16th Raymond N. Castle Student Research Conference

Table of Contents

Welcome from the Castle Conference Committee

Dear Colleagues and Friends,

Welcome to the 16th Raymond N. Castle Student Research Conference hosted by the University of South Florida. In honor of Dr. Raymond N. Castle, this Conference was created to promote his goals of scientific collaboration and science education.

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

We are especially proud of the research done by all students in the department, both graduate and undergraduate. With the continued success of the Raymond N. Castle Student Research Conference and to more clearly promote scientific collaboration, we have expanded our invitation for presentation to students in other Natural Science Departments as well as Colleges and Universities in Tampa and the surrounding areas. Today, we have an opportunity to hear from students in chemistry related disciplines from around Florida. Chemistry research will be highlighted with our special guest, Dr. Catherine Fenselau. 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. Fenselau will be giving a presentation on her exciting research and experience in the field of chemistry.

Lastly, we would like to thank all that chose to volunteer their time and efforts, particularly the judges, and Dr. Shi for helping us plan and coordinate this year's conference. In addition, we are grateful for the financial support that allows us to host this conference and owe special thanks to Dean and Barbara Martin, Tampa Bay Local Section of the American Chemical Society, University of South Florida College of Arts and Sciences, as well as the multiple other sponsors and affiliates who have generously contributed to this event. Most importantly, this conference would not exist without the efforts of those of you presenting your research today. Therefore, we gratefully acknowledge you and your research advisors, as well as all in attendance. Thank you all and we hope you enjoy and learn from the 16th Raymond N. Castle Student Research Conference.

Sincerely,

The Castle Conference Committee

16th Raymond N. Castle Student Research Conference Committee

Committee Members

Zachary Shultz (Chair)
Elena Bray
Bo Song
Jamie Nunziata
AJ Sonja
Alejandro Rivera Nicholls
Chuan Shan
Ruixuan Gao
Sylvia Singh
Imalka Marasinghe Arachchilage

Staff & Faculty Support

Mike Shi, PhD
Kimberley Fields, PhD
Marie Bourgeois, PhD

Web Support

Brant Tudor
Douglas Franz

Program Cover Design

Adam Hogan

Specials Thanks

16th Raymond N. Castle Student Research Judges

University of South Florida

Juan Del Valle, PhD
Emre Seyyal, PhD
Rong Zhang, PhD
Theresa Evans-Nguyen, PhD
Ioannis Gelis, PhD
Laura Anderson, PhD
James Leahy, PhD
Kimberly Fields, PhD
Maria Bourgeois, PhD
Kenneth Caswell, PhD
Ellen Leahy, PhD
John Kuhn, PhD
Ushiri Kulatunga
Christine Tang
Brian Space

USF Moffitt Cancer Center

Justin Lopchuck, PhD

Florida Southern University

Deborah Bromfield Lee, PhD
Jarrod Eubank, PhD

Saint Leo

Jerome Williams, PhD

Southeastern University

Ralph N. Salvatore, PhD

University of Tampa

Olesani Sode, PhD

University of Central Florida

Gang Chen, PhD
Yulia Gerasimova, PhD

Retired Personnel

Robert Litman, PhD

Building Map

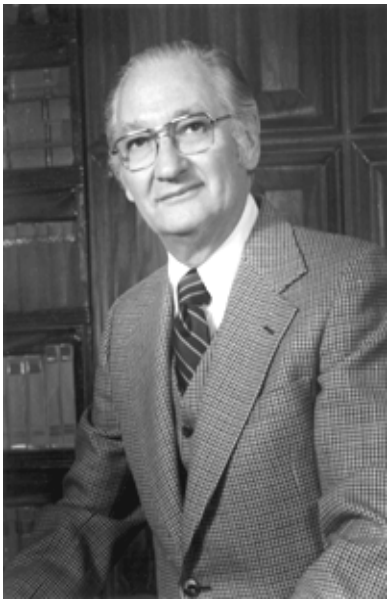
Schedule of Events

Saturday, March 24th, 2018

8:00 AM	-	9:00 AM	Welcome Session - *Registration and Breakfast*	Chemistry Courtyard
9:00 AM	-	10:45 AM	Morning Talk Session I & II *Graduate Student Presentations*	CHE 301 & CHE 302
10:45 AM	-	11:00 AM	Break	
11:00 AM	-	11:15 AM	Castle Conference Welcome	CHE 100
11:15 AM	-	12:15 PM	Plenary Speaker - Dr. Catherine Fenselau	CHE 100
12:15 PM	-	1:00 PM	Lunch *Sponsored by the ACS Tampa Bay Local Section*	Chemistry Courtyard
12:30 PM	-	1:00 PM	ACS Tampa Bay Local Section General Body Meeting	CHE 100
1:00 PM	-	3:00 PM	Poster Session *Graduate and Undergraduate Presentations*	CHE 1st Floor Classrooms
3:00 PM	-	3:15 PM	Break	
3:15 PM	-	5:00 PM	Afternoon Talk Session *Graduate Student Presentations*	CHE 100
5:00 PM	-	5:15 PM	Break	
5:15 PM	-	5:30 PM	Awards Ceremony	CHE 100

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.

Castle Conference Plenary Speaker
Dr. Catherine Fenselau

University of Maryland, College Park

Biological Mass Spectrometry: Observations on its Evolution

In this lecture, aspirations, advances in instrumentation, successful applications and Nobel prizes will be reviewed as part of the evolution of biological mass spectrometry, with illustrations from the laboratory of the speaker.

Biography

Catherine Fenselau was one of the first trained mass spectrometrists to join the faculty of an American medical school (Johns Hopkins). She was given the job description to "exploit mass spectrometry in biomedical research." In early work she pioneered MS investigations of intact microorganisms, analysis and novel reactivities of drug conjugates with glucuronic acid and glutathione, and benchmark analyses of zinc fingers and metallothioneins. Her laboratory reported early determinations of gas phase peptide basicities including the first measurement of arginine's proton affinity, target capture in ion molecule reactions, and the stability of α-helices and β-sheets in the gas phase. Her group introduced enzyme-catalyzed O-18 labeling, Asp-selective acid cleavage and the use of nanoparticle pellicles into proteomic workflows, and since 2000 they have exploited proteomic strategies to investigate mechanisms of tumor resistance to chemotherapy and immunotherapy.

Her contributions to mass spectrometry and its biomedical applications have been recognized by awards from the American Chemical Society, the International Mass Spectrometry Foundation, the American Society for Mass Spectrometry, the American Society for Pharmacology and Experimental Therapeutics, the Human Proteome Organization, the Pittsburg Conference, and others. She was associate editor of Analytical Chemistry for 26 years and the founding editor of Biomedical Mass Spectrometry (now Journal of Mass Spectrometry). She is a past president of ASMS, founding president of US HUPO, and was senior vice president of international HUPO.

She has published more than 380 peer reviewed research papers and book chapters, and about one hundred and forty undergraduates, graduate students and post-doctoral fellows have received training in Dr. Fenselau's laboratories.

Fenselau grew up in Nebraska, received her A.B. from Bryn Mawr College and earned a Ph.D. from Stanford University. Presently she is Distinguished University Professor of Chemistry & Biochemistry at the University of Maryland, Affiliate Professor of Bioengineering, and a member of the Greenebaum Cancer Center.

Dr. Dean and Barbara Martin

Special Thanks

Dr. Dean F. Martin is Distinguished University Professor Emeritus and Director of the Institute for Environmental Studies at the University of South Florida, where he has been a member of the faculty since 1964. Dr. Martin received his B.A., with Honors, from Grinnell College (1955), where he met his future wife

Barbara while both were chemistry majors. They were married in 1956 while both attended Pennsylvania State University as graduate students and in 1958 Dr. Martin received his Ph.D. and Mrs. Martin her Master's degree. In 1958-59, he was a National Science Foundation Post-Doctoral Fellow at University College, London after which he returned to the States and accepted a faculty position at the University of Illinois, Urbana-Champaign, as Instructor and Assistant Professor of Inorganic Chemistry (1959-1964). He received (1969-1974) a Career Development Award from the Division of General Medical Sciences, NIH, to study the chemistry and chemical environment of algal toxins. In 1970-71, he was a Visiting Professor of Physiology and Pharmacology at Duke University Medical Center.

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

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

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

Sponsors

Tampa Bay Local Section

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

IKA® Works, Inc.
2635 Northchase Pkwy. SE
Wilmington, NC 28405
Phone: 800-733-3037

Pro Copy
5219 E. Fowler Ave.
Tampa, FL 33617
Phone: (813) 988-5900

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

USF Department of Chemistry
4202 E. Fowler Ave., CHE 205
Tampa, FL 33617
Phone: (813) 974-9676

Graduate Talks Morning Session I (CHE 301)

GT-1.1 9:00 - 9:20 AM **Wishrawana Sarathi Ratnayake**

A typical protein kinase C inhibitors (ICA-1 specific to PKC-ι and ζ-Stat specific to PKC-ζ) repress epithelial to mesenchymal transition in melanam

GT-2.1 9:20 - 9:40 AM **Brian O'Flynn**

Arylalkylamine N-acetyltransferases in Tribolium Castaneum: A possible target to control crop destruction

GT-3.1 9:40 – 10:00 AM **Geoffrey M. Gray**

Structural Studies of Spider Silk Dope

GT-4.1 10:00 – 10:20 AM **Ying He**

G-Quadruplex Formation from H8 Modified Guanosine Derivatives: From Structure to Function

GT-5.1 10:20 - 10:40 AM **Bo Song**

Self-assembly of Supramolecular Norias based on Sequence-specific Ligand

Graduate Talks Morning Session II (CHE 302)

GT-1.2 9:00 - 9:20 AM **Gaurav Verma**

Utilization of the stable soc-MOF platform for one pot Strecker synthesis

GT-2.2 9:20 – 9:40 AM **Yanbin Zhang**

Synthesis and characterization of covalently linked G-quadruplex

GT-3.2 9:40 - 10:00 AM **S M Anisul Islam**

Protein Kinase C-ζ stimulates colorectal cancer cell carcinogenesis via PKCζ/Rac1/Pak1/β-Catenin signaling cascade

GT-4.2 10:00 - 10:20 AM **Yiming Li**

Dispersion and Separation of Single-walled Carbon Nanotubes by Supramolecule

GT-5.2 10:20 - 10:40 AM **Garrett Craft**

Comparing 3D-Printed PA12 Parts Produced via Extended Sintering Timespans to Parts Produced by Conventional Methods.

Graduate Talks Afternoon Session (CHE 100)

GT-06 3:15- 3:35 PM **Briana Aguila**

Lower Activation Energy for Catalytic Reactions through Host-Guest Cooperation within Metal-Organic Frameworks

GT-07 3:35- 3:55 PM **Chiyu Wei**

Iodine catalyzed diazo activation to access radical reactivity

GT-08 3:55- 4:15 PM **Fiona L. Kearns**

PETase: Characterization of a plastic-degrading enzyme

GT-09 4:15 - 4:35 PM **Yassin Elbatrawi**

A submonomer-based approach towards Piperazic acid (Piz) natural products. The total synthesis of L-156,373

GT-10 4:35 - 4:55 PM **Linda Barbeto**

Studies Aimed at the Synthesis of Antileishmaniasis Agents

The Barbara and Dean F. Martin Poster Session
CHE 101A

Graduate: Group GP All Disciplines

The Jianfeng Cai Poster Session
CHE 103

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

The ACS Tampa Bay Local Section Poster Session
CHE 101A

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

GRADUATE TALKS

XX-YY **Yassin Elbatrawi** [1], Juan Del Valle [1]
[1]Department of Chemistry, University of South Florida

A submonomer-based approach towards Piperazic acid (Piz) natural products. The total synthesis of L-156,373

The piperazic acid (Piz) residue is found in a number of biologically active natural products and there exist numerous methods for its synthesis and incorporation into host peptides. Most approaches introduce pre-formed orthogonally protected Piz residues, synthesized in many steps, onto a growing peptide chain. L-156,373, a cyclic hexapeptide and oxytocin antagonist isolated from Streptomyces silvensis, features two consecutive enantiomeric forms of the Piz residue. Here, we present our efforts towards the first total synthesis of L-156,373 and its analogues via a sub-monomer-based electrophilic amination approach. Our strategy relies on a tandem SN2 cyclization to afford both Piz residues in one step and employs L- and D- glutamic acid residues as chiral synthons. This approach provides a means to introduce Piz and δ-oxo piperazic acid (Oxopiz) residues into host peptides using readily available amino acid building blocks.

XX-YY **Geoffrey M. Gray** [1], Arjan van der Vaart [1]
[1]Department of Chemistry, University of South Florida

Structural Studies of Spider Silk Dope

Spider dragline silk possesses a unique combination of strength and elasticity. Its main constituents are two proteins (MaSp1 and MaSp2), that are stored in a high concentration (30-50%) dope before the silk is spun into a fiber. The dope is thought to form micelles that aggregate into liquid crystals, but the microstructure of the proteins in the dope remains unclear. To help elucidate secondary structure characteristics, enhanced sampling simulations were performed on several common dragline silk sequence motifs at various concentrations, including in octanol to mimic a high concentration solution. Additional pulling experiments were performed to assess structural changes that occur under spinning-like conditions. Results show that the motifs resemble random coils under aqueous conditions, while showing some turns and helices in octanol. Pulling showed an increase in the polyproline II helical content, consistent with the idea that these structures form as part of the spinning process.

XX-YY **Ying He** [1]
[1]Department of Chemistry, University of South Florida

G-Quadruplex Formation from H8 Modified Guanosine Derivatives: From Structure to Function

G-quadruplex (GQ) has been developed extensively over the past decades. It has been reported that GQs could be used in many directions of chemical, material and biological researches, including supramolecular hydrogel, molecular switch and ionophores. One general approach to achieve structurally rigid G-monomer is the modification of C-8 position by fixing the sugar syn/anti conformation. However, according to literature, the studies of C-8-modified G-quadruplexes are rare, mainly due to the challenges associated with the substrate synthesis. Herein, we report the new synthesis of 8-aryl guanosine and fluorescent active 8-triazole guanosine and their selfassembly property in solid state and in solution. Through cation templation (Mn+= Na+, K+, Ba2+, Pb2+, Sr2+, La3+), discrete self-assembled G-quartet structures were formed. Both structurally novel and functional enriched G-quartets are achieved using this new system.

XX-YY **S M Anisul Islam** [1], Rekha Patel [1], Mildred Acevedo-Duncan [1]
[1]Department of Chemistry, University of South Florida

Protein Kinase C-ζ stimulates colorectal cancer cell carcinogenesis via PKCζ/Rac1/Pak1/β-Catenin signaling cascade

Colorectal cancer (CRC) is the second most common cancer due to therapy resistant cancerous cells. The exact mechanisms of cell growth, survival, metastasis and inter & intracellular signaling pathways involved in CRC is still a significant challenge. Hence, investigating the signaling pathways that lead to colorectal carcinogenesis may give insight into the therapeutic target. In this study, the role of atypical Protein Kinase C (aPKC) on CRC was investigated by using two specific inhibitors of aPKC. The cell lines tested were CCD18CO normal colon and LOVO metastatic CRC cells. The inhibition of aPKCs did not bring any significant toxicity on CCD18CO normal colon cell line. Although PKC-ι is an oncogene in many cancers, we found the overexpression of PKC-ζ and its direct association with Rac1. Our findings suggest that the PKC-ζ may be responsible for the abnormal growth, proliferation, and migration of metastatic LOVO colon cancer cells via PKC-ζ/Rac1/Pak1/β-Catenin pathway.

XX-YY **Yiming Li** [1], Guifei Huo [2], Xiaomin Qian [1], Xiaopeng Li [1]
[1] Department of Chemistry, University of South Florida, Tampa FL 33620, USA
[2]School of Chemistry and Molecular Engineering , East China Normal University, Shanghai, 200062,China

Dispersion and Separation of Single-walled Carbon Nanotubes by Supramolecule

Carbon nanotubes have many potential applications due to their superb mechanical and electrical properties. However, many of the applications were limited by their polydispersity and their poor solubility in both aqueous and non-aqueous solvents. Here we report a new discrete supramolecular metallacycle functionalized with an alkynylplatinum(II) bzimpy moiety, and it displayed well dispersion and

separation of single-walled carbon nanotubes (SWNT). Bundled SWNT can be effectively dispersed in acetonitrile by sonication in the presence of the supramolecule. Characterization such as fluorescence spectroscopy, transmission electron microscopy (TEM) and scan electron microscopy (SEM) measurements provide evidence for individually dispersed carbon nanotubes. TEM also revealed that SWNT with diameter around 2 nm could be selectively extracted from mixed SWNT with different diameters.

XX-YY **Brian O'Flynn** [1]
[1]Department of Chemistry, University of South Florida

Arylalkylamine N-acetyltransferases in Tribolium Castaneum: A possible target to control crop destruction

The red flour beetle (T. castaneum) is probably the most common secondary pest of all grain commodities in the world. This large-scale destruction results in substantial economic damage due to loss of the market price of product and decreased nutritional value. One possible route to develop a novel type of insecticide for T. castaneum is based on the study of arylalkylamine N-acyltransferases (AANATs). These promiscuous enzymes (members of the GCN5-related N-acetyltransferase (GNAT) family) are vital to T. castaneum as they are involved in melanism, as well as hardening of the cuticle. In addition, the N-acylarylalkylamines are suggested to act as potent neurotransmitters. Presented here is a mechanistic analysis and crystal structure of Tc-AANAT0, which was determined to catalyse the formation of short chain N-acylarylalkylamines, with acetyl CoA functioning in the role of acyl-donor.

XX-YY **Wishrawana S. Ratnayake** [1], Christopher A. Apostolatos [1], Mildred Acevedo-Duncan [1]
[1]Department of Chemistry, University of South Florida

Atypical protein kinase C inhibitors (ICA-1 specific to PKC-ι and ζ-Stat specific to PKC-ζ) repress epithelial to mesenchymal transition in melanam

Melanoma is one of the fastest growing cancers in the United States, reported a 14% increase in new cases in 2017 compared to 2016. Atypical PKCs contains two structurally and functionally distinct isozymes in human; PKC-ι (iota) and PKC-ζ (zeta) and they play critical roles in cancer development. We believe that aPKCs play an important role in cell motility of melanoma by inducing EMT. In the current study, we have investigated the effects of novel PKC-ι inhibitor [4-(5-amino-4-carbamoylimidazol-1-yl)-2, 3-dihydroxycyclopentyl] methyl dihydrogen phosphate along with its nucleoside analog on cell migration and invasion of two malignant melanoma cell lines compared to a normal melanocyte cell line. Both inhibitors decreased the levels of total and phosphorylated levels of PKC-ι. Furthermore, both inhibitors increased the levels of E-cadherin and RhoA while changing phosphorylated Vimentin levels thereby preventing the Vimentin intermediate assembly. Immunoprecipitation and immunofluorescence showed a strong interaction of PKC-ι and Vimentin.

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

Self-assembly of Supramolecular Norias based on Sequence-specific Ligand

In the past few decades, coordination-driven self-assembly as a bottom-up approach has witnessed a rapid growth in building giant structures. Challenges still remain, however, within the construction of giant structures in terms of high efficiency and complexity from simple precursors. In biological systems, the shapes, complexity and functions of DNA- and protein-based assemblies are encoded by the defined sequence of nucleotides and amino acids. Inspired by this phenomenon, we herein introduced the concept of “programming of sequence-specific ligands” and designed a series of linear building blocks with specific sequence through the bridging of terpyridine ligands with Ru(II) coordination. The resulting structures were characterized via multi-dimensional mass spectrometry analysis (ESI-MS, TWIM-MS) as well as a series of NMR (1H, COSY, NOESY) analysis. Moreover, the larger size supramolecules N4 and N5 formed amazing supramolecular pattern on HOPG surface, which was observed using STM.

XX-YY **Gaurav Verma** [1], Sanjay Kumar [1], Wenyang Gao [1], Zheng Niu [1], Lukasz Wojtas [1], Shengqian Ma [1]
[1]Department of Chemistry, University of South Florida

Utilization of the stable soc-MOF platform for one pot Strecker synthesis

The development of new heterogeneous catalysts is of paramount importance because many industrial and chemical processes require the use of such species. Also, these offer an advantage over the homogeneous catalysts due to their reuse and recyclability. The metal organic frameworks (MOFs) have received considerable attention recently as heterogeneous catalysts due to their tunable open metal centres, functional organic linkers and accessibility of the pores for active guest species. Herein, we report an Indium based MOF with soc (square octahedral) topology that exhibits a very high surface area (~2500 m2/g) and shows good catalytic activity in the one pot multicomponent Strecker reaction for the synthesis of alpha-aminonitriles.

XX-YY **Chiyu Wei** [1], Pan Li [1]
[1]Department of Chemistry, USF

Iodine catalyzed diazo activation to access radical reactivity

An unprecedented iodine catalyzed diazo activation is disclosed herein under either photo- or thermal-initiated conditions. The mechanistic

studies revealed the formation of an iodo-substituted alkyl radical as the key intermediate, which represents a novel approach to enable diazo radical reactivity. This metal-free diazo-activation strategy were successfully applied into olefin cyclopropanation and epoxidation with excellent yields. Further extension to substituted pyrrole synthesis under thermal-initiated conditions demonstrates the unique reactivity using this method over typical metal-catalyzed conditions.

XX-YY **Yanbin Zhang** [1], Ying He [1], Xiaodong Shi [1]
[1]Department of Chemistry, University of South Florida

Synthesis and characterization of covalently linked G-quadruplex

We report herein the design and synthesis of covalently linked guanosine derivative as the building block to construct a G-quadruplex with unique properties. The subunit of G-quadruplex, G-quatet, was based on H-bond assembly, and the designed G-quadruplex was formed by covalently linked G-quatet. The structure showed enhanced stability since the covalent bond between G-quatet layer.

GRADUATE POSTERS

XX-YY **Sami Abdulkadir** [1], Jianfeng Cai [1]
[1]Department of Chemistry, University of South Florida

Modulation of angiogenesis through rationally designed γ-AApeptide helical mimetic of VEGF

Angiogenesis, formation of new blood vessels from existing vascular network, is modulated mainly through vascular endothelial growth factors (VEGF). This is an important process in healing and development. Abnormalities in angiogenesis, most notably, sustained angiogenesis, is a hallmark of cancer cells. Tumor vascular proliferation leads to tumor growth and metastasis and it is for this reason that the prospect of affecting this process has gained considerable interest in the fight against cancer. X-ray crystal structure of VEGF bound to its receptor-VEGFR indicate a helix structure on VEGF (residues 17 - 25) is an essential binding interface. In this research we describe the design and synthesis of γ-AApeptide, a helical peptidomimetic of the VEGF helix region. Preliminary testing on human cell lines show that the first VEGF mimic synthesized promotes cell proliferation. Currently we are testing receptor binding and activity in human umbilical vein endothelial cells (HUVEC).

XX-YY **Nicole E. Avalon** [1], Lucas Bishop [2], Alison E. Murray [2], Bill J. Baker [1]
[1]Department of Chemistry, University of South Florida, Tampa, FL
[2]Division of Earth and Ecosystem Sciences, Desert Research Institute, Reno, NV

Predictive Databases, Computational Peptide Sequencing, and Secondary Metabolite Identification from a New Antarctic Pseudovibrio species

Antarctic invertebrates are rich sources of secondary metabolites with high potential for bioactivity. Often present within the genome of invertebrate-associated bacteria are biosynthetic gene clusters(BGC) responsible for the biosynthesis of non-ribosomal peptides, polyketides, as well as other compounds. In this project, mass spectrometry is used to validate the compound predictions from computational databases by confirming the presence of predicted peptides based on the genomic sequencing results of Pseudovibrio sp. Tun.PSC04-5.I4, isolated from the Antarctic tunicate Synoicum adareanum. Proteomic analysis was performed using nanoelectrospray and a hybrid quadrupole-Orbitrap Q Exactive Plus mass spectrometer. Preliminary data has been used for de novo peptide sequencing and custom database searches, with particular focus on fragments of possible permutations of the predicted peptide using PEAKS 8.5 software(Bioinformatics Solutions, Inc.). These indicate the presence of at least one of five predicted non-ribosomal peptides in the bacterial extract, with variable post-translational modifications.

XX-YY **Lindsay Blume**
[1]Department of Chemistry, University of South Florida

Synthesis and Antibacterial Testing of Alkyl Thiosulfonates

Methicillin-resistant Staphylococcus aureus (MRSA) is an increasing concern in the medical community. The use of common antibiotics like penicillins and cephalosporins to treat MRSA has continued to decline in effectiveness. Our laboratory has developed a number of new families of anti-MRSA antibacterial compounds. My project is to investigate eight initial S-alkyl thiosulfonates. I will present the results so far obtained toward the synthesis, characterization, and antimicrobial testing.

XX-YY **Elena Bray**
[1]Department of Chemistry

The Treatment of Toxoplasmosis using FKBP Ligands: Synthesis and Analogs of Shield-1

Toxoplasmosis is a disease caused by Toxoplasmosis gondii. T. gondii is a protozoan parasite that infects more than 60 million people in the world chronically and is listed by the CDC as one of five Neglected Parasitic Infections. T. gondii causes symptoms ranging from asymptomatic to death, with immunocompromised people being the most at risk for severe symptoms. The protozoan goes through active and dormant phases, depending on which stage of the life cycle it is in. The current treatment can only eradicate the active form of the protozoan, while the dormant form stays in the body forever. Shield-1 is a FKBP ligand that can be used to study the transcription factors of the protozoan in active and dormant phases. Analogs of Shield-1 have been synthesized to maximize the binding and pharmacokinetics of Shield-1 with the binding domain.

XX-YY **Justin Goodwin** [1], Christopher F. Cain [1], Juan Del Valle [1]
[1]Dept. of Chemistry, University of South Florida

Synthetic studies toward the 4-alkylideneproline natural products eleganine A and 17-nor-excelsinidine

Eleganine A is a monoterpene indole alkaloid capable of inducing apoptosis in HuH-7 cancer cells. 17-Nor-excelsinidine, a novel member of the Akuammiline family of alkaloids, possessing an unusual 1-azoniatricyclo [4.3.3.0] undecane core structure and has shown activity against adenovirus and HSV. Of interest from a synthetic standpoint, these molecules possess an ethylidene proline moiety found in only a handful of other natural products, including lucentamycin A, as well as isodomic Acids G and H. Here, we describe our progress toward the total synthesis of eleganine A and 17-nor-excelsinidine starting from L-serine as a chiral progenitor. Our synthetic strategy involves formation of the ethylidene proline fragment via nickel-catalyzed reductive Heck-type cyclization and generation of the indole ring through Larock heteroanulation.

XX-YY **Selam Hagos** [1], Bill Baker [1]
[1]Department of Chemistry, University of South Florida

Chemical Investigation of Antarctic Sponges

In terms of significant contributions of nature to the biomedical sciences, marine sponges have been an important source of potential drugs for diseases like cancer, infectious, and inflammatory diseases. Secondary metabolites isolated from sponges are structurally diverse and have shown interaction with important biological receptors, many of which have implications for human disease. In this project, several red/orange sponges collected over the years from different sites of Antarctica, underwent Nuclear Magnetic Resonance (NMR) spectroscopy guided fractionation. Using ELSD (Evaporative Light Scattering Detector) and UV detectors, Normal phase MPLC (Medium Pressure Liquid Chromatography) followed in sequence by RP HPLC(Reverse Phase High Pressure Liquid Chromatography) separations obtained several chemically interesting fractions and pure compounds. Structure elucidation of the pure compounds was performed using one-and-two-dimensional NMR. These pure compounds and future isolates will be subjected to bioassay against Zika virus, ESKAPE pathogens and Clostridium difficile.

XX-YY **Shahedul Islam** [1]
[1]Department of chemistry, USF

Short Metallo-peptides and peptoids: A look into the oxidative reactivity

Since the discovery in early 1990's peptoids have come a long way to show immense potential in myriad of applications that includes antibacterials,anticancers, antitumors , anti-alzeimers to drug delivery systems etc. The emergence of peptoids from peptides has practically added an edge to the field of peptidomimetics. This study sheds light on the comparison between peptides and peptoids in terms of their catalytic activity in oxidation when interacting with biologically available metals , such as copper(II). Minimalistic metallo-peptide and peptoid; acylated FHFH and metallo peptoid ɣ-AA-FHFH with metal binding motif two Histidines ; as available in different metalloproteins were designed and synthesized to study their catalytic activity in oxidation. 3,5- Di-tert- butylcatechol(DTBC) is chosen as a primary substrate . As hydrogen Peroxide(H_2O_2) can also interact with Di-Cu center to exhibit different pathway,the H_2O_2 effect is also examined . Kinetic data as well as NMR data suggests both the DTBC and H_2O_2 binding with Cu(II) center and the binding of one substrate affects the binding of another one.

XX-YY **Taranjot Kaur** [1]
[1]Department of Chemistry, University of South Florida

Label Free Biosensors for Thyroid Detection

Functional abnormality of Thyroid is a common day problem in clinical practices. Thyroid diseases are deeply involved with the metabolism in our body. Hence, the detection of thyroid stimulating hormone (TSH), Thyroxine (T4), and Triiodothyronine (T3) is critical for disease early intervention and the prevention of pandemics. In this study, GO@Ag nanocomposites based electrochemical immunosensors had been

fabricated and employed for highly sensitive and cost effective detection of thyroid hormones (T3 and T4). The fabrication proceeded through the modification of screen printed carbon electrode (SPE) with rGO-Ag. These rGO-Ag modified graphene electrodes were then biointerfaced with the thyroid hormones. rGO-Ag nanocomposites were used as receptor materials for binding the iodized compounds though electrostatic interaction between Ag+ and I- ions rather than using enzyme-linked immune sorbent assays (ELISA) technique. The obtained results showed a promising performance of NPs based biosensor for the thyroid detection with fairly good sensitivity and selectivity.

XX-YY **Sofia Kokkaliari** [1], Bill J. Baker [1]
[1]Department of Chemistry, University of South Florida

Chemistry of Marine Tunicates Collected from Antarctica

Marine organisms have attracted the interest of the scientific community in the past few decades. Aspiring from this development, research has been directed towards Antarctic organisms, due to the unique ecosystem. In this project, we attempted to isolate new compounds from Antarctic invertebrates and especially tunicates, which have been the source of multiple new and active compounds. The tunicates were collected in numerous locations in the waters of Antarctica and at different depths. After extraction, a sequence of MPLC (medium pressure liquid chromatography) and HPLC (high pressure liquid chromatography) purification procedures were performed. The process was guided using proton NMR, and the compounds with the most interesting profile were isolated, identified and will be submitted in various bioassays to determine their activity.

XX-YY **Vasantha Kumar M. V.** [1], Brian Blagg , Ioannis Gelis [1]
[1]Department of Chemistry

NMR Spectroscopy: Insights into Protein–Ligand Interactions.

Biological macro-molecules, mainly proteins, mediate essential functions through their physical interactions with other target molecules such as ligands, proteins and nucleic acids. Some of these interactions are transient in nature, making them difficult to detect by other spectroscopic technique such as X-ray crystallography. NMR spectroscopy offers the Saturation-transfer difference (STD) NMR experiment, which accurately determines weak and strong ligand protein interactions, their relative affinities, Kd. In addition, the interaction between a receptor protein and a peptide where one of the Cysteine residue of the peptide is selectively attached to a paramagnetic ligand tag (MTSL tag) to identify the binding surface on the protein. In our studies we have put our efforts understand the interaction between full length HSP90a with few ligands (anticancer properties) using STD NMR. We have also studied the interaction between p38a with C-terminal peptide called N32 (with and without MTSL) using 2D HSQC experiments.

XX-YY **Qi Lai** [1], Qing Liu
[1]University of South Florida

Developing Triazole-Imidazole (TAIM) as Novel Fluorescence Probe for Selective Ag+ Cation Detection within PPb Scale

The 1,2,3-triazole-imidazole derivatives (TA-IM) were prepared as novel fluorescence probes. The design principle was based on the incorporation of electron rich imidazole with electron deficient triazole to enhance molecular dipolement between two aryl rings. Excellent florescence emission was received both in organic solvent and in aqueous media. Screening metal binding ability revealed excellent selectivity of this new class of compounds toward Ag+ cation in aqueous solution, giving linear detecting within nM limit.

XX-YY **Xuming Li** [1], Shuyao Zhang [1], Jin Wang [1]
[1]Department of Chemistry, University of South Florida

Highly Efficient and Stereoselective Thioallylation of Alkynes

The research works on highly efficient and stereoselective thioallylation of alkynes using gold redox catalyst and without the utility of external strong oxidant. The study shows that our method gives good yield in a broad scope.

XX-YY **Anne-Claire Limon** [1], Ala Anzhari [2], Jessie Adams [3], Anthony Sanchez [3]
[1]Department of Chemistry
[2]Department of Global Health
[3]Department of Cell Biology, Microbiology, and Molecular Biology

New alcyopterosins and steroids isolated from an undescribed Antarctic coral

The chemical investigation of an undescribed Antarctic coral has led to the isolation of two different kinds of bioactive compounds. After

lyophilization of the organism, two different extractions were performed: the first one used a methylene chloride: methanol (1:1) mixture, and the second one used methylene chloride only as solvent in a Soxhlet extraction. After a partition followed by normal phase Medium Pressure Liquid Chromatography, stages of normal phase and reverse phase High Performance Liquid Chromatography purifications revealed to two kinds of new bioactive compounds: new acetylated sesquiterpenoids with alcyopterosin scaffolds from the first process and new acetylated steroids from the second. One and two-dimensional nuclear magnetic resonance, mass spectrometry, X-ray crystallography, and circular dichroism were the methods performed to elucidate the structures. Furthermore, biological testing against Leishmania sp. and ESKAPE pathogens, Zika virus, Clostridium difficile, and HeLa cancer cells were performed to extend the scope of drug discovery potential.

XX-YY **Anne-Claire Limon** [1], Jessie Adams [2], Rahmy Tawfik [2]

[1]Department of Chemistry

[2]Department of Cell Biology, Microbiology, and Molecular Biology

New secondary metabolites isolated from epigenetically modified fungi for anti-infective drug discovery

Whether from tropical or lower latitude ecosystems, the chemical survival mechanisms used by fungi offer a potential axis for research to find new drugs. Epigenetic regulation is a key mechanism to orchestrate the expression or suppression of gene activity; hence, manipulating these mechanisms offers new opportunities to express down-regulated secondary metabolite genes and has the potential to generate new potent and novel metabolites. After an ethyl acetate:water partition, the crude extracts were fractionated on normal phase MPLC. Then, stages of normal phase and reverse phase HPLC purifications have already brought forward known and new bioactive compounds and the work is still ongoing and fruitful. With the pool of isolated compounds, one and two-dimensional nuclear magnetic resonance, mass spectroscopy, and X-ray crystallography are providing the data necessary to elucidate the structures and characterize the stereochemistry involved. Further biological testing is being performed to extend the scope of drug discovery potential.

XX-YY **Faeez Mahzamani** [1], Edward Turos [1]

[1]Department of Chemistry, University of South Florida

Ciprofloxacin-Based Antibacterial Homopolymer Nanoparticle Emulsions for Antibacterial Applications

We investigate for the first time a method for forming polyacrylate nanoparticles using N-acryloyl ciprofloxacin for its construction. The procedure entails a free radical induced emulsion polymerization of the ciprofloxacin acrylate as the sole monomer in water to produce a stable emulsion containing nanoparticles of highly uniform size and morphology with an average diameter of 970 nm and average surface charge of -63 mV. The nanoparticles were found to be capable antibacterials with minimum inhibitory concentration values against Staphylococcus aureus and Escherichia coli comparable to that of free ciprofloxacin, with essentially no observable cytotoxicity.

XX-YY **Faeez Mahzamani** [1], Ashleigh Bachman [1], Kristy Flores [1], Edward Turos [1]

[1]Department of Chemistry, University of South Florida

Poly(Menthyl Acrylate) Homopolymer Nanoparticle Emulsions as Drug Delivery Vehicles

We explore a method of forming homopolymer nanoparticle emulsions as drug delivery vehicles using menthyl acrylate as the monomer. The poly(menthyl acrylate) homopolymer nanoparticle emulsion provided greater stability compared to the previous copolymer models investigated in our laboratory. The resulting homopolymer emulsions exhibited a decrease in cytotoxicity, and a significant increase for loading of penicillin G. The nanoparticle emulsions exhibited similar minimum inhibitory concentration activity against both S.aureus and MRSA.

XX-YY **Imalka Marasinghe Arachchilage** [1]

[1]Department of Chemistry, University of South Florida

A novel approach to develop laccol polymer and laccol-styrene blends via cationic polymerization to produce radiation hard materials

In recent years lacquer chemistry stimulated more attention from scientific community due to its environmental friendly applications. A novel approach is introduced to develop polymers using laccol extracted from Vietnamese lacquer sap (Rhus succedanea). In nature, lacquer polymerization is induced via enzymatic radical initiation. Herein, monomer was polymerized via cationic initiation via an aluminum chloride-ethyl acetate (AlCl3.EtOAc) initiator complex. This approach was further developed by polymerizing blends of laccol and styrene designed for use in radiation hard materials. The IR and NMR data evidence reactions with the trans conjugated double bonds in the side chain of laccol monomer accompanying the polymerization. Molecular weight build up was measured by GPC on partially cured laccol polymers and laccol-styrene blends. Fully cured samples were cross linked and this was clearly observed in the rheology data. Further, an increase in hardness was observed after the gamma irradiation using Co-60 gamma irradiator.

XX-YY **Jacob M. Mayers** [1], Randy W. Larsen [1]
[1]Department of Chemistry, University of South Florida

Photophysical study of Ruthenium (II) Tris (1,10-Phenanthroline) encapsulated in zirconium based Uio-66 and derivatives

Uio-66 metal organic frameworks are thermally stable porous materials that provide an excellent environment for the encapsulation of photoactive guests. The guest of particular interest is Ruthenium (II) Tris-(1,10-Phenanthroline) (RuPhen) due to the relatively long lifetime and photostability of this class of complexes. Presented here is a photophysical study of RuPhen encapsulated Uio-66 MOFs and derivatives. The RuPhen encapsulated in each of the MOF frameworks were fit to a biexponential decay function. A bathochromatic shift is also observed in both the steady state emission and FT-IR spectrum of each framework. The consequences of adding an amine or hydroxyl substituent to the organic ligand exhibits photophysical changes different from the parent Uio-66 such as lower lifetimes and longer wavelength emissions. Electron transfer or intermolecular hydrogen bonding between the RuPhen and the amine or hydroxyl substituent might be a plausible explanation of such spectroscopic variation. It is shown that the photophysical properties

XX-YY **Arjan van der Vaart** [1]
[1]Department of Chemistry, University of South Florida

Flexibility of Lesion Containing DNA

Ionization radiation damages DNA by oxidizing bases, and these distortions can be removed by variety of glycosylases resulting in an apyrimidinic (AP) site. Subsequent AP endonucleases cut out the remaining nucleotide creating a lesion in the strand. This nick in the phosphodiester backbone causes considerable flexibility which has been linked to an increased affinity for repair enzymes. The flexibility and behavior of a control, single strand AP site and an AP site with a lesion were investigated by molecular dynamic simulations. Implications for damage repair will be discussed.

XX-YY **Alfredo Peguero-Tejada** [1], Arjan van der Vaart [1]
[1]Department of Chemistry, University of South Florida

Assessing the intrinsic secondary structure propensity of chameleon sequences

Chameleon sequences can adopt both α-helical and β-sheet conformations depending on the protein in which they are found. The extent to which this polymorphism is intrinsic or context driven is not fully understood. Characterizing the relative stability between the different structural states of these sequences would allow for more intelligent drug design and shed light on the observed structural plasticity of sequences. The present study addresses this issue by calculating the conformational free energy difference between α-helical and β-sheet conformations via the confinement method, which links thermodynamic states of interest by transforming them into sets of independent harmonic oscillators. The results of this study will yield a library of conformational free energy differences as a function of various chameleon peptide sequences.

XX-YY **Swetha Ramani**
[1]Department of Chemistry, University of South Florida

Effect of Cobalt based mixed Chalcogenides as catalysts for Oxygen Reduction Reaction

Cobalt based selenides/sulphides and their mixed phases CoSe(1-x)Sx were synthesized using a facile solvothermal technique. With increasing sulphur content, CoSe(1-x)Sx undergoes a phase change from hexagonal to cubic. Pure CoSe showed nanosheets and dendritic structures. As the sulphur substitution increased, the average number of nanosheets decreased significantly. With 0.25 sulphur substitution, sheets along with nanoparticles were present. while with 0.5 sulphur, little/no sheet like structures were observed. Only nanoparticles were seen with sulphur substitution >75%. The best ORR activity was shown by Pure CoSe and Co9S8 followed by CoSe0.75S0.25 with very small change in diffusion limited current. The η1 of CoSe was achieved at a remarkable 0.767 V. The improvement in the onset in pure phases can be associated with a lower tafel slope of 44mV/decade for CoSe or 56mV/decade for Co9S8. As a result, ORR activity is shown to be better at pure Cobalt Chalcogenides than mixed Chalcogenides.

XX-YY **Benjamin M. Rathman** [1], Juan R. Del Valle [1], Jessie Adams [2], Lindsay N. Shaw [2]
[1]Department of Chemistry, University of South Florida
[2]Department of Cell Biology, Microbiology and Molecular Biology, University of South Florida

Backbone Aminated Gramicidin S Analogues with Antimicrobial and Antiamyloidogenic Activity

Gramicidin S (GS) is a naturally occurring β-sheet-like cyclic decapeptide from Bacillus brevis that possesses antimicrobial activity against gram-positive and gram-negative bacteria. While GS is very potent it also causes hemolysis of human erythrocytes; therefore significant effort has been devoted to improving its selectivity for bacterial over mammalian cells. Here we report the synthesis and biological evaluation of N-

aminated analogues of GS. Their antimicrobial activity was assayed against a panel of drug-resistant gram-positive and gram-negative bacteria known as ESKAPE pathogens, and their cytotoxicity measured using human red blood cells. Several N-aminated analogues not only showed improved antimicrobial activity but also reduced hemolytic activity. GS also has antiamyloidogenic activity and we have preliminary data which suggests N-aminated analogues show greater inhibition of the fibrilization of amyloid-beta (Aβ1-42). We believe the improved therapeutic index and inhibition of fibrilization is due to the increased stabilization of the β-Sheet that N-amination affords.

XX-YY **Sabrina M. Rosa-Ortiz** [1], Arash Takshi [1]

[1]Department of Electrical Engineering, University of South Florida

Low Temperature Soldering Surface-Mount using Hydrogen Assisted Copper in an Electroplating Bath

Low-temperature soldering procedure represents a useful method by using copper growth for soldering electronic components on a printed circuit board allowing modification of thickness and morphology. To accelerate the soldering process hydrogen assisted electroplating method was employed to solder a surface-mount component to a PCB track at room temperature. Formation of irregular deposits by electrodeposition was obtained by using an aqueous solution containing CuSO4 and H2SO4 in de-ionized water. During the experiment electrolysis was observed, allowing hydrogen ions to interact with Cu2+ ions in order for the plating to take place. The hydrogen bubbles released after the electrolysis caused the structure of the electroplated layer to be more porous, but with remarkable mechanical strength suitable for use as interconnect on PCBs. The morphology of copper deposits based on the interaction with hydrogen and the deposition of the plating material has being confirmed by using a Scanning Electron Microscopy technique.

XX-YY **Sylvia Singh** [1], Alekyha Nimmagadda [1], Ma Su [1], Minghui Wang [1], Peng Teng [1], Jianfeng Cai [1]

[1]Department of Chemistry, University of South Florida

Lipidated α/α-AA heterogeneous peptides as antimicrobial agents

With an increase of resistance in bacteria there is an urgent need for alternative treatment methods that will complement conventional antibiotics. Focus has been drawn to Host Defense Peptides (HDPs) and their efficacy as potential antibiotic agents. Herein we reported on the development of lipidated α/α-AA heterogeneous peptides as HDP mimetics. These compounds showed potent antimicrobial activity toward both Gram-positive and Gram-negative bacteria, and they also displayed excellent selectivity as they only have limited hemolytic activity. Fluorescence microscopy suggested that the mechanism of action of these heterogeneous peptides is bacterial membrane disruption, which is believed to be the major reason it is difficult for bacteria to develop resistance. Time kill studies suggested that these compounds could rapidly eradicate bacteria. Moreover, these compounds could also clear biofilm formed by bacteria. These findings suggested that lipidated α/α-AA heterogeneous peptides, as a new class of peptidomimetics, are promising antibiotic agents combating antibiotic resistance.

XX-YY **Yetunde Oluwatosin Sokefun** [1], Dr. Babu Joseph [1], Dr. John Kuhn [1]

[1]Department of Chemical and Biomedical Engineering, University of South Florida

The effect of nickel and magnesium loadings on the activity, selectivity and stability for catalytic dry reforming of biogas using Pt/cerium-zirconium

CO2 reforming of methane is a technology that converts biogas (CH4 and CO2) into valuable syngas. With the right processing syngas can then be converted to various chemicals and liquid fuels. Typical operating temperatures for CO2 reforming of methane range from 600-900oC. Previous studies by our research group showed that high activity can be achieved at low temperature (450oC) using Pt-doped Ni/Mg catalyst supported on cerium-zirconium mixed oxide. Our current work involves evaluating the role of Pt, Ni, and Mg on the catalyst and determining if all components are necessary. Elimination of unnecessary metals will lead to reduction in overall cost and synthesis time. Performance will be based on activity, selectivity, and stability results from the CO2 reforming experiments. Two sets of supported metal catalysts series were prepared. A series contained no Ni metal; 0.16%Pt-0.5%Mg-Ce0.6Zr0.4O2, 0.16%Pt-1%Mg-Ce0.6Zr0.4O2, 0.16%Pt-2%Mg-Ce0.6Zr0.4O2 while the other contained no Mg; 0.16%Pt-0.67%Ni-Ce0.6Zr0.4O2, 0.16%Pt-1.34%Ni-Ce0.6Zr0.4O2, 0.16%Pt-2.68%Ni-Ce0.6Zr0.4O2

XX-YY **Tracess Smalley** [1]

[1]Department of Chemistry, University of South Florida

An investigation of the potential effects of the atypical PKC-ι inhibitor ICA-1 on ovarian cancer proliferation and survival, in estrogen dependent

Ovarian cancer is the most lethal gynecological cancer diagnosis. There is no efficient screening process for ovarian cancers and the average stage of diagnosis is stage III. Atypical PKCs (PKC-ζ and PKC-ι/λ) have been shown to be overexpressed in various malignant cells lines and to be linked to pathways for cellular proliferation and survival. Many investigations suggest that the hormone estrogen regulates cellular proliferation in an ERα dependent manner. Little research shows the effects of estrogen on ERα and β negative cells and its role in cellular proliferation. In this investigation, ovarian cell lines (HEY, COV644, T80) were treated with the atypical PKC-ι inhibitor ICA-1 nucleoside variant in two different systems, with and without estrogen, and assayed to determine the effects on proliferation and cellular survival. These assays included protein quantification, cell proliferation, and wound healing. Our preliminary data suggests that PKC-ι is a novel target in

carcinogenesis and inhibition of this protein decreases the rate of proliferation. Our results also suggest that estrogen has a significant effect on cell proliferation, even in estrogen receptor negative cells.

XX-YY **Ma Su** [1]
[1]Department of Chemistry, University of South Florida

Membrane-Active Hydantoin Derivatives as Antibiotic Agents

Hydantoin (imidazolidinedione) derivatives such as nitrofurantoin are small molecules that have aroused considerable interest recently due to their low rate of bacterial resistance. However, their moderate antimicrobial activity may hamper their application combating antibiotic resistance in the long run. Herein, we report the design of bacterial membrane-active hydantoin derivatives, from which we identified compounds that show much more potent antimicrobial activity than nitrofurantoin against a panel of clinically relevant Grampositive and Gram-negative bacterial strains. These compounds are able to act on bacterial membranes, analogous to natural host-defense peptides. Additionally, these hydantoin compounds not only kill bacterial pathogens rapidly but also prevent the development of methicillinresistant Staphylococcus aureus (MRSA) bacterial resistance under the tested conditions. More intriguingly, the lead compound exhibited in vivo efficacy that is much superior to vancomycin by eradicating bacteria and suppressing inflammation caused by MRSA-induced pneumonia in a rat model, demonstrating its promising therapeutic potential.

XX-YY **Santana A.L. Thomas** [1], D. Kyle [3], Y. Kee [2], N. Wilson [4], B.J. Baker [1]
[1]Department of Chemistry, University of South Florida
[2]Department of Cellular, Molecular and Microbiology, University of South Florida
[3]University of Georgia
[4]Western Australian Museum

The Chemical Investigation of Deep- Sea Antarctic Corals and their Potential in Drug Discovery

Secondary metabolites have attracted interest in drug discovery because of their biological effect on other organisms, as opposed to primary metabolites which exert their biological effect intracellularly. The chemical diversity of secondary metabolites has been the frontier of drug discovery. A recent report quantified more than 28,000 marine natural products reported over 6 decades and approximately 10% of these were reported as bioactive. This demonstrates the potential of marine natural products as a good source of drugs for human diseases. This project describes the isolation of secondary metabolites from three species of Antarctic deep sea corals. They all displayed diversity amongst the terpene chemical class. Although these compounds are related biosynthetically they have shown specificity to biological effects as seen in through biological screen against infectious diseases.

XX-YY **Lei Wang** [1], Dr. Xiaopeng Li [1]
[1]Department of Chemistry, University of South Florida

Stepwise Self-Assembly of Heterometallic Macrocycles Based on Terpyridine Ligand

Coordination between organic ligands and metal ions has been widely used to construct supramolecules in the field of self-assembly. However, rational design and synthesis for discrete heterometallic macrocycles have been less explored so far. Here, we utilized a stepwise strategy to design a hexagonal metallomacrocycle based on the coordination of terpyridine ligand and three different metal ions. The metallo-ligand was achieved via connection of terpyridine motifs by Ru2+, and the supramolecular macrocycle was constructed in almost quantitative yield by stepwise self-assembly of 6 metallo-ligands with 6 Fe2+ (or Cr2+) and 12 Zn2+. Both 1D and 2D NMR spectroscopy, electrospray ionization mass spectrometry (ESI-MS), traveling-wave ion mobility mass spectrometry (TWIM-MS), and transmission electron microscopy (TEM) have been used to characterize the supramolecules. More study about tuning the florescence properties of the supramolecules is currently under the way.

XX-YY **Lulu wei**, Ma Su, Alekhya Nimmagadda, Minghui Wang
[1]Department of chemistry, University of South Florida

short sulfono lipo-a/γ -AAlipidated hybrid peptides with antimicrobial activity

we designed and developed short sulfono lipo-a/γ -AAlipidated hybrid peptides. These sequences, bearing lysine γ-AA peptide building blocks, a lysine amino acid, and hydrophobic lipid tail which is a more economical synthetic process. These compounds were reported to interact with bacteria membrane and bacteria killing. The lead sequences display potent and broad-spectrum antimicrobial activity against a series of Gram-positive and Gram-negative bacteria.

XX-YY **Bingjie Yang** [1], Bill J. Baker [1]
[1]Department of Chemistry, University of South Florida

Bioassay-guided isolation of mangrove fungal secondary metabolites against Leishmania

Marine secondary metabolites are known for their structural diversity and bioactivity. Mangrove plants live at the marine margin and consequently harbor both terrestrial and marine endophytic fungi. The interaction between mangrove fungi and the mangrove plant can modify the way that plant responds to the environment, which leads to the consideration that mangrove fungi are possible sources to screen for new products. In this project, mangrove endophytic fungi are cultured using three different treatments. Two treatments utilize epigenetic modulators to promote the expression of latent biosynthetic pathways. These methods use 5-azacytidine as a DNMT (DNA methyltrasferase) inhibitor and sodium butyrate as a HDAC (Histone deacetylase) inhibitor. The third treatment is the control culture with no epigenetic modulator agents. Crude extracts prepared from each mature culture are fractionated using chromatographic techniques. Using Leishmania donovani bioassays to guide each fractionation step results in the isolation of bioactive compounds that target the parasite.

XX-YY **Teng Yuan** [1]
[1]Department of Chemistry, University of South Florida

Gold-Iron combined catalysis in regioselective aldol reaction

Aldol condensation is a well-known named reaction which provides an easy way of constructing C-C bond. However, due to its mechanism, self-condensation is hard to control. Therefore, here we report a protocol to realize cross aldol condensation via vinyl gold species.

XX-YY **Shuyao Zhang** [1], Pan Li [1], Jing Wang [1], Chiyu Wei [1], XIaodong Shi [1]
[1]Department of Chemistry, University of South Florida

Iodine catalyzed diazo activation to access radical reactivity

An unprecedented iodine catalyzed diazo activation is disclosed herein under either photo- or thermal-initiated conditions. The mechanistic studies revealed the formation of an iodo-substituted alkyl radical as the key intermediate, which represents a novel approach to enable diazo radical reactivity. This metal-free diazo-activation strategy were successfully applied into olefin cyclopropanation and epoxidation with excellent yields. Further extension to substituted pyrrole synthesis under thermal-initiated conditions demonstrates the unique reactivity using this method over typical metal-catalyzed conditions.

XX-YY **Yanbin Zhang** [1], Ying He [1], Xiaodong Shi [1]
[1]Department of Chemistry, University of South Florida

Synthesis and characterization of covalently linked G-quadruplex

We report herein the design and synthesis of covalently linked guanosine derivative as the building block to construct a G-quadruplex with unique properties. The subunit of G-quadruplex, G-quatet, was based on H-bond assembly, and the designed G-quadruplex was formed by covalently linked G-quatet. The structure showed enhanced stability since the covalent bond between G-quatet layer.

UNDERGRADUATE POSTERS

XX-YY **Kurrdeige Alexander** [1], Dr. Deborah Bromfield Lee [1]
[1]Chemistry, Biochemistry & Physics

Synthesis of the Isoindolinone Moiety of Stachybotrin D: Incorporating Greener Methods

The human immunodeficiency virus (HIV) is a debilitating viral infection that can negatively affect the individual as well as a nation's economy and workforce. Stachybotrin D is a phenylspirodrimane extracted from Stachybotrys chartarum MXH-X73 found to inhibit the reverse transcription activity of wild type HIV-1 as well as five other non-nucleoside reverse transcriptase inhibitor-resistant HIV strains. This greener synthesis involved the esterification of a benzoic acid derivative, protection of aromatic hydroxyl groups, and Mannich/lactamization aminoalkylations. Esterification of benzoic acid derivatives using a microwave resulted in 85-94% yields. By developing a successful and greener synthesis of Stachybotrin D larger quantities of this natural metabolite may be produced for further study into its biological activity. Additionally, this research may advance current research into solving the dreadful antibiotic resistance crisis and drug shortages.

XX-YY **Juan Argüelles** [1], Edwin Rivera [1]
[1]INTERDISCIPLINARY NMR FACILITY, UNIVERSITY OF SOUTH FLORIDA

Quantitative NMR Analysis of a series of Amines

Quantitative NMR (qNMR) is a common application of Nuclear Magnetic Resonance (NMR) spectroscopy alongside structure elucidation. The percentage of contaminants present in an industrial sample of TRIS Amino crystals will be determined using three independent methods. First, qNMR will be used to find concentration based on an external standard. Second, a calibration curve of standard amine concentrations will be generated and used to find the concentration. Third, Complete Reduction to Amplitude-Frequency Table (CRAFT) will be used to recreate the spectrum of the individual components. The results of these three methods will determine their relative effectiveness as quantitative methods and against other analytical techniques such as Gas Chromatography (GC).

XX-YY **Bryce Bader** [1], Benjamin Pollard [1], Lee Woodcock [1]
[1]Department of Chemistry, University of South Florida

Optimizing Boron parameters for the CHARMM general force field using force matching methods

The current iteration of the CHARMM general force field (CgenFF), a molecular mechanical level of theory, lacks parameters for boron and boron containing compounds. As such, boron containing systems cannot be studied with the current force field. Here we seek to generate boron parameters for CGenFF with a force matching method for the antifungal drug tavaborole. Small molecules, like tavaborole, can be used for simulations, in which configurations are sampled. We seek to validate boron parameters by seeing if simulation results are similar using new parameters from simulations and comparing to the simulation results from the semiempirical method used for force matching. A way to do this is using free energy perturbation (FEP) and Bennet's Acceptance Ratio (BAR) to see if a successful connection exists between the two levels of theory. Free energy calculations obtained from vFEP will give a hint for the success of these two theories.

XX-YY **Dakota Becker-Greene** [1], Anne-Claire Limon [1], Bill Baker [1]
[1]Department of Chemistry, University of South Florida

Isolation of Novel Compounds from the Octocorallia Carijoa (Telesto) riisei

Secondary metabolites help sessile marine organisms adapt to their environment, while deterring and defending against predators. This makes secondary metabolites suitable for development of new drugs to counteract issues of drug-resistant infectious diseases. Carijoa (Telesto) riisei is a soft octocoral that was extracted from Hawaii in 1986 and was found to be a viable source of novel compounds. Three of the isolated punaglandins demonstrated potent anti-tumor and anti-inflammatory biological activities. Punaglandins and pregnane steroids are two of the primary compounds isolated from C. riseii collected from Clearwater, Florida in 2014, and displayed similar known chemistry with additional potential for novel chemodiversity. Nuclear Magnetic Resonance guided medium-pressure and high-performance liquid chromatography, mass spectroscopy, and x-ray crystallography are implemented for purification and structure elucidation purposes. In addition, novelty of the compounds and bioactivity against multiple drug-resistant pathogens will be assessed.

XX-YY **Bryan Benitez** [1], Teng Yuan [1]
[1]Department of Chemistry, University of South Florida

Synthesis of Chiral N2-Substituted Cyclic Triazole Ligand

The formation and use of cyclic azide structres, substituted triazole, has been documented as far back as 1961. A more recent version of this synthesis dubbed Click chemistry has been used countless times to create substituted triazole structures often in either the N1 or N3 substituted forms. This proposed synthesis path aims to push triazole ligand synthesis towards the formation of not only chiral cyclic structures but also N2 substituted triazole structures. The primary applications are hypothesized to include lewis acid catalyzed reactions. This synthesis route will allow for ring size control and is also included in additional synthesis paths allowing for very selective reaction pathways.

XX-YY **Melissa Bikowitz** [1 2], Md Rezaul Karim, Ernst Schonbrunn, PhD
[1]Department of Chemistry, University of South Florida
[2]Department of Drug Discovery, Moffitt Cancer Center

Structural studies of TRIM28 protein by X-ray crystallography

Transcription intermediary factor 1-beta (TRIM28) is a ubiquitously expressed nuclear co-repressor involved in transcriptional regulation, cellular differentiation, proliferation and DNA damage repair. It is a member of the tripartite motif family of proteins and contains a C-terminal PHD-type zinc finger domain along with a bromodomain (BRD). The objective of this project is to determine the high resolution crystal structure of the TRIM28 PHD-BRD module for structure-based drug design purposes and to gain structural insights into the recognition of acetylated histone bookmarks and regulation of target gene expression. The human TRIM28 gene fragment encoding the PHD-BRD module was cloned into

a modified pET28 vector containing both solubility and affinity tags. Induction studies were performed to optimize the overexpression levels of the target protein. A large scale culture followed by FPLC purification yielded > 95 % pure protein suitable for crystallization screening campaigns and biochemical studies.

XX-YY **Luiza Brabo-Catala** [1], Enlin Lo [2], Dr. George Philippidis [1]
[1]Patel College of Global Sustainability, University of South Florida
[2]Department of Biomedical and Chemical Engineering, University of South Florida

Effects of enzymatic hydrolysis using Cellic® CTec2 and CTec3 on pretreated sweet sorghum bagasse

Lignocellulosic biomass is a renewable raw material for the biofuels and bioproducts industries. Even though the cost of most biomass species is low, the enzymatic degradation of cellulose into fermentable sugars by cellulase enzymes is challenging and costly. In this study, we assessed the hydrolytic potential of the cellulases Cellic® Ctec2 and CTec3 (Novozymes) by using filter paper as model substrate in acetic buffer (pH 5.0) and monitoring glucose release. Sweet sorghum bagasse was first pretreated with concentrated phosphoric acid at conditions that were optimized in one of our previous studies. The pretreated material was hydrolyzed utilizing 40 filter paper units of enzyme in acetic buffer (10% solids loading) at 50ºC and shaken at 50 rpm. Samples were taken at 0, 12, 24, 48 and 72 hours of hydrolysis and analyzed to compare the glucose release. The performance of the two commercial enzymes and the cost implications will be discussed.

XX-YY **Andrew Cabage**, Mi Zhou, Jianfeng Cai [1]
[1]Department of Chemistry, University of South Florida

Peptidomimetics of APC Cdc20 and BIM

Peptidomimetics are a widely used technique for numerous applications. Employing this technique in studying protein-peptide interactions has been extensive. In our study, we employed peptidomimetics to study the interactions between the pro-apoptotic protein BIM and APCCdc20; a component of the Anaphase-promoting complex (APC). Cdc20 is a protein that forms complexes with APC, and this complex has most expression during the mitotic phase. Because APCCdc20 is most active during the mitotic phase, the significantly lowered expression of BIM during this phase was linked to the interaction between the complex and the pro-apoptotic protein. Unfortunately, this complex is unstable, so this study employs peptidomimetics in order to find a possible alternative α-helix that is more stable, but also retains the behavior of the original protein. We will use a “staple” to link two turns of the α-helix and study the resulting changes in behavior.

XX-YY **Isel Perez Cabrera** [1], Ethan Zheng [1], Shahedul Islam [1], Dr. Li-June Ming [1]
[1]Department of Chemistry, University of South Florida

Exploration of Pre-Equilibrium Kinetics and Oxidation Chemistry of Cu(II)-Tetracyline

The binding activity of electron-rich functional groups of Tetracycline (TTC) with transition metal ions such as Mg2+, Ni2+, Co2+, and Cu2+ have been heavily studied for the last decade. Currently, the binding activity of cupric ions and TTC are known; however, their potential for enzyme-like behavior is unknown, especially considering its multiple chelation sites (i.e. β-diketone, enol, and carboxamide moiety). By using colorimetric analysis, a Michaelis-Menten plot that illustrates pre-equilibrium conditions of the enzyme-substrate to enzyme-product complexes and the substrate affinity to the enzyme can be used to describe the catalytic character of Cu(II)-TTC in oxidizing 3,5-di-tertbutylcatechol (DTBC) to 3,5-di-tertbutylquinone (DTBQ). The implications of this inquiry include elucidating the influence of Cu(II)-TTC in its binding with other di-oxygen species such as hydrogen peroxide and explore its role in oxidative stress mechanisms.

XX-YY **Emmanuel Cruz** [1]
[1]Department of Chemistry, USF

Novel Cannabinoid Analog Synthesis

A popular cannabinoid, tetrahydrocannabinol Δ9 (THC), is found in cannabis and is known to bind well to cannabinoid receptors and express medicinal properties. THCΔ9 studies have shown β Amyloid disaggregation, anti-inflammatory effects, and modulation of immune system functionality, but the many metabolites of THC invalidate the studies. To mitigate these issues, a seven-membered ring analogue of THC was synthesized. The objective of the seven-membered ring THCΔ9 (7THC) is to reduce the possibility of aromatization and metabolization. From this compound, we hope to further determine pharmacological pathways, increase in-vivo half-life, and tune THC’s therapeutic effects. These differences are hoped to increase therapeutic ability and help to better define the ways that THC interacts with the brain in vivo.

XX-YY **Emma Doukmak** [1], James Leahy [1]
[1]Department of Chemistry, University of South Florida

Novel Synthesis of Inosine Analog EdI for Labeling Malarial DNA

Malaria is a deadly parasite-borne illness which affects over 200 million people worldwide each year, particularly in sub-Saharan Africa and South Asia. The most common parasite associated with malaria, P. falciparum, uses inosine in place of guanosine in its DNA. Therefore, it is possible to test for the presence of malarial DNA in cell cultures using fluorescent markers attached to synthetic inosine analogs such as 7'Deaza-2'-deoxy-7-ethynyl inosine, (EdI). Progress toward the completion of a three-step synthesis of EdI will be discussed.

XX-YY **Evans-Nguyen, Theresa** [1], Vuppala, L. Sinduri [1], Nguyen, Ding [1]
[1]Department of Chemistry, University of South Florida

A Gas Chromatography Experiment for Elementary Analytical Students

Our goal is to design a gas chromatography (GC) experiment that is mimicking a real-world application of GC and is fitting the objective of an Elementary Analytical Chemistry course. Separation techniques include gas chromatography, liquid chromatography, and capillary electrophoresis are the main objectives in the analytical chemistry course. Therefore, the students in this course should have hands-on experience about at least one of those techniques. In the forensic laboratory, GC is extremely useful for the determination of blood alcohol concentration (BAC) because it can provide results with high accuracy and precision. We are constructing an experiment where the students will use GC to determine the concentration of ethanol in a blood sample, specifically, cow's blood. In addition, we are developing a procedure which could help the students to accomplish the goal within the time limit of the laboratory.

XX-YY **Robert Feeney**, Shaina Linsky, Zachary Shultz, James Leahy [1]
[1]Department of Chemistry, University of South Florida

Progress Towards an Enantioselective Total Synthesis of Membranolide

Natural products have provided inspiration for the development of a wide range of pharmaceuticals. The membranoid family of marine natural products, isolated from the Antarctic Sea sponge *Dendrilla membranosa*, has shown promising anti-parasitic and antibacterial properties in Leishmaniasis and methicillin resistant Staphylococcus aureus (MRSA) assays. These compounds share a common structural core and mainly differ by oxidation states at varying carbons. We set out to develop synthetic methodology to access the parent natural products and to generate structural analogs for further biological evaluation. With membranolide as our key template, methods have been developed to construct the common core of the membranoids. The challenging quaternary carbon stereocenter as well as the uniquely substituted phthalide core has become attainable. The racemic synthesis of membranolide and progress towards the enantioselective synthesis will be discussed.

XX-YY **Alexander Filosa** [1], Dr. Xiaopeng Li [1], Heng Wang [1]
[1]Department of Chemistry, University of South Florida

Bottom up formation of a tetrakis terpyridine porphyrin ligand and self assembly of zinc supramolecule

The purpose of this research is to create a 5,10,15,20-tetrakis(3-([2,2':6',2"-terpyridin]-4'-yl)phenyl)-7H,8H-porphyrin starting with isopthalaldehyde. The yield of this porphyrin-terpyridine ligand was significantly improved compared to other similar studies in literature. Once the porphyrin is synthesized and confirmed through Mass Spectrometry and NMR, Zinc(II) is coordinated with the terpyridine to perform self-assembly to create a library of supramolecules, including trimers, tetramers and pentamers. Trimers have the highest prevalence among the mixture of structures which indicates that trimers form the most stable complex. The zinc terpyridine complex will be characterized by Mass Spectrometry, NMR, TEM and SEM.

XX-YY **Claire Freij** [1], Jason Perman [1], Shengqian Ma [1]
[1]Department of Chemistry, University of South Florida

Disrupting the Hydrogen Bonds in a Copper Adenine Complex

It is challenging to maintain a porous structure sustained by hydrogen bonds which extend between the donor and acceptor groups of adenine as similarly observed in DNA. The adenine ligands coordinating with Cu(II) generate a square building block motif. Through hydrogen bonding, the motif generates a tetragonal and porous structure which collapses upon the removal of its mother liquor. The main objective of this project is to disrupt the hydrogen bonds with new hydrogen bonds in order to increase the porosity of the material. Co-crystallization can be used in order to disrupt the hydrogen bonds, which is carried out through a guest-exchange process. Heterosynthon type hydrogen bonding is expected to improve the overall structural integrity of the material and allow for its complete evacuation for surface area studies. Powder X-ray diffraction is used to evaluate the original material as well as its competing hydrogen bonding molecule complex.

XX-YY **Rebeca Gonzalez Jauregui** [1], Cassandra Ly [1], Vanessa R. Ralph [1], Scott E. Lewis [1]
[1]Department of Chemistry, University of South Florida

Identifying reflective learning approaches among general chemistry students

Learning theories and research literature indicates the importance of reflective thought in academic success. This presentation explores the ability of a brief online survey to characterize reflective thought among students in general chemistry. The survey was intended to have students reflect upon their processes on select items from a recently completed exam on stoichiometry and mole concept. Student responses were coded based on their ability to accurately reflect on their own processes and their ability to metacognitively identify how another student may have attempted the same problem. Measures of reflectivity, or lack thereof, may serve to inform instructors and researchers on the thought processes students engage on the targeted assessment items and inform efforts to better assist struggling students.

XX-YY **Yaima Guzman** [1], Edwin Rivera [1], Micheal Williams [1], Arthur Maknenko [1]
[1]USFINMRF, Department of Chemistry

Monitoring Glycolysis by Solution State Nuclear Magnetic Resonance in Selectively Enriched 13C and Natural Abundance 1H and 31P

Nuclear Magnetic Resonance (NMR) spectroscopy enhances the practical understanding of the underlying molecular structure of compounds. This research hopes to improve the understanding of complex biochemical enzymatic reactions, such as glycolysis. Students will have the opportunity to perform 1H, 13C, and 31P experiments to observe the formation of the glycolytic by-product 13C-enriched ethanol and the reduction in glucose and ATP signal intensities. Students will learn how NMR spectroscopy can be used to further understand enzymology, regioselectivity, reaction kinetics, and the biochemical process of glycolysis.

XX-YY **Julie Harmon** , Yesenia Perez, Alejandro Rivera
[1]Department of Chemistry, University of South Florida

Incorporation of Hydrogen Bonding Properties into Aliphatic Polyimides by Urea Linkages

Assembled by imide moieties, polyimides are resistant to extreme thermal environments, versatile, and light weighted, which make them utilizable in aerospace and biomechanical devices. A series of aliphatic polyimides were remodeled with isocyanate at different quantifications to increment the hydrogen bonding within these polymeric compounds. A polyurea prepolymer with amine ends was synthesized and then linked with dianhydrides to create a Polyimide-Polyurea copolymer. The isocyanate was incorporated in the middle of the polymer backbone to improve the intramolecular bonding effect between the chains. The polyimides were characterized for structural identification to confirm the presence of intramolecular bonding and were tested through tensile testing, TGA, rheology, and dynamic mechanical analysis to determine the thermal and mechanical properties affected by hydrogen bonding.

XX-YY **Aaron T. Hendricksen** [1], Nicole E. Avalon [1], Bill J. Baker [1 2]
[1]Department of Chemistry, University of South Florida
[2]Center for Drug Discovery and Innovation (CDDI), University of South Florida

Biosynthetic Potential of Pseudovibrio sp.

Bacterial natural products afford an invaluable source of bioactive compounds of high interest for development as novel pharmaceutical agents. These small molecules are biosynthetically produced through modular polyketide synthases (PKS) and non-ribosomal peptide synthetases (NRPS). These are multifunctional megaenzymes that serve as templates to program natural product assembly in a primarily linear manner. The polyketide palmerolide A, which has potent anticancer activity was isolated from the Antarctic tunicate Synoicum adareanum. Structural features of palmerolide A are suggestive of a bacterial origin. A Psuedovibrio sp. bacterial symbiont of S. adareanum was investigated through a bottom-up proteomic analysis, comparing in silico PKS/NRPS pathways with experimental tandem mass-spectrometry data. Retro-biosynthetic predictive resources including antiSMASH and PRISM were used to annotate gene products found within Pseudovibrio sp. Herein, the techniques and analysis of these predictive resources are described, as well as the efficacy of their application for further biosynthetic potential of similar natural products.

XX-YY **John Hurst**, Dr. Dean F. Martin
[1]Department of Chemistry, University of South Florida

NSAID Removal from Aqueous Solutions by Metallolig Chelated Complexes

Acetaminophen is one of the most commonly produced NSAIDs (Non-Steroidal Anti-Inflammatory Drug) in the United States. Today it is the most commonly used over-the-counter medication with a production volume of about 75-000-80,000 metric tons per year. With such wide spread production and usage of acetaminophen the concentration in the environment increases significantly. Octolig is a type of polyethyledediimine attached to silica gel. It has the ability to remove anions. Many NSAIDs like acetaminophen bond with other organic and biological compounds

in the environment; however the pKa is too high for an efficient extraction, thus transition metal derivatives chelated to Octolig were used, specifically cobalt and zinc. These transition metal complexes are known as metalloligs, were tested for a more efficient method of acetaminophen removal.

XX-YY **Dr. James Leahy** [1], Mikaela Griffith [1], Roy Blackburn [1]
[1]University of South Florida

Synthesis of Hsp70 Inhibitor for Treatment of Alzheimer's Disease

In general, Alzheimer's disease can be described as a neurodegenerative disease which results in the afflicted suffering from various forms of cognitive impairment. It is ultimately fatal as patients begin to experience difficulties even talking, walking and eating with the accompanying loss of brain cells and subsequent body functions. While there is still much debate surrounding the exact cause of Alzheimer's disease, its occurrence has been linked to the aggregation of aberrant tau protein in the brain as a result of activity of the molecular chaperone heat shock protein 70 (Hsp70). This project will be focused on the synthesis of an analogue of the Hsp70 inhibitor JG-98 – the original of which was shown to decrease the levels of aberrant tau. As such, should this project be successfully completed, the synthesized analogue may play a role in the future of treatment of Alzheimer's disease.

XX-YY **Eun Lee** [1], Ashleigh Bachmann [1], Arthur Maknenko [1], Edwin Rivera [1], Cole Cerrato [1]
[1]USFINMRF, Department of Chemistry, University of South Florida

Molecular Dynamics measured by the coalescence of the 1H NMR signals of Dimethylacetamide (DMAc) as a function of temperature: Proposed Lab Exercise

1D 1H measurements by NMR spectroscopy are essential in undergraduate chemistry education. While students learn how to interpret spectra and gain basic practical experience in lower-level courses, they typically do not have the opportunity to gain insight into the more specialized applications of NMR spectroscopy. As a foundation of the physical chemistry course, students are taught about Gibbs' Free Energy and molecular dynamics. This laboratory exercise facilitates learning these advanced thermodynamic concepts. Students will observe the effect of temperature on Gibbs' free energy and the intramolecular dynamics. By studying the effect of temperature (20-65°C ± 1 °C) on the 1H NMR spectrum of methyl groups of dimethylacetamide (DMAc) and by proposing simulations (DNMR3 or Mexico software), students will be able to correlate the NMR measurements with the physical properties of molecules and gain further comprehension into topics taught in CHM 4410.

XX-YY **Shengqian Ma** [1], Jason Perman [1], Alejandro Gonzalez [1]
[1]Department of Chemistry, University of South Florida

Development of Paddle Wheel Motif for More Resilient Structures

The "paddle wheel" motif is renowned when discussing metal organic frameworks due to its profound structural attributes, in creating unparalleled porous materials. Historically, carboxylate-based ligands are utilized as primary functional groups coordinating with distinct metal centers to achieve structural control and integrity. To differentiate the physical and chemical properties, purine ligand analogs are synthesized to alter the typical paddle wheel materials. These new metal organic frameworks could prove to be of physiological importance, due to similarities of natural molecules within the biological system. Materials were analyzed via single-crystal XRD, H1 NMR, and GC-MS, upon synthesizing 9-(tetrahydro-2H-pyran-2-yl)-adenine as the precursor to develop the tri-purine ligand.

XX-YY **Min-Lee MacDonald** [1]
[1]Department of Chemistry, University of South Florida

Synthesis of Silver Nanoparticles (AgNPs) for General Chemistry Laboratory

A laboratory protocol for the synthesis of silver nanoparticles using various reducing agents has been developed for use in a general chemistry laboratory. The effects of varying the amount of reducing agent, silver nitrate, and sodium citrate on the size of the nanoparticles were tested using a UV-Vis spectrophotometer. Further considerations as to the cost of the materials used, waste-management, and safety of available chemicals, were examined and adjusted to be suitable for a general chemistry laboratory. The purpose of this project was to create a feasible method for introducing lower-level undergraduate chemistry students to nanoparticle synthesis and size control, in response to growing interest in the field of nanotechnology.

XX-YY **Angelica McCaskey** [1], Brian O'Flynn [2], James Leahy [1], David Merkler [2]
[1]Department of Chemistry, University of South Florida
[2]Department of Biochemistry, University of South Florida

Coenzyme A Assays and Arylalkylamine N-acetyltransferases (AANATs)

Coenzyme A acts as a carrier for neurotransmitters throughout the body. Studying it can lead to discoveries about signal transmission and control. To that end, varying forms of coenzyme A were created such as a desulfurized coenzyme A and coenzyme A attached to an acetyl and a neurotransmitter, in this case tryptamine. The forms were created to subtly change the response that the neurotransmitter normally solicits while simultaneously observing how coenzyme A delivers the neurotransmitter if it is covalently bound to a covalent linker. Specifically, the varying forms were produced to measure how AANATs are inhibited. A pheromone was also produced to attract weevils to observe certain fatty acid amides and their specific trafficking with enzymes.

XX-YY **Truc Nguyen** [1], Jhon Figueroa [1]
[1]Department of Chemistry, University of South Florida

Introduction of Electrochemistry to General Chemistry Laboratory

Electrochemical cells are constructed based on the differences in reduction potentials between different electrodes for the conversion between chemical and electrical energies. This project aims to improve the student's understanding in electrochemistry through the introduction of this concept to General Chemistry II laboratory. Through constructing multiple galvanic cells, the students investigate different metal-pairs and concentrations to find the combination which produces the highest electrical potential. In addition, the students can measure the reduction potentials of each metal half-cell when it is paired with an inert electrode. Instead of beakers or test tubes, the project utilizes well plates to reduce the required volumes of electrolytes, which subsequently reduces the production of waste. Therefore, the experiment is more cost-effective and safe while still generates reproducible results. After the experiment, the student should be able to describe common electrochemical concepts such as anode, cathode, electrode, salt bridge, and path of current.

XX-YY **Owen O'Grady** [1], Xiaopeng Li [1], Heng Wang [1], Bo Song [1]
[1]Department of Chemistry, University of South Florida

Introduction of Cobalt and Ruthenium Based Catalysts Into Novel Supramolecular Structure

Cobaloximes are a series of compounds that have the general formula CoR(dmgH) 2 L, where dmgH is dimethylglyoxime and R and L are ligands occupying the axial positions. Members in this class of molecules have been shown to successfully catalyze hydrogen evolution. Another coordination compound that has been used to successfully catalyze water oxidation are Ru(bda) complexes where bda is 2,2'- bipyridine-6,6'-dicarboxylic acid. The goal of our research is to incorporate these metal complexes into novel supramolecular structures. Supramolecular structures are compounds comprised of molecular subunits that interact non-covalently. The ligand synthesized for the formation of the designed supramolecule contains a terpyridine-based motif (which has been exploited for many supramolecular structures) and a solitary pyridine for the site of catalyst binding. We aim to self-assemble a stable supramolecular structure connected with the target coordination compounds, and test the catalytic ability of these novel materials.

XX-YY **Nolan R. Otto** [1], Matthew W. Scales [1], Ralph N. Salvatore, Ph.D. [1]
[1]Department of Natural Sciences, Southeastern University

Efficient Synthesis of Cyclopropylacetylene, a Crucial Synthetic Intermediate for Efavirenz (Sustiva™), an HIV-1 Reverse Transcriptase Inhibitor

Cyclopropylacetylene (CA) has become an attractive synthetic target due to increasing demand as a building block for Efavirenz (Sustiva™), which is a potent inhibitor of the human immunodeficiency virus type-1 (HIV-1) nonnucleoside reverse transcriptase. Although a variety of syntheses have been reported, CA is the most expensive raw material, uses combinations of toxic, difficult to handle reagents, results in incomplete conversions and low yields/purity that render the overall preparations inefficient. Thus, it is desirable to discover new routes to produce CA on a large scale that improve upon these limitations. In our laboratories, efficient syntheses of cyclopropylacetylene were achieved from either cyclopropyl methyl ketone or via an intramolecular ring closure of 5-chloro-1-pentyne in the presence of a strong base (cesium hydroxide). Different reaction pathways were investigated to avoid the concomitant formation of side products. In addition, to explore the versatility of these conditions, various heterocyclic analogs were also prepared.

XX-YY **Cody Phoenix, Briana Aguila** [1]
[1]Department of Chemistry, University of South Florida

Use of an extended amidoxime ligand in porous aromatic frameworks to capture and remove Uranium in contaminated water.

Due to our modern existence and the use of nuclear power, uranium has been introduced to the bodies of water found all over the world. Thanks to other dedicated researchers, we have found that the effective way of extracting uranium from sea water is to combine of PAF-1 and amidoxime. PAF-1 is known to be stable under harsh conditions, be reusable and has a very large surface area; combining this with the most effective uranium extracting ligand makes for a strong combination. We plan to build on this idea and elongate the amidoxime ligands in hopes

that it may be that much more effective and efficient. In order to elongate the ligands, we plan to attach an ethylamine group to the PAF-1 and the amidoxime onto its end. The elongation of this ligand will increase its surface area and allow the framework to be more flexible and efficient.

XX-YY **Iva Radeva**, Linette Harding [1]
[1]Department of Chemistry, University of South Florida

Proteasomal Inhibition Study of a Copper Complexing Ligand Using Synthesized 2-{[(Carbamoylsulfanyl)acetyl]amino}benzoic Acid

Cancer cells and tissues are known to accumulate larger concentrations of copper compared to that of normal cells. Elevated copper ion levels, as well as copper-ligand complexes, have been shown to inhibit proteasome activity, subsequently leading to apoptotic cell death. Our lab previously identified a potential copper-chelating proteasome inhibitor, 2-{[(Carbamoylsulfanyl)acetyl]amino}benzoic acid, via virtual screening of an NCI Diversity Set and enzyme inhibition assays. The benzoic acid derivative was synthesized and tested for effectiveness of proteasome inhibition.

XX-YY **Dane Randol** [1], Dr. Jin Wang [1], Dr. Xiaoping (Michael) Shi [1]
[1]Department of chemistry , University of South Florida

Reactions of vinyl thiophenes: Gold-based catalysis, exploration of intermolecular and intramolecular syntheses

ABSTRACT: Gold-based catalysts are extremely useful reagents in modern synthetic chemistry. As recent studies have proven, these catalysts boast substantial gains in efficiency over other catalysts, specifically in syntheses involving alkynes reacted with certain electron-rich species. Using a gold catalyst, a vinylic thiophene substrate was synthesized in high yields which was then used as a building block for molecules with additional functionality. The scope of this material was explored and new derivatives were created using synthetic techniques which afford selective intramolecular rearrangements and additions of other functional groups or atoms. Other reactions were investigated which aimed to add functionality to the substrate, while leaving the vinyl thiophene intact. After successful reactions, the possible industrial applications of the products were explored.

XX-YY **Selena Rashid** [1]
[1]Department of Chemistry, University of South Florida

The Usage of Metal Organic Frameworks as a Method of Drug Delivery Using Caffeine and Melatonin

Metal organic frameworks are synthetic organic molecules that can act as drug carrier systems to hold and deliver drug . Metal organic frameworks may offer the possibility of in vivo treatments and can hold a high amount of the drug, and deliver this drug over extended periods of time and offer a more controlled release of drug. The particular metal organic framework that will be utilized within this experiment is NH2-Mil-101-Fe, which will be synthesized using centrifugation and separation techniques. The pore size of this synthesized MOF will be tested prior to the loading of any drug. The metal organic framework will then be loaded with caffeine within one trial, and melatonin within the other, and the subsequent loading efficiency of each of these drugs within the metal organic framework will be tested after each drug has fully attached to the synthesized MOF.

XX-YY **Wishrawana Ratnayake** [1], Christopher Apostolatos [1], Sloan Breedy [1], Mildred Acevedo-Duncan [1]
[1]Department of Chemistry, University of South Florida

Atypical protein kinase C iota and zeta are crucial oncogenes for prostate cancer cell migration and invasion

Prostate cancer is the most common cancer among men and reported 161,360 new cases and 26,730 deaths in 2017. We believe that aPKCs (PKC-ι and PKC-ζ) play an important role in malignancy of prostate carcinoma (PC) by inducing epithelial-mesenchymal transition. Both PKC-ι and PKC-ζ are over expressed in PC cells. In the current study, we have investigated the effects of siRNA knockdown of aPKCs on PC cell migration and invasion compared to normal cells. PC cell migration and invasion were significantly reduced while altering the levels of E-cadherin, NF-κB p65, Vimentin, β-catenin and CD44. Immunofluorescence microscopy, electron microscopic techniques, and flow cytometry were used in the study. We also found that PKC-iota and PKC-zeta knockdown induced apoptosis in PC cells. Overall, results show that aPKCs are essential for prostate carcinoma progression and metastasis, and they could be used as effective therapeutic targets.

XX-YY **Alysha Reichel** [1], Haohan Zhao [2], Chuanhai Cao [2]
[1]Department of Chemistry, University of South Florida
[2]Department of Pharmaceutical Sciences, University of South Florida

Poly(ethylene glycol) Methyl Ether-block-Poly(lactide-co-glycolide) Polymer as Delivery System for Melatonin

Drug therapies have been around for centuries to help cure a multitude of ailments. Of these drug therapies, drug delivery systems have been a more modern approach to help cure illnesses. A PEG-PLGA compound will be used to form a micellular drug delivery system around a hydrophobic molecule, which is Melatonin in this case. The micelle formation will first be proven by using Sudan Black B, a hydrophobic dye, in place of the drug to attempt to encapsulate. The size of the micelles will then be determined by dynamic light scattering, where the desired range of diameters for the micelle are from 20-100nm. Toxicity of the drug delivery system will be tested against the "bare" molecule, as well as tested by LC-MS to determine the amount of drug the molecules contains per micelle. Animal models will be used at the last stage of testing.

XX-YY **Jessica Rose**
[1]Department of Chemistry, University of South Florida

UTSA-100 for Removal of Acetylene in Acetylene/Ethylene Mixtures

Ethylene is one of the most widely used raw chemicals, mainly in the production of polymers and other chemicals. During ethylene production, a process called cracking occurs with ethane, propane and other hydrocarbons. This produces trace amounts of acetylene within the ethylene, which, even at a small impurity percentage, can cause many negative side effects. Acetylene causes harm to the end products of ethylene, for example, acetylene acts as a catalyst during ethylene polymerization, which reduces the quality of the resulting polyethylene. The microporous MOF, UTSA-100, shows to have excellent potential in acetylene uptake within acetylene/ethylene mixtures. UTSA-100 takes on a three-dimensional shape and open zigzag nanochannels. The unit cell consists of 6-connected binuclear Cu2(COO)4 units attached via 3-connected ATBDC2- anions. This formation results in a (3,6)-connected apo-type network. A computational analysis was done to determine the sorption of acetylene in UTSA-100.

XX-YY **Quintan T. Rossow** [1], Reed W. Roberts [1], Aaron J. Todman [1], Mark E. Steury [1], Nathaniel J. Jordan [1], Lucas Kline [1]
[1]Department of Natural Sciences, Southeastern University

Applications of the Cesium Effect: Synthesis of de Novo Peptidomimetics as Potential Anticancer Agents

Numerous physiological and pathological stimuli induced programmed cell death (apoptosis), and the Bcl-2 family of oncoproteins plays a central role in this regulation. Proteins such as Bcl-2 are known to inhibit apoptosis, and uncontrolled cell survival due to Bcl-2 overexpression has been proven to make a significant contribution to tumor formation. With this in mind, we have directed our attention toward the synthesis of a variety of non-peptide inhibitors of oncoprotein Bcl-2. Recently, we have disclosed efficient protocols leading to the synthesis of carbazate and dithiocarbazate peptidiomimetics, respectively. This study is now being extended to the synthesis of other de novo analogs with similar structural features to natural proteins, that may interrupt protein-protein interactions. Utilizing our aforementioned protocols, various scaffoldings are being employed for the development of novel artificial biomolecules, which may have interesting biological behaviors in the disruption of protein-protein interaction and hold potential applications in clinical chemotherapy.

XX-YY **Nicholas Schofield** [1], Jacob R. Hobby [1], Josue F. Deslauriers [1], Tori Scheffler [1], Ralph N. Salvatore, Ph.D. [1]
[1]Department of Natural Sciences, Southeastern University

Organobarium Chemistry: Synthesis of 3,4-dihydroxyphenylacetaldehyde (DOPAL): a Potential Target for Neuroprotective Therapy in Parkinson's Disease

3,4-dihydroxyphenylacetaldehyde (DOPAL), an important biogenic aldehyde, serves as a critical endogenous toxin which triggers dopamine (DA) neuron loss in Parkinson's disease (PD). Despite the immense biochemical significance of DOPAL, attempts to synthesize this compound in pure form have been met with grave difficulty. In fact, most methods lack detailed experimental procedures, full characterization, and suffer from extremely low product yield (~4%). Therefore, considerable effort to produce DOPAL in a higher yield would be clearly warranted. In an effort to mitigate these problems, we have directed our attention toward a more efficient synthesis of DOPAL using organobarium reagents. These novel reagents, standardized against various carbon-carbon bond forming reactions fundamental to organic synthesis, were then applied toward the total synthesis of DOPAL. These studies may provide important insight on future drug action to combat PD and, when the scope of this research is expanded, may aid in the treatment of other disorders.

XX-YY **Dr. Lindsey Shaw, Dr. James Leahy, Leugim Quintana**
[1]Department of Chemistry, University of South Florida

The Fight Against Bacteria

The growing concerns over antibiotic-resistant bacteria have led to research into the development of novel molecules with the potential of fighting bacteria via a new mechanism. After a library of molecules was screened, this compound was selected for its potent biological activity against bacteria. Theoretical steps were taken so this novel molecule could be synthesized to uncover its underlying mechanism of action.

XX-YY **Dr. Xiaodong Michael Shi** [1], Shuyao Zhang [1], Shasline Gedeon [1]
[1]Department of Chemistry, University of South Florida

Synthesis of Triazole-Ru(II) complexes and Investigation of Potential Reaction Properties

Prevalent in the field of synthetic organic chemistry are Grubbs catalysts which are successions of metal carbene complexes. Named after Robert H. Grubbs, Grubbs catalyst is used for olefin metathesis which is the rearrangement of substituents and formation of new carbon-carbon double bonds formed by a four-ring opening intermediate starting from two olefin substrates. Ruthenium-based complexes can proficiently catalyze ring closing metathesis (RCM) of dienes having terminal olefins. Exploration of metathesis activity of vinylcarbene ruthenium complexes continues. This project is a continuing report where triazole ligands are used mainly because of their properties of being a good sigma-donor and a good pi-receptor. These are good properties because they allow for increased stability of the Ru(II) catalysts. To move forward, focus is being placed into the synthesis of multiple triazole-Ru(II) complexes that'll be analyzed for stability and any significant properties that can be used for other lines of research.

XX-YY **Christian Stanley** [1], Anne-Claire Limon [1], Bill Baker [1]
[1]Chemistry Department, University of South Florida

Chemical investigation of bioactive metabolites from the Octocoral Carijoa (Telesto) riisei for use in drug discovery

Marine invertebrates develop chemical mechanisms within their metabolism to compensate for their sessile nature and help them avoid predation. In 1967, the chemical investigation of a Hawaiian Telestacean octocoral, Carijoa (Telesto) riisei, yielded the punaglandins: novel and highly functional prostaglandins exhibiting anti-inflammatory/ antitumor activity. Similar analyses of a Floridian C. riisei also led to isolation of three punaglandins exhibiting bioactivity comparable to their Hawaiian counterpart. These findings inspired the current conjecture that interesting chemistry may present itself within the uninvestigated aqueous fractions of the Floridian C. riisei. Methods of extraction, separation, and purification were subsequently developed to investigate these fractions with primary focus given to isolating interesting and potentially novel compounds. Following multiple rounds of liquid-liquid partitions, Nuclear Magnetic Resonance-guided purification was implemented via medium pressure and high performance liquid chromatography techniques. Future isolates will be assayed to evaluate their activity against resistant pathogens and their potential use in pharmaceuticals.

XX-YY **Brooke Stark** [1], Dr. Xiaopeng Li [1], Lei Wang [1]
[1]Department of Chemsitry, University of South Florida

Aggregate-induced emission of a tetraphenylethene-based macrocyclic molecule with bridged triple bonds

Aggregate-induced emission is a recently developed field of chemistry involving molecules that are non-luminescent in solution, but can emit light to great extents upon the formation of aggregates within high concentrations. The phenomenon is characteristic of propeller-shaped molecules, such as tetraphenylethene (TPE), and is possible due to the restriction of their intramolecular rotations. A derivative of TPE was utilized in the experiment as the core molecule with the attachment of four terpyridine structures, in which each has a acetylene with Triisopropylsilyl ether (TIPS) group. Upon the completion of this step, the TIPS will be deprotected in order for the triple bonds to become locked and form a bridge between a neighboring terpyridine. The fluorescent and AIE capabilities of this macrocyclic molecule is to be further tested.

XX-YY **Brittany Urban** [1], Jhon Figueroa, Ph.D. [1]
[1]Department of Chemistry, University of South Florida

Improving Safety Culture at the University of South Florida

A recent American Chemical Society report regards safety as "a positive value- it prevents injuries, improves productivity and outcomes, and saves lives." The most significant aspect of safety is each individual's perception of safety. Safety culture is a term that is most commonly associated with safety. Safety culture is defined as something that encompasses an organization's shared values, assumptions, and beliefs that are specific to workplace safety. Safety culture starts with each individual. This project focuses on faculty, staff, and students in academia. The goal of this project is to determine the level of safety culture at the Department of Chemistry at USF and develop a plan to improve it. This will be done through a safety survey administered to students in undergraduate chemistry labs, safety inspections conducted in undergraduate chemistry labs, interviews with various professors regarding safety and Chemistry lab incident reports from EH&S.

XX-YY **Gustavo Velasquez** [1], Vanessa R. Ralph [1], Scott E. Lewis [1]
[1]Department of Chemistry, University of South Florida

Lessening Disparities In Student Performance Related to Assessment Design

Research literature has shown that Math SAT is related to academic performance in General Chemistry, with students with lower Math SAT

scores more likely to struggle in the course. Mole concept and stoichiometry were identified as the two topics on which these disparities in academic performance were most pronounced. Differential student performance on individual assessment items of these topics result in higher effect sizes as measured by Cohen's d. Items with high effect sizes suggest at-risk students struggle significantly more on a particular item than their not at-risk peers. This study seeks to identify characteristics of assessment items in these topics that evidently exacerbate or ameliorate the differences between these two groups. The data suggests large influences on the context and presentation of information provided within each assessment item. Practical suggestions for writing assessment items that serve to improve student performance overall and lessen effect sizes amongst students.

XX-YY **Dylan Wallis** [1], Brian O'Flynn [1], David Merkler [1]
[1]Department of Chemistry, University of South Florida

An Investigation of Mechanistically Important Amino Acids in Tribolium Castaneum Arylalkylamine N-acetyltransferase 0 Using Site-Directed Mutations

Arylalkylamine N-acetyltransferases (AANATs) catalyze the synthesis of N-acylarylalkylamides using an acyl-CoA and an arylalkylamine. In humans, serotonin-NAT performs the rate-limiting step in melatonin synthesis. AANATs are also important in the deactivation of neurotransmitters in many organisms and the sclerotization of the cuticle in insects. An understanding of these proteins could lead to novel pesticides as well as targeted therapeutics in humans. One variant of these proteins was discovered in Tribolium castaneum, the number one stored grain pest in the world, and designated TcAANAT0. TcAANAT0 has been cloned and expressed using Escherichia coli and characterized using kinetic experiments. Several amino acid residues that are suggested to be important were then identified and investigated using alanine scanning. Several of these residues were found to be catalytically important to the enzyme insofar as the site-directed mutagenesis had a noticeable effect on the activity.

XX-YY **Jill Wegner**, Dr. Jhon Figueroa
[1]Department of Chemistry, University of South Florida

General Chemistry Laboratory Development: Organic Compounds vs. Energy as it Pertains to Fuel and Renewable Resources

Various organic compounds like alcohols (methanol, ethanol, propanol, butanol, and pentanol) can be used as energy for fuel and renewable resources. An example of this is when filling up gasoline for automobiles, only ten-percent of ethanol is used in the blended petroleum mixture. The goal is to find the lowest energy in the form of standard enthalpy of combustion by determining the number of carbon atoms in these alcohols, in volumes of twenty-milliliters versus thirty-milliliters (for consistency); the alcohols are to be heated up inside a spirit lamb burner, where the mass of the alcohol is burnt or released as a gas, using the burner to heat up one-hundred-grams of water inside the calorimeter, and to determine temperature rising approximately thirty-three degrees Celsius via by a digital thermometer.

XX-YY **Christian Yang**, Grant Lawrence, Dr. James Leahy, Dr. Dennis Kyle
[1]University of South Florida

Metabolic Labeling of Malaria Virus DNA via Inosine Analog

Malaria is a mosquito-borne disease that is caused by protozoan parasites of the Plasmodium genus. Symptoms include chills, fevers, headaches, nausea, and weakness. Malaria is also very prevalent in countries that are less developed. There are numerous drugs in development targeting the various malaria life stages due to the possible increase of drug-resistant malaria parasites. To ensure the efficacy, potential drug applications, and the dynamics of the malaria life cycle, the method of metabolic labeling will be performed utilizing a synthesized purine derivative, inosine analog. The analog contains a crucial substituent group allowing it to perform click chemistry reactions. The possibilities with these reactions are countless, ranging from fluorometric to specific metabolic labeling assays. The successful synthesis of this compound would effectively impact the drug development and other treatments towards the malaria virus.

XX-YY **Richard Zeitler**, Chiyu Wei [1], Mike Shi [1]
[1]Department of Chemistry, University of South Florida

Novel Chiral Ligands: Combining Organic Catalysis and Transition Metal Catalysis

The focus of my research project was the development of a novel, chiral ligand that integrates both organocatalysts and transition metal catalysts to achieve desirable stereoselectivity, reactivity, and versatility. Traditionally, organic catalysis is highly efficient for stereochemistry; however, due to the limited reactivity, organocatalysts usually suffer from low efficiency and from the need for high catalyst loading. Transition metal catalysts, on the other hand, give excellent versatile reactivity for many challenging chemical transformations; however, achieving good stereo selectivity can be challenging due to the difficulty associated with the transition state arrangement. In this study, a new combination of organocatalyst reaction sites and transition metal cation binding sites was designed. It is our expectation that this newly integrated catalyst will

promote challenging transformations better than the sum of its parts. The performance of the catalyst has been evaluated with the elucidation of the important factors that controlled.

About the Cover