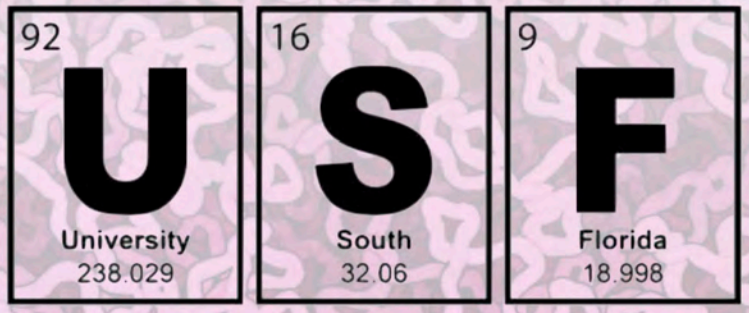
19th Raymond N. Castle
Student Research Conference



CHEMISTRY

– April 10, 2021 –

19th Raymond N. Castle Student Research Conference

Saturday, April 10th, 2021

Department of Chemistry, University of South Florida

In Loving Memory of Barbara B. Martin and Professor Julie Harmon

Barbara B. Martin (1934 — 2021)

Professor Julie Harmon (1949 — 2021)

Table of Contents

Agenda

Check-in and Chair's Welcome *(https://tinyurl.com/rff5pmc)*	09:45am - 10:00am
Section A (Undergraduate) *(https://tinyurl.com/msuuberz)*	10:00am - 01:00pm
Section B (Analytical and Physical) *(https://tinyurl.com/pjrrrcbt)*	10:00am - 01:00pm
Judge Meeting *(https://tinyurl.com/5x63k2sa)*	01:00pm - 01:15pm
Award Announcement (Sections A & B) *(https://tinyurl.com/vzc2t73w)*	01:15pm - 01:25pm
Section C (Biochemistry) *(https://tinyurl.com/3efyxdpe)*	01:30pm - 04:30pm
Section D (Organic) *(https://tinyurl.com/77amd7pc)*	01:30pm - 04:30pm
Judge Meeting *(https://tinyurl.com/n5k54abf)*	04:30pm - 04:45pm
Award Announcement (Sections C & D) *(https://tinyurl.com/byzbpkss)*	04:45pm - 05:00pm

Remembering Raymond N. Castle

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.

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 attending 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 coordination chemistry in natural water systems, including problems of red tide and aquatic weeds. Currently, they are investigating the removal of metals and organic compounds from water by means of supported chelating agents. 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.

Section Breakdowns

Section A (Undergraduate) (https://tinyurl.com/msuuberz)

Intermission	*10:00am - 10:20am*
Sims, Makayla	*10:20am - 10:40am*
Larese, Austin L.	*10:40am - 11:00am*
Beck, Zully	*11:00am - 11:20am*
Intermission	*11:20am - 11:40am*
Wolfe, Brielle	*11:40am - 12:00pm*
Sierra, Connor	*12:00pm - 12:20pm*
Niess, Isaiah	*12:20pm - 12:40pm*
Intermission	*12:40pm - 01:00pm*

Section B (Analytical and Physical) (https://tinyurl.com/pjrrrcbt)

Ahmed, Mohammed Muzammil	*10:00am - 10:20am*
Warrensford, Luke	*10:20am - 10:40am*
Nunziata, Jamie	*10:40am - 11:00am*
Young, Jessica	*11:00am - 11:20am*
Intermission	*11:20am - 11:40am*
Laud, Melyse	*11:40am - 12:00pm*
Tudor, Brant	*12:00pm - 12:20pm*
Swanson, Dina	*12:20pm - 12:40pm*
Orndorff, Paul	*12:40pm - 01:00pm*

Section C (Biochemistry) (https://tinyurl.com/3efyxdpe)

Ni, Ruidong	*01:30pm - 01:50pm*
Islam, Shahedul	*01:50pm - 02:10pm*
Xue, Songyif	*02:10pm - 02:30pm*
Noor, Radwan Ebna	*02:30pm - 02:50pm*
Intermission	*02:50pm - 03:10pm*
Wang, Minghui	*03:10pm - 03:30pm*
Bhandari, Suzeeta	*03:30pm - 03:50pm*
Khalid, Khandker Mohammad	*03:50pm - 04:10pm*
Gao, Ruixuan	*04:10pm - 04:30pm*

Section D (Organic) (https://tinyurl.com/77amd7pc)

Dietrick, Sarah	*01:30pm - 01:50pm*
Zhang, Zhanpeng	*01:50pm - 02:10pm*
Matar, Angelie	*02:10pm - 02:30pm*
Sakib, Mohammad Nazmus	*02:30pm - 02:50pm*
Intermission	*02:50pm - 03:10pm*
Astalos, Aaron	*03:10pm - 03:30pm*
Tang, Qi	*03:30pm - 03:50pm*
Herrera, Kristin	*03:50pm - 04:10pm*
Williams, Michael	*04:10pm - 04:30pm*

Abstracts (Section A - Undergraduate)

Dr. Karl Landsteiner made many contributions to pathological anatomy, histology and immunology

Dr. Karl Landsteiner made many contributions to pathological anatomy, histology and immunology. He is best remembered and honored for his discovery in 1901 and studies of blood groups, for which he received the Nobel Prize in 1930.

Presented by: Makayla Sims *(Undergraduate, Analytical Chemistry)*

Ligand Photodissociation of Heteroleptic Ruthenium (II) bis-(2,2'-bipyridine)(X)2 Complexes Encapsulated in the Zn(II)-based Metal Organic Framework, USF-2

Metal-organic frameworks (MOFs) are a class of porous materials composed of inorganic molecular building blocks (MBBs) and organic linkers. Drug delivery applications of MOFs are of interest as these materials can have a high loading of biologically active molecules in the large cavities of the porous material. Presented here is the encapsulation of four heteroleptic ruthenium(II) bis(2,2'-bipyridine)2(X)2 complexes (X = acetonitrile (ACN), 6,6'-dimethyl-2,2'-bipyridine (DMBpy), pyridine (Py), and 4-aminopyridine (4-aminopy) within the zinc(II)/benzene tricarboxylic acid MOF, USF-2 as a proof of concept for the encapsulation of photoactive guest molecules and photorelease of the attached ligand(s) (X). The photorelease of the attached ligands inside USF-2 was determined optically using steady-state absorption methods. The results indicate photorelease of both RuBpy(ACN)2 and RuBpy(Py)2 while no release is observed for DMBpy and 4-aminopy ligands.

Presented by: Austin L. Larese *(Undergraduate, Inorganic Chemistry)*

Efficient Synthesis of Cyclopropylacetylene, a Crucial Synthetic Intermediate for Efavirenz Using Chlorinating Reagents (PCl5 and Ph3PCl2)

Cyclopropylacetylene (CA) is a key intermediate in the synthesis for the HIV reverse transcriptase inhibitor Efavirenz, an antiviral drug used to treat HIV. CA is an expensive raw material, difficult to obtain, employed in the preparation of medicaments to combat AIDS. The efficient process for the preparation of CA is described, in which cyclopropyl methyl ketone is chlorinated with PCl5 and the 1,1-dichloro-1-cyclopropylethane isolated, and then dehydrochlorinated with potassium tert-butoxide in toluene to form CA. However, the chlorination protocol was found to take place with appreciable cyclopropyl ring opening. For this the employment of dichlorotriphenylphosphorane-Ph3PCl2-as a mild chlorinating agent is predicted to give a mixture of 1-chloro-1-cyclopropylethene and I,I-dichloro-1-cycloproplehtane. Treatment with a strong base is expected to produce CA at higher yields with significant reduction of ring opening. Additional synthetic routes will also be presented.

Presented by: Zully Beck *(Undergraduate, Organic Chemistry)*

Spectroscopic Analysis of Heme Proteins Mineralized in a Zeolitic Imidazole Framework

The possible structural and functional changes to heme proteins upon encapsulation within a Metal-Organic Framework (MOF) directly impact their ability to be considered for future biological products/materials. Through the encapsulation of Cytochrome C (Cc), Microperoxidase (MP-11), and N-acetyl Microperoxidase (N-Acetyl MP-11) by mineralization within a Zeolitic Imidazole Framework (ZIF-8), the conformational changes of heme proteins due to MOF encapsulation can be examined. Ultraviolet-Visible spectroscopy is used to ensure the protein has been encapsulated while transient absorption is used to probe at the conformational changes and functionality of the heme protein in ZIF-8. One of the main functions of Cc, MP-11, and N-acetyl MP-11 that will be examined extensively is the binding and releasing of small ligands, specifically, nitric oxide and carbon monoxide.

Presented by: Brielle Wolfe *(Undergraduate, Inorganic Chemistry)*

Application of in-Silico High Throughput Screening to Identify Coral Natural Products with Highest Binding Potential to Human Cancer Protein Targets

Marine invertebrates are an underexplored yet promising source of new natural products, many of which have demonstrated pharmaceutical potential. The abundance of compounds that researchers must study can be made less overwhelming by using virtual screening programs, for example, Schrodinger's Glide. We utilized this program to examine the structural compatibility and predict the binding potential of coral natural product ligands and target proteins commonly associated with various human cancers. By using in-silico high throughput screening methods of increasing selectivity and assessing their binding potential, we identified coral compounds hits for various cancer proteins that may merit further investigation.

Presented by: Connor Sierra *(Undergraduate, Organic Chemistry)*

Effects of the Various Treatments on the Biofuel Production of the Marine Diatom Navicula

Microalgal biofuels are one of the most promising areas of green technology in modern research. This study looks into the effects of a few different treatments of the marine diatom Navicula and the effects that the treatments have on the lipid content of the algae. The diatoms were cultured in four different media containing a basic culture media with a single variable nutrient. The four cultures consisted of a control treatment and three variable treatments. The three variable treatments consisted of a serine treatment, a tryptophan treatment, and a titanium treatment. The various treatments were cultured and harvested, and the lipid content was analyzed using carbon nuclear magnetic resonance spectroscopy (C13 NMR).

Presented by: Isaiah Niess *(Undergraduate, Biochemistry)*

Abstracts (Section B - Analytical and Physical)

Novel, simple, robust, ultra-small electrochemical sensor for real-time detection of Cd (II) in the environment

Heavy metal contamination is a rising global health concern; thus, it is critical to developing robust, cheap metal sensors with good selectivity and sensitivity. This study reports a novel, nanometer-scale electrochemical metal sensor based on ion transfer between two immiscible electrolyte solutions (ITIES) to detect Cd(II) in aqueous samples. We calibrate our sensor in various matrices and show its capability to withstand the complicated matrices without fouling. Furthermore, we show our sensor can detect Cd(II) dissolved in a water sample collected from Indian River Lagoon, Melbourne, FL; thus, demonstrating its power as an environmental monitoring tool. We find the limit of detection of the unmodified sensor to be 0.5 ppm. Our ultra-small electrode will enable us to study the kinetics of ion transfer across ITIES; thus, allowing us to modify the sensor to enhance the sensitivity and selectivity.

Presented by: Mohammed Muzammil Nishar Ahmed *(Graduate, Analytical Chemistry)*

CIFDock: A Novel CHARMM-based Induced Fit Docking Method

Docking studies play a critical role in the current workflow of drug discovery. However, limitations may often arise through factors including inadequate ligand sampling, a lack of protein flexibility, scoring function inadequacies and difficulty in retaining explicit water molecules. Herein, we present a novel CHARMM-based induced fit docking workflow that can circumvent these limitations by employing all-atom force fields coupled to enhanced sampling molecular dynamics procedures. Self-guided Langevin dynamics simulations are used to effectively sample relevant ligand conformations, side chain orientations, crystal water positions, and active site residue motion. We validated the CIFDock procedure by performing cross-docking studies using a data set of 21 pharmaceutically relevant proteins. Results obtained were comparable to, or in some cases improved upon, commercial docking program data.

Presented by: Luke Warrensford *(Graduate, Physical Chemistry)*

Structure-Activity Relationship of STING Compounds

Stimulator of Interferon Genes (STING) is an important transmembrane protein involved in innate immune response to foreign or damaged DNA or RNA in a cell's cytosol. When a cell is infected with an intracellular pathogen, STING acts as a sensor that triggers the production of type I interferon, which then promotes an anti-inflammatory response. Enhancers of STING can increase the immune response to the abnormal DNA of tumor cells and inhibitors of STING can help treat autoimmune disorders where there may be an overly aggressive immune response to self-DNA. Through molecular modeling studies performed by the Guida group, we have been

able to identify several compounds that have been active toward the STING pathway. Our goal for this project is to assess the structure-activity relationship of molecules that have had a positive response toward STING along with the synthesis of new analogs to test their enhancing or inhibiting activity.

Presented by: Jamie Nunziata *(Undergraduate, Organic Chemistry)*

Retention of equilibrium concepts among students in analytical chemistry

Retention of general chemistry concepts is important as evidence of meaningful learning and is also relied upon for instruction of upper-level chemistry courses. To investigate retention of chemical equilibrium concepts an assessment was administered to students at the start of an analytical chemistry class at four post-secondary institutions. To explore the role of factors that may promote retention, survey questions were given to accompany the assessment. Factors investigated include the pedagogy used in general chemistry, the time passed since taking general chemistry and outside of class experiences such as tutoring general chemistry. Results indicate a varying amount of retention depending on the specific equilibrium concept. This presentation will detail the topics within chemical equilibrium that students exhibit relatively high or low retention and the student experiences that were found to relate to retention

Presented by: Jessica Young *(Graduate, Chemistry Education)*

A novel, ultra-fast multi-bore carbon fiber microelectrode for simultaneous detection of multiple neurotransmitters

Increased progression rate of neurodegenerative diseases is a global burden; hence it is critical to expand the studies related to these illnesses. In this study, we fabricate a new, multi-bore CFM with four sensing elements capable of simultaneously detecting four neurotransmitters. We use fast-scan cyclic voltammetry to test our sensor in a mixture of dopamine (DA), ascorbic acid (AA), serotonin (5-HT), and Cu(II) ions. Interestingly, we find that DA and AA contribute to an improved sensitivity for Cu(II) detection. Conversely, we find that 5-HT detection is not feasible with Cu(II). These findings may be presumably due to two reasons; 1. increased number of surface-active sites on the secondary film formed by AA, DA, and their products, and 2. those sites being fully occupied by Cu(II) ions, thus leaving no space for 5-HT adsorption. Our findings will improve the understanding of co-transmitters and interactions with external stimuli, hence contributing to more efficient drugs.

Presented by: Melyse Laud *(Graduate, Analytical Chemistry)*

Parallel Computation of Discrete Feynman Path Integrals

Feynman Path Integrals can be approximated through a discretization process and doing so renders their computation highly amenable for use on parallel hardware. The form of the resulting model is mathematically identical to a system of point masses connected into loops via harmonic springs, allowing the use of classical algorithms to by employed in the simulation of properties such as nuclear quantum effects. Unexpected effects and difficulties in sampling the configuration space of these classical/quantum loops are explored.

Presented by: Brant Tudor *(Graduate, Physical Chemistry)*

Novel Fentanyl Analog Screening using Mass Defect Filtering

Fentanyl analogs are a challenge for forensic laboratories to identify because illicit producers modify compounds as bans for specific drugs go into effect. This creates a moving target for laboratories who struggle to keep up with detecting the latest analog due to lack of certified reference material and validated methods. Fentanyl analogs are made by making small changes in the functional groups of the fentanyl molecule therefore the analogs should have similar mass defects to the original compound. This research uses mass defect analysis as a non-targeted method to screen for novel analogs using a mass defect filter on unfragmented ions, searching for precursor ions based on the observed fragment ions, and using mass defect filtering on the fragment ions. Data will be taken using Agilent triggered MS/MS acquisition mode at 10, 20 and 40 V collision energies (CE) simultaneously using fentanyl analog screening kits obtained from Cayman Chemical with over 100 fentanyl analogs.

Presented by: Dina Swanson *(Graduate, Analytical Chemistry)*

Sequence effects of uracil damaged DNA

Uracil is a common type of lesion in damaged DNA. This damage arises from either spontaneous deamination of cytosine or errors in the replication process. Excision of uracil from the genome is carried out in the base excision repair (BER) process by uracil DNA-glycosylase (UDG). It is hypothesized that UDG activity is depended on the intrinsic deformability of the base steps neighboring the uracil. To shine a light upon this issue, the behavior and deformability of a diverse set of uracil-damaged DNA sequences have been studied using molecular dynamics (MD) simulations. Bending and torsional persistence lengths along with individual base step parameters have been examined to provide insight into sequence effects and their influence on repair enzymes.

Presented by: Paul Orndorff *(Graduate, Physical Chemistry)*

Abstracts (Section C - Biochemistry)

Reasearch on catalytic mechanism of Mammalian peptidylglycine α-amidating monooxygenase (PAM) by (R,S)-N-acyl-α-hydroxyglycines

Peptidylglycine α-amidating monooxygenase (PAM) catalyzes the oxidative cleavage of glycine extended peptides at their terminus. (R)-N-acyl-α-hydroxyglycine is regarded as the reaction intermediate. So (S)-N-acyl-α-hydroxyglycine can be regarded as a promising inhibitor for PAM. By synthesis and seperation (R,S)-N-acyl-α-hydroxyglycines, we could get more details about catalytic mechanism of PAM.

Presented by: Ruidong Ni *(Graduate, Biochemistry)*

Inhibiting Cu(II)-Tetracycline mediated Oxidation

Tetracycline (TC) isolated from the S. aureofaciens, S. rimosus, and S. viridofaciens is a widely used antibiotic in animal production. There are significant presence of Tetracyclines in the soil via feces, urine and manure utilization. Our study presents the inhibition of Copper bound Tetracycline by natural products like Salicylic acid , Benzoic acid and another cyclic peptide antibiotic Bacitracin available in the envirinment.

Presented by: Shahedul Islam *(Graduate, Inorganic Chemistry)*

Inhibition of NHR/CHR of Gp41 protein-protein interaction using α Helix-Mimicking sulfono-γ-AApeptide inhibitors.

Peptides, including small molecules and antibodies, have attracted much attention in the last decade and are currently employed developing new medicines. Despite the substantial progress, their intrinsic drawbacks, including short in vivo half-lives and poor membrane permeability, still limit their development. Peptidomimetics could offer opportunities to overcome these drawbacks. Here, we design a series of helical sulfono-γ-AApeptides with entire unnatural backbones for their ability to structurally and functionally mimic MTSC22 which is an effective bioactive peptide of HIV fusion inhibitor. Right now, the IC50 of the most potent helical homogeneous sulfono-γ-AApeptides in our design is at low nanomolar range. Our study reveals that homogeneous sulfono-γ-AApeptides could be used for the development of next generation of potent anti-HIV agents. These homogeneous sulfono-γ-AApeptides peptidomimetics could be a new strategy to modulate a myriad of protein-protein interaction and may pr

Presented by: Songyi Xue *(Graduate, Organic Chemistry)*

Study of the Protein Dynamic Properties of Class A β-lactamases by NMR Spectroscopy

The molecular-level information of Extended-spectrum β-lactamases (ESBLs) of different Enterobacteriaceae (e.g. E.coli, K. pneumoniae) is currently limited to structural studies performed by X-ray crystallography. To gain further insights into the structure and function of ESBLs, it is also essential to fully understand their dynamic and chemical properties in solution. Here, we have applied NMR spectroscopy to study the backbone dynamics of two members of class A β-lactamases. The 15N relaxation experiments with different T1, T2 delay times as well as HSQC, NOE were performed at multiple fields. The dynamics data obtained were analyzed using the Lipari and Szabo model-free approaches. The experiments provide information on longitudinal (R1) and transverse relaxation rates (R2), generalized order parameter (S2), conformational exchange, spectral density mapping, and total correlation time for internal motions. The results discussed here indicate a highly ordered protein structure.

Presented by: Radwan Ebna Noor *(Graduate, Biochemistry)*

Modular Design of Membrane Active Antibiotics: From Macromo-lecular Antimicrobials to Small Scorpion-like Peptidomimetics

Infections caused by multidrug-resistant bacteria are emergent in recent decades, leading to escalating interest in host-defense peptides (HDPs) to reverse this dangerous trend. Inspired by the modular design in bioengineering, herein we re-port a new class of small amphiphilic scorpion-like peptidomimetics based on this strategy. These HDP mimics show potent antimicrobial activity against both Gram-positive and Gram-negative bacteria without drug resistance but with high therapeutic index. Membrane-compromising action mode was suggested to be their potential bactericidal mechanism. Pharmaco-dynamics experiments were conducted in a murine abscess model of MRSA infections. The lead compound 12 showed impressive in vivo therapeutic efficacy with 99.998% (4.7log) reduction in skin MRSA burden, significantly higher bactericidal efficiency than ciprofloxacin, as well as good biocompatibility. The results highlight the potential of these HDP mimics as novel antibiotic therapeutics.

Presented by: Wang Minghui *(Graduate, Biochemistry)*

Spatial Analysis of Lipids in D. Melanogaster by Matrix Assisted Laser Desorption/Ionization Mass Spectrometric Imaging

Mass spectrometric imaging (MSI) has evolved as a useful technique for the spatial analysis of intact molecules in situ. As such, Matrix Assisted Laser Desorption Ionization (MALDI) is widely used for the purpose. Herein, we use MALDI-MSI to provide spatially resolved distribution of lipids in Drosophila melanogaster sections. Organism was embedded in 5% carboxymethyl cellulose (CMC) to prepare intact 20 μm cryo-sections. MSI was done in positive ionization

mode using 2,5-dihydroxybenzoic acid (DHB) as matrix which was sprayed with an airbrush to achieve uniform distribution of matrix across the tissue sections. Taking into account possible matrix interference at low mass region, and presence of isobaric compounds in biological samples, additional MS/MS experiment was performed on some of the identified lipids for their structural elucidation.

Presented by: Suzeeta Bhandari *(Graduate, Biochemistry)*

Prevalent PKC-ι/ζ signaling is crucial for apoptosis inhibition and invasiveness of glioblastoma through upregulation of 14-3-3 and Smad2/3.

Glioblastoma (GB) is an aggressive form of cancer derived from astrocytes and often found in brain or spinal cord. Poor prognosis of GB has limitations in current therapeutics mainly due to the development of resistance. Our results demonstrated that atypical protein kinase C-iota and zeta (aPKC-ι/ζ) levels were over-expressed in U-87 and T-98 cells and GB tissue samples compared to normal brain cells/tissues which is correlated with increased invasiveness. The present study shows the downstream effects of siRNA knockdown of PKC-ι/ζ on the expression of aPKCs, E-cadherin, Vimentin, p-Vimentin, 14-3-3 and p-14-3-3, BAD, p-BAD, Pdk1, Akt1, c-Raf, Tak1, Smad2/3 and p-Smad2/3. Downregulation of Vimentin, p-Vimentin (S33 and S56) indicated the downregulation of epithelial-mesenchymal transition (EMT) and acquisition of epithelial characteristics. Proteolytic E-cadherin fragment of 80 kDa indicates the reduction of cancer progression. Result also indicated that SNAIL1, SLUG and PRRX1 transc

Presented by: Khandker Mohammad Khalid *(Graduate, Biochemistry)*

Antimicrobial peptides mimicking polycarbonates with broad antibacterial activity

Bacterial infection is still threatening global health nowadays due to the lack of new antibacterial drug development and the abuse of traditional antibiotics results in the drug resistance of bacteria. Inspiring by the host defense peptide, cationic charged polycarbonates are designed which show activity against both Gram-positive and Gram-negative bacteria with different tail lengths. The introduction of amino acid side chain also increases bioavailability which makes them potent for clinical application.

Presented by: Ruixuan Gao *(Graduate, Biochemistry)*

Abstracts **(Section D - Organic)**

Natural Product Drug Discovery against SARS-CoV-2 proteins vi in-silico screening

A selection of isolated marine natural products were screened as potential inhibitors against the SARS-CoV-2 virus using rigid docking methods. Four proteins critical to viral function were selected as targets of the study: the main protease (Mpro), the papain-like protease (PLpro), the transmembrane protease (TMPRSS2), and the RNA-dependent RNA-polymerase (RdRp). Schrodinger's rigid docking program, Glide, was used to screen structures of published coral compounds from MarinLit and isolated novel natural products (NPs) from National University of Ireland, Galway (NUIG) and the Bill Baker lab at USF. Theaflavin, Integracin, a family of Characellide compounds, and a selection of other marine natural products exhibited excellent predicted binding affinity to these protein targets and have persisted onto in-vitro biological assay screening.

Presented by: Sarah Dietrick *(Graduate, Organic Chemistry)*

Supramolecular helical polymer: construction and further investigation

We plan to construct a helical polymer. We designed a monomer structure with two terminal alkyne protons on both side arm. Terpyridine and pyridinium structures were also included in the monomer structure so that we can do some topological study as well as find some antibacterial application.

Presented by: Zhanpeng Zhang *(Graduate, Organic Chemistry)*

Optimizing the Development of ACK1 Inhibitors to Use as Therapeutic Cancer Agents

Activated CDC42-associated tyrosine kinase 1 (ACK1) is an enzyme encoded by the TNK2 gene. The interactions of this enzyme are seen in lung, leukemia, ovarian, and prostate cancers. Utilizing a fragment-based drug design, ACK1 inhibitors are made from three fragments coupled together by Buchwald-Hartwig amination reaction. Once the fragments are designed, the compound is docked to suitable models of ACK1 (PDB 4EWH) with the software Schrodinger. The final purified products are screened by a 33P HotSpot assay to evaluate the compounds' ACK1 inhibition. The most potent analogs are then evaluated through cell viability (UKE1 and MB-231) assays (MTT) to determine GI50 and EC50 values. This fragment-based model has optimized the development of ACK 1 inhibitors (IC50 13.8-36.4 nM). These analogs can be used as therapeutic agents against different cancers. Evaluating SAR will help optimize the process of choosing an A-ring and B-ring for future compounds.

Presented by: Angelie Matar *(Graduate, Organic Chemistry)*

Studies of New Synthetic Ketogenic Molecules

Ketosis is a metabolic state where liver produces small molecules called ketone bodies, that most cells in the body can use as a source of energy. Other than working as a source of energy during prolonged fasting or carbohydrate restriction ketosis has already an established treatment for epilepsy and type 2 diabetes. Although, a good amount of research was done on ketogenic diet recent times, the field of synthesis of novel ketogenic compounds was neglected. Our endevour was to find synthetic routes and characterization of some new small ketogenic molecules.

Presented by: Mohammad Nazmus Sakib *(Graduate, Organic Chemistry)*

ICA-1: Synthesis of a Selective PKC-ι Inhibitor and its Analogues

In the past years, the atypical isoform protein kinase iota (PKC-ι) was found to be an oncogene expressed in multiple types of cancers. PKC-ι is required in the growth of human cancer cells and is involved in growth, invasion and survival. ICA-1 has been proven to selectively inhibit PKC-ι activity over its closely related isoform protein kinase ζ (PKCζ) with an IC-50 of 0.1μM with no cytotoxic properties. The focus of this study was to synthesize ICA-1 and analogues of ICA-1 with an improved inhibition activity towards PKC-ι.

Presented by: Aaron Astalos *(Graduate, Organic Chemistry)*

N-B substituted polycyclic aromatic hydrocarbon via gold catalysis

Polycyclic aromatic hydrocarbons (PAH) has unique physical properties, and plays an important role in material science due to the delocalized electrons in the aromatic system. Polycyclic aromatic hydrocarbons containing N-B bond as C=C double substitution is attractive though, less concerned, mainly because of synthetic challenge. In this work, we developed a new method to achieve various benzotriazole-cyanoborane complexes. Under the catalysis of gold, stable fluorescent benzotriazole azaboranes N-B substituted polycyclic aromatic hydrocarbon was successfully synthesized with high yield and good functional group tolerance. The tunable fluorescent properties of these compounds highlight the potential application in material science.

Presented by: Qi Tang *(Graduate, Organic Chemistry)*

An Ongoing Investigation of Endophytic Mangrove Fungi for Antimicrobial Natural Products

Mangrove endophytes are rich in natural products with antibacterial and antifungal properties. In this ongoing project, an in-house library of endophytic fungi isolated from mangroves is investigated to isolate and characterize new and novel compounds active against the ESKAPE pathogens and Candida albicans. To prevent re-isolating previously discovered compounds,

tandem mass spectrometry and nuclear magnetic resonance spectroscopy dereplication strategies were employed, including GNPS molecular networking and use of databases such as SMART NMR and MarinLit. If a known bioactive toxin is identified, it is chromatographically edited out of the extract using preparative LCMS and the edited fraction is resubmitted for bioassay to determine if activity is conserved. One organism in particular, EG12-35E-2, is highlighted in this presentation as it has undergone most arms of the workflow process, from fungal growth to pure compound isolation.

Presented by: Kristin Herrera *(Graduate, Organic Chemistry)*

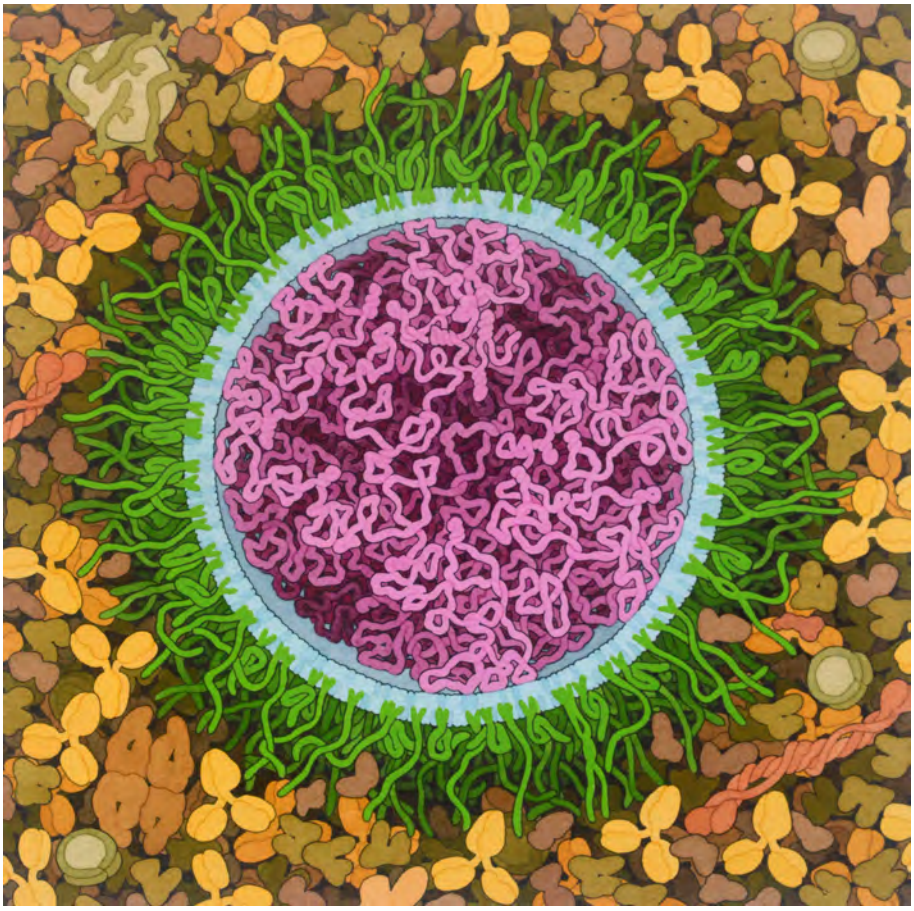
Synthesis of a Novel Compound for Inducing Ketosis on a Normal Diet

The recent popularity of high-fat, low-carbohydrate 'ketogenic' diets among the public as a weight-loss tool has led to an expansion of research into both the health benefits of the diet and methods for conferring those benefits through supplements instead of strict adherence to the diet. A synthetic compound developed by our lab has been shown to elevate ketone body concentrations in the blood (ketosis) more effectively than compounds currently being studied.

Presented by: Michael Williams *(Graduate, Organic Chemistry)*

About the Cover

SARS-CoV-2 mRNA Vaccine, 2020



Messenger RNA (mRNA) vaccines developed for the COVID-19 pandemic are composed of long strands of RNA (magenta) that encode the SARS-CoV-2 spike surface glycoprotein enclosed in lipids (blue) that deliver the RNA into cells. Several different types of lipids are used, including familar lipids, cholesterol, ionizable lipids that interact with RNA, and lipids connected to polyethylene glycol chains (green) that help shield the vaccine from the immune system, lengthening its lifetime following administration. In this idealized illustration, all of the lipids are arranged in a simple circular bilayer that surrounds the mRNA and the PEG strands have both extended and folded conformations.

Illustration by David S. Goodsell, RCSB Protein Data Bank;
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Judges

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