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<th>Name</th>
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<th>Advisor</th>
<th>Coauthors</th>
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<td>Liam Twight</td>
<td>California State University at Long Beach</td>
<td>AE1</td>
<td>Chlorine radical and chloramine reactivity with wastewater species in support of advanced oxidation processes</td>
<td>Stephen P Mezyk</td>
<td>Kylie D Couch</td>
<td>The UV photolysis of chlorinated compounds as a potential Advanced Oxidation Process (AOP) treatment is of interest to many U.S. water utilities that maintain a chloramine residual in their wastewater treatment systems. In some wastewater treatment and water reuse systems chloramines are deliberately added before the reverse osmosis (RO) process to control membrane biofouling. Chloramines can readily pass through the RO membranes and this could impact a downstream UV/H2O2 AOP. Both direct photolysis and indirect reaction of produced HO· radicals with mono- and dichloramine will produce Cl· radicals. In this project Cl· atom kinetics with a suite of wastewater chemical contaminants, such as nitrosamines and estrogenic steroids will be measured using the methodology established for 1,4-dioxane. In addition to Cl· kinetics with a variety of contaminants, Cl· kinetics with wastewater constituent species such as bicarbonate, nitrate, and nitrite will be measured. Furthermore, efficiencies of these radical reactions will be determined using steady-state radiolysis plus LCMS/NMR techniques. The measurement of these kinetic parameters will provide quantitative understanding of the feasibility of this alternative AOP radical treatment.</td>
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<td>Couch Kylie</td>
<td>California State University at Long Beach</td>
<td>AE1</td>
<td>Effect of base modification on the photolytic production of reactive oxygen species in natural water samples</td>
<td>Stephen P Mezyk</td>
<td>Garrett McKay, Fernando Rosario-Ortiz</td>
<td>Photolysis of dissolved organic matter (DOM) produces reactive oxygen species (ROS) such as the hydroxyl radical (•OH), singlet oxygen (1O2), and triplet dissolved organic matter (3DOM*). Reactions with ROS are significant degradation mechanisms of organic contaminants in natural water systems. Reactions with the •OH radical occur quickly (10^8-10^10 M^-1 s^-1) with most organic contaminants, while 'O2 and 'DOM* are more discriminating oxidants. One of the mechanisms for •OH radical formation in these systems is through photo Fenton reactions that involve photo reduction of Fe(III) to Fe(II), which further reacts with photochemically produced hydrogen peroxide (H2O2). The contribution of the photo Fenton processes to •OH radical formation from effluent organic matter (EfOM) were assessed for two wastewater samples by employing a simple base modification procedure that removed up to 90% of total iron (determined by ICP-MS) and by using bovine liver catalase to quench photochemically formed H2O2. There was little to no change in •OH radical formation rates between the non base modified and base modified wastewater samples. However, addition of catalase quenched •OH radical formation to a greater extent (up to ~21%) for the non base modified (iron-rich) sample relative to the base modified sample (up to ~5%). Additionally, fluorescence, size exclusion chromatography, alkalinity tests, and total organic carbon analysis were done to further characterize differences in EfOM quality before and after base modification. Size exclusion chromatography showed that there was removal of higher molecular weight DOM during base modification. There was an increase in quantum yields for ROS after base modification.</td>
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As the demand for energy increases, the search for an alternative fuel source intensifies. Fossil fuels are not only becoming increasingly expensive, they are causing damage to the environment. An ideal system is based on a biological source through which alternative fuels are produced by natural processes, resulting in a net 0 carbon footprint. Clostridium beijerinckii is a bacteria that facilitates ABE fermentation, where carbohydrates are anaerobically converted into acetone, ethanol, and butanol. From the 92 C. beijerinckii isolates found in fecal samples, 5 different strains (L34A, L34B, L31C, L32C, and L35A) yielded the necessary biochemical pathways for ABE fermentation to occur, however the extent to which ABE products are formed is unknown. NMR spectroscopy, a powerful analytical approach for qualitative and quantitative elucidation of unknown compounds, would be an ideal platform for screening the different strains for these fermentative pathways. By taking advantage of the inherently quantitative nature of NMR, the production of acetone, butanol, and ethanol can easily be accomplished. For this study, the 5 strains were screened for ABE products and efficiency of the bacteria for ABE fermentation quantified using NMR. It was found that strains L34A, L31C, and L32C definitively contained butanol.

The cancer-causing action of the alkaloid-derived nitrosamines (R\textsuperscript{1}R\textsuperscript{2}CH\textsubscript{2}NNO) found in unburned tobacco, tobacco smoke, and smokeless tobacco products has been investigated for many years. In the human body cytochrome P450 activation of these nitrosamine species initially occurs by catalytic reaction of this enzyme to form an a-nitrosamine radical (R\textsuperscript{1}R\textsuperscript{2}C\cdot HN-NO). This nitrosamine radical either combines with a hydroxyl radical (\cdot OH) within the P450 catalytic site to form the DNA-alkylating a-hydroxynitrosamine (R\textsuperscript{1}R\textsuperscript{2}C(OH)HN-NO), or undergoes loss of nitric oxide. However, nitrosamine chemical activation can occur without P450 being involved. This alternative pathway also requires the initial formation of the a-carbon radical, by reaction of a reactive oxygen species such as the hydroxyl radical, with subsequent reaction with oxygen to form the nitrosamine peroxyl radicals (R\textsuperscript{1}R\textsuperscript{2}C(O\textsuperscript{2}O\cdot )HN-NO). To date, the formation of the carbon-centered a-nitrosamine radical has been well characterized. However, there has been very little study of the peroxyl radical formation chemistry, particularly for the tobacco-specific nitrosamines. The measurement of these kinetic parameters will provide mechanistic insights into the importance of the alternative peroxyl radical formation pathway for nitrosamine carcinogenesis relative to the P450 pathway.

In the Orange County Water District (OCWD) Advanced Oxidation Process (AOP) UV illumination of hydrogen peroxide (H\textsubscript{2}O\textsubscript{2}) is used to create the powerful oxidizing hydroxyl radical (\cdot OH) which non-selectively destroy any chemical contaminants remaining after their primary, secondary, microfiltration (MF) and reverse osmosis (RO) treatments. However, they also add chloramines (NH\textsubscript{2}Cl, NH\textsubscript{2}Cl\textsubscript{2}, NCl\textsubscript{3}) to prevent membrane fouling. These chloramines also pass into the AOP, where they significantly impact the AOP efficiency by lowering the efficiency of OH production and scavenging of the \cdot OH radicals. The mode of chloramine production is through adding a concentrated (12.5%) basic hypochlorite solution through a single-point feeder pipe into the wastewater stream. The reaction of hypochlorite with the ammonia in the waste stream is slow (half-life on the order of seconds due to the low levels of ammonia present), allowing unwanted side-reactions of hypochlorite/chloramine species to occur; notably with the major treated wastewater constituents of dissolved organic matter (DOM). It has been shown that the organic chloramines produced have practically zero disinfection potential, so the overall formation
of these halogenated by-products is of major concern. In this work, we have determined the extent of organic chloramine production through chloramine reaction with prototypical organic constituents and quantified the kinetics of all three chloramine species reactions with a range of organic species, particularly nitrogen-containing compounds. The measured reactivity was correlated with different classes of studied chemicals. These data can be used to estimate the extent of organic chloramine formation under real-world treatment conditions.

Biogenic volatile organic compounds (BVOCs) are organic chemical compounds produced by nature and emitted into the atmosphere. The overall research goal is to identify and quantify the BVOC emissions that affect the climate and air quality. The specific focus of this project is to quantify BVOCs present within local vegetation in order to identify potential high BVOC-emitters. Leaves from three native and two nonnative plants were taken approximately every month since July of 2014 from the vicinity of the Loyola Marymount University campus. Terpenes (a class of BVOCs produced by plants) were then extracted from the freeze-dried samples for analysis using gas chromatography-mass spectrometry. The results will show seasonal trends in the monoterpene (C_{10}H_{16}) and sesquiterpene (C_{15}H_{24}) content within the leaves, specifically focusing on the BVOC response to temperature fluctuation and rainfall. Preliminary data suggests that reducing the stress caused by drought provides additional resources for the biosynthesis of terpenes.

Ion Selective Electrodes (ISE) are used regularly in analytical chemistry to determine concentration of ions in solutions. These electrodes however, are either too expensive ($300+ per unit) or too complex to develop for a classroom level laboratory experiment. We have developed techniques reducing the cost and complexity for designing and performing classroom laboratory ISE experiments for Cu^{2+} electrodes. These experiments involved not only reducing costs of the electrodes themselves, but also reducing the costs of the metering equipment required in a classroom setting. The ISEs created were a membrane type using Cu^{2+} complexed with 4-(4-Nitrophenylazo)resorcinol (Azo Violet), and homogeneously mixed into a thin layer of plasticized PVC. The success of each electrode was determined first by calibration, then by measurement of a separate "unknown" standardized solution. Each electrode was also tested for interference by taking measurements of solutions with possible interfering ions. Measurements were also taken using different meters to verify accuracy of less expensive meters. A small cohort of Quantitative Analysis student volunteers successfully executed a draft ion selective electrode experiment based on this research.

Aerosol particles, although a small component of all atmospheric constituents, play a key role in the chemistry of the atmosphere. The composition of aerosol particles directly affects whether particles are present in the solid or liquid phase, the interaction with solar and terrestrial radiation, and the ability to form clouds. Particle composition is inherently varied depending on the source from either natural (e.g., ocean generation of sea salt particles) or anthropogenic (e.g., meat cooking generation of soot particles) sources. It is important to identify atmospheric reactants and identify the reaction products that form to fully comprehend the effect aerosol particles have on climate. In this study, the reaction of a prevalent dicarboxylic acid, succinic acid (C_{4}), with hydroxyl radicals, an established atmospheric oxidizer, is examined to determine the reaction products formed as a function of oxidant concentration and reaction time. Aqueous phase mixtures of succinic acid with varying concentration of hydrogen peroxide were photolyzed to generate hydroxyl radicals for 0 to 120 min. Nine
photooxidation products were identified and quantified using gas chromatography coupled to a mass spectrometer (GC-MS) and GC coupled to a flame ionization detector (GC-FID), respectively. In conditions of excess hydroxyl radicals, shorter chain dicarboxylic acids such as malonic (C3) and oxalic (C2) acids were formed, in agreement with previous measurements. However, as hydroxyl radical concentrations decreased and photolysis of the reactant dominated, larger chain compounds such as the succinic acid dimer (C7) were formed. Previous studies have not explored the concentration dependence of this reaction and have not observed the larger carbon chain reaction products. Reaction products and corresponding proposed mechanisms will be discussed as the results provide insight into the chemistry occurring in the atmosphere and the resulting effect on climate.

Atmospheric aerosol particles have a large and indeterminate effect on the Earth’s climate. Incoming solar radiation and outgoing terrestrial radiation can directly interact with aerosol particles which can scatter or absorb the radiation. This process can result in either a cooling effect on the Earth’s surface, where incoming solar radiation is scattered back to space or a warming effect, where outgoing terrestrial radiation can be absorbed and reemitted back to the Earth’s surface. Radiative transfer calculations, a quantification of the radiative effects, are dependent on absorption and extinction parameters and are dependent on the chemical composition and phase of the aerosol particle. Therefore, it is necessary to be able to quantify how much of what type of aerosol and in what phase is present in order to fully understand the climate effects. Although the composition of aerosol particles is highly variable given numerous sources from both anthropogenic (man-made) and natural origins, organic compounds can account for nearly 50% of the aerosol mass. Dicarboxylic acids are a prevalent component of the organic aerosol. In this study, the optical properties of short chain C2–C6 α, ω-dicarboxylic acids are measured using infrared radiation representative of terrestrial radiation. Five particular acids- oxalic, malonic, succinic, glutaric, and adipic acid, and mixtures thereof, have been characterized from 1500–1000 cm⁻¹ using a Fourier transform infrared (IR) spectrophotometer with an attenuated total reflectance cell (FTIR-ATR) as a function of both phase and concentration. In the aqueous phase, observed changes in the absorption spectra of the individual acids and mixtures with concentration are generally in agreement with Beer’s Law and the additive properties. However, deviations from Beer’s Law become evident as solutions of the acids, and mixtures, are dried to a solid. In particular, the even carbon chain acids are more greatly affected than the odd carbon chain acids. Changes in the infrared region with corresponding phase change and resulting implications for being able to accurately identify and quantify compounds present.

Mercury is a persistent pollutant in the environment, with significant impacts on ecosystem and human health. Since the 1950’s, concentrations of mercury have been increasing, especially in the marine ecosystem. Surface ocean (top 100 meters) mercury concentrations have increased by as much as 200%. Mercury is known to bioaccumulate throughout the ecosystem; higher trophic levels have higher concentrations of mercury. While there is currently a large body of research on high trophic organisms, e.g. tuna and swordfish, knowledge is lacking on producers and mercury. *Macrocystis pyrifera* (giant brown kelp) is a foundational organism in the marine community, and is the organism we have selected as a biosentinel. We hypothesize that kelp will exhibit higher levels of mercury in more polluted areas, such as ports. We also hypothesize that kelp sampled from beaches more heavily affected by the recent Refugio oil spill in Santa Barbara County. The purpose of this study is...
to highlight the differences between point source and non-point source pollutants and their effects on environmental mercury, as well as establish *M. pyrifera* as a biosentinel organism.

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<th>Ashley Le-Pham</th>
<th>California State University, Fullerton</th>
<th>B1</th>
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<th>Structure-Function Studies of Deinococcus radiodurans ADP Glucose Pyrophosphorylase: Role of Ser48 in Allosteric Regulation</th>
<th>Dr. Christopher Meyer, Jeries Qoborsi, Leo Ong</th>
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Adenosine Diphosphate Glucose Pyrophosphorylase (ADPG PPase) is an allosterically regulated enzyme that functions as the rate-limiting step of starch synthesis in plants and glycogen synthesis in bacteria. Because starch is a source of renewable and biodegradable carbon, ADPG PPase is an attractive target for protein engineering to increase biomass yield in crops. The microbial versions of this enzyme are quite diverse in their regulatory and physical properties; some of these properties would be useful to incorporate into transgenic crops to enhance starch production. Little is known about the enzyme from *Deinococcus radiodurans* (*D. rad*), an extremophile that is resistant to ionizing radiation and harsh growth conditions. When comparing the amino acid sequence of this enzyme to other characterized ADPG PPases, it was noted that position 48 differed with a serine substituted for alanine in a region known to be important for allostery. To probe the role of Ser-48, the S48A enzyme was generated by site-directed mutagenesis and the recombinant altered *D. rad* ADPG PPases successfully expressed in *E. coli* and purified via a scheme that includes anion exchange chromatography, size exclusion chromatography, and affinity chromatography. Initial studies on the S48A enzyme in the absence of activators have shown a dramatic 20-fold increase in the apparent affinity for the substrate ATP, a 3-fold increase in apparent affinity for the cofactor magnesium, and a 4-fold increase in V\textsubscript{max} compared to wild-type. Interestingly, in the presence of the activator FBP there was no change in the apparent binding affinity for substrates or V\textsubscript{max} compared to WT which displays a 14-fold increase in V\textsubscript{max} and 12-fold and 3-fold increase in apparent affinity for ATP and magnesium, respectively. In the presence of F6P, there was a 9-fold difference in V\textsubscript{max} and a 12-fold and 2-fold increase in apparent binding affinity for ATP and magnesium, respectively. The alanine substitution appears to result in an enzyme form that is partially activated but relatively insensitive to activators. Complete kinetic and physical characterization of the S48A enzyme is in progress. Supported in part by NSF BIO MCB grant #0448676.

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<th>Rachel Oldfield</th>
<th>California State University, Bakersfield</th>
<th>B1</th>
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<th>Identification of Histidine-303 as the Catalytic Base of Lysyl Oxidase via Site-Directed Mutagenesis</th>
<th>Karlo M. Lopez</th>
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Lysyl oxidase (LOX) is a copper-dependent amine oxidase enzyme that activates the formation of cross linkages of collagen and elastin in connective tissues. Recent discoveries have also found LOX to act as a tumor suppressor while playing a paradoxical role in the spread of cancer. Although LOX is an essential biological enzyme, very little is known about the mechanism by which it carries out its function. The major focus of our work is to understand the mechanism whereby LOX carries out catalysis. In particular, we are interested in determining if histidine at position 303 is the catalytic base of LOX. To accomplish our goals, we propose three mutations to LOX: isoleucine (H303I) to remove the catalytic activity of the enzyme, and aspartate (H303D) and glutamate (H303E) to introduce an amino acid that can also act as catalytic base and therefore maintain the activity of the enzyme. All of the mutations were generated via site-directed mutagenesis and verified by sequencing. Overexpression of H303I yielded 4.65 mg of enzyme per liter of media and H303D yielded 5.27 mg of enzyme per liter of media. Total copper incorporation for H303I was calculated to be 68% and H303D had no copper detected. No catalytic activity was detected for both H303I and H303D when compared to the wildtype. Current experiments are underway to
characterize the H303E mutant. The ability to determine whether or not histidine-303 plays a crucial role in lysyl oxidase before now has only been proposed, although the results of these mutations will provide valuable data for which conclusions can be made.

As patients with Alzheimer’s disease show decreased levels of acetylcholinesterase (AChE) activity and increased levels of butyrylcholinesterase (BChE) activity, the development of potent and specific BChE inhibitors has received much attention. Many types of inhibitors have been developed, including organophosphates, to reverse side effects from decreased acetylcholine levels resulting from increased BChE activity. Building on previous tests of dialkyl phenyl phosphates as BChE-specific inhibitors, we tested bisphosphates as inhibitors, as the two phosphate groups may interact with the active site and a peripheral binding site. We evaluated a series of tetraalkyl bisphosphates by determining the effect of varying inhibitor concentration on BChE and AChE activity. All molecules tested were selected for BChE and lengthening the alkyl chains from ethyl to butyl increased potency. Substitution of the two bridging oxygen atoms with sulfur in the tetrabutyl background led to an ~100-fold better inhibitor, while the same oxygen to sulfur substitution did not affect the $K_i$ value in the tetraethyl background. We are currently investigating if sulfur substitution at other positions in the bisphosphate compounds lead to potent and selective BChE inhibitors.

Oxidative damage to DNA plays a role in the progression of many diseases, including cancer. This damage is observed primarily at the DNA base guanine (G) because it is the most easily oxidized base. The Flash-Quench technique is a method that is used for selective guanine oxidation in double-helical DNA and it can induce DNA-protein crosslinking. Glutathione is a small cysteine-containing peptide responsible for redox buffering in the cell. Here, we investigated whether it might be possible for glutathione, to play a role in diminishing DNA damage (e.g. DNA-protein crosslinks) by engaging in redox repair of the 1-electron oxidized guanine base. Samples containing Ru(phen)$_2$dpzp 2+ [phen = phenanthroline, dpzp = dipyridophenazine], Co(NH$_3$)$_5$Cl$_2^+$, histone protein, salmon sperm DNA and glutathione (reduced form) were irradiated for 0-240 seconds with 442 nm light to effect guanine damage. The % crosslinked was determined by the chloroform extraction assay: NaCl and SDS were added to the samples to disrupt noncovalent interactions between DNA and protein, then the proteinaceous material was extracted into 24:1 chloroform:isoamyl alcohol. After centrifuging, the aqueous phase containing unreacted DNA was assayed at 260 nm by UV spectroscopy. Our results showed as the irradiation time increased, the absorption of free DNA decreased; consistent with crosslinking. Less DNA-protein crosslinking was observed when glutathione was present in the samples. We also used the gel shift assay: pBR322 plasmid was seen to migrate to the wells upon flash quench treatment in the presence of histone, but this behavior is strongly inhibited by glutathione. Lastly, we investigated whether or not glutathione interfered with the quenching process by doing emission spectroscopy experiments. We found that glutathione only slightly interfered with the quenching of Ru(phen)$_2$dpzp 2+, indicating that it most likely reacts with the guanine radical directly.
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<td>Immortal Plants: Isolation of Arabidopsis thaliana Flowering Locus T and Lipid Transfer Protein 3/4 Loss-of-Function Mutants</td>
<td>Dr. Robert Luis Vellanoweth</td>
<td>We seek to understand the biochemistry of lifespan determination in Arabidopsis thaliana, a model plant. Plants will be generated with three nonfunctional signal-carrying molecules: lipid transfer proteins (LTP) 3 and 4, and flowering locus T protein (FT), to create a plant that never flowers or exhibits delayed flowering. LTP3/4 RNAi knockdown mutants isolated in our lab showed a perennial-type growth pattern, producing many flowers and seeds and living over six times longer than wildtype plants. Additionally, FT and LTP 3 and 4 are up-regulated during the floral transition and have lipid-biding domains, suggesting they carry a lipid signal that may be the true flowering hormone. Double-mutants were created by crossing FT and LTP3/4 RNAi mutants to yield heterozygous FT and LTP3/4 RNAi plants. After these plants self-crossed, seeds were collected and grown on sulfadiazine/kanamycin agar plates to select for double-mutants. Genomic extractions will be used to confirm genotypes after the plants bolt. These plants exhibit unusual phenotypes compared to wildtype plants, such as asymmetrical, bushy rosettes and rosette-like patterns growing on shoots. A double-mutant that did not bolt was previously isolated and confirmed through genomic extraction. Studying senescence in Arabidopsis will provide applications in longevity or fruit production of agricultural plants.</td>
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<td>2</td>
<td>The therapeutic benefit of TMZ through alteration of methylation status of proteins</td>
<td>Tieli Wang, Anthony Joseph Diaz, Sheva Saif, Amanda Picker and James Gallo</td>
<td>Temozolomide (TMZ) is an alkylating agent used for clinical treatment of glioblastoma multiforme, an aggressive type of brain tumors and metastatic melanomas. It has been reported that the antitumor effect of TMZ on tumor cells rely on the spontaneous production of its degradation metabolites at physiology pH and the therapeutic benefit of TMZ involves reactions with methylation of guanine nucleotides in DNA. This DNA methylation in turn inhibits their correct utilization by base pairing, prevents cells from dividing and triggers the tumor cell death. However, the interaction of TMZ with proteins is not well documented. Like phosphorylation, ubiquitylation and acetylation of proteins which have been extensively studied, methylation of amino acid residues especially Arg and Lys in proteins is also an important posttranslational modification of proteins. It plays essential roles in regulating structure, function and localization of a protein. In the present study, we examined the methylation reaction of proteins by TMZ using proteomic technology and protein biochemistry. Our results showed that the TMZ/its metabolite methylidyazinium ion methylated the amino acid, peptide and proteins at physiological pH. Methylation of proteins will increase functional diversity of the proteome and have effects on all aspects of cell biology and pathogenesis. Identification and understanding of methylation modification of proteins is critical in the study of cancer treatment and prevention. We hope the study will contribute to our understanding the TMZ anticancer drug activity against human cancer in order to develop novel targeted molecular strategies.</td>
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<td>3</td>
<td>Sequence-specific nucleic acid detection based on blockade of a nanopore in a thin glass membrane</td>
<td>Harold Monbouquette, Allison Yorita</td>
<td>A new platform for sequence-specific nucleic acid (NA) detection with binary response has been demonstrated. The detection of nucleic acid sequences is useful for diagnosing the presence of bacteria, (especially those proven to be harmful to public health). Most existing methods are complex and require special reagents, as they rely on polymerase chain reaction (PCR) for target sequence amplification and/or fluorescence or enzyme labels. In our previous work, we described our first-generation, PCR-free, label-free system based on polystyrene beads conjugated with uncharged peptide nucleic acid (PNA) as sequence-specific probes, and demonstrated a detection limit of 10 FM. A drawn glass pipette tip served as the micropore and was placed between two buffer-filled chambers, one of which contained the uncharged bead-PNA conjugates. In the presence of target NA sequence, the bead-PNA conjugates acquire enough negative charge to become mobile by hybridizing the NA sequence of...</td>
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interest. Upon pore blockade by the beads, a change in the pore conductance occurs, which is reflected in a step-decrease in current that signals the presence of the target nucleic acid.

At lower concentrations of NA where fewer target NA molecules hybridize per bead, smaller beads are expected to have a higher mobility. By decreasing both the size of the pore and the beads, lower detection limits may be achieved. We fabricated thin (1 μm or thinner) glass membranes in which a nanopore is milled with a focused ion beam (FIB). This device has proven capable of distinguishing between complementary and non-complementary sequences of ssDNA at various bead sizes. Currently, we are working towards detecting E.coli 16S ribosomal RNA as the target sequence with the bead-PNA probes. With this device, we achieved at least a 1 pM detection limit. These results indicate that this work could give rise to a diagnostic platform for the rapid, sensitive, and cost-effective detection of NA of specific sequence.

Robert Ontiveros
California State University, Fullerton

Identification and Characterization of a Minimal Functional Splicing Regulator PTBP1

Niroshika Keppetipola
J. Doan, E. S. Adams, A. L. Hernandez, D. L. Black

In higher eukaryotes, alternative splicing of a single gene transcript into multiple final mRNA isoforms contributes significantly to increasing the diversity of the cellular proteome. The process of alternative splicing is regulated partly by RNA binding proteins that bind pre-mRNA transcripts to modulate splice site selection. Disease related splice variants have been identified in many neurodegenerative diseases and cancers, underscoring the importance of alternative splicing. Polypyrimidine Tract Binding Protein 1 (PTBP1) is a well-characterized RNA binding protein that acts primarily as a splicing repressor. PTBP1 contains four RNA Recognition Motifs (RRMs) joined via three linker regions that bind to pyrimidine rich sequences with varying affinity and structural preferences. PTBP1 regulates the alternative splicing of several cancer related genes including pyruvate kinase and FGFR2. Abnormal overexpression of PTBP1 is implicated in splicing deregulation in glioma and ovarian cancer as well as Alzheimer’s disease. Several different models for PTBP1 mode of action has been proposed and atomic details of each RRM bound to a CUCUCU hexamer are available from NMR structure studies. However, no single model explains how full-length PTBP1 binds a target exon to exert its function. A detailed atomic understanding how PTBP1 binds to its target RNA and the role of each RRM during exon inclusion/exclusion will unravel the mode of PTBP1 function and provide a rational for therapeutic targets for those diseases relate to splicing misregulation. PTBP1 crystallization trials have been hindered by the flexible linker 1 and 2 regions. The aim of this study is to identify and characterize a minimal functional PTBP1. A series of PTBP1 mutants were created with deletions in linker 1 (Δ19, Δ29, Δ37, Δ40) as well as linker 2 (Δ21, Δ44, Δ53, Δ68). Mutants were tested in vivo for protein expression and splicing repression activity using reporter minigenes in mouse neuroblastoma cells (N2A). Western blots indicate that the mutants are well expressed. Splicing assays reveal that the shortest construct (linker 1Δ40 and linker 2 Δ68) maintains splicing repression activity similar to full-length PTBP1. The minimal PTBP1 protein was cloned into a bacterial expression plasmid and tested for recombinant protein expression. Our results indicate that the recombinant minimal PTBP1 protein is soluble and well expressed. We are currently further genetically engineering the minimal construct to pursue x-ray crystallography studies.
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<td>Marissa Gionet-Gonzales</td>
<td>University of California, Riverside</td>
<td>IMPT 1 Fabrication of Silica Nanofibers for Nucleic Acid Extraction</td>
<td>Wenwan Zhong, Luis Jimenez, Kenneth Flack</td>
<td>DNA extraction is a vital technique in biology often used in the diagnosis of diseases, and DNA and RNA research. Commercially available silica coated iron oxide beads are able to extract as low as 1 fmol of DNA. However, silica nanofibers should better extract DNA because of their larger surface area. Silica fibers are also cheaper to produce than the silica beads, making them more economical as well as extraction efficient. In this research, silica nanofibers were produced via the sol-gel electrospinning method. Tetraethyl orthosilicate, a precursor of silica, was first treated with acid to produce silica, and then polyvinyl alcohol (PVA), an easily electrospun polymer, was added before electrospinning to increase the entanglements. After electrospinning, the fibers were calcinated to remove solvents and PVA. These fibers were then used in DNA extraction from a buffer solution or serum. After eluting the extracted DNA from the fibers, the DNA was quantified via real time PCR. These results showed that the DNA recovered from the fibers was higher than the silica beads and other fibers at 1 nM (50 fmol). This indicates that these fibers recovered a higher concentration of DNA and proves that silica nanofibers are able to extract DNA more efficiently. The use of silica fibers in DNA and RNA extraction can potentially increase detection of disease and lower the cost and time of biological and medical research that rely on extraction.</td>
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<td>Sahar Naghibi</td>
<td>University of California, Riverside</td>
<td>IMPT 2 CVD Growth and Characterization of TMD Materials on Patterned and Non-Patterned Substrates</td>
<td>Ludwig Bartes, Brandon Davis, Ariana Nguyen, Velveth Klee, I-Hsi Lu, Edwin Preciado, David Barroso, Aimee Martinez</td>
<td>Two-dimensional transition metal dichalcogenides (TMDs) are promising new materials because of their direct-bandgap and semiconducting capabilities present at the monolayer limit. Through chemical vapor deposition (CVD) I am able to synthesize monolayer MoS2 onto patterned and non-patterned SiO2 substrates. This method yields single domain &quot;islands&quot; and continuous films, which range from μm to cm scale growth. Through the use of patterned substrates, the transistor channel-length is defined independent of the lithographic lateral resolution. These CVD growth methods of MoS2 on the vertical sidewalls of micron- and nano-scale pillars fabricated out of SiO2 is possible. Optical characterization with Raman and photoluminescence spectroscopy verify single-layer growth of MoS2 on and off the patterned substrate, leading to the possibility for preliminary transport measurements of pristine MoS2.</td>
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<tr>
<td>Irene Diep</td>
<td>California State University Long Beach</td>
<td>IMPT 3 Lithium Sulfur Rechargeable Batteries</td>
<td>Irene Diep, Eduardo Pardo, Ngoc Tran, John Duong</td>
<td>Lithium sulfur rechargeable battery is a potential game-changer in rechargeable Lithium Battery technology. In addition to being very low cost due to the abundance of sulfur, it also has a higher theoretical specific capacity, helping the battery to last much longer. Incorporating carbon nanomaterials to prolong the life of lithium sulfur batteries has been a new, effective strategy in the last five years. A recent study has incorporated graphene oxide to encapsulate sulfur. Our project explores the use of graphene halides to replace graphene oxide, due to high cost of commercial graphene oxide. The graphene halides used in this study could be made through a simple, cheap ball-mill process. Our study shows that out of the halides, graphene-iodide performed the best. We believe this may be due to its higher surface area. The Li/S batteries made with graphene iodide performed remarkably well in cycle performance when compared to graphene oxide.</td>
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selective fluorides. New Pd-catalysis, and chemical biology. Despite their promise, there are few methodologies to synthesize aromatic sulfonyl compounds, but the susceptibility of reductive breakage of S-Cl bond lowers the efficiency of the required halide substitution step. In contrast, sulfonyl fluorides provide a more stable and chemoselective alternative to sulfonyl chlorides due to their resistance to hydrolysis, thermal stability, and selective reactivity with a variety of nucleophiles. The burgeoning interest in sulfonyl fluorides have led to applications in synthesis, organometallic catalysis, and chemical biology. Despite their promise, there are few methodologies to synthesize aromatic sulfonyl fluorides with various O- and N-based electrophiles to synthesize a variety of sulfonylated compounds, but the susceptibility of reductive breakage of S\(^{VI}\)-Cl bond lowers the efficiency of the required halide substitution step. In contrast, sulfonyl fluorides provide a more stable and chemoselective alternative to sulfonyl chlorides due to their resistance to hydrolysis, thermal stability, and selective reactivity with a variety of nucleophiles. The burgeoning interest in sulfonyl fluorides have led to applications in synthesis, organometallic catalysis, and chemical biology. Despite their promise, there are few methodologies to synthesize aromatic sulfonyl fluorides. New Pd- and Zn-mediated routes to aryl sulfonyl fluorides will be discussed, focusing on trends in the selective reactivity of electronically and sterically diverse aromatic sulfonyl fluorides with various O- and N-
nucleophiles. Sulfonate esters and sulfonamides were generated in good to excellent yields. Future studies will focus on applications in chemical biology and organometallic catalysis.

Peptide-based polymers have various applications including drug delivery agents, biomaterials, and in the regeneration of cell tissue. There are several advantages to utilizing peptides because their sequences are easily manipulated, they are compatible with aqueous environments, and have distinct biological functions including cell targeting. Reversible addition-fragmentation chain transfer (RAFT) polymerization is a 'green' living free radical technique that is able to withstand numerous reaction conditions. However, there are several issues involved in RAFT polymerization as monomers become more complex, including slow reaction time, poor control, and a need for multi-step reactions. One way to circumvent these shortcomings is by incorporating microwave technology into RAFT polymerization. This project aims to efficiently prepare peptide-based polymers by introducing microwave heating into the polymerization of complex peptide monomers. Eight pentapeptide monomers with varying characteristics including hydrophilic, hydrophobic, and zwitterionic were synthesized via SPPS utilizing Fmoc/tBu methodology followed by purification and characterization through High performance liquid chromatography (HPLC) and mass spectrometry (MS). Preliminary polymerization was conducted with simple monomers such as aminopropyl methacrylamide (APMA) and dimethylaminopropyl methacrylamide (DMAPMA) to investigate optimum reaction conditions. Once reaction conditions are optimized for these simple monomers, peptide-based monomers will be utilized in the polymerization to compare conventional and microwave heating. Overall, microwave-assisted RAFT polymerization will allow for a more efficient and natural method of preparation of peptide-based polymers that will have the potential to be utilized for numerous applications, such as drug delivery agents and biomaterials.

SNAAP® is a promising synthetic design for the preparation of esters and ethers by alkylation with sulfonimidates. The alkylation of alcohols is similar to the Williamson Ether Synthesis, but requires acid catalysis rather than substitution by alkoxides. Isopropylation of acids, alcohols and phenols utilizing the isopropyl sulfonimidate (N-1-adamantyl-O-isopropyl-4-nitrobenzenesulfonimidate) are favorably executed in good yields in a one-pot method with common organic solvents at room temperature. Products created contain retention of configuration, as no racemization or molecular rearrangement occurs. Yet, the real beauty of this, lies in the starting material, the sulfonimidate, as when you react with an acid or phenol or alcohol, the side product is the sulfonamide, which is the precursor to the sulfonimidate. One could say that this is green chemistry.

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N-1-Adamantyl-O-Isopropyl-4-Nitrobenzenesulfonimidate
Alzheimer’s disease (AD) has been associated with irregular levels in the cholinergic system. In the AD brain, concentration of the neurotransmitter acetylcholine (ACh) is observed to decrease. Because ACh is hydrolyzed by acetylcholinesterase (AChE) and butyrylcholinesterase (BChE), current anti-AD medications have focused on inhibiting both enzymes, especially AChE as a form of restoring ACh levels and thus cognition. Our research focuses on the synthesis of organophosphates that can display inhibition against BChE, since this enzyme has received less attention but its inhibition could play a major role in balancing the cholinergic system levels considering its activity is observed to be elevated in the AD brain. Previously, we established that the dialkyl phenyl phosphates are BChE-selective inhibitors. Based on these studies, we decided to synthesize similar compounds containing modifications in the aromatic moiety, such as addition of substituents to the phenyl ring or replacement of the phenyl ring with a naphthyl ring or a benzyl group. The inhibition studies of these dialkyl aryl phosphates (DAAP’s) showed that di-n-butyl 2-naphthyl phosphate and di-n-butyl 3,5-dimethyl phenyl phosphate were the two most potent inhibitors with $K_I$ values of 1.6 $\mu$M and 1.8 $\mu$M, respectively. The DAAP’s with substituents on the phenyl ring and those with the naphthyl moieties all exhibited significantly higher inhibitory properties against BChE compared to the unsubstituted analog (di-n-butyl phenyl phosphate; $K_I = 99.7$ $\mu$M). Positional isomers displayed differences on inhibition due to their preferred binding modes resulting from steric interactions with the active site groups and differential modes of binding. These results have provided insight into the design of new, more effective organophosphorus BChE inhibitors.
**Poster Abstracts**

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<tr>
<td>Farnaz Aghabarari</td>
<td>California State University Northridge</td>
<td>1</td>
<td>Anal/Env</td>
<td>Optical properties of internally mixed synthetic sea salt / glucose aerosol using cavity ringdown spectroscopy</td>
<td>Farnaz Aghabarari</td>
<td>Maryam Ghiyassee, Daniel B. Curtis</td>
<td>Atmospheric aerosols have a profound impact on climate by directly interacting with incoming solar radiations. Particles can contribute directly and indirectly to global climate change by absorbing radiative forcing, or scattering radiative forcing. Sea spray aerosols are one of the main three types of aerosols which represent the largest effect on climate. However, sea spray aerosols contain more than one compound. There are many different organic compounds in sea spray aerosols which glucose and carbohydrates are the most common ones. Research on synthetic sea salt shows that the refractive index of synthetic sea salt matches the refractive index of sea water aerosols very well. In this research, method of cavity ring down spectroscopy is used to measure the effects of organic compounds, specifically glucose, on the refractive index of synthetic sea salt in order to better understand the effect of sea spray aerosols on climate. In this experiment different concentrations of synthetic sea salt mixed with glucose solutions are made as follows: 0.1wt% samples of synthetic sea salt and glucose, 1:1 ratio solution mixture of synthetic sea salt mixed with glucose, and 1:4 ratio solution mixture of glucose ad synthetic sea salt. Primary results for this experiments indicates value of n and k for each solution as follow: 1.502 – 0.000, 1.539 – 0.007, 1.548 – 0.045, and 1.547 – 0.000, respectively. The errors in some results in this experiment are mostly due to the high concentration of the solutions.</td>
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<tr>
<td>Kelly Araujo</td>
<td>Mount Saint Mary’s University</td>
<td>2</td>
<td>Anal/Env</td>
<td>Correlation study between weather and PAH concentrations: Bio-monitoring of pine trees near the I-405 freeway in west Los Angeles</td>
<td>Stephanie Castillo, Megona Ligot, Angeline Camille Bautista, Yeneri Torres, Stephannie Jimenez, Ellisha Davis</td>
<td></td>
<td>PAHs (polycyclic aromatic hydrocarbons) are organic compounds consisting of two or more fused aromatic hydrocarbon rings. PAHs are unwanted byproducts occurring in carbon soot during incomplete combustion. They are air pollutants part of the Particulate Matter family (particles ranging between 2.5 to 10 microns in diameters) harmful to our health and monitored daily by the EPA (Environmental Protection Agency). PAHs are known to cause DNA mutations, cancer and birth defects. PAHs were bio-monitored through the Italian Blue Cyprus Pine tree leaves nearby the I-405 N Freeway. High traffic, and the presence of crevices found on the outer leaf make it suitable for PAHs to settle in. The PAHs were extracted using a Soxhlet apparatus and analyzed via Gas Chromatography Mass Spectrometer (GCMS). A SIM (Selected Ion Monitoring) table was specifically used to search for the 16 EPA known PAHs within the spectrum. With the PAH and PM values (collected daily from AQI (Air Quality Index)) the quotient ratio was mathematically determined, then graphed to see the correlation between two different seasons. Since PAHs are a component of the PM values their settlement on the environment should occur at the same rate. Samples collected from the I-405 from May through April showed a correlation between the amount of PAH and PM2.5 values. Within our results, we find discrepancies from the trend lines when both values are inversely</td>
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proportional, however, we were able to link this to occurring rain events. We are currently furthering our daily quotient ratio correlation by running samples throughout the different seasons of the year.

Homocysteine, cysteine, cysteinyl-glycine, and glutathione are significant aminothiols which have been implicated as risk factors in atherosclerosis and other vascular diseases. Rapid determination of these aminothiols is, thus, desirable. Following reduction of the disulfides with tri-n-butylphosphine, a widely used method utilizes derivatization with ammonium 7-fluoro-benzo-2-oxa-1,3-diazole-4-sulfonate (SBD-F) as a fluorogenic probe prior to reversed-phase HPLC analysis. We report the results of microwave-enhanced synthesis of the fluorescent derivatives at temperatures ranging from 90-110 °C. Utilizing microwave heating, we reduced the derivatization time at all temperatures from 1 h to less than 4 min. Standard solutions produced rectilinear calibration curves with correlation coefficients >0.99 for all four aminothiols. We compared the results obtained for the four aminothiols extracted from mouse heart, chicken plasma, and chicken liver using traditional heating and microwave heating. Statistical differences were evaluated for the concentrations of aminothiols determined after the different heating methods. We also report the results of recovery experiments and differences in calibration sensitivities between the two methods.

PAHs (polycyclic aromatic hydrocarbons) are organic compounds consisting of two or more fused aromatic hydrocarbon rings. PAHs are unwanted byproducts occurring in carbon soot during incomplete combustion. They are air pollutants part of the Particulate Matter family (particles ranging between 2.5 to 10 microns in diameters) harmful to our health and monitored daily by the EPA (Environmental Protection Agency). PAHs are known to cause DNA mutations, cancer and birth defects. PAHs were bio-monitoring through the Italian Blue Cyprus Pine tree leaves nearby the I-405 N Freeway. High traffic, and the presence of crevices found on the outer leaf make it suitable for PAHs to settle in. The PAHs were extracted using a Soxhlet apparatus and analyzed via Gas Chromatography Mass Spectrometer (GCMS). A SIM (Selected Ion Monitoring) table was specifically used to search for the 16 EPA known PAHs within the spectrum. With the PAH and PM values (collected daily from AQI (Air Quality Index)) the quotient ratio was mathematically determined, then graphed to see the correlation between two different seasons. Since PAHs are a component of the PM values their settlement on the environment should occur at the same rate. Samples collected from the I-405 from May through March showed a correlation between the amount of PAH and PM2.5 values. Within our results, we find discrepancies from the trend lines when both values are inversely proportional, however, we were able to link this to occurring rain events. We are currently furthering our daily quotient ratio correlation by running samples throughout the different seasons of the year.

Significant improvements in analytical chemistry technology have allowed trace metal analyses in complex matrices with here-to-fore unmatched speed and sensitivity, at low cost. Thus, our group has investigated measuring trace amounts of Pb in a Ca-rich aqueous matrix, to utilize these recent
improvements. We will discuss our procedure, equipment used, and results in the context of investigating Pb as a potential contaminant in Ca dietary supplements derived from oyster shells.

Tetraethyl Lead was utilized in large quantities starting in the 1920s to make gasoline combustion engines more efficient. White Pb was used as a widely dispersed ingredient of paint, and Pb aerosols are a persistent byproduct of coal fired power generation. Fuel combustion, and the weathering of paint, released fine Pb particles into the atmosphere, where smaller particles were dispersed into various environmental repositories. Specifically, Pb pollutants remain, to this day, in aquatic systems impacted by previous and continuing release of Pb. Oysters are at risk of contamination as they directly feed from the Pb-impacted ocean water. Oysters are a type of filter feeder, which draw in surrounding water, trapping Pb. As Pb is chemically similar to Ca, Pb can be incorporated into the oyster’s shells. Dietary Ca supplements which derive their Ca carbonate from oyster shells thus was presumed by our team to have contain Pb replacing shell Ca.

Yellow prussiate of soda (YPS) is a chemical added to table salt to prevent caking. When YPS is acidified (as in the stomach), or heated (as in a transportation mishap), hydrogen cyanide (HCN) is produced. HCN is a powerful biotoxin. The current investigation developed a technique which could detect HCN released from table salt samples containing YPS. HCN detection was via a detector tube technology using a color change in the packing of the tube to indicate the presence and concentration of HCN released from a test sample. The presentation will examine procedures and results in detail.

Mercury levels in recent decades have been on the rise due to the expanding use of fossil fuels. Elemental mercury becomes airborne and gets deposited into the oceans where microbial processes oxidize it to methyl mercury, which then bioaccumulates in fish. Fish consumption becomes a source of mercury, which is harmful to human health. This study focuses on the difference in mercury levels of wild caught salmon and farmed salmon, where the salmon is raised in a controlled environment. Salmon samples were tested using thermal decomposition, amalgamation and then atomic absorption spectroscopy. The results for Wild Sockeye averaged 7.512 (±0.195) ppb and Farmed Atlantic averaged 1.108 (±0.166) ppb.

The purpose of this project was to design, assemble, and calibrate a multicomponent device capable of instantaneous and cost-effective enzyme kinetic analysis. First, it was used in comparison with the abilities of UV Spectrophotometer. After ascertaining the range and accuracy of its fluorescence detection, the device was modified for the analysis of the well-studied double hydrolysis of the substrate Fluorescein-di-β-D-Galactopyranoside (FDG) by the enzyme β-Galactosidase.

Designed as a lightweight alternative to bulky analysis equipment, the apparatus utilized a variety of methods to cut down on sample size, time, waste and cost. The materials were channeled through a droplet-based system of microfluidic tubing, and a 3 mL syringe was used as a Continuously Stirred Tank Reactor. The fluorescein product of the reaction was isolated by a layer of Streptavidin beads,
which immobilized all other components within the reactor. A photo diode detector recorded the absorbance of the outlet stream, which could be coupled and compared with data from COMSOL Multiphysics simulations. Data analysis included calculation of the Michaelis-Menten constant.

The experiment as a whole provided insight into the immense potential for high-throughput Labs on a Chip modeled after this design. Further work will continue to scale down and eliminate errors in this process. The benchtop-scale model could be helpful for facilitating research, not only on β-Galactosidase, but any number of fluorescein-labeled materials. Measurements of aerosol optical properties such as the complex refractive index can be used to improve climate models and remote sensing measurements of atmospheric particulate matter and therefore improve our understanding of aerosol effects on climate. Sea-spray aerosol is one of the most ubiquitous particle types in the atmosphere, yet few measurements of the refractive index exist. This research describes a measurement of the extinction properties and complex refractive index of dry sea spray aerosol at a wavelength of 532 nm using continuous-wave cavity ring down spectroscopy and retrieval by comparison with Mie theory. The aerosol particles were generated in the laboratory by nebulizing and drying samples of authentic seawater collected from the Pacific Ocean at the California coastline, USA. The average retrieved complex refractive index was $m=1.51 + 0.00i$, similar to the bulk measurements in the literature. Measured refractive indices did not vary with sampling location within the uncertainty of the measurement. In addition, a commercially available synthetic sea salt sample was measured and the retrieved refractive index was a good match to the authentic samples.

Salt marshes play an important role in the sequestration and exchange of organic carbon in coastal aquatic ecosystems. Organic carbon in these tidally forced wetlands is primarily a result of inputs from allochthonous terrestrial material, and loss processes that include microbial degradation, photodegradation, and export. Dissolved organic matter (DOM) levels and functionality in salt marshes often determines the degree of nutrient uptake, light availability, and overall carbon cycling. DOM chemical and physical functionality changes as the material is processed and transformed by both microbial and photochemical processes. In southern California, intertidal wetlands are often impacted by oil through marine spills, natural seeps, coastal wells, and contaminated storm water runoff. This adds an additional level of complexity to understanding the physical, chemical and biological transformation of DOM in these systems. The degree to which oil products are significant sources of organic carbon is not clear and transformations of oil products in salt marshes are poorly characterized. In this work we have used optical properties to track the photochemical changes in a range of oil products in the laboratory, from heavy crude oils to distillates from a number of different sources. Data from three dimensional excitation-emission fluorescence spectra and associated fluorescence indices, including measures of humification, will be presented and discussed.
Ammonia Borane (AB) has high hydrogen density (19.6 wt. %), and can, in principle, release up to 3 equivalents of H₂ under mild catalytic conditions. A limited number of catalysts are capable of non-hydrolytic dehydrogenation of AB beyond 2 equivalents of H₂ under mild conditions, but none of these is known directly to derivitize borazine, the product formed after 2 equivalents of H₂ are released. We present here a high productivity ruthenium-based catalyst for non-hydrolytic AB dehydrogenation that is capable of borazine dehydrogenation, and thus exhibits among the highest H₂ productivity reported to date for anhydrous AB dehydrogenation. At 1 mol% loading, (phen)Ru(OAc)₂(CO)₃ (1) affects AB dehydrogenation through 2.7 equivalents of H₂ at 70°C. We further demonstrate that catalyst 1 has unprecedented ability to dehydrogenate borazine in isolation. This is important both because borazine derivatization is productivity-limiting in AB dehydrogenation and because it is a fuel cell poison that is commonly released in H₂ production from this medium.

Polycyclic aromatic hydrocarbons (PAHs) are molecules composed of two or more fused hydrocarbon rings. PAHs are created as the bi-products of the incomplete combustion of organic materials. PAHs are volatile compounds whose characteristics pose concerns about long-term risk of exposure in highly populated cities such as Los Angeles, CA. In comparison, particulate matter (PM) is the sum of all products of pollution including PAHs, dust, pollen, and smoke. Both PAHs and PM are of concern to the U.S. Environmental Protection Agency (EPA) due to their known harmful effects on human health. The EPA provides the public with data records of PM, which allowed this study to further quantify PAH molecules in the atmosphere while also comparing to the EPA's PM findings. Through the bio-monitoring of Blue Italian Cypress trees, PAH quantification in Los Angeles was obtained. This tree of study was chosen because it was evergreen, abundant, and its leaf scale like structure provided a larger surface area for PAH accumulation. Utilizing a Soxhlet extraction technique, PAHs were extracted from leaves, the extract were then evaporated under mild vacuum close to dryness, resuspended in fresh solvent, and analyzed through Gas Chromatography Mass Spectroscopy. All 16 PAHs of EPA interest were successfully identified and quantified at all 3 locations of interest. The results had shown discrepancies within the hypothesis proposed where PAH concentration in the residential area would be higher than that of the secluded hillside. Due to this inconsistency, further investigation was done to prove that weather conditions such as wind, rain, humidity, etc. take effect on concentrations of PAHs daily. The experimental PAH concentrations and the obtained PM values were then scaled to the same magnitude for the purpose of trend demonstration. The difference quotient, which measures the average rate of change of concentration over the interval of time, was then applied for all PAH and PM values and then analyzed. The preliminary results validated an overall correlating trend between the EPA's PM value curve and our experimental PAH concentration curve. For future direction, this project will continue to monitor PAH concentration from Italian Blue Cypress trees and identify a comparison to the EPA's daily PM values to uncover a long term trend.
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<td>Chidinma Abanobi</td>
<td>California State University, Fullerton</td>
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<td>Characterization of Homologs Showing Evolutionary Relationships with Methylobacterium extorquens AM1 Dihydromethanopterin Reductase A (DmrA)</td>
<td>Chidinma Abanobi, Mark Burton, Madeline Rasche</td>
<td>Methanogens are major contributors to the microbial production of methane, which is correlated with the greenhouse effect and human obesity. Inhibition of tetrahydromethanopterin (H4MPT) biosynthesis, an important coenzyme and one-carbon carrier in methanogens, can diminish the production of methane without inimically affecting beneficial bacteria in the host organism. Aerobic α-proteobacteria, such as Methylobacterium extorquens AM1, also produce H4MPT, and the enzyme DmrA catalyzes the last reaction of the biosynthetic pathway: the reduction of (H2MPT) to H4MPT. Homologs currently labeled as DAG kinases from Methylobacterium variabile, and Hyphomicrobium nitrativorans were produced heterologously in Escherichia coli. The purified enzymes were tested using an enzymatic assay that measures the NADPH-dependent reduction of H2MPT to H4MPT. In the absence of both MvaDAG1 and HniDAG, no changes in the absorbance at 340nm were observed, but when active MvaDAG1 and HniDAG were added to the reaction mixture, a decrease in A340 occurred, which is evidential that MvaDAG1 and HniDAG catalyze the NADPH-dependent reduction of H2MPT. These results provide evidence that MvaDAG1 and HniDAG are likely to be H2MPT reductase rather than diacylglycerol kinase and that they should be renamed as DmrA. Previous studies from our lab led us to hypothesize that lipid transfer proteins (LTPs) shuttle signals from seeds to meristems that mediate senescence. Our aim is to clone, express, and purify the LTP4 so that we may use the protein to analyze the bound lipids from wild-type and ltp4 mutant leaves and seeds of A. thaliana. We expect to characterize a lipid molecule that is accumulated in LTP mutant leaves and seeds. The result of this study would give insight to the importance of lipid transfer proteins in the development and senescence of A. thaliana.</td>
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<td>Jacopo Airapetyan</td>
<td>California State University Los Angeles</td>
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<td>Expression of Arabidopsis thaliana recombinant LTP4 in Escherichia coli</td>
<td>Dr. Vellanoweth Robert, Yasmin Homayoun</td>
<td>Dr. Vellanoweth Robert, Yasmin Homayoun</td>
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<td>Dorith Anda</td>
<td>California State University, Fullerton</td>
<td>15</td>
<td>Crystallization of Orf22 from Methylobacterium extorquens AM1 for X-Ray Structure Determination</td>
<td>Dorith Anda and Tiana Le, Herbert Axelrod and Madeline Rasche</td>
<td>Methanogens are microorganisms that synthesize methane. The synthesis of methane requires a cofactor called tetrahydromethanopterin (H4MPT). Many aerobic bacteria utilize H4MPT to consume methane or methanol. Complementation studies indicate that Orf22 from Methylobacterium extorquens AM1, a homolog of Methanocaldococcus jannaschii 1099 (MJ1099), catalyzes one of the reactions in H4MPT biosynthesis. In contrast, a recent biochemical study suggests that MJ1099 plays a role in methanofuran biosynthesis, which is a carbon dioxide reduction cofactor needed to synthesize methane. However, bacterial methanol oxidation does not involve in reducing CO2. To enhance our understanding of whether Orf22 in bacteria has multiple functions similar to those of MJ1099, the purpose of our investigation is to determine the X-ray crystal structure of Orf22. For the structure determination, here we report on the purification and crystallization of Orf22. Orf22 was purified by nickel-affinity chromatography followed by gel filtration column chromatography. Sodium dodecyl sulfate polyacrylamide gel electrophoresis (SDS-PAGE) showed the protein to be more than 90% pure. Dynamic light scattering (DLS) showed that the protein solutions concentrated to 2.6 mg/ml or 6.8 mg/ml solution were 100% pure without aggregation. Crystallization has been achieved from droplets containing 32% 2-methyl-2,4-pentanediol (MPD). More extensive screening of crystallization conditions is now underway at the Macromolecular Crystallography Core Technology Center at UCLA using a TPP LabTech Mosquito nanodispenser robot to increase the dimensions of the crystal for X-</td>
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ray data collection. Obtaining a 3D structure of Orf22 should initiate a better understanding of its controversial role in cofactor biosynthesis.

**Johanna Bautista**
California State University of Los Angeles

16 Biochem

**RBP-Expression Vector, RBP Purification and Antibody Production to Further Understand the Role of RNP Multi-Protein Complexes in Storage Protein mRNAs Transport**

**Thomas Okita, Ph.D and Robert Luis Vellanoweth, Ph.D**

Rice accumulates two major classes of storage proteins, prolamines and glutelins. Storage proteins accumulate in different subcellular locations: the ER-lumen to form protein body-I (PB-I) and protein storage vacuole (PSV, PB-II). Earlier studies have demonstrated that prolamine RNAs are transported to the PB-ER that bound the PB-I, while glutelin RNAs are transported to adjacent interconnecting cisternal-ER. Subsequent studies show that storage protein RNA transport is a multistep processes requiring several cis-elements located in the coding sequence and 3'UTR of the prolamine and glutelin RNAs. We have identified eight RBPs that may serve as potential RNA localization transactors. To generate antibodies to these RBPs, we have expressed and purified the recombinant protein by immobilized metal affinity chromatography (IMAC). Results depicting the expression of four recombinant RBPs will be presented. Overall, results from our study will accelerate our understanding of how the RNP transport complex is formed and remodeled during mRNAs movement to specific cellular locations in rice endosperm tissue.

**Ana Chan**
California State University, Long Beach

17 Biochem

**Investigating the Catalytic Role of a Conserved Non-Active Site Residue in Triosephosphate Isomerase**

**Jason Schwans**

**Anna Nguyen** (Anna Nguyen and I, Ana Chan, are both presenting together), Nessa Seangmany

Triosephosphate isomerase (TIM) is a glycolytic enzyme that catalyzes the reversible isomerization of dihydroxyacetone phosphate and glyceraldehyde-3-phosphate. TIM has served as a model system to study enzyme function, and previous studies have investigated the catalytic roles for three active site residues: K13, H95, and E167. In addition to the residues that directly contact the substrate, E97 is conserved in all known TIM sequences. Previous studies reported the E97Q mutation in TIM from Plasmodium falciparum decreased $k_{cat}$ ~4000-fold relative to wild type, suggesting an important catalytic role for this residue. To investigate further the catalytic role of E97 and to evaluate if E97 mutations lead to similar effects in TIM from another organism, we evaluated the effect of E97 mutations in TIM from Trypanosoma brucei brucei. Following generation of the constructs via site-directed mutagenesis, we overexpressed the enzymes in Escherichia coli, purified using ion-exchange chromatography, and characterized the mutants using Michaelis-Menten kinetics. Our results show the E97Q mutation in TBB decreased $k_{cat}$ ~40-fold, suggesting the residue plays an important role in catalysis, but the rate decrease was significantly less than that observed in P. falciparum. Structures show that although the active site residues are conserved, the residues surrounding E97 differ in TBB and Plasmodium TIM. The mutations may lead to different structural rearrangements in TIM from the two sources. We are currently investigating the physical basis for the different effects from the mutations and evaluating the role of E97 in positioning K13, as structures show the Glu residue is situated near K13. These results will further our understanding of the catalytic role of residues that surround the active site.
West Nile Virus (WNV) is a flavivirus carried by various species of mosquitoes that can be transmitted to animals and humans through mosquito bites. Transmission of the disease can be life threatening as it causes meningitis, encephalitis, and damage to the Central Nervous System (CNS). At this time, there are no known treatments or vaccinations. Current research of WNV has been focused on the NS2B-NS3 protease. This 36 kDa serine protease contains a His-Asp-Ser catalytic triad in NS3, which is vital for the replication of the West Nile Virus. NS2B is a cofactor needed in order for it to be active. The inhibition of this protease is a strong target for drug development. Fluorescence Resonance Energy Transfer (FRET) assays were used with a synthetic peptide substrate containing a K-K-R sequence, 7-Methoxycoumarin-4-acetic acid (MCA) fluorophore, and 2,4-Dinitrophenyl (DNP) quencher molecules to study the inhibitory properties on the WNV protease. The kinetic parameters of the activity of NS2B-NS3 are $K_m = 3.29 \mu M$, $V_{max} = 2.53 \text{ RFU/S}$, and $k_{cat} = 84.47 \text{s}^{-1}$. In this study, the inhibitor "Z" was tested and the IC$_{50}$ value was determined to be 50 μM. However, inconsistencies in data led to speculations of aggregation of the inhibitor. Varying concentrations of dimethyl sulfoxide (DMSO) and temperatures were assayed to prevent aggregation and to improve the consistency of data between trials. The Z inhibitor shows partial inhibition, however further studies are required to determine which part of the structure of the inhibitor is most effective in inhibiting the protease for drug development.

Methane is a potent greenhouse gas and is released into the atmosphere by methane-producing microorganisms (methanogens) in the rumen of cattle. Tetrahydromethanopterin (H$_4$MPT) is an essential coenzyme in methane biosynthesis and functions as a carrier of one-carbon (C1) compounds. It has previously been shown that inhibiting enzymes of H$_4$MPT biosynthesis can halt the methanogenesis process. The first step of H$_4$MPT biosynthesis is catalyzed by 4-(β-D-ribofuranosyl)aminobenzene-5’-phosphate (RFA-P) synthase, and analogs of the substrate p-aminobenzoic acid (pABA) have been developed that prevent the growth of methanogens in culture at a minimal inhibitory concentration of 0.1 µM. Design of more potent inhibitors could be facilitated by detailed knowledge of the active site through protein crystallography. However, the structure of RFA-P synthase remains unknown. Attempts to create a computational model of RFA-P synthase using homoserine kinase as the template were unsuccessful due to the inability to model a pABA binding site. Therefore, the goal of this research is to produce, purify, and crystallize a heat stable RFA-P synthase from Methanocaldococcus jannaschii. RFA-P synthase was produced with an N-terminal histidine tag in Escherichia coli cells and purified to homogeneity by carrying out a 65°C heat treatment followed by nickel affinity chromatography. Native polyacrylamide gel electrophoresis (PAGE) produced a single 316-kDa band, consistent with a quaternary structure of about eight 37-kDa subunits. This result is in contrast with a previously reported 70-kDa homodimer structure, determined by size exclusion chromatography. Although the protein precipitated at concentrations approaching 10 mg/mL, RFA-P synthase remained soluble up to 6 mg/mL, suitable for initial protein crystallography attempts. Determination of the three-dimensional structure of RFA-P synthase will be
useful for predicting the mechanism of the enzyme and designing more effective methanogen inhibitors to mitigate greenhouse gas production.

Curli fibers are known to be involved in bacterial adhesion to surfaces, cell aggregation, and biofilm formation. Curli belongs to a class of fibers known as amyloids. Curli assembly requires 5 proteins, CsgA, CsgB, CsgE, CsgF, and CsgG. CsgA and CsgB are the major structural components of curli. CsgG is an outer membrane protein responsible for the secretion of CsgA and CsgB to the extracellular surface. CsgE and CsgF are thought to be chaperon proteins in which are responsible for transport of CsgA and CsgB in the periplasm. Research done on curli identified functional interactions between CsgG and CsgE during curli secretion. Recent crystal structure of CsgG indicated the transmembrane segment of the protein adopts a β-sheet structure. However, not much is known regarding the interactions between CsgG and the other curli assembly proteins. The ultimate goal of our study is to characterize the membrane associated structure of CsgG, to gain insight on how its structure contributes to its function in curli formation, and to determine any interaction with CsgE.

Recent studies have shown that while acetylcholinesterase (AChE) activity remains unchanged or declines in patients with Alzheimer’s disease, butyrylcholinesterase (BChE) activity is increased. Thus, use of molecules that selectively inhibit BChE has attracted attention as a potential therapeutic for Alzheimer patients. Previous studies suggested dialkyl phenyl organophosphates may be effective and selective BChE inhibitors, but effects of modifications on the aryl group were not reported. We evaluated a series of dialkyl aryl organophosphates as selective BChE inhibitors, as the molecules provided an attractive scaffold to readily introduce substituents and develop more potent inhibitors. The inhibition constant ($K_I$) and IC\textsubscript{50} value were determined for each inhibitor using established kinetics assays. Our results show incorporation of alkyl groups on the aryl moiety led to better inhibitors relative to the dibutyl phenyl phosphate for all inhibitors tested, but inhibition properties were dependent on the number and location of the methyl group(s). Increasing the size of aryl substituent to a naphthyl group led to better inhibition with the 2-naphthyl analog showing a 10-fold lower $K_I$ value compared to the 1-naphthyl analog. Experiments to evaluate the connectivity of the alkyl substituents and the aryl group suggest the contribution of the aromatic moiety to inhibition is affected by the identity of the alkyl chains. These results identified molecules with improved inhibition properties compared to the previously reported dialkyl phenyl phosphate and begin to dissect the structural features responsible for inhibitor binding.

Helicobacter pylori, the cause of most gastritis cases, thrives in the highly acidic pH of the human stomach. The heat shock protein Hsp60 is one of the most abundant proteins observed in H. pylori. Since the structure and sequence of Hsp60 are similar to those of the chaperonin from E. coli, GroEL, it is hypothesized that their functions are similar as well. However, unlike GroEL which binds to ATP, Hsp60 from H. pylori binds to GTP. In a previous
study, it was shown that the binding of GTP caused alpha-crystallin, a protein in the eye lenses that functions as a molecular chaperone, to be less stable. Here, we investigated the effect of GTP on the chemical stability of *H. pylori* Hsp60. A mutant of Hsp60 containing a tryptophan replacement at residue 202 was purified and used for fluorescence studies. Fluorescence spectroscopy was used to determine whether the binding of GTP stabilized or destabilized the protein against urea denaturation. It was shown that Hsp60 has a low stability against urea denaturation and that the binding of GTP had a destabilizing effect on the Hsp60 mutant.

In living systems, arginine is able to take the form of three different methylated species: monomethylated (MMA), symmetrically dimethylated (SDMA), and asymmetrically dimethylated (ADMA) arginine. Separation of SDMA from ADMA is a challenge as both derivatives are the same size and differ only in their placement of methyl groups. Thin layer chromatography (TLC) is a method for separating and identifying non-volatile mixtures. Using traditional TLC methods and a silica plate as the stationary phase, we separated the three different methylated arginine derivatives including ADMA from SDMA. The solvent ratio was optimized to a ratio of: (2:0.5:4:5:1 ratio of 30% NH₄OH : CHCl₃ : CH₃OH : H₂O). Once the silica plate is spotted with known standards (MMA, SDMA, ADMA), each in their own lane, an acid hydrolyzed mixture of proteins can be spotted in a separate lane. By capillary action, the solvent will separate the mixture. A final spray with ninhydrin will detect primary and secondary amines for final identification.

Lysyl oxidase (LOX) is a copper-dependent amine oxidase that has been implicated in playing a paradoxical role in cancer. Expression of the LOX gene was found to inhibit the transforming activity of the H-ras oncogene in NIH 3T3 fibroblasts. Ras proteins are involved in transmitting signals within cells and are the most common oncogene in human cancers. It was hypothesized that the activity of LOX can be controlled through the use of mechanism-based inhibitors in MDA-MB-231 breast cancer cells. Selective inhibitors for lysyl oxidase were synthesized and assayed for cell viability using breast cancer cells. The inhibitors synthesized were the meta and para derivatives of 4-nitrobenzyl β-APN, the para derivative of 4-bromobenzyl β-APN, and the dibenzyl derivative of β-APN. A three-day viability assay following the treatment of cancer cells with these derivatives revealed that cells treated with the meta derivative of 4-nitrobenzyl β-APN, the para derivative of 4-bromobenzyl β-APN, and the dibenzyl derivative of β-APN had a significant decrease in cell viability when concentrations greater than 500 μM were used. The para derivative of 4-nitrobenzyl β-APN, however, had little effect on the viability of the cells. These results indicate that the meta derivative of 4-nitrobenzyl β-APN, the para derivative of 4-bromobenzyl β-APN, and the dibenzyl derivative of β-APN are successfully targeting the cancer cells, although it remains to be seen whether or not the inhibitor is selectively targeting lysyl oxidase. Normal breast cells are currently being tested in order to ensure that the inhibitory effect is only present in cancer cells.
Bacteria have developed antibiotic resistance creating the need for natural alternatives. Herbs, a class of natural products, have been shown to inhibit bacterial growth in various studies. In this study, antibacterial properties of seven herbs were tested on *Bacillus megaterium*, *Enterobacter aerogenes* and *Enterococcus faecalis*. The herbs in the study were extracted with methanol, filtered, rotovaporated and dissolved in dimethyl sulfoxide (DMSO). Bacteria were grown in tryptic soy broth and incubated overnight. The samples were then diluted to match a 0.5 McFarland standard to ensure a fixed bacteria density. Samples were composed of 1500μL of diluted bacteria with 20μL of herb samples, and incubated/shaken at 37°C for 45 minutes. The percent transmittance of each sample was measured at a wavelength of 625nm hourly until the control decreased to less than 50%. Percent inhibition was determined by normalizing the percentage transmittance of the sample at 50% of the normalized control.

*Bacillus megaterium* exhibited the greatest inhibition with the herbs (41-67%). In contrast, *Enterobacter aerogenes* had an inhibition of 33-58%, and *Enterococcus faecalis* had an inhibition of 11-27%. The minimum inhibition concentration (MIC) for catnip on *Bacillus megaterium* was 0.014g/mL. In the future, additional MIC values will be determined and additional bacteria will be tested. This study has demonstrated the potential for herbs to be effective antibacterial agents.
can inhibit oxidative DNA damage. The flash-quench technique is a method that is used for guanine oxidation and it can induce DNA-protein crosslinking. In the flash quench technique, the intercalator, Ru(phen)2dppz2+ [phen = phenanthroline, dppz = dipyridophenazine], is excited with a laser and gives an electron to the quencher, Co(NH3)5Cl2+. The intercalator takes an electron from guanine, creating the guanine radical, which then reacts with protein. In our experiment, samples containing Ru(phen)2dppz2+, Co(NH3)5Cl2+, histone protein, calf thymus DNA and either water or green tea were irradiated for 0 - 2 minutes with blue laser light from a HeCd laser to effect guanine damage. The extent of crosslinking was determined by the chloroform extraction assay, whereby protein and DNA-protein crosslink is extracted away from unreacted DNA. Our results showed as the irradiation time increased, the absorption of free DNA decreased less in the presence of green tea, consistent with inhibition of DNA oxidation. In addition, agarose gel electrophoresis experiments of samples containing pUC19 DNA showed that the free DNA band persisted at dilutions of green tea up to 400:1. In future work, experiments will be carried out to determine a more accurate concentration range for the antioxidant effects of the green tea and to identify the molecular components responsible; analogous experiments with small peptides suggest that phenols could produce the inhibitory effect by reducing guanine radicals.

The goal of our project is to construct and test biosensors that can detect metal uptake and ROS formation in human HeLa and neuroblastoma cells. The motivation for this project comes from several recent studies that suggest accumulation of excess metals in cells can cause an increase in the production of reactive oxygen species (ROS) that are implicated in many diseases, including cancer and neurodegenerative disorders. We previously constructed two luciferase reporter plasmids (pMtn-luc2 and pSOD-hRluc) containing the Drosophila metallothionein and superoxide dismutase promoters, respectively, and evaluated their responses to low and high concentrations of Cu, Fe, and Zn in Drosophila S2 cells. We found that all three metals induced similar levels of Mtn-luc2 reporter activity; however, the SOD-hRluc reporter showed a much higher induction in response to Fe and Zn than in response to Cu. This suggested that Fe and Zn induced higher levels of ROS than Cu in S2 cells. We recently introduced the Drosophila Mtn-luc2 and SOD-hRluc constructs in human HeLa and SHSY-5Y neuroblastoma cells and performed luciferase assays in order to see if they could function as metal and ROS biosensors in these cells. In HeLa cells, the luminescence response of the Mtn-luc2 reporter to Fe was approximately 200-fold and 150-fold higher than that induced by Cu and Zn, respectively. For the SOD-hRluc reporter, Cu induced a slightly higher but statistically significant luminescence response compared to Fe and Zn. Similarly, in SHSY-5Y cells, the response of the Mtn-luc2 to Cu was weaker, while that of the SOD-hRluc was stronger. These results suggest that Cu may be a strong ROS inducer in HeLa and SHSY-5Y cells, and that the Mtn and SOD promoters from Drosophila can also function as metal and ROS sensors in human neuroblastoma cells, which to our knowledge, has not been demonstrated before.
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<td>Shannon Yang</td>
<td>Mount Saint Mary's University</td>
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<td>Studying the Effect of Manganese Import on Mutation Rates in Escherichia coli</td>
<td>Paul Lee, Ph.D, Michell Garcia, Ivy Gasparyan, Yvette Nowry, Rochelle Nevarez, Nancy Tran</td>
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<td>Under excessive amounts of hydrogen peroxide a cell will activate genes to protect itself against oxidation. In Escherichia coli, one of these genes codes for mntH, a manganese import protein. Manganese is a redox cofactor and is thought to help protect proteins from oxidative damage. We wish to understand the role manganese may have in DNA damage and repair. To study this, we have attempted to knockout the mntH gene in a reporter strain of E. coli which is sensitive to DNA mutation. We used the Lambda Red system, a special recombination system, to insert a linear piece of DNA containing the kanamycin gene into the E.coli's genomic DNA, replacing the mntH gene. Using the new strain of E. coli without the gene, we will observe how many colonies grow on Lac media plates and compare this to the reporter strain of E. coli that does not have the gene deleted. For this reporter strain, growth on Lac media plates is an indicator of high mutation rates. These experiments will allow us to have a greater understanding of the role manganese has in E. coli. We were successful in creating the insert that would replace the gene and transforming the reporter strain with a plasmid containing the recombination system. We are currently in the process of transforming the bacteria with the insert that will replace mntH.</td>
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<td>Radiance</td>
<td>University of California, Irvine</td>
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<td>Strategies to block the Neurite Outgrowth Inhibitor, Nogo</td>
<td>Melanie Cocco, Ali Alhoshani, Verna Vu, D'Artagnan Greene, Katayoun Yazdi-Nejad, Raymond Chu, Sung (David) Kim</td>
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<td>Thompson</td>
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<td>Damaged axons in the central nervous system (CNS) aren't able to regenerate, in contrast to cells in the peripheral nervous system (PNS). Studies have shown that this is partly due to interactions between myelin-associated inhibitors and their receptors, which are present in myelin in the CNS but not in the PNS. When the interactions between the 66 amino-acid loop of Nogo (Nogo-66) and the Nogo-66 receptor (NgR1) are disrupted neurite growth increases. Consequently, this domain has been targeted to treat spinal cord injury, stroke and other neuronal degenerative conditions. A possible way to prevent binding between Nogo-66 and NgR1 is through the use of aptamers. These are single-stranded oligonucleotides that fold and present unique three-dimensional structures. Using aptamers rather than antibodies has many advantages including low cost, ease in identification, excellent shelf-life, simple storage and manufacturing. The systematic evolution of ligands by exponential enrichment (SELEX) is a method used to find aptamers that bind to the target with high affinities. The Cocco laboratory now has a library of aptamers that bind Nogo-66. In this poster, we will present functional assays and biophysical studies of the aptamers alone and bound to Nogo-66.</td>
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<td>Armando Bolnanos</td>
<td>College of the Desert</td>
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<td>Investigation of Possible Reactions between Alkali Metals and Cyclosiloxanes</td>
<td>Armando Bolanos, Jesus Jimenez, Salvador Hernandez, Haide Vela-Alvarez</td>
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<td>This projects is the study of possible reactions of Alkali metal ions with cyclosiloxane, specifically octamethylcyclohexasiloxane (D4) and decamethylcyclopentasiloxane (D5), common ingredients in several household beauty products. Crown ether are used to increase the solubility of insoluble substances, especially potassium ions. Since 18- Crown- 6 rings react with potassium ions and similarity between the structures of crown ether and cyclosiloxane, we hypothesize that cyclosiloxane may react similarly with metal ions ( Li+, K+, Cs+, Rb+). Our group mixed various concentrations of Alkali metals ions with the two cyclosiloxane and conducted flame test to confirm each reaction.</td>
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Large oil spills in the ocean are catastrophic events which pose a threat to the environment and marine life. This project was inspired by the Deepwater Horizon oil spill that occurred in April 2010, and is relevant to the recent Santa Barbara oil spill from May 2015. Currently, oil dispersants containing carbon-based surfactants are commonly used for clean-up. Surfactants help the oil disperse into droplets, encouraging more efficient bioremediation by microorganisms. Our objective is to synthesize novel phosphorus-based surfactants. Phosphorus is a vital element for life, so it is anticipated that phosphorus-based surfactants could increase the growth of bioremediating organisms and generate phosphates as bi-products as they decompose, thus providing a more environmentally friendly alternative. Our three-step synthetic route involves hypophosphite esters and a palladium-catalyzed hydrophosphinylation with bromoalkenes, followed by a reaction with a tertiary amine. The Dean-Stark method, which allows for the removal of water during esterification, has shown high yields of hypophosphite esters in step one of our project with 31P crude NMR yields ranging from 80-95% using primary and secondary alcohols such as heptanol and 2-pentanol, respectively, in toluene. Results from the Pd-catalyzed hydrophosphinylation between the 2-pentyl ester and 5-bromo-1-pentene show that our target product is synthesized with two conformations due to, we believe, the unselective addition of the bromoalkene onto the phosphorus center. Purification began with a work-up involving a series of washes, followed by flash chromatography, and TLC analysis of the collected fractions. Similar fractions were then combined, and two compounds were isolated. Proton and phosphorus NMR spectra reveal that the compounds obtained are most likely the expected 2 isomers of the 2-pentyl (5-bromo-pentyl) phosphinate. Further analysis with higher power NMR will be conducted to clearly identify the isolated compounds and the scope of the reaction will be expended to various classes of esters.
separate from the online survey to further provide opportunities for the selected students to elaborate on these factors. Quantitative data from the online survey were analyzed statistically, while interview audio recordings were transcribed and coded. Demographic survey results show that the majority of respondents were females, upperclassmen, and Asian, Hispanic, or White, respectively. 53% of all students reported having a job with 89% of those students working between 1 and 30 hours per week. When asked about academic performance, most students reported that they felt they had performed neither adequately nor poorly. 85% of students reported that they were confident that they would graduate with a STEM degree. Interview responses corroborated survey results. Results of this study will help ascertain the types of programs and practices that could alleviate the factors that affect student persistence in STEM majors.

Michael Baird
UC Riverside
37 Inorg/Mat Synthesis of Copper(II) Complexes with Potential for Antitumor Activity

Jack Eichler

The harmful side effects associated with the chemotherapeutic Cisplatin (cisdiamminedichloroplatinum(II)) and other platinum-based anticancer drugs have motivated research for new drugs based on other transition metals, including copper. Copper(II) is thought to be safer than other transition metal ions because it is regulated by homeostasis and has a range of biological functions. While copper can be toxic at high levels of exposure, it has a much larger permitted daily exposure (PDE) than platinum. The search for copper-based anticancer drugs is bolstered by research that has shown their effectiveness against several cancerous cell lines. The promising results of copper drugs and the potential for less severe side effects make it an excellent candidate as a cancer therapeutic. In an effort to build on recently developed copper-based anticancer compounds, I have targeted heteroleptic coordination complexes containing a bipyridine (bipy) and an L-tyrosine (tyr) ligand along with bis complexes containing two equivalents of bipy ligands. The syntheses of these complexes were performed by adding an equivalent of each appropriate ligand to a copper(II) ion. For the heteroleptic complexes, copper (II) nitrate was reacted with an equivalent of tyr and bipy. For the bis complexes, a \([(\text{bipy}) \text{CuCl}_2]\) complex was reacted with an equivalent of a bipy compound. \([(\text{4,4’-dimethylbipy})_2\text{CuCl}_2]\), \([(\text{6,6’-dimethylbipy})_2\text{CuCl}_2]\), \([(\text{4,4’-dimethylbipy})(\text{tyr})\text{CuNO}_3]\), and \([(\text{4,4’-dimethylbipy})(\text{tyr})\text{CuNO}_3]\) have been synthesized. Mass spectroscopy has confirmed that the ligands in each case are bonded to the copper center. X-ray crystallography is being processed for each of the compounds, although preliminary data indicates that the ligands have bonded as expected. Combustion analysis is still being processed for each compound. Future work will focus on determining the in vitro antitumor activity of the reported compounds against A549 lung cancer cells. These results will be compared with previous complexes in which copper was coordinated by one polydentate ligand. After these complexes are fully characterized and tested for cytotoxicity, similar copper complexes using alkyl substituted bipy and phen ligands will be synthesized. Promising results and the potential for improvement makes research in copper chemistry an exciting and ever-changing field. I hope to contribute by synthesizing new compounds and exploring their pathways in the search for a new anticancer drug.
The probing of periodic solids by coupled neutron scattering and dynamic pair distribution function (DPDF) analysis (collected at the Spallation Neutron Source at Oak Ridge National Lab) is a newly emerging and robust field of physical chemistry and condensed matter physics focused on elucidating molecular vibrations without the aid of expensive computational tools or the study of a large family of materials. Recently, group theoretical methods have been used to analyze DPDF and is currently being further developed for use in describing other periodic solids. Utilization of this technique to investigate the crystal structure of La₄Ru₂O₁₀ (LRO), a particularly interesting ruthenate compound which exhibits an orbital order transition at 160K, coincident with a structural shift from triclinic (P-1bar) to monoclinic (P-2 1/c), can provide a better understanding of highly correlated temperature dependent transitions in solids. Shown here are pair distribution function (PDF) refinements of LRO of neutron powder diffraction data that indicate that the local structure of LRO differs from the long range structures at temperatures 100K, 140K, 180K and 300K. PDF refinements glean information on the physical changes in spatial arrangement at lengths on the order of angstroms (10⁻⁹ m) intended on describing the crystalline structural changes responsible for the orbital order transition. These initial PDF studies are an integral first step to the analysis of the phonon structure of LRO via the DPDF as the local structure dictates the observable phonons and must be known before embarking on normal mode analysis.

Graphene, a two-dimensional carbon allotrope which forms a hexagonal lattice, is a highly promising material for future electronic and solar uses. Graphene is thin, transparent, flexible, has the ability to resist heat, and most importantly the ability to conduct electricity. Due to graphene’s lack of a band gap, there is a higher mobility of electrons within the lattice making it an excellent candidate for future electronics. By combining materials such as transition metal dichalcogenides (TMD) with graphene, we have the possibility to control the on/off state. Through chemical vapor deposition (CVD), we demonstrate the synthesis of thin layer graphene grown on top of the copper foil by utilizing argon, hydrogen, and methane. After the film has been formed, the underlayer of copper foil is etched away by using a mixture of ammonium persulfate and water in order to obtain the transparent layer of graphene. After the extraction of the metal underlayer, the graphene is transferred to a metal free substrate such as silicon dioxide (SiO₂) to be able to combine with other materials. Utilizing transferred graphene on SiO₂, monolayer TMD films such as molybdenum disulfide (MoS₂) can be combined with graphene for investigation of the heterostructure properties. Nanoparticles are unique in the fact that they have properties that make them applicable in many different areas such as catalysis, microelectronic, magnetic materials, information storage, etc. Nickel in particular has applications in catalyst and conducting magnetic material, but synthesis of metal nanoparticles such as nickel tend to be difficult due to its fast oxidizing nature. In this research we synthesized nickel nanoparticles using NiCl₂•6H₂O as the metal precursor, PVP as the capping agent, and Triethylene glycol as the reducing agent. As far as we know, this methodology has not been applied for the synthesis of Ni nanoparticles. Here, we tried various ratios of NiCl₂•6H₂O and
compared the size and the shape of the nanoparticles synthesized, which was done by means of Transmission Electron Microscopy. Data showed that the nanoparticles synthesized were on average 3.8 nm in diameter.

As computer processors continue to decrease in size and increase in power, they also are generating substantially more heat. As a result, there is need to keep pace with this advancement by the development of materials that can rid the processor of excess heat in order to ensure reliable operation. While graphene has garnered much attention over the past several years for its thermally and electrically conductive properties, it remains prohibitively expensive for use in a mass-market application. However, graphene oxide, a single layer of exfoliated graphite oxide, is considerably more cost effective and warrants exploration into its ability to conduct heat as a filler material for thermal interface materials. We prepared graphene oxide and tested, via Laser Flash Analysis, the effects it has on thermal interface materials thermal conductivity. We found that there was a positive correlation between the concentration of GO and the thermal conductivity measured. However at the higher concentrations there was not as much of an impact on the peak thermal conductivity, yet there was less sharp a decrease in the conductivity which warrants further investigation.

Ever since the initial development of ferrofluids in the 1960s, numerous methods have been investigated for fabricating iron oxide nanoparticles. A group of these methods rely on the slow bottom-up precipitation of iron oxide nanoparticles out of solution. Though past research suggests faster solution mixing rates could yield larger particles, the relationship between rate variations in the mixing process and the final qualities of the resultant ferrofluid is quantitatively unclear. Furthermore, while synthesis techniques may qualitatively caution against mixing that is too fast or too slow, the actual limits and range of rates that form viable nanoparticles is unknown. For many applications in sensitive fields like medicine and magnetic hyperthermia, consistent quality and stability of the ferrofluids fabricated is of paramount importance. Thus, this work aims at quantitatively exploring how different mixing rates of the precursor solutions affect the end properties of the ferrofluid and iron oxide nanoparticles. Characterization of the nanoparticles is done with X-ray diffraction (XRD) and transmission electron microscopy (TEM). For maximal heat generation capabilities, we wish to particularly identify rates that yield nanoparticle sizes between 10 and 14 nm in diameter.

Among various two-dimensional materials, transition metal dichalcogenides (TMDs) have attracted much interest because they provide tunable and direct-bandgap semiconducting properties at the single-layer limit. The presence of the direct bandgap in single-layer MoS₂, coupled with strong photoluminescence is of interest for optoelectronics. Through chemical vapor deposition (CVD) the synthesis of monolayer MoS₂ onto pre-patterned silicon dioxide (SiO₂) and sapphire substrates is possible. This method yields single domain islands and continuous films, which range from microns to millimeter scaled growth. Organized growth of monolayer MoS₂ is achieved onto lithographically...
Michelle Wurch, I-Hsi Lu and Ludwig Bartels

patterned substrates and sapphire. The growth of MoS$_2$ on sapphire allows for controlled orientation of the MoS$_2$ islands. Optical characterization such as Raman and photoluminescence spectroscopy verifies the integrity of the single-layer growth. This holds fundamental significance to the further development in nanoelectronics and optoelectronics.

David Ortega
CSULB 44
Inorg/Mat
Catalytic activity of Palladium nanoparticle-graphene oxide hybrids for fuel energy applications
Dr. Young-Seok Shon

Various processes and chemicals reactions have been studied in order to produce efficient and cost effective synthetic fuel. One such process is the Fischer-Tropsch Synthesis (FTS), which is a collection of chemical reactions which uses metal catalysts to convert CO and H$_2$ gas into hydrocarbon chains which can be used as an alternative fuel source. The FTS usually requires the use of Co, Rh, or Pt metals and high reaction temperature over 200 °C for successful fuel formation. Another well-known process is the methanol fuel synthesis from CO by metal-catalyzed hydrogenation. In this poster, ω-carboxylate-S-alkanethiolate-capped Pd-nanoparticles (PdNP), a hybrid of PdNP and graphene oxide (PdGO), and PdGO heated to 300 °C (PdGO 300) will be used as catalysts in the hydrogenation of various carbonyl compounds. It is anticipated that the catalyst PdGO 300, with the removal of thiolate ligands from the catalyst surface and the support by GO, might be able to convert aldehydes into alcohols, an intermediate in the Fischer-Tropsch Synthesis, due to the enhanced catalytic activity and stability of the PdGO hybrids. Synthesis of PdNP was performed involving a phase transfer of the ligand ω-carboxylate-S-alkanethiolate onto the nanoparticles using excess tetraoctylammonium bromide (TOAB). The synthesis of PdGO involved a 1:1 mixture of PdNP with GO. Hydrogenation of aldehydes was performed in D$_2$O using the Personal Reaction Station from J-KEM Scientific, with a constant flow of H$_2$ (g) via a balloon system. The reaction was monitored using H-NMR of the reaction mixtures ran at 3, 12, and 24 hours and the extent of hydrogenation was analyzed. The catalytic hydrogenation reactions performed at room temperature and atmospheric pressure for both propionaldehyde and acetaldehyde using PdNP, PdGO and PdGO 300, were all unsuccessful. Due to the acidic conditions produced by D$_2$O and GO, gem-diols of the respective aldehydes were produced. In order to increase the effectiveness of PdGO and PdGO 300 for the carbonyl hydrogenation, the reaction conditions including solvent, temperature, and pressure may need to be changed.

Eduardo Pardo
California State University, Long Beach 45
Inorg/Mat
Investigation of Graphene Halide in Sulfur Cathodes for Li/S batteries
Dr. Ted Yu Irene Diep, Ngoc Tran, Duy Do, John Duong, Jon Tafel, Christopher Lindley

Lithium sulfur rechargeable battery is a potential game-changer in rechargeable Lithium Battery technology. In addition to being very low cost due to the abundance of sulfur, it also has a higher theoretical specific capacity, helping the battery to last much longer. Incorporating carbon nanomaterials to prolong the life of lithium sulfur batteries has been a new, effective strategy in the last five years. A recent study has incorporated graphene oxide to encapsulate sulfur. Our project explores the use of graphene halides to replace graphene oxide, due to high cost of commercial graphene oxide. The graphene halides used in this study could be made through a simple, cheap ball-mill process. Our study shows that out of the halides, graphene-iodide performed the best. We believe this may be due to its higher surface area. The Li/S batteries made with graphene iodide performed remarkably well in cycle performance and capacity when compared to graphene oxide.
Nayeli Pelayo  
University of La Verne  
46 Inorg/Mat  
Pt Nanoparticle Synthesis  
Nayeli Pelayo  
Ricardo Morales  
Approximately one-fifth of everything we use either contains platinum or requires platinum in its manufacture. Platinum is highly used in many industrial applications and new uses for platinum are constantly developed. Some industrial uses of platinum include automobile catalyst, petroleum industry, jewelry, hard discs, electronics, medicine, etc. Due to the high demand and price elevation of platinum the development of high performance catalysis is important. My research consists of preparing tetrahedral-shaped platinum nanoparticles in colloidal solution from H2PtCl6. I am using PVP as the capping polymer via H2 reduction. The samples are characterized via TEM. Different concentration ratios are prepared for the characterization of tetrahedral-shaped Pt nanoparticles. So far a 1:1 and 1:2 Pt to PVP ratio have been conducted but more concentration ratios will be prepared for further analysis.

Grant Rose  
UCLA  
47 Inorg/Mat  
Conductive Polymer and Lithium Titanate-based Flexible Batteries  
Bruce Dunn  
Chun-Han Lai  
A flexible Li-ion battery was fabricated using P3HT polymer, carbon nanotubes, and activated carbon as the cathode and Lithium titanate and reduced graphene oxide as the anode. Composition, thickness, and annealing conditions were varied to produce the optimum physical and electrical properties, chiefly flexibility, durability, and capacity. The final goal is to produce batteries that can perform consistently under bending and be integrated with flexible photovoltaics. While LTO is a common Li-ion battery anode, the use of P3HT in cathodes has just begun to be explored. This research primarily aims to develop a composite cathode that combines the flexibility of conductive polymers with the higher capacities of traditional materials. Ideally, this will result in flexible materials systems that nevertheless show high capacity and rate for use in a variety of applications including wearable electronics. Half-cell testing revealed capacities of ~120 mAh/g for the anode and ~30 mAh/g for the cathode. The final cell used LiPF6 as the electrolyte, ITO film as the current collector, and was packaged in Kapton and Mylar tape. The first cells produced showed rapid breakdown of performance before reaching the ideal charging potential due to contact problems and unknown side reactions.

Zachary To  
University of California, Riverside  
48 Inorg/Mat  
Growth of Molybdenum Disulfide through Chemical Vapor Deposition on Silicon Dioxide Substrates  
Ludwig Bartels  
Molybdenum disulfide (MoS2) is a transition metal dichalcogenide (TMD) that exhibits a direct bandgap at the monolayer limit. Monolayer MoS2 is grown through the process of chemical vapor deposition (CVD) in a tube furnace. Powdered sulfur and molybdenum trioxide are used as the chalcogen and transition metal precursors, respectively. The precursors are placed into two separate alumina crucibles and are situated at specific regions in the tube furnace for growth. The furnace is slowly annealed to ~680°C and an inert gas, such as nitrogen, is used as a carrier gas to deposit the monolayer MoS2 onto the SiO2 substrate. Raman and photoluminescence spectroscopy are two characterization methods used to determine the quality of the grown materials. In monolayer form, MoS2 exhibits a direct bandgap at 1.85 eV, which has interesting optical properties, which can be applied to future electronics.

Michelle Wurch  
University of California  
49 Inorg/Mat  
Lithographically-Patterned Substrates for Seeding Monolayer MoS2  
Ludwig Bartels  
Edwin Preciado, I-Shi (Daniel) Lu, Brandon Davis, Wafer-scale growth of single-layer transition metal dichalcogenide (TMD) films, such as molybdenum disulfide (MoS2), is desirable for integration at the industrial level, however, results have shown that the resultant films are not single-crystalline. Grain boundaries, present in the films, lead to a decrease
Ingrid Liao, Sahar Naghibi, Aimee Martinez, Ludwig Bartels

in charge-carrier mobility. In this work, we propose the use of geometric, periodically-arrayed, topographic patterns to direct the island growth of MoS2 in specified areas. Because these islands are small, single-layer crystallites, they are the perfect size to fit into transistor channel regions. By lithographically patterning and etching SiO2 substrates in a cleanroom environment, we see preferential, homogeneous growth over a majority of the patterns. The growth has been characterized as monolayer using Raman, photoluminescence spectroscopy and atomic force microscopy (AFM).

Ongoing research for alternative anticancer drugs address the limitations of Cisplatin treatment. A major limitation to cisplatin therapy is development of drug resistance which leads to cancer progression. The investigation of copper (II) complexes potential anticancer agent is a growing area of research due to lower toxicity compared to platinum, and because there are numerous reports that have shown that copper (II) complexes have potent antitumor activity. Cancer cells often possess higher levels of GSH, hence the stability of metal based drugs is often correlated to redox stability. The research presented herein describes recently synthesized copper (II) complexes possessing polypyridyl ligands and the correlation between in vitro antitumor activity and redox stability.

As a growing number of chiral, non-racemic bioactive molecules flood the pharmaceutical industry, the importance of efficient enantioselective synthesis and purification of these compounds also increases. Enantioselective organocatalysis has emerged as a powerful synthetic tool complementary to traditional metal-containing catalytic transformations. Organocatalysis has several noteworthy advantages over traditional metal-containing catalysis. For example, some metals are highly toxic and may build up in biological systems over time, whereas there are typically fewer toxicity issues with organocatalysts. Also, organocatalysts can be tolerant of air and water, and the reactions are typically easy to perform. Taking this into account, we have developed the asymmetric Brønsted acid catalysis of the Friedel Crafts reaction of sesamol, a naturally occurring component of sesame oil that shares the chemical structure of many pharmaceutical compounds, with Boc-protected-benzaldimines using axially chiral bisphosphorylimides. Currently, bisphosphorylimides are underutilized despite their notable potential for catalysis. The chemical scaffold of bisphosphorylimides is highly structured and ordered, mimicking the active site of an enzyme. The long-term objective is the enantioselective synthesis of bioactive natural products, unnatural amino acids, and other various building blocks useful in the synthesis of chiral bioactive molecules.

Previous studies have confirmed that Wnt/beta-catenin is a conserved signal transduction pathway that contributes to several biological processes essential for cancer initiation and development. Recent data suggests pre-cancerous cells express the protein beta-catenin when they become cancerous cells by Wnt stabilization and nuclear localization. Several proteins participate in a multiprotein "destruction complex" that targets the proto-oncogene beta-catenin for ubiquitin-mediated proteolysis. To inhibit beta-catenin formation, a library of small molecules were designed to target inhibition of the destruction complex activity. An important area of investigation involves
analyzing how each compound targets beta-catenin levels to influence cell proliferation. We hypothesize that small molecules that reduce beta-catenin levels can potentially function as anti-cancer drugs. To test this hypothesis, various small molecules with modified structures were synthesized and purified. To assess and quantify cell proliferation, the fluorescence-based CyQuant assay was used to measure DNA content. The Hela cell lines were maintained for 24 hours containing 10 μM of each respective drug. Beta-catenin protein levels in the cells were accomplished with the TOPflash assay. Our recent findings show that several molecules that contain a specific structural motif show promising results to reduce beta-catenin levels. For instance, small molecules with long alkyl chain substituents with a polar end have consistently shown better results than those with a smaller alkyl chain. Recent studies have also indicated that a commonly used anthelmintic showed potential as an anti-cancer drug and lowered beta-catenin levels dramatically. Structural analysis of this anthelmintic shows a greater rigidity not present in our original drug library. A next generation of drug compounds will therefore focus on molecules with similar functionalities but greater rigidity. Docking studies will compare the results of the original drugs to those of the new series to determine the best method to increase phosphorylation of beta-catenin, thereby generating more potent anti-cancer drugs.
prepare different peptide-based polymers with different properties and structure. The monomer, dimethylaminopropyl methacrylamide (DMAPMA), was polymerized with microwave-assisted RAFT and conventional heating, and then characterized by nuclear magnetic resonance (NMR). The DMAPMA was used to determine optimal conditions for more complex and expensive peptide monomers. The results of conventional and microwave heating were compared, and observed that microwave heating was more efficient. Based on these results, the polymerization of peptide monomers via microwave-assisted RAFT is further encouraged and offers an opportunity to further expand interest in peptide-based polymers composed of different compositions and structures with a greener chemistry outlook.

Iris Marquez
California State University, Long Beach

Kensaku Nakayama, Ph. D
Trina Tran, Jeanette Gonzalez, and Jason Schwans, Ph. D

I. Organic Inhibition Study of Butyrylcholinesterase with Optically Active Butyl Cholinyl Phenyl Phosphate

Kensaku Nakayama, Ph. D
Trina Tran, Jeanette Gonzalez, and Jason Schwans, Ph. D

The enzyme class known as the cholinesterases exists in two forms: the butyrylcholinesterases (BChE) and acetylcholinesterases (AChE). Both classes are capable of hydrolyzing the neural transmitter acetylcholine. Among those who suffer from Alzheimer’s disease (AD), the activity of BChE is found at levels 40–90% above normal, while AChE is observed to decrease 45% from normal levels. BChE activity steadily rises for AD patients with increasing severity of the disease. The imbalance of cholinesterases in the brain of a patient with AD leads to memory loss and neurocognitive dysfunction. Thus, compounds that are selective inhibitors of BChE are receiving more attention recently as potential therapeutics for the treatment of cognitive loss associated with AD. In our group, a wide structural range of organophosphates are being investigated as BChE-selective inhibitors. In this study, we investigated optically active organophosphorus compounds with a cholinyl group as potential BChE inhibitors.

We first prepared (S)-butyl cholinyl phenyl phosphate (46.2% ee) and determined it to possess a Ki value of 7.2 µM. A racemic mixture of butyl cholinyl phenyl phosphate was found to afford a Ki value of 10.6 µM. This poster describes the synthesis of (R)-butyl cholinyl phenyl phosphate for further Ki studies to establish the enzyme’s enantioselectivity toward the two enantiomeric inhibitors. The results of these studies will help identify the precise three-dimensional interactions between BChE and the inhibitors, which will allow us to design future chiral inhibitors.

Nikolay Maslov
CSU San Bernardino

Developing chemical inhibitors to investigate the function of falcilysin, an essential malarial protease

Jeremy Mallari
Nikolay Maslov, Hannah Feijzic, Cindee Nguyen, Bradley Kuwahara, Obiel Hernandez, Teodulo Crisanto, Ruby Aispuro

The protozoan parasite Plasmodium falciparum is the cause of over 500,000 cases of human malaria per year, mostly occurring in South Africa. All clinical symptoms of the disease are caused by parasite infection of the host’s red blood cells (RBCs). Falcilysin (FLN) is a metalloprotease expressed by the parasite—it is necessary for the development of the P. falciparum in the host RBC, but its function is poorly understood. We are developing competitive inhibitors of FLN based on a sulfonyl piperazine hydroxamic acid scaffold. Previous studies in our lab have shown that this class of compounds has good inhibitory activity against both recombinant FLN and cultured P. falciparum. We are currently testing the effects of different substituents on inhibitor potency in order to optimize this scaffold against FLN. Our team synthesized inhibitors through a 4-step route and purified them by a combination of liquid extraction and flash chromatography. Compound structures were confirmed by
NMR spectroscopy. In future experiments, we will use these inhibitors to block FLN activity in cultured *P. falciparum*. This will enable us to study FLN-null phenotypes and to better understand the biological role of FLN.

Transition metals and their complexes have been extensively employed in catalysis due to their high reactivity and selectivity. Best known examples are rhodium-based Wilkinson's catalyst and various palladium complexes, which are used in many reactions such as hydrogenation, isomerization, decarboxylation, etc. Recently, a novel discovery of palladium nanoparticle (PdNP) catalysts has proposed that this new group of catalay has several advantages such as less ligand dissociation and easier separation over the currently available ones. Our laboratory has also shown that the reactivity and selectivity of alkanethiolate-capped PdNP in certain environment was influenced by the interaction between the substrates and the ligands on the metal surface. In this study, octanethiolate-capped palladium nanoparticle catalysts (C8PdNP) are synthesized and examined for i) the chemoselective hydrogenation of styrene derivatives with reducible functional groups such as nitro, fluoro, chloro, and bromo and ii) the cis-trans isomerization of stilbene derivatives. The obtained results thus far indicated that C8PdNP has an excellent chemoselectivity for terminal alkene groups during the hydrogenation of styrene derivatives comparable to Wilkinson's catalyst and Pd complexes. Additionally, the cis-trans isomerization of stilbene derivatives could be further optimized by increasing the temperature and minimizing the amount of solvent, surpassing the activity and selectivity of most other transition metal catalysts used for this purpose. Considering the mild reaction conditions and the easy separation of PdNP catalysts, these features of highly selective catalytic properties of C8PdNP might help to discover novel synthetic routes for functional materials and fine chemicals.

All medications that have been developed for the treatment of Alzheimer's disease—the most prevalent form of dementia in the U.S.—inhibit the neurotransmitter-degrading enzyme acetylcholinesterase (AChE) and butyrylcholinesterase (BuChE). Recent studies against acetylcholinesterase have suggested bisphosphates as potential bivalent inhibitors. An attractive feature of organophosphate inhibitors is that the size of substituents can be readily varied within an organophosphate scaffold. Based on our earlier studies with dialkyl phenyl phosphates as BuChE-specific inhibitors, we synthesized and assayed a library of tetraalkyl bisphosphates and a few representative bisthiophosphates as bivalent inhibitors. These bivalent organophosphates connect two phosphate moieties through a linker chain of varying length. The inhibitory concentration 50% (IC50) values were determined for each analog. To evaluate if the analogs were selective for BuChE, the inhibitory properties of the analogs against both BuChE and AChE were determined. All molecules tested were selective for BuChE and lengthening of the alkyl chains from ethyl to butyl generally increased potency against BuChE. The substitution of two oxygen atoms of the linker chain with sulfur atoms led to an approximately 100-fold more potent inhibitor in the tetrabutyl scaffold compared to the tetraethyl scaffold, suggesting the longer alkyl chains are necessary for differences in binding.
interactions between the bisphosphates and bisthiophosphates. These results identify new selective and potent BuChE inhibitors. Current work involves the synthesis of a library of bisthiophosphate analogs to uncover the molecular factors responsible for the increased inhibition.

In Alzheimer’s Diseases (AD) patients, there is an increase in butyrylcholinesterase (BChE) activity which hydrolyzes the neurotransmitter, acetylcholine. This increase in hydrolytic activity leads to abnormally low concentrations of acetylcholine which causes the symptoms of AD, decline in cognitive, behavioral, and global functioning. The goal of our project is to synthesize a library of choline-containing organophosphates with varying alkyl chains in order to evaluate their inhibitory effects against BChE. The cholinyl organophosphate inhibitors were derived from alkyl diphenyl phosphates which are synthesized from commercially available diphenyl chlorophosphates. Previous cholinesterase inhibitors we studied lacked the cholinyl group and instead had a phenyl group and two alkyl substituents. Introduction of the cholinyl group to the organophosphate inhibitors was done to mimic the binding interaction between BChE and acetylcholine. This poster will report on the effects of varying the alkyl group chain length as well as introducing methyl groups in various positions on the phenyl ring on BChE inhibition. We have found that as the alkyl chain length increases, the inhibitory potency increases as well.

Bioluminescence is an imaging technique used to non-invasively image biological processes in vivo. This process utilizes an enzyme (luciferase), which catalyzes the oxidation of a small molecule substrate (luciferin) resulting in emission of a photon of light. Bioluminescence is useful for macroscopic imaging small mammals such as mice due to its inherent low background. Previous work has been limited to using only naturally occurring luciferase:luciferin systems in bioluminescence imaging. Native luciferase systems are limited to only two commonly occurring, orthogonal systems. I am working on developing new luciferase enzymes which utilize novel luciferin analogs in order to expand the number of luciferase:luciferin pairs. A region of the luciferase gene, coding for amino acid phenylalanine, was targeted. We found that a site directed mutation in this region yielded emission of a photon of light, two orders of magnitude times more than the wild type enzyme luciferase when bounded to luciferin. Semi-rational techniques were used to design new luciferase libraries; these include a combination of random mutagenesis and site directed mutagenesis. The mutant enzymes were evaluated through screening for improved light emission. Generating new luciferase:luciferin pairs will broaden the utilization of bioluminescence imaging in order to improve visualization of cellular processes in whole organisms.

Boron trifluoride (BF₃) combines with water very readily and forms the stable BF₃·hydrate (BF₃·H₂O) complex which has been shown to be superacidic. Many of the reactions BF₃·hydrate catalyzes is by superelectrophilic activation, the further protonation of non-bonding electron pairs of a monocation that lead to dications which are substantially more reactive than their parent monocation. We are currently studying BF₃·hydrate as a potential replacement for trifluoromethanesulfonic acid (triflic acid), the superacid of choice for studying superacid catalyzed
reactions that proceed by superelectrophilic activation. A major drawback of triflic acid is its expense, which limits the opportunity to conduct many of these novel transformations on a larger scale. In comparison, BF$_3$ monohydrate is cheap since it is readily available by bubbling inexpensive BF$_3$ gas into water. We will present our preliminary results on the superacid catalyzed condensation reactions of 2-carboxybenzaldehyde with arenes catalyzed by BF$_3$ monohydrate and compare the reactivity with triflic acid.

The pragmatic application of peptide therapeutics is a novel field, delegating advantageous characteristics such as high specificity, low toxicity, and relatively high biocompatibility. While peptide-based drugs allocate highly beneficial therapeutic effects, several debilitations exist, such as issues related to enzymatic degradation. Studies have shown that covalent attachment of a saccharide will essentially allot an increased circulation half-life, solubility of the peptide moiety, and biocompatibility. Our group has synthesized a novel hybrid of biomaterials, that constitute a starch, a peptide, and a linker molecule with reactive thiols, dibromomaleimide, azide and alkyne moieties. Each component was prepared separately and covalently attached through thiol conjugation and a copper(I)-catalyzed alkyne-azide cycloaddition “click” reaction. In previous studies, the starch would be conjugated to the peptide; these initial experiments posed several challenges in NMR characterization due to the relatively prodigious size of the starch moiety compared to the tripeptide. To circumvent these issues, we investigated the utility of the fluorine-based small molecule linker for thiol exchange analyzed by $^{19}$F NMR. Our prospective work includes the conjugation of a peptide to our starch-linker complex. We hope to utilize these hybrid conjugates for peptide delivery systems, or as therapeutic coating on biomedical devices.

In order to expand the toolbox of bioluminescence, a large amount of luciferin analogs is required. In past years, our group has reported the synthesis and emission properties of heterocyclic luciferins with benzimidazole and imidazoline. Previously, I have synthesized a brominated analog of D-luciferin and a series of brominated luciferin precursors. My final aim is to generate a new series of sterically- and electronically- modified luciferin analogues to be used for multicomponent imaging.
Tachysterol is an important factor in the vitamin D photo equilibrium. Although it has long been known that tachysterol and its derivatives have several biological functions in the body, its photochemical reactivity and role in the photochemical equilibrium is not well understood. It can be expected that tachysterol's photochemistry is determined by the presence of rotational conformers. To study the equilibrium of its conformers, we carry out replica-exchange molecular dynamics. Based on the generated Boltzmann ensemble, we simulate its absorption spectrum and assess its photochemical reactivity by real time non-adiabatic dynamics based on time-dependent density functional theory. We find that the broad absorption spectrum arises from mainly four different ground state rotamers. We see a strong dependency of reaction channels on the dihedral angle conformation. Only cis-E-cis rotamers have been found to produce previtamin D via double bond isomerization. Tachysterol's large extinction coefficient and low previtamin D quantum yield suggest that it plays a major role in the quenching of previtamin D production upon extended sun exposure.

Nuclear Magnetic Resonance (NMR) is a very important and useful technique in science and medicine, forming the basis of several Nobel prize winning discoveries and inventions, including the life-saving Magnetic Resonance Imaging (MRI) technology. NMR can probe into the nuclei of almost all atoms and inform us about molecular structures, motions, proximities of atoms, and rates of reactions.

Deuterium has a spin quantum number of 1 and a distorted nuclear charge density which creates a quadrupole moment which interacts with the electrical field gradients around the nucleus. This quadrupolar interaction dominates the solid state deuterium NMR Spectra. Deuterium line shapes are very sensitive to molecular motion and provide valuable information about them.

We are investigating the molecular motion of D2O in Gypsum where presence of water in Gypsum causes it to have fire retardants properties. Using algorithms in Dr. Alan Benesi's new book "A Primer in NMR Theory with Calculations in Mathematica" we are simulating the rotation rates of deuterium nuclei for water in gypsum. When compared to the experimental spectrum our results indicate that the D2O in Gypsum at ambient temperature performs a 2 site hop about the bisector angle of 54.80 at the rate of 107Hz or higher. The Quadrupole Coupling Constant and the asymmetry parameter used are 120KHz and 0 respectively.
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|                       |                                                  |        |                                                                       | Monolayer transition metal dichalcogenides (TMDs) are semiconducting materials with desirable optical and electrical properties, making them great candidates for microelectronics and spintronics. Unlike graphene, TMDs such as Tungsten disulfide (WS2) and molybdenum disulfide (MoS2) have the unique property of transitioning from an indirect to a direct bandgap at the single-layer limit. Chemical vapor deposition (CVD) is utilized to synthesize monolayer WS2 and MoS2 with direct bandgaps of 1.95eV and 1.85eV respectively, over several types of silicon dioxide substrates. The TMD growth and quality is characterized by means of Raman and photoluminescence (PL) spectroscopy. The photo-induced electrocyclic ring-opening reaction of 1,3-cyclohexadiene (CHD) to 1,3,5-hexatriene in an argon matrix is studied from a theoretical/computational perspective. The study is performed with ab initio non-adiabatic molecular dynamics based on time-dependent density functional theory. Particularly, we are interested in the effects that argon matrix has on the photochemical dynamics and subsequent hot ground state reactions. Due to the fully quantum mechanical description of the system we are able to describe the electronic effects as well as the steric effects of the matrix on CHD. A main focus of our study is to describe energy dissipation from the initially photoexcited CHD to the surrounding argon atoms. The study serves as a model system for photoreactions in the condensed phase. With the removal of a single atom from a small cluster, a noticeable difference is seen in the generated optical spectra. Using analytical Time Dependent Density Functional Theory (TDDFT), excitation energies of increasing sizes of gold clusters, alongside their truncated counterparts, were calculated. Fast Fourier Transform (FFT) was conducted on these results to produce optical spectra-the physical observable. The ratios of optical spectra for each set of gold clusters were superimposed, and a change in the absorbance was visible. Nuclear Magnetic Resonance (NMR) is a very important and useful technique in science and medicine, forming the basis of several Nobel prize winning discoveries and inventions, including the life-saving Magnetic Resonance Imaging (MRI) technology. NMR can probe into the nuclei of almost all atoms and inform us about molecular structures, motions, proximities of atoms, and rates of reactions. We are investigating the molecular motion of D2O in Gypsum where presence of water in Gypsum causes it to have fire retardants properties. Using algorithms in Dr. Alan Benesi’s new book "A Primer
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Deuterium has a spin quantum number of 1 and a distorted nuclear charge density which creates a quadrupole moment which interacts with the electrical field gradients around the nucleus. This quadrupolar interaction dominates the solid state deuterium NMR Spectra. Deuterium line shapes are very sensitive to molecular motion and provide valuable information about them.

In the past years we studied zeolites as a possible medium for enriching the enantiomeric excess of solutions. Zeolite lattices being achiral, do not prefer one enantiomer over the other, and adsorb both enantiomers equally well. However, if the D- and L- enantiomers adsorb together as a heterodimer, the enantiomeric excess of the solution they leave behind is augmented. We used NMR to explore the adsorption behaviors of D-, L- and DL- N-acetyl Leucine, Alanine and Methionine into Zeolite NaY. The solid state NMR spectra of the pure D- and L- acetyl Leucine showed the same results as the racemic mixture of N-acetyl-DL-Leucine, indicating a preference to form microcrystals of pure D and L forms. In contrast differences in the solid state NMR spectra are observed for N-Acetyl -DL-Methionine and N-acetyl-DL-Alanine from their pure enantiomers. This implied that both form a mixed crystal. However when adsorbed onto the zeolite, N-Acetyl Methionine and N-acetyl-Alanine exhibit the same behavior as its Leucine counterpart indicating that they are adsorbed as homodimers. NMR line widths of all compounds show a 10 fold increase when adsorbed in NaY indicating restricted molecular motion. Recently, in order to investigate this behavior further we decided to study the same set of systems with molecular modelling. We will present the results of computer simulations regarding the dynamics and energetics of the enantiomer-zeolite interactions.

An initial brown carbon mixture was reacted by combining 0.5 molar glyoxal and 0.5 molar glycine. After 6 months of reacting, the brown carbon solution was used to make two additional solutions. The second solution was made from the initial brown carbon solution and 0.5 molar hydrogen peroxide and the third solution was made identical to the second but also was treated with 7 hours photolysis. By analyzing the brown carbon solution without hydrogen peroxide or photolysis and then additional solutions under conditions with only the addition of hydrogen peroxide and then the addition of hydrogen peroxide and photolysis, the effects of each condition on the refractive index can be evaluated. It is important to study the optical properties of organic aerosols to better understand the effects they have on the atmosphere, environment and global climate conditions. Brown carbon is likely to absorb, contributing to the global climate change. The three different brown carbon solutions were analyzed using cavity ringdown spectroscopy. The measured refractive indices were determined by minimizing the difference between the measured extinction efficiency and the...
Mie calculated extinction efficiency. More experimentation and analysis is needed to explain the optical properties of brown carbon in the atmosphere. The refractive index of brown carbon with hydrogen peroxide is affected when it undergoes photolysis. Preliminary results suggest that the addition of hydrogen peroxide and photolysis with an ultraviolet lamp reduces $k$, the imaginary part of the refractive index. The decrease in absorption of the aqueous solution of brown carbon with hydrogen peroxide and photolysis is consistent with the decrease in $k$, the imaginary part of refractive index.

Large oil spills in the ocean are catastrophic events, which pose a great threat to marine life and the environment. Our project was influenced by the Deep Water Horizon Oil Spill in April 2010, and the recent Santa Barbara Oil Spill in May 2015. Releasing a carbon-based solvent/surfactant mixture (dispersant) into the ocean allows for bioremediation while decomposing the toxic compounds found in oil. Our objective is to synthesize a phosphorous-based surfactant due to their environmentally friendly properties. Our three-step synthetic route involves hypophosphite esters and a palladium-catalyzed hydrophosphinylation with bromoalkenes, followed by reaction with a trimethylamine. We have established Step-1 of our three-step process by synthesizing long-chain hypophosphite esters, employing two different methodologies: transesterification and direct esterification. The direct esterification method only utilizes toluene as a solvent, in comparison to the transesterification method that involves a broader solvent scope (Acetonitrile, Hexane, Toluene, Cyclohexane) along with a silicon derivative. Percent yields from both routes have been compared. Primary alcohols do not display any methodology preference; however, secondary alcohols, such as cyclohexanol, have resulted in favoring the direct esterification, most likely due to steric hindrance. Transesterification gave higher percent yields with the one-pot two-step method than the one-pot one-step because it allows for a complete formation of the intermediate ethyl ester. The Dean-Stark synthesis has provided high percent yields for the formation of long-chain hypophosphite esters, allowing us to continue with Step 2, the Pd-catalyzed hydrophosphinylation with bromoalkenes.

Biological activity in the anoxic sediments of the Salton Sea marshes produce and release hydrogen sulfide ($\text{H}_2\text{S}$). As the geochemistry of sulfur and selenium are similar, it is postulated that hydrogen selenide ($\text{H}_2\text{Se}$) could also form in, and escape, from the marshes. Previous work at College of the Desert has investigated the occurrence of $\text{H}_2\text{Se}$ near the Salton Sea. Specifically, there is documented evidence of $\text{H}_2\text{S}$, which is probably "patchy" of $\text{H}_2\text{Se}$, is released from the marshes. Previous work at College of the Desert has investigated the occurrence of $\text{H}_2\text{Se}$ near the Salton Sea. Specifically, there is documented evidence of $\text{H}_2\text{S}$, which is probably "patchy" of $\text{H}_2\text{Se}$, is released from the marshes. A reasonable approach to find $\text{H}_2\text{Se}$ could be to find the location of $\text{H}_2\text{S}$ release. Their release point could serve as a location to sample for $\text{H}_2\text{Se}$. Our group has designed and built a $\text{H}_2\text{S}$ sensor equipped drone which, when deployed in the marshy areas of the Salton Sea, could pin point $\text{H}_2\text{S}$ sources. These sources then could be analyzed for $\text{H}_2\text{Se}$ specific collection technology to confirm the proposed parallel release of $\text{H}_2\text{S}$ and $\text{H}_2\text{Se}$.
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<td>In our efforts to progress anti-tumor Structure-Activity Relationship studies of caged garcinia xanthones, the syntheses of analogs were prepared and optimized. Through the utility of a range of starting materials and reagents, we were successful in developing total synthetic reaction pathways that add functional groups on the A-ring of the pharmacophore backbone – cluvenone. These model complexes provide insight to the synthesis of highly-functionalized heterocyclic xanthones, and Claisen/Diels-Alder cascade reaction. The synthetic findings are showcased, and model analogs have been characterized via multinuclear magnetic resonance spectroscopy and X-ray crystallography.</td>
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<td>Microfluidic fuel cells (MFCs) utilize co-laminar flow to maintain separation between fuel and oxidant streams in place of a polymer membrane. However, parasitic energy losses due to the requirement of continuous flow present significant challenges to the implementation of such fuel cells. Recently, Esquivel, et al, demonstrated the first MFC on paper using methanol as fuel and air as oxidant. Such a paper MFC takes advantage of the capillary action of paper to induce and maintain laminar flow without any requirement of external pumping. Our paper MFC device produced a maximum power density of 2 mW/mg Pd with 30% hydrogen peroxide, and 1 mW/mg Pd with 3% hydrogen peroxide; in both cases 5 M potassium formate was used as the fuel. A maximum power density of 2.5 mW/mg Pd was achieved with 10 M potassium formate. A hybrid device using formate oxidation and silver ion reduction resulted in significantly higher power density, 18 mW/mg Pd. The recent increase in atmospheric carbon dioxide is concerning due to its impact on global climate. However, state of the art alternative energy has limited availability, while storage and transport of electrical energy is challenging. One solution to these challenges is to store electrical energy in liquid fuels for on-demand conversion to energy. Formate is a promising liquid for energy storage because its conversion from carbon dioxide only requires reduction without the formation of a carbon-carbon bond; this is possible through electrochemical reduction on metals such as Sn. We have reduced sodium carbonate solution to sodium formate using a tin electrode in a three electrode cell and a two electrode cell using a potentiostat to maintain potential control. It is known that carbon dioxide can be reduced on tin to a primary product of formate because the carbon dioxide does not strongly adsorb to the tin surface. In the case of other metals, such as zinc, carbon dioxide adsorbs strongly to the surface and the primary product is CO. We then transitioned to the electrolysis and fuel cell device so that formate is regenerated using solar power.</td>
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<td>Brenna C. Biggs, Chau Hua, Christopher Nguyen, Salvador Mayoral</td>
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<td>The recent increase in atmospheric carbon dioxide is concerning due to its impact on global climate. However, state of the art alternative energy has limited availability, while storage and transport of electrical energy is challenging. One solution to these challenges is to store electrical energy in liquid fuels for on-demand conversion to energy. Formate is a promising liquid for energy storage because its conversion from carbon dioxide only requires reduction without the formation of a carbon-carbon bond; this is possible through electrochemical reduction on metals such as Sn. We have reduced sodium carbonate solution to sodium formate using a tin electrode in a three electrode cell and a two electrode cell using a potentiostat to maintain potential control. It is known that carbon dioxide can be reduced on tin to a primary product of formate because the carbon dioxide does not strongly adsorb to the tin surface. In the case of other metals, such as zinc, carbon dioxide adsorbs strongly to the surface and the primary product is CO. We then transitioned to the electrolysis and fuel cell device so that formate is regenerated using solar power.</td>
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Oxygenated hydrocarbons are ubiquitous in the atmosphere with levels ranging from low ppt (acetaldehyde) to low ppb (methanol). As an OH sink and an atmospheric HOx and ozone source, oxygenated hydrocarbons have a direct impact on the oxidative capacity of the atmosphere. The oceans are one of the largest sources of uncertainty in current atmospheric budget estimates of these species. A better understanding of the processes that produce and destroy these species in seawater would improve our understanding of the role of the oceans in cycling these species into or out of the atmosphere. We have measured the degradation rate of ethanol in unfiltered and filtered southern California coastal waters. Rates were determined by following the concentrations of D-6 labelled ethanol in spiked (nM levels) seawater in 100ml glass syringes as a function of time. Concentrations were determined by isotope dilution purge and trap gas chromatography mass spectrometry. Rates in 0.2um filtered seawater were not measurable. Degradation rates in unfiltered seawater were first order and ranged from 0.046 to 0.32 hr$^{-1}$. Bacteria levels were also measured in all samples. Ethanol degradation rates scale with bacteria levels. Variability as a function of time, rainfall and other water quality parameters will be discussed.

Mercury is a known neurochemical toxin to human health. Previous studies have been done on mercury concentrations in cigarettes but very few recent ones in the US. Nearly 17.8% of adults in the United States smoke cigarettes today making the mercury concentration in tobacco of possible importance to human health. This study is intended to examine cigarettes as a viable method of Mercury ingestion in humans. The top two brands sold in the US were studied, including Marlboro and Newport; both regular and menthol varieties. American Spirit Teal cigarettes were also studied as an organic branded cigarette. This data was gathered through the techniques of Thermal Decomposition, Catalytic Conversion, Gold Amalgamation, and Atomic Absorption Spectroscopy. A previous study done on mercury in cigarettes in 2008 found an average of 13 (±1.3) ppb (ng/g) Hg in a whole cigarette out of 30 cigarettes on three different non-specified brands. When compared to this study out of 302 samples (50 cigarettes) we found a 19% difference with an average value of 15.5 (±0.5) ppb Hg. The average concentrations in ppb found in the Marlboro, Newport, Newport Menthols, and American Spirit were found to be 16.4 (±2.5), 13.8 (±2.7), 13.5 (±1.7), and 18.3 (±2.9) respectively. Decorative metallic bands on the American Spirit and Newport Non-Menthol cigarettes were found to have anomalous concentrations of 170.6 (±51.9) and 408 (±274.5) ppb Hg. The implications of these results could be used as a possible indicator for climate change, or it could be used as evidence of manufacturing reform. Further studies on human Hg level changes after smoking cigarettes should be conducted to see if cigarette smoking is a reasonable pathway for mercury accumulation. An important novel study could be to analyze the mercury concentrations of electronic cigarettes as their popularity has been on the rise.

A nanometer-sized Pt electrode is becoming a routine tool in nano-electrochemistry research, but, the dissolution of Pt in aqueous solution is quite common and the rate of the dissolution of Pt is related to the current density on the electrode. Measurement on a nanometer-sized Pt electrode in...
solution containing very dilute electroactive species can effectively decrease the current on the electrode and thus decrease the extent of the dissolution of Pt electrode. So far, a commercial potentiostat which has a peak-peak noise of less than 10 fA is not common. In this paper, a homemade potentiostat, which has a peak-peak noise of less than 5 fA, has been made. By using the instrument, voltammograms with a limiting current of less than 20 fA can be obtained on a nanometer-sized electrode in solution containing micro molar Ferrocenemethanol. Our results show that the standard rate constant of the oxidation of Ferrocenemethanol measured in micro molar Ferrocenemethanol solution is a little greater than that measured in mili molar Ferrocenemethanol solution, which indicates that kinetic parameter may be affected by the amount of electroactive molecules being measured.

Mitragynine is a natural component that is found in the Kratom leaves. Mitragynine has been used by many Asian countries as an herbal supplement over the centuries. It is commonly consumed in the form of tea beverage that is made from the leaves of Kratom. Although mitragynine is not an opioid, it affects the same receptors as an opioid does, but at a lower affinity. Mitragynine has been used as an analgesic to stop inflammation and diarrhea. Since mitragynine affects the same receptors as opioids, it is also used for treatment of opioid and alcohol withdrawal in order to counter the withdrawal symptoms. In some countries, Kratom leaves tea is being used as the base to prepare the “Kratom Cocktails that contains a mixture of other drugs including codeine, alcohol, and various opioids. It is currently up for debate as to whether or not to add mitragynine to one of the DEA lists. More tests must be done to find out the long-term effects of mitragynine use. The purpose of this study was to extract mitragynine from Kratom plants and determine the corresponding concentration of mitragynine. A liquid-liquid extraction method is used to extract mitragynine and the extraction efficiency was determined. Mitragynine was detected with a reverse-phase high performance liquid chromatography at 223 nm. The mobile phase consists of a mixture of acetonitrile and 0.05% formic acid (50:50 v/v) adjusted to pH = 5. Peroxisome proliferator-activated receptor gamma coactivator 1-alpha (PGC-1 alpha) a protein involved in maintaining glucose levels is modified by protein arginine methyltransferase 1 (PRMT1). In particular, PGC-1 alpha contains arginine residues that become methylated and are implicated in the pathogenesis of obesity and diabetes. PRMT1 is one of nine mammalian enzymes that transfer methyl groups to proteins. In this study, we bacterially expressed glutathione S-transferase-tagged (GST)-PRMT1 for the purpose of carrying out methylation reactions on PGC-1 alpha. Optimization was achieved with BL21 E. Coli cells using 1M Isopropyl beta-D-1 thiogalactopyranoside (IPTG) and a 5 hour induction. After expression, the cells were lysed by sonication and GST-PRMT1 was batch purified and eluted with 1M of glutathione. GST-PRMT1 was then resolved on a 12% trisglycine SDS PAGE gel resulting in a band corresponding to the molecular weight of 71 kDa, indicative of GST-PRMT1. These results indicate that these conditions are optimal for GST-PRMT1 expression and purification. We next plan to express GST-PGC-1 alpha which has a molecular weight of 98 kDa, by
similar methods and conditions. Upon expression and purification of both PRMT1 and PGC-1alpha, a methylation reaction between these two proteins will be carried out in order to identify the arginine residues that become methylated in PGC-1alpha and for further studies into the mechanism of the development of diabetes and obesity.

The metabolomics of microorganisms that inhabit spacecraft assembly facilities are important facets to planetary protection and astrobiology. As per NASA policy, the cleanliness of all Mars-destined spacecraft (and associated facilities) must be carefully controlled to reduce microbial contamination and to minimize the probability of detecting false positive signals of life during exploration. Despite these robust policies, however, spacecraft assembly facilities harbor a low abundant yet diverse inventory of microorganisms, with the Acinetobacter being among the most abundant bacteria. In this presentation, we will provide molecular and biological evidence that Acinetobacter radioresistens 50v1, which was isolated from the preflight Mars Odyssey orbiter, metabolizes/degrades spacecraft cleaning reagents such as ethanol, 2-propanol, and Kleenol-30. Gas chromatography-mass spectrometry (GC-MS) studies confirm that ethanol is a sole carbon source under minimal conditions, with 13C-labeled ethanol being incorporated into metabolites such as TCA/glyoxylate cycle intermediates, amino acids, monosaccharides, and disaccharides. Further, mixtures of 2-propanol and ethanol manifest reproducible changes in glutamate and aspartate abundances, which suggests metabolic adjustments to osmotic stress. However, biochemical analyses on cell-free extracts support the enzymatic oxidation of 2-propanol by a membrane-bound and NAD+/PQQ-dependent alcohol dehydrogenase. Additionally, preliminary GC-MS analyses suggest that Kleenol-30 is degraded by A. radioresistens 50v1 when grown in ethanol mixtures. Therefore, these combined results suggest that the spacecraft cleaning reagents serve as carbon and energy sources and, hence, influence the microbial ecology dynamics within the spacecraft assembly facilities.

The extremotolerance of forward contaminants are critical measurements for planetary protection and astrobiology, as the microorganisms that inhabit spacecraft may contaminate extraterrestrial environments and compromise the integrity of life detection missions. Despite the robust cleaning protocols utilized during spacecraft assembly, spacecraft harbor a low abundant yet diverse inventory of microorganisms. The Acinetobacter are among the most abundant bacteria within these communities, potentially due to metabolism of the spacecraft cleaning reagents (e.g., ethanol and isopropanol). In this presentation, we will describe the survivabilities, catalase specific activities, and metabolomics of oxidative stress for Acinetobacter radioresistens 50v1, which was isolated from the preflight Mars Odyssey orbiter. When cultured on minimal media (0.2x M9) containing 16 mM ethanol (0.1% v/v) and 26 µM Fe, which serve as the sole carbon source and transition metal, the 50v1 strain shows an appreciable tolerance towards 10 mM hydrogen peroxide (~2.5-log reduction from ~10⁸ cfu/mL) and catalase specific activities of ~40 Units/mg, which are predominantly found in the insoluble fraction after cell lysis; comparisons to values obtained under carbon and metal-rich conditions will be discussed. Additionally, preliminary gas chromatography-mass spectrometry
analyses of cell extracts obtained under nutrient rich conditions show the presence of several metabolites that change abundance upon peroxide exposure. Hence, these combined studies suggest that the environmental conditions of the assembly facilities promote oxidative stress and that the resulting biochemical adaptations of spacecraft-associated microorganisms, such as the Acinetobacter, may increase the probability of contamination for Mars.

The catalase activities from environmental samples are important parameters for soil microbiology, as this enzyme serves as a proxy for oxidative stress. To date, the most commonly used methods for measuring catalase activities from soil samples include permanganate titrations, fluorometric assays, and manometric methods. However, these combined methods are unsuited for field-based assays, generate copious amounts of chemical waste, and are often incompatible with organic-rich soils. In this presentation, we will describe the use of a field-amenable and low-cost water displacement assay to measure the catalase specific activities from black-crusted biological soil crusts (BSCs) obtained from the Mojave National Preserve. Specifically, we have analyzed differing successional stages and vertical subsections of BSCs obtained from sites possessing differing BSC surface coverages. Benchtop analyses provided the specific activities of 3.7±0.3 and 3.4±0.1 µkat/g soil for pedicelled BSCs (from the high and intermediate surface density sites), 0.28±0.10 and 0.36±0.26 µkat/g soil for sub-surface samples of pedicelled BSCs (from the high and intermediate surface density sites), 1.2±0.3 µkat/g soil for non-pedicelled BSCs, and undetectable activities for the non-BSC control soils. Currently, we are measuring the apparent Michaelis-Menten constants for these differing BSC samples, which, along with a comparison of field and benchtop values, will be discussed. Thus, when considered together, our results indicate that catalase activity is ~10-fold higher in the top layer of the BSCs and suggest that the successional stages of BSCs have differing metabolic activities.

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Investigating the Catalytic Role of a Conserved Non-Active Site Residue in Triosephosphate Isomerase

Triosephosphate isomerase (TIM) is a glycolytic enzyme that catalyzes the reversible isomerization of dihydroxyacetone phosphate and glyceraldehyde-3-phosphate. TIM has served as a model system to study enzyme function, and previous studies have investigated the catalytic roles for three active site residues: K13, H95, and E167. In addition to the residues that directly contact the substrate, E97 is conserved in all known TIM sequences. Previous studies reported the E97Q mutation in TIM from Plasmodium falciparum decreased $k_{cat}$ ~4000-fold relative to wild type, suggesting an important catalytic role for this residue. To investigate further the catalytic role of E97 and to evaluate if E97 mutations lead to similar effects in TIM from another organism, we evaluated the effect of E97 mutations in TIM from Trypanosoma brucei brucei. Following generation of the constructs via site-directed mutagenesis, we overexpressed the enzymes in Escherichia coli, purified using ion-exchange chromatography, and characterized the mutants using Michaelis-Menten kinetics. Our results show the E97Q mutation in TBB decreased $k_{cat}$ ~40-fold, suggesting the residue plays an important role in catalysis, but the rate decrease was significantly less than that observed in P. falciparum. Structures show that although the active site residues are conserved, the residues surrounding E97 differ in TBB.
and *Plasmodium* TIM. The mutations may lead to different structural rearrangements in TIM from the two sources. We are currently investigating the physical basis for the different effects from the mutations and evaluating the role of E97 in positioning K13, as structures show the Glu residue is situated near K13. These results will further our understanding of the catalytic role of residues that surround the active site.

Protein folding is central to the organization of living matter. In-vitro protein folding studies typically employ chemical denaturants and linear extrapolation methods to characterize the energy landscapes and conformations accessed under native solution conditions. However, in-vivo folding pathways may be very different from those populated using such approaches. Novel methods which enable the study of protein folding under more physiologically relevant conditions are required. Of all physiological folding environments, the one provided to nascent polypeptides during translation by the ribosome is the first and arguably the most important for directing the protein folding pathways populated in-vivo. Single molecule fluorescence resonance energy transfer (smFRET) can be used to directly probe the distributions, dynamics, and transient intermediates populated during biomolecular folding. This approach requires the attachment of pairs of fluorescent dyes to specific sites in the protein system under study. Unfortunately, creating dual-labeled proteins for smFRET remains a significant challenge. Here we describe a simple and efficient in-vitro “tag-and-modify” method for generating large-libraries of dual-labeled proteins suitable for smFRET protein folding studies. This approach involves first the introduction of alkyne-bearing unnatural amino-acid (UAA) tags into nascent protein chains using a purified and reconstituted in-vitro translation system; next dyes are attached to the UAA tags using a ligand accelerated and anaerobic variant of copper click chemistry. Using this approach we show that libraries of protein constructs can be made and screened by smFRET to study their folding properties. We also show that dual-labeled ribosome-bound nascent chains suitable for smFRET-based studies of protein folding on the ribosome can also be generated using this approach. A major benefit of this in-vitro approach to smFRET sample generation is its highly parallelizable nature.

Oxidative damage is involved in the formation of free radicals, which can cause various diseases. In DNA, this damage is observed primarily at guanine because it is the most easily oxidized base and one form of oxidative damage is DNA protein crosslinking. Here, we examined whether green tea can inhibit oxidative DNA damage. The flash quench technique is a method that is used for guanine oxidation and it can induce DNA-protein crosslinking. In the flash quench technique, the intercalator, Ru(phen)2dppz2+ (phen= phenanthroline, dppz= dipyridophenazine), is excited with a laser and gives an electron to the quencher, Co(NH3)5Cl2+, histone protein, calf thymus DNA and either water or green tea were irradiated for 0-2 minutes with blue laser light from a HeCd laser to effect guanine damage. The extent of crosslinking is extracted away from unreacted DNA. Our results showed as the irradiation time increased, the absorption of free DNA decreased less in the presence of green tea, consistent with inhibition of DNA oxidation. In addition, agarose gel electrophoresis experiments of
samples containing pUC19 DNA showed that the free DNA band persisted at dilutions of green tea up to 400:1. In future work, experiments will be carried out to determine a more accurate concentration range for the antioxidative effects of the green tea and to identify the molecular components responsible; analogos experiments with small peptides suggest that phenols could produce the inhibitory effect by reducing guanine radicals.

Disruption of cholinesterase activity has been implicated in neurodegenerative diseases such as Alzheimer’s. While acetylcholinesterase (AChE) activity decreases or remains unchanged, butyrylcholinesterase (BChE) activity is found to increase in Alzheimer’s patients. Multiple classes of BChE-specific inhibitors have been evaluated as potential therapeutics to manage the progression of neurodegenerative diseases, and previous studies identified molecules bearing aromatic and carbamate groups as potent inhibitors. We postulated Fmoc-amino acids may provide an attractive starting point to develop a new class of inhibitors, as the amino acid analogs contain aromatic and carbamate groups. We determined the effect of Fmoc-amino acids on BChE activity and identified Fmoc-Leu-OH, Fmoc-Trp-OH, and Fmoc-Lys-OH as the most effective inhibitors. The inhibition constants (K_i values) for the analogs were ~100-200 mM. Experiments with AChE showed the analogs did not affect activity, suggesting the compounds are specific for BChE.

We next tested Fmoc-amino acids bearing side chain modifications and identified Fmoc-Trp bearing a t-butoxycarbonyl on the indole side chain (Fmoc-Trp(Boc)-OH) led to an inhibitor with a K_i value of 20 mM. As amino acids provide a convenient scaffold to synthesize an array of analogs, we are currently determining if short peptides bearing Fmoc-amino acids are potent and specific BChE inhibitors.

Cell-cell interactions are involved in many physiological processes. The dysregulation of these interactions can result in numerous disease states including infections and cancer. Despite their importance to human health, cell-cell interactions are difficult to study in vivo with conventional imaging tools. To visualize cell-cell interactions on a whole animal scale, the need for new general strategies to selectively and noninvasively visualize cellular interactions has arisen. A strategy using bioluminescence imaging is well suited for sensitive, noninvasive visualization at the macroscopic level. Bioluminescence imaging utilizes enzymes (luciferases) that generate light through the oxidation of their small molecule substrates (luciferins). Therefore, no excitation light source is required, and almost no background signal is produced, making bioluminescence well suited for whole animal imaging. While bioluminescence is a powerful technique, cell location can only be approximated due to its low spatial resolution. To address this issue, the Prescher lab aims to engineer new bioluminescent tools to produce light only when two cell populations are in close proximity or direct contact. To monitor direct cell-cell contacts, we plan to develop tools based on bioluminescent protein complementation. Complementation strategies utilize “split reporters” that reassemble to produce signal upon direct contact. We aim to monitor direct cell-cell contacts by tethering "split" luciferase fragments to cell surfaces using transmembrane domains. Investigations of orientation and tether length/rigidity could provide a more sensitive readout on direct cell-cell
The Polypyrimidine Tract Binding Protein 1 (PTBP1) is an RNA binding protein that binds to pre-mRNA sequences containing mixtures of C and U nucleotides. It plays an important role in the alternative splicing of RNA. Additionally, PTBP1 is also involved in stabilizing mRNA, mRNA transport, and polyadenylation. PTBP1 contributes to the splicing regulation of many gene transcripts, including those involved in cancer. It functions to inhibit the inclusion of target cassette exons. Atomic details of how PTBP1 binds to its target RNA to repress the inclusion of cassette exons hinge on obtaining a crystal structure of the full length of PTBP1 bound to a target RNA. PTBP1 consists of an N-terminal region and four RNA binding domains connected via three linker regions. The contribution of each RNA binding domain during exon repression is not completely understood. The N-terminal domain of PTBP1 has a nuclear localization sequence and is required for nucleocytoplasmic shuttling. However, this region has an unstable flexible structure in solution and hinders protein crystallization. My project aims to clone an N-terminal deletion mutant (Δ48) of PTBP1 into the bacterial expression vector pQE80L. If successful, I plan to transform BL21 DE3 Escherichia coli cells with the N-terminal deletion construct for over-expression of the mutant protein for crystallization trials.

Patricia Souza Marimon, Davi Assuncao, Rafael Lima De Morais, Tanya Espino, Sharon Patray

Curli, a type of proteinaceous cell surface filament, found on enteric bacteria such as E. Coli and Salmonella, are thought to play an important role in host cell adhesion and invasion. Assembly of curli is thought to involve six proteins: CsgA, CsgB, CsgC, CsgE, CsgF, and CsgG. Of these CsgE and CsgF are thought to be periplasmic chaperone proteins that play a vital role in the assembly of CsgA into Curli fibers. We have found that CsgF is able to prevent the aggregation of CsgA as well as human Islet Amyloid Polypeptide (hIAPP) suggesting that CsgE may be able to prevent aggregation of amyloidogenic polypeptides in general. We sought to determine the nature of any CsgF-hIAPP interaction using four cysteine mutants of CsgF labeled with the environment sensitive fluorescent probe IAEDANS, as well as using the extrinsic fluorophore ANS.

Amy Tran

Protein phosphorylation, a reversible modification, plays a central regulatory role in various cellular processes, such as proliferation, differentiation, migration, etc. Thus, over- or under-activation of kinases (the enzymes that carry out phosphorylation) can result in various pathological conditions. Cyclin-dependent kinase 5 (CDK5) is a proline-directed serine/threonine kinase. Unlike other members of this family, CDK5 is activated by p35 and p39 rather than by cyclins and is primarily involved in the regulation of cell migration rather than the cell cycle. CDK5 over-activation/over-expression has been implicated in several pathologies including cancer cell metastasis and neurodegeneration. Therefore, investigating mechanisms that regulate CDK5 activity remains a crucial area of study with far-reaching implications in pathological understanding and therapeutics. Here, we show and characterize the ability of CDK5 to auto-phosphorylate - a possible mechanism to modulate its own activity. Our results showed a slower migrating band only in case of CDK5 WT expressed with contacts. Preliminary data suggests that increased linker length and rigidity facilitate split luciferase complementation.
but not in case of its kinase-dead counterpart. Since phosphorylated proteins show retarded electrophoretic mobility on SDS-PAGE, we reasoned the slower migrating CDK5 band to be the phosphorylated form of the kinase. Also, since the kinase-dead CDK5 did not show any additional bands, we concluded that increased levels of CDK5 phosphorylation must be due to auto-phosphorylation. The ability of CDK5 to auto-phosphorylate potentially represents a previously unknown auto-regulatory mechanism. Our current and future goals include identifying the auto-phosphorylation site(s) on CDK5 and generating phosphomimetic and non-phosphorylatable mutations to characterize the effect of phosphorylation on its activity.

Human apolipoprotein E (apoE) is a 34-kDa 299 residue exchangeable apolipoprotein that plays a critical role in lipid transport and cholesterol metabolism in the plasma and brain through its ability to interact with the LDL-receptor family of proteins. The APOE gene polymorphism results in three different alleles which produce the common protein isoforms apoE2, apoE3, and apoE4, respectively; these isoforms differ in amino acids at positions 112 and 158. They possess remarkable structural flexibility and bear the ability to exist in lipid-free and lipoprotein-associated states. Whereas apoE3 is considered to be the anti-atherogenic protein, apoE4 is considered a risk factor for developing Alzheimer’s disease (AD) and cardiovascular disease (CVD). Here we investigate the structure and organization of apoE3 or apoE4 on reconstituted high density lipoprotein (rHDL) particles using a combination of chemical cross-linking and mass spectrometry (MS). Reconstitution of POPC with recombinant apoE3 or apoE4 yielded a heterogeneous mixture of HDL particles as revealed by non-denaturing PAGE. The mixture was subjected to gel filtration on an FPLC to obtain discrete uniformly sized particles. rHDL/apoE4 or rHDL/apoE4 were subjected to chemical cross-linking using dimethylsuberimidate (DMS), a lysine specific cross linker. SDS-PAGE revealed the presence of ~70 kDa and ~35 kDa bands corresponding to dimeric and monomeric apoE, respectively. The dimers represent inter-molecularly covalently cross-linked apoE, while the monomers likely represent a mixture of intra-molecular and non-cross linked species. The monomeric and dimeric bands were subjected to in-gel digestion with AspN and GluC followed by MALDI-MS. We are currently in the process of analyzing the mass spectral data. Taken together, mass spectral data and cross-linker distance constraints allow us to create a low-resolution model of organization of apoE3 and apoE4 discoidal HDL particles by identifying intra and inter-molecular crosslink between the apoE molecules. The significance of this study is that it offers an innovative approach to obtain insight into the structure and organization of apoE on large lipoprotein complexes, Further, it allows us to identify potential differences between the two isoforms from a structural perspective and determine distinguishing features that contribute to the role of apoE4 in developing CVD and AD.
individuals affected by ALS is between 250-1600 repeats. But even though it is known that ALS is caused by these extended repeats, the exact mechanism for the disease is still being investigated.

The Qin research group uses a biophysical tool-kit to study nucleic acids such as DNA, RNA, and DNA/RNA-protein complexes called site-directed spin labeling (SDSL). A stable nitroxide radical (the spin-label) is attached at a specific location along the DNA or RNA and then Electron Paramagnetic Resonance (EPR) is used to detect the signal emitted from the free electrons on the spin-label. This signal can give us relevant structural and dynamic information about the sample. The data taken using continuous wave-EPR was used to confirm (using the SDSL method) that in K+, a GQ forms. Furthermore, we were able to see that when annealed in a Li+ solution, the GQ either didn’t form, or was not as stable as within the K+ solution. Once it was determined that the GQ formed, intramolecular distances were taken and analyzed. From these distances, we can use the raw measurements and molecular modeling to describe the conformation of the GQ.

Alzheimer’s disease (AD) is a chronic neurodegenerative disease and is the most prevalent form of dementia. Progression of AD occurs concomitantly with an increase in both the levels of brain butyrylcholinesterase (BuChE) activity, neurotoxic β-amyloid plaques and neurofibrillary tangles. The result is loss of cognitive function. This study focuses on the effect of bis-phosphates as inhibitors of BuChE. Bis-phosphates were synthesized with varying length in linkers and different alkyl groups. In sodium phosphate buffer at pH 7.5, tetrabutyl propyl, tetrabutyl 3-hexenyl and tetrabutyl pentyl bis-phosphates are good inhibitors of BuChE. The relative IC50’s are 0.79 µM, 1.20 µM and 2.69 µM. However, in HEPES at pH 7.5, tetrabutyl propyl, tetrabutyl 3-hexenyl and tetrabutyl pentyl bis-phosphates were significantly less inhibitory. The effect of pH on inhibitory activity was then evaluated. In sodium phosphate buffer there was no significant change in the inhibitory activity of 10^{-4} M tetrabutyl propyl bis-phosphate as a function of pH. However, when assayed in HEPES (4-[(2-Hydroxyethyl)-1-piperazineethanesulfonic acid), the activity of the enzyme was stimulated as the pH increased. Subsequent experiments showed that the stimulatory activity was due to the buffer and not the inhibitor. Interestingly, HEPES, MOPS (3-(N-morpholino)propanesulfonic acid), MES (2-(N-morpholino)ethanesulfonic acid), and PIPES (piperazine-N,N'-bis(ethanesulfonic acid)) showed similar stimulatory effects on BuChE activity.

Endoplasmic Reticulum (ER) is a site of many important cellular functions including proper protein folding, post-translational modifications and maintaining Ca2+ homeostasis in virtually every mammalian cell. Perturbations in these functions lead to activation of a cellular stress response known as the unfolded protein response (UPR). Once activated, its main function is to re-establish normal ER function by decreasing general translation and increasing production of chaperones as well as ER-associated degradation of unfolded proteins. Initially, cells try to maintain homeostasis by promoting cyto-protective signaling. However, if normal ER function cannot be restored in a timely
manner, cells commit to apoptosis. Cancer cells are susceptible to ER stress due to intrinsic and extrinsic factors such as elevated glucose metabolism and hypoxia. However, unlike normal cells, cancer cells manage to survive and recover from ER stress. An overexpression of GRP78 (78kDa Glucose-Regulated Protein) in cancer cells has been reported to be a key element in their survival. GRP78 is a stress-inducible luminal ER chaperone that facilitate protein folding and assembly. In addition to being found in the ER lumen, its expression has been reported to be shown in the cytosol and cell surface as well. Our preliminary data revealed GIV (Go-Interacting Vesicle associated protein), an enhancer of Akt activation and cell migration, as a novel binding partner of GRP78. Interestingly, the Akt pathway is known to promote several other downstream responses, including cell survival and angiogenesis. We hypothesize that the mechanism of cancer cell survival during ER stress is dependent on the interaction of GIV and GRP78, which promotes cell survival signaling via the Akt pathway.