The 14th Annual ACS-SA Undergraduate Research Symposium

Abstracts

Department of Chemistry and Biochemistry
University of California, San Diego

Thursday, May 21, 2020
3PM – 6PM
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How to Use this Booklet

Dear Symposium Presenter, Judge, or Attendee,

The teams at ACS-SA and the Department of Chemistry are excited to host this virtual symposium to continue to provide an opportunity for our students to build their presentation skills and highlight the impressive undergraduate research conducted at UCSD.

This booklet is your doorway to the event as it contains links to all parts of the event. The next page consists of a comprehensive list of links for the event. These are also interspersed throughout the booklet for your convenience.

The posters can be viewed via the google drive links provided and are sorted by division. The presentations of the posters can be viewed via the Zoom links provided. The Open Presentation Discussion from 4-5 pm will occur in presenters’ own Zoom rooms. These rooms can be found in the document listed in the List of Links on the next page.

Any questions that arise about how to participate in this event can be sent to acssa@ucsd.edu.

Best,

The 2020 Symposium Team
List of Links
The following hyperlinks will take you to the posters and presentations for this event

All Posters

Biochemistry Division Posters

Inorganic/Organic Division Posters

Physical/Analytical Division Posters

3 pm - Poster Presentations via Zoom:

Biochemistry Group 1 Presentations
Andrew Ecker, Kaushik Ganapathy, Tyler Lam & Shushruth Kallutla, Jori Mills

Biochemistry Group 2 Presentations
Nael Mousa, Kendrick Nguyen, Kailash Venkatraman

Biochemistry Group 3 Presentations
Dalida Warda, Matthew Yu, Robin Yu

Inorganic/Organic Group 1 Presentations
Hayley Fong, Hannah Martin, Ningkai Zheng & Catherine Arceo

Inorganic/Organic Group 2 Presentations
Kun Yong Jeoung, Kien Malarney, Shenghua Yang

Physical/Analytical Group 1 Presentations
Po Jui Chu, Duyen Dang, Reece James, Shouying Lin

Physical/Analytical Group 2 Presentations
Catherine Mullenmeister, Gordon Peiker, Cindy Tan, Christina Trinh

4pm - Open Presentation Discussion Links

5pm - Keynote Address and Awards Ceremony
Dr. Klosterman earned his doctoral degree in Organic Chemistry from the University of Zürich and earned his M.S. in organic chemistry at UCSD. His primary research area is in Chemical Education with research interests in visuospatial and representational competency.
# Table of Presenters

## Biochemistry Division

**Presentation Group 1**
1. Andrew Ecker  
2. Kaushik Ganapathy  
3. Tyler Lam & Shushruth Kallutla  
4. Jori Mills

**Presentation Group 2**
5. Nael Mousa  
6. Kendrick Nguyen  
7. Kailash Venkatraman

**Presentation Group 3**
8. Dalida Warda  
9. Matthew Yu  
10. Robin Yu

## Inorganic/Organic Division

**Presentation Group 1**
1. Hayley Fong  
2. Hannah Martin  
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4. Kun Yong Jeoung  
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## Physical/Analytical Division

**Presentation Group 1**
1. Po Jui Chu  
2. Duyen Dang  
3. Reece James  
4. Shouying Lin

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5. Catherine Mullenmeister  
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8. Christina Trinh
Biochemistry Division

Posters:
https://drive.google.com/drive/folders/1B6OxiMj86RGbHMFeElIeKnDdaUsSORpd?usp=sharing

Group 1
Virtual Presentation:
https://ucsd.zoom.us/j/95637112157
  1. Andrew Ecker
  2. Kaushik Ganapathy
  3. Tyler Lam & Shushruth Kallutla
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Group 2
Virtual Presentation:
https://ucsd.zoom.us/j/98973082524
  5. Nael Mousa
  6. Kendrick Nguyen
  7. Kailash Venkatraman

Group 3
Virtual Presentation:
https://ucsd.zoom.us/j/94548703392
  8. Dalida Warda
  9. Matthew Yu
  10. Robin Yu
Novel heterologous expression of cryptomaldamide in a cyanobacteria host

Andrew Ecker and William Gerwick
Principal Investigator: Dr. William Gerwick

Cyanobacteria produce many bioactive specialized metabolites including toxins and other natural products that represent potential drugs and drug leads. However, in many cases it is difficult to obtain sufficient quantities of these compounds for structural and biological characterization, and it can be difficult to study the biosynthetic gene clusters (BGCs) required for their production because of difficulties in identifying or growing the producing organism or because of a lack of genetic tools available for the producing organism. To overcome these problems, we have developed genetic methods and tools in model cyanobacterial strains for the heterologous expression of cyanobacterial natural product BGCs. Here, we report the expression of cryptomaldamide from a Moorea producens strain JHB BGC in the heterologous host Anabaena. For several reasons, we engineered the filamentous cyanobacterium. Fully segregated Anabaena clones containing the putative cryptomaldamide BGC in NS2 were shown by LC-MS/MS to produce cryptomaldamide, thereby demonstrating that this BGC is indeed responsible for production of cryptomaldamide and that Anabaena is a suitable heterologous expression host. The cryptomaldamide produced by the heterologous host was then isolated to be confirmed by NMR and used to quantify the production of cryptomaldamide by LCMS. Due to the significantly larger amount of cryptomaldamide now available, biological assays were performed to test the compounds ability as a novel natural product drug candidate for its antimicrobial activity.

Virtual Presentation: https://ucsd.zoom.us/j/95637112157
Digital Poster:
https://drive.google.com/open?id=1B6OxiMj86RGbHMFeeIlIeKnDdaUSORpd

Biochemistry #1
Proteins form the building blocks of human life. A protein can be thought of as a sequence of 20 amino acids, selected by nature over billions of years to perform useful functions for human survival. However, natural selection does not allow for the synthesis of proteins with exotic functions, such as those which could prevent diseases ranging from color-blindness to cancer.

Current experimental techniques such as directed evolution use structural insights to help mutate proteins, albeit being laborious and lacking rationale as to why certain mutations seem to work.

Furthermore, such methods are unable to provide any insights when a protein structure is unavailable. In this project, we demonstrate an open source python software infrastructure that uses information entropy derived from an input protein sequence to identify residues that are amenable for performing biologically relevant mutations. Upon receiving an input protein sequence, the software then performs comparisons with similar sequences in protein databases such as the UniProt Knowledgebase. Subsequently, the software then computes the associated information-entropy for each residue in the sequence and then displays these intuitions through bar plots and interactive 3D homology models. To demonstrate the validity of our infrastructure, we show consistency in key insights derived from our infrastructure to results obtained through intensive directed evolution experiments. We envision that our software infrastructure could not only help bioinformaticians gain insights on mutation hotspots on protein sequences quickly, but also serve as feature to future machine learning workflows which could predict relevant mutations given a protein sequence.

Virtual Presentation: https://ucsd.zoom.us/j/95637112157
Digital Poster: https://drive.google.com/open?id=1B6OxiMj86RGbHMFeElJcKnDdaUsSORpd

Biochemistry #2
Students’ perceptions of BiochemAR: An augmented reality tool for teaching molecular visualization in biochemistry

Tyler Lam, Shushruth Kallutla (co-presenter), and Thomas Bussey
Principal Investigator: Dr. Thomas Bussey

Understanding the relationship between macromolecular structure and function is a core learning outcome in nearly all biochemistry courses; however, instructors are largely limited to using two-dimensional images in order to teach students about three-dimensional molecules. New technologies may be able to enhance students’ ability to grasp key visuospatial elements of three-dimensional macromolecular structures, such as a sense of scale or the effects of conformational changes on both local and macromolecular levels. To address the current gap in instructional tools available for teaching macromolecular structure, a new augmented reality (AR) application was implemented in a trial in order to gain initial insights into how the technology will be used by students and how it compares to other conventional two-dimensional representational tools. In this poster, we will discuss our phenomenographic methodology for data analysis as well as our preliminary results of students’ perceptions of the technology and the biochemistry content.

Virtual Presentation: https://ucsd.zoom.us/j/95637112157
Digital Poster: https://drive.google.com/open?id=1B6OxiMj86RgHMFPeElIeKnDdaUsSOPd

Biochemistry #3
Understanding how group A Streptococcus evades the immune system

Jori Mills, Kuei-Chen Wang, Piotr Kolensinki, and Partho Ghosh

Principal Investigator: Dr. Partho Ghosh

Group A Streptococcus (GAS, S. pyogenes) is a major bacterial pathogen responsible for over 500,000 deaths annually and is among the top 10 agents of infectious causes of death. A significant aspect of GAS that makes it a deadly pathogen is its capacity to evade the immune response. A key but poorly understood mechanism for its immune evasion is the binding of human immunoglobulin G (IgG) antibodies through the Fc domain to the bacterial surface. This masks GAS from the immune system and is carried out by the surface-associated GAS protein M1.

This project sought to gain a better understanding of the M1/IgG-Fc binding interaction. Utilizing PCR and mutagenic deletion four new constructs of the M1 protein were created, expressed in E. coli, and purified through nickel affinity chromatography. These four constructs, the native protein, and three previously created M1 constructs were tested by a coprecipitation assay for binding to the IgG-Fc fragment to determine the Fc-binding site in M1 protein. The results showed that the hypervariable region (HVR) at the N-terminus of the M1 protein as well as the S domain, which is spatially distant from the HVR in the coiled-coil structure of the M1 protein, were both necessary for interaction with IgG-Fc. Furthermore, when the B-domain of the M1 protein, which is between the HVR and S domain, was removed, binding did not occur in shorter constructs but did occur in the longest construct. Overall, the results demonstrate the necessity of the HVR and S domains of the M1 protein for binding to IgG-Fc, and the possible influence of the B domain in this interaction.

Virtual Presentation: https://ucsd.zoom.us/j/95637112157
Digital Poster: https://drive.google.com/open?id=1B6OxiMj86RGbHMFeElleKndDaUSsORapd

Biochemistry #4
Biological macromolecules must sample a variety of conformational space to perform their important cellular functions. As such, a molecular-level understanding of the motions that occur as proteins sample between these conformational states is important in achieving a complete understanding of a protein’s role in the larger biological context. Cryogenic electron microscopy (CryoEM) has proven to be useful to investigating dynamic protein complexes in near-native environments. Indeed, conformationally heterogeneity is preserved during EM sample preparation and a single cryoEM data collection is capable of yielding multiple conformationally distinct structures. However, despite algorithm advancements, most datasets yield a single high-resolution structure that only represents ~10% of the data with the remaining 90% being discarded during processing. In order to better capture more conformational states from cryoEM data and quantify their dynamics, we first need to better understand how dynamics manifest in EM data. To achieve this goal, we have generated simulated EM data using all-atom molecular dynamics (MD) simulations of well-studied EM specimens. Using atomic snapshots along these simulations, we used a combination of “in-house” developed scripts together with other available computational methodologies to generate simulated EM densities from each of the simulation snapshots that we collected. Following the MD to EM conversion we have added various noise models to these snapshots and, through comparisons to the raw EM data that was published we have yielded a simulated EM reconstruction that is nearly indistinguishable. From this simulated EM data, we have generated 2D projections from each snapshot in order to better quantify how different conformational states manifest in the data. Through careful analysis of these simulations and simulated EM data, yielding structures of multiple confirmations, we will be able to better quantify the number of conformational states a given protein samples and obtain insight on the how much of the conformational landscape we can access. This methodology will benefit the broader EM community and increase our ability to better investigate information pertaining to dynamics and conformational heterogeneity that is often dismissed during high-resolution processing.

Virtual Presentation: https://ucsd.zoom.us/j/98973082524
Digital Poster: https://drive.google.com/open?id=1B6OxiMj86RGbHMFeElIeKnDdaUsSORpd

Biochemistry #5
Using computational algorithms to correct high-order aberrations in CryoEM

*Kendrick Nguyen*, Hoang Nguyen, and Mark Herzik
Principal Investigator: Dr. Mark Herzik

Recent technological advancements in modern cryogenic electron microscopy (cryoEM) have culminated in the so-called “EM resolution revolution” and allowed researchers to determine high-resolution structures of biological specimens that had been previously deemed intractable by other methodologies. Despite these advances, numerous limitations that can hinder the true attainable resolution of a biological specimen far beyond the theoretical limits remain. Indeed, there exists a large discrepancy between the resolution obtained from the biological specimens (e.g., ~2 Å resolution) and the information limits of the transmission electron microscopes (TEM) (~0.02 Å resolution). It has been speculated that the electromagnetic lenses of the TEM cause aberrations that deform the image to such an extent that considerable loss of important high-resolution information results. Although some of these aberrations can be corrected for by installing aberration-correcting lenses on the TEM, these lenses are prohibitively expensive for the broader EM community. Recently, algorithms have been developed to computationally correct for these higher-order aberrations caused by the TEM to improve the attainable resolution of the cryo-EM reconstructions. Here I present a thorough investigation into the extent for which we can computationally recover important high-resolution information that was originally lost during imaging. Through these efforts, we improve the overall resolution of the 3D reconstruction and inform on the prevalence of these aberrations in modern cryoEM. A more complete understanding of the extent and prevalence of these higher-order aberration and how we can correct for them using computational algorithms will help push the resolution limits of cryoEM closer to the theoretical limit without significantly incurred additional costs. Together, these efforts can lead to improved 3D reconstructions from cryoEM data and provide better platforms for structure-based drug design.

Virtual Presentation: [https://ucsd.zoom.us/j/98973082524](https://ucsd.zoom.us/j/98973082524)

Digital Poster: [https://drive.google.com/open?id=1B6OxiMj86RGbHMFeElIeKnDdaUsSORpd](https://drive.google.com/open?id=1B6OxiMj86RGbHMFeElIeKnDdaUsSORpd)

Biochemistry #6
Elucidating the structure of the Virion RNA Polymerase from the PhiKZ bacteriophage

Kailash Venkatraman, Sean Reardon, Erica Birkholz, Joseph Pogliano, and Tatiana Mishanina

Principal Investigator: Dr. Tatiana Mishanina

The dawn of the post-antibiotic era has cultivated a widespread increase in the presence of multidrug-resistant bacteria over the past fifty years. An alarming number of bacterial strains are showing significant resistance to antibiotics, which makes infections harder and more costly to treat. One emerging alternative is the use of bacteriophages, viruses that infect and kill bacteria, as a means to combat antibiotic resistant bacterial infection. The jumbo bacteriophage PhiKZ, which infects Pseudomonas aeruginosa, is one example of an ideal candidate for phage therapy. Previous studies have demonstrated that PhiKZ is able to complete infection independent of the host bacterial RNA Polymerase (RNAP) enzyme. Instead, transcription of the PhiKZ genome is completed by two unique RNAPs encoded by the PhiKZ genome, one of which is delivered as a protein to the host via the virion (thus called “virion RNAP”, or vRNAP), and the other is transcribed by vRNAP as part of the early phage genes inside the infected bacteria (“non-virion RNAP”, nvRNAP). Partial biochemical characterization of the non-virion RNA Polymerase (nvRNAP) has been done in previous work. However, the virion RNA polymerase (vRNAP) has yet to be purified or structurally characterized. In collaboration with the Pogliano lab at UCSD, we are working toward recombinant expression of the vRNAP in E. coli, its purification and elucidation of its structure using cryo-EM. In my presentation, I will discuss our past and ongoing trouble-shooting efforts to optimize the production of vRNAP in E. coli. The structure and biochemical understanding of this novel RNAP will not only expand the existing repertoire of molecular machines that organisms use to perform transcription but will also guide future in vivo imaging work into the mechanism of phage infection. Ultimately, if we understand how the jumbo phage infects and kills bacteria, we can tune this process for phage therapy.

Virtual Presentation: https://ucsd.zoom.us/j/98973082524
Digital Poster: https://drive.google.com/open?id=1B6OxiMj86RGbHMFeElIeKnDdaUsSORpd

Biochemistry #7
Oncogenic fusion protein BCR-FGFR1 relies on Grb2 and PLC Gamma for activation

*Dalida Warda, Malalage Nicole Peiris, April Meyer, and Daniel Donoghue*

Principal Investigator: Dr. Daniel Donoghue

The breakpoint cluster region- fibroblast growth factor receptor 1 (BCR-FGFR1) fusion protein results from the t(8;22) (p11;q11) chromosomal translocation. BCR-FGFR1 is a driver of acute myeloid leukemia (AML), atypical chronic myeloid leukemia (aCML), and 8p11 myeloproliferative syndrome (EMS). This study focuses on examining the protein-protein interactions required for the oncogenic activity of BCR-FGFR1. We found that BCR-FGFR1 relies on interactions with growth factor receptor bound protein 2 (Grb2) and phospholipase C gamma-1 (PLC-γ) for activation, as seen through cell transformation and downstream cell signaling analysis. BCR-FGFR1 interacts with Grb2 via Y177 and interacts with PLC-γ via Y766. Cells expressing BCR-FGFR1 showed a decline in transforming ability when either Y177 or Y766 were mutated to phenylalanine. Furthermore, cells expressing BCR(Y177F)-FGFR1(Y766F) were unable to activate PLC-γ or STAT3 signaling, indicating that these pathways play a key role in BCR-FGFR1 driven oncogenesis. Additionally, cells expressing BCR-FGFR1 were sensitive to treatment with PLC-γ inhibitor, U73122. Hence, this study suggests that interactions with Grb2 and PLC-γ are important for the oncogenic activation of BCR-FGFR1. Furthermore, inhibition of PLC-γ could serve as a potential therapeutic target in patients with BCR-FGFR1 driven cancers. Overall, this work establishes critical protein-protein interactions with Grb2 and PLC-γ that mediate BCR-FGFR1 directed hematologic malignancies.

Virtual Presentation: [https://ucsd.zoom.us/j/94548703392](https://ucsd.zoom.us/j/94548703392)

Digital Poster: [https://drive.google.com/open?id=1B6OxiMj86RGbHMFeElIeKnDdaUsSORpd](https://drive.google.com/open?id=1B6OxiMj86RGbHMFeElIeKnDdaUsSORpd)

Biochemistry #8
Protein kinases serve an integral role in cardiac development, function, and disease. Previous clinical studies have shown that certain atypical α-protein kinases, including α-protein kinase 2 (ALPK2), are important for normal development and function of the heart via regulation of WNT signaling. More specifically, a recent study on zebrafish found that ALPK2 depletion results in severe cardiac defects. In this study, we investigated the role of ALPK2 in the mammalian heart by first generating two independent global ALPK2 knockout (ALPK2 gKO) mouse lines using CRISPR/Cas9. Physiological and biochemical analyses of ALPK2 gKO mice used to determine the functional, morphological, and molecular differences showed that ALPK2 gKO mice continued to exhibit normal cardiac development and function up to one year of age. Furthermore, there were no differences in WNT signaling found in neonatal ALPK2 gKO mice. Based on the results, we concluded that ALPK2 is not essential for mammalian heart function and development.
Developing a recombinant nitrogenase expression system in Azotobacter vinelandii

Robin Yu, Hannah Rutledge, Laura Williamson, Alkane Xu, and Akif Tezcan
Principal Investigator: Dr. Akif Tezcan

Biological nitrogen fixation by the enzyme nitrogenase is mediated by two metalloproteins: a homodimeric iron protein and a heterotetrameric molybdenum iron protein (MoFeP). Obtaining MoFe protein has only been done through expression in its native organism, as recombinant expression in non-native species such as E. coli has yet to be successful. The nitrogenase of Azotobacter vinelandii (Av) has been extensively studied because the organism is relatively easy to grow and produces more nitrogenase than other organisms. However, Av nitrogenase doesn’t encompass all the structural variations among molybdenum nitrogenases. We are developing a modular recombinant expression system for MoFeP using Av. A deletion strain plasmid was first constructed via blunt-end ligation that contains two Av overlap regions flanking a kanamycin resistance gene. This plasmid was successfully transformed into the Av chromosome via double homologous recombination to produce a MoFeP deletion strain that lacks nitrogen fixation ability. A second plasmid (rescue plasmid) has been constructed with the MoFeP genes (nifDK) of Gluconacetobacter diazotrophicus in place of the kanamycin resistance cassette. Multiple construction methods were attempted to successfully achieve the rescue plasmid. Transformation of the rescue plasmid into the Av deletion strain is still ongoing.

Virtual Presentation: https://ucsd.zoom.us/j/94548703392
Digital Poster: https://drive.google.com/open?id=1B6OxiMj86RGbHMFeElJeKnDdaUsSORpd

Biochemistry #10
Inorganic/Organic Division

Posters:  
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Group 1  
Virtual Presentation:  
https://ucsd.zoom.us/j/96710939211  
1. Hayley Fong  
2. Hannah Martin  
3. Ningkai Zheng & Catherine Arceo

Group 2  
Virtual Presentation:  
https://ucsd.zoom.us/j/95446864473  
4. Kun Yong Jeoung  
5. Kien Malarney  
6. Shenghua Yang
Melanins are of significant research interest due to their ubiquity in nature as well as their high versatility for application. Polydopamine (PDA) serves as a synthetic mimic to melanin. Unlike previous efforts made to isolate and purify melanin, synthesis of polydopamine is facile, sustainable, and highly reproducible. Despite decades of study, researchers have yet to elucidate the polymeric structure and synthetic mechanisms. Previous work has proposed that aliphatic amines mechanistically favor Schiff-base formation, indicated by 1H NMR and FTIR spectroscopic studies; thus, we speculate that Tris buffer is incorporated into the structure of PDA via imine formation. Preliminary characterization of the material by SQUID magnetometry and ICP Mass Spectrometry suggests that the magnetic behavior of the material is notably sensitive to the iron concentration of the polymer, while variations in the Tris concentration appear to affect the coupling strength between metal ions. The synthetic methodology to prepare these materials is described herein.

Virtual Presentation: https://ucsd.zoom.us/j/96710939211
Digital Poster: https://drive.google.com/drive/folders/1uY608-iugli6xc_wkhWAz7FBJqDFE86q?usp=sharing

Inorganic/Organic #1
Space-filling organic chemistry models: An entirely 3D printed CPK molecular model set

Hannah Martin and Jeremy Klosterman
Principal Investigator: Dr. Jeremy Klosterman

Ball and stick (BS) molecular models are widely used in organic chemistry for teaching connectivity, bond angles, and the stereochemistry of organic molecules. However, BS models do not accurately convey the reality of atomic radii or bond lengths, yet understanding the steric size and shape of molecules is essential for predicting the reactivity and selectivity in organic reactions. 3D printing has become increasingly accessible and has enabled widespread access to custom 3D printed models, yet accurate and flexible molecular model sets remain few. This project aimed to create an inexpensive and accessible Corey Pauling Kolton (CPK) molecular model set with accurate atomic radii. This fully 3D printed model set physically represents the steric s of any organic molecule for organic chemistry students to learn from and use to predict reactivity. Each atom was designed using Autodesk Fusion 360 from spheres based on updated and accurate atomic radii. Flat bonding surfaces were cut at the average bond radii, based on modern crystallographic data, and a female connector socket stamped into each bonding surface. The Koltun connector, designed to hold atoms at the correct distances while also allowing for bond rotation, was adapted for 3D printing from common thermoplastics. Students can hold and interact with these models to tangibly experience molecular steric and its effects when examining the conformations and reactivity of organic molecules. Additionally, these 3D printed molecular models can be printed at large scale for supplemental lecture demonstrations.

Virtual Presentation: https://ucsd.zoom.us/j/96710939211
Digital Poster: https://drive.google.com/drive/folders/1uY608-iugli6xc_wkhWAz7FBJqDFE86q?usp=sharing

Inorganic/Organic #2
Eumelanin is a type of melanin pigment commonly found in biological systems like the shells of insects. Polydopamine (PDA), a synthetic mimic of eumelanin, has many applications such as drug delivery and sensing hydrocarbons. A more detailed understanding of PDA would be helpful to our research on the thermal conductivity and the effects of radiation. Also, further understanding of PDA could contribute to our research on thermal conductivity and the effects of radiation. PDA can be synthesized by oxidizing dopamine in an aqueous solution. However, PDA’s polymerization can be affected by pH and oxygen concentration, which can change properties of PDA nanoparticles such as size.

To mimic the natural conditions found within biological systems, PDA nanoparticles were added to a chitosan polymer matrix. Then, using drop casting and doctor blade casting methods, PDA-chitosan films were prepared and studied using UV-Vis spectroscopy. The films were studied to monitor the effects of particle size to obtain a better understanding of PDA’s structure.

Our study of PDA is part of a multi-collaborative project consisting of several different labs at several different universities. The labs that we are closely collaborating with are studying thermal conductivity and the effect of radiation on PDA-chitosan films.

Virtual Presentation: https://ucsd.zoom.us/j/96710939211
Digital Poster: https://drive.google.com/drive/folders/1uY608-iugli6xc_wkhWAz7FBJqDFE86q?usp=sharing

Inorganic/Organic #3
Development of fluorescent probes for the detection of tau in Alzheimer’s Disease

Kun Yong Jeoung, Kristine L. Teppang, and Jerry Yang
Principal Investigator: Dr. Jerry Yang

Alzheimer’s Disease (AD) currently affects 5.8 million Americans and with no current treatments available, there is a need for chemical tools for detection. Pathological hallmarks of AD precede clinical symptoms by years. These include accumulations of misfolded proteins (amyloids) such as β-Amyloid (Aβ) and tau, with tau better correlating with AD disease progression. Despite the development of tau fluorescent probes in the field, many suffer from poor selectivity (binding to other amyloids) and low brain uptake. Many of these probes are based off Aβ binders since they both share high β-sheet content, however precedence in literature has shown that the extension of conjugation of known Aβ probes results in selectivity towards tau. Previously, the Yang lab has developed aryl cyano amide (ARCAM) and amino-aryl cyanoacrylate (AACA), fluorescent probes that bind to Aβ in solution and in AD postmortem tissue. ARCAM and AACA are environmentally sensitive molecular rotors that demonstrate fluorescence enhancement when bound to the β sheet region of amyloids. In this presentation, I will present ongoing efforts to extend the π conjugations of ARCAM and AACA by utilizing Aldol or Wittig chemistry to modulate the probe’s selectivity towards tau. I will present both synthesis and characterization of new probes in solution with recombinant amyloids, and some preliminary results on their ability to stain tau in AD brain tissue. The development of these probes can be useful in a research setting and contribute to increased understanding about tau and its role in pathogenesis.

Virtual Presentation: https://ucsd.zoom.us/j/95446864473
Digital Poster: https://drive.google.com/drive/folders/1uY608-iugli6xc_wkhWAz7FBJqDFE86q?usp=sharing

Inorganic/Organic #4
Expanding the ligand scaffold for photochemical cycloadditions

*Kien Malarney and Valerie Schmidt*

Principal Investigator: Dr. Valerie Schmidt

Four-membered heterocycle containing oxygen and nitrogen atoms play an important role in synthetic, biological, and materials chemistry. Methods for synthesizing such heterocycles typically involve reactions with limited substrate scope or stoichiometric waste. More recent methods involve nucleophilic or transition metal catalysis. Among these recent strategies for accessing these heterocycles is a photochemical [2 + 2] cycloaddition between an imine or carbonyl compound and an olefin to produce the azetidine or oxetane, respectively. We sought to expand the substrate scope of this reaction through the rational design of ligand scaffolds and synthesis of strained olefins. Accordingly, we synthesized tris-(3-mesityl-pyrazolyl)-borate (TpMes) and tris-(3-(2-furyl)-pyrazolyl)-borate ligands. These ligands are of interest due to reports of TpMesCu coordinating simple olefins that do not coordinate the parent hydro-tris-pyrazolylborate copper catalyst. We propose that these compounds will aid in expanding the substrate scope of this reaction and in providing mechanistic insight.

Virtual Presentation: https://ucsd.zoom.us/j/95446864473
Digital Poster: https://drive.google.com/drive/folders/1uY608-iugli6xc_wkhWAz7FBJqDFE86q?usp=sharing

Inorganic/Organic #5
Synthesis of an emissive cytidine analogue (mthC)
Shenghua Yang, Paul T. Ludford III, and Yitzhak Tor
Principal Investigator: Dr. Yitzhak Tor

Fluorescence spectroscopy has long been viewed as a valuable tool in observing dynamics of biomolecules. Nucleic acids present a unique challenge. While the native nucleosides possess only negligible fluorescence, monitoring nucleosides and nucleotides have been made possible with the aid of fluorescent nucleoside analogues. Whereas fluorescent properties are usually unpredictable, we envisioned that through adding substituents to the thiophene ring of the previously synthesized thieno[3,4-d]pyrimidine scaffold, improved fluorescent features may be achieved.

In this work, a methylated analogue (mthC) is prepared through a nine-step synthesis. As envisioned, the molecule possesses red shifted absorption and emission compared to its unmethylated counterpart (thC). I will describe efforts towards synthesis and purification of the target molecule, as well as how the generation of this molecule may lead to further refinement of the photophysical features of emissive nucleosides.

Virtual Presentation: https://ucsd.zoom.us/j/95446864473
Digital Poster: https://drive.google.com/drive/folders/1uY608-iugli6xc_wkhWAz7FBJqDFE86q?usp=sharing

Inorganic/Organic #6
Physical/Analytical Division

Posters: https://drive.google.com/drive/folders/1huFFbND-kMnppysb1edY3H5I7x15HE28?usp=sharing

Group 1
Virtual Presentation: https://ucsd.zoom.us/j/96877019028
  1. Po Jui Chu
  2. Duyen Dang
  3. Reece James
  4. Zhuoying Lin

Group 2
Virtual Presentation: https://ucsd.zoom.us/j/93826094066
  5. Catherine Mullenmeister
  6. Gordon Peiker
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  8. Christina Trinh
Base editing is the latest genome editing technology that enables the conversion of one base pair into another at a precise genomic locus of interest through the chemical modification of a targeted nucleotide. One such class of base editors are the adenine base editors (ABEs) which facilitate efficient A:T to G:C base pair conversion at specific sites. Due to the lack of naturally occurring DNA-editing enzymes, ABEs were engineered through extensive evolutionary methods, starting from an RNA-editing enzyme, tRNA adenosine deaminase (TadA). Seven rounds of evolution and fourteen amino acid changes transformed the TadA enzyme into an efficient DNA-editor.

However, recent research has shown that this mutated TadA variant still preserves the RNA-editing activity of the native protein. This makes ABEs less viable as therapeutic agents. Hence there is a pressing need to find amino acid mutations that can abrogate this native RNA-editing activity of TadA enzyme. We are using molecular dynamics simulations to understand how these TadA variants interact with both DNA and RNA. Our research has shown that the initial mutations involved in the development of ABEs leads to structural and functional changes that not only increase the activity of the enzyme on DNA but also enable it to edit RNA substrates more efficiently. With this atomistic understanding of the interactions of ABEs with both RNA and DNA we can help guide experiments to design better base editor enzymes which selectively edit DNA with high efficiency.

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Physical/Analytical #1
Sea spray aerosols (SSA) have been shown to have a major impact on our climate, yet its composition and climate relevant properties are still poorly understood. Specifically, primary aerosols are generated mechanically through the breaking of waves via bubble bursting, suspending particles into the air above the ocean surface. Secondary marine aerosols (SMA) are formed through the nucleation of semi-volatile organic compounds. Many marine VOCs are directly emitted by marine biology such as phytoplankton, bacteria, and viruses, usually due to environmental stresses, quorum sensing, defense mechanisms, light initiated metabolisms, and more. Abiotic VOCs are formed without the help of biology via interfacial photochemistry of organic surfactants at the sea surface microlayer (SSML). These photochemically produced VOCs have been recently highlighted as a large potential source of gas phase species in our atmosphere—potentially driving climate processes. In this mesocosm study, bulk seawater from a controlled phytoplankton bloom was collected, where its headspace was analyzed using an Orbitrap mass spectrometer with a modified atmospheric pressure chemical ionization probe. The results present preliminary temporal compositional changes of the gaseous phase of seawater throughout a bloom cycle with respect to changes in biology.

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Physical/Analytical #2
The impact of phytoplankton organic emissions on sea spray aerosol phase state

Reece James, Paul Ryan Tumminello, Sarah Amiri, Kimberly Prather, and Jonathan H. Slade
Principal Investigator: Dr. Jonathan H. Slade

With the prevalence of larger and longer-lived phytoplankton blooms worldwide, discerning the climatic effect of their emissions in sea spray aerosol (SSA) has become increasingly important. SSA is the largest contributor to global aerosol mass and mainly composed of sea salt, organic carbon, and biological material. Organic carbon can adopt amorphous phase states (liquid, semisolid, or solid) that vary depending on its chemical composition (oxygen-to-carbon ratios and molecular weight), ambient temperature, and relative humidity. While phase state impacts gas-to-particle conversion processes, heterogeneous chemistry, and atmospheric phenomena, such as ice nucleation, it is currently unknown how bulky biomolecules emitted from phytoplankton affect the phase state of SSA during various stages of phytoplankton blooms. Phytoplankton abundance and its link to SSA phase state has been studied based on wave-breaking mesocosm experiments in conjunction with the National Science Foundation Center for Aerosol Impacts on Chemistry of the Environment. Phaeocystis has been identified as the dominant species in the induced bloom. Tracking the life cycle and intercellular competition between bacteria and phaeocystis species has led to the identification of chrysolaminarin, mucopolysaccharides, and monosaccharides as potential important organic emissions that impact SSA phase state. In our work we use an electrical low-pressure impactor, an extractive electrospray ionization high-resolution time-of-flight mass spectrometer and a scanning electrical mobility spectrometer to directly infer transient variations in SSA phase state and composition over the course of the bloom. Our analysis indicates, for the first time, a direct link between phytoplankton bloom organic emissions and SSA phase state.

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Physical Analytical #3
Using scanning electricity mobility spectrometer (SEMS) to study size distribution and physical properties of marine aerosol as a function of biological activity, oxidative exposure and relative humidity

Zhuoying Lin, Adam W. Cooper, Paul R. Tumminello, Samantha Kruse, and Jonathan H. Slade
Principal Investigator: Dr. Jonathan H. Slade

Aerosols influence climate both directly via the scattering of light and indirectly via the formation of clouds. A major source of atmospheric aerosol originates from marine environments, either through direct (primary) emission as sea spray or indirectly (secondary) via gas-to-particle conversion of marine-derived gases. While marine aerosol represents the greatest source of particulate mass to the atmosphere, its chemical and physical properties as a function biological activity in sea water and age in the atmosphere are poorly understood. In the Sea Spray Chemistry and Particle Evolution (SeaSCAPE) 2019 summer study, three types of marine aerosol---primary (nascent), secondary and oxidatively aged marine aerosols---were sampled from a mesocosm in a wave channel over the course of two months, and their number concentrations and size were tracked as a function of biological activity, oxidative exposure (equivalent atmospheric aging) and relative humidity using a scanning electricity mobility spectrometer (SEMS). SEMS charges the entering particles and sorts them by diameter based on charge-to-size differences. It counts them via light scattering after condensational growth in a condensation particle counter, yielding near-real time (2 min) size distributions from 5 nm to 859 nm. Preliminary results show the number concentration of aerosols increase with increasing oxidative age and relative humidity, and their total mass depends on biological activity in the seawater. These measurements reveal a dynamic relationship between the composition of marine aerosol, ocean biological activity and atmospheric age, which may be useful to better understand the impact of marine aerosol on Earth’s climate.

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Physical/Analytical #4
Secondary Marine Aerosols (SMA) are formed through the release of volatile gases into the atmosphere. These gases are oxidized and condense to form particles that can serve as "seeds" for cloud droplet formation, known as Cloud Condensation Nuclei (CCN). To characterize the CCN activity of Secondary Marine Aerosol, we simulated aging of gases released over the course of a phytoplankton bloom in a Potential Aerosol Mass Oxidative Flow Reactor (PAM-OFR). Over the course of the bloom, both the number concentration and CCN activity of SMA changes. The results indicated that as the oxidative exposure in a PAM-OFR cycle increases, representing increased aging intensity, SMA exhibited increased cloud condensation nuclei activity in super-saturated conditions. The hygroscopicity parameter, a quantitative measure of water uptake ranged from k=0.3-0.7 as oxidation increased. Due to the complex chemical composition of SMA we then developed simplified model systems using pure standards of common SMA precursors to better understand the CCN behavior of this aerosol. In sub-saturated conditions, the uptake of water by SMA can be represented by the hygroscopic growth factor. By oxidizing common SMA precursors, such as α-pinene the shift in particle diameter due to the uptake of water can be examined. The hygroscopic growth factor of α-pinene was found to be 1.12 ± 0.04 at 90% relative humidity. These results provide insight into the hygroscopic properties of SMA in both sub-saturated and super-saturated relative humidity conditions, further informing how Secondary Marine Aerosol can affect the number and size of cloud droplets. Understanding these aerosol-cloud interactions is important as they impact cloud properties such as precipitation and albedo.

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Physical/Analytical #5
Changes in the O–H stretching region of water as a function of temperature using micro-Raman spectroscopy with and without the presence of ice nucleating particles

Gordon Peiker, Liora Mael, Heidi Busse, and Vicki Grassian

Principal Investigator: Dr. Vicki Grassian

Ice nucleating particles (INP) lead to the formation of atmospheric ice and mixed phase clouds which play a critical role in many atmospheric processes such as radiative forcing and the global hydrological cycle. The immersion freezing pathway resulting from interactions between INPs and condensed water is a particularly important yet poorly understood process. In order to understand a freezing event, an understanding of interactions between water and the INP prior to freezing is key. Raman spectroscopy was used in combination with a temperature and relative humidity-controlled cell to investigate spectral changes in water at various temperatures. Changes in the O-H stretching region of water provide information about the interaction between INPs and water prior to freezing. The broad O-H stretching peak was deconvoluted in order to investigate how the interactions between INPs and water change relative to pure water. This method was applied to both water in contact with lipopolysaccharide (LPS), a poor INP, and with Snomax, a well-known, commercially available biological INP with high activity. Comparisons between spectral behavior of 3-micron sized substrate deposited pure water drops and these mixed systems as a function of temperature can be used to gain a better understanding of the water-INP interactions on a molecular level. Future studies will work to extend this technique to more marine relevant systems and potentially use this information to help categorize and predict the ice nucleating behavior of different systems.

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Physical/Analytical #6
Sea spray aerosol (SSA), generated from oceanic wave breaking, can affect the climate by altering Earth’s radiative budget and influencing cloud formation by acting as cloud condensation nuclei and participating in ice nucleation. SSA, the largest contributor of atmospheric aerosol mass, also serves as a long-range transporter of oceanic constituents. Current analytical techniques for understanding SSA molecular composition result in low time resolution or only provide partial composition analysis. In this work, an Extractive Electrospray Ionization High-Resolution Time-of-Flight Mass Spectrometer (EESI-HR-ToF-MS) is utilized as an online, soft ionization method that reduces analyte fragmentation, minimizes thermal desorption, and improves time resolution from traditional hard ionization and offline techniques. In this study, the molecular composition of nascent SSA, generated from a Marine Aerosol Reference Tank (MART) over the course of an induced phytoplankton bloom in sampled oceanwater, is analyzed using the EESI-HR-Tof-MS. The MART produces SSA by mimicking the wave breaking of natural waves. In this work, we present the observed changes in molecular composition of SSA over the course of the bloom. We also report overall trends, including weighted average molar masses, H:C/O:C ratios, and variation due to changes in relative humidity. This study contributes to the further understanding of nascent SSA molecular composition, as well as provides another example of the many capabilities of the EESI-HR-ToF-MS.

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Physical/Analytical #7
Minimal media expression and spectroscopic characterization of azurin with isotopically substituted L-Trp-d5

Christina Trinh, Joel Rivera, and Judy Kim
Principal Investigator: Dr. Judy Kim

The blue copper protein, azurin, is a model protein used to study the role of amino acid radical intermediates in electron transfer reactions. Azurin contains a single tryptophan residue in a hydrophobic pocket of the protein that undergoes a photo-induced proton coupled electron transfer reaction to generate a long lived neutral radical. Previous work has shown that the quantum yield of the tryptophan neutral radical is reduced when isotopically substituted tryptophan (L-Trp-d5) is incorporated into the protein. The observed isotope effect may be correlated to a lower fluorescence intensity of the deuterated isotopologue. A quantitative study on the fluorescence quantum yield of L-Trp-d5 in azurin has not been pursued due to a lack of protein sample. In this work, a minimal media expression protocol was optimized to produce azurin in high yield, but this high yield was not reliably reproduced. It was determined that overnight expression, at room temperature significantly increased protein yield and that minimal media could be used to control the metal content of the protein sample without the need for re-metalation. Spectroscopic characterization of the protein sample confirmed that L-Trp-d5 was successfully incorporated into azurin. Fluorescence quantum yield values at different excitation wavelengths are also reported but additional measurements are needed to obtain reliable values.

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Physical/Analytical #8
We are grateful for the time, expertise, and encouragement from our faculty, postdoc, and graduate student judges from the UC San Diego Department of Chemistry and Biochemistry.

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