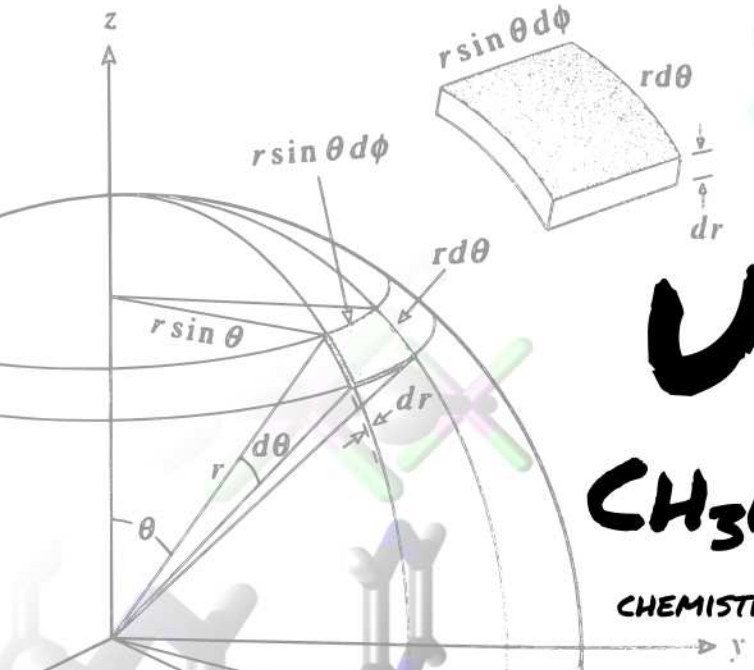
11TH Raymond N. Castle Student Research Conference

April 20, 2013



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11th Raymond N. Castle Student Research Conference

April 20, 2013

University of South Florida

4202 E. Fowler Ave

Tampa, FL 33620

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Proceedings Table of Contents

Welcome from the Castle Conference Committee

Dear Colleagues and Friends,

Welcome to the 11th 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, Sir Fraser Stoddart. 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 Sir Stoddart will be giving an interdisciplinary presentation entitled *Mingling Art with Science*.

Lastly, we would like to thank all that chose to volunteer their time and efforts, particularly the judges, and Dr. Patricia Muisener and Dr. Edward Turos 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 the Tampa Bay Local Section of the American Chemical Society, 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 11th Raymond N. Castle Student Research Conference.

Sincerely,

The Castle Conference Committee

11th Raymond N. Castle Student Research Conference Committee

Committee Members:

Danielle Demers (Co-Chair)
Joseph Gill (Co-Chair)
Christian Cioce
Michael Doligalski
Yaqiong (Rosemary) Li
Jordany Maignan
Hasnaa Mouttaki
Ranjani Muralidharan
Siqi Sun
Christie Tang
Jingran Tao
Brant Tudor
Justin White
Christi Whittington
Kia Williams

Special Thanks To:

Faculty Advisors:

Dr. Patricia Muisener
Dr. Edward Turos

Office Staff:

Cheryl Graham
Linda Lowe
Kimberly Read

Building and Parking Map

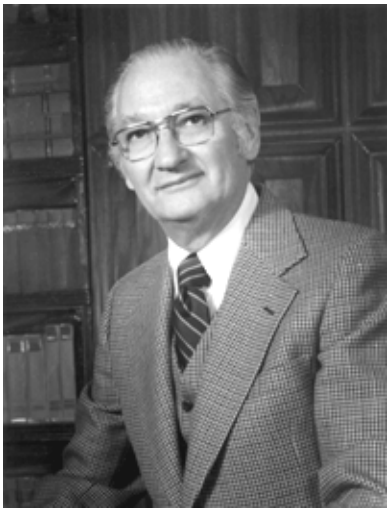
Schedule of Events

Saturday, April 20, 2013

7:45 AM	-	8:25 AM	**Welcome Session** - *Registration and Breakfast*	BSF Lobby
8:25 AM	-	8:30 AM	**Castle Conference Introduction**	BSF 100
8:30 AM	-	10:40 AM	**Morning Talk Session I** *Graduate Student Presentations*	BSF 100
10:40 AM	-	10:50 AM	**Break**	
10:50 AM	-	12:05 PM	**Plenary Speaker - Sir Fraser Stoddart** *Mingling Art with Science*	BSF 100
12:05 PM			**Lunch** *Sponsored by the Tampa Bay Local Section of ACS*	BSF Lobby
1:00 PM	-	3:00 PM	**Poster Session** *Graduate and Undergraduate Presentations*	CHE 1st Floor Classrooms
3:00 PM	-	3:10 PM	**Break**	
3:10 PM	-	5:35 PM	**Afternoon Talk Session II** *Graduate Student Presentations*	BSF 100
5:35 PM	-	5:45 PM	**Break**	
5:45 PM	-	6:00 PM	**Awards Ceremony**	BSF 100

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.

Sir Fraser Stoddart

Plenary Speaker

The academic career of **Fraser Stoddart**, who was born in the capital of Scotland on Victoria Day in 1942, can be traced through thick and thin from the Athens of the North to the Windy City beside Lake Michigan with interludes on the edge of the Canadian Shield beside Lake Ontario, in the Socialist Republic of South Yorkshire, on the Plains of Cheshire beside the Wirral, in the Midlands in the Heartland of Albion, and in the City of Angels alongside the Peaceful Sea. He was raised, an only child, on a mixed-arable farm a dozen miles south of Edinburgh. His formal education began with his attending the local village school in Carrington, Midlothian when he was four. A rigorous introduction to the three Rs – namely, reading, writing and arithmetic – made it relatively easy for him to make the transition to Melville College, a high school in the middle of Edinburgh. He went to Edinburgh University in 1960 and graduated with a BSc degree in 1964. During his time as an postgraduate student in the Department of Chemistry he cut his teeth in research investigating the nature of plant gums of the *Acacia* genus within the School of Carbohydrate Chemistry under Professor Sir Edmund Hirst.

In March 1967, Stoddart took his leave of the Chemistry Department at Edinburgh with a PhD degree to spend the next three years as a National Research Council of Canada Postdoctoral Fellow at Queen's University with Professor J. K. N. Jones. No sooner had he arrived in Kingston, Ontario than a communication appeared in the *Journal of the American Chemical Society* by Charles Pedersen describing the synthesis of dibenzo[18]crown-6 in excellent yield as a consequence of the templating action of potassium ions. This seminal event marked the beginning of Fraser's fascination with chemistry beyond the molecule, which, combined with his interest in templation, has led to the template-directed synthesis, based on molecular recognition and self-assembly processes, of a wide range of mechanically interlocked molecules (e.g., catenanes and rotaxanes), bistable variants of which have found their way into molecular electronic devices and drug delivery systems.

Fraser met Norma Scholan (BSc chemist/PhD biochemist) in 1966 while he was a postgraduate student and they started their married lives in Canada in 1968. In 1970, they returned to the United Kingdom so that Fraser could take up an Imperial Chemical Industries (ICI) Fellowship at Sheffield University where he worked briefly with Professor W. D. Ollis before being appointed as a Lecturer in Chemistry. After spending a three-year sabbatical (1978–1981) at the ICI Corporate Laboratory in Runcorn he returned to Sheffield where he was promoted to a Readership in Chemistry. It was during his time at ICI that Stoddart developed his long-standing interest in bipyridinium units (constituents of the ICI herbicides Diquat and Paraquat) as redox-addressable building blocks for incorporation into bistable catenanes and rotaxanes. In 2013, Fraser expects to publish his 1000th paper: he has trained >350 graduate and postdoctoral students of which >80 have subsequently embarked on successful independent academic careers.

In 1990, he took up the Chair of Organic Chemistry at Birmingham University where he was Head of the School of Chemistry (1993–97) before moving to the University of California, Los Angeles (UCLA) as the Saul Winstein Professor of Chemistry in 1997. In 2002, Fraser became the Director of the California NanoSystems Institute (CNSI) and assumed the Fred Kavli Chair of NanoSystems Sciences. He joined the faculty at Northwestern University in 2008 as a Board of Trustees Professor of Chemistry and Director of the Center for the Chemistry of Integrated Systems (CCIS).

Stoddart was appointed by Her Majesty Queen Elizabeth II as a Knight Bachelor in her 2007 New Year's Honours List for services to chemistry and molecular nanotechnology. In this same year, he won the King Faisal International Prize in Science. In 2010, he was the recipient of a Royal Medal, granted by her Majesty Queen Elizabeth II and presented by Prince Philip, Duke of Edinburgh.

Fraser's and Norma's daughters, Fiona and Alison, were born in 1973 and 1976, respectively: they are both PhD chemists! In 2004, Norma succumbed to a 12-year battle with breast cancer. Fiona lives with her Australian husband and their two children in Belmont, MA while Alison, who is a Senior Editor with *Nature Materials*, lives in Waterbeach, UK with her Chinese husband and their three sons. To learn more about the life and works of **Fraser Stoddart**, read about "Big and Little Meccano" in *Tetrahedron* **2008**, *64*, 8231–8263.

Dr. Dean F. 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.

Dr. Solomon T. Weldegirma

Special Thanks

Dr. Solomon T. Weldegirma received his B.S., with Honors, from Asmara University, Eritrea in 1989. He focused his graduate studies on extraction of active compounds from natural products through organic chemistry, earning his M.S. in 1995 from Addis Ababa University, Ethiopia. During this time, he worked in the Food Industry heading up Research, Quality Control, and Development Departments, with companies that shared his passion for the importance of natural products. Under the guidance of Professors Frode Rise and Lise-Lotte Gundersen, Dr. Weldegirma received his Ph.D. in Synthetic Organic Chemistry from the University of Oslo, Norway, in 2004, where he studied indolizine compounds as possible inhibitors for a variety of targets. In 2005, he took a Post- doctoral fellowship under Dr. Bill Baker here at the University of South Florida, studying degradation of natural products.

Since 2006, Dr. Weldegirma has shared his love of organic chemistry with students at the University of South Florida as the Organic Chemistry Laboratory Coordinator and Instructor of Organic Chemistry. As Coordinator, Dr. Weldegirma authored the experimental manuals, Experimental Organic Chemistry Laboratory Manual: CHM 2210L and CHM 2211L, to further the laboratory curriculum. Proceeds from the sale of these manuals were donated to the Castle Student Research Conference. We would like to thank him for his generosity in support of the Castle Conference.

Judges

American Chemical Society Tampa Bay Local Section

Eric Ballard, Ph.D.
Sid White, Ph.D.

Florida Southern College

Deborah Lee Bromfield, Ph.D.

James A. Haley Veteran's Hospital

Andrea N. McCray, Ph.D.

St. Leo University

Darin Bell, Ph.D.
Jess Jones, Ph.D.

University of Tampa

Eric Werner, Ph.D.
Michelle Leslie, Ph.D.

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Laura Anderson, Ph.D.
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Laurent Calcul, Ph.D.
Ryan Cormier, Ph.D.
Xin Cui, Ph.D.
Kimberly Fields, Ph.D.
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Ioannis Gelis, Ph.D.
Wayne Guida, Ph.D.
Julie Harmon, Ph.D.
John Koomen, Ph.D.
Mohanraja Kumar, Ph.D.
Randy Larsen, Ph.D.
James Leahy, Ph.D.
Xiao (Sheryl) Li, Ph.D.
Vicky Lykourinou, Ph.D.
Shengqian Ma, Ph.D.
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Robert Potter, Ph.D.
Brian Space, Ph.D.
Edward Turos, Ph.D.
Arjan van der Vaart, Ph.D.
Solomon Weldegirma, Ph.D.
Lukasz Wojtas, Ph.D.
Juanjuan Yin, Ph.D.
Michael Zaworotko, Ph.D.

Thank you to all of our judges for donating your time today to promote research and collaboration!

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Graduate Talks Morning Session I (BSF 100)

Session Chair: Christi Whittington

8:30- 8:45 AM **Joseph B. Gill**

Ligand Effect on Stereoselectivity of Asymmetric Cyclopropanation by Co(II)-Based Metalloradical Catalysis

8:45- 9:00 AM **Youngran Ji**

Metal Organic Materials (MOMs) for Enantioselective Heterogeneous Asymmetric Catalysis Promoted by Chiral Phosphoric Acid

9:00- 9:15 AM **Jingran Tao**

Asymmetric Intermolecular Olefin Aziridinations with Azides via Co(II)-Based Metalloradical Catalysis (MRC)

9:15- 9:30 AM **Kristen A. Jeffries**

Long-Chain N-Acylglycines: A Study of Their Biosynthetic Pathways

9:30-9:40 AM **Break**

9:40-9:55 AM **Christopher Lee Lizardi**

Modular and Divergent Synthesis of Novel Chiral Porphyrin Ligands

9:55-10:10 AM **Michael Veri**

Isolation and Identification of Antibiotics from Bacterial Sources via Dead-live Co-culture

10:10- 10:25 AM **Adrián Villalta-Cerdas**

Use of Problem Solving to Elicit Self-explaining in General Chemistry

10:25-10:40 AM **Daniel R. Dempsey**

Characterization of Recombinant Arylalkylamine N-acetyltransferase from Drosophila Melanogaster

Graduate Talks Afternoon Session II (BSF 100)

Session Chair: Kia Williams

3:10- 3:25 PM **Geoffrey Gray**

Free energy simulation studies of ribonucleotide substituted DNA

3:25- 3:40 PM **Ning Ma**

Unexpected DNA intercalation of a doubly linked Cy3 dye

3:40- 3:55 PM **Stephen Burd**

Pore size control for highly selective carbon capture

3:55- 4:10 PM **Andrew R. Powers**

Recent advancements to the Inorganic Click (iClick) reaction methodology leading to the synthesis of a small library of trinuclear, hetero-metallic Pt^{II}/Au^{I}_2 complexes

4:10- 4:25 PM **Tony Pham**

Theoretical Investigations of CO_2 and H_2 Sorption in an Interpenetrated Square-Pillared Metal-Organic Material

4:25- 4:35 PM **Break**

4:35- 4:50 PM **Katherine Forrest**

Computational Insights into Tuning Adsorption Mechanisms in Metal Organic Materials with rht Topology

4:50- 5:05 PM **Christian Tang**

Inhibition studies against oxidation stress caused by Cu-β-amyloid (Aβ) complexes of Alzheimer's Disease

5:05- 5:20 PM **Ranjani Muralidharan**

Study of formic acid electrooxidation by platinum deposited from haloplatinate complexes on Au by Electrochemical Surface Enhanced Raman Spectroscopy

5:20- 5:35 PM **Sameh Elsaidi**

Pore size control in diamondoid metal organic frameworks to optimize CH_4 and CO_2 sorption performance

The Barbara and Dean F. Martin Poster Session
CHE 103
Session Chair: Christie Tang

Graduate:	GP	All Disciplines
Undergraduate:	AN	Analytical
Undergraduate:	CO	Computational

The Clear Springs Land Poster Session
CHE 101
Session Chair: Hasnaa Mouttaki

Undergraduate:	CE	Chemical Education
	IN	Inorganic
	NP	Natural Products

The Solomon T. Weldegirma Poster Session
CHE 101A
Session Chair: Yaqiong (Rosemary) Li

Undergraduate:	BIO	Biochemistry/Biophysical
	OR	Organic

Graduate Talks

GT-01 **Joseph B. Gill**[1], X. Peter Zhang[1]
[1]Department of Chemistry, University of South Florida

Ligand Effect on Stereoselectivity of Asymmetric Cyclopropanation by Co(II)-Based Metalloradical Catalysis

Cyclopropanes, the smallest type of carbocycles, have attracted a large amount of attention in the past decade due to both their unique reactivities and structural properties. Significant progress has been made on the asymmetric construction of the cyclopropane structure from readily available olefins by transition metal-catalyzed carbene transfer reactions. The majority of existing catalytic systems have focused on the formation of the more thermodynamically stable trans-cyclopropanes. Few catalysts have been developed for the formation of the less stable cis-cyclopropanes. To this end, we have been in the process of developing Co(II)-based metalloradical systems for asymmetric cyclopropanation enabling synthesis of either cis- or trans-cyclopropanes while controlling enantioselectivity. We have shown that the steric and electronic environments of porphyrin ligands can be fine-tuned to effect the outcome of Co(II)-catalyzed metalloradical cyclopropanation, including both diastereoselectivity and enantioselectivity.

GT-02 **Youngran Ji**[1], Zhuxiu Zhang[1], Michael J Zaworotko[1], Jon C. Antilla[1]
[1]Department of Chemistry, University of South Florida

Metal Organic Materials (MOMs) for Enantioselective Heterogeneous Asymmetric Catalysis Promoted by Chiral Phosphoric Acid

Construction of catalytically active chiral MOMs having nanoscopic channels was achieved with well designed homochiral tetra- and octacarboxylate ligands. One of the materials, ocMOM-1, was found to exhibit improved enantioselective organocatalysis (as high as 84% ee) over the parent ligand in the context of transfer hydrogenation of a series of benzoxazines.

GT-03 **Jingran Tao,** Hongjian Lu[1], Joshua Ruppel[1], X. Peter, Zhang[1]
[1]Department of Chemistry, University of South Florida

Asymmetric Intermolecular Olefin Aziridinations with Azides via Co(II)-Based Metalloradical Catalysis (MRC)

Asymmetric olefin aziridination reactions via metalloradical catalysis (MRC) with azides has attracted research interest because of its fundamental and practical importance. The resulting aziridine units are recurrent motifs in biologically important molecules and can serve as versatile precursors in organic synthesis. The [Co(D_2-Por*)] have emerged as a new class of catalysts for asymmetric aziridination. These metalloradical catalysts have been shown to be highly effective for the asymmetric intermolecular aziridination of a broad scope of substrates with different classes of azides with excellent to good enantioselectivity.

GT-04 **Kristen A. Jeffries**[1], Daniel R. Dempsey[1], Anita Behari[1], Ryan Anderson[1], Gabrielle Garbade[1], David J. Merkler[1]
[1]Department of Chemistry, University of South Florida

Long-Chain N-Acylglycines: A Study of Their Biosynthetic Pathways

The fatty acid amides (FAAs) are a broad family of cell signaling lipids with members that include the N-acylamino acids, the N-acyldopamines, the N-acylethanolamines, and the primary fatty acid amides. Long-chain N-acylglycines (NAGs), a subfamily of the N-acylamino acids, have recently been reported in mammalian sources and their biosynthesis is not completely understood. Two proposed pathways for the biosynthesis of the NAGs include a glycine-dependent route and an N-acylethanolamine-dependent route. It has been proposed that the enzyme catalyzing the biosynthesis of NAGs via the glycine-dependent route is a glycine N-acyltransferase. In vivo and in vitro experiments provide insight into the biosynthesis of NAGs in two model systems, mouse neuroblastoma cells and Drosophila melanogaster. Identification and quantification of FAAs by LC-QTOF-MS, feeding studies with heavy labeled metabolites, and activity screening with recombinant enzymes aid in the determination of the enzyme responsible for the synthesis of long-chain NAGs *in vivo.*

GT-05 **Christopher Lee Lizardi**[1], Li-Mei Jin[1], X. Peter Zhang[1]
[1]Department of Chemistry, University of South Florida

Modular and Divergent Synthesis of Novel Chiral Porphyrin Ligands

meso-Functionalized porphyrins have promising applications in the fields of medicine (photodynamic therapy), materials (dye-sensitized solar cells), and catalysis (asymmetric organic synthesis). Accordingly, it would be highly desirable to develop new synthetic tools for modifying the meso-positions of the porphyrin ring with different functionalities. A new synthetic route has been established for the design and synthesis of novel D2-symmetric chiral porphyrins that have potential as supporting ligands in metal-based catalysis. A series of chiral porphyrin ligands were synthesized from new generation chiral bromoporphyrin synthons with bromo substituents on the meso-positions and pre-installed chiral amide moieties. Through the use of well-known cross-coupling methodologies, including Buchwald, Suzuki, Sonogashira and others, a wide array of chiral porphyrin ligands have been accessed, which were unattainable through conventional methods. The goal of this project is to prepare the corresponding Co(II) complexes of these chiral porphyrins, and explore their applications as chiral catalysts for asymmetric atom/group transfer

GT-06 **Michael Veri**[1], Shivangi Patel[1], Stephanny Reyes[1], Fiona Kearns[1], Bill Baker[1,2]
[1]Department of Chemistry, University of South Florida; [2]Center for Drug Discovery & Innovation, University of South Florida

Isolation and Identification of Antibiotics from Bacterial Sources via Dead-live Co-culture

Natural product isolation from microbial sources has been a rich source for years resulting in many compounds of clinical significance. The "golden age" of antibiotics resulted in diminished antimicrobial research, yet the surge in resistant microbes has resulted in renewed interest in this field. Novel methodology is necessary to elicit chemical responses from existing microbial stores. This project focuses on the natural competition that arises between organisms. By growing existing stores in the presence of metabolites from common human pathogens, novel antibiotics will be produced. These can then be isolated, identified and taken to a clinical setting with further research.

GT-07 **Adrián Villalta-Cerdas**[1], Santiago Sandi-Urena[1]
[1]Department of Chemistry, University of South Florida

Use of Problem Solving to Elicit Self-explaining in General Chemistry

The prevalent trend in chemistry instruction relies on what Lemke (1990) described as the classroom game which posits students in a passive role. In this model, the instructor does all the explaining, and learning is trivialized to knowing the correct answers and being able to produce them when prompted. Educational psychology research has shown that activities that elicit self-explaining improve learning and enhance learning in the sciences. In science self-explaining refers to the student's generation of inferences about how and why actual/hypothetical phenomena take place. Research findings suggest that self-explaining influences many aspects of cognition, including acquisition of problem-solving skills, and conceptual understanding. Although, there is empirical evidence for the link between self-explaining and learning, there is a need for research conducted in the context of real college science learning environments. This study intends to fill that void by studying the effect of different self-explaining tasks on learning chemistry concepts

GT-08 **Daniel R. Dempsey**[1], Kristen A. Jeffries[1], Anne-Marie Carpenter[1], Jason D. Bond[1], David J. Merkler[1]
[1]Department of Chemistry, University of South Florida

Characterization of Recombinant Arylalkylamine N-acetyltransferase from Drosophila Melanogaster

Fatty acid amides are an emerging class of cell signaling molecules that are composed of N-acyl arylalkylamines, N-acyl amino acids, N-acyl ethanolamines, and primary fatty acid amides. A direct pathway for the biosynthesis of fatty acid amides has remain elusive, however; one proposed pathway is the acylation of an amino donor by an N-acyltransferase enzyme. Arylalkylamine N-acetyltransferase (AANAT) catalyzes the formation of N-acetyl arylalkylamines from the corresponding acetyl-CoA and arylalkylamine which is the penultimate step in the biosynthesis of melatonin. Our hypothesis is that AANAT or an AANAT hetero-functional homolog will be responsible for catalysis of both the short and long chain N-acyl arylalkylamines. Eight putative Drosophila melanogaster AANAT enzymes have been identified and are hypothesized to have an important role in the biosynthesis of the N-acyl arylalkylamines. Characterization of these enzymes is critical in elucidating how these important signaling molecules are biosynthesized.

GT-09 **Geoffrey Gray**[1], Arjan van der Vaart[1]
[1]Department of Chemistry, University of South Florida

Free energy simulation studies of ribonucleotide substituted DNA

The incorporation of ribonucleotides into DNA during replication results in structural destabilization and a higher susceptibility to cleavage. While X-ray studies suggest a transition from B to A DNA upon any amount of ribonucleotide incorporation, NMR studies suggest a more complex behavior that also depends on the amount of substitution. To assess the effect of ribonucleotide substitution on the helicity of DNA, we performed free energy simulations of the B to A transition for DNA with various degrees of ribonucleotide incorporation. Results of these simulations and possible biological implications will be discussed.

GT-10 **Ning Ma**[1], Arjan van der Vaart[1]
[1]Department of Chemistry, University of South Florida

Unexpected DNA intercalation of a doubly linked Cy3 dye

To reduce the uncertainty in extracting molecular distances from FRET experiments on DNA, our collaborators developed a new linking strategy thought to rigidify the Cy3 dye in an orientation parallel to the DNA axis. In order to verify the assumptions of this strategy and confirm if rigidification is really achieved, we performed simulations of the Cy3-DNA complex. Starting from the hypothesized parallel orientation, in four out of five unbiased molecular dynamics simulations, the dye rotated 90° and intercalated into the DNA. Pathways and barriers for the process were subsequently obtained from atomistic free energy simulations. Our simulations indicate significant problems with the new linking strategy and suggest the need for two state models to interpret FRET measurements on this system.

GT-11 **Stephen Burd**[1], Michael Zaworotko[1]
[1]Department of Chemistry, University of South Florida

Pore size control for highly selective carbon capture

Metal-Organic Materials (MOMs) or Porous Coordination Polymers (PCPs) have gained vast attention over the past decade in terms of design and application. PCPs including square grids pillared with anionic linkers exhibiting pcu topology are highly amenable to crystal engineering strategies and thus serve as platforms for systematic investigation of gas sorption. Their modularity gives exquisite control over pore size and functionality, and we have developed this platform in which we have observed highly selective carbon capture in narrow pore pillared grids based upon saturated metal centers (SMCs). Structural and separation properties will be addressed.

GT-12 **Andrew R. Powers**[1]; Trevor J. Del Castillo[1], Xi Yang[1], Khalil A. Abboud[1], Adam S. Veige[1]
[1]Department of Chemistry, University of Florida

Recent advancements to the Inorganic Click (iClick) reaction methodology leading to the synthesis of a small library of trinuclear, hetero-metallic Pt^{II}/Au^{I}_2 complexes.

A prototypical example of Click chemistry (high-yield, thermodynamically driven reactions which utilize simple molecular building blocks to create more complex species through the formation of new heteroatom bonds) is based on the Huisgen 1,3-dipolar cycloaddition of azides to alkynes, in which the reaction is very effectively catalyzed by copper. While this reaction motif is quite prolific, analogous cycloaddition reactions utilizing azides or acetylides originating within the coordination sphere of a metal are much less prevalent. This talk will focus on the application of an inorganic version of this click reaction (iClick), and will highlight the advancements towards the creation of new multimetallic systems. In particular, the synthesis and characterization of a series of hetero-metallic Pt^{II}/Au^{I}_2 complexes will be discussed.

GT-13 **Tony Pham**[1], Katherine A. Forrest[1], Patrick Nugent[1], Ashley Mullen[1], Michael J. Zaworotko[1], Brian Space[1]
[1]Department of Chemistry, University of South Florida

Theoretical Investigations of CO_2 and H_2 Sorption in an Interpenetrated Square-Pillared Metal-Organic Material

Simulations of CO_2 and H_2 sorption were performed in [$Cu(dpa)_2SiF_6$-i], a metal-organic material consisting of an interpenetrated square grid of Cu^{2+} ions coordinated to 4\',4\'\'-dipyridylacetylene rings and pillars of SiF_6^{2-} ions. The simulated CO_2 and H_2 sorption isotherms and calculated isosteric heats of adsorption, Qst, were in excellent agreement with the corresponding experimental measurements. It was observed that the Qst for CO_2 increases as a function of uptake. Compared to an empty structure, the presence of a sorbed CO_2 molecule within a channel provides a more energetically favorable site for incoming CO_2 molecules. The modeled structure at CO_2 saturation shows a loading of 8 CO_2 molecules per unit cell. The CO_2 molecules can be seen alternating between a vertical and horizontal alignment within a channel. H_2 saturation corresponds to 10 H_2 molecules per unit cell for the studied structure. Moreover, there were two observed binding sites for hydrogen sorption.

GT-14 **Katherine Forrest**[1], Tony Pham[1], Amy Cairns[1], Mohamed Eddaoudi[1], Michael Zaworotko[1], Brian Space[1]
[1]Department of Chemistry, University of South Florida

Computational Insights into Tuning Adsorption Mechanisms in Metal Organic Materials with rht Topology

Computational examination was undertaken to characterize the alteration of gas adsorption mechanisms in rht metal-organic materials (MOMs), due to inclusion / removal of functional groups. A first principles study of Cu PCN-61 and Cu TPBTM, the latter replacing the former's strait alkyne carbon chain with amide functionality, revealed significant differences in electron density in areas distant from the variant functional groups. Most notably, open metal sites have distinctly shifted charge distributions. Grand Cannonical Monte Carlo gas adsorption simulations revealed that these changes result in dramatic shifts in favored occupation sites inside the MOM. A difference not limited to the expected direct alkyne / amide adsorption. Notably, open metal adsorbed gas molecules in variant structures are found to favor metals in differing environments, resulting in divergent bi-layer adsorption mechanisms.

GT-15 **Christian Tang**[1], William Tay[1], Giordano da Silva[1], Alaa Hashim[1], Li-June Ming[1]
[1]Department of Chemistry, University of South Florida

Inhibition studies against oxidation stress caused by Cu-β-amyloid (Aβ) complexes of Alzheimer's Disease

High level of redox-active metal ions such as Cu^{+2} and Fe^{+3} are observed in Alzheimer's disease (AD) plaques; indicating potential metal-induced reactive oxygen species (ROS) which can contribute to oxidative stress in the brain and cause neuron death. Significant oxidative activity toward catechol oxidation by Cu^{2+}-Aβ was observed. Therefore, by inhibiting the oxidative activities caused by Cu-Aβ complexes may possible lessen oxidative stress in AD. Since catechol oxidation by Cu-Aβ complexes following enzyme-like kinetics, the inhibition efficacies against the oxidation can be monitored. Flavonoids, vitamin B6, curcumin and synthetic triketone compounds were used to study their inhibitions toward oxidation activities. NMR and kinetics studies were used to investigate the structure-activity relationship.

GT-16 **Ranjani Muralidharan**[1], Xiao Li[1]
[1]Department of Chemistry, University of South Florida

Study of formic acid electrooxidation by platinum deposited from haloplatinate complexes on Au by Electrochemical Surface Enhanced Raman Spectroscopy

Platinum modified gold surface has a great potential as anode catalyst in the formic acid fuel cells. By this study, we aim to understand the effect of the deposition solutions employed in the deposition of platinum on gold surface (Pt/Au), towards electrooxidation of formic acid. Electrochemical studies show that Pt/Au surface prepared from chloroplatinate is most active in oxidizing formic acid followed by bromoplatinate and iodoplatinate solutions. Moreover, the type of precursor haloplatinate solution, not only affects the amount of Pt deposited on the Au surface, but also modifies the surface structure of the deposits. Interestingly, real time in situ surface enhanced raman spectroscopy (SERS) with potential control has revealed a novel formate intermediate at 300cm-1 in the electrooxidation process. Thus by electrochemical SERS, we were able to show that the haloplatinate deposition solutions have a dramatic effect on the catalytic activity of Pt/Au surfaces, for formic acid electrooxidation.

GT-17 **Sameh Elsaidi**[1,2], Mona H. Mohamed[1,2], Lukasz Wojtas[1], Michael J. Zaworotko[1]
[1]Department of Chemistry, University of South Florida, [2]Chemistry Department, Alexandria University, Egypt

Pore size control in diamondoid metal organic frameworks to optimize CH_4 and CO_2 sorption performance

We report the study of a family of seven diamondoid (**dia**) metal-organic materials (MOMs) that are sustained by Co(II) cations linked by one of three rigid ligands: 4-(2-(4-pyridyl)ethenyl)benzoate, **1**, 4-(pyridin-4-yl)benzoate, **2** and 4-(pyridin-4-yl)acrylate, **3**. Pore size control in this family was exerted by two approaches: changing the length of the linker ligand from **1**-**3**; using solvent to control the level of interpenetration in nets based upon **1** and **3**. The resulting MOMs, dia-8i-**1**, dia-5i-**3**, dia-7i-**1**, dia-4i-**3-**a, dia-4i-**3**-b, dia-4i-**2** and dia-4i-**1**, exhibit 1D channels with pore limiting diameters (PLDs) of 1.64 Å, 2.90 Å, 5.28Å, 8.57, 8.83Å, 11.86 Å and 18.25Å, respectively. We selected **dia** nets for study for the following reasons: their 1D channels allows study of the impact of pore size in when pore chemistry is similar or identical (in the case of polymorphs); their saturated metal centers (SMCs) eliminate open metal sites from dominating sorbent-solvate interactions and possibly masking the effect of pore size. Our data reveals that smaller pore size leads to stronger interactions as determined by the isosteric heat of adsorption (Q_{st}) and the steepness of the adsorption isotherm in the low pressure region. The porous MOM with the smallest PLD suitable for physisorption, dia-7i-**1**, was thereby found to exhibit the highest Q_{st} for CO_2 and CH_4. Indeed, its gravimetric selectivity for CO_2 over N_2 is 52.1 at 298K and 1atm, its IAST selectivity for a 10:90 CO_2:N_2 mixture is 41 and it exhibits a Q_{st} value for CH_4 of 22.5 kJ/mol. These values are considerably higher than those found in COFs and other MOMs with UMCs. These results therefore further validate the critical role that PLD plays in gas adsorption by porous MOMs.

The Barbara and Dean F. Martin Poster Session Abstracts

Graduate:

GP-01 **Siqi Sun**[1], Xiao Li[1]
[1]Department of Chemistry, University of South Florida

Preparation of Magnetite Fe_3O_4/Ag Nanostructure for Surface Enhanced Raman Spectroscopy

Melatonin plays an important role in Alzheimer's disease as an antioxidant and as a neuroprotector. This study involves developing a novel substrate of Fe_3O_4/Ag magnetic nanostructures which will be employed for melatonin detection by Surface Enhanced Raman Spectroscopy (SERS). Fe_3O_4/Ag nanostructures were synthesized, and their surface morphology and structure were characterized by using transmission electron microscopy, scanning electron microscopy and energy dispersive spectroscopy. Fe_3O_4 nanoparticles with size of 10 nm are coated with silver as shell, and the shell thickness of nanostructures becomes tunable through the adjustment of the ratio between Fe_3O_4 to silver precursor salts. The sensitivity and reproducibility of the nanostructures were tested using Rhodamine 6G and 4- aminothiophenol in SERS. These Fe_3O_4/Ag nanostructures offer the advantage of both extraction and detection of biologically impartment molecules.

GP-02 **Michael Doligalski**[1], Priyesh Jain[1], Rajesh Nair[1], Mohanraja Kumar[1], Lori Hazelhurst[1], Mark L. McLaughlin[1]
[1]Department of Chemistry, University of South Florida

Pharmacokinetic analysis of a novel multiple myeloma therapy, MTI-101, with tandem mass spectrometry

MTI-101 is a novel cyclic peptide with activity against multiple myeloma, a plasma cell cancer in the bone marrow. Pharmacokinetic (PK) analysis is necessary to determine the in vivo half-life for development of this promising therapy. A unique multi reaction monitoring (MRM) transition was established for MTI-101 (749.9→270.2) and an internal peptide standard (769.4→342.0). After a simple extraction of the peptide from 57BL/CalRiij mouse serum, the extracts were chromatographed and quantified with the LC-MS/MS system (Agilent 1260 HPLC and 6460 triple-quadrupole with Jet-Stream Electrospray ionization source). Seven time points ranging from 0 min to 60 min were assessed for peptide concentration. Application of the standard calibration curve and a best fit model indicate that free MTI-101 has a short half-life in vivo. This study establishes a framework for further analysis of various bioconjugated analogs developed to extend the half-life of MTI-101.

GP-03 **Benjamin Van Norman**[1], Dimitra Keramisanou[1], Mai Mohamed[1], Ioannis Gelis[1]
[1]Department of Chemistry, University of South Florida

Assembly mechanism of Cdc37-Kinase complexes in Cancer Signaling

Cdc37 is a gain-of-specificity co-chaperone of Hsp90 specializing in the recruitment of protein kinases to the Hsp90 machinery. Mutated, upregulated or otherwise oncogenic kinases are highly unstable or mal-folded proteins, exhibiting increased affinity and high functional dependence to the Cdc37·Hsp90 complex. As a consequence, cancer cells become "addicted" to Cdc37·Hsp90 that permits oncogenic substrates to escape proteasomal degradation, accumulate in the cell and mediate signaling pathways responsible for promoting the malignant transformation. The exact mechanism by which Cdc37 functions as a gain-of-specificity co-chaperone recognizing Hsp90 substrates remains elusive. Our long term goal is to provide a comprehensive molecular understanding of this decisive step, by unraveling the specificity determinants on both Cdc37 and kinases using Nuclear Magnetic Resonance (NMR) spectroscopy. Ultimately, we anticipate translating the gained knowledge into new strategies for the rational design of drug candidates with pleiotropic effects on multiple signaling pathways involved in cancer.

GP-04 **Yuri Pevzner**[1], Daniel N. Santiago[1], Wesley H. Brooks[1], Wayne Guida[1,2], H. Lee Woodcock[1]
[1]Department of Chemistry, University of South Florida; [2]Drug Discovery Department, H. Lee Moffitt Cancer Center and Research Institute

Development of the CHARMM Interface and Graphics Portal as a Platform for Computer Aided Drug Design

Web-based front end interfaces to scientific applications are important tools that allow researchers to utilize a broad range of software packages with just an internet connection and browser. One such interface, CHARMMing (CHARMM interface and graphics), allows researchers to take advantage of functionality of the powerful and widely used molecular software package CHARMM. CHARMMing incorporates tasks such as molecular structure analysis, energy minimization, molecular dynamics and other techniques commonly used by computational life scientists. We are extending CHARMMing's capabilities to incorporate common drug discovery tasks that include docking, virtual screening and virtual target screening. As part of this undertaking docking and scoring protocols based on the latest CHARMM protein, nucleic acid and small molecule force fields are being developed and evaluated.

GP-05 **Christi L. Whittington**[1], Randy W. Larsen[1], H. Lee Woodcock[1]
[1]Department of Chemistry, University of South Florida

Time Dependent Density Functional Theory on Zn(II)tetrakis(N-methylpyridyl)porphyrin

Metal organic frameworks (MOFs) are a class of rigid and nanoporous solid-state materials, composed of metal carboxylate clusters linked by organic ligands. There are numerous applications suitable for MOFs including biomimetic catalysis. The scaffold of regular, repeating cavities potentially mimics protein pockets and can be useful for encapsulating catalytic molecules in a protein-like matrix with the added benefit of protecting the catalyst from degradation. To this end, we have previously encapsulated the photoactive guest Zn(II)tetrakis(N-methylpyridyl)porphyrin (ZnT4MPyP) into cavities of a MOF formed from Zn(II) benzene-1,3,5-tricarboxylate. It has been shown that the ZnT4MPyP photophysical properties differ in the restricted environment from the porphyrin in solution. In this study, Zn(II)tetrakis(phenyl)porphyrin (ZnTPP) and Zn(II)tetrakis(pyridyl)porphyrin (ZnTPyP) were utilized as model systems to elucidate the electronic effects of porphyrin encapsulation by time-dependent density functional theory (TD-DFT) calculations. Results will be presented on differences in electronic structure of the porphyrins due to encapsulation and in solution.

GP-06 **Jacqueline L. von Salm**[1], Margaret O. Amsler[2], Charles D. Amsler[2], Craig F. Aumack[2], James B. McClintock[2], Ryan M. Young[1], Bill J. Baker[1,3]
[1]Department of Chemistry, University of South Florida; [2]Department of Biology, University of Alabama at Birmingham; [3]Center for Drug Discovery & Innovation, University of South Florida

Chemical Sequestration and Resilience of an Antarctic Amphipod: the First of its Kind

Macroalgae such as *Plocamium cartilagineum* have evolved to produce secondary metabolites as a powerful defense mechanism, of which prominent mesograzers, such as amphipods, take advantage by seeking refuge in the algae. The chemistry produced by *P. cartilagineum* has been well investigated over the past four decades showing that the most prominent natural products produced are polyhalogenated monoterpenes. A particular amphipod species, *Paradexamine fissicauda*, not only inhabits the algae, but also ingests it as a food source. This rare behavior was investigated to show that *P. fissicauda* has utilized the defensive chemistry of *P. cartilagineum* by sequestering the compounds upon ingestion. Analysis of the hydrophobic extracts of *P. cartilagineum* fed amphipods was done via GC/MS QToF. The resulting data shows that compounds prevalent in *P. cartilagineum* are found in the amphipod extracts, making *P. fissicauda* the only known crustacean to sequester defensive chemistry from its diet.

GP-07 **Dan Utic**[1], Chad Dickey[3], Jinwal Umesh[3], Dennis Kyle[4], Tina Mutka[4], Luis Perez-Mena[1], Bill J. Baker[1,2]
[1]Department of Chemistry, University of South Florida; [2]Center for Drug Discovery & Innovation, University of South Florida, [3]Byrd Alzheimer's Institute, [4]College of Public Health, University of South Florida

Novel Compound Search of Endophytic Microbes from Florida Everglades Mangroves.

In our ongoing quest to discovery novel compounds we have collected and isolated several hundred endophytic microbes from mangroves of the Florida Everglades. Mangroves have proven to be a rich repository of diverse microbial populations harboring unique secondary metabolites. In an effort, which will hopefully yield novel drug treatments, microbial extracts were tested for activity against, M.R.S.A., Malaria, the Alzheimer's tao protein, and fungi. Several extracts have shown promise both in activity and in NMR characterization. Our efforts are currently focused on the purification and elucidation of the active compounds.

GP-08 **Aleksandra Karolak**[1], Arjan van der Vaart[1]
[1]Department of Chemistry, University of South Florida

Development of a Novel Coarse-Grained Model for Protein-DNA Binding

We are developing a new coarse-grained model to simulate the complex binding process of transcription factors and other sequence-specific DNA-binding proteins. The binding of these proteins is coupled to protein folding and DNA bending. The protein part of the model is based on an existing Gō-model, using one bead per amino acid. DNA bases are modeled by three beads per base, and DNA deformations are described by the shift, slide, rise, roll, twist and tilt parameters. Interactions between proteins and DNA will partly be modeled by statistical potentials derived from known protein-DNA structures. A progress report on the development of the model is given.

GP-09 **Qigan Cheng**[1], Silke Evdokimov[1], Xue Xu[1], Jennifer Le[1], X. Peter Zhang[1]
[1]Department of Chemistry, University of South Florida

Asymmetric Olefin Cyclopropanation with α-Halodiazoacetates via Co(II)-Based Metalloradical Catalysis: Effective Synthesis of Chiral Cyclopropyl Halide

The cobalt(II) complex of the D2-symmetric chiral porphyrin 3,5-Di^{t}Bu-ChenPhyrin, [Co(P1)], has proven to be an effective catalyst for catalyzing asymmetric olefin cyclopropanation with α-chlorodiazoacetates and α-bromodiazoacetates. The [Co(P1)]-mediated metalloradical cyclopropanation is suitable for a wide range of aromatic and aliphatic olefins with varied steric and electronic properties, providing the corresponding halogenated cyclopropanes in high yields with excellent diastereo- and enantioselectivity.

GP-10 **Fenger Zhou**[1], Courtney DuBoulay[1], Michael Doligalski[1], Wayne Guida[1], Mark L. McLaughlin[1]
[1]Department of Chemistry, University of South Florida

Synthesis of [1,2,4]triazine Nucleus as a New Kinase Inhibitor Template

A novel 3-(1H-imidazol)-1,2,4-triazin-6(1H)-one scaffold was designed as a new kinase inhibitor analog mimicking the bioactive conformation of the well-known diaminopyrimidine motif. Described herein are our development activities that led to the efficient preparation of this new [1,2,4] triazine scaffold. The key transformations include the efficient cyclization of imidazole-2-carbothioamido methyl ester with hydrazine to form 3-(1H-imidazol)-4,5-dihydro-1,2,4-triazin-6(1H)-one, followed by oxidation to afford 3-(1H-imidazol)-1,2,4-triazin-6(1H)-one. We believe these [1,2,4] triazine based analogs are potential candidates as inhibitors of anaplastic lymphoma kinase (ALK).

GP-11 **Ali Husain**[1] Kirpal S. Bisht[1]
[1]Department of Chemistry, University of South Florida

Design and the Synthesis of Novel water-soluble pseudo- Cyclodextrin Resorcin[4]arenes (CDRs)

Water soluble pseudo-cyclodextrin resorcin[4]arenes (CDRs) were envisioned by decorating the upper rim of resorcinarenes with sugars. The resulting CDR would have a hydrophobic cavity surrounded by a hydrophilic shell. The CDRs were synthesized via Cu(I)-catalyzed Azide-Alkyne Cycloaddition (CuAAC) reaction of appropriately modified resorcinarene and glucose derivatives. The utility of the CDRs has been demonstrated as a phase transfer catalyst in CuAAC reactions of hydrophobic substrates which can now be carried out in aqueous media. The CDRs mediated CuAAC reactions were much faster and afforded the desired 1,4-disubstituted 1,2,3-triazole products.

GP-12 **Garrett Craft**[1], **Mike Nguyen**[1], Mona Hasan[1], Julie Harmon[1]
[1]Department of Chemistry, University of South Florida

Investigating the Swelling Characteristics of a Smart Synthetic Hydrogel System for Use as a Chemotherapeutic Drug Delivery Platform

Hydrogels are defined as hydrophilic three dimensional polymeric systems which can absorb large quantities of water without dissolving in the solvent. Hydrogels also possess properties which render them uniquely qualified in their application as biomaterials; they are the most life-like of all synthetic materials, with physical characteristics such as high water content, soft texture and high permeability. In this incipient study, the swelling characteristics of the three-dimensional lattice of the synthetic hydrogel N-isopropylacrylamide (NIPAm)-co-2, 3-dihydroxypropyl methacrylate (GMA) with N, N'-methylenebisacrylamide as crosslinker will be investigated towards the formulation of a drug delivery platform. Such a hydrogel platform is envisioned for use in the slow release of chemotherapeutic agents as triggered by changes in environmental parameters characteristically found near a tumor.

GP-13 **Tamalia Julien**[1], Julie Harmon[1]
[1]Department of Chemistry, University of South Florida

Self-Healing Characteristics of Polycarbonate urethane (PCPU) using FTIR

Polycarbonate urethane (PCPU) is of interest for biomedical uses because of its bio-stability, resistance to hydrolysis and absence of vulnerable ether linkages. Our PCPU was synthesized using methylene bis (4-cyclohexylisocyanate), 1,4- butanediol and a polycarbonate polyol containing 1, 6-hexanediol and 3-methyl-1, 5-pentanediol. This particular PCPU was designed to exhibit optimum toughness, ultimate elongation and tensile strength. In addition, we found that it undergoes self-healing upon rupture without the use of additives or self-healing agents. Herein we discuss hydrogen bonds which break during rupture and reform during self-healing. This is documented via FTIR analysis.

GP-14 **Iredia D. Iyamu**[1], Katja Nacheva[1], Sameer S Kulkarni[1], David Flanigan[1], Megan Barber[1], Hong-Gang Wang[1], Roman Manetsch[1]
[1]Department of Chemistry, University of South Florida

Multi-fragment Screening of Protein-protein Interaction Modulators via Sulfo-click Kinetic Target-guided Synthesis

Although protein-protein interactions possess significant biological importance, identification of small protein-protein interaction modulators (PPIMs) remains challenging due to the flexible nature of proteins. Several fragment-based approaches have been used to identify ligands with good ligand efficiencies, but failure to provide insight into efficient fragment evolution has made the drug discovery process complicated. Herein, we report the development of a drug discovery approach that generates only biologically active compounds, known as kinetic target-guided synthesis (TGS). A sulfo-click reaction between thio acids and sulfonyl azides was successfully employed for Bcl-xL-and Mcl-1-templated screenings. After obtaining encouraging results, efforts were made to increase the throughput of kinetic TGS by approximately 100-fold. The development, high throughput and use of the new kinetic TGS will be discussed.

GP-15 **Cynthia Lichorowic**[1], Tina Mutka[1], Dennis Kyle[2], Roman Manetsch[1]
[1]Department of Chemistry, University of South Florida [2]College of Public Health, University of South Florida

Development of an ICI56,780 Probe for Mechanism of Action Studies

With the exception of 8-aminoquinolines, very few antimalarial compound series have demonstrated activity against the exoerythrocytic (EE) stages in the liver as well as erythrocytic and gametocyte stages. Previously, it has been reported that quinolone ester ICI56,780 produced a radical cure (eradicate dormant EE parasites) in Plasmodium cynomologi infected rhesus monkeys, however, rapid induction of resistance hampered its further development. Many of these studies were conducted over 20 years ago without an adequate evaluation in current preclinical efficacy models or without assessing physicochemical properties of the compounds. Herein we describe a limited structure-activity relationship study on ICI56,780 analogues and the development of a photoaffinity probe to study the mechanism of action of ICI56,780.

GP-16 **Vishwani Persaud-Sharma**[1], Shu-Feng Zhou[1]
[1]College of Pharmacy, University of South Florida

Characterization of Particle Size and Chemical Profiling of Electronic Cigarette Refill Cartridge Fluid

With claims as a healthful substitute, the electronic cigarette(EC) serves as an alternative for smoking consumers.The purpose of this study is to experimentally examine the purity of the EC fluid in terms of chemical profiling & particle size characterization to establish safety profile parameters via HPLC,LC/MS,&TEManalysis. Base EC fluid sans additives was primarily analyzed by HPLC in its unaltered state, however, no rational data was observed. As a result, EC fluid was dissolved & re-analyzed as a1% EC solution via the use of 1:1 acetonitrile & methanol. Similar conditions were used for LC/MS analysis with a binary gradient of 1mM ammonium acetate & pure acetonitrile observed at 230nm.Both HPLC&LC/MS data were obtained through the use of a C18 column whereas particle size &zeta potential characterizations were obtained through TEM analysis. As observed by TEM analysis, the particle size of the flavored EC samples ranged from 0.90 to 1.70 nm.

GP-17 **J. R. Maignan[1]**, C. L. Lichorowic[1], T. S. Mutka[1], A. N. LaCrue[2], D. E. Kyle[2], R. Manetsch[1]
[1]University of South Florida, Department of Chemistry, College of Arts and Sciences, Tampa, FL, United States
[2]University of South Florida, Global Health, College of Public Health, Tampa, FL, United States

Synthesis, Antimalarial Activity, and Physicochemical Properties of 7-(2-Phenoxyethoxy)-4(1H)-quinolones

There are a few antimalarial classes which possess activity against blood stages of malaria. However, very few compound classes have been shown to be active against the liver, blood, and gametocyte stages of the parasite's life cycle. It has been reported that quinolone ester ICI56,780 is active in eradicating dormant exoerythrocytic parasites in *Plasmodium cynomologi* infected rhesus monkeys. This discovery was stalled due to the rapid resistance induction that appeared. Because of recent advances in preclinical efficacy models and ease of assessing physicochemical properties, this class of compounds, which was worked on more than 20 years ago, has been revisited. Herein, structure-activity relationship and structure-property relationship studies of ICI56,780 analogues are discussed. The results suggest that ICI56,780 and analogues thereof have potential for the development of a novel chemotype to treat multidrug resistant malaria, to eradicate EE stages, to block transmission, and to eradicate malaria.

GP-18 **Danielle Demers[1]**, Jeremy Beau[1], Tina Mutka[3], Dennis Kyle[3], Bill J. Baker[1,2].
[1]Department of Chemistry, University of South Florida, [2]Center for Drug Discovery and Innovation, University of South Florida, [3]Department of Global Health, University of South Florida

Metabolomic Manipulation of Marine Fungi Through Epigenetic Modification via Histone Deacetylase Inhibition

Recent studies have shown marine fungi to be interesting targets of natural product investigation due to their ability to be grown under a variety of conditions that alter secondary metabolite production. Epigenetic modification via the histone deacetylase (HDAC) inhibitor sodium butyrate has been shown to increase production of metabolites of interest as well as previously unidentified compounds. In the spring of 2012, a collection of endophytic fungi was isolated from Florida mangroves. Crude extracts of these isolates were investigated for antibacterial activity. This study illustrates examples in which modified versus unmodified crude extracts yielded both differing bioassay results and metabolomic profiles.

GP-19 **Matt Battistini**[1], David J. Merkler[1]
[1]Department of Chemistry, University of South Florida

Activity Based Protein Profiling of Extremophilic Bacteria

Our group has developed a novel activity based probe (ABP) which enriches soluble proteins that bind adenine nucleotide derivatives; it can be used to profile disease states in eukaryotic systems by identifying aberrantly expressed biomarkers or investigate evolutionary divergence in similarly related bacterial cells. By utilizing modern comparative genomic strategies, activity based protein profiling (ABPP) and high-resolution mass spectrometry in tandem with isobaric tagging for absolute protein quantitation, we hope to elucidate genetic and proteomic differences that allow bacteria to thrive in extreme temperatures. This will be achieved by studying thermophilic and psychrophilic strains of bacteria within the same genus Bacillus.

Undergraduate:

AN-01 **Douglas M. Franz**[1], Dean F. Martin[1]
[1]Department of Chemistry, University of South Florida

What can be done when an apparently useful invention turns out to be a bad idea

The substantial use of bisphenolacetone (BPA) in the plastics industry has led to the ubiquitous presence of the material in the environment and in our bodies. BPA has been shown to be an endocrine disrupter and its removal from the environment is desirable; it has been strictly monitored or banned in many countries already. Our research investigates means of removing BPA model compounds (BPA itself poses an extreme eye hazard) from aqueous solutions by means of metal derivatives of a polyethylenediimine bonded to high surface-area silica gel called Octolig(R). In preliminary experiments, the metal derivatives Cuprilig (Copper II) and Cobaltilig (Cobalt II) show promise in removing BPA model compounds more effectively than Octolig(R). Octolig(R) and its derivatives have been shown to remove metals, nutrient anions, dyes, pharmaceuticals, and other chemicals from aqueous solution and is optimized at specific pH\'s for specific contaminants.

AN-02 **Hannah Feig**[1], Robert Tykot[1]
[1]Department of Anthropology, University of South Florida

Trace Element and Sourcing Analysis of Prehistoric Ceramics from Northwest Florida using Portable X-ray Fluorescence Spectrometry

Portable X-ray fluorescence spectrometry (pXRF) is a useful analytical technique in archaeology in the source determination of materials used to create ceramics. The non-destructive technique uses an X-ray beam to excite electrons and measures energy of secondary X-rays, generating a plot of elemental composition in parts per million (ppm). Analyzing trace elements Rb, Sr, Y, Nb, and Zr can give indication as to where ceramics materials originated. This research aims to use new pXRF settings to obtain more accurate sourcing data. Pottery samples from northwest Florida were reanalyzed using new settings, then compared to previously obtained data on the same sample set. A linear correlation unique to each element was found and can be used to translate between data sets without reanalysis. This study is important for better understanding prehistoric trade routes and past peoples, contributes to sourcing studies previously done at USF, and is helpful for optimizing pXRF methods.

AN-03 **Mohammad K Hamdan**[1], Abdul Malik[1]
[1]Department of Chemistry, University of South Florida

Magnetite Fe_3O_4/Ag Nanostructures with tunable silver shell

Surface enhanced Raman spectroscopy (SERS) is an effective technique in chemical and biomedical study. When molecules are adsorbed on the nano-size metal surface, the Raman signals are strongly enhanced. This study involves developing a novel SERS substrate of Fe_3O_4/Ag magnetic nanostructures which will be employed for biomarker detection and sample pre-concentration. Fe_3O_4 nanoparticles with size of 10 nm have been prepared successfully in aqueous micellar medium at 80°C. To make Fe_3O_4 sensitive in SERS, Fe_3O_4 are coated with silver as shell, and the shell thickness of nanostructures becomes tunable through the adjustment of the ratio between Fe_3O_4 to silver precursor salts. Surface morphology and structure of these nanostructures were characterized by using transmission electron microscopy (TEM), scanning electron microscopy (SEM) and energy dispersive spectroscopy (EDX).

AN-04 **Mona Hasan**[1], Garrett Craft[1], Julie Harmon[1]
[1]Department of Chemistry, University of South Florida

Optimization of Polyimide Performance in Gel Permeation Chromatography

Known for their flexibility and exceptional heat resistance, polyimides are highly favored components currently applied in Lithium Ion batteries of newer credit cards used for protecting funds. These polymers, synthesized using diamines and dianhydrides, act both as binders and separators in the battery apparatus to promote effective energy transfer and efficient battery use. Constructing these thin, fully functional polyimides for maximum applicability involves the need for polymer analysis using GPC (Gel Permeation Chromatography). However, Polyimides' high polarity and distinct solubility creates a challenge for preparation and analysis. With the introduction of 0.06M LiBr (Lithium Bromide) in NMP (N-Methyl-2-pyrrolidone), both complications cease to exist as liquid polymer samples having limited interaction with the polar GPC silica are now accessible. This technique grants the potential to enhance the reproducibility of poliyimide synthesis for batteries. Additionally, through analysis, applications of these batteries can further extend to cell phones, medical equipment, or even implants.

AN-05 Sungyub Han[1], **Janet Mara**[1,2], Xiao Li[1]
[1]Department of Chemistry, University of South Florida; [2]Department of Physics, University of South Florida

Fabrication of Silica Core Silver Shell Nanoparticle as a SERS Active Substrate

Core-shell nanoparticles with dielectric materials (SiO_2) have attracted much interest due to the application to biological sensing, photonic crystal, catalysis, surface enhanced Raman scattering (SERS) and so on. Since surface plasmon resonance frequency of core-shell nanoparticle is tunable by changing the size of core and the thickness of the shell, core-shell nanoparticle can exhibits excellent SERS activity. In this work, SiO_2 core Ag shell nanoparticle is synthesized using combination methods of a seed-mediated growth process and a further silver reduction step. We assemble core-shell nanoparticles on a glass slide to test its SERS activity with Rhodamin 6G molecule. We concluded from our results that under our conditions, SiO_2/Ag nanoparticle is a highly active SERS substrate compared to Ag nanoparticle.

AN-06 **Rebeca Pupo**[1], Abdul Malik[1]
[1]Department of Chemistry, University of South Florida

In-tube solid phase microextraction of naphthalene using a capillary coated in Germania-based sol-gel stationary phase

Solid Phase Microextraction (SPME) is an advantageous, widely-used extraction technique that provides a solventless method for sampling, sample preconcentration, and introduction to chromatographic techniques. Capillary microextraction (CME), also called in-tube SPME, allows for better handling of the technique and higher loading capacity of the extraction phase. The inner surface of a fused silica capillary was coated with sol-gel Germania-based extraction phase, prepared with a triblock copolymer (PPO-PEO-PPO), providing thermal stability with parts per billion limits of detection. An aqueous sample of naphthalene was passed through a capillary using a gravity-fed liquid dispenser. The capillary was connected to the GC injection port and to a GC column using a press-fit glass connector. Thermal desorption was performed by increasing the temperature of the injection port; the extracted analyte was carried through the column, then to the FID via the Helium-gas mobile phase. Excellent extraction capabilities and limits of detection were obtained.

AN-07 **Gabrielle Vaz**[1], Rongfu Huang[1], Xiao Li[1]
[1]Department of Chemistry, University of South Florida

The Enhancement of Cotinine & 3-hydroxy-cotinine using Au/Ag Nanoparticles in SERS

Metal nanoparticles are typically used to amplify the Raman signal of target molecules in Surface Enhancement Raman Spectroscopy (SERS). This experiment utilizes a gold core silver shell (Au/Ag) nanoparticle as the enhancement agent and compares the results to the pure silver nanoparticles for effectiveness of maximizing the enhancement factor of the detection of the target molecules. There were two target molecules, cotinine and 3-hydroxy cotinine (metabolites of nicotine). The methodology involved the formation of the core-shell structure at various concentrations with increasing shell size, and a stable core size of around 50nm (6 total core shell structures were formed with varying amounts of AuCl). The structures were confirmed using SEM imaging. SERS is conducted using the various core-shell sizes and selecting the one with the highest enhancement factor. The novel core-shell structure resulted in a larger enhancement of the signal of the target molecules when compared to silver nanoparticles.

AN-08 **Zachary Shultz**[1], **Emre Seyyal**[1], Minhphuong Tran[1], Abdul Malik[1]
[1]Department of Chemistry, University of South Florida

Germania-Silica Hybrid Sol-Gel Materials for Solvent-Free Enrichment of Environmentally Important Compounds by Capillary Microextraction

Solid phase microextraction media hyphenated on-line with high performance liquid chromatography analysis allows for a solvent-free sample preparation method that has been previously proven to be mechanically and chemically durable. Two novel germania-silica hybrid sol-gel extraction media were prepared using sol-gel technology. Tetraethoxygermane (TEOG) was used as the precursor in the creation of a sol-gel network via hydrolytic condensation on the walls of a 40cm segment of 250µm diameter fused silica capillary. Each extraction medium contained a silica linked organic ligand incorporated into the polymeric network to create micro-environments aiding in non-covalent capture of an analyte. (2-(3-cyclohexenyl)ethyltrimethoxysilane and phenyltrimethoxysilane were chosen for comparison due to their π orbital distributions and similarity in overall structure which enhances specificity to carcinogenic compounds common in environmental samples. There is promising applicable use in environmental and biomedical sample analysis for carcinogenic compounds such as harmful PAHs, phenols, and most compounds containing π orbitals.

AN-09 **Aaron Garrison**[1], Sungyub Han[1], Xiao Li[1]
[1]Department of Chemistry, University of South Florida

Synthesis of Si-Au Nanoparticles for Use as SERS Substrates

Surface Enhanced Raman Spectroscopy (SERS) can be an effective tool for quantitative analysis of biological samples. When a Raman-active analyte is adsorbed onto the surface of, in this case, metallic nanoparticles, enhancement of Raman signals can be observed by up to several orders of magnitude. This permits the detection of compounds at concentrations too low to yield signals via alternative methods. Cotinine and trans-3-hydroxycotinine, metabolites of nicotine, can be found in the urine of smokers. Our goal is to synthesize a colloidal solution of bimetallic nanoparticles (NPs) that, when used as a SERS substrate, will yield enhancement of Raman signals greater than that of our previously produced monometallic Au nanoparticles, thus lowering the detection limits of these molecules.

AN-10 **Alex Cole**[1], Jacqueline von Salm[1], Hasnaa Mouttaki[1], Bill Baker[1,2]
[1]Department of Chemistry, University of South Florida; [2]Center for Drug Discovery & Innovation, University of South Florida

Solid phase analytical separation of organic molecules utilizing MOF HKUST-1

Metal Organic Frameworks (MOFs) have recently received much attention as tools for analytical separation. HKUST-1 is a three dimensional crystalline structure synthesized with organic linker benzene-1,3,5-tricarboxylic acid and a copper metal node. MOFs have previously proven apt for gas separation and adsorption. MOFs will be used as a new form of solid phase separation for natural product research, where small molecule isolation is of primary interest. The window sizes for HKUST-1 are approximately 11 Å, and 8.5 Å, ideal for separation of various molecules and potentially filtration of unwanted natural byproducts such as highly polar sugars, salts, and highly non-polar fatty acids from natural products of interest. Assorted compounds, ranging from 100-950 amu were loaded onto a column packed entirely with HKUST-1, subject to multiple MPLC trials and monitored with LC/MS.

CO-01 **Fiona L. Kearns**[1], Sai Lakshmana Vankayala[1], Bill J. Baker[1,2], Henry Lee Woodcock[1]
[1]Department of Chemistry, University of South Florida; [2]Center for Drug Discovery & Innovation, University of South Florida

Computational Ecology: Elucidating novel chemical defense mechanisms of Antarctic Sea Sponges

In 2000, the novel secondary metabolite erebusinone was isolated from the Antarctic sea sponge, Isodictya erinacea. The compound's observed molt inhibition capacity and chemical similarity to known endogenous molt inhibitor xanthurenic acid led researchers to postulate its potential as a chemical defense mechanism. We propose erebusinone inhibits select cytochrome P450s along the ecdesteroidogenesis pathway in a manner similar to xanthurenic acid. This hypothesis will be validated via computational modeling. Because neither the sequence nor crystal structure of crustacean P450s along the ecdysteroidogenesis pathway are known, homology models must be constructed. A protein key to the ecdysteroidogenesis pathway has been modeled. The model has been refined and tested with a combination of structural prediction tools and Molecular Dynamics simulations. Docking studies have been carried out to determine key interactions between xanthurenic acid, erebusinone and P450 heme binding sites.

CO -02 **Lindsay Fatjo**[1], Wayne Guida[1, 2]
[1]Department of Chemistry, University of South Florida; [2]Drug Discovery Department, H. Lee Moffitt Cancer Center and Research Institute

Virtual Screening of the Ring Domain of MDM2

The goal of my research project is to prove the validity of virtual screening and docking scores of different ligands. With any success it will aid potential drug research by looking into different ways the amount of MDM2 and MDMX regulate the production and amount of P53. This research relates to the effect of these components and cancer studies. I am hoping to find energetically favorable ligands to dock to the ring in MDM2 that will better control P53 regulation. By controlling the regulation of P53 it will aid in the use of better drugs to help fight cancer.

CO -03 **Helen W. German**[1], Raymond J. Terryn III[1], Nathaniel Price[1], J. Clayton Baum[1], Mark J. Novak[1]
[1]Department of Chemistry, Florida Institute of Technology

Computational Elucidation of Energetic Trends for DNA Intercalation.

The prediction of general energetic trends from intercalation of polycyclic aromatic compounds with DNA can provide insight into these pertinent interactions, as well as improve synthetic drug design. Compounds chosen for this study are nucleoside base pairs (AT, GC) and 4-azatryptanthrin. Since there is no established crystal structure for this interaction, an alternative computational starting place is necessary. Since dispersion forces have been shown to drive optimal orientation based on π-stacking, this method utilizes the electrostatic potential (ESP) maps of both interacting species generated using DFT. The simplicity of relying on visual alignment of ESP maps could lead to a significant decrease in the time cost and the consideration of dispersion forces increases confidence in the resulting insight. Results indicate a slight preferential intercalation of 4-azatryptanthrin for the GC over the AT base pair which is beneficial for sequence targeting in drug design.

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

Development of a new and transferable water model for heterogenous simulations.

There are a large number of computational models for water however they are most often fit to reproduce bulk thermodyanmic data and therefore aren't necessarily representative of the true potential surface. This becomes especially important in heterogeneous simulations where previous models have no guarantee of accuracy. Therefore a new water model based on gas phase data, ab initio calculations and a simple potential model is developed and compared to previous models. Preliminary results show reasonable agreement with experiment.

CO -05 **Michael Trent Kemp**[1], Arjan van der Vaart[1]
[1]Department of Chemistry, University of South Florida

Effects of methylation on DNA hydration properties

DNA methylation protects the genome and controls genome transcription, regulating such processes as gene expression, protection from non-self DNA, and X-chromosome inactivation. To help understand the structural origins of this epigenetic control, we performed a study of the effects of methylation on DNA structure, dynamics and hydration. The DNA sequence 5'-CCGTCGACGG-3' was simulated in explicit water, using various methylation patterns for the CG steps. Differences in structural and hydration properties and possible biological implications are discussed.

The Clear Springs Land Poster Session Abstracts

NP-01 **Keith T. Zimmerman**[1], Ryan M. Young[1], Bill J. Baker[1,2]
[1]Department of Chemistry, University of South Florida; [2]Center for Drug Discovery & Innovation, University of South Florida

Synthesis of Anti-plasmodial Meridianin A Analogs

The malaria parasite *Plasmodium sp.* kills approximately 2,000-3,000 people per day and resistance to the once widely used drug chloroquine has spread to most areas affected with the disease, so new drugs are required to overcome this resistance. Preliminary screening for anti-malarial activity demonstrated that the marine natural product, meridianin A (1) isolated from the sponge *Psammopemma sp.*, inhibited growth of *P. falciparum*. Several 3-pyrimidylindole compounds were synthesized and screened for anti-plasmodial activity.

NP-02 **Mfonobong Inyang[1], Carla O'neale[1], Lindsay Vacca[1],** Danielle Demers[1], Bill J. Baker[1,2]
[1]Department of Chemistry, University of South Florida; [2]Center for Drug Discovery & Innovation, University of South Florida

Epigenetic Manipulation of Mangrove Endophytes

It is well known that marine fungi exhibit secondary metabolites that serve as defense mechanisms to protect the organism from predation and infection. These metabolites often have the potential to be used as therapeutic agents against many infectious diseases. Studies have revealed that these fungi contain gene clusters that code for the production of secondary metabolites. Epigenetic modifiers can be used to activate those gene clusters that might be silenced or down-regulated and enhance secondary metabolite production. In this study, endophytic fungi samples collected from Florida mangroves were isolated and grown under modified and unmodified conditions. Epigenetic modification via the histone deacetlyase (HDAC) inhibitor sodium butyrate was employed to promote the production of secondary metabolites. Compounds were extracted via MeOH extraction (3x) and EtOAc partitions. Crude extracts underwent 96 well plate and LCMS sample preparation and were subjected to bioassay and metabolite investigation.

NP-03 **Shikha Sharma[1]**, Juanjuan Yin[1], Shu-Feng Zhou[1]
[1]Department of Pharmaceutical Sciences, College of Pharmacy, University of South Florida

Preparation and biological evaluation of novel β-cyclodextrin based estrone conjugate drug complex in the treatment of estrogen receptor-positive breast cancer

The paradigm of using pharmaceutical carriers has been well established over the past decade, both in pharmaceutical research and in the clinical setting. Drug carriers are expected to facilitate targeted delivery of specific ligand-modified drugs and drug carriers into poorly accessible areas, the therapeutics accumulate in pathological sites via the passive and active tumor targeting. Active targeting which based on the attachment of specific ligands to the surface of pharmaceutical carriers to recognize and bind pathological cells is advanced among various approaches to specifically target drug-loaded carrier systems to required pathological sites in the body. In our study, cyclodextrin-based nanosystem with functional compositions and biological properties has been investigated for drug delivery applications. β-Cyclodextrin was vectorized by estrone which could target tumor cell-surface estrogen receptors. The estrone was conjugated to β-cyclodextrin with reductive amination through multi-step reactions. The novel estrone acid attached cyclodextrin drug was obtained and purified, the structure were rigorous characterized by HR-MALDI-MS, 1H-NMR, 13C-NMR, g-COSY, HMBC and HSQC. The drug complex was obtained through molecular recognization by mixed solvent precipitation, and the guest therapeutic agents is cytotoxic doxorubicin prodrug obtained by the reaction of adamantly chloride and doxorubicin hydrochloride in which the adamantly group acts as a perfect candidate for the host-guest combination. The host-guest association was determined by induced circular dichroism (ICD). The in vitro drug uptake and releasing profiles have been greatly enhanced compared with non-targeting drug complex. Cyclodextrin-based estrogen conjugated drugs may represent a new group of compounds for the treatment for estrogen receptor-positive tumors.

NP-04 **Luis Perez-Mena**[1] Dan Utic[1] Bill J. Baker[1,2]
[1]Department of Chemistry, University of South Florida; [2]Center for Drug Discovery & Innovation, University of South Florida

Extraction and Elucidation of Tau-Protein Active Compounds from Endophytic Mangrove Microbes within the Florida Everglades

Tau proteins modulate stability of microtubules within the central nervous system and cause dementias in humans when defective; they play a role in the development of fibrous plaque and eventual neuronal death within brain regions that coordinate cognition in Alzheimer's disease (AD). AD progression arrest shows promise in newly-found Tau-inhibitory natural products. Several fungal samples were isolated from everglades mangroves, grown in enriched media, epigenetically modified with histidine deacetylase (HDAC) to incur the production of secondary metabolites, and tested for activity against the tau protein. All samples with effective hits against the protein were scaled up, and their secondary metabolites were isolated using appropriate solvents and techniques. The crude extracts were then purified into fractions through MPLC and HPLC, based on the sample's UV light absorption and evaporative-light-scattering signals. The isolated active compounds involved were studied for their characteristic structures, composition, and potential to hinder the onset of Alzheimer's disease.

NP-05 **Marie Cherline Atilus**[1]**, Athena Failla**[1]**, Margarita Gianniosis**[1], Enoemem Okpokpo[1], Bill J. Baker[1,2]
[1]Department of Chemistry, University of South Florida; [2]Center for Drug Discovery & Innovation, University of South Florida

Isolation of Microorganisms from the Florida Keys for the Development of a Diverse Natural Product Library

Natural product libraries are an essential component in the discovery of bioactive metabolites for natural product isolation. These archives commonly consist of plant, bacterial, and fungal sources which supply a variety of bioactive compounds. A research expedition to the Florida Keys was completed on August 10th, 2012, for the purpose of developing the CDDI Chemodiversity facility natural product inventory. Ninety-five samples of marine organisms (sponges, corals, tunicates, and algae), sediments, seawater, and endophytic samples from mangroves were transferred to the laboratory for the isolation of bacteria and fungi via various media. Specifically, slow-growing microorganisms, including actinomycetes and myxobacteria, were the main focus during isolations. The pure isolates will be extracted and then prepared for screening submission in a 96 well-plate format. Finally, these will be distributed to different collaborators for biological evaluation in order to identify new active metabolites against parasitic, viral, neurological, and cancerous diseases.

NP-06 **Emily Trebour**[1] Laurent Calcul[2], Vicki Muise[1], Eliane Ubalijoro[1], Timothy Geary[1], Bill J. Baker[1,2]
[1]Department of Chemistry, University of South Florida; [2]Center for Drug Discovery & Innovation, University of South Florida

Utilization of Yeast-Based Multiplex Assay to Screen Natural Products as Potential Targets for Endectocidal Drug Development

In many developing countries, neglected diseases such as parasitic infections are still a major issue of medical concern. The objective of the yeast based multiplex project is to identify new compounds that could be potential targets for developing anthelmintic medications. Sacchromyces cerevisae strains were genetically mutated to express receptors from Drosophila melanogaster and Caenorhabditis elegans that are functionally essential to survival. These yeast strains were subjected to high through-put screening methods, testing compound binding affinity to the specific neuropeptide receptors. More than 4,000 crude extracts from various fungal and bacterial sources, as well as, 66 pure compounds from diverse origins have been screened. Optimally, by this method we will be able to design drugs which target multiple receptor sites, thereby reducing the likelihood of nematodes and other parasites from developing resistance to the medication.

NP-07 **Nathaniel O Johnson[1]**, Chris Witowski[1], Bill J. Baker[1,2]
[1]Department of Chemistry, University of South Florida; [2]Center for Drug Discovery & Innovation, University of South Florida

Secondary Metabolites of Antarctic Marine Endophytes

Studying the medicinal effects of secondary metabolites of microorganism has been central to drug discovery for many years. This project studies the secondary metabolites of endophytes isolated from invertebrates collected in April 2011 at Palmer Station in Antarctica. Samples were plated on Saboraud Dextrose Agar (SDA), Trypticase Soy Agar (TSA), marine SDA, and TSA with epigenetic modifiers, and incubated at 0°C. Two fungi, PSC11-37-M13C-1 and PSC11-37-M15B-1.1, were first grown on SDA then scaled up in one and three liters of broth (respectively). After three weeks, mycelia and broth were freeze dried and extracted with methanol. Crude extracts were separated using butanol/water partitions. Organic fractions were separated into ten and eight fractions for PSC11-37-M13C-1 and PSC11-37-M15B-1.1, using medium pressure liquid chromatography. Utilizing high pressure liquid chromatography and mass spectrometry, several compounds were isolated and structure determination will be performed using nuclear magnetic resonance spectroscopy.

NP-08 **Michael Field[1]**, Ryan Young[1], Bill J. Baker[1,2]
[1]Department of Chemistry, University of South Florida; [2]Center for Drug Discovery & Innovation, University of South Florida

Colonial Morphology

Morphology is a systematic description of an organism's characteristics. Colonial morphology is the macroscopic description of bacterial, and fungal colonies that grow on media. In the chemiodiversity lab there is little interest in the identity of the microbes used in natural product development. However keeping consistent, and systematic records of isolated microbes allows researchers to continue working with microbes that have interesting chemical properties. Without consistent colonial morphology, and record keeping it can be difficult to re-isolate certain microbes. Colonial morphology gives a guide on how colonies should appear in a media, and whether or not researchers have researchers have re-isolated the correct microbe. This paper will describe a systematic method for describing colonies isolated on media.

NP-09 **Stephanny Reyes[1], Shivangi Patel[1]**, Michael Veri[1], Bill J. Baker[1,2]
[1]Department of Chemistry, University of South Florida; [2]Center for Drug Discovery & Innovation, University of South Florida

Isolation of Secondary Metabolites from Bacterial Sources

As a response to microbe-microbe interactions, bacteria produce chemical defenses in an attempt to survive and outcompete neighboring organisms.The goal of this study is to produce microbial responses from cultures of bacteria and determine if these chemicals are potent enough to inhibit the growth of pathogens. To accomplish this task, cultures of bacteria are grown from surface to bottom sediments obtained from Palmer Station, Antarctica and other labs in different regions of Florida. After culturing, the bacteria is isolated and frozen. After freezing, the organisms are lypholized, extracted, and ran through a micro filter. The resulting solution undergoes Medium Pressure Liquid Chromatography (MPLC) and the desired 50 mg/ml concentration for the fractions obtained from the MPLC are made. A Kirby-Bauer disk diffusion assay is then performed using concentrated paper discs composed of the fractions to determine of any of the fractions inhibit the growth of the pathogen. If so, ^{1}H NMR and HPLC is performed on the specific fraction to obtain its structure. So far, 58 organisms have been grown and 40 organisms have been Kirby-Bauer assayed. Of these, 27 fractions from a total of 14 organisms had 36 hits across all pathogenic organisms tested. One formula of a compound found was $C_{18}H_{31}N_3O_5$. For now, we are still working on determining structures of all isolated compounds and determining if they are "new" compounds.

NP-10 Chris Witowski[1], **Ella Cortinas**[1] Alan Maschek[1] Charles Amsler[1] Jim McClintock[1] Bill J. Baker[1,2]
[1]Department of Chemistry, University of South Florida; [2]Center for Drug Discovery & Innovation, University of South Florida

Principal Component Analysis of the Antarctic Sponge Dendrilla membranosa Secondary Metabolome

The sponge Dendrilla membranosa (D. membranosa) is common on the benthos around the Western Antarctic Peninsula (WAP) and is easily recognized by its yellow cactus-like bulbs. Chemical defenses are employed by D. membranosa and many other sessile Antarctic marine invertebrates to deter predation and fouling. Diterpenoids, like tetrahydroaplysulphurin and membranolide, have been reported as feeding deterrents against known sponge predators. Four sampling sites were chosen around Palmer Station, Antarctica, each containing a deep and shallow sponge samples for comparison. Purified crude extracts were analyzed via LC/QToF-MS to quantify feeding deterrent concentrations and subjected to Principle Component Analysis (PCA) to determine metabolic variations between location and depth.

NP-11 **Amit P. Patel**[1], Christopher G. Witowski[1], Bill J. Baker[1,2]
[1]Department of Chemistry, University of South Florida; [2]Center for Drug Discovery & Innovation, University of South Florida

Extraction, Isolation, and Structural Determination of Marine Natural Products for Use as Potential Medically Relevant Lead Compounds

Natural products chemistry is currently one of the most potent sources of potential drug candidates. The purpose of this research was to locate potential drug candidates from endophytes hosted within the tissues of marine invertebrates and mangrove trees for use against a variety of human-afflictions such as MRSA and cancer cells. The experimentation focused on polarity based separations via classical chromatographic methodology, bio-guided fractionation and structural elucidation through spectroscopic techniques such as NMR spectroscopy, X-ray crystallography, and Mass Spectroscopy. Current testing has yielded three chemicals of potential medicinal interest that are currently undergoing structural determination.

NP-12 **Andrew Shilling**[1], **Mallory Belcher**[1], **Pedro Zamora**[1], **Dennis Trautman**[1], Laurent Calcul[2]. Bill J. Baker[1,2]
[1]Department of Chemistry, University of South Florida; [2]Center for Drug Discovery & Innovation, University of South Florida

Generation of Microorganism Library

The project's mission is to emphasize the significance of generating a microbe library, which supplies the CDDI with natural product samples for screening. Such library has the potential to lead researchers toward new discoveries by providing a unique chemical and biological supply of microbes. The library can also initiate new collaborations between researching facilities, which share a common interest for advanced scientific breakthroughs relating to microorganisms. The project started off with specimen collections during a diving excursion at the Florida Keys Marine Lab, in the summer of 2012. Such collections were variable from sediments to numerous marine organisms (i.e. algae, soft coral, and sponges). Each representation of microbe went through numerous courses of isolations which resulted in over ~ 1400 pure isolates. The next step is to produce extractions, preparative LCMS, and 96-welled fraction plates for screening purposes, leading to the deconvolution of the microbe library.

NP-13 **Riley Bednar**[1], **Shaney Penas**[1], Chris Witowski[1], Bill J. Baker[1,2]
[1]Department of Chemistry, University of South Florida; [2]Center for Drug Discovery & Innovation, University of South Florida

Metabolic Screening and Titer Enhancement of a Solid State Co-Culture

Secondary metabolites are an invaluable reservoir for pharmaceutical compounds, particularly for new antibiotic leads. Competition for resources among organisms often elicits the production of secondary metabolites as a defensive measure to ward off antagonists. Such interactions result in the activation or overexpression of biochemical pathways leading to the biosynthesis of new compounds, analogues or titer enhancement of minor metabolites. Solid-state co-culturing offers a unique method to trace the identity, quantity, and point-of-origin of secondary metabolites produced during exploitative competition. Aspergillus niger and an endophytic fungus from the Caribbean sponge Xestospongia muta were co-cultured on agar plates and their regions of interaction and individual mycelium were extracted. Compounds will be isolated and elucidated using Nuclear Magnetic Resonance (NMR) guided fractionation, and the metabolomic indices of confrontations will be compared across samples by use of Liquid Chromatography Quadrapole Time of Flight analysis (LC-QToF).

NP-14 **Stephanie Villalobos**[1], Danielle Demers[1], Bill J. Baker[1,2]
[1]Department of Chemistry, University of South Florida; [2]Center for Drug Discovery & Innovation, University of South Florida

Chemical Investigation of Antarctic Tunicates Lissoclinum sp. and Aplidium cf. variabile

This experiment is concentrated on two tunicates, Lissoclinum sp. and Aplidium cf. variabile collected at Palmer Station in Antarctica. Many marine invertebrates produce secondary metabolites during their life cycle. Exploring the secondary metabolites of organisms from such a remote part of the world could yield undiscovered compounds. Processing the tunicates is done through a series of techniques. The samples are freeze-dried then extracted in two different solvents. After this the crude extracts can be separated by MPLC to then be divided up into fractions based on relative polarity. A 1H NMR spectrum can then be obtained for each fraction. After this the samples go through HPLC for purification, through LCMS for a mass, and back through NMR to get proton and carbon spectra of the purified fractions. Going through these steps aids in the structure elucidation of the secondary metabolites. The goal of this research is to discover new compounds.

NP-15 **Christopher E. Konig**[1], Jacqueline von Salm[1], Ryan Young[1], Daniel N. Santiago[1], Wayne Guida[1,3], Bill J. Baker[1,2]
[1]Department of Chemistry, University of South Florida; [2]Center for Drug Discovery & Innovation, University of South Florida, [3]Drug Discovery Department, H. Lee Moffitt Cancer Center and Research Institute

Measuring chemical diversity of CDL148, NCID1 and AntiMarin via custom 2D-fingerprinting and Tanimoto similarity

Natural products and secondary metabolites are validated by nature. Such produced and commonly toxic compounds are often used for chemical defense by the living organism and are a rich source for drug discovery. Here, an attempt is made to measure the degree of chemical diversity exhibited by the Center for Drug Discovery and Innovation's (CDDI's) 148 natural products (CDL148), the National Cancer Institute's Diversity Set 1 (NCID1 containing 2,000 small diverse molecules), and AntiMarin (AM containing 62,830 marine, terrestrial and marine microbial natural products). A custom 2D fingerprint is created based on 60 descriptors computed by Schrödinger Suite's QikProp software. The normalized frequencies of the computed Tanimoto coefficients are plotted over their respective range. The results indicate that CDL148 is similarly diverse to NCID1 and that both are moderately less diverse than AntiMarin. These results are part of CDDI's NIH (R01) Research Grant Proposal for infectious disease drug discovery.

NP-16 **Haddjatou Jallow**[1], Ryan Young[1], Bill J. Baker[1,2]
[1]Department of Chemistry, University of South Florida; [2]Center for Drug Discovery & Innovation, University of South Florida

Development of a more effective method for the collection of Mangrove-rich Endophytes

Endophytes are non-parasitic fungal and bacterial species living under the epidermal cell layer of Mangrove parts. Due to their production of bioactive metabolites, which have been found to be useful in the treatment of cancer, malaria, and other infectious diseases, interest in endophytes has grown. Taxol, found in each yew (*Taxus*) species but was originally isolated from *Taxus brevifolia*, is the world's first billion dollar anticancer drug. Mangroves are complex and dynamic ecosystems varying in salinity, water level, low O_2 and nutrient availability and are mostly found in the tropical and subtropical regions of the world. The current collection methods used are the 5 types of media petri-dish method for short term growth, and 20% glycerol: water solutions for long term storage. Cryo tubes are much smaller and manageable, so this study is based on the development of an efficient method they can be used in the collection and growth of endophytes from around the world. This would be done by varying the surface area, aeration level, and media volume in the Cryo tubes. Data would be collected and analyzed to determine what the most ideal set-up would be.

IN-01 **Erick A. Barnum**[1], Naga K. Duggirala[1], Lukasz Wojtas[1], Michael J. Zaworotko[1]
[1]Department of Chemistry, University of South Florida

New Composition of Lithium Benzoate with Proline (LBEPRO) to Improve Brain Bioavailability

The 1:1 cocrystal of proline with lithium benzoate salt crystallizes from hot water to afford a novel ionic cocrystal (LBEPRO). The composition of the ionic cocrystal was characterized by single crystal x-ray diffraction. Lithium is currently used as an active pharmaceutical ingredient's (API), in medication of bipolar disorder. Currently available lithium salts have poor bioavailability as the uptake of lithium to the other organs is more compared to brain. We hypothesize that the new lithium complex with proline will be transported to the brain over other organs via an active transporter mechanism and LBEPRO is a potential material to improve the brain bioavailability of lithium.

IN-02 **Vanessah L. Rhodus**[1], Patrick S. Nugent[1], Michael J. Zaworotko[1]
[1]Department of Chemistry, University of South Florida

Synthesis of Porous Metal Organic Materials with Various Hexafluorometalate Pillars and Bipyridyl Ligands for Gas Separation and Storage

Porous Metal Organic Materials (MOMs) have the potential to address a wide variety of technological challenges in the context of gas storage and separation, heterogeneous catalysis, and drug delivery. The judicious choice of organic and inorganic building blocks can afford robust, predictable network topologies which are fine-tunable in terms of pore size and surface functionality. This research focuses on a MOM platform known as pillared square grids in which the metal node, organic linker, or inorganic pillar may be systematically varied while preserving the topology of the network. Herein we report the synthesis and gas separation properties of six square grid variants containing assorted hexafluorometalate pillars and varied bipyridyl ligands. Through our strategy of pillar and ligand substitution in this platform, we hope to gain insight concerning the relationship between subtle structural variation (i.e. tuning of framework electrostatics) and CO_2 selectivity.

IN-03 **Shelby Register**[1], Patrick Nugent[1], Michael J. Zaworotko[1]
[1]Department of Chemistry, University of South Florida

Synthesis of Metal Organic Materials for Ion Exchange and Gas Adsorption

Porous metal organic materials (MOMs), which form via the self-assembly of metal nodes and organic linkers, have become increasingly important towards the future of gas storage and separation, among other applications. The goal of this project is to examine the carbon capture properties of variations on a 2D layered grid through the measurement of CO_2, CH_4 and N_2 adsorption isotherms. A MOM with the formula $([Ni(bipy)_2(NO_3)_2]\cdot 2\ arene)_n$ [bipy= 4,4'-bipyridine] was synthesized via slow diffusion with varying arene solvents to create porous layered square grids containing arene guest molecules in the cavities. Through powder and single crystal X-ray diffraction we have confirmed the structure. Through post-synthetic modification, via ion exchange, we will exchange the nitrate groups in the axial positions of the nickel ion nodes for other ions. CO_2 adsorption measurements of different variations of the grid will be taken to examine the effect of grid composition on carbon capture.

IN-04 **Kyle McDonald**[1], Patrick Nugent[1], Michael J. Zaworotko[1]
[1]Department of Chemistry, University of South Florida

Controlling Crystallization of Metal-organic Materials for Gas Storage and Separations

Metal-organic materials (MOMs), constructed via self-assembly of metal nodes and organic linkers, offer the potential to address vital challenges in the realm of gas storage and separations. Some MOM platforms make use of pillaring ligands linking metal-organic sheets to form 3D-scaffolds, thereby increasing porosity and stability to loss of guest species. We report herein a series of pillared sheet MOMs, $[Co(bpy)_2(SiF_6)]$, $[Co(bpy)_2(TiF_6)]$, $[Co(bpy)_2(SnF_6)]$, and $[Co(bpy)_2(ZrF_6)]$ (bpy= 4,4'-bipyridine), synthesized via room temperature diffusion and solvothermal methods from readily available starting materials. These MOMs exhibit high relative CO_2/N_2 and CO_2/CH_4 uptake in comparison to other MOMs with similar surface areas, relevant to carbon capture and alternative fuels. Alternative synthesis methods have been examined. By systematically varying the MF_6 pillar and length of the linker, we aimed to examine the effect of subtle changes in framework composition on CO_2 adsorption selectivity for energy-related applications.

IN-05 **George Pitt**[1], Sameh Elsaidi[1], Michael Zaworotko[1]
[1]Department of Chemistry, University of South Florida

Pore size control in diamondoid nets to optimize pore size for CH_4, H_2 and CO_2 sorption

Metal organic materials (MOMs) are typically comprised from metal ions or metal clusters with 3 or more points of connection (nodes) and organic ligands or metal clusters that serve as linkers. MOMs have emerged as a class of porous materials with great potential for a wide range of applications, including gas storage, heterogeneous catalysis and drug delivery. The drive behind the development of MOMs is their extraordinary surface area and their modular nature, which makes for tunable pore dimensions and surface functionality. In this study we focus upon study the effect of pore size on the isosteric heat of adsorption of various gases using diamondoid nets. Pore size control in this family was exerted by two approaches: changing the length of the linker; using solvent to control the level of the interpenetration of such nets. Our results reveal how pore size plays an important role in gas adsorption by MOMs.

IN-06 **Kimberly Faeh**[1], Nagakiran Duggirala[1], Michael Zaworotko[1]
[1]Department of Chemistry, University of South Florida

Synthesis of Novel Ionic Cocrystals of Lithium Salts and Amino Acids

Lithium has been shown fight suicidal thoughts in patients with depression, bipolar and other psychotic diseases. Ionic cocrystals can be synthesized in order to improve the drug's solubility and bioavailability in the brain. Coordinating lithium salt with an amino acid is believed to aid passage through the blood brain barrier. Previous studies have been done to obtain ionic cocrystals of lithium chloride, lithium bromide and lithium nitrate with various amino acids. The following study aims to synthesize and characterize ionic cocrystals of lithium saccharinate and lithium oxalate with various amino acids by evaporation in DI water. The resulting crystals are analyzed using single crystal and powder X-ray diffraction, TGA, and FTIR to show that they are novel cocrystals of the three compounds. These novel cocrystals can then be further tested in rat studies to determine the efficacy of the cocrystal as a drug.

IN-07 **Katherine R. Johnson**[1], Melanie P. Masden[1], Eric J. Werner[1]
[1]Department of Chemistry, Biochemistry and Physics, University of Tampa

Solution Thermodynamic and Relaxometric Studies of Schiff Base/Pyridine Lanthanide Complexes

Contrast agents utilizing gadolinium(III) are often used to enhance the images produced from an MRI scanner. When injected, such agents are bound by water molecules within human tissue and cause an increase in the relaxation rate of water protons, improving image contrast. The effectiveness of any contrast agent can be related to the number of bound water molecules (q) that coordinate to the metal. Current commercial agents have q values of one water molecule, resulting in low proton relaxation rate enhancements. In this study, a tripodal pyridine/Schiff base ligand for Gd(III) was synthesized to produce a novel MRI contrast agent. The so-called TRIPy ligand effectively binds Gd(III) and Eu(III) and allows for additional coordinated water molecules. The metal complexes were characterized via UV-Vis, IR, and fluorescence spectroscopy. Relaxometric and thermodynamic stability studies were also conducted and will be discussed in light of potential imaging applications.

IN-08 **Wesley Boyette**[1], **Zohrab Kotchounian**[1], Alexander Schoedel[1], Lukasz Wojtas[1], Michael J. Zaworotko[1]
[1]Department of Chemistry, University of South Florida

A Highly Versatile Class of Ionsdaleite-type Networks Through Metal-organic Pillaring of Functionalized Kagome Layers

Metal-organic materials (MOMs) assembled from metal-based building blocks and organic linkers have attracted much interest due to their large pore dimensions and enormous structural diversity. In comparison to their inorganic counterparts (e.g. zeolites), MOMs can be modified to tailor pore dimensions and functionality for specifically targeted properties. Herein we present a crystal engineering strategy based upon a 2-step synthetic process for the construction of a family of binodal frameworks. In this context our previously reported trigonal prismatic Primary Molecular Building Block (tp-PMBB-1) serves as a metal-organic pillar that, when combined with 2-D kagome lattices, generates 3-periodic networks. All nets exhibit Ion-e (Ionsdaleite) topology and possess functionalized hexagonal nanopores. Examples of functionality affecting both surface area and Qst for CO_2 and CH_4 will be presented. This, together with the use of simple, inexpensive ligands, renders tp-PMBB-1-Ion-e a fine-tunable MOM platform which can potentially be used for industrial applications.

IN-09 **Austin Weyant**[1], Naga K. Duggirala[1], Lukasz Wojtas[1], Michael J. Zaworotko[1]
[1]Department of Chemistry, University of South Florida

Ionic Cocrystals of Lithium for Targeted Brain Delivery

Lithium is used in treating bipolar disorder but is limited in its delivery to the brain due its poor permeability to cross the blood brain barrier. As amino acids are known to cross the blood brain barrier, we hypothesize lithium salts coordinated with amino acids can improve the brain bioavailability. In an effort to improve the delivery of lithium to the brain, novel ionic cocrystals of lithium salicylate with 4-hydroxyproline and beta-alanine (LIS4HPR, LISBAL) have been synthesized and characterized. These compounds could potentially be used to reduce the oral dosage needed for therapeutic levels and consequently, reduce the peripheral toxicity of lithium and its associated side effects.

IN-10 **Katherine Somodi**[1], Matthew Andrus[1], Olivia Risset[1], Pedro Quintero[2], Khalil Abboud[1], Daniel Talham[1]
[1]Department of Chemistry, University of Florida; [2]Department of Physics, University of Florida

The Effect of the Surface on Physical Properties Changes in RbjCok[Fe(CN)$_6$]l·n H2O Prussian Blue Analogues

Prussian blue analogues (PBAs) are a class of magnetic coordination polymers. In some, the magnetic response can be switched with external stimuli such as light or temperature. Cobalt hexacyanoferrate (CoFe) PBA, $A_jCo_k[Fe(CN)_6]_l \cdot n$H2O (A = alkali metal), undergoes a charge transfer induced spin transition (CTIST), Fe^{III}(LS)-CN-Co^{II}(HS) to Fe^{II}(LS)-CN-Co^{III}(LS), leading to a change in magnetization. We aim to demonstrate how the particle surface influences the CTIST. Working with hollow and heterostructured CoFe PBA particles we can tune the structural properties. Recent work has focused on defining the surface using hollow PBA particles. Varying the thickness of the hollow particles allows for the physical changes such as the CTIST to be correlated to surface effects. Defining the surface and altering properties by changing the physical environment of particles could provide new approaches to tuning the behavior of light switchable magnets.

IN-11 **Mary E. Garner**[1], Amrita B. Mullick[1], Sudarsan Venkatramani[1], Adam S. Veige[1]
[1]Department of Chemistry, University of Florida

Design and Synthesis of Functionalized Gold-N-Heterocyclic Carbenes for Aptamer Conjugation.

Current metal-based anti-cancer agents display a high level of instability and lack the selectivity to be deemed therapeutically valuable. We seek to solve this problem by first developing potent gold-N-heterocyclic carbene (Au-NHC) complexes with enhanced selectivity and stability. Next, using cancer-specific aptamers generated by the cell SELEX process, we will increase the targeting ability of our Au-NHC drugs by preparing Au-NHC aptamer conjugates. This work outlines our progress in the rational design, synthesis, and characterization of our novel Au-NHC pre-aptamer complexes. So far we have developed a reliable route to synthesize a water stable and water soluble carboxylate modified Au(III)-NHC complex and performed preliminary cytotoxicity studies using CEM (T-cell leukemia) and Ramos (Burkitt's Lymphoma) cell lines. We will continue to evaluate our complexes for stability under a variety of conditions, assess their cytotoxicity, carry out aptamer conjugation and perform cell viability studies.

CE-01 **Aryan Beharry**[1], Nardo Munoz[1], Sophie Cene[1], Cristian Ariza[1], Myles Johnson[1], Priya Patel[1], Rene Salazar[1]
[1]College of Public Health, University of South Florida

Desired qualifications for landing an environmental/occupational health job in Florida

A career in Environmental/Occupational Health (EOH) focuses on the control of various hazards and their impact on humans in work and non-work settings. A study was carried out to evaluate the types of EOH jobs available by region, the qualifications required by employers, and salary. This study utilized various job-listing websites to identify available jobs throughout Florida. Job-specific details were collected from specified regions and recorded on a spreadsheet. The research showed that there were 104 jobs available in the north, 96 in the central, and 20 in the south. A bachelor's degree was typically the minimal level of education necessary for qualifying for an EOH job in Florida. These results confirm that education increases the opportunity for finding an EOH job in Florida and also indicate that someone who wants to work in Florida would have a better opportunity of attaining a job in the north and central regions.

CE-02 **Matthew Sestilio**[1], Todd A. Gatlin[1], Adrian Villalta-Cerdas[1], Santiago Sandi-Urena[1]
[1]Department of Chemistry, University of South Florida

Participation of Foreign Educated Faculty in Undergraduate Education

Chemistry faculty demographics have changed considerably over the past three decades. Although minorities and women continue to be underrepresented in faculty positions, the proportion of foreign-born professors has increased substantially. The diversity that this brings is celebrated and in terms of research it pays dividends. It also gives students access to a global perspective that may be beneficial in their professional practice. However, in most cases these professors have completed their K-16 education in educational systems substantially different from that in the US and the influence of this unfamiliarity has seldom been discussed. Moreover, chemistry assistant professors receive little to no instructional training before immersing in undergraduate education. There is very little work done to investigate the consequences that unfamiliarity with the system, lack of training, conflict of expectations, cultural and communication factors and other related aspects may have on foreign-born professors and undergraduate students' experiences.

CE-03 **Patrick McKeny**[1], Todd A. Gatlin[1], Santiago Sandi-Urena[1]
[1]Department of Chemistry, University of South Florida

Ratemyprofessors.com: General Chemistry Students' Contribution and Use Patterns

Online rating websites such as Ratemyprofessors.com (RMP) influence college professor and course selections. However, their use often sparks skepticism among instructors because of the self-selected nature of raters. Prior research on this topic in chemistry education concluded that RMP might be used as a valid source of supplemental information for evaluating instruction. The objectives of this study were to determine students' motives behind contributing to the site and to determine how students use the site to inform their decision making process. 500 General Chemistry students over the course of two years completed a 50-question survey addressing RMP use patterns. Findings suggest the majority of students use RMP and found it useful. Contributors' motives varied but were quite different from commonly held conceptions (e.g. They post to rant.). The contention is put forth that chemistry departments and professors may find a valuable supplemental source of information in RMP data.

The Solomon T. Weldegirma Poster Session Abstracts

BIO-01 **Ryan Anderson**[1], **Anita Behari**[1], Kristen A. Jeffries[1], David J. Merkler[1]
[1]Department of Chemistry, University of South Florida

Identification and Quantification of Fatty Acid Amides in Drosophilia melanogaster by Liquid Chromatography – Mass Spectrometry

The members of the fatty acid amide (FAA) family include the N-acylethanolamines, the N-acylamino acids, the N-acyldopamines, and the primary fatty acids. The FAAs have been found to perform an array of biological roles as cell signaling molecules in various mammalian species. We have expanded our knowledge of these FAAs in a non-mammalian organism. A novel panel of FAAs has been identified in Drosophilia melanogaster (fruit flies). The FAAs were extracted with organic solvents, purified with solid phase chromatography, and analyzed by LC-QTOF-MS. The FAAs were then quantified using standard curves. These data allow for further studies involving the elucidation of the biosynthetic pathways of FAAs in diverse model systems. Understanding these metabolic relationships and characterizing the enzymes in these pathways will lead to ultimate insight into what these molecules do and how they can aid in the development of therapeutics.

BIO -02 MuSeong Kim[1], **Faysal Rifai**[1], Elisa Marangon[1], Cedric Marrouatc[1], Julie Harmon[1]
[1]Department of Chemistry, University of South Florida

Zero Dimensional Copper Nanoballs Dispersed in Methacrylate Polymers

Zaworotko and his researchers classify metal-organic materials, MOMs, containing metals and organic ligands arranged in various ways [1]. The simplest are discrete, zero dimensional structures are metal-organic polyhedra nanoballs and polygons. More extended structures are coordination polymers with periodicity in one, two and three dimensions, referred to as 1D, 2D and 3D, and the nanoballs were sonicated polymerized within them. A comparison study was made between the hydrophobic PMMA-NB and hydrophilic PHEMA-NB nanocomposites. The composites were analyzed via differential scanning calorimetry, microhardness and dielectric analysis. The dodecyl groups significantly alter the solubility of the nanoballs, imparting hydrophobicity to the surface of the nanoball. Structure property relations are discussed in terms of interactions between the polymer matrices and nanoball surfaces and interiors. This work forms the basis for future applications in mechanical properties.

BIO -03 **Solianna Herrera**[1]**, Patrick McKeny**[1], Justin Moses[1], Lijune Ming[1]
[1]Department of Chemistry, University of South Florida

Sol Gel Encapsulation and Characterization of the Oligopeptide Thiostrepton

We present an overview of a method for entrapment of biomolecules using Sol-Gel as an immobilization matrix. Although the employment of Sol-Gels for the use of enzyme entrapment shows promise in a variety of applications, traditional bio-encapsulating methods still face challenges such as; retention of reactivities, stability, volume, and surface area of particles. In the following experiments the Ogliopeptide Thiostrepton, along with various transition metals, were encapsulated. Herein we observe how the use of this relatively new method was used for preferences in formation of the gel structure, activity, and matrix interactions with the complexes.

BIO -04 **Stepan Shumyak**[1], Juanjuan Yin[1], Shu-Feng Zhou[2]
[1]Department of Chemistry, University of South Florida, [2]College of Pharmacy, University of South Florida

Synthesis and biological evaluation of novel Î²-cyclodextrin based folic acid receptor targeting drug complex for the therapy of cancer

Targeting nanoparticles hold tremendous potential as effective drug delivery systems in the treatment of tumor. Cyclodextrin's nanosystem with functional compositions and biological properties have been investigated for drug delivery applications in this study. β-Cyclodextrin was vectorized by folic acid which could target tumor cell-surface folate receptors. The folic acid was conjugated to β-cyclodextrin with an amide bond through multiple step reactions. The drug complex was obtained through molecular recognition by mixed solvent precipitation, and the guest therapeutic agent was a cytotoxic doxorubicin prodrug obtained by the reaction of adamantyl chloride and doxorubicin hydrochloride; where the adamantyl group serves as a perfect candidate for the host-guest interaction. The in vitro drug uptake and releasing profiles were found to be greatly enhanced compared to non-targeting drug complex by using confocal microscopy and flow cytometry. Cyclodextrin based folate conjugated drugs could be potential candidates for the treatment for FR-positive cancers.

BIO -05 **Gabrielle J. Garbade**[1], Kristen A. Jeffries[1], David J. Merkler[1]
[1]Department of Chemistry, University of South Florida

Fatty Acid Amides: Identification and Quantification in N18TG2 Mouse Neuroblastoma Cells

Fatty acid amides (FAA) are endogenous signaling lipids that have various biological functions in mammalian species. The biosynthetic pathways of FAAs are not completely understood. Studying these pathways can lead to potential therapeutic answers for a number of diseases. Previous research with FAAs was performed using gas chromatography-mass spectrometry (GC-MS), which allowed researchers to identify and quantify a panel of FAAs with limitations. With today's technological advances, liquid chromatography- quadrupole time-of-flight mass spectrometry (LC-QTOF-MS) is available and was utilized in this lipidomic experiment. A panel of endogenous FAAs was identified and quantified in N18TG2 mouse neuroblastoma cells. FAAs were extracted from the cells, purified, analyzed by LC-QTOF-MS, and quantified with standard curves. We were able to identify novel FAAs that were not detectable by GC-MS. For future studies, the N18TG2 cells will be fed heavy labeled fatty acids for further elucidation of the biosynthetic pathways of FAAs.

BIO -06 **Luis R. Saavedra Román**[1], Elizabeth Remily-Wood[1], John Koomen[1,2]
[1]Department of Chemistry, University of South Florida, [2]Moffitt Cancer Center

Detecting NRAS mutations in Melanoma using Liquid Chromatography-Multiple Reaction Monitoring Mass Spectrometry

Melanoma is the most serious type of skin cancer. The Ras family of oncogenic proteins is critical in cancer due to their role in cell signaling and apoptosis regulation. In melanoma, the second most common alteration is mutation of N-RAS (position 61 in 15-20% of patients). N-RAS mutation detection is important for therapy selection, but is difficult to confirm at the protein level with existing techniques. Through use of liquid chromatography-multiple reaction monitoring mass spectrometry (LC-MRM), expressed NRAS proteins will be screened after digestion with various enzymes to determine the best peptide-based detection method for wild type NRAS gene and possible mutations (Q61R, Q61K, Q61L, Q61H). Tryptic digestions produce peptides too long for LC-MRM analysis, other enzymes which cleave shorter fragments will be explored. Results from this study can improve N-RAS mutation detection in patients and serve as a model to confirm other mutations.

BIO -07 **Ratna Suthar**[1], Stanley M. Stevens Jr. [1], M. Cecilia N. Nunes[1]
[1]Department of Cell Biology, Microbiology and Molecular Biology, University of South Florida

Proteomic insight on quality changes in response to high-temperature stress in organic and conventional strawberry fruit

Consumers perceive that organic produce is of higher quality than conventional produce. However, few studies have effectively compared both selections by taking into consideration critical factors such as the area of production, cultivar and maturity at harvest. This study compares quality of organic and conventional strawberries in response to high-temperature stress. Data will be collected using two methods of evaluation: physicochemical and proteomic analysis. Correlation between data will allow investigation of enzymatic pathways associated with degradation of quality attributes. The goal of this study is to provide fundamental insight into factors that affect the proteome. Preliminary physicochemical results showed organic strawberries were more sensitive to temperature stress by exhibiting a higher phenolic content, decreased firmness, and development of darker pigments. Further analysis will compare ascorbic acid content, individual sugars, and proteomic data. Identifying biomarkers of fruit quality will provide the foundation for further research in extending shelf-life of horticultural products.

BIO -08 **Daniel Hennessey**[1], Michael Moses[1], Ioannis Gelis[1]
[1]Department of Chemistry, University of South Florida

Expression of Cdc37 and Chromatographic Isolation to Observe Protein Interactions Using NMR

The decision of whether to enter the eukaryotic cell cycle is made in G1, a period during which cells respond to both positive and negative growth signals. The ultimate recipients of these signals are cyclin-dependent protein kinases (Cdk) that regulate passage through sequential cell cycle transitions. D-type cyclins are induced by mitogens and activated Cdk4/cyclin D complexes are thought to phosphorylate the retinoblastoma susceptibility protein (Rb), thereby facilitating G1 progression. Cdc37 is a co-chaperone that is thought to assist in the formation of the Cdk4/cyclin D complex, and significant efforts have been dedicated to understanding the involvement of the co-chaperone in the complex formation. NMR spectra from single and double-labeled Cdc37, ^{15}N and $^{15}N/^{13}C$ respectively, have been obtained to be analyzed and interpreted.

BIO -09 **Brittany Metz**[1], Micheal Doligalski[1], Mohanraja Kumar[1]
[1]Department of Chemistry, University of South Florida

Synthetic Cyclic Peptide Characterization using HPLC, Circular Dichroism Spectroscopy, and mass spectrometry

Cyclic peptidomimetics that undergo β-sheet conformation have recently been studied as a possible way to disrupt interaction between improperly folded proteins in various amyloid diseases. Amyloid diseases include Huntington's, Parkinson's, Alzheimer's, and various cancers. β-sheets is very prominent in these type of diseases causing proteins to aggregate. A cyclic peptidomimetic was synthesized using solid-state Fmoc chemistry, and characterized using HPLC and mass spectrometry. The conformation of the cyclic peptidomimetic was analyzed using circular dichroism spectrometry. Circular Dichroism will tell if the peptidomimetic is a β-sheet. If the peptidomimetic is a β-sheet, than further research will be done on it's potential drug capabilities.

BIO -10 **Nicholas J. Cotter**[1], Darin Bell[1]
[1]Department of Chemistry, Saint Leo University

Boosting the microcidal capabilities of ethyl alcohol on Staphylococcus aureus by utilizing synergy between two fatty acids: palmitic acid and linolei

Ethanol, a common disinfectant used in laboratory, industrial, and even residential settings, is a widely used and mostly harmless chemical. Even against Staphylococcus bacteria, ethanol has been proven an effective agent in combating this type of bacteria. Although, in recent years, the rise of MRSA (methicillin-resistant Staphylococcus aureus) has shown that antibiotics are proving to be more and more difficult to successfully eliminate bacterial infections caused by MRSA. However, linoleic acid and palmitic acid, two organic fatty acids, show microcidal effects towards S. aureus and often show synergy with related fatty acids. By testing the microcidal effectiveness of each of these compounds on S. aureus cultures at varying molar quantities and also testing mixtures of these two compounds at varying molar quantities, boosted effectiveness towards the bacteria may be achieved.

BIO-11 **Michael Moses**[1], Daniel Hennessey[1], Mai Mohamed[1], Dimitra Keramisanou[1], Ioannis Gelis[1]
[1]Department of Chemistry, University of South Florida

NMR assignment of full-length hsCdc37

Cdc37 is a 90 kDa dimeric protein that acts as a substrate specificity co-chaperone for the Hsp90 machinery, recruiting oncogenic protein kinases to Hsp90 for folding, stabilization and activation. To understand the role of Cdc37 in cancer biology we initiated a high resolution biophysical study. The large content of intrinsically disordered regions in Cdc37 suggests that NMR is the most appropriate tool to study its function; however, the molecular weight of the full-length dimer falls well above the limit of “conventional” biomolecular NMR. To circumvent this limitation we use Methyl-TROSY NMR in combination with a domain parsing approach. Isolated domains and domain fragments of Cdc37 have been cloned into appropriate expression vectors, labeled by expression in E. Coli and purified by standard techniques. The resulting spectra exhibit excellent sensitivity and resolution and provide the basis for future functional studies.

OR-01 **Stacia Gorniak**[1], **Charlotte Wilkinson**[1], Kerriann Greenhalgh[1], Edward Turos[1]
[1]Department of Chemistry, University of South Florida

Synthesis of Lidocaine-conjugated Polyacrylate Nanoparticles

Nanoparticles have been studied for their ability to encapsulate active drugs to increase solubility and bioactivity in the body. Polyacrylate nanoparticles have a distinct structure that allows for both encapsulation and the polymerization of drug conjugates into the backbone of the nanoparticle. The goal of this research is to create a polyacrylate nanoparticle emulsion wherein lidocaine molecules are conjugated to the polyacrylate framework. Lidocaine acrylate is synthesized, purified, and polymerized in solution with butylacrylate and methylmethacrylate monomers while in water to form the nanoparticle emulsion. This nanoparticle emulsion can then be used as a form of wound covering that also reduces pain. The data from this project will be able to assist in the synthesis of other drug-conjugated polyacrylates for use in both topical wound care and intravenous applications.

OR-02 **Andrea Lemus**[1], Linda Barbeto[1], James W. Leahy[1]
[1]Department of Chemistry, University of South Florida

Novel Organic Compounds to Target Heat Shock Proteins in Leishmania Parasites

Leishmaniasis is a neglected disease prevalent in developing countries caused by protozoa of the genus Leishmania. The disease is transmitted to humans through the bite of sand flies that carry the microorganism. The most common symptom of leishmaniasis is the appearance of large sores in the skin at the site of the insect bite. No vaccine currently exists and there are limited effective treatments, some of which are toxic. The goal of our research project is to synthesize a novel organic compound that will target heat shock proteins, which appear to aid the protozoan differentiation, based on a screening campaign conducted in the laboratories of Professor Dennis Kyle. We are working on a convergent synthesis of active molecules that will allow the rapid analysis of chemical activity in order to determine molecules with optimal activity and pharmacokinetic properties.

OR-03 **Jesse Revenis**[1], Frankie Costanza[1], Jianfeng Cai[1]
[1]Department of Chemistry, University of South Florida

Antimicrobial Polymers Synthesized Using mPEG-amine To Polymerize N-carboxyanhydrides

The widespread use and abuse of antibiotics for medical and agricultural purposes has lead to increasing bacterial resistance, which can bring an end to modern medicine if alternatives don't become available. This problem has lead to the development of polymers that kill bacteria by exploiting the difference in charge between human and bacterial cell membranes. Our polymers were created using mPEG-amine to polymerize N-carboxyanhydrides (NCAs) in a single chain manner. PEG allowed us to create a library of new block and random polymer nanoparticles that can be used as antibacterial agents. Our polymers showed activity against MRSE, Klebsiella Pneumoniae, Bacillus Subtilis, and Pneumonia Aeruginosa. In the future, we are going to use a structure that can initiate polymerization from various sites on the initial reacting polymer, instead of polymerizing in a single chain manner. Hopefully, this will increase the branching of the polymer and we will have better antimicrobial activity.

OR-04 **Thiago Arzua**[1], Li-Mei Jin[1], Christopher Lizardi[1], X. Peter Zhang[1]
[1]Department of Chemistry, University of South Florida

Highly Efficient Synthesis of Fluoroazocompounds by Metalloradical Catalysis

Azocompounds are organic compounds used component of liquid crystal, and are also connected to the biosynthesis of certain steroids. Their photochemistry is especially important with fluoroazocompounds, a class of azocompounds that still has difficulties in being synthesized. The best current method requires the catalytic oxidation of anilines under basic conditions. Such method suffers from low yields, with side products and a poor substrate scope. It is, thus, desirable to develop a more efficient method of synthesis. This project presents a highly effective catalytic system, based on a Co(II) metalloradical catalyst, which uses fluoroaryl azides as nitrogen source, producing the corresponding fluoroazocompound in high yields. Preliminary results point to an environment friendly new method of azocompounds synthesis – since N2 is the only byproduct –that occurs at mild conditions. Being broad and simple, this new synthesis protocol could be a step into a new type of photochemistry, with countless practical applications.

OR-05 **Sean Johnson**[1], Qigan Cheng[1], X. Peter Zhang[1]
[1]Department of Chemistry, University of South Florida

Design and Synthesis of Chiral Porphyrin Linkers for Construction of Metal-Porphyrin Frameworks

Metal-porphyrin frameworks (MPFs), a unique class of metal-organic frameworks (MOFs) based on the use of porphyrins and metalloporphyrins as the organic linkers, have been recently studied due to their great potential for various applications. To our knowledge, there have not been systematic accounts of using chiral porphyrin linkers for construction of chiral MPFs (MP*Fs). MOFs have been shown with useful applications in many areas, such as catalysis, separation, and gas storage. The use of chiral organic linkers in MPFs may lead to interesting applications in asymmetric catalysis and chiral separation. In view of unique properties of chiral porphyrins, we have been in the process of building MP*Fs and exploring their applications as heterogeneous asymmetric catalysts for synthesis of pharmaceutically important chiral molecules. This project aims at the design and synthesis of new chiral porphyrins that will been incorporated as linkers for construction of MP*Fs. To this end, chiral porphyrins containing additional carboxylic acid functionalities have been prepared through modern synthetic methods. In collaboration with Prof. Ma's group, these chiral porphyrin carboxylate compounds are being used as the linking units for construction of the frameworks. These MP*Fs will be explored for applications in asymmetric catalysis.

OR-06 **Victoria Wharton-Lake**[1], Faeez Mahzamani[1], Edward Turos[1]
[1]Department of Chemistry, University of South Florida

A Study of the Optical Properties of Chiral Polymer Nanoparticles

As more and more bacteria become resistant to medication, researchers are faced with finding new ways to combat this phenomenon. Within recent years, one of these methods has been the use of polyacrylate nanoparticle emulsions as a drug delivery method. Using this nanoparticle model we aim to introduce chirality into a nanoparticle system. A series of emulsions containing various ratios of D and L menthol acrylate were composed and run through the polarimeter and circular dichroism in order to study the optical properties. The findings are expected to have a linear trend with increasing chirality. However, since circular dichroism has never been used to observe these nanoparticles, the results should add to further characterization. From the findings, a chiral antibiotic will be introduced into the most optimal emulsion mixture with the hope of finding preferential uptake of one enantiomer of the antibiotic into the nanoparticle emulsion.

OR-07 **Monica Macahuachi**[1], Faeez Mahzamani[1], Edward Turos[1]
[1]Department of Chemistry, University of South Florida

Analysis of emulsion stability and uniformity of chiral polymer nanoparticles

The advancement of polyacrylate nanoparticles provides an innovative vehicle for drug delivery. It promotes the performance of insoluble aqueous antibiotics and strengthens the bio-activity of older classes of antibiotics. This presentation investigates the stability and uniformity of various synthesized chiral polymer nanoparticles to determine which variation of the polymer exhibits the most stable and homogeneous characteristic. A variety of chiral menthol-styrene nanoparticles were prepared by emulsion polymerization that differed by ratios of the monomer components. Through dynamic light scattering analysis we will be able to measure the size and zeta potential to determine the characteristics of each sample. These results may ensure a viable and uniform emulsion suspension of chiral nanoparticles for the potential use as a drug delivery vehicle that may possess efficient properties to separate a racemic mixture of antibiotics.

OR-08 **Marcus Farmer**[1], Jon Antilla[1]
[1]Department of Chemistry, University of South Florida

Evaluation of the True Catalyst in the Chiral Phosphoric Acid Literature

In 2010, two groups (Ishihara and List) reported the purification procedure for C2 symmetric, binol derived chiral phosphoric acids provided not the pure acid, but a mixture of the acid and various alkali and alkaline metal phosphate complexes. As a result, many of the catalyst loadings reported in the literature are too high as only a fraction of the compound is actually catalyzing the reaction and in some cases, it is the metal phosphate complex that is the active catalyst in the reaction. The purpose of this work has been to survey some important reactions published in the Antilla group and to elucidate the true catalyst so that the reaction efficiency can be improved and the mode of activation for these reactions can be properly understood.

OR-09 **Jennifer Le**[1], Xin Cui[1], Yang Hu[1], Silke Evdokimov[1], X. Peter Zhang[1]
[1]Department of Chemistry, University of South Florida

Asymmetric Synthesis of Amitifadine: A New Approach via Co(II) Metalloradical Catalysis

Amitifadine, an azobicyclo[3.1.0]hexane, is an investigational antidepressant that functions as a triple reuptake inhibitor of serotonin, norepinephrine, and dopamine. The existing synthesis, developed by Merck scientists in 2006, for Amitifadine requires a chiral starting material, suffers from moderate diastereoselectivity, and involves a difficult recrystallization process. To address these weaknesses, this work aims to develop a new synthesis using only achiral starting materials and cobalt(II) porphyrin catalyzed asymmetric cyclopropanation developed by the Zhang group as the key step. The structures of intermediates were confirmed using NMR spectroscopy, HPLC, and X-ray crystallography. Results indicate that this new method can achieve efficient synthesis of the product with high enantiopurity and diastereocontrol. This work provides direct evidence for the application of the cobalt(II) metalloradical catalysis towards drug development.

OR-10 **James Giarrusso**[1], Jordany Maignan[1], Tina Mutka[1], Dennis E. Kyle[2], Roman Manetsch[1]
[1]Department of Chemistry, University of South Florida, [2]College of Public Health, University of South Florida

Synthesis, Antimalarial Activity, and Physicochemical Properties of 7-(2-Phenoxyethoxy)-4(1H)-quinolones

Malaria is one of the deadliest diseases man has ever faced. About 40% of the world's population is at risk with over 600,000 deaths occurring last year. Current drugs are available, however increasing resistance of the parasite that causes the disease and the mosquito vector has caused a need for novel drugs to combat this threat. Over 20 years ago, quinolone ester, ICI56,780 was found to be active in rhesus monkeys, the gold standard. However, the poor solubility of the drug and the sudden adaptation of the parasite to resist the drug caused the quinolone ester to be abandoned. Due to technological advances, compounds can be more readily assessed by preclinical efficacy trials, and their physicochemical properties measured. Our structure-activity relationship and structure-property relationship data of ICI56,780 suggest that the molecule and its analogues could prove effective in the treatment of malaria by addressing the molecule's solubility, stability, and resistance issues.

OR-11 **Andrea A. Lemus[1], Catherine Costa[1], Marilyn Medina[1], Piero Carletti Bonomo[1]**, Ankush Kanwar[1], Benjamin J. Eduful[1], Linda Barbeto[1], James Leahy[1]
[1]Department of Chemistry, University of South Florida

Work Toward the Discovery and Synthesis of Novel Antileishmanial Agents

Leishmaniasis is a neglected disease prevalent in developing countries caused by protozoa of the genus Leishmania. The disease is transmitted to humans through the bite of sand flies that carry the microorganism. The most common symptom of leishmaniasis is the appearance of large sores in the skin at the site of the insect bite. No vaccine currently exists and there are limited effective treatments, some of which are toxic. The goal of our research project is to synthesize a novel organic compound that will target heat shock proteins, which appear to aid the protozoan differentiation, based on a screening campaign conducted in the laboratories of Professor Dennis Kyle. We are working on a convergent synthesis of active molecules that will allow for the rapid analysis of structure-activity relationships in order to determine molecules with optimal activity and pharmacokinetic properties.

OR-12 **Vidya Hanuman**[1], Priyesh Jain[1], Anthony Gebhard[1], Rajesh Nair[1], Lori Hazelhurst[1], Mark L. McLaughlin[1]
[1]Department of Chemistry, University of South Florida

Improving the Pharmacokinetics of Bioactive MTI-101 Using Pegylation

Existing therapeutic agents to treat Multiple Myeloma (MM) have been able to cure the disease causing apoptosis but it's possible for the cancer to develop pathways that avoid apoptosis and become multi-drug resistant. Recently Hazlehurst and co-workers have reported an all d-amino acid peptide HYD1 that induces necrotic cell death in MM. Optimization of linear HYD1 led to the finding of novel cyclic peptide MTI-101 that was found to induce necrosis of MM cells. However, pharmaco-kinetics studies indicated poor half-life of MTI-101. Previous studies have shown that coupling of peptides to pegylating agents and antibodies improves the half-life of the drug. We aim to use this strategy and synthesize several pegylating reagents to prolong the half-life of the cyclic MTI-101 peptide conjugate. The pegylating reagents will be characterized using MALDI-TOF. This ongoing project seeks to induce necrotic cell death of MM tumors using MTI-101 which will help treat MM.

OR-13 **Kevin Ihrig**[1], Arthur Maknenko[1], Kirpal Bisht[1]
[1]Department of Chemistry, University of South Florida

Synthesis of Glucosamine Derived Glycolipid

Glycolipids are biomolecules that organisms synthesize from fatty acids and carbohydrates using enzymes. However the availability of the glycolipds, which have interesting properties, is limited to the ones occurring naturally. Synthetic efforts to make glycolipids involve complex reaction schemes with several protecting/de-protecting steps. Using in-vitro enzyme catalysis offers opportunities for synthesis of non-natural glycolipids without complex synthetic reaction schemes and in fewer steps. In here we describe our efforts towards the synthesis of glucosamine based glycolipids using in-vitro enzyme catalysis.

OR-14 **Brian Guedes**[1], Yi Liang[1], Priyesh Jain[1], Mark McLaughlin[1]
[1]Department of Chemistry, University of South Florida

The Synthesis of Beta Turn Promoters for Cyclopeptidomimetics

An outgrowth of drug-resistant tumor cells is an immense problem in attempting to successfully cure multiple myeloma. HYD1, a particular peptide consisting of 10 D-amino acids, has shown an ability to promote necrotic cell death while inhibiting integrin-mediated ECM adhesion in multiple myeloma. Based on HYD1, our goal then has been to synthesize novel beta turn promoters that will act as linkers in generating a unique cyclic peptide with the tendency to adopt a β-hairpin conformation. The subsequent approach has revolved around those structures that are derivatives of a modified prolinol precursor. Moving forward we expect to produce distinct cyclic peptides capable of enhancing the disruption of cellular adhesion in multiple myeloma.

OR-15 **Trang Tran**[1], Si Yi[1], Jon Antilla[1]
[1]Department of Chemistry, University of South Florida

Enantioselective Nucleophilic Addition of Oxindole Derivatives to Imines catalyzed by Chiral VAPOL Calcium Phosphate

We disclosed a novel-high yielding and highly enantioselective chiral zinc VAPOL-phosphate catalyzed Mannich-reaction of 3-substituted oxindoles with benzoyl imine. The reaction condition, which reacts these two substrates in DCM under room temperature by using chiral zinc VAPOL phosphate as catalyst showed effective for this catalytic enantioselective Mannich reaction.

OR-16 **Christa Creech**[1], Mukul Kanauja[1], Corey P. Causey[1]
[1]Department of Chemistry, University of North Florida

Design and Synthesis of an Activity-based Protein Profiline (ABPP) Reagent for the Investigation of Newly Discovered AMPylator Enzymes.

Post translational modifications have long been recognized as a means by which protein structures, and subsequent functions, can be altered. Recently, reports of a novel PTM have emerged in the literature. This modification, termed AMPylation, results from the transfer of the adenosyl monophosphate moiety of ATP to a threonine and tyrosine residues in protein substrates, with concomitant release of pyrophosphate. While the transfer of phosphate groups from ATP to proteins has been extensively studied, these new reports offer the first examples of transfer of the AMP portion. The goal of this work is to develop molecular probes that target AMPylators in an effort to gain insight into the catalytic mechanisms and substrate specificities of these enzymes. Current efforts are focused on the synthesis of a new ATP analog that will serve as a useful ABPP reagent to target this family of enzymes.

OR-17 **Mikhail Marchenko**[1], Christiam Campero[1], Corey P. Causey[1]
[1]Department of Chemistry, University of North Florida

Design and Synthesis of an Activity-based Protein Profiling (ABPP) Reagent Targeting Agmatine Deiminase Enzymes

The agmatine deiminase family of enzymes is a potential target for the development of therapeutic agents for the treatment of some bacterial infections. Agmatine is a small naturally occurring molecule that arises from the enzymatic decarboxylation of, arginine. Agmatine deiminase enzymes (AgDs) are involved in the breakdown of agmatine in vivo. These enzymes are responsible for the hydrolytic conversion of agmatine into N-carbamoyl putrecine and ammonia. This project is focused on the synthesis of an Activity-Based Protein Profiling (ABPP) probe that will fluorescently label agmatine deiminase enzymes; this probe will allow us to set up a florescence polarization screen experiment. In short, with this probe, we will be able to quickly screen thousands of molecules in search of one (or a few) that provide better inhibition of this enzyme family.

OR-18 **Bri Gordon**[1], Steven T. Shipman[1]
[1]Division of Natural Sciences New College of Florida

Waveguide Chirped-Pulse Fourier Transform Microwave Spectra of Small Alkylthiols

The microwave spectra of three small alkylthiols (ethanethiol, 1-propanethiol, and 2-propanethiol) were measured from 8.7—26.5 GHz with waveguide chirped-pulse Fourier transform microwave spectroscopy (CP-FTMW) at ~250 K. All three of these alkylthiols can be either trans or gauche with respect to the C-S bond, and both conformers are present in reasonable abundance for each molecule. In fact, transitions from the 34S isotopically-substituted species are also easily seen in natural abundance. These molecules have been previously studied but our spectrometer is significantly more sensitive than prior instruments and we have been able to extend these prior fits to substantially higher values of the J rotational constant.

OR-19 **M. Christian Metzger**[1], Steven T. Shipman[1]
[1]Division of Natural Sciences New College of Florida

Waveguide Chipred-Pulse Fouier Transform Microwave Spectra of Isopropylamine ane 2-(methoxy-^{13}C)-ethanol

The methoxy-^{13}C isotopomer of 2-methoxyethanol was synthesized through the sodium hydride catalyzed reaction of ethylene glycol with iodomethane. The pure rotational spectra of isopropylamine and this isotopomer were recorded from 8.7 - 26.5 GHz at -20ºC with a waveguide chirped-pulse Fourier transform microwave spectrometer. Previous literature values for the ground state of trans-isopropylamine have been refined by the assignment of 132 peaks to an RMS of 80 kHz, but excited vibrational states could not be fit due to the lack of strong transitions in the observed range. An automated spectral fitting program and previous assignments of the naturally abundant species by Maria Phillips will be used to fit the ground and several excited vibrational states of the all-gauche conformer of 2-(methoxy-^{13}C)-ethanol. Progress on this species and both trans and gauche isopropylamine will be presented.

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