8th Raymond N. Castle Student Research Conference April 2010

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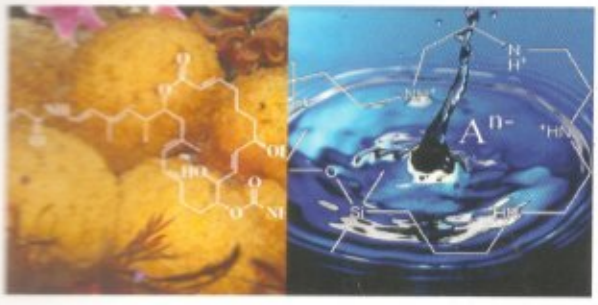

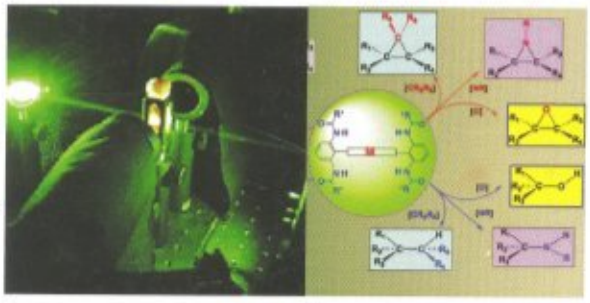

8th Raymond N. Castle Student Research Conference

Proceedings Table of Contents

Welcome from the Castle Committee

Dear Colleagues and Friends,

Welcome to the 8th Raymond N. Castle Student Research Conference. 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. Today, we have an opportunity to hear from over 100 students and our special guest, Dr. Lyle W. Castle. 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. Lyle W. Castle is able to return to USF and speak at the conference in honor of his father.

Lastly, we would like to thank all members of the Chemistry Department that chose to volunteer their time and efforts, particularly the judges and Dr. Patricia Muisener and Dr. Brian Space for helping us plan and coordinate this year's conference. We are grateful for the financial support that allows us to host this conference and owe special thanks to the University of South Florida College of Arts and Sciences, the Tampa Bay 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 8th Raymond N. Castle Student Research Conference.

Sincerely,

The Castle Conference Committee

8th Raymond N. Castle Student Research Conference Committee

Committee Members:

Todd Gatlin (Co-Chair)
Christi Whittington Young (Co-Chair)
Biplob Bhattacharya
Christian Cioce
Kimberly Fields
Joseph Gill
Priyesh Jain
Chungsik Kim
Wiliam Maza
Sreya Mukherjee
Meagan Small
Melissa (Missy) Topper
Carissa Vetromile
Justin White
Tarah Word
Xue (Snow) Xu
Mingzhou Zhou

Faculty Advisors:

Dr Patricia Muisener
Dr Brian Space

Web Support:

Tony Green

Schedule of Events
Saturday, April 17, 2010

Time	Event
8:00-8:30	Welcome Session - Registration and Breakfast NES Lobby
8:30-8:45	Castle Conference Introduction CHE 100
8:45-11:30	Morning Session – Graduate Student Oral Presentations CHE 100
11:30-11:45	Break
11:45-12:45	Plenary Speaker – Dr Lyle W Castle CHE 100
12:45-1:45	Lunch NES Lobby
1:15-2:45	Poster Session – Graduate and Undergraduate Presentations NES Hall and Classrooms
2:45-3:00	Break
3:00-5:45	Afternoon Session – Graduate Student Oral Presentations CHE 100
5:45-6:00	Break
6:00-6:15	Awards Ceremony CHE 100

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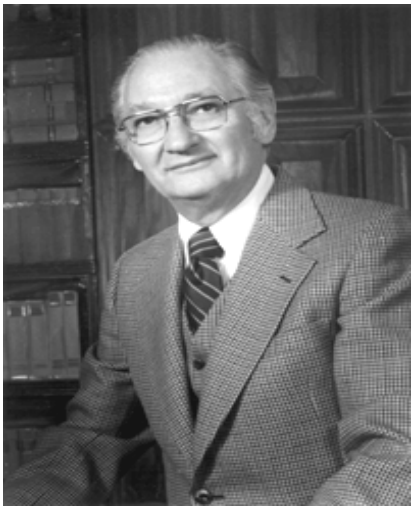
Professor Raymond N. Castle

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. Lyle W. Castle

Plenary Speaker

Dr. Lyle Castle earned a Bachelor's degree in Chemistry from Southern Utah University, a Master's degree from the University of Nebraska and a Doctoral degree in Organic Chemistry from the University of South Florida in 1992, working under the direction of Dr. Milton Johnston Jr. Dr. Castle joined the Chemistry Faculty at Idaho State University in 1994, and currently serves as Professor and Dean of Academic Programs at Idaho State University – Idaho Falls. He was appointed Dean of Academic Programs in Spring 2008. ISU – Idaho Falls currently serves nearly 3,000 students and places strong emphasis on science and engineering programs.

Throughout his career, Dr. Castle's research has largely focused on organic and organometallic synthesis, with special interest in the synthesis of heterocyclic compounds. Recent work involved the synthesis and characterization of heterocyclic compounds with potential application as photosensitizes for solar energy conversion devises. He has published numerous works in the field of heterocyclic chemistry and was named Cambridge's Who's Who in Professional of the year in Heterocyclic Chemistry in 2006.

Along with research, Dr. Castle has dedicated much time and effort towards teaching and preparing students for future careers in the sciences. He previously acted as Principal Investigator for an NSF funded grant to introduce FTNMR techniques and experiences into the general chemistry curriculum.

In September 1999, Dr. Castle took over as CEO and President of Hetero Corporation, and Editor-in-chief of the *Journal of Heterocyclic Chemistry.* His father, Raymond N. Castle, formally held both positions. The *Journal of Heterocyclic Chemistry* currently publishes six issues a year and is in its 46th year of publication.

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 arsenic by means of supported chelated iron compounds. 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. 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 four grandchildren.

Graduate Talks Morning Session Schedule (CHE 100)

Session Chair: Kimberly Fields

8:45- 9:00 AM Chungsik Kim
Ylide Chemistry via Co(III) Corroles: Axial Ligand Effect of N-H Insertion Reactions with Diverse Diazocompounds

9:00- 9:15 AM Mingzhou Zhou
The Design and Synthesis of Non-Peptidic α-helix Mimics Targeting MDM2-P53 Protein-Protein Interaction

9:15- 9:30 AM Mike McIntosh
Elucidating the Reaction Mechanism and Electrochemical Behavior of Ellagic Acid, a Natural Polyphenolic Antioxidant

9:30- 9:45 AM Sridhar Reddy Kaulagari
Design and Synthesis of Novel Phospho-Tyrosine Mimetics

9:45-10:00 AM Jingran Tao
Cobalt(II) Porphyrin Catalyzed Intramolecular C-H Amination Reaction with Carbonyl Azides

10:00-10:15 AM Break

10:15-10:30 AM Priyesh Jain
Design and Synthesis of Novel Cyclic III Peptide as β1 Integrin Inhibitor

10:30-10:45 AM Seongmin Hong
Gold Nanoparticles, Effect Substrates of Surface Enhanced Raman Spectroscopy

10:45-11:00 AM Jeremy Beau
Investigations of Antimalarial and Antibiotic Compounds from Mangrove Endophytes

11:00-11:15 AM Gajendra Ingle
Chiral BINOL Phosphoric Acid Catalyzed Addition of Diphenyl Phosphine Oxides, and Thiols to Imines

11:15-11:30 AM Melissa Topper
The Design and Synthesis of Novel α-Helical Mimetics Based on Functionalized Piperazine Units for the Antagonist Disruption of p53/MDM2 Binding Interactions

Graduate Talks Afternoon Session (CHE 100)

Session Chair: William Maza

3:00- 3:15 PM Roger Bass
Self-Healing Shape-Memory Polyurethane Containing Single and Multiwalled Carbon Nanotubes

3:15-3:30 PM Brent Hilker
Improving Electrical and Thermal Properties of Poly(methyl methacrylate) (PMMA) Utilizing Zinc(II) Mono-pinacolborane diphenylporphyrin (Zn(II)Bpin-DPP)

3:30-3:45 PM Christian Cioce
Computational Design of a Co-Por Carbene Catalyst

3:45-4:00 PM Cynthia Nwachukwu
Electrospun BSA Nanofibers: Integrin Binding with Fibronectin, Focal Adhesion Component and Cell Adhesion Strength

4:00-4:15 PM Abe Stern
New Methods for Parameterizing Simulation of Metal-Organic Materials

4:15-4:30 PM Break

4:30-4:45 PM Ranjani Muralidharan
Pt Modified Au Surfaces, Anode Catalysts for the Electro Oxidation of Formic Acid

4:45-5:00 PM Daniel Santiago
Validation of Virtual Counter Screening

5:00-5:15 PM Ramakanth Ananthoji
Effect of Substituent Groups on Thermal Stability of Sulfonyl, Carbonyl and Phosphonyl Azides

5:15-5:30 PM Mu Seong Kim
Dielectric Anylsis of PHEMA and PMMA Composites with OC12 Nanoball

5:30-5:45 PM William Maza
Ion Sensing Using a Novel Functionalized Metalloporphyrin: Spectroscopic Studies of Nitrite/Nitrate Binding to Zn(II)[3,5-DitBu-IbuPhyrin]

Graduate Talks

Morning Session (CHE 100)

M-01 8:45-9:00

Chungsik Kim[1], C Ludwin[1], EK Carter[1], X Peter Zhang[1]
[1]Department of Chemistry, University of South Florida

Ylide Chemistry via Co(III) Corroles: Axial Ligand Effect of N-H Insertion Reactions with Diverse Diazocompounds

Cobalt(III) corroles were found to be an efficient catalysts for intermolecular N-H insertion reactions with a variety of alipathics, aromatics, and amides with up to 99% yields. The catalytic reactions are extremely dependent on the fifth coordinated ligand. The cobalt(III) corroles complexes are versatile catalysts working with diverse diazo-compounds with good to high yields.

M-02 9:00-9:15

Mingzhou Zhou[1], Hyun Joo Kil[1], Melissa Topper[1], Laura Anderson[1], Jillian M McLaughlin[1], Daniel N Santiago[1], Frank R Fronczek[1], Wayne C Guida[1], Mark L McLaughlin[1]
[1]Department of Chemistry, University of South Florida

The Design and Synthesis of Non-Peptidic α-helix Mimics Targeting MDM2-P53 Protein-Protein Interaction

The p53 tumor suppressor protein plays a paramount role as the activator of the apoptosis (programmed cell death) in damaged cells. MDM2 is the major regulator of p53. MDM2 can directly bind to the wild-type p53 thereby inhibiting the activities of p53. The binding interactions between the two proteins, shown by crystallographic study, are formed between one α-helical structure from p53 and the deep hydrophobic pocket at the NH_2-terminal of MDM2. Therefore, the design and synthesis of the small molecules capable of binding to the MDM2 pocket could prevent the binding between MDM2 and p53, thus activate apoptosis. Protein p53 forms an α-helical structure that binds to MDM2, so it is reasonable to expect the α-helical peptides to be potent inhibitors of MDM2. However, peptides are usually unsuitable for intracellular targets. Following the previously reported non-peptidic α-helix mimics, we present the design and synthesis of non-peptidic molecules, containing the mixed structures of amino acids, pyrimidines, and triazoles.

M-03 9:15-9:30

Mike McIntosh[1], Tien Teng Ong[1], Xiao Li[1]
[1]Department of Chemistry, University of South Florida

Elucidating the Reaction Mechanism and Electrochemical Behavior of Ellagic Acid, a Natural Polyphenolic Antioxidant

Ellagic acid is a polyphenolic compound found in strawberries, raspberries, pomegranates, walnuts, pecans, etc. Like many other polyphenols, it exhibits beneficial antioxidant properties, which relates to the molecule's ability to scavenge harmful free radicals and reactive oxygen species. Particular anticarcinogenic properties relating to the prevention of DNA mutation have also been proposed among its benefits. In its protonated state, Ellagic acid is relatively insoluble in aqueous media, making it a difficult

candidate for study. There are currently no studies using modern electrochemical techniques that focus on studying Ellagic acid in purely aqueous media. Per the relatively low solubility of Ellagic acid, analytical methods require the detection of Ellagic acid at low micromolar or nanomolar concentrations. In this project, electrochemical methods are used to characterize Ellagic acid in aqueous media using in house, cheaply made carbon fiber ultramicroelectrodes (UMEs). It is demonstrated that both Differential Pulse Voltammetry (DPV) and Cyclic Voltammetry (CV) are economical methods for the detection of Ellagic acid. In addition, specific properties of Ellagic acid were also investigated such as its redox behavior at different pH levels, diffusion coefficient, and solubility.

M-04 9:30-9:45

Sridhar Reddy Kaulagari[1,2], Mark L. McLaughlin[1,2]
[1]Department of Chemistry, University of South Florida; [2]H. Lee Moffitt Cancer Center and Research Institute

Design and Synthesis of Novel Phospho-Tyrosine Mimetics

Protein phosphorylation is a post translational modification of proteins in which a serine, a threonine or a tyrosine residue is phosphorylated by an enzyme, kinase. Phosphorylation of proteins is a reversible and very important regulatory mechanism that occurs in both prokaryotes and eukaryotes. Phosphorylation turns many protein enzymes on and off, preventing or causing many diseases such as diabetes, cancer and rheumatoid arthritis. The phosphorylation on tyrosine residues of proteins is essential for transmission of signals for cell growth, proliferation and differentiation. Protein tyrosine phosphatases (PTPs) in concert with protein tyrosine kinases (PTKs) regulate many signal transduction pathways by regulating the degree of phosphorylation of tyrosine residues within the protein. While the roles and mechanisms of protein tyrosine kinases are well documented, our present understanding of protein tyrosine phosphatases is very less. In this regard we still have much more to understand about PTPs. Here we propose the design and synthesis of novel protein tyrosine phosphatases mimetics which we hope could be very helpful in significantly improving the current understandings about the roles and mechanisms of the PTPs. These proposed tyrosine phosphatases inhibitors are believed to work effectively in treating the diseases by modulating the phosphorylation in signal transductions pathways.

M-05 9:45-10:00

Jingran Tao[1], Hongjian Lu[1], Yang Hu[1]
[1]Department of Chemistry, University of South Florida

Cobalt(II) Porphyrin Catalyzed Intramolecular C-H Amination Reaction with Carbonyl Azides

Starting from readily available alcohols and phenols, a series of alkoxyl carbonyl azides were synthesized in a two step one-pot reaction in moderate to high yield. These azides were subjected to the designed multifunctional Co(II) Porphyrin to give intramolecular C-H amination product. Using azides as the uique nitrene source, desired 2-oxo-1, 3-oxazolidine derivatives formed without the need of terminal oxidants or other additives, generating nitrogen gas as the only byproduct.

M-06 10:15-10:30

Priyesh Jain[1], David B Badger[1], Ted J Gauthier[1], Anthony Gebhard[2], Lori A Hazlehurst[3], Mark L McLaughlin[1,4]

[1]Department of Chemistry, University of South Florida; [2]Molecular Pharmacology and Physiology, School of Biomedical Science, College of Medicine, University of South Florida; [3]Molecular Oncology, H Lee Moffitt Cancer Center & Research Institute; [4]Drug Discovery Department, H Lee Moffitt Cancer Center & Research Institute

Design and Synthesis of Novel Cyclic III Peptide as β1 Integrin Inhibitor

Standard chemotherapy treatments have been unsuccessful to eliminate Minimal Residual Disease (MRD) while treating leukemia and multiple myeloma patients. This relapse in cancer and leukemia arises due to emergence of drug resistance that decreases chemotherapy sensitivity. MRD is usually found in the bone marrow. Previous studies have shown that cellular adhesion of leukemia and multiple myeloma to extracellular matrix (ECM) component, fibronectin via β1 integrin is responsible for increased drug resistance. Integrin contains 17 α and 18 β subunits. VLA-4 (α4β1) and VLA-5 (α5β1) are most common integrin receptors found in multiple myeloma (MM), acute myeloid leukemia (AML) and chromic myelogeneous leukemia (CML). Thus inhibition of β1 integrin mediated cell adhesion has been of great interest to various research groups. Previous studies have shown that a D-amino acid peptide HYD1 inhbits β integrin mediated adhesion of myeloma cells to extracellular matrix. Herein we propose the synthesis of cyclic III (Integrin Interaction Inhibitor) peptide which inhibits β1 integrin mediated cell adhesion. The extended conformation of the cyclic peptide is believed to increase the bio-activity of the parent linear peptide.

M-07 10:30-10:45

Seongmin Hong[1], Xiao Li[1]

[1]Department of Chemistry, University of South Florida

Gold Nanoparticles, Effect Substrates of Surface Enhanced Raman Spectroscopy

The synthesis of nano metallic structures has been an active research area for many decades, because of the importance of these materials in catalysis, photography, electronics, photonics, information storage, optoelectronics, biological labeling, imaging and sensing. The essential properties of nano metallic structures can be modified by controlling their size, surface area, pH, shape, crystallinity and structure. Surface Enhanced Raman Spectroscopy (SERS) is one of the most promising techniques that requires the use of nano-structured metals, especially gold and silver. In this research, the gold nanoparticles with different size were synthesized by varying the initial concentration of hydrochlorauric acid ($HAuCl_4$), reducing agents such as hydroxylamine and sodium citrate, and temperature of solvent. The synthesized gold nanoparticles were then characterized by Scanning Electron Microscope (SEM) and UV-visible spectroscopy. At last, their corresponding SERS enhancement is tested using 4-nitrothiophenol as a standard. When there is the same number of gold nanoparticles, higher SERS enhancement was observed as the size of gold nanoparticles increases. Interestingly, with the same surface area of gold nanoparticles, the highest SERS enhancement was achieved around an average size of 50 nm of gold nanoparticles. This directly indicates…

M-08 10:45-11:00

Jeremy Beau[1], Hoangmy Chau[1], Nida Mahid[1], Lindsey Shaw[2], Tina Mutka[3], Dennis E. Kyle[3], and Bill J. Baker[3]
[1]Department of Chemistry, University of South Florida; [2]Department of Biology CMM, University of South Florida; [3]Department of Global Health, University of South Florida

Investigations of Antimalarial and Antibiotic Compounds from Mangrove Endophytes

Recent studies have shown that within the leaves, bark, roots and seeds of mangroves exists an immense world of endophytic organisms. These microscopic communities are complex, providing a great diversity of secondary metabolites with special functions that combat the microbe-plentiful seawater. These secondary metabolites have the potential to be potent and highly selective drugs. As part of our screening program for drug leads against drug-resistant bacteria and protozoan parasites, we developed a collection of mangrove-endophytic microbes. This talk will present the results of the bioassay-guided fractionation of the extracts of several endophytes, that yielded a series of compounds bearing both anti-plasmodial and antibiotic activity.

M-09 11:00-11:15

Gajendra Ingle[1], Y Liang[1], M Mormino[1], Jon Antilla[1]
[1]Department of Chemistry, University of South Florida

Chiral BINOL Phosphoric Acid Catalyzed Addition of Diphenyl Phosphine Oxides, and Thiols to Imines

Amino phosphoric acids are biologically important. The absolute configuration of phosphonyl compounds strongly influences their biological properties. However, other compounds with N, P hetero-atoms, like amino phosphine oxides have not been exploited for their biological properties due to lack of direct enantioselective synthetic route. Therefore, we have developed a new enantioselective method to synthesize α -amino phosphine oxides by addition of diphenyl phosphine oxide to imines catalyzed by chiral phosphoric acids. 9-anthryl BINOL phosphoric acid (catalyst), acetonitrile and dichloromethane (solvents) at ambient temperature produced the highest yields and enantioselectivity. A wide variety of functional groups are tolerated. Aliphatic imines produced good yields and enantioselectivity. Synthesis of amino- thio aminals is accomplished by addition thiols to N-acyl imines. After screening various catalyst and solvents 2,4,6-$(i\text{-}Pr)_3C_6H_2$ BINOL and toluene produced the highest yields and ee. Chiral N, S aminals could be used as building blocks for synthesis of the sulfur containing natural product, Fusaperazines.

M-10 11:15-11:30

Melissa Topper[1], Hyun Joo[1,2], Courtney DuBoulay[2], Frank Fronczek[3], Vasudha Sharma[2], Mark L McLaughlin[1,2]
[1]Department of Chemistry, University of South Florida; [2]Moffitt Research Cancer Center, Drug Discovery Program; [3]Department of Chemistry, Louisiana State University

The Design and Synthesis of Novel α-Helical Mimetics Based on Functionalized Piperazine Units for the Antagonist Disruption of p53/MDM2 Binding Interactions

The p53 protein promotes tumor eradication upon activation, making it an attractive target in cancer therapies. A reported 50% of all human cancers display aberrant activation of the MDM2 oncoprotein, which directly promotes tumorgenesis by inactivating the transcriptional activity of wild type p53. Previously

reported crystallographic analysis of the p53/MDM2 complex infers that the p53 protein forms an amphipathic α-helix whose hydrophobic face interacts within a hydrophobic cleft in the NH_2-terminal domain of the globular MDM2. This suggests that the synthesis of small molecule antagonists of p53/MDM2 binding interactions, capable of reactivating wild type p53 function, represents a promising therapeutic strategy in pharmaceutical discovery. Presented is the design, synthesis, and analysis of a novel class of proteomimetics based on an α-helix mimetic scaffold derived from a functionalized piperazine unit. These scaffolds are designed to mimic the hydrophobic face of two turns of an α-helix with key aromatic and hydrophobic residues in the ith, ith+3, and ith+7 positions while maintaining desired drug like properties.

Afternoon Session (CHE 100)

A-01 3:00-3:15

Roger Bass[1], Julie Harmon[1]
[1]Department of Chemistry, University of South Florida

Self-Healing Shape-Memory Polyurethane Containing Single and Multiwalled Carbon Nanotubes

A one of kind polycarbonate polyurethane (28203) was discovered that demonstrates both shape memory and self healing properties that are superior to any self healing elastomer or elastomer-like materials described in literature to date. It was discovered that 28203 samples that were ruptured during destructive testing could be pressed back together and that upon pressing together an instantaneous bond was formed between the two halves. The ruptured surfaces literally stick to each other. This was an interesting phenomenon because the material was designed not to exhibit the usual tendency of polyurethanes to block (stick to itself) when pressed together. Testing was conducted to compare the self-healing properties of neat material and composite materials containing 1 w/w% SWCNT/MWCNT and it was found that at ambient temperature, material containing CNTs healed at 24 hour timeframe retained 60-75% of its original break strength. When the material is healed at slightly elevated temperatures but kept below the melting temperature of the included soft segments (50C), the material retains >85% of its original break strength. Based on the preliminary data surrounding the healing ability of this unique material, a patent application has been filed.

A-02 3:15-3:30

Brent Hilker[1], Kimberly B Fields[1], Abraham Stern[1], Brian Space[1], X Peter Zhang[1], Julie P Harmon[1]
[1]Department of Chemistry, University of South Florida

Improving Electrical and Thermal Properties of Poly(methyl methacrylate) (PMMA) Utilizing Zinc(II) Mono-pinacolborane diphenylporphyrin (Zn(II)Bpin-DPP)

Poly(methyl methacrylate) (PMMA) composites were made from a polar metalized porphyrin [5-(4',4',5',5'-tetramethyl[1',3',2']dioxaborolan-2'-yl)-10,20-diphenylporphyrinato]zinc(II) (Zn(II)Bpin-DPP). Differential Scanning Calorimetry (DSC) showed that porphyrin acted as an antiplasticizer raising the glass transistion temperature (T_g) from 105°C to 123°C. Dielectric Analysis (DEA) was performed in the frequency range of 0.3Hz-100KHz between 150-270°C. Permittivity (ε'), loss factor (ε'') and dielectric response of beta (β), alpha (α), and conductivity relaxations were studied. The electric modulus formalism is used to reveal the β,

α, and conductivity relaxations. The apparent activation energies (E_a) for the molecular relaxations are presented. AC (σ_{AC}) and DC (σ_{DC}) conductivity are also evaluated.

A-03 3:30-3:15

Christian Cioce[1], Jonathan L Belof[1], X Peter Zhang[1], Brian Space[1], H Lee Woodcock[1]
[1]Department of Chemistry, University of South Florida

Computational Design of a Co-Por Carbene Catalyst

In this integrative study we investigate the rational design of a carbene-containing cobalt porphyrin-based catalyst implemented in a cyclopropanation reaction. The use of chemistry-based supercomputing applications offer great insight to exploit critical physical properties during the design process.

A-04 3:45-4:00

Cynthia Nwachukwu[1,3], Nathan Gallant[2,3]
[1]Department of Chemical and Biomedical Engineering, University of South Florida; [2]Department of Mechanical Engineering, University of South Florida; [3]Cellular Mechanotransduction and Biomaterials laboratory, University of South Florida

Electrospun BSA Nanofibers: Integrin Binding with Fibronectin, Focal Adhesion Component and Cell Adhesion Strength

The structural and mechanical properties of a surface often play an integral part in the determination of the cell adhesion strength and design parameters for creating a biodegradable electrospun scaffold. This electrospun protein scaffold serves as an extracellular matrix to which adhesion interaction exist with cells via cell surface integrins. This interaction is vital in regulation cell differentiation, growth and migration. Nanofibers composed of the globular proteins bovine serum albumin (BSA) and fibronectin were produced by electrospinning from a solution consisting of 10% BSA, β-mercaptoethanol, trifluoroethanol (TFE), deionized water ($dH_2O)_2$, and various concentrations of fibronectin. Fibers based on BSA were selected due to its abundance in blood and its non-adhesive nature. Therefore, the nanofibers produced via the spinning process are expected to resist protein fouling and non-specific adhesion. The incorporation of fibronectin is expected to support integrin receptor-mediated cell adhesion, would not be considered foreign and be rejected by the body when used for biomedical applications. We will demonstrate the ability to manipulate ligand receptor interaction, the properties of the electrospun fibers, the concentration of the fibronectin which when viewed during immunofluorescence analysis should show the specific binding site to which integrins can bind and finally control and the…

A-05 4:00-4:15

Abe Stern[1], Brian Space[1]
[1]Department of Chemistry, University of South Florida

New Methods for Parameterizing Simulation of Metal-Organic Materials

Computer simulation of metal-organic materials can impose challenges to conventional condensed-phase classical simulation techniques. Parameterization of the electrostatics is one area that has been particularly neglected, yet one of the most important interactions to describe correctly. Previous studies employ gas-phase parameterization techniques that fail to account for the periodicity present in metal-organic

frameworks. Here, we present a novel method to fit atomic point charges for the purposes of classical simulation that reproduces the fully periodic electrostatic potential.

A-06 4:30-4:45

Ranjani Muralidharan[1], Xiao Li[1]
[1]Department of Chemistry, University of South Florida

Pt Modified Au Surfaces, Anode Catalysts for the Electro Oxidation of Formic Acid

Present formic acid fuel cell efficiency is limited by the low kinetics at both the cathode and anode, thus inciting the need for effective catalysts which will improve the formic acid electrooxidation process. Current work involves investigating this process by the sub monolayer deposition of Pt on Au surface. The results revealed that Pt/Au assists in oxidizing formic acid at potentials as low as 0.2V as compared to plain Au (1.0V). Also, that the oxidation currents obtained is 100 times higher than on Au. This affirms the enhanced catalytic activity of Pt/Au for formic acid oxidation. Finally, the nature of the reaction intermediates formed during the electrooxidation is explored using Surface Enhanced Raman Spectroscopy.

A-07 4:45-5:00

Daniel Santiago[1], Ashley Durand[1], MinhPhuong Tran[2], Rachel G Scherer[1], Shen-Shu Sung[3], Wayne C Guida[1,2], Wesley H Brooks[1]
[1]Molecular Modeling and Virtual Screening Core, Drug Discovery Program, H. Lee Moffitt Cancer Center & Research Institute; [2]Department of Chemistry, University of South Florida; [3]Milton S. Hershey Medical Center, Pennsylvania State University

Validation of Virtual Counter Screening

The growing number of protein coordinate data has created a vast source of data; various projects attempt to take advantage of this information to discover new targets for a given small molecule. Here we present a method for comparing the binding affinities of one ligand against a protein library. Indeed, scoring functions may not be perfect in calculating binding affinities of a library of small molecules that is docked into one protein structure; however, we normalize our library of protein structures in efforts to minimize scoring function error as well as improve accuracy of defining a protein "hit." We use a calibration set of diverse ligands that are known to have at least weak binding affinity and dock them to each structure in our library to produce statistics. Given a ligand, these statistics allow the distinction of potential protein targets for drug repositioning, toxicity, metabolic degradation, and focusing focused libraries.

A-08 5:00-5:15

Ramakanth Ananthoji[1], Adrien Etienne[1], Hongjian Lu[2], Jingran Tao[2], Peter Zhang[2], Julie P Harmon[1]
[1]Polymer Chemistry Research group, University of South Florida; [2]Organic Chemistry Research group, University of South Florida

Effect of Substituent Groups on Thermal Stability of Sulfonyl, Carbonyl and Phosphonyl Azides

Organic azides are of vital importance to the scientific world in many ways. Azides are used as a way to introduce amine groups in many reactions in organic chemistry. They are also very popular for their participation in "click reactions". Low molecular weight azides are very unstable and the studies on the thermal stability of organic azides are still scarce because of their high reactivity and explosive nature. A

thermal stability study of this category can reveal vital information such as the range of the temperature where reactions can be planned, knowledge of subsequent rearrangements, cyclization reactions, melting point, energy of decomposition and safety precautions for an exothermic process. Hence the knowledge of thermal stability is considered as an important tool in organic chemistry for various reactions involving azides. Here we present the thermal stability studies of three different types of azides namely sulfonyl, carbonyl and phosphonyl azides in terms of decomposition temperature, energy of decomposition and T_{max}. The effect of substituent groups on their thermal stability for the azides is also studied using differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA).

A-09 5:15-5:30

Mu Seong Kim[1], Julie Harmon[1]
[1]Department of Chemistry, University of South Florida

Dielectric Anylsis of PHEMA and PMMA Composites with OC12 Nanoball

A self assembled nanostructure with OC_{12} 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. The effect of interactions between OH nanoballs with above mentioned polymers on dielectric properties was studied earlier. The present work deals with the interactions of OC_{12} nanoballs with polymers and that there is an effect on dielectic properties. The dielectric permittivity (ε') and loss factor (ε") measured via Dielectric Analysis (DEA) in the frequency range 1Hz to 100 kHz and between the temperatures -150 to 150°C. 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.

A-10 5:30-5:45

William Maza[1], Xin Cui[1], Chungsik Kim[1], X Peter Zhang[1], Randy W Larsen[1]
[1]Department of Chemistry, University of South Florida

Ion Sensing Using a Novel Functionalized Metalloporphyrin: Spectroscopic Studies of Nitrite/Nitrate Binding to Zn(II)[3,5-DitBu-IbuPhyrin]

The development of effective sensor elements relies on the ability of a chromophore to bind an analyte selectively and then report the binding through a change in spectroscopic signal. In this report the ability of Zn(II)[3,5-DitBu-IbuPorphyrin] (ZnDtBIP) to selectively bind nitrite ions over nitrate ions is examined. The results of Benesi-Hildebrand analysis reveals that ZnDtBIP binds nitrite ions with an association constant of 101.0 M^{-1} versus 80.9 M^{-1} for nitrate ions. In contrast, the association constants for nitrite and nitrite ion binding to unsubstituted Zn(II)tetraphenyl porphyrin (ZnTPP) are found to be 739.4 M^{-1} and 133.9 M^{-1}, respectively. Interestingly, nitrogenous ligands in the fifth coordination site of the Zn(II) center enhance both the binding and selectivity of nitrite ions with bulkier N-heterocycles providing the most significant enhancement. These results will be discussed within the context of both steric flexibility of the substituted porphyrin as well as electron factors associated with the central Zn(II) ion.

The Barbara and Dean F Martin Graduate Poster Session

Analytical, Chemical Education, and Physical (NES North Hall)

GP-01 Christi Young[1], Alfredo Cardenas[2]
[1]Department of Chemistry, University of South Florida; [2]Center for Computational Life Sciences and Biology, Institute for Computational Engineering and Sciences, University of Texas at Austin

Analysis of Molecular Dynamics Simulations of Influenza A NS1 RNA Binding Domain

The RNA binding domain of the Non-structural protein 1 (NS1) of influenza A virus, a homodimer, was studied using molecular dynamics simulations. The simulations were performed with NAMD at 298K in explicit water with force field CHARMM22. The effect of a salt solution on the domain was determined by comparison of five explicit water and nine 0.1M explicit KCl and water simulations. Flexibility of key residues in the RNA binding cavity was studied. There are eighteen possible initial structures for the simulations, of which the first NMR PDB structure was chosen. RMSD values for the possible structures were compared against average structures from the simulations and structures from normal mode analysis.

GP-02 Todd Gatlin[1], Santiago Sandi-Ureña[1]
[1]Department of Chemistry, University of South Florida

Proposed Design and Validation Strategy of an Instrument for the Assessment of College Students' Epistemological Sophistication

Research is heavily dependent upon data collection, measurement techniques and instruments. Surveys and questionnaires are a common form of instrument used and developed in chemical education research. However, as in all areas of chemistry, when new research questions arise, instruments often have to be adapted or developed in order to collect reliable data. One current area of interest in our group is personal epistemology (one's views about the nature, limits, and certainty of knowledge). Students' views of knowledge have been closely associated with their self-regulation, problem-solving performance and identity formation—relevant aspects of becoming scientists. Prior work suggests that adequately designed laboratory environments promote epistemological conflict and epistemological reflection. These two components are considered precursors for the development of sophisticated views of knowledge. However, in order to determine if students actually develop sophisticated views of knowledge as a result of the laboratory experience, data would have to be gathered before and after the experience. Thus, a reliable instrument is needed. For this purpose, we have undertaken the design and development of an epistemological sophistication inventory, ESi. This presentation will discuss the proposed design, validation strategy, and future use of ESi.

GP-03 Butch Knudsen[1], Julie P Harmon[1]
[1]Department of Chemistry, University of South Florida

The Dispersion of Functionalized Nanotubes in Polymers

Polymers play an important role in our lives affecting everything from your drinking glass to the space program. With the changing needs of the latter, new and better polymers are in demand. One way to

improve the physical properties of polymers is the dispersion of a nano material. In this case, functionalized carbon nanotubes (FCNT) were dispersed in the polymer poly(4-methyl-1-pentene), PMP. However, dispersion of the nanotubes can be tricky. Previously techniques such as sonication have been used but this resulted in only a temporary solution as the tubes would agglomerate after only a short time. This limitation can be overcome by covalently bonding organic side chains to the FCNT with the process of reductive alkylation. Once functionalized these FCNT dissolve easily in common organic solvents and stay in solution making their dispersion in a polymer easy to achieve.

GP-04 Wen-shan Chang[1], Megan Small[1], Dean F Martin[1]
[1]Department of Chemistry, University of South Florida

Use of Model Compounds to Study Removal of Pharmaceuticals Using Octolig®

The existence of pharmaceuticals in the environment has some adverse effects, and may pose threat to the organisms in the environment. The possibility of removing certain pharmaceuticals from wastewater was tested using Octolig® commercially available material with polyethyldiamine moieties covalently attached to high-surface area silica gel. Selected drug models compounds were subjected to column chromatography in efforts to effect removal by means of ion encapsulation, the effectiveness of which would depend upon having appropriate anionic functional groups. The experimental results suggested that the model compounds, Rose Bengal, Eosin Y, Erythrosine and ZPS, were success to be encapsulated by Octolig®. Methylene Blue with quaternary ammonium groups was (statistically) unsuccessful. In contrast, complete success was attained for removal of each of three xanthenylbenzenes (Rose Bengal, Eosin Y, Erythrosine) that have both phenolic and carboxylic acid groups. In addition complete success was attained for ZPS (zinc phthalocyaninetetrasulfonate) and Lissamine Green B with sulfonate anions present. In addition, test of real pharmaceutical compound had been applied on Amoxicillin, and the result indicates that Octolig® can be used to remove this compound.

GP-05 Cynthia Nwachukwu[1,3], Nathan Gallant[2,3]
[1]Department of Chemical and Biomedical Engineering, University of South Florida; [2]Department of Mechanical Engineering, University of South Florida; [3]Cellular Mechanotransduction and Biomaterials laboratory, University of South Florida

Electrospun BSA Nanofibers: Integrin Binding with Fibronectin, Focal Adhesion Component and Cell Adhesion Strength

The structural and mechanical properties of a surface often play an integral part in the determination of the cell adhesion strength and design parameters for creating a biodegradable electrospun scaffold. This electrospun protein scaffold serves as an extracellular matrix to which adhesion interaction exist with cells via cell surface integrins. This interaction is vital in regulation cell differentiation, growth and migration. Nanofibers composed of the globular proteins bovine serum albumin (BSA) and fibronectin were produced by electrospinning from a solution consisting of 10% BSA, β-mercaptoethanol, trifluoroethanol (TFE), deionized water ($dH_2O)_2$, and various concentrations of fibronectin. Fibers based on BSA were selected due to its abundance in blood and its non-adhesive nature. Therefore, the nanofibers produced via the spinning process are expected to resist protein fouling and non-specific adhesion. The incorporation of fibronectin is expected to support integrin receptor-mediated cell adhesion, would not be considered foreign and be rejected by the body when used for biomedical applications. We will demonstrate the ability to manipulate ligand receptor interaction, the properties of the electrospun fibers, the concentration of the

fibronectin which when viewed during immunofluorescence analysis should show the specific binding site to which integrins can bind and finally control and the…

GP-06 Parul Jain[1], Niloofar Ghazi-Moghaddam[1], Julie P Harmon[1]
[1]Department of Chemistry, University of South Florida

Novel Strategy for Sample Preparation used in the Detection of Biomarkers Via Induction Based Fluidics

Matrix-assisted laser desorption/ionization-Time of flight (MALDI-TOF) is a accurate and sensitive technique for the identification of biomolecules. Analysis of proteins and peptides by MALDI-TOF is affected by sample formulation and spotting onto a MALDI target. Here we used a novel technique, induction based fluidics (IBF), to analyze its effectiveness during sample preparation. It is a simple and contact free technology that offers a method of spotting samples kinetically by delivering precise volumes. We have produced bovine serum albumin samples with increased uniformity and a greater signal to noise ration by depositing in an electric field. In this study, the common “dried droplet” method is compared to electric field enhancement (EFE) sample preparation technique. Transmission electron microscopy and a polarizing optical microscope were used to contrast the EFE and dried droplet method. In addition, we used surface profilometry to demonstrate the evenness of the EFE samples.

GP-07 Sungyub Han[1], Seongmin Hong[1], Xiao Li[1]
[1]Department of Chemistry, University of South Florida

Simultaneous Detection of Tobacco-Related Biomarkers by SERS

Detection of tobacco-related biomarkers in biological samples has long been a great challenge. As the most specific component of smoke, nicotine is metabolized mainly to cotinine, and then cotinine is further metabolized to trans-3'-hydroxy cotinine and other metabolites. Since cotinine and 3'-hydroxy cotinine have longer plasma half-life (18-20 and 4-8 h, respectively) than that of nicotine (ca. 1-2 h), they are more suitable biomarkers for real time measurements. In addition, thiocyanate can also serve as a biomarker to distinguish smokers from nonsmokers. In this work, we aim to simultaneously detect three tobacco-related biomarkers: cotinine, trans 3'-hydroxy cotinine and thiocyanate using surface enhanced Raman spectroscopy (SERS). First, the effect of pH and ionic strength on the SERS enhancement is investigated. With the strong enhancement generated by Ag nanoparticles, detection of cotinine, trans 3'-hydroxy cotinine or thiocyanate in nanomolar region has been achieved. More importantly, despite of the similar chemical structure of cotinine and trans-3'-hydroxy cotinine, SERS can successfully distinguish these two chemicals. This is the first time that an optical spectroscopic method is used to detect multiple tobacco-related biomarkers.

GP-08 Erica Turner[1], Scott S. Segro[1], Abdul Malik[1]
[1]Department of Chemistry, University of South Florida

Sol-Gel Mixed Germania-Silica Poly(ethylene glycol) Monoliths for Capillary Microextraction On-line Coupled to High-Performance Liquid Chromatography

A sol-gel method was developed to create novel germania PEG-based hybrid orgranic-inorganic materials for use in capillary microextraction (CME). Sol-gel reactions were carried out within fused silica capillaries (0.32 mm I.D.) to fabricate monolithic capillaries. While monoliths have inherent advantages over

conventional coatings in the preconcentration of analytes, problems arise due to their cracking tendency. Crack free sol-gel germania PEG monolithic beds were successfully immobilized within fused silica capillaries through extension of sol-gel condensation reaction to the capillary walls. This monolith was very porous and able to withstand liquid-phase operations involving elevated pressures. Detection limits in the nanogram/liter range were accomplished with CME sol-gel germania PEG monolithic capillaries coupled to high performance liquid chromatography (HPLC) with UV detection.

GP-09 Kellen Danley[1], Arjan van der Vaart[1]
[1]Department of Chemistry, University of South Florida

Vibrational Analysis of Catabolite Activator Protein in the Apo and Holo States

Catabolite activator protein (CAP), which activates transcription by binding to specific sites of DNA, is allosterically regulated by cyclic AMP (cAMP). NMR studies of the apo and cAMP-bound states of the protein showed that cAMP-binding induces large conformational changes, but the pathway and specific mechanism of the change are still unknown. To further understand the transition, we performed a vibrational analysis of the apo and holo structures using normal mode and block normal mode analyses. The low-frequency modes demonstrated the anticipated flexibilities of the recognition helices involved in DNA-binding in the active state. Our calculations showed how the motions of the DNA and cAMP-binding domains are coupled, giving insight into plausible pathways of the transition.

GP-10 Meagan Small[1], Kirpal S Bisht[1], Randy W Larsen[1]
[1]Department of Chemistry, University of South Florida

Photophysical Characterization of a Novel Resorcinarene-Based Cavitand

Cavitands are a class of cyclic oligomers whose backbones are comprised of four repeating functionalized aromatic rings that are bridged on the upper and lower rims to form a hydrophobic cavity. Cavitands have been exploited in a wide range of host-guest and biomimetic applications because of their ability to oordinate a metal with open sites for small molecules and the versatility of the functional groups that can be substituted onto the backbone. The work presented here is the initial photophysical characterization of a novel resorcinarene-based cavitand functionalized with imidazole arms. The cavitand shows a absorption maximum at λ=280 nm and is determined to bind copper (II) ions in a 1:1 cavitand : Cu^{2+} stochiometry with a dissociation constant of K_D= 8.6 ± 0.2 uM. The model system has the potential to provide detailed Cu-CO bond energies that are hard to obtain in vivo.

Bioorganic, Natural, and Organic (NES South Hall)

GO-01 Wai Sheung Ma[1], Tina Mutka[2], Dennis E Kyle[2,3], Lilian Vrijmoed[4], Bill J Baker[1,3]
[1]Department of Chemistry, University of South Florida; [2]Department of Global Health, University of South Florida; [3]Center for Molecular Diversity in Drug Design, Discovery and Delivery, University of South Florida; [4]Department of Biology and Chemistry, City University of Hong Kong

Malaria Screening and the Chemical Investigation of Endophytic Fungal Extracts

Malaria bioassay guided screening and the chemical investigation of the crude endophytic fungal extracts has lead to the isolations of a series of known cytochalasins; along with the discovery of a few new compounds, including a new cytochalasin, a simple carboxylic acid, and two potentially new compounds of unknown class. Majority of the cytochalasins display outstanding inhibition to chloroquine-resistant reference strain (W2) Plasmodium falciparum with IC_{50} ranging from 13 ng/mL to 121 ng/mL. The structures of the compounds and the associated anti-malarial activities isolated will be presented.

GO-02 Chandan Barhate[1], Bill Baker[1]
[1]Department of Chemistry, University of South Florida

Isolation and Structural Determination of Biologically Active Compounds from Marine Bacteria

Marine organisms both flora and fauna are excellent sources of associated bioactive microorganisms which are active especially against drug resistant bacteria. Methicillin resistant Staphylococcus aureus (MRSA) and VRE infection is considered to be one of the main causes of death among the hospital-acquired infectious diseases, and has led to many thousands of deaths and additional expenditure. Recent studies have identified the existence of vancomycin-resistant and teicoplanin-resistant S. aureus. Thus, there is urgency for the development of new drugs effective against MRSA. The number of vancomycin-resistant isolates of S. aureus or Enterococcus (VRSA and VRE) causing disease is steadily increasing. Cultivation of a marine Streptomyces sp isolated from marine algae shown potential biological activity against MRSA (zone of inhibition=3 mm) and VRE (zone of inhibition=2mm). Further investigation of compounds by sophisticated structural determination techniques like MS and 2D NMR spectroscopy may prove marine bacteria to be one such important source of compounds with useful clinical applications infections those caused by MRSA and VRE.

GO-03 Sujeewa Ranatunga[1], Hua Yang[2], Said M Sebti[2], Juan R Del Valle[2]
[1]Department of Chemistry and Biochemistry, New Mexico State University; [2]Drug Discovery Department, H Lee Moffitt Cancer Center and Research Institute

Synthesis of Potential Akt Inhibitors using a Bicyclic Proline-Based Scaffold as the Peptidomimetic Core

Akt is a serine/threonine protein kinase that modulates cell proliferation, apoptosis, and angiogenesis and is known to be activated or amplified in many human malignancies. Among other proteins, Akt selectively phosphorylates GSK3β activating downstream protection from apoptosis. The operative protein-protein interaction involves recognition of the β-strand peptide domain of GSK3β. The Design of peptidomimetic Akt inhibitors based on the GSK3β extended conformation is as a promising approach for drug discovery. We have synthesized novel GSK3β peptidomimetics that featured an extended dipeptide surrogate

scaffold. The design, synthesis, incorporation of proline-based bicyclic core structure into potential Akt inhibitors, and their preliminary biological activity will be presented.

GO-04 Tao Liang[1], Jon Antilla[1]
[1]Department of Chemistry, University of South Florida

Brønsted Acid Catalyzed Enantioselective Pinacol Rearrangement

The first example of chiral phosphoric acid catalyzed enantioselective pinacol rearrangement of indole derivatives with up to 90% yield and 95% ee.

GO-05 Biplob Bhattacharya[1], Silvia Robles[1], Edward Turos[1]
[1]Department of Chemistry, University of South Florida

N-Thiolated β-Lactams: Altering Microbiological Activity and Bacterial Cell Targeting with C3 Ring Functionality

The main objective of this project is to check any change in inhibitor activity if the side chains were water-soluble polar groups like amino acids. This project also includes studying the effect of side chain structure and polarity at the C3 position of N-Thiolated β-Lactams on solubility and antibacterial activity. Our primary objective is to see if there is a correlation between chain length and polarity at the C3 position of N-Thiolated β-Lactams on the antibacterial activity. The project started to diverge and now we are looking at different moieties like carbohydrates and PEG attached to N-Thiolated β-Lactams.

GO-06 Andrii Monastyrskyi[1], R Matthew Cross[1], David L Flanigan[1], Tina Mutka[2], Jeremy Burrows[3], Dennis E Kyle[2], Roman Manetsch[1]
[1]Department of Chemistry, University of South Florida and Center for Molecular Diversity in Drug Design, Discovery and Delivery; [2]Global Health, University of South Florida; [3]Medicines for Malaria Venture

Design of Novel 4(1H)-quinolones Targeting Multi-Drug Resistant P. falciparum Malaria

Malaria is one of the most devastating parasitic diseases of man with over 1 million deaths per year. Despite the availability of several antimalarial drugs, treatment has become increasingly complicated with widespread drug resistance. 4(1H)-quinolones including endochin were known causal prophylactic (kill growing liver stage parasites) and potent erythrocytic stage agents in avian malarial models, but not against parasites in mammals. However, these studies were conducted over 30 years ago without adequate evaluation in current preclinical efficacy models. A series of endochin and WR 197236 analogs obtained from the Walter Reed Army Institute of Research (WRAIR) chemical inventory were initially screened in an erythrocytic stage assay with multidrug resistant isolates D6 and TM90-C2B of P. falciparum in vitro. Surprisingly, several of these compounds had remarkable potency (low nM). Structural similarities of the quinolones with naptho-quinones and related atovaquone analogs led to further evaluation of the 4(1H)-quinolones against atovaquone resistant P. falciparum. The results not only indicated potent erythrocytic stage activity of these compounds but interestingly, the cross resistance seen with atovaquone was not found to be complete across the series. These results encouraged us to further investigate the series of 4(1H)-quinolones as antimalarial agents.

GO-07 Sameer Kulkarni[1], Niranjan Namelikonda[1], Xiangdong Hu[1], Kenichiro Doi[2], Hong-Gang Wang[2], Roman Manetsch[1]
[1]Department of Chemistry, University of South Florida; [2]Department of Pharmacology, Penn State College of Medicine

Kinetic Target Guided Synthesis for the Identification of Bcl-XL-protein Interaction Modulators

In the recent years, protein-protein interactions have been identified to possess significant biological importance and targeting certain protein-protein interactions has been shown to have therapeutic effects. The discovery of numerous small molecules interfering with Bcl-XL-protein complexes has introduced a practicable route for inducing apoptosis in cancer cells. Herein, we report our progress towards the development of a novel drug discovery method that generates only biologically active compounds, an approach known as kinetic target guided synthesis (TGS). We discovered that an amidation reaction between thio acids and sulfonyl azides can be employed for Bcl-XL-templated screening to identify inhibitors of Bcl-XL itself. The target protein, Bcl-XL, displayed selective formation of bidentate compounds from different libraries of fragments bearing complementary reactive functionalities. The hit compounds have been synthesized and tested for their capability to modulate Bcl-XL-protein interactions using conventional biological assays.

GO-08 Matt Lebar[1], Bill Baker[1]
[1]Department of Chemistry, University of South Florida

Isolation and Synthesis of Meridianin A, Synthesis and Structure Reassessment of Psammopemmin A

We have isolated meridianins A, B, C, and E from the Antarctic tunicate Synoicum sp. In the process of verifying the resemblance to that of psammopemmins. The psammopemmins are alkaloids bearing similar structures to the meridianins, but reported from the Antarctic sponge Psammopemma sp. To verify the structure originally proposed for psammopemmin A, the compound was synthesized. By comparing the ^{1}H and ^{13}C NMR data of reported and synthetic psammopemmin A with that of meridianin A, we infer that the correct structure of psammopemminA isolated from Psammopemma sp. is actually that of meridianin A.

GO-09 Faeez Mahzamani[1], Leigh West[2], Danielle Gergeres[1], Praveen Ramaraju[1], Edward Turos[1]
[1]Department of Chemistry, University of South Florida; [2]FCoE-BITT, University of South Florida

5-amino Salicylic Acid Bound Nanoparticle for the Treatment of Inflammatory Bowel Diseases

As a therapeutic drug, 5-amino salicylic acid (5-ASA) is used for the treatment of inflammatory bowel diseases. In an attempt to reduce the extremely large dosage required for 5-ASA to be effective, the drug is placed into a polymer (butyl acrylate, styrene) based nanoparticle to increase its effectiveness. Covalently bound and encapsulation methods are used to load the therapeutic drug into the nanoparticle. Acryloyl amino 5-ASA is used for covalently binding to nanoparticle, and acetyl amino 5-ASA is used for encapsulation in the nanoparticle. After purification, Dynamic light scattering data shows that the drug containing nanoparticles are stable. Bacterial testing show a slight increase in antibacterial activity, unique for a therapeutic drug; HT-29 human colonic cells are used for cytotoxicity tests, and SEM images are used to capture the effects of the nanoparticle on human colonic cells.

GO-10 Kurt Van Horn[1], Anuradha Srivastava[1], Dennis Kyle[2], Roman Manetsch[1]
[1]Department of Chemistry, University of South Florida; [2]College of Public Health, University of South Florida

Anti-leishmanial Activity of a New Series of Quinazolines

A new series of 2,4-disubstituted quinazolines has been synthesized and tested for in vitro activity against Leishmania mexicana axenic amastigotes and L. donovani intracellular amastigotes. The Topliss scheme was loosely followed in order to see if an accurate structure activity relationship (SAR) study could be evaluated to bring to fruition a usable lead compound. This study led to several compounds in the low micromolar range for EC_{50} in the L. donovani intracellular amastigote assay.

GO-11 Jordany Maignan[1], Richard Cross[1], Andrii Monastskyi[1], Tina Mutka[2], Dennis Kyle[2], Roman Manetsch[1]
[1]Department of Chemistry, University of South Florida; [2]College of Public Health, University of South Florida

The Development and Use of an HPLC-based Assay to Determine Aqueous Solubility of Compounds with Biological Activity

A drug molecule on its path to its biological target encounters a variety of obstacles of physical, physicochemical and/or biochemical nature attenuating the drug uptake and activity. In the past, countless drug discovery projects focusing solely on biological activity experienced serious or terminal obstacles at later development stages related to formulation, pharmacokinetics, metabolism and/or toxicity. Consequently, drug discovery programs made considerable efforts to develop and implement assays to test “drug-likeness” as early as possible. Structure is then correlated to common drug properties (structure-property relationships or SPRs) in a similar fashion as structure is directly correlated to activity (structure-activity relationship or SAR). Thus in a modern approach, activity and property data are together helping drug discovery programs refocus their efforts on molecules meeting acceptable activity and property parameters. Currently, the Manetsch laboratory is developing various classes of compounds as antimalarial, antibacterial, antileishmanial, and/or anticancer agents. Herein, we report the development and optimization of a HPLC-based assay to routinely determine the aqueous solubility of compounds displaying biological activity.

GO-12 Xue Xu[1], Hongjian Lu[1], Joshua Ruppel[2], Peter Zhang[1]
[1]Department of chemistry, University of South Florida 2Hamilton College

Design and Synthesis of Cobalt(II) Porphyrin Catalysts for Stereoselective IntraMolecular Cyclopropanation

Metalloporphyrins have been shown to catalyze many fundamental and practically important chemical transformations, including an assortment of atom/group transfer reactions, such as oxene, nitrene, and carbene transfers. Our group has shown that cobalt porphyrin-based carbene transfer reactions are some of the most selective and practical catalytic systems developed for cyclopropanation. Supported by a family of D2-symmetric chiral cobalt porphyrins, herein I report some recent progress on stereoselective carbene transfer reactions.

The Clear Springs Land Undergraduate Poster Session

Analytical and Biochemical (NES 106)

AB-01 Rebecca Burt[1], Kimberly Fields[1], Whittney Burda[2], Natasa Dragicevic[2], Cynthia Bucher[3], Alberto van Olphen[3], Patrick Bradshaw[2], Lindsey Shaw[2], Peter Zhang[1]
[1]Department of Chemistry, University of South Florida; [2]Department of Cell Biology, Microbiology, and Molecular Biology, University of South Florida; [3]Department of Global Health, University of South Florida

Biomedical Applications of Porphyrins and Small Molecules

Porphyrins are organic compounds commonly found in nature and in the human body. Heme containing proteins, such as hemoglobin, myoglobin, and cytochromes, are a few examples of porphyrins in the human body. The focus of this project is the possible biomedical uses of lab synthesized porphyrins in the treatment of disease and infections; particularly Methycillin Resistant Staphylococcus aureus (MRSA) infections, Alzheimer's disease, and influenza. For each disease specific porphyrins and porpyhrin derivatives were selected based on chemical properties and structures. The compounds were then diluted in DMSO and delivered for testing. A total of about 250 different porphyrins and related organic compounds were screened. Approximately 50 porphyrins and related compounds have shown to inhibit the growth of several strains of Staphylococcus aureus. Further testing is underway to determine the mechanism of action of these compounds. The preliminary testing of the compounds in the Alzheimer's lab show that approximately 15 porphyrins and related compounds are effective in treating mitochondrial cells that express the β-amyloid precursor protein (N2aAPP cells). Furthermore, the effectiveness of these compounds in treating this protein in Caenorhabditis elegans, a model eukaryotic, organism will be tested. Preliminary testing on influenza is still in progress.

AB-02 Sonia Almonte[1], Erica Turner[1], Abdul Malik[1]
[1]Department of Chemistry, University of South Florida

Germania-Based Sol-gel Monolithic Columns with a Positively Charged Organic Ligand for Capillary Microextraction Coupled Chromatographic Separation

A sol-gel method was developed to create germania-based sorbents for capillary microextraction. Capillaries (320µm i.d.) were pre-treated before fabrication of the monolithic capillaries via sequential rinsing of methylene chloride, methanol and water to form silanol groups on the capillary surface upon conditioning within a gas chromatograph (GC) oven. Monoliths have inherent advantages over conventional coatings in the preconcentration of analytes. However, significant problems arise due to the tendency of cracking under pressure, shrinking of the bed and monolithic cladding during the drying process. Monoliths are a compromise between loadability, permeability, and mass transfer kinetics. Due to the better mass transfer properties of a monolithic skeleton over distinct particles, high flow rates and high speed separations are possible. A successfully monolithic column was prepared containing a positively-charged sol–gel silicate by hydrolyzing and co-polymerizing N-octadecyldimethyl[3-(trimethoxysilyl)propyl] ammonium chloride (C_{18}-TMS NH_4^+ Cl^-) with tetraethoxygermane(TEOG) on the stationary phase, providing electrostatic interaction sites for charged compounds. Vital information can be derived from the data collected such as how efficient the monolithic column is extracting these charged compounds and whether it can withstand obstacles that monolithic columns can endure such as cracking, shrinking and cladding.

AB-03 Nishal Patel[1], Erica B Turner[1], Abdul Malik[1]
[1]Department of Chemistry, University of South Florida

Sol-Gel Mixed Germania-Silica Poly(ethylene glycol) Monoliths for Capillary Microextraction Coupled to Gas Chromatography

A novel mixed-mode Germania-silica based monolith was prepared for gas chromatography (GC). Tetraethoxygermane (TEOG) was used as a precursor to create a sol-gel monolithic network within a fused silica capillary. Polyethylene glycol (PEG, MW=600) was used as a polymer to chemically bind the sol-gel network to the silanol groups on the inner capillary surface. The Germania-silica based monolithic capillary will be used for the extraction of polar compounds (alcohols, phenols, amines) using capillary microextraction hyphenated with GC flame ionization detection (FID). This monolithic capillary should provide high temperature resistance, solvent resistance, and stability in extreme pH, characteristics determined in a Germania coated capillary (Fang, Li; S. Kulkarni; K. Alhooshani; A. Malik. Analytical Chemistry. 2007, 79, 9441-9451). Unlike a coated capillary, however, a monolithic capillary has a higher surface area due to the solid porous bed, thereby allowing for a higher sample loading, higher sensitivity and lower limits of detection.

AB-04 Jared Tur[1], Erica Turner[1], Abdul Malik[1]
[1]Department of Chemistry, University of South Florida

Germania-Based Sol-Gel Monoliths for Capillary Microextraction

Germania-based sol-gel monoliths using an organic ligand containing sol-gel active sites were developed for capillary microextraction (CME), gas chromatography (GC) and, high performance liquid chromatography (HPLC). These Sol-gel monoliths have the potential to become a highly effective stationary phase for microextration on a range of highly-polar to non-polar molecules. The precursor, tetraethoxygermane (TEOG) was used with the organic ligand, poly (ethylene glycol) (PEG MW:600) to create a sol-gel network via hydrolytic polycondensation reactions performed within a fused silica capillary. To our knowledge, this is the first time in which a Germania-based monolith has been used as sorbent in chromatographic separations or sample preparation. These capillaries will be further tested to extract trace concentrations of polycyclic aromatic hydrocarbons, aldehydes, ketones, alcohols, phenols, and free fatty acids from aqueous solutions. In addition these sol-gel monoliths will be tested for stability under high temperatures and aggressive solvents.

AB-05 Martha L Fuentes[1], MinhPhuong Tran[1], Sheshanka Kesani[1], Abdul Malik[1]
[1]Department of Chemistry, University of South Florida

Preparation of a Sol-Gel Silica and Poly Propylene Glycol Coated Capillary

In this research, a sol-gel based silica capillary was prepared for capillary microextraction. An alkoxide of silica, Tetramethoxysilane (TMOS), was used as the sol-gel precursor and poly propylene glycol (PPG) as a sol-gel active polymer. The sol-gel silica PPG coated capillary was utilized for capillary microextraction hyphenated on-line with High Performance Liquid Chromatography (HPLC) for extracting different analytes including polycyclic aromatic hydrocarbons, ketones, alcohols and phenols. Concluding chemical analysis by HPLC showed how promising sol-gel silica PPG-coated capillary can be when applied in the extraction of contaminants in environmental aqueous samples.

AB-06 Christopher Lizardi[1], Eileen Schulman[1], Bryan Vo[1], Darius Wynn[1], Dean F Martin[1]
[1]Department of Chemistry, University of South Florida

Removal of Selected Nuisance Anions by Octolig®

Octolig®, a commercially available immobilized ligand (IMLIG), has been studied for its effectiveness in removing nuisance anions. The material consists of polyethylenediamines covalently linked to high surface-area silica, and has a high affinity for transition metal ions. Previous research indicated that anions could be removed quantitatively from aqueous solutions using the metal derivatives of Octolig® as packing in column chromatography. The present study focused on the results with Octolig® alone. Quantitative removals (>99%) were obtained for arsenate, chromate, paramolybdate, selenious acid, and fluoride. Boric acid was not removed by under similar conditions, but previously the copper(II) derivative of Octolig® had been partially successful. A mechanism of removal is proposed.

AB-07 Robin Fulton[1], Abdullah Alhendal[1], Abdul Malik[1]
[1]Department of Chemistry, University of South Florida

Preparation of a Polar Hybrid Organic-Inorganic Germania-based Coating for Capillary Microextraction by Sol-gel Chemistry

Germania-based sol-gel coating was prepared for the extraction of moderately polar and polar analytes by Capillary Microextraction technique which is a solvent free method widely used in trace analysis. Sol-gel Chemistry was utilized to immobilize the coating on the inner surface of a 250 µm inner diameter fused-silica capillary by chemical bonds. These chemical bonds made the coating (1) stationary and un-effected by the organic solvents used for rinsing the capillary, (2) resistant to the high temperatures while performing Gas Chromatography analysis. After performing the extraction by a laboratory-made gravity fed dispenser which allowed the sample to pass through the coated capillary, the capillary was connected to the GC injection port, the temperature of the injection port was raised to 250 °C to completely desorb the extracted analyte. A two-way press-fit connector was used to connect the capillary to the GC column. The detection of the analyte was done by a Flame Ionization Detector (FID).

AB-08 Stephi Pofahl[1], Wesley Brooks[2]
[1]Department of Chemistry, University of South Florida; [2]Moffitt Cancer Center

Effect of Putrescine on SAM Decarboxylase Activity for Cancer Research and Drug Development

Cancer is a worldwide health issue. In 2007, there were an estimated 12 million deaths worldwide, 1.7 million of which were in North America. Polyamines such as, putrescine, spermidine and spermine are organic compounds that have two or more amino groups. They are present in all eukaryotic cells and have increased levels in neoplastic cells. The interest in polyamines and their regulation is a target for pharmaceutical research in cancer. The biosynthetic reaction from the decarboxylation of S-adenosylmethione (AdoMet) is tightly regulated, once decarboxylated by the enzyme S-adenosylmethionine (AdoMetDC) can no longer act as a methyl donor. AdoMetDC is used to provide aminopropyl groups in synthesis of spermine from putrescine by enzyme spermidine synthase. The final product spermine, from spermidine reacting with spermine synthase has shown to decrease polyamine synthesis. The inhibition activities of these polyamines are under investigation for targeting by chemotherapeutic agents. The purpose of this study is to develop novel compounds that inhibit AdoMetDC.

AB-09 Lorenzo Rodriguez[1], Dean F Martin[1]
[1]Department of Chemistry, University of South Florida

Removal of Lithium from Solutions Using Octolig®

TEEDA (tetraethylethylenediamine) has been used before to remove lithium cations from tandem organic reactions. An attempt was made to achieve a similar feat using a commercial product called Octolig® that consists of polyethylenediamine moieties covalently bound to silica gel. Octolig®'s polyethylenediamine units are similar in structure to TEEDA. The hypothesis was that Octolig® should be able to remove lithium cations from solution as well. Our initial attempt used water as the solvent because water is environmentally-safe. Three solutions were prepared with a concentration of 100 ppm Li: $LiNO_3$ and LiCl in deionized water, and LiCl in well water. Each solution was passed through a chromatography column (dimensions 2 cm x 30 cm) packed with 62.8 cm3 of Octolig®. The lithium concentrations of both composite effluent samples and the standard solutions were determined indicating 0% removal. Presumably the lithium cation has too much affinity for water, preventing it from interacting with the Octolig®. Future work will involve trying non-aqueous solvents such as ethers. Given the growing need for lithium in electric and hybrid-electric vehicles, finding a method to remove lithium is of critical importance.

AB-10 Jorge Vega[1], Sharon Spencer[1], Brent Hilker[1], Julie P Harmon[1]
[1]Department of Chemistry, University of South Florida

Blister Agent Analog Sequestration using Porphyrins and Polymer Hydrogels

Polymer hydrogel systems are investigated as a media to make a useful composite with meso-tetra(m-hydroxy phenyl)porphyrin (4(m-OHP)P) to sequester and ultimately photo-catalytically destroy sulfur and nitrogen mustards. Hydroxyethyl methacrylate (HEMA), vinylpyrrolidinone (VP), ethylene glycol dimethacrylate (EGDMA) in three copolymer composite mixtures are synthesized with 4(m-OHP)P in varied mol%. Samples were then purified via soxhelet extraction to remove unreacted reagents. Freeze dried composite samples were monitored for uptake of thioanisole, a sulfur mustard analog, using UV|Vis spectroscopy.

AB-11 Niloofar Ghazi-Moghaddam[1], Parul Jain[1], Julie Harmon[1]
[1]Department of Chemistry, University of South Florida

Signal and Morphological Differences in IBF vs Micropipet Deposits

The novel technique of induction based fluidics (IBF) is a contact-free small volume deposition method, in which inductively charged droplets are launched and dynamically directed to a target. Matrix-assisted laser desorption /ionization–Time of flight (MALDI-TOF) is an accurate and sensitive technique for the identification of biomolecules, but the analysis of proteins and peptides by MALDI-TOF is affected by sample formulation and spotting onto a MALDI target. The effectiveness of IBF sample preparation for MALDI-TOF was evaluated by analyzing signal to noise ratios and morphology of bovine serum albumin deposits. In this study, the common "dried droplet" method of micropipetting was compared to the electric field enhancement (EFE) preparation technique, which yielded greater sample uniformity and signal enhancement in the IBF spots. Transmission electron microscopy and a polarizing optical microscope were used to contrast the EFE and dried droplet deposits, as well as surface profilometry used to demonstrate the eveness of the EFE samples.

AB-12 Sibel Demirel[1], Daniel Leyva[1], Ruben Durand[1], Vicky Lykourinou[1], Li-June Ming[1]
[1]Department of Chemistry, University of South Florida

Mechanistic Studies of Catalytic Activity of Cu(II)-Bound Copolymers in Oxidation of Catechols, DNA Cleavage and Modeling of Antioxidant Activity of Natural Products

Copper (II)-bound copolymers can catalyze the oxidation of catechol, mimicking 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 or phenyl. We investigate the catalytic activity of two linear copolymers containing a hydrophobic or a hydrophilic functional group (from styrene or acrylamide) and a metal binding functional group (e.g. vinylpyridine). The 1:1 Cu(II) complexes of these copolymers exhibit a significant catalytic activity in oxidation of catechol derivatives in air and H_2O_2 and toward DNA cleavage with H_2O_2 or O_2 (under reduction conditions). Our study will focus on the cooperativity between catechol derivatives and H_2O_2 in the proposed oxidation mechanism where H_2O_2 gives further activation to observed substrate oxidation. In addition, some specificity has been seen by the two different copolymers towards peroxide binding. Moreover, reactive oxygen species such as H_2O_2 and O_2 occurring naturally in the body and can be further activated by redox-active metal ions. The interaction of these Cu(II)–copolymer complexes with H_2O_2 or O_2 can generate substantially more active intermediates responsible for the significant oxidative activities observed…

AB-13 Krit Setthi[1], Erica B Turner[1], Abdul Malik[1]
[1]Department of Chemistry, University of South Florida

Sol-Gel Mixed Germania-Silica Poly(ethylene glycol) Monoliths for Capillary Microextraction (CME) Coupled to Gas Chromatography (GC)

A novel mixed-mode Germania-silica based monolith was prepared for gas chromatography (GC). Tetraethoxygermane (TEOG) was used as a precursor to create a sol-gel monolithic network within a fused silica capillary. Polyethylene glycol (PEG, MW=600) was used as a polymer to chemically bind the sol-gel network to the silanol groups on the inner capillary surface. The Germania-silica based monolithic capillary will be used for the extraction of polar compounds (alcohols, phenols, amines) using capillary microextraction hyphenated with GC flame ionization detection (FID). This monolithic capillary should provide high temperature resistance, solvent resistance, and stability in extreme pH, characteristics determined in a Germania coated capillary (Fang, Li; S. Kulkarni; K. Alhooshani; A. Malik. Analytical Chemistry. 2007, 79, 9441-9451). Unlike a coated capillary, however, a monolithic capillary has a higher surface area due to the solid porous bed, thereby allowing for a higher sample loading, higher sensitivity and lower limits of detection.

AB-14 Christian Barbosa[1], Sumit Handa[1], David Merkler[1]
[1]Department of Chemistry, University of South Florida

Expression of Human Peptidylglycine α-Hydroxylating Monoxygenase in E. coli

Peptidylglycine α-hydroxylating monooxygenase (PHM) is a part of bi functional enzyme Peptide α-amidating monooxygenase (PAM) that catalyze the O^{2-}, ascorbate, and copper-dependent hydroxylation of glycine α-carbon in a C-terminal glycine-extended precursor peptide. Subsequent dealkylation by another enzyme leads to the formation of amidated peptide and glyoxylate. PHM is expressed in higher level

eukaryotes, and is part of hormones activation system, since ~50% of all mammalian peptide hormones are α-amidated. The purpose of this study is to overexpress PHM in E. coli, using codon optimized sequence for E. coli. In an attempt to maximize production for better characterization and further analysis, E. coli was cultured in different growth conditions and media. Many parameters were altered, including temperature, growth media content, length of induction, etc. The expressed protein was analysed using SDS-PAGE and western-blotting, and purified by immobilized metal ion affinity chromatography (IMAC). This purification method was analyzed for efficiency and efficacy of PHM overexpression.

AB-15 Jordan Anderson[1], Arun B Kumar[1], Anthony Melendez[1], Roman Manetsch[1]
[1]Department of Chemistry, University of South Florida

Design of a Small Molecule Inhibitor of β-Secretase

β-Secretase is an enzyme found in the brain that is responsible for the cleavage of amyloid precursor proteins to amyloid β-peptide, which forms plaques on the brain. Brains of patients afflicted with Alzheimer's Disease can have plaque and β-Secretase protein concentrations double that of a healthy brain. This makes β-Secretase an ideal target for a small molecule inhibitor. After virtual screening of the NCID-2 library on a β-Secretase model, a molecule was found to bind at the active site with a score of -9.73. This molecule resembled molecules of a library of 150 compounds previously synthesized and characterized. Using a Fluorescence Resonance Energy Transfer (FRET) assay the 150 compounds were screened at initial concentrations of 100, 50 and 25 μM. The compounds with the largest percentage inhibition at these concentrations were then screened at different concentrations (1000–0.01 μM) to determine the IC_{50} values of each compound. With this approach, three compounds were found to inhibit β-secretase ABK-2-171, ABK-2-172, and ABK-2-274, with respective IC_{50} values of 12.3 ± 1.9 μM, 14.4 ± 3.8 μM, and 19.0 ± 13.8 μM.

AB-16 Kathryn Ballance[1], MinhPhuong Tran[1], Abdul Malik[1]
[1]Department of Chemistry, University of South Florida

Germania-based Sol-gel Coating for Capillary Microextraction of Aqueous Trace Analytes with High-performance Liquid Chromatography

A sol-gel germania poly(propylene glycol) (PPG-425) coating was developed for capillary microextraction coupled with high-performance liquid chromatography (HPLC). Tetraethoxygermane (TEOG) was used as the sol-gel precursor and PPG-425 was chosen as the sol-gel active polymer to exploit its ability to extract components from complex matrices. The PPG-425 allows for the preconcentration of polar analytes containing hydroxyl, carboxyl, cyano and amino groups, and heterocyclic compounds with nitrogen and oxygen heteroatoms, which can then be analyzed using high-performance liquid chromatography (HPLC). The sol-gel coating was formed via hydrolysis and polycondensation reactions. This coating was then chemically bonded to the inner surface of a 250μm fused silica capillary using sol-gel chemistry. This sol-gel germania PPG-425 coated capillary expected to improve sensitivity and selectivity for the extraction of trace pollutants in aqueous environmental samples and provide a direct path to preconcentrate analytes from complex matrices. Its effectiveness is demonstrated through the successful extractions of alcohols, ketones, amines, aldehydes, and polycyclic aromatic hydrocarbons.

Inorganic and Physical (NES 103)

IP-01 Jennifer Drozd[1], Catherine Geiser[1], Michael Zaworotko[1]
[1]Department of Chemistry, University of South Florida

Cocrystal Synthesis of Malic Acid

To expand the knowledge of the synthon bonding properties of carboxylic acids, an excess of cocrystals must be synthesized and analyzed. A well formulated list of fifteen cocrystal formers combined with numerous experimental synthesizing methods will formulate the bonding statistics needed to develop conclusions on synthon bonding habits of the six chosen carboxylic acids. With these statistics, the cocrystal forming properties of carboxylic acids will be readily accessible thus expanding upon the library of suitable cocrystal formers. Among the six chosen acids, malic acid provides beneficial biological aspects such as improved immunity, healthier skin and increased energy. Malic acid, naturally found in tart foods such as apples, is nontoxic and abundant. By using many methods to crystallize malic acid with a cocrystal former, a cocrystal ultimately formed by ways of slow evaporation. Nicotinamide and malic acid, dissolved in a 1:1 molar ratio in methanol proved to be a cocrystal through extensive analysis.

IP-02 Jacob Weissman[1], Daniel Santiago[1,2], Wayne C Guida[1,2]
[1]Department of Chemistry, University of South Florida; [2]Molecular Modeling and Virtual Screening Core, Drug Discovery Program, H. Lee Moffitt Cancer Center & Research Institute

Comparison of Low Mode Fluctuations for Flexible Docking

Few computational methods provide unbiased rigid docking without spending expensive computational time for simulations. Normal Mode Analysis (NMA) could be the bridge between speed and accuracy. Large-scale normal low modes were compared to identify the pertinent normal modes that define protein-ligand binding. 17 CDK2/Cyclin A structures were chosen from the Protein Data Bank (PDB) because Cyclin A (which is necessary for CDK2 function) is attached, the resolution was less than 2.6 Å, a structure generated by X-ray crystallography, and their structures were complete. PDB structure 1H26 was chosen for NMA and cross-docking because of its lowest resolution of the ligand-less structures. Each of the remaining 16 structures was prepared for docking using Schrödinger molecular modeling applications. Ligands of each PDB structure were self-docked to the original protein and cross-docked to the 1H26 structure—cross docks yielded modes differing with worse poses and docking scores—illustrating the need for flexible docking. RMSD values calculated for the low modes of the 555 residues (297 CDK2 and 258 Cyclin A residues) of PDB 1H26 allowed for the important normal low modes to be determined, as the active site residues should undergo greater fluctuation in modes of interest.

IP-03 Arthur Pettygrove[1], Tien Teng Ong[1], George Norton[1], Michael J Zaworotko[1]
[1]Department of Chemistry, University of South Florida

The Study of Potential Cocrystal Formation between Lithium Chloride and Six Neutral Amino Acids

Cocrystals have emerged as a class of crystalline forms that offer potentially beneficial different physical properties than a single Active Pharmaceutical Ingredient (API). With regards to pharmaceutical cocrystals, they can greatly increase the number of crystal forms of a given API. In this research project, it is desired to

ascertain if cocrystals can be formed between lithium chloride and six different neutral amino acids. The amino acids, L-valine, L-alanine, L-leucine, L-isoleucine, N,N-dimethylglycine, and betaine are all neutral amino acids that become zwitterions in solution. Lithium chloride is being targeted because it does not cause suicidality as a side effect as compared to other commercially available antidepressant drugs. Due to lithium's narrow therapeutic index, it is desired to make cocrystals of lithium chloride in order to modulate the concentration of lithium cations in solution (solubility) to treat suicidality.

IP-04 Alyssa Rigolo[1], Roger Bass[1], Julie Harmon[1]
[1]Department of Chemistry, University of South Florida

Comparison of Two Polyurethanes Containing Single and Multiwalled Carbon Nanotubes

Nanocomposites of 2 different shape memory polymers with increasing weight percentages of single and multiwalled carbon nanotubes were mechanically tested and the results and conclusions are presented. Each type of carbon tube affects each polyurethane differently suggesting a difference in interface.

IP-05 Nicholas Zoumberos[1], R Luebke[1], L Wojtas[1], Mike Zaworotko[1], Mohamed Eddaoudi[1]
[1]Department of Chemistry, University of South Florida

Control of Coordination Isomers Using Structure Directing Agents

The synthesis of metal-organic frameworks (MOFs) constructed from single-ion molecular building blocks (MBBs) currently utilizes ligands which hetero-chelate to a metal ion to create a rigid MBB which can then be used to form an extended 3d framework. Due to multiple possible coordination configurations of the ligands around the metal a variety of possible MBBs can be created by each specific ligand and metal combination. The selection of the coordination isomer leading to the desired MBB is essential in the rational synthesis of a framework featuring a desired topology. This poster presents a potential method of rational synthesis of target MBBs using organic bases as structure directing agents to direct the coordination configuration.

IP-06 Crystal Tenn[1], Arjan van der Vaart[1]
[1]Department of Chemistry, University of South Florida

Normal Mode 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. Domain 2 bends and the alpha-helices of domain 3 refold into ß-sheets, which are inserted into the membrane. To elucidate the pathway and triggers for these conformational changes, we performed normal mode analysis on two monomeric PFO structures. 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 stability of the alpha-helices of domain 3 was assessed by molecular dynamics simulations in implicit solvent.

IP-07 Matthew Turtzo[1], Vicki Lykourinou[1], Li-June Ming[1]
[1]Department of Chemistry, University of South Florida

Iron Metallopolymers as Catalysts for Oxidative Cleavage of Catechol

Polymerization of monomers containing the desired arrangement of functional groups within a metallopolymer creates a unique microenvironment similar to the active site of an enzyme wherein specific chemical reactions may be catalyzed. It is believed that a suitable catalyst for the oxidative cleavage of catechol (dihydroxybenzene) can be generated by modeling the active site of the soil bacterial enzyme catechol dioxygenase, which is responsible for conversion of dihydroxybenzene into nonaromatic, acyclic compounds. The active site of the enzyme $[FeIII(His)_2(Tyr)_2]$ contains an iron(III) atom covalently bound with two nitrogen atoms from histidine moieties and two oxygen atoms from tyrosine moieties. This iron atom within the active site adopts a trigonal bipyrimidal geometry wherein the fifth coordination position is occupied by a hydroxyl group. The catechol dioxygenase active site has been modeled through the creation of a metallopolymer containing iron(III) coordinated to both 4-vinylpyridine and 4-vinyl phenol within the repeating unit. The structure of the metallopolymer and its effectiveness as a catalyst for the oxidative cleavage of catechol will be reported.

IP-08 Joelle Mendez- Hinds[1], Jason Perman[1], Mike Zaworotko[1]
[1]Department of Chemistry, University of South Florida

The Investigation and Synthesis of Metal Organic Materials as Pertaining to HTriNA, a Ligand Derived From Solid State Synthesis

Material science is addressing many of society's concerns for energy and technology, and Metal Organic Materials (MOMs) are at the forefront for discovery and application. MOMs are promising candidates for both gas storage and separation based on construction strategies utilizing molecular building blocks, making new materials with high surface area that are stable to vacuum. MOMs are constructed from two components: 1) an organic ligand which influences size and, through polarization or hydrogen bonding, could favor molecular recognition, and 2) the metal component which can affect luminescence, redox active sites, and magnetism. HTriNA (Trimellitic Nicotinic Acid) is a condensation product prepared via cocrystal controlled solid-state synthesis from grinding and heating trimellitic anhydride and 4-aminopyridine to a total of 4 hours at 265 °C, efficiently achieving yields of 90% or better. HTriNA was reacted with different metals under various conditions producing permanently porous isostructural metal organic materials, which are currently being investigated for hydrogen storage.

IP-09 Patrick Howland[1], Jason A Perman[1], Michael J Zaworotko[1]
[1]Department of Chemistry, University of South Florida

Cocrystal Controlled Solid-State Synthesis of H4BIPA-TC, a Molecule Used for the Construction of a 3-periodic Porous Metal-Organic Material

Metal-Organic Materials (MOMs) are comprised of metal clusters and multi-dentate organic ligands producing a variety of structures, from discrete to 3-periodic. Luminescence, redox active sites, and magnetism are a few of the properties the metal cluster may contribute, while size and molecular recognition can be influenced by the organic ligand in the MOM. An additional feature for many of these materials is the retention of porosity under total evacuation. This allows for the exchange of various gases

including hydrogen or carbon dioxide, both used for energy storage and sequestration, respectively. H_4BIPA-TC was synthesized by cocrystal controlled solid-state synthesis (C3S3) and was used to construct a porous 3-periodic framework with copper. Initial results suggest the material retains its structure after the removal of solvent molecules and allows for the absorption of nitrogen gas at 77 K for surface area analysis.

IP-10 Anna Cardwell[1]
[1]Department of Chemistry, University of South Florida

Natural Product Cocrystals

To further comprehend the concept of the supramolecular synthon, a research plan involving an extensive amount of cocrystal formers was devised. The two different types of synthons are heterosynthons and homosynthons. A supramolecular heterosynthon involves two different functional groups hydrogen bonding. Melatonin, a naturally occurring hormone produced by the pineal gland in mammals has been proven to improve sleep quality, is the chosen compound to bind with a list of various cocrystals formers. A supramolecular homosynthon involves two identical functional groups hydrogen bonding to one another. Lactic acid is an ingredient found in yogurt, cottage cheese and butter and has beneficial effects on the skin as a cleanser. Lactic acid is the chosen compound to demonstrate a homosynthon containing carboxylic acid functional groups. Lactic acid was ball milled with glutaric acid on a 1:1 ratio and provided different experimental data from the starting carboxylic acid compounds.

Organic (NES 104)

O-01 Petoria Gayle[1], Sameer Kulkarni[1], Xiangdong Hu[1], Hong-Gang Wang[2], Roman Manetsch[1]
[1]Department of Chemistry, University of South Florida; [2]Department of Pharmacology, Penn State College of Medicine

Protein-Protein Interaction Modulators & Role of Target Guided Synthesis

Protein-protein interactions are necessary for basic biological functions. However, modulators to certain protein-protein interactions can have therapeutic effects. We are focusing on the disruption of the interactions between anti-apoptotic proteins, such as Bcl-XL and pro-apoptotic proteins. Bcl-XL is the main regulator of apoptosis, or programmed cell death. Over expression of anti-apoptotic proteins has been commonly observed in cancer cells. This over-expression results in the suppression of apoptosis, leading to uncontrolled growth of cells, a phenomenon known as tumor growth. We are targeting the anti-apoptotic protein Bcl-XL using a fragment-based drug discovery approach known as Target-Guided Synthesis (TGS). In this approach, the biological target (Bcl-XL in this case) acts as a template onto which the fragments can bind and form a covalent bond, leading to a potential inhibitor of that target itself. These fragments generally consist of complimentary reactive functional groups. After investigating various reactions, an amidation reaction between sulfonyl azides and thio acids was employed for this purpose. So far, several acyl sulfonamides have been identified as potential inhibitors of Bcl-XL, using this approach. We believe that this approach will be utilized for targeting various protein-protein interactions in the future.

O-02 Edward Keshishian[1], Ali Hussain[1], Kirpal Bisht[1]
[1]Department of Chemistry, University of South Florida

Synthesis of Resorcinarene with Modified Functionality

Cavitands are being extensively researched due to the capability of these molecules to polymerize, catalyze, and encage guest molecules of complementary size and shape. Resorcinarenes, a particular type of cavitands, are cyclic tetramers formed by an acid catalyzed condensation reaction of resorcinol with aldehydes. Functionality can be added to resorcinarene derivatives by using different reactants, which would give the molecule a variety of new chemical applications. In this experiment cinnamic acid was methylated to form an ester and catalyzed by boron trifluoride etherate (BF_3*$O(C_2H_5)_2$) to make the resorcinarene. The reduction of this tetra ester resorcinarene would add new functionality, such as selectivity associated with the type of molecules that can be encapsulated. The results indicate that this tetramer has potential as a precursor to form novel compounds.

O-03 Michael Mormino[1], Gajendra Ingle[1], Jon Antilla[1]
[1]Department of Chemistry, University of South Florida

Chiral Phosphoric Acid Catalyzed Addition of Thiols to Imines

Chiral N, S acetal functional groups are found in several natural products, including penicillin. We have developed a new method for the synthesis of chiral N, S acetals by the addition of thiols to N-acyl imines. After screening various catalyst and solvents, 2,4,6(i-Pr)$_3C_6H_2$ BINOL and toluene produced the highest yields and ee. The rate of nucleophilic addition of thiolss to N-acyl imines is extremely fast. Reaction completion has been found to occur in less than one minute. 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 substrates also gave excellent yield and enantioselectivity.

O-04 Lindsay Kulczynski[1], Sridhar Reddy Kaulagari[1,2], Mark L McLaughlin[1,2]
[1]Department of Chemistry, University of South Florida; [2]H Lee Moffit Cancer Center & Research Institute

Design and Synthesis towards New Potential PTP1B Inhibitor

Reversible phosphorylation of tyrosine residues on proteins is the cornerstone of many cell signaling events. Protein tyrosine phosphatases (PTPs) work in coordination with protein tyrosine kinases (PTKs) to maintain the phosphorylation on tyrosine residues balanced. Phosphorylation can either turn on or off proteins. The shift in the equilibrium to either side, excessive phosphorylation or under phosphorylation, leads to many diseases like obesity, type II diabetes besides many cancers. Due to the plethora of phosphatases, kinases, and the very little difference among them, it is very challenging to selectively inhibit the desired phosphatase without interrupting other phosphatases. Selectivity and the cell permeability are the main problems for the current inhibitors therefore, cannot be used as effective drugs in human beings. Here we are proposing a potent new inhibitor and the efforts to synthesize. The proposed inhibitor is a sulfonic acid derivative of phenylalanine. The para-toluenesulfonylchloride was protected as sulfonamide with suitable amine and treated with butyl lithium and sulfur dioxide to get sulfinic acid. Oxidative chlorination, followed by ring closure in presence of base, gave bissulfonamide which can be brominated through Friedal-Crafts bromination, and further S_N2 reaction with $NO_2CH_2CO_2Et$ to displace the bromide. The compound would further undergo Clemmensen's reduction…

O-05 Kornwalee Wiangkham[1], Ryan Cormier[1], Edward Turos[2]
[1]Department of Chemistry University of South Florida; [2]Center for Molecular Diversity in Drug Design, Discovery, and Delivery, University of South Florida

Synthesis, Characterization, and Biological Activity of Poly(vinyl benzoate) Nanoparticles Containing N-Acylated Ciprofloxacins

Fluoroquinolone antibiotics such as Ciprofloxacin ("Cipro") have been an effective treatment for life-threatening bacterial infections. However, the steady increase in deadly bacteria having fluoroquinolone-resistance has placed an urgent demand for new antibiotics that are effective against these drug-resistant pathogens. Our laboratory is developing novel antibiotics as well as drug delivery platforms for overcoming these sorts of bacterial infections, and one area of interest is the development of N-acylated ciprofloxacin analogues in combination with poly(vinyl benzoate) nanoparticles (also discovered in our lab). This poster highlights our progress on these investigations.

O-06 Anthony Melendez[1], Arun Kumar[1], Jordan Anderson[1], Roman Manetsch[1]
[1]Department of Chemistry, University of South Florida

Synthesis of 1,3-Disubstituted Isopropanols as Potential Small Molecule Inhibitors for BACE-1 and Protein-Protein Interaction

Herein we illustrate the synthesis of a novel library of 1,3-disubstituted isopropanols using the epoxide ring opening reaction. Eighteen epoxides synthesized in the lab were reacted with a series of twenty-three commercially available thiophenols in various combinations. One hundred and sixty 1,3-disubstituted isopropanols were synthesized. The products were purified via column chromatography then characterized with mass spectroscopy, ^{1}H NMR, and ^{13}C NMR. This library is being tested in the inhibition of protein-protein interaction such as Bcl-xL, Mcl-1 and the enzyme BACE-1.

O-07 Kathryn Rutherford[1], Priyesh Jain[1], Ted J Gauthier[1], Daniel N Santiago[1], Sergiy I Borysov[2], Mark L McLaughlin[1,3]
[1]Department of Chemistry, University of South Florida; [2]Department of Molecular Medicine, Johnnie B. Byrd, Sr. Alzheimer's Center and Research Institute; [3]Drug Discovery Program, H. Lee Moffitt Cancer Center & Research Institute

Synthesis of cyclic β-hairpin as Aβ peptide fibrillogenesis inhibitors

Alzheimer's disease (AD) is believed to be caused by abnormal self-assembly of amyloid-β peptides. These fibrillar masses are primarily formed by aggregation of proteolytic cleavage products of Amyloid Protein Precursor (APP) and consist of 40-42 amino acids. These Aβ peptides are disordered in monomeric state but form fibrils with ordered beta-sheet conformation upon aggregation. Disruption of Aβ aggregation has been a major area of research in treating Alzheimer's disease. Previous studies have shown that the hydrophobic portion of Aβ peptide (Leu-Val-Phe-Phe-Ala) is responsible for aggregation. Herein we present the synthesis of cyclic β-hairpin peptides that bind specifically to this hydrophobic region and prevent β-sheet aggregation. We believe that the cyclic β-hairpin caps the growing fibril and prevents further oligomerization and can even solubilize preformed Aβ fibrils. To increase the bioavailability of these peptides, we have attempted to synthesize morpholine derivatives of lysine and serine and incorporate them into the non-recognition strand of the cyclic peptide.

O-08 Isabella Garriga[1], Ritch Williams[1], Meghanath Gali[2], Kirpal S Bisht[2]
[1]Department of Biology, University of South Florida; [2]Department of Chemistry, University of South Florida

Introductory Organic Chemistry Research

Current research includes performing and learning various organic transformations like reduction of esters, oxidation of alcohols and esterification. Reduction of ester functional groups is achieved by LiAlH4. These alcohols have been converted to aldehyde via oxidation by Dess-Martin periodinane reagent or Pyridinium chlorochromate. Esterification of alcohols is performed by using catalysts like DMAP in the presence of DCC. While performing these reactions, thin layer chromatography (TLC) is used to analyze reactions. TLC is useful to identify any impurities that may be present from the reaction as well. Purification of products is performed by using column chromatography, which has similar principles as TLC, and is especially useful to isolate more than one product from a mixture.

O-09 Chris Ludwin[1], C Kim[1], X Peter Zhang[1]
[1]Department of Chemistry, University of South Florida

Design and Synthesis of Chiral Corroles

The corrole is an analogue of the porphyrin macrocycle, and has demonstrated a variety of applications, such as use in photodynamic therapy for location and effective treatment of breast cancer cells, and also for reversing the process of arteriosclerosis, making it a viable candidate for the treatment of heart disease. On top of these medicinal uses, the corrole has also been shown to be useful for performing many catalytic reactions such as cyclopropanation, epoxidation, and N-H insertion reactions. First introduced in the mid 60's, corrole research was limited due to lack of a reasonable method of synthesis. The first practical corrole syntheses were performed in 1999, through condensation of pyrrole and an aldehyde, followed by ring-closing oxidation. In recent years, an even more efficient method to synthesize the corrole has been developed by Gryko. Using this aforementioned technique, multiple variations of A2B corroles were synthesized, and then subsequent cross coupling and metalation reactions were performed on the products to give chiral corroles capable of asymmetric catalytic reactions.

O-10 Andre Daley[1], Ruizhi Wu[1], Ali Husain[1], Kirpal S Bisht[1]
[1]Department of Chemistry, University of South Florida

Synthesis of Seven-membered Cyclic Carbonate Monomer from L-Tartaric acid

Polymers from renewable resources, which are biodegradable and biocompatible, have been an attractive area of research. For the monomer synthesis, enantiomerically pure functional seven-membered cyclic carbonate (5S,6S)-dimethyl-5,6-isopropylidene-1,3-dioxepin-2-one (ITC) was synthesized from L- tartaric acid in a four steps process. The first step involved the esterification of both acid groups in acidic condition using methanol as a reagent and as a solvent, along with PTSA (p-Toluenesulfonic Acid) as an acid catalyst. The second step is the protection of both diol groups of the diester using 2,2-dimethoxy propane as a protecting agent, PTSA as an acid catalyst, and toluene as the solvent. In the third step both diester groups were reduced into primary alcohols using LAH as a reducing agent, and THF as a solvent. The ketal protected diol was obtained and used for the final step in which triphosgen was used as a reagent, pyridine as a base, and THF as a solvent to produce the seven-membered ring poly carbonate monomer.

O-11 Mijal Guevara[1], Carolina Lopez[1], Ali Hussain[1]
[1]Department of Chemistry, University of South Florida

Formation of Bridged-Resorcinarene: Tetrabromoresorcinarene

The synthesis of the bridged resorcinarerne was accomplished in three steps. To begin with, condensation of 2-methyl-resorcinol and one equivalent of heptaldehyde catalyzed by hydrochloric acid in ethanol led to the octahydroxyresorcinarene. The product, a white solid, was filtered and washed with cold ethanol and water. The resulting product was then treated with dibromomethane/K_2CO_3 in DMF as a solvent to form the bridged resorcinarene product. The bridged resorcinarene was then brominated (using NBS as a reagent, and AIBN as an initiator) in benzene to yield the tetrabromoresorcinarene. Future research with include nucleophilic substitution of the bromine to yield new interesting compounds.

O-12 Lisa Luong[1], R Matthew Cross[1], Justin Sargent[1], Jordany Maignan[1], Tina Mutka[2], Dennis E Kyle[2], Roman Manetsch[1]
[1]Department of Chemistry, University of South Florida; [2]College of Public Health, University of South Florida

1,2,3,4-Tetrahydroacridones as Potential Inhibitors of Atovaquone-Resistant and Atovaquone-Susceptible P. falciparum isolates TM90-C2B and W2

Malaria is one of the most significant parasitic diseases affecting mankind today, exceeding 200 million annual cases worldwide. This disease has been a serious issue due to the emergence of drug resistance against common chemotypes such as atovaquone. This project focuses on the preparation of 1,2,3,4-tetrahydroacridones that can be tested for their activity against P. falciparum isolates TM90-C2B (an atovaquone resistant parasitic strain) and W2 (an atovaquone susceptible parasite). The research aims to utilize structure-activity relationship (SAR) studies of the benzenoid ring of the 1,2,3,4-tetrahydroacridone scaffold by following the Topliss operational scheme. 1,2,3,4-tetrahydroacridones are generated through a multi step synthesis that involves the cyclization of substituted anthranillic acids by refluxing in phosphorus oxychloride ($POCl_3$) with cycloalkanones to produce various 9-chloro -1,2,3,4-tetrahydroacridines. Subsequent hydrolysis in acetic acid gives the respective 1,2,3,4-tetrahydroacridone. Since the 1,2,3,4-tetrahydroacridone contains some similar structural properties to naphthoquinolone and ubiquinone (important features in the parasite's energy generation), it is hypothesized that 1,2,3,4-tetrahydroacridones are potential inhibitors of the parasite's respiration. Once compounds are synthesized they are screened in vitro against blood stage P. falciparum. Based on the data collected, it is found that the most active…

O-13 John Markantonis[1], Ali Hussein[1], Kirpal Bisht[1]
[1]Department of Chemistry, University of South Florida

Synthesis of a mono-brominated resorcin[4]arene

Synthesis of a mono-brominated resorcin arene from 2-methyl resorcinol through electrophilc aromatic substitution is a three step synthesis involving the formation of an octahydroxy resorcin arene from 2-methyl resorcinol, a rigid bowl shaped resorcin arene through bridging of the hydroxy groups in the octahydroxy product, and the monobromination through bromination of one of the methyl groups on the resorcin arene. Bromine can serve as a good leaving group for further substitution on the upper rim of the cavitand.

Natural (NES 102)

N-01 Minh Cong Nguyen[1], Charles Harter[1], Matt Lebar[1], Tina Mutka[2], Dennis Kyle[2], Bill Baker[2]
[1]Department of Chemistry, University Of South Florida; [2]College of Public Health, University of South Florida

Screening Microorganisms for Anti-Malarial Compounds

Malaria is a potentially fatal disease that affects 190-300 million people a year and results in 708,000-1,003,000 deaths. Malaria, a parasitic protist, with the most lethal strain in humans being Plasmodium falciparum. P. falciparum have developed strains that are resistant to antimalarial drugs, which is why research for alternative treatments are necessary. Antarctic microorganisms are a unique and unexplored potential source for compounds bearing anti-malarial properties. Over 1000 endophytic microorganisms have been isolated from Antarctic marine invertebrates. The Antarctic microorganisms were grown in differential marine broth. Organic chemicals produced by the organisms were extracted from the broth and lysed cells using polystyrene beads (XAD 17). Methanol was used to strip organic chemicals from the beads to give a crude residue. This dried residue was re-dissolved in dimethylsulfoxide (DMSO) and transferred to 96-well plates for analysis of biological activity. The bioassay determines if any microorganisms are producing anti-malarial compounds. A portion of the 96 well plates has been assayed to date, resulting in the identification of several partially active microbes. The active microbes were cultured on a larger scale to identify what compounds are responsible for the anti-malarial activity. Purification of the extracts resulting from these scale-ups is ongoing.

N-02 Vanessa Santos[1], Cynthia Mehler[1], Stephanie Holdener[1], Heather Trinder[1], Alexander Williams[1], Jackie Salm[1], Samantha Landolfa[1], Roberto Lopez[1], Tiffany Lanham[1], Minh Cong Nguyen[1], Anangamanjari Pedapudi[1], Michele Summerville[1], Hoangmy Chau[1], Elisa Herrera[1], Matt Lebar[1], Charles Harter[1], Tina S Mutka[2], Dennis E Kyle[2], Bill J Baker[1]
[1]Department of Chemistry, University of South Florida; [2]Center for Molecular Diversity in Drug Design, Discovery and Delivery, University of South Florida

Malaria: Drugs, Disease, and Obstacles in Malaria Parasites

Malaria is an infectious disease caused by a eukaryotic protist of the genus Plasmodium. This mosquito-borne disease is widespread in tropical/subtropical regions. According the the Medicines for Malaria Venture (MMV) website, Malaria kills a child under 5 every 40 seconds. Malaria parasites start to multiply within red blood cells, causing symptoms that are similar to the common cold. The disease will, if untreated, proceed to coma and death. Drug resistant strains of P. falciparum are spreading rapidly, heightening the need for antimalarial drugs. A substantial understanding of malaria parasite biology is the only way potential vaccines can be developed. Various species of fungi and bacteria have displayed the ability for removal of early parasite forms from circulation. 70,000 samples of fungi and bacteria currently being examined for a mechanism of resistance against malaria in widespread red blood cell mutations. These organisms are gathered, cultured, and placed into MeOH for a minimum of 24 hours to remove the crude extract. The solvent Dimethyl Sulfoxide (DMSO) is then used to dissolve the crude extract for bio-assay. Occasionally, biomolecules of these organisms return to be an active against malaria and are isolated to be tested as drug candidates.

N-03 Rosemary Persaud[1], Jason Cuce[1], Bill J Baker[1,2]
[1]Department of Chemistry, University of South Florida; [2]Center for Molecular Diversity in Drug Design, Discovery and Delivery, University of South Florida

Isolation and Further Chemical Investigation of Ecdysteroids from Synoicum Adareanum

Ecdysteroids, hormones responsible in the regulation of molting, metamorphosis, reproduction, and diapauses in crustaceans, were first isolated in the 1950's. Evidence suggests that some of these compounds possess pharmacological properties. In fact, there are several plant species among traditional medicines that contain ecdysteroids. The tunicate Synoicum adareanum, contains six known ecdysteroids and represents first tunicate reported to yield ecdysteroids. Previous studies have shown that the S. adareanum ecdysteroid abeohyousterone exhibits considerable cytotoxicity against leukemia, colon, and lung cancer cell lines. This paper describes the isolation of the six known ecdysteroids from S. adareanum as the basis of continuing studies of their pharmacological activity.

N-04 Hoangmy Chau[1], Jeremy Beau[1], Bill Baker[1]
[1]Department of Chemistry, University of South Florida

Isolation and Chemical Extraction of Endophytes from Rhizophora Mangle for Bioactivity against S. aureus

Rhizophora Mangle are plants that grow around salty bodies of water. They are unique because they are able to flourish in soil that is unstable and low in oxygen. R. mangle depend on chemical and biological defenses in order to protect themselves from pathogens. They do this through a symbiotic relationship with endophytes. Endophytes are bacteria and fungi that live symbiotically within the R. mangle. The endophytes benefit from the R. mangle because the R. mangle provide the endophytes with nutrients. The endophytes, in turn, provide the R. mangle with protection from certain bacteria or fungi by releasing chemicals. These compounds can be chemically extracted and isolated in order to discover new drugs that are active against pathogens. Staphylococcus aureus is bacteria that can be responsible for serious illnesses such as pneumonia and meningitis. Through our experiments, we have chemically extracted and isolated a chemical compound that is active against S. aureus. The chemicals released by a particular R. mangle endophyte (P4-08) were extracted and chemically isolated. The isolation was done by the Medium Pressure Liquid Chromatography and High Pressure Liquid Chromatography methods in order to obtain a pure compound. A series of experiments were run on the pure…

N-05 Garrett Craft[1], Wai Sheung Ma[1], Bill J Baker[1]
[1]Department of Chemistry, University of South Florida

Endophytes in the Search for Novel Malaria Drugs

Plants often host and exploit symbiotic endophytic fungal populations within their tissues to ward off predation via potent fungal secondary metabolites, with such fungi gaining a continual source of plant carbohydrate in return. These fungal metabolites, known collectively as mycotoxins, are extracted, isolated and assayed in this study to address whether inhibition of a drug-resistant form of malaria is manifested. With 84 strains of endophytes originating from Hong Kong mangroves screened, seven demonstrated activity and 10 resulting fractions maintaining former activity of >67% inhibition across all four replicates of both low and high test concentrations. This poster summarizes and presents the extraction and isolation procedures employed in this study, along with NMR spectra and assay data.

N-06 Ryan Baker[1], Charles Harter[1], Matt Lebar[1], Raymond Chowmond[3], Tina Mutka[2], Dennis Kyle[2], Cedric Pearce[4], Lilian Vrijmoed[3], Bill Baker[1]
[1]Department of Chemistry, University of South Florida; [2]College of Public Health, University of South Florida; [3]Department of Biology, City University of Hong Kong; [4]Mycosynthetix

Antimalarial Constituents of Fungi

Malaria, a vector borne plasmodium parasite, is responsible for 200-300 million infections each year in mostly developing nations according the The World Health Organization. The two most common species, Plasmodium falciparum and Plasmodium vivax, are becoming resistant to all forms of treatment. Thus a need exists for new drug therapies. The chemical constituents of approximately 70,000 fungi were extracted in methanol and bioassayed at a 30µg/ml concentration to determine which microbes were producing anti-malarial compounds. The extracts showing the highest level of activity were then separated into fractions based on polarity using Medium Pressure Liquid Chromatography with a gradient solvent system (hexane to ethyl acetate to methanol). The resulting fractions were assayed again. The fractions that remained active against malaria were further purified using High Pressure Liquid Chromatography. The resulting pure compounds were identified via Nuclear Magnetic Resonance spectroscopy, Mass Spectroscopy and re-screened against malaria.

N-07 Jayesh Gopal[1], Bill J Baker[1], Matthew Lebar[1]
[1]Department of Chemistry, University of South Florida

Florida Marine Tunicates

Antarctic marine tunicates have been previously studied, with special note being given to their ability to sequester metals such as vanadium, manganese, and nickel. The environment of Antarctica is known for being one of the most pure, pollution-free areas in the world, making it a possibility that its marine tunicates store metals differently from tunicates found elsewhere. For this reason Florida tunicates must also be studied and their mechanism of storage compared to that of Antarctic tunicates. The tunicates are freeze-dried and their minerals extracted using a hot concentrated acid mixture. The practical application of this is the possible use of tunicate-derived chelators in medicine, such as in diabetes medication and antibiotics.

N-08 Elisa Herrera[1], Jeremy Beau[1], Bill Baker[1]
[1]Department of Chemistry, University of South Florida

Isolation of a Potential New Anticancer Compound

Recent studies depict that mangroves contain a diversity of endophytic organisms producing secondary metabolites that combat environmental pathogens. These secondary metabolites have the potential to be developed into highly selective drugs that may help against diseases in humans. One such case is a fungal endophyte found in the roots of the Floridian Rhizophora mangle (red mangrove) from our Key Largo collection named KL-07-26-2A. Its crude extract showed activity against cell line Colon 38 from a bioassay done at Henry Ford Cancer Center. Thus, the sample was regrown at a larger scale, freeze-dried and extracted. The crude was then fractionated using Medium Pressure and High Pressure Liquid Chromatography (MPLC and HPLC). The fractions obtained from these techniques were then analyzed via Nuclear Magnetic Resonance to determine what types of compounds are present that could potentially aid in the development of anticancer drugs.

N-09 Tony Kurian[1], Jeremy Beau[1], Dennis Kyle[2], Bill J Baker[1]
[1]Department of Chemistry, University of South Florida; [2]Department of Global Health, University of South Florida

Isolation of Endophytic Fungi from Exostema Caribaeum and Extract Screening for Antimalarial Activity

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. Exostema caribaeum, or Caribbean Princewood, is indigenous to Florida, Mexico and the Caribbean and 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. Endophytes can produce compounds providing survival value to the host plant that can also have medicinal value. 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. Voucher specimen was deposited to the USF Herbarium. Two trees were donated to USF Botanical Gardens. 79 fungi were isolated. The chemicals they produced were extracted and are currently being screened for antimalarial activity. Compounds in active samples will be isolated and their structures determined. The fungi that produced them will be identified.

N-10 Morgan Pyne[1], Kristen Pyne[1], Alex Gonzalez Jacobo[1], Charles Harter[1], Bill Baker[1]
[1]Department of Chemistry, University of South Florida

Project MMV

As part of the Baker Lab, we are part of Project MMV (Medicines for Malaria Venture). This lab is set out to find a new cure to fight against malaria. With malaria affecting millions of people worldwide annually, a new medicine to fight it would be a breakthrough. The lab started out with roughly 70,000 organisms that were found and collected from extreme environments around the world. Once the samples are collected, they are brought back to the lab, where they are then covered in methanol. The methanol helps to separate the polar compounds out of the specimen. These are the compounds that we are interested in. The methanol is then removed from the vial and placed into a clean vial where it is left to dry, leaving just the crude polar compounds in the vial. Then, DMSO is added to the vial, which makes a solution of the compounds, allowing them to be placed into a deep well plate and an assay tray in order to be analyzed. The compounds are then shipped to another lab where they are assayed. If any are positive to fight malaria…

N-11 Franka Co[1], Jeremy Beau[1], Bill J Baker[1]
[1]Department of Chemistry, University of South Florida

Discovery of Anti-P. aeruginosa Compounds from Mangrove Endophytes

Pseudomonas aeuriginosa is a bacterium that is disease causative in both animals and humans, thriving off of abnormal environments such as one with little to no oxygen. Those with compromised immune systems are number one targets and there is evidence that it is beginning to develop an antibiotic resistance. In our recent efforts of finding new drugs from endophytic organisms from Floridian mangroves, we have isolated a candidate that is active against P. aeruginosa. This bacterial endophyte, EG09-14B-3, was isolated from the Everglades. This paper presents the results and progress of this project.

N-12 Steven Austin[1], Jeremy Beau[1], Bill J Baker[1]
[1]Department of Chemistry, University of South Florida

Studies of Natural Products for Drug Discovery

Natural products research represents the discovery of molecules to study and screen against a wide variety of illnesses. A new area of interest in our group is the kingdom Fungi. Easily collected, cataloged, and cultured, the natural product compounds from fungi can be studied in the laboratory. Due to their high degree of biodiversity, fungi contain many active compounds that can be tested against an illness in a bioassay. Once activity has been determined, purification, along with various spectroscopy methods can be used to isolate a single active compound. Finally, this active compound can be further studied to develop new drugs to combat illness. This paper reports on the collection, isolation, archival and results of the preliminary screening of fungi from Floridian Mangroves.

N-13 Nida Mahid[1], Jeremy Beau[1], Halie Miller[2], Lindsey Shaw[2], Bill J Baker[1]
[1]Department of Chemistry, University of South Florida; [2]Department of Biology CMMB, University of South Florida

Natural Products from Mangrove Endophytes

Endophytes are microorganisms, either fungi or bacteria that live within plant cells. They have symbiotic relationship with the host. It has been shown in recent literature that extremely valuable compounds can be extracted from endophytes with potential medical uses. Once samples are collected they are surface sterilized and microbes are collected and plated from inside the sample. Samples are than isolated, archived and regrown in broth. Once grown in broth the secondary metabolites are extracted using ethyl acetate, butanol and dichloromethane. Those crude extracts are then tested against MRSA, VRE, Pseudomonas aeruginosa and many other infectious agents. One of the secondary metabolite extracted was macrolactin A, exhibitng potent activity against MRSA. This paper reports on these processes used to obtain natural products from endophytes as well as the identification of the bacterium responsible for the production of macrolactin A.

N-14 Alyssa Greenawalt[1], Alejandro Mendez[1], Daria Yunina[1], Lori Hammer[1], Jessica Kastory[1], Matt Lebar[1], Charles Harter[1], Bill Baker[1]
[1]Department of Chemistry, University of South Florida

Undergraduate Work Assisting the Medicines for Malaria Venture

Medicines for Malaria Venture (MMV Project), a non-profit, public-private organization, was established in Switzerland in 1999 by the Gates Foundation and Exxon Mobile. The goal is to create a low cost anti-malarial drug that will put a halt to Malaria and eventually exterminate any future sightings of this disease. MMV Project tests biodiverse organisms' (terrestrial and marine) ability to produce an anti-malarial vaccine. These organisms can develop specific defenses against predation, which once controlled, can become a potent drug. Ensuring the use of clean equipment and the method of methanol transfers are imperative, enabling the research to continue at a constant pace. Vials are thoroughly scrubbed and cleaned curtailing fungus residue contamination of future samples. Assays are tested with Methanol to extract the specific molecules providing the biodefense technique. Organisms are tested using the dried crude extract against specific concentrations of the malarial parasite that will show a positive or negative test. Out of the original 70,000 organisms tested, there might be seven to ten possible drugs which could change the lives of many.

Judges

American Chemical Society Tampa Bay Local Section
Eric Ballard, Ph.D.
Eric Steimle, Ph.D.

H Lee Moffitt Cancer Center and Research Institute
Juan Del Valle, Ph.D.
Jinsoo Kim, Ph.D.
Young B. Kim, Ph.D.

Department of Chemistry, University of South Florida
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Thank you to all of the judges for donating their time today to promote Chemistry research!