2025 Herty Undergraduate Research Symposium

Speaker presentations will be held at the GGC Belonging Center (Building B, Room 100).
Student poster presentations will be held in the GGC Building B Atrium.

12:30 PM	**Registration & Poster Set-Up (GGC Building B Atrium)**
1:30 - 1:35 PM	**Introductory Remarks: Dr. Ajay Mallia, GGC**
1:35 - 1:40 PM	**Welcome: Dr. Joseph Ametepe, Interim Dean, SST, GGC**
1:40 - 1:45 PM	**Introduction of the 2025 Herty Medalist: Dr. Chavonda Mills, Provost, GGC**
1:45 - 2:30 PM	**Herty Award Address: “Learning to ask Questions: The Basis for Scientific Discovery,” Dr. James D. Martin, 2025 Herty Awardee, NC State University**
2:30 - 2:45 PM	**Break**
2:45 - 4:15 PM	**Undergraduate Student Poster Session / Reception**
4:15 - 4:25 PM	**Break**
4:25 - 5:00 PM	**“Finding Joy from Discovery: Our Journey as Scientists”, Dr. Gracy Wingkono, The Coca-Cola Company, Atlanta**
5:00 - 5:15 PM	**Poster Award Ceremony & Concluding Remarks, Dr. Sang Park, Chair, Department of Chemistry, GGC**

Herty Awardees

2025	James D. Martin	North Carolina State University
2024	John A. McLean	Vanderbilt University
2023	C. David Sherrill	Georgia Institute of Technology
2022	H. N. Cheng	U.S. Department of Agriculture, New Orleans
2021	Anne-Frances Miller	University of Kentucky
2020	Susan D. Richardson	University of South Carolina
2019	Lisa McElwee-White	University of Florida
2018	Sandra Rosenthal	Vanderbilt University
2017	Rigoberto Hernandez	Georgia Institute of Technology and Johns Hopkins University
2016	Brooks H. Pate	University of Virginia
2015	David Beratan	Duke University
2014	Luigi G. Marzilli	Louisiana State University
2013	David G. Lynn	Emory University
2012	Alvin L. Crumbliss	Duke University
2011	R. Mark Wightman	University of North Carolina at Chapel Hill
2010	Ken B. Wagener	University of Florida
2009	Craig L. Hill	Emory University
2008	Gregory H. Robinson	University of Georgia
2007	Luis Echegoyen	Clemson University
2006	Gary B. Schuster	Georgia Institute of Technology
2005	Dennis C. Liotta	Emory University
2004	Michael T. Crimmins	University of North Carolina, Chapel Hill
2003	Alan G. Marshall	Florida State University
2002	Lanny S. Liebeskind	Emory University
2001	F. Ivy Carroll	Research Triangle Institute
2000	James C. Powers	Georgia Institute of Technology
1999	Richard D. Adams	University of South Carolina
1998	Gordon L. Nelson	Florida Institute of Technology
1997	Fredric M. Menger	Emory University
1996	David W. Boykin	Georgia State University
1995	R. Bruce King	University of Georgia
1994	William D. Ehmann	University of Kentucky
1993	Leon H. Zalkow	Georgia Institute of Technology
1992	Isiah M. Warner	Emory University
1991	Ernest L. Eliel	University of North Carolina, Chapel Hill
1988	Jett C. Arthur, Jr.	Milliken Research Corp. Spartanburgh, SC
1987	Charles K. Bradsher	Duke University
1986	Lockhart E. Rogers	University of Georgia
1985	Raymond B. Seymour	University of Southern Mississippi
1984	Eugene C. Ashby	Georgia Institute of Technology
1983	Albert Padwa	Emory University
1982	Norman L. Allinger	University of Georgia
1981	Jacob H. Goldstein	Emory University

1980	Irwin Fridovich	Duke University
1979	Mary E. Carter	Southern Regional Research Center, USDA, New Orleans
1978	George B. Butler	University of Florida
1977	William L. Marshall	Oak Ridge National Laboratory
1976	Henry C. R. McBay	Morehouse College
1975	Mary L. Good	Louisiana State University
1974	John Montgomery	Southern Research Institute, Birmingham
1973	D. Stanley Tarbell	Vanderbilt University
1972	Kent C. Brannock	Tennessee Eastman Company, Eastman Kodak, Kingsport, TN
1971	S. William Pelletier	U. of Georgia, Athens
1970	Robert E. Lutz	University of Virginia
1969	George L. Drake, Jr.	Southern Regional Research Center, USDA, New Orleans
1968	Charles N. Reilley	University of North Carolina at Chapel Hill
1967	G. H. Cartledge	Chemistry Division, Oak Ridge National Laboratory
1966	James E. Copenhaver	University of South Carolina
1965	Charles T. Lester	Emory University
1964	S. Y. Tyree, Jr.	University of North Carolina at Chapel Hill
1963	Jack Hine	Georgia Institute of Technology
1962	Charles R. Hauser	Duke University
1961	Howard E. Skipper	Southern Research Institute, Birmingham, AL
1960	Arthur E. Wood	Mississippi College
1959	C. Harold Fisher	USDA, New Orleans
1958	Lucius A. Bigelow	Duke University
1957	S. J. Floyd	
1956	M. P. Etheridge	Mississippi State
1955	Frank J. Soday	The Chemstrand Corp., Decatur, AL
1954	John R. Sampey	Furman University
1953	Raymond W. McNamee	Carbide & Carbon Chemical Company, WV
1952	Alton E. Bailey	Humko Company, Inc., Tennessee
1951	J. T. MacKenzie	American Cast Iron Pipe Company, Alabama
1950	R. W. Bost	University of North Carolina
1949	Osborne R. Quayle	University of Georgia
1948	W. F. Rudd	Medical School of Virginia
1947	E. Emmett Reid	Johns Hopkins University
1946	W. A. Lazier	Southern Research Institute
1945	P. M. Gross	Duke University
1944	J. E. Mills	Sonoco Products Company
1943	J. H. Yoe	University of Virginia
1942	T. R. Leigh	University of Florida
1941	W. F. Hand	Mississippi State College
1940	J. Sam Guy	Emory University
1939	F. K. Cameron	University of North Carolina
1938	C. E. Coates	Louisiana State University

1937	J. L. Howe	Washington and Lee University
1936	W. H. MacIntire	University of Tennessee
1935	F. P. Dunnington	University of Virginia
1934	Charles H. Herty (1867–1938)	Herty Laboratory
1933	Fred Allison	Alabama Polytechnic Institute, Alabama

Herty 2025 Poster Presentation Abstracts

Institutions Represented

- Georgia Gwinnett College
- Georgia State University
- Georgia Institute of Technology
- University of North Georgia
- Kennesaw State University
- Georgia College & State University
- Emory University
- Oxford College of Emory University

Analytical Chemistry

Poster # 1

Presenter:	Alexandra Tokos
PI:	Wathsala Medawala
Institution:	Georgia College & State University Department of Chemistry, Physics, and Astronomy
Title:	Quality Assurance and Comparative Analysis of Trace Elements of In-store and Online Purchased Cosmetic Products

Cosmetic products such as lip gloss, concealer, foundation, blush, bronzer, highlighter mascara, eyeliners, eyebrow pencils, and other personal care are widely used globally to enhance beauty and boost human self-confidence. The sales of cosmetics products are over a billion dollars globally. Nonetheless, cosmetics can be potentially contaminated with toxic elements such as lead, cadmium, and many other harmful elements. In addition, the potential for cosmetics to be adulterated and counterfeited by cosmetic manufacturers for financial gain is worrisome. Health implications of toxic elements, necessitate analysis of cosmetic products for quality assurance. This study was aimed at conducting quality assurance and comparative analysis of trace elements of cosmetics products. In-store cosmetic products, including lip gloss, foundation, mascara, blush, and eyeliners, were collected through donations from peers towards to project. The online cosmetic products were purchased from Amazon. Each product was treated with fixed ratio amounts of HNO_3 and H_2O_2 to promote efficient digestion and identification of individual elements through a microwave digestion system. Digested products were then filtered through gravity filtration to isolate the components. Samples were analyzed through Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES), an analytical instrument used to qualify the presence of heavy metals. ICP-OES promoted sensitive and accurate trace elements of cosmetic products in ppm when compared to standards containing target metals and created a spectrum for contents found in each product. A future study includes analyzing digested samples through Atomic Absorption Spectroscopy (AAS) to quantify results of the presence of heavy metals.

Poster # 2

Presenter:	Stacie Rigli
PI:	Joshua Driver
Co-author:	Daygan Wasson
Institution:	University of North Georgia

Title: Influence of Sun Protection Factor on Sunscreen Degradation After Exposure to UVA Radiation Utilizing UV-Vis Spectroscopy

UVA rays make up about 95% of the total UV radiation that reaches Earth. UVA can have significant effects on the health of human skin, such as skin aging, wrinkling, sunspots, and contributions to skin cancer. The goal of this experiment was to determine the degradation rates in the UVA range in 30 and 70 SPF sunscreen utilizing UV-Vis spectrophotometry. The degradation rate of the sunscreen products for the 30 SPF was 5.41×10^{-4} min^{-1} which was much quicker than the 70 SPF which was 2.81×10^{-4} min^{-1}. The lower SPF degraded roughly twice as fast (30 SPF *vs*. 70 SPF). These data indicate that the UVA blocking ability of the 70 SPF sunscreen is more effective than the 30 SPF sunscreen to prolonged UV exposure. Researching UVA is crucial as it may lead to more regulations in an underestimated field and help contribute to more effective sunscreen development.

Poster # 3

Presenter:	Jayden Kypri
PI:	Wathsala Medawala
Co-Authors:	Edward Lisic & Xiaohua Jiang
Institution:	Georgia College & State University Department of Chemistry, Physics, and Astronomy

Title: Synthesis, characterization, and bioactivity of Alloxan Benzyl Thiosemicarbazide (ALL-BzTSC) and its Palladium Complex on Topoisomerase IIa

According to the NCI, in 2025, there will be an estimated 618,000 deaths caused by cancer, a merciless illness caused by mutated cells undergoing quick, unchecked cell proliferation. One path for treatment of cancer is the targeted inhibition of Topoisomerase IIα's active site. This enzyme is part of a subclass of human Topoisomerase enzymes that participate in the relieving of supercoils upstream of DNA Helicase during replication; as a result, Topoisomerase IIα's activity in unchecked prolific cell division is heightened, which makes it a prime target for cancer drug research. Thiosemicarbazones (TSC) are a class of chelating organic compounds that can form metal complexes with Cu^{2+} and Pd^{2+} that competitively inhibit Topoisomerase IIα, acting as a key anti-cancer agent, as shown in the literature. This study will focus on the synthesis and characterization of alloxan benzyl thiosemicarbazide (ALL-BzTSC), its palladium complex, and the bioactivity of the compounds on Topoisomerase IIα through enzyme assays using varying concentrations. In this poster, synthesis, characterization, and enzyme inhibition assays for the TSC and its metal complexes will be discussed.

Poster # 4

Presenter:	Audrey Anggraeni
PI:	Wei Zhou
Institution:	Kennesaw State University

Title: Analysis of Turmerone Compounds in Various Turmeric Food Samples and Supplemental Products using GC/MS

Turmeric (*Curcuma longa*) is a plant belonging to the ginger family Zingiberaceae. Native to South and Southeast Asia, the golden-yellow spice has been cultivated for dyes, spices, and a variety of health benefits since ancient civilization. Turmerone compounds (curcumene, non-aromatic turmerone, aromatic turmerone, and curlone) are responsible for turmeric's vibrant color, anti-inflammatory and antioxidant properties. With these benefits, turmeric has been added into supplement capsules, immunity shots, and pain relief topical solutions. Turmeric is also widely used in traditional herbal medicine to help with diseases such as asthma and arthritis. We are interested in identifying and evaluating turmerone compounds in ground turmeric, turmeric supplement capsules, and turmeric rhizomes. Ethanol was selected as the extracting solvent. Sonification for 10 minutes was used to improve extraction. Extracted solutions from various samples have been analyzed using gas chromatography-mass spectroscopy (GCMS, Agilent-QP2010). Aromatic tumerone, non-aromatic tumerone, curlone, and curcumene have been identified as the four major turmerone compounds across all samples. They were eluted at 16.01 minutes, 16.23 minutes, 17.71 minutes, and 9.98 minutes, respectively. Their relative abundance of each compound varied among our tested samples.

Poster # 5

Presenter:	Eduardo Vega
PI:	Misael Romero-Reyes
Institution:	Georgia Gwinnett College

Title: Investigating the Viability and Capacity of Wood as a Sustainable Water Filter through the Absorption of Methylene Blue and Bacteria

In this study, the capacity of wood is tested when used as a means for effective, sustainable water filtration. Both the absorption of methylene blue and bacteria were tested throughout these experiments. Two separate 10 mg/L methylene blue solutions were made from deionized water and lake water. This concentration is higher than what is most commonly found naturally. A modified Büchner vacuum filtration system is used in these experiments to run water through the wood and to collect the filtered product. The results of these experiments show that wood can effectively remove methylene blue with an absorption rate of at least 93%. The resulting absorption rate of bacteria is between 20% and 70% on average. More careful testing will be done to confidently gauge the capacity of wood in the sense of bacterial absorption. The results of this study show that wood could be used as an effective and sustainable water filter.

Biochemistry

Poster # 6

Presenter:	Thais Arslanbekov
PI:	Ronghu Wu
Co-authors:	Longping Fu
Institution:	Georgia Institute of Technology School of Chemistry & Biochemistry

Title: Global analysis of newly synthesized proteins in monocyte and macrophage response to bacterial infection

Monocytes and macrophages are essential components of the innate immune system, playing distinct but interconnected roles in recognizing and responding to bacterial infection. While transcriptomic approaches provide insight into mRNA expression, they do not fully capture post-transcriptional regulation or translational dynamics. This study aims to globally quantify newly synthesized proteins in monocytes and M1/M2 macrophages during bacterial infection, using metabolic labeling and click chemistry-based enrichment using dibenzocyclooctyne (DBCO) beads. Following macrophage polarization with phorbol 12-myristate-13-acetate (PMA) and differentiation bacterial lipopolysaccharide (LPS) and INF-γ stimulation for M1, and IL-4 stimulation for M2, newly synthesized proteins are selectively metabolically labeled, enriched via biotin-streptavidin pulldown, and analyzed using stable-isotope labeling and non-canonical amino acid incorporation and LC-MS/MS. We expect to identify polarization-dependent differences in protein synthesis, revealing key regulators of immune activation. Understanding translational changes in response to infection provides mechanistic insights into macrophage function and immune modulation, which could inform novel therapeutic strategies targeting bacterial infections and inflammatory diseases.

Poster # 7

Presenter: Yinan Chen
PIs: Ajay Mallia, Neville Forlemu, Simon Mwongela
Institution: Georgia Gwinnett College

Title: Investigating Time-Dependent Microwave-Assisted Extraction of Cyclotide as a Potential Biopesticide

Insect pests are responsible for significant crop loss. This research investigates the use of cyclotides (cyclic peptides) as potential biopesticides. This study involved both computational and experimental methods. Molecular docking simulations revealed that hydrophilic cyclotides, specifically 2M86, have significantly stronger binding affinity (–73.63 kcal/mol) with insect proteins than benchmark pesticides like ivermectin (–7.844 kcal/mol). Experimentally, cyclotides were extracted from *Viola hederacea* using microwave-assisted extraction for 30, 45, and 60 minutes. These extracts were tested on caterpillars, where growth inhibition mass was observed when the extraction groups only had 15.25%, 14.84%, and 13.87% mass growth compared to the 38.29% for the control group. The percent increase decreased as the extraction time increased. Aggregation trends were analyzed using UV-Vis spectroscopy, showing an increase in absorbance from the beginning until around 48–72 hours post-extraction along with visible precipitate formation. These findings affirm cyclotides' insecticidal potential and aggregation behaviors from the literature, providing insights into time-dependent microwave-assisted extraction.

Poster # 8

Presenter:	Dominic Kassing
PI:	Annette Neuman
Co-author:	Latonia Taliaferro-Smith
Institution:	Oxford College of Emory University

Title: Investigation on the antibiotic effect of superior-class traditional Chinese medicinal herbs on *Escherichia Coli*

Escherichia coli (*E. coli*) is a common gram-negative, polymorphic bacterium found in the gastrointestinal tract. The presence of *E. coli* can lead to colibacillosis, which can induce pain, diarrhea, vomiting, and fever. One of the most common treatments for colibacillosis and other bacterial infections is the use of antibiotics; however, the overuse of antibiotics has led to the prevalence of antimicrobial resistance. Thus, in response, alternate treatments to current antibiotics should be explored. The treatments examined in this study are Chinese medicinal herbs cited in the Divine Farmer's Classic of Materia Medica. These herbs were classified as superior-class herbs, having the best results and the least side effects. In this study, herbs were prepared as extracts and dry root powders. The extracts were prepared using maceration in ethanol and made at a concentration of 0.167 g/mL. The dry roots were prepared by powdering each herb in a blender. Using the agar well diffusion method, antimicrobial effect was analyzed by the measurement of each herb's zone of inhibition with a negative control of ethanol or sand for the extracts and dry roots, respectively. The results showed that all five herbs displayed a significant antimicrobial effect above the negative controls in both extract and powder form. Two of the herbs, Rhizoma Acori Graminei and *Rehmannia glutinosa*, showed the greatest effect in both powder and extract form, showing that they are the most promising for further testing and potential future antibacterial treatments. Further analysis provided evidence that there may have been active compounds lost in extraction, as the powders displayed higher antimicrobial activity when factoring in the activity of the ethanol. Further studies with different extraction methods could help verify this. Despite this, each of the five herbs has the potential to be studied further in the pursuit of new avenues of medical treatments.

Poster # 9

Presenter: Adithi Penmesta
PI: Raquel Lieberman
Co-author: Elijah Dunn
Institution: Georgia Institute of Technology

Title: Structural Characterization of Myocilin Coiled-Coil Interactions with Myosin Regulatory Light Chain

Myocilin is a secreted glycoprotein localized to the extracellular matrix of the eye, yet its biological function remains poorly understood. Mutations in MYOC are strongly associated with elevated intraocular pressure, but the biological function remains unclear, partly due to limited structural information (Saccuzzo *et al.*, 2024). This project seeks to characterize the structure of the coiled-coil (CC) domain of myocilin using nuclear magnetic resonance (NMR) spectroscopy, with a focus on its interaction with myosin regulatory light chain 2 (MYL2). A yeast two-hybrid screen previously identified MYL2 as a potential binding partner (Wentz-Hunter *et al.*, 2024). MYL2 is a muscle protein essential for contractility, and knockout models exhibit cardiac and skeletal muscle defects. To probe this interaction, both proteins were purified and analyzed using gel electrophoresis and NMR spectroscopy. Gel electrophoresis results revealed that MYL2 stabilizes the myocilin CC domain by protecting it from proteolytic degradation over time. NMR spectroscopy further demonstrated specific binding between the two proteins, with smaller peak shifts suggesting weak or high-timescale interactions. Ongoing optimization of these experiments will enable characterization of specific atomistic interactions, providing insight into the structure of the coiled coil domain and potential biological function of myocilin.

Poster # 10

Presenter: Lorenzo Layug
PI: Katherine Davis
Co-authors: Kirklin McWhorter, Manik Sharma & Tiffany Alvarez
Institution: Emory University

Title: Biochemical and Computational Approaches Reveal Insights into the Novel Reactivity of a Vanadium-dependent Bromoperoxidase from *Corallina pilulifera*

Vanadium-dependent haloperoxidases (VHPOs) utilize a pentavalent orthovanadate cofactor to catalyze the oxidation of halide ions by hydrogen peroxide, generating hypohalous acids (H-OX) that facilitate halogenation reactions. The bromoperoxidase from *Corallina pilulifera* (CpVBPO), for example, has demonstrated broad catalytic versatility across a wide range of pH values, temperatures, and organic solvents. This adaptability positions CpVBPO as a promising biocatalyst for the sustainable functionalization of industrially relevant molecules.

Most recently, our collaborators in the Biegasiewicz Lab achieved the catalytic conversion of carbonyl compounds to diazo derivatives *via* hydrazone intermediates at ambient conditions. However, they observed a surprising disparity between the reaction rates of (E)- and (Z)-hydrazone isomers: the (E)-hydrazone reached optimal yield in 6 hours, while the (Z)-hydrazone required 18 hours to attain a comparatively lower maximum yield.

To elucidate the underlying factors contributing to this discrepancy, we performed molecular docking studies using AutoDock. As the active site of CpVBPO forms at the interface of the homodimer, we focused our efforts on the associated hydrophobic pocket. Gratifyingly, the reactive nitrogen of the (E)-hydrazone was placed within 6 Å of the vanadate cofactor, suggesting a favorable orientation for catalysis. The (Z)-hydrazone, by contrast, docked further from the metal, near the opening of the binding pocket. Superimposition of the (Z)-hydrazone onto the docked (E)-hydrazone conformation indicates steric hindrance between D335 and A336 of the enzyme and the reactive nitrogen of the (Z)-isomer. Subsequently, molecular dynamics was performed on the docked structures, revealing that the (Z)-hydrazone adopted a more flexible position within the active site compared to the (E)-isomer. Both site-directed mutagenesis and microscale thermophoresis were utilized to highlight critical residues within the active site and determine binding constants for different substrates. Taken together, these findings provide a structural basis for the observed difference in reaction rate between the substrates.

Poster # 11

Presenter: Ting Du
PI: Jenny J. Yang
Institution: Georgia State University

Title: Purification and characterization of hProCA32.collagen1 for MRI-based liver fibrosis detection

Early diagnosis of liver fibrosis is a significant clinical challenge. Using invasive methods such as liver biopsy for detection may lead to potential complications. While, in non-invasive detection methods, magnetic resonance imaging (MRI) technology shows certain technical advantages over ultrasound imaging and ultrasound elastography. The main way to improve the effectiveness of MRI imaging is the use of effective contrast agents. Traditional gadolinium contrast agents have problems with potential toxicity and insufficient targeting. Therefore, this study aims to investigate the purification and characteristics of the novel human collagen-targeting protein MRI contrast agent hProCA32.collagen1, focusing on optimizing the purification process and exploring whether the new contrast agent is safer and more effective. These proteins were analyzed by SDS-PAGE, mass spectrometry, ELISA and relaxation analysis. The results showed that the contrast agent showed strong signal attenuation in T_2 weighted MRI contrast imaging and had good targeting specificity. Meanwhile, following the previous FPLC SP purification steps, this experiment also found that the protein yield decreased significantly from lysis to heat treatment and after centrifugation with PEI. Therefore, the precipitate obtained after centrifugation was also analyzed and SDS-PAGE images were obtained. Further analysis is still needed to achieve high recovery and high purity of target protein.

Poster # 12

Presenter: Li Xu
PI: Jenny J. Yang
Institution: Georgia State University (Chemistry)

Title: Enhanced Purification and Binding Optimization of hProCA32.collagen1 for Improved MRI Detection of Liver Fibrosis

Liver fibrosis, characterized by the excessive accumulation of collagen and extracellular matrix, is a common consequence of chronic liver diseases (CLD). Early detection is crucial for halting or potentially reversing fibrosis, which can significantly improve patient outcomes. This study emphasizes the importance of early diagnosis and the development of non-invasive detection methods for liver fibrosis and related conditions. While Magnetic Resonance Imaging (MRI) is a powerful tool for visualizing internal organs, its effectiveness is often limited by the current contrast agents available. To address this issue, researchers have developed hProCA32.collagen1, a protein-based contrast agent with high specificity for human collagen type I. This agent’s strong affinity for collagen I enhances tissue targeting, allowing for improved imaging precision and reduced dosage. To purify the proteins, different methods such as lysis, heating, PEI, dialysis and FPLC were used to separate other kinds of proteins. Finally, to verify that isolated proteins were the ones desired for this study, SDS-PAGE was used to visualize the results; Bradford assay was used to determine the concentration of the proteins and ELISA was used to determine additional characteristics such as binding affinity.

Chemistry Education

Poster #13

Presenter: Nicole Reyes
Co-PIs: Paula Nolibos & Brynna Quarles
Institution: University of North Georgia

Title: Using pre- and post-activity assessments to measure student achievement in organic chemistry I through collaborative learning jigsaw activities

Mastering the comprehension of complex topics in organic chemistry requires a combination of skills: memorization of names and reactions, spatial awareness of structures, arrow pushing in mechanisms, and multi-step synthetic sequences. Spectral interpretation to elucidate the structure of a molecule is also an important step in synthesizing information from the entire semester. The overall goal for this project was to evaluate interactive exercises developed to help students work towards mastery of these common challenging concepts by using pre-activity and post-activity quizzes to better analyze the overall effectiveness of the activity as well as how certain skills related to the topic were improved. Specifically, this project emphasized four major concept areas: the qualitative "ARIO" (Atom, Resonance, Inductive, Orbital) framework in order to analyze acid/base chemistry, the use of cards to arrange the steps of a reaction mechanism, a concept map activity reaction webs to visualize all the reactions covered in the course, and a new jigsaw spectroscopy activity. All activities require students to collaborate in small groups and to rotate to different groups throughout the activity. Students were individually given an initial assessment to gauge understanding before the interactive activity. After a collaborative activity, students were then given the same individual assessment to evaluate the impact of these collaborative learning activities on their overall conceptual understanding. Our results show that student achievement increased in most topics assessed.

Poster #14

Presenter: Sara Lupu
Co-PIs: Paula Nolibos & Brynna Quarles
Institution: University of North Georgia

Title: A scaffolded guided inquiry activity and assessment metrics for mastery of organic functional group recognition

Comprehension of complex organic chemistry topics requires a combination of skills: memorization of functional groups, chemical names and reactions, spatial awareness of structures, arrow pushing in mechanisms, and multi-step synthetic sequences. As part of a comprehensive realignment of the course, the authors have previously developed a number of collaborative learning activities in the topics of acid/base chemistry, spectroscopy, and chemical reactions. We now seek to design an activity to be employed with the first week of the course in order to allow students to not only practice the identification of functional groups, but to also become acquainted with the active learning nature of the course and get to know other students. Students will be assigned to groups of three and given a set of cards that each show the structure of common medicinal drugs and/or biologically significant compounds. In the first part of the activity, the compounds have highlighted functional groups that students must correctly name, while in the second part, students have to first identify and then name the functional groups in the molecule. Student participants were asked to provide feedback via an anonymous survey after completing the exercises, and the activity's efficiency was monitored via pre-activity and post-activity quizzes.

Overall, the student response to the activities was positive, as they indicated that they felt more confident in their knowledge of functional groups than they did prior to the active learning engagement while the quizzes show more quantitatively that student knowledge improved after the activity

Computational Chemistry

Poster #15

Presenter: Sara Dixon
PI: Shina Caroline
Co-authors: Lynn Kamerlin & Bruno di Geronimo
Institution: Georgia Institute of Technology

Title: Tracing the evolution of substrate specificity in LMW-PTPs and ArsCs

At the origin of evolution, ancient enzymes were thought to be versatile and promiscuous. Through genetic mutation, proteins evolve to acquire activity with new substrates, higher efficiency, or novel functions. Our current research explores the hypothesis that, despite differing functions, sequences, and substrates, low molecular weight protein tyrosine phosphatases (LMW-PTPs) and thioredoxin-coupled arsenate reductases (ArsCs) share a common ancestor that later evolved substrate specificity, as shown by their similar mechanisms and structure, including the conserved active site P-loop. We performed ancestral sequence reconstruction (ASR) on a combined database of the families to investigate the development of specificity for phosphate derivatives or arsenate ions. Analyzing key sites for structural conservation and catalytic residues revealed that the reconstructed common ancestor contained ArsC-specific reducing cysteines, which only mutated in the branch from which all LMW-PTPs evolved. Although the P-loop remained mostly conserved, ancestors with the ArsC cysteines consistently featured a serine at a key position, while those without often had a bulkier, nonpolar residue, suggesting the active-site serine may play a critical role in distinguishing between phosphate derivatives and arsenate. Further conventional molecular dynamics (MD) studies reveal that the common ancestor has a stronger affinity for the LMW-PTPs' substrate than that of ArsCs, revealing a potential for dual-functionality. By bridging evolutionary insights with practical applications, this research can drive enzyme engineering for efficient and sustainable bioremediation of arsenic and phosphate pollutants.

Poster #16

Presenter: Doyeon Yoon
Co-PIs: Ajay Mallia, Neville Forlemu & Simon Mwongela
Institution: Georgia Gwinnett College

Title: Optimizing Aminoquinoline Derivatives to Target SARS-CoV-2 Proteins

Limited vaccine distribution worldwide highlights the growing need for accessible resources to combat SARS-CoV-2. One potential solution is developing antiviral drugs using 4-aminoquinolines, which its derivatives have been historically used to treat Spanish flu, fever, and malaria. This study investigates the efficacy of optimized aminoquinoline derivatives by targeting proteins that may contribute to COVID-19. Molecular docking was used to quantitatively score the binding affinity of the designed molecules, as well as calculating ADME properties. 240 with a substitution of CH_2CO_2H displayed the strongest binding affinity of -10.91 kcal/mol out of all optimized ligands.

Environmental Chemistry

Poster #17
Presenter: Claire Park
PI: Ajay Mallia
Institution: Georgia Gwinnett College

Title: Investigating the Effects of Sodium Dodecyl Sulfate (SDS) Surfactant on Nitrates in Water

Nitrate contamination in drinking water disproportionately affects low-income communities reliant on private wells, which lack EPA regulation. Existing treatment methods, such as ion exchange and reverse osmosis, are often inaccessible due to high cost and maintenance requirements. This study explores the potential of sodium dodecyl sulfate (SDS), an anionic surfactant, to reduce nitrate concentrations in water by leveraging its micelle-forming properties. Nitrate levels were quantified through both direct and indirect analytical methods, with indirect UV-Vis spectrophotometry ultimately used for greater accuracy. Results showed a decrease in observed nitrate concentrations with the addition of 1 mM and 10 mM SDS, though unexpectedly, 1 mM SDS yielded a greater reduction than 10 mM SDS. This result contradicts expected micelle behavior, since SDS's critical micelle concentration (CMC) was calculated to be 6.82 mM at 22 °C, suggesting that factors such as zinc interference may have influenced the outcome. Additional surface tension analysis revealed that $NaNO_3$ at 1 μM and 1 mM concentrations decreased the CMC of SDS, while 125 mM $NaNO_3$ inhibited micelle formation altogether. These findings indicate that while SDS may alter apparent nitrate concentrations through surfactant–ion interactions, further studies are needed to clarify the mechanism and practical viability of surfactant-based nitrate remediation.

Organic Chemistry

Poster #18

Presenter:	Jagruti Goli
PI:	M.G. Finn
Co-author:	Evan Scislowicz & Jimin Hwang
Institution:	Georgia Institute of Technology

Title: Development of Azanorbornadiene Self-Cleavable Linkers and Evaluation of Their Release Kinetics

Pyrroles were investigated as potential substitutes for furans in Diels-Alder (DA) and retro-Diels-Alder (rDA) chemistry, facilitating the use of azanorbornadienes (ZNDs) as self-cleavable linkers. ZNDs were prepared by incorporating various substituents (*e.g.*, N-sulfonyl, N-acyl, ester, aliphatic, aromatic groups) into pyrroles, enabling the electron-rich ring to undergo DA condensation with electron-poor alkynes. The subsequent conjugate addition of thiols resulted in adducts that underwent rDA fragmentation at rates ranging from minutes to several months based on the nature of the substituents and solvent system used. Intriguingly, ZNDs were found to be much harder electrophiles than ONDs, displaying diverse reactivity patterns with amines and alcohols alongside the conventional thiol nucleophile that is frequently employed in OND Michael reactions. The tunable fragmentation kinetics of ZND compounds makes them promising linkages for potential applications in controlled drug delivery systems.

Poster #19

Presenter:	Long Nguyen
PI:	Misael Romero-Reyes
Co-authors:	Kristy Zhou & Daniel Babalola
Institution:	Georgia Gwinnett College

Title: Most Efficient Wood Grit to Filter Microbial Present Water

Many of Earth's natural water sources contain *E. coli*, a bacterial contaminant that can pose serious health risks. *E. coli* can cause illnesses that can result in serious health complications. Therefore, being able to filter as much *E. coli* out of water is desirable. We developed a method of filtering water using wood, which removes a significant number of bacteria. The goal of this study is to identify which wood dust grit would give the lowest number of *E. coli* remaining. To do this, we filtered water through different wood sized grits. All filtrations are done through K-cups for consistency. 60, 80, and 120 grit wood dust is created by being sanded from cedar wood. *E. coli* containing water is pipetted into a K-cup with 1 of 3 types of wood grit size above a Büchner funnel/filtering flask. This step is repeated 4 extra times with separate apparatus. A micropipette is used to transfer the filtered water into petri dishes. These petri dishes are incubated and then counted to see how many *E. coli* colonies have grown within the incubation period. So far, 120 grit wood dust limits the amount of *E. coli* colonies the most in comparison with the other grit sizes. The outcome of this research may provide a low-cost alternative for people living close to dangerous water sources for filtration. Further research is being done with higher grit sizes of wood to optimize results for *E. coli*.

Physical Chemistry

Poster #20

Presenter: Sabrina Dini
Co-PIs: Ajay Mallia, Neville Forlemu & Simon Mwongela
Institution: Georgia Gwinnett College

Title: Molecular Dynamics and Surface Tension Analysis of Ionic Surfactant–Nitrate Interactions

Nitrate contamination in groundwater remains a challenge in many parts of the world. The micellization of surfactants in the presence of nitrates may offer an approach for water purification. Examination of how sodium nitrate influences the critical micelle concentration (CMC) and aggregation of two ionic surfactants, sodium dodecyl sulfate (SDS) and cetyltrimethylammonium bromide (CTAB), tests this hypothesis. Surface tension measurements were used to determine the CMC of SDS at 22 °C under varying concentrations of sodium nitrate.

In parallel, molecular dynamics simulations were run using CTAB to assess micelle formation and stability at different concentrations. The addition of 1 mM sodium nitrate reduced the CMC of SDS to 5.7 mM, whereas 1 µM sodium nitrate increased the CMC to 6.8 mM, relative to the control CMC of 6.6 ± 0.12 mM. CTAB simulations across all tested systems exhibited stability, with root mean square deviation (RMSD) values remaining below 5 nm. Visual molecular dynamics revealed micelle aggregation at 0.33 and 0.44 mM CTAB.