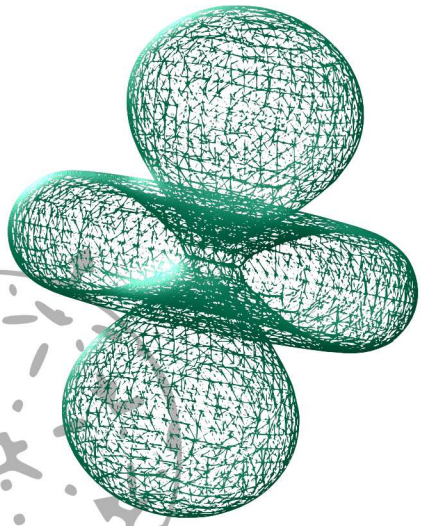
10th Raymond N. Castle Student Research Conference

April 21, 2012



USF

University of South Florida
Department of Chemistry
4202 E. Fowler Avenue, CHE105
Tampa, Florida 33620

http://chemistry.usf.edu

10th Raymond N. Castle Student Research Conference

Proceedings Table of Contents

Welcome from the Castle Conference Committee

Dear Colleagues and Friends,

Welcome to the 10th Raymond N. Castle Student Research Conference hosted by the University of South Florida. In honor of Dr. Raymond N. Castle, this Conference was created to promote his goals of scientific collaboration and science education.

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

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

Lastly, we would like to thank all that chose to volunteer their time and efforts, particularly the judges, and Dr. Patricia Muisener and Dr. Arjan van der Vaart 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 Agilent, Tampa Bay Local Section of the American Chemical Society, University of South Florida College of Arts and Sciences, and University of South Florida ResearchOne, as well as the multiple other sponsors and affiliates who have generously contributed to this event. Most importantly, this conference would not exist without the efforts of those of you presenting your research today. Therefore, we gratefully acknowledge you and your research advisors, as well as all in attendance. Thank you all and we hope you enjoy and learn from the 10th Raymond N. Castle Student Research Conference.

Sincerely,

The Castle Conference Committee

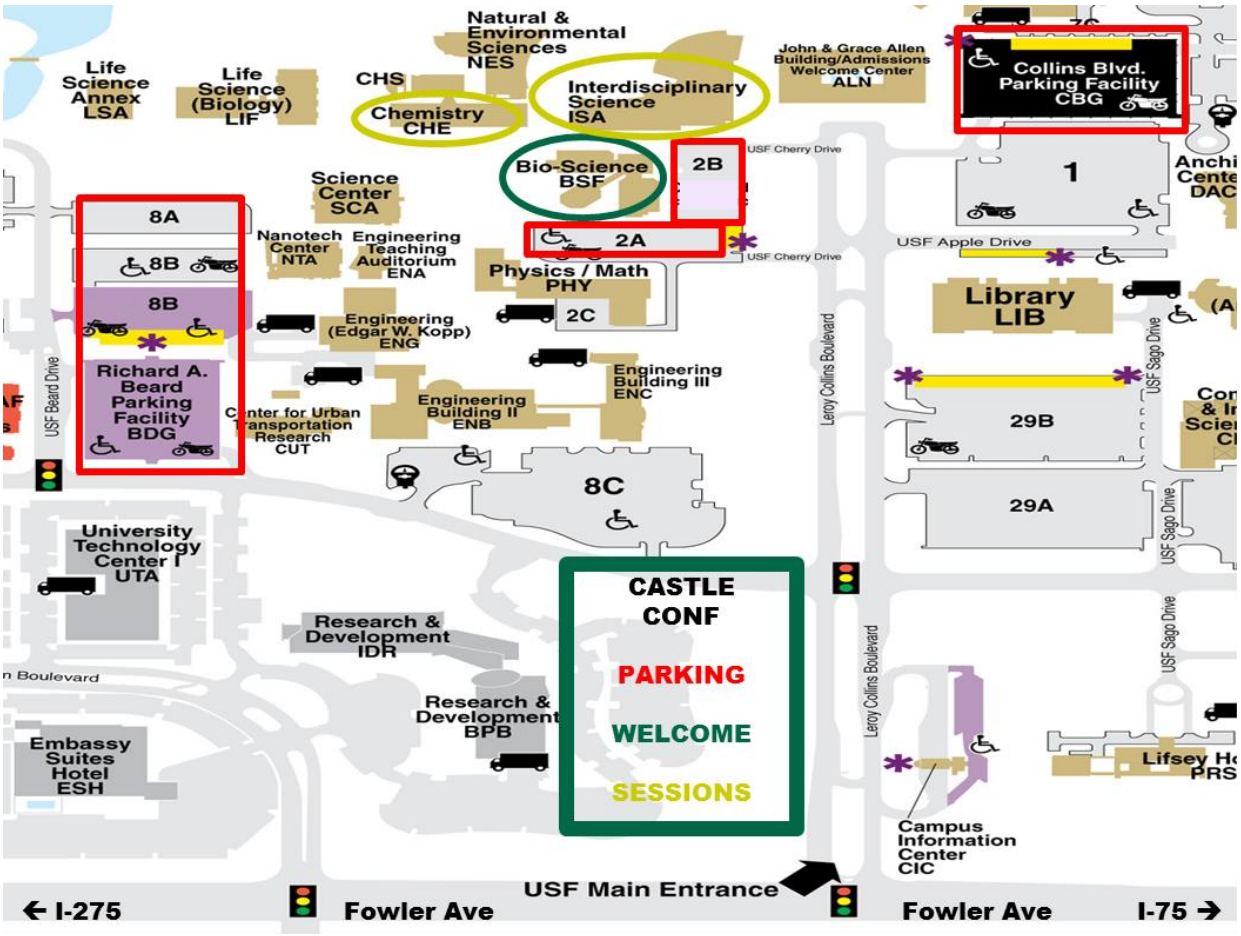
10th Raymond N. Castle Student Research Conference Committee

Committee Members:
Christi Whittington (Chair)
William Maza (Co-Chair)
Rachel Alessio
Christian Cioce
Kristin Costelow
Jason Cuce
Danielle Demers
Joseph Gill
Alaa Hashim
Seongmin Hong
Mu Kim
Yaqiong (Rosemary) Li
Silke Lopez de Mesa
Hasnaa Mouttaki
Ranjani Muralidharan
Justin White

Faculty Advisors:
Dr. Patricia Muisener
Dr. Arjan van der Vaart

Web Support:
Christian Cioce

Building Map



Schedule of Events

Saturday, April 21, 2012

8:00 AM	-	8:30 AM	**Welcome Session** - *Registration and Breakfast*	BSF Lobby
8:30 AM	-	8:45 AM	**Castle Conference Introduction**	ISA 1051
8:45 AM	-	10:30 AM	**Morning Talk Sessions I & II** *Graduate Student Presentations*	ISA 1051 & ISA 1061
10:30 AM	-	10:45 AM	**Break**	
10:45 AM	-	12:00 PM	**Plenary Speaker - Dr. Kim Janda** *Creating Successful Vaccines Against Drugs of Abuse*	ISA 1051
12:00 PM	-	3:00 PM	**Lunch** *Sponsored by Agilent*	BSF Lobby
12:00 PM	-	3:00 PM	**Poster Session** *Graduate and Undergraduate Presentations*	CHE 1st Floor Classrooms
3:00 PM	-	3:15 PM	**Break**	
3:15 PM	-	5:00 PM	**Afternoon Talk Sessions I & II** *Graduate Student Presentations*	ISA 1051 & ISA 1061
5:00 PM	-	5:15 PM	**Break**	
5:15 PM	-	5:30 PM	**Awards Ceremony**	ISA 1051

Professor Raymond N. Castle

1916 – 1999

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

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

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

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

Dr. Kim D. Janda

Plenary Speaker

Dr. Kim D. Janda received a Bachelor of Science degree in Clinical Chemistry from the University of South Florida in 1980. He then joined the Chemistry program at the University of Arizona as a graduate student where he received a Master of Science degree in 1983 and Doctor of Philosophy degree the following year, 1984. While at the University of Arizona, Dr. Janda's research focused on new synthetic methods in the synthesis of the anti-tumor agent Deoxybouvardin. Dr. Janda later accepted a post-doctoral position in the Department of Molecular Biology at the Scripps Research Institute in La Jolla, California.

In 1991, Dr. Janda was offered an Associate Professor position in the Department of Molecular Biology at the Scripps Research Institute in La Jolla, where he continues today, earning a full-tenured Professorship in 1996. Dr. Janda currently holds joint appointments in the Department of Molecular Biology at Scripps as well as the Skaggs Institute for Chemical Biology (also in La Jolla, California). Dr. Janda is also the Director of the Worm Institute of Research and Medicine located at the Scripps Research Institute in La Jolla.

Dr. Janda's on-going research covers a range of topics, including the biochemistry and mechanisms of action of addictive substances, as well as development of immunopharmacotherapies for treatment of addiction, detection, sequestration, and mitigation of chemical/biological warfare agents, development of oncological therapeutic agents, elucidation of mechanisms of intercellular communication between bacteria, design and synthesis of catalytic antibodies, and development of phage display technologies, to name a few. His many honors and awards include an Alfred P Sloan Fellowship in 1993, Arthur C Cope Scholar Award in 1999, and Elected Fellow of the American Association for the Advancement of Science in 2003. Dr. Janda has helped start three companies and has published more than 400 peer-reviewed works over his illustrious career.

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.

James A. Haley Veteran's Hospital

Andrea N. McCray, Ph.D.

University of Tampa

Eric Ballard, Ph.D.
Glenroy (Dean) Martin, Ph.D.
Eric Werner, Ph.D.

Florida International University

Jaroslava Miksovska, Ph.D.

Florida Southern College

Kim Fields, Ph.D.

Florida State University

A. Carl Whittington, Ph.D.

University of South Florida – St. Petersburg

Leon Hardy, Ph.D.

University of South Florida – Tampa

Laura Anderson, Ph.D.
Bill Baker, Ph.D.
Jianfeng Cai, Ph.D.
Ying-Hua Chung, Ph.D.
Wayne Guida, Ph.D.
Sheeba Varghese Gupta, Ph.D.
Julie Harmon, Ph.D.
Jess Jones, Ph.D.
John Kuhn, Ph.D.
Dennis Kyle, Ph.D.
Randy Larsen, Ph.D.
Xiao (Sheryl) Li, Ph.D.
Vicky Lykourinou, Ph.D.
Shengqian Ma, Ph.D.
David Merkler, Ph.D.
Patricia Muisener, Ph.D.
Robert Potter, Ph.D.
Rebecca O'Malley, Ph.D.
Santiago Sandi-Urena, Ph.D.
Justin Spiriti, Ph.D.
Srinivas Tipparaju, Ph.D.
Jeremiah Tipton, Ph.D.
Edward Turos, Ph.D.
Arjan van der Vaart, Ph.D.
Solomon Weldegirma, Ph.D.
Lukasz Wojtas, Ph.D.
H. Lee Woodcock, III, Ph.D.
Juanjuan Yin, Ph.D.

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

Sponsors

Tampa Bay Local Section

Tampa Bay Section of the American Chemical Society
4202 E. Fowler Ave., CHE 205
Tampa, FL 33620
Phone: (813) 974-2144

USF College of Arts & Sciences
4202 E. Fowler Ave., CPR 107
Tampa, FL 33620
Phone: (813) 974-2804

Agilent Technologies
5301 Stevens Creek Blvd
Santa Clara, CA 95051
Phone: (877) 424-4536

McAlister's Deli
11402 N. 30th Street
Tampa, FL 33612
Phone: (813) 341-1160

Alpha Graphics
4209 W Kennedy Blvd.
Tampa, FL 33609
Phone: (813) 289-4663

Clear Springs Land Company, LLC
690 E. Davidson Street
Bartow, FL 33830
Phone: (863) 534-1292

USF Research One
3702 Spectrum Blvd, Suite 175
Tampa, FL 33612
Phone: (813) 974-5570

Affiliates

Cengage Learning
P.O. Box 6904
Florence, KY 41022
Phone: (800) 487-8488

Fisher Scientific
300 Industry Drive
Pittsburgh, PA 15275
Phone: (800) 766-7000

Sigma-Aldrich Corp.
3050 Spruce St.
St. Louis, MO 63103
Phone: (800) 521-8956

Graduate Talks Morning Session I (ISA 1051)

Session Chair: Justin White

8:45- 9:00 AM **Daniel Dempsey**
Recombinant expression and characterization of the glycine N-acyltransferase family

9:00- 9:15 AM **Christi L. Whittington**
Nitrate/nitrite selectivity of Zn(II) porphine

9:15- 9:30 AM **Chelsea D. Frost**
Cardiac hormones are c-Jun-N-Terminal kinase 2-inhibiting peptides

9:30- 9:45 AM **Break**

9:45-10:00 AM **Aleksandra Karolak**
Importance of local interactions for the stability of inhibitory helix 1 of Ets-1 in the apo state

10:00-10:15 AM **Sumit Handa**
1-deoxy-D-xylulose-5-phosphate synthase (DXS) from Plasmodium vivax, a crucial enzyme required for survival of malaria parasite

Graduate Talks Morning Session II (ISA 1061)

Session Chair: Rachael Alessio

8:45- 9:00 AM **Jordany R. Maignan**
Synthesis, antimalarial activity, and physicochemical properties of 7-(2-Phenoxyethoxy)-4(1H)-quinolones

9:00- 9:15 AM **Yuri Pevzner**
Development of the CHARMM Interface and Graphics web portal as a platform for computer aided drug design

9:15- 9:30 AM **Chris Witowski**
Enhanced secondary metabolite production by microbial co-cultures

9:30- 9:45 AM **Break**

9:45-10:00 AM **Adrian Villalta-Cerdas**
Self-explaining experiences in large enrollment general chemistry courses

10:00-10:15 AM **Kurt S Van Horn**
Studies on 2,4-diaminoquinazolines as anti-parasitic agents

10:15-10:30 AM **Sai Lakshmana**
Unlocking the binding and reaction mechanism of hydroxyurea substrates as biological nitric oxide donors

Graduate Talks Afternoon Session I (ISA 1051)

Session Chair: Jason Cuce

3:15- 3:30 PM **Tao Liang**
Chiral Brønsted acid catalyzed pinacol rearrangement

3:30- 3:45 PM **Xue Xu**
Co(Porphyrin) catalyzed asymmetric dihydrofuran formation. Developed from "unwanted"

3:45- 4:00 PM **Ali Husain**
Synthesis of pseudo-cyclodextrin resorcin[4]arene via click chemistry

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

4:15- 4:30 PM **Rachael Alessio**
Removal of Bisphenol A model compounds and related substances using Octolig®

4:30- 4:45 PM **Silke Lopez de Mesa**
Co(II) porphyrin-catalyzed inter- and intramolecular cyclopropanation with halodiazoacetates

4:45- 5:00 PM **Arun Babu Kumar**
Design and synthesis of ambient light stable 3-trifluoromethyl-3-aryldiazirine photo probes

Graduate Talks Afternoon Session II (ISA 1061)

Session Chair: Hasnaa Mouttaki

3:15- 3:30 PM **Wenyang Gao**
Construction of metal-triazolate frameworks based upon bifunctional ligands

3:30- 3:45 PM **Matthew J. Andrus**
Properties of a non-equilibrium state of the photoactive magnet K0.2Co1.3[Fe(CN)6]•1.6H2O

3:45- 4:00 PM **Christian R Cioce**
Development of accurate and transferable potential energy functions for methane and nitrogen

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

4:15- 4:30 PM **Yao Chen**
Exploration of mesoporous MOFs as new platforms for biocatalysis application

4:30- 4:45 PM **Tony Pham**
Computational studies of CO_2 sorption in an ultramicroporous metal-organic framework

4:45- 5:00 PM **Andrew Powers**
Extension of 1,3-dipolar cycloaddition reactions to azides and acetylides both within metal coordination spheres: Development of the iClick reaction

The Barbara and Dean F. Martin Poster Session
CHE 103
Session Chair: Christi Whittington

Graduate:	Group GP	All Disciplines

The Clear Springs Land Poster Session
CHE 101
Session Chair: William Maza

Undergraduate:	Group ABC	Analytical, Biochemistry, Chemical Education,
	Group CIP	Computational, Inorganic, and Physical

The Solomon T. Weldegirma Poster Session
CHE 101A
Session Chair: Kristin Costelow

Undergraduate:	Group BO	Organic
	Group NP	Natural Products

Graduate Talks

GT-01 **Daniel Dempsey**[1], David J. Merkler[1]
[1]Department of Chemistry, University of South Florida

Recombinant expression and characterization of the glycine N-acyltransferase family

Fatty acid amides are an interesting class of cell signaling molecules that are composed of N-acylglycines, N-acyldopamines, N-acylethanolamines, and primary fatty acid amides. Strong evidence suggests that these molecules are interrelated biosynthetically however a direct pathway still remains elusive. There are two proposed pathways for the formation of long chain N-acylglycines which include the glycine dependent route (R-CO-CoA+ NH_2-CH_2-COOH → R-CO-NH-CH_2-COOH + CoA) and the ethanolamine dependent route (R-CO-NH-CH_2-CH_2-OH → R-CO-NH-CH_2-CHO → R-CO-NH-CH_2-COOH). It is hypothesized that the predominant pathway for the formation of N-acylglycines is the conjugation of glycine to the long chain acyl-CoA thioester. Four putative mammalian glycine N-acyltransferase enzymes have been identified and are hypothesized to have an important role in long chain N-acylglycine biosynthesis. Complete characterization of these enzymes is critical for a full understanding of the biosynthetic pathway for the production of the fatty acid amides.

GT-02 **Christi L. Whittington**[1], William A. Maza[1], H. Lee Woodcock, III[1], Randy W. Larsen[1]
[1]Department of Chemistry, University of South Florida

Nitrate/nitrite selectivity of Zn(II) porphine

Selectivity of small molecule binding to metalloporphyrins is important for numerous applications in biology and industry, ranging from sensors to highly efficient catalysts. Of specific interest is the selectivity of nitrite/nitrate associated with Zn(II) porphyrins, as this system may serve as a model for the binding selectivity of Zn-metal clusters towards a wide range of nitrogen oxides. To explain selectivity of nitrite over nitrate by Zn(II)[5,10,15,20-tetraphenyl porphyrin] (ZnTPP), and an increase in affinity for both nitrite and nitrate when pyridine is present as a proximal base, the interactions of a model for ZnTPP, Zn(II) Porphine (ZnP), with nitrite, nitrate, and pyridine were examined computationally using Density Functional Theory (DFT). The preference of nitrite binding is rationalized through the metal-to-ligand orbital interactions. These results provide new insights into the electronic nature of porphyrin-ligand interactions.

GT-03 **Chelsea D. Frost**[1], Omar Santana[1,2], Jennifer Nguyen[2], Jennifer Guerrero[1], David L. Vesely[1]
[1]Departments of Medicine, James A. Haley VA Medical Center; USF for Health Sciences; [2]Department of Biology, Wichita State University, Wichita, KS

Cardiac hormones are c-Jun-N-Terminal kinase 2-inhibiting peptides

Derived from the same 126-aa prohormones, four cardiac peptides, namely vessel dilator, long-acting natriuretic peptide (LANP), kaliuretic peptide, and atrial natriuretic peptide (ANP) have potent anticancer effects. The effects of these four cardiac hormones on proliferatory human c-Jun-Nterminal kinase 2 (JNK2) were examined in human small cell lung cancer and human prostate cancer cells. Vessel dilator, LANP, kaliuretic peptide and ANP maximally reduced expression of JNK2 by 89%, 88%, 77%, and 89%, respectively in human small cell lung cancer cells. In human prostate adenocarcinoma cells, JNK2 was maximally decreased 76%, 84%, 57%, and 26% secondary to vessel dilator, LANP, kaliuretic peptide, and ANP, respectively. These results indicate that the four cardiac hormones are significant inhibitors (by up to 89%) of JNK2 -mediated signaling in human small cell lung cancer cells and up to 84% in human prostate adenocarcinoma cells as part of their anticancer mechanism(s) of action.

GT-04 **Aleksandra Karolak**[1], Arjan van der Vaart[1]
[1]Department of Chemistry, University of South Florida

Importance of local interactions for the stability of inhibitory helix 1 of Ets-1 in the apo state

DNA binding induces the unfolding of inhibitory helix 1 (HI-1) in the Ets-1 human transcription factor. To investigate the local interactions that stabilize HI-1 in the apo state, we performed simulations of various Ets-1 constructs. Our results show that the HI-2 and H4 helices stabilize the helical state of HI-1 through specific residue-residue contacts and macrodipolar interactions. The importance of these contacts has been verified by simulations on Ets-1 mutants. Our calculations indicate the importance of local interactions for the stability of the HI-1 helix in the apo protein.

GT-05 **Sumit Handa**[1], Divya Ramamoorthy[1], Tyler Spradling[1], Wayne C. Guida[1], David J. Merkler[1]
[1]Department of Chemistry, University of South Florida

1-deoxy-D-xylulose-5-phosphate synthase (DXS) from Plasmodium vivax, a crucial enzyme required for survival of malaria parasite

Isopentenyl pyrophosphate (IPP) and dimethylallyl pyrophosphate (DMAPP) are the precursor for isoprenoids, which is the largest family of biologically active compounds. These are comprised of ubiquiniones, sterols, dichols, triterpenes, prenylated proteins, chlorophyll, etc. The mevalonate pathway (MVA) was considered as the sole source of IPP and DMAPP for many years, and recently it has been discovered that MVA exist only in eukaryotes, archae, and few eubacteria. An alternate pathway also exists in many eubacteria, green algae, protozoa, and plants. The mevalonate-independent pathway or Non-mevalonate pathway (NMVA) is considered as a target for the development of novel antibacterial, herbicides and anti-malarial because of the nonexistent of this pathway in higher organisms. In this report the first rate determining enzyme 1-deoxy-D-xylulose-5-phosphate (DXS) of NMVA pathway from Plasmodium vivax has been explored. This enzyme has been over-expressed in E.coli without the signaling sequence and transit sequence.

GT-06 **Jordany R. Maignan**[2], C. L. Lichorowic[1,2], T. S. Mutka[2], A. N. LaCrue, D. E. Kyle, R. 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

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.

GT-07 **Yuri Pevzner**[1], H. Lee Woodcock[1]
[1]Department of Chemistry, University of South Florida

Development of the CHARMM Interface and Graphics web 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 a browser. One such interface, CHARMMing (CHARMM interface and graphics), allows researchers to take advantage of the 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 include virtual screening and docking protocols as well as virtual target screening, by which a potential drug candidate can be screened against a library of proteins for potential off-target hits. Such additions would allow researchers to utilize CHARMMing as a drug design platform in addition to its existing capabilities as a molecular simulation front-end.

GT-08 **Chris Witowski**[1], Bill J. Baker[1]
[1]Department of Chemistry, University of South Florida

Enhanced secondary metabolite production by microbial co-cultures

Microorganisms are a rich source of bioactive natural products beneficial in drug discovery. Competitive interactions are a prominent factor in secondary metabolite production. However, typical isolated cultivation techniques do not harness the complete chemical diversity found in their natural environment. Recently, microbial mixed fermentations have been employed to increase yields of previously described metabolites and induce production of novel secondary metabolites. Isolation of a marine endophytic fungus from a *Xestospongia muta* sponge has been shown to inhibit the growth of *Aspergillus niger*, a common foodstuff and laboratory mold contaminant. A co-culture technique of both fungi was utilized and lead to increased metabolite production from pure cultures. The research herein describes the methods and preliminary results from the co-cultures.

GT-09 **Adrian Villalta-Cerdas**[1], Santiago Sandi-Urena[1]
[1]Department of Chemistry, University of South Florida

Self-explaining experiences in large enrollment general chemistry courses

The prevalent trend in chemistry instruction relies on the “classroom game” which posits students in a passive role. In this model, the instructor does all the explaining (thinking), and learning is trivialized to knowing the correct answers (memorizing) and being able to produce them when prompted (regurgitating). Engaging learners in active self-explaining of scientific observations and statements is a promising method to enhance authentic learning. In the present study self-explaining refers to student's generation of inferences about causal connections between objects and events. This study probes the effect of different self-explaining tasks on learning chemistry topics. The conditions used include: solving problems without explaining, explaining solutions to problems, explaining agreement with others' solutions, explaining solutions for others to use, and explaining others' wrong reasoning. These conditions are observed in the naturalistic classroom ecology of a large enrollment General Chemistry course. Preliminary results and ongoing work will be discussed.

GT-10 **Kurt S Van Horn**[1], Xiaohua Zhu[2], Trupti Pandharkar[2], Karl Werbowetz[2], Michael Wang[3], Roman Manetsch[1]
[1]Department of Chemistry, University of South Florida; [2]Division of Medicinal Chemistry and Pharmacognosy, Ohio State University; [3]Department of Pharmaceutical Chemistry, University of Kansas

Studies on 2,4-diaminoquinazolines as anti-parasitic agents

Leishmaniasis is a systemic protozoan disease which has been affected by drug resistance and toxicity effects in current drug therapies. Resistance and long treatments have been a problem with the mainstay antimonials; Amphotericin B has had troubles with formulations and extended treatments and resistance has been encountered in vitro with the first orally bioavailable anti-leishmanial Miltefosine. Because of this, we have synthesized and analyzed the anti-leishmanial activity of a set of 2,4-diaminoquinazoline analogues. These compounds have been found to display single digit micromolar or high nanomolar inhibitory activity against intracellular Leishmania donovani in vitro and also possess selectivity indexes >20 (toxicity against J774 macrophages/activity against intracellular L. donovani), making these compounds interesting leads. Initial in vivo testing has been undertaken in murine models and one compound, KVH 14, has shown to reduce liver parasitemia 36% at an intraperitoneal dose of 15 mg/kg/day for 5 days starting day 7 post-infection.

GT-11 **Sai Lakshmana**[1], H. Lee Woodcock[1], Jacqueline Hargis[1]
[1]Department of Chemistry, University of South Florida

Unlocking the binding and reaction mechanism of hydroxyurea substrates as biological nitric oxide donors

Hydroxyurea is the only FDA approved treatment for sickle cell disease. It is believed the primary mechanism of action is associated with the pharmacological elevation of nitric oxide in the blood; however, the exact details of this are still unclear. In the current work we investigate the details of this process on an atomic scale using a combination of flexible-ligand / flexible-receptor virtual screening methods coupled with energetic interaction decomposition analysis. Utilizing these methods, we are able to elucidate the previously unknown substrate binding modes of a series of hydroxyurea analogs to hemoglobin and the concomitant structural changes of the enzyme. We identify a backbone carbonyl that forms a hydrogen bond with bound substrates. Our results are consistent with kinetic and EPR measurements of hydroxyurea-hemoglobin reactions and a full mechanism is proposed that offers new insights into the possibly of improving substrate binding and/or reactivity.

GT-12 **Tao Liang**[1], Jon Antilla[1]
[1]Department of Chemistry, University of South Florida

Chiral Brønsted acid catalyzed pinacol rearrangement

The pinacol rearrangement has long been known to be difficult to control in terms of regioselectivity and stereoselectivity. In this work, we found that indolyl diols can be treated with chiral phosphoric acids to effect a regio- and enantioselective pinacol rearrangement with high efficiency (yield up to 99%, ee up to 96%).

GT-13 **Xue Xu**[1], Xin Cui[1], Peter Zhang[1]
[1]Department of Chemistry, University of South Florida

Co(Porphyrin) catalyzed asymmetric dihydrofuran formation. Developed from "unwanted"

The asymmetric dihydrofuran formation, a side reaction from Co(Porphyrin) catalyzed cyclopropanation was discovered and further studied. Based on the understanding of reaction mechanism, we were able to tune the reaction toward dihydrofuran formation, thus, high yield of dihydrofuran was isolated with excellent enantioselectivity.

GT-14 **Ali Husain**[1], Kirpal Bisht[1]
[1]Department of Chemistry, University of South Florida

Synthesis of pseudo-cyclodextrin resorcin[4]arene via click chemistry

Several water-soluble pseudo-cyclodextrin resorcin[4]arene were synthesized via Cu(I)-catalyzed Huisgen 1,3-dipolar cycloaddition. Three different resorcin[4]arene derivatives (tetraazide and tetraalkyne with rigid bowl shape structure and octaalkyne with open flexible system) were synthesized as intermediate. Moreover, two different glucose sugar derivatives were prepared by introducing azide and alkyne functional groups on the anomeric position. These resorcin[4]arene intermediates were coupled with the sugar glucose derivatives via 1,2,3-triazole linkages resulting in three new water-soluble multivalent sugar resorcin[4]arenes. All click coupling reactions were well studied and proceed in a short period of time with excellent product yield. All three sugar resorcin[4]arenes were characterized by NMR spectroscopy. Since these sugar resorcin[4]arenes have similar structure to cyclodextrin, we are interested in studying these macromolecules and their activities as cyclodextrin. Different studies in the future can be done with these resorcin[4]arenes such as separation, enantioselective catalysis, phase-transfer catalysis and other studies.

GT-15 **Rachael Alessio**[1], Dean F. Martin[1]
[1]Department of Chemistry, University of South Florida

Removal of Bisphenol A model compounds and related substances using Octolig®

Bisphenol-A, a widely used raw material in the plastics industry, is released to the environment during the manufacturing process and by leaching from consumer products. Recent studies suggest that low-dose amounts of Bisphenol-A may have adverse health effects on humans. The possibility of removing Bisphenol-A from natural water sources or from solvents used to extract the material from consumer products before they enter the market has been studied. The use of model compounds and related substances (4-isopropylphenol, 4-(t-butyl) phenol, and nitrophenols) have been used to study their removal from aqueous solutions using column chromatography and Octolig®, a commercially available material with polyethylenediamine moieties covalently bonded to high-surface area silica gel. The experimental results suggest that 2-nitrophenol and 4-nitrophenol can be successfully removed while 3-nitrophenol, 4-isopropylphenol, and 4-(t-butyl) phenol did not yield a high percent removal. A look at the pK_a of the compounds provides an interesting explanation of the results.

GT-16 **Silke Lopez de Mesa**[1], X. Peter Zhang[1]
[1]Department of Chemistry, University of South Florida

Co(II) porphyrin-catalyzed inter- and intramolecular cyclopropanation with halodiazoacetates

New methods for facile synthesis of diversified cyclopropanes are in demand because of the general utility of these chemical moieties both as selectively reactive intermediates and as substituents in a variety of pharmaceutically and biologically relevant compounds. We have developed a synthetic route towards chiral halogenated cyclopropanes derived from halogenated diazo-compounds undergoing metalloradical-mechanism reactions in the presence of D2-symmetric chiral Co(II)-substituted porphyrin catalysts. Exquisite chemical and chiral selectivity of these reactions can be achieved by steric and electronic reaction control through the choice of porphyrin substituents. Our results indicate that the desired cyclopropanes can be obtained via this method in quantitative yield with up to 99% enantiomeric excess.

GT-17 **Arun Babu Kumar**[1], Roman Manetsch[1]
[1]Department of Chemistry, University of South Florida

Design and synthesis of ambient light stable 3-trifluoromethyl-3-aryldiazirine photo probes

3-trifluoromethyl-3-phenyldiazirine offers very good selectivity and resistance against pseudo-labeling but its photo labiality is such that photodecomposition occurs even under ambient light conditions. This character of 3-trifluoromethyl-3-phenyldiazirine makes its use cumbersome, restricted to constant darkness. Herein, we have developed a photolabel that has very good selectivity and pseudo-labeling resistance as 3-trifluoromethyl-3-phenyldiazirine but enhanced stability to ambient light condition. The development of this photolabel is of immense significance since the cumbersome ordeal of working in darkness, when dealing with diazirine photolabels, could be completely eliminated.

GT-18 **Wenyang Gao**[2], Wuming Yan[2], Rong Cai[2], Lukasz Wojtas[1], Xiaodong Shi, Shengqian Ma[1]
[1]Department of Chemistry, University of South Florida; [2]Department of Chemistry, West Virginia University

Construction of metal-triazolate frameworks based upon bifunctional ligands

Metal-organic frameworks (MOFs) have been promoted into promising candidates with potential applications in gas storage, separation, heterocatalysis, sensor and other areas, due to their intriguing topologies and structural tunability. Carboxylate- and pyridine-based ligands have been predominantly employed for MOF construction. So far however, among the reported various MOFs, 1,2,3-triazolate frameworks have been rarely developed. To combine the merits of 1,2,3-triazolate group with the diverse coordination nature of the carboxylate group, we designed two bifunctional ligands featuring both 1,2,3-triazolate and carboxylate donor groups and constructed two kinds of Metal-Triazolate Frameworks (MTAFs) exhibiting very interesting gas separation and water-stability properties.

GT-19 **Matthew J. Andrus**[1], Matthieu F. Dumont[2], Yitzi M. Calm[2], Elisabeth S. Knowles[2], Mark W. Meisel[2], Khalil A. Abboud, Daniel R. Talham[1]
[1]Department of Chemistry, University of Florida; [2]Department of Physics, University of Florida

Properties of a non-equilibrium state of the photoactive magnet K0.2Co1.3[Fe(CN)6]•1.6H2O

Prussian blue analogues (PBAs) form a class of magnetic coordination polymers some of which exhibit photo-induced changes in magnetism. The PBA K0.2Co1.3[Fe(CN)6]•1.2H2O (CoFe) is known to exhibit a charge transfer induced spin transition (CTIST) that can be induced by light, temperature, or pressure. This is described as a charge transfer from Fe^{III}(LS)-CN-Co^{II}(HS) to Fe^{II}(LS)-CN-Co^{III}(LS) followed by a change in spin state on the cobalt ion. We have previously demonstrated a cooling rate dependence in which a meta-stable strained high spin state can be attained at low temperature. Similar to the low spin state it is photoactive but exhibits changes not previously observed. The chemical and physical properties of this meta-stable state will be reported.

GT-20 **Christian R Cioce**[1], Keith McLaughlin[1], Brant Tudor[1], Giovanni Quiel[1], Jonathan L Belof[2], Brian Space[1]
[1]Department of Chemistry, University of South Florida; [2]Lawrence Livermore National Laboratory

Development of accurate and transferable potential energy functions for methane and nitrogen

Methane, a greenhouse gas, and nitrogen, a major atmospheric constituent, are two of several environmentally relevant gases studied today, as the world "goes green." The need for separation and sequestration of all environmentally threatening gases has been, and is still, highly desired. Metal-organic frameworks (MOFs) are a class of materials which can offer solutions, but accurate simulation of these systems remains a challenge. Herein we present both accurate and transferable potential energy functions for methane and nitrogen which bring new meaning to precision modeling.

GT-21 **Yao Chen**[1], Vasiliki Lykourinou[1], Tran Hoang[1], Li-June Ming[1], Shengqian Ma[1]
[1]Department of Chemistry, University of South Florida

Exploration of mesoporous MOFs as new platforms for biocatalysis application

Metal-organic frameworks (MOFs) have emerged as a new class of materials with tailor-made functions. That the interior of MOFs can be decorated with various organic functional groups for specific interactions with biomolecules makes them attractive as host matrix materials to stabilize proteins and/or enzymes for biocatalysis. Recent developments in mesoporous MOFs have enabled the immobilization of larger enzymes into a crystal lattice, and serve as a new platform to facilitate the study of enzymatic reactions in an otherwise unnatural environment. A series of biomolecules have been examined with several different mesoporous MOFs. For the first time, MP-11, myoglobin and cytochrome c have been successfully immobilized into a mesoporous MOF, exhibiting a hierarchy of pore dimensions. Immobilization of the larger enzyme in large pores and efficient diffusion of substrates through smaller channels is feasible and presents superior catalytic performance compared to mesoporous silica materials.

GT-22 **Tony Pham**[1], Katherine A. Forrest[1], Patrick Nugent[1], Stephen Burd[1], Michael J. Zaworotko[1], Brian Space[1]
[1]Department of Chemistry, University of South Florida

Computational studies of CO_2 sorption in an ultramicroporous metal-organic framework

SIFSIX-3-Zn is an ultramicroporous square-pillared metal-organic framework (MOF) that is composed of a square grid of [{Zn(pyrazine))2}n] and pillars of SiF_6^{2-} ions. Grand Canonical Monte Carlo (GCMC) methods were used to simulate CO_2 sorption in SIFSIX-3-Zn over a wide range of temperatures and at pressures where the experimental CO_2 uptake is saturated. CO_2 sorption was simulated in SIFSIX-3-Zn using highly accurate and transferable nonpolar and polar potentials. The simulated CO_2 sorption isotherms were found to be in outstanding agreement with experimental data. All calculated isotherms show a trend toward a characteristic uptake value based on the loading of one CO_2 molecule per unit cell. The calculated isosteric heats of adsorption (Q_{st}) suggest that SIFSIX-3-Zn has a CO_2 Q_{st} value greater than 40 kJ/mol. The modeled structure shows a favorable interaction between the carbon atoms of CO_2 molecules and the equatorial fluorine atoms of SiF_6^{2-} ions.

GT-23 **Andrew Powers**[1]
[1]Department of Chemistry, University of Florida

Extension of 1,3-dipolar cycloaddition reactions to azides and acetylides both within metal coordination spheres: Development of the iClick reaction.

The Huisgen 1,3-dipolar cycloaddition of organic azides to organic acetylides and the copper catalyzed variant, are powerful carbon-nitrogen bond forming reactions. These reactions are utilized in many aspects of synthetic chemistry, and represent a premier example of Click chemistry. The analogous cycloaddition reaction within the coordination sphere of a metal is much less prevalent, and prior to 2011, all literature examples involved an organoazide adding to a metal-bound acetylide, or an organoacetylide adding to a metal-bound azide. The synthesis of 1,5-bis-triphenylphosphinegold(I) 1,2,3-triazolate via an unprecedented inorganic click (iClick) reaction between PPh_3-Au-N_3 and PPh_3-Au—C≡CPh marks the first example in the literature in which both the azide and acetylide participating in the cycloaddition reaction are within metal coordination spheres. The mechanism of this reaction and the extensions of this reaction methodology to other inorganic systems is discussed.

The Barbara and Dean F. Martin Poster Session Abstracts

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

Formic acid electrooxidation at platinum-modified gold surface: a combined study by electrochemistry and surface enhanced raman spectroscopy

Present Formic acid fuel cell efficiency is limited by low kinetics at the anode indicating the need for effective catalysts to improve the formic acid oxidation. As a prerequisite, we investigated the nature of adsorbed species and reaction intermediates formed in this process. Current work involves the electrooxidation of formic acid and study of the intermediates including formate at platinum-modified gold surface by combination of electrochemistry and in situ Surface enhanced Raman Spectroscopy (SERS).The oxidation currents obtained on Pt/Au electrode is higher than that on bare Pt surface and 200 times higher than that on bare Au surface. The electrochemical results affirm the enhanced catalytic activity of Pt/Au for formic acid oxidation. Furthermore, the SERS formate peak which appears at 300 cm-1 showed a characteristic stark effect. A unique relationship has been observed between the formic acid oxidation currents and the relative SERS intensity of this formate adsorbate on Pt/Au.

GP-02 **Sheshanka Kesani**[1], Dr.Abdul Malik[1]
[1]Department of Chemistry, University of South Florida

Sol-gel niobia material for capillary microextraction

A sol-gel derived polytetrahydrofuran bonded niobia coating was developed for capillary microextraction (CME) hyphenated online with High performance liquid chromatography (HPLC). Niobium pentaethoxide was used as a sol-gel precursor, polytetrahydrofuran as a sol-gel active polymer to develop a CME coating to extract analytes of environmental and biological interest. Additionally a sol-gel derived molecularly imprinted (MIP) niobia material is being developed for precocentration of amyloid beta peptide, which is main component in amyloid plaques in the brains of Alzheimer's patients. As a proof of principle study for the above molecularly imprinted coating first a tryptophan imprinted sol-gel niobia material is being developed. The sensitivity of the coating would be evaluated by extracting tryptophan and phenylalanine. The MIP niobia material could provide an effective means to preconcentrate amylodegenic proteins. Such a preconcentration technique coupled to HPLC could be utilized for early diagnosis of diseases like Diabetes II, Parkinson's disease and Medullary carcinoma.

GP-03 **Chelsea D. Frost**[2], Jennifer P. Nguyen[1], Meghan L. Lane[2], William P. Skelton[3], Michelle Skelton[2], David L. Vesely[2]
[1]Department of Biology, Wichita State University, Wichita, Kansas; [2]Departments of Medicine, James A.Haley VA Medical Center; University of South Florida; [3]University of Florida College of Medicine, Gainesville, Florida

Novel dual inhibitors of vascular endothelial growth factor and VEGFR2 receptor

Derived from the same 126-aa prohormone, four cardiac peptides — vessel dilator, long-acting natriuretic peptide (LANP), kaliuretic peptide (KP), and atrial natriuretic peptide (ANP) — have potent anticancer effects.Four cardiac hormones were evaluated for their ability to directly decrease VEGF/VEGFR2 levels, which are linked to tumor angiogenesis. Response levels were measured by ELISAs in three human cancer cell lines. Over a concentration range of 100 pM to 10 µM, the four peptides downregulated the VEGFR2 receptor in human pancreatic adenocarcinoma, small-cell lung cancer, and prostate cancer cells by at least about half of its basal values. VEGF in human pancreatic carcinoma, small-cell lung cancer, and prostate cancer cells was decreased by an average of about a quarter of its basal values. These four cardiac hormones are the first dual inhibitors of VEGF and the VEGFR2/KDR/Flk-1 tyrosine kinase receptor, presenting a novel means of limiting tumor growth.

GP-04 **Kristen A. Jeffries**[1], David J. Merkler[1]
[1]Department of Chemistry, University of South Florida

Determination of the enzyme responsible for the biosynthesis of long-chain N-Acylglycines in vivo

The fatty acid amides are a broad family of cell signaling lipids. Members of this family include the N-acylamides (NAMs), the N-acylamino acids (NAAs), the N-acyldopamines (NDAs), the N-acylethanolamines (NAEs), and the primary fatty acid amides (PFAMs). Long-chain N-acylglycines (NAGs), a subfamily of the NAAs, have recently been reported in mammalian sources. The metabolism of short chain NAGs is known, however the biosynthetic pathways of long chain NAGs are 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 (GLYAT). Herein, two different GLYATs have been identified in mouse neuroblastoma cells; cells known to produce NAGs. Determination of the enzyme responsible for the biosynthesis of NAGs in vivo is crucial for a full understanding of the metabolism of these molecules.

GP-05 **William A Maza**[1], Randy W. Larsen[1]
[1]Department of Chemistry, University of South Florida

A non-radiative method for measuring donor/acceptor distances using photoacoustic calorimetry: PAC-FRET

Förster resonance energy transfer (FRET), widely used as a method through which to probe conformational dynamics and distances in biological and biomimetic systems, has traditionally been measured using a variety of radiative techniques. In the steady-state these measurements can be complicated by inner-filter effects associated with either the excitation or emitted energy of the donor due to ground-state absorption by the acceptor. In this report, a non-radiative method for measuring FRET between a donor and acceptor is presented using photoacoustic calorimetry, PAC. FRET efficiencies and donor/acceptor distances are measured between the donor (rhodamine B, RB) and acceptor (indigo carmine, IC) with PAC and compared to the same values found by steady-state emission. It was found that at lower concentrations of IC (~24 μM) in a 6 μM RB solution, the FRET distances measured by steady-state emission and PAC were found to be within experimental error.

GP-06 **Khoa Pham**[1], Jaroslava Miksovska[1]
[1]Chemistry and Biochemistry Departement, Florida International University

Conformational changes associated with Ca^{2+}/Mg^{2+} binding to EF-hands of DREAM protein

Downstream Regulatory Element Antagonistic Modulator (DREAM) belongs to neuronal calcium sensors (NCS) family that interact with Ca^{2+}/Mg^{2+} through an EF-hand binding motif. DREAM directly controls activity and assembly of potassium voltage channels and regulates c-fos/prodynorphin gene transcription by binding to DRE sequence in Ca^{2+} dependent manner. Determination of dynamics and energetics of conformational changes associated with Ca^{2+}/Mg^{2+} binding to DREAM is essential for understanding the regulatory and functional mechanism of Ca^{2+} signaling by NCS. DREAM possesses single Trp located in hydrophobic vicinity between EF-2 and EF-3 that is an ideal probe for monitoring ligand-induced structural changes. Ca^{2+} binding induces conformational changes in Trp vicinity based on the blue shift and decrease in Trp emission intensity of the full length and truncated DREAM constructs. Mg^{2+} binding increases Trp emission intensity in truncated DREAM suggesting Mg^{2+} binds to EF3/EF4 in this construct. The impact of Ca^{2+}/Mg^{2+} on DREAM stability will be discussed.

GP-07 **Sumit Handa**[1], Divya Ramamoorthy[1], Tyler Spradling[1], Wayne C. Guida[1], David J. Merkler[1]
[1]Department of Chemistry, University of South Florida

Reaction mechanism and substrate binding study of D. radiodurans 1-deoxy-D-xylulose-5-phosphate synthase

Non-mevalonate pathway (NMVA) is the sole source of isoprenoids synthesis in eubacteria and apicomplexian parasites. 1-deoxy-D-xylulose-5-phosphate Synthase (DXS), the first enzyme catalyzes the rate determining step of NMVA pathway, and its critical for the organism which utilizes this pathway for survival. DXS catalyzes a thiamine pyrophosphate and Mg^{2+}/Mn^{2+} dependent condensation of pyruvate and D-glyceraldehyde-3-phopshate to form 1-deoxy-D-xylulose-5-phosphate (DXP). In this study reaction mechanism of substrate binding is studied using steady-state kinetics (double reciprocal studies, product inhibition, and dead end inhibition) and rational mutant design. This study suggests that binding of substrate in DXS follows random sequential pathway, where binding of substrate is independent with respect to each other.

GP-08 **Ge Bai**[1,3], Shruti Padhee[1], Youhong Niu[1], Rongsheng E. Wang[1], Qiao Qiao[1], Robert Buzzeo[2]
[1]Department of Chemistry, University of South Florida; [2]Department of Biology, CMMB, University of South Florida; [3]Byrd Alzheimer's Institute, University of South Florida

Cellular uptake of an α-AApeptide

Some short and cationic peptides such as the Tat peptide can cross the cell membrane and function as vectors for intracellular delivery. Here we show that an α-AApeptide is able to penetrate the membranes of living cells from the extracellular environment and enter the endosome and cytoplasm of cells. The efficiency of the cellular uptake is comparable to Tat peptide (48-57) of the same length and is unexpectedly superior to the α-peptide with identical functional groups. The mechanism of uptake is similar to that of the Tat peptide through endocytosis by an energy-dependent pathway. Due to the easy synthesis of the α-AApeptides, their resistance to proteolytic hydrolysis, and their low cytotoxicity, α-AApeptides represent a new class of transporters for the delivery of drugs.

GP-09 **MinhPhuong Tran**[1], Emre Seyyal[1], Abdul Malik[1]
[1]Department of Chemistry, University of South Florida

Tantala-based sol-gel coating for capillary microextraction

In sample preparation and separation field, silica-based materials have shown poor stability under extreme pH environments as they pertain to various applications. To overcome such limitations, a tantala-based sol-gel material has been developed to provide stable performance. In this work, we describe the in-situ creation of sol-gel tantala-octadecyl coatings covalently bonded to the inner surface of fused-silica capillaries and their performance in the extraction and preconcentration of a wide variety of compounds via sol-gel capillary microextraction.

GP-10 **Erum Qayyum**[1], John Kuhn[1]
[1]Department of Chemical & Biomedical Engineering, University of South Florida

The role of oxygen as a reactant: Aluminum phosphate as a catalyst for dimethyl ether (DME) formation

Acid catalysts are employed in the methanol dehydration to dimethyl ether (DME). However, acid catalysts such as alumina and silica/alumina come with their own sets of problems for the reaction — they are responsible for the formation of unsaturated hydrocarbons and contribute to coking. Aluminum phosphate was synthesized and studied as a possible catalyst for DME formation. To eliminate or minimize side reactions and increase catalyst activity over silica/alumina and alumina, we investigated methanol oxidation towards DME by varying the different partial pressures of oxygen over a range of temperatures (448-623 K) while keeping the rest of the reactants constant.

GP-11 **Walter G. Gonzalez**[1], Jaroslava Miksovska[1]
[1]Department of Chemistry, University of South Florida

Ca^{2+} and Mg^{2+} induced conformational changes on DREAM (Downstream Regulatory Element Antagonist Modulator) measured by extrinsic hydrophobic probes

DREAM is a multifunctional calcium sensor protein involved in regulation of gene expression and Kv4-channel activity in neuronal cells. Spectroscopic studies of the Ca^{2+} triggered conformational transition in DREAM using ANS extrinsic hydrophobic probes. Fluorescence emission spectra of the ANS-DREAM complexes show an increase in ANS emission intensity for Ca^{2+} and Ca^{2+}/Mg^{2+} bound DREAM consistent with an overall decrease in surface polarity. The dissociation constants were determined to be: K_d1,8-ANS=145±15 μM for the apoform and K_d1,8-ANS= 45±2 μM for Ca^{2+} DREAM. Two binding sites for both ANS isomers were identified using fluorescence lifetime measurements. We propose that one binding site is partially solvent exposed and exhibits a shorter lifetime, τ1,8-ANS=5.9 ns, whereas the second site is buried within the protein matrix with τ1,8-ANS=17.6ns. Moreover, computational simulation of ligand binding support the two site binding model with one site located between EF-3/4 and the second site near Trp169.

GP-12 **Tarah Word**[1], Randy W. Larsen[1]
[1]Department of Chemistry, University of South Florida

Probing the thermodynamics and kinetics of Cytochrome-c surfactant-protein folding by CO photo-initiation methods

Sodium Dodecyl Sulfate (SDS) is known to bind to Cytochrome-c (Cyt-c) resulting in a partial denaturation of the protein, which produces a molten globule (MG) state. However, the nature of the surfactant—protein interaction as well as the SDS concentration dependence of such interactions is still not fully understood. In order to elucidate the mechanism through which surfactant-protein interactions induce denaturation, we have examined the time resolved thermodynamics and kinetics of folding associated with Cyt-c in the presence of SDS. More specifically, time resolved photothermal methods and transient absorption spectroscopy are utilized to probe Cyt-c folding in the presence of SDS. The data obtained from these studies will provide the framework needed to construct enthalpy and molar volume profiles for the earliest events in the folding process.

GP-13 **Luisana Astudillo**[1], Sophie Bernad[2], Valérie Derrien[2], Pierre Sebban[2], Jaroslava Miksovska[1]
[1]Chemistry Department, Florida International University, Miami, FL; [2]University Paris XI, Orsay, France

Impact of the disulfide bond on structural dynamics in vertebrate hexacoordinate hemoglobins

Neuroglobin (Ngb) and cytoglobin (Cygb) belong to the hexacoordinate hemoglobins superfamily. Ngb has a neuro-protective role under hypoxic-ischemic insults; whereas Cygb was proposed to protect cells against oxidative stress. To understand the impact of the disulfide bond on structural dynamics in Ngb and Cygb, we determined kinetics and thermodynamics for CO photo-release and rebinding to both proteins in the presence and absence of the disulfide bond (Ngbred and Cygbred). Our PAC data indicate that CO photo-release from Ngb and Ngbred is monophasic (τ<50 ns) and the disulfide bond impacts the structural volume change upon CO escape. CO migration from the heme pocket of Cygb produces biphasic kinetics with τ_1<50 ns and τ ~150 ns at 20 °C, whereas CO escape from Cygbred occurs within 50 ns suggesting that the disulfide bond strongly modulates the ligand migration pathway. These results suggest different mechanisms of ligand migration in vertebrate hexacoordinate hemoglobins.

GP-14 **Parul Jain**[1], Jennifer Wedebrock[1], Alcantar Norma[2], Julie Harmon[1]
[1]Department of Chemistry, University of South Florida; [2]Department of Chemical and Biomedical Engineering, University of South Florida

Thermal and electrical properties of polycarbonate and BEDO-TTF /polycarbonate films

In the last few decades, there has been growing interest in conductive polymers and composites due to an array of potential applications. Bis (ethylenedioxy) tetrathiafulvalene (BEDO-TTF) is a potential candidate for the preparation of crystalline organic metals, superconductors and metal like composites. The present study addresses the effect of BEDO-TTF on electrical, thermal, and dielectric behavior of Bisphenol A-Polycarbonate and dye doped films, which were produced by the solution casting technique. These films have the potential to be used in sensor or photovoltaic applications. Dielectric analysis (DEA) study revealed multiple transitions in neat and dye doped PC films. The beta relaxation process below Tg exhibited an Arrhenius behavior, whereas above Tg it showed William-Landel-Ferry (WLF) temperature dependence. This study also showed a separation of conductivity and viscoelastic relaxations.

GP-15 **Katherine Forrest**[1], Tony Pham[1], Ashley Mullen[1], Jonathan L. Belof[2], Christian R. Cioce[1], Brian Space[1]
[1]Department of Chemistry, University of South Florida; [2]Lawrence Livermore National Laboratory

Computational study of CO_2 sorption mechanisms in square SiF_6 pillared metal-organic materials

Grand Canonical Monte Carlo (GCMC) simulations were undertaken to characterize CO_2 sorption mechanisms in a square pillared grid metal-organic material (MOM). This MOM is composed of pyrazine linkers which are coordinated to Zn^{2+} ions, forming a 2D square net. Nets are layered using SiF_6^{2-} pillars coordinated axially to the metal centers. $Zn(pyrazine)_2SiF_6$ is notable for rapid, highly preferential CO_2 sorption with room temperature isotherms reaching a maximal loading of 1 CO_2 per unit cell at 0.1 atm. Simulation results at temperatures ≥ 273 K produced isotherms and isosteric heats in good agreement with experiment and revealed a single favored sorption site. At lower temperatures, experimental uptake was negligible, while simulated results produced loading beyond the 1 CO_2 per unit cell maximum. This deviation is attributed to the loading of a secondary sorption site, showing significant occupation only at lower temperatures, which is predicted to dynamically hinder further CO_2 sorption.

GP-16 **Anthony J. D'Angelo**[1,2], Emre Demirocak[2]
[1]Department of Chemical Engineering; University of South Florida; [2]Clean Energy Research Center; University of South Florida

Metal doping and crosshe-linking of grapne-based materials for hydrogen storage

The need for a renewable energy to replace automobile gasoline has become more critical in the past decade. Hydrogen has been proven to be a viable fuel source for automobile usage. Storage of hydrogen at room temperature must be optimized by increasing the surface area and having an adsorption enthalpy between 20-40 KJ/mol. Graphene (G) sheets and graphene oxide (GO) sheets will be utilized as a matrix for hydrogen storage by cross-linking with Boronic ester organic spacers in order to increase surface area. Various solvothermal reaction conditions will be investigated to determine optimum conditions. Metal decorating of Calcium and Platinum on the G/GO matrix will be utilized to enhance Kubas interactions and adsorption enthalpies. Characterization tests of XRD, BET, adsorption enthalpy test, PCT, and FT-IR are employed to optimize and compare the materials in order to develop a suitable storage material.

GP-17 **Yolanda Daza**[1], John N. Kuhn[1]
[1]Department of Chemical and Biomedical Engineering, University of South Florida

Carbon dioxide reduction by oxygen absorption on strontium doped lanthanum cobalt perovskite-type oxides

In 2010, the world estimate carbon dioxide emissions were 30.6 Gt, which constitutes an all-time high. From this number, the US is responsible for emissions around 5 Gt. To prevent a continuous increase, new techniques need to be developed. Perovskites materials have been used as electrodes in fuel cells and conductors. These types of materials, ABO_3, have oxygen deficiencies. In the present work, strontium doped lanthanum cobalt perovskite in different proportions was synthesized to evaluate its properties as a carbon dioxide reductor with temperature programmed techniques. In order for the reduction reaction to take place, an unfavorable Gibbs energy must be overcome. Results showed that $La_{0.75}Sr_{0.25}CoO_3$-σ was the most active catalyst in the reduction of carbon dioxide. Further studies are currently being performed to improve the carbon dioxide conversion using these materials.

GP-18 **David Butcher**[1], Takashi Yonetani[2], Jaroslava Miksovska[1]
[1]Department of Chemistry and Biochemistry, Florida International University, Miami FL; [2]Perelman School of Medicine, University of Pennsylvania, Philadelphia PA

Time-resolved thermodynamics for diatomic ligand interactions with hemoglobin-effector complexes

Heterogenous effectors were shown to modulate allosteric affinity of human hemoglobin for diatomic ligands. To fully understand the impact of the effector binding on the structural and functional properties of hemoglobin we have used photoacoustic calorimetry to probe the time-resolved volume and enthalpy changes associated with the carbon monoxide and oxygen photo-dissociation from hemoglobin-effector complexes. The analysis of photoacoustic traces reveal that L35 association to oxyhemoglobin diminishes the temperature dependence of the observed volume changes and leads to an increase in the reaction enthalpy change coupled to the oxygen photo-dissociation. More pronounced changes in reaction volume and enthalpy were observed for the ligand dissociation from the hemoglobin:inositol hexakisphosphate complex and were attributed to the increased electrostriction effect.

GP-19 **Edward Ofori**[1], Comfort Boateng[2], Jagan R. Etukala[1], Mellissa R. Jacob[2], Larry A. Walker[2], Seth Y. Ablordeppey[1,2]
[1]Florida A & M University; [2]University of Mississippi

Benzothieno- and phenylthio-quinolonium salts: New lead compounds against opportunistic infections.

The incidence and severity of human opportunistic infections (OIs) continues to be alarming in developing countries and especially Sub-Saharan Africa. The AIDS epidemic and the use of powerful immunosuppressants in cancer chemotherapy and organ transplantation have increased the number of people infested. With the emergence of resistance to current drug therapy for OIs, it is imperative to search for new agents to combat OIs. Previous studies in our labs and from others have indicated that the indoloquinoline alkaloid, Cryptolepine, and its analogs possess interesting anti-infective activities. However the toxicity profile of Cryptolepine is less than desired. To improve the potency and toxicity profile of Cryptolepine, we began to explore changes in its tetracyclic structure resulting in the identification of 3-substituted-quinolinium salts as a novel antifungal/antibacterial lead. Several analogs have been synthesized and evaluated for their anti-infective properties against Candida albicans, Cryptococcus neoformans, Aspergillus fumigates and MSRA.

GP-20 **Christopher Lee Lizardi**[1], X. Peter Zhang[1], Hongjian Lu[1], Jingran Tao[1], Joshua Ruppel[1]
[1]Department of Chemistry, University of South Florida

Catalyst design of Co(II) porphyrins and their application to C-H aminations

A library of novel porphyrin catalysts has been designed and synthesized for use in enantioselective and chemo-selective catalytic activation of C-H bonds. With Co(II) as the active metal site, the porphyrin ligand/Co metal catalytic system is able to transform a variety of simple organic precursors into value added amines, diamines, sulfonamides, and cyclophosphoroamidates amongst others. The C-H amination reactions are able to functionalize tertiary, secondary, and even primary C-H bonds through intramolecular amination and tertiary and secondary C-H bonds through intermolecular amination. The ability of this Co(II) porphyrin system is realized via a stepwise radical pathway, which generates a key nitrene intermediate. Following principles of green chemistry, the catalyst system is chemoselective, transforms abundant feedstock reagents, and produces nitrogen gas as the only byproduct.

GP-21 **Sidney Bolden**[1], Seth Y. Ablordeppey[1]
[1]Department of Pharmacy and Pharmaceutical Sciences, Florida A&M University

Design, synthesis, and evaluation of novel 3-substituted thiobenzyl quinolinium salts as anti-infective agents

Worldwide, there are over 33 million people living with AIDS and inevitably all of them will be affected by life-threatening opportunistic infections (incl. *Candida albicans*, *Aspergillus fumigates*, and *Cryptococcus neoformans*). Currently, immuno-compromised patients may be given Amphotericin B and/or Fluconazole as antifungal treatment. Currently, isosteres of the natural product cryptolepine have been shown to be more active against a broader spectrum of microorganisms. The proposed research focuses on open chained 3-substituted thiobenzyl quinolinium salt analogs of cryptolepine. These analogs have been designed using CoMFA molecular modeling, synthesized using microwave assisted synthesis, and evaluated in vitro against a broad spectrum of fungal species. ^{1}H-NMR was used to characterize the compounds and CHN elemental analysis was used to determine purity of the final products before in vitro testing against the most prevalent OI's. The activities of some of the compounds have shown better potency than Amp B, the gold standard drug.

GP-22 **Todd A. Gatlin**[1], Santiago Sandi-Urena[1]
[1]Department of Chemistry, University of South Florida

Learning from teaching: Impact on graduate teaching assistants' self-image and epistemological beliefs

Graduate teaching assistants (GTAs) play a prominent role in chemistry laboratory instruction. However, their role in laboratory instruction education has too often been overlooked in educational research. This presentation reports on a cross-case analysis of two studies designed to investigate how graduate students in two independent and very different learning environments constructed their GTA self-image and what factors contributed to this process. Thirteen GTAs from an expository-based program and eleven GTAs from an inquiry-based program participated in this study. Findings suggest that GTAs' construction of their self-image is shaped through the interaction of several factors: prior experiences, training, beliefs about the nature of knowledge and laboratory work, and involvement in the laboratory setting. Findings from this study can assist introductory chemistry laboratory instructors and coordinators to re-consider, when applicable, their GTA training and continuous support, and may place laboratory reform in a new light of appreciation.

GP-23 **Mubarak O Ameen**[1,4], Laurent Calcul[1], Tina Mutka[2,3,4], Dennis E. Kyle[2,3,4], Cedric Pearce[3,4], Bill J. Baker[1]
[1]Department of Chemistry, University of South Florida; [2]College of Public Health, University of South Florida; [3]Mycosynthetix, Hillsborough, N.C.; [4]Department of Chemistry, University of Ilorin, Ilorin, Nigeria

Isolation of antimalarial principles from fungi

Malaria is a parasitic disease that involves high fevers, shaking chills, flu-like symptoms, and anemia. It is caused by a parasite that is passed from one human to another by the bite of infected *Anopheles* mosquitoes. Pregnant women, patients with HIV/AIDS, non-immune travelers, and in high transmission areas children under five years of age are in high risk of contracting malaria. Thus there is a need to identify novel drug classes since the malaria virus is continuously becoming more and more resistant to drugs. A bioassay-guided fractionation of extracts from the fungi supplied by Mycosynthetix, Inc. has yielded fractions that significantly inhibited the replication of malaria parasite and demonstrated low cytotoxicity. The active fractions were purified using high performance liquid chromatography and further examined by spectroscopic and spectrometric techniques.

GP-24 **Haifan Wu**[1], Shruti Padhee[1], Youhong Niu[1], Ge Bai[1], Yaqiong Li[1], Jianfeng Cai[1]
[1]Department of Chemistry, University of South Florida

Identification of cyclic γ-AApeptides with potent and broad-spectrum antimicrobial activity

Antimicrobial peptides (AMP) have attracted increasing interest because they have the potential to be developed into a new generation of antibiotic agents, which circumvent emerging drug-resistance that occurs with conventional antibiotic treatment. Non-natural antimicrobial oligomeric peptidomimetics hold great promise due to their enhanced potency and in vivo stability. Here we report the design, synthesis, and evaluation of γ-AApeptides based cyclic antimicrobial peptidomimetics. These cyclic γ-AApeptides show very potent broad-spectrum activities against fungi, and a series of clinically-relevant Gram-positive and Gram-negative bacteria, including pathogens that are unresponsive to most antibiotics. These results suggest cyclic antimicrobial γ-AApeptides that have the potential to emerge as a new class of novel antibiotic therapeutics. The findings will also shed further light on the design and optimization of other non-natural antimicrobial oligomers in the future.

GP-25 **Sameer S. Kulkarni**[1], Xiangdong Hu[1], Kenichiro Doi[2], Hong-Gang Wang[2], Roman Manetsch[1]
[1]Department of Chemistry, University of South Florida; [2]Department of Pharmacology, Penn State College of Medicine

Kinetic target guided synthesis for the identification of protein-protein interaction modulators of the Bcl-2 family

Although protein-protein interactions possess significant biological importance, identification of small molecules modulating specific protein-protein interactions remains challenging due to the flexible nature of proteins. Several fragment based approaches have been established to identify fragments with good ligand efficiencies, but fail to provide insights into efficient fragment linkage, complicating the drug discovery process. Herein, we report the development of a novel drug discovery approach that generates only biologically active compounds, kinetic target guided synthesis (TGS). An amidation reaction between thio acids and sulfonyl azides was successfully employed for Bcl-XL-templated screening to identify novel inhibitors of anti-apoptotic protein Bcl-XL. After obtaining encouraging results, this approach was extended to another important protein, Mcl-1. Gratifyingly, some high quality TGS hits were identified and displayed biological activity, comparable with the reported inhibitors of Mcl-1. This validates the kinetic TGS approach as a reliable platform for identification of novel protein-protein interaction modulators.

GP-26 **Chandan Barhate**[1], Alan Maschek[3], C. D. Amsler[2], J. B. McClintock[2], Umesh K. Jinwal[4], Bill J. Baker[1]
[1]Department of Chemistry, University of South Florida; [2]Department of Biology, University of Alabama at Birmingham, Birmingham, AL USA 35294; [3]University of Utah, Department of Medicinal Chemistry, Salt Lake City, UT 84112; [4]Department of Pharmaceutical Sciences, USF College of Pharmacy

Microtubule-associated tau protein reducing activity of Polyhalogenated monoterpenes

Accumulation of tau protein is a hallmark of several neurodegenerative diseases collectively known as tauopathies. A major tau related disorder is Alzheimer's disease and to a lesser extent Parkinson's disease. Screening of organic extracts of *Plocamium cartilagineum* showed considerable reduction in tau protein level. Further purification of extract yielded two acyclic monoterpenes, Anverene (1) and (1E,5E)-1,8-Dibromo-3,4,7-trichloro-3,7-dimethyl-1,5-octadiene and one cyclic monoterpene (1R,2R,4R)-2,4-dichloro-1-((E)-2-chlorovinyl)-1-methyl-5-methylenecyclo hexane (2). Structures and absolute stereochemistry of acyclic monoterpenes were confirmed by single crystal X-ray analysis. Drug screening in cell culture models for tau protein reducing level shows promising results.

GP-27 **Sri Krishna Nimmagadda**[1], Zuhui Zhang[1], Jon C. Antilla[1]
[1]Department of Chemistry, University of South Florida

One-pot synthesis of chiral 1,3-Oxazolidines via intramolecular cyclization of hemiaminal intermediates

Chiral 1,3-Oxazolidines are synthesized by intramolecular cyclization of hemiaminal intermediates. The reaction proceeds in one-pot by the nucleophilic addition of 2-Chloroethanol to N-benzoyl Imines catalyzed by BINOL derived magnesium phosphates, followed by cyclization under mild basic conditions. A wide range of substrates have been demonstrated using this methodology to give products in excellent yields and enantioselectivities.

GP-28 **Xue Xu**[1], Shifa Zhu[1], Xin Cui[1], Peter Zhang[1]
[1]Department of Chemistry, University of South Florida

Highly asymmetric cyclopropanation reactions by Co(II)-based metalloradical catalysis

Metal-catalyzed asymmetric olefin cyclopropanation with diazo reagents stands as one of the most general approaches for the synthesis of optically active cyclopropane derivatives. Cobalt (II) complexes of D2-symmetric chiral amidoporphyrins [Co (D2-Por*)] were first introduced in 2004, now they have emerged as a new class of catalysts for asymmetric cyclopropanation. These metalloradical catalysts have been shown to be highly effective for asymmetric inter- and intra-molecular cyclopropanation with different classes of carbene sources, particularly including acceptor/acceptor-substituted diazo reagents, and excellent diastereoselectivity and enantioselectivity.

GP-29 **Faeez Mahzamani**[1], Edward Turos[1], Denis Kyle[2]
[1]Department of Chemistry, University of South Florida; [2]Department of Global Health, University of South Florida

Use of Clodinafop as an anti-malarial drug

The focus of this project is the synthesis of Clodinafop and its derivatives for treatment of malaria. Clodinafop is part of the Oxyphenoxy propionic acid family of herbicides traditionally used for treatment of spring wheat. Preliminary studies indicate strong positive results against the malaria parasite, combined with low oral toxicity. Derivatives of Clodinafop are currently being developed in hopes of increasing its effectiveness against the malaria parasite.

GP-30 **Michael Veri**[1], Fiona Kearns[1], Shivangi Patel[1], Bill Baker[1]
[1]Department of Chemistry, University of South Florida

Antibitotics from environmental bacteria

Bacterial infections resistant to current available antibiotic courses are becoming more prevalent and kill between fifty and a hundred thousand people every year. This study uncovered a method of isolating novel natural product based antibiotics from bacterial sources. This dead/live study is unique and utilizes several of the most problematic pathogens currently seen in medical science. Original antibiotic scaffolds that have not seen wide use against known pathogens provide the highest probability of success in fighting these infections and natural products chemistry provides the best chance of obtaining these working compounds. The methodology presented has screened over 150 organisms collected from around the world and screens an additional 25 organisms every week. While novel antibiotics have yet to be uncovered, the lottery that is natural products promises results.

The Clear Springs Land Poster Session Abstracts

ABC-01 **Caitlin E. Howell**[1,2], Jiazhi Sun[2,3], Shefung Zhou[2], Kevin B. Sneed[4]
[1]Department of Chemistry, University of South Florida; [2]Department of Pharmaceutical Sciences, University of South Florida; [3]Department of Molecular Medicine, University of South Florida; [4]Department of Pharmacotherapeutics and Clinical Research, University of South Florida

Computational identification and characterization of off-target TKI binding

Tyrosine Kinase Inhibitors (TKIs) are an important group of FDA-approved cancer-treating drugs that have the potential for off-target binding. Repositioning these FDA approved drugs is a cost-effective and time-efficient way to approach drug discovery and can potentially lead to the discovery of a drug that can treat multiple diseases. Through a previous collaborative effort the binding energies of many ligands to specified binding sites (found using an established chemical-protein interactome) were compared by a ZZ_score. This project focuses on employing computational methods to understand how these ligands with relatively good ZZ_scores bind and compares their binding energies of these ligands to the binding energies their respective naturally-occurring ligands. This comparison indicates which ligands may successfully inhibit the activity of the protein. This project focuses on the binding of sorafenib, dasatinib, and crizotinib to various proteins although several other FDA-approved TKIs are also of interest for further study.

ABC-02 **Dana Robertson**[1], Sheshanka Kesani[1], Abdul Malik[1]
[1]Department of Chemistry, University of South Florida

Forensic trace analysis using sol-gel molecular imprinting and capillary microextraction coupled to chromatography

Forensic trace analysis is the study of minimal evidence amounts and their probable origin; with applications in drug and disease testing, DNA analysis, etc. The objective of this experiment is to extract a target analyte (*o*-cresol) from a sample solution of closely related phenols. This may be achieved by using a molecularly imprinted capillary tube coated with a silica based sol-gel. The cavities created by the imprinting should separate the target analyte from the sample, which can later be extracted from the cavities with a solvent (ethanol). This pre-concentrated solution will then run through an HPLC and analyzed using UV-Vis spectroscopy to confirm the presence of the target analyte and absence of the remaining compounds. This experiment could prove to be a widely-applicable technique for compound identification and analysis in the field of forensic chemistry.

ABC-03 **Sayeef Mirza**[1,2], Bin Fang[2], John Koomen[1,2]
[1]Universisty of South Florida; [2]Moffitt Cancer Center

Quantifying differential protein expression in drug resistant multiple myeloma

Mass spectrometry analysis of differential protein expression in chemotherapy-resistant multiple myeloma may explain the development of resistance to different clinical treatments. A pipeline method was developed using gel-based protein fractionation followed by peptide sequencing with liquid chromatography coupled to tandem mass spectrometry (GeLC-MS/MS) for proteome cataloging. Liquid chromatography coupled to multiple-reaction monitoring mass spectrometry (LC-MRM) assays were then developed for quantification of selected protein biomarkers and selected peptides in cell lysates of doxorubicin resistant multiple myeloma (Dox40). Increased expression of specific proteins emphasizes certain biological pathways associated with doxorubicin resistance in multiple myeloma. Therefore up-regulation of proteins associated with resistance was conveyed using LC-MRM; with additional development, it may be translated to patient assessment using companion biomarkers to evaluate therapeutic response and the development of drug resistance. These efforts may pave the way for more effective treatments for multiple myeloma and may be utilized in future biomarker discovery studies.

ABC-04 **Aaron Garrison**[1], Sungyub Han[1], Xiao Li[1]
[1]Department of Chemistry, University of South Florida

Synthesis of SiO_2-Ag and SiO_2-Au core-shell nanoparticles for use as SERS substrates

Our goal is to synthesize a colloidal solution of bimetallic nanoparticles that, when used as a SERS substrate, will yield enhancement of Raman signals greater than that of our previously produced Ag nanoparticles, thus lowering the detection limits for pyridine, our SERS probe. The use of bimetallic nanoparticles has been shown to produce a greater effect than monometallic nanoparticles on the increase of surface plasmon resonance signal. Based on our previous success with 50-60 nm SiO_2@Ag nanoparticles we intend to synthesize the SiO_2@Au ones. We will limit the size of SiO_2@Au to less than 60 nm while maintaining similar parameters for SiO_2 core synthesis.

ABC-05 **Cheryl H McCane**[1], Dean F Martin[1]
[1]Institute for Environmental Studies, Department of Chemistry, University of South Florida

Evaluation of the removal of selected aqueous food dyes by Octolig®

Good and cogent reasons exist for the removal of food dyes from natural water systems. This study was concerned with evaluating the ease or possibility of removing the ions of selected FD&C food dyes from water by column chromatography on Octolig® medium. This material is a commercially available polyethyleneimine covalently attached to a high-surface-area silica gel (CAS Registry No. 404899-06-5). Previous research suggests a mechanism for removal of certain anions [J. Environ. Sci. Hlth., 44A: 1545-1550]. Utilizing UV-visible spectrophotometry absorbance was measured to indicate percent removal. Analysis of initially collected results indicates a potential for 99.5 ± 0.3% removal.

ABC-06 **Brittany G Kociuba**[1]
[1]Florida Institute of Technology

Sythesis and intercalative analysis of Tryptanthrin analogues

Tryptanthrin (indolo [2, 1-b] quinazoline-6, 12-dione) is a naturally occurring compound that has shown to have potent anti-parasitic activity. However its mechanism of action is currently unknown. As such we have synthesized a series of Tryptanthrin analogues to investigate their potential interaction with DNA. Presented here are results of a DNA intercalation assay utilizing a pGEM plasmid. Interestingly, a wide range of intercalative ability was observed for a series of similar structural analogs.

ABC-07 **Darrell Cole Cerrato**[1], Vicky Lykourinou[1], John Williams[1], Li-June Ming[1]
[1]Department of Chemistry, University of South Florida

Describing metal binding of Thiostrepton by examining metal-TSN enzymatic activity

The antibiotic, thiostrepton (TSN), has metal binding capabilities that are not fully known. There are several moieties that are potentially responsible for TSN's binding capability. To describe the metal binding capability of TSN, the rates of enzymatic activity of metal-TSN complex was measured against a substrate. One of the challenges of examining the metal-TSN complex was the different polar properties of the metals and TSN. Thus, several solvent systems were compared to ensure the activity trends were comparable. It was found that free copper and apo-TSN have very small turnover rates compared to the CuTSN complex, indicating that any enzymatic activity is largely due to the complex and not any free copper or unbound TSN. The data shows that TSN has multiple binding sites for copper and potentially other metals based on turnover rate and catalytic efficiency. The ideal ratio of the different metals to TSN is still being determined.

ABC-08 **Juan C. Gonzalez**[1], Elizabeth Remily-Wood [2], John Koomen[2]
[1]Department of Chemistry, University of South Florida; [2]H. Lee Moffitt Cancer Center, Tampa, Fl

Comparing enzymatic digestion methods for quantitative proteomics

In the majority of proteomics experiments, proteins are digested with trypsin, a robust enzyme which reproducibly cleaves peptides with both the desired basicity and molecular weight for mass spectrometry analysis. However, trypsin's specificity (cleavage C-terminal to lysine and arginine) can be limiting when examining specific biological questions, because it can cleave fragments either too large or small for effective mass analysis. Therefore, the goal of this experiment is to complement trypsin digestion with alternative digestion methods for quantitative proteomics. Tests were conducted with alternate proteolytic enzymes, including pepsin, glutamyl endoproteinase (Glu-C), and chymotrypsin. These enzymes which cleave proteins at different amino acids can be used to detect other regions of protein sequence that are not observed in tryptic digests, providing additional opportunities to detect and quantify protein expression, mutation, and modification. Proteins were quantified in-solution of different cell lysate digests.

ABC-09 **Elizabeth D'Esposito**[1], Erin Fagan[1], Vasiliki Lykourinou[1], Li-June Ming[1]
[1]Department of Chemistry, University of South Florida

Complex formation and catalytic activities of Cu(II)-bound copolymers: Kinetic studies of the effect of polymer functionality on oxidative activity

Copper (II)-bound copolymer complexes provide a more versatile alternative to small complexes for development of catalysts capable of activating O_2 and H_2O_2 and form active intermediates capable of oxidation of catechol derivatives of phenolic substrates. These copolymers mimic the activity of enzymes such as tyrosinase and catechol oxidase. The catalytic behavior of these copolymers has been attributed to functional groups in the polymeric chain namely pyridine and amide or phenyl. We observed that oxidative activity is dependent on chemical properties of the polymeric functional groups. Herein we present the investigation of complex formation of two linear copolymers containing a hydrophobic or hydrophilic functional group (styrene to acrylamide) with Cu(II) and their catalytic activities exhibited by these different metallopolymers using catechol derivatives in air and in the presence of H_2O_2.

ABC-10 **Faysal Rifai**[1], Mu Seong Kim[1], Julie Harmon[1]
[1]Department of Chemistry, University of South Florida

Poly (Carbonate Urethane) (PCPU) metal organic composites with different methods of formation

This project focused on designing, processing and testing novel polymer composites for use in biomedical applications and using different methods of formation. PCPU was chosen because this class of polymers is known to be biocompatible. The specific aim was to strengthen physical properties an ultra-soft PCPU matrix with metal organic nanoball fillers. Nanoballs were sonicated in polymer solutions in order to disperse them effectively. The composites were rapidly precipitated from the organic based solution by flooding the solution with water. After drying in vacuum oven, samples were compression molded. The characterization procedures used were differential scanning calorimetry, dynamic mechanical analysis, optical microscopy and Shore A hardness testing. These techniques allowed us achieve the aim of optimizing the physical properties of the composites. Mechanical testing illustrated that Nanoballs can be used to tune mechanical properties. This work is an important step in the design of ultrasoft materials for biomedical devices.

ABC-11 **Brodie A. Reiger**[1], Dean F. Martin[1]
[1]Department of Chemistry, University of South Florida

Kamlet Laboratories and Miles Laboratories correspondence, 1941-1945: A search for credit

We used the Kamlet Papers Collections [cf. Martin, D. F. and B. B. Martin, Florida Scient. 2007, 70 40-44] in the USF Tampa Library Special Collections Department to learn if Dr. Jonas Kamlet received appropriate credit for his idea and his patent for rapid and convenient analysis for glucose in urine and blood involving a pill called “Clinitest”. Jonas Kamlet took the idea to Miles' Walter Compton, MD, who did not know what to do with it (according to Edna Yanveh Kamlet Rogers, wife of Dr. Kamlet). More recent statements by a former employee of Miles Laboratories claim that the test was ”developed by Dr. Compton”[C&EN, 2011,89(34): 51]. It is evident that Dr. Kamlet did not (in our opinion) receive appropriate credit, but available correspondence indicated that it was not an issue with him.

ABC-12 **Tyler J. Spradling**[1], Sumit Handa[1], David Merkler[1]
[1]Department of Chemistry, University of South Florida

Purification and inhibition of 1-Deoxy-D-Xyulose-5-Phosphate synthase (DXS)

The mevalonate-independent or non-mevalonate pathway for isoprenoid synthesis is one of the last evolutionary pathways discovered during last decade. Presence of this pathway in eubacteria and protozoa makes this pathway an interesting pathway for the discovery of novel antibiotics and antimalarials. 1-deoxy-D-xyulose-5-phosphate synthase (DXS) is the first enzyme involved in this pathway, which catalyzes the thiamine pyrophosphate and Mg2+ condensation of pyruvate and glyceraldehyde-3-phosphate to form 1-deoxy-D-xylulose-5-phosphate (DXP). Subsequently DXP is utilized by the second enzyme 1-deoxy-D-xylulose-5-phosphate reductoisomerase (DXR) to convert DXP to 2C-Methyl-D-erythritol-4-phosphate (MEP) and also utilizes NADPH. N-terminal His6 tag DXS and DXR were expressed in E. coli and purified using affinity chromatography. A high throughput spectrophotometric assay was developed to screen the large library of compounds.

ABC-13 **Kevan Sharp**[1], Patrick McKeny[1], Todd Gatlin[1], Adrian Villalta-Cerdas[1], Santiago Sandi-Urena[1]
[1]Department of Chemistry, University of South Florida

Clarifying the credentials: Judging criteria of ratemyprofessors.com as an instruction assessment tool

Online rating websites such as Ratemyprofessors.com (RMP) influence college professor and course selections. However, often their validity sparks skepticism among instructors because of the self-selected nature of raters. The objective of this study was to determine whether or not there are significant differences between students who contribute chemistry ratings to RMP and those who do not. A sample of 270 General Chemistry II students completed a 50-question survey addressing RMP use patterns and student characteristics. Findings revealed that there was no significant difference between the two groups in seven comparison criteria: GPA, major, class status, course load, learning/grade orientation, gender or previous chemistry course grade. These findings are in agreement with other reports. This work presents further findings concerning factors that influence students' decisions about rating instructors. The contention is put forth that institutions and professors may find a valuable supplemental source of information in RMP data to evaluate instruction.

ABC-14 **Solianna Herrera**[1], Sachel Villafuente[1], Jennifer E. Lewis[1]
[1]Department of Chemistry, University of South Florida

Degree of success in reaching underrepresented minority students with an active learning curriculum for biochemistry

Historically, NSF has been concerned about inclusion of underrepresented minority students in STEM. Since 2009, an NSF-funded project, "Active Learning in Biochemistry" works with a biochemistry student population at 14 different institutions across the United States. Hopefully this project has met NSF's goals in reaching minority students. It is important to determine how the percentage of minority students participating in this project compares to the overall national averages of STEM graduates. Demographic data from a paper-and-pencil survey was collected from 8 participating institutions during the 2009-2011 years. CHI-square analyses support our conclusions as to whether this project reaches underrepresented minority students in 3 categories: sex, race, and ethnicity. We report the extent to which this project falls short of the optimum. In the absence of specific remediative strategies we are unlikely to make progress towards the inclusion of minority students in STEM.

CIP-01 **Chelsea Tieu**[1], Arjan van der Vaart[1]
[1]Department of Chemistry, University of South Florida

Simulations of the Perfringolysin O pore-forming toxin

The bacterial toxin perfringolysin O is a member of the family of cholesterol dependent cytolysins which form large pores in cell membranes. Upon binding and oligomerization on the cell membrane, the α-helices in domain 3 refold into β-sheets, which insert themselves into the membrane, resulting in a ~150 Å wide pore. We performed biased molecular dynamics simulations to investigate the activation mechanism of this process. In the simulations, we artifically moved domain 3 away from the rest of the protein in order to establish the contacts important for refolding. Results of the simulations and implications for the mechanism will be discussed.

CIP-02 **Kristina T. Gemayel**[1], Simin Falsafi[2], William Price[1]
[1]University of South Florida, Saint Petersburg; [2]West Virginia University

Computational analysis of double bond migrations and MS3 fragmentation of nitrile-terminated PPI dendrimer ions

Due to unique physical and chemical properties, dendrimers have a wide range of potential applications and several promising uses as chelating agents, chemical sensors, site-specific host-guest chemistry, and controlling gene and drug delivery systems. Related to this study, the nitrile-terminated poly-propylene imine (PPI) dendrimer ions create a unique environment that is both aprotic and polar, conditions which are suitable for various reaction environments. Understanding the gas-phase chemistry and transition states of these PPI dendrimers allows for insight into the fundamental organic chemistry properties and reactions that dominate these particular molecules.

CIP-03 **Charles Doerner**[1], Leon Hardy[1], Lewis Rubin[2]
[1]Department of Mathematics, University of South Florida, Saint Petersburg; [2]USF Health

A proposed structure for beta-carotene oxygenase 2

Carotenoids are organic pigments naturally occurring in plants and some algae and bacteria. Because they cannot be synthesized, humans must obtain these pigments from food or other sources. Beta-carotene oxygenase 2 (BCO2) is an enzyme involved in carotenoid cleavage, a process which produces vitamin A (retinol) and aids in its function. The BCO2 protein structure has not been determined by x-ray crystallography, therefore a computationally obtained theoretical structure may give us insight about the relationship between the protein's form and function.

CIP-04 **Charles Doerner**[1], Leon Hardy[1]
[1]Department of Mathematics, University of South Florida, Saint Petersburg

The molecular dynamics of BAX peptide and its interaction with a POPC membrane

Bcl-2-associated X protein, or BAX, is a pro-apoptotic protein involved in a variety of cellular processes. A member of the Bcl-2 gene family, including pro- and anti-apoptotic proteins, it has been implicated in a number of cancers and autoimmune diseases. BAX is found in the cytosol, but when given the apoptotic signal, undergoes a conformation shift and interacts with organelles, primarily the mitochondrial outer membrane. It is believed to trigger the opening of voltage dependent anion channels, however growing evidence suggests the protein forms a pore, called a mitochondrial apoptosis-inducing channel (MAC), in the membrane. The BAX peptide exists as a wild-type with several mutant forms. Each differs only by an identical side-by-side pair of amino acids, substituted for another pair in the mutants. We modeled the wild-type, which has paired Lysines, interacting with a POPC membrane.

CIP-05 **Geoffrey Gray**[1], Arjan van der Vaart[1]
[1]Department of Chemistry, University of South Florida

Molecular dynamics for the development of selective RXR agonists

The retinoid X receptor (RXR) is a nuclear receptor important in cancer and Alzheimer's disease. To help rationalize the design of new RXR agonists, we performed molecular dynamics simulations of bound and unbound states of the protein. Analyses were performed to assess the availability of hydrophobic and hydrophilic areas for binding. From the simulations, important structural and energetic contributions to the binding process were identified.

CIP-06 **Juan C. Baso**[1], Geoffrey Gray[1], Arjan Van Der Vaart[1]
[1]Department of Chemistry, University of South Florida

Molecular dynamics studies of retinoid X-receptor's and their interaction with Bexarotene analogues

Bexarotene is an FDA approved retinoid X-receptor (RXR) agonist that is used in the treatment of cutaneous T-cell lymphoma (CTCL) and shows promise for treatment of Alzheimer's disease. Based on previous docking studies, halogenated derivatives showed improved binding affinity over non-halogenated analogues. Following up on the previous study, a molecular dynamics study is being conducted using the CHARMM program, which has allowed for insight into the behavior of the protein pocket as it interacts with the ligand over time.

CIP-07 **Erik Nevicky**[1], Patrick Nugent[1], Mike Zaworotko[1]
[1]Department of Chemistry, University of South Florida

Synthesis and characterization of novel copper paddle wheel complexes to be used in Methacrylate polymers

The polymer Methacrylate holds an important role in contact lens construction. It has been seen, however, that the secondary building units called copper paddle wheels alter the physical properties of this polymer through supramolecular forces. Therefore, the production of copper paddle wheels with varying R groups is essential to further this research. The use of layering, refluxing, evaporating, and cooling various copper and ligand solutions were implemented in order to grow crystals of copper paddle wheels for characterization. Once successfully synthesized and characterized, experiments were repeated to obtain a large quantity to be sent off, mixed with Methacrylate, and changed properties measured. The synthesis of new paddle wheel complexes will be used in future research for inorganic and polymer chemistry.

CIP-08 **John T. Williams**[1]
[1]Department of Chemistry, University of South Florida

Zn coordination with thiostrepton (TSN) and its hydrolysis of biological substrates

Metal coordination and common antibiotics is not a well investigated area. Many common pharmaceuticals products and their potential for metal bonding go un-researched and there potential catalytic effects go undetected. One particular antibiotic that has shown the ability to coordinate with multiple metals is thiostrepton (TSN). Thiostrepton has shown the ability to coordinate with Cu, Co, Ni, Pb and now Zn. Under UV-Vis spectroscopy, Zn has been shown to interact with TSN in ratios of 1:1 to 1:6. It is the hope of this investigation to determine the binding coordination of Zn and TSN in various its various ratios as well as the possible hydrolytic capacities that the metal ligand compound exhibits towards various biological substrates, such as DNA, in an attempt to determine and bring to life the significance of metalloantibiotics.

CIP-09 **Nicholas P. Dovellos**[1], Patrick Nugent[1], Mike Zaworotko[1]
[1]Department of Chemistry, University of South Florida

Crystal engineering

Attempting to create Cu(II) Paddlewheels via heuristical and various forms of experimentation. Methods include layering and refluxing while altering solvents used and metal salts. Should successful crystals be created they will then be placed into polymethacrylate polymer containing pHEMA and GMA polymers in order to test the response of the paddlewheel additive. My work is to create as many variations of the Cu paddlewheel in hopes that one of the crystals will provide the ventured outcome. Our overall mission is to create a polymer which can retain water left outside an aqueous environment and improve in tension/overall durability.

CIP-10 **Erik Madsen**[1], Patrick Nugent[1], Michael J. Zaworotko[1]
[1]Department of Chemistry, University of South Florida

Expanding modularity of the pillared grid metal organic material (MOM) platform via novel node metal incorporation

The pcu-type SiF_6-pillared grid platform originally emerged from a series of Cu and Zn MOMs reported by Kitagawa, Hosseini, and Zaworotko. Some Cu variants of this class have exhibited high specific surface area as well as high uptake of and selectivity for energy-related gases. We report herein the synthesis and structural features of five Cd variants of SiF_6-pillared grid MOM: $[Cd(pyz)_2(SiF_6)]n$ (pyz = pyrazine), 1; $[Cd(bpy)_2(SiF_6)]n$ (bpy = 4,4'-bipyridine), 2; $[Cd(bpe)_2(SiF_6)]n$ (bpe = 1,2-bis(4-pyridyl)ethylene), 3; $[Cd(bpeth)_2(SiF_6)]n$ (bpeth = 1,2-bis(4-pyridyl)ethane), 4; and $[Cd(abp)_2(SiF_6)]n$ (abp = 4,4'-azobipyridine), 5. MOMs 1-5 are composed of $[Cd(L)_2]^{2+n}$ sheets that are pillared by SiF_6^{2-} to form neutral 3D frameworks possessing nanoscale square or rhombic channels.

CIP-11 **Matthew Chrzanowski**[1], Xi-sen Wang[1], Shengqian Ma[1]
[1]Department of Chemistry, University of South Florida

Epoxidation of olefins catalyzed by cadmium based metal-metalloporphyrin framework

The past decade has seen significant advances in the field of metal-organic frameworks. Over the past year, Dr. Shengqian Ma's research lab at USF has been working to develop a novel, new species of metal-organic frameworks constructed using porphyrin ligands known as metal-metalloporphyrin frameworks (MMPFs). MMPFs look to capture the versatility and utility of porphyrins that exist in nature and combine it with the stability, structure, and selectivity of MOFs.

CIP-12 **Kyle McDonald**[1], Patrick Nugent[1], Michael J. Zaworotko[1]
[1]Department of Chemistry, University of South Florida

Expansion of a Pillared Metal-Organic Material Platform for Gas Storage and Separations

Crystalline Metal-Organic Materials (MOMs) are constructed by a self-assembly process using metal nodes and organic linkers. Pillaring linkers can be utilized to expand 2D MOMs into 3D scaffolds, thereby increasing their porosity and stability to loss of guest species. MOMs of this class have shown a high Q_{st} for CO_2 and thus are ideal for the separation of CO_2 from N_2 or CH_4, which is relevant to carbon capture and alternative fuels. We herein report a novel pillared grid MOM, $[Co(bipy)_2(SiF_6)]_n$, synthesized via solvent diffusion at room temperature from $CoSiF_6$ and 4,4'-bipyridine. This MOM crystallizes in the tetragonal space group P4/mmm and exhibits CO_2/N_2 and CO_2/CH_4 relative uptakes of 18.3:1 and 7.3:1, respectively, at 298 K and 1 atm, with a BET surface area of 1076 m^2g^{-1}. Isostructural derivatives of this class of MOM are being synthesized with varying linkers in order to investigate pore size on affinity for energy-related gases.

CIP-13 **Jeremy Dovel**[1], Wenyang Gao[1], Shengqian Ma[1]
[1]Department of Chemistry, University of South Florida

UV-VIS determination of cobalamin adsorption to lanthanide meso-porous metal organic frameworks

Terbium, yttrium, and cadnium based MOF's were synthesized; each having an exceptionally large pore size. First, a Cobalamin absorbance standard curve was established with an R^2 of 0.9993. A very dilute concentraton of cobalamin (Vitamin B-12) was then mixed with each MOF and the concentration was monitored every 30 minutes by UV-VIS absorbance. The UV-VIS determination of cobalamin adsorption in each MOF is currently underway.

CIP-14 **Veronica Valencia**[1], Yao Chen[1], Tran Hoang[1], Shengqian Ma[1]
[1]Department of Chemistry, University of South Florida

Kinetics of biomolecules into new types of porous materials

Porous metal organic frameworks (MOFs) show great promise for the use of biocatalysis due to their high porosity. A study of the kinetics of the diffusion of biomolecules into new types of MOFs provided proof of the properties of these porous materials. Our project studied the initial rate of uptake, as well as the diffusion rate, of Cytochrome C on Bio-MOF-100 and Tb MOF, under different conditions.

CIP-15 **Brittany P. Gordon**[1], Steven Shipman[1]
[1]Department of Chemistry, New College of Florida

Waveguide chirped-pulse Fourier transform microwave (CP-FTMW) spectrum of ethanethiol and the new 18.3-26.5 GHz circuit

The microwave spectrum of ethanethiol at 0°C was measured from 8.7-26.5 GHz with waveguide chirped-pulse Fourier transform microwave spectroscopy (CP-FTMW). The existing spectrometer could collect data from 8.7-18.3 GHz. A new circuit was built to extend the range of the spectrometer from 18.3 to 26.5 GHz. The first molecular signal we observed with this new instrument was of ethanethiol. The spectrum consists of contributions from ^{34}S and ^{13}C isotopomers of the trans and gauche isomers. Preliminary analysis of the spectrum of the ground state trans normal species, ^{34}S, and ^{13}C have been accomplished using starting constants from the literature in the fitting programs SPFIT , SPCAT, SVIEW, and ASCP.

CIP-16 **Christopher B Fryman**[1], Julie P. Harmon[1]
[1]Department of Chemistry, University of South Florida

Metalorganic hydrogel composites with enhanced strength

$[Cu(II)_2(Benzenecarboxylate)_4(Axial\ Ligand)_2]$ paddlewheels with H-bonding functional groups are utilized as fillers in poly(hydroxyethyl)methacrylate (PHEMA) and copolymers of HEMA with glycerol methacrylate (GMA). Hydrogels are hydrophilic polymers that swell when exposed to polar solvents. Monomer structure can be tuned to optimize the degree is swelling; as hydroxyl content is increased, the degree of swelling increases. HEMA contains one hydroxyl group, GMA contains two hydroxyl groups. Neat GMA swells to the point of network tearing due to swelling pressure. USF scientists have shown that metalorganic paddlewheel increase hydrogel strength, glass transition temperature and hardness of such composites. The degree of solubility of the Cu(II) paddlewheels in HEMA, 1:1 HEMA/GMA, and GMA composites will be determined by sonicating the Cu(II) paddlewheels in the monomer solutions and polymerizing. Ethanol extraction will determine any leaching of the paddlewheel from the matrix. Equilibrium water sorption will be characterized and any matrix tearing will be noted.

CIP-17 **Jennifer Wedebrock**[1], Julie Harmon[1]
[1]Department of Chemistry, University of South Florida

Powder x-ray diffraction and differential scanning calorimetry of Poly (Carbonate Urethane) Carbon-nanotube composites

A novel ultra-flexible polycarbonate-polyurethane (PCPU) has been shown to exhibit enhanced self-healing and enhanced mechanical properties when nanotubes are incorporated into the matrix. PCPU composites with 1% by weight single-walled carbon nanotubes (SWCNT) and 1% by weight multi-walled carbon nanotubes (MWCNT) were sonicated into the matrix. Samples were prepared by two techniques: water coagulation and solvent evaporation. The goal of this methods project is to examine the crystallinity in neat PCPU and in its composites with SWCNT and MWCNT using powder x-ray diffraction and differential scanning calorimetry. Examination of crystallinity in these composites is expected to contribute to an understanding of the healing process, which would help in the development of potential applications for both PCPU and its composites.

CIP-18 **Mona Hasan**[1], Mu Seong Kim[1], Julie Harmon[1]
[1]Department of Chemistry, University of South Florida

Evaluating the potential of synthesized PCPU composites

With its unique composition of both a hard and soft surface, PolyCarbonate-Polyurethane (PCPU) is well known for its durability and stability. However, little research has been done on the resulting properties when combining PCPU and nanotubes, compounds known for their exceptional conductivity of electricity. Through sonication and water coagulation, the synthesis of PCPU with various concentrations of either SWNT (Single-Walled Nanotubes) or MWNT (Multi-Walled Nanotubes) is possible. The resulting features of these synthesized rubber-like composites are to be examined by conducting both the Differential Scanning and Calorimetry (DSC) and hardness tests. Evaluating these tests will determine both the possible distinctive attributes of the novel substances and the extent of changes noted in correlation with various concentrations of the different nanotubes used. These composites could carry the potential of becoming a multi-functional tool in many scientific fields, particularly in those requiring substances that are durable, stable, yet easily conductible.

CIP-19 **Kevin S. O'Connell**[1], Christi L. Whittington[1], H. Lee Woodcock[1], Randy W. Larsen[1]
[1]Department of Chemistry, University of South Florida

Effects of confinement on the electronic properties of the ruthenium(II) trisbipyridine excited state ^{3}MLCT

Ruthenium polypyridine complexes have advantageous photochemical properties such as excited state reactivity, relatively long luminescence, and efficient light absorption. The photophysics of these complexes differ based upon environment. The current computational study focuses on understanding the properties of free and encapsulated ruthenium(II) trisbipyridine. Excited state quantum calculations will shed light on the electronic properties that lead to altered geometries and extended fluorescence lifetimes. Density functional theory (DFT) was used to explore both constrained and relaxed geometries of the ground and excited states. Results presented here will be discussed in the broader context of excited state confinement effects.

The Solomon T. Weldegirma Poster Session Abstracts

BO-01 **Jennifer Le**[1], Silke Lopez de Mesa[1], Xue Xu[1], Peter Zhang[1]
[1]Department Of Chemistry, University of South Florida

Applications of cobalt (II) porphyrin catalyzed cyclopropanation of halodiazoacetates

Cyclopropane rings are found in many drugs such as the anti-cancer drug Taxol; and are generally useful in synthetic organic chemistry. Halogenated cyclopropanes are even more useful because halogenated compounds may be suitable substrates for substitutions, eliminations, or cross-coupling reactions. At least 3600 biologically important halogenated compounds have been documented, ranging from the pollutant PCDD to plant hormones. Using our cobalt (II) porphyrin catalyst we have developed a direct method to obtain monohalogenated cyclopropane rings from halodiazoacetates with high diastereo- and enantio- selectivity. Full characterization of the products was done using methods such as HNMR, CNMR, IR, GC/MS, and HPLC. Finally, we used the halogenated cyclopropane products as starting materials to synthesize chiral complex cyclopropylidene intermediates useful for a wide variety of further transformations.

BO-02 **Jacob Pierce**[1], Faeez Mahzamani[1], Luke Gill[1], Edward Turos[1]
[1]Department of Chemistry, University of South Florida

Menthol-based chiral polyacyrlate nanoparticles

Polyacrylate polymers can be modified to create specific function and therefore can serve as customizable frameworks. Enantiomerically pure polyacrylate nanoparticles were prepared by mini-emulsion polymerization of a homogenized mixture of acrylated L-menthol and styrene in the presence of surfactant (sodium dodecyl sulfate) and a radical initiator (potassium persulfate). Samples of poly(Menthyl-acrylate-styrene) nanoparticles were synthesized using 10 -100 v/v % of Menthyl-acrylate relative to Styrene with both 3% and 5% SDS surfactant. The stability, particle size, mass, and optical activity of these nanoparticles were investigated. Copolymerization of the chiral monomer with the achiral monomer induced optical activity in the nanoparticles. The increasing concentration of MtA correlated to a linear increase in optical activity of the nanoparticles up to the maximum value, and demonstrated the possibility of molecular level control of chiral material design. Our study extends to D-Menthol as well as racemic menthol nanoparticles obtained under the same parameters.

BO-03 **Alexander Gonzalez-Jacobo**[1], Carrie Waterman[1], Laurent Calcul[1], Chris Witowski[1], Dennis Kyle[2], Bill Baker[1]
[1]Department of Chemistry, University of South Florida; [2]College of Public Health - Global Health, University of South Florida

Determination of anti-malarial properties of delta-lactam derivatives from MSX232697

The Medicines for Malaria Venture seeks to obtain a new treatment for malaria that is simple to recreate and is of lower cost margin than the currently available drugs. Over 50,000 fungal samples were screened for anti-malarial properties, and those showing promise were further analyzed. The extraction and purification of compounds from sample MSX232697 was performed using methanol extractions, liquid partitions, medium-pressure liquid chromatography (MPLC), and HPLC. NMR and mass spectrometry (MS) were used to characterize these compounds and to elucidate their structures. The basic structures of the two compounds of interest were found to be delta-lactam derivatives. The final purified products will be submitted for bioassay and the results will determine whether the compounds are viable for future drug development.

BO-04 **Johana Andrea Trejos**[1], Noella Cortinas[1], Christopher Witowski[1], Bill J. Baker[1]
[1]Department of Chemistry, University of South Florida

Secondary metabolite enhancement of endophytes in competing co-cultures

Microbes in nature interact with one another using a diverse array of chemicals however most laboratory cultivation techniques (pure cultures) do notproduce this chemical diversity. Known as secondary metabolites, these compounds play an important role in mechanisms of self-defense, symbiosis,and natural selection. Bioactive natural products are important in modern medicine and the development of therapeutic drugs, with microbes being responsible for many potent anti-bacterial and anti-fungal compounds. Co-cultures of Aspergillus niger and marine endophytes were grown to examine interactions between organisms and compounds responsible for inhibition. Kirby-Bauer disk diffusion assays were used to test for bioactivity of the various extracts, and Liquid Chromatography- Mass Spectrometry (LCMS) profiling was employed to analyze secondary metabolites. The goal was to discover any differences between the isolated and co-culture methods by examining the ring of inhibition produced by culture extracts.

BO-05 **Megan M Barber**[1], Katya P Nacheva[1], Iredia D Iyamu[1], Roman Manetsch[1]
[1]Chemistry Department, University of South Florida

Multi-fragment screening of protein-protein interaction modulators via sulfo-click kinetic target-guided synthesis

Screening of fragments using kinetic target-guided synthesis (TGS) and in situ click chemistry is a relatively new process that can be beneficial to the development of potential protein-protein interaction modulators (PPIMs). Kinetic TGS using in situ click chemistry allows for multiple fragments to be screened simultaneously against one protein target assembling biologically active bidentate ligands. We have previously shown that potent PPIMs can be identified using a kinetic TGS by means of the sulfo-click reaction between thio acids and sulfonyl azides. Using liquid chromatography with triple quadrupole mass spectrometry detection, we have been able to screen reliably up to 300 fragment combinations in a single well. We began a screening initiative of a reactive fragment library leading to a potential 1710 acylsulfonamide components against the anti-apoptotic proteins Bcl-xL and Mcl-1. Preliminary results demonstrate the new kinetic TGS method accelerates the screening process compared to standard assays.

BO-06 **Patrick M. Wieruszewski**[1,2,3], Kenneth R. Graham[1,2,3], Romain Stalder[1,2,3], Dinesh G. Patel[1,2,3], Danielle H. Salazar[1,2,3], John R. Reynolds[1,2,3]
[1]The Center for Macromolecular Science and Engineering; [2]Department of Chemistry, University of Florida; [3]George and Josephine Butler Polymer Research Laboratory

Tailor-made additives to control morphology in organic photovoltaics

With increasing demands for electricity, organic photovoltaics (OPVs) are becoming a popular alternative to renewable energy due to their light weight, flexibility, and inexpensive processing. We report the use of an asymmetric triisobutylsilyl containing tailor-made additive to controllably tune morphologies of thin film organic photovoltaics. Molecular bulk heterojunction (BHJ) OPVs were prepared using an isoindigo-thiophene containing oligomer and its asymmetric tailor-made additive as the donor, with a fullerene derivative as the acceptor. Transmission electron microscopy and atomic force microscopy were used to probe film morphology and show precise control of donor and acceptor domain sizes. Additionally, an analogous symmetrical tailor-made additive was also synthesized and incorporated in BHJ OPVs to show whether the asymmetry of the additive alone leads to morphological control. We believe tailor-made additives can be prepared for various electroactive materials to fine tune morphology and achieve reproducibly high power conversion efficiencies in OPVs.

BO-07 **Niles Gunsalus**[1], Jordany Maignan[1], Richard Matthew Cross[1], Roman Manetsch[1]
[1]Department of Chemistry, University of South Florida

In situ click chemistry as a tool for lead discovery of inhibitors demonstrating species selectivity

The use of in situ click chemistry to facilitate lead discovery has only recently been developed. In situ click chemistry enables enzymes to selectively construct their own inhibitors from reactive fragments within the enzyme binding subsites. Previously, it has been demonstrated in the self-assembly of potent inhibitors of mouse and eel acetylcholinesterases (AChEs) with IC50s in the femto- to picomolar ranges using variations of azido-tacrine/acetylene fragments. Here, we demonstrate for the first time the use of in situ click chemistry to effectively design inhibitors displaying selectivity to AChE of one species over another. Eleven azido-tacrines were combined with twenty-one isoquinoline alkynes and incubated with AChE from mice and Drosophila melanogaster. It was observed that fragment combinations assembled selectively into triazoles depending on the AChE utilized. Results were confirmed by LC-MS of the crude incubation mixtures and the triazole products were compared to isomerically pure triazole samples synthesized in the laboratory.

BO-08 **Brian D Guedes**[1], Yi Liang[1], Mark McLaughlin[1]
[1]Department of Chemistry, University of South Florida

Solid phase synthesis and isolation of peptide nucleic acid monomers, unnatural analogs of DNA with potential use in gene therapy drug discovery

Peptide Nucleic Acids are utensils — structurally resembling DNA — which have been modeled to assist various DNA- and RNA-binding oligonucleotides. PNA monomers contain a pseudopeptide backbone composed of repeated units of N-(2-aminoethyl) glycine moieties where the various nucleobases are attached via methylenecarbonyl linkers. One drawback with PNA usage is its poor uptake in vitro by eukaryotic or prokaryotic cells; to remedy this, our investigation was directed towards PNAs based on cysteine residues (CPNAs). In order to synthesize PNA monomers, the ethylene diamine precursor was treated with either the Fmoc- or Boc-based monomer synthesis pathway. In particular, the monomer synthesis was accomplished with several steps of alkylation, mesylation, and hydrolysis. Throughout the synthetic process, various methods were used to examine and isolate the necessary compound. This included column and thin layer chromatography, simple and reflux distillation, suction filtration, extraction, and hydrogenation. There are no results to report at this time.

BO-09 **Matthew R McCord**[1], Mark Novak[1]
[1]Department of Chemistry, Florida Institute of Technology

Novel substrates for soybean lipoxygenase

Research in the last decade has uncovered fascinating new chemistry of the enzyme soybean lipoxygenase, type I (SBLO-I). In addition to its traditional 1,4-pentadiene substrates, the enzyme has been found to catalyze reactions of monounsaturated fatty acids, producing β-unsaturated enones. The presence of a hydroperoxide intermediate was confirmed by reactions carried out in the presence of a reducing agent, capturing the intermediate in the form of a chiral allylic alcohol. The production of two different chiral allylic alcohols suggests a regiospecific rearrangement, possibly similar to the Mislow-Evans. Future SBLO-I studies will be aided greatly by the creation of synthetic analogs for natural substrates. We have successfully synthesized two such substrates and carried out SBLO-I catalyzed reactions. One substrate is analogous to 12-Z-octadecenoic acid. The other incorporates a conjugated diene system. Both of these substrates represent a new chapter in lipoxygenase chemistry.

BO-10 **Bert L. Hudson**[1], Laurent Calcul[1], Charles D . Amsler[1], James B. McClintock[2] , Bill J. Baker[1]
[1]Department of Chemistry, University of South Florida; [2]Department of Biology, University of Alabama at Birmingham

Isolation of Palmerolides from Antarctica tunicate Synocium adareanum

The marine life off the coast of Antarctica is unique from the rest of the world due to the strong circumpolar current which isolates the continent and its surrounding waters. The organisms that have evolved in this landscape have developed the use of uncommon secondary metabolites which can represent potential new chemical scaffolds. Previous studies of the Antarctic tunicate Synoicum adareanum collected off the Antarctic Peninsula led us to isolate and identify a series of polyketide macrocycles related to the melanoma-selective cytotoxin palmerolide A. Most of these palmerolides showed strong cytotoxic properties but Palmerolide A remains the most potent one. Our goal is to extract compounds from S. adareanum on a higher scale in order to re-isolate the palmerolide series and submit them to diverse bioassays at our collaborators' laboratories.

BO-11 **Emilio Bucheli**[1], Courtney Smith[1], Laurent Calcul[1], Chad A. Dickey[2], Umesh K. Jinwal[2], Bill J. Baker[1]
[1]Department of Chemistry, University of South Florida; [2]Alzheimer's Institute, University of South Florida

Large scale isolation of diarylheptanoid tau-reducing (+)-S-Myricanol from Myricacerifera and derivatives generation

Alzheimer's disease is caused by the formation of soluble tau intermediates and amyloid β peptides. There are an estimated 5.1 million Americans that suffer from Alzheimer's disease and this number is rising in line with the aging population. Previous bioassay-guided fractionation of Myrica cerifera identified S-(+)-myricanol as a strong tau-reducing agent that may represent a novel scaffold for drug development targeting tau turnover in Alzheimer's disease. A larger scale extraction from the bayberry root bark provided enough pure S-(+)-myricanol to generate semi-synthetic derivatives. Bioassay screening for anti-tau efficiency using a variety of natural products to treat M17 neuroblastoma cells identified bayberry extract as a potent tau-reducer lacking cellular toxicity. Synthetic derivatives formed from myricanol were submitted to the Alzheimer's Institute for further evaluation of tau-reducing potential.

BO-12 **Jason A. Gomez**[1], C. Eric Ballard[1]
[1]Department of Chemistry, Biochemistry, and Physics, University of Tampa

Transition metal catalyzed aerobic oxidation at sp^3-hydridized carbon: Catalytic homocoupling of indene

In recent years, transition metals, such as copper, have been used to catalyze aerobic oxidative coupling reactions has received much attention. Many of these studies have focused there attention on bond formation at sp- and sp^2-hybridized carbon or a to a carbonyl group. In this poster, we describe our studies examining homo-coupling of indene as a model for the homocoupling of formally "sp^3-hybridized" carbon. A variety of copper sources were examined in the model system. Reactions were conducted under dry air or under dry oxygen. Analysis of the crude reaction mixtures was made using GC-MS. The optimal results for this work will be described.

BO-13 **Brendan M. Riley**[1], C. Eric Ballard[1]
[1]Department of Chemistry, Biochemistry, and Physics, University of Tampa

Preparation of 2-substituted indoles via solvent-assisted ring opening of styrene oxides in trifluoroethanol

The alkylation of 4,7-dihydroindole using a solvent-assisted ring opening of various styrene oxides in 2,2,2-trifluoroethanol will be presented. The reaction is regioselective at both the C-2 position of 4,7-dihydroindole and the benzylic position of the styrene oxide. Oxidation of the 2-substituted product with 1,4-benzoquinone restores the aromaticity of the indole nucleus.

BO-14 **Stephanie J. Meyers**[1], Edith J. Banner[1]
[1]Department of Chemistry, Florida Southern College

Synthesis of pyrrole analogs in hopes of producing LQT3-specific class 1b antiarrhythmic drugs

Voltage-gated sodium channels are responsible for the depolarization of excitable cells including cardiac myocytes. Several mutations in the gene (SCN5A)coding for the α-subunit for these channels are linked to the autosomal dominant Type 3 Long QT syndrome (LQT3), a condition characterized by ventricular arrhythmias due to persistent late sodium current. Class 1b antiarrythmic drugs such as lidocaine, ranolazine, mexiletine and other lidocaine analogs bind to the Phe1759 of the α-subunit and stabilizes the inactivated state of Nav1.5. The goal of this study is to prepare pyrrole analogs similar to these class 1b drugs in hopes of finding agents that could alleviate the effects of LQT3 as specific inhibitors of Nav1.5 current. The efforts for the synthesis of these analogs will be described.

BO-15 **Michael G. Mormino**[1], Gajendra Ingle[1], Jon C. Antilla[1]
[1]Department of Chemistry, University of South Florida

Chiral phosphate salt-catalyzed asymmetric ring-opening of meso-epoxides with TMS-azide: Access to enantioenriched 1,2-amino alcohols

Chiral 1,2-amino alcohols are rich in synthetic utility. They are found as both structural motifs in a multitude of natural products, as well as precursors to versatile ligands for asymmetric catalysis. Currently, chiral chromium salen complexes developed by Jacobsen provide the practical catalytic option for generation of chiral 1,2-amino alcohols. In search of new catalytic routes for enantioselective ring-opening of meso-epoxides with TMS-azide and aromatic amines, herein we explore chiral BINOL phosphate salts as alternative catalysts for this transformation.

BO-16 **Marcus Farmer**[1], Jon Antilla[1]
[1]Department of Chemistry, University of South Florida

Asymmetric catalytic halogenation of enamides and enecarbamates

Asymmetric halogenation of ketones is a formidable challenge in catalysis with no general solution available to-date. Our preliminary results show that chiral alkaline metal phosphates efficiently catalyze the chlorination of enamides and enecarbamates with moderate enantioselectivity and good yields. Hydrolysis of the imine formed in the reaction provides α-chloroketones. Further optimization may provide excellent enantioselectivity and a general catalytic approach to the preparation of α-chloro ketones.

BO-17 **Brennan Hyler**[1], Shawn Larson[1], Jon Antilla[1]
[1]Department of Chemistry, University of South Florida

Halogen-free Heine reaction

The asymmetric conversion of the aziridine to the oxazoline is a useful tool in asymmetric synthesis. Known as the Heine reaction, the aziridine changes its configuration through isomerization. The intramolecular ring expansion occurs primarily in the presence of nucleophiles such as NaI or other halogen sources. The goal of my undergraduate research is to generate optically pure oxazolines from the corresponding racemic aziridines, via enantioselective catalysis rather than nucleophilic halogenation. To promote the acquisition of chiral product, enantioselective catalysts are used to hinder the intramolecular attack on one side of the aziridine plane; thus, preferentially favoring the other position. I have developed a method that does not use nucleophilic halogenation; this method readily isomerizes aziridines to oxazolines in substantial yield.

BO-18 **Yasmine Yousef**[1], Mark Novak[1]
[1]Department of Chemistry, Florida Institute of Technology

Approach to the enantioselective synthesis of Achilleol A utilizing Oxidosqualene Lanosterol Cyclase

Rational design of an internally modified ester is an important step for the enantioselective synthesis of Achilleol A utilizing Oxidosqualene Lanosterol Cyclase (OSLC). A key step is the sterification of a homoallylic alcohol with an appropriate carboxylic acid. Although we have accomplished the production of the homoallylic alcohol in 6 steps from an allylic chloride we desired a more efficient synthesis of the homoallylic alcohol. Consequently, we are proposing to use a modification of Yamamoto's activated barium chemistry as an alternative approach. Presented herein is an improved method for the synthesis of our surrogate substrate eliminating several steps. The surrogate substrate was then successfully cyclized to produce a key intermediate in the Achilleol A synthesis.

BO-19 **Jennifer Tejiram**[1], Kristin Costellow[1], Bill Baker[1]
[1]Department of Chemistry, University of South Florida

Extraction and chromatography of macroorganisms

This research focuses on extracting basic chemical components from marine macroorganisms and analyzing these samples against critical diseases to observe any counteractivity. The goal is to synthesize strongly counteractive components and utilize them for medical purposes. The manner in which these samples are extracted are as such: The crushed sample is cycled through three extractions of Methanol and Dichloromethane (dash 6) and then cycled through three extractions of Methanol and Water (dash 7) to pull out the natural product of the samples that may be sent on for further analysis. The major findings of this research are inconclusive as of yet however it is expected that any random sample may be an inhibitor of a particular disease. It is concluded that this research would yield samples with properties that fight the diseases that would need to be analyzed further for verification.

BO-20 **Jordan Edlinger**[1], Ryan Cormier[1] Edward Turos[1]
[1]Department of Chemistry, University of South Florida

Preparation and biological evaluation of chiral ciprofloxacin carbamates

The focus of this research is to synthesize a library of chiral carbamate ciprofloxacin derivatives and to evaluate their antimicrobial activities against an array of bacteria, including methicillin-resistant Staphylococcus aureus and Escherichia coli to determine the differences in activity between each enantiomer. Effects of each enantiomer on encapsulation efficiencies in chiral nanoparticles, particle size and their antimicrobial activity will be studied.

BO-21 **Javier Narvaez**[1], Glenroy Martin[1]
[1]Department of Chemistry, Biochemistry and Physics, University of Tampa

Biocoversion of formestane by Beauveria Bassiana ATCC 7159

Formestane is a biologically active steroid in the class of aromatase inhibitors. It is used in the treatment of breast cancer and ovarian cancer in postmenopausal woman. It suppresses the production of estrogen by inhibiting the aromatase enzyme which converts androgens into estrogens. In an attempt to increase its bioavailability the bioconversion of formestane by Beauveria bassiana was attempted. The three metabolites showed activities against the MCF7 cell lines and their identities were determined by chemical and spectroscopic means.

BO-22 **Amirali Aminmadani**[1], Ali Hussain[1], Steven Thach[1], Kirpal Bisht[1]
[1]Department of Chemistry, University of South Florida

Bridged and octamethoxy resorcinarenes in separation chemistry

Resorcinarenes are known macrocyclic tetramers that can easily be synthesized from cyclocondensation reactions of resorcinol or methyl resorcinol with various aliphatic or aromatic aldehydes under acidic conditions. Recently, octahydroxyl resorcinarene was synthesized by our group and tested as a sol-gel extraction phase in capillary microextraction for the extraction of ketones, aldehydes, alcohols, phenols and PAH's in collaboration with Dr. Malik's group. A promising affinity of octahydroxyl resorcinarene coatings toward different analytes was observed with ng/L limits of detection. Here in, we synthesized opened-cavity and bridged cavity resorcinarene macromolecules with tetrahydroxyl groups on the lower rim. Our goal is to study the roles of different molecular cavities in capillary microextraction coupled to gas chromatography, execute detailed studies on the importance of the molecular interactions of the cavities and inclusions toward different analytes, and study how the addition of the resorcinarenes to conventional coatings can enhance their selectivity and performance in microextraction.

BO-23 **Rosalinda Medina**[1], Stephen Girgis[1], Priyesh Jain[2], Sirisha Reddy Thambuluru[1], Lori A. Hazlehurst[1,2], Mark L. McLaughlin[1,2]
[1]Department of Chemistry, University of South Florida; [2]Drug Discovery Program, H. Lee Moffitt Cancer Center & Research Institute

Cyclo-proteomimetics targeting protein-protein interactions

Inhibiting therapeutically important protein-protein interactions has been a tremendous challenge for medicinal chemists. The most common secondary structural elements of proteins such the α-helix, β-sheet, β-turn, etc. can be mimicked. This creates the opportunity to rationally design inhibitors of protein-protein interaction (PPI). Herein, we describe cyclic beta-hairpin peptide-like scaffolds that mimic the recognition of diverse targets, such as integrin mediated extracellular matrix-cell adhesion in multiple myeloma, p53-MDM2, Rb-Raf and an amyloid beta fibrillogenesis inhibitor. Novel beta turn promoters that increase the propensity of cyclic peptides to adopt beta-sheet structures are highlighted. Herein we propose a novel peptidomimetic scaffold for disrupting cellular adhesion of acute myelogenous leukemia and multiple myeloma cells to the extracellular matrix components (ECM) of the bone marrow microenvironment.

NP-01 **James Vogler**[1], Chandan Barhate[1], Bill Baker[1]
[1]Department of Chemistry, University of South Florida

Isolation and structural determination of Bostrycin and Fusaquinon B from mangrove fungi

To date, billions of dollars have been spent to find an antimicrobial agent active against Plasmodium falciparum. P. falciparum originated and is most prevalent in Southeast Africa, where more than half of P. falciparum deaths worldwide occur. The aim of this research was to isolate compounds from mangrove fungi active against P. falciparum and determine whether the use of epigenetic modifiers on mangrove fungi induced production of previously 'silenced' compounds. Mangrove fungi were chosen as the experimental organism because they produce a vast array of pharmaceutically active secondary metabolites. The mangrove fungi were collected from Matheson Hammock Park and Long Key, Florida. Two compounds, Bostrycin and Fusaquinon B, have been isolated from the original mangrove fungi scale up and are both non-pharmaceutically active anthracene derivatives.

NP-02 **Amit P. Patel**[1], James Vogler[1], Chandan Barhate[1], Bill J. Baker[1]
[1]Department of Chemistry, University of South Florida

Extraction, isolation, and structural determination of biologically active marine mangrove endophytic fungi

Every year, approximately 250 million individuals are afflicted by malaria, resulting in nearly a million deaths, despite the fact that malaria is easily curable. A major issue in combating malaria is finding a cure that is both cost effective and capable of eradicating the rapidly adapting Plasmodiums that cause malaria. Marine natural products chemistry serves as an ideal front from which a cure to malaria may be found because of the diversity of compounds produced by marine organisms as well as the potential for cheaper production of effective compounds. This research focuses on endophytic mangrove fungi. These fungi reside in various parts of mangrove trees and produce compounds that prevent the growth of other organisms. Through the use of bioassay, methanol extraction, and liquid chromatography, various compounds can be discovered and isolated. Currently, an active polyketide has been discovered and is undergoing structural determination.

NP-03 **Novia Leverentz**[1], Ryan Young[1], Bill Baker[1]
[1]Department of Chemistry, University of South Florida

Synthesis and biological application of Simulium Pheromone

Current primitive efforts to monitor populations of Simulium yahense, carriers of the nemotode Onchocera volvulus (responsible for the neglected disease onchocerciasis), rely on human bait to verify nemotode presence after a two-year incubation period. An alternative synthetic method is proposed which would rely on compounds that mimic chemical signals used by this species in oviposition aggregation. The synthesis process would provide a safe, inexpensive, compact, species and gender specific way to monitor fly populations. S. yahense eggs were analyzed via SPME for potential target molecules. One compound, 2-cyclohexanone, 2-(3,3-dimethyl-5 oxocyclohexl)-5,5-dimethyl, was identified as a molecule of interest. This project was designed to synthesize 2-cyclohexanone, 2-(3,3-dimethyl-5 oxocyclohexl)-5,5-dimethyl through three reactions and determine whether the synthesized chemical will elicit selective S. yahense population response upon exposure as an alternative to human bait.

NP-04 **Sharon Zachariah**[1], Vinutha Rattehalli[1], Amir Mostatabzadeh[1], Chandan Barhate[1], Bill Baker[1]
[1]Department of Chemistry, University of South Florida

Isolation of secondary metabolites from endophytic fungi

Endophytes are fungi that reside in plants and exhibit mutual interactions with the host. Although the mechanisms and principle features of these interactions are unknown, the isolation of secondary metabolites produced by these endophytic fungi remains of high interest within the field of natural products chemistry. Since MRSA is resistant to antibiotics produced from beta-lactams, endophytic fungi metabolites can be utilized to combat the spread of bacteria. Terrestrial and marine fungi obtained from Matheson-Hammock Park were grown on petri dishes containing sabouraud-dextrose broth (SDB). These fungi are found to be active against Methicilline-resistant Staphylococcus aureus (MRSA). The active fungi (MHP 19A2, 7A1, 1A) were inoculated and grown on SDB and potato-dextrose broth (PDB). Increased growth was observed on PDB and therefore used as the primary media. Metabolite production was observed and further analyzed through MPLC, HPLC, and NMR. Final isolations were analyzed for activity and bioassayed against strains of bacteria.

NP-05 **Nathaniel O Johnson**[1], Bill Baker[1]
[1]Department of Chemistry, University of South Florida

Secondary metabolites of an Antarctic marine endophyte

Studying the medicinal effects of secondary metabolites from microorganism has been central to drug discovery for many years. This project aims to study the secondary metabolites of an endophyte isolated from an anemone 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. PSC11-37-M13C-1, a blue-gray fungus, was first grown on SDA then scaled up in one liter of broth. Following three weeks of growth, mycelia and broth was freeze dried and extracted with methanol. This crude extract was separated using a butanol/water partition. The organic fraction was separated into ten fractions 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-06 **Karna Sheth**[1], Jeffrey Joseph[1], Laurent Calcul[1], Dennis E. Kyle[2], Cedric Pearce[3], Bill J. Baker[1]
[1]Department of Chemistry, University of South Florida; [2]College of Public Health, University of South Florida; [3]Mycosynthetix, Hillsborough, NC

Extractions and separations of anti-malarial fungal samples

The Medicine for Malaria Venture (MMV) is a worldwide project in which our laboratory partners with USF Health (Tampa), Mycosynthetix (Hillsborough, NC), City University of Hong Kong, and National Taiwan Ocean University to find new and affordable drugs effective against malaria. More than 200 million people worldwide are affected by malaria, a mosquito-borne disease of the genus Plasmodium, killing over 700,000 each year. In total, 70,000 different fungi samples have been tested against malaria (P. falciparum 3D7). Our goal is to extract and separate active fungal samples using bioassay-guided fractionation with solvent extraction and chromatography, purify and identify active compounds through spectroscopic and spectrometric techniques. We will present extraction from Mycosynthetix fungal samples which led to isolation of moderately active compounds with low cytotoxicity (A549).

NP-07 **Young Pak**[1], Jeremy Beau[1], Bill Baker[1]
[1]Department of Chemistry, University of South Florida

Sturcture-activity-relationship of Meridianin A

The ongoing search for bioactive metabolites produced by Antarctic marine invertebrates has resulted in isolation of several previously characterized aminopyrimidine substituted indole alkaloids. These compounds were initially isolated from the tunicate, Aplidium meridianum, and named meridianins. Meridianin A has shown modest activity against malaria with an IC_{50} of 12 μM, but its cytotoxicity was high (15 μM), thus it would not be a good drug candidate. My research deals with continuing discovery of new meridianin analogs with the aim of increasing activity against malaria while decreasing cytotoxicity through this structure-activity-relationship study using combinations of fluorine, chlorine, bromine, methoxy, and o-benzylic substitutions at the indole C-1, C-5, and C-6 positions.