quartz crystal microbalance and are adequately represented by the Flory-Huggins model. The data were reported using a Quartz crystal microbalance in a newly designed flow system constructed in the lab.

GP-17 **Jenin Jedian**[1], Kirpal Bisht[1]
[1]Department of chemistry, usf

Synthesis of potential anti-cancer Jak2 kinase inhibitor

Janus Kinase (Jak2) is a tyrosine kinase that plays a key role in numerous signaling pathways (1). Jak2 forms association with growth factor and cytokine receptors and upon its activation, it phosphorylates substrates a signal producer and activator of transcription called STATs that modulate gene transcription (1). Jak2 mutation called Jak2-V617F was found in many myeloproferative neoplasm MPN patients, which causes overproduction of blood cells of the myeloid lineage. Previously, our group was able to synthesis a small molecule called G6 that inhibits Jak2-mediated pathogenic cell growth using in Vitro cell culture, in vivo models, and ex vivo patient samples(1). G6 is known to inhibit the proliferation of human erthrolukemia HEL cell in vitro and in vivo (1).G6 greatly reduces the growth of Jak2-Val616phe mutated human pathological cells isolated from the bone marrow of a polycythemia vera patient with IC50 VALUE of 50Nm (2). Jak2 inhibitors were a subject for extensive studies in the last years, due to the fact that there are no effective therapies beside palliative treatment (1). Our current goal in to make G6 more stable molecule and as a result more effective drug. Using in silico drug discovery approach, we designed a potential anticancer drug that have structural similarity with G6 and shows more stability. We are using click chemistry and Mannich condensation reaction to design multiple synthetic routes to obtain the target drug. References: 1- Rebekah Baskin,a M

GP-18 **Andrea Lemus**[1], Shreya Patel[1], Ronald Swonger[1], James Leahy[1]
[1]Department of Chemistry, University of South Florida

Synthesis of New Compounds to Improve Degradation of Tau for Alzheimer's Disease

Alzheimer's disease is a neurodegenerative disorder that causes memory and behavior problems. It is not a normal part of aging, there is no cure, and it is unknown how to stop the progression. Some of the symptoms in Alzheimer's are: difficulty remembering new information, mood changes, and difficulty speaking and swallowing. Research shows that plaques of beta-amyloid build up in the spaces between nerve cells and tangles of tau build up inside cells. The combination of plaques and tangles combine to block cell communication and build to the progression of AD. Worldwide research efforts are underway to create new treatments for the disease to delay progression or to prevent it entirely. Our target is the Heat Shock Protein 70 (Hsp70) family. In collaboration with researchers in the USF Byrd Alzheimer's Institute, we have been working to create new set of compounds that use Hsp70 to enhance the degradation of tau.

GP-19 **Jacob Mayers**[1], Randy Larsen[1]
[1]Department of Chemistry, University of South Florida

Photophysical study of Ruthenium (II) Tris-(2,2'-bipyridine) encapsulated within Uio-66 metal organic frameworks containing functionalized linkers

Uio-66 metal organic frameworks are thermally stable porous materials that provide an excellent environment for the encapsulation of photoactive guests. The guest of particular interest is Ruthenium (II) Tris-(2,2'- Bipyridine) (RuBpy) due to the relatively long lifetime and photostability of this class of complexes. Presented here is a photophysical study of RuBpy encapsulated Uio-66 MOFs and derivatives. The RuBpy encapsulated in each of the MOF frameworks were fit to a biexponential decay function. A bathochromatic shift is also observed in both the steady state emission and absorbance spectrum of each framework and these results also support the quenching of the photoactive RuBpy guest by the frameworks composed of BDC-NH 2 and BDC-OH ligands. It is shown that the photophysical properties of RuBpy be altered through the adjustments of the Uio-66 framework by modifying the organic linkers supporting the inorganic Zr 6 O 4 (OH) 4 clusters.

GP-20 **Christopher R. McKeithan**[1], Randy W. Larsen[1]
[1]Department of Chemistry, University of South Florida

Ruthenium(II) tris(2,2'-bipyridine) Encapsulated within a novel Cobalt Metal Organic Framework Exhibits Guest to Host Photoinduced Electron Transfer

Here the photophysical properties of [Ru(2,2'-bipyridine)3]2+ (RuBpy) encapsulated within a previously reported framework, RWLC-2, with a substituted SBU constructed of cobalt in place of zinc, herein, RWLC-2 (Co), are reported. Altering the composition of the RWLC-2 SBUs yields a material that possesses photophysical properties distinct from those observed in the original material. Upon deconvolution of the fluorescence decay data, two phases were resolved, one being that of the laser~3-6 ns, and the second being a temperature dependent phase corresponding to the decay of the triplet metal to ligand charge transfer state (3MLCT) with a lifetime of~5-12 ns. The lifetimes observed in RWLC-2 (Co) suggests a nonradiative decay pathway not present in those lifetimes observed in RWLC-2. In this context, the proposed mechanism of nonradiative quenching for the 3MLCT is the result of photoinduced electron transfer originating from *Ru(II)Bpy2+ to Ru(III)Bpy3+ to Co3III(O) to CoIICo2III(O).

GP-21 **Jessica Martin**[1], Randy Larsen[1]
[1]Department of Chemistry, University of South Florida

Photophysical Characterization of Photocatalytic Rhenium(I) materials for CO2 reduction

The continual rise of atmospheric CO2 concentrations, largely due to combustion of fossil fuels, is a serious global problem. Despite advancements in chemical materials, CO2 concentrations are still increasing. The goal of this study is to design Rhenium(I) based photocatalysts that can capture and reduce CO2 to C1-based fuels and industrial feedstock chemicals. The first step in development of these catalysts is the synthesis and characterization of the parent ClRe(CO)3(2,2'-bipyridine). The optical spectrum shows absorbance bands in the 360-380 nm region (ReX(CO)3 -> bpy 1MLCT), 290-295 nm region (ligand based π -> π^*) and 235-245 nm region (Re -> CO 1MLCT). The emission spectrum when excited at 370nm shows a λmax between 600-605nm. The second step involves encapsulating this Rhenium(I) catalysts into a stable, porous metal-organic framework, USF2, and analyzing the photophysical properties of the encapsulation. Our efforts to determine lifetimes, structural and other physical information are described herein.

GP-22 **Alfredo Peguero**[1], Arjan van der Vaart[1]
[1]Department of Chemistry, University of South Florida

Conformational Analysis of AX/XT DNA Base Steps via Molecular Dynamics Simulations

An accurate and efficient implementation of the six DNA base pair parameters as order parameters for enhanced sampling simulations is presented. The parameter definitions are defined by vector algebra operations on a reduced atomic set of the base pair, and correlate very well with standard definitions. Application of the model is illustrated by umbrella sampling simulations of propeller twisting within AT/AT, AA/TT, and AC/GT steps and their uracil analogs. Strong correlations are found between propeller twisting and a number of conformational parameters, including buckle, opening, BI/BII backbone configuration, and sugar puckering. The thymine methyl group is observed to notably alter the local conformational free energy landscape, with effects within and directly upstream of the thymine containing base pair.

GP-23 **Nicole Azbill**[1], Randy Larsen[1]
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Photo-Release of Tryptamine and Tyramine from [Ru(II) bis(2,2'-bipyridine)]$^{2+}$ complexes Encapsulated within a Polyhedral Zn(II)-Trimesic Acid Metal-Organic Framework: A Photo-Dynamic Therapy Model

Implantable drug delivery systems (IDDSs) are a significant technology, useful in controlled and targeted delivery of bioactive molecules (BAMs) to desired tissues. Metal-organic frameworks (MOFs) are solid, porous materials capable of functioning as hosts for guest molecules. Previous work has shown that guest molecules include photoactive compounds such as ruthenium bipyridine (RuBpy) complexes. MOFs used to encapsulate compounds that photorelease BAMs upon light exposure would be a novel form of photodynamic therapy (PDT). In this "proof of concept" study, [Ru(2-2',bipyridine)$_2$(tyramine)$_2$]$^{2+}$(RuTyra) and [Ru(2-2',bipyridine)$_2$(tryptamine)$_2$]$^{2+}$ (RuTryp) were synthesized, and then encapsulated within the polyhedral Zn(II)-trimesic acid MOF, USF2. The loading of RuTyra and RuTrypt were both observed to be 5% in USF2. The photorelease of tyramine and tryptamine from the RuBpy complex via optical light was confirmed by measuring the absorbance and emission over time. The measurement for quantum yields of photorelease from USF2 and the determination of the crystal structures are in-progress.

GP-24 **Ankush Kanwar**[1], Tommy W. McGaha Jr. [1], James W. Leahy[1], Dennis E. Kyle[1]
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Synthesis and evaluation of Xanthurenic analogs for impeding transmission of Plasmodium falciparum from host to vector

The need for new anti-Malarial drugs is greater than ever before owing largely to the emergence of multidrug resistance in common pathogens as well as the rapid emergence of new infections. Malaria is one of the most common infectious diseases which affect large populations, especially in less developed countries. *Plasmodium* is the parasitic protozoa that cause malaria. The life cycle of *Plasmodium* involves two hosts (mosquito and mammals). During the life cycle, gametocytes (mature sexual stage) are present in the blood of infected vertebrate hosts while gametogenesis (activation of mature gametocytes) and formation of diploid zygotes only occur in the midgut of vector mosquitoes. It has been reported that the process of gametogenesis is induced by various factors such as pH and temperature change. Xanthurenic acid, which is present in the head and midgut of the mosquito, also plays an important role in the differentiation of the parasite. Xanthurenic acid and a series of analogs have been synthesized with the aim of impeding the transmission of malaria.

GP-25 **Bo Song**[1], Xiaopeng Li[1]
[1]Department of Chemistry, University of South Florida

Self-Assembly of 2D and 3D Star of David

The Star of David, recognized as symbol of modern Jewish identity and Judaism, has fascinated chemists due to its unique beauty and complexity. Over the past few decades, several strategies, including stepwise self-assembly as well as template-directed synthesis have been manipulated on the journey toward this fancy structure. We herein designed a single step self-assembly of 2D and 3D Star of David using a tetratopic pyridyl ligand with 180° diplatinum(II) acceptor and naked Pd 2+, respectively. 2D Star of David structure was achieved by the self-assembly of tetratopic pyridyl-based ligand with 180° diplatinum(II) acceptor at 1:2 ratio, while the 3D Star of David was achieved by the self-assembly of ligand and Pd 2+ in 1:1 ratio. It is noteworthy that alkane chains were introduced into the ligand to improve solubility for the 3D structure. The molecular compositions, shapes and sizes of supramolecular complexes were unambiguously characterized via multi-nuclear (1H, 13C, 31P) and multi-dimensional (COSY, NOESY, DOSY) NMR techniques, electrospray ionization-mass spectrometry (ESI-MS) as well as ion-mobility mass spectrometry (IM-MS). AFM and TEM were employed to directly visualize individual supramolecules. Finally, the stabilities of the 2D and 3D structures were measured and compared using gradient tandem-mass spectrometry (gMS 2). The high stability of 3D Star of David was correlated to its high density of coordination sites (DOCS).

GP-26 **Lei Wang**[1], Xiaopeng Li[1]
[1]Department of Chemistry, University of South Florida

Self-Assembly of molecular fractals

Fractals are defined as natural phenomenon or mathematical set which display a repeating pattern. Such structures widely occur in the field of art, science and engineering. Driven by the thought to interpret the concept of fractal from a micro point of view, chemists have endeavored in the construction of molecular fractals during the past few years, while only a few examples were reported, especially for the extended molecular fractals. In the light of our previous success in coordination-driven self-assembly, we herein designed and constructed four extended molecular fractals based on the self-assembly of terpyridine-based ligands. All the ligands were synthesized from a disubstituted triphenylamine unit, which worked as a specific angle controller. The smallest ligand was easily achieved by direct Sonogashia coupling of disubstituted triphenylamine units with terpyridine motifs, while the largest one was constructed based on the smallest one, followed by stepwise connections between terpyridine and Ru2+. Four supramolecular fractals were obtained in almost quantitative yields by precise coordination of terpyridine units and Zn2+ ions. Characterization of the architectures were accomplished via both 1D and 2D NMR spectroscopy, electrospray ionization mass spectrometry (ESI-MS), traveling-wave ion mobility (TWIM) mass spectrometry, and transmission electron microscopy (TEM). As triphenylamine units have been widely used in photoreceptor devices and organic light-emitting diodes due to their unique photoelectrochemical characteristics, the supramolecular fractals were expected to have potential applications in optoelectronic fields. Higher-generation fractal architectures are currently underway.

GP-27 **Yiming Li**[1], Xiaopeng Li[1]
[1]Department of Chemistry, University of South Florida

Post-assembly Functionalization of Supramolecular Ring-in-ring Structure via Click Chemistry

The use of a strain-promoted click reaction in the post-self-assembly functionalization of a supramolecular ring-in-ring structure . The coordination-driven self-assembly of a 120°double layer tetraterpyridine ligand and differnet trans metal ions forms molecular ring-in-ring hexagon bearing terminal alkyne. These species undergo post-selfassembly [3+2] Huisgen cycloaddition with a variety of azides to give functionalized ensembles under mild conditions.

UNDERGRADUATE POSTERS

AN-01 **Ronelle Bailey**[1], Christina Manusco[1], Ifeoluwa Ayodeji[1], Theresa Evans-Nguyen[1]
[1]Department of Chemistry, University of South Florida

DART with Differential Mobility Spectrometry-Mass Spectrometry for Pre-filtration of Organic Analytes

Separation and analysis of molecular ions within a portable setting are studied in detection and analysis of organic materials. For on-site screening of organic materials for forensic investigations, rapid separation of organic mixtures requiring minimal sample preparation is ideal. In this work, differential ion mobility (DMS) provides post-ionization differentiation and filtration of caffeine prior to mass spectral analysis. When utilized prior to mass analysis, DMS provides ion filtration on the order of milliseconds, enhancing the detection accuracy of the system. As an ionization technique Direct Analysis in Real Time (DART) allows for the ionization of gas, liquid and solid samples at atmospheric pressure and requires minimal sample preparation. This work aims to couple the pre-filtration capabilities of DMS with the versatile sample ionization method of DART before subsequent ion trap mass analysis.

AN-02 **Stephanie Asher-Leonard**[1], C. R. McKeithan[1], Dean F. Martin[1]
[1]Department of Chemistry, University of South Florida

Removal of Acetaminophen from Aqueous Solution with Selected Metalloligs

Pharmaceutically active compounds in water sources is an emerging environmental concern. Pharmaceutical agents are used for treatment of human conditions, veterinary medicine, aquaculture, and livestock production, providing ample opportunity for environmental infiltration. These compounds have been detected in municipal water sources and downstream from wastewater treatment plants. Though wastewater treatment can be effective in removal of pharmaceuticals, it was not engineered for this purpose, and removal rates vary. Octolig®, a polyethylenediimine covalently attached to high surface area silica, has demonstrated efficacy in purification for certain pharmaceuticals. Previous studies have found acidity to be a strong indicator of purification potential, as compounds with higher pKa necessitate higher pH solution for the target compound to dissociate to anionic form, which also likely deprotinates Octolig®, rendering it inactive for ion encapsulation. Acidity issues may be offset by transition metal-bonded Octolig® derivatives, allowing removal of acetaminophen, the most widely used analgesic in the U.S.

AN-03 **Jonathan Gomogda**[1], **Disha Thadhani**[1], Garrett Craft[1], Julianne Harmon[1]
[1]Department of Chemistry, University of South Florida

The Effects of PEG Molecular Weights on Starch Networks

Polyethylene glycol (PEG) is a polyether utilized as a hyperosmotic agent in nursing homes and is frequently delivered in thickened liquids to patients with dysphagia. However, its presence reduces the viscosity of liquids thickened with starch gels to dangerous levels, presenting the risk of aspiration and resultant pneumonia, as described in previous work. A TA Instruments AR 2000 rheometer will be used to further analyze the resulting viscosity of various PEG molecular weights, starch, and/or xanthan gum thickener combinations and to characterize their interactions. Variables such as molarity, solubility, and time will be studied to determine the structural effects they have on the starch network and why PEG thins down the viscosity.

AN-04 **Victoria Lear**[1], Tamalia Julien[1], Julie Harmon[1]
[1]Department of Chemistry, University of South Florida

Conductive Ultrasoft Thermoplastic Polyurethane/Lithium Electrolyte Composite

Due to the instability of lithium ion batteries a novel polymer, polycarbonate polyurethane (PCPU) combined with lithium salt was analyzed for its ability to be a highly conductive electrolyte that does not easily degrade. PCPU has a Shore A hardness of 64, whereas not many polyurethanes can reach such soft grades and maintain processability. This is due to the PCPU's composition of a hard segment, providing stability, and soft segment allowing the polymer to flow at high temperatures instead of degrading. Through incorporation of lithium salts, lithium hexafluorophosphate (LiFPO4) and lithium bromide (LiBr), this composite could lead to an innovative, ultra-soft, conductive polymer electrolyte film. The characterization methods that will be used include Differential Scanning Calorimetry (DSC), Fourier transform infrared spectroscopy (FTIR), and Four Point Probe.

BC-01 **Zachary Sannasardo**[1]
[1]Department of Chemistry, University of South Florida

Effect of Repetitive Mild Traumatic Brain Injury and Voluntary Drinking on Neuronal Cytokines

Cytokines are a group of proteins, glycoproteins, and peptides secreted by immune cells that regulate the inflammatory response. Consumption of alcohol following traumatic brain injury has been associated with negative long-term effects and increased levels of pro-inflammatory cytokines in the brain. The aim of this experiment is to measure the effect of voluntary alcohol consumption on the expression of cytokines IL -1, IL -6, IL -10, MCP-1 and TNF over an 8 week time interval after repetitive mild traumatic brain injury (mTBI). Mice were subjected to 4 mild brain injuries followed by voluntary alcohol exposure for 0, 2, 4, 6, or 8 weeks. Brain tissue was extracted and cytokine levels were measured using enzyme-linked immunosorbent assay (ELISA). Preliminary results show that there was no significant change in MCP-1 levels 4-days after mTBI. Additionally, there was no significant change in MCP-1 levels one week after mTBI compared to the 4-day non-injury group. However, this data is limited and no significant claims can be made until additional data is obtained.

BC-02 **Daniel Joseph**[1]
[1]Department of Chemistry, University of South Florida

Synthesis of Alanine Based Peptidomimetic and Analysis through X-ray crystallography

Peptidomimetics are biological compounds that mimic the structure of naturally occurring peptides. Peptidomimetics are usually composed of altered amino acids sequenced with a variety of chemical subunits. These compounds serve an imperative role in biological research as they possess greater stability than traditional peptides due to their synthetic nature. The focus of this research project is to properly synthesize a peptidomimetic with ligand binding capabilities and later analyze its tertiary structure through X-ray crystallography.

BC-03 **Andrea Bernat**[1], Ying He[1], Xiaodong Shi[1]
[1]Department of Chemistry, University of South Florida

Guanosine Quadruplexes

Guanosine quadruplexes have several applications in the fields of structural biology, medicinal chemistry, supramolecular chemistry, and nanotechnology, where their structure and function are observed and analyzed. The purpose of our research project is to synthesize the well-designed sugar and non-sugar guanosine derivative to study the self-assembling of different substrates. We used organic synthesis to synthesize the target molecule (different guanosine derivatives) and set up the self-assembly reactions to answer the questions that show how the conformation difference will change the self-assembly ability. The results were analyzed via ESI-MS and 1H NMR. In conclusion, both sugar G-Quadruplexes and nonsugar G-Quadruplexes were formed and MS and NMR were used to analyze the structure after self-assembling from the monomer with the presence of the cation.

BC-04 Frank Zamudio[1], **Corbin Rodier**[1], Anjanet Loon[1], Khawla Benyamine[1], Carlos Osorno[1], Shayna Smeltzer[1]
[1]USF Health Byrd

Peripheral Inflammation in TDP-43 pathology

TDP-43 is a protein found to be associated with Frontotemporal dementia and Amyotrophic Lateral Sclerosis. Past studies have supported the relationship between TDP-43 and inflammatory response molecules such as IL-6. To study the interaction of peripheral immune response on TDP-43, 9 month old WT and TAR4 mice were injected with 500 µg/kg or saline intraperitoneally 5 times over 15 days. After the 15th day, brain tissue was collected for further treatment. From this experiment, it was found that overexpression of TDP-43 when coupled with peripheral inflammation lead to deficits in learning and memory. All though alteration to inflammatory receptors and kinases occurred, the changes were not different between mice models. LPS exacerbates TDP-43 induced pathology by impairing memory and increasing neurotoxicity in the brain.

BC-05 **Mary Weinrich**[1]
[1]Department of Chemistry, University of South Florida

Analysis of unusual Tribolium castaneum dopamine N-acetyltransferase (aaNAT0) substrates via double-reciprocal kinetic analysis

Tribolium castaneum, or the red flour beetle, is an indo-Australian pest that causes commercial loss in stored grains. BLAST was used to compare the T. castaneum genome to Drosophila melanogaster in order to assess whether Arylalkylamine N-acetyltransferases (aaNATs) were expressed, and two Dopamine N-acetyltransferases were found; timezymes, from the GNAT family, found in many insects that is believed to contribute to circadian rhythm and chitin formation through acetylation of amino acids, neurotransmitters, and likely similar compounds with a free amine group. In order to understand one of these proteins, aaNAT0, it was overexpressed in Escherichia coli and purified using affinity chromatography. From there, a screening assay was performed in order to determine the specificity of the enzyme to unusual substrates, and analyze the subsequent kinetic activity using double reciprocal analysis.

BC-06 **Michael Winstead**[1]
[1]Department of Chemistry

The Role of Connective Tissue Growth Factor in Ethanol Induced Liver Fibrosis

Expanding the current treatment options of chronic liver fibrosis and cirrhosis would provide a great benefit to humanity. The investigation of liver fibrosis, in particular the role of connective tissue growth factor (CTGF) in advancing the mechanism, is of particular interest due to recent studies indicating a reduction of fibrotic tissue upon deletion of CTGF on several organs. The growth factor can be rendered denatured by the administration of a viral vector grown in human embryonic kidney cells (HEK cells). Injecting mice with this vector has shown to not decrease the survivability of mice over a period of six days, showing potential to reduce fibrotic activity without diminishing the health of a specimen suffering from ethanol induced liver fibrosis. The fibrotic levels of liver tissue samples are being evaluated qualitatively by comparing the relative amount of scar tissue buildup of control and CTGF knock-out mice.

BC-07 **Brittney Kahler**[1]
[1]Department of Chemistry, University of South Florida

Proposed Coiled Coil through Design and Synthesis of γ-AApeptides

Sequences of coiled coil γ-AApeptide backbones were synthesized using Fmoc solid phase synthesis. The secondary and tertiary structure was observed and identified using circular dichroism, 2-D NMR, and X-Ray Crystallography. Unnatural peptide backbones have the capability to mimic secondary and tertiary structures of natural peptides with enhanced chemodiversity and resistance to enzymatic hydrolysis. By synthesizing and observing the conformational structures of these γ-AApeptides, we can better predict the reaction of natural peptides within cellular processes.

BC-08 **Shirley Figueroa Gonzalez**[1], Tania Cruz Arevalo[1], Celia Osorio Cantillo[1], Jose I. Ramirez Domenech[1], Edmy Ferrer Torres[1]
[1]Science and Technology, Interamerican University of Puerto Rico, Ponce, PR, United States

Effect of the interaction of ZnO nanoparticles and the gentamicin in growing populations of Staphylococcus aureus

This study aims to prove the effectiveness of ZnO nanoparticles as an antimicrobial agent against Staphylococcus aureus, and their potential to enhance antibiotic effectiveness by combining nanoparticles with the antibiotic Gentamicin. In this study, the impact of ZnO nanoparticles in bacteria (S.aureus) was evaluated by the bacterial growth curve based on the number of cells versus time. The effect of these nanoparticles in the form and size of the bacteria were analyzed microscopically. The synthesis of ZnO nanoparticles were achieved via the precipitation method which was applied using zinc sulfate 0.1 M and NaOH as precursors with PVP used as stabilizer. The surfactant employed to control the nanoparticle size was tetramethylammonium hydroxide (TMAH). Characterization was done through UV-vis optical absorption, Infrared Spectroscopy (FT-IR) and Dynamic Light Scattering (DLS). The optical studies show the characteristic absorption band around 370 nm and DLS analysis shows a diameter size of 35 nm.

BP-01 **AnneMarie VanderSchouw**[1], Timothy Odom[1], Fengyu She[1], Dr. Jianfeng Cai[1]
[1]Department of Chemistry, University of South Florida

Conformational Study of γ-AA Peptide in Solution

Two synthetic peptide sequences were designed for synthesis, based on previously observed helical structures. The peptides will be formed with a combination of γ-AA and unmodified amino acids. The folding of this sequence will be observed for helical conformation to predict trends in right-handed and left-handed helices.

BP-02 **Dylan Grassie**[1], Randy W. Larsen[1]
[1]Department of Chemistry, University of South Florida

Structural and Spectroscopic Characterization of Heme Proteins Mineralized within the ZIF-8 Metal Organic Framework

The ability to encapsulate bioactive molecules and enzymes within porous solid state materials has long been of interest in the development of hybrid materials for industrial applications. Metal organic frameworks (MOFs) are of particular interest for encapsulation of these molecules due the presence of regularly porous cavities of tunable dimensions, ease of synthesis, and functionalizable interiors. Recently the ability to mineralize various proteins within several zeolitic imidazole frameworks (ZIFs) has been demonstrated in which the MOF grows around the protein creating large protein encapsulated cavities. These materials have been shown to have unique catalytic activity which is promising for industrial reactions. The most widely investigated material is ZIF-8 formed from Zn(II) ions and 2-methyl imidazole. Here we report protein structural studies to determine the impact of mineralization on the three dimensional structure of myoglobin (Mb), cytochrome c (Cc), and Microperoxidase-11 (MP-11).

BP-03 **Anthony G. Giacalone**[1], Dr. Randy W. Larsen[1]
[1]Dr. Randy W. Larsen Lab
[2]Department of Chemistry, University of South Florida

Encapsulation of Ruthenium (II) Complexes possessing Photo-releasable Bioactive Molecules (BAMs) within Zn(II) and Fe(III) Metal Organic Frameworks

Metal organic frameworks (MOFs) are a class of porous materials composed of organic ligands linked through metal clusters (molecular building blocks or MBBs) that have exceptional potential to serve as platforms for a wide array of applications including novel drug delivery. Drug delivery applications for MOMs are of increasing interest as these materials can contain a high weight percent of biologically active compounds within the large interior cavities while the relatively small pore sizes enables effective time release. Here we describe the development of a novel photodynamic therapy application of MOMs in which a Ru(II)(2,2'-bipyridine)2(BAM)2 (BAM = Bio-Active Molecule) cluster is encapsulated within the cavities of the Zn (II)-based polyhedral MOM, USF2, and water stable Fe (III) MOF's. Exposure of the new materials to white light results in the photo ejection of the BAM and subsequent egress to the bulk solvent through the exterior pores.

CE-01 **Devon Mitchell**[1]
[1]Department of Chemistry, University of South Florida

NKCC1 and its impact on hearing loss treatment

This study was done to show a potential mechanism of aldosterone treatment on the NKCC1 cotransporter. Previous research associated with the use of aldosterone as a potential treatment with hearing impacts the NKCC1. Currently there are no treatments for hearing loss and the use of aldosterone is showing promise as a potential solution, but we aren't sure of the mechanism that the aldosterone enacts on the NKCC1. The exploration of NKCC1 in the body as well as its impact on hearing loss is key to figuring this out.

CO-01 **Zachary Dyott**[1], Adam Hogan[1], Brian Space[1]
[1]Department of Chemistry, University of South Florida

Toward Next-Generation Force Fields: Atom Typing as a Viable Parametrization Tool

Next-generation force fields strive for complete transferability between molecular systems for simulations. We are investigating the applicability of atom typing in analyzing the transferability of point multipole polarizabilities and dispersion coefficients for a diverse set of molecules found in both petroleum and byproducts of petroleum cracking. This set represents a large ensemble of chemically distinct atoms of the same element as well as distinct patterns of connectivity and hybridization. Through recursive and single-point calculations, the constrained and unconstrained fits to the energetics of these molecules will reveal information about the transferability of the parameters in question. Pending results, development of next-generation force fields for the purposes of gas sorption simulations for metal-organic frameworks (MOFs) may continue.

CO-02 **Luciano Laratelli**[1]
[1]Department of Chemistry, University of South Florida

Comparison of Many-Body Polarizability Potentials With Lennard-Jones and Stockmayer Potentials in Grand Canonical Monte Carlo Simulation

Grand Canonical Monte Carlo (GCMC) code was developed, and tested in order to reproduce important, seminal results in computational chemistry (in particular de Leeuw et. al, The Journal of Chemical Physics 93, 2704 (1990),) confirm the validity of the acceptance conditions utilized in Massively Parallel Monte Carlo (MPMC,) and compare the effects of a many-body polarizability potential with that of the pure Lennard-Jones potential, as well as its well-known embedded point dipole modification, the Stockmayer potential.

CO-03 Tony Pham[1], Katherine Forrest[1], **Matthew Mostrom**[1], Joseph R. Hunt[2], Jeurgen Eckert[1], Brian Space[1]
[1]Dept. of Chemistry, University of South Florida
[2]Department of Chemistry and Biochemistry, University of California–Los Angeles

The Rotational Dynamics of H2 Adsorbed in Covalent Organic Frameworks

Inelastic-neutron-scattering (INS) and theoretical studies were carried out on H2 adsorbed in two covalent-organic-framework (COF) materials. Molecular simulations of H2 adsorption in COF-1 revealed that the H2 molecules occupy the region between two eclipsed layers of the COF, with the most favorable binding site in COF-1 located between two B3O3 clusters of the eclipsed layers. Two distinct H2 binding sites were identified in COF-102. Two-dimensional quantum rotation calculations for H2 adsorbed at the considered sites in both COFs resulted in rotational transitions that agree with those in the corresponding INS spectra. Calculation of the rotational potential energy surface for H2 bound at the most favorable adsorption sites in COF-1 and COF-102 revealed unusually high rotational barriers attributed to the B3O3 rings. The values for these barriers are greater than or comparable to those of some metal–organic-frameworks (MOFs) that possess open-metal sites. This study demonstrates for the first time the rotational dynamics of H2 adsorbed in COFs.

CO-04 Christian Cioce[1], **Alejandro Navas**[1], Adam Hogan[1], Brian Space[1]
[1]Department of Chemistry, University of South Florida

Designing PHAST2 Potentials for Heterogeneous Environments

A variety of simulation models has been used to approximate the interatomic and intermolecular potential energy for chemical systems. One such model is PHAST (Potentials with High Accuracy, Speed and Transferability), and it has proven useful for reproducing bulk thermodynamic properties of several gaseous systems. The pair potentials which comprise the PHAST family are additive and include electrostatic energy, polarization energy, and dispersion-repulsion energies. To improve upon the PHAST model, a new potential family, PHAST2, has been developed. PHAST2 replaces the Lennard-Jones 12-6 repulsion-dispersion function with the sum of a Tang-Toennies dispersion function and an exponential repulsion term. This new potential family's ability to reproduce ab initio calculations in heterogeneous environments is demonstrated. Also, ab initio energies were calculated for helium clusters of MOF-like local geometries to show that best-fit dispersion-repulsion pairwise parameters are geometry dependent. This geometry dependence may aid heterogeneous noble-gas simulation.

CO-05 **N. A. Clough**[1], F.L. Kearns[1], P.S. Hudson[1], H.L. Woodcock[1]
[1]Department of Chemistry, University of South Florida

Evaluation of the ANIKIN-ME Neural Network Potential with Respect to Dipeptide Simulations

A neural network based potential, derived from the Accurate NeurAl networK engINe for Molecular Energies (ANIKIN-ME), was recently shown to accurately predict ab initio single-point energies for small organic compounds based only on atom identity and atom position. The work undertaken in the current study seeks to evaluate the applicability of such potentials in molecular dynamics and Monte Carlo simulations, achieving a desired level of accuracy while reducing computational cost. Dipeptide models of serine and alanine will be used in classical molecular dynamics, SCC-DFTB based dynamics and non-equilibrium simulations to generate torsion maps. The atom identities and coordinates from the resulting trajectory data will be given as input to the neural network potential in order to generate additional torsion maps. Comparing the maps will allow for the determination of accuracy, reduction in time costs and possible applications of the neural network potential.

CO-06 **Alexis Johnson**[1], Brian Space[1]
[1]Department of Chemistry, University of South Florida

Monte Carlo Simulations of H2, CO2 and CH4 in Al-soc-MOF-1

Metal-organic frameworks provide alternative solutions to environmental and energy issues common in industry. Gas storage in nanoporous materials has become a lucrative technology. One of these materials, Al-soc-MOF-1, meets the DOE dual target of gravimetric and volumetric methane storage. Computer simulations provide a platform to examine the mechanism of gas adsorption at the atomistic level. Monte Carlo simulations, by referencing only the potential energy of the system, allow sorbates to settle in the most statistically favorable positions in the system. The different force fields employed in these simulations exemplify the range of interactions between sorbates and MOFs that are necessary to quantitatively replicate adsorption. Preliminary results for gas adsorption using UFF parameters reveal unusual over-adsorption for all CO2 and H2 models. This suggests that alternate Lennard-Jones parameters that take into account varying chemical environments must be employed in the simulation of this material.

CO-07 **Nicole Stewart**[1], David M. Rogers[1]
[1]Department of Chemistry, University of South Florida

Interface Interactions in Solvated Pyrophyllite Clay

Shale gas is being increasingly tapped as an alternative to traditional petroleum drilling. Hydraulic fracturing has proven effective in the release of petroleum and natural gases from pores in shale clays. However little is known about the mechanism of and driving forces behind this release. Nanoscale flows are highly dependent upon the nature of interactions between the flow and interface. Molecular dynamics simulations of a nanoscale fracture in pyrophyllite clay is used to investigate these solvent-interface interactions. Simulation data is analyzed to determine the water orientation profile at the clay interface and the electrostatic interactions between the clay layers. The relationship between these factors and the amount of swelling in the clay system provides information on the structure and energetics of this process.

CO-08 **Andrew Apugliese**[1], Fiona L. Kearns[1], H. Lee Woodcock[1]
[1]Department of Chemistry, University of South Florida

Computational Exploration of Lymphatic Filariasis Treatments

Lymphatic Filariasis (LF, a.k.a. elephantitis) is one of sixteen Neglected Tropical Diseases, which primarily affect populations in poverty with inadequate sanitation. Currently, there are 947 million people in 54 countries at risk for becoming infected with LF. LF is caused by nematodes that enter human lymph nodes after being transferred from mosquitoes. In the lymph nodes, they prevent proper circulation of water and cause swelling of lower extremities. The steroidal compound, 20-hydroxyecdysone (20E), binds to the ecdysone receptor (EcR) in LF causing nematodes to incite transcription of developmental genes. It has been shown that the EcR can be targeted to trigger premature release of nematode progeny and therefore prevent further passage of the disease. The current work is a computational screening of compounds identified

from PubChem Database, ProBiS Ligands, and Torrey-Pines screening results. Our objective is to virtually propose potential LF treatments and identify vital chemical moieties.

CO-09 **Brittany Thiessen**[1], Geoffrey M. Gray[1], Dr. Arjan Van Der Vaart[1]
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Secondary Structure Adopted by Peptide Sequences in Dragline Spider Silk

Spider dragline silk is one of the strongest natural materials known to man, yet despite the many possible applications the secondary structure of the noncrystalline regions is still unclear. To investigate this structure, computer simulations were performed of common repetitive motifs found in most dragline silks in both water (high dielectric, representative of the dope) and octanol (low dielectric, representative of the solid fibrous state). Results indicate that these motifs were generally unstructured in aqueous solvent, while a greater degree of secondary structure was adopted in the low dielectric solvent. Turns and helices were the two most common structural elements. A comparison of calculated and experimentally measured NMR chemical shifts, and possible implications for the silk spinning process will be discussed.

IN-01 **Solomon Tesfaye**[1]
[1]Departmant of Chemistry, University of South Florida

Aza-macrocycles combined with MOFs as Potential Candidates for Molecular Recognition

The Aza-macrocycle combined with metal ions to create a unique kind of metal organic framework that is intended to be used for molecular recognition. Two different kinds of aza-macrocycle will be employed 1,4,7-Triazacyclononane and 1,4,7,10-tetraazacyclododecane (TACN and Cyclen). These two macrocycles will be combined with Copper, Nickle, and Cobalt ions and tested for molecular recognition properties. 1,4,7,10-tetraazacyclododecane- N, N', N'', N'''-tetra-p-isophthalic acid was synthesized and characterized using powder x-ray diffraction, single x-ray diffraction and thermogravimetric analysis. This macrocyclic based MOF is pours in nature and it works as a cation ion receptor. By incorporating the properties of the metal ion with the aza-macrocycle ligand shows intriguing properties.

IN-02 **Jesse David**[1], Darrell Cole Cerrato[1]
[1]Department of Chemistry, University of South Florida

Heavy Metal Beets: Inhibition of metal-mediated oxidative stress by betanin from sugar beets

Antioxidants have been a tool of evolutionary biology long before the interest in popular science and are commonly found in plants and single-celled organisms. Combating oxidative stresses in organisms, including free radicals and peroxides, allows for prevention of diseases associated with oxidative stress. Sugar beets (Beta vulgaris) produce betanin, a secondary metabolite, which has been shown in previous studies to bind to ambient metals which are commonly responsible for many types of oxidative stress. To examine how betanin might prevent oxidation and peroxidation in its natural growth medium, the soil, a metal-binding antibiotic produced by a soil-dwelling bacteria was used. Thiostrepton (TSN), produced by Streptomyces azureus, has been shown to bind to metals, especially copper (II), and to perform oxidative and peroxidative chemistry in its bound state. Using Michaelis-Menten fitting, this study shows that betanin can significantly inhibit metal-mediated oxidative processes caused by CuTSN.

NP-01 **Victoria Mischley**[1,3], **Victoria Dukharan**[1,3], Santana Thomas[1,3], Christopher Rice[2], Dennis Kyle[2], Bill Baker[1,3]
[1]Department of Chemistry, University of South Florida
[2]College of Public Health, University of South Florida
[3]Center for Drug Discovery and Innovation, University of South Florida

Potential Answer to Amoebic Infections: Isolation of Secondary Metabolites from Mangrove Fungal Endophytes

The purpose of this project is to isolate secondary metabolites that are active against Naegleria fowleri and Acanthamoeba. Although secondary metabolites are not necessary for survival, they are used as a means of defense against prey and pathogens. Specifically, in plants, fungal endophytes can produce secondary metabolites. In this project, mangrove plants are collected and the fungal endophytes are isolated. Once the fungal endophytes are isolated, the fungal endophytes are introduced to epigenetic modifiers that increase the potential of the secondary metabolites being produced in the lab. These fungal endophytes can potentially have secondary metabolites that can defend against other types of microbes. Once the secondary metabolite has been extracted, it is screened through bioassay against Naegleria fowleri and Acanthamoeba. We have identified some crude extracts that show activity against N. fowleri and Acanthamoeba which, by bioassay guided fractionation, we will isolate to discover pure bioactive compounds.

NP-02 **Christian Stanley**[1,2], Anne-Claire Limon[1,2], Bill J. Baker[1,2]
[1]Department of Chemistry, University of South Florida
[2]Center for Drug Discovery and Innovation, University of South Florida

Isolation of Alcyopterosin compounds from an Antarctic coral for use in drug discovery

Corals are sessile marine organisms that develop unique secondary metabolites to avoid predation and indemnify them for their immobility on the ocean floor. These unique secondary metabolites can be further developed as novel drugs for human biological systems. During a 2013 collection trip, an Antarctic coral, Gersemia sp, (NBP13-37), was obtained for study. Through methods of extraction, isolation, purification and elucidation, potentially bioactive compounds within this Antarctic coral have been isolated. Samples from NBP13-37 were freeze-dried before being subjected to multiple rounds of Soxhlet extraction and liquid-liquid partitioning to separate terpenoid compounds. Further purification and analysis via Medium Pressure Liquid Chromatography (MPLC) and High Pressure Liquid Chromatography (HPLC) were performed. Nuclear Magnetic Resonance Spectroscopy (NMR) piloted the advancement of this extraction process towards purity. Future isolates will be subjected to assays to evaluate their activity against resistant pathogens in order to assess their potential use in pharmaceuticals.

NP-03 **Aaron T. Hendricksen**[1], **Devin M. Thornton**[1], Alison H. Hughes[1], Bill J. Baker[1]
[1]Department of Chemistry, University of South Florida

Chemical Diversity of Antarctic Nudibranch Austrodoris kerguelenensis and the Extraction and Analysis of their Secondary Metabolites

Hendricksen T. Aaron, Thornton M. Devin, Hughes H. Alison, Baker J. Bill The Nudibranch Austrodoris kerguelenensis is distributed widely around the Antarctic coast and continental shelves. The species produces compounds belonging to a class of known diterpene glyceride esters, implicated as a chemical defense in nudibranchs. The present chemical investigation of secondary metabolites afforded by A. kerguelenensis collected near Palmer Station on the Western Antarctic afforded a suite of 19 such compounds, aptly named palmadorin A-S. The isolation of secondary metabolites was achieved using a series of chromatographic techniques, including Thin Layer Chromatography (TLC), Medium-Pressure and High-Performance Liquid Chromatography (MPLC and HPLC, respectively). -Structure elucidation and determination of stereochemistry were performed using a combination of one- and two-dimensional Nuclear Magnetic Resonance (NMR) spectroscopy and wet chemical analytical methods. Separation techniques of Thin Layer and

NP-04 **Dakota Becker-Greene**[1], Anne-Claire Limon[1], Bill Baker[1,2]
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[2]Florida Center for Drug Discovery & Innovation

Isolation of Natural Products from an Antarctic Coral Species for Application to Drug Discovery

Drug over-usage produces resistance of infectious agents, and promotes the spread of disease. The original drug is progressively rendered ineffective, requiring development of a new drug to combat the more resistant strain of the disease. In extreme environments, like the Antarctic, coral species have molecular and physical adaptations, such as the production of secondary metabolites, that allow for optimal function. This research focuses on the extraction, isolation, purification, and identification of compounds from an Antarctic marine coral, NBP13-37. The primary goal is to isolate novel bioactive compounds for drug discovery purposes. Coral samples collected during diving trips in Antarctica were freeze-dried, then processed through Soxhlet extraction, liquid-liquid partition, and multiple chromatographic techniques. The progression of these samples towards purity was guided by NMR spectroscopy. Upon elucidation, compound bioassays will be performed to assess bioactivity towards resistant infectious diseases, which could be a source of compounds for drug discovery.

NP-05 **Sun Fai Lau**[1], Allison H. Hughes[1], Bill J. Baker[1]
[1]Department of Chemistry & Center for Drug Discovery and Innovation, University of South Florida

Natural Product Extraction of Antarctic Nudibranch, Austrodoris kerguelenensis

Nudibranchs are soft-bodied, marine molluscs that inhabit seas worldwide. These organisms produce defensive secondary metabolites which could have application in drug discovery efforts. A 2007 bulk extract from nudibranchs has been partitioned with hexane and methanol:water solvents to remove lipids and sugars. Chromatographic techniques will be utilized to purify compounds using NMR-guided isolation. High performance liquid chromatography is a routine instrumental technique used to separate the different compounds in the sample. General structures of secondary metabolites include alkaloids, phenylpropanoids, polyketides and terpenoids. Structure elucidation will be achieved using 1D and 2D NMR experiments and mass spectrometry. Pure compounds will be tested for anti-cancer and anti-parasitic activity within a range of diseases including various cancers, malaria, and leishmaniasis.

NP-06 **Cynthia Grim**[1], Andrew Shilling[1], Bill Baker[1]
[1]Department of Chemistry, University of South Florida

Isolation of Bromotyrosines from Order Verongida

Marine invertebrates produce astounding variety in their natural products. Sponges from Verongida are in particular known for producing a class of secondary metabolites called bromotyrosines. Bromotyrosines contain fragments that resemble their namesake, tyrosine, but which also are brominated and oftentimes substituted with additional rings or functional groups. Chemical extraction of Aiolochroia crassa and subsequent study by HPLC, NMR, and MS led to the isolation of multiple pure compounds, one of which has been identified as fistularin-3. Additional screening will be done to investigate the bioactivity of any compounds found.

OR-01 James W. Leahy[1], **David Herrera-Perez**[1], **Aaron Astalos**[1]
[1]Department of Chemistry, University of South Florida

Treating Malaria: Synthesis of an Anti-Plasmodium Analog of Aurachin D

Malaria is a dangerous disease that is found in the tropical and subtropical areas of the world that is spread by the female of the Anopheles species of mosquitoes. The malaria parasite, from the genus Plasmodium, has two different growth cycles. In a human host, the parasite multiplies and destroys the red blood cells it inhabits. Based on previous research, it was discovered that Aurachin D, a natural product made by myxobacterium Stigmatella aurantiaca was active in inhibition of the malaria causing parasites. The purpose of this research is to develop an analog of Aurachin by performing a synthesis of the compound 3-isopentyl-2-methylquinolin-4(1H)-one and performing a series of lead optimization studies to measure the greatest activity against the Plasmodium parasite.

OR-02 **Shreya Patel**[1], Ron Swonger[1], Andrea Lemus[1], James Leahy[1]
[1]Department of Chemistry, University of South Florida

Alzheimer's Treatment Through the Synthesis of Rhodanine Compounds to Enhance Tau Degradation Alzheimer's Treatment Through the Synthesis of Rhoda

Alzheimer's disease (AD) is a type of dementia that causes problems with memory and behavior. Its symptoms slowly develop and worsen over time to the point that performing daily tasks becomes difficult for the patient. Evidence shows that the causes of AD are beta-amyloid plaques and tau tangles. These plaques and tangles block nerve cell communication. Currently, there are treatments that slow its symptoms, but no cure. Research is being performed all over the world to create new treatments for AD to delay progression or completely prevent it. One possible target for treatment is the Heat Shock Protein 70 (Hsp70) family. Hsp70 is a set of molecular chaperones that bind to misfolded proteins to send to lysosomes. In collaboration with researchers in the Byrd Alzheimer's Institute, we have been working to create new set of rhodanine compounds through organic synthetic pathways that use Hsp70 to improve the tau degradation.

OR-04 **Anthony Kanowitz**[1], Linda Barbeto[1], James Leahy[1]
[1]Department of Chemistry, University of South Florida

Studies Aimed at the Synthesis of Hsp 90 Inhibitors as Antileishmaniasis Agents

Leishmaniasis is a disease transmitted by sandflies carrying the protozoan Leishmania. Leishmaniasis is responsible for twenty- to fifty-thousand deaths a year; therefore, it is imperative that low cost and low toxic drugs are discovered. The chaperone protein Hsp 90, when inhibited, can disrupt the life-cycle of Leishmania. In 2012 the Kyle group identified an initial lead through an axenic amastigote assay; this initial lead was a derivative of tetrahydroindazole. Inactivity of the methyl groups after their removal lead us to investigate different analogs and compare activity. Using novel quinazoline to optimize the synthesis, and to allow for easier analog manipulation, lead us to many different analogs to test their IC50s. The initial novel, quinazoline, will be the basis for analog testing and had an IC50 of 650 nM. A synthesis of many different analogs like a Carbon-modified tetrahydroindazole core was done, among others, and results showed increased IC50s.

OR-05 **Bernard Dankyi**[1], **Christian Yang**[1], Ankush Kanwar[1], James W. Leahy[1]
[1]Department of Chemistry, University of South Florida

Synthesis of Anti-malarial Agents

Malaria is a mosquito-borne disease that is caused by protozoan parasites of the Plasmodium genus. Currently, it is the fourth leading cause of death in the world, also being very prevalent in countries that are less developed. During the malaria life cycle, two hosts are included, which would be the mosquito and the mammal. The mature sexual stage of the parasite, also known as the gametocytes, are only found in the infected mammalian hosts. Gametogenesis and the formation of diploid zygotes actually occur in the gut lumen of infected mosquitos. A tryptophan metabolite, Xanthurenic acid (XA), is also found within the gut of the mosquito, which has been shown to be the trigger that induces gametogenesis. The goal of preventing the transmission of malaria and determination of the biological mechanism that is responsible for this chemical signaling pathway using XA as well as other.

OR-06 **Ousman Jallow**[1], **Arianna Rashedi**[1], Melissa Chin[1], Benjamin Eduful[1], David Khan[2], James Leahy[1]
[1]Department of Chemistry, University of South Florida
[2]Department of Molecular Medicine, University of South Florida

Synthesis of Quinazoline Scaffold for the Treatment of Alzheimer's Disease.

Alzheimer's disease (AD) is the most widespread neurodegenerative disorder and the leading cause of dementia affecting more than 44 million people worldwide. Two highly toxic proteins, -amyloids and tau, have been associated with the progression of AD. We have identified a protein known as Slingshot (SSH1) known to contribute to both -amyloids and tau formation via a complex mechanism. Our job as chemists is to block the pathway by synthesizing compounds that are able to do so. Hence, our research focuses on the synthesis of compounds that can inhibit SSH1. We conducted virtual screening of several compounds by docking them into the catalytic pocket of SSH1 and identified a compound of the type: thiazolyl-dihydropyridine-carboxylic acid, capable of inhibiting SSH1. Through organic synthetic strategies we have been pursuing a lead optimization campaign based on the initial hit. A number of compounds have been synthesized and tested for activity against SSH1.

OR-07 **Jeffrey Jacobson**[1], Zachary Shultz[1], James Leahy[1]
[1]Department of Chemistry, University of South Florida

Synthesis of Possible E.S.K.A.P.E. Pathogen Medication

The World Health Organization has deemed antimicrobial resistance as one of the three greatest threats to mankind in the 21st century. The most common group of organisms contributing to this hazard are the E.S.K.A.P.E. pathogens. Research done at the Torrey Pines Institute for Molecular Studies proved the ability to synthesize a new group of molecules that have biological activity against these microbes, which includes the molecule of interest in this work. The synthesis used a novel approach, "Tea Bag" methodology, in which molecules are attached to solid support resin contained in a sealed mesh bag. Although this method was extremely efficient in the synthesis of millions of molecules, it was not a practical way to synthesize large quantities of these molecules. The synthetic route in this work will allow for greater quantities of the molecule in question to be produced and tested against these pathogens.

OR-08 **Emmanuel Cruz**[1]
[1]Department of Chemistry, University of South Florida

Novel Synthesis of Cannabinoids with Emphasis in Prospective Therapeutic Effects

The human cannabinoid receptor one (CB1) is not fully understood in its connections to disease, particularly Alzhemier's, cancer, and the infection of Naegleria Fowleri. To test the interactions of the human CB1 receptor with cannabinoids, the full stereoselective synthesis of tetrahydrocannabinol delta 9 (THCΔ9), cannabidiol (CBD), and select analogs of each are developed to probe and test for beneficial properties on select models. The synthesis can occur through a variety of newly introduced mechanisms. The analogs derived are strategically manipulated to determine cannabinoid interaction with the blood-brain-barrier (BBB), CB1 receptor, and metabolites within the cellular matrix. Cannabinoids have a range of antimicrobial, anti-oncogenic, and analgesic properties, which deems their exploration valuable. Due to the permeability of cannabinoids to the BBB, speculations on fluorescence-tagging, molecular-probing, radiolabeling, and other medicinal technologies are discussed.

OR-09 **Grant Lawrence**[1], Zachary Shultz[1], James Leahy[2]
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Enantioselective Total Synthesis of Cannabidiol – Facile Route to Analog Development

Cannabidiol (CBD) is the non-psychoactive sibling compound to Δ9-tetrahydrocannabinol (THC) and shows similar viability as a widespread therapeutic. Unique properties of cannabinoids show potential applications as a neuroprotectant against neurodegenerative and neuropathic diseases, as well as an anti-inflammatory, pain reducer, etc. Lack of psychoactivity also increases viability to be an approved potential drug versus THC. An enantioselective synthesis for the core cannabinoid structure has been developed and modified to give a route for potential analog development of CBD.

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Synthesis and Characterization of Heterocyclic Ferrocenyl Chalcones and their Potential Biological Applications

The study of bio-organometallics has become of interest and although results have been varied, in numerous reported cases the substitution of one of the phenyl groups of a chalcone by a ferrocene has enhanced the bioactivity of potential molecules. The role of ferrocene is a topic of broad research discussion, but its ability is highlighted due to its physical and chemical properties such as lipophilicity, size, and the capability to undergo reversible oxidation-reduction. Literature shows that ferrocenyl chalcones exhibit a wide array of biological activity as antimalarial, antitumor, and antioxidant agents among others. Therefore, products bearing bromothiophene, pyrrole, and pyrazole substituents have been synthesized by solvent-free base catalyzed Claisen-Schmidt reaction with moderate to good yields. Electrochemical analysis shows the chemically reversible redox abilities of these compounds. In-vitro drug assay for Plasmodium berghei resulted in non-efficient inhibition at a nano molar scale for the synthesized compounds.

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The Synthesis and Characterization of avant-garde Supramolecular pseudo-telechelic polyimides

2-ureido-4[1H]-pyrimidinone, UPy, is a monomer unit that has propitious properties such high association constants, adaptability and ease of purification. It exhibits thermo-reversible behavior; noncovalent bonds respond to stimuli. Structures containing UPy are precursors in supramolecular polymers with self-healing properties. The noncovalent interaction of interest in UPy is hydrogen bonding. It creates four hydrogen bonds, forming a monomer network. This enables chain extension, strengthens the backbone, causes a high degree of polymerization and increases crosslinking. Here, a series of aliphatic polyimides were end capped with UPy to introduce H-bonding sites into the backbone. Furthermore, the addition of UPy units will yield high performance polyimides with hydrolytic stability, wear resistance and adhesive strength. These materials are suitable for microelectronic and aerospace applications. UPy was synthesized in a one-step reaction with Hexamethylene diisocyanate and 2-amino-6-methylpyrimidin-4-ol. Different stoichiometric ratios of UPy were added to determine how addition of H-bonds affected thermal and mechanical properties.

About the Cover

The crystal structure shown on the cover is that of diaporthalasin, a cytochalasin derivative with known anti-bacterial activity. Kamthong et al.[1] isolated the pentacyclic lactam from an endophytic fungus living symbiotically within a sponge collected at Pak Meng beach, Thailand. The *Diaporthacaea* sp. produces a suite of anti-bacterial compounds but has not yet been shown to have anti-fungal activity. The Baker lab focuses on the isolation of small molecules from the marine environment to identify new scaffolds with bioactivity against the ESKAPE bacterial pathogens, neglected tropical disease, and a plethora of other diseases and infections in need of new treatments.

1. Khamthong N., Rukachaisirikul V., Phongpaichit P. S., Sakayaroj J. (2014) An antibacterial cytochalasin derivative from the marine-derived fungus *Diaporthacaea* sp. PSU-SP2/4, *Phytochemistry Letters* **10:5-9**.