

TABLE OF CONTENTS

ANALYTICAL/BIOANALYTICAL CHEMISTRY.....	5
POSTER #1 – ANALYTICAL/BIOANALYTICAL	5
Presenter: Elijah Holloway	5
Title: Study of Output Spectrum and Optimization of the Composition of Toluene-Based Liquid Scintillator	5
POSTER #2 – ANALYTICAL/BIOANALYTICAL	5
Presenter: Leah Eubanks	5
Title: Buffer-Free Quantification of Iron in Ferrous Sulfate Supplements Using Cyclic Voltammetry	5
POSTER #3 – ANALYTICAL/BIOANALYTICAL	6
Presenter: Huynh Phuong	6
Title: Determining the Optimal Nanodisc Lipid to Protein Ratio for Lipid Mixes of Varying Lipid Head Groups	6
POSTER #4 – ANALYTICAL/BIOANALYTICAL	6
Presenter: Andrew Sunshine	6
Title: One-Step Attomolar Quantification of SARS-CoV2 RNAs with Aptamer-Based Electrochemical Sensors	6
POSTER #5 – ANALYTICAL/BIOANALYTICAL	7
Presenter: Jeanne Cooper	7
Title: Comparison of Traditional and Microwave-Assisted Extraction Methods and Purification of Cyclotides	7
POSTER #6 – ANALYTICAL/BIOANALYTICAL	8
Presenter: Callie Goins	8
Title: Investigating IR Switching Capabilities of Dioxythiophene-Based Conjugated Polymers	8
POSTER #7 – ANALYTICAL/BIOANALYTICAL	9
Presenter: Bakai Sheytov	9
Title: Investigating the Optimal Kinetic Parameters of Exonuclease III to Create a Next-Generation Robust, Self-Avoiding Rolling Motor Biosensor	9
POSTER #8 – ANALYTICAL/BIOANALYTICAL	10
Presenter: Diana Kem	10
Title: UV-Vis absorption and Steady-State Fluorescence Studies of Cyclotides: A Comparison of the Photophysical Properties of Cyclotides with Vancomycin Hydrochloride	10
POSTER #9 – ANALYTICAL/BIOANALYTICAL	11
Presenter: Voytek Tarnowski	11
Title: Comparative Analysis of Secondary and Tertiary Amine Desalination Extraction Efficiencies Based on Molecular Characteristics	11
BIOCHEMISTRY	12
POSTER #10 –BIOCHEMISTRY	12
Presenter: Lydia Kenney	12
Title: Structural Characterization of Clathrate Binding Proteins	12
POSTER #11 –BIOCHEMISTRY	13
Presenter: Hyein Kang	13
Title: Optimizing Purification of Collagen Targeted Protein MRI Contrast Agent for Early Detection	13
POSTER #12 –BIOCHEMISTRY	14
Presenter: Andrew Schilling	14
Title: Supramolecular Polymers Promote the Non-enzymatic Generation of Proto-Nucleic Acid Oligomers	14
POSTER #13 –BIOCHEMISTRY	14
Presenter: Kenneth Liu	14
Title: Biophysical Characterization of Previously Intractable Myocilin Olfactomedin Mutants	14

POSTER #14 –BIOCHEMISTRY	15
Presenter: Dulciana Davis	15
Title: Discovery of Macrocyclic Ribosomal Peptides from <i>Glechoma hederacea</i> (Ground Ivy).....	15
POSTER #15 –BIOCHEMISTRY	16
Presenter: Katelynn Powell	16
Title: The Effects of Benzothiazole-Derivatives on the TDP-43 Protein in ALS Patients	16
POSTER #16 –BIOCHEMISTRY	16
Presenter: Sarah Clark.....	16
Title: Identification of an Antimicrobial Compound from <i>Pseudomonas protegens</i> CHA0	16
POSTER #17 –BIOCHEMISTRY	17
Presenter: Jon Dudkin	17
Title: Comparing Growth in Common Lab Media of Vmax™ X2 and BL21(DE3) <i>E. coli</i>	17
POSTER #18 –BIOCHEMISTRY	17
PI: Jeremy Olson.....	17
Title: Novel Efficient Synthesis of Caged Coumarin Chromophores	17
POSTER #19 –BIOCHEMISTRY	18
Presenter: Kha Minh Nguyen.....	18
Title: Determination of the Optimal Lipid to Protein Ratio (LPR) for Nanodisc Formation with Varying Tail Features.....	18
ENVIRONMENTAL/GREEN CHEMISTRY	19
POSTER #20 – ENVIRONMENTAL/GREEN CHEMISTRY.....	19
Presenter: Tram Nguyen	19
Title: Experimental Study and Modeling of Thermodegradation During Torrefaction.....	19
of Raw and Potassium Impregnated Beech Wood (Part 1)	19
POSTER #21 – ENVIRONMENTAL/GREEN CHEMISTRY.....	20
Presenter: Harris Carlisle	20
Title: Chemical Investigations of Organics and Metabolites in the Chattahoochee River	20
POSTER #22 – ENVIRONMENTAL/GREEN CHEMISTRY.....	20
Presenter: Starr Jenkins	20
Title: Catalytic Aerobic Oxidation of Benzylic Amines to Imines Utilizing a Sustainable Copper/TEMPO System	20
POSTER #23 – ENVIRONMENTAL/GREEN CHEMISTRY.....	21
Presenter: Raven Nicole Stanlet.....	21
Title: Implications for Disproportionate 1,4-Dichlorobenzene Exposures Among Communities of Color	21
POSTER #24 – ENVIRONMENTAL/GREEN CHEMISTRY.....	21
Presenter: Olivia Kapwadi	21
Title: Analyzing the Disproportionate Effect of Pesticide Exposure in Communities of Color.....	21
POSTER #25 – ENVIRONMENTAL/GREEN CHEMISTRY.....	22
Presenter: Chaunie Banks	22
Title: Analyzing Pesticide Residue Exposure to Communities of Color Through Use of Shampoos and Conditioners.....	22
POSTER #26 – ENVIRONMENTAL/GREEN CHEMISTRY.....	22
Presenter: Chaunie Banks	22
Title: Analyzing Pesticide Residue Exposure to Communities of Color Through Use of Shampoo and Conditioner	22
POSTER #27 – ENVIRONMENTAL/GREEN CHEMISTRY.....	23
Presenter: Katheryn Foust.....	23
Title: Mapping Microfibers in Lake Allatoona Water.....	23
POSTER #28 – ENVIRONMENTAL/GREEN CHEMISTRY.....	23
Presenter: Nadine Abrahamse	23
Title: Culture-Based Strategies for Marine Bacteria Natural Product Discovery.....	23
POSTER #29 – ENVIRONMENTAL/GREEN CHEMISTRY.....	24
Presenter: Alexa Luna.....	24
Title: Carotenoid Extraction Using an Emerging Green Approach.....	24

ORGANIC CHEMISTRY	25
POSTER #30 – ORGANIC CHEMISTRY	25
Presenter: Ashley Goehrig	25
Title: Organic Chemistry Concept Maps: An Interactive Approach to Helping Students	25
Review Organic Chemistry I Reactions	25
POSTER #31 – ORGANIC CHEMISTRY	25
Presenter: Dahnielle Milton	25
Title: Use of Dioxiranes in the Epoxidation of Oleochemicals	25
POSTER #32 – ORGANIC CHEMISTRY	26
Presenter: Corina Paun	26
Title: Biofuel Synthesis, Characterization, Blend Performance, and Combustion Analysis	26
POSTER #33 – ORGANIC CHEMISTRY	26
Presenter: Mason Jones	26
Title: Synthesis and Characterization of a Furfural Derived Semi-Rigid Diol	26
POSTER #34 – ORGANIC CHEMISTRY	27
Presenter: Byron Fisher	27
Title: Gelation and Photophysical Studies of Aminophenylalkanamides as Low Molecular Mass Gelators	27
POSTER #35 – ORGANIC CHEMISTRY	27
Presenter: Jessica Budwitz	27
Title: A Diels–Alder Disconnection of <i>para</i> -Quinones	27
POSTER #36 – ORGANIC CHEMISTRY	28
Presenter: Jeremy Norton	28
Title: Synthesis, Self-Assembly, Gelation Studies, and Steady-State Fluorescence properties of Anthraquinonylalkanamides-Based Low Molecular Mass Gelators	28
POSTER #37 – ORGANIC CHEMISTRY	28
Presenter: Nguyen Le	28
Title: Steady-State Excitation and Emission, and Gelation Properties of Alkyloxycoumarin Derivatives as Low Molecular Mass Gelators	28
POSTER #38 – ORGANIC CHEMISTRY	29
Presenter: Joshua Leonora	29
Title: Synthesis, Characterization, Steady-State Fluorescence and Gelation Properties of Coumarin-Linked Cholesteryl Derivatives	29
POSTER #39 – ORGANIC CHEMISTRY	29
Presenter: Romy Doan	29
Title: Synthesis, Characterization, and Steady-State Fluorescence Properties of 2-(benzylidene)-1-Indanone Derivatives	29
POSTER #40 – ORGANIC CHEMISTRY	30
Presenter: Ken Aratame	30
Title: Fluorinated Indolenine-Based Squaraine Near-Infrared Dyes: Synthesis, Characterization, and Optical Properties	30
INORGANIC/ORGANOMETALLIC CHEMISTRY	31
POSTER #41 – INORGANIC/ORGANOMETALLIC CHEMISTRY	31
Presenter: Katelin Gary	31
Title: N-Heterocyclic Carbene Complexes of Nickel: An Examination of Synthetic Options and Target	31
POSTER #42 – INORGANIC/ORGANOMETALLIC CHEMISTRY	31
Presenter: Justin Bindewald	31
Title: Structural Properties of Iron(0) Nanoparticles in Micellar Solutions and Deep Eutectic Solvents	31
POSTER #43 – INORGANIC/ORGANOMETALLIC CHEMISTRY	32
Presenter: Andrea Mancia	32
Title: Catalytic Oxidation of Propene through Transition Metal Modified α -MnO ₂ Catalysts Decreases Conversion Temperature	32
POSTER #44 – INORGANIC/ORGANOMETALLIC CHEMISTRY	33
Presenter: Annaleena Hansen	33
Title: Synthesis of Cæsium Bismuth Sulfide Compounds, a Precursor to Lead Free Perovskites	33

POSTER #45 – INORGANIC/ORGANOMETALLIC CHEMISTRY	34
Presenter: Janae Burks	34
Title: Synthesis of Uranium Organometallic Precursors for Laser Irradiation	34
PHYSICAL/COMPUTATIONAL CHEMISTRY	35
POSTER #46 – PHYSICAL/COMPUTATIONAL CHEMISTRY	35
Presenter: Jane Yoo.....	35
Title: Computer Aided Anti-Malarial Drug Design Targeting <i>Plasmodium falciparum</i> Glutathione S- Transferase	35
POSTER #47 – PHYSICAL/COMPUTATIONAL CHEMISTRY	36
Presenter: Kathryn Monheim	36
Title: Synthesis of Fluorescent Dyes for Incorporation into Silica Nanoparticles.....	36
POSTER #48 – PHYSICAL/COMPUTATIONAL CHEMISTRY	36
Presenter: Oluwaseun Omodemi.....	36
Title: Computational Study of N ₄ H ⁺ /N ₄ D ⁺ Raman Vibrational Spectra.....	36
POSTER #49 – PHYSICAL/COMPUTATIONAL CHEMISTRY	37
Presenter: Mary Kate Smith	37
Title: Anionic Polymerization of Styrene in Flow	37
POSTER #50 – PHYSICAL/COMPUTATIONAL CHEMISTRY	37
Presenter: Sara Sarasiya	37
Title: Synthesis and Optical Characteristics of Perimidine-Containing Squaraine Dyes	37
POSTER #51 – PHYSICAL/COMPUTATIONAL CHEMISTRY	38
Presenter: Aneri Amin.....	38
Title: Solution Structures of Novel Cyclotides Sequences (alca 1 and alca 2) Using Homology Modeling and Molecular Dynamics Simulations	38
POSTER #52 – PHYSICAL/COMPUTATIONAL CHEMISTRY	39
Presenter: Uyen Ta.....	39
Title: Yb-Doped-Fiber-Laser Femtosecond Pulse Compression with Double-Pass Gratings and Filters	39
POSTER #53 – PHYSICAL/COMPUTATIONAL CHEMISTRY	39
Presenter: Imani Rogers	39
Title: Synthesis, Activity, and Characterization of Pd/Al ₂ O ₃ Catalysts for Methane Combustion Under Stoichiometric Conditions.....	39
POSTER #54 – PHYSICAL/COMPUTATIONAL CHEMISTRY	40
Presenter: Erica Browne.....	40
Title:Comparing Computational Methods: Calculating Vertical and Adiabatic Excitation Energies in Flavin.... 40	40
POSTER #55 – PHYSICAL/COMPUTATIONAL CHEMISTRY	41
Presenter: Rahul Pandit	41
Title: Molecular Docking and Fine-Tuning Ligands for Drug Discovery Purposes (COVID-19).....	41
POSTER #56 – PHYSICAL/COMPUTATIONAL CHEMISTRY	42
Presenter: Laila Belpalme	42
Title: Cyclotide Interactions with the Lipid Bilayer	42

Georgia Gwinnett College welcomes presenters and attendees from over 20 institutions with regional, national and international representation.

Analytical/Bioanalytical Chemistry

Poster #1 – Analytical/Bioanalytical

Presenter: Elijah Holloway
PI: Dmitriy Beznosko
Institution: Clayton State University

Title: Study of Output Spectrum and Optimization of the Composition of Toluene-Based Liquid Scintillator

Liquid scintillator is widely used as a medium for the detection of charged particles for numerous applications in science, medicine, and other areas. The composition of scintillator affects not only its performance, but also the cost of the components. The spectrum of the output scintillator light also affects what detectors can be used in conjuncture with this scintillator formula. Optimization of this composition provides the ability to design particle detectors with a certain light yield and emission spectra of the detection medium or maximize the light yield while optimizing the expenses. This work presents the component optimization for the toluene-based liquid scintillator that uses PPO as a fluor and POPOP as a secondary shifter. The light yield vs. concentration and the changes in the output spectra will be presented. Future plans include light attenuation measurements.

Poster #2 – Analytical/Bioanalytical

Presenter: Leah Eubanks
PI: Isaac Agyekum
Institution: University of North Georgia - Gainesville Campus

Title: Buffer-Free Quantification of Iron in Ferrous Sulfate Supplements Using Cyclic Voltammetry

Recent interest in introducing electrochemical techniques at the undergraduate level has necessitated the development of highly informative yet simple to understand laboratory experiments. We herein present a simple buffer-free cyclic voltammetry experiment using a three-electrode system to quantify elemental iron in over-the-counter ferrous sulfate supplements. Several student learning outcomes captured in this cost-effective lab include an introduction to a three-electrode system and the basic principles of cyclic voltammetry; sample preparation through acid digestion; statistical evaluation of experimental data; and propagation of error in the determination of the mass of iron in each tablet. The advantage of using the method of standard addition to a single solution compared to multiple solutions with a constant volume is strongly emphasized.

Poster #3 – Analytical/Bioanalytical

Presenter: Huynh Phuong
PI: Khue Nguyen
Co-Author: Kerry Strickland
Institution: Mercer University

Title: Determining the Optimal Nanodisc Lipid to Protein Ratio for Lipid Mixes of Varying Lipid Head Groups

Nanodiscs are individually-packaged lipid bilayers that mimic the native lipid environment of cellular membranes. Efficient nanodisc formation relies on optimal lipid to protein ratios (LPRs). However, there is little data on the optimal LPRs for generating nanodiscs of specific lipid combinations. Our research focuses on determining the optimal LPR for nanodiscs of specific lipid combinations of varying head groups. Phospholipid head groups act as access codes to mediate biological functions through lipid-protein interactions. First, we will study the lipid selectivity of MSP to confirm nanodisc formation is only dependent on the optimal LPR. Currently, membrane scaffold protein (*i.e.* MSP1D1), used to make nanodisc, has been expressed and purified from BL21(DE3) *E. coli* cells. Nanodiscs of a single, well-characterized lipid are being generated (*i.e.* DMPC). Next, nanodiscs of lipid mixtures with varying head groups will be tested and analyzed by size exclusion chromatography (SEC) and transmission electron microscopy (TEM). Generating nanodiscs of specific lipid combinations allows for the study of membrane protein structures and functions, which give insights into lipid specificity during nanodisc formation.

Poster #4 – Analytical/Bioanalytical

Presenter: Andrew Sunshine
PI: Gangli Wang
Co-Author: Sarah Ake
Institution: Georgia State University

Title: One-Step Attomolar Quantification of SARS-CoV2 RNAs with Aptamer-Based Electrochemical Sensors

The recent SARS-Cov-2 highlights the shortcomings of PCR as a quantitative tool. Real time quantitative PCR calculates the initial concentration of target sequence based on the number of PCR cycles (C_q) before the target sequence is detectable. Exponential amplification of the target results in exponential amplification of error. An aptamer-based electrochemical sensor was developed to allow the direct detection and quantification of dilute concentrations of SARS-Cov-2 e-gene RNA. Initial results suggest the sensor is reliably detects concentrations as low as 10 aM.

Poster #5 – Analytical/Bioanalytical

Presenter: Jeanne Cooper
PIs: Ajay Mallia and Simon Mwangela
Co-Author: Diana Kem
Institution: Georgia Gwinnett College

Title: Comparison of Traditional and Microwave-Assisted Extraction Methods and Purification of Cyclotides

Cyclotides are pharmaceutically active cyclic peptides containing 29 – 31 amino acid residues of which there are six cystine residues forming three disulfide bridges. The present study describes the extraction and purification of cyclotides from Australian violet (*Viola hederacea*) plants and compares the efficiency of traditional solvent extraction to microwave-assisted extraction methods, which optimize green chemistry principles by reducing time and harmful solvents used. Traditional extraction was optimized using a solvent extraction of fresh plants through two methods of either ethanol (20 %) or methanol (50 %), water, dichloromethane, and chloroform which produced yields of 3 – 4 %. Microwave extraction utilized only water as the solvent and extracted cyclotides in a quarter of the time with similar yields of 3 % when considering the mass ratio of fresh to dried plant. Additionally, crude cyclotide product has been purified using C18 solid-phase extraction cartridges and analyzed through high performance liquid chromatography (HPLC) using a C18 column and a binary gradient solvent system of water and acetonitrile. The cyclotides are further purified *via* Prep-HPLC. Results of HPLC analysis and purification will be discussed.

Poster #6 – Analytical/Bioanalytical

Presenter: Callie Goins
PI: Eric Shen
Co-Authors: Austin L. Jones, Anna M. Österholm and John R. Reynolds
Institution: Georgia Institute of Technology

Title: Investigating IR Switching Capabilities of Dioxythiophene-Based Conjugated Polymers

Electrochromic materials that can effectively switch between a highly transmissive and a highly absorptive state upon user-controlled application of an applied voltage in the visible, near-infrared, and mid-infrared regions of the electromagnetic spectrum have been of interest due to their potential application in areas such as military camouflage, transportation, and traffic visualization. Specifically, developing materials with large optical contrasts in the 3-5 micron and 8-12 micron wavelength ranges would allow for on-demand switching at wavelengths where IR detectors operate. Metal oxides have shown excellent switching in the 3-5 μm range, but they do not exhibit large contrast in the 8-12 μm range. Few conjugated polymers have been investigated for IR switching, and previously investigated devices incorporating conjugated polymers have not exhibited large optical contrast in the mid-IR region. Here, we explore the mid IR-switching capabilities of two dioxythiophene-based donor-acceptor conjugated polymers. While these polymers have been widely explored for their visible color switching properties, little existing work has been done to investigate their mid-IR switching properties. These systems were selected based on their strong performance as electrochromic materials, having demonstrated fast switching between a highly transmissive oxidized state and a highly absorptive neutral state within seconds, and reversible switching for hundreds to thousands of switches, both of which are important properties as mid-IR switching materials. First, we determined the relationship between the mid-IR transmittance and the thickness of thin-films spray-coated onto gallium arsenide, an IR-transparent substrate, to determine if there is an optimal film thickness to afford the highest possible contrast. These thin films demonstrated strong contrast in both the 3-5 μm range and the 8-12 μm range. Next, prototype reflective devices were constructed, demonstrating significant contrast in the 3-5 μm range. The spectral contrasts of these polymers are found by applying voltages ranging from -1 to 1 V, a relatively small window for full device operation. We believe that these materials are promising candidates for applications requiring on-demand and user-controlled adaptive mid-IR switching.

Poster #7 – Analytical/Bioanalytical

Presenter: Bakai Sheyitov
PI: Khalid Salaita
Co-Authors: Yusha Imtiaz, Alisina Bazrafshan and Khalid Salaita
Institution: Emory University

Title: Investigating the Optimal Kinetic Parameters of Exonuclease III to Create a Next-Generation Robust, Self-Avoiding Rolling Motor Biosensor

DNA machines come in various sizes ranging from the micro to the nanoscale. These synthetic constructs harness the chemical and mechanical properties of biomolecules to conduct computing, drug delivery, and even diagnostics. A prominent advancement in this field was the development of the "rolling" motor system, which used the enzymatic capabilities of RNaseH to consume an RNA-laden "fuel" monolayer to propel the motor system, a 5 micron bead with multivalent DNA legs, with super diffusive, self-avoiding, processive motion. This system has been used as a blueprint to create systems from logic gates to COVID-19 biosensors. However, despite its programmability, the RNA-based system still suffers from being wholly dependent on the stability of its RNA monolayer. To update the design and create a fully DNA-based system, we must now employ another nuclease system, Exonuclease III. Our group has done much work to uncover the kinetic parameters of RNaseH, but little has been yet to elucidate ExoIII's potential in our design. Thus, this project aims to show the kinetic capabilities of ExoIII in both solution and surface-bound conditions to determine its optimal conditions to achieve an even more efficient and stable rolling motor system.

Poster #8 – Analytical/Bioanalytical

Presenter: Diana Kem
PIs: Ajay Mallia and Simon Mwangela
Co-Author: Jeanne Cooper
Institution: Georgia Gwinnett College

Title: UV-Vis absorption and Steady-State Fluorescence Studies of Cyclotides: A Comparison of the Photophysical Properties of Cyclotides with Vancomycin Hydrochloride

Cyclotides are plant-based cyclic peptides characterized by six cysteine residues, flanked by a diverse set of amino acids which in turn form three disulfide bonds. Observed pharmaceutical and insecticidal properties present potential applications in both agriculture and medicine. Vancomycin hydrochloride is a glycosylated peptide antibiotic with broad-spectrum usage. The current study explores steady-state excitation and emission properties of cyclotides compared with vancomycin hydrochloride. Additionally, aggregation and self-assembly of vancomycin in water, phosphate, and borate buffer solutions are explored through photophysical studies. Time-dependent photophysical studies of cyclotides in water will be presented.

The UV-Vis absorption spectrum of cyclotides exhibit λ_{\max} values at 268 nm and 318 nm at concentrations of 10, 20, 40, 60, and 80 ppm. The steady-state emission spectrum (excitation wavelength 435 nm) showed an emission maximum centered at 355 nm. Additionally, a Stokes shift of approximately 80 nm is observed. Furthermore, the UV-Vis absorption spectrum of vancomycin exhibits λ_{\max} at 282 nm. The steady-state emission spectrum (excitation wavelength 282 nm) displays an emission maximum centered at 325 nm. A Stokes shift of 43 nm is observed between the excitation and emission spectra. Findings validate the fluorescing capabilities of cyclotides; highlighting their potential usage in biological staining. Optical studies reveal that vancomycin exhibits aggregation in borate buffer with increasing concentrations.

Poster #9 – Analytical/Bioanalytical

Presenter: Voytek Tarnowski
PI: Seungjin Lee
Co-Authors: Cristin Colona and Jonathan McKinney
Institution: Georgia Gwinnett College

Title: Comparative Analysis of Secondary and Tertiary Amine Desalination Extraction Efficiencies Based on Molecular Characteristics

As the world population continues to increase, the demand for purified, potable water will increase proportionally. Densely populated cities not only have greater water demands, but also produce more industrial wastewater. Desalination of hypersaline industrial brines could provide a source for clean drinking water, while also treating wastewater. Current desalination technologies include evaporative distillation and membrane methods, but high energy consumption and inability to efficiently process high total dissolved solids (TDS) levels make them less attractive options. Temperature swing solvent extraction (TSSE) is an effective alternative method characterized by membrane-less, low-energy, cost-effective desalination. The technique utilizes low-temperature heat and a low-polarity solvent in combination with temperature-dependent water solubility. The focus of this study was to compare the extraction efficiencies of secondary and tertiary amines using their volumes, mass, and moles as a basis for comparison. Extraction experiments were conducted for each amine using both 1 M and 4 M NaCl brines across all trials. Secondary amines were found to extract the largest quantities of product water compared to tertiary.

Biochemistry

Poster #10 –Biochemistry

Presenter: Lydia Kenney
PIs: Raquel Lieberman
Co-Authors: Dustin Huard, Abigail Johnson, Manlin Xu, Sheng Dai, JC Gumbart,
Zixing Fan and Jennifer Glass
Institution: Georgia Institute of Technology

Title: Structural Characterization of Clathrate Binding Proteins

Clathrates are crystalline ice cages that contain gas molecules, and some, including methane clathrate, are capable of supporting life. We hypothesize that clathrate-dwelling organisms produce clathrate binding proteins (CBPs) to enable survival in such a harsh environment in a manner analogous to organisms that make antifreeze proteins (AFPs) to survive in freezing conditions. Through the metagenomic analysis of deep-sea sediments found off the coasts of Oregon and Japan, genes harboring an amino acid motif (TxxxAxxxAxx, where x is any amino acid) found in Type I AFPs were identified as potential CBPs. The corresponding proteins were then expressed and purified, and five hypothetical clathrate-binding proteins were produced. Four of these proteins (CbpA_{2,3,5,6}) were shown to bind to and change the morphology of THF clathrate, a model system for gas clathrates. Excitingly, the CbpAs also inhibited the growth of the more biologically relevant methane clathrate. A fragment of CbpA₃ active against methane clathrate was then crystallized, and the structure was solved using X-ray crystallography. The protein structure provides a starting point to tease apart the mechanism of activity of this new class of proteins and will give insight into the survival strategies of clathrate-dwelling organisms. In addition, CbpAs can be utilized as green gas clathrate inhibitors, as gas clathrate inhibition is a billion-dollar industry.

Poster #11 –Biochemistry

Presenter: Hyein Kang
PI: Jenny Yang
Co-Authors: Brenda-Ruth Mimba and Dongjun Li
Institution: Georgia State University

Title: Optimizing Purification of Collagen Targeted Protein MRI Contrast Agent for Early Detection

hProCA32.collagen 1 protein is a newly developed promising MRI contrast agent used to detect small, early stages of liver tumors and other liver diseases like liver fibrosis and cirrhosis. To prepare hProCA32.collagen protein for pre-clinical and clinical applications and facilitate drug discoveries, we need to develop an optimized expression and purification process with high yield. hProCA32.collagen contains two cysteine residues, and the formation of an intra-disulfide bond is required for its targeting capability. However, there is a challenge to the formation. Inter-disulfide bonds result in protein aggregation and disulfide bond shuffling. In this study, we first report the expression of hProCA32.collagen using an *E.coli* expression system with an average yield of cell pellets of 6 g/L with desired protein expressed. The goal of the purification was to purify the protein in order to separate hProCA32.collagen from other unwanted host cell proteins and refold the protein down to its monomeric form while increasing the protein yield after the purification process. The purification process was optimized by changing the FPLC purification column from the Q column to the SP column and adjusting the buffer pH from 7.4 to pH 5.5 and pH 6.0. As a result, using the FPLC purification with an SP column with pH 6.0, dimers, high oligomers, and other impurities were significantly decreased, and the sample mainly consisted of about 80% monomer. The purified protein exhibits high MRI contrast capability with high relaxivity, r_1 , and r_2 , which are several folds of clinically approved contrasts. Further optimizing this process for purification and formulation will facilitate the early detection of cancer and other diseases by non-invasive MRI.

Poster #12 –Biochemistry

Presenter: Andrew Schilling
PIs: Nicholas Hud, Suneesh Karunakaran and Gary Schuster
Institution: Georgia Institute of Technology

Title: Supramolecular Polymers Promote the Non-enzymatic Generation of Proto-Nucleic Acid Oligomers

The means by which biological informational polymers arose are currently unknown. The RNA world hypothesis implies that RNA oligomers emerged nonenzymatically, yet demonstration of such a process remains difficult. Alternatively, RNA may be a molecular descendent of proto-RNA, which in turn may be a descendant of an original polymer or contained nucleobases with an intrinsic capability to base pair at the monomeric level. Here we report prebiotically plausible heterocycle functionalized peptides (PNAs) as proto-RNA candidates. Interactions with opposing non-canonical nucleobases lead to hexad supramolecular assembly and upon conditions of condensing agents, polymers form. These PNAs spontaneously self-assemble to promote long and selectively supramolecular linear oligomers relative to non-assembled PNAs. These results highlight a possible pathway by which simple, self-assembling molecules could selectively and favorably elongate to form primitive informational polymers.

Poster #13 –Biochemistry

Presenter: Kenneth Liu
PI: Raquel Lieberman
Co-Author: Hailee Scelsi
Institution: Georgia Institute of Technology

Title: Biophysical Characterization of Previously Intractable Myocilin Olfactomedin Mutants

Mutations of myocilin are causative for 10-33% of juvenile open angle glaucoma cases, making it a leading cause of pediatric blindness. Known disease mutations are primarily found in the C-terminal olfactomedin domain (OLF) of myocilin and are highly destabilizing. While some of the more mild disease mutants have been recombinantly expressed and characterized in *E. coli*, the most severe mutations have resisted all attempts at purification. Using an algorithm designed to enhance recombinant protein folding in *E. coli*, we designed a highly stable mutated OLF scaffold. Borrowing ideas from protein engineering, we have inserted the most destabilizing disease mutations into the more stable OLF scaffold. We have successfully expressed and characterized these mutants in the engineered OLF. Our results show promise in allowing us to shed light on the structural and biophysical factors that may play a role in glaucoma pathogenesis.

Poster #14 –Biochemistry

Presenter: Dulciana Davis
PI: Roland Kersten
Institution: University of Michigan

Title: Discovery of Macrocyclic Ribosomal Peptides from *Glechoma hederacea*
(Ground Ivy)

Transcriptome mining is an effective tool for identifying bioactive macrocyclic peptides from plants by searching peptide biosynthetic genes. Transcriptome mining of genes encoding the BURP domain, a plant-specific peptide cyclase, has previously identified the anti-cancer bicyclic peptide moroidin in Japanese Kerria. Moroidins feature a 1.ring with a leucine-Cb-tryptophan-indole-N1-crosslink and a 2.ring with a tryptophan-indole-C2-histidine-imidazole-N2-crosslink. We hypothesize that moroidin anti-cancer activity is due to the 2.ring in the moroidin core peptide motif, and aim to find moroidin analogs with a different 2.ring-crosslink.

Using BURP domain mining of the moroidin core peptide as a strategy to find anti-cancer macrocyclic peptides, we identified a novel peptide, Glechomin, from *Glechoma hederacea* (Ground ivy) with a hypothetical macrocyclic bond *via* a C-terminal tryptophan-indole instead of a histidine-imidazole. This project aimed to isolate, purify, and structurally elucidate the chemical novelty of glechomin. Previously established peptide isolation techniques from the Kersten lab were used to purify the peptide fractions from *G. hederacea*, and preliminary structural elucidation was performed with ¹H-NMR. ¹H-NMR results showed that two indole amines were present in glechomin, which suggest a different macrocyclic crosslink in glechomin compared to the C-N-bond forming the 2.ring of moroidin. 2D-NMR studies are ongoing to structurally elucidate the full 2D structure of glechomin.

Poster #15 –Biochemistry

Presenter: Katelynn Powell
PI: Kerri Taylor
Co-Authors: Alisha Kennedy, Destini Thornton, Harris Carlisle, Shyrisse Ramos, John Gorden, Daniel Unruh, David Goode, Alexandra Taraboletti, Monica Frazier and Kerri Shelton
Institution: Columbus State University

Title: The Effects of Benzothiazole-Derivatives on the TDP-43 Protein in ALS Patients

Amyotrophic lateral sclerosis (ALS) is a progressive neurodegenerative disease that affects nerve cells in the brain and spinal cord. Motor neurons run from the brain to the muscles and impact voluntary muscle action where patients can lose the ability to speak, eat, move, and breathe. Riluzole is the only FDA-approved oral drug for ALS that has been shown to have little to no effects on the treatment and is a known benzothiazole compound. Using a series of substituted benzothiazoles that have been synthesized, this study will test these compounds on U2OS, SH-SY5Y, and HEK293T cells with overexpressed TDP-43 protein aggregates and their effects with each other. TDP-43 is a protein that is commonly found within the nervous system of sporadic ALS patients, and causes rapid pathogenic activities. During this process the cells will be analyzed for rate of growth in hopes of creating a cell model that will demonstrate an alternative therapeutic option for treating ALS.

Poster #16 –Biochemistry

Presenter: Sarah Clark
PI: Royce Dansby-Sparks
Co-Authors: Samantha Balboa and Leslie Hicks
Institution: University of North Georgia

Title: Identification of an Antimicrobial Compound from *Pseudomonas protegens* CHA0

The rise of multi-drug resistant pathogens and the dwindling availability of effective antibiotics requires the discovery of novel antimicrobial compounds to combat this global threat. Natural products, such as antimicrobial peptides, have played an indispensable role in the discovery of new antibiotics. The soil-based bacterium, *Pseudomonas protegens* CHA0, is known to secrete insecticides and fungicides, but its antibiotic abilities have not been fully assessed. The secretome of *P. protegens* CHA0 was investigated for the presence and efficacy of antibiotic compounds. Bacterial supernatant was harvested and fractionated using reversed-phase liquid chromatography. The fractions were subsequently assayed for antibiotic activity against *Escherichia coli*. Active fractions were then analyzed via LC-MS/MS. The MS/MS characterization confirmed that the bioactive fractions contained a known antimicrobial secondary metabolite, pyoluteorin. Further biological characterization is needed to determine the mechanism

of action and assess the spectrum of activity against other pathogens. These results highlight the significance of natural products as sources of antibiotics.

Poster #17 –Biochemistry

Presenter: Jon Dudkin
PI: Grace Kelley and Kerry Strickland
Institution: Mercer University

Title: Comparing Growth in Common Lab Media of Vmax™ X2 and BL21(DE3) *E. coli*

Vibrio natriegens (Vmax™ X2, *V. nat*) has been recently discovered as a promising chassis for molecular biology and biotechnology due to its fast generation time and genetic tractability. Although *V. nat* has been pushed in the synthetic biology field as a standard chassis for laboratory use in recent years, there are still a multitude of barriers that prevent the cell line from achieving its full potential. One of these barriers is the lack of a robust and well-characterized workflow and toolkit. This study aims to further develop the current *V. nat* toolkit, by exploring and quantifying growth of the *V. nat* strain in a variety of common lab media. Vmax™ X2 (glycerol stocks) were grown in 10 different lab media over 6 hours at two temperatures to determine optimal growth conditions. Our findings suggest that Vmax™ X2 outgrows BL21(DE3) *E. coli* in a multitude of common lab media. Future work will include further improvement of *V. nat* workflow, including transformation and protein expression optimization.

Poster #18 –Biochemistry

Presenter: Seth McDonald
PI: Jeremy Olson
Institution: University of North Georgia

Title: Novel Efficient Synthesis of Caged Coumarin Chromophores

It is known that conjugated coumarin compounds can extend the wavelength of light they absorb by adding particular electron donating and withdrawing groups to the base coumarin molecule. Coumarins can be synthesized using simple starting materials and act as caging chromophores when adding a biologically active molecule such as proline or glutamic acid. Once in contact with ultraviolet or visible wavelengths of light, these compounds may become uncaged. Unfortunately, most of these organic synthesis schemes are rather extensive and require several inputs and producing several intermediates. However, further research has found a neo-synthetical process that requires only two steps to make the caged coumarin chromophores. Comparatively, the novel scheme appears much more efficient than the previously accepted coumarin synthesis. Currently, this neo-synthetical process is being used to cage simple biological molecules such as proline, and in the future will be used to cage other biologically active molecules such as glutamic

acid and gamma amino butyric acid (GABA). This improved synthesis combined with extended conjugation, leads to increased efficiency and applications of caged chromophores.

Poster #19 –Biochemistry

Presenter: Kha Minh Nguyen
PI: Kerry Strickland
Institution: Mercer University

Title: Determination of the Optimal Lipid to Protein Ratio (LPR) for Nanodisc Formation with Varying Tail Features

The major structural components of cell and organelle membranes are lipids and membrane proteins. Membrane proteins are one of the largest subcategories of proteins and are associated with the lipid bilayer, representing a major drug target with applications in the fields of proteomics and biomedicine. The study of membrane proteins and lipid-protein interactions has been revolutionized by nanodisc technology. Nanodiscs are a synthetic model membrane system created using a membrane scaffold protein (*i.e.* MSP1D1); however, the optimal LPR in nanodisc formation has been determined for only a few synthetic lipids. This project will determine the optimal LPR for several combinations of lipids with different hydrocarbon chain lengths and saturation levels. Determination of these optimal LPRs for various lipid compositions will allow for the direct study of lipid structural features on membrane protein structure and function, especially in the presence of drug therapies. A high expressing MSP1D1 colony was selected after Western blot determination and MSP1D1 was purified *via* His-tag affinity chromatography using Fast Protein Liquid Chromatography (FPLC). Nanodiscs of a single, well-characterized lipid were generated to ensure proper function of MSP1D1. Future work will include improving the purification of MSP1D1 and determining the optimal LPR for lipids in various mixtures.

Environmental/Green Chemistry

Poster #20 – Environmental/Green Chemistry

Presenter: Tram Nguyen
PI: Rafael Quirino
Co-Authors: Larissa Richa, Anelie Pétrissans, Daniela Florez, Romain Remond, Baptiste Colin,
Vanessa Fierro, Alain Celzard and Mathieu Pétrissans
Institution: Georgia Southern University

Title: Experimental Study and Modeling of Thermodegradation During Torrefaction of Raw and Potassium Impregnated Beech Wood (Part 1)

The untreated wood material cannot be used directly in construction or the carpenter industry since it undergoes several degradations due to the hydrophilic character of the material and is vulnerable to the attacks of fungi. Chemical treatments like the use of biocide or preservation of this material pose a great threat to the environment and to the people who live nearby. Meanwhile, heat treatment such as torrefaction is an inexpensive but more environmentally friendly and sustainable way to upgrade the wood material's properties. Despite the intense development of industrial processes, a reliable tool is needed to control transformation progress and certify the final quality of the torrefied wood. A numerical tool simulating the wood transformation pathway could give recommendations to companies concerning process intensity (temperature and residence time). However, the thermal diffusivity represents a great obstacle to finding a unified kinetic model for wood torrefaction. In this work, the thermal diffusivity and thermal conductivity of beech wood treated at 180 °C, 220 °C, and 235 °C with the duration varying from 90 minutes to 240 minutes were measured on the hotplate and compared with the pre-treated samples. Initial results show a correlation in the thermal diffusivity of the material with the temperature and duration. This result suggests thermal diffusivity can be added to the previous two-step kinetic model for wood torrefaction of Di Blasi.

Poster #21 – Environmental/Green Chemistry

Presenter: Harris Carlisle
PI: Kerri Taylor
Co-Authors: Kari Goodwin, Elizabeth Klar and Kerri L. Shelton
Institution: Columbus State University

Title: Chemical Investigations of Organics and Metabolites in the Chattahoochee River

Water is quite vital to daily living and impacts life on a micro to macroscale. Our project seeks to conduct water analysis of the Chattahoochee River and its tributaries to determine the components in the water. The Columbus Water Works (CWW) facility in Columbus, GA is noticing chlorinated hydrocarbons, such as chloromethane, chloroethane and dichloromethane, after the disinfection process of the water. High levels of such compounds are identified post rain. Presently, the facility is treating the water with NaClO₄ (sodium perchlorate), and noticed issues in their effluent, meaning it is coming from their facility's two locations, roughly 4.3 miles apart. Chemical Testing will be utilized to identify the organic compounds located in the influent and effluent water of the two plants. The aim is to identify what organic compounds are found in the influent water and help Columbus Water Works finalize a modified treatment procedure to remove the organics during water purification.

Poster #22 – Environmental/Green Chemistry

Presenter: Starr Jenkins
PI: Omar Villanueva
Institution: Georgia Gwinnett College

Title: Catalytic Aerobic Oxidation of Benzylic Amines to Imines Utilizing a Sustainable Copper/TEMPO System

The synthesis of imines from benzyl amines is an essential reaction in chemical research. Imines are highly sought-after intermediates or products in various biologically relevant and biologically active compounds. Traditionally, imine synthesis involves toxic reagents or harsh reaction conditions; finding alternative pathways to make these reactions more sustainable through catalysis remains a critical tool in synthesizing these organic compounds. This research looks at implementing the catalytic oxidation of benzyl amines to imines using sustainable green methods. Additionally, this research explores implementing these sustainable tools in an undergraduate organic chemistry laboratory. This presentation will highlight our current work to employ a protocol adapted from contemporary research literature that can provide undergraduate students with practical experience of a modern, “green” oxidation method. In addition to the practical aspects, the experiment allows and encourages student discussion and exploration of sustainable reactions, a topic underrepresented in the contemporary undergraduate organic chemistry curriculum.

Poster #23 – Environmental/Green Chemistry

Presenter: Raven Nicole Stanlet
PI: Laurel A. Royer
Co-Authors: Pamela Leggett-Robinson and Nichole Powell
Institution: Carinalis Consulting and Research, PLR Consulting,
Oxford College of Emory University

Title: Implications for Disproportionate 1,4-Dichlorobenzene Exposures Among Communities of Color

Disproportionate chemical exposures among communities of color is a topic of concern as highlighted in research publications and the ongoing work of environmental justice organizations. Socioeconomic factors can exacerbate exposures as many people of color live, work, and play in spaces that increase the potential for acute and chronic exposure to chemicals. Systemic inaccessibility to safe living spaces and “healthier” chemical agents in cleaning and personal care products can increase the risks. One such chemical with limited research is 1,4 –Dichlorobenzene (1,4–DCB). 1,4–DCB has also been identified in Feminine Hygiene Products (FHPs) including those that are more commonly used by women of color such as douches. This study investigates the ways 1,4–DCB impacts women of color disproportionately through the use of FHPs.

Poster #24 – Environmental/Green Chemistry

Presenter: Olivia Kapwadi
PI: Laurel Royer
Institution: American Chemical Society

Title: Analyzing the Disproportionate Effect of Pesticide Exposure in Communities of Color

A recent study by Donley confirmed the decades-long theory of disproportionate exposure to pesticides in communities of color. This exposure can be occupational; through food and water, or in the home. 2 pesticides from this study, DDT and 2,4-D showed significant concentrations in the blood and urine of Black and Mexican individuals compared to White individuals. Results showed a high storage content of DDT's metabolite DDE in adipose(fat) tissue, and a linkage between these pesticides and cancer onset, as well as generational exposure through gestation, although DDT was banned for use in 1972. 2,4-D was also determined as a possible carcinogen. However, its metabolite was found in the urine, indicating that exposure came from the parent 2,4-D. These past, present, and future implications reaffirm the notion of unfair exposure in communities of color, and the effects that follow suit.

Poster #25 – Environmental/Green Chemistry

Presenter: Chaunie Banks
PIs: Laurel A. Royer, Pamela Leggett-Robinson and Nichole Powell
Institution: Carinalis Consulting and Research, PLR Consulting,
Oxford College of Emory University

Title: Analyzing Pesticide Residue Exposure to Communities of Color Through Use of Shampoos and Conditioners

Many hair products that are available in today's market include common chemicals that are primarily tested on straight hair for fighting lice bugs, which do not commonly attach to curly hair types. Although these products are efficient for straight hair, the chemicals present are harmful to African American hair, thus causing disparities in dandruff prevalence, hair loss/breakage, and dry, itchy scalp. The chemicals present in shampoos and conditioners (regardless of hair type considerations) are pesticide residues. Such common pesticide residues are Sodium Lauryl Sulfate and Methylisothiazolinone. This study investigates excessive residue exposure and the disparities for communities of color through use of hair care products.

Poster #26 – Environmental/Green Chemistry

Presenter: Chaunie Banks
PIs: Laurel Royer, Pamela Leggett-Robinson and Nichole Powell
Institution: Oxford College of Emory University

Title: Analyzing Pesticide Residue Exposure to Communities of Color Through Use of Shampoo and Conditioner

This project represents an analysis of Environmental Protection Agency (EPA) registered pesticides found in shampoos and conditioners, and the effect the chemicals have on African hair. The topic was studied to understand if Communities of Color are appropriately exposed to these chemicals. Literature reviews, fact sheets, and physical hair product labels were reviewed to determine the necessity of these pesticides in the hair products. The makeup and structure of Afro hair was researched to understand the effect these chemicals have on the hair strands and scalp. There are data presented that represents the African American community, particularly Black women, and the common negative hair experiences faced. There was no experiment conducted, this study represents an investigation and analyzation to create an informative poster. Studies of Afro hair properties; what is needed; and what is avoidable to take proper care of the hair type will be continued. Ways to provide a platform for more transparent communication of proper hair health for communities of color will also be addressed.

Poster #27 – Environmental/Green Chemistry

Presenter: Katheryn Foust
PI: Marina Koether
Institution: Kennesaw State University

Title: Mapping Microfibers in Lake Allatoona Water

Microfibers were found during a water study at six beach locations on Lake Allatoona. This lake is manmade, fed by a river and flows into a river *via* a power plant and dam. A wastewater plant discharges into the lake. Five plankton nets were used at each location to skim the water and retain the microfibers. After digestion, microfibers were counted by microscopy. Results ranged from 7.3 - 14.2 microfibers/m³. These results indicate that a concentration gradient of microfibers exists based on the distance from the wastewater plant.

Poster #28 – Environmental/Green Chemistry

Presenter: Nadine Abrahamse
PI: Neha Garg
Co-Authors: Monica Monge and Jessica Deutsch
Institution: Georgia Institute of Technology

Title: Culture-Based Strategies for Marine Bacteria Natural Product Discovery

Stony coral tissue loss disease (SCTLD) is an illness devastating Scleractinian corals, spreading rapidly through the coast of Florida and down into the Caribbean. This work focuses on bacterial interspecies cross-talk as a driver for secondary metabolite production in an attempt to develop possible treatments for SCTLD. One strain of *Vibrio coralliilyticus*, a known coral pathogen associated with SCTLD, has been isolated from healthy Atlantic corals. Data from cocultures has provided insight into metabolome changes resulting from interactions of *V. coralliilyticus* and other marine-derived bacteria. In an untargeted metabolomics approach, natural product databases and molecular networks have aided in identifying secondary metabolites that are inhibited and upregulated in coculture. Results from this analysis workflow could lead to essential discoveries about how the microbiome of a coral could be manipulated to fight a disease like SCTLD.

Poster #29 – Environmental/Green Chemistry

Presenter: Alexa Luna
PIs: Alexandria Focsan and Gopeekrishnan Sreenilayam
Institution: Valdosta State University

Title: Carotenoid Extraction Using an Emerging Green Approach

Carotenoids are the pigments found in plants which have been proven to be excellent antioxidants. These pigments could potentially scavenge free radicals within the human body produced by common metabolic reactions. An overwhelming amount of free radicals in the body is what leads to oxidative stress which can cause a number of degenerative chronic diseases. These supplements are currently being extracted using volatile organic solvents (VOS). These solvents pose plenty of risk to the environment, are very dangerous to work with in larger quantities, and are not very economical. Deep eutectic solvents (DES), on the other hand, are organic solvents composed of biodegradable compounds which are much safer for the environment. This extraction method is fairly new but most definitely worth exploring.

In this project, four different choline chloride based DES's were used to extract the pigments from spinach leaves and then analyzed using an HPLC with YMC C30 Carotenoid column. These results were then compared with spinach leaves extraction data obtained from six commonly used VOS's (acetone and others). Identity of various pigment peaks in the HPLC chromatogram were assigned as mentioned in the literature. In the future, quantitative extraction efficiency of DES vs VOS will be mapped after constructing the calibration curves for significant peaks in the HPLC chromatogram.

Organic Chemistry

Poster #30 – Organic Chemistry

Presenter: Ashley Goehrig
PI: Paula Nolibos
Institution: University of North Georgia

Title: Organic Chemistry Concept Maps: An Interactive Approach to Helping Students Review Organic Chemistry I Reactions

Organic chemistry topics are focused on learning to name organic compounds, spatial orientation, arrow pushing mechanism, organic reactions and logical synthetic sequences. In this activity we focus on providing students with a different approach to integrate all the reactions covered in an organic I course. We sought to design an interactive, cooperative activity in which students could practice the reactions covered using concept maps. The activity was broken into two parts. In the first part, each group of 2 – 3 students receive a partial concept map and a zip lock bag with the pieces needed to complete the concept map. During the second part, all groups work together to intertwine all concept maps together. Students were asked to provide feedback *via* a survey at the end of the class period. Overall, the student response was positive, indicating that they felt more confident about their knowledge of the reactions covered than they did prior to the class period.

Poster #31 – Organic Chemistry

Presenter: Dahnielle Milton
PI: Davita McTush Camp
Institution: Spelman College

Title: Use of Dioxiranes in the Epoxidation of Oleochemicals

Human exposure to hazardous materials from consumer products has been a growing concern over the past several decades. Human exposure to these materials is widely variable but ubiquitous in the general population and in subpopulations. Some of the hazardous chemicals include phthalates, dioxins, parabens, and bisphenol reagents to name a few. These chemicals are found in many everyday products such as food, food containers, detergents, toys, pesticides, and cosmetics. More importantly, studies have shown that these chemicals have caused health concerns including developmental, reproductive, brain, and immunity issues amongst the general population. Phthalates are amongst these hazardous materials; are widely used and are endocrine disruptors that can interfere with the human body's hormones known as the endocrine system. This project will explore the synthesis of epoxy-fatty acids and epoxy-vegetable oils, necessary alternatives to phthalates, by utilizing the very reliable and efficient oxidizing agents dimethyldioxirane and ethylmethyldioxirane.

Poster #32 – Organic Chemistry

Presenter: Corina Paun
PIs: Neelam Khan, Sang Park and David Pursell
Co-Authors: Jasmin Mena, Pedro Rodriguez-Romero, Tyler Rockey and Jessica Taza
Institution: Georgia Gwinnett College

Title: Biofuel Synthesis, Characterization, Blend Performance, and Combustion Analysis

Biofuel was synthesized from peanut oil trans-esterification and characterized for suitability as an alternative fuel. Biofuel was blended with commercial diesel and used to power a 5-kW diesel generator. The biofuel, its blends, and exhaust gasses and particles were characterized using FT-IR, GC-MS, AFM, and viscometry. This research is ongoing.

Poster #33 – Organic Chemistry

Presenter: Mason Jones
PI: Rahul Shahni
Institution: University of North Georgia

Title: Synthesis and Characterization of a Furfural Derived Semi-Rigid Diol

A semi-rigid diol monomer that bridges the gap between flexible aliphatic chain and rigid aromatic counterparts replaces BPA in the production of polyesters and polycarbonates with outstanding thermal and mechanical properties. Bio-advantaged chemicals such as furfural and malonic acid have been utilized as non-petroleum-based feedstocks towards biomass derived compounds. In this study, 2-furanarylic acid (FAA) was synthesized from furfural and malonic acid *via* Knoevenagel condensation; and is followed by environmentally friendly [2+2] solid-state photoreactions to afford *rac*-3,4-di-2-furanyl-1,2-cyclobutanedicarboxylic acid (CBDA-2). The dicarboxylic acid (CBDA-2) was further reduced using sodium borohydride in the presence of an electrophile to the corresponding semi-rigid 3,4-(furan-2-yl)-cyclobutane-1,2-diol (CBDO-2). The structure of FAA, CBDA-2, and CBDO-2 were characterized using spectroscopic techniques. CBDO-2 showed the potential to function as a semi-rigid building block for polymeric materials with desired thermal and mechanical properties.

Poster #34 – Organic Chemistry

Presenter: Byron Fisher
PI: Ajay Mallia
Institution: Georgia Gwinnett College

Title: Gelation and Photophysical Studies of Aminophenylalkanamides as Low Molecular Mass Gelators

To understand the relationship between molecular structure and the molecular properties, six aminophenylalkanamide derivatives were synthesized. The synthesized compounds differ in the location of the substituent alkylamine group and the length of the alkyl chain. In pursuit of understanding the similarities and differences of the aminophenylalkanamides derivatives, a series of analytical techniques were used. These techniques included TLC plate analysis, IR spectroscopy, UV-Vis spectroscopy, and fluorescence spectroscopy. A gelation study of the compounds of interest was also conducted. From the rendered studies, it was found that the 2-(aminophenyl)tetradecanamide only formed gels with silicone oil, carbon tetrachloride, and dimethyl sulfoxide as the solvent.

Poster #35 – Organic Chemistry

Presenter: Jessica Budwitz
PI: Christopher Newton
Institution: University of Georgia

Title: A Diels–Alder Disconnection of *para*-Quinones

The *para*-quinone motif is present within a wide array of settings, including reagents, dyes, and bioactive natural products. Consequently, efficient strategies toward the synthesis of this motif are of significant importance, especially with respect to highly convergent ring-forming approaches. An overview of the state-of-the-art with respect to such approaches is presented, highlighting our recent contribution leveraging the Diels–Alder reactivity of 2,5-*bis*(*tert*-butyldimethylsilyloxy)-furans. Alkenic and alkynic dienophiles, including arynes, provide direct access to either *para*-hydro or benzoquinones, respectively. Extension to diene-transmissive reactivity, the total synthesis of the natural product indanostatin, and the synthesis of *para*-aminoquinones from the corresponding pyrrole derivatives demonstrates the generality of our methodology. Our most recent unpublished contribution concerning the development and optimization of a > 20 g scale approach to the 2,5-*bis*(*tert*-butyldimethylsilyloxy)furan motif, followed by reaction with benzyne, will also be presented.

Poster #36 – Organic Chemistry

Presenter: Jeremy Norton
PI: Ajay Mallia
Co-Authors: Terukimi Hayashi and Erica Lee
Institution: Georgia Gwinnett College

Title: Synthesis, Self-Assembly, Gelation Studies, and Steady-State Fluorescence properties of Anthraquinonylalkanamides-Based Low Molecular Mass Gelators

Anthraquinones can be found in various herbs and have been known to exhibit many biological functions. Cleavage of DNA by irradiation of substituted anthraquinones is also reported. The present study discusses the synthesis and gelation studies and steady-state excitation and emission properties of anthraquinonylalkanamides as low molecular mass gelators. Low molecular mass gelators are viscoelastic materials that can be considered an important class of soft materials. The gelator molecule aggregate *via* weak intermolecular interactions such as hydrogen bonding, Van der Waals interactions, and π - π stacking to form a three-dimensional fibrillar network that can trap a large amount of liquid. Anthraquinonylalkanamides with varying alkyl chain lengths have been synthesized and characterized. Correlations between the molecular structures of the anthraquinonylalkanamide gelators and the properties of their gels, as well as fluorescence properties will be presented.

Poster #37 – Organic Chemistry

Presenter: Nguyen Le
PI: Ajay Mallia
Co-Author: Joshua Leonora
Institution: Georgia Gwinnett College

Title: Steady-State Excitation and Emission, and Gelation Properties of Alkyloxycoumarin Derivatives as Low Molecular Mass Gelators

Molecular gels are a class of soft materials that play an essential role in biomedical applications, such as drug-delivery systems, sensors, and injectable gels. Also, fluorescent molecular gels have potential applications in sensing since its light-emitting. Coumarin derivatives have been reported to find application in medical imaging. In the present study, a series of four alkylated coumarin derivatives were prepared from 7-hydrocoumarin and 4-hydrocoumarin; 7-dodecyloxycoumarin (7C12), 7-decyloxycoumarin (7C10), 4-dodecyloxycoumarin (4C12), and 4-decyloxycoumarin (4C10); and characterized using spectroscopic (NMR, IR, UV-Vis, Fluorescence) and thermal analysis (MP, DSC). Gelating ability of the synthesized compounds in various polarity liquids as well as the steady state fluorescence properties of the synthesized compounds will be presented.

Poster #38 – Organic Chemistry

Presenter: Joshua Leonora
PI: Ajay Mallia
Co-Author: Nguyen Le
Institution: Georgia Gwinnett College

Title: Synthesis, Characterization, Steady-State Fluorescence and Gelation Properties of Coumarin-Linked Cholesteryl Derivatives

Coumarin derivatives are known to exhibit pharmacological properties. In the present study coumarin-linked cholesteryl derivatives have been prepared from 7-hydrocoumarin and 4-hydrocoumarin. All the synthesized compounds were characterized using spectroscopic and thermal methods. UV-Vis, fluorescence properties, gelation studies of the synthesized compounds will be presented.

Poster #39 – Organic Chemistry

Presenter: Romy Doan
PIs: Ajay Mallia and Joseph Sloop
Co-Authors: Madeline Faass
Institution: Georgia Gwinnett College

Title: Synthesis, Characterization, and Steady-State Fluorescence Properties of 2-(benzylidene)-1-Indanone Derivatives

Chalcones consist of at least two aromatic rings connected using an α , β -unsaturated ketone and are reported to have biological and therapeutic properties. In the present study, three derivatives of 2-(benzylidene)-indan-1-one have been synthesized by the condensation reaction between 1-indanone and the corresponding benzaldehyde derivative and characterized. All the synthesized compounds were characterized using thermal (melting point, DSC) and spectroscopy studies (IR, NMR, UV, fluorescence). Characterization data will be presented.

Poster #40 – Organic Chemistry

Presenter: Ken Aratame
PI: Maged Henary
Co-Author: Stefanie Casa
Institution: Georgia State University

Title: Fluorinated Indolenine-Based Squaraine Near-Infrared Dyes: Synthesis, Characterization, and Optical Properties

Fluorinated drugs have been shown to exhibit unique pharmacological properties in literature. These include tissue selectivity, cell uptake, and improved solubility. Such improvements have led to an increase in fluorinated drugs on the market. One class of drugs, squaraine-based fluorophores, could particularly benefit. Currently, there is a pressing need for advanced dyes that exhibit high optical activity in the near-infrared window. The associated improvements of fluorination in terms of tissue selectivity and solubility could lead to exciting biodistributive and optical performance. To explore the effects of fluorination, two fluorine-containing squaraine dyes in the near-infrared region were synthesized. Furthermore, preliminary computational analysis and optical properties of the dyes were obtained.

Inorganic/Organometallic Chemistry

Poster #41 – Inorganic/Organometallic Chemistry

Presenter: Katelin Gary
PI: Ryan Meier
Co-Authors: Meghan Richter and Gina Diodati
Institution: University of North Georgia

Title: N-Heterocyclic Carbene Complexes of Nickel: An Examination of Synthetic Options and Target

Organometallic catalysts are used throughout industry, but many are not cost-efficient or use easily accessible materials. This study focuses on creating an organometallic catalyst that shows similar behaviors to catalysts containing palladium and platinum while being cheaper to produce. The process involves the synthesis of the ligand group 1,3-di(2-picoly)imidazolium chloride for the further purpose of coordinating a Ni²⁺ metal ion. This ligand, 1,3-di(2-picoly)imidazolium chloride, reacts with strong bases to form a carbene which allows for the organometallic catalyst to form with Ni. This study explores different synthetic routes to forming these catalysts.

Poster #42 – Inorganic/Organometallic Chemistry

Presenter: Justin Bindewald
PI: Ajay Mallia
Institution: Georgia Gwinnett College

Title: Structural Properties of Iron(0) Nanoparticles in Micellar Solutions and Deep Eutectic Solvents

Iron(0) nanoparticles are reported to have strong reducing properties that can react and remove a wide variety of water contaminants. This study investigates the properties of iron(0) nanoparticles suspended in sodium dodecyl sulfate micellar solutions and deep eutectic solvents using spectroscopic (UV-Vis, and IR), dynamic light scattering, and surface tension studies. Iron(0) nanoparticles were prepared by the reduction of iron(II) sulfate in ethanol with sodium borohydride. We noted that the addition of varying concentrations of iron(0) nanoparticles did not significantly affect the surface tension of the sodium dodecyl sulfate solutions, whereas drastic changes in UV-spectra were observed. A systematic comparison of dynamic light scattering and spectroscopic studies of iron nanoparticles in sodium dodecyl sulfate solutions as well as in deep eutectic solvents will be presented.

Poster #43 – Inorganic/Organometallic Chemistry

Presenter: Andrea Mancina
PI: Anne Grior-Fendler
Co-Author: Weidong Zhang
Institution: Université Claude Bernard Lyon 1

Title: Catalytic Oxidation of Propene through Transition Metal Modified α -MnO₂ Catalysts Decreases Conversion Temperature

Volatile organic compounds (VOCs) have been a growing source of indoor and outdoor pollution due to their production of ground-level ozone and negative health effects on those exposed. Catalytic oxidation is a method to remove VOCs by oxidizing them into CO₂ and water at lower, safer temperatures using catalysts, such as metal oxide catalysts. A common metal oxide catalyst, MnO₂, has often been used in oxidizing different VOCs; however recent studies have shown that doping MnO₂ with transition metal cations can enhance the activity of the MnO₂ catalyst, specifically α -MnO₂. α -MnO₂ is a promising catalyst due to its particular morphology which includes a (2 x 2) tunnel of 4.6 Å that is able to accommodate metal cations. Thus, we explored this enhancing effect by modifying α -MnO₂ with the cations Fe³⁺, Co²⁺, Ni²⁺, Cu²⁺, Y³⁺, La³⁺, Ce³⁺, and studied how these changes facilitated the oxidation of a common VOC, propene. The doped catalysts were prepared *via* a redox precipitation method, and characterized using X-ray diffraction (XRD); Fourier-transform infrared spectroscopy (FTIR); Raman spectroscopy; nitrogen (N₂) adsorption-desorption analysis; hydrogen temperature-programmed reduction (H₂-TPR), and oxygen temperature-programmed desorption (O₂-TPD). Lastly, the catalytic performance was tested using an online gas chromatography (GC) system. It was found that the Fe-MnO₂ catalyst had the best performance for the complete oxidation of propene with T90 of 205 °C at a space velocity of 60,000 mL/g•h. The characterization data highlighted that the catalysts had changes in their surface structures, lattice composition, and redox ability due to the metal cation doping, likely explaining their ability to catalyze the oxidation reaction of propene. These results have indicated that the doping of metal cations into a metal oxide catalyst such as MnO₂ aids the oxidation of propene and provides complete oxidation at lower temperatures that are safer and more efficient for industrial use.

Poster #44 – Inorganic/Organometallic Chemistry

Presenter: Annaleena Hansen
PI: Sidney Creutz
Co-Author: Tom Boggess
Institution: Mississippi State University

Title: Synthesis of Cæsium Bismuth Sulfide Compounds, a Precursor to Lead Free Perovskites

A major topic of research in recent years has been lead halide perovskites, for their impressive power conversion efficiencies when applied to the structure of a solar cell. However, due to the toxicity of lead and the poor overall stability of lead halide perovskites, a specific interest in synthesizing lead free, more stable perovskites has been conducted. One option in achieving a lead free perovskite, is a mixed anion approach, with the chemical formula CsBiChX_2 , where Ch is a chalcogenide and X is a halide. Unfortunately, a direct synthesis route is not feasible and a cæsium bismuth sulfide (CsBiS_2) precursor is required. Two major synthesis pathways were investigated to form CsBiS_2 . In the first pathway, the reagents cæsium hexamethyldisiloxane, bismuth hexamethyldisiloxane, diethylthiourea, and oleylamine were combined and reacted. The other pathway utilized cæsium dicyclohexyldithiocarbamate, bismuth diethyldithiocarbamate, and oleylamine. To characterize and confirm a successful synthesis, powder x-ray diffraction (PXRD), as well as transmission electron microscopy (TEM) were performed. By comparing the bulk CsBiS_2 x-ray pattern, it was determined that by using the dithiocarbamate precursors, there was great potential that the correct material was made. To further study the compatibility of the dithiocarbamate precursors, the concentration of reagents, molar stoichiometry, and solvent were also altered and researched. After CsBiS_2 is successfully made and characterized, the goal is to achieve a perovskite structure through a halide anion exchange.

Poster #45 – Inorganic/Organometallic Chemistry

Presenter: Janae Burks
PIs: Bradley C. Childs (Lawrence Livermore National Laboratory) and
Michelle Gaines (Spelman College)
Co-Authors: Maryline G. Ferrier; Michelle M. Greenough; Kiel S. Holliday
Institutions: Spelman College and Lawrence Livermore National Laboratory

Title: Synthesis of Uranium Organometallic Precursors for Laser Irradiation

Uranium (IV) tetraiodide organometallic complexes are unique coordination compounds used to create uranium ceramics under extreme thermal conditions. These materials can be incorporated into next generation nuclear fuel as well as storage of nuclear materials. However, they are challenging to synthesize because uranium is an actinide metal that has a high reactivity in its metallic state. In syntheses, this creates an unstable environment under most conditions. This research focused on synthesizing uranium (IV) tetraiodide, complexed with (1,4) dioxane. The synthesis was conducted on a Schlenk line to maintain an air and water-free environment. Once synthesized, the precursors were exposed to laser irradiation, to convert them into a uranium ceramic. The final products were characterized *via* X-ray diffraction and scanning electron microscopy, which showed evidence of conversion to the ceramic product. This research will help provide more insight for creating larger quantities of uranium complexes for future applications.

Physical/Computational Chemistry

Poster #46 – Physical/Computational Chemistry

Presenter: Jane Yoo
PI: Neville Forlemu
Institution: Georgia Gwinnett College

Title: Computer Aided Anti-Malarial Drug Design Targeting *Plasmodium falciparum* Glutathione S-Transferase

Plasmodium falciparum Glutathione S-Transferase (PfGST) and Glutathione S-transferase alpha 2 (GST A2-2; human GST) are critical enzymes that protect cells against cytotoxic compounds. The structural differences in the active sites of PfGST and GST A2-2 makes these enzymes attractive targets for drug development against the world scourge that is malaria. With 200 million cases and 600,000 deaths annually, there is a growing need for the development of effective, less toxic and less expensive antimalarial agents. This is in part due to growing resistance to chloroquine and artemisinin-based antimalarials as a result of the multiple mutations engineered by *Plasmodium falciparum*, the causative agent of Malaria.

In this study, Computer Aided Drug Design (CADD) was used to design ligands that can selectively target PfGST. Specifically, the interactions between 9 current antimalarial drugs with GST were modeled using AutoDock Vina and Chimera. The initial binding data show that all the ligands formed stable complexes with the GST, with binding affinities ranging from -5.7 to -8.45 kcal/mol. The most energetically favorable complexes involved the benchmark drug artemisinin. However, all the ligands modeled were more tightly bound to GST A2-2 compared to PfGST.

To mitigate this, new ligands were designed by varying molecule polarity with functional group substitutions and structure rigidification based on the artemisinin pharmacophore. Of nearly 70 ligands designed, four (D48, D50, D61, and D63) matched or exceeded the binding affinity of artemisinin to PfGST. Of these four, D63 had the most favorable binding energy (-9.27 kcal/mol) while also closing the gap of the score difference between the ligands to PfGST and GST A2-2 most effectively. This suggest molecules with the D63 framework can selectively enhance binding to PfGST.

Poster #47 – Physical/Computational Chemistry

Presenter: Kathryn Monheim
PI: Suri S. Iyer
Co-Author: Tianwei Jia
Institution: Georgia State University

Title: Synthesis of Fluorescent Dyes for Incorporation into Silica Nanoparticles

The Iyer group focuses on developing a point of care diagnostic strategy for the early detection of pathogens. To this end, our research examined the synthesis of Janelia Fluor 549 for incorporation into 30 – 100 nm silica nanoparticles. We synthesized Janelia Fluor according to the procedure reported by Lavis *et al.* and modified it to attach the dye to a silica nanoparticle. This dye is highly fluorescent with a quantum yield of 0.88, and an extinction coefficient of $101,000 \text{ M}^{-1}\cdot\text{cm}^{-1}$, giving it a brightness of $88,880 \text{ M}^{-1}\cdot\text{cm}^{-1}$. The conjugation to a suitable precursor and subsequent fabrication of the dye encapsulated silica nanoparticle will be the focus of this presentation.

Poster #48 – Physical/Computational Chemistry

Presenter: Oluwaseun Omodemi
PI: Martina Kaledin
Co-Authors: Janiyah Riley and Ramsay Revennaugh
Institution: Kennesaw State University

Title: Computational Study of $\text{N}_4\text{H}^+/\text{N}_4\text{D}^+$ Raman Vibrational Spectra

This work focuses on developing theoretical techniques to study Raman spectra that are complementary to experimental studies. Raman spectroscopy is practical when identifying symmetrical vibrations that are IR inactive in molecules whose vibrations tend to be infrared dark. Computational cost and efficiency are of great significance when developing computational techniques for robust systems, such as biological molecules. Hence, we developed and tested a polarizability tensor surface in the analytical form that is used to calculate the Raman spectra. The computational method and level of theory was CCSD(T)/aug-cc-pVTZ(H:sp, N:spd) to generate data points. This method yields relatively low Root Mean Square error (RMS) as compared to a full CCSD(T)/aug-cc-pVTZ treatment. A comparison of harmonic vibrational spectra to molecular dynamics (MD) and driven molecular dynamics (DMD) suggests a presence of anharmonic features in the region between 500-2000 cm^{-1} corresponding to the asymmetric parallel proton transfer overtone, $2\nu_4$. Additionally, a Fermi resonance was identified using the DMD analysis near 2400 cm^{-1} , attributed to the N-N symmetric stretch, ν_1 and the perpendicular proton transfer overtone, $2\nu_6$.

Poster #49 – Physical/Computational Chemistry

Presenter: Mary Kate Smith
PIs: Eric Huddleston and Zane Miller
Institution: University of North Georgia

Title: Anionic Polymerization of Styrene in Flow

Flow chemistry offers many advantages over traditional batch chemistry such as increased control over fluid dynamics, thermal transport properties, and kinetics due to high surface area to volume ratios. Additionally, anionic polymerization offers control over molecular weight and molecular weight distribution. The anionic polymerization of styrene with *sec*-butyllithium as an initiator using a reactor comprised of simple laboratory tubing, commercially available fittings and T-connectors with fluids driven by syringe pumps is presented. The polymeric products are characterized by ¹H NMR, TGA/DSC, and IR spectroscopy.

Poster #50 – Physical/Computational Chemistry

Presenter: Sara Sarasiya
PI: Maged Henary
Institution: Georgia State University

Title: Synthesis and Optical Characteristics of Perimidine-Containing Squaraine Dyes

NIR molecular probes offer two major advantages over small molecules, which emit at visible wavelengths. First, biological tissues have lower absorption in NIR light than light; this enables NIR light to penetrate deeper into tissue than the compounds emit light at visible wavelengths, thus enabling the assessment of data from deeper structures. Second, less autofluorescence is present at the NIR compared to visible wavelengths, enabling higher signal-to-background ratios. Therefore, molecular probes that emit light within the NIR region are expected to be suitable for bioimaging.

Perimidine-based squaraine dyes have shown absorbance over 800 nm. Numerous squaraine dyes have been synthesized over the years, but they have not been able to utilize the full NIR window. The use of 2,3-dihydro-1H-perimidines heterocycle has generated compelling results in optical properties. The larger conjugated heterocycle allows for red shift in absorbance beyond 800 nm. Herein, we are reporting the synthesis and characterization of the red shifted probes.

Poster #51 – Physical/Computational Chemistry

Presenter: Aneri Amin
PI: Neville Forlemu
Institution: Georgia Gwinnett College

Title: Solution Structures of Novel Cyclotides Sequences (alca 1 and alca 2) Using Homology Modeling and Molecular Dynamics Simulations

Cyclotides are plant-based peptides with exceptional stability and structural features that has rendered them amenable for fine tuning for development of pharmaceutical therapies, environmentally friendly pesticides, and important biological activities. Their self-aggregation, functional complexes with proteins and lipid bilayer membranes are at the center of their widespread applications. However, structural characterization is still a key obstacle in fully understanding and functionalization of cyclotides. In this study, we apply computational tools including homology modeling, molecular dynamics simulations and molecular docking to study solution structures of two novel cyclotides (alca 1 and alca 2), and possible supramolecular complexes formed. The three-dimensional coordinates alca 1 and alca 2 homology models were obtained from templates with sequence identity ranging from 65-70 %. The cyclic cystine knot (disulfide bridge system) in all models built (SwissModel and Robetta servers) was conserved with the root mean square deviation (RMSD) of 0.864 Å for alca 1 and 0.880 Å for alca 2. The backbone cyclization of the models with the best Q-mean scores was done manually using the UCSF Chimera build tool. The cyclized models were then energy minimized and equilibrated in an NPT ensemble for 1 ns, followed by 100 ns production dynamics. Unbiased simulations indicate a radius of gyration of 8.425 Å for alca 1 and alca 2, consistent with other cyclic peptide structures solved by NMR (Nuclear Magnetic Resonance). The disulfide bond network distances range from 1.9 to 2.20 Å and the non-conserved residues in N-terminus fluctuate the most (as expected). However, these are not the most stable structures for alca 1 and alca 2, due to a high protein RMSD and incomplete sampling that will be addressed with enhanced free energy MD methods. The dimerization and aggregation of cyclotides was also modeled using the peptide docking module of MOE (Molecular Operating Environment) and all atom MD (Molecular Dynamics) simulations. Cyclotides with different physicochemical properties formed docked poses (dimers) with binding affinities ranging from -9.0 to -4.0 kcal/mol. Dimers were stabilized by local favorable contact independent of the overall charge of the monomers. The potential for stable dimers and aggregation from unbiased MD may suggest that aggregation to supramolecular complexes is critical for cyclotide activity.

Poster #52 – Physical/Computational Chemistry

Presenter: Uyen Ta
PI: Melanie Reber
Co-Author: Nicholas Cooper
Institution: University of Georgia

Title: Yb-Doped-Fiber-Laser Femtosecond Pulse Compression with Double-Pass Gratings and Filters

Ultrafast lasers are an effective tool in pump-probe spectroscopy, imaging, micromachining, *etc.* In this project, we characterize a new method to conveniently compress ultrafast laser pulses by about a factor of three. By adjusting degrees of filters, and quarter- and half-wave plates, the magnitude of the group delay dispersion is minimized to yield the most compressed pulse. Using the Knox method to measure laser dispersion, the group delay dispersion could be quantified at different intracavity double-pass grating compressor separation. We successfully compress temporal 120 fs from Yb-doped fiber laser to 41-43 fs pulse. In the future, the pulse will be used in the cavity-enhanced transient absorption spectrometer (CETAS) to study molecular dynamics in quantum mechanical systems of different molecules and clusters.

Poster #53 – Physical/Computational Chemistry

Presenter: Imani Rogers
PIs: Anil Banerjee,
Co-Authors: Austin Clance and Kristina Armstrong
Institution: Columbus State University

Title: Synthesis, Activity, and Characterization of Pd/Al₂O₃ Catalysts for Methane Combustion Under Stoichiometric Conditions

Through studies on lowering greenhouse gasses, catalytic combustion of methane at low temperatures under stoichiometric conditions has proven to be suitable. A Pd catalyst (3.3 wt.% Pd) on γ -alumina support was prepared by a slurry-incipient wetness-vortex method. The catalyst was calcined at 500 °C and 850 °C to study the effect of calcination temperature on methane conversion. The activity (% conversion of methane) of each catalyst was determined in a fixed-bed temperature-controlled catalytic reactor by flowing a gas mix (1 % methane, 2 % oxygen, and balance nitrogen) at 250 – 400 °C. The catalyst calcined at 850 °C showed much higher activity at 300 – 400 °C compared to the same catalyst calcined at 500 °C. The better activity of the catalyst calcined at 850 °C is due to a lower activation energy. In recent studies, it is the opposite result of methane combustion under lean conditions. Characterization of each catalyst was provided by pulse chemisorption, temperature-programmed reduction, and x-ray photoelectron spectroscopy. The data provided for the characterization will provide particle size, and metal correlation between activity and properties of the catalysts at the calcined temperatures produced.

Poster #54 – Physical/Computational Chemistry

Presenter: Erica Browne
PI: Samer Gozem
Institution: Georgia State University

Title: Comparing Computational Methods: Calculating Vertical and Adiabatic Excitation Energies in Flavin

Spectrophotometry is a widely used tool in biochemistry due to its quick and accurate identification and quantification of biological macromolecules such as proteins, nucleic acids, carbohydrates, *etc.* UV-visible spectroscopy directly probes the energy required to excite a molecule from its ground state to an excited state. It arises from the Bohr frequency condition, which states that the wavelength absorbed by an atom is directly related to the difference in the energy between its quantized energy levels. Modern chemical quantum methods make it possible to predict molecules' UV-visible spectra without the need for laboratory experiments in the traditional sense. Therefore, there is potential to apply computational chemistry tools in the field of biochemistry, particularly to understand the molecular origin of absorption spectra and how they are influenced by their surrounding environment (*e.g.*, confirmation of a protein or DNA stacking, *etc.*). This study focuses on lumiflavin, a derivative of riboflavin (vitamin B₂). Our lab recently predicted lumiflavin's UV/vis spectrum in its five redox and protonation states in various solvents using a widely used quantum chemical method: B3LYP. In this work, our goal was to compute the vertical and adiabatic excitation energy of flavin's redox states with the CAM-B3LYP method and compare the results to our previously predicted B3LYP data. Although CAM-B3LYP incorporates a long-range correction factor that is supposed to improve the results of B3LYP, the comparison showed that CAM-B3LYP overestimated both the vertical and adiabatic excitation energy, which in turn reduced the agreement with the experiment. Further research must be conducted to understand the limitations of CAM-B3LYP in this case.

Poster #55 – Physical/Computational Chemistry

Presenter: Rahul Pandit
PI: Neville Forlemu
Institution: Gwinnett Georgia College

Title: Molecular Docking and Fine-Tuning Ligands for Drug Discovery Purposes (COVID-19)

The COVID-19 pandemic and its impact on society exemplify the need for rapid development of antiviral drugs, especially in response to more virulent, drug-resistant diseases. In this study, Computer Aided Drug Design (CADD) was used to model ligands targeting critical SARS-CoV-2 protein receptors: Non-Structural-Protein-5 (Mpro)(1UG1), Transmembrane Serine Protease 2 (7MEQ), and Janus Kinase 2 (6VN8). Current antiviral drugs like Fusion Inhibitors (Baricitinib and Nafamostat Mesylate), Protease Inhibitors (Lopinavir, Atazanavir, and Darunavir), and Reverse Transcriptase Inhibitors (Favipiravir and Ribavirin) were all modeled as benchmarks. The 3-D structures of the proteins and antivirals were downloaded from the PDB and DrugBank Databases respectively. The interactions between antivirals and SARS-CoV-2 receptors were characterized with molecular docking using AutoDock Vina and Chimera. The details of the molecular interactions were described with Discovery Studio's 2D Ligand interaction tool. The docking data identified the antiviral drug Nafamostat and receptor Mpro with a strong binding affinity (-11.3 kcal/mol) as targets for Pharmacophore-Based Drug Design (PBDD). The PBDD framework was used to design 54 molecules, with candidates 49 – 53 showing a strong affinity (-10.7 to -11.3 kcal/mol) with Mpro. The interactions are stabilized with hydrogen bonding interactions between residues A-5(LYS), B-125(VAL), and B-127(GLN) and Hydrogen 17, Hydrogen 18, and Oxygen 3 respectively. In addition, the ADMET properties of candidate 52 determined from SwissADME are acceptable based on the Lipinski rule of 5.

Poster #56 – Physical/Computational Chemistry

Presenter: Laila Belpalme
PI: Neville Forlemu
Institution: Georgia Gwinnett College

Title: Cyclotide Interactions with the Lipid Bilayer

As bacterial resistance to antibiotics continues to increase, there is a resurgence on research to characterize and functionalize antimicrobial peptides, like cyclotides, for the development of more effective drugs. Cyclotides are unique plant miniproteins, with distinctive structural features including a macrocyclic backbone and cyclic cystine knot of three disulfide bonds between 6 conserved cysteine residues. These unique features enhance their tolerance to chemical, thermal and enzymatic degradation along with a plethora of biological applications. In this study, USCF Chimera was employed to highlight and analyze the physicochemical properties of the cyclotide structures available in the protein data bank. Twenty cyclotides were studied, with varying net charges and mostly found to be amphipathic in nature. The cyclotides extracted from *Violaceae* (the bracelet subfamily) displayed the most hydrophobicity. The solubility of all the cyclotides explored ranged from 0.546 to 0.799 as computed from predictive algorithm Protein-Sol.

The Lipid Bilayer has been identified as the major target for the cyclotides involved in plant defense. To study such interactions, the CHARMM-GUI system generator tool was used to build and equilibrate multiple cyclotide/bilayer systems. Specifically, 10 model systems with lipids prevalent in bacteria, human and other parasites (POPG, POPE, POPC) with a positively charged cyclotide and a cyclic trypsin inhibitor (5WOW). The goal of building these systems is to examine the interactions between various kinds of cyclotides with different lipid membranes found in bacteria and in humans.