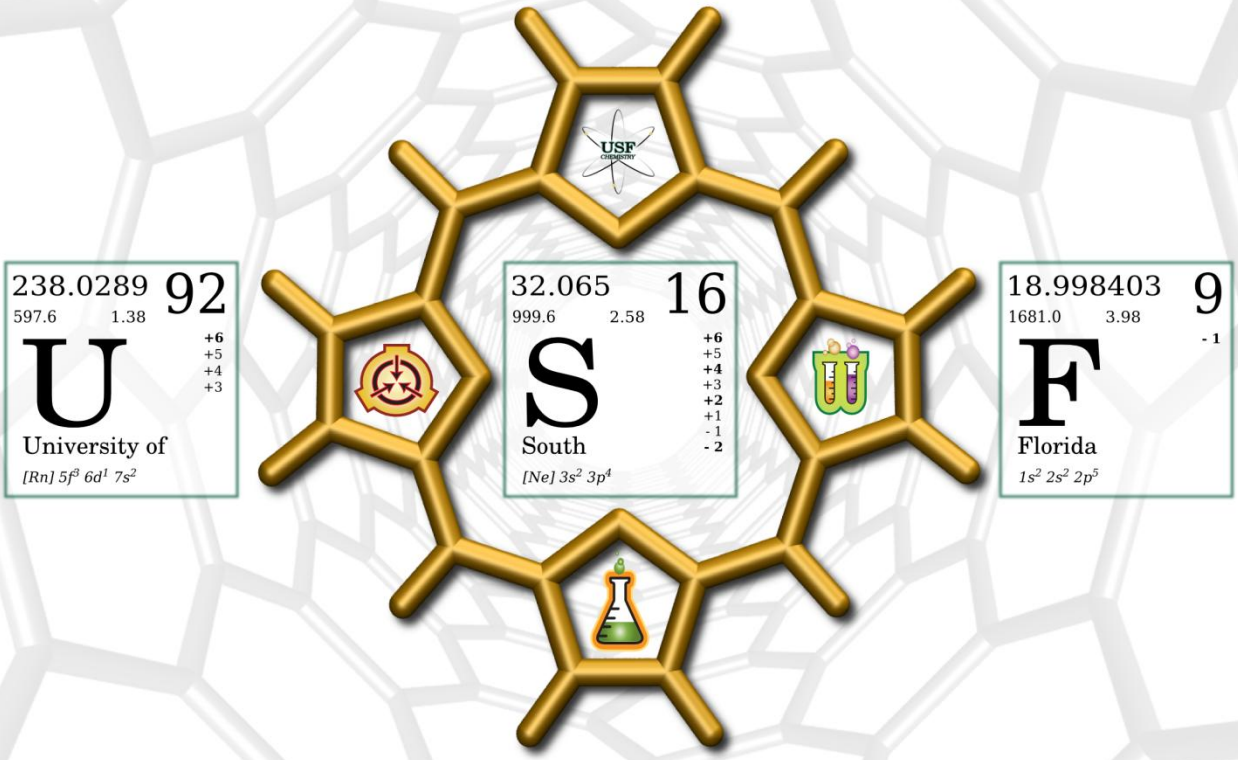
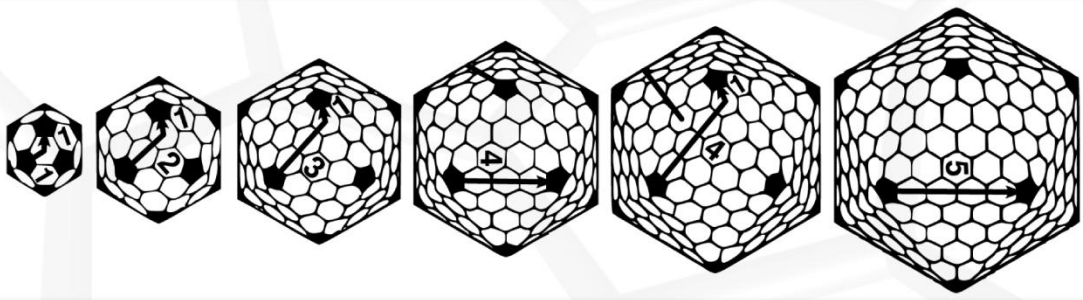
9th Raymond N. Castle Student Research Conference

April 9, 2011





9th Raymond N. Castle Student Research Conference

Proceedings Table of Contents

Welcome from the Castle Committee

Dear Colleagues and Friends,

Welcome to the 9th 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 chemistry and physics students from USF-Tampa, USF-St. Pete, and the University of Tampa. Chemistry research will be highlighted with our special guest, Dr. Charles L. Brooks, III. 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. Charles Brooks will be giving a presentation on one aspect of his exciting research.

Lastly, we would like to thank all members of the Chemistry Departments of USF-Tampa, USF-St. Pete, and UT that chose to volunteer their time and efforts, particularly the judges, Dr. Patricia Muisener and Dr. H. Lee Woodcock for helping us plan and coordinate this year's conference. In addition, we are grateful for the financial support that allows the us to host this conference and owe special thanks to the University of South Florida College of Arts and Sciences, the Tampa Bay Local Section of the American Chemical Society, and the multiple 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 9th Raymond N. Castle Student Research Conference.

Sincerely,

The Castle Conference Committee

9th Raymond N. Castle Student Research Conference Committee

Committee Members:

Christi Whittington Young (Chair)
Wiliam Maza (Co-Chair)
Rachel Alessio
Janelle Arjoon
Christian Cioce
Jason Cuce
Shradda Desai
Naga Duggirala
Todd Gatlin
Joseph Gill
Parul Jain
Sridhar Kaulagri
Ushiri Kulatunga
Justin Moses
Ranjani Muralidharan
Shruti Padhee
Prajit Pillai
Jingran Tao
Justin White

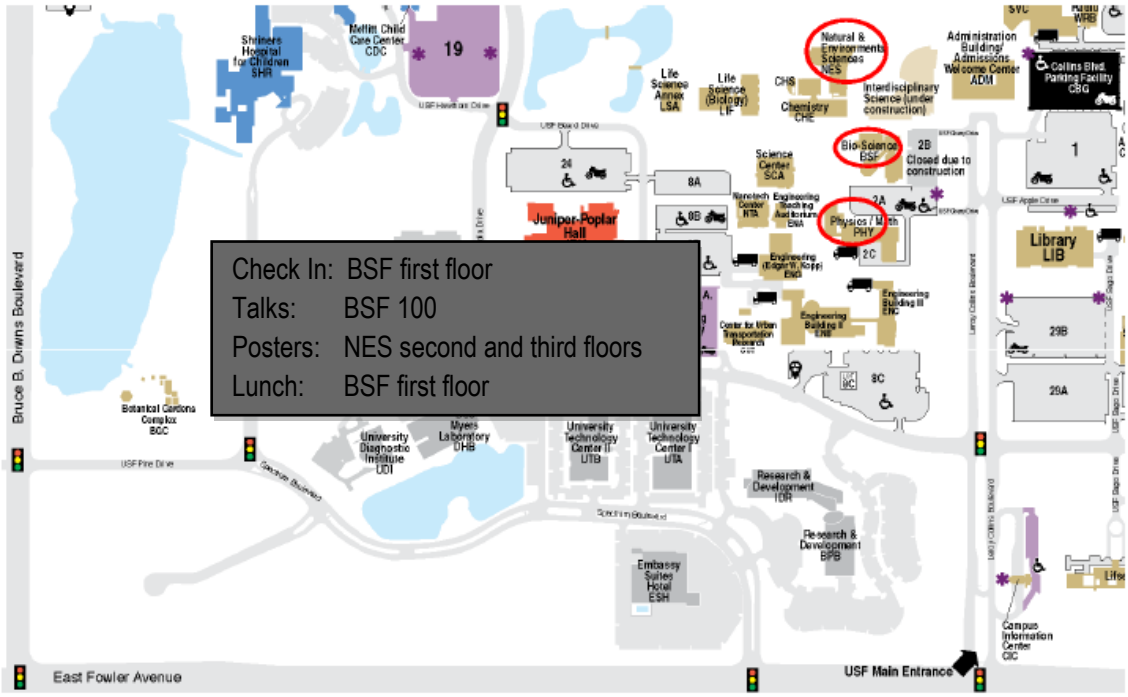
Faculty Advisors:

Dr Patricia Muisener
Dr H Lee Woodcock III

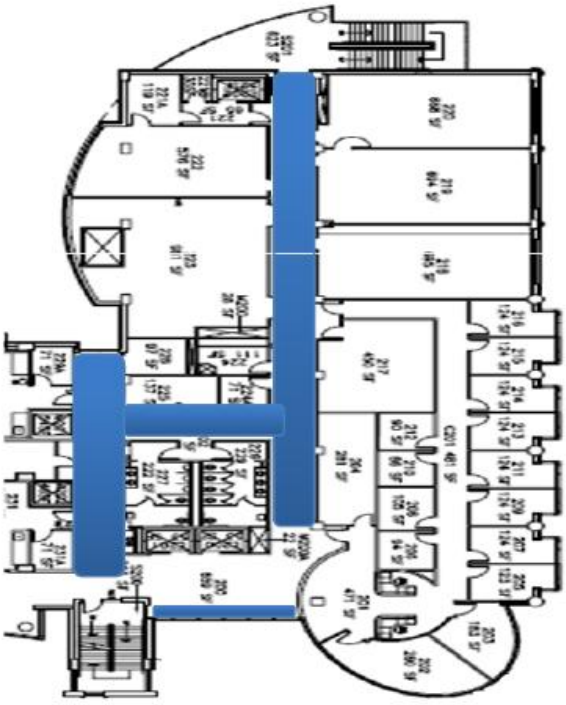
Web Support:

Jeremy Beau

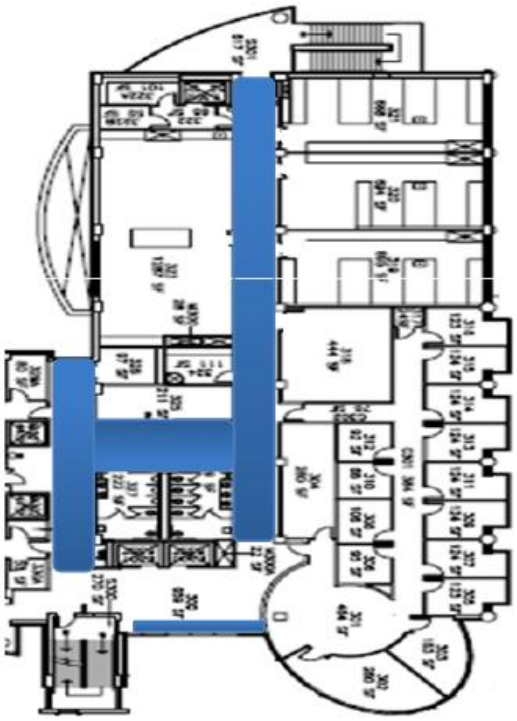
Building Maps



Second Floor Poster Session
4:45 PM – 6:15 PM



Third Floor Poster Session
11:15 AM – 12:30 PM



Schedule of Events
Saturday, April 9, 2011

8:00 AM	-	8:30 AM	**Welcome Session - Registration and Breakfast**	BSF 102 and Lobby
8:30 AM	-	8:45 AM	**Castle Conference Introduction**	BSF 100
8:45 AM	-	9:45 AM	**Talk Session I**	BSF 100
9:45 AM	-	11:00 AM	**Plenary Speaker - Dr. Charles L. Brooks III**	BSF 100
11:00 AM	-	12:15 PM	**Poster Session I**	NES 3rd Floor
12:15 PM	-	1:15 PM	**Lunch**	BSF 102 and Lobby
1:15 PM	-	2:45 PM	**Talk Session II**	BSF 100
2:45 PM	-	3:00 PM	**Break**	BSF 102 and Lobby
3:00 PM	-	4:00 PM	**Talk Session III**	BSF 100
4:00 PM	-	5:15 PM	**Poster Session II**	NES 2nd Floor
5:15 PM	-	5:45 PM	**Awards Ceremony**	BSF 100

Professor Raymond N. Castle

1916 – 1999

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

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

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

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

Dr. Charles L. Brooks III

Plenary Speaker

Dr. Charles Brooks received a Bachelor of Sciences degree from Alma College in the physical sciences in 1978 and then pursued graduate studies at Purdue University under the direction of Professor Stephen A. Adelman. His graduate work focused on the development of non-equilibrium statistical mechanical theories for reactions on surfaces, in solids and in liquids using molecular timescale generalized Langevin (MTGLE) theory which earned him a Ph.D. in 1982. Postgraduate work was done at Harvard University with Professor Martin Karplus between the years of 1982 and 1985 where he focused on theoretical and computational biophysics. Dr Brooks was the recipient of an NIH Postdoctoral Fellowship between 1983 and 1985.

In 1985 Professor Brooks joined the Chemistry Faculty of Carnegie Mellon University. He rose through the academic ranks at CMU, being promoted to Professor of Chemistry in 1992. He received an Alfred P. Sloan Research Fellowship in 1992 and during this period, 1992-1993, spent a sabbatical year working at the Karolinska Institute in Stockholm Sweden and The Scripps Research Institute in La Jolla California. Professor Brooks moved his research group to The Scripps Research Institute in 1994. Very recently (2008), Professor Brooks became more in touch with his roots by moving to the University of Michigan, where he holds the positions of Warner-Lambert/Parke-Davis Professor of Chemistry and Professor of Biophysics.

Professor Brooks has received a number of honors and awards. In 1997 he was recognized for his pioneering work in computational biophysics with a Computerworld Smithsonian Award, which includes a permanent exhibit of his work in the Smithsonian Institute in Washington D.C. In 2002 he was inducted as a Fellow of the American Association for the Advancement of the Sciences. Early in 2011 he was named one of the Top 100 Chemists, 2000-2010 by Thomson Reuters.

Professor Brooks' service to the scientific community includes several stints on review panels for the NIH and NSF, reviewing for all of the major scientific journals, as well as founding and serving on the Steering and Oversight Committees of the La Jolla Interfaces in Sciences Interdisciplinary Training Program and the Center for Theoretical Biological Physics. He currently directs an NIH funded research resource center for Multiscale Modeling Tools in Structural Biology (MMTSB). He is an Editorial Board Member for the journals *Proteins* and *Molecular Simulation*. Since January 2004 he has been the North American Editor for the *Journal of Computational Chemistry*. His Curriculum Vitae includes approximately 240 papers, including the book *Proteins: A Theoretical Perspective on Dynamics, Structure and Thermodynamics*, which was a collaborative effort with M. Karplus and M. Pettitt.

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, a position he has held since 2006. As Coordinator, Dr. Weldegirma authored the experimental manual, *Experimental Organic Chemistry Laboratory Manual: CHM 2210L and CHM 2211L*, to further the laboratory curriculum. Proceeds from the sale of the manual were donated to the Castle Conference this year. We would like to thank him for his generosity in support of this year's Castle Student Conference.

Judges

American Chemical Society Tampa Bay Local Section

Eric Ballard, Ph.D.
Eric Steimle, Ph.D.

University of Tampa

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

University of South Florida- St. Petersburg

Leon Hardy, Ph.D.

University of South Florida- Tampa

Mildred Acevedo-Duncan, Ph.D.
Kirpal S. Bisht, Ph.D.
Jianfeng Cai, Ph.D.
Laurent Calcul, Ph.D.
Xin Cui, Ph.D.
Jarrod Eubank, Ph.D.
Alicia Garcia, Ph.D.
Wayne Guida, Ph.D.
Julie P. Harmon, Ph.D.
Milt Johnston, Ph.D.
Mohanraja Kumar, Ph.D.
Xiao (Sheryl) Li, Ph.D.
Vicky Lykourinou, Ph.D.
Shenggian Ma, Ph.D.
Abdul Malik, Ph.D.
Roman Manetsch, Ph.D.
Andrea McCray, Ph.D.
Patricia Muisener, Ph.D.
George Patargias, Ph.D.
Robert Potter, Ph.D.
Brian Space, Ph.D.
Arjan van der Vaart, Ph.D.
Carrie Waterman, Ph.D.
Lukasz Wojtas, Ph.D.
H. Lee Woodcock, Ph.D.

Thank you to all of the judges for donating their time today to promote research and collaboration!

Sponsors

Tampa Bay Local Section

Tampa Bay Section of the American Chemical Society
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Affiliates

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4500 Turnberry Drive
Hanover Park, IL 60133
Phone: (800) 766-7000

Graduate Talk Session I (BSF 100)

Session Chair: Justin White

8:45 - 9:00 AM **Shraddha Desai**
PKC-ı promotes glioblastoma cell survival by phosphorylating and inhibiting BAD through a phosphotidylinositol 3-kinase pathway

9:00 - 9:15 AM **Katherine A Forrest**
Characterization of hydrogen sorption in *rht*-based metal-organic frameworks

9:15 - 9:30 AM **Biplob Bhattacharya**
Altering microbiological activity and bacterial cell targeting with C3 ring functionality of N-Thiolated ß-Lactams using protected amino acid

9:30 - 9:45 AM **Prajit P. Pillai**
A novel PKC-ı inhibitor abrogates cell proliferation and induces apoptosis in neuroblastoma

Graduate Talk Session II (BSF 100)

Session Chair: William Maza

1:15 -1:30 PM **Chengliang Jiang**
Germania-based Sol−gel Poly(dimethyldiphenylsiloxane) Stationary Phase for Capillary Gas Chromatography

1:30 - 1:45 PM **Daniel N Santiago**
Flexible docking via large-scale low-frequency modes

1:45 - 2:00 PM **Mike McIntosh**
Connecting oxidation state and redox potential of cobalt porphyrin derivatives with their catalytic activity in organic synthesis

2:00 - 2:15 PM **Divya Ramamoorthy**
Identification of a new binding site in FabH using molecular dynamics simulations and validation by docking studies

2:15 - 2:30 PM **Abdullah A Alhendal**
Sol-gel resorcinarene sorbent for capillary microextraction coupled to gas chromatography

2:30 - 2:45 PM **SaiLakshmana Vankayala**
Unlocking the binding and reaction mechanism of hydroxyurea as a biological nitric oxide donor

Graduate Talk Session III (BSF 100)

Session Chair: Jason Cuce

3:00 - 3:15 PM **Pankaj Jain**
Allylation and propargylation of aldehydes

3:15 - 3:30 PM **Andrii Monastyrskyi**
Synthesis and evaluation of 4(1H)-Quinolone prodrugs targeting multi-drug resistant P.falciparum malaria

3:30 - 3:45 PM **Jeremy Beau**
Black fly pheromones and the eradication of Onchocerciasis

3:45 - 4:00 PM **Katya P. Nacheva**
Fluorescent Properties and Resonance Energy Transfer of 3,4-bis(2,4-difluorophenyl)-maleimide

The Barbara and Dean F. Martin Poster Session I

Poster Session I (11:00 AM – 12:15 PM, NES 3rd Floor)

Session Chairs: Prajit Pillai and Rachel Allesio

Graduate:	Group GP	All Disciplines
Undergraduate:	Group CIP	Computational, Inorganic, and Physical

The Clear Springs Land Poster Session II

Poster Session II (4:00 PM – 5:15 PM, NES 2nd Floor)

Session Chairs: Joey Gill and Shraddha Desai

Undergraduate:	Group ABC	Analytical, Biochemistry, and ChemEd
Undergraduate:	Group BO	Organic and Bioorganic
Undergraduate:	Group NP	Natural Products

Graduate Talks (BSF 100)

GT-01 **Shraddha Desai**(1), Prajit Pillai(1), Hla Win-Piazza(1), Mildred Acevedo-Duncan(1,2)
(1)Department of Chemistry, University of South Florida; (2)James A. Haley Veteran's Hospital

PKC-ι promotes glioblastoma cell survival by phosphorylating and inhibiting BAD through a phosphotidylinositol 3-kinase pathway

The focus of this research was to investigate the role of protein kinase C-iota (PKC-ι) in regulation of BAD, a pro-apoptotic BH3-only molecule of the Bcl-2 family in glioblastoma. PKC-ι co-localized and directly associated with BAD, as shown by immunofluorescence, immunoprecipitation and Western blot. Furthermore, in-vitro assay showed that PKC-ι directly phosphorylated BAD at S112, S136 and S155 which in turn induced inactivation of BAD and disrupted BAD/Bcl-XL dimer. PKC- ι knockdown by siRNA exhibited a corresponding reduction in BAD phosphorylation suggesting that PKC- ι may be a BAD kinase. Since, PKC-ι is a downstream mediator of the PI (3)-kinase, we hypothesize that glioma cell survival is mediated via a PI (3)-kinase. Treatment with PI (3)-kinase inhibitors, Wortmannin, LY294002 and PDK1 siRNA, inhibited PKC-ι activity and subsequent phosphorylation of BAD. Thus, our data suggests that glioma cell survival occurs through a novel PI (3)-kinase/PDK1/ PKC-ι /BAD mediated pathway.

GT-02 **Katherine A Forrest**(1), Tony Pham(1), Jonathan L Belof(1,2), Abraham C Stern(1,3), and Brian Space(1)
(1)Department of Chemistry, University of South Florida; (2)Lawrence Livermore National Laboratory; (3)Department of Chemistry, University of California - Irvine

Characterization of hydrogen sorption in rht-based metal-organic frameworks

This research involves computational parameterization, Monte Carlo simulation, and determination of chemical behavior of hydrogen sorption in metal-organic frameworks (MOFs). Three sets of hydrogen parameters were used for simulation in PCN-61, a framework with *rht* topology, at 77K. *Rht* MOFs are notable for their high surface area and consist of several distinct polyhedral cages: truncated tetrahedral, truncated octahedral, and cuboctahedral. Sorbate potentials were selected to evaluate the importance of van der Waals, stationary electrostatic, and induction energetics in modeling this type of system. Including all of the above energy contributions produced results in good agreement with experimental isotherms. Neglecting polarization effects (common practice in MOF sorption simulation) resulted in a 10% drop in uptake at 1 atm. Further examination revealed a preferential sorption site, corresponding to dipoles ranging from 0.25-0.45 debye, which remains unsaturated without induction contributions. Two secondary sorption sites were identified, which displayed occupancy with all potentials.

GT-03 **Biplob Bhattacharya**, Edward Turos
Department of Chemistry, University of South Florida

Altering microbiological activity and bacterial cell targeting with C3 ring functionality of N-Thiolated ß-Lactams using protected amino acid

The main objective of this research project is to evaluate the antibacterial properties of N-thiolated ß-lactams bearing polar substituents at the C3 position of the ß-lactam ring. Our primary objective is to determine if a correlation exists between chain length and polarity of amino acid side chains and the in vitro antibacterial activity towards methicillin-resistant Staphylococcus aureus (MRSA).

GT-04 **Prajit P Pillai**(2), Shraddha R Desai(2), Rekha Patel(1), Mini Sajan(1,2), Robert Farese(1,2), David Ostrov(3) and Mildred Acevedo-Duncan(1,2)
(1)James A Haley Veterans Hospital; (2)Department of Chemistry, University of South Florida; (3)University of Florida

A novel PKC-ι inhibitor abrogates cell proliferation and induces apoptosis in neuroblastoma

Protein kinase C-iota (PKC-ι) confers resistance to drug-induced apoptosis in cancer cells. The acquisition of drug resistance is a major obstacle to good prognosis in neuroblastoma. The focus of this research was to identify the efficacy of [4-(5-amino-4-carbamoylimidazol-1-yl)-2, 3-dihydroxycyclopentyl] methyl dihydrogen phosphate (ICA-1) as a novel PKC-ι inhibitor in neuroblastoma cell proliferation and apoptosis. ICA-1 inhibited the activity of PKC-ι with an IC50 of approximately 0.1μM. Furthermore, our data shows that neuroblastoma cells proliferate via PKC-ι /Cdk7/cdk2 cell signaling pathway and ICA-1 mediates its antiproliferative effects by inhibiting this pathway. ICA-1 (0.1μM) inhibited the in-vitro proliferation of BE(2)-C neuroblastoma cells by 58% (P=0.01) as well as induced apoptosis in these cells. Interestingly, ICA-1 did not affect the proliferation of normal neuronal cells, suggesting its potential as a chemotherapeutic with low toxicity. Hence, our results emphasize the potential of ICA-1 as a novel PKC-ι inhibitor and chemotherapeutic agent for neuroblastoma.

GT-05 **Chengliang Jiang**, Abdullah Alhendal, Li Fang, MinhPhuong Tran, Erica Turner, Abdul Malik
Department of Chemistry, University of South Florida

Germania-based Sol−gel Poly(dimethyldiphenylsiloxane) Stationary Phase for Capillary Gas Chromatography

For the first time, capillary columns with germania-based sol-gel stationary phase were developed for high-resolution capillary gas chromatography (GC). Coating, immobilization, and deactivation of these columns were accomplished in a single step. Tetramethoxygermane was used as the sol- gel precursor and hydroxyl-terminated poly(dimethyldiphenylsiloxane) (PDMDPS) as the sol-gel active organic component . The performance of the prepared columns was evaluated using Grob test mixture, TC-WAX probe, and a series of nonpolar, moderately polar, and highly polar analytes. Van Deemter plot was constructed using methyl dodecanoate (k=6.9) as the test probe. Column efficiency on the order of 3300 theoretical plates per meter was achieved using helium as the carrier gas. Sol-gel-coated germania PDMDPS stationary phase provided fast and efficient GC separations at relatively low temperature. They provided sharp peaks for nonpolar and moderately polar analytes whereas acid peaks were tailing. This suggests that GC column with germania-based PDMDPS stationary phase needs further deactivation.

GT-06 **Daniel N. Santiago**(1), Jacob H. Weissman(1), and Wayne C. Guida(1,2,3)
(1)Department of Chemistry, University of South Florida; (2)Drug Discovery Program, H. Lee Moffitt Cancer Center and Research Institute; (3)Center for Molecular Diversity in Drug Design, Discovery and Delivery

Flexible docking via large-scale low-frequency modes

In silico techniques have been used in drug discovery to predict which small molecules are likely to be developed into an effective drug. Grid-based docking programs have been at the forefront of this approach with limited success despite its popular use. One such barrier hampering present efforts is the initial use of a rigid protein structure with a bound inhibitor, which will bias docking studies towards the pharmacophores of the bound ligand as well as the conformation of the target. A combination of grid-based docking with normal mode analysis minimizes this bias by producing a likely conformation of each protein-ligand docking. 40 small molecules, having X-ray structures with cyclin-dependent kinase 2, were docked with this protocol into unbound CDK2 (PDB 1H26). Results were as successful as ~1 RMSD compared to X-ray poses as determined by best docking score. With refinement, this protocol has potential to be comparable to current techniques.

GT-07 **Mike McIntosh**, Delilah Jewel, Xiao Li
Department of Chemistry, University of South Florida

Connecting oxidation state and redox potential of cobalt porphyrin derivatives with their catalytic activity in organic synthesis

Cobalt porphyrins act as catalytic reagents for organic syntheses (e.g. cyclopropanation) by assisting electron transfer. This early stage study will attempt to demonstrate and describe the derivative porphyrin's effects on central cobalt's redox potential and its oxidation state's role in the catalysis of organic synthesis reactions. Using well known catalytic agents and their respective reactions, cyclic voltammetry with platinum ultramicroelectrodes are used to investigate this activity.

GT-08 **Divya Ramamoorthy**, Wayne C Guida
Department of Chemistry, University of South Florida

Identification of a new binding site in FabH using molecular dynamics simulations and validation by docking studies

Biomembranes are made up of fatty acids, which supply energy. There are two main types of fatty acid synthase; FAS I and II. Fatty acid synthesis, FASII governs the synthesis of fatty acids in plants and bacteria; FAS I is employed by animals. The significant differences in structural organization, and role played by fatty acids between bacteria and humans make FASII an opportune target for antibacterial drug discovery. FabH is a key-condensing enzyme of the type II FAS system. Currently known inhibitors of FabH are developed to address the active site; the mode of action is extensively studied to develop a model for active-site inhibitor design. The formation of dimer is very important for proper functioning of the FabH enzyme. This suggests that the dimer interface of FabH may itself be targeted, which could possibly result in catalytically inactive monomers. The aim of this study is to elucidate the structural details in the interface region by means of MD simulations, to derive valuable information for structure-based design of inhibitors.

GT-09 **Abdullah Alhendal**, Abdul Malik
Department of Chemistry, University of South Florida

Sol-gel resorcinarene sorbent for capillary microextraction coupled to gas chromatography

Octahydroxy resorcinarene with a hexyl ligand was utilized in the synthesis of a silica-based sol-gel organic-inorganic hybrid coating for sample preconcentration by capillary microextraction (CME) coupled to gas chromatography (GC). Tetraethoxysilane (TEOS) was chosen as a sol-gel precursor to create a cross-linked sol-gel network via acid-catalyzed hydrolytic polycondensation reactions. In situ creation of the sol-gel coating chemically bonded to inner surface of fused silica capillary was accomplished via condensation of the sol-gel active sites on the network with the surface silanol groups. FTIR spectroscopic data suggested the chemical bonding of the resorcinarene moiety to the sol-gel network. These coatings demonstrated excellent thermal stability (up to 350 °C). For extraction, aqueous samples were passed through the sol-gel resorcinarene coated capillaries. Traces of PAHs, ketones, phenols, amines, and alcohols were successfully extracted from aqueous samples providing parts per trillion level detection limits. Sol-gel resorcinarene coated capillaries showed excellent extraction reproducibility (RSD <8.3%).

GT-10 **Sai Lakshmana Vankayala**, Wayne C Guida, H. Lee Woodcock
Department of Chemistry, University of South Florida

Unlocking the binding and reaction mechanism of hydroxyurea as a biological nitric oxide donor

Hydroxyurea is the only FDA approved treatment of 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 atomic level details of this process using a combination of flexible-ligand / flexible-receptor virtual screening (i.e. induced fit docking, IFD) coupled with energetic analysis that decomposes interaction energies at the atomic level. Using these tools we were 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. Our results are consistent with kinetic and EPR measurements of hydroxyurea-hemoglobin reactions and a full mechanism is proposed that offers new insights into possibly improving substrate binding and/or reactivity.

GT-11 **Pankaj Jain** and Jon C. Antilla
Department of Chemistry, University of South Florida

Allylation and propargylation of aldehydes

The catalytic enantioselective allylation and propargylation of aldehydes is a long-standing problem with considerable interest to the chemical community. We wish to disclose a new high yielding and highly enantioselective chiral Brønsted acid-catalyzed allylboration and propargylation of aldehydes. The reaction is shown to be highly general, with broad substrate scope that covers aryl, heteroaryl, α,ß-unsaturated, and aliphatic aldehydes. The reaction conditions were also shown to be effective for the catalytic enantioselective crotylation of aldehydes. We believe that the high reactivity of the allyl and allenyl boronate is due to protonation of the boronate oxygen by the chiral phosphoric acid catalyst.

GT-12 **Andrii Monastyrskyi**, Tina S. Mutka, Fabian Saenz, Alexis LaCrue, Dennis E. Kyle, Roman Manetsch
Department of Chemistry, University of South Florida

Synthesis and evaluation of 4(1H)-Quinolone prodrugs targeting multi-drug resistant P.falciparum malaria

4(1H)-Quinolones and 1,2,3,4-tetrahydroacridones (THAs) are known to possess causal prophylactic activity (kill growing EE stage parasites) and potent erythrocytic stage inhibition in avian malaria models, but not against malaria parasites in mammals. Recently, the Manetsch laboratory has synthesized and identified 4(1H)-quinolones and THAs displaying excellent in vitro activity against *P. falciparum* and adequate in vivo activity in *P. berghei* infected mice. Subsequent pharmacokinetic studies with compound RMMC_146 suggest that the aqueous solubility is the major reason for RMMC_146's poor bioavailability and moderate in vivo activity. Herein, we describe the development of a prodrug approach to circumvent the observed boavailability issues. 4(1H)-Quinolones have been derivatized via esterification or alkyloxycarbonyloxymethylation (AOCOM). The prepared prodrugs have then been tested for chemical stability at different pHs, aqueous solubility as well as regeneration of active parent compound in vitro and in vivo.

GT-13 **Jeremy Beau**(1), TJ McGaha(2), Raymond Noblet(2), Thomas Unnasch(3) and Bill Baker(1)
(1)Department of Chemistry, University of South Florida; (2)Department of Entomology, University of Georgia; (3)Department of Global Health, University of South Florida

Black fly pheromones and the eradication of Onchocerciasis

Onchocerciasis, or river blindness disease, is a parasitic disease caused by infection from the nematode *Onchocerca volvulus*. The parasite is transmitted to humans by black fly vectors of the genus *Simulium*. Most of the infections occur in central Africa, with significant incidence also in Central and South America. According to the WHO an estimated 18 million people suffer from onchocerciasis. The current method for monitoring the spread employs human bait, which is neither optimal nor ethically sound. The need for a new monitoring method is very important. It was noticed that gravid flies are attracted to egg masses recently deposited by flies of the same species. This paper describes our efforts to isolate and identify the pheromone responsible for this attraction, and then plan to develop as bait for a field trap for monitoring vector pressure. In the long term, field traps may be useful in eradication of the disease.

GT-14 **Katya P. Nacheva**, William Maza, David Z. Mayer, Frank R. Fronczek, Randy W. Larsen, Roman Manetsch
Department of Chemistry, University of South Florida

Fluorescent Properties and Resonance Energy Transfer of 3,4-bis(2,4-difluorophenyl)-maleimide

A fluorescent compound 3,4-bis(2,4-difluorophenyl)-maleimide from the 3,4-diaryl-substituted maleimides was synthesized and determined to have a Stokes shift of 140 nm (?abs = 341 nm, ?em = 481 nm), a high fluorescent quantum yield (?fl 0.61) and an extinction coefficient of e(340) = 48,400 $M^{-1}cm^{-1}$. For the first time we present the successful implementation of a 3,4-diaryl-substituted maleimide molecule as a donor component in FRET experiments.

The Barbara and Dean F Martin Poster Session I

GP-01 **Sachel M. Villafañe**, Jennifer E. Lewis
Department of Chemistry, University of South Florida

Understanding attitude: Preliminary results from an attempt to look beyond the average response

A four-factor career decision-making self-efficacy instrument was used to examine students' confidence toward career decision-making self-efficacy (CDMSE) within the first few weeks of an introductory college chemistry course. The scores from the instrument had good internal consistency and there was some evidence for factorial validity, but it was still difficult to interpret the results. Since the overall student response for each factor was around seven on a 10-point continuum scale, differences among students are being sought. Results from these analyses and the implications of this preliminary work is discussed.

GP-02 **Susana S. Lopez**, Todd A. Gatlin, and Santiago Sandi-Urena
Department of Chemistry, University of South Florida

Phenomenological approach to understanding learning in the laboratory

Despite having been described as a powerful tool for investigating the academic chemistry laboratory, phenomenology has been seldom used for this purpose. Understanding the meaning of the laboratory experience as lived by the participants may facilitate access to a realm of information otherwise overlooked. This approach informs not only about gains and benefits but more importantly about processes that promote learning in the laboratory. In this work, we present findings from phenomenological studies describing participants' experiences in a general chemistry laboratory course. These studies are part of a larger research program designed to use the same methodology across multiple learning environments. It is our premise that this approach will contribute towards identifying the factors that promote learning in the lab, which may then inform the design and implementation of lab experiences.

GP-03 **Todd A. Gatlin**, Santiago Sandi-Ureña
Department of Chemistry, University of South Florida

Learning from teaching: GTAs' development of scientific skills through general chemistry laboratory instruction

There is sound consensus among chemistry educators regarding the potential of laboratory instruction in promoting students' scientific literacy. Lab related education research has focused on the implementation of different instructional approaches whose effectiveness is typically assessed based on students' achievement and perceptions. An implied assumption is that the effectiveness is an intrinsic property of the instructional methodology and not of the learning environment that represents the unique shared experience of participants in the lab. Our proposal is to explore multiple laboratory learning environments to discern the common factors that promote significant learning and scientific development. Once identified, these factors can be adopted by and adapted to real laboratory experiences. In this study, we compare and contrast graduate teaching assistants' experiences (GTAs) in a non-typical laboratory program with GTAs' experiences in a typical one. For this purpose, we conducted independent phenomenological studies. Findings and implications from this work will be presented.

GP-04 **Ushiri Kulatunga**, Jennifer Lewis
Department of Chemistry, University of South Florida

Level of argumentation in general chemistry I peer-led sessions

Our research focuses on the use of Toulmin's scheme to study argumentation in Peer-Led Guided Inquiry (PLGI) sessions for general chemistry I. Data was collected by videotaping one or two small groups in a single peer-led session throughout the course of a semester. Analysis is focused on the strength of the argument and the participation patterns of the group members in constructing the argument. This poster presents findings based on analysis of data from two groups in two different sessions. Findings on comparison of the two groups on the level of argumentation as well as comparison of arguments with and without peer leader intervention for both groups are presented.

GP-05 **Shruti Padhee**, Yaogang Hu, Youhong Niu, Ge Bai, Frankie Costanza, Jianfeng Cai
Department of Chemistry, University of South Florida

AA peptides as antimicrobial peptidomimetics

The emergent resistance of bacteria against conventional antibiotics has motivated the search for novel antimicrobial agents. Nature abounds with a number of antimicrobial peptides that are part of our innate immune system and protect us against a variety of pathogenic bacteria. While they are broad-spectrum in their activity and show less drug-resistant induction, their intrinsic lack of metabolic stability limits their potential therapeutic applications. Herein we describe the development of novel broad-spectrum bioactive antimicrobial peptidomimetics-AApeptides. Substitution of nucleobases yields AApeptides that are resistant to proteolysis and capable of mimicking peptides. AApeptides showing antibacterial activity were prepared by synthesizing cationic amphipathic antibacterial peptide mimics of varying lengths. The therapeutic potential of these AApeptides were accessed by conducting antibacterial assays against a series of both gram-positive and gram-negative bacteria. The toxicity of the AA-peptides was evaluated against human erythrocytes and these AApeptides were found to be almost non-hemolytic up to 100 ug/ml.

GP-06 **Perry Mitchell, Jr.**, Jacob Shafer, Sumit Handa, David J. Merkler
Department of Chemistry, University of South Florida

N-acyltyramines & N-acyltyrosines as substrates for tyrosinase

The objectives of this study are to measure and compare the kinetic parameters of synthesized N-acyltyramine and N-acyltyrosine substrates with tyrosinase. Additionally, the tyrosinase-generated oxidation product from an N-acylated substrate was characterized. Tyrosinase is a highly studied and widespread enzyme with several important biological functions including the production of precursors to cell pigments and the cell-signaling N-acyldopamines and has been implicated in cancer. A kinetic study of these N-acylated substrates may provide greater insight into the biosynthesis of the N-acyldopamines. Kinetic data was obtained using standard oxygen electrode methodology. Synthesis of the novel substrates utilized a modified Schotten-Baumann synthesis method. These derivatives included acetyl, propanoyl, butyryl, pentanoyl and hexanoyl N-acylated tyramines and tyrosines. Kinetic results show that tyrosinase has some preference for the N-acetyl derivatives of tyramine and tyrosine compared to tyramine. The tyrosinase-generated oxidation product of N-acetyltyramine was 1-acetyl-2,3-dihydro-1H-indole-6,7-dione, a quinone.

GP-07 **Yuri Pevzner**(1,2), Daniel N. Santiago(1,2), Wesley H. Brooks(1,2), Wayne C. Guida(1,2), and H. Lee Woodcock(1)
(1)Department of Chemistry, University of South Florida; (2)HTS & Chemistry Core, H. Lee Moffitt Cancer Institute & Research Institute

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 counter screening methodology by which a potential drug candidate can be screened against a library of proteins for potential off-target hits as well as fragment based de Novo approach to designing drug molecules. Such additions will allow researchers to utilize CHARMMing as a drug design platform in addition to its existing capabilities as a molecular simulation front-end.

GP-08 **Tony Pham**, Katherine A. Forrest, Brian Space, Jonathan L. Belof, Abraham C. Stern
Department of Chemistry, University of South Florida; SMMARTT

Hydrogen Adsorption of Isoreticular (3,24)-connected Metal-Organic Framework, PCN-61, using Massive Parallel Monte Carlo (MPMC)

Hydrogen adsorption in a novel isoreticular (3-24)-connected metal-organic framework, PCN-61, was simulated using Massive Parallel Monte Carlo (MPMC) and using the grand canonical ensemble (μ, V, T). Monte Carlo simulation of hydrogen adsorption in PCN-61 was performed using three different H2 potentials: BUCH, BSS Nonpolar, and BSS Polar. The hydrogen adsorption isotherms at 77K and up to 1 atm were produced for each model, and they were compared to the isotherm that was produced via experiment. The BUCH and BSS Nonpolar models under adsorbed by ~20% and ~10%, respectively, compared to experimental data, while the BSS Polar provided a good fit for the experimental isotherm. These results show the importance of electrostatic interactions of hydrogen adsorption in PCN-61. Specifically, stationary electrostatics and induction parameters are vital to adsorption mechanics.

GP-09 **Christian R Cioce**(1), Brant Tudor(1), Jonathan Belof(1,2) and Brian Space(1)
(1)Department of Chemistry, University of South Florida; (2)Lawrence Livermore National Laboratory

Methane potential energy function

A many-body polarizable methane (CH_4) potential energy function is currently being developed for use in heterogeneous systems. The intermolecular potential is derived from first principles, and will be suitable for transferability to exogenous systems. A total of 800 points for 8 different angular orientations of the CH_4-CH_4 dimer on the potential energy surface (PES) were calculated at the CCSD(T) level of theory with aug-cc-pVTZ/aug-cc-pVQZ basis sets extrapolated to the complete basis set limit. The analytic form of the potential energy function will be suitable for methods of statistical physics, such as Monte Carlo or Molecular Dynamics simulation.

GP-10 **Courtney J. Du Boulay**, Mary Falatek, Wayne C. Guida
Department of Chemistry, University of South Florida

Using BREED to generate novel inhibitors of MDM2/MDMX

A certain docking regiment using Schrödinger's GLIDE software applied to published inhibitors of MDM2 produces scores linearly correlating with published IC_{50} values (R^2 value = 0.6). Using the correlated equation, one finds that the minimum docking score -9 Kcal/mol should achieve 1μm IC_{50} value. With the BREED genetic algorithm, fragments of known inhibitors are "breed", exchanging fragments of the inhibitors along overlapping bonds within docked positions bound to MDM2 and MDMX proteins producing a new generation of potential inhibitors. The "BREED"ing process allows for some flexibility in bond angles, 15 degrees, and position, 1Å. From approximately 40 inhibitors, this methodology generates 14,000 new molecules. The resulting inhibitors' docking scores produced 10 molecules that meet the desired scoring criteria.

GP-11 **Aleksandra Karolak**, Arjan van der Vaart
Department of Chemistry, University of South Florida

Replica exchange simulations of the inhibitory helix of the ETS-1 transcription factor

Binding of the human transcription factor Ets-1 to its DNA target sequence induces the unfolding of inhibitory helix 1 (HI-1). We performed replica exchange simulations of various HI-1 constructs to investigate the local interactions that stabilize HI-1 in the apo state. Our results indicate that the presence of the HI-2 and H4 helices stabilize the helical state of HI-1. In addition, we identified mutants that increased the stability of the HI-1 helix.

GP-12 **Mu-Seong Kim**, J. Perry, M.J. Zaworotko and Julie P. Harmon
Department of Chemistry, University of South Florida

Dielectric analysis of PHEMA and PMMA composites with OC12 nanoball

A self assembled nanostructure with OC12 functionality has been incorporated into two polymeric systems: poly(1-hydroxyethyl methacrylate) (PHEMA) and poly(methylmethacrylate) (PMMA). This nanoparticle is rhombihexahedral in shape and possesses 24 saturated 12 carbon chains on the surface. This work deals with the interactions of OC12 nanoballs with polymers and there is effect on dielectric properties. The dielectric permittivity (e´) and loss factor (e´´) measured via Dielectric Analysis (DEA) in the frequency range 1Hz to 100 kHz and between the temperature -150 to 150. The electric modulus formalism was used to reveal α, β, γ and conductivity relaxations. The activation energies for the relaxations are presented. Nanocomposites were also characterized by differential scanning calorimetry (DSC) to determine glass transition temperatures.

GP-13 **Sreya Mukherjee**, Lukasz Wojitas, Dr.Michael Zaworotko
Department of Chemistry, University of South Florida

Tailoring solubility using cocrystals

Caffeine, a natural alkaloid found in various plants, has shown efficacy against Alzheimer's disease (AD). Deposition of protein ß-amyloid (Aß) is believed to be the cause of AD pathogenesis. Caffeine has shown to be able to suppress Aß deposition in brain and thereby revert AD pathogenesis. It has a short half life, so tailoring solubility to achieve a sustained dosage form is a desirable goal. Thus, crystal engineering using the "supramolecular synthon" approach was used, to develop a series of caffeine cocrystals. Aqueous dissolution profiles of caffeine and its cocrystals were generated and concentration was measured using HPLC-UV/vis spectrophotometry. All the cocrystals exhibited a decrease in the solubility of caffeine. The dissolution profile also showed that some cocrystals depicted a smooth plateau showcasing their possibility of being used as a sustained dosage of caffeine and suggests that the new forms might be more suitable for oral delivery than pure caffeine.

GP-14 **Parul Jain**(1), Julie Harmon(1) , Alcantar Norma(2)
(1)Department of Chemistry, (2)Department of Chemical Engineering, University of South Florida

Preparation and Characterization of Bis (ethylenedioxy) tetrathiafulvalene/Iodine doped polycarbonate films

This study focuses on the fabrication of polycarbonate films doped with bis (ethylenedioxy)tetrathiafulvalene (BEDO-TTF) and complexed with iodine. These conductive polymer films were analyzed via differential scanning calorimetry (DSC), dielectric analysis (DEA), UV-Vis spectrometry (UV-Vis) and optical microscopy. Thermal studies showed a decrease in glass transition temperature as the concentration of the soluble dye, BEDO-TTF, increased. Optical images depicted the development of conductive network with respect to optimum iodine exposure time and dye concentration. Dielectric analysis (DEA) in the frequency range 1Hz to 100 KHz revealed the alpha, secondary and conductivity relaxations. These films showed a clear dependency of the bis(ethylenedioxy)tetrathiafulvalene content on conductivity and structural relaxations.

GP-15 **Justin K White**, H. Lee Woodcock
Department of Chemistry, University of South Florida

The Off-Path Simulation Method: A New Technique that Mixes Chain-of-Replica Methods with Umbrella Sampling-like Approaches

Free energy is typically referred to as the most important quantity in chemistry, with computational approaches offering unique insight into the effects that govern chemical and biochemical processes. In this work we will introduce a new chain-of-replica method that uses an umbrella sampling-like approach to determine the potential mean force (PMF) and present examples. The Off-Path Simulation method (OPS) uses multiple distance restraints to sample orthogonal directions of a discretized reference energy pathway. OPS was applied to calculate the torsional free energy of butane, and the dissaccharide maltose (vacuum and solvated). Calculated values from the OPS method are compared to published theoretical work to verify the validity of the novel method.

GP-16 **Shawn E. Larson**(1), Guilong Li(2), Gerald B. Rowland(3), Denise Junge(1), Rongcai Huang(1), H. Lee Woodcock(1), and Jon C. Antilla(1)
(1)Department of Chemistry, University of South Florida; (2)Department of Chemistry, Sun Yat-Sen University, Guangzhou, China; (3)Department of Chemistry, Mississippi State University

Catalytic asymmetric aza-Darzens reaction with vaulted biphenanthrol magnesium phosphate salt

Conditions for a catalytic asymmetric aza-Darzens aziridine synthesis mediated by a vaulted biphenanthrol (VAPOL) magnesium phosphate salt is described. Using simple substrates this methodology explores the scope and reactivity of a new magnesium catalyst for an aziridination reaction capable of building chirality and complexity simultaneously.

GP-17 **Sujeewa Ranatunga**(1,2), Jinsoo Kim(1), Juan R Del Valle(1)
(1)Drug Discovery Department, H. Lee Moffitt Cancer Center and Research Institute; (2)Department of Chemistry & Biochemistry, New Mexico State University

Exploring an enolate-Claisen rearrangement route to lucentamycin A and related 3-alkyl-4-alkylideneprolines

Lucentamycins A-D are non-ribosomal tripeptides isolated from the marine bacteria Nocardiopsis lucentensis. The most biologically active of these structures, lucentamycin A, exhibits significant cytotoxicity toward HCT-116 human colon cancer cells in vitro (IC50 = 0.20 μM). Structural elucidation revealed unique tripeptides harboring a polysubstituted central 4-ethylidene-3-methylproline (Emp) residue unprecedented in the natural product literature. Interestingly, the proline-containing analogue of lucentamycin A shows no significant cytotoxicity against HCT-116 cells indicating that the central Emp residue is crucial for bioactivity. We utilized ethyl lactate as a chiral progenitor and an enolate-Claisen rearrangement as the key step to install the relative stereochemistry of the core. Comparison of physical data of synthetic and natural products suggests the need for structural revision. Here, we will present our synthetic studies toward the natural product and expansion of the enolate-Claisen methodology to synthesize 3-alkyl-4-alkylideneprolines in addition to a series of analogs.

GP-18 **Faeez Mahzamani**, Mandi Leming, Rehana Murani, Edward Turos
Department of Chemistry, University of South Florida

Synthesis of Clodinafop-propargyl and analogs for use as antimalarial drug

The main focus of this project is to develop and enhance the activity of clodinafop-propargyl as an antimalarial drug. Clodinafop-propargyl is currently produced and marketed as an herbicide used in Wheat fields. However, during a wide search for new anti-malarial drugs, clodinafop-propargyl displayed activity against the malaria parasite and low cytotoxicity in mammals. Though the exact mode of action is not known in the parasite, the drug is known for inhibiting the enzyme Acetyl-CoA carboxylase(ACC), which in turn inhibits fatty acid synthesis. Clodinafop is important synthetically because it is composed of 3 core structures, which can be substituted for any other functional group needed. By creating analogs of the main drug, we hope to increase its activity and understand the mode of action.

The Barbara and Dean F Martin Poster Session I

CIP-01 **Crystal A Tenn**, Arjan van der Vaart
Department of Chemistry, University of South Florida

Analysis of the bacteriological toxin perfringolysin O

Perfringolysin O (PFO) belongs to a group of bacterial toxins known as cholesterol-dependent cytolysins. PFO contains four domains and binds membrane-bound cholesterol with domain 4. Upon binding it oligomerizes into a circular pre-pore, which collapses and forms a ~ 150 Å wide pore in the membrane. Pore formation involves large conformational changes and trans-membrane insertions from domain 3. Our calculations showed that the motion of domains 3 and 4 is coupled, causing domain 3 to swing away from the rest of the protein. In addition, we identified the hinge for the buckling motion of domain 2. The alpha-helices of domain 3 and the full protein were both assessed by molecular dynamics simulations in implicit EEF1 solvent, in order to compare their stability. Secondary structure and RMSD analyses confirm quantitative results of the tests. Further solvents and a contact analysis further the understanding of the conformational changes.

CIP-02 **Stephen D. Burd**, Jason A. Perman, Michael J. Zaworotko
Department of Chemistry, University of South Florida

Pillared porous metal organic materials with modular square channels by design

Metal Organic Materials (MOMs) are a broad class of coordination polymers that have been of growing interest for their applications in gas storage, separations, catalysis and ion exchange. These crystalline materials are constructed using metal nodes and organic ligand linkers to produce new structures with unrivaled surface area and permanent porosity. Structures that contain the same network topology but differ in dimensions and functionality can serve as platforms to systematically evaluate multiple properties. Investigation into synthesizing three isoreticular MOMs using an identical metal and pillaring agent with variants of the 4,4'-bipyridyl linker is desired to determine how pore size affects gas sorption and diffusion.

CIP-03 **Juan Baso**, **Mark LaBossiere**, Arjan van der Vaart
Department of Chemistry, University of South Florida

Docking of bexarotene analogs to the retinoid X-receptor

Bexarotene is an FDA approved Retinoid X Receptor (RXR) agonist that is used in the treatment of cutaneous T-cell lymphoma and shows promise for treatment of Alzheimer's disease. To help identify compounds with less severe side-effects and stronger Alzheimer activity, we performed docking studies of bexarotene analogs to the RXR receptor. Our studies suggest that structural analogues of bexarotene which possess fluoro and nitro groups ortho to the carboxylic acid group exhibit the highest binding affinity.

CIP-04 **Jeff Hernandez**, **Tatyana Jeune**, **Liliana Pimentel**, **Witny Aguy**, **Marjorie Jeune**, Bernard Knudsen, and Julie Harmon
Department of Chemistry, University of South Florida

Rheometry of covalently functionalized single walled carbon nanotubes dissolved in poly(4-methyl-1-pentene)

Raw carbon nanotubes are covalently functionalized using reductive alkylation with a dodecyl group to render them easily soluble in the same organic solvents as low molecular weight poly(4-methyl-1-pentene). The polymer and the functionalized nanotubes are dissolved together in carbon tetrachloride then the solvent is removed leaving the functionalized nanotubes uniformly dispersed in the polymer matrix. The physical characteristics are then probed with rheometry.

CIP-05 **Kyle A McDonald**, Jason A Perman, and Michael J Zaworotko
Department of Chemistry, University of South Florida

Synthesis of water stable Metal Organic Materials for anion and guest exchange applications

Crystalline Metal-Organic Materials (MOMs) are constructed using metal nodes and organic linkers by a self assembly process. Charged, porous MOMs are promising candidates for exchange with counter ions and small molecules, such as organophosphates and organosulfates. Removal of these toxic anions from aqueous environments is important for industrial waste remediation. In addition, MOMs have the potential to enable the controlled release of nutrients into the soil via guest/ion exchange. With these applications in mind, water stable square grid MOMs composed of cobalt or nickel and 4,4'-bipyridil linkers will be targeted. These materials will be synthesized with and without guest molecules present for the purpose of investigating guest/ion exchange.

CIP-06 **Jennifer Wedebrock**, **Daniel Lopez**, Parul Jain, Julie Harmon
Department of Chemistry, University of South Florida

Preparation and characterization of thin polycarbonate films for vapor sensors

Thin films made from polymers have many potential applications in the area of sensors. A thorough analysis of the properties of such films will reveal ways to apply them most effectively. The main goal of this project is to characterize thin films made from bis(ethylenedioxy-)tetrahiafulvalene (BEDO-TIF) dye- with bisphenol polycarbonate. Polycarbonate will be purified by solution precipitation, dried and ground into powder. This powder will be mixed with a solution of the dye in dichloromethane. Films will be cast for testing. Structure-property relations will be determined, using differential scanning calorimetry and UV/Visible spectroscopy and 4 point probe analysis.

CIP-07 **Thanhha Nguyen**, Tien Teng Ong, Michael Zaworotko
Department of Chemistry, University of South Florida

Cocrystal engineering of active pharmaceutical ingredients

Pharmaceutical cocrystals represent new crystal forms of APIs which are traditionally restricted to polymorphs, salts and solvates/ hydrates. They allow the tailoring of the physicochemical properties of the API while retaining the molecular structure. That the cocrystal is a new composition of matter dictates a change in the thermodynamic solubility and dissolution rate according to the Noyes Whitney equation. Since multiple cocrystals can exist for a particular API, the number of cocrystals is potentially greater than the combined numbers of polymorphs, salts, solvates and hydrates for an API. These inevitably inverted the drug discovery funnel and generate a myriad of crystal forms for the selection of the optimal crystal form to be possible. We shall report the synthesis, solid state characterization of new pharmaceutical cocrystals.

CIP-08 **Shivani Vora**, **Irvin Singh**, Ramakanth Ananthoji, Julie P. Harmon
Department of Chemistry, University of South Florida

Absorption analysis of a blister agent analog using polymer hydrogels

Blister agents are chemical compounds that induce severe skin, eye and mucosal pain and irritation. This research focuses on sequestering a blistering agent analog, thioanisole in hydrogels. A series of polyHEMA, hydroxyethyl methacryalte hydrogels with tunable crosslinkers, ethylene glycol dimethacrylate (EGDMA), diethylene glycol dimethacrylate (Di-EGDMA), triethylene glycol dimethacrylate (Tri-EGDMA), tetraethylene glycol dimethacrylate (Tet-EGDMA) and neopentyl glycol dimethacrylate (NP-EGDMA) were synthesized by varying the mol % of each crosslinker. Crosslinkers were chosen to vary crosslink spacing. The absorption of thioanisole in methanol by these hydrogels was characterized with ultra-violet visible (UV-vis) spectroscopy. The thermal stability of the hydrogels was characterized via differential scanning calorimetry (DSC).

CIP-09 **Peter M Jordan**, Patrick Nugent, Jason Perman, Michael Zaworotko
Department of Chemistry, University of South Florida

Synthesis of Metal Organic Materials from Iron and 1,2-Bis(4-pyridyl) Ethane

Metal Organic Materials (MOMs) are crystalline polymeric structures that form via self assembly of metal ion nodes and organic linkers. These materials can exhibit permanent porosity and they have proven widely applicable in areas such as gas storage, separation, and catalysis. We have synthesized a series of MOMs by means of room temperature solvent diffusion and by varying conditions. Iron was used as the metal ion node and the ligand used was 1,2-Bis (4-pyridyl) Ethane. The goal of this research is to produce 2-dimensional square MOMs using Iron (II) and Iron (III) and to study ion/guest exchange in an aqueous environment. Characterization methods include x ray powder and single crystal crystallography and IR spectroscopy for the study of ion/guest exchange.

CIP-10 **Aves N Bukhari**, Justin Moses, Li-June Ming
Department of Chemistry, University of South Florida

Analysis of oligopeptide antibiotic Thiostrepton with regards to metal binding and its effects on interaction and catalysis of DNA

Thiostrepton (TSN) is an antibiotic that inhibits protein synthesis in bacteria. Copper has previously been shown to interact with TSN using UV-Vis spectroscopy with a proposed 4:1 metal to TSN ratio, although the location for this interaction is unknown. TSN has been demonstrated to interact with ribosomal proteins and influences interaction with RNA, as such it was theorized that TSN may also have the potential to interact with DNA. It is thought that other metal ions may interact, and this study is intended to explore metal binding and their influence on DNA. Preliminary results indicate that apo-TSN is inactive towards DNA, whereas Cu4-TSN is capable of both hydrolytic and oxidative DNA cleavage.

CIP-11 **Andrea Salas**, Le Meng, Shengqian Ma
Department of Chemistry, University of South Florida

Exploration of Cobalt Imidazolate Framework for Fuel Cell Application

Fuel cell applications have a bright future as a power source for zero-emission automobiles, since they convert chemical energy in hydrogen to high-efficiency electrical energy with water as the only by-product. The expense of Pt and Pt-based catalysts interferes with its advancement, particularly at the site of the cathode for oxygen reduction reaction (ORR). Research in Dr. Ma's laboratory focuses on the development of non-precious ORR cathode catalysts to replace the Pt-based materials currently used. Recently, we've focused on the exploration of porous Co-based imidazolate frameworks as precursors for ORR catalysts, in which each Co atom coordinated to four nitrogen atoms of imidazolate ligands serves as the catalytic active site. We have obtained four new Co-imidazolate framework structures, which possess interesting zeolite topologies of SOD and RHO. Future work will focus on checking the surface areas of the obtained materials and preparing them into ORR catalysts for fuel cell tests.

CIP-12 **Evan T Vickers**, Patrick Nugent, Jason Perman, Mike Zaworotko
Department of Chemistry, University of South Florida

Metal-organic frameworks

In coordination polymers a metal cation, called a node, is connected to an organic ligand, called a linker. The linkers that are used are able to be bonded to more than one metal cation and in doing so it creates a network of 1D, 2D, or 3D grid system. Within these network grid systems, properties can be manipulated to the point in which molecules can be stored. Molecules are able to be stored because the grid systems formed have pores that attract the molecules by way of intermolecular forces. Molecules stored can be regulated through different conditions such as temperature, solvent mixing, and using different metal and ligand combinations. Once the function of the coordination polymer is fully investigated, it may be used commercially for materials.

CIP-13 **Daniel A. Velez**, Gabriel A. Goenaga, Ann V. Call, Di-Jia Liu, Le Meng, and Shengqian Ma
Department of Chemistry, University of South Florida

Introduction to fuel cell: The use of Co imadazolate frameworks accessible to gas diffusion through a porous framework

Using Co imadazolate frameworks we are trying figure out a way to convert chemical energy into electrical power in high efficiency rates, which will allow for hydrogen fuel cell vehicles. We try to accomplish this trough macromolecules of high surface area materials such a porous activated carbons. Right now platinum group metals (PGM) are the common catalyst materials of choice, so the idea is to move away from those because of their high cost and low reserves, and instead we are trying to find the most efficient oxygen reduction reaction (ORR) at the cathode of a proton exchange membrane fuel cell (PEMFC) because it creates a very important electrocatalytic reaction.

CIP-14 **Demetrios Kiriopoulos**, **Kevin Moore**, **Jessica Ruekberg**, Leon Hardy and Deby Cassill
Department of Environmental Science, Policy & Geography, University of South Florida - St. Petersburg
How to model and setup a molecular dynamics simulation of the Stat3 monomer

Signal transducer and activator of transcription 3, or Stat3, is a protein that enters a cell's nucleus from the cytoplasm. In doing so it mediates the expression of a variety of genes, which plays a role in both cell growth and apoptosis. Here we focus on the monomer which is phosphorylated in response to cell stimuli, forming a homodimer that acts like a pair of pliers as it transports DNA. After we build a model of the monomer and characterize it, we describe how to set up a molecular dynamics simulation using NAMD, an MD code, and visualize results with VMD.

CIP-15 **Jessica L Nicola**, Patrick Nugent, Jason A Perman, Michael J Zaworotko
Department of Chemistry, University of South Florida

Sequestration of hydrophobic and hydrophilic molecules using metal-organic materials

Metal-organic materials (MOMs) have become a topic of great importance in recent years. This is due in part to their adjustable porosity for applications in separation, sorption, and catalysis. MOMs are comprised of metal nodes and organic ligand linkers. In this context, we have explored the use of copper(II) nodes with bypyridyl ligands to generate MOMs with high free volume and molecular recognition features that target both hydrophobic and hydrophilic molecules. 1,2-Di(4-pyridyl)ethylene and meso-α,ß-Di(4-pyridyl) glycol (DPYG) are similar in size, but differ in functional moieties. Synthesis and structures of MOMs using these ligands will be described.

CIP-16 **Christopher Carlson**(1), Jarrod F. Eubank(1), Hasnaa Mouttaki(1), Mohamed Eddaoudi(1,2)
(1)Department of Chemistry, University of South Florida; (2)Advanced Membranes & Porous Materials Center, King Abdullah University of Science and Technology

A systematic design strategy to porous chiral MOF platforms for potential applications

Systematic study of adsorption properties through structural design of pillared square grid metal-organic frameworks (MOFs) and encapsulation of porphyrin and similar molecules for potential applications is underway. The 3D systems are composed of 2D square grids of copper paddlewheels bridged by camphorates and pillared by bipyridyl-type ligands, which vary in length and functionality. Unique bow-tie shapes of sheet windows prevents interpenetration and gas sorption; thereby, the system is a controlled environment where pores between layers differ while the grid remains constant, allowing variance of pore size and functionality of one pore type to be studied in a logical fashion (i.e. changing pillars). In some cases, inter-layer spaces are sufficient to allow small molecules. The four-fold symmetry is ideal for functionalized porphyrin-like molecules, and experiments are underway, with catalysis and separation studies following. Encapsulated materials will be compared to the original materials to note variance in surface area, gas uptake/diffusion, etc.

CIP-17 **Michael D. Glidden** and Martin Muschol
Department of Physics, University of South Florida

Characterization of lysozyme protofibrils via rotational dynamics measurements with a custom-built depolarized dynamic light scattering apparatus

Rotational diffusion measurements with Depolarized Dynamic Light Scattering (DDLS) provide detailed information on nanoparticle size and shape anisotropy. We attempt to utilize DDLS for characterizing fibril assembly of the ß-amyloid protein, lysozyme. We have obtained polarized and depolarized correlation functions for lysozyme protofibrils using a custom-built DDLS instrument. The depolarized correlation function for the protofibrils displayed slow decay modes not found in the polarized geometry. These slow modes result from short bursts ("pings") in scattering intensity that arise from large aggregates diffusing through the laser beam. Their presence was omitted from autocorrelation algorithmically by a novel software program, DEPING. The success of DEPING suggests that the pings, arising from number fluctuations, are potentially separable from the weak depolarized background. The algorithm is therefore a potential step towards a novel instrument that is capable of simultaneously measuring both the number and concentration fluctuations of a molecular system.

The Clear Springs Land Undergraduate Poster Session II

ABC-01 **Allan E Chavez** and Dean F Martin
Institute for Environmental Studies, Department of Chemistry, University of South Florida

Removal of aqueous ammonium ion by chromatography with Cobaltilig

A convenient method for removal of ammonia from water seems desirable, and the possibility of using Cobaltilig seemed appropriate. This material is a composite of aqueous cobalt chloride and Octolig®, a commercially available, polyethyleneimine covalently attached to a high-surface-area silica gel (CAS Registry No. 404899-06-5) [J. Environ.. Sci. Hlth 2008, 43, 1296]. Presumably under the conditions of synthesis, the product was converted to the cobalt(III) state. Samples of the composite in a chromatography column [1.9 cm (id) x 30 cm], were treated with dilute aqueous sodium hydroxide to convert the material to the hydroxide form, washed with water, then subjected to chromatography with a 6 ppm ammonium ion (as ammonium chloride). Best results to date indicate 94% removal, based on HACH kit analyses. Implications will be considered.

ABC-02 **Eileen Schulman**, Christi Young, and Dean F Martin
Department of Chemistry, University of South Florida

Efforts to Remove Bisphenol A using model compounds from aqueous solutions using column chromatography with Octolig®

Synthesized from phenol and acetone, Bisphenol A (BPA) is used to make polycarbonate plastics and epoxy resins. From production, an excess of BPA can contaminate the water supply and cause health problems. We are investigating the potential of Octolig®, an immobilized ligand that has entrapped anions in previous studies, to remove BPA. The long-term goal was to determine if BPA would form an anion which the immobilized ligand would trap. After considering the MSDS for BPA, we chose to begin with model compounds with similar properties to BPA. Using phenol and column chromatography, it appears that Octolig® will trap the phenol anion when the hydrogen atom of the hydroxyl group is removed by control of the solution pH value. Even though more studies need to be done, Octolig® does show promise to work to remove BPA if one of the phenolic hydrogens can be removed at a reasonable pH.

ABC-03 **Daniel T Lee**, Sungyub Han, Xiao Li
Department of Chemistry, University of South Florida

Optimize the SERS activity of Ag nanoparticles

Surface-Enhanced Raman Spectroscopy (SERS) is a valuable analytical tool which benefits from the strong enhancement generated when chemicals adsorbed on a roughened metal surface. Two variables were tested for the effect on the SERS activity of silver nanoparticles, the most commonly used substrates. Optimal SERS activity was obtained when Ag nanoparticles were synthesized at 95° C instead of at boiling temperature as reported. The effect of pH was also tested by adjusting the solution pH to varying levels before the addition of the reducing agent. The solution was later returned to a pH of 7 after the synthesis. Interestingly, a pH of 10 provided the highest SERS intensity. Such results are important to further improve the sensitivity of SERS.

ABC-04 **Cheryl H McCane** and Dean F Martin
Institute for Environmental Studies, Department of Chemistry, University of South Florida

Evaluation of the removal of aqueous halides by Octolig®

Cogent reasons exist for removal of halide ions from natural water systems. This study was concerned with evaluating the ease or possibility of removing fluoride, chloride, and bromide ions from water by column chromatography with Octolig®, a commercially available, polyethyleneimine covalently attached to a high-surface-area silica gel (CAS Registry No. 404899-06-5). Previous research suggested a mechanism for removal of certain anions [J. Environ. Sci. Hlth., 44A: 1545-1550]and subsequent research indicated the efficacy for removal of fluoride ion [J. Environ. Sci. Hlth.45A:1144-1149] and further unpublished research indicated bromide was not removed under similar conditions. Plotting percent removal as a function of charge/ion volume ratio suggested perhaps 20% removal might be anticipated for chloride ion. As seen by completed unpublished research, nearer 10% of Cl- ions were removed. These results suggest a relationship between ionic charge distribution and percent removal. Research has been expanded to study ion-removal in collected well water.

ABC-05 **N. Nabar** and Dean .F. Martin
Department of Chemistry, University of South Florida

Studies on the removal of Lissamine Green B (LGB) from soil in comparison with contemporary approaches

Vast amounts of chemical dyes (around 106 tons) are made annually worldwide. Dye effluents make their way into runoff and wastewater, eventually settling in soil. Previous extraction methods, including electrochemical methods using Fenton's reagent, have had limited success and are not cost efficient. We examined the efficacy of dye removal using a kaolin-clay model for soil and Lissamine Green B (LGB) dye. The removal of LGB from a LGB/kaolin mixture was recorded after a 24 hour extraction with hot water using a Soxhlet apparatus. Previously, aqueous LGB removal was achieved using column chromatography with commercially available Octolig®, a polyethyldiamine molecule attached to a high surface area silica gel. The results indicated 100% removal of LGB from kaolin using successive 24-hour Soxhlet extractions. Removal of dyes using hot water and/or chromatography with Octolig® could provide a safe, large-scale solution to treating soils contaminated with dyes or other organics with suitable functional groups.

ABC-06 **Inga Sergienko**, Mu-Seong Kim, Peter Zhang and Julie P. Harmon
Department of Chemistry, University of South Florida

Methacrylate Polymer- Porphyrin Interactions Characterized By DSC for Thermal Property

A zinc(II) 2,6-dichloro-diphenyl porphyrin has been incorporated into two polymeric systems: poly(2-hydroxyethyl methacrylate) (PHEMA) and poly(methyl metacrylate) (PMMA). Polymer and polymer composites with 0.1 and 0.5 wt% of porphyrins were polymerized by bulk polymerization. This work characterizes the interactions between porphyrin and the polymers revealing interesting effects related the polymer substituents. Nanocomposites were characterized by differential scanning calorimetry (DSC) to determine glass transition temperatures. The hardness was also measured by a microhardness test characterize mechanical properties.

ABC-07 **Delilah Jewel**, Michael McIntosh, Xiao Li
Department of Chemistry, University of South Florida

Investigation of the electrochemical properties of cobalt tetraphenylporphyrin and select derivatives via cyclic voltammetry

Metalloporphyrin design and synthesis is a field of great potential for applications in catalysis and medicine. In this study, cobalt tetraphenylporphyrin (Co(TPP)) and two derivatives are characterized via cyclic voltammetry using a Pt ultramicroelectrode-based three electrode system. The effect of derivatization of Co(TPP) on the electrochemical properties of the compounds is analyzed.

ABC-08 **Sibel Demirel**, **Elizabeth Desposito**, **Erin Fagan**, Vicky Lykourinou, Li-June Ming
Department of Chemistry, University of South Florida

Mechanistic studies of catalytic activity of Cu(II)-Coordinated Copolymers with various functional groups in DNA Cleavage and oxidation of Catechol substrates

Copper (II)-bound copolymers offer a more versatile alternative to small complexes towards the development of catalysts for oxidation of catechol capable of mimicking the activity of enzymes such as tyrosinase and catechol oxidase. The catalytic behavior of these copper-bound copolymers has been attributed to the functional groups in the polymeric chain namely pyridine and amide, carboxylic acid or phenyl. Moreover we observed that the oxidative activity is modulated by the chemical properties of the polymeric functional groups. We investigate the catalytic activity of three linear copolymers containing a hydrophobic or hydrophilic functional group (from styrene to acrylamide and acrylic acid) and a metal binding functional group (from vinylpyridine). The 1:1 Cu(II) complexes of these copolymers exhibit a significant catalytic activity toward catechol derivatives in air with or without H_2O_2 and toward DNA cleavage with H_2O_2. The interaction of these Cu(II)–copolymer complexes with H_2O_2 can generate very active intermediates responsible for the significant oxidative activities we observed.

ABC-09 **E. Kathleen Carter**(1), Kent W. Steely(1), Stanley M. Stevens(1,2)
(1)Department of Cell Biology, Microbiology and Molecular Biology CMMB, University of South Florida; (2)Proteomics Facility, Florida Center of Excellence for Biomolecular Identification and Targeted Therapeutics (FCoE-BITT)

Identification of enzymes selective for nitrated tyrosine in rat liver mitochondria lysate via mass spectrometry

Tyrosine nitration is a posttranslational modification that is the result of oxidative stress. Nitration can be used to monitor disease onset, progression and outcome as well as other components of cell signaling. The nitration and denitration process of tyrosine has been proposed to be the result of selective enzymatic activity. Isolation of this proposed enzyme has been investigated using tyrosine and nitro-tyrosine affinity columns. Rat liver mitochondrial lysate was passed through the columns and showed a stronger affinity for the nitrated tyrosine column than the tyrosine column based on protein assay suggesting enzymatic selectivity. Further analysis of the proteins extracted from the affinity columns will be performed using mass spectrometric techniques. Isolation of such enzyme will lead to further investigation and confirmation of this posttranslational modification as a cell signaling mechanism.

ABC-10 **Juan C. Gonzalez**(1), Umut Oguz(2), John M. Koomen(2)
(1) Department of Chemistry, University of South Florida; (2)H. Lee Moffitt Cancer Center

Comparing enzymatic digestion methods for quantitative proteomics

The purpose of this study is to examine a new direction in the digestion of proteins. Traditionally, proteins are digested with Trypsin and require overnight incubation. Trypsin cleaves C-terminal to lysine and arginine, but in some cases this specificity is limiting because it can cleave fragments, which could be either too large or small for effective mass analysis. We have conducted tests with another proteolytic enzyme, pepsin. Utilization of pepsin instead of trypsin during the digestion could reduce digestion times and enable selection of a different cleavage reagent for samples that are not amenable to tryptic digestion. As another alternative, we will also analyze glutamyl endoproteinase (Glu-C). Five standard proteins will be evaluated MALDI MS to determine sequence coverage and reproducibility of digestion. Both enzymes have the potential to give more choices in sample management and enable analysis of sequences that are difficult to analyze after tryptic digestion**.**

ABC-11 **Adam A. Bergin**, **Austin A. Gower**, Todd A. Gatlin, Susana S. Lopez, Santiago Sandi-Urena
Department of Chemistry, University of South Florida

Tapping the goldmine: Use of RateMyProfessors.com as an instruction assessment tool

Online instructor evaluations have gained influence on professor and course selections at universities. However, those in academia often view these websites validity with skepticism and dismiss them without consideration of their reliability and accuracy. RatemyProfessors.com (RMP) is the most popular of such evaluation tools and houses a wealth of qualitative and quantitative elements regarding instruction, professors, and the learning process from the viewpoint of the student. The purpose of this study is to utilize RMP to develop a qualitative analysis model to interpret student's entries and construct a profile of General Chemistry instruction at our institution. The analysis included a random sampling of ten comments for each of the six current General Chemistry professors at USF submitted between 2008-2010. Findings revealed seven categories that emerged as important pertaining to students' learning environment. The validation of the online RMP data will use statistical analysis to test its convergence with the Student …

ABC-12 **Danielle E. Babb**, Yao Chen, Shengqian Ma
Department of Chemistry, University of South Florida

Metal-Organic Frameworks: A biochemical approach

The use of porous Metal-Organic Frameworks (MOFs) has gained the interest of many chemists and biochemists for the many possible applications they possess. This class of highly porous structures enables them to be possible efficient methods for gas storage, catalysis and drug delivery. Designing MOFs to incorporate guest drug molecules is the long term goal. This study is currently focused on finding the right combination of conditions, nontoxic metals, ligands, and stable structure to make the pore walls of MOFs functional for these future purposes.

ABC-13 **Kevin Kresofsky** and J. Michelle Leslie
Department of Chemistry, Biochemistry, and Physics, The University of Tampa

Gold(III)-catalyzed hydration of an aryl alkyne. A new, question-driven experiment for the undergraduate organic chemistry laboratory

Although the chemistry of alkynes is a major topic in the first semester of sophomore organic chemistry, there are currently very few laboratory experiments that explore this topic. Hydration is a useful method for the functionalization of terminal alkynes, and has thus found considerable use in synthesis. Classically, this hydration reaction requires the combination of strongly acidic conditions and the presence of a mercuric ion catalyst. While these conditions often produce the desired carbonyl compound in good to excellent yield, the environmental problems associated with mercury presents significant drawbacks. In this experiment, students investigate the use of a gold(III) catalyst for the hydration of phenylacetylene. From the results of the experiment, students are asked to examine two questions: 1) Does the gold catalyst efficiently catalyze the hydration of phenylacetylene? 2) What is the regiochemistry of the hydration reaction?

BO-01 **Arthur Maknenko** and Kirpal S. Bisht
Department of Chemistry, University of South Florida

Glycolipid analogs via a chemo enzymatic approach

Hexanoate ß-D-glucopyranoside (glucose-1-hexanoate) and 4-O-(a-D-glucopyranosyl)-1-hexanoate ß-D-glucopyranoside (maltose-1-hexanoate), facilitate the study of more complex biologically derived analogs which have been isolated from eukaryotic yeast and prokaryotic bacteria. Since a direct coupling route between a mono or a disaccharide and an ester is fretted with numerous protection/de-protection steps, a chemo enzymatic route is conceived. The carbohydrates were per acetylated while the methyl 6-hydroxyhexanoate derived from e-caprolactone was attached to the anomeric position of the ß-D-glucose pentaacetate or ß-D-maltose octaacetate by a boron trifluoride etherate catalyzed reaction. After the coupling, the acetylated products were de-protected and yielded glycolipids which were confirmed using 1H NMR. A further enzymatic modification of these compounds may produce structures which are mimics of the naturally occurring glycolipids.

BO-02 **Michael G. Mormino**, Gajendrasingh K. Ingle, Jon C. Antilla
Department of Chemistry, University of South Florida

Chiral phosphoric acid catalyzed addition of mercaptans to N-acyl imines: Synthesis of chiral N,S-acetals

Chiral N,S acetal functional groups are found in many natural products, including penicillin. We have developed a new method for the synthesis of chiral N,S acetals by the addition mercaptans to N-acyl imines. After screening various catalyst and solvents, 2, 4, 6 (i-Pr)3C6H2 BINOL and toluene produced the highest yields and ee. The rate of nucleophilic addition of mercaptans to N-acyl imines is extremely fast. The chiral N,S acetal products were obtained in quantitative yields and excellent enantioselectivity, even with 0.005 mol% of catalyst loading. A wide variety of functional groups on the N-acyl imine substates also gave excellent yield and enantioselectivity. Also, aliphatic and aromatic thiols were found to be excellent nucleophiles for this addition reaction.

BO-03 **Shannon Collins**, **Jacob Pierce**, Faeez Sisan Mahzamani, Edward Turos
Department of Chemistry, University of South Florida

Analytical studies of enantiomerically pure polyacrylate nanoparticles

Control of polymer synthesis at the molecular level enables the development of specific properties and therefore purposeful design. Polyacrylate polymers can be modified to create specific function, and therefore, can serve as tailorable frameworks. Enantiomerically pure polyacrylate nanoparticles were prepared by miniemulsion polymerization of a homogenized mixture of acrylated L-menthol (MtA) and styrene (St) in the presence of the surfactant (sodium dodecyl sulfate) and a radical initiator (potassium persulfate). Six samples of poly(MtA-co-St) nanoparticles were synthesized using 10, 20, 30, 40, 50, and 60 v/v% of MtA relative to St. The stability, particle size, and optical activity of the 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 a maximum value, and demonstrated the possibility of molecular level control of chiral material design.

BO-04 **Joshua A. Stramiello**, Priyesh Jain, Yi Liang, Mark L. McLaughlin
Department of Chemistry, University of South Florida

An ether-peptidomimetic amino acid as a cyclic beta-hairpin promoter for inhibition of p53-MDM2 interactions

The protein p53 is a naturally occurring tumor suppressor found at relatively low levels in normal cells, yet higher levels are common in cells exposed to stress, which must be regulated through negative inhibition by MDM2. Overexpression of MDM2 can completely inhibit p53 and lead to the uncontrollable proliferation of tumors that are chemotherapeutically resilient and non-apoptotic. Cyclic beta-hairpin peptides are being used to imitate the alpha-helix of p53 for inhibition of p53-MDM2 interactions, effectively leading to normal cell apoptosis in tumor cells through increased levels of uninhibited p53. Herein a design is presented for synthesis of a beta-hairpin "turn-promoter," which, upon cyclization, promotes side chain conformations that mimic the i, i+4, and i+7 residues of the N-terminal alpha-helix of p53. Incorporation of an efficient, low-cost, low-waste procedure for production of an effective alpha-hairpin "turn-promoter" will better facilitate research of medicinal cancer treatments.

BO-05 **Vladimir Salamakha**, Xin Cui, Peter Zhang
Department of Chemistry, University of South Florida

Design and Synthesis of a new generation of chiral cobalt(II) Porphyrin Catalysts

The previously synthesized Co-3,5-t-butyl-ChenPhyrin catalyst was used in the process of synthesizing new cobalt (II) corphyrin catalysts in the attempt to increase the enantioselectivity and yield of cyclopropanation and C-H insertion reactions. Two ligands which contain novel amido building blocks were synthesized using the method mentioned above to design new cobalt (II) porphyrin catalysts. These catalysts are produced at very high yields. Thus far, the newly designed cobalt (II) porphyrin catalysts have shown high yields and high enantioselectivity for C-H insertion reactions.

BO-06 **Edward Keshishian**, Ali Husain, Kirpal S. Bisht
Department of Chemistry, University of South Florida

Rim modification of resorcinarenes

Resorcinarene cavitand are cyclic tetramers formed by an acid catalyzed condensation of resorcinol and aldehydes that are being extensively investigated due to their capability to catalyze, polymerize and encapsulate guest molecules. Synthesis of resorcinarenes derivatives selectively modified on the upper or lower rim may add unique properties. The purpose of this project is to form resorcinarenes that can serve as stable platforms for further chemical modifications. Upon addition of 2-methyl resorcinol and heptaldehyde, a resorcinarene with eight hydroxyl groups was obtained. After bridging the hydroxyl groups, the upper rim was brominated and methyl p-hydroxy benzoate was attached with high yields (>90%). Another resorcinarene derivative having ester functionality on the lower rim was synthesized using trans-methyl 2,4-dimethoxycinnamate and boron trifluoride etherate ($BF_3{\cdot}O(C_2H_5)_2$). Both of these tetramers could serve as precursors for more complex cavitand structures.

BO-07 **Corey A. Francis**, Ali Husain and Kirpal S. Bisht
Department of Chemistry, University of South Florida

Tetrabromo resorcinarene synthesis from 2-methyl resorcinol

Resocinarenes are known as cyclic tetramers that can be easily synthesized from an acid-condensation reaction of resorcinol with an aldehyde. Present work focuses on the synthesis of tetrabromo resorcinarene using 2-methyl resorcinol as starting material. Octahydroxy resorcinarene was synthesized via condensation of heptaldehyde with 2-methyl resorcinol. The adjacent hydroxyl groups were bridged with a methylene group to make the resorcinarene cavitand, a rigid- bowl-shaped structure. The benzyl carbon was then bromonated to form tetrabromo resorcinarene. Tetrabromo resorcinarene has multiple bromine substituents that are viable for reactions. The bromine is known as a good leaving group in which all bromine on the upper rim of the resorcinarene can be easily substituted under nucleophilic substitution reaction.

BO-08 **Cyrus A Vahdatpour**, Meg Gali, Kirpal Bisht
Department of Chemistry, University of South Florida

Synthesis of (3r, 5s)-3,5-diacetoxycyclopent-1-ene

Synthesis of (3R, 5S)-3,5-Diacetoxycyclopent-1-ene involves a multistep reaction mechanism from the starting material dicyclopentadiene. This multistep reaction is catalyzed by enzyme PS30 to form the final product. This mechanism will be discussed through focusing on this enzyme's catalytic property. The purpose for this synthesis is to use this compound as a precursor for further evaluation in other various research purposes. Some of the techniques used for the organic synthesis were fractional distillation, column chromatography, thin lay chromatography, and vacuum filtration. In this experiment the following reactions will be discussed; the reaction from dicyclopentadiene to its monomer, cyclopentadiene to cyclopentene epoxide, from cyclopentene epoxide to cyclopentene diacetate, and then cyclopentene diacetate to (3R, 5S)-3,5-Diacetoxycyclopent-1-ene.

BO-09 **Sirisha R Thambuluru**, Priyesh Jain(1), Phillip Murray(1), Srikumar Chellappan(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

Novel linkers inducing ß-Hairpin structures in cyclic Raf1 peptides

The world is still plagued by many disease that are not curable, innovation and progress in synthesis of new drugs is necessary in order to treat these diseases. Our body produces retinoblastoma tumor suppressor protein (Rb) which regulates the cell cycle movement from G(1) phase to S phase and problems with regulation leads to the growth of tumor cells. A progression in tumor growth is led by an increase in Raf1-Rb binding interactions, so by targeting this interaction the tumor cell growth could be suppressed. The focus is placed on a 10-18 amino acid residue in the Raf-1 which regulates the Rb-Raf1 interaction and the inhibition of this interaction using a linear Raf-1 peptide ISNGFGFK. Herein we propose a synthesis of novel linkers or turn promoters which induce ß-hairpin structures in cyclic peptides, and these cyclic peptides in turn inhibit the Rb-Raf1 interactions.

BO-10 **Young J. Pak**, Jeremy Beau, Bill J Baker
Department of Chemistry, University of South Florida

Structure-activity-relationship study of Meridianin A

The ongoing search for bioactive metabolites produced by Antarctic marine invertebrates has resulted in the 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 IC50 of 12 μM but its cytotoxicity was also high (15 μM), thus it would not be a good drug candidate. We are developing analogs of meridianins with the aim of increasing the activity against malaria, while decreasing the cytotoxicity. This poster will describe the progress of this structure-activity-relationship study using fluorine, chlorine and bromine substitutions at the C-6 position of the indole.

BO-11 **Nick M Cramer**, Biplob Bhattacharya, Edward Turos
Department of Chemistry, University of South Florida

Synthesis and analysis of monosaccharide-coupled β-lactams

Methicillin resistant *Staphylococcus aureus* (MRSA) is a strain of bacteria which has become highly resistant to β-lactam antibiotics like penicillin and cephalosporins. The motivation of the MRSA research lab, lead by Dr. Turos, is to create and test the activity of new β-lactam derivatives. Typically, when long hydrophobic chains are attached to β-lactam rings, the antibiotic activity significantly decreases against MRSA. However, there has been limited research with attached hydrophilic groups, such as monosaccharide-coupled β-lactam rings. The activity of the monosaccharide-coupled β-lactam rings produced in Dr. Turos' lab have not been tested with MRSA because the synthesis of the antibiotics is incomplete. Finalization of the antibiotic synthesis and analysis of their activity against MRSA will be finished by the end of the semester. If the activity against MRSA increases, the derivatives will be further explored.

BO-12 **Darius W Wynn**, Hongjian Lu, X.P. Zhang
Department of Chemistry, University of South Florida

Selective Intramolecular C-H Amination through the Metalloradical Activation of Azides: Synthesis of Indole diamines under Neutral and Nonoxidative Conditions

Co(II) catalyzed reactions are an efficient means of synthesizing organic substrates in neutral and nonoxidative conditions. This work will investigate the efficacy of Co(II) porphyrin catalysts at synthesizing 1,3 diamines. Various organic substrates fixed with a sulfamoyl azide moiety were catalytically treated with 2 mol% of a select Co(II) catalyst under N_2 gas to measure the catalyst's ability facilitate intramolecular C-H amination. Previous investigations by Zhang et. al revealed that intramolecular C-H amination achieved yields of up to 99% and as low as 83% after catalytic treatment of the sulfamoyl azide substrate under investigation. These results showcase the catalytic power of Co(II) porphyrins as effective agents in facilitating intramolecular C-H amination. The implications will greatly contribute to the ease of synthesis of natural products and pharmaceutical drug candidates.

BO-13 **Roy Elias**, Roger Bass, Julie Harmon
Department of Chemistry, University of South Florida

Polycarbonate polyol effects on self-healing and mechanical characteristics

Polyurethanes have been recently discovered to have unique properties including the ability to self-heal. These compounds were created to be non-blocking, that is will not stick to themselves, yet will reattach to a ruptured portion of themselves. Self healing materials can have a tremendous impact on industry, and can also be used in several biomedical applications. Optimizing the self healing and strength of the polyurethanes is thereby an obvious goal. Investigations included discovery of the effects of using different polyols featuring distinct functional groups on the ability to self heal. Resulting mechanical characteristics were controlled by altering the ratios of the building blocks of polyurethanes including; diisocyanates, long-chain polyols, and short chain polyols which were used as polymer chain extenders. Results of several mechanical tests are discussed.

BO-14 **Jonathan L Dodson**, Yang Hu, Peter X. Zhang
Department of Chemistry, University of South Florida

Methodologies of asymmetric intramolecular C-H amination via Co(por) catalysis

Recently, newly formed chiral asymmetric Co(II)-porphyrins have been shown to catalyze a broad range of substrates to produce high-yielding, enantiopure compounds that have a large utility in chemical and pharmaceutical industries. Investigation of this exciting process is reported herein, in hopes that a better understanding will be gained, and the scope of this catalysis may be broadened into a general method.

NP-01 **Donata Vaiciunaite**(1), **Elizabeth A. Luffman**(1), and **Alexander Gonzalez-Jacobo**(1), Dennis Kyle(2), Laurent Calcul(1), Carrie Waterman(1), Bill J. Baker(1)
(1)Department of Chemistry, (2)Department of Global Health, University of South Florida

Drug Discovery: The Process Behind the MMV Project

Malaria is one of the most pervasive diseases in the world, affecting approximately 300-500 million people each year. Finding new small molecules to treat this problematic disease was approached by utilizing natural products from microbes in biologically rich areas. This project has screened 70,000 species of fungi for antimalarial activity. Fungi containing active crude extracts were scaled-up, extracted with methanol and separated using a hexane to methanol gradient on MPLC. The MPLC fractions were then submitted for antimalarial and cytotoxicity screening. The bioassay guided fractionation has lead to the isolation of several active pure compounds using HPLC, MS, and NMR. This research is still in progress due the high number of active MPLC fractions for which active compound have yet to be found.

NP-02 **Alexander Williams**(1), Jackie Salm(1), Jeremy Beau(1), Tina Mutka(1), Dennis Kyle(2) and Bill J. Baker(1)
(1)Department of Chemistry, (2)Department of Global Health, University of South Florida

Discovering New Anti-Malarial Compounds

Malaria is a vector-borne infectious disease; which means it is carried by a vector until it is transferred to a human. According to the World Health Organization (W.H.O.), in 2006 an estimated 247,000,000 people were infected and 891,000 people died from malaria. Malaria is becoming more resistant to current drug treatments, thus the need for new anti-malaria drugs is urgent. A collection of 400 fungal and endophytic organisms collected from the Everglades are being screened for biological activity towards malaria. The compounds are extracted in methanol, the extracts are dissolved in dimethyl sulfoxide (DMSO) to determine the biological activity of the extracts. The extracts that show anti-malarial properties are then grown in large quantities. This poster reports the progress of this research.

NP-03 **Samantha L. Landolfa**(1), Jason R. Cuce(1), Dennis E. Kyle(2), Bill J. Baker(1)
(1)Department of Chemistry, (2)Department of Global Health, University of South Florida

Secondary metabolites from the Antarctic sponge Isodictya setifera and their potential as drug leads

The Antarctic region is of particular interest to natural products chemists because it remains relatively unexplored and possesses a wealth of unique biodiversity. Organisms that thrive in this region must produce different chemical defenses to survive in the harsh polar environment, making their secondary metabolites potentially useful as drugs for human disease. These compounds often have very complex structures, making their syntheses difficult and impractical. With this knowledge, secondary metabolites from the Antarctic sponge *Isodictya setifera* are being isolated. The chemical isolation studies were performed by macroorganism extraction followed by chromatographic separation and purification of metabolites guided by proton nuclear magnetic resonance (NMR) spectroscopy. The isolates were screened in malaria, leishmaniasis, and cytotoxicity bioassays. Based on the bioassay data, extracts of interest were then be further purified by high performance liquid chromatography to identify individual compounds and determine their structures using NMR spectroscopy and mass spectrometry.

NP-04 **Morgan L Pyne**(1), Laurent Calcul(1), Bill J Baker(1), Dennis Kyle(2), Lillian Vrijmoted(3), Ka-Lai Pang(4)
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Isolation and identification of polyketides from antimalarial Taiwanese fungal extracts

This project, supported by Medicine's for Malaria Venture (MMV), is aimed at finding an alternative and affordable cure for malaria. Since the malaria parasite, Plasmodium falciparum, is continuously becoming more resistant to current drugs, discovering novel products could save millions of lives annually. In this project, which started off with approximately 70,000 fungal samples from diverse environments, we focused on about 5000 south-east Asian extracts (Taiwan and Hong-Kong). The extracts have been evaluated against Plasmodium falciparum and those that demonstrated activity against the parasite were examined through bioguided chromatographic methods and were analyzed by spectroscopic and spectrometric techniques. Overall, we are trying to find original isolates that have high antimalarial activity, while not harming the host, expressed by a low cytotoxicity. We will discuss the isolation of two known polyketides: acremonisol A and 3,4-dimethyl-8-methoxy-3,4-dihydroisocoumarin extracted from the active National Taiwan Ocean University collection No. 2009 and 1455, respectively.

NP-05 **Peter D. Silverman**, **Anaisy Pargas**, **Juan G. Escobar**, **Sharon Zachariah**, Carrie Waterman, Bill Baker
Department of Chemistry, University of South Florida

Isolation of fungal compounds as a source of antimalarial drugs

Malaria kills hundreds of thousands of people in impoverished countries throughout the world and current treatments are becoming less effective due to resistance. The goal of the Medicines for Malaria Venture (MMV) was to find antimalarial compounds from fungal extracts using bioassay guided fractionation. 70,000 species of fungi were screened and scaled-up if they demonstrated activity. The scale-ups were extracted with methanol and separated with medium pressure liquid chromatography (MPLC). The MPLC fractions were then submitted for bioassay to screen for both antimalarial and cytotoxic properties. Further isolation and identification of pure compounds was followed through by other members of the lab using high pressure liquid chromatography (HPLC), mass spectrometry (MS), and nuclear magnetic resonance (NMR). Currently, several known compounds have been found to possess strong antimalarial activity, but are also cytotoxic.

NP-06 **G. Scott Johnson**, Kristen Costelow, Jeremy Beau, Bill Baker
Department of Chemistry, University of South Florida

Mangrove endophytes

It has been found that there is a plethora of endophytes living within the bark and leaves of the Red (*Rhizophora mangle*), White (*Languncularia racemosa*), and Black (*Avicennia germinans*) Mangroves. An endophyte is either a bacterial or fungal organisms that lives within plants. Other studies have found that some of the mangrove endophytes have promising results for new potential drugs to combat infectious diseases. This poster demonstrates the field collection techniques and isolation and archiving of the endophytes. This process gives rise to a renewable resource for ongoing screening of the endophytes.

NP-07 **Garrett M Craft**, Jason Cuce, Bill J Baker
Department of Chemistry, University of South Florida

Analyzing the lipophilic extract of sponge-encrusted echinoderms in search of novel small molecule metabolites

Sponges are well known for being treasure troves of chemistry. As sessile invertebrates—with many completely lacking any form of physical protection—they subsequently must rely on secondary metabolites to reduce both predation and competition stresses in the form of encroachment and settling of other benthic fauna. Therefore, a sample of Antarctic sea stars encrusted in a sponge was extracted in whole, utilizing both lipophilic (1:1 DCM:MeOH) and hydrophilic (1:1 H2O:MeOH) solvent systems in hopes of finding novel secondary metabolites that may lend the sea star a survival advantage against predation from the encrusted sponge's chemistry. Focus was directed towards the lipophilic crude due to the majority of the compounds extracted in hydrophilic solvents being characteristically either inactive or biopolymers. Nuclear magnetic resonance (NMR) and mass spectroscopy (MS) were employed in the identification and elucidation of compounds of interest.

NP-08 **Amit P. Patel**, **James B. Vogler**, Chandan Barhate, Bill J. Baker
Department of Chemistry, University of South Florida

Determination of chemical activity of secondary metabolites produced by marine mangrove epiphytes

MRSA and VRE have become pathogens of concern over the past decade due to their resistance to many antibiotics. It has become vital to unearth compounds deadly to these pathogens to avoid the possibility of an incurable epidemic. Naturally produced compounds are excellent candidates for study due to the lack of preparation required and their inclination to display chemical activity. The focus of this research is to observe the chemical activity of secretions produced by fungi residing in mangroves on the pathogens MRSA, VRE, *C.albicans*, and malaria. The secretions that were found to be effective on pathogens were then divided into the individual compounds to determine the compound of activity. Through the study of sixty fungi over six months, this research yielded three compounds deadly to MRSA, VRE, and *C.albicans*. This study not only revealed chemically active compounds, but the effectiveness of investigation in naturally produced marine compounds.

NP-09 **Nida Mahid**, Jeremy Beau, Bill Baker
Department of Chemistry, University of South Florida

Epigenetic regulation in endophytic fungi acquired from mangrove trees

Gene regulation gives the cell control over structure and function. Epigenetics is an upcoming concept which studies chemical changes made to DNA without actually changing the genotype. Direct DNA cytosine methylation is associated with strong silencing of gene clusters in fungi. Studies show that a variety of new compounds can be acquired from fungi once those silent bio-synthetic pathways are active. To study the effects of Azacitidine, fungal samples were isolated and cultured from Floridian mangroves collected in Everglades City, Florida. We hypothesized that if we expose our three samples to Azacitidine, it would activate previously silent bio-synthetic pathways thus producing diverse array of secondary metabolites when compared to the unmodified controls. LCMS data confirmed our hypothesis. Results of the modified samples had different peaks when compared to the unmodified controls.

NP-10 **Jeffrey Joseph**, **Karna Sheth**, **Heather Trinder**, Laurent Calcul, Dennis E. Kyle, Bill J. Baker
Department of Chemistry, University of South Florida

Extractions and separations of anti-malarial fungal samples

The Medicine for Malaria Venture (MMV) is a world wide project in which our laboratory is partnered with different organizations including USF Health, Mycosynthetix (Hillsborough, NC), the City University of Hong Kong, and National Taiwan Ocean University. More than 200 million people worldwide are affected by malaria, killing over 700,000 each year. In total, 70,000 different samples of fungi have been tested against malaria. In this poster, we will present the fungal extraction process for Mycosynthetix samples. Our aim is to process the active fungal samples using various separation techniques such as solvent extraction and chromatography. The resulting fractions are submitted in 96 well plates to USF Health for malaria and cytotoxicity screening. The overall goal of this project is to find new drugs that are effective against malaria and show low cytotoxicity.

NP-11 **Quinn Colburn**, **Aklil Hiruy**, **Saiteja Mallipeddi**, Calcul Laurent, Dennis E. Kyle, Bill J. Baker
Department of Chemistry, University of South Florida

Bioguided Fractionation of Antimalarial Extracts from Fungi

The Medicines for Malaria Venture (MMV) project aims at identifying compounds that are active against *Plasmodium falciparum*, the major protist that causes malaria. Every year, there are about 250 million malaria cases and nearly one million deaths reported worldwide. 70,000 fungal samples from various parts of the world have been screened against Malaria. The active fungi were scaled-up and extracted. The extracts were fractionated using chromatography and the fractions were prepared into 96 well plates, and submitted to USF health for anti-malarial and cytotoxic evaluation. If any fractions exhibit anti-malarial properties and low cytotoxicity, further experiments are performed to isolate and identify compounds that could be developed into anti-malarial drugs.

NP-12 **Steven Austin**, Jeremy Beau, Bill J. Baker
Department of Chemistry, University of South Florida

Anti-MRSA compounds from Floridian mangroves

Mangrove trees that thrive in the coastal areas of the Florida Everglades are constantly tested by environmental factors such as winds, tides and microbial organisms from the sea water that surrounds them. Studies based in China and India have found that mangrove trees contain endophytic fungi that live within the bark, stem, leaves, and roots of the tree. These fungi have been shown to produce secondary metabolites that can be tested for antibiotic activity. After isolating and screening several hundred fungal samples from a summer trip in the canals of Everglades City, FL., a select few extracts showed promising anti-Methicillin-resistant *Staphylococcus aureus* activity. Bioassay guided fractionalization using MPLC and HPLC of each extract led to the isolation of the single active fraction from each extract. This poster presents a report of the screening results as well as the active molecules obtained from each isolated fraction.

NP-13 **Tony J. Kurian**, Jeremy Beau, Dennis Kyle and Bill J. Baker
Department of Chemistry, University of South Florida

Search for antimalarial natural products from endophytes associated with the Caribbean Princewood

Each year, one million people die from Malaria and 300-500 million people contract it. Drug-resistant strains of *Plasmodium falciparum* are emerging so there is a need for new treatments. Caribbean Princewood has traditionally been used against Malaria. Modern research confirms that stem and bark extracts of Princewood exhibit antimalarial activity. Endophytes are microbes living in plant species, and recent studies have shown that endophytes may harbor useful chemical activity. This study analyzes the endophytic fungi associated with *E. caribaeum* to determine if they yield antimalarial compounds. This is a relatively novel approach, and a review of the pertinent literature indicates that this has not been previously investigated. *E. caribaeum* samples were collected in Plantation Key, Florida. 79 fungi were isolated. The chemicals they produced were extracted and screened for antimalarial activity. Active compounds will be isolated and their structures elucidated utilizing chromatography and NMR techniques.