Poster Presentation Abstracts - Session 1

Name	Institution	Poster#/Area	Title	Advisor	Coauthors	Abstract
Claire Page	UCLA	1 Biochem	Unexplored Hybrid Polyketide Synthase Motif Reveals Unprecedented Dimethyltransferase and *cis*-Acting Thioesterase Activity	Yi Tang	Leibnez Hang	Fungal polyketides represent a large portion of modern pharmaceuticals, however little is known about the chemistry of fungal polyketide biosynthetic enzymes. Due to recent work in fungal genome sequencing, a multitude of uninvestigated fungal polyketide synthase genes have been found and grouped into families according to homology. One family of highly-reducing polyketide synthases (HRPKS) is particularly interesting because it has an adjoined domain with strong similarity to carnitine *o*-acyltransferase (cAT). We report the first characterization of one such HRPKS-cAT enzyme from *Trichoderma virens*. This enzyme shows unprecedented activity of dimethyl transferase and cis-acting thioesterases to produce a polyketide-polyol conjugate with a rare *gem*-dimethyl component. *In vitro* characterization of the enzyme shows it catalyzes the production of the *gem*-dimethyl moiety through two convergent routes. In the first route, the ACP-bound polyketide chain is directly dimethylated. In the second route, the second methylation occurs after the monomethylated product is released from the ACP. The dependence of the second route on the presence of the cAT domain and ACP suggests the second round of methylation is assisted by the retro-transacylation of the α-monomethyl polyketide back onto the ACP.
Carisse Geronimo	CSU Bakersfield	2 Biochem	Fluorescence Studies of Lysyl Oxidase	Karlo Lopez		Lysyl oxidase, an extracellular enzyme, is responsible for catalyzing the formation of crosslinks between elastin and collagen. Its mechanism is a key contributor in the stability and proper development of organisms, especially for skin and connective tissues in humans. Much research has been done in recent years to discover more about its physical characteristics. One way of analyzing the structure of proteins is through fluorescence spectrophotometry; the emission of light by each protein sample is indicative of its relative degree of exposure to water. An excitation-emission matrix (EEM) has been produced for each of the following variations of lysyl oxidase (LOX): pLOX02 (wild-type), pLOX09 (with solubility tag Nus-A), as well as pLOX20 (H303D mutant) and pLOX21 (H303E mutant). The preliminary results show excitation-emission maxima of (336 nm, 276 nm) for pLOX02, (341 nm, 282 nm) for pLOX09, (339 nm, 280 nm) for pLOX20, and (340 nm, 284 nm) for pLOX21. When compared to the wild-type, it is suggested that larger emission wavelengths (relatively less energetic emissions) indicate a protein that is more exposed to water/less tightly packed. These data can be used to piece together the structural influences of different mutations/variations of lysyl oxidase.

Lisa Situ	UCLA	3 Biochem	Adenovirus Protein E4ORF6/7 Alters Oxidative Metabolism of Human Epithelial Cells Through Interaction with Cellular E2F-1	Heather Christofk	Shivani K. Thaker,and Heather R. Christofk	Cancers and viruses reprogram cellular metabolism to promote biosynthesis of macromolecules that support proliferation and replication. Strong selection pressure for efficiency enables viruses to accomplish similar metabolic changes as those seen in cancers by activation of only the most critical nodes pivotal to anabolic metabolism. Our research uses adenoviral infection as a model to highlight key transcription factors and metabolic genes that may also be relevant for metabolic reprogramming in the cancer context. Notably, many human tumors decrease oxygen consumption rate (OCR) even in aerobic conditions. Our lab has shown that adenovirus infection also decreases OCR in human breast epithelial (MCF10A) cells. Although the mechanisms by which cancers and viruses inhibit OCR are currently unknown, if a decrease in OCR confers a growth advantage, then identification of key regulators can point to therapeutic targets. Adenovirus protein E4ORF6/7 binds cellular transcription factor E2F-1 to activate adenoviral genes. Because E2F-1 inhibits oxidative metabolism, we hypothesize that the interaction between E4ORF6/7 and E2F-1 decreases OCR during infection. We performed shRNA-mediated E2F-1 knockdown, which increased OCR and protein levels of the electron transport chain (ETC). We stably overexpressed wildtype or mutant E4ORF6/7, with the mutant being unable to bind E2F-1. Overexpression of wildtype E4ORF6/7, but not mutant E4ORF6/7, decreased OCR. Furthermore, wildtype E4ORF6/7 overexpression increased E2F-1 levels while decreasing levels of specific ETC subunits. Our experiments suggest that E4ORF6/7's ability to decrease OCR relies on direct interaction with E2F-1. Our work thus highlights a potential mechanism through which adenovirus infection alters host oxidative metabolism.
Katia Lopez	UCLA	4 Biochem	Characterization of a Novel Aged-Protein Repair Pathway in Saccharomyces cerevisiae Yeast	Steven Clarke	Rebeccah Warmack and Steven Clarke	The spontaneous chemical reactions that damage biomolecules are a hallmark of the aging process. The non-enzymatic isomerization and racemization of asparaginyl and aspartyl residues to L-isoaspartyl residues is a common type of protein damage in aging organisms. Most of these organisms are able to repair some of this damage through the protein-l-isoaspartyl (d-aspartyl) O-methyltransferase (PCMT), which methylates D-aspartyl and L-isoaspartyl residues specifically, leading to the reformation of L-aspartate. Although the enzyme is present in almost all organisms, it has been of great interest that the budding yeast Saccharomyces cerevisiae does not express this protein but is able to maintain very low levels of L-isoaspartyl residues in comparison to organisms with PCMT. This indicates the presence of a potentially novel protein repair mechanism. Incubation of S. cerevisiae protein extracts revealed an increased accumulation of L-isoaspartyl damage in the presence of the metal chelator ethylenediaminetetraacetic acid (EDTA). These results suggest that at least one of the proteins responsible for L-isoaspartyl damage repair in yeast may be a metal dependent protease or peptidase. Examination of L-isoaspartate levels from individual single metal dependent protease knockout strains, however, did not reveal any strains with increased accumulation of L-isoaspartyl residues. Further metal rescue experiments directed towards finding the metal co-factor of our protein of interest revealed that this repair protein is most likely dependent on magnesium or calcium, possibly suggesting a non-proteolytic pathway since yeast cells do not contain proteases activated by these ions.

Andrew Smith and Gaston Moorhead	USD	5 Biochem	Progress towards the development of novel nucleic acid-based therapeutics.	Anthony J. Bell	Gaston Moorhead	The objective of this study was to evaluate the viability of using intramolecular four-way junctions (4WJs) for use as therapeutic inhibitors against the DNA-binding cytokine, High Mobility Group B1 (HMGB1). Reports suggest HMGB1 should be considered a lupus biomarker because the protein is linked with several key stages of pathogenesis[1, 2]. The strategy to use 4WJs to target HMGB1 is grounded in classic in vitro studies that show HMGB1 binds to cruciform/bent DNA with a very high affinity [3-5]. Our initial studies focus on investigating the nuclease stability of 4WJs. Three 4WJs are currently being evaluated; two 4WJs referred to as iJ1 and J4 are composed of natural DNA with thymine-thymine end caps. The final 4WJ referred to as tDNA is composed DNA with thiol linkages vs. phosphate bonds. The presence of end caps in i-J1 and J4 are intended to enhance nuclease stability by preventing favorable contacts with nucleases. The thiol linkages in tDNA are known to enhance stability because these bonds are not recognized by nucleases. Nuclease digestion assays are conducted at 20o and 37o C using nucleases that digest double (DNase I, LExo, and Exo III) and single stranded DNA (Exo V and T5 Exo). Our preliminary reports show that as expected the presence of thymine end-caps and thiol linkages enhance the relative nuclease resistance of intramolecular 4WJs vs. unmodified DNA 4WJs.

Edward Njoo and Larry Palato	LMU	6 Biochem	Determining Amyloidogenicity in Islet Amyloid Polypeptide (IAPP) Across Mammalian Species	David A. Moffett	Larry Palato, Shannon Pilcher, Dillon Rinauro, Angela Tun, Kate Menefee, and David A. Moffet	It is estimated that 25.8 million children and adults in the United States have diabetes, approximately 8.3% of our population with nearly 2 million new cases each year. While the cause of type 2 diabetes remains unknown, it is known that as the disease progresses, patients lose pancreatic β cells (the cells that produce insulin) with up to 45% loss of pancreas mass in severe cases of the disease. It is believed that the protein, IAPP, is one of the agents responsible for this massive death of β cells. For unknown reasons, IAPP accumulates in the pancreas where it aggregates into a variety of toxic forms that are known to kill β cells. It has been known that the IAPP of mice and rats does not aggregate and that these two species do not develop type-II diabetes; however, the IAPP of monkeys, humans, and cats does aggregate and these species do develop type-II diabetes. To determine if a correlation exists between amyloidogenecity of IAPP and the propensity for an individual to develop type-II diabetes, a list of mammals that do and do not develop diabetes has been compiled. By determining the amyloidogenicity of the IAPP sequences of these animals, we expect to find a correlation between the ability to contract diabetes with the propensity of IAPP to aggregate.
America Hidalgo	Cal Baptist U.	7 Biochem	Antioxidant Activity Study in Agave Using 1,1-diphenyl-2picrylhydrazyl (DPPH) radical Assay	Y. Hu	M. A. Hamrick, I. Davis-Ward, and Y. Hu	Agave is a popular plant in the hotter climates of the southwestern United States and Mexico. It is well known for its nutritional, industrial and medicinal applications. In this study, we investigated the antioxidant activity in fresh Agave by using a 1,1-Diphenyl-2-picryl hydrazyl (DPPH) radical assay. Fresh Agave was collected at San Manuel Reservation in early April, 2016. Samples were sorted for quality, maturity, field heat removed, cooled, weighed into whirl pack bags, treated with liquid nitrogen, stored in ultra-low at -80° and studied in September, 2016. The results show an IC50 value of 2.20 mg/mL for the fresh Agave. The IC50 of the reference, ascorbic acid, is 0.146 mg/mL. The antioxidant activity of Agave is relatively high compared to other plant derived species studied in the area, such as yucca blossom (21.85 mg/mL) and stinging nettle (414.42 mg/mL). Further research is proposed to investigate how a cooking method will influence the antioxidant activity of the agave.

Martin Amezcua	CSU Fullerton	8 Biochem	Synthesis and Evaluation of Small Molecule Inhibitors as Therapeutics against BoNT/A	Nicholas Salzameda	Sandra Beltran, Ricardo Cruz, and Nicholas Salzameda	The Botulinum neurotoxin serotype A (BoNT/A) is a metabolic byproduct of the Clostridium botulinum bacteria and is responsible for causing Botulism, a paralytic disease. The neurotoxin is the most lethal toxin known to man. Its potency and ease of extraction from the bacteria cause a major concern that it can be used as a bioterrorism weapon and in warfare. The BoNT/A is composed of a heavy chain (HC), and a light chain (LC). Upon exposure, the HC binding domain binds to neural cells, while the HC aids the LC into the cytosol. The LC is a zinc metalloprotease, and its metal ion active site is responsible for cleaving SNARE proteins. Cleaving of the SNARE protein is an irreversible process that terminates neurotransmissions and results in flaccid paralysis, which can lead to death. Current available therapeutics such as intensive care and physical therapy are not readily available for large scale infections. Therefore, it is vital to develop alternative therapeutics against BoNT/A. Previously, the laboratory discovered an inhibitor that contained four major components to the scaffold: (1) Hydroxamic acid, (2) Isoleucine, (3) Sulfonamide bond, and (4) 4-Chlorobiphenyl, that had good inhibition. We hypothesized that increasing the amino acids on the scaffold would increase its affinity for the enzyme. The amino acids were coupled to the resin in varied sequences for analysis, the 4-chlorobiphenyl 4-sulfonyl chloride was added to give the sulfonyl-amide bond, and the small molecule was cleaved from the resin with trifluoroacetic acid. In hindsight, chlorobiphenyl ring system and sulfonamide bond were altered to study its impact on inhibition. Fluorescence Resonance Energy Transfer assay was utilized to evaluate the molecules as inhibitors. The sequences containing isoleucine-phenylalanine, isoleucine-valine, and isoleucine-isoleucine displayed 84% or greater inhibition of the BoNT LC at a concentration of 15 μM. Changing the chlorobiphenyl ring system and the sulfonamide bond on the molecules had a decrease in inhibition of over 50%, a significant decrease. The decrease in inhibition confirmed the importance of the sulfonamide bond and the chlorobiphenyl component of the molecule.

Harrison Shawa	UCLA	9 Biochem	How are proteins in the eye lens protected against isomerization-associated damage during the aging process?	Steven Clarke	Binsen Li, Rebeccah Warmack, and Steven Clarke	As a mammal ages, amino acids in their long-lived eye lens proteins can racemize and isomerize. These modifications can damage the proteins and lead to the decline in visual integrity that accompanies aging. Eye lens fiber cells lack protein turnover machinery, thus the proteins must remain for the entire lifespan of an individual, and the damaging modifications can accumulate. The isomerization of L-aspartyl residues to form L-isoaspartate is an especially prevalent form of spontaneous damage. In a majority of tissues, the protein carboxyl methyltransferase (PCMT) and its cofactor S-adenosylmethionine repair this damage. We have discovered that this enzyme is present and active in the lens, but damaging levels of L-isoaspartate still increase greatly with age. Despite the accumulation of L-isoaspartate with age, lens PCMT activity remains constant. Our data suggests that the concentration of PCMT actually increases, but still is unable to repair many L-isoaspartate sites. Both L-isoaspartate accumulation and PCMT activity appear to be consistent across the different regions of the lens, but only specific proteins appear to be receiving the majority of the enzyme's repair activity.

Christian Totoiu	UCI	10 Biochem	Engineering the Human Insulin Receptor for Integration into a Real-time Insulin Biosensor	Gregory A. Weiss	Sen, S. R.; Majumdar, S.; Crawley, E; Piercy, M.; Gabriel, K. N., Weiss, G. A.	Type I diabetes (T1D) affects 1.25 million Americans and is predicted to affect approximately 5 million, by 2050.[1] Disease management involves frequent glucose monitoring and insulin administration. The artificial pancreas (AP) uses control algorithms to automate and link continuous glucose monitoring with insulin administration. While glucose is directly measured in these devices, the control algorithm indirectly and belatedly estimates insulin levels, thus increasing a patient's risk of hypoglycemia (excessive blood insulin) or hyperglycemia (insufficient blood insulin). Direct insulin monitoring would allow for faster regulation and more accurate glucose control. Therefore, we aim to develop a continuous, real-time insulin biosensor for AP devices. To mimic nature's real-time insulin detection system, our biosensor is engineered from the wildtype human insulin receptor (wtInR). Novel InR variants were designed using a combination of wtInR insulin binding sites and supporting domains. The variants were built using ligation independent cloning and were expressed in E. coli and through M13 bacteriophage-display. Insulin binding was examined using enzyme-linked immunosorbent assays (ELISA). Since insulin binding causes conformational changes in the wtInR, we incorporated Förster Resonance Electron Transfer (FRET) in our InR variants to relay its insulin-dependent conformational changes as a light signal. This signal can then be captured by a photodetection system in the AP device and exact insulin levels can be quantitatively analyzed. Thus far, our results demonstrate that our InR variants bind monomeric insulin. Our lab's research is directed towards creating and analyzing corresponding FRET-based variants in functional and kinetic assays, in preparation for future in vivo device studies. Our insulin receptor biosensor can make devices, such as the AP, safer and more effective for the millions of T1D patients that will depend on it. Furthermore, the promise of such biomimetic sensors opens doors to continuous real-time in vivo sensing of regulatory components in numerous other diseases.
Rochelle Radzyminski	UCI	11 Biochem	Elucidating Structure Dependency and Genetic Determinants in Phage and Amoebae Interactions with Pseudomonas aeruginosa	Albert Siryaporn		Pseudomonas aeruginosa is a multidrug resistant pathogen that exploits immune-weakened hosts including hospital patients, such as those on breathing machines or with wounds and burns. We are most interested in the central role of the opportunistic pathogen P. aeruginosa in patients with cystic fibrosis (CF). P. aeruginosa cells are found in high density communities known as biofilms, which secrete polymers that obstruct antibiotic diffusion into the biofilm. Thus, we look to use bacteriophage therapy as an alternative treatment for CF. We hypothesize that biofilm organization contributes to its susceptibility to being lysed by phage, and that the structure is influenced by physiological and metabolic conditions. Through fluorescence microscopy time-lapses of phage-bacteria interactions, we have found that phage not only lyses non-resistant bacteria, but also inhibits regular cell functions of resistant bacteria. Phage prevents the division of cells. At the end of a 24-hour period, bacteria cells grow into long, worm-like structures. A spike in fluorescence intensity occurs prior to rapid phage lysis, which

					appears to correspond with an increase in protein translation—another effect of phage on cell functions. These altered functions are significant because they may potentially inhibit the bacteria's virulence, which we will test for with subsequent virulence assays. We are also infecting a 100,000-mutant transposon insertion library for P. aeruginosa with phage and DNA sequencing the resistant cells to determine the genetic determinants involved in biofilm clearing. As we continue varying the oxygen levels, pH, nutrient availability, and substrate stiffness to mimic the CF lung, we will gain a better understanding of the biofilm structure's role in its resistance to antibiotics. This, in conjunction with our DNA sequencing of resistant cells, will allow us to look towards alternative CF treatments using phage.
Michele Ramos Correa	CSU Northridge	12 Biochem	Comparing Expression of Genes Involved in Carbohydrate Metabolism in Wild-Type and LPL-Knock-Down Muscle Cells	Jheem Medh	Lipoprotein Lipase (LPL) catalyzes the hydrolysis of triglycerides into glycerol and free fatty acids (FFA). Thus, LPL regulates the entry of FFAs into skeletal muscle tissue, which is an insulin-responsivetissue. When LPL activity is high it releases FFA that are oxidized for energy, but when LPL activity is low, muscle cells oxidize glucose for energy. Hence, the downregulation of LPL forces the muscle cells to use glucose for energy and in turn, can make the cell more insulin-sensitive. We want to study the effects of LPL levels in L6 rat skeletal muscle cells on insulin action. We used wild type L6 cells and LPL-deficient (LPL-KD) cells to compare the expression of different genes that play important roles in the metabolic actions of insulin. We used reverse transcriptase polymerase chain reaction and agarose gel electrophoresis to quantify gene expression in these cells. Preliminary gel results confirmed a role for LPL in the regulation of genes involved in carbohydrate metabolism.

Hannah Fejzic, Kayla Garcia, Simbarashe Peresuh, Kaythryn Rager,	CSU San Bernardino	13 Biochem	Using Drosophila Reporters to Evaluate Metal Uptake, ROS Production, and Chelation in Drosophila S2 Cells and Human HeLa and Neuroblastoma Cells	Yu Jung Kim		The goal of our project is to determine the rates of metal uptake and reactive oxygen species (ROS) production in DrosophilaS2 cells and human HeLa and neuroblastoma cells using a Drosophila metal- and ROS-sensitive luciferase reporter. An additional goal was to use these reporters to examine the effects of metal chelation in ROS production in these cells since metal chelators are suggested as potential therapeutics for neurodegenerative diseases. First, we performed time course experiments to estimate the rates of metal uptake and ROS production in S2 cells by measuring the luciferase signals from the Mtn and SOD promoters after treating the cells with Cu, Fe, and Zn for different time periods. From this study, we found that the luciferase signal from the Mtn promoter construct increased linearly over time when the cells were treated with Cu and Zn, but not with Fe. This trend was also observed with the SOD promoter construct. For our chelation tests, we used EDTA, citrate, and histidine because they have been suggested as potential therapeutics for neurodegenerative diseases. We performed the chelation experiments in Drosophila S2 cells and human HeLa and SHSY cells by measuring the luciferase activities from the Mtn and SOD promoters in cells treated either with Cu, Fe, or Zn in the presence or absence of EDTA, histidine, or citrate. Of the nine metal-chelator combinations tested in S2 cells, the only combination that led to a significant decrease in Mtn-luciferase activity was Zn and citrate, which correlated with a corresponding decrease in SOD-luciferase activity. The same effect was observed in HeLa and SHSY-5Y cells with the Mtn promoter construct. Additionally, we found that in HeLa cells treated with Cu and histidine, there was a 2-fold decrease in Mtn-luciferase activity relative to cells treated with histidine alone.
Luis Pena	CSU Dominguez Hills	14 Biochem	Using proteomic technology to study the DNA methylation	Tieli Wang	Maria Nava, Sheva Saif , Anthony Diaz, Arumugam Thangavel, and Tieli Wang	DNA methylation has been shown to affect chromatin structure and influence histone methylation. Hypermethylation of the promoter of methylguanine methyltransferase (MGMT) in glioma brain cancer patients is used as a favorable prognostic biomarker and increases drug sensitivity since a lower amount of the enzyme is available to repair TMZ-induced lesions. In this presentation, we studied the methylation of DNA using proteomic technology. DNA methylation reaction by temozolomide was compared with the one using formaldehyde in the presence of sodium cyanoborohydride. Both reactions showed the similar methylation pattern. We found that anticancer drug temozolomide and formaldehyde can produce dimethylated DNA at the amine group.

Sam Mahdi	CSU Northridge	15 Biochem	Structural and dynamic differences influence the affinity of RGS4 and RGS7 for $G\alpha_{i1}$	Karin Crowhurst

Misregulation of signal-transmitting G proteins is linked to many neurological diseases, such as Parkinson's and Huntington's. Regulators of G protein signaling (RGS proteins) are responsible for accelerating the deactivation of G proteins. RGS4 selectively targets Gαi; however, studies have shown that RGS7 targets primarily Gαo, with lower affinity (and selectivity) for Gαi1. Considering that residues in the RGS4 and RGS7 binding sites differ at only two positions (F33 and Y82 for RGS7, and Y34 and R84 for RGS4), it is not fully understood why the difference in Gα selectivities exist. We hypothesize that protein motions are important contributors to the contacts between Gαi1 and the "box" domains of RGS4 and RGS7, and that these motions influence the selectivity and affinity of each RGS for this specific Gα. Our goal for this project was therefore to use NMR and SPR spectroscopies to probe these motions and to test the effect of RGS7 mutations on its interactions with Gαi1. Previous HD exchange and backbone dynamic data have indicated apo RGS7 primarily exhibits ps-ns timescale motion and is more flexible overall, whereas RGS4 has µs-ms timescale motion. To determine whether these dynamic differences or the 2 differing residues within the binding site play roles in affinity and/or selectivity, we recorded backbone dynamics on apo RGS7-F33Y and RGS7-Y82R and ran SPR on Gαi1 binding to RGS7, RGS4, and both RGS7 mutants. RGS7-F33Y showed decreased ps-ns timescale motion and no structural change when compared to WT. RGS7-Y82R showed no change in dynamics, except at the site of the mutation, but showed structural change around the mutation site due to charge-charge repulsion caused by the positively charged amine of arginine. SPR unexpectedly showed the highest KD value for RGS4 and the lowest KD value for RGS7. Overlays of apo and holo structures of RGS4 show that it undergoes significant conformational change upon binding to Gαi1, whereas the conformation of RGS7 is already close to optimal for binding. Furthermore, RGS7-F33Y showed a faster rate of binding than RGS7 due to the increased rigidity of the mutant. RGS7-Y82R showed a decreased rate of binding due to structural changes, but also a decreased rate of dissociation due to the increased stability of the hydrogen bond from arginine. SPR and relaxation data of apo RGS4, RGS7 and both mutants indicate dynamic and structural differences affect the affinities of RGS4 and RGS7 for Gαi1.

Omair Qureshi	USC	16 Biochem	Investigating mechanism of target DNA recognition by a CRISPR-Cas9 nuclease	Peter Z. Qin		The type II RNA-guided CRISPR-Cas9 nuclease, which has revolutionized genome engineering, targets double-stranded DNA at sites determined by the complementarity between a single-stranded region of RNA and a segment of the target DNA (designated as the protospacer), as well as a short protospacer-adjacent-motif (PAM). It has been established that the Cas9/RNA complex first recognizes the DNA at the PAM, then initiates unwinding of the PAM-adjacent segment of the protospacer. With a cognate target, formation of Watson-Crick base pairing between the unwound DNA and the single-strand guide segment of the RNA allows further unwinding of the DNA duplex, eventually enabling formation of an R-loop structure that stabilizes the ternary Cas9/RNA/DNA complex for cleavage. Unwinding of the target DNA to allow R-loop formation and hybridization between the DNA protospacer and sgRNA guide is a hallmark step of the CRISPR-Cas9 mechanism. The mechanism of DNA unwinding by Cas9, which is critical in discriminating a correct vs. an incorrect DNA target, is investigated and reported through a combination of biochemical and biophysical assays. Specifically, DNA constructs containing nicks or gaps within either the target strand or non-target strand protospacer region are evaluated for their impact on ternary complex formation. Preliminary findings suggest that discontinuity at various sites along the non-target strand protospacer region of the target DNA do not impede complex formation. Further experiments are currently underway to determine how discontinuity within the target strand protospacer region of the DNA duplex affects ternary complex formation and DNA targeting. This study will lay the foundation for examining DNA elements that contribute to Cas9 recognition and target specificity, which will facilitate further investigation on the overall mechanism of CRISPR-Cas9 as well as its applications in genome editing.
Cyrus Jin	UCLA	17 Biochem	Kinetic Characterization of PRMT1 and 5	Steven Clarke	Kanishk Jain, Steven Clarke	Histone H4 is an important target for gene regulation through posttranslational modifications such as arginine methylation. Protein arginine methyltransferase (PRMT) 5 is known to symmetrically dimethylate histone H4 R3, which can result in silencing of certain genes. Additionally, various studies report the link between levels of PRMT7 and symmetric dimethylarginine (SDMA) at histone H4 R3 catalyzed by PRMT5. We tested the hypothesis that histone H4 R17 and/or histone H4 R19 affect PRMT5's ability to methylate H4 R3, a mark of gene repression, by being monomethylated by PRMT7. Phosphocellulose paper binding assays were used to optimize linear reaction conditions and calculate kinetic parameters for the histone H4 wild-type N-terminal peptide (1-21) and peptides with the R17 and R19 residues mutated or chemically modified. Results indicate positive cooperative behavior for PRMT5 as well as the importance of R17 in affecting catalytic activity and reducing its allosteric nature once monomethylated. Similar studies were conducted with PRMT1 as a control and because it asymmetrically dimethylates H4 R3. Likewise, PRMT1 exhibits positive cooperative behavior and R17 affects PRMT1-mediated methylation on H4 R3. However, the positive cooperativity of PRMT1 remains when using the R17 monomethylarginine substrate, highlighting the unique link between PRMT5 and PRMT7.

Ning Liu	UCLA	18 Inorg/Mat	Photo-responsive hydrogel materials based on Au NP-incorporated thermal-responsive hydrogel PNIPAM	Ximin He	Through billions of year of evolution, living forms have developed many self-adaptive capabilities in order to respond to ambient environment in an energy efficient way, such as self-regulated temperature and pH value in animals, heliotropism in plants. However, self-adaptive functionalities are rarely exhibited in synthetic material systems. This project focuses on developing an intelligent material system that is capable of detecting and tracking an incident light source self-adaptively with high-energy efficiency. Here we developed a photo-thermal-responsive hydrogel by incorporating photonic absorbers in the materials system by physical trapping. In specific, PNIPAM was selected to provide thermal responses owing to its well-known phase transition around its Lower Critical Solution Temperature (LCST). On the other hand, gold nanoparticles (Au NPs) were developed as photo-absorption particles that can convert incident photonic energy into thermal energy that elevates the temperature. PNIPAM hydrogel will expel water content at temperatures above human body temperature (around 32℃), and experience dramatic shrinkage at even higher temperature. Therefore, upon radiation, PNIPAM/AuNP nanocomposite will shrink at the position where light incidents, and gradually propagate to the adjacent regions, creating a special gradient of both temperature and deformation. AuNP were fabricated via citrate synthesis method under different conditions to provide controllable photonic absorbance. UV-visible spectroscopy was then employed to characterize the absorbance and wavelength of AuNP. By far, a set of reliable recipes for several concentrations of AuNP has been developed for one particular absorption wavelength to facilitate the production of PNIPAM/AuNP micropillars with a range of AuNP concentrations. We also modify the surface of AuNPs with different linkers to covalently bond with the hydrogel, to study their effects on PNIPAM/AuNP interface on the thermal conductivity. Further optimization of the materials system will be conducted in near future. The optimization should include more detailed AuNP design, such as geometry, surface treatment, etc. to manipulate physical properties of the material system in absorption wavelength, mechanical (flexural modulus) and thermal properties (thermal conductivity). The project would pave the way toward a class of smart, self-adaptive, multi-stimuli-responsive material system that could benefit wide scope of applications, such as all-optical photonics, optoelectronics, low noise communications and stimuli guided biomedical applications.
Karen Tom	CSU Fullerton	19 Inorg/Mat	Synthesis of Potential Ionic-Conducting Materials XAgTa4O11 (X: Na, K, Cs, Rb)	Allyson Fry-Petit	Silver tantalates with the structure, AgTa4O11, appear to have promising applications for materials development of ion transporters, particularly for use in batteries. XAgTa4O11 (X: Na, K, Cs, Rb) have adopted a similar structure to that of the known P21/n monoclinic compound, NaAgNb4O11. Distinctive pores in the known structure of NaAgNb4O11 exist that house the sodium and silver ions, further stimulating interest in the potential ion conducting properties of the proposed system of NaAgTa4O11 analogs. XAgTa4O11 (X: Na, K, Cs, Rb) have been synthesized using a flux growth technique followed by standard solid state techniques. X-ray powder diffraction and Rietveld refinement were used to successfully refine the structures of the proposed system of conducting materials. Due to the lack of d orbital electrons, in the proposed NaAgTa4O11 analogs, molybdenum was doped into the K analog with the hopes that KAgTa4-xMoxO11 has a greater chance of consisting of conductive properties, which are necessary to realize ion conduction as well.

Pedro Pena Rodriguez	UCR	20 Inorg/Mat	Optoelectrical Characterization of MoS2	Ludwig Bartels	Miguel Isarraraz and Daniel Lu	Since the discovery of graphene, 2D materials have been extensively researched. Unlike graphene, transition metal dichalcogenides (TMDs), such as molybdenum disulfide (MoS2), exhibit a direct bandgap at the monolayer limit. This makes them ideal for optoelectronic devices. We utilize chemical vapor deposition (CVD) for the growth of monolayer MoS2, which we characterize by scanning photocurrent microscopy (SPCM). By optically exciting the MoS2 devices, we study the photoconductive nature of the material. Preliminary results show that photocurrent is localized near the contacts, showing that these contact-material interfaces play a large role in these 2D materials.
Alexander Malinick	University of La Verne	21 Inorg/Mat	Synthesis of Fe/Mn Bimetallic Magnetic Nanoparticles	Ricardo Morales		Cancer treatment can be just as deadly as the cancer itself. A noninvasive cancer treatment would not only save lives but also save patients from the suffering that chemotherapy can cause. Magnetized nanoparticles can solve the suffering caused by chemotherapy via drug delivery to the targeted area. With the aid of nanoparticles, chemotherapy will become precise and affect only the targeted area via magnets, thus making the process much less harmful. In this experiment, nanoparticles were synthesized at various ratios of iron (II), iron (III), and a mix between manganese (III) and manganese (II). These two metals were selected due to the low toxicity and proximity in the periodic table. In this study different ratios were selected with the goal of yielding the smallest, most uniform particles and to study the difference in magnetic properties. The samples were analyzed by means of transmission electron microscopy (TEM) to determine the size and shape of nanoparticles. Qualitatively, all tested samples showed magnetic properties; however, the 2:1 Fe2+:Mn3+ samples showed the most. At this point, the type of metal to metal ratio seems to affect the magnetic properties of the sample.

Luis Garay	CSU Fullerton	22 Inorg/Mat	Non-cooperative Octahedral Tilting Transition of Double-Perovskites Ca2SrWO6 and Sr2.9Ca0.1WO6	Allyson Fry-Petit		Double-perovskite oxides A2B'B"O6 are derivatives of the basic perovskite structures of the form ABO3. In this experiment, the structures of two known perovskites were investigated to determine if they adopt a non-cooperative octahedral tilting (NCOT) structure. The double perovskite Ca2SrWO6 was reported to share the cooperative structure of the basic perovskite Ca3WO6 with the space group P21/n. The converged Rietveld refinement of Ca2SrWO6 suggested that the correct formula is SrCaCaWO6, indicating that Sr, due to its relatively large size, occupies the A/A' site. Attempts to lower the space group symmetry of Ca2SrWO6 from P21/n to P1 produced bond valence sum averages that closely matched the oxidation state of each atom, suggesting that the previously reported structure was not able to chemically describe the structure. Further data analysis of Ca2SrWO6 indicated that the Cc space group, which is the high-temperature NCOT structure of the Sr3WO6 compound, was a better fit than the cooperative structure of Ca3WO6. Further investigation into the ability to control the structure of NCOT compounds was explored through calcium doping of NCOT Sr3WO6. Doping of calcium of 0.033% showed that the high-temperature NCOT structure observed in Ca2SrWO6 could be induced in Sr3WO6 without the application of temperature, but instead the application of chemical pressure. The full solid solution between Sr3WO6 and Ca2SrWO6 was investigated to probe the effect of chemical pressure on NCOT compounds further. Neutron diffraction data is currently being collected to allow for a more accurate determination of the structures of Ca2SrWO6 and Sr2.9Ca0.1WO6.
Donghyeok Kim	UCLA	23 Inorg/Mat	Homogenous Amplified Digital Immunoassay	Dino Di Carlo	Donghyuk Kim, Omai Garner, Aydogan Ozcan, and Dino Di Carlo	Today, healthcare concerns continue to stress the importance of an accurate, early diagnosis of diseases. The challenge lies in providing a simple, quick, and reliable detection of biomolecular markers (e.g., nucleic acids or proteins) in physiological samples. Herein, we present homogenous entropy-driven biomolecular assay (HEBA)1, an amplified assay which can detect various biomolecules in a robust and rapid one-pot reaction. We use an easily-programmable DNA machinery that catalytically2 drives a series of DNA hybridization/displacement reactions (Fig.1A) which generate an amplified signal in presence of an analyte (i.e., protein or nucleic acid). We demonstrate the utility of HEBA by using viral protein, viral RNA, and microRNA as analytes. Consequently, HEBA was able to successfully detect these molecules within 10 minutes without any washing steps or additional instrumentation (e.g., thermal control) in either a buffer or physiological fluids (i.e., undiluted blood and plasma). Furthermore, HEBA provided fM level limit of detection for all examined analytes (Fig.1B and 1C and 1E), which is orders of magnitudes higher compared to conventional, alike methods (Fig.1E) Lastly, we exploited HEBA in a digital assay format using a microfluidic well array, by which we achieved successful detection of a few tens of viral protein molecules (Fig. 1D). Further development of HEBA we believe will lead to a development of new advanced, point-of-care diagnostics

Annie Wong and Danish Pirzada	UCR	24 Inorg/Mat	Effect of Electrodeposition Variables on the Topography and Photoelectron Kinetics of Zinc Oxide Nanorods grown on Graphene	Ashok K. Mulchandan	Claudia Villarreal, Ashok K. Mulchandan	The growth of verticallyaligned zinc oxide nanorods (ZVNRs) has recently gained interest due to the possibility of growing high quality singlecrystalline 2D semiconductors with large surface area. ZnO is largely applied as electron acceptor material in a variety of solar energy harvesting devices, including dyesensitized solar cells. This work focuses on the growth of these caxis oriented ZVNRs on carbonbased flexible graphene. The application of large area graphene grown by chemical vapor deposition is being investigated as the transparent conductor in the ZnO photoanodes. The robust optoelectronic properties of graphene and the abundance of raw materials for its production makes it an attractive replacement to the commonly used fluorine-doped or indium tin oxide (FTO and ITO respectively), which are not only costly and brittle but also derived from conflict minerals. The main objective of this research is to study how the geometry of the ZVNRs on graphene affects the performance of this hybrid as photoanode platform. The ZVNRs are grown by electrodeposition on graphenecoated glass. Variations in the deposition conditions such as precursor concentration, temperature, time, applied potential, speed of mixing and the use of additives seem to have an observable effect on the geometry of the ZVNRs. By tuning the electrodeposition conditions we are able to obtain distinct geometries and achieve our ultimate goal of a hybrid optoelectronic material with efficient charge separation, fast charge transfer, and low electron interfacial recombination. ZVNR/G was characterized using various analytical methods: Xray diffraction, Raman spectroscopy, scanning electron microscopy and UVvisible transmittance spectroscopy measurements. We then used the ZVNR/G platform to fabricate dyesensitized solar cells and measure their performance. The internal resistance elements and charge transfer kinetics were determined with the techniques of open circuit voltage decay and electrochemical impedance spectroscopy. This way, the electrodeposition variables were correlated to the kinetics of photoelectrons generated in the hybrid.
Derek Deming	Concordia University	25 Org	Spectroscopic Measurements of Brown Carbon in Atmospheric Pollutants in Southern California	John W. Kenney, III		Recent studies have shown that organic aerosols are one of the major constituents of air pollution in both urban and rural environments. These organic aerosols are referred to as brown carbon (BrC).[1] BrC is a byproduct of incomplete combustion of fuels, biomass burning/decay, mobile vehicle emissions, stationary factory emissions, and emissions from common household appliances such as stoves and furnaces. Benzene (C6H6), toluene (C6H5CH3), and xylene (C8H10) are laboratory chemicals that are also constituents of atmospheric BrC. Each of these known BrC compounds was diluted into water to duplicate the characteristics of atmospheric BrC. These solutions were measured and analyzed spectroscopically using an ultraviolet-visible (UV) spectrophotometer. The control solutions provided reference spectra in the near-UV. Environmental air samples were collected via a water capture technique on the Concordia University campus and were measured and analyzed spectroscopically. Depending on the local weather conditions at the point of sample collection, some of the environmental samples displayed similar spectra compared to the laboratory control BrC solutions. Based on this preliminary study, it was verified that UV-visible spectroscopy can be used to detect BrC in the atmosphere. This initial study suggested that weather conditions may affect BrC levels at a given site. Future experimental studies will consider correlations between BrC levels and weather factors such as prevailing winds from Los Angeles toward Concordia University, Irvine and heavy dew conditions.

Giovanna Cano	CSU Fullerton	26 Org	Synthesis of Peptidomimetics for Inhibition of NS2B-NS3 Protease	Nicholas Salzameda	West Nile virus infection (WNV) has been shown in some cases to lead to the development of neuroinvasive conditions. The CDC estimates that about 1% of the estimated US incidences of WNV lead to a neuroinvasive condition such as meningitis or encephalitis. As of 2016, 2,038 cases of WNV infection were reported to the CDC with 1,140 of these cases presenting neuroinvasive conditions. Currently, there are no vaccines or therapeutic methods to treat WNV. The virus is composed of (+)ssRNA and a viral envelope which infects the host cell. The encapsulated RNA is translated into three structural and seven nonstructural peptides that are essential for viral replication in host cells. One of these components is the NS2B-NS3 protease, which contains serine protease, nucleoside triphosphate, and helicase activity necessary for cleaving the structural and nonstructural portions of the polyprotein of the new viral components.. Stopping the protease's enzymatic activity thereby ends WNV replication. Through organic synthesis our research focuses on the development of arginine and lysine peptidomimetics. Our current research has yielded inhibition of the NS2B-NS3 protein protease. As improvements are made these compounds are then tested through competitive enzyme assays to find better inhibition at lower concentrations. The results of these enzyme assays could lead to treatments for WNV.
Natalia Neris and Angelica Carmona	Mount Saint Mary's University	27 Org	Transesterification of Hypophosphorous Esters: A Methodology Study	Sylvine Deprele	Large oil spills in the ocean are catastrophic events, posing a great threat to marine life and the environment. Our project was influenced by the Deep Water Horizon oil spill in April 2010. Releasing a carbon-based solvent/surfactant mixture into the ocean allows for bioremediation and the decomposition of 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 a trimethylamine reaction. We have established step 1 of our three-step process by synthesizing long-chain hypophosphite esters, employing two different methodologies: one-pot one-step and one-pot two-step. The transesterification method involves varying classes of alcohols (primary, secondary, and tertiary), broad solvent scope (acetonitrile, hexane, toluene, and cyclohexane) and varying equivalence of alcohol (2, 4, and 6) along with a silicon derivative. In a one-pot one-step synthesis we add the alcohol, concentrated H_3PO_2 , and TEOS all at once in the selected solvent and let it reflux for 2 hours. In a one-pot two-step synthesis we add the concentrated H_3PO_2 and TEOS and let it reflux for 2 hours, and then add the alcohol for a total reflux time of 4 hours. The results for one-pot one-step and one-pot two-step showed that the best conditions were 4 equivalence of alcohol in acetonitrile and toluene yielding 31P crude NMR yield range of 32% to 88% product. Future directions include product yield optimization and hydrophosphinylation of the esters synthesized under Pd/Ni catalyzed conditions.

Ronnie Garcia	UCLA	28 Org	Efficient Synthesis of Pentiptycene: Symmetric Organic Building Blocks for New Material	Miguel Garcia-Garibay		Iptycenes are a group of molecules that have many applications due to their rigid symmetrical structures. Triptycenes, a member of the iptycene family, have been used as building blocks for molecular machines,1 polymers,2 and other materials.3 Extended analogs of triptycenes called pentiptycenes have the similar promise, but they have not been explored as extensively, in part due to their difficult and inefficient syntheses. Current strategies involve the laborious introduction of functional groups at the beginning of the synthesis, with a low-yielding step near the end, which causes much of the early work to be wasted. This work addresses those issues by formulating a high yielding, divergent synthetic pathway where the low-yielding construction of the pentiptycene scaffold is accomplished via a quinone intermediate before adding the functional groups to create the desired derivatives. Previously reported synthesis of the pentiptycene quinone works in 100mg,4while the new method developed shows a 70% yield regardless of the scale of the reaction. The pentiptycene quinone is then reduced to the hydroquinone and alkylated to form the pentiptycene scaffold for later functionalization. The alkylation, which is necessary for solubility purposes, is most effective in the absence of oxygen because the hydroquinone can be oxidized back to the quinone, which separates poorly from the desired product. Thus, a reaction closed to the environment raises the yield of the synthesis. Optimizing the synthesis will provide access to a variety of functionalized pentiptycenes, which have potential uses in solid-state machinery and materials applications.
Katrina Ngo and Susan Andersen	SDSU	29 Org	tCc – A New Family of Fluorescent Nucleosides	Byron Purse	Dillon D. Burns and Byron Purse	Fluorescent nucleotides can act as useful molecular probes as well as fluorescent markers for the study of nucleic acids, but brighter probes are needed for new applications including fluorescence microscopy. Previous work done in our group on nucleoside analogues has led to the development of a new generation of modified fluorescent analogues known as tricyclic cytosines (tC), which are able to participate in normal G:C base pairs in DNA while functioning as molecular probes. The properties of these tC compounds led us to propose a new structure for fluorescent nucleotide design, tCc. We hypothesize that tCc compounds will be the most fluorescent of the cytidine analogues because of the stronger conjugated system that exists within the molecule. We used an efficient series of synthetic reactions to construct the molecule, and we characterized the intermediates and products using 1H NMR spectroscopy and mass spectrometry. The main ring system of the molecule was built using a series of reactions that included the Vilsmeier reaction and the Knoevenagel condensation for critical C–C bond forming steps. The unique carbon-carbon bond linking the sugar to the nucleobase was achieved by utilizing the Heck reaction and our nucleoside analogue was confirmed via NMR spectroscopy and mass spectrometry. Initial observations show that the parent tCC compound is fluorescent, but further tuning will be needed to maximize its brightness. In the future, we intend to synthesize derivatives consisting of various electron withdrawing and electron donating groups to further tune the conjugation. Future steps include transforming our nucleosides into nucleoside phosphoramidites and incorporating them into DNA using solid-phase synthesis.

Christian Moreno	Cal Poly Pomona	30 Org	Toward the Synthesis of Cyclic Carbonates Based on FAME Derivatives	Michael F.Z. Page	Victor Wyatt and Michael F.Z. Page	Vast amounts of petroleum is used every day to generate electricity, fuel our vehicles, and form plastics. Biodiesel is a renewable, clean-burning diesel alternative that could assist in reducing U.S. dependence on foreign petroleum and help meet our current energy needs. Fatty acid methyl esters (FAMEs) are synthesized through a transesterification between a triacylglyceride and methanol in the presence of a catalyst. Previously, the Page group synthesized green polyurethanes from seed oils with varying equivalents of polyols from FAMEs that were crosslinked with petroleum-based diisocyanate. Isocyanates can cause skin irritation, asthma, and bronchitis. In 2015, Hybrid Coating Technologies won the Presidential Green Challenge for designing a hybrid non-isocyanate polyurethane. This non-isocyanate β-hydroxyurethane formed from a reaction between cyclic carbonates and aliphatic polyamines. Currently, the Page group plans to synthesize a non-isocyanate polyurethane using waste oil FAMEs as the only starting materials. The proposed synthesis involves a conversion of the alkene within the fatty chain to a cyclic carbonate. In the preliminary steps methyl oleate (1) is converted to epoxide 2 with a key 1H chemical resonance at 2.889 ppm. In the subsequent step, 2 will eventually be converted to cyclic carbonate 3. Following characterization, 3 will be primed to be polymerized with a polyamine from another related FAME derivative; ultimately leading to a diisocyanate-free polyurethane material.
Masis Parunyan, Elenie Philippas, Jennifer Jensen	CSU Northridge	31 Org	Understanding the metabolic transformations of resveratrol by human enzymes	Gagik Melikyan		Experimental research suggests that the metabolic oxidation of resveratrol, a polyhydroxylated stilbenoid found in red wine, by cytochrome P450 enzymes (CYPs) of the human digestive system may have severe deleterious health effects. Enzymatic transformations of resveratrol and its 3’-hydroxylated derivative piceatannol were investigated by exposing them to human esophageal and hepatic CYPs (CYP4F3, 3A4, 1A1, 4F12, 2C8, 2C9, 2E1, 2A6, 2C18). Metabolic profiles were studied by using high-pressure liquid chromatography (HPLC) method. Gradient elution was applied to enhance separation between resveratrol and its hydroxylated derivatives, establishing a reliable qualitative method for the identification of structurally related metabolites. Resveratrol-derived piceatannol was oxidized in vitro to yield the carcinogenic orthoquinone, 4-[(E)-2-(3,5-dihydroxyphenyl)ethenyl]benzene-1,2-dione, characterized by 1 H/ 13C NMR spectroscopy and mass spectrometry. Stability studies indicate that in an environment mimicking physiological conditions this quinone may have a lifetime of several days or even weeks. The negative ramifications for public health will be discussed along with the prudence of selling resveratrol to the general public as a food supplement.

Sarah Baker	CSU Fullerton	32 Org	The Intramolecular reactions of Oxime and Oxime Ether Radicals and Radical Cations using Alkenes as a Potential Nucleophile or Radical Trap	H. J. Peter de Lijser	Nicholas R. Armada, Emmie Ho, Andrew S. Petit, and H. J. Peter de Lijser	The formation of radicals and radical cations result from oxidative processes. When oxidation of oximes and oxime ethers occur, iminoxyl radicals and oxime radicals are produced. The reactivity of these intermediates is largely unexplored and to learn about the fundamental reactivity of iminoxyl radicals and oxime ether radical cations, we have begun an investigation on intramolecular reactions of oximes and oxime ethers using built-in alkenes as a potential nucleophile or radical trap. Previously, built-in alkynes were found to act as radical traps whereas aromatic rings were found to act as nucleophiles. This project explores the reactivity of alkene functional groups under similar oxidative conditions. We hypothesize that the alkene functional group may act as a nucleophile and as a radical trap to form the cyclized product. Photolysis of the substrate at 420 nm with 9,10-dicyanoanthracene (DCA) as the photosensitizer leads to the formation of the iminoxyl radical (oxime) or radical cation (oxime ether) intermediate that can then cyclize. Studies on the PET reactions of the vinyl oxime (1a) and oxime ether (1b) did not show any evidence of cyclization. Preliminary results suggest that cyclization occurs at the nitrogen for the 2-isopropenyl derivative for both the oxime (2a) and the oxime ether (2b). NMR analysis of both reactions upon irradiation at 420 nm in the presence of DCA for up to 4 hours shows the formation of new products over time; the product mixtures of the oxime and oxime ether show very distinct similarities suggesting that the products formed are very similar. The NMR results are consistent with structures formed using a cyclization pathway. The exact identity of the cyclic product formed in these reactions is unclear and further analysis of the reaction mixtures is being completed using NMR and GC/MS. Computational studies are being performed to obtain mechanistic insights into why the presence or absence of a methyl group on the alkene group has such a pronounced impact on the reaction. The results of these studies, as well as those of the E- and Z-propenyl derivatives (3a, 3b, 4a, and 4b) will be discussed.
Catherine Taylor	CSU Fullerton	33 Org	Synthesis of Complex Ring Systems via Photoinduced Oxidative Cyclization Reactions of Benzaldehyde Oximes and Oxime Ethers	H. J. Peter de Lijser	Abdullah Alshreimi, Mimi Le, and H. J. Peter de Lijser	The use of oxidative cyclization with radical or radical ion intermediates is a potentially useful and efficient strategy to achieve the synthesis of novel heteroaromatic structures. Oxime ethers with built in aromatic groups have been shown to undergo a cyclization reaction in which the aromatic ring acts a nucleophile attacking the oxime ether radical cation. Using this same methodology, aromatic nucleophiles with built in heteroatoms could lead to potential new synthetic pathways of interesting and complicated heteroaromatic ring systems. To determine whether heteroaromatic rings can be used as nucleophiles under oxidative cyclization conditions, we prepared a series of benzaldehyde oximes and oxime ethers substituted with heteroaromatics rings containing nitrogen, oxygen, and sulfur. The purified oximes and oxime ethers were subjected to photooxidation processes in controlled conditions and were monitored by GC/MS and NMR for product formation. The result from these studies suggest that the oximes formed their parent aldehydes but did not show signs of cyclization. Several oxime ethers were found to yield what is believed to be a cyclized product via nucleophilic attack by the heteroaromatic ring on the nitrogen of the oxime ether. The most promising results were obtained with the thiophenyl derivatives of the oxime ethers. To further determine if the thiophenyl oxime ether derivatives did in fact cyclize, the reaction is being optimized so the product can be isolated and characterized. In the process of synthesizing the furanyl and thiophenyl oxime derivatives an unknown, possibly cyclized, side product is formed. These side products are being analyzed and characterized. The mechanistic pathway of this product formation is also being investigated.

Huy T Bui	Cal Poly Pomona	34 Org	A Study of Molybdenum Catalysts for the Deoxydehydration Reaction	Alex John	Nathan W. Green, Alex John	We report a study on molybdenum catalysts of the type LMoO2 supported over ancillary ligands for converting vicinal diols into olefins. Fossil resources which include natural gas, coal, and petroleum are currently the primary energy and material feedstock. Unfortunately, these resources are finite and have adverse environmental effects. Researchers are working towards identifying and utilizing renewable and sustainable resources such as wind, sun, water, and biomass to accommodate our current and future energy and material needs. A fundamental difference between biomass and petroleum is that biomass, such as cellulose, is highly functionalized whereas petroleum is of hydrocarbon nature. Therefore, being able to convert molecules that have characteristics of biomass to those that are hydrocarbon-like is a critical step in efforts to incorporate biomass-derived into chemical processes. A promising reaction in this direction is deoxydehydration (DODH), that transforms a vicinal diol into an olefin. In the recent past, rhenium (Re) has been the metal of choice for its efficiency as a catalyst in the DODH reaction. However, it is not economically feasible and its low abundance in the earth's crust adds to the concern. Alternatively, molybdenum (Mo) is a reasonable substitute for Re in the DODH reaction because of its similar chemical properties and low cost. The focus of this project is to synthesize and explore the reactivity and selectivity of various molybdenum catalysts (LMoO2) supported over salan type ligands for the DODH reaction. Deoxydehydration studies using these molybdenum catalysts will be discussed.
Stephannie Jimenez and Stephania Luna	Mount Saint Mary's University	35 PhysAnal/Theory	A Correlation Study Between Particulate Matter and PAH Concentrations: The Bio-monitoring of Pine Tree Leaves	Sylvine Deprèle		Polycyclic aromatic hydrocarbons are organic compounds composed of two or more fused benzene rings. They are naturally found in the environment but, can also be man-made. PAHs are created through an incomplete combustion reaction with an unknown amount of oxygen, resulting in unwanted byproducts such as carbon monoxide and PAHs. They are detrimental to our health because they are carcinogenic, teratogenic, and mutagenic. PAHs are inherent in particulate matter, which is a mixture of solid particles and liquid droplets in the air. Due to their toxic properties, it is important to qualify as well as quantify PAHs. Here, we propose the bio-monitoring of PAHs through pine tree leaves from the Italian Blue Cyprus tree in two designated areas near the I-405 Freeway and on the Mount Saint Mary's University campus. PAHs were extracted via a continuous Soxhlet extraction, further processed and analyzed by the Gas Chromatography Mass Spectrometer (GCMS). A Selected Ion Monitoring (SIM) table was used to search for the 16 most common PAHs found in the sample (Environmental Protection Agency (EPA) standard was used for reference). Through a series of calculations, the concentration of the PAHs were graphed and compared with the values of PMs reported by the EPA. Since PAHs fall within the family of particulate matter, a direct correlation between the concentration of PAHs and PM values reported was expected. Samples collected from the freeway and campus area showed a direct correlation with few discrepancies that can be linked to weather patterns. Analysis of the data confirmed that our campus location, on top of a hill, displays higher levels of PAHs than the I-405 freeway area. For future directions, we will continue to monitor PMs and PAHs during different seasons and analyze previous data acquired to finalize the quantification and qualification of PAH and PM concentrations found within the designated areas.

Rahia Solomon	Mount Saint Mary's University	36 Phys/Anal/Theory	Enantiomeric interactions of amino acids adsorbed in zeolites: An investigation using Solid-State NMR and Molecular Modelling	Deniz Cizmeciyan	In the past years we studied zeolites as a medium for enriching the enantiomeric excess of solutions. Zeolite being achiral, do not prefer one enantiomer over the other. 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. Recently, in order to investigate this behavior further we decided to study the same set of systems with molecular modelling. As a starting point, considering only Van der Waals interactions, we investigated how these amino acids were fitting into the zeolite cage. We found that Alanine gets adsorbed better than Leucine and Methionine. We will present the results of computer simulations regarding the dynamics and energetics of the enantiomer-zeolite interactions.
Taehoon Ha	CSU San Marcos	37 Phys/Anal/Theory	Extraction of the Active Component of Kratom Leaves	Karno Ng	Kratom, also known as Mitragyna speciosa, is a tropical evergreen tree in the coffee family. It is native to Southeast Asia. Kratom leaves have been used for hundreds of years in traditional medicine to relieve the pain. The leaves can be chewed in raw and can also be processed into tablets and capsules. In the recent years, there is an increase of uses of Kratom leaves as a recreational drug. The primary active alkaloid substance, Mitragynine, found in the Kratom leaves affects the same receptor as the opioids such as heroine, morphine, and codeine. Consumption of Kratom leaves can lead to psychotic symptoms and mental addition. The potential effects of Kratom leaves on humans draw international concerns. In some countries such as Finland and Hungary, the use and/or importation of Kratom leaves are restricted. The Drug Enforcement Agency (DEA) had initiated an attempt to move Kratom to controlled substance list (Schedule 1) in 2016. The purpose of this study is to develop an efficient extraction method for mitragynine from Kratom leaves. One gram of crushed Kratom leaves were soaked in methanol and sonicated. At the end of the soaking period, solvent was evaporated under vacuum to yield the methanol extract that is rich in alkaloid. The methanol extract was mixed with 90% acetic acid and the content was partitioned between the aqueous and petroleum ether. The aqueous layer is collected and basified with Na2CO3 to pH 9. The alkoloid was then extracted into chloroform. The extract was washed with distilled water and dried over Na2SO4 anhydrous. The extract was then loaded to the packed silica column and eluted with chloroform. The elute is evaporated and the resulting extract was dissolved in 1.5 mL of methanol and then filtered through a 0.45 mm syringe filter prior to injection to HPLC with a C-18 column. The sample is eluted isocratically with a mobile phase of 0.05% formic acid and acetonitrile at pH 5.0 (50:50, v/v), flow rate = 1.0 ml/min. Mitragynine is detected at 223 nm.

Laura Marsalla	CSU Fullerton	38 Phys/Anat/Theory	Understanding the Reactivity of Iminoxyl Radicals with Built-In Alkynyl Radical Traps	Andrew Petit	Peter de Lijser, Andrew Petit	Recently, the de Lijser lab used photoinduced electron transfer (PET) to prepare reactive radical cations and iminoxyl radical intermediates from oxime derivatives containing a built-in alkynyl group. They used nuclear magnetic resonance (NMR) to monitor the reaction mixture and look for evidence of intramolecular cyclization. Their results suggest that once the iminoxyl radical forms, the alkynyl group can act as a radical trap causing intramolecular cyclization. Isolation of the cyclized products has been difficult, preventing their experimental characterization. In order to aid in the identification of the cyclized products, we calculated NMR chemical shifts for a series of possible products using computational chemistry. Our results suggest that five-membered heterocyclic exo products were formed via intramolecular cyclization of the iminoxyl radical.
Zachary To	UC Riverside	39 Phys/Anal/Theory	Growth of Monolayer Molybdenum Disulfide Through Chemical Vapor Deposition on Silicon Dioxide Substrates	Ludwig Bartels		Transition metal dichalcogenides (TMDs), such as molybdenum disulfide (MoS2), have been gaining popularity due to their semiconducting properties at the monolayer limit. The research goal is to find and optimize a facile method to grow consistent MoS2 using a chemical vapor deposition tube furnace. Characterization methods such as raman and photoluminescence spectroscopy are used to assess the quality of the growth. Raman spectroscopy is used to observe the molecular vibrations, and photoluminescence measures the band-gap by exciting the electrons in the valence band with light. Monolayer MoS2 exhibits a direct band-gap at 1.85 eV, and shows promising spintronic and optoelectronic properties. The application of TMDs can create electronics flexible, energy efficient, and faster electronics.

Adan Garcia	CSU San Marcos	40 Phys/Anal/Theory	Extraction and Detection of Cancer Treatment Drug with Phenytoin in Biological Samples	Karno Ng	Karno Ng	Among patients with cancer, in particular brain tumors, seizures can become a daily routine in their everyday lives. To counter-act the seizures, an antiepileptic drug such as phenytoin is administered to act as an anticonvulsant that is in essence a muscle relaxant. Dexamethasone is classified as a corticosteroid and has many uses in cancer treatment. One of the uses of dexamethasone among cancer patients is to decrease the amount of swelling around the tumor. Dexamethasone is also used for the treatment of nausea caused by chemotherapy. In addition, dexamethasone is used as a cancer treatment for a variety of cancers, such as leukemia, lymphoma, and multiple myeloma. Phenytoin and dexamethasone are frequently administrated concurrently to brain cancer patients. A previous study has shown that phenytoin serum concentration decreases when it is administrated concurrently with dexamethasone.1 Thus, it is important to monitor the concentration of these two drugs in biological samples, in order to ensure that the proper dosages are administrated to the patients. The purpose of this study is to develop an effective extraction and detection method for dexamethasone and phenytoin. A reverse phase high performance liquid chromatography (HPLC) method with UV/VIS detection has been developed to separate phenytoin and dexamethasone at 219 nm and 241 nm respectively from urine samples. The mobile phase consists of a mixture of 0.01 M KH_2PO_4, acetonitrile and methanol adjusted to pH 5.6 (48:32:20) and is pumped at a flow rate of 1.0 mL/min. Calibration curves were prepared for phenytoin and dexamethasone. The calibration curves show good linearity (r^2 >0.99). The detection limit for phenytoin and dexamethasone is 0.625 g/mL and 0.053 g/mL respectively. An efficient solid phase extraction method with the use of C-18 cartridges on urine samples was developed. The percent recovery for phenytoin and dexamethasone is 90.46% and 89.53% respectively.
Katey McCoy	CSU Fullerton	41 Phys/Anal/Theory	Measurement of the Hygroscopic Growth of Brown Carbon Mixtures using a Tandem Differential Mobility Analyzer	Paula K. Hudson	Ali Saad, Damaris Chavez and Paula K. Hudson	Atmospheric aerosols are small particles that can affect climate by directly absorbing and scattering solar radiation. Further, aerosol particles have the ability to act as cloud condensation nuclei (CCN) through the uptake of water. Depending on the amount of water an aerosol absorbs as a CCN, it could form highly reflective white clouds which would then have a cooling effect on climate as incoming sunlight is reflected back into space. However, the degree of cooling is dependent on the aerosol particle composition. Brown carbon, one type of aerosol, can be formed in a number of ways but is commonly formed by reacting an aldehyde, glyoxal, with a nitrogen containing compound such as glycine or ammonium sulfate. Given that these three particular compounds used to form brown carbon have different water uptake properties, and that reactants and products can change with atmospheric processing, it is important to study the hygroscopic properties of brown carbon aerosol. In this study, a tandem differential mobility analyzer (TDMA) is used to measure the hygroscopic growth, the uptake of water, of brown carbon aerosol particles by measuring the particle size before and after exposure to relative humidity. The hygroscopic growth of brown carbon samples generated from mixtures of glyoxal and glycine, or glyoxal and ammonium sulfate, in mole ratios of 1:1, 1:0.5, 0.5:1, before and after photolysis, were measured to determine the effects of various compositions of brown carbon and their ability to act as CCN. In general, the hygroscopic growth of brown carbon generated from ammonium sulfate mixtures are higher than glycine mixtures which would result in the formation of more reflective clouds and a stronger cooling effect. This study provides information to be used by climate modelers to improve the predictive capability of climate change due to different brown carbon sources.

Poster Presentation Abstracts - Session 2

Name	Institution	Poster#/Area	Title	Advisor	Coauthors	Abstract
Sylvia Alejo	UCI	1 Biochem	Filter binding assay generates a binding affinity constant of aptamer and Nogo-66, which corresponds to therapeutic application to neural growth in mouse primary neurons	Melanie Cocco	Verna Vu, Ali Alhoshani, Melanie Cocco	Injury and deterioration of adult mammalian neurons in the central nervous system has long been thought of as impervious to any treatment in comparison to peripheral nerves. Reticulon-4 contains a 66 residue region called Nogo-66 that binds to the Nogo receptor 1 (NgR1); this interaction is responsible for nerve growth inhibition (GrandPre et al., 2000, Fournier et al. 2001). Through a systematic evolution of ligands by exponential enrichment (SELEX) procedure, tight binding aptamers were selected for Nogo-66 (Jayasena et al., 1999). This was done by subsequent steps of selection and amplification of single-stranded DNA from a randomly generated library of ssDNA oligonucleotide. Thus, it is hypothesized that the aptamer sequenced is able to disrupt the Nogo-66/NgR1 interaction. Functional assays were conducted using mouse primary neurons which showed a significant increase in axonal growth. Further analysis was done by determining the binding affinity of the aptamer to Nogo-66 using a filter binding assay. The aptamer was tagged with γ-32P that was then incubated with increasing concentration of Nogo-66. These results show that aptamer and Nogo-66 binding occurs in the nanomolar range making our selected aptamer a potential therapeutic molecule. The use of aptamers, with its three-dimensional structure that rivals antibody binding, is justified by its cost-effective approach in terms of labor and reproducibility. These oligonucleotides are much more easy to identify, manufacture and store as future therapeutic drugs than antibodies. Pilot studies are underway to test the efficacy of the aptamer on animal models.
Nikolay Maslov	CSU San Bernardino	2 Biochem	Developing chemical inhibitors to investigate the function of falcilysin, an essential malarial protease	Jeremy Mallari		The protozoan parasite Plasmodium falciparum causes approximately over half of million fatal cases of malaria per year, mostly occurring in Africa. Falcilysin (FLN) is a metalloprotease expressed by the parasite—it is necessary for its development in the host red blood cell. However, its function is poorly understood. We are developing competitive inhibitors of FLN with a piperazine hydroxamic acid-based scaffold. Previous studies in our lab have shown that this class of compounds has good inhibitory activity against recombinant FLN and cultured P. falciparum. Our team is synthesizing inhibitors through a 4-step route and purifying them with a combination of extraction and flash chromatography. Eight of the compounds were tested for inhibition in a FRET-based substrate cleavage assay. During this study, we have identified several features important for inhibitor against FLN. Specifically, introduction of an amide group at the N4 position leads to a significant improvement in activity compared to similar amines. This strategy produced our most potent inhibitor against FLN so far (IC50 < 10 µM).

Randall Ortega	CSU Fullerton	3 Biochem	Purification and Preliminary Crystallization of a Bacterial Dihydromethanopterin Reductase (DmrA) Involved in Tetrahydromethanopterin Biosynthesis in Methylobacterium extorquens	Madeline E. Rasche	Madeline E. Rasche	The one-carbon metabolism of methane-producing archaea and methylotrophic bacteria requires the cofactor tetrahydromethanopterin (H4MPT), an uncommon tetrahydrofolate analog. In archaea, the final step of H4MPT biosynthesis is the reduction of dihydromethanopterin to H4MPT by dihydromethanopterin reductase X (DmrX). Curiously, no DmrX homolog exists in the genome of the bacterium Methylobacterium extorquens AM1. Instead, the final reaction is catalyzed by DmrA, a homolog of bacterial dihydrofolate reductase (DHFR). This finding has led to the hypothesis that DmrA evolved from duplication and mutation of an ancestral dhfr gene. To gain insight into evolutionary changes that may have altered the substrate specificity from dihydrofolate to dihydromethanopterin, computational modeling and crystallography studies were initiated. Using DHFR as a template, ICM-Pro was able to predict the overall protein fold of DmrA and the NADPH binding site, but was unsuccessful in modeling a dihydromethanopterin binding site. Therefore, in preparation for crystallography, we developed a strategy to increase the solubility of recombinant DmrA and decrease its potential for aggregation. Shortening the N-terminal histidine tag from six to four histidines and storing the cells at pH 8 instead of pH 6.8 allowed purification of a single quaternary structure. Following nickel affinity chromatography and desalting, a protein concentration of 4.11 µg/µL was obtained. SDS-PAGE showed greater than 95% purity with a main band at 17 kDa, while a single band at 396 kDa was obtained by native PAGE. A preliminary crystallization trial resulted in successful light precipitation using buffer containing 0.1 M Tris hydrochloride, 2.0 M Ammonium sulfate, pH 8.5 with a 2:1 ratio of sample:buffer. However, a crystallization screen with 288 conditions resulted in no precipitate or crystals, indicating that a higher protein concentration might be beneficial for crystallography. Future research will focus on identifying protein concentration, salt, and buffer conditions suitable for DmrA crystallization and structure determination.
Caroline Aziz	Chapman University	4 Biochem	Partial Amino Acid Sequence and Anti-Cancerous Activity of a Lipid Transfer Protein from Fennel (Foeniculum vulgare) Seeds	Aftab Ahmed	Rukhsana Lalani, Mekdes Megeressa, Umesh T. Sankpal, Riyaz Basha, and Aftab Ahmed	Fennel (Foeniculum vulgare) is a biennial Egyptian medicinal plant with an aromatic odor that belongs to the family Apiaceae (Umbelliferae). Fennel seeds are commonly used in traditional medicine as they are known to have anti-inflammatory, anti-fungal and anti-cancer activities. The major constituents of the fennel seeds are sugars, minerals, essential fatty acids, proteins and fibers. Although, there are numerous studies on the medicinal properties of essential oils of the fennel seeds, they are not much focused on the proteins and peptides. The objective of current project is to fully characterize the primary structure of proteins and to test their biological activities. We present here the preliminary data on the amino acid sequence of lipid transfer protein (LTP) from fennel seeds and its biological (anti-cancer) activity using human cancer cells. The proteins were extracted in Tris/HCl pH 8.0 buffer and successfully purified by two dimensional liquid chromatography (2D-LC), using gel filtration chromatography followed by reverse phase HPLC (RP-HPLC). The purity of isolated LTP protein was judged by the SDS gel electrophoresis. The purified protein was loaded on to the PVDF disc and sequenced by automated amino acid sequencer, model PPSQ-31A (Shimadzu). The partial amino acid sequence of intact LTP protein was successfully established up to 23 amino acid residues. The amino acid sequence search was performed by Protein BLAST which confirmed it as a lipid transfer protein. The Cell viability assay was performed on the isolated LTP protein using the CellTiter-Glo (Promega). The results of the assay demonstrated anti-proliferative activity against prostate (PC3) and breast (MCF7) cancer cell lines, showing a decrease in cell viability approximately 30% and 60% in PC3 and MCF7 cell lines respectively.

Lucy Chen	Chapman University	5 Biochem	Extraction and Purification of Proteins from Turmeric (Curcuma longa) Root	Aftab Ahmed	Rukhsana Lalani and Aftab Ahmed	Herbal medicines have been in use since ancient times for the treatment of various ailments. According to WHO about 80% of the world population relies on plant-based herbal medicine. Despite the advancements in modern medicine, traditional medicines involving the use of plants have gradually been accepted as a complementary medicine throughout the world. Turmeric is one such plant that plays an important role as a common spice and also well-known for its medicinal properties. In South Asian countries such as India and Pakistan, turmeric is often used to treat diseases such as gastrointestinal disorders, arthritis, depression, asthma, and diabetic wounds. This plant has also been extensively studied for its anti-tumor, antimicrobial, and antioxidant activity. In this poster, we are presenting the preliminary data on the extraction and purification of proteins from of turmeric (Curcuma longa), which belongs to the plant family of Zingiberaceae. Proteins were extracted from powdered turmeric in 20 mM Tris/HCl pH 8, 50 mM sodium acetate pH 5.2, 10 mM sodium phosphate pH 7 and 0.1% acetic acid in water. Purification of proteins was carried out using gel filtration chromatography using Sephacryl-S200 10/60 column. Fractions were pooled and analyzed by Tris/Tricine gel electrophoresis. Further purification was successfully achieved by reverse-phase HPLC using Aeries Protein (4.6x25 mm) column. Further work is in progress to establish the complete primary structure of the purified proteins using the automated Edman sequencing technique.
Brandon Yeshoua	University of Southern California	6 Biochem	Combining Antibacterial Antibodies to Enhance Opsonophagocytosis of Acinetobacter baumannii	B. Spellberg	B. Pascual, T. B. Nielsen, B. Spellberg	We are developing monoclonal antibodies (MAbs) as a novel therapeutic approach to highly antibiotic-resistant Acinetobacter baumannii infections. A. baumannii is highly diverse, with an estimated >100 serotypes. As a result a combination MAb regimen will be necessary to cover sufficient clinical isolates to establish a viable therapeutic. One concern about combining multiple MAbs targeting a single pathogen is the potential for antagonism to occur, as one MAb may interfere with binding of another MAb to its epitope target. We investigated the effect (synergistic, antagonistic, or neither) on opsonophagocytosis upon combining two anti-Acinetobacter baumannii monoclonal antibodies (MAbs) in vitro: MAb C8 and MAb 39. We first used flow cytometry to select strains of the bacterium A. baumannii that were bound by both, either, or neither antibody (Table 1). After selecting suitable strains, we then performed a phagocytosis assay using RAW 264.7 mouse macrophages to quantify the variable uptake of bacteria due to antibody opsonization. We were able to confirm that combining the two antibodies for opsonophagocytosis enabled macrophages to phagocytize pathogens to which only one of the MAbs bound, and that antagonism between the MAbs was not observed. Thus, combining MAbs is a viable approach to targeting A. baumannii, which will enable coverage of multiple serotypes without antagonism. We seek to confirm these results in vivo.

Ervin Irimpan	UCI	7 Biochem	Structure of CDI toxin reveals a novel bacterial member of the RNase A superfamily	Celia W. Goulding	Gaëlle Batot, Karolina Michalska, Greg Ekberg, Grazyna Joachimiak, Robert Jedrzejczak, Gyorgy Babnigg, Christopher S. Hayes, Andrzej Joachimiak, Celia W. Goulding	Contact Dependent growth Inhibition (CDI) is one mechanism that Gram negative bacteria utilize to communicate with each other. The CdiA protein is a large cell surface protein that delivers its C-terminal toxin domain (CdiA-CT) to neighboring bacteria cells upon cell to cell contact. CDI+ bacteria can express a cognate immunity protein (CdiI) which binds tightly to its cognate toxin thereby rendering the toxin inactive. Our collaborators solved the X-ray crystal structure of the CdiA-CT/CdiI toxin-immunity pair from Yersinia kristensenii. The toxin (CdiA-CT) has structural homology to the mammalian RNase A superfamily, however, the toxin did not retain the characteristic disulfide bonds and has little to no sequence similarity to RNase A paralogs. In my laboratory, we purified wild-type toxin alone along with a series of mutations to probe their role in its predicted RNase function. We showed that the toxin did possess RNase activity and mutational analysis of His175, Arg186, Thr276 and Tyr278 show that these residues contribute to its activity. We also demonstrated that CdiI inhibits the toxin's RNase activity. The CdiA-CT toxin from Y.kristensenii is the first non-vertebrate protein found to possess the RNase A superfamily fold, and homologs of this toxin have been discovered throughout bacterial secretion systems which are associated with inter bacterial communication in many Gram-negative and Gram-positive bacteria.
Sarah Castillo	Mount Saint Mary's University	8 Biochem	Characterization of Glutathione Inhibition of Oxidative DNA-Protein Crosslinking	Eric Stemp	Mary Bekarian, Sarah Castillo, Mary Safaeipour, Maritza Sanchez, Juliette Jauregui and Eric Stemp	Glutathione is a small cysteine-containing peptide responsible for redox buffering in the cell. Here, we investigated whether it might be possible for glutathione, a strong reductant, to inhibit DNA damage (e.g. DNA-protein crosslinks) by engaging in redox repair of the 1-electron oxidized guanine base as formed by the flash-quench method. Samples containing Ru(phen)2dppz 2+ [phen = phenanthroline, dppz = dipyridophenazine], Co(NH3)5Cl2+, histone protein, calf thymus DNA were irradiated for 0-240 seconds in the absence or presence of glutathione with 442 nm light to effect guanine damage. In the chloroform extraction assay, we found that the 260 nm absorption of free DNA decreased with increasing irradiation time, consistent with crosslinking, and that the crosslinking plateaued at a higher value when the histone concentration was increased. In a separate experiment, the DNA samples were also subjected to ultrafiltration to remove the glutathione, which was then analyzed by reversed phase HPLC. Separation of the reduced and oxidized glutathione was observed by monitoring absorbance at the 220 nm wavelength. As irradiation time increased, the intensity of the oxidized glutathione peak increased, consistent with the redox repair mechanism described above. Furthermore, we compared the effect of reduced and oxidized glutathione in our samples via the gel shift assay and it was observed that the oxidized form had little to no effect on reducing the crosslinking, while the reduced form decreased crosslinking. 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)2dppz 2+ , indicating that it most likely reacts with the guanine radical directly.

Daniel A. Coello	CSU Dominguez Hills	9 Biochem	Histone methylation status by temozolomide in tumor cells	Tieli Wang	Hugo Mora, Maria Nava, Lili Nyugen, Anthony Diaz, Amanda Parker, James Gallo, and Tieli Wang	Histone methylation is a well-known mechanism of epigenetic regulation. The epigenetic event is a potential driver of acquired chemo-resistance. Temozolomide (TMZ) is a methylating agent used for clinical treatment of several types of cancers and remains as the main chemotherapy agent based on its ability to increase the median survival of the patient. In our previous study, we have found that TMZ was able to methylate recombinant histone using the proteomic technology. In this presentation, we are interested in identifying the histone methylations status following the TMZ treatment in brain and triple negative breast cancer cells to find out whether TMZ will alternate the histone methylation status in tumor cells using western blot analysis. Our results showed that histone methylation was decreased as we increase the concentration of TMZ in brain tumor cells while the histone methylation status was not significantly affected by TMZ in triple negative brain cancer cells. The results indicate that histone associated proteins may be a target of TMZ in brain tumor cells but not in triple negative breast cancer cells.
Rima Sanyal	Chapman University	10 Biochem	Structure Activity Relationship Studies of a Diarylpentanoid that Induces Reactive Oxygen Species in Prostate Cancer Cells	Marco Bisoffi	Justin O'Neill and Marco Bisoffi	Prostate cancer, or prostatic adenocarcinoma has been shown to thrive on the high concentrations of androgen secreted by the testicular and adrenal glands. Curcumin analog and diarylpentanoid ca27 (5-bis(2-hydroxylphenyl)-1,4-pentadien-3-one) has been shown to induce reactive oxygen species (ROS) which have been shown to down regulate the androgen receptor in prostate cancer cells and thus impede tumor progression. Curcumin, ca27, various other analogs with a hydroxyl (OH) group at different positions (ortho-meta-para) on the aryl rings, and analogs of ca27 without any OH groups or Michael acceptor groups were used to treat LNCaP prostate cancer cells to determine the amount of ROS induced. LNCaP cells were incubated in black 96-well plates with the compounds at multiple concentrations alongside DMSO as a control and hydrogen peroxide as a standard ROS. ROS induction was determined via dichlorofluorescein (DCF) mediated fluorescence and glutathione (GSSG/GSG) detection assay. DCF data was normalized using Hoechst dye. Our preliminary data shows that all analogs analyzed induce more ROS than curcumin and that analog c58 (OH group at meta position on aryl groups) showed the lowest oxidant potential, indicating that the presence of Michael acceptors and the position of OH groups determine the potential of diarylpentanoids to induce ROS and down-regulate the androgen receptor. It is expected that our structure activity relationship (SAR) studies will identify pharmacophores that can be used in further drug development efforts towards a therapeutic strategy against prostate cancer.

Quang-Minh Dang	UCI	11 Biochem	Understanding the Roles and Functions of Cryptochrome in Magnetoreception	Albert Siryaporn	Many eukaryotic organisms detect magnetic fields, but the molecular mechanisms of magnetoreception are unknown. Recent work hypothesized that Cryptochrome 1 (Cry1) is a magnetosensor. We test this hypothesis by creating a custom and working model for Eukaryotic Cryptochrome in bacteria. We constructed a chimera of Cry1 with CpxA, a two-component system histidine kinase, in E. coli. Two-component systems are signal transduction pathways in which histidine kinases phosphorylate response regulators, which are typically transcription factors, and can be observed with activation of fluorescent proteins. Thus, a Cry1 two-component system hybrid system in E. coli represents a way to probe magnetoreception using a finely tuned signal transduction pathway. To characterize the photon and magneto-responsive characteristics of Cry1, we will use blue light activation and a two-component system reporter. A photoresponse is considered any measurable chemical or biological response to light and magnetoresponse is a response that allows an organism to perceive a magnetic field for purposes of direction and orientation. This research aims to test the expression of the reporter system under several blue light activation and magnetic fields in vivo in order to learn more about the functions of cryptochrome. Light activation involves measurements in lux for illuminance and magnetic activations measurements in tesla for magnetic flux density. We will also use a directional evolutionary approach to insert CpxA at random locations in Cry1 and screen for a magneto-response and optical response. Much of the preliminary work has been completed and the results are encouraging for an implementation of our testing techniques.
Denny Biju and Diana Rios	CSU Bakersfield	12 Biochem	The Impact of Roasting Level on the Phenolic Acid Profile of Coffee	Sarah Forester	According to the American Cancer Society, cancer is becoming one of the leading causes of death in the United States, affecting more than a million people each year. Oral cancer is one of the most common types of cancer in the United States for both men and women. More than 59,000 men and women are diagnosed with oral cancer, and part of the treatment includes consuming a healthy diet rich in phenolic compounds. Phenolic acids are a class of phenolic compounds that are produced by plants in response to ultraviolet light, pests and disease. Chlorogenic, caffeic, and gallic acids are particularly abundant in coffee, a widely consumed beverage. Consumption of these coffee-derived components could have many beneficial health effects including prevention of oral cancer. The concentration of these phenolic compounds are dependent on roast levels of coffee. In this study, the anticancer activities of various freeze dried coffee beverages were compared, differing only in their roast treatments. The different roasting stages selected for this study were “Green”, “Cinnamon”/Blonde, “City”/Medium, “Full City”/Medium-Dark, and “Full City Plus”/Dark. The freeze-dried coffee samples were re-suspended in water and methanol. The total phenolic content and total antioxidant activity of each extract was also determined by the Folin-Ciocalteu, HPLC (high pressured liquid chromatography), and ORAC (oxygen radical absorbance capacity) assays, respectively. Data collected from the Folin-Ciocalteu method showed that the “Cinnamon”/Blonde roasted coffee contains the most amount of phenolic compounds, which likely helps in the inhibition of the cancer cell growth 50% more than the other coffee extracts experimented upon. Observed data, through HPLC, displayed high peak areas at 280 nanometers (mAUs) for caffeic acid and gallic acid in the “Cinnamon”/Blonde roasted coffee and high peaks of chlorogenic acid were observed in the “Green” roasted coffee. The “Cinnamon”/Blonde also showed the most amount of total antioxidant activity compared to the other extracts according to the data collected from the ORAC assay. In conclusion, the consumption of lighter roasted coffee (“Cinnamon”/Blonde), along with a healthy and balanced diet, may contribute to the prevention of oral cancer.

Minh Vy Tran Nguyen	Mount Saint Mary's University	13 Biochem	Determination of The Effect of Meringue Under Different Conditions	Eric Stemp		Meringue is commonly used in various dessert recipes. The formation of meringue is created via the blending of liquid protein from raw egg whites, whipping creams and chickpea liquid and air from the atmosphere. The stability of the meringue may be affected due to the ingredients that are available and the additional acidic contents added to the protein mixture. One common acidic addition is cream of tartar and vinegar. The cream of tartar is also known as potassium bitartrate which is a potassium acid salt of tartaric acid that has the ability to break the protein component and stabilize the meringue. In this study, we examine how the different protein, fat and acidity components control the meringue's stability. The procedure includes the exactly similar volume of room-temperature mixtures of egg white, whipping cream and chickpea solution are mixed with different amount of cream of tartar and vinegar. As the result, the stiff meringue forms faster with egg white and chickpea liquid. However, the whipping cream takes longer to form the stiff meringue. The meringue's stability is promoted depend on the protein, fat and acidity ratio. In future experiments, we hope to use NMR spectroscopy to examine the physical and chemical properties of molecules present in egg white, whipping cream and chickpea solution.
Mai Abdusamad	UCLA	14 Biochem	Characterization of Zyg11A as a Novel Mitotic Protein	Jorge Torres	Jorge Torres and Ankur Gholkar	During mitosis, cells are highly regulated to ensure proper formation of the mitotic spindle and equal chromosome segregation. As a disturbed mitotic spindle is a feature of many cancer cells, one approach in cancer treatment has been to target the spindle assembly to trigger apoptosis. To identify proteins involved in the mitotic spindle assembly, a proteomic analysis of co-purified microtubule aster proteins was previously performed. Of the 592 proteins identified by mass spectrometry, Zyg11A emerged as a potential key player in cell division as previous literature has shown that down-regulation of Zyg11A has been linked to defects in chromosome condensation and cytoplasmic organization. While Zyg11A has been identified as a member of the Cullin-2 E3 ligase complex that regulates several key processes of cell division, the specific role of Zyg11A is unknown. Preliminary immunofluorescence data indicates that Zyg11A localizes to the nuclear envelope, the microtubules and the cytokinetic bridge. This suggests that it may have a crucial role in cell division, particularly during spindle assembly. To better understand Zyg11A's role in cell division, we performed pulldowns of tagged Zyg11A to identify protein interacting partners by mass spectrometry. Further functional analysis of these proteins may prove vital to understanding of Zyg11A's role in cell division and subsequently discovering new therapeutic targets for cancer treatment.

Nguyen Pham	UCLA	15 Biochem	A conserved putative kinase is required for coenzyme Q biosynthesis: Functional insights from yeast genetics	Catherine F. Clarke	Catherine F. Clarke	Coenzyme Q (ubiquinone or Q) is an essential lipid functioning as electron carrier in the electron transport chain during cellular respiration. At least 11 Coq polypeptides involved in the Q biosynthetic pathway have been characterized in Saccharomyces cerevisiae. Several of the Coq polypeptides essential for efficient Q biosynthesis organize into a high weight molecular complex localized to the inner mitochondrial membrane, designated the 'CoQ-synthome'. Coq8 was identified as an atypical kinase responsible for sustaining the stability of the CoQ synthome. Overexpression of COQ8 has been shown to restore steady state levels of Coq proteins in several of the yeast coq null mutants. However, the specific function of Coq8 remains unknown. Previously, a mutant yeast strain harboring the coq8-3 allele was shown to encode the A197W substitution within the conserved kinase motif 1, and was suspected to disrupt the putative kinase activity of Coq8p. The yeast coq8-3 mutant lacks Q, is respiratory deficient, and does not grow on non-fermentable media. The yeast coq8-3 mutant exhibits a dramatic decrease in the steady-state levels of the Coq4 and Coq9 polypeptides. To gain insight into Coq8 function, the coq8-3 mutant was selected for further investigation. Six spontaneous revertants were isolated from the coq8-3 mutant. Each of the six revertants was able to grow on a non-fermentable carbon source and retained the parental coq8-3 point mutation. Analysis of the six revertants by LC/MS-MS revealed Q6 content was restored. Three out of six revertants appeared to contain recessive secondary mutations, while one revertant displayed a dominant supressor mutation as demonstrated by complementation tests. Here we report our investigation of the spontaneous revertants with recessive suppressor mutations. Elucidation of how they function to restore Q biosynthesis in the coq8-3 mutant may help clarify the function of Coq8 in Q biosynthesis. This research was supported by NSF MCB-1330803.
Emmie Ho	CSU Fullerton	16 Biochem	Computational Studies of The Intramolecular Cyclization of the Radical Cations of E/Z 2-Propenylbenzaldoxime	Andrew Petit		The functional groups –C=NOH and –C=NO-R are commonly found in pharmaceutical and pesticides. Compounds containing these functional groups are known as oximes and oxime ethers respectively. Oxime ether radical cations and iminoxyl radicals are the reactive intermediates produced by the oxidation of oximes and oxime ethers. When oximes and oxime ethers are metabolized, radicals are formed in the cells, which could cause harmful reactions that damage tissues and DNA. The reactivity of oxime ether radical cations and iminoxyl radicals is still relatively unexplored. Dr.de Lijser's lab has been using photochemistry to oxidize oximes and oxime ethers and produce reactive radical cation intermediates that can undergo further intramolecular reactions. Based on the results, they found that aryl groups and alkynyls group act as nucleophiles and radical traps respectively; and formed cyclized products. Alkene groups have the ability to act as either nucleophiles or radical traps. The alkene with no methyl group (2- vinylbenzaldoxime ether) and alkene with one methyl group cis (2-isopropenylbenzaldoxime methyl ether, 2-isopropenylbenzald-oxime) both yield similar cyclization products The de Lijser lab also considered the isomers 2-(E)-propenylbenzaldoxime methyl ether, 2-(E)-propenylbenzaldoxime, 2-(Z)- propenylbenzaldoxime methyl ether, and 2-(Z)-isopropenylbenzaldoxime. These (E/Z)-propenyl alkenes seem to all produce the same product, however the NMR data appears to be inconsistent with the cyclized products observed with the other alkenes. Because the de Lijser lab has not yet been able to isolate the product of the oximes and oxime ethers containing a propenyl group, we use computational chemistry to help to solve the problem by calculating the NMR chemical shifts and J coupling constants of many possible products. We also mapped out the radical cation minima as well as the transition states connecting them. Although we have not yet definitively identified the

						product, out results have ruled out many different possibilities as well as improved our understanding of the mechanism by which the alkene oxime and oxime ther radical cations undergo intramolecular cycilzation.
Kevin Ye	University of Southern California	17 Inorg/Mat	Perovskite Chalcogenides for Solar Energy Conversion.	Jayakanth Ravichandra		As the energy needs of the planet are likely to double within the next 50 years, alternative forms of energy are being explored to supplement the Earth's depleting oil reserves. Solar energy remains a strong candidate, with the Sun feeding 10,000 times more energy than the global population's consumption in a year. Hence, photovoltaics can be a suitable renewable source of energy. However, a major limitation of the leading photovoltaic material, crystalline silicon, is its poor absorption characteristics. This leads to the need for 180–300 μm thick wafers to absorb sunlight instead of a few hundreds of nanometers for materials with higher absorption characteristics. Thus, it is crucial to develop high performance and cost effective functional materials to enable sustainable, large scale photovoltaics. Transition metal perovskite chalcogenides are a new class of versatile semiconductors with high absorption coefficients and high luminescence efficiency. First principle calculations show that these materials are promising candidates for optoelectronic applications in the visible and IR wavelengths. These perovskite materials were made using a one-shot synthesis with iodine as a catalyst. Polycrystalline samples were synthesized with experimental band gap values in the visible light range, as determined by photoluminescence measurements. Three distinct phases of perovskites were characterized, with one of the phases approaching the external luminescence efficiency of single crystals such as InP and CdSe. By studying the mechanism of their synthesis and resulting physical properties, the use of the perovskite chalcogenides for harvesting solar energy shall be explored
Marisol Herrera-Ruiz	UCR	18 Inorg/Mat	Growth and Characterization of NbSe2 Monolayer Film	Ludwig Bartels	Darrick Wang, Michael Valentin, Sahar Naghibi, Ariana Nguyen, Velveth Klee, I-His Lu, Edwin Preciado, Ludwig Bartels	Niobium diselenide has become an attractive material for making nano superconducting quantum interference devices. Charge density wave (CDW) distortions have been observed in transition metal dichalcogenides (TMDs) and only the monolayer limit displays the superconducting characteristic. Here, NbSe2 is synthesized through chemical vapor deposition (CVD) on SiO2/Si substrates to achieve atomically thin crystalline structures. Compared to mechanical exfoliation, CVD ensures more consistent and scalable growth that can be easily adopted by the semiconductor industry. NbSe2 displays the E2g and A1g Raman signals at 238 and 228 cm-1, respectively. A direct band gap at 1.34eV emerges at the monolayer limit. The successful growth of this new TMD material promises the advancement of nano quantum devices.

Jonathan Stoffel	Cal Poly Pomona	19 Inorg/Mat	Investigation of the reduction of cobalt nitrosyl complexes	S. Chantal E. Stieber		Carbon dioxide (CO2) is oftentimes a focus for pollution remediation, however, lesser known pollutants such as nitrogen oxides (NOx) pose a similar threat. While biological cycles convert NOx into less harmful inert gasses, the conversion is carried out at an unfavorable rate to diminish the atmospheric levels to a favorable level. This project aims to synthesize cobalt metal complexes that have the capability to react with NOx species. These transition metal centers may be able to provide insights towards characterization of intermediates in the biological cycle. The long-term goal of this project is to utilize the metal complex to transform NOx species in chemical conversions.
Naneh Vartan, Danyal Cave, Jaki Liu, and Jason Hernandez	Pasadena City College	20 Inorg/Mat	Nanotechnology in Chemical Education: DNA Origami and nanoART	Jillian L. Blatti	Danyal Cave, John Garcia, Jiaqi Liu, Felix Monge, Frieda Schwebel, Ellen Chan, Jason Hernandez, Jillian L. Blatti	Through the Early Career Undergraduate Research Program (eCURe) at Pasadena City College, we are involved in interdisciplinary research projects at the cutting edge of science, at the art- science interface, and those that can be translated into lessons to inspire K-12 students. Our goal is to make advanced scientific research accessible to all students through simplification, using affordable materials, and implementing effective teaching pedagogies, such as active learning, group work, and employing hands-on manipulatives to illustrate concepts. We used nanoART and DNA origami to introduce students to nanotechnology in a creative and engaging way. DNA origami, the nanoscale folding of DNA into 2D and 3D shapes, emphasizes the interdisciplinary nature of science, bringing together chemistry, biology, and computer science, which is important to show in modern science curricula, beginning early in one's education. We chose to design a 2D DNA origami shamrock as a platform for our lesson plan, as its symmetrical shape allows for easy design. The DNA origami shamrock was designed using free, open-source software (caDNAno.org; cando-dna-origami.org), facilitating scalability of the lesson. The DNA origami shamrock was imaged using Atomic Force Microscopy (AFM), which can be accessed remotely1. After implementing the lesson in an underrepresented high school in Los Angeles and analyzing assessment data, it was clear that DNA origami and nanoART generated student interest and lead to greater understanding of nanotechnology. By teaching students science in context, showing them how it can be applied towards solving current global challenges, and introducing them to careers in these fields, they become motivated to use their science education to change the world.

Chien-Fu Frank Huang	UCLA	21 Inorg/Mat	Controlling the Morphology of Polymer Solar Cells using Sequential Processing	Benjamin J. Schwartz	Taylor J. Aubry, Matthew T. Fontana, Benjamin J. Schwartz	Organic solar cells are a potential solution for resolving energy needs because of their low cost, flexibility, light weight, and ease of manufacturing. The donor material, usually a conducting polymer, absorbs sunlight to create a bound electron hole pair known as an exciton. To separate the exciton, the donor material must be paired with an acceptor material, usually a fullerene derivative. The donor and acceptor material must create a sufficiently mixed, bicontinuous and interpenetrating network, known as a bulk-heterojunction (BHJ), to efficiently split the excitons. Here we carefully control the morphology of PTB7 and PCBM based BHJs using a new processing technique, Sequential Processing (SqP), and study the effects on charge transfer with photoluminescence quenching measurements. With SqP, the active layer is formed through separate and sequential depositions of the donor and acceptor layers. The formation of a mixed active layer is therefore dependent on the swelling of the underlying donor polymer by the acceptor solution and inter-diffusion of the acceptor. Additionally, co-solvent blends for acceptor deposition extend the work to any polymer system by tuning the ratio of swelling to non-swelling solvents in the blend. Building on prior group work, we study the use of solvent blends of swelling solvent 2-chlorophenol (2-CP) paired with non-swelling co- solvent isopropyl alcohol (IPA) so that the solvent blend may optimally swell the polymer acceptor, PTB7 without dissolution. [1] By tuning the fraction of 2-CP to IPA in the fullerene casting solution, we observe the evolution from a quasi-bilayer structure to a well-mixed active layer, as evidenced by increased PL quenching, to dissolution of the polymer under layer. The optimal ratio of solvents is between 60-70% 2-CP (40-30% IPA, respectively). This work will now be extended to BHJ solar cells that employ perylene diimides (PDIs), commonly used as car paints, as alternative acceptors because of their even lower cost and strong absorption in the visible spectrum.
Ashish Streatfield	Pomona College	22 Inorg/Mat	Mechanistic Investigation of SO2 Insertion into Organopalladium (II) Complexes using Solid SO2 Adducts and Lewis Acids	Nicholas D. Ball		Metal-catalyst incorporation of sulfur dioxide (SO2) into organic molecules using bench-stable SO2 is of intense interest as an atom-economical way to access sulfonylated compounds, often in one reaction vessel. Compared to the intensive literature regard of SO2 insertion in metal-carbon bonds using gaseous SO2, comparable studies of SO2 migratory insertion using bench-stable SO2 reagents like DABSO and DMAP·SO2 are rare. Investigations of SO2 insertion of model organopalladium (II) complexes using DABSO and various Lewis acids will be discussed. Intermediates isolated and characterized by NMR spectroscopy provide evidence of SO2 migratory insertion compared to the NMR of literature reactions involving gaseous SO2 insertion. Future studies will focus on selective SO2 aryl C–Pd bond and alkyl C–Pd bond insertion and demonstrating the elementary steps of Pd-catalyzed sulfone and sulfonyl fluoride formation.

Sooihk Ro	UCLA	23 Inorg/Mat	Yttrium and indium alkoxide complexes as redox switchable catalysts	Paula L. Diaconescu	Alexander Laughlin, Paula L. Diaconescu	The activities of redox-switchable yttrium and indium alkoxide complexes supported by a ferrocene-based ligand during ring-opening polymerizations of L-lactide and trimethylene carbonate are investigated. Switching the metal complexes in situ between their oxidized and reduced states with redox reagents changes the rate of polymerization of L-lactide and trimethylene carbonate. The yttrium and indium alkoxide complexes showed opposite behavior in the polymerization of monomers. The activities of various metal complexes were investigated as a function of the ligand substituents.
Tate Reuter	UCLA	24 Inorg/Mat	Ferrocene Chelating Heteroscorpionate Compounds	Paula Diaconescu	Mark Abubekerov and Paula Diaconescu	Ferrocene-chelating heteroscorpionate compounds based on [fc(PPh2)(BH[(3-R-5-R'-1-H)2pz]2)] (fc = 1,1'-ferrocenediyl, pz = pyrazole), are studied and characterized for their role in the catalysis of block copolymerization. The ferrocene scaffold supports the heteroscorpionate adduct that binds late transition metals. A zinc complex, [fc(PPh2)(BH[(3,5-Me-1-H)2pz]2)]ZnCl, was synthesized previously and shown to exist in a dimeric state. Herein, the substituents on the pyrazole fragments of the scorpionate are replaced with bulkier groups to force a steric interaction. The aim is to produce a catalyst in the monomeric state that can be characterized and utilized in biodegradable polymer synthesis with potential for redox switchability.
Paul Chong	UCLA	25 Inorg/Mat	B 12(OR) 12 r eagents as tunable one-electron oxidants	Alexander M. Spokoyny		We report the discovery that perfunctionalized icosahedral dodecaborate clusters of the type B 12(OCH 2A r) 12 (Ar = Ph or C 6F 5) can act as powerful metal-free photooxidants. These cluster compounds, when irradiated with blue LED light, exhibit excited state reduction potentials as high as ~3 volts vs. SCE, making them the strongest molecular photo oxidants known to date. Photo-excitation occurs as a result of charge transfer between low-lying orbitals of the benzyl substituents and an unoccupied orbital delocalized throughout the boron cluster core. We show that these species are able to participate in electron transfer processes with a broad range of electron-rich and electron-deficient styrene substrates, initiating their polymerization at cluster loadings as low as 0.005 mol%. Furthermore, photo-excitation of B 12(OCH 2C 6F 5) 12 in the presence of isobutylene, a less activated olefin, results in the production of highly branched poly(isobutylene). This work introduces a new class of robust, metal-free photo-redox reagents capable of mediating chemical transformations.

Michael Pardo	CSU Long Beach	26 Org	Development of an Aboriginal Chemical Process to Make Biodiesel	Sergio Mendez	James Borgese and Sergio Mendez	This research project can potentially benefit impoverished, rural communities that have a need for substitutes or supplements to petroleum fuels. We have developed an “aboriginal” chemical process to make biodiesel with the following constraints: minimal cost, reactants are readily available from local area, relatively simple chemistry, and that it be environmentally friendly. The two reactants for this process would be an oil and ethanol derived from local plants. High purity ethanol was distilled from palm wine using tapioca as a hygroscopic agent. Since the biodiesel transesterification reaction requires a catalyst, we utilized waste egg shells that were calcined into calcium oxide, a heterogeneous catalyst. FTIR spectroscopy was used to confirm the synthesis of biodiesel.
Nicole Lukasko and Megan Chisesi	Cal Poly San Luis Obispo	27 Org	Investigation of Artemisia californica and Umbellularia californica Antibacterial Compounds.	Jennifer Carroll	M. Chisesi, J. Carroll, A. Yep, J. Yost	California Native Americans used a variety of native plant species to treat fevers, wounds, and bacterial infections. The leaves of native Californian plants contain a variety of terpenoids, alkaloids, flavonoids, cyanogens, and tannins, all of which have been shown to be active against bacteria, fungi, viruses, and protozoa. We obtained plant extracts of Umbellularia californica (California bay laurel) and Artemisia californica (California sagebrush) through steam distillation and tested them against Escherichia coli, Bacillus subtillis, and Staphylococcus epidermidis. Extracts of A. californica were active against both Gram positive species, B. subtillis and S. epidermidis. A previous study identified two flavonoid compounds active against E. coli (Gram negative), but the compounds active against Gram positive bacterial species have yet to be elucidated. We found that the U. californica extract was effective against both Gram positive and Gram negative species. While the active compounds have yet to be clearly identified, we validate the use of these species to fight microbial infections of both Gram negative and Gram positive bacterial species.
Jocelyn Ochoa	CSU Long Beach	28 Org	Synthesis of Enantioenriched Butyl Cholinyl Phenyl Phosphate Iodide and its Inhibition Against Butyrylcholinesterase	K. Nakayama	T. Tran, M., J. Gonzalez, J. Schwans, and K. Nakayama	It has been shown that patients with Alzheimer’s disease (AD) have abnormal activity levels of the two cholinesterases, acetylcholinesterase (AChE) and butyrylcholinesterase (BChE). AChE tends to decrease its activity by up to 45%, while BChE activity increases by 40-90%. Current AD treatment attempts to inhibit AChE activity with the aim of restoring cholinergic levels and consequently, cognition of AD patients. Our laboratory has been interested in the synthesis and study of compounds that target the other cholinesterase, BChE. Previous work from our laboratory indicated that dialkyl aryl phosphates were potent inhibitors of BChE, among which analogs containing a cholinyl moiety showed greater inhibition with inhibition constant (KI) values down to 0.6 µM. Since these cholinyl-group containing phosphates possess a chiral center, we decided to synthesize enantiomerically enriched forms of these phosphates. Employing chiral auxiliary 2-(methoxymethyl)-(2S)-pyrrolidine, (S)-butyl cholinyl phenyl phosphate (54% ee) was prepared in 4 steps: reaction between the chiral auxiliary and diphenyl chlorophosphate; treatment with 2-dimethylaminoethanol; reaction with 1-butanol under acidic conditions; and finally methylation with methyl iodide. The KI value of this compound was determined to be 7.2 µM while its racemic form had a KI value of 10.6 µM. This poster presents the synthesis of the enantioenriched (R)-butyl cholinyl phenyl phosphate. By comparing the KI values of the two enantiomers, we will be able to determine the key interactions involved between each enantiomer and BChE. This should assist in the future design of BChE inhibitors.

Gregory Dawson	SDSU	29 Org	The Cinchona-Alkaloid Catalyzed Nucleophilic Dynamic Kinetic Resolution of Atropisomeric Aryl-Naphthoquinones	Jeffrey Gustafson	Sean Maddox, Nick Roschester, Gregory Dawson, Jeffrey Gustafson	Atropisomerism is a form of chirality that arises from the hindered rotation about a bond, resulting in rotational enantiomers. BINOL and BINAP are two examples of privileged ligands in enantioselective catalysis that contain a stable chiral axis. The mild, enantioselective synthesis of these ligands has only recently been reported; and few general strategies exist to enantioselectively synthesize diverse atropisomeric scaffolds. A general enantioselective synthesis towards diverse enantioenriched atropisomeric ligands would provide access to catalysts with unique geometries and structural properties. Herein, we disclose a dynamic kinetic resolution of biaryl naphthoquinone atropisomers via the nucleophilic addition of thiophenol proximal to the chiral axis. Various biaryl naphthoquinone atropisomers were amenable to this strategy, often yielding enantiomeric ratios of greater than 90:10. The resulting enantioenriched 1,4-dimethoxynaphthoquinone atropisomers can be further modified to contain desirable functional groups in catalysis (i.e. amines phosphines) with high enantioretention.
Valeria Garcia	SDSU	30 Org	Structural Optimization of Atropisomeric Pyrrolopyrimidine Structures	Jeffrey Gustafson	Sean Toenjes, Jeffery Gustafson	Kinase proteins are abundant in the human genome and their aberrant activity can lead to various life threatening diseases. Consequently, a dense amount of medicinal research has been focused in the development of effective kinase inhibitors. Even though kinase proteins are widely accessible, the targeted active sites of each are highly conserve. As a result, the kinase inhibitors bind not only to the target active sites, but also to off-target sites, leading to unwanted side effects. A wide variety of kinase inhibitors exist in the form of atropisomers, an extended form of chirality that compromises of at least one rotational axis between two aromatic centers. Many of these kinase inhibitors exist as rapidly interconverting atropisomeric racemic mixtures. From these mixtures only a single atropisomeric conformation binds to the targeted active site, while the other conformation binds to off-target sites. n research done by the Gustafson lab, atropisomerism is exploited to increase kinase inhibition selectivity of Pyrrolopyrimidine based compounds. In the report, they rigidified a biaryl axis by adding steric bulk adjacent to the axis and found the (R)-conformer to be 5x more selective towards RET kinase than the (S)-conformer after subjecting the conformers to a partial kinome screen. One drawback to this work was a loss in potency from the parent compound (no steric bulk). To fully exploit the strategy of spatial pre-organizing an inhibitor as a selectivity filter, the analogs need to be optimized for both potency and selectivity. To accomplish this, we first identified potential analogs by screening various substituent combinations (Figure 1) of the (R)- configuration against RET using MOE, a molecular modeling software. The docking results sorted by dihedral angles (determinant of R and S) and then ranked by both binding score (potency) and ΔR/S (atropisomer preference) in order to establish priority molecules to synthesize. The optimized molecules were synthesized and their R and S conformers (separated via HPLC) were screened in vitro against RET using ADP-Glo kinase inhibition assay. Preliminary in vitro data (consistent with in silico studies from MOE) demonstrated that any loss of potency from the parent compound may be regained while maintaining RET's atropisomer preference.

Micaelle Morales, Corey Myers, and Luis Salazar	CSU Bakersfield	31 Org	A One-Pot Environmentally Benign Synthetic Route for Isoxazoline Derivatives	Danielle Solano		The avail of isoxazoline rings in pharmaceuticals entails a greener method for the synthesis of these heterocycles. Isoxazolines are widely synthesized for their biological effects as anticancer, antibacterial, anti-HIV and anti-inflammatory agents. The standard synthetic route of these heterocycles involves the use of toxic solvents such as dichloromethane (DCM). The Solano Research Group has developed an environmentally benign and more efficient method for isoxazoline synthesis, which replaces the use of dichloromethane for water as the main solvent. The synthetic protocol employed in the green method uses sodium dodecyl sulfate (also known as SDS, a common ingredient in soap) as a surfactant and water as the reaction medium for the formation of the isoxazoline ring. This one-pot method occurs via the reaction of an aldehyde to form a nitrile oxide intermediate which then undergoes 1,3-dipolar cycloaddition with a dipolarophile. The micelles created by the SDS form a hydrophobic cavity that makes it possible for organic compounds to dissolve and cause the reaction to occur. The research focuses on testing a variety of dipolarophiles and elucidate their scope of the reaction.
Alejandro Torres	CSU Fullerton	32 Org	Synthesis of Small Molecule Inhibitors for The NS2B/NS3 Protease	Nicholas Salzameda		West Nile Virus (WNV) infects millions of people every year globally via mosquito bites. Approximately 1% of WNV cases lead to a fatal neurological condition. Currently, there are no vaccines or other therapeutic methods to treat WNV infections. The WNV contains positive, single-stranded RNA in a viral envelope invade host cells through endocytosis. Cleavage of the viral polypeptide by the NS2B-NS3 protease leads to active structural and nonstructural proteins in host cells that result in WNV replication. The NS2B-NS3 protease is a therapeutic target for WNV infections by inhibiting the NS2B-NS3 protease, a small molecule inhibitor could prevent the enzymatic activity, thereby ending WNV replication in host cells. Our research focuses on the development of small molecule inhibitors featuring arginine mimetics. The synthesis of these mimetics is accomplished through a multi-step synthesis from 1,4-cyclohexanedione to 5 varying arginine mimetics. The arginine mimetics will be coupled to various carboxylic acids to produce a library of compounds that will be screened for NS2B-NS3 protease inhibition.
Jillian Dawley and Ryan Ellson	Chapman University	33 Org	Synthesis and evaluation of dye derivatives as G-quadruplex-stabilizing molecules	Jeremy McCallum	Nicolas Ventigan, Jeremy McCallum	DNA G-quadruplexes represent a new, promising target of anticancer therapies. G-Quadruplexes have been shown to stop unrestricted cell growth in cancerous cells by inhibiting the enzyme telomerase from extending DNA length. The goal of our research is to synthesize novel molecules that stabilize the G-quadruplex structure. Through the derivatization of azobenzene and indigo based dyes, a small library of novel organic compounds was synthesized in 2-3 steps. These compounds were purified, characterized, and then tested for G-quadruplex stabilizing abilities by measuring changes in melting point curves of telomeric DNA as measured by circular dichroism. Several of the drugs increased the melting temperature of the DNA, demonstrating that these core structures possess the ability to stabilize the telomeric G-quadruplex structure.Through the derivatization of azobenzene and indigo-based dyes, a small library of G-quadruplex ligands was synthesized and characterized. Compounds with various tertiary amine side chains were synthesized in 2-3 steps in good yields. Moderate G-quadruplex stabilization, as measured by changes in DNA melting curves, was achieved with several compounds. These dye derivatives represent new core structures that have G-quadruplex stabilizing properties and the potential for novel anticancer therapies.

Justin Hathaway	CSU Dominguez Hills	34 Phy/Anal/Theor	Maker's Electrochemistry: Building a Low-Cost Potentiostat for Cyclic Voltammetry	Barbara Belmont	This poster is a progress report on a research project to build a low cost potentiostat for use in undergraduate electrochemistry cyclic voltammetry experiments. Cyclic voltammetry is a potentiometric method that is useful for studying electrochemical reactions that create currents. The technique is used to quantify chemical compounds, discover reaction kinetics, and elucidate reaction mechanisms. The instrument used for cyclic voltammetry experiments is a potentiostat, which linearly varies an electrode potential over a specific range at a specific rate, while monitoring the current that develops. Commercially, potentiostats and some variation of voltammetry or chronoamperometry are the foundation of myriad chemical sensors such as glucose sensors, on-chip protein biosensors, and gas sensors. Even though extremely useful in biomedical and industrial hygiene applications, little is said of cyclic voltammetry or potentiostats in the undergraduate chemistry laboratory curriculum. One of the reasons for this is that cyclic voltammetry measurements can be tedious and unforgiving. Another reason is that the measurement equipment can be very expensive, with most laboratory potentiostats retailing for $5000 to >$10000. Our research group has previously demonstrated that the open source “Cheapstat” device coupled with screen-printed electrodes is suitable for an undergraduate cyclic voltammetry experiment, for a startup cost of $160. To incorporate a student-built measurement system into the experiment, we are now developing a low cost potentiostat using open source software, the Arduino family of micro-controllers, and the Texas Instruments LMLP 91000 programmable analog front-end chip. A successful project will provide an opportunity for students to become more familiar with both electrochemistry and electronics/computer interfacing, for a re-usable student kit startup cost of less than $30.
Regina Cordova	Mount St. Mary's University	35 Phy/Anal/Theor	Investigating Motion via Deuterium Line shape simulations	Deniz Cizmeciyan	Deuterium is a nucleus which is Nuclear Magnetic Resonance (NMR) active and has a spin quantum number of 1 which gives rise to a non-spherically symmetric nuclear charge density. The distortion of the charge density is the cause of deuterium’s 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 which are called Pake Patterns are very sensitive to molecular motion and provide valuable information. We are investigating the molecular motion of D2O in Gypsum where presence of water in Gypsum might cause it to have fire retardants properties. Using algorithms in Dr. Alan Benesi’s book “A Primer in NMR Theory with Calculations in Mathematica” we are simulating the rotation rates of deuterium nuclei for water in gypsum. Our results indicate that the D2O in Gypsum at 220C performs a 2 site hop about the bisector angle of 54.80 at the rate of >5x107Hz. The Quadrupole Coupling Constant and the asymmetry parameter η, used are 216KHz and 0.15 respectively. At 00C the line shape is similar with the same parameters. At -250C, the lineshape shows some broadening with a QCC of 223kHz and η of 0.13. Our goal is to simulate deuterium spectra for many temperatures to be able extract the activation energy for this motion from an Arrhenius plot.

Eileen Lek	UCR	36 Phy/Anal/Theor	Construction of a Cavity Enhanced Absorption Spectrometer for HONO Detection	Jingsong Zhang	Mixtli Campos and Jingsong Zhang	Nitrous acid (HONO) is a major source of reactive hydroxyl radicals that react with other trace species to form ozone and peroxyacetalnitrate in the troposphere. Given that HONO plays an important role in the subsequent formation of ozone, it is critical to study its presence in the atmosphere. Thus, the development of sensitive instrumentation such as the Cavity Enhanced Absorption Spectrometer (CEAS) allows for the detection of ambient HONO. The construction process of the CEAS consisted of aligning the light emitting diode with two bi-convex lenses and two high reflectivity mirrors. A helium neon gas laser was utilized for the alignment in order to optimize mirror reflectivity capacity. An adjustable iris was included in the setup to reduce the background noise and therefore increase the signal to noise ratio. Additionally, a flow system of N2, NO2, and HONO was constructed and installed into the CEAS setup for calibration. HONO was continuously generated from a reaction setup of NaNO2, HCl, and Ar(g) and flowed into the CEAS cavity. Experiments were conducted by alternating a background N2 measurement with stepwise dilution concentrations of HONO. By statistically analyzing the preliminary measurements in the wavelength range of 340 nm – 390 nm, the CEAS yielded a mirror reflectivity of 97.31% with the lowest detection limit of 800 ppbv for HONO. From the calculations, the sensitivity of the CEAS must be improved either by reconfiguring the light emitting diode setup or making additional adjustments to the high reflectivity mirrors. A lower detection limit of HONO must be achieved before the instrument is sensitive enough to measure ambient levels of HONO. Future work is focused on improving the CEAS setup design by identifying the underlying factors that contribute to a statistically significant difference in the CEAS measurements.
Courtney Mayhew	CSU Channel Islands	37 Phy/Anal/Theor	Analysis of Rice Determining if it is a Significant Source of Mercury to Humans	Simone Aloisio		Mercury is a persistent, global and toxic contaminant. The more common organic species, methylmercury has been a public health concern for decades because of its high toxicity and readily biomagnifies in food chains. High levels of mercury and methylmercury can accumulate in rice grains; recent literature has identified rice as a bioaccummulator plant species of methylmercury. This work presents the results of mercury measurements of different types of commercially available rice. The results of this study suggest that the consumption of rice can be a significant source for exposure to mercury and methylmercury in the human body. The concentrations of mercury were measured by thermal decomposition, amalgamation followed by atomic absorption spectroscopy. The samples collected for analysis were different types of rice including brown, white and organic ranging from short grain and long grains. Average mercury concentrations in white short grain: 6.9 ± 3.5 ppb, brown short grain: 9.4 ± 2.6 ppb, brown short grain organic: 9.2 ± 3.3 ppb, white jasmine rice: 5.4 ± 3.4 ppb, brown jasmine rice: 2.8 ± 1.4 ppb, brown long grain rice: 12.5 ± 1.3 ppb, and brown long rice organic: 8.2 ± 4.1 ppb. While the concentrations of mercury in these rice samples seems to be low. Mercury concentrations per serving of rice are one sixth of chunk white tuna. Since rice is a dominant staple crop for more than half the world’s population, however, rice may be a significant source of mercury in humans.

Samantha Tsumaki	CSU Dominguez Hills	38 Phy/Anal/Theor	Cis-3-hexenol in Kabocha (*Cucurbita maxima*)	Barbara Belmont	Parliment et. al. has reported cis-3-hexenol to be present as a major component in the volatile fraction of Connecticut-grown pumpkins (Cucurbita pepo). This alcohol, which is found in many plants, is responsible for the scent of freshly cut grass, and plays a major role in the flavor and fragrance of cooked pumpkin. We hypothesize that the Japanese pumpkin, kabocha (Cucurbita maxima), will also contain cis-3-hexenol, and have undertaken an investigation to assess this hypothesis using GC-MS of extracts of cooked and uncooked kabocha.
Jaclyn Pittman	SDSU	39 Phy/Anal/Theor	Measuring Metal Complexation Capacity of Unknown Fulvic Acid Substances via Capillary Electrophoresis	Christopher Harrison	MPXA, a lignite-derived agricultural product, is used to complex and deliver key micronutrients to plants. The fulvic and humic substances in MPXA more easily allow for the chelation of metals that would otherwise be difficult to deliver to the plants. The MPXA provides an effective alternative to traditional fertilizers and has been shown to promote more plant growth with less product. In order to maximize the efficacy and economy of this product, it is crucial the MPXA- metal ratio be optimized. For this reason, the extent to which MPXA complexes important plant micronutrients, such as calcium, magnesium, and zinc, must be determined. This specific analysis of MPXA can be performed by way of capillary electrophoresis (CE), an analytical tool used to separate aqueous phase ions. MPXA will deprotonate and become anionic in aqueous solutions, possessing an electrophoretic mobility specific to the compound. Due to CE's lack of differentiation of polymers of different sizes, MPXA migrates in a single peak, regardless of the size of the polymer, during the separation, in the absence of metal. When the metal is added and binds to the MPXA, the cationic charge of the metal reduces the overall anionic charge of the MPXA, thereby reducing the electrophoretic mobility of the complex. This leads to two results: the migration time of the complex is increased, and the separation produces two peaks of MPXA, one with and one without the metal. Increasing the amount of metal mixed with MPXA and quantifying the differences between the two peaks allow us to evaluate the extent of complexation. Two complementary approaches have been employed for the analysis of MPXA complexation; micellar electrokinetic chromatography separation, with the cationic surfactant cetyltrimethylammonium bromide, and capillary zone electrophoresis, with the cationic surfactant didodecyldimethylammonium bromide as a capillary coating. These two approaches facilitate this unique study of the agricultural product MXPA. Results from both methods are compared and presented for evaluation of the complexation of several important plant micronutrient metals with MPXA.

Stephanie Salas	Cal Poly Pomona	40 Phy/Anal/Theor	Analysis of Chloride, Nitrate, and Sulfate in Water Samples	Yan Liu	Water is a crucial and essential part of an everyday life for a human. Inorganic species such as sulfate, chloride, and nitrate in water are closed related to the anthropogenic and biogenic activities. For example, sulfate and nitrate are the major components in the acid rain, while chloride may come from industrial sources. Therefore, my project is to determine the concentration of chloride, nitrate, and sulfate in water samples.In order to determine the concentration of the desired ions in water, a calibration curve must first be made with standard solutions with concentrations of 2, 4, 6, 8, and 10 ppm. The solutions were transferred into the Ion Chromatography instrument vials and loaded into the auto-sampler of the IC instrument. A triplicate run for each solution was carried out, and the peak height and areas of each anion was recorded. It was determined that the migration of chloride was 4.1 min, the migration time of nitrate was 6.7 min, and the migration of sulfate was 10.8 min, respectively. Due to the strong rain storms during the winter months, the concentrations of the inorganic ion species were to be highly affected in water. Fourteen different water samples were retrieved from the Water Analysis graduate course. The samples came from various locations such as a river, rain barrel, or water served at a restaurant. The same procedure was done to the sample solutions as it was performed for the standard solutions with the triplicate run for each; it was found that each sample had distinctive concentrations of each anion being analyzed.
Phan Phu	Cal Poly Pomona	41 Phy/Anal/Theor	Quantifying NO Activation and Coordination Modes in Nickel and Cobalt Complexes by X-ray Emission Spectroscopy	S. Chantal E. Stieber	Nitrous oxide (N2O) is the third most potent greenhouse gas and has global warming potential 310 times higher than carbon dioxide. Reducing the concentration of N2O is chemically challenging, however biological systems can reduce N2O through chemical reactions at copper centers within enzymes. Understanding the mechanism of nitrous oxide formation would be a significant benefit for pollutant control and also of possible environmental significance. This project aims to explore activation modes relevant to the conversion of N2O to NO. We investigated how metal compounds interact with NO species through synthesis, X-ray emission spectroscopy (XES) and calculations. XES probes transitions from filled valence orbitals and can be used to inform ligand identity, metal ligand bonding, and metal spin state. While XES is a sensitive probe for the identification of metal-bound ligands and the quantification of small-molecule bond activation, the method is still being developed. We have used XES in combination with computational chemistry to understand chemical interactions between NO and nickel, and to quantify NO activation and coordination modes. Cobalt has also shown sensitivity toward N2 reduction and reactivity toward NO, so synthesis of Co-N2 and Co-NO complexes is underway in our laboratory to be used for future XES studies. The XES development in this work offers new techniques for characterizing complex systems and understanding mechanisms of N2O reduction.

Morning Oral Presentation Abstracts

Name	Institution	Session/Area	Title	Advisor	Coauthors	Abstract
Hillary Belo Gonzalez	CSU Dominguez Hills	Analytical	Exploring Methyl Paraben Content of Fresh Blueberries	Barbara Belmont		Online sources have cited that methylparaben, an ester of p-hydroxybenzoic acid, can be naturally found in plants, including blueberries and thale cress. However, primary literature sources containing data supporting the natural occurrence of methylparaben in blueberries has not been found. Methylparaben is widely used as a preservative in foods and cosmetics. Thus, the conclusion that it may be found in blueberries may be due to its use in commercial extracts. Furthermore, previous student research into the presence of methylparaben in blueberries using HPLC-MS concluded that methylparaben cannot be found in blueberries at a concentration detection limit of 1 ppm. This study expands on the previous student research by lowering the concentration detection limit. GC-MS analysis of concentrated blueberry extracts showed that methylparaben was not found fresh blueberries at a concentration detection limit of 0.1 ppm. Future studies include lowering the concentration detection limit even further by freeze-drying fresh blueberries, exploring the methylparaben content of different blueberry species, other berries, and organic blueberries.
Monna Tabarani	CSU Fullerton	Analytical	Comparison of GC and HPLC Analytical Techniques for the Determination of Atmospherically Relevant Reaction Products	Paula Hudson	Christine Wang, Paula Hudson	Atmospheric aerosol are small solid or liquid phase particles suspended in the air that play a key role in the chemistry of the atmosphere. Aerosol particles can be generated from anthropogenic and biogenic sources. Organic compounds, specifically dicarboxylic acids, comprise as much as 2% of the total aerosol mass originating from both sources. Further, aerosol particle composition can change while in the atmosphere through reaction with solar radiation or other atmospheric compounds. It is important to not only identify atmospheric reactants but also identify the reaction products that form to fully comprehend the effect aerosol particles have on climate. The aqueous phase photolysis of a prevalent dicarboxylic acid, succinic acid (C4), with hydroxyl radical, a prevalent atmospheric oxidizer, was performed in order to determine the photo-oxidation products as a function of hydroxyl radical concentration. It is common, in the atmospheric community, to analyze aerosol samples using gas chromatography coupled to a flame ionization detector (GC-FID). However, this method requires samples to be dried and chemically derivatized prior to analysis, a process where more volatile reaction products could be lost or could result in inaccurate concentrations due to incomplete derivatization. In this study, the methods of high performance liquid chromatography (HPLC), which requires no additional sample preparation, and GC-FID were used to independently identify and quantify photo-oxidation products. Results show that for samples that underwent the drying step, a lower concentration of more volatile products like oxalic acid were detected.

Ruby Moran and Stephanie Cortez	Mount Saint Mary's University	Analytical	A Correlation Study Between Particulate Matter and PAH Concentrations through the Bio-Monitoring of Pine Tree Leaves	Syvine Deprèle		PAHs are polycyclic aromatic hydrocarbons composed of two or more fused hydrocarbon rings. These compounds are a result of an incomplete combustion in which a hydrocarbon reacts with an unknown amount of oxygen to produce carbon dioxide, water, and unwanted by-products: carbon monoxide and PAHs. Exposure to PAHs are prevalent in forest fires, tar, car exhaust, and smoke. They are detrimental to our health because they are carcinogenic, teratogenic, and mutagenic. PAHs are inherent in particulate matter; particulate matter is a mixture of solid particles and liquid droplets in the air. Due to their deleterious properties, it is important to qualify as well as quantify PAHs. Herein, we propose the bio-monitoring of PAHs through pine tree leaves from the Italian Blue Cyprus tree in two designated areas near the I-405 Freeway and on the Mount Saint Mary's University (MSMU) campus. PAHs were extracted via a continuous Soxhlet extraction, further processed and analyzed by the Gas Chromatography Mass Spectrometer (GCMS). A Selected Ion Monitoring (SIM) table was used to search for the 16 most common PAHs found in the sample. Through a series of calculations, the concentration of the PAHs were graphed and compared with the values of PMs reported by the EPA. Since PAHs fall within the family of particulate matter, a direct correlation between the concentration of PAHs and PM values reported was expected. Samples collected from the freeway and campus area showed a direct correlation with few discrepancies that can be linked to weather patterns. Analysis of the data confirmed that the MSMU campus location displays higher levels of PAHs than the I-405 freeway area. For future directions, we will continue to monitor PMs and PAHs during the spring season and analyze previous data acquired to finalize the quantification and qualification of PAH and PM concentrations found within the designated areas.
Azin Saebi	UCLA	Biochem 1	Development of Carborane-Based Histone Deacetylase Inhibitors	Alexander M. Spokoyny	Jonathan C. Axtell, Rafal M. Dziedzic, Joshua L. Martin, Timur Katsnelson and Alexander M. Spokoyny	Carbon-rich molecules have been historically utilized as building blocks for assembly of complex molecular architectures due to the vast development of methods for fine-tuning their properties. Yet, the classical toolbox of 2D aromatic building blocks presents inherent topological limitations, which sometimes is referred to as "molecular flatland". Carboranes (C2B10H12), the three-dimensional aromatic analogues of benzene, introduce a potentially powerful solution for addressing this limitation by offering an inherently rigid, three-dimensionally defined scaffold available for dense functionalization. Here, the dense functionalization of carboranes is exploited in biological systems, in order to develop a library of isoform-specific small molecule inhibitors targeted toward histone deacetylase (HDAC) enzymes. HDAC enzymes are critical regulators of gene expression and their aberrant regulation in the brain has been linked to many neurological disorders. Currently, our understanding of such HDAC- mediated disorders is limited due to lack of adequate means for measurement of HDAC expression and function in the brain. Furthermore, over 19 isoforms of HDAC proteins are expressed in the body that are differentially involved in diseases, yet there is no method for selective tracking and *in vivo* quantification of each in the brain. Incorporation of carboranes in the design of the inhibitors is aimed to 1) facilitate higher binding selectivity of the molecule toward its target HDAC isoform via tuning the carborane-protein interactions and 2) confer the desired hydrophobicity for blood-brain barrier penetration. The recent advancements in the field of boron cluster chemistry by our group and others have granted access to new methods for selective vertex functionalization, providing a potential mean for synthesis of these HDAC inhibitors. In this presentation, we demonstrate the latest advancements in synthesis of the carborane-based HDAC inhibitors.

Imagine Davis-Ward and Madison Hamrick	Cal Baptist University	Biochem 1	Antioxidant Activity Study in Agave Using 1,1-diphenyl-2picrylhydrazyl (DPPH) radical Assay	Y. Hu	America Hidalgo, Y. Hu	Agave is a popular plant in the hotter climates of the southwestern United States and Mexico. It is well known for its nutritional, industrial and medicinal applications. In this study, we investigated the antioxidant activity in fresh Agave by using a 1,1-Diphenyl-2-picryl hydrazyl (DPPH) radical assay. Fresh Agave was collected at San Manuel Reservation in early April, 2016. Samples were sorted for quality, maturity, field heat removed, cooled, weighed into whirl pack bags, treated with liquid nitrogen, stored in ultra-low at -80° and studied in September, 2016. The results show an IC_{50} value of 2.20 mg/mL for the fresh Agave. The IC_{50} of the reference, ascorbic acid, is 0.146 mg/mL. The antioxidant activity of Agave is relatively high compared to other plant derived species studied in the area, such as yucca blossom (21.85 mg/mL) and stinging nettle (414.42 mg/mL). Further research is proposed to investigate how a cooking method will influence the antioxidant activity of the agave.
Kelly Araujo	Mount Saint Mary's University	Biochem 1	The Effect of Peruvian Teas on Mammalian Cells	Luiza Nogaj	Desarey Morales, Sylvine Deprèle, and Luiza Noga	Two compound families were analyzed within this research: polycyclic aromatic hydrocarbons and polyphenols. Polycyclic aromatic hydrocarbons (PAHs) are organic compounds consisting of two or more benzene rings. These compounds are known to be teratogenic, mutagenic, and carcinogenic. We are exposed to these compounds through dermal absorption, consumption, and inhalation. Polyphenols are organic chemicals, characterized by the presence of multiple phenol structural groups. They are antioxidants that help prevent degenerative diseases and free radical damage. Polyphenolic compounds are found in abundant quantities within our food sources, including teas. This study involved extracting polyphenols from medicinal Peruvian teas using various solvent systems through a Soxhlet apparatus. The tea extracts were subjected to a chloroform extraction to remove excess caffeine and pigments, followed by an extraction with ethyl acetate. All samples were concentrated, filtered and re-suspended in the proper solvent/buffer. Extracts were further analyzed by Gas Chromatography/Mass Spectrometer (GCMS) prior to their addition to HeLa cells and subsequent incubation for 24 hours. A MTT assay was performed to test the effects of the tea extracts on cell viability. Our findings determined that three active teas that consist of herbal remedies aimed towards potential aide in illness, gave consistent and positive results with cell viability. All teas displaying activity were extracted in ethanol/acetone and specifically blended for natural relief in nerves, prostate, and stomach acid/diuresis medical problems. Further experimentation will subject the extracts to fractioning via column chromatography, where, based on polarity, one whole tea extract will be separated in parts and further analyzed.

Kristen Fregoso	Mount Saint Mary's University	Biochem 1	The effects of Ebenaceae diospyros & Annona muricata on Mammalian Tissue Culture	Luiza Nogaj and Sylvine Deprele	Natural products have been used in medicine as a treatment for numerous diseases such as cancer. *Annona muricata,* the soursop, is an angiosperm that is cultivated in humid environments. For this reason, the soursop is a plant that is used in many third world countries as a primary source of treatment against cancer. *Ebenaceae diospyros*, the persimmon, is an angiosperm that has displayed benefits for diabetes and renal dysfunction when accompanied with other compounds like green tea leaves. Both of these species contain phytoconstituent compounds such as polyphenols and alkaloids. Phytoconstituents are compounds in plants known for their color and odor that may contribute to the beneficial effects of these plants. The objective of this study is to examine the effects of soursop and persimmon extracts on the viability of mammalian tissue culture. Our results show that soursop extracts with and without skin decreased HeLa cell viability using an MTT assay, a cytotoxicity assay, and an apoptosis kit. However, persimmon extract has shown no effect on cell viability. GC/MS analysis identified many compounds present in the soursop extracts that could serve as potential candidates for further anti-cancer analysis. Additional biological and chemical analysis is necessary to examine specific active compounds present in the soursop that contribute to this effect.
Monica Kirollos	UCLA	Inorg 1	Developing Atomically Precise Boron Cluster-Based Nanoparticles via Perfluoroaryl-thiol Nucleophilic Aromatic Substitution Chemistry	Alexander M. Spokoyny	Undesirable protein-protein interactions (PPIs) within the body have been known to lead to numerous diseases,1 and over the past few decades, research on multivalent nanoparticles such as gold nanoparticles has yielded promising results.2 However, many of these systems have important fundamental limitations that inhibit their full potential, such as the lack of precise control over their sizes and compositions.3 Therefore, our lab has focused on creating atomically precise organomimetic cluster nanomolecules (OCNs). Furthermore, since all the bonds are fully covalent, the synthesized OCNs are stable under biological conditions.4 This method shows how dodecaborate clusters perfunctionalized with pentafluoroaryls can be efficiently conjugated with various thiols through nucleophilic aromatic substitution (SNAr) under mild conditions. The pentafluoroaryl-terminated linkers can be further extended through Suzuki cross-coupling reactions, and the different lengths of the aryl linkers used for the cluster synthesis allow facile tuning of the OCNs. The results show that OCNs exhibited increased stability in comparison to thiol-capped gold nanoparticles. Lastly, this assembly strategy also allowed us to create glycosylated OCNs, which was capable of multivalent interactions with a model protein.

Yi Shen	UCLA	Inorg 1	Zirconium Complexes Supported by Ferrocene-Based Ligand as Redox Switches for Hydroamination Reactions	Paula L. Diaconescu	Scott M. Shepard, Paula L. Diaconescu	The activity of zirconium complexes supported by ferrocene-based ligand for ring opening polymerization reactions is well studied in previous work by Diaconescu group. Here we report the synthesis of (thiolfan*)$Zr(NEt_2)_2$ (thiolfan*= 1, 1'-bis(2,4-di-*tert*-butyl-6-thiophenoxy) ferrocene), and its activity in hydroamination reactions. Switching the metal complex *in situ* between its oxidized and reduced states with redox reagents resulted in selectivity for the two catalytically active species. We found that the reduced form of (thiolfan*)$Zr(NEt_2)_2$ can catalyze hydroamination reactions of primary aminoalkenes, whereas the oxidized form, [(thiolfan*)$Zr(NEt_2)_2$][BAr^F] can catalyzed hydroamination reactions of secondary aminoalkene. We also found that both the reduced and oxidized forms of the zirconium complex can catalyze intramolecular hydroamination of primary alkyl aminoalkynes with different rates.
Alexander Laughlin	UCLA	Inorg 1	Substituent Effects on Redox-Switchable Catalysis for Orthogonal Polymerizations of Biodegradable Block Copolymers	Paula L. Diaconescu	Soohik Rho, Jonathan Brosmer, Paula Diaconescu	Control over the rate of ring-opening polymerization has been realized via redox-switchable catalysis. In this vein, biodegradable block copolymers have been synthesized. By altering the ligand scaffold, new modalities of control may be accessible. Therefore, a series of ferrocene-based proligands, phosfen = 1,10-di(2-tert-butyl-6-diphenylphosphiniminophenoxy)ferrocene) with altered substituents para to the phenoxide group are being synthesized to investigate the reactivity of their yttrium and indium complexes. The electron-donating or electron-withdrawing nature of these modifications may allow for a greater scope of viable monomeric precursors.
Joshua Martin	UCLA	Inorg 1	Cage-Walking: Vertex Differentiation by Palladium- Catalyzed Isomerization of B(9)-Bromo-meta-Carborane	Alexander M. Spokoyny		We report the first observed Pd-catalyzed “cage-walking” process featuring a metal B-bound carboranyl moiety. As such, isomerization of 9-Br-meta-carborane during Pd-catalyzed cross-coupling enables formation of B–O and B–N bonds at all boron vertices (B(2), B(4), B(5), and B(9)) of meta-carborane via a proposed “cage-walking” mechanism. Experimental and theoretical studies suggest this isomerization mechanism is strongly influenced by the steric crowding at the Pd catalyst by either a biaryl phosphine ligand and/or substrate. Ultimately, this isomerization process can provide a unique pathway to preferentially introduce functional groups at the B(2) vertex using B(9)-bromo-meta-carborane as the sole starting material through substrate control.
Cassidy Feltenberger	USC	Materials/Theory	Synthesis and Applications of Singlet Fission Dimer Ligands on PbS Nanocrystals for Use in Organic Photovoltaics	Mark E. Thompson		One of the most apparent issues in modern technologies that have gained the attention of scientists globally is the necessity for effective and affordable renewable energy sources. The application of organic photovoltaic units is a promising, viable and sustainable method of utilizing solar energy. One current challenge facing the progression and widespread application of organic photovoltaics is the low efficiency of these units. Singlet fission, a process by which the absorption of a single photon by an organic semiconductor results in the formation of two triplet excitons, has been studied as a mechanism to increase energy harvesting efficiencies in organic photovoltaics. During efforts to understand the process of singlet fission more thoroughly, tetracene dimers including ortho-bis-ethynyltetracenyl-benzene (o-BETB) were synthesized and their photophysical properties measured. After identifying and confirming that o-BETB exhibits singlet fission at a significant rate, the challenge becomes harvesting the energy from the two triplet excitons into useful energy, rather than wasted thermal or light energy.

				Previous studies have reported triplet energy transfer from organic acene molecules to inorganic nanocrystals by way of Dexter energy transfer. By synthesizing an organic ligand that exhibits singlet fission, can be directly attached to the nanocrystal material, and can be altered in the length between the coupled chromophores and the nanocrystal, the energy transfer from the organic ligand to the inorganic semiconductor material will ideally become more efficient. The synthetic process of creating an o-BETB analog that maintains the molecule's physical properties but also creates a mechanism for attachment to PbS nanocrystals consists of several steps. Currently, the proposed synthetic scheme for the o-BETB analog has been completed up to the step prior to the addition of the coupled tetracene chromophores, which will allow for the molecule to exhibit singlet fission. Finally, the singlet fission dimer will be attached to the nanocrystal material by reacting the terminal thiol groups with the PbS nanocrystals. Provided that the energy of the two triplet excitons resonates with the bandgap energy of the PbS nanocrystal material, energy transfer will ideally occur.
Paul Robinson	UCLA	Materials/Theory	Borides: Bonding, Hardness, and Anisotropy" is in the discipline of Theoretical & Computational Chemistry	Anastassia Alexandrova
				Since pre-historic times, there has been a need for ultra-hard materials to be used for tools. Until recently, mostly carbides were used as such materials, though they are not ultra-hard. The hardest materials known are diamond and cubic boron nitride, but they are very expensive. Also, diamond turns into carbides upon contact with ferrous metals at high T, making manufacturing of cutting tools problematic. Recently, it was discovered that borides of heavy transition metals are ultra-hard; they can scratch diamond in certain crystallographic orientations. It is exceptionally exciting as it offers a new route to ultra-hardness that could be fundamentally free of the limitations of diamond-like materials. The understanding of ultra-hardness was in its rudimentary stage, however, and, as a result, many of their properties remained unexplained and unpredictable. We will discuss several borides, WB4, ReB2, OsB2, SmB6. Our chemical bonding insight into these materials is local and cluster-based. We will show how hitherto unsuspected M-B bonding contributes to boride superhardness, and explains the counterintuitive anisotropy of the stiffness against sheer stress of WB4. We will explain why the (B)n sheets change from flat to extremely bent in the series: TiB2, ReB2, OsB2. We note that in general, it is not understood why the geometries of the B-network within borides can be anything from chains to sheets to cages, depending on the metal. Finally, we will explain the outstanding question of mixed valency in SmB6. In this solid, Sm exists in the oxidation states of +2 and +3 in a 50/50 mix. We show how that phenomenon emerges, without ever engaging in the change of the nature of the occupied electronic states. All presented results are new and unpublished.

Alexis Rochelle Basa	CSU Los Angeles	Materials/Theory	Chemotactic Behavior on Paper Microfluidic Platforms	Frank Gomez	Grenalynn Ilacas, Ayusman Sen, and Frank A. Gomez	Microfluidics serves as a prominent platform for the design and development of a myriad of devices owing to their reduced reagent consumption rate and short sampling-to-result time. Chemotaxis is the movement of materials, particularly biological species, in response to the influence of chemical stimulation. Recently, chemotactic behavior in poly(dimethylsiloxane) (PDMS)-based microfluidic platforms in the separation of enzyme species has been described. We hypothesize that paper is a better platform for proving chemotaxis. Herein, we describe for the first-time chemotactic behavior on a microfluidic paper analytical device using as a model enzyme-substrate system glucose oxidase (GOx) and glucose. Glucose oxidase and glucose migrate through chromatography paper and chemotaxis is proven by examining varying intensities of color, which signify chemotactic movement of GOx to glucose or lack thereof. Color, on-chip, is achieved by the addition of horseradish peroxidase (HRP) to catalyze the reaction between the product of glucose and GOx, hydrogen peroxide, and potassium iodide. Our results show that, with the appropriate microfluidic arrangement, molecular chemotaxis can afford products not obtainable under other experimental conditions and that can be predicted by modeling and simulation. Microfluidic paper analytical devices are easily fabricated by patterning hydrophobic materials in hydrophilic paper. They are low cost, compatible with biological samples, and have shown promise as platforms for various applications and in resource-limited settings. Current work is focused on optimizing the design of the microfluidic paper analytical device and its application to enzyme separations.
Parastoo Ali Pour	UCI	Materials/Theory	Tuning particle wettability for the formation of bicontinuous interfacially emulsion gels	Ali Mohraz	Max Kaganyuk and Ali Mohraz	μ μExperimentally discovered in 2007, bicontinuous interfacially jammed emulsion gels (bijels) are a new class of multiphase soft materials that exhibit a peculiar microstructure comprised of two independently continuous fluid domains separated by a monolayer of jammed particles, as seen in Figure 1. This unique morphology makes bijels ideal soft matter templates for the synthesis of a variety of advanced materials for energy and health care applications. Bijels are prepared by the spinodal decomposition of two partially miscible liquids, which is halted by the jamming of near neutral-wetting colloidal particles at the fluid interfaces. Successful formation of bijels requires the wetting properties of the colloidal particles to be carefully tuned to make them neutrally wetting with respect to the two fluids. The specific binary fluid system that I work with is water and 2,6-lutidine, and the particles are monodispersed silica particles tagged with fluorescent dye and synthesized through a modified Stober method in our laboratory. The silica synthesis occurs in two steps. The initial step is the coupling of a fluorescent dye, Rhodamine B Isothiocyanate (RITC) with 3-Aminopropyltriethoxysilane (APS). Fluorescent silica particles are produced in the second step through the reaction of this aps-dye conjugate with Tetraethyl Orthosilicate (TEOS), resulting in particles with surface chemistry as schematically depicted in Figure 2. However, the surface coverage and number of different ligands bonding to the particle surfaces can vary depending on the amount of each reagent present in the reaction, which, in turn, affects the particle's wettability by each fluid. Thus, a more systematic study is necessary to study the effects of each reagent in the silica synthesis process and to determine the optimal amounts and ratios of the reagents in the reactions to achieve near neutral-wetting particles. Our preliminary results suggest that hydrophilicity increases with increasing the APS amount in the initial reaction, which presumably displaces surface hydroxyl groups with amine groups (see Figure 2). In this talk I will discuss the systematic experiments performed to determine the effects of RITC, TEOS, and APS on particle wettability and bijel formation

Ifeh Akano, Matthew De Silva, Jeremy Armas	Cal Poly San Luis Obispo	Materials/Theory	Characterization of the mechanical stability of chemically functionalized carbon nanotubes by scanning probe microscopy	Gregory Scott	Chemically functionalized carbon nanotubes have received a great deal of interest in recent years because of their potential use in a variety of electronic, materials, sensing, and biomedical applications. Many methods for functionalizing carbon nanotubes have been developed, yet the local effects of functionalization chemistry are not well understood. The addition of functional groups can affect the material properties including the mechanical stability of the carbon nanotubes. We have found that when nanotubes are acid-treated to create carboxylic acid functional groups as a starting point for the addition of many different functional moieties, the materials can be degraded controllably under mild conditions (i.e. normal scanning conditions) by a scanning tunneling microscope (STM). In order to optimize cutting conditions, we are currently constructing a high-vacuum STM system to reduce the noise produced in ambient conditions. Through this research, we propose that the degree of functionalization of carbon nanotubes can be optimized as function of reaction time with acid. This covalent functionalization allows for low-voltage template cutting of carbon nanotubes by STM. Because identification of functional groups by scanning probe microscopy can be difficult, we covalently attach gold nanoparticles to the sidewalls of the carbon nanotubes via a thiol bridge. In addition to STM and AFM measurements, chemical modification is verified by Raman, UV-Vis, and FT- IR spectroscopic techniques
Ricardo S. Cruz	CSU Fullerton	Organic I	Small Molecule Inhibitors for the Botulinum Neurotoxin	Nicholas T. Salzameda	The Botulinum neurotoxin (BoNT) is secreted and/or can be easily extracted from the *Clostridium botulinum* bacteria. The neurotoxin is one of the most lethal toxins known to man with a LD_{50} of about 1 ng/kg of body weight. The potency of the toxin and its ease of extraction from the bacteria makes BoNT a threat for use as a biological weapon. BoNTs are composed of a heavy chain (HC) and a light chain (LC), which are held together by disulfide linkage. The LCs are a zinc metalloprotease, which are responsible for the cleaving of Soluble N-ethylmaleimide-Sensitive-factor Attachment Receptor (SNARE) proteins in the axon terminal. Cleaving of these protein complex results in failure of neurotransmissions that lead to botulism, a deadly muscle-paralysis causing disease. Cleavage of the SNARE protein is irreversible; therefore, treatments are needed to prevent botulism. Current treatments for BoNT intoxication are designed for pre-exposure through the use of antibody vaccines. Currently available treatments are not designed to deal with a large infected population, are inefficient with long delays between exposure and treatment, and if accessible the cost is immense. Consequently, if the toxin is dispersed worldwide such as in a terrorist attack or utilized in warfare, those infected would not be treated in time. Our lab focuses on small molecule therapeutics to inhibit this protease and treat the disease. Previously, our laboratory discovered a biphenyl sulfonamide isoleucine hydroxamic acid inhibitor for the BoNT LC. We have expanded on this inhibitor by increasing the number of amino acids in the scaffold while maintaining the biphenyl sulfonyl N-terminal and the hydroxamic acid at the C-terminal. We hypothesized that increasing the number of amino acids would improve binding to the protease. The new inhibitors were created via a solid phase synthetic strategy with Hydroxylamine Wang Resin. Amino acids were coupled to the resin in specific sequences and the sulfonyl chloride was added to give the sulfonyl-amide bond. The library of inhibitors was evaluated using a Fluorescence Resonance Energy Transfer assay and in silico docking was performed to visualize and develop optimization routes based on possible binding interactions of lead molecules with active site residues.

Sandra Rodriguez	CSU Fullerton	Organic I	Structure activity relationship study of isoleucine sulfonamide hydroxamic acid inhibitors for the Botulinum Neurotoxin	Nicholas T. Salzameda		Botulism, a severe paralytic disease caused by the botulinum neurotoxin (BoNT), is produced by the bacterium Clostridium botulinum . The BoNT is composed of heavy (HC) and light (LC) chains. The LC, a zinc metalloprotease, cleaves SNARE proteins which can cause fatal muscle paralysis. BoNT is the most poisonous toxin known to man and due to its ease of production, there are concerns the neurotoxin could be used for bioterrorism. Our laboratory is working on inhibiting the BoNT LC as a novel treatment option due to lack of viable treatment options for large populations. In our previous studies, we designed molecules that successfully inhibited the BoNT LC. These molecules were composed on a functionalized amino acid with a biphenyl ring, sulfonamide bond and a hydroxamic acid. The 3 step synthetic route begun with the coupling of isoleucine, a Suzuki coupling to build the biphenyl structure and hydrolysis to form the hydroxamic acid. We sought to study how substituents on the biphenyl affect inhibition alongside with the importance of the sulfonamide. Based on an enzymatic assay, the position and number of chlorine on the biphenyl ring drastically affected inhibitor activity. Additionally, due to stereochemistry, D-isoleucine resulted in greater inhibition than L-isoleucine. When D-Isoleucine was replaced L-Isoleucine, the sulfonamide small molecule with 2-chloro phenyl ring increased inhibition from 50% to 90% and the benzofuran molecule increased inhibitor activity from 61% to 94%.
Kevin Kossick	CSU Northridge	Organic I	N,N-diarylbenzimidazolium Compounds	Taeboem Oh		Axially chiral N,N-diarylbenzimidazolium salts may be useful enantioselective hydrogen bonding Diels-Alder cycloaddition catalysts, as well as NHC ligands for enantioselective metal catalysis. A new route to N,N-diarylbenzimidazolium salt synthesis was studied by combining copper catalyzed cross coupling arylation of the 1-position nitrogen, followed by the employment of diaryliodonium reagents for the arylation of the 3-position nitrogen. We also investigated the barrier of rotation around the benzimidazole-aryl bonds via variable temperature proton NMR spectroscopy. It has been determined that naphthyl and 2-isopropyl N-substituted moieties can induce axial chirality, both having approximately a 70 kJ/mol energy barrier. Other substituted aryl groups will be investigated in future studies to find an optimal barrier of rotation for their potential use as catalysts.
Garry Leonard	California State University Northridge	Organic I	Synthesis of 2,6-diarylpyridine and 2,6-diaryllutidine for atrope isomerism investigations	Tae Oh	Carolina Yulek, Tae Oh	To explore the atrope isomerism of 2,6-diarypyridine systems, we have synthesized 2,6-diarypyridine via palladium coupling. 2,6-(2-Methylphenyl)pyridine was shown to have atropismerism with a barrier of 9.4 Kcal/mole as examined by DNMR. We also examined 2,6-(3-methylphenyl)pyridine and 2,6-(dinaphth-1-yl)pyridine was examined. We next proceeded to synthesize the 2,6-(diaryl)-3,5-dimethylpyridine to examine its barrier to rotation.

Emil Samson	UCI	Organic I	Two-Tiered Force Sensing via Tandem Mechanophore Activation	Zhibin Guan	Recently, significant effort has gone into the design of mechanophores, which are molecules that rupture at one specific covalent bond upon an applied force. A small library of these molecules has been synthesized to become visually active, release small molecules, or undergo molecular remodeling when stressed. Thus, mechanophores have the potential to identify stress concentration, dissipate energy, and sense the presence of acid. To further the utility of mechanophores, we are en route to creating an elastomeric material capable of multi-level force sensing via tandem mechanophore activation. The proposed material will exhibit color changes when exposed to specific amounts of force to easily identify stress build up. To obtain force sensing properties, a two-tiered network containing both spiropyran (SP) and a HCl-generating mechanoacid will be fabricated. Without any applied force, the material is colorless. Under low force (X), the material turns purple due to the ring opening of SP to its zwitterionic merocyanine (MC) isomer. Under high force, the material turns yellow as the HCl mechanophore is activated to protonate the MC isomers. Through tandem activation of these mechanophores, we anticipate a material with facile visualization of damage via distinct color changes.
Vivian Lee and Ann Gonzalez	Mount Saint Mary's University	Organic 1	Surfactant Synthesis of Hypophosphite Esters Involving Phosphorus Chemistry	Sylvine Deprele	The recent Deepwater Horizon oil spill impacted the wildlife, causing rise in algae blooms and affected the wildlife. Two carbon based oil dispersants, Corexit 9527A® and 9500A® that were used as clean up methods contained toxic components, thus harming the marine life. This led us to focus on synthesizing an environmental friendly, phosphorous-based surfactant. Our research involves a three step synthesis. In Step 1, a long, nonpolar chain is attached to a hypophosphorus acid to form hypophosphorus esters through direct esterification. This process is done with the Dean-Stark apparatus, which allows water to be removed as it accumulates during esterification. Step 2 involves elongating the nonpolar chain with a bromoalkene and a palladium catalyst to produce alkyl (5-bromo-pentyl) phosphinate. This product is then reacted with a trimethylamine in step 3. Results show that nonanol, cyclohexanol, heptanol and 2-octanol respectively yield of 50%, 61%, 54% and 54% for Step 2. We are currently working on the isolation of the products in order to specifically identify between the linear and branched products. It is expected that both linear and branched products will form from the hydrophosphinylation step. Concurrently, we are working on achieving higher product yields and expanding the scope of alcohols used for this study. Future directions include using different alcohols and equivalences to maximize step 1 and step 2 product formation.

Afternoon Oral Presentation Abstracts

Name	Institution	Session/Area	Title	Advisor	Coauthors	Abstract
Ellisha Davis	Mount Saint Mary's University	Biochem 2	The Extraction of Polyphenols from Peruvian teas and the effect of the tea fractions on HeLa cells	Luiza Nogaj	Sylvine Deprèle and Luiza Nogaj	Polyphenols are a group of naturally occurring organic compounds, consisting one or more phenol rings. Anti-carcinogenic health benefits of polyphenols have been observed due to their antioxidants properties and ability to modulate enzyme activity and cell signals. The intake of polyphenols activate enzymes for detoxification, therefore, stimulating defenses within toxic environment. Polyphenols were extracted from various Peruvian Tea mixtures which advocate to treat medical problems. The extractions were performed by using a Soxhlet setup with solvent mixtures of ethanol and acetone at a 1:1 ratio and water. The samples were then washed with chloroform to remove caffeine and pigments, followed by ethyl acetate to separate the polyphenols. The samples were further concentrated, filtered and subjected to Gas Chromatography Mass Spectrometer (GC-MS) analysis after re-suspension in a solvent. The samples were added to HeLa cells and an MTT assay was performed on the cells to analyze the anti-carcinogenic effects of the tea extractions from each tea mixture. It was found that the tea mixture made to alleviate nervous system cancer (Tea 1EA) and the tea to alleviate prostate cancer (Tea 5W) demonstrated accurate correlations to inhibit cell growth, and were therefore further analyzed. The tea extractions were fractioned by flash column chromatography using a solvent gradient from non-polar to polar. GC-MS analysis and a 24-hour incubation of MTT assay on the HeLa cells were repeated on fractions 1-8 obtained from Tea 1EA and 2-8 obtained from Tea 5W. Our results show, one fraction from Tea 1EA, fraction 6, displayed a trend for lowering cell viability in HeLa cells as the concentration of the fraction increased, and two fractions, fraction 3 and 4, from Tea 5W followed this trend. A compound table provided by the GC-MS showed the presence of polyphenol derivatives and PAHs in the effective fractions from Tea 1EA and Tea 5W. In future experiments, standards of polyphenols found in the effective fractions will be inserted into the HeLa cells to analyze their effects. In addition, cytotoxicity assay will be performed using the samples.

Patricia Perez and Melissa Martinez	Mount Saint Mary's University	Biochem 2	DNA-Protein Crosslinking via Green Tea	Eric Stemp	Oxidative damage is involved in the formation of free radicals, which can cause various diseases. In DNA, this damage is observed primarily at guanine (G) because it is the most easily oxidized base and one form of oxidative damage is DNA-protein crosslinking. Here, we examined which brands, conditions and concentrations of green tea are most effective in preventing oxidative DNA damage. Oxidation was effected by the flash-quench technique, a method that is used for guanine oxidation and that 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 0-4 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 with tea that was stored at cold temperatures showed that the free DNA band persisted at dilutions of green tea up to 1:10000. Additionally, a pro-oxidative effect was observed at high tea concentrations. 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, as well as examine the damage seen at high concentrations of tea; analogous experiments with small peptides suggest that phenols could produce the inhibitory effect by reducing guanine radicals.

Christine Hua	UCI	Biochem 2	Novel Luciferase-Luciferin Pairs for Multi-component Imaging	Jennifer Prescher	Krysten Jones, William Porterfield, Colin Rathbun	Bioluminescence imaging (BLI) is a powerful technique for visualizing cells and other biological processes *in vivo*. This technology relies on enzymes (luciferases) that catalyze light emission through oxidation of their small molecule substrates (luciferins). Since no excitation light source is required, bioluminescence provides an extremely high signal-to-noise ratio, making it well-suited for sensitive imaging applications. Despite its versatility, BLI has been confined to tracking only one cell type at a time, since the most optimal luciferases bind the same small substrate. To address this limitation, we report an approach to engineer selective (i.e, orthogonal) bioluminescent probes. We imposed site-directed mutagenesis to craft mutant luciferases that can selectively process synthetic luciferin analogs. Libraries of mutant enzymes were screened using a two-tiered process against chemically modified luciferins to identify unique enzyme-substrate pairs. We additionally applied our screening strategy to evaluate a mutant luciferase library designed by statistical coupling analysis (SCA) methods. From our preliminary data on both the site-directed (SD) and SCA libraries, we identified functional mutants that were robust light-emitters when combined with distinct luciferin analogs. Furthermore, the results provided insight into SD and SCA library designs, suggesting that diverse mutagenesis approaches may enable practical evolution of orthogonal pairs. Based on their substrate selectivity, these orthogonal luciferase-luciferin partners hold potential for broader applications in multicellular imaging and rapid expansion of the bioluminescence toolkit.
Johanna Bautista	CSU Los Angeles	Biochem 2	Analysis of lipid transfer proteins in *Arabidopsis thaliana* by means of epitope tags to decipher the role of LTP4's lipid in plant senescence	Robert Luis Vellanoweth		RNAi knock down of two lipid transfer proteins that are up-regulated during the bolting stage in *Arabidopsis thaliana* produce a mutant plant that continues to flower after having already completed senescence and apparent death. We hypothesize that these LTPs carry a lipid signal that mediates meristem death. The objective of this work is to insert an epitope tagged lipid transfer protein 4 (LTP4) gene into the *Arabidopsis thaliana* plant which will allow us to use a reagent to specifically pull out this lipid carrying protein for analysis. We expect that this approach will uncover the identity of the LTP4-bound lipid. Also, using the epitope tag on the LTP4 protein, we will track the process in which the LTP4 protein carries the unknown lipid through the plant in senescence. Currently, the binary vectors have been constructed and the floral dip method has been used to insert the modified gene. Selection for the modified plants is underway. This will give us our final transgenic plants that will have an epitope tagged LTP4 gene and allow us to uncover the unknown lipid signal.

Jenny Lee	UC San Diego	Biochem 3	The Role of Cyclic di-AMP in Synechococcus elongatus	Susan S. Golden	Cyclic di-AMP (c-di-AMP) has recently been elucidated as the newest member of the nucleotide signaling family, and has been found to have broad distribution and importance. Our work in the Golden lab has shown the presence of c-di-AMP and the responsible enzyme in the cyanobacteria, Synechococcus elongatus PCC7942, which is a model organism for photosynthesis and the circadian clock. We have identified putative c-di-AMP interacdting proteins using a pull-down assay, and following up on the findings from unbiased screens, I created targeted mutations of the genes encoding for these proteins and assayed the mutants for phenotypes shared by the cyclase responsible for c-di-AMP production. This work will vastly improve our understanding of the signaling molecule's role in a photsynthetic organism such as S. elongatus.
Jeff Wang	UCLA	Biochem 3	Interaction Between Spire and Rab GTPases and its Effect on the Developing Drosophila Oocyte	Margot Quinllan	Mammalian Spire, an actin nucleator, and mammalian Rab GTPases, effectors for membrane trafficking have been shown to interact directly. Drosophila Spire has a putative rab-binding sequence, the Spir-box, located in the C-terminal half of the protein. Initial fertility assays testing flies lacking the Spir-box, showed a fertility decrease of about 50%, supporting the idea that interaction between Drosophila Spire and Drosophila Rabs is functionally significant. Specifically which Rab(s) remains unclear. Here we investigate which Drosophila Rabs interact with Drosophila Spire and whether it is through direct or indirect means. Based on data showing Rab 6 and Rab 11 interactions in mammalian systems and Rab expression patterns in the developing oocyte, we chose to probe for binding interactions starting with Rabs 5, 6, and 11. Binding interactions were tested through an in vitro GST pulldown assay with GST tagged Rab 5, 6 and 11 and C-terminal constructs of Spire. So far the pulldown assay does not indicate a direct interaction. Further optimization of experimental conditions will allow for a more conclusive assessment of the presence or absence of a direct interaction. However, this raises the possibility of indirect interactions or the requirement of additional components to stabilize the complex. Co-IP experiments from ovary lysate will be performed to probe for indirect binding between Spire and Rab 5, 6 or 11. Once specific Rabs have been identified, the complex will be further characterized biochemically with the long-term goal of modifying the binding sites in vitro and determining the functional consequences of these changes in vivo.

Katayoun Yazdi-Nejad	UCI	Biochem 3	DNA EXTRACTION FROM APTAMER-TREATED MICE AND REAL-TIME PCR ANALYSIS OF THE EXTRACTS	Melanie Cocco		The inability of the axons in the central nervous system (CNS) to regenerate and regrow is the main reason why CNS injuries remain permanent and incurable. The complex of Nogo-A, a protein localized on the membrane of the oligodendrocytes, and NgR1, Nogo-A's receptor on the axons, is known to cause inhibition of the axonal regeneration. In order to inhibit the formation of this complex, DNA apatamer sequences are designed to block Nogo-A and stop it from binding to NgR-1. After successful in- vitro trials, this study is aiming at determining whether or not aptamers can be detected in the brain tissue of Multiple Sclerosis (MS) model mice that were retro-orbitally injected with the aptamer periodically after MS-disease onset. By using Real-Time PCR techniques, we were able to show that retro-orbital injection of the aptamers does not result in the presence of them in the brain tissue. This might be due to the presence of the blood brain barrier (BBB), which aptamers should pass before getting to the brain. For future research, it can be studied whether or not coupling the apatemrs with BBB- penetrating proteins can successfully take the aptamers into the brain tissue and enhance the axonal regeneration.
Andrew Smith	USD	Biochem 3	Progress towards the development of novel nucleic acid-based therapeutics.	Anthony J. Bell	Anthony J. Bell	The objective of this study was to evaluate the viability of using intramolecular four-way junctions (4WJs) for use as therapeutic inhibitors against the DNA-binding cytokine, High Mobility Group B1 (HMGB1). Reports suggest HMGB1 should be considered a lupus biomarker because the protein is linked with several key stages of pathogenesis[1, 2]. The strategy to use 4WJs to target HMGB1 is grounded in classic in vitro studies that show HMGB1 binds to cruciform/bent DNA with a very high affinity [3-5]. Our initial studies focus on investigating the nuclease stability of 4WJs. Three 4WJs are currently being evaluated; two 4WJs referred to as i- J1 and J4 are composed of natural DNA with thymine-thymine end caps. The final 4WJ referred to as tDNA is composed DNA with thiol linkages vs. phosphate bonds. The presence of end caps in i-J1 and J4 are intended to enhance nuclease stability by preventing favorable contacts with nucleases. The thiol linkages in tDNA are known to enhance stability because these bonds are not recognized by nucleases. Nuclease digestion assays are conducted at 20o and 37oC using nucleases that digest double (DNase I, Exo, and Exo III) and single stranded DNA (Exo V and T5 Exo). Our preliminary reports show that as expected the presence of thymine end-caps and thiol linkages enhance the relative nuclease resistance of intramolecular 4WJs vs. unmodified DNA 4WJs.

Loi Nguyen	CSU Fullerton	Inorg 2	The Effect of Ionic Radii on the Formation of NCOT Perovskites	Allyson M. Fry-Petit		Perovskites with their robust structures have many intriguing properties, such as piezoelectricity, pyroelectricity, nonlinear optic response, and ferroelectricity which can make them useful in such technologies as memory devices, photovoltaics, and light-emitting diodes (LEDs). The Fry-Petit group has suggested that double perovskites, AA'BB'X6 adopt non-cooperative octahedral tilting (NCOT) structure when differences in ionic radii (ΔIR), ΔIRB-B' ≥ 0.50Å, ΔIRA-A' < 20% and ΔIRcounter ions < 0.50Å are satisfied. This suggests that Ca3WO6, Ba3WO6 and Ba2CaMoO6 should all possess NCOT structures despite being reported as cooperative structures. Powder X-ray diffraction and Rietveld refinement are used to probe the structure of Ca3WO6. The Cc space group gives a better goodness of fit and more accurate bond valence sum than the P21/n refinement. Ba2CaMoO6 is a tilted perovskite at room temperature, however low temperature data shows splitting of diffraction peaks indicative of a NCOT structure. Analysis of neutron powder diffraction data on both compounds is under way to corroborate these findings. This research explores the structure-property relationships toward the design of new materials. Fully understanding the structures helps control the properties of novel materials for desired purposes.
Kelci Skinner	CSUCI	Inorg 2	Giant Brown Kelp as Biosentinel of Environmental Mercury Differs Geographically	Simone Aloisio	Jeyla S. Fendi, Simone Aloisio	Mercury in its organic and inorganic forms is a global health concern, and persists as a pollutant in the marine environment. It is projected to increase over time due to global climate change, making it a matter of interest. As mercury enters the aquatic system it is converted into its organic form, methylmercury. This form is one that biomagnifies and becomes toxic as it travels up the food chain. Our study investigated establishing Macrocystis pyrifera (giant brown kelp) as a biosentinel of environmental mercury due to being a fast-growing producer that is both widespread and abundant. This species has the potential to serve as an indicator of current levels of mercury in the ocean surface, through the contributions of non-point and point source pollution. The study area included kelp forests off of the coast of Southern California from Santa Barbara, Ventura, Los Angeles, Long Beach and Santa Rosa Island. Mercury was quantified in samples through thermal decomposition, followed by amalgamation and atomic absorption spectroscopy. Results showed high levels of mercury near the Port of Long Beach (avg: 125.5 ppb, std: 25.1) and low levels in Ventura County (avg: 0.36 ppb, std: 0.2). Anthropogenic factors as well as point source pollution could be the reason for varying concentrations among beaches. Santa Rosa Island had moderate levels of mercury (avg: 46.1 ppb, std: 9.8), which may be a result of upwelling and unique ocean currents from surrounding waters. The implications of this study showed that there are locational differences affecting the concentrations of mercury in Giant Brown Kelp. This must be taken into consideration when using this species as a bioindicator for mercury analysis.

Madeline Riffel	UCLA	Inorg 2	Polymerization through Redox Switchable Catalysis	Paula L. Diaconescu	Junnian Wei, Paula L. Diaconescu	Polymers are used in everyday life and the chemistry of polymerization has been around since before the early 1900s. However, synthetic chemists have not been able to achieve the same control over the polymer structure as nature has. Redox switchable catalysis is a new area that could lead to sequence-controlled polymers. We are researching the use of catalysts, such as (thiolfan)AlO^{t}Bu, that can switch between their oxidized and reduced states during reactions. Certain chain-forming monomers have been found to polymerize in one redox state, but not the other. By using this selectivity, the composition of polymers can be manipulated.
Kevin Swartz	UCLA	Inorg 2	Physical Characterization of Multi-Block Copolymers and the Effect of Increasing Block Numbers	Paula L. Diaconescu	Mark Abubekerov, Paula Diaconescu	The synthesis of multiblock copolymers using a zinc scorpionate complex with a redox switchable ferrocene backbone is described. Practical methods for casting films of the corresponding block copolymers using a volatile solvent are described. The Young's modulus, ultimate tensile strength, and the elongation at break of the polymers were measured to illustrate changes in the mechanical properties as the block numbers of a certain monomer increased. Differential scanning calorimetry (DSC) was used to determine the glass transition, and melting temperatures of the polymers.

Shannen Guarina	CSU Northridge	Organic 2	The CH/π-coordination as a conformational tool for accelerating spontaneous radical coupling reactions	Gagik Melikyan

We found that introducing a methyl group beta to a cobalt-complexed propargyl radical dramatically accelerates the spontaneous radical coupling. The parent reaction was discovered in 2003 (Org. Lett. 5, 3395) and consists of the temperature-dependent conversion of diamagnetic propargyl cations to paramagnetic propargyl radicals π-bonded to a dicobalthexacarbonyl core. Replacing an alpha phenyl nuclei with vinyl groups allowed for projection of the radical center within an allylic triad (alpha-to-gamma), and also for introducing substituents along the carbon framework (α-, β-, γ-). While α- and γ-methyl groups yielded requisite propargyl cations, β-methyl group "failed" to produce an expected cation, undergoing instead the spontaneous radical dimerization reaction even at -20°C! Kinetic studies revealed that in comparison with an alpha-phenyl propargyl cation, spontaneous reaction is accelerated by at least 132 times (<5min vs 660min). The tentative mechanism of the acceleration effect will be discussed alleging a CH/π-coordination between a methyl group and an aromatic hexagon located at the acetylenic terminus. The scope of the reaction yielding E,E-γ,γ-dimers in a highly stereoselective manner and in good yields, was expanded by altering the nature of the substituents at the triple bond, as well as the location of the alkyl groups along the allylic triad. Dimeric cobalt-complexes were oxidized with ceric ammonium nitrate to yield polysubstituted 3E,7E-diene-1,9- decadiynes in four-step synthetic sequences. Computation data will be presented to corroborate experimental findings, and to also make predictions with respect to the nature and bulkiness of the beta substituents that could have an accelerating impact upon the rate of the spontaneous reaction.

Elen Artashyan	CSU Northridge	Organic 2	Cobalt-mediated radical cyclizations: Novel gateway to linearly fused carbocycles	Gagik Melikyan	The coordination of triple bonds with a dicobalthexacarbonyl core has long proven to be an efficient way of stabilizing the alpha cations, precluding an unwanted acetylene-allene rearrangement, and stereodirecting propargyl radicals in inter- and intramolecular reactions. The latter can be carried out with topologically diverse acetylenic diols in which the triple bonds are positioned either within, or outside a carbocycle. The second type of substrates constitutes the focal point of our study. The requisite bis-cobalt complexes of 1,9- decadiyne-3,8-diols were synthesized in four steps from commercial dicarboxylic acid dichlorides such as adipoyl chloride, or in five steps from commercial carboxylic acids such as phenylene dicarboxylic acid. With a flexible carbon tether between triple bonds, diastereomeric diols were chromatographically inseparable, while a rigidity introduced by a phenyl group allowed for isolation of individual d,l- and meso-diastereomers, and their characterization by means of X-ray crystallography. The generation of bis-cations was carried out by a reverse addition protocol, in a low-polarity medium, in order to optimize the formation of the six- membered ring. As reducing agents, zinc and cobaltocene were used, each in its specific temperature domain (Zn +20°C; Cp2Co -78°C). Diastereoselectivity of cyclization reactions was dependent upon the topology of substrates, rigidity of the carbon tether, configuration of diynediols, nature of reducing agents, and reaction temperature. Propargyl bis-cations were studied by means of low-temperature multinuclear NMR spectroscopy in an attempt to correlate the configuration of intermediate ionic species with that of the requisite diols and radical cyclization products. The project provides access to linearly fused polycarbocycles and paves way for targeted synthesis of novel estrogen mimics and estrogen receptor modulators.

Ciara Ordner	Cal Tech	Organic 2	Synthesis of Chiral Tetrahydropyrans by a Tandem Sakurai Allylation/Intramolecular 6-Exo-Tet Cyclization	Julie L. Hofstra	Sarah E. Reisman and Julie L. Hofstra	Heterocycles are ubiquitous in a variety of bioactive natural products, many of which have found use as potential drug targets. The potency of these molecules with regards to treating disease is often dependent upon their chirality. While several methods have been developed to synthesize a variety of chiral heterocycles, we propose a new method that utilizes chiral allyl silane substrates and proceeds through a stereospecific cascade reaction. The synthesis of a variety of chiral allyl silanes containing pendant electrophiles was achieved via a nickel-catalyzed cross-coupling method recently developed in our laboratory. We have since shown that these allyl silanes can provide the desired tetrahydropyran heterocyclic product under Lewis acid-catalyzed conditions. This mechanism proceeds through an intermolecular Sakurai allylation followed by an intramolecular 6-exo-tet cyclization. We report on the development and optimization of this cascade reaction and envision using this method to access a variety of other chiral heterocycles, including tetrahydrofurans, piperidines, pyrrolidines, and butyrolactones.
Hector Alarcon	Cal Poly Pomona	Organic 2	Deoxydehydration of Biomass-Derived Carbohydrates to Olefins using Molecular Vanadium Catalysts	S. Chantal E. Stieber		Future risk of fossil fuel depletion and documented climate change serve as incentives for studying alternative and sustainable sources of energy and chemical feedstock. Biomass from dry plant matter is the most abundant raw material on earth and is currently industrially underutilized. By removing oxygen from biomass, chemical feedstock could be generated that would otherwise be obtained from fossil fuels through cracking. This work aims to improve the conversion of vicinal diols to alkenes with new vanadium catalysts. New vanadium complexes were synthesized using two different bidentate N-heterocyclic carbene ligands. Results were compared to previous reports by establishing reproducibility for reported reactions with commercially available vanadium salts prior to testing new vanadium catalysts. Successfully improving the conversion of 1,2 cyclohexanediol could be useful in a transition to larger scale DODH conversion of glycols to useful hydrocarbons.

Annabelle Cantu	CSU Long Beach	Organic 3	Palladium(II)-Catalyzed Directed anti-Hydrochlorination of Unactivated Alkynes with In Situ Generated HCl	Keary Engle		A regioselective anti-hydrochlorination of unactivated alkynes is reported. The reaction utilizes in situ generated HCl as both the Cl- and H+ source and is catalyzed by palladium(II) acetate. Removable picolinamide and aminoquinoline bidentate directing groups are used to control the regioselectivity of the chloropalladation step and stabilize the resulting vinylpalladium(II) intermediate for subsequent protodepalladation. This method provides access to a broad array of substituted vinyl chlorides in excellent yields and with high regioselectivity. The reaction proceeds under mild conditions and is compatible with catalyst loadings as low as 25 ppm.
Kristine Claudine Teppang	SDSU	Organic 3	Monitoring DNA Duplex Formation with a Chemically Modified Tricyclic Cytidine Analogue	Byron Purse	Dillon Burns, Raymond Lee, Melissa Lokensgard, Byron Purse	Fluorescent nucleoside analogues are valuable molecular probes in biochemistry and biophysics. With structural similarities to their native counterparts in DNA, they maintain conventional Watson-Crick hydrogen bonding characteristics. These fluorescent analogues can act as fluorescent labels or be utilized in photophysical studies to report a variety of properties such as environmental changes and detection of DNA abasic sites. Due to the need for a variety of molecular probes, the Purse lab is investigating the relationship between structural and photophysical properties to provide an expanded tool kit of practical fluorescent probes with various applications. Contrary to many fluorescent nucleoside analogues available, tricyclic cytidine (tC and tCO) derivatives maintain their brightness when incorporated into duplex DNA. Our group has made chemical modifications to the tC and tCO scaffold and studied the effects of electron donating and electron withdrawing substituents on photophysical properties by means of fluorescence spectroscopy. By investigating their photophysical properties when incorporated into oligonucleotides, we can explore patterns for a systematic design of future fluorophores. The Purse lab has recently discovered a new analogue that has a distinct fluorescence response to the formation of duplex DNA. Unique other fluorescent nucleoside analogues, 8-diethylamino-tC (8-DEA-tC) becomes notably brighter once incorporated into double-stranded DNA. Quantum yield measurements of 8-DEA-tC show up to a twenty fold increase in quantum yield from nucleoside to duplex formation where base pairing protects the analogue from quenching by excited state proton transfer. Abasic and mismatch studies reveal that correct Watson-Crick base pairing is required and that the fluorescence-turn on effect is largely dependent on neighboring bases. Due to its ability to report on DNA duplex formation, we are investigating the analogue's use as a probe for enzymatic DNA synthesis.

Tyler Liebel	Cal Poly Pomona	Organic 3	Collaborative Approaches towards the Synthesis of Polyurethanes from Waste Oils	F. Z. Page	Tyler Liebel, Francisco Leyva, Christian Moreno, Victor Wyatt, Michael F Z. Page	Petroleum is a finite resource used ubiquitously as a fuel and in the manufacture of plastic materials. Due to the growing concerns regarding the environmental impact and future of petroleum as a chemical feedstock, extensive efforts have focused on providing alternative innovations that still meet consumer needs in a sustainable manner. Previously, in the Page group, seed oils have been chemically modified and cross-linked using diisocyanate to form carbamates. Diisocyanate, however, is acutely toxic and exposure often causes severe respiratory problems in addition to being a detriment to the environment. The goal of this project is to synthesize a diisocyanate-free, 100% green polyurethane using waste oils from the USDA. One of the key intermediates is the synthesis of a fatty acid methyl ester (FAME) derivative with two amine moieties. In the first step, the alkenes of compound 1 are converted to diols through hydroboration-oxidation, which display a key 13C NMR resonance at 71.9 ppm. In the subsequent step, compound 2 is oxidized turning the alcohol groups into ketones using Dess-Martin periodinane, which display a key 1H resonance at and 2.29 ppm (2H, t) and 13C NMR resonance at 211.6 ppm. Currently, the project is finalizing the synthesis of compound 4 through a reductive amination using Raney-Nickel in the presence of H2 gas. Diamine 4 will be polymerized with another FAME derivative that contains cyclic carbonates (compound 5) resulting in a 100% green polyurethane.
Justin Min	UCR	Organic 3	Direct and Indirect Impacts of Black Lights on Secondary Organic Aerosols formed from Oxidation of 1-methylnapthalene	Roya Bahreini		Directly emitted air pollutants react with atmospheric oxidants such as hydroxyl (OH.) radicals to form secondary organic aerosols (SOA). This uncontrolled, multigenerational oxidation in the atmosphere yields secondary products that form SOA species. The optical properties of SOA are not well characterized although SOA species contribute to a significant amount of direct radiative forcing. In addition, it is uncertain how stable the absorbing components of aerosols are in the presence of sunlight. In this investigation, we considered the oxidation of 1-methylnapthalene and the changes in optical properties of SOA aged in the presence and absence of black lights. SOA reactions with varying light intensities were measured and compared with experiments where lights were constant after the injection of 1-methylnapthalene. We used a 2 m3 Teflon chamber flanked with black lights at the peak radiation of λ = 350 nm; OH. Radicals were generated from the photolysis of H2O2. In these experiments, we measured aerosol absorption and scattering coefficients at 375 nm, aerosol size distribution and composition, and concentration of gas phase tracers. To characterize the differences in gas phase oxidation conditions among different experiments and the subsequent changes in aerosol composition, we compared the decay rate of 1-methylnapthalene and investigated changes in the oxidation state of carbon in SOA. The oxidation state of carbon was then related to the optical properties and mass absorption efficiency.