Poster Presentations

A1) Analyzing Size and Structural Effects on Photocatalytic Efficiency of CdSe Nanoparticles

Emilio Aguilar, Kayla Lee, Chloe Peak, Michael Enright

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Growing concerns over climate change have driven the urgent need to transition from petroleum-based energy sources to renewable alternatives, increasing the demand for renewable carbon-based feedstocks to produce high-value commodity chemicals. Semiconductor nanoparticles, such as quantum dots and nanorods, have emerged as promising photocatalysts for driving organic transformations, including biomass valorization, a process that selectively cleaves specific bonds within lignin to extract valuable molecular components. In this study, we investigate the use of CdSe quantum dots and nanorods with varying sizes and morphologies for the photocatalytic degradation of biomass model substrates. The electronic properties and redox potentials of these nanomaterials can be precisely tuned by adjusting their size and surface chemistry, while their increased surface area compared to molecular catalysts enhances substrate interactions, electron transfer, and overall catalytic efficiency. To assess the influence of nanoparticle size and structure on photocatalytic performance, we compare a series of CdSe nanoparticles based on their surface area, crystal phase (zinc blende or wurtzite), and efficiency in selectively cleaving C–O bonds in model substrates that resemble biomass. Photocatalysis experiments incorporated different bandpass filters, and for one sample, varying light intensities were also explored to assess their impact on catalytic efficiency. This study provides insights into the structure-activity relationship of CdSe nanomaterials for biomass valorization and demonstrates how differences in nanoparticle size and morphology influence their photocatalytic performance.

A2) Structure-function of dual NAD-kinase/NADP-phosphatase enzymes from extremeophiles

Haneen Alkabbani, Eric Greene

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Organisms maintain distinct pools of reducing equivalent molecules in the cell where NADH is associated with anabolic reactions (energy harvesting) and NADPH is associated with catabolic reactions (energy utilizing). Often, these pools need to be altered for adaptation to new cellular conditions or when engineering hosts to produce (energy utilizing) high level of high value compounds. This project focuses on the expression and characterization of a dual function NAD kinase/NADP phosphatase

enzyme that can directly alter levels of NAD(H) and NADP(H) in the cell. To achieve this, we designed and cloned expression plasmids bearing synthesized genes. We expressed the bifunctional enzymes in E. coli and purified each to homogeneity and kinetic characterization is underway. Future directions include mutation studies and cryoEM structural determination to further elucidate enzyme function and adaptation mechanisms. The structure-function relationships forged herein will represent the first for this unique class of enzymes that are the only known to directly rebalance NAD(P) (H) pools in the cell and offer a promising avenue to manipulating reducing equivalents towards bioengineering efforts.

A3) Computation of Substituent Effects on Neutral Enediyne Cyclizations

Benjamin F Gherman

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Enediyne-containing compounds have the potential to form diradicals upon either a C1C6 (Bergman) or C1-C5 cyclization. The importance of these diradicals is in their ability to cleave hydrogen atoms off of DNA, which has implied characteristics for cancer treatment. In order to study this reactivity, a computational study of the substituent effects on the cyclization reactions of enediynes, benzannelated enediynes, and quinoxalenediynes was conducted. The quinoxalenediynes contain N-heterocycles which may make their reactivity different compared to the enediynes and benzannelated enediynes. The substituents tested were H, electron-withdrawing (F, CF3), and electrondonating (OCH3, NH2). Computations were done using density functional theory (DFT) with the BLYP, B3LYP, and mPW1PW91 functionals (each used in prior computational studies on enediynes). These methods were used to calculate the activation enthalpy ΔH‡ and reaction enthalpy ΔHr for both reaction pathways (C1-C6 and C1-C5). For each type of enediyne compound, Hammett plots of activation enthalpy and reaction enthalpy versus the substituent Hammett σp parameters were made. Results showed that both quinoxalenediynes and benzannelated enediynes had higher reaction enthalpies for C1-C5 compared to C1-C6. However, due to the proximity of the alkyne phenyl substituents on the quinoxalenediynes, there was a higher activation enthalpy for the C1-C6 compared to the C1-C5. Overall, C1-C6 products are more stable than C1C5 due to aromaticity in the new six-membered ring. With data for activation and reaction enthalpies varying little with different substituents, substituent effects on the neutral enediyne cyclizations were minimal.

A4) Protein corona formation on functionalized fullerenes

Rebecca Gardner, Rebecca An, Claire Alford, Samira Billow, Maciej Serda, Korin E. Wheeler

SANTA CLARA UNIVERSITY

Due to their versatile applications in nanomedicine and targeted drug delivery, fullerenes—hollow spherical nanoparticles with an alternating hexagonal and pentagonal carbon structure—have become a new area of interest to researchers in biotechnology and biomedicine-related fields. Fullerenes' applications in targeted therapeutics are particularly important because they can deliver many kinds of molecules, from drugs to nucleic acids. This specific and more efficient delivery system would mitigate harmful effects on healthy cells and reduce the side effects of aggressive treatments like chemotherapy. When exposed to biological media, fullerenes form a coating of proteins called a protein corona that dictates their properties and biological interactions. By manipulating the fullerenes' functionalization, the corona surface proteins can guide the particle to the desired tissues and cells. Despite yielding promising results as targeted carriers, competitive protein adsorption and corona formation in fullerenes have not been fully understood. This study provides insight into these particle-protein interactions and demonstrates the effect of functionalization on the protein corona population. We analyze the human serum protein corona across biologically active modified fullerenes: Fullerol (C60(OH)24) and Erlotinib-treated conjugates (Gd@C82 EDA-ERL and C70BUT-ERL). Zeta potential and dynamic light scattering characterized changes in fullerene surface chemistry and agglomeration by changing stability in blood plasma across various pH conditions. LC-MS/MS proteomics identified hundreds of proteins in each fullerene corona, yielding very different populations. Further bioinformatic analysis provided insight into relative abundance, biophysical property trends, and potential impacts of nano drugs on metabolic pathways. Through characterizing fullerene coronas, we can better predict fullerene behavior and efficacy in vivo to further the development of targeted carriers.

A5) Application of 3D Printing in Nuclear Targetry to Aid New Element Discovery

Jacklyn M. Gates , Rodney Orford, and Nicholas E. Esker

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Target thickness plays a crucial role in the production and study of exotic heavy elements at the Berkeley Gas-filled Separator (BGS) of Lawrence Berkeley National Laboratory's (LBNL) 88-inch cyclotron facility. An inconsistent target thickness can limit the production of isotopes or lead to the synthesis of different isotopes entirely, making it a crucial variable to understand in nuclear science experiments. We have successfully designed a system to quickly and accurately measure targets down to hundredths of a micron. To do this, we quantified the energy loss of an alpha particle moving through a target compared to open vacuum. This energy loss was then compared to SRIM Monte Carlo simulation

data to determine a final target thickness. A mixed alpha source consisting of 239Pu, 241Am, and 244Cm was used and observed with a PIPS detector mounted on 3D printed arms inside a custom vacuum chamber. 3D printing is a common method for rapidly manufacturing custom parts used in nuclear science experiments. Printed parts that are used under vacuum require special consideration as they are prone to having air trapped in their interior volume, which is problematic as it can cause excessive outgassing or a catastrophic structural failure of the part. It was determined that a gyroid infill has superior performance under vacuum and was utilized for parts in the target thickness chamber. These parts experienced no failures under extensive use and proved the efficacy of 3D printing for our purposes. These findings were then used in additional projects including mounting detectors in the BGS and the production/analysis of thin film targets, opening new possibilities for what our group is capable of. In this talk, we will discuss the results of our target thickness measurements and the applications of 3D printing in nuclear targetry.

A6) Investigation of Target Thickness to Aid New Element Discovery

Allan Ard, Jacklyn Gates, Rodney Orford

SAN JOSE STATE UNIVERSITY

Target thickness plays a crucial role in the production and study of exotic heavy elements at the Berkeley Gas-filled Separator (BGS) of Lawrence Berkeley National Laboratory's (LBNL) 88-inch cyclotron facility. This facility has a well established history of utilizing beam-target reactions to characterize the properties of super heavy elements and has continued to push far from stability on the nuclide chart. An inconsistent target thickness can slow the production of isotopes or lead to the synthesis of different isotopes entirely. This makes super heavy element experiments extremely difficult and demand high levels of precision to be successful.

This project focuses on the development of a procedure for accurately measuring target thickness at the cyclotron lab to increase the efficacy of super heavy element experiments. Measuring target thickness was previously impossible and required outsourcing to Lawrence Livermore National Laboratory or other campus divisions. Our newly constructed apparatus enables the Heavy Element Group at LBNL to quickly and accurately measure target thickness for BGS experiments without outside aid. To measure target thickness, we quantified the amount of energy loss an alpha particle experiences moving through a target compared to open vacuum. A mixed alpha source consisting of 239Pu, 241Am, and 244Cm was used and observed with a PIPS detector inside a custom vacuum chamber. This energy loss was then compared to SRIM Monte Carlo simulation data to estimate a final target thickness.

A Ti foil was initially measured due to its known thickness of 2.032 microns, which was confirmed by our calculated thickness of 2.031 microns This result helped us to characterize the thickness of several additional Bi targets that will be used in future experiments involving radioactive targets.

A7) CRISPRi Knockdown of J-domain Proteins in Pseudomonas putida

Gwen Libozada, Melanie Martinez, Kanika Kolpe, Jason Do, Aryan Shah, Harsita Kumar, Jared Raab, Sanjana Ramesh, Misty Ramos, Megan Badrak, Taylor Arhar

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Bacteria face a variety of stressful conditions in their environments, and to adapt to these conditions, bacteria rely on J-domain proteins (JDPs). These molecular cochaperones play a pivotal role in maintaining protein integrity and function in stressful conditions. Previous studies have highlighted the importance of JDPs in the Pseudomonas genus as they often rely on several JDPs like DnaJ, CbpA, and DjlA to increase stress tolerance. However, little is known about the specific role each of these chaperones has in bacterial survival under stress. This project specifically focuses on understanding the role of DnaJ, CbpA, and DjlA in the growth and survival of Pseudomonas putida. Using Mobile CRISPRi, we will knock down expression of these proteins and assess their impact on bacterial growth and survival. Our approach includes cloning guide sequences targeting the three JDPs into Mobile CRISPRi vectors, followed by triparental matings to build the knockdown strains. This study will elucidate which JDPs are essential for specific environmental pressures and increase our comprehension of bacterial proteostasis networks. P. putida is related to Pseudomonas aeruginosa, a dangerous pathogen that causes infections in humans. Therefore, our work in P. putida may potentially reveal novel targets for antimicrobial development and enhance our understanding of microbial stress adaptation.

A8) Chiral Recognition in Lanthanide(III) Complexes Using Spectroscopic Methods

Daniel Ariza, Kim Rivera,Tylaire Ocampo,Darlyn Gonzalez,Gilles Muller

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Many biomolecules in nature display chiral characteristics, existing in two enantiomeric forms. One form may be beneficial, while the other can be harmful to biological systems. As a result, determining the chirality of a molecule and effectively separating or resolving its enantiomers is essential before introducing it into a living organism. To facilitate this process, there is a need for more sensitive tools and techniques. Circularly Polarized Luminescence (CPL) spectroscopy proves to be a valuable tool for chiral recognition due to its heightened sensitivity to chiral environments and its ability to differentiate between two chiral species in solution. The present study investigates how spectroscopic methods can be employed to examine the disruption of racemic equilibria in luminescent lanthanide(III) complexes, caused by the introduction of biomolecules such as L-amino acids.

A9) Life on Earth... from Space

Stephen Ball, Nourdean Shraim, Dr. Andro Rios

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Determining the origin of metabolism is one of the most significant problems in prebiotic chemistry. The discovery of this process would be a profound step towards finding the origin of life itself. Our research aims to verify the hypothesis that a major component of a primitive metabolism, the pyruvate reaction network (PRN), was present in meteorites before they fell to Earth. In other words, we want to find evidence that metabolismadjacent reactions occurred on the early Earth.
Under certain conditions, pyruvate molecules may combine to form compounds that can undergo further reactions with each other or break down back into pyruvate. Building off of previous work, we are searching for evidence that the PRN has been an active presence in carbonaceous chondrites – carbon-containing meteorites that, in some cases, landed on Earth billions of years ago.
Using gas chromatography–mass spectrometry (GC–MS), we have conducted many comparative analyses. Using pyruvate-based chemical standards made in our lab, we carry out reactions under simulated prebiotic conditions – generating the PRN – and compare chemical data of their products with that/those of meteorites - records of the early Solar System. To enhance volatility and thermal stability for GC-MS analysis, we use tert-butyldimethylsilyl (TBDMS) reagents to derivatize the compounds, allowing for better chromatographic separation, more predictable fragmentation patterns, and easier detection of PRN products. We compare mass spectra and chromatographic data of meteoritic samples with data from samples of lab-generated reactions. We have determined some compounds to be identical across meteoritic and lab-generated samples. This supports our hypothesis that the PRN we see in our laboratory reactions also occurs in meteorites. Our results showcase one match identified as zymonic acid as well as four yet-unidentified matches within the GC-MS spectral data.
In our research, we are seeing mounting evidence that carbonaceous chondrites, with no contamination by Earth-based life , can harbor a series of complex pyruvate-based reactions. If true, this will strengthen the case for a prebiotic PRN, and provide new avenues into the study of the origin of metabolism as well as life itself.

A10) H-Bond Networks Described by Exhaustive Model Set of BIV TAR RNA Binding Tat Peptide

Brooke Bellinghausen, Ethan Suwandi, Brooke Lustig

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The interaction between viral-encoded regulatory proteins with RNA target sequences controls gene expression among lentiviruses, notably the human immunodeficiency (HIV) and bovine immunodeficiency virus (BIV). BIV is structurally similar to HIV but provides a

simpler interaction model between the trans-activator of transcription protein (Tat) and RNA trans-activation response element (TAR). Initial theoretical considerations of the effect of peptide flexibility on binding affinity may reveal potential clinical approaches for treatment. Building on our earlier approach of introducing flexibility to increase binding stability, we considered the K75G, R78G, and K75G-R78G mutant Tat peptides in addition to the wild-type (WT). In a novel fashion, we exhaustively generate a set of 273 RNA targets with peptides flexibly docked for each (resulting in some 300 thousand stable complexes). More recently we filtered 3D secondary structures by heat maps of Rg (radius of gyration) and Gridscore (DOCK6), leaving selected RNA targets with WT and mutant flexibly docked peptides. Extensive sampling for WT and mutants strongly suggests the multiplet (u10:a13-u24) is largely intact. In addition, there is some evidence of extended peptide structures as well as opening of the TAR g11-c25 pair as well as possible alternative stem stackings. Originally, we selected from WT and each mutant, stable DOCKed complexes for molecular dynamics (MD) over 200ns time scales. Here mutant structures have significantly more metastable states relative to the WT as well as a variety of alternative RNA secondary structures. This is consistent with glycine mutants being more flexible and hence more available for a variety of alternative contacts. Interestingly, R78G and K75G- R78G binding often displays decoupling of the g11-c25 RNA base pair. And the binding of mutant peptides indicated a variety of alternative hydrogen bond networks. Waters that mediate via their hydrogen bonding to adjacent ribonucleotides and amino acids (bridging waters) were also found to correlate with the extension of the peptide, increasing interactions with the hairpin loop. Longer MD time scales are suggested to better explore the correlation of stabilizing interactions with relatively large-scale events such as the opening of the BIV TAR g11-c25 pair.

A11) Ensemble Modeling of Switch-Like and Related Regions in Sirtuins

Brooke Bellinghausen, Britney Nguyen, Richard Pearson, Shwethal Sayeeram Trikannad and Brooke Lustig

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Protein function is inextricably linked to protein flexibility and mechanics, where fluctuations are a function of sequence and environment. Research focused on protein conformational switches promises to help advance the development of biosensors, engineered proteins, and novel therapeutics. In our research, we use three sequencebased descriptors with the potential to guide us to interesting biologically relevant, switch-like regions within proteins. The descriptors are six-term sequence entropy (E6), residue disorder propensity (IsUnstruct), and predicted secondary structure variability (Vkabat). These key descriptors are among the best performing of all sequence-based predictors indicated by logistic regression. A simple direct method of analysis has these three parameters displayed as overlays with respect to sequence, describing sequence regions that are correlated. Then we can evaluate these overlay patches by calculating Vkabat from secondary structures for an ensemble of at least twenty model structures generated via I-TASSER, C-I-TASSER, AlphaFold2 and RoseTTAFold. So for hSIRT-1, a lysine deacylase that plays important roles in regulating cellular pathways, the

most viable set among the regions of interest originally derived from the overlays of sequence-based descriptors are 186-193, 295-298, 447-452, and 279-286 (ranked best to least).

Our methodology for evaluating the switch-like regions does seem reasonably robust with respect to changes in the structure prediction methods used, such as exchanging the models generated from RaptorX for those generated by AlphaFold2 not changing the regions' ranked order. Interestingly, all four ranked regions are accessible to key features involving binding and regulation, where the 186-193 region has been verified experimentally as modulating allosteric effects. Also, the ensemble of 3D models indicates an additional helix in proximity to a nearby three-helix structure that includes the possible 186-193 switch. Interestingly, initial modeling of Xenopus SIRT4 sequence compared to a related hSIRT1 X-ray structure suggests the formation of a similar transient helix in what appears to be also in a highly disordered region. Our findings suggest integrating such computational approaches to experiment may facilitate the identification of key residues in enzymes and other proteins for therapeutic drug targeting and other applications.

A12) Studies Towards Synthesis of (-)-Ardeemin Using Convergent Electrochemical Radical Cyclization

Enguun Boldbaatar, Tim Chyrklund, Herman Nikolayevskiy

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Multidrug resistance (MDR) in cancer cells is a major cause of chemotherapy failure, contributing to over 90% of related deaths. Reversing MDR represents a promising strategy to extend the effectiveness of existing chemotherapeutic agents. (−)-Ardeemin, a natural product first isolated from Aspergillus Fischeri, has been shown to reverse MDR through inhibition of efflux pumps but further research development has been limited by its low natural abundance and the poor yields from total synthesis. This study aims to improve the efficiency of (−)-Ardeemin synthesis through a convergent approach that employs a one-electron electrochemical radical cyclization as the key transformation to construct the central ring system. To evaluate the feasibility of this step, we are developing a model system that omits the substituted indole. An advanced intermediate toward this model compound has been successfully synthesized in approximately 50% yield over 3 steps with structure and purity confirmed by NMR analysis. Future work will focus on completing the synthesis of the model system and optimizing the key radical cyclization step, ultimately enabling application of this strategy toward the total synthesis of (−)-Ardeemin.

A13) Testing Aromaticity of Soils as a Function of Moisture and Depth in TerrestrialAquatic Interfaces

Carlo Borea, Amrita Bhattacharyya

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Terrestrial-aquatic interfaces (TAIs) are dynamic regions where land meets water. TAIs are home to incredibly complex biogeochemical systems within the ecosystem, yet little is known of the effects of regional parameters, like soil moisture and depth, on the aromaticity of soils in TAIs. Aromatic compounds, an important component of soil organic matter (SOM), influence soil properties like sorption, decomposition, water retention, redox reactions, and soil fertility and stability. An aromaticity index delegates a numerical value to quantify the concentration of aromatic compounds as a response to specific changes. This research aims to construct an aromaticity index using SUVA (Specific UV-vis Absorbance) analysis that will quantify the effects of soil moisture and extraction depth on the concentration of aromatic compounds in TAIs. An SUVA analysis was performed on soils collected at five depths from a floodplain and hillslope region in East River, CO, to capture how proximity to the river can affect the distribution of aromatic organic compounds. Preliminary data show that aromatic carbon concentration steadily decreases with depth and increases with moisture content, yet carbon absorbance values in TAIs are significantly influenced by other variables besides depth and moisture. This aromaticity index will aid in understanding SOM decomposition patterns, which play a major role on greenhouse gas emissions at TAIs, and thereby providing more accurate predictions as soils are subject to change.

A14) Development of Assays for the Evaluation of a “Reverse Prodrug” DNA-Alkylator

Stella Bronzini, Christine Albrecht, Herman Nikolayevskiy

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Traditional DNA-damaging chemotherapy agents remain the most used in cancer treatment due to their potent antiproliferative effects on malignancies. Among these, DNA alkylators are a key subclass that destabilizes DNA by forming covalent adducts with nucleotides, specifically targeting the N7 position of guanine. Despite their efficacy against cancer cells, DNA-damaging agents often cause collateral damage to healthy cells, resulting in tissue damage and chemotherapy side effects. To address this challenge, our lab is working on the development of DNA alkylators equipped with DNAtargeting elements, such as amino numonafides (AN). These compounds are designed to selectively deactivate in healthy cells while remaining active in cancer cells.
Evaluating the efficacy of such compounds requires optimized biological assays such as gel electrophoresis, which assesses DNA-alkylating activity by analyzing the migration of damaged DNA fragments, and UV-Vis spectroscopy, which quantifies DNA intercalation using the Benesi-Hildebrand equation. This study attempts to explore the effects of DNA

purification buffers, and DNA extraction methods on the yield of pRSETA-GFP and calf thymus plasmid DNA. One goal is to optimize the pRSETA-GFP plasmid DNA for gel assays by investigating how heat/incubation time, the concentration of NaOH for denaturation, and DNA extraction quality impact the results of gel electrophoresis experiments. Initial studies suggest that the concentration of NaOH has a larger influence on denaturation than time or temperature. Additionally, UV-Vis assays show that the 6-AN compound has a lower Kd value compared to 5-AN, suggesting a higher DNA-binding affinity and increased DNA-damaging potential against calf thymus plasmid DNA. Further assay optimization is planned to expand our understanding of DNA damage induced by off-switchable DNA alkylators.

A15) Unusual chemical and physical properties in metal-verdazyl coordination compounds

Anna Buryachenko, Shoug Almutairi, Danh Hoang, Wilson Lee, Jesus Tamayo, David J. R. Brook

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The redox active terpyridine analog 1,3-dipyridyl-5-isopropyl-6-oxoverdazyl shows a wide variety of unusual phenomena with transition metals. Physical phenomena include strong magnetic exchange, valence tautomerism, spin crossover, equilibria between localized and delocalized forms. In addition coordination compounds can show important chemical reactivity such as water oxidation under mild conditions. We present a summary of the various observed phenomena and attempt to rationalize them based on a close match between ligand and metal orbital energies, and a short metal ligand distance

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A16) Identifyinig E3 Ubiquitin Ligases for Human CENP-A using CRISPR-Cas9 Knockout

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The nucleosome is the repeating unit of chromatin composed of histone proteins assembled in an octameric core and wrapped in DNA.The canonical histones H2A, H2B, H3, and H4 make up the nucleosome and several variants including H3.3 and CENP-A.Histones undergo a diverse range of post-translational modifications to regulate cellular processes.Yet the method of histone degradation in humans remains elusive.Previous studies revealed yeast histones are targeted for degradation by the ubiquitin-proteasome system (UPS) but no specific E3 ligases involved in histone homeostasis have been identified in humans. Knowing this we can infer the process is likely conserved in higher eukaryotes. CENP-A and H3.3 are the focus of this project.CENP-A plays a vital role in localizing the human centromere for proper cell division.Overexpression of CENP-A is common in many cancers so learning more about how it is degraded is of high clinical

relevance.The modification of interest ubiquitylation requires an enzymatic cascade involving enzymes E1, E2, and E3. E3 ubiquitin ligases responsible for polyubiquitinating proteins to target them for degradation.This project aims to perform an arrayed CRISPR-Cas9 knockout screen using an sgRNA library targeting human E3 ubiquitin ligases and observe histone level changes to identify ligases involved in degradation.We will focus on human H3.3 to create expression clones for use in our knockout.We already have a bicistronic lentiviral vector containing XbaI and BamHI cloning sites followed by a 3XGS linker, EGFP, a self-cleavable linker, and a nuclear-localized mCHERRY sequence. Additionally we have a HEK293T cell line expressing GFP-tagged H3.3 and nuclear-localized mCHERRY.The next step is a pilot screen of 20 E3 ligases using pools of 3 sgRNA sequences per gene.Fluorescence microscopy will be used to observe Relative Fluorescence Units (RFU) for GFP and mCHERRY.RFU will be analyzed for each ligase to assess if it impacts histone levels.If knocking out a specific E3 ligase results in a higher GFP signal relative to mCHERRY we can infer that it is involved in targeting histones for degradation.We expect to produce pilot data defining which E3 ligases target CENP-A for degradation to investigate their role in cancer.This project is clinically significant due to CENP-A's role in cell division a process dysregulated in many cancers.This data will benefit epigenetic researchers and provide insight into a poorly understood molecular behavior.

A17) Surface Film Formation via Acid-Catalyzed Polymerization of Carbonyl Species in Sulfate-Rich Aerosols

Sean Colina, Kaitlyn Nguyen, Aishwarya Deepak, Anureet K. Chahal, Ethan Guidicotti, Rianna Farahani, Kathy Tong, Thuy Tran, Thomas Nelson, Annalise Van Wyngarden

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Aerosols in the upper troposphere and lower stratosphere (UT/LS) consist primarily of water and sulfuric acid (40 – 80 wt%), formed from photo-oxidation of sulfur dioxide. Current climate models incorporate the cooling effects of UT/LS sulfate aerosols due to their ability to scatter solar radiation. However, recent atmospheric measurements indicate that many UT/LS aerosols also contain a substantial amount of organic compounds (5 – 50 wt%), which could alter their climate-forcing properties.
Furthermore, we have previously shown that the reactions of relevant organic aerosols, such as propanal, methylglyoxal, and glyoxal, in sulfuric acid generate highly-colored surface films, potentially altering optical and cloud-forming properties of these aerosols. Since atmospheric concentrations of propanal alone are too low to produce a significant amount of aerosol surface film, products of cross-reactions between multiple aldehydes would be required. To determine whether these cross-reactions are likely to occur in UT/LS aerosols, mixtures of propanal with other common aerosol organic species (glyoxal and methylglyoxal) in sulfuric acid were prepared. Surface films formed on these multiple-aldehyde mixtures, and were chemically analyzed using Attenutated Total Reflectance FTIR and Nuclear Magnetic Resonance (NMR) spectroscopies. Preliminary results show evidence of cross-reaction products in propanal/glyoxal and propanal/ methylglyoxal films.

Therefore, these reactions have the potential to produce significant organic aerosol mass, which could partition into surface films and impact optical, chemical, and/or cloud-forming properties of aerosols.

A18) Capsaicin and Capsazepine Interactions with Lipid Membranes

Hannah Cowe, Ayush Kris, Grace Stokes

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Capsaicin is the compound responsible for the painful burning sensation in chili peppers. Similar to its synthetic antagonist, capsazepine, it interacts with Transient Receptor Potential Vanilloid 1 (TRPV1). TRPV1, a transmembrane channel protein, participates in the detection of harmful stimuli, offering insights into pain reception. Using second harmonic generation (SHG), we measured the binding affinities and surface densities of both compounds to better understand their interactions with lipid membranes. Our study focused on investigating these interactions with supported lipid bilayers at physiologically relevant drug concentrations. Fluorescence anisotropy was used to monitor changes in the fluidity and phase transition of lipid membranes upon interaction with capsaicin and capsazepine. By utilizing model liposomes mimicking human cell membranes, we varied lipid phase, cholesterol content, and head group charge to quantify how binding behavior changed with lipid composition. By studying the effects of these small molecule drugs on membrane fluidity and lipid structure, our work provides insight into how these compounds modulate membrane properties, which potentially affect their biological functions and the conformation of membrane-bound receptors.

A19) Gingerol Analogs as Allosteric Activators of the Sarcoendoplasmic Reticulum Calcium ATPase

Shiffany Asha Devaraja, Dr. Stefan Paula, Jastina Makeyenko, Dr. James Miranda

CALIFORNIA STATE UNIVERSITY, SACRAMENTO

The sarco/endoplasmic reticulum calcium ATPase (SERCA) resides in the sarco/endoplasmic reticulum (SER) membrane and pumps calcium ions from the cytosol into the lumen of the endoplasmic reticulum, undergoing a conformational change between its E1 and E2 states during the catalytic cycle. Alleviating SER stress by up regulation of calcium-ion transport by SERCA, can help treat many chronic conditions like cardiovascular disease, diabetes, cancer and neurodegenerative disorders. Previous research has identified the natural compound gingerol as an activator of SERCA. To explore this further, analogs of gingerol were tested via an enzyme activity assay. In parallel, to enzyme assays, an online tool named Morphinator was used to help model the transition of SERCA between its two known conformations in fifteen steps. The highest

energy state was then used for global protein docking studies with gingerol-10, which had been found to produce the most significant SERCA activation in the assays.

Our findings are a valuable contribution to current efforts focused on alleviating SER stress via SERCA activation by small molecules.

A20) Inhibition of the Sarcoendoplasmic Reticulum Calcium ATPase by Naphthoquinones

Aubrei Drennan, Sydni Sobata, Stefan Paula Ph. D

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The Sarco/Endoplasmic Reticulum Calcium ATPase (SERCA) is a vital transmembrane protein responsible for tightly regulating intracellular calcium concentrations - an essential function for maintaining cellular homeostasis. Operating as a calcium ion pump, SERCA actively transports Ca^{2+} ions from the cytosol into the sarcoplasmic or endoplasmic reticulum following muscle contraction. This process is energy-dependent and is driven by the hydrolysis of ATP, highlighting SERCA's critical role in calcium signaling and muscle relaxation.
Given SERCA's significance in physiological processes and disease states, it could come out as an important therapeutic target. In this context, a series of nine naphthoquinone-based compounds were screened for their inhibitory activity against SERCA. Among these, several compounds demonstrated particularly strong inhibitory potencies, standing out as promising candidates for further study. Structure–activity relationship insights suggest that specific substituents may enhance or diminish inhibitory effectiveness, pointing to a potentially modifiable scaffold for drug development. To explore the molecular interactions in greater depth, computational docking analyses for some of the compounds were conducted. These in silico studies provided valuable information on the binding affinities and interaction modes of the potent inhibitors within the SERCA binding pocket, further supporting their potential as lead compounds for future therapeutic applications targeting calcium dysregulation.

A21) Development of a nitroreductase sensitive prodrug for 5-hydroxy γ-pyrone based covalent inhibitors

Isabella Escutia, Herman Nikolayevskiy

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Covalent inhibitors have garnered attention in drug discovery campaigns for their ability to irreversibly bind target proteins, resulting in permanent inactivation, even with low binding affinity. Yet, the possibility of nonspecific binding and off-target toxicity remains an issue, necessitating focused efforts to increase selectivity. The Williams group recently reported

that derivatives of kojic acid can covalently bind the Cys 468 site of Stat3-dependent cancer cells. These hydrolytically unstable molecules appear to function as Michael acceptor prodrugs, forming an active electrophile via proton transfer from the 5-hydroxy substituent of the γ-pyrone core to an aniline leaving group. Biological assays of capped 5-hydroxy γ-pyrones noted a decrease in activity and complete stability in aqueous solutions. This work, with the incorporation of prodrugs, explores the 5-hydroxy site to improve selectivity and the stability of this class of molecules. The synthesis involved an analog of the Williams compound with the 5hydroxy group protected as a p-nitrobenzyl carbonate. The reduction of p-nitrobenzyl carbonate would result in a p-amino group, triggering self-degradation. In future studies, HPLC will be used to assess the rate of self-degradation upon treatment with nitroreductatse, typically amplified in hypoxic tumor cells.

A22) On Extending the AIIR Method to CBS-apno and W1BD Methods

Tafai Muck

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In 2016, the AIIR (Averaged Isogyric, Isodesmic Reaction) method, using G4 calculations, was shown to be able to calculate H-R bond enthalpies with a Mean Average Deviation (MAD) of 0.5 kcal/mol over a set of 31 molecules for which experimental values are know to within 0.1 kcal/mol. The method uses the known H-X bond enthalpy (calculated from data in the Active Thermochemical Tables (ATcT) and the calculated reaction enthalpy for the reaction

X + H-R --> H-X + R

For several choices of an abstracting species X, to calculate the H-R bond enthalpy. This project seeks to extend the AIIR method to include calculations at the CBS-apno and W1BD levels of theory. Results of these efforts will be presented.

A23) Expression, Purification, and Characterization of Recombinant, TEV-cleavable Human Serum Amyloid A1

Justine Garcia, Mark Borja

CAL STATE EAST BAY

Serum amyloid A-1 (SAA1) is a small acute-phase protein that is upregulated during inflammatory responses, which occur in conditions such as acute infections, tissue injury, and particularly in heart attacks. SAA1 is primarily associated with high-density lipoprotein (HDL) and is believed to replace the resident apolipoprotein A-I (apoA-I) during inflammation, potentially leading to a decrease in cholesterol efflux capacity and a loss of

antioxidant function. The objective of this study is to explore whether SAA1 can displace apoA-I from HDL particles in vitro, thereby shedding light on the mechanisms underlying its observed in vivo behavior. To achieve this, an engineer codon-optimized, mature human SAA1 (hSAA1) expression construct was created using the pET-30a vector. The construct included an N-terminal 6His tag and a tobacco etch virus (TEV) protease cleavage site. We expressed His-TEV-hSAA1 in E. coli and purified the protein using nickel affinity chromatography. Following the TEV protease cleavage, the protein is further purified by passing over a second nickel column to remove the TEV protease and 6His tag, with the final product confirmed as pure hSAA1 by SDS-PAGE analysis.

A24) Successful E. Coli Expression, Purification, and Characterization of Human Serum Amyloid A1

Justine Garcia, Mark Borja

CAL STATE EAST BAY

Serum amyloid A-1 (SAA1) is a small acute-phase protein that is upregulated during inflammatory responses, which occur in conditions such as acute infections, tissue injury, and particularly in heart attacks. SAA1 is primarily associated with high-density lipoprotein (HDL) and is believed to replace the resident apolipoprotein A-I (apoA-I) during inflammation, potentially leading to a decrease in cholesterol efflux capacity and a loss of antioxidant function. The objective of this study is to explore whether SAA1 can displace apoA-I from HDL particles in vitro, thereby shedding light on the mechanisms underlying its observed in vivo behavior. To achieve this, an engineer codon-optimized, mature human SAA1 (hSAA1) expression construct was created using the pET-30a vector. The construct included an N-terminal 6His tag and a tobacco etch virus (TEV) protease cleavage site. We expressed His-TEV-hSAA1 in E. coli and purified the protein using nickel affinity chromatography. Following the TEV protease cleavage, the protein is further purified by passing over a second nickel column to remove the TEV protease and 6His tag, with the final product confirmed as pure hSAA1 by SDS-PAGE analysis.

A25) Optimizing Lithium Sulfure Batteries with Metal Organic Frameworks

Lisette Garcia Martinez, Daryl Miranda, Jack Lee, Lamija Kovacevic, Sofia Marquez, Tosif Aliyev, Philip T. Dirlam

SAN JOSE STATE UNIVERSITY

Lithium-sulfur (Li-S) batteries are a promising new electrochemical energy storage technology that could demonstrate over three times the capacity of current lithium-ion batteries. By obtaining successful results Li-S batteries can be incorporated into vehicles, modern technology and grid-level systems for renewable energy storage. However, there

are certain challenges that limit their ability to perform at a commercially viable level. These challenges arise from the inherent solubility of lithium polysulfide redox products, poor redox kinetics, and the electrically insulating nature of elemental sulfur. To address these issues, research on incorporating metal-organic frameworks (MOFs) into Li-S batteries has been undertaken . These MOF's are extended porous materials that have metal ions coordinated to organic "linker" molecules. We demonstrate the use of conductive, layered topology MOFs with tunable pore sizes to improve Li-S cycle lifetime, capacity retention, and rate capability. Furthermore, we demonstrate improved synthetic procedures for target organic linker compounds and techniques and strategies for fabrication of Li-S cathodes with corresponding MOF inclusions.

A26) Computational Investigation of MnO_2 Polymorph Phase Transitions

Nicole Adelstein, Bo Wang

SAN FRANCISCO STATE UNIVERSITY

Manganese dioxide (MnO_2) is a promising material for electrochemical technologies due to its abundance and electrochemical versatility. In this study, we investigate the thermodynamic and kinetic properties of various MnO_2 polymorphs—specifically the α, β, γ, and δ crystal structures—through computational analysis. Our focus lies in determining how the elastic properties affect phase transformations. Leveraging code developed by our collaborators at livermore, we simulate phase transitions and energy landscapes between polymorphs. This computational insight is intended to guide experimental synthesis carried out by our team's graduate researchers. Our hypothesis is that through this combined theoretical-experimental approach, we can control which crystal structure is present after synthesis or operation.

A27) Biophysical Studies of Peptoid-Lipid and Peptide-Lipid Interactions

Kasiet K. Temiralieva, Hannah A. Cowe, Wanyu (Mary) Xiang, Elliott J. Anderson, Jwwad Javed, Amelia A. Fuller, Grace Y. Stokes

SANTA CLARA UNIVERSITY

Peptoids are N-substituted glycine oligomers, which can serve as peptide and smallmolecule drug mimics. Our goal is to gain a molecular-level understanding of how the chemical structure of a peptoid impacts how strongly it adsorbs to a lipid membrane. We study phospholipid monolayers using a Langmuir trough in the presence of varying amounts and types of peptoids to better understand how the physical structure of the lipids change due to peptoid adsorption and intercalation. We have also obtained pressure-area isotherms of peptoid monolayers to quantify a peptoid's physical properties

(such as surface packing density) at the air-water interface.

A28) Allosteric Regulation of Human Glutamine Synthetase Revealed by Cryo-EM and Molecular Dynamics

Cyrina Joy Geluz, Markus C. B. Tecson, Haneen Alkabanni, Hiroki Yamamura, Eric R. Greene

SAN FRANSISCO STATE UNIVERSITY

Glutamine synthetase (GS) is a ubiquitous enzyme whose activity is dependent on forming an oligomeric complex. Here, we investigated the allosteric regulation mechanisms of human glutamine synthetase using cryogenic electron microscopy (cryo-EM), molecular dynamics (MD) ensemble fitting, and structural bioinformatics, we present an allosteric network across key interfaces in the GS complex whose disruption can modulate GS activity. Importantly, mutations to this interface impact the loop that closes over the active site. We further, found conserved structural variability in this active site loop across phylogenetically diverse organisms. These results provide novel insights into the oligomeric state-dependent regulation of glutamine synthetase that can facilitate the development of targeted therapeutic approaches for disorders related to glutamine synthetase dysfunction.

A29) Stabilizing Gold Nanospheres for Biological Applications with Peptoid Capping Ligands

Hanna Goldberg, Joseph Hong, Maggie Batek, Isabella Matusich, Nikhila Raman, Amelia Fuller

SANTA CLARA UNIVERSITY

Colloidal gold nanoparticles (AuNPs) are versatile materials with wide-ranging applications in nanomedicine as biosensors, diagnostics, and therapeutics. To function in physiologically relevant aqueous conditions, AuNPs must be surface-modified with capping ligands to resist agglomeration through electrostatic or steric repulsions. Peptoids (N-substituted glycine oligomers) serve as ideal AuNP capping ligands due to their ease of preparation, versatile functionalization, and biocompatibility, including proteolytic stability and low immunogenicity. A long-term goal of our laboratory is to characterize the physicochemical features of peptoid capping ligands that modulate AuNP colloidal dispersion. In this poster, we detail our work to study peptoid capping ligands that prevent the agglomeration of AuNPs. This includes the preparation and evaluation of 100 short peptoid sequences as capping ligands for 10 nm AuNPs. Our initial findings have revealed important sequence and structural features of peptoids that effectively solubilize AuNPs. We report peptoid-capped AuNP stabilization across a range of physiologically

relevant conditions including varied pH and salt concentrations, as well as provide a direct comparison to the behavior of peptide-capped AuNPs.

A30) Investigating Safer and More Sustainable Methods for Synthesizing InP Shells to Strengthen Optical Performance of Near Infrared Emissive InAs Quantum Dots

Alexander Gomez, Marcello Garbo, Trang Le, Michael Enright

SAN FRANCISCO STATE UNIVERSITY

Colloidal indium arsenide quantum dots (InAs QDs) have near-infrared optical properties that enable potential applications in building integrated photovoltaic systems. By taking advantage of their strong visible light absorption and near-infrared emission, we can envision using InAs QDs to absorb sunlight before reemitting it at energies optimal for solar cell performance. The quantum yield, a measurement of the absorbance and reemission performance, of InAs QDs alone is low. However, it can be greatly enhanced by supporting it in a shell of indium phosphide (InP) to create a protected core/shell QD. Most strategies for making good quality InP shells are costly and unsafe, using dangerous and expensive materials. This research has developed significantly safer procedures to grow high quality InP shells to greatly improving the optical performance of the near infrared emissive InAs quantum dots.

A31) Zinc-Mediated Palladium-Catalyzed Cross-Coupling of Silyl Enol Ethers to Aryl Halides for the Synthesis of Quaternary Homobenzaldehydes

Angelina C. Graf, Liv R. Alleyne, Ashlynn B. Van Lare, Ritter V. Amsbaugh, Ravi M. A. Kotamraju, and Benjamin J. Stokes *

SANTA CLARA UNIVERSITY

A central area of research interest in our group is the development of reactions involving small organic molecules containing benzylic quaternary carbons, which are ubiquitous in pharmaceuticals and biomolecules. One area of recent focus has been the development of reactions of versatile quaternary homobenzaldehydes, but the synthesis of these aldehydes has been complicated by the lack of an established direct synthesis as well as the relative sensitivity of the aldehyde functional group itself. Herein, we describe our efforts to address this need through the optimization of a procedurally simple and safe direct synthesis of these aldehydes in a single step, namely a palladium-catalyzed cross-coupling between in situ-generated zinc enolates and aryl halides using Buchwald pre-catalysts under inert (air-free) conditions.

A32) Enhancing Photocatalytic C–O Bond Cleavage in Biomass Model Substrates

Using $CuAlS_2$/ZnS Quantum Dots

Gabriela Vazquez

SAN FRANCISCO STATE UNIVERSITY

This study investigates the development of type-II core-shell quantum dots as photoredox catalysts. $CuAlS_2$/ZnS core-shell quantum dots (QDs) are unique due to the large, >0.5 eV energy offsets in the conduction and valence bands of the two materials. Here we seek to understand the impact of a type-II heterostructure on a quantum dot's ability to act as a photoredox catalyst by exploring a model electron-transfer redox process - selective C–O bond cleavage in biomass model substrates. Monodisperse quantum dots with tunable $CuAlS_2$ core sizes and ZnS shell thicknesses are synthesized through a one-pot hot injection method, resulting in quantum dots capped with long-chain, non-polar ligands. However, the non-polar nature of these ligands limits photocatalytic efficiency and disallows homogeneous catalysis in polar solvents. In addition to developing size-tunable $CuAlS_2$/ZnS quantum dots, we also explore new strategies for ligand exchange to assess the value of a quantum-confined, type-II heterostructures in contrast to their single material counterparts.
This research aims to explore biphasic ligand exchange processes on $CuAlS_2$/ZnS quantum dots to enhance photocatalytic yields. We hypothesize that ligand exchange with a polar ligand containing a cyano functional group will improve catalytic performance and enhance substrate compatibility. By optimizing synthesis and ligand exchange protocols, this work advances the green chemistry potential of $CuAlS_2$/ZnS, contributing to the reduction of the carbon footprint by seeking to reduce our reliance on oil for carbon feedstocks.

A33) Exploring Structural Features and Synthetic Strategies for Peptoid Ligands for Gold Nanosphere Functionalization

Joseph Hong, Hanna Goldberg, Maggie Batek, PI: Amelia Fuller

SANTA CLARA UNIVERSITY

The Fuller lab is exploring the use of peptoids (N-substituted glycine oligomers) to functionalize the surface of gold nanospheres for varied applications of these nanomaterials in aqueous solutions. Peptoids are synthetic analogs of peptides, sharing the amide backbone, but the key differentiation lies in the location of the side chains: in peptoids, these are bonded to the backbone nitrogen as opposed to the α-carbon in peptides. The synthesis of peptoids is straightforward and is carried out on resin. In this poster, we will present our modular design of peptoids for synthesis, based on peptides previously used to functionalize the surface of gold nanospheres and stabilize dispersions of these in aqueous solutions. Like these peptides, peptoids are composed of a charged

hydrophilic region, a hydrophobic core, and a thiol anchor region that interacts with the gold nanomaterial surface In order to investigate the important structural features of peptoid analogs of peptide surface ligands, multiple analogs have been synthesized. Here we present the specific structural features of these analogs and the varied synthetic approaches we have used to prepare a diverse library of peptoids for further evaluation. More specifically, we have focused our efforts on the preparations of peptoids with different sulfur-containing anchor groupsand on peptoids that include branched architectures installed by selective side chain modifications.

A34) Investigating the effect of ubiquitin on protein amyloid formation

Jeslyn Hopham, Angelika Paige Caraballo, Natalie Dinh, Emiliano Lopez Ruiz, Hannah Nicole Suazo, Johan Villalpando, Regina Leyva, Emma Carroll

SAN JOSÉ STATE UNIVERSITY

Ubiquitin is a small protein that is covalently attached to lysine residues of other proteins as a posttranslational modification (PTM); typically, ubiquitination condemns protein to proteasomal degradation. A hallmark of cancers and neurodegenerative diseases is formation of highly stable (hard to break down) pathological amyloid protein aggregates. Interestingly, these amyloid aggregates are heavily ubiquitinated. Prior research has revealed that ubiquitin can destabilize the fold of the protein it is attached to, but only at certain sites. Thus, we hypothesize that ubiquitin-induced protein destabilization and unfolding may play a role in driving formation of pathological amyloid species in disease states. To address this question, we utilize a biochemically reconstituted ubiquitination system and model proteins for ubiquitin-induced destabilization and amyloid formation: barstarK2, barstarK60, and barstarK78. Here, the barstarK(n) nomenclature where the value of “n” defines the position of a lysine (K) residue. In barstarK2 and barstarK60, ubiquitin is known to destabilize the protein, but, by contrast, has no effect on barstarK78. Moreover, barstar has been shown to form inducible amyloid aggregates in vitro under low pH/high temperature conditions. We will use these differences in barstarK(n)’s sensitivity to ubiquitination and ability to induce amyloid formation to test whether site-specific ubiquitination can influence barstar amyloid formation rate and propensity, which we will track with Thioflavin T dye and microscopy. Since protein folding principles are universal, we can apply our observations to gain further insight on disease associated amyloid formations that form under the same process. We expect these studies will shed light on whether ubiquitin can modulate protein energy landscapes to promote pathological misfolding, including providing a basis to understand mechanisms of amyloid formation in neurodegenerative diseases and cancer.

A35) Effects of Methionine-Oxidation on the Self-Association of Human and Canine Apolipoprotein A-I Using SEC-MALS

Isaias Iniguez-Sandoval, Jacqueline Tavares-Suchil, Linda M. Roberts, PhD

CALIFORNIA STATE UNIVERSITY, SACRAMENTO

Apolipoprotein A-I (apoA-I) is the major protein of HDL (high density lipoprotein) whose primary role is to remove excess cholesterol from the body. Previous studies suggest methionine-oxidized apoA-I readily leads to the formation of amyloid, a deleterious insoluble aggregate that has been linked to cardiovascular disease and other neurodegenerative ailments. Human apoA-I has a natural propensity to self-associate into dimers, trimers, and larger oligomers. Recent studies have pointed to the loss of self-association, through methionine-oxidation, as a possible precursor to amyloid formation.Canine apoA-I, which contains only one methionine residue (vs 3 in human apoA-I), has been found in the vasculature of older dogs. We are seeking to explain how canine apoA-I, with fewer sites of oxidation, forms amyloid deposits in this relatively shorter-lived species. Here, we use SEC-MALS (size exclusion chromatography coupled with multi-angle light scattering) to determine the size and distribution of oligomers in methionine-reduced and –oxidized apoA-I. Reduced versions of the human and canine proteins show significant differences in oligomer distributions. Human apoAI has overall more oligomeric diversity with no substantial preference for any selfassociative species. In contrast, canine apoA-I has a strong preference for trimeric association, while also showing a significant decrease in oligomeric diversity compared to its human counterpart. Preliminary SEC-MALS data on oxidized species will be presented.

A36) Development of Analytical Methods for the Kinetic Analysis of 5-Hydroxy-γ-pyrone Prodrugs

Ashley Joban, Clifford Leung, Herman Nikolayevskiy

UNIVERSITY OF SAN FRANCISCO

Substituted 5-Hydroxy-γ-pyrone derivatives are the core of many anticancer and antibacterial compounds. In these compounds, a benzylic leaving group ortho to the hydroxyl group enables their function as prodrugs by converting them into potent Michael acceptors after the leaving group is lost. This process is rate-limited by the electronics of the leaving group, with electron-donating groups (EDGs) accelerating loss and electron-withdrawing groups (EWGs) slowing it down. Current generations of these inhibitors lack selectivity between bacterial and cancer cells. Our research aims to adjust the electronics of leaving groups to selectively target cancer cells by triggering the conversion of an EWG (NO_2) to an EDG (NH_2) using nitroreductase, which can be overexpressed in cancer cells. To investigate this, the kinetics of cysteine addition to nitro-containing prodrugs were studied using High-Performance Liquid Chromatography (HPLC), which detected steady but inconsistent cysteine adduct formation. Ongoing work involves synthesizing a

Fluorescence Resonance Energy Transfer (FRET) donoracceptor pair to further study these kinetics, with the donor on cysteine and the acceptor on the γ-pyrone core. Overall, the goal is to study the electronics of these leaving groups, therefore improving the selectivity of γ-pyrone-based prodrugs, thus increasing therapeutic precision.

A37) Dilution-Driven Speciation Changes in Glyoxal Polymers During Cloud Formation on Aerosol Particles

Mateo Johnson, Alejandro Municio, Esmeralda Mendoza Corrales, Kimberly Houghton, and Annalise Van Wyngarden

SAN JOSE STATE UNIVERSITY

Atmospheric aerosols influence climate by interacting with radiation (scattering and/or absorbing) and by serving as nucleation sites. Glyoxal polymers are common components of atmospheric aerosols. Upon dilution during cloud formation, glyoxal can undergo hydration, hydrolysis, and polymerization reactions, potentially altering the aerosol properties and their climate impacts. It is unknown which polymers decompose on the timescale of typical cloud droplet formation and evaporation. Therefore, water uptake during cloud formation was simulated through a 100-fold rapid dilution of 40wt% glyoxal, and the speciation and kinetics were monitored via high-resolution QTOF Mass Spectrometry. Overall, results indicated the decomposition of larger glyoxal polymers into smaller polymers and monomers post-dilution. Furthermore, polymer speciation changes continued for hours after dilution, indicating that the timescale for many polymer reactions is substantially longer than typical cloud droplet lifetimes. Therefore, polymer speciation reaction rates should be taken into account in future modeling of chemical changes in aerosols during cloud formation.

A38) Benchmarking Density Functional Theory Methods for Metalloenzyme Reactions and Enzyme Catalyzed Reactions

Andrew Kai, Tiffany Nguyen, Robin Grotjahn

SANTA CLARA UNIVERSITY

Understanding enzymatic reaction mechanisms at the molecular level relies heavily on the accuracy of electronic structure methods. Density Functional Theory (DFT) is widely used for investigating the key steps in enzymatic reactions due to its excellent ratio of accuracy to computational cost. While benchmark studies of DFAs for small transition metal complexes have been available for some time, more practically relevant benchmark sets involving larger systems from real-world applications have only emerged recently. This study systematically benchmarks a range of DFT functionals across a set of metalloenzyme and enzyme-catalyzed reactions (ECR). The metalloenzyme model

reaction energies and barrier heights (MME55) test set published by Wappett and Goerigk contains 10 different enzymes, representing eight transition metals (both open and closed shell systems with sizes up to 116 atoms) and provides DLPNO-CCSD(T)/CBS reference values. The ECR benchmark set published by Sirirak et al. contains 20 small model reactions of commonly studied enzymatically catalyzed reactions for which we devise new CCSD(T)/CBS reference values. This study focuses on the relatively new class of local hybrid functionals (LHs), which incorporate a realspace dependent admixture of exact (Hartree-Fock like) exchange. The top performing functional for both test sets was the strong-correlation range-separated local hybrid (scRSLH) ωLH23tdb with an MAE of 2.56 and 0.73 kcal/mol for the MME55 and ECR benchmark sets, respectively. For comparison, the performance of MP2 and B3LYP is 5.7 and 4.0 kcal/mol for MME55 and 1.2 and 1.7 kcal/mol for ECR, respectively. It also surpasses the ωB97M-V functional (MAEs of 2.7 and 0.74 kcal/mol, respectively) making sc-RSLHs the most reliable choice for the study of the energetics of enzymatic reactions at rung-4 hybrid cost. Efficient seminumeric implementations of LHs are available in the Turbomole program.

A39) Investigating Chemical Inducers of PTEN Misfolding and Amyloid Formation

Tess Kempner, Jennifer Nguyen, Belle Okere, Jay Thompson, Regina Leyva Roman, Johan Villalpando Farrach, Nathaniel Bazan, Emma Carroll

SAN JOSE STATE UNIVERSITY

Protein aggregation into toxic amyloid fibrils underlies diseases including neurodegeneration and numerous cancers. PTEN (phosphatase and tensin homolog deleted on chromosome 10) is a phosphatase and critical tumor suppressor protein that regulates a broad range of pro-cell growth signaling pathways, with tumor suppressor activity occurring principally via dephosphorylation of phospholipid second messengers. Interestingly, PTEN has been observed to accumulate in filamentous amyloid aggregates in cancer cells. PTEN amyloid formation represents a toxic, misfolded state that likely contributes to loss-of-function phenotypes and cytotoxicity observed in cancer; however, the cellular environmental factors driving transformation of PTEN to its amyloid state remain poorly understood. Here, we report a new strategy for recombinant purification of PTEN from E. coli that overcome persistent hurdles in the field to recombinant PTEN purification. These results enable investigation of PTEN conformation, dynamics, and misfolding in vitro. With pure PTEN, we are developing a high-throughput screening platform to test systematically the chemical determinants of PTEN amyloid formation in the cellular environment using metabolite libraries. While it is long established that mutations can alter a protein’s energy landscape, leading to oncogenesis, the influence of cellular metabolic state and PTMs on this landscape is equally significant, yet largely unexplored. Our approach will enable exploration of the potential for components of the cellular environment, including cancer-associated metabolites, to induce amyloid transformation from soluble PTEN. We expect that our studies will enable mechanistic models of PTEN aggregation and inform drug development efforts to prevent PTEN loss

of function in oncogenesis.

A40) Greenhouse Gas Emissions and Iron Redox Chemistry in Terrestrial-Aquatic Interfaces: A Case Study from the East River Floodplains, Colorado

Kiana Keyhani, Hermes Ruiz, Amrita Bhattacharyya

UNIVERSITY OF SAN FRANCISCO

Terrestrial-aquatic interfaces (TAIs), which represent dynamic transition zones between land and water, act as biogeochemical (BGC) hotspots for elemental cycling and greenhouse gas (GHG) emissions. Riverine floodplains are examples of TAIs that can function either as carbon sources or sinks. However, there is limited understanding of how seasonal variations in moisture levels impact GHG dynamics such as CO2 and CH4 emissions in floodplains and their relationship with iron (Fe) redox processes. Using a suite of analytical tools, we measured methane and carbon dioxide fluxes during both flooded and drained seasons, along with Fe(II) concentrations in bulk sediment samples. Our findings indicate that CH4 flux decreased by approximately 50% from the flooded to the drained season, while CO2 flux increased nearly tenfold during the same transition. Soils with higher Fe(II) indicated more reduced conditions and emitted a higher amount of CH4. Our data on GHG emissions and soil redox chemistry in TAIs have provided valuable insights into climate change and global carbon cycle studies.

A41) Cardiac Eco-Polymer

Dina Khabaz 1, Shalen Ardeshna 1, Allison Lee 2, Rachel Lee 2, Alberto Lizarraga Herrera 2

UNIVERSITY OF CALIFORNIA, BERKELEY

The shortage of organs for transplantation is a critical global issue, with demand far surpassing supply. Our aim is to address this challenge by harnessing the potential of bioprinting, a cutting-edge technology that uses 3D printing to create compatible tissues and organs. Bioprinting combines cellular bioinks and hydrogels to build threedimensional structures, with the ability to create functional, patient-specific tissue constructs. By using a patient’s own cells, bioprinted organs could eliminate the risk of rejection and remove the need for lifelong immunosuppression, presenting a promising solution to the transplant crisis.

We are developing a model tricuspid heart valve to be bioprinted. The GelMA hydrogelbased scaffold was designed in CAD based on a combination of a human tricuspid valve and current bioprosthetic options. It serves as the foundation for creating durable and functional tissue structures. As this hydrogel scaffold is printed, we’ve seeded it with mouse cardiac fibroblast and cardiomyocytes which then grow across the scaffold.

We've run simulations to ensure the valve would perform as expected in the body and have characterized the properties of our hydrogel at different concentrations to determine the ideal one for this application. A key strength of this approach is the integration of CAD, which allows for precise and customizable scaffold geometries, ensuring optimal functionality in each patient's case.

The project aims to ease the burden on organ donation waitlists by developing a feasible replacement in cases of tricuspid valve failure, such as complications following surgery or conditions like Ebstein's Anomaly.

A42) Exploring Surfactant – Beta Cyclodextrin Interactions via Thermodynamic Properties

Alexia Rios, Jasslyn Salazar, Steve Bachofer

SAINT MARY'S COLLEGE OF CALIFORNIA

The cationic surfactants – tetradecyltrimethylammonium bromide (TTAB), dodecyltrimethylammonium bromide (DTAB), and decyltrimethylammonium bromide (C10TAB) – and β-cyclodextrin (β-CD) binding interactions were investigated under a thermodynamic lens by use of isothermal titration calorimetry (ITC). The aim of this study was to understand how these surfactants interact with the hydrophobic pocket of β-CD while also characterizing thermodynamic parameters: the binding constant (Kb), enthalpy (ΔH), entropy (ΔS), and Gibbs free energy (ΔG). The experiments were completed at room temperature (25°C), with plans for future thermal studies. Binding was explored across different surfactant and β-CD concentrations, and experimentally maintaining the surfactant-to-cyclodextrin molar ratio of 2:1, yet a 1:1 binding ratio is known in existing literature. This data was obtained below the Critical Micelle Concentrations (CMCs) —3.5 mM (TTAB), 17 mM (DTAB), and 67 mM (C10TAB) and the ITC thermograms gave insight into the binding energetics. These findings provide a better understanding of surfactant–cyclodextrin complexes and offer applications in drug delivery and encapsulating molecular technologies.

A43) Faceted Copper Nanocubes for Selective CO_2 Reduction to High-Value Products

Jonah Glass-Hussain

SAN FRANCISCO STATE UNIVERSITY

To ensure an environmentally sustainable economy, we must reduce our reliance on petroleum. This project seeks to move away from a petroleum-based economy by exploring CO_2 reduction as an alternative carbon feedstock. Copper nanoparticles can be used to electro-catalytically reduce CO_2 to carbon-based products, however, this process is typically nonselective. Here, we seek to improve CO_2 reduction selectivity on copper by

deploying highly faceted copper nanocrystals on electrodes to guide selectivity towards high-value C_{2+} products such as ethylene. Characteristics such as shape, size, structure, and other exposed facets of the nanocrystal are fine-tuned to affect the catalytic selectivity of copper in self-assembled superlattices. Currently, our work has focused on synthesis, scale-up and purification strategies for copper nanocubes and nano-octahedra and investigating methods for deposition such as spin coating and drop casting. Characterized by distinct, strong plasmonic properties present near 600-650 nm by UV-Vis as well as SEM imaging, we demonstrate the successful scale-up and deposition of concentrated copper nanocrystals. These concentrated batches will be used to deposit copper nanoparticles on electrodes for selective reduction of CO_2 and ultimately pave the way for more sustainable and environmentally friendly practices.

B1) Synthesis of MIL-100 (Fe) and Fe3O4@MIL-100(Fe) for the oxidation of organic contaminants

Emily Lam, Hannah Miller, Dr. Jacqueline Houston

CALIFORNIA STATE UNIVERSITY SACRAMENTO

MIL-100 (Fe) is a metal organic framework (MOF) that is high in surface area, porous, stable at high temperatures, and recyclable. MIL-100 (Fe) has the potential to be used as a photocatalyst in oxidation reactions, which will aid in the degradation of organic contaminants. It offers an inexpensive, nontoxic, and ecofriendly alternative to traditional metal catalysts. Fe3O4@MIL-100(Fe) offers the same advantages with a magnetic iron oxide core to improve ease of separation from solution. The synthesis of MIL-100 (Fe) and Fe3O4@MIL-100(Fe) were accomplished via hydrothermal methods. The materials were characterized by XRD and IR. The oxidation of common organic dyes using MIL-100 (Fe) and Fe3O4@MIL-100(Fe) as a catalyst was examined using UV-vis. We found that oxidation of the dye reached relative completion after two days. The MOF also facilitated greater efficiency as the degradation of the dye was several folds faster than without the catalyst. Future work will focus on the kinetics of oxidation, the photocatalyzed oxidation using the two MOFs, and exploring oxidation reactions of other organic contaminants. Since the MIL-100 (Fe) catalyst oxidizes organic dyes of similar structure, we hypothesize that the MIL100(Fe) catalyst will also oxidize birth control hormones. The goal is to develop a ‘green’ catalyst for the cost effective and efficient removal of organic contaminants from wastewater.

B2) Analyzing Carbon Dioxide Flux in Relation to Seasonal and Spatial Variations at East River, Colorado

Amber Le, Hermes Ruiz, Kenneth Celis, and Amrita Bhattacharyya

UNIVERSITY OF SAN FRANCISCO

Terrestrial-aquatic interfaces (TAIs), transition zones between land and water, are biogeochemical hot spots in natural ecosystems that promote greenhouse gas (GHG) emissions. There is limited quantitative data on how GHG flux - the rate of exchange of GHG between the atmosphere, land, and water sources - is influenced by seasonal changes, creating knowledge gaps in understanding how moisture patterns affect SOM (soil organic matter) decomposition, which increases GHG flux and emission rates. To investigate these effects on GHG emissions, the East River in Colorado, which serves as an exemplary TAI, was analyzed to see how spatial and moisture gradients influence carbon dioxide flux. Soils from the river were sampled along a vegetation gradient from the floodplain (area closest to the river) to the hillslope (area furthest from the river) during the river's flooded (moistest) and drained (driest) seasons. Carbon dioxide flux was measured using LI-COR Trace Gas Analyzer (LI-7810), which recorded the gas exchange between the soil and the atmosphere over 24 hours in triplicates. Data presents that CO2 flux is highest during the drained season, suggesting that dryer climates promote SOM decomposition. Fourier transform infrared spectroscopy (FTIR) was used to characterize SOM, revealing that floodplain samples contained higher organic matter content, which may create favorable conditions for decomposition. Understanding how these factors drive GHG emissions at TAIs is critical, as climate change is expected to intensify drier conditions. The resulting increase in SOM decomposition underscores the vulnerability of TAIs to environmental shifts. Future research can build on these findings to develop land management strategies to mitigate climate change.

B3) Assessing his-tag Cleavage in Apoliprotein A-I Using TEV Protease

Amanda Lee and Dr. Linda Roberts

CALIFORNIA STATE UNIVERSITY, SACRAMENTO

Apoliprotein A-I (ApoA-I) is the major protein of the high-density lipoprotein. It is important for reverse cholesterol transport which removes cholesterol from tissues and transports it to the liver for waste. ApoA-I, like most proteins expressed in E. coli., has a His-Tag, a string of six histidine amino acids at the N-terminus. This allows for easy purification with immobilized metal affinity chromatography (IMAC). The His-Tag can be removed after purification using TEV Protease. This enzyme recognizes a specific sequence (Glu-Asn-Tyr-Leu-Phe-Gln-Gly) and cleaves between the Gln and Gly residues. It cleaves with high specificity and is active at lower temperatures. This project will determine the optimal conditions for removing the His-tag from human and canine apoA-I. The conditions to be tested include time and temperature of incubation with TEV and different buffer conditions. Following incubation with TEV, cleaved samples will be electrophoresed using SDS-PAGE to determine the completeness of the reaction. This research will be conducted on both human and canine apolipoprotein A-I.

B4) Electrophilic Aromatic Brominations using Sodium Bromide and Sodium Perborate: A Green Chemistry Experiment

Paula Luna, Elizabeth M. Valentín, Ph.D.

SAINT MARY'S COLLEGE OF CALIFORNIA

Electrophilic aromatic substitution (EAS) reactions are taught in the second semester of organic chemistry. The nitration of acetanilide and methyl benzoate is traditionally used in the organic chemistry laboratory to teach regioselectivity of aromatic substitutions. This experiment introduces bromination as a safer, greener alternative. Bromine was generated in situ from sodium bromide and sodium perborate to yield 4bromoacetanilide in excellent yields. Students used melting point, NMR, and GC/MS to determine the regioisomer formed. The present work focuses on expanding this sustainable method for selective bromination of benzene derivatives, expanding its use to derivatives containing electron-withdrawing groups.

B5) Polymers as Frameworks for Metal Complexes: Synthesizing Single Chain Nanoparticles for Catalyzed Reactions

Felix Ma, Osvaldo Garcia, Jose Ramirez, Tony Mo, Madalyn Radlauer

SAN JOSE STATE UNIVERSITY

Single Chain Nanoparticles (SCNPs) are emerging as promising synthetic enzyme mimics for catalyzed reactions, and offer a microenvironment that is expected to have enhanced catalytic efficiency and selectivity. Our project involves synthesizing two types of SCNP scaffolds whose properties govern how, and to what degree, its polymer components collapse into a nanostructure of desired conformation. For our multi-step synthesis of SCNPs, we chose two types of Chain-transfer agent (CTA) precursors: trithiocarbonate and dithiobenzoate. The isolated homo- and copolymer components of our macroCTA, as well as the A-block macroCTA (i.e. hydrophilic copolymer poly(OEGMA-co-AEMA) appended to a CTA backbone), were synthesized in a simplified system. This success warranted a chain extension experiment wherein tBA and NIPAM were adducted to the A-block macroCTA to create the A-B diblock polymer via reversible addition-fragmentation chain transfer (RAFT) polymerization. Obtaining a collapsed structure through crosslinking is enabled by the Michael Addition reaction of A-block active sites provided by each AEMA repeat unit and the crosslinking agent TMT, as well as intramolecular hydrogen bonding at sites contributed by each B-block NIPAM repeat unit. This phenomena is corroborated by a decreased hydrodynamic volume observed in gel-permeation chromatograms. Our future work involves determining the merits of the unique steric environments offered by the two CTAs in our aminolysis and thiol-ene click reactions, as well as incorporating a ligand host for a catalytic transition metal.

B6) Synthesis of a Photoaffinity Probe to Identify Target Proteins in Pseudomonas aeruginosa

Kseniya Maiseyeva, Laura Miller Conrad, PhD

SAN JOSE STATE UNIVERSITY

Pseudomonas aeruginosa is a Gram-negative pathogen known for causing opportunistic infections, particularly in immunocompromised individuals and patients with implanted medical devices. With rising antibiotic resistance, targeting bacterial virulence factors such as pyocyanin provides a promising therapeutic alternative. Previous work in the Miller Conrad lab identified small molecule antipyocyanin analogs that reduce pyocyanin production through an unknown mechanism. This project focuses on synthesizing a novel photoaffinity probe containing both a photoreactive diazirine ring and a terminal alkyne. Upon UV activation, the diazirine ring enables covalent bonding with target proteins, while the alkyne is available for biotin tagging and subsequent target enrichment via affinity purification. The final goal is to deliver a sufficient amount of the synthesized probe for the photoaffinity assay, enabling identification of low-abundance protein targets involved in pyocyanin regulation. Successful identification of these targets has the potential to increase our options to treat the infections caused by P. aeruginosa.

B7) Synthesis of a three-fold symmetric copper(2+) complex supported by the heptaamine ligand TAL

Anna Solis-Rodriguez, Cole Carnahan, Edwin Marriottherzog, Dr. Wan-Yi “Amy” Chu

SAINT MARY'S COLLEGE OF CALIFORNIA

This project aimed to isolate a three-fold symmetric copper(II) complex supported by the heptaamine ligand N,N-{2-Bis[2-(3-aminopropylamino)ethyl]aminoethyl}-1,3propanediamine (TAL). Three-fold symmetric copper complexes supported by polyamine ligands have been shown to be promising candidates to extract phosphates from surface waters. Excess phosphates in surface waters can lead to detrimental environmental consequences such as eutrophication. Given our group’s interest in developing environmental remediation strategies for phosphate pollution in surface waters, we sought to analyze the structure and properties of a copper complex supported by TAL to better understand how their structures and solution dynamics affect phosphate binding efficacy. García-España and coworkers previously reported on the synthesis of TAL as the hexahydrobromide salt, TAL·6HBr. While they were able to show the generation of a [Cu(TAL)]2+ complex in situ in neutral aqueous solutions, a copper complex was not isolated. The previously reported TAL·6HBr did not react with copper(2+) precursors in non-aqueous media, presumably due to all the amine binding sites being protonated by HBr. We developed a new procedure to remove the hydrobromide and isolated an acid-free TAL ligand. Addition of KOH to TAL·6HBr afforded the TAL ligand in

86% yield. This hydrobromide-free TAL was reactive to CuCl2, and the [Cu(TAL)]Cl2 complex was isolated as a blue solid with 45% yield by mixing TAL with the CuCl2 in methanol followed by precipitation using diethylether. The ligand was analyzed using NMR spectroscopy. In the future, we will further analyze the [Cu(TAL)]Cl2 using ESI-MS and X-ray crystallography.

B8) Hyperbranched Glycodendrimers for use in Broad Spectrum Antiviral Therapeutics

Brooke Milam and Ally Bridge

CSUS

Viral infections have long been an issue in our society. While strides have been made toward confronting these diseases, preventatives, and treatments remain hyper-specific. This significantly reduces patient outcomes, especially when infected with a novel virus. There is an overwhelming need for nonspecific therapies in the form of broad-spectrum antiviral therapeutics. Previous studies show that there is a class of molecules capable of behaving in such a manner. Sulfoglycodendrimers are branching, globular molecules that may inhibit the binding and entry of many viruses to host cells. These viruses interact with a class of cell surface molecules called heparin sulfate proteoglycans (i.e. Human Immunodeficiency Virus, SARS-CoV-2, and Ebola). In prior studies, it has been shown that the amount of branching present in these molecules may affect the level of binding and inhibition seen. This study seeks to develop a new set of sulfoglycodendrimers that are hyperbranched to test their antiviral capabilities through multistep organic synthesis. Final molecules are to be analyzed with nuclear magnetic resonance to verify identity and characterize the molecules.

B9) Evaluating Cu(II) Binding to Holothuroidin-2 using Electronic Absorption Spectroscopy

Clarissa Molina-Rodriguez, Isabella Wang, Keana Davis, Tiffany Nguyen, Michael Stevenson

UNIVERSITY OF SAN FRANCISCO

Antibacterial resistance is a growing issue in the medical field due to the inability to develop novel drugs at a faster rate than bacteria develop resistance against them. An attractive alternative is antimicrobial peptides (AMPs) for their immunomodulatory properties, ease of synthesis, and their ability to disrupt cell membranes and slow evolution of antibacterial resistance. The metal binding abilities of AMPs are also important for their potential positive modulation of previously discovered AMP properties; however, the binding effects are generally underexplored. The peptide Holothuroidin-2 (H2), derived from the marine animal Holothuria tubulosa, was chosen to investigate for its broad spectrum activity. H2 possesses the Amino-Terminal Cu(II) and Ni(II) (ATCUN)

binding motif that coordinates Cu(II) with backbone amide nitrogens, a histidine side chain at the third position, and a free amino-terminus. H2 has the ability to bind to Cu(II), an essential micronutrient with fluxional concentrations during infections. Additionally, previous studies have shown this metal-binding motif affects reactive oxygen species generation and improves bacterial inhibition, making the analysis of Cu(II) binding at this site important in antibacterial resistance research. Direct titrations of Cu(II) into H2, using electronic absorption spectroscopy, found specific metal-peptide interactions. Coupled with previous isothermal titration calorimetry data, this study indicates Cu(II) binds to the ATCUN motif with physiologically relevant nanomolar affinity. Future studies will focus on the competition for H2 between Cu(II) and other metals with the potential to modulate antimicrobial activity and bind to H2.

B10) Diabetes interactive demonstration, based on Nopales effect on glucose uptake.

Riley Neikirk, Rimah El Bayouk, Vasty Ortiz

SONOMA STATE UNIVERSITY

Diabetes is a chronic condition that affects millions of people around the world, including children, yet many young people do not understand what it is or how to manage it. This research project aims to develop an interactive and engaging demonstration that will teach children about the condition. This demonstration will include creative visuals that teach children how sugar intake works and the body's response and teach kids how to stay healthy. The goal is to raise awareness, reduce fear, and promote empathy among children, whether they live with diabetes or want to be a supportive friend. Through this project, we hope to make health education more engaging and inclusive for young learners.

B11) Characterizing the Sequence Determinants of a Novel Interaction Between the E. coli Molecular Chaperones DnaK and CbpA

Donna Quach, Quynh Nguyen, Stephanie Virgen, Andrea Mateo, Samantha Chin, Hanh Nguyen, Ryan Dana, Vinh Chau, Samantha Ramirez, Taylor Arhar.

SAN JOSE STATE UNIVERSITY

The heat shock protein 70 (Hsp 70) is a central molecular chaperone protein that maintains protein homeostasis by regulating the folding and translocation of "client" proteins. J-domain proteins (JDPs) are a conserved class of co-chaperones that preselect client proteins and allosterically regulate their binding to Hsp70. JDPs collaborate with Hsp70s by engaging in one or more protein-protein interactions. In eukaryotes, some JDPs bind to a highly conserved EEVD motif at the C-terminus of Hsp70; this interaction is required for client refolding. The E. coli homolog of Hsp70, DnaK, has been observed to

engage in a similar C-terminal interaction with the JDP CbpA despite lacking the EEVD motif. To investigate this interaction between DnaK and CbpA, fluorescence polarization (FP) and differential scanning fluorimetry (DSF) were performed on CbpA and a peptide corresponding to the DnaK C-terminus. Truncations of the DnaK peptide were used to identify a region of ten residues that is sufficient for binding to CbpA. A single point mutation in the DnaK peptide (F631A) ablated binding to CbpA. Future work will utilize alanine scanning to investigate the relative roles of the remaining 9 amino acids. Saturation binding, measured by FP, will be used to determine the affinity of this interaction. Ultimately, these results will allow us to test the role of this interaction in DnaK functions, such as ATPase activity and client refolding.

B12) Ultrafast Modification of Copper Chlorophyllin by Magnetic Induction Heating for Water Electrodisinfection by Selective Reduction of Oxygen to Hydrogen Peroxide

Alex Nguyen, John Tressel, Shaowei Chen

UC SANTA CRUZ

The two-electron oxygen reduction reaction ($2e^-$ ORR) is becoming a promising way to produce hydrogen peroxide (H_2O_2) in an environmentally friendly way, which can then be used to disinfect water on-site. In this study, scientists used magnetic induction heating—basically heating with electricity—for just a few seconds to modify a material called sodium copper chlorophyllin. This process created nanocomposites (tiny materials) called CuNC, where important copper-nitrogen (CuN_4) structures are still present and supported by a carbon framework. They confirmed the structure using several advanced techniques like electron microscopy and spectroscopy. When tested in electrochemical reactions, these CuNC materials were shown to effectively turn oxygen into hydrogen peroxide in alkaline (basic) solutions. The best-performing sample was made at 400 amps for 10 seconds and produced nearly 90% hydrogen peroxide. This material also worked well for cleaning water—breaking down dye pollutants like methylene blue and killing harmful bacteria like E. coli. This research shows that magnetic induction heating is a fast and useful method to make high-performance materials for water treatment and other uses.

B13) Computational Study of Heavy-Atom Tunneling in Biosynthesis: Model Systems for the Cope Rearrangement

Amanda Nilsen, William Karney

UNIVERSITY OF SAN FRANCISCO

Exploration of heavy-atom tunneling can be the key to further understanding the kinetics behind biochemical reactions. Though recent literature reports numerous examples of heavy-atom tunneling, there is a gap in knowledge for biosynthetic examples. In this

study, two examples of biosynthetic reactions are computationally probed to evaluate the contributions of heavy-atom tunneling with the goal of adding to a growing body of evidence for tunneling in biosynthesis. We studied the biosynthesis of dictyoxepin and the tricyclic analogue for dimethylallyltryptophan synthase, both of which involve a Cope rearrangement – a [3,3] sigmatropic shift – combined with opening of a three-membered ring. This provided an opportunity for comparison of how different structural factors impact the tunneling contributions for similar reactions. The probability of heavy-atom tunneling in this reaction was estimated using density functional calculations (M06-2X/ cc-pVDZ), with direct dynamics and the small curvature tunneling approximation. Both reactions exhibited high-rate constants, providing the basis for speculation that heavyatom tunneling plays a role in many biosynthetic pathways involving Cope rearrangements with three membered rings. It also allows us to show that the exothermicity of a reaction pathway has a higher contribution to rate constants than the mass of the atoms. Due to these findings, we speculate that heavy-atom tunneling plays a role in many biosynthetic pathways leading to natural products with a three-membered ring structure. This work adds to a growing appreciation that the kinetics of biochemical reactions are influenced not only by hydrogen tunneling, but also substantially by heavyatom tunneling.

B14) Toward reliable amino acid decarboxylation procedures for compound-specific stable oxygen isotope analysis of individual amino acids

Vivian C. Norris, Jennifer A. Tripp

UNIVERSITY OF SAN FRANCISCO

Oxygen isotope analysis is a useful tool for tracing migration patterns and resource use in ecological and archaeological studies. Tissue samples from bones and teeth are currently employed in analysis, but mineral preservation is often poor and such samples cannot be obtained from living organisms. Oxygen isotope analysis of proteins would enable testing of tissues such as bone collagen, hair and feathers. Meaningful oxygen isotope analysis cannot be conducted on proteins without pretreatment: oxygen atoms in carboxylic acid groups of amino acids are exchangeable with those in surrounding water, and the sample may be contaminated with oxygen atoms from the burial environment or laboratory. However, oxygen atoms in hydroxyl side chains are nonexchangeable and must be derived from consumed food or water. A method for decarboxylation of an amino acid without disruption of the hydroxyl group would therefore prove valuable. L-serine and L-threonine were selected for analysis due to their non-exchangeable, water-derived hydroxyl side chains and presence in keratin and collagen. An exploration of published amino acid decarboxylation procedures was conducted to optimize yield and product isolation. Mass spectrometry analysis showed peaks corresponding to the mass-to-charge ratio of 1-amino-2-propanol (product) following the decarboxylation procedure, indicating successful conversion of reactant to product. Peaks corresponding to L-Threonine remained in the reaction mixture until after the extraction procedure, indicating only partial conversion. Disappearance of reactant peaks after extraction indicates successful

removal of unreacted L-Threonine. Difficulties emerged in extracting the product from the reaction mixture. Future research will explore alternative purification methods.

B15) Natural Products from California Native Plants: Grindelia stricta and Emmenanthe penduliflora.

Natalie Kapfenstein, Owen Huang, Serena Choo, Nathalie Alfaro, William Pham, Ayden Latta, Kristy Chow, Skyler Burgess, Seiji Takeshita, Roy K. Okuda.

SAN JOSE STATE UNIVERSITY

Relatively little is known about the natural product chemistry of California Native Plants. A search of the chemical literature indicates that many species in our region have not been investigated. Among the plants that we have investigated are Grindelia stricta (Gum Plant, Fig 1) and Emmenanthe penduliflora (Whispering Bells, Fig 2). We have successfully grown both plants in the SJSU Greenhouse on top of Duncan Hall and under grow lights in the basement – G. stricta from propagation from cuttings, and E. penduliflora from seeds. In both cases, extracts from the plants exhibit a prominent spot in TLC (thin-layer chromatography) analysis that is visible under UV light. We will report the current status of our efforts to isolate and characterize the major natural products from these plants.

B16) Synthesis of verdazyl radical substituted carboranes and metallocarboranes

Khason Ong, Taylor Jackson, Nadia Palomares, Nicholas Adams, David J. R. Brook

SAN JOSE STATE UNIVERSITY

Carboranes are remarkable icosohedral cluster compounds containing boron, carbon and hydrogen. Replacement of one of the BH vertices with metal atoms gives metallocaboranes; stable clusters that can also have unpaired electrons. Though they have been known for over fifty years, there are few studies of carboranes and metallocarboranes with other paramagnetic substituents. We report the synthesis and characterization of a verdazyl substituted carborane through deprotonation with butyl lithium followed by in situ reaction with ethyl formate, and 2,4diisopropylcarbonohydrazide to give a tetrazane. Subsequent oxidation gives the corresponding free radicals. We also report approaches to verdazyl substituted metallocarboranes through removal of a BH vertex followed by reaction with metal triflates.

B17) Synthesizing star polymers as copper catalyst supports

Hannah Pell, Naomi Oluseyi-Oke, Sadaf Omar, Madalyn Radlauer

SAN JOSE STATE UNIVERSITY

Using star polymers as supports for copper complexes, we aim to develop specialized architectures and properties to maximize catalytic activity and long-term viability of the supported copper catalysts. Star polymers are large molecules that consist of linear polymer chains attached to a crosslinked core, giving them a star-like shape. We synthesize these polymers via RAFT (reversible addition-fragmentation chain transfer polymerization) which allows for control over the polymer size and dispersity. In this process, we utilize the arms-first approach, in which the arms of the star, also called macroCTAs, are synthesized first. Then, macroCTAs are tied together into a star through a core-forming reaction between the macroCTAs, crosslinker units, and spacer units. The first macroCTA we have investigated was synthesized via the homopolymerization of the tert-butyl-acrylate (tBA) to make the PtBA macroCTA (P = poly). All of our polymeric materials are characterized by gel permeation chromatography (GPC) to determine the size and dispersion, and nuclear magnetic resonance spectroscopy (NMR) to confirm the chemical composition and purity. In order to incorporate copper complexes into these star polymers, we have synthesized a tridentate pyridyl-bisimine ligand precursor with two pendent alkene groups that can double as a crosslinker in the core-forming reaction of the star polymers. Our current work includes refining RAFT parameters for macroCTA and star polymer syntheses using tBA and other monomers - including reagents, reaction conditions, and solvents. Our next steps involve using the pyridyl-bis imine ligand precursor as our crosslinker to form stars capable of supporting copper centers. We will purify the crosslinked polymers and metalate the ligand precursors in the core of the star polymer. This final modification will yield copper-functionalized star polymers—"copper stars"—which are expected to act as efficient, recyclable catalysts with versatile applications in organic transformations and material science. Using star polymers as supports for copper complexes, we aim to develop specialized architectures and properties to maximize catalytic activity and stability.

B18) Mixed-valence thiophene/verdazyl systems.

Yvonne Pham, Sophia Crudo, Yousuf Mufti, David Brook

SAN JOSÉ STATE UNIVERSITY

Molecules containing groups with closely matched oxidation/reduction potentials can have interesting and unusual electronic properties. These include low energy electron transfer processes that result in absorption in the near IR as well as thermal equilibrium between different electronic structures (valence tautomerism) and spin states. We are working on the synthesis of a series of verdazyl radical substituted oligothiophenes in which the redox potential of the thiophene units is modified through the inclusion of ethylenedioxy

substituents with the goal of matching the oxidation potential of the thiophene chain to the verdazyl. One electron oxidation of the tetrathiophene system gives mixed valence systems which show multiple electronic absorptions in the near IR. We ascribe these to intervalence charge transfer (IVCT) and Donor-Acceptor (DA) transitions involving a verdazylium cation. We also report synthetic approaches to systems with longer thiophene chains.

B19) Electrocyclizations that Yield Natural Products: Computational Study of Tunneling and Kinetic Isotope Effects

Benjamin Quinn, William Karney

UNIVERSITY OF SAN FRANCISCO

Many natural products contain structures arising from 6 electrocyclizations—reactions previously not thought to commonly occur under typical biological conditions. Examples of such secondary metabolites include (+)-occidentalol and dictyolene. The inclusion of these seemingly unfavorable reactions in biosynthetic pathways prompted us to investigate alternative pathways. Heavy-atom tunneling was computationally studied as a possible explanation for faster-than-expected electrocyclization rates, using substrates modeled after four different natural products. The model systems were separated into two subcategories: acyclic substrates and cyclic substrates. The method and basis set combination M06-2X/def2-TZVP was employed after comparing computed barrier heights with experimental activation energies. The investigation included geometry optimizations, vibrational frequency calculations, rate constant calculations with (kSCT) and without (kCVT) tunneling, as well as 12C/13C kinetic isotope effects to generate experimentally testable predictions. Based on the results, we predict that roughly 30% of the rate of electrocyclization in numerous model systems is due to tunneling. The rates were found to be faster for cyclic substrates, such as those leading to the natural products (+)-occidentalol and dictyolene, as compared to the acyclic models. These preliminary results suggest that significant heavy-atom tunneling occurs in biosynthetic pathways involving electrocyclic ring closures.

B20) Green chiral amines

Angel Quintero, Sawyer Bruzza-Omen, John Kolonay, Olivia Hoy, Dave Ball

CALIFORNIA STATE UNIVERSITY, CHICO

Chemical reactions, both in academic and industrial settings, are largely done in organic solvents that result in wastefulness and a negative impact on the environment. A more environmentally conscious approach can be taken through inspiration in biological enzymes, in the fact that they exist in an aqueous environment, and use surfactant to

create micelles in an aqueous solution. These micelles would work using the same principle as biological enzymes by taking place in water and have reactions occur inside of the micelles where the concentration of the reactants dramatically increases which increases the reaction rate. Our team has been working with chiral amines reacting with varying benzaldehydes to create imines, which is a valuable reaction in pharmaceutical settings. These reactions were done in both organic solvent and in a surfactant/water solution, with the goal of comparing their percent yields to assess which method produces the most product. Our results conclude that using surfactant increases percent yields when compared to using organic solvent, which results in a more environmentally friendly way to conduct reactions. These results will hopefully lead chemistry towards a more green approach that will decrease the use of harmful organic solvents and decrease waste using the power of micelles.

B21) Evaluating the efficacy of antibiotic adjuvants in Pseudomonas aeruginosa

Ramya Rajesh (author), Ryan Shamoon (co-author), Dr. Laura Miller Conrad (PI)

SAN JOSE STATE UNIVERSITY

Pseudomonas aeruginosa is an opportunistic gram-negative pathogen that primarily affects immunocompromised patients. It has the potential to develop resistance to multiple classes of antibiotics. Polymyxins are a class of antibiotics used for treatments as a last resort for multidrug resistant infections. Unfortunately, polymyxin resistance is also increasingly encountered. Antibiotic adjuvants help the antibiotic work more effectively. Our goal is to develop antibiotic adjuvants to combat antibiotic resistance. Here we characterized the efficacy of potential adjuvants with a static minimum inhibitory concentration assay, where active adjuvants were able to enable colistin to kill P. aeruginosa at a lower dose.

B22) Expansion Mass Spectrometry

Dalia Riad, Jason Guerrero, Laura Sanchez, Lydia Kisley

UC SANTA CRUZ

High-grade serous ovarian cancer (HGSOC) a highly aggressive, quick, and asymptomatic ovarian cancer (OC) subtype. HGSOC follows a distinct metastasis pattern. Despite its name, it originates from epithelial cells that undergo deleterious mutations. We aim to explore the environmental factors and chemical cues that drive metastasis to specific tissues. To explore chemical gradients we use matrix-assisted laser desorption/ionization mass spectrometry imaging (MALDI-MSI), which is a soft ionization technique that gives spatial information on analytes of interest in the form of a 2D-ion image. However, commercialized MALDI instruments currently lack the capability for

single-cell imaging, achieving maximum resolution of only 10μm x 10μm. HGSOC prone epithelial cells range in size from 8μm-12 μm falling short in the range of current MALDI instrumentation (approx two data points). Our goal is to physically expand these epithelial cells on the surface of hydrogels, to increase the number of data points, and to create a metabolomics map of a single cell. I have been working with my mentor to specifically modify the surface of the double crosslinked hydrogel to allow for 2D cell adhesion by utilizing sulfo-SANPAH and fibronectin (FBN). Fibronectin, an extracellular matrix protein, was tested for its ability to contribute to the cell adhesion and growth of cells. FBN is covalently bound to the sulfo-SANPAH which allows the cells to bind to the hydrogel's surface. These adhesion steps are important for the cell line to overcome the physical stress of being stretched and prevent cell death or detachment before MSI analysis. I will present our optimization results, visualization with red fluorescent protein (RFP) tagged OVCAR8 HGSOC human cells, and preliminary MSI data of stretched and adhered cells towards the development of Expansion Mass Spectrometry.

B23) The First Total Synthesis of Lorneic Acid F and H and their Inhibition Activity against PDE5

Claudia G. Lucero

CALIFORNIA STATE UNIVERSITY SACRAMENTO

The lorneic acids are a group of molecules that have been extracted and isolated from different strains of bacteria. Eleven different lorneic acids(A-K) have been identified, all of which share a base structure consisting of a tri-alkyl substituted aromatic ring. The lorneic acids show potential for treating erectile dysfunction and hypertension, due to the observed phosphodiesterase(PDE5) inhibition of lorneic acids A and B. The greater PDE5 inhibition activity of lorneic acid A was linked to one of its conjugated double bonds, and this specific double bond and its position in the molecule is also present in lorneic acid F. I have completed the first total synthesis of lorneic acid F in four steps from 2-bromo-5-methyl-benzaldehyde with an overall percent yield of 38%. Lorneic acid F has also been tested for its PDE5 inhibition and was found to have PDE5 inhibition stronger than that of lorneic acid B, but weaker than lorneic acid A. I am also working on the optimization of the first total synthesis of lorneic acid H from 2-bromo-5-methylbenzaldehyde with a total yield of 25% in 5 steps. The bioactivity of lorneic acid H is currently under investigation. The key step to both syntheses includes a palladium catalyzed Suzuki cross coupling between an aryl bromide and a vinyl borane to introduce the carboxylic acid side arm present in the natural products.

B24) Synthetic Studies Towards the Synthesis of an Off-Switchable Intercalator

Kat McIntyre, Haley Roach, Herman Nikolayevskiy

UNIVERSITY OF SAN FRANCISCO

Treating and targeting cancer cells has been a complex issue that has utilized many different approaches, one notable example being the use of DNA intercalators. DNA intercalators are planar molecules that insert between the base pairs of double-stranded DNA. In doing so, intercalators interrupt the hydrogen bonding between the strands, causing breakage and signaling apoptosis within the cell. While this technology has been around for a while, there has yet to be a development of an intercalator that is able to selectively combat cancer cells. In this project we combine the use of a DNA intercalator, a planar molecule, with a self-immolative spacer that upon appropriate stimuli, will change the planarity, thus changing its ability to intercalate. The importance of this study is to synthetically confirm the formation of the non-planar product. Our 5 step synthetic approach involves the transformation of a chloro-bromobenzoic acid to a non-planar heterocyclic molecule utilizing a Curtius Rearrangement and a Suzuki Cross-Coupling reaction as key transformations. All successfully synthesized intermediates have been confirmed by NMR and IR spectroscopy. Future work includes the use of our synthesized non-planar molecule as a negative control in DNA binding experiments. During future assays, stimuli such as pH or redox will be tested to induce conformational changes within our planar molecule.

B25) Synthesis of ArnA Adjuvants to Potentiate Colistin in Pseudomonas aeruginosa

Brandon Sanchez Rodriguez, Oluwakemisola Kaka, and Laura Miller Conrad, PhD

SAN JOSE STATE UNIVERSITY

The rise of multi-drug-resistant bacteria like Pseudomonas aeruginosa is an evergrowing threat to public health. This situation has led to increasing reliance on lastresort antibiotics like colistin. Even though colistin is an effective solution, it can also pose a threat due to the negative side effects that go along with the use of it. An enhancement of efficacy would widen the therapeutic index so that lower dosages can be used for the same result without causing side effects. One promising approach is with the use of adjuvants, which are compounds that can increase the effectiveness of antibiotics. Our research focuses on designing and synthesizing adjuvant analogs to identify new compounds that are more efficient at potentiating colistin. These adjuvants are synthesized by an initial acylation reaction step followed by an SN2 reaction to form the final adjuvant product. The development of these new adjuvant analogs could lead to additional options for the treatment of P. aeruginosa infections.

B26) Selective Activation of Bonds via PCET in Amine-Functionalized Photoactive Complexes

Olivia Sargent, Derik Seymour Jr., Glenn P. A. Yap, Meaghan M. Deegan

SANTA CLARA UNIVERSITY

Excited state proton coupled electron transfer (PCET) may proceed with a photo-excited compound acting as both a proton and electron acceptor. PCET is well-understood in many fundamental energy systems in biology, such as photosynthesis and oxygen reduction in ATP synthesis. PCET can be performed similarly for small molecules with hydrogen-bonding interactions between a catalyst and a substrate typically controlling reactions. However, there is a lack of research on how to replicate PCET reactions on non-polar bonds to activate and transform bonds that are otherwise chemically inert toward this type of reactivity. For this study, we describe the synthesis of a series of amine-appended rhenium and ruthenium complexes that demonstrate PCET reactivity. We describe how these compounds our proposed approach to controlling the selective activation of non-polar bonds by these systems. To synthesize novel complexes, simple procedures were modified and the number of amine functional groups appended to the complexes have been modified. X-ray crystallography and NMR spectroscopy were used to verify the identity of these novel complexes. Ongoing fluorescence quenching studies demonstrate the reactivity of these systems toward PCET reactivity.

B27) Accommodating New Geometries in PVD for Nuclear Target Fabrication

Melanie Segura Guerrero, Justice Wilkes, Nicholas Esker

SAN JOSE STATE UNIVERSITY

The SJSU Nuclear Target Research Group investigates low-energy nuclear reactions with a focus on the synthesis of heavy isotopes. A key component of these experiments is the use of high-quality thin films, which serve as both the reaction site and a source of nucleons. Current capabilities include target production, through physical vapor deposition (PVD), on standard 3” x 1” glass slides. These coated slides are subsequently sectioned and mounted onto small circular frames - a process that imposes significant limitations on usable surface area and limits the target geometry.

To address these limitations, our group is developing alternative fabrication methods that enable the production of non-standard geometric targets. In our latest work, we implemented a novel approach that utilized polyethylene film as a sacrificial backing substrate, replacing the standard glass slide. Banana-shaped target frames backed with polyethylene were placed directly into the vacuum chamber, and approximately 1000 μg/cm² of bismuth was deposited onto the polyethylene surface. This method enables

deposition onto complex geometries and significantly expands the flexibility of nuclear target fabrication.

B28) Probing Amino Acid Chirality with Lanthanide (III) Complex

Zachary Smay, Jenna Dinh, Maggie Huang, and Gilles Muller

SAN JOSE STATE UNIVERSITY

Chirality plays a critical role in medicine, as drug molecules need to selectively bind to specific proteins in the body to be effective. The research focuses on using lanthanide(III) complexes as a tool to probe the chirality of biological molecules like amino acids. The project aims to investigate how experimental conditions affect the mixture of amino acids using steady-state and time-resolved luminescence techniques, along with circularly polarized luminescence spectroscopy (CPL).

B29) Investigating the Prebiotic Chemistry of Acyl Phosphates Through Chemical Synthesis

Vicky Ta, Tara Vaddiraj, Andro C Rios

SAN JOSE STATE UNIVERSITY

The origin of life on Earth is a question that remains unanswered. Our group is interested in bridging this gap by investigating the abiotic origins of metabolic chemistry through the exploration of small molecules that could have been present on the early Earth. Pyruvate is a central metabolite found in meteorites that is hypothesized to have participated in a network of prebiotic chemical reactions that helped spawn compounds associated with primary metabolism and high energy species such as acyl phosphates. One molecule of interest to our research is methylsuccinic acid, a meteoritic compound that has previously been identified to form from a decarboxylation of a core pyruvate reaction network derivative. We are aiming to understand how prebiotic decarboxylation reactions can drive the formation of high energy species, such as acyl phosphates, analogous to how decarboxylation reactions drive metabolism in extant life. Acyl phosphates are hydrolytically unstable species but can be isolated or monitored in situ by LC-MS or NMR. We aimed to obtain methylsuccinyl phosphate through a phosphorylation reaction using a methylsuccinic anhydride precursor. This was initially done using two different methods reported in the literature: an aqueous reaction in 0.17M phosphate buffer at pH 10, and an anhydrous phosphorylation reaction using triethylammonium phosphate and triethylamine in acetonitrile. Initial attempts with either approach to verify product formation proved challenging and was suspected to be tied to a rapid reformation and subsequent hydrolysis of a five-membered ring. This was supported by the differences observed in our successful synthesis with glutaric anhydride, a six-membered ring anhydride. Exploring

reaction conditions to optimize the production of methylsuccinyl acyl phosphate, we decided to incorporate the use of succinic anhydride and maleic anhydride to serve as reaction analogs. We found that for these reactions, the concentration of phosphate buffer needed to be increased to 1M to successfully produce maleyl and succinyl phosphate, which was confirmed by NMR. Further experimentation of methylsuccinyl phosphate is required through this method, as well as the anhydrous synthesis in order to obtain isolated yields. Overall, efforts to identify and synthesize acyl phosphates enables further exploration of metabolite generating reactions originating from pyruvate under prebiotic conditions, a key step in uncovering the origins of life.

B30) Recombinant Expression of Zebrafish ApoA-I

Jacqueline Tavares-Suchil, Linda M. Roberts, PhD

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Apolipoprotein A-I (apoA-I) is the major protein component of high-density lipoprotein (HDL), whose main role is to transport excess cholesterol from the bloodstream into the liver for excretion. Methionine-oxidized human apoA-I misfolds, forming amyloidogenic fibrils and consequently amyloid, an insoluble protein aggregate found in human arterial plaque. Methionine-oxidation has been shown to abolish the protein's natural selfassociation into oligomers, implying that this inherent self-association is protective towards amyloid formation. Species comparisons can lend insight into structure-function relationships and the factors that make these go awry, as in amyloid formation. Due to its use as a model organism for human physiology, development, and biochemistry, we sought to express and purify zebrafish apoA-I to study its structural and lipid-binding properties. A zebrafish apoA-I clone in a pET-20b+ expression vector was obtained (Genscript) and used to transform pLysSBL21(DE3) E. coli cells. A pilot expression at 37°C was conducted to determine the optimal time of incubation. The results indicated maximum expression occurred at 4 hours post-induction with 0.5M IPTG. Zebrafish apoA-I was observed to be substantially less soluble than apoA-I constructs previously used in the lab. Future experiments will explore lower expression temperatures as well as optimal recovery of protein from the insoluble cell lysis fraction.

B31) Alzheimer's Stage Classification and Progression Prediction Using Cross-Modal Vision Transformers

Aditya Krishnan, Liza Tinku Jose, Tushar Kotamraju, Srihita Ramini, Himani Manjunath

UNIVERSITY OF CALIFORNIA, DAVIS

Alzheimer's Disease remains a critical challenge in medical research due to its complex, multifactorial progression and lack of definitive early-stage diagnostics. This project,

addresses the need for accurate classification and prediction by leveraging multimodal data from the Alzheimer's Disease Neuroimaging Initiative (ADNI) - a landmark study launched in 2004 and widely recognized as a gold standard in Alzheimer's research.

Our work includes two complementary models: one that classifies cognitive impairment stages (cognitively normal, mild cognitive impairment, or Alzheimer's dementia), and another that predicts the likely rate of disease progression for each individual. The dataset integrates structural imaging (such as MRI and PET scans), clinical assessments (including MMSE and CDR scores), and biospecimen-based features.

The backbone of our method is a multimodal machine learning model using crossmodal Vision Transformers. This architecture employs cross-attention mechanisms to learn complex relationships between data types and prioritize the most relevant features for classification. Unlike traditional early- or late-fusion models, our transformer-based approach adapts dynamically to missing or noisy data and learns more context-aware, interpretable representations. The model implementation and data loading is done in Python using PyTorch, Pandas, Scitkit-learn, etc. Imaging data - particularly hippocampal and cortical volumes - plays a pivotal role due to its strong correlation with neurodegeneration. We compute the mean, standard deviation, and average volume changes across patients, and these measurements are reviewed in collaboration with a radiologist to ensure anatomical accuracy.

Developed in close collaboration with clinicians from the UC Davis Medical School, this project is grounded in real-world clinical relevance. Their input has guided the selection of clinically meaningful features and helped validate model predictions in a healthcare context. By bridging clinical knowledge with advanced machine learning, our work supports both early diagnosis and individualized treatment planning for patients with Alzheimer's Disease. By uncovering new biomarker combinations and offering a holistic view of disease progression, this project contributes to more effective, personalized care and paves the way for future innovation in neurodegenerative disease research.

B32) Comparing the Effects of Different Small Molecules on SIRT1 Activity

Jenny Trieu Dang, Isabella Perez, Crystal Garcia, Kalia Castro, Tejaswini Jagannathan, Ningkun Wang

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Sirtuin 1 (SIRT1) is an NAD+-dependent lysine deacetylase. It is part of the sirtuin family and is associated with many age-related diseases, such as neurodegeneration, diabetes, and cardiovascular-related diseases. SIRT1 activity can be modified by sirtuin-activating compounds (STACs) by activation or inhibition. Resveratrol is a widely studied STAC that was believed to have SIRT1 activating effects; however, further studies have shown that resveratrol can act as either an activator or an inhibitor depending on the substrate sequence identity. Our project aims to determine if this substrate-dependent regulatory

effect is true with other small molecule modulators of SIRT1. Through protein purification and enzyme-coupled assays, we compare resveratrol and piceatannol, another small molecule with a similar structure, in their ability to modulate SIRT1 activity against several peptide substrates, namely Ac-p65 in this study.

B33) Examining Cellular Iron Homeostasis of Highly Glycolytic T cells Utilizing Sorting by Interfacial Tension (SIFT)

Aria Trivedi, Paul Abbyad

SANTA CLARA UNIVERSITY

Microfluidics uses small volumes of fluids to study many different biological applications, enabling researchers to analyze chemical and biological samples on a micro scale. The Abbyad lab developed the technique of Sorting by Interfacial Tension (SIFT) which allows sorting to occur based on the cell metabolism. This technique, which is useful to sort cells of the same type, is label-free, passive, and fixation-free. SIFT allows for the sorting of cancer versus non-cancer cells, activated versus naïve T cells, high versus low glycolysis cells, and much more. Our lab is able to adjust the pH threshold of selected droplets which allows for sorting the most metabolically active cells within a given population which can provide important insights on how metabolism affects other cellular processes within a single cell type.

Activated T cells, in comparison to naïve T cells, undergo a metabolic reprogramming needed for differentiation which is regulated by iron. This leads to an increase in glycolysis and anabolic and mitochondrial metabolism in which SIFT allows for the separation of activated T cells based on their metabolism. Following sorting, cells are examined for varying levels of labile iron uptake indicating different levels of iron homeostasis. Iron plays an important role in the proliferation of cells and mitochondrial metabolism. Labile iron, stored in the cytosol, is strictly regulated by iron homeostasis preventing oxidative damage. Examining how metabolism affects iron homeostasis at a single-cell level provides more insights into potential underlying mechanisms of how iron regulation affects T cell function which is currently not well understood.

B34) ATP Binding and Hydrolysis by a Bacterial Methionine ABC Importer

Emiko Uohara, Maile Gardner, Janet Yang, Benjamin Quinn

UNIVERSITY OF SAN FRANCISCO

ATP-binding cassette (ABC) transporters are membrane proteins that use ATP binding and hydrolysis to facilitate the active transport of molecules across cellular membranes. In all kingdoms of life, regulating the movement of molecules across cellular membranes aids in maintaining homeostasis by importing essential nutrients and exporting toxins.

Defective ABC transporters are linked to diseases such as cystic fibrosis and Alzheimer's disease. The ABC transporter of interest in the Yang Group is the MetNI transporter, a methionine importer in Escherichia coli. This research focuses on ATP binding and hydrolysis at the highly-conserved nucleotide-binding domains (NBDs) of the MetNI system. We have measured the ATPase activity of MetNI mutations and their effects on ATP hydrolysis using solution-based kinetic assays. Additionally, we have used isothermal titration calorimetry (ITC) to measure the thermodynamics of ATP binding. Here, we present preliminary results of our findings, which may ultimately be broadly applicable to other ABC transporters as well.

B35) Fluorescent Chalcone Scaffold for Nematicidal Mechanism Studies

Alyson Marks, Shayla Verma, Carolynn Arpin

CALIFORNIA STATE UNIVERSITY, CHICO

Plant-parasitic nematodes are a serious threat to agriculture, causing significant crop damage and economic losses of over 100 billion dollars annually by feeding on roots, reducing nutrient uptake, and increasing susceptibility to other diseases. With the wellknown risks of traditional commercial-use pesticides like its tendency to contaminate food, water, and soil, and as a contributor to human chronic health problems like cancer, it is pertinent that we need to turn to safer and greener methods that are also still effective. At CSU Fresno, Dr. Alejandro Calderón-Urrea and his team tested and identified novel nematicides containing a chalcone scaffold. These chalcones are a safe and effective method to eradicate nematodes, however their specific mode of action in killing the nematodes remains unknown. This initiated our collaboration with the Calderón-Urrea lab, where our contribution is to chemically synthesize three chalcone nematicides coupled with a fluorescent tag. These fluorescent chalcones would then enable the Calderón-Urrea lab to use fluorescence microscopy to view and follow the compounds while inside the nematodes, thus helping to elucidate the compounds' mode of action. We have worked to synthetically couple three different fluorescent tags onto the chalcones, and this presentation will involve obstacles we have faced, compounds we have successfully synthesized, and where this work is headed next.

B36) Production of Thin Film Polymer Targets for Light-Ion Nuclear Reactions

Phu G. Vo, Sofia V. Malmhall, Nicholas E. Esker

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Deuterons, or hydrogen atoms with an additional neutron (2H, often designated as D), are a crucial component in understanding light-ion nuclear reactions, which have important implications in the field of nuclear astrophysics. However, hydrogen is a gas, making it

difficult to prepare for experimental nuclear reaction studies. To perform these studies, we produce thin film depositions of plastics, which are called “targets” in nuclear science, for bombardment at particle accelerators. In particular, deuterated polyethylene targets (monomer is C2D4) are often used as the primary source of deuterium targets for accelerator experiments. Polyethylene has the highest ratio of hydrogen to carbon, which is beneficial for reducing the amount of unwanted reactions with the beam. The scope of this research involves developing a simple and costeffective method of producing deuterated polyethylene targets through solvent casting. We utilized low-density polyethylene (monomer: C2H4) during the development of our process, instead of deuterated polyethylene, due to the high cost associated with C2D4. To begin, we dissolve a measured amount of low-density polyethylene pellet from Sigma-Aldrich in a mixture of xylenes. The target thickness is a crucial parameter for nuclear reaction study and it is determined by the initial amount of polyethylene. After heating for sufficient time to allow the polymer precursor to mix, we pour the xylenepolyethylene solution onto a microscope slide. Then, the slides are transferred into a preheated oven to allow the xylene to evaporate and the polyethylene film to clarify. Once cooled, the films are then removed using tweezers and their thickness is measured using alpha-particle energy loss measurements using an alpha spectrometer. Knowing the thickness precisely is important for our nuclear reaction studies. Alpha spectroscopy measures the energy loss of alpha particles (α) emitted from 148Gd alpha source at a known energy of 3.183 MeV. By measuring the energy loss as it travels through the polyethylene film, we can deduce their thickness. Using our current method, the targets were within 30% of the desired thickness across the thin film, which is sufficient uniformity for our nuclear reaction studies. In the future, we plan on applying this research to investigate approaches that can increase target uniformity as well as produce uniform deuterated polyethylene targets at our desired thickness.

B37) Elucidating the metal binding site and imparted structural changes on the antimicrobial peptide Holothurodin 2

Isabella Wang, Clarissa Molina-Rodriguez, Keana Davis, Micheal Stevenson

UNIVERSITY OF SAN FRANCISCO

Resistance to traditional antibiotics is a growing concern in the healthcare field resulting in millions of deaths worldwide. An attractive alternative is antimicrobial peptides (AMPs) which are short peptides expressed in the innate immune system of many organisms. Holothuroidin 2 (H2) is an AMP found from the Mediterranean sea slug (Holothuria tubulosa) and contains multiple potential metal binding motifs (ASHLGHHALDHLLK). Cu(II) is predicted to bind at the amino terminal Cu(II) and Ni(II) (ACTUN) binding motif and Zn(II) at the HXXXH motif. Given that infections may cause changes to local concentrations of Cu(II) and Zn(II), understanding how these metals interact with H2 is imperative. To probe the location of metal binding, nuclear magnetic resonance (NMR) spectroscopy was employed. The results provide a general location of Cu(II) and Zn(II) binding at or near histidine residues. To further probe the specific

locations of metal binding, two-dimensional (2D) NMR is used to elucidate specific coordinated residues. With this insight, the precise location of metal binding will be ascertained and related to previously measured binding thermodynamics.

B38) Inhibition of the LuxI homolog in Chromobacterium subtsugae

Mia Guraydin, Natalie Hendrix, Laura Miller Conrad

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Morbidity and mortality rates continue to rise for hospital-acquired infections, highlighting our need to combat increasingly antibiotic-resistant strains. One way to approach antibiotic resistance involves the disruption of quorum sensing (QS) in bacteria. [2] QS is utilized by both Gram-positive and Gram-negative bacteria. The pathway mediates cell-to-cell communication to regulate energetically costly behaviors such as biofilm formation, motility and production of virulence factors, which enable bacteria to colonize a host. [1] Successful inhibition of QS would reduce pathogenicity without affecting microbial growth. The strategy should impose less selective pressure to develop resistance, unlike the high selective pressure to develop resistance promoted by traditional antibiotics. The antivirulence approach should allow the immune system to more effectively overcome bacterial infection on its own or in conjunction with traditional antibiotics.Gram-negative bacteria often use acyl-homoserine lactones (AHLs) as signals to communicate. After AHL synthesis, typically by a LuxI-type synthase, the signal can diffuse out of the cell or is actively transported. At high cell density, the concentration of signal is high enough to bind to a LuxR homolog, leading to upregulation of virulence factors as well as transcription of luxI and luxR. [2,3] The goal of this project is to synthesize and assay potential small molecule inhibitors of the LuxI homolog in Chromobacterium subtsugae, CviI, to prevent the production of signal. With no signal, the QS pathway should turn off to reduce virulence. Although C. subtsugae rarely infects humans, this bacterium is a good model organism, as its quorum sensing pathway is relatively simple. In addition, activation of QS can be quantified by colorimetric assays based on the production of violacein, a purple virulence factor synthesized at high cell density. Here we tested potential inhibitors for their ability to inhibit violacein production in wild-type C. subtsugae. We screened for inhibitors targeting CviI by running a second assay in ΔcviI mutants with exogenous AHL added, where we expected CviI inhibitors to be effective in the wild-type strain but show no violacein-reducing activity in the mutant. Our long-term goal is to translate our results to target Pseudomonas aeruginosa, an opportunistic pathogen currently considered by the World Health Organization as one of the largest antibiotic-resistant threats to human health.

B39) Correlation of EEG Signals and Other Data to Map Unique Patterns for Motor Control

Jeffrey Liu, Waqas Khalid

UC BERKELEY

We propose a novel end-to-end model to map EEG data to locomotive outputs to enable a generalizable paradigm for EEG-controlled robotics. Existing models in fields such as robotics have achieved such end-to-end models using techniques such as reinforcement learning, which are suitable for the challenges of low signal-to-noise data and emergent use cases. Existing classifiers for EEG data rely on vague task labeling, which makes them unsuitable for a general-purpose model capable of mapping new movements and actions. A model which instead maps EEG data to quantitative positional data enables multi-task learning, which makes such a model generalizable to not only different neural inputs but also to control of robotic and mechatronic systems. Examples of systems enabled by such a model include rehabilitative TBI recovery apparatuses (linking brain signals with motor stimulated movement), neurologicallyoperated industrial heavy machinery, and general-purpose brain-computer interfaces (particularly for those with limited physical articulation - paraplegia).

B40) Exploring Amyloid Fibril Formation and Fragmentation Pathways via Network-based Hamiltonian Models and Molecular Dynamics Simulations

Joshua Gadingan, Huy Dang, Bailee Rusconi, David Andreasyan, Jason Kim, Hrishikesh Joshi, Dianoosh Sabetnejad, Dhairya Vyas, Alan Wong, Barry Wong, Andrew Ly, Srinitha Sridharan, Joel Vinod, Gianmarc Grazioli

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Amyloid fibrils, characterized by their conserved cross-β secondary structure along the fibril growth axis, are implicated in numerous protein misfolding diseases, including Alzheimer’s disease. Despite extensive experimental studies, including X-ray crystallography and atomic force microscopy (AFM), key aspects of fibril self-assembly and mechanical properties remain unclear due to limitations in replicating physiological conditions and accessing atomistic details. This research combines two computational approaches—Network Hamiltonian Models (NHMs) and Molecular Dynamics (MD) simulations to enhance our understanding of amyloid fibril structures by exploring both their self-assembly and mechanical behavior. Network Hamiltonian models are notoriously difficult to parameterize using conventional optimization techniques. Thus, we optimized NHMs using a genetic algorithm to simulate the self-assembly of amyloid fibrils. These coarse-grained models address the substantial timescale gap between the slow experimental observations of fibril formation and the shorter, computationally feasible

timescales of atomistic simulations. Our methodology involves evolving NHMs through generations of parameter sets, using simulated evolution and selective breeding to enhance fibril formation yields across different amyloid topologies, thus providing insights into the self-assembly process. Second, we employed MD simulations with enhanced sampling techniques to investigate the mechanical properties of amyloid fibrils. Using Steered MD, we applied artificial forces to fibrils derived from the crystal structure of human insulin chain B (PDB ID: 3hyd) to simulate their mechanical response under conditions analogous to AFM experiments. Our simulations generated stress-strain curves that aligned closely with AFM measurements, validating our in-silico approach to probing the mechanical integrity of amyloid fibrils and supporting the relevance of crystallographic structures in a physiological context. By integrating NHMbased self-assembly simulations with atomistic-level mechanical testing through MD, our combined efforts provide a more comprehensive understanding of amyloid fibril dynamics. This dual approach not only advances the modeling of fibril formation mechanisms but also offers a robust framework for assessing the structural stability and mechanical properties of amyloid fibrils, contributing to the broader goal of unraveling the complexities of amyloid-related diseases.

B41) Optimizing Lithium Sulfur Batteries with Metal Organic Frameworks

Lisette Garcia Martinez, Jack Lee, Daryl Miranda, Lamija Kovacevic, Sofia Marquez, Tosif Aliyev, Philip T. Dirlam

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Lithium-sulfur (Li-S) batteries are a promising new electrochemical energy storage technology that could demonstrate over three times the capacity of current lithium-ion batteries. By obtaining successful results Li-S batteries can be incorporated into vehicles, modern technology and grid-level systems for renewable energy storage. However, there are certain challenges that limit their ability to perform at a commercially viable level. These challenges arise from the inherent solubility of lithium polysulfide redox products, poor redox kinetics, and the electrically insulating nature of elemental sulfur. To address these issues, research on incorporating metal-organic frameworks (MOFs) into Li-S batteries has been undertaken . These MOF’s are extended porous materials that have metal ions coordinated to organic “linker” molecules. We demonstrate the use of conductive, layered topology MOFs with tunable pore sizes to improve Li-S cycle lifetime, capacity retention, and rate capability. Furthermore, we demonstrate improved synthetic procedures for target organic linker compounds and techniques and strategies for fabrication of Li-S cathodes with corresponding MOF inclusions.

B42) Discovering Chemical Determinants of p53 Amyloid Formation

Anushree Bhattacharya, Kashish Airen, Chester Alhambra Jr, Katherine Hoang, Trang Pham, Lazarus Cobb, Sophia Crudo, Vicky Ta, Tara Vaddiraj, Andro Rios, Emma Carroll

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Protein aggregation into toxic amyloid fibrils underlies diseases including neurodegeneration and numerous cancers. p53 is a critical transcription factor and tumor suppressor protein that regulates a broad range of cellular processes, but has been observed to accumulate in filamentous amyloid aggregates in cancer cells. p53 amyloid formation likely contributes to loss-of-function phenotypes observed in cancer; however, the cellular environmental factors driving transformation of p53 to its amyloid state remain poorly understood. Here, we develop a system to test the chemical determinants of p53 amyloid formation systematically. Using purified recombinant p53, we will explore the potential for components of the cellular environment, including cellular metabolites that are responsible for p53 activity and stabilization. Through Differential Scanning Fluorimetry (DSF) experiments, we are investigating the role of pyruvic acid and 4-hydroxy-4-methyl-2-oxoglutaric acid (HMOG) in inducing p53 stabilization or destabilization. Next, we are also interested in screening endogenous metabolite libraries to study the physiological conditions that facilitate p53 propensity to unfolding or misfolding. We expect that our results will enable mechanistic models of p53 aggregation and inform drug development efforts to prevent p53 loss of function in oncogenesis.

B43) Developing methods to investigate the role of ubiquitin in destabilization and misfolding of the cancer-associated proteins p53 and PTEN

Nivita Susendran, Nate Bazan, Jasmin Ho, Katherine Martinez, Tiffany Nguyen, Amie Trinh, Emma Carroll

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Ubiquitin is a protein posttranslational modification (PTM) typically appended to lysine residues of substrate proteins to target them for degradation by the proteasome. The model protein Barstar displays differential sensitivity to ubiquitination depending upon the exact site of attachment; ubiquitin destabilizes barstar‚Äôs fold when attached to some locations but has no effect when attached to others. However, it remains unknown if these effects occur across the proteome, including for critical signaling proteins like tumor suppressors that are known to be regulated by ubiquitination and misregulated in cancer. Here, we use biophysical methods to measure the effect of ubiquitin on the thermodynamic stability of two tumor suppressor proteins, p53 and PTEN. We have developed biochemical techniques to attach ubiquitin to p53 and PTEN. Using purified ubiquitinated proteins, we systematically analyze the effect of ubiquitin attachment at

different locations and the effect of ubiquitin on p53 and PTEN function and proteasomal degradation. To expand these studies, we have also created a Differential Scanning Fluorimetry (DSF) platform to identify fluorogenic dyes that are specific for individual ubiquitin proteoforms. In this process, we screened a library of dyes to identify hits that specifically recognize monoubiquitin and/or K48- and K63-linked polyubiquitin chains. We envision that these dyes will be useful for rapid detection of ubiquitin proteoforms in biological systems and to monitor protein degradation in real-time in a more accessible manner than protein imaging methods. It is known that p53 and PTEN are often misregulated and lead to the proliferation of cancer; the role of ubiquitin signaling in this misregulation will be crucial to understanding this process thus leading to better treatments. Understanding the patterns of ubiquitination will help identify key enzymes and pathways involved in tumor progression and uncover potential therapeutic targets.

B44) Enhancing Photocatalytic C–O Bond Cleavage in Biomass Model Substrates Using $CuAlS_2$/ZnS Quantum Dots

T. Fay Harris, Gabriela Vazquez, Michael Enright

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This study investigates the development of type-II core-shell quantum dots as photoredox catalysts. $CuAlS_2$/ZnS core-shell quantum dots (QDs) are unique due to the large, >0.5 eV energy offsets in the conduction and valence bands of the two materials. Here we seek to understand the impact of a type-II heterostructure on a quantum dot's ability to act as a photoredox catalyst by exploring a model electron-transfer redox process - selective C–O bond cleavage in biomass model substrates. Monodisperse quantum dots with tunable $CuAlS_2$ core sizes and ZnS shell thicknesses are synthesized through a one-pot hot injection method, resulting in quantum dots capped with long-chain, non-polar ligands. However, the non-polar nature of these ligands limits photocatalytic efficiency and disallows homogeneous catalysis in polar solvents. In addition to developing size-tunable $CuAlS_2$/ZnS quantum dots, we also explore new strategies for ligand exchange to assess the value of a quantum-confined, type-II heterostructures in contrast to their single material counterparts. \nThis research aims to explore biphasic ligand exchange processes on $CuAlS_2$/ZnS quantum dots to enhance photocatalytic yields. We hypothesize that ligand exchange with a polar ligand containing a cyano functional group will improve catalytic performance and enhance substrate compatibility. By optimizing synthesis and ligand exchange protocols, this work advances the green chemistry potential of $CuAlS_2$/ZnS, contributing to the reduction of the carbon footprint by seeking to reduce our reliance on oil for carbon feedstocks.

B45) Correlation of EEG Signals and Other Data to Map Unique Patterns for Motor Control

Jeffrey Liu, Waqas Khalid

UC BERKELEY

We propose a novel end-to-end model to map EEG data to locomotive outputs to enable a generalizable paradigm for EEG-controlled robotics. Existing models in fields such as robotics have achieved such end-to-end models using techniques such as reinforcement learning, which are suitable for the challenges of low signal-to-noise data and emergent use cases. Existing classifiers for EEG data rely on vague task labeling, which makes them unsuitable for a general-purpose model capable of mapping new movements and actions. A model which instead maps EEG data to quantitative positional data enables multi-task learning, which makes such a model generalizable to not only different neural inputs but also to control of robotic and mechatronic systems. Examples of systems enabled by such a model include rehabilitative TBI recovery apparatuses (linking brain signals with motor stimulated movement), neurologically-operated industrial heavy machinery, and general-purpose brain-computer interfaces (particularly for those with limited physical articulation - paraplegia).

B46) Correlation of EEG Signals and Other Data to Map Unique Patterns for Motor Control

Jeffrey Liu, Waqas Khalid, Humayd Zameer

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