Abstracts

Department of Chemistry and Biochemistry
University of California, San Diego

Natural Sciences Building Atrium
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4PM – 7PM
Professor Alina Schimpf earned her undergraduate degree in Chemistry and Mathematics from Boise State University. She then went on to pursue a PhD in Chemistry at the University of Washington. As an NSF Fellow, she studied the electronic and impurity doping of colloidal semiconductor nanocrystals. Subsequently, Dr. Schimpf completed her postdoctoral studies at the Massachusetts Institute of Technology (MIT). While at MIT, she worked on conductive metal-organic frameworks. Dr. Schimpf was awarded the American Chemical Society Division of Inorganic Chemistry Young Investigator Award in 2015. She then joined the Department of Chemistry and Biochemistry at UCSD in 2016. Her current research interests are in the field of spectroscopy, inorganic chemistry, and nanoscale materials.
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A new face of ASB9 cullin ring ligase

Rachel Blake, Czarina Goingco (co-presenter), Ryan Lumpkin, Chris Condon, and Elizabeth Komives
Principal Investigator: Dr. Elizabeth Komives

The ASB9-Cullin E3 ligase is responsible for targeting substrate proteins for proteasomal degradation through the transfer of Ubiquitin by a covalent attachment to a lysine residue on the target protein. This ligase belongs to the ECS-type (ElonginBC-Cullin-SOCS-box) Cullin RING E3 ubiquitin ligase (CRL) family; within these complexes, the ASB (Ankyrin and SOCS box) protein acts as the substrate recognition site. There are 18 different ASB proteins which have the capability to recognize 10-15 substrates each. Once a substrate is bound, and tagged by Ubiquitin (Ub), the ligase will create a chain of Ub’s through K48 polyubiquitin linkages. Following polyubiquitination, the substrate-protein is degraded by the 26S proteasome. This mechanism of proteolytic degradation is responsible for the maintenance of proper cellular function.

In a pull-down assay, Gamma enolase (ENO2) was found to associate with ASB9, and therefore identified as a potential substrate of the ASB9-Cullin E3 ligase. ENO2 was expressed in E. coli and purified using Ni-NTA and Size Exclusion Chromatography (SEC). Possible association of ENO2 to ASB9 was evaluated through incubation of ENO2, ASB9, Elongins B and C (ELOB/C) and subsequent SEC. Further analysis of fractions collected through SEC with SDS-PAGE indicated the possible formation of a ENO2-ASB9-ELOB/C complex.

Biochemistry #1
Dynamics of the catalytically inactive full-length human urokinase-type plasminogen activator

Yueyi Chen, Constanza Torres-Paris, and Elizabeth Komives

Principle Investigator: Dr. Elizabeth Komives

The urokinase-type Plasminogen activator (uPA) is a serine protease that catalyzes the rate limiting step in the fibrinolysis process of anticoagulation. The uPA cleaves the inactive zymogen, plasminogen, to its active form, plasmin, which can cleave and dissolve fibrin blood clots. The uPA has three domains: the EGF-like domain, the kringle domain and the protease domain. The uPA is synthesized as a low-activity zymogen and cleavage by plasmin results in the active conformation, making a positive activation feedback loop. Recent studies suggested that the activity of the serine protease domain was related to a decrease in dynamics in the protease domain. However, whether that is true for the full-length uPA has not been fully characterized. Moreover, the role of the EGF and the kringle domains on the dynamics of the protease domain remains unknown. Last year, we expressed and purified the protease domains of the murine and human uPA, and human full-length uPA and studied the dynamics of uPA upon plasmin cleavage. Full-length human uPA can cleave itself into a two-chain form in the absence of plasmin, which is a potential drawback to the later experiments on the protein dynamics. Therefore, I cloned a catalytically inactive mutant using mutagenesis PCR and I expressed and purified this full-length human uPA mutant in E.coli for the first time by refolding. I am also carrying out plasmin-activation assays the catalytically inactive uPA and comparing the dynamics with wild-type uPA using hydrogen-deuterium exchange. These experiments will enable us to characterize how the dynamics of uPA influence its activation.

Biochemistry #2
Heart failure (HF) is a pandemic of epic proportions—affecting the lives of 26 million people across the globe. As medical treatments progress, and lifespans increase, so does the demand for better treatment options of the world’s most deadly disease. A major protein target for development of new therapeutics of patients suffering HF is the cardiac isoform of the Sarco/Endoplasmic Reticulum Ca2+-ATPase (SERCA2a) which is responsible for regulation of cytoplasmic calcium. SERCA is responsible for sequestering between 70-90% of calcium in response to Ca2+-release, and thus, plays a major role in the contraction-relaxation cycle of the heart. Its dysfunction has been directly linked to abnormal heart tissue that causes HF. In the present study, we use computational methods to better understand how competitively binding nucleotide substrates such as 2’-deoxy-ATP (dATP) affect the regulation and action of SERCA in its calcium clearing action. We begin our investigation with Gaussian Accelerated Molecular Dynamics (GaMD), a tool that explores the conformational landscape of SERCA in response to interactions with ATP and dATP. Using unique confirmations from MD, we then employ Brownian Dynamics (BD) simulations to better understand Ca2+ and nucleotide association differences. Specifically, we determine association rates (K_{on}) to develop a kinetic landscape model of SERCA regulation. Finally, we have developed a method for the analysis of the salt-bridge occupancy of the respective domains, in order to understand how the Nucleotidate (N), Phosphorylation (P), and Actuator (A) domain dynamics are affected by the presence of nucleotides.
pH low insertion peptide (pHLIP) has a structure that is finely
tuned to respond to the pH of its environment. At neutral pH
(~7.4), the peptide binds to membranes interfacially and
adopts a random coil structure. In acidic pH; however, the
peptide undergoes a significant structural change and inserts
into the membrane bilayer as a transmembrane α-helix. The
pH sensitive structure of pHLIP makes it a potential means of
drug delivery to acidic cancer cells which are commonly
observed in hard tumors. While these aspects have drawn
attention to the peptide, little is still known about how the
lowered pH induces the structural changes. The goal of this
study is to apply molecular dynamics (MD) to compare and
contrast pHLIP’s interactions within a POPC lipid bilayer at
different charged states of its aspartic and glutamic acid
residues. We observed that the peptide tends to have less
helical tendency and insertion propensity in its charged state,
in agreement with experimental measurements. We also
observed that, in charged state, the peptide induces a large
deformation into the bilayer by allowing water molecules to
penetrate the membrane hydrophobic core. Overall, the
simulations show a more tumultuous nature when the pHLIP
peptide has charged aspartic acid and glutamic acid residues
than when these amino acids are neutralized with protonation
which occurs in an acidic environment.

Biochemistry #4
Cytotoxicity of Light-Activated Ferrocene Compounds
Andrea Gonzalez, Pauline Olsen, Polin Ivanova, and Joseph O’Connor
Principal Investigator: Dr. Joseph O’Connor

Cancer is a complex disease that pervades the lives of an innumerable amount of people. The complexity of the disease has led to the research of therapies that can treat many types of cancer. Several successful therapies have been discovered and implemented, but there is still a need for new therapies. Cisplatin was the first successful anticancer metallotherapy and has been used for several decades to treat a variety of tumors, but still has side effects such as resistance in cancer cells along with heavy metal toxicity. Ferrocene has proved to be an interesting alternative due to its low cost and biological properties. The O’Connor research group has been synthesizing light-activated benzoyl-ferrocene derivatives that release free iron(II), which allows for a photodynamic therapy effect. It is hypothesized that the benzoyl-ferrocene derivatives cause cell death by oxidizing the iron(II) to iron (III) by the Fenton and Haber-Weiss reaction in the cell causing cell death. The results of previous experiments have led to the synthesis of two new derivatives that have more lipophilic character and are hypothesized to have a higher potency than the previous derivatives tested.

Biochemistry #5
Co-culturing marine cyanobacteria with antagonistic organisms leads to altered expression of bioactive secondary metabolites

Aurora C. Guild, Evgenia Glukho, and William Gerwick
Principal Investigator: Dr. William Gerwick

Antagonistic interaction between co-cultured organisms has been a productive method by which to activate normally silent secondary metabolite biosynthetic gene clusters. To this end, we performed co-culture experiments with non-axenic, tropical filamentous cyanobacteria in order to evaluate their influence on each other. As identified by 16S rRNA sequencing, two of the cultures were Leptolybya species (ASF and ISB) while the others were Moorea producens (PAL and JHB) and Moorea bouillonii. All five cultures were isolated from original field collections made in shallow waters near Jamaica (JHB), Palmyra atoll (PAL), American Samoa (ASF), Papua New Guinea (PNG) and Sulawesi (ISB), and have been maintained in culture for between 4 and 24 years. These cultured cyanobacteria have previously been established as producers of a number of potent biologically active natural products such as hectochlorin, the jamaicamides, palmyramide A, leptochealin, the fagaaluamides, cryptomaldamide and curacin D. These four cyanobacteria were co-cultured in a matrix comprised of all possible pairs, and then were further co-cultured with Candida albicans with the intention of up-regulating the production of an antifungal secondary metabolite. The crude extracts from each experiment were analyzed by mass spectrometry, MS2-based molecular networking, UV spectrophotometry, biological activity to cancer cells in culture, and antifungal activity bioassays.
NFkB is a family of transcription factors of which the RelA-p50 heterodimer plays key role in regulating the immune response. Of the two transcription factors, RelA, also known as p65, is the one that contains a transcription activation domain (TAD). This TAD is predicted to be intrinsically disordered according to the amino acid sequence, and it is predicted to not have a fixed three dimensional structure. In order to get a better perspective of how common disordered TADs are in nature, 111 Homo sapiens transcription factors were sorted and analyzed through prediction algorithms. We started with the DBD transcription factor prediction database, which was derived by analyzing genomic sequences for the presence of a DNA binding domain. All 111 transcription factors’ amino acid sequence in this project were obtained from this database. The sequences were then analyzed with PONDR and 9aaTAD. PONDR is a web-based predictor for disordered sequences, whereas 9aaTAD is a transactivation domain predictor. Both web based predictor analyses use protein sequences as input. Seventy-three transcription factors were predicted to be disordered and predicted to be a transactivation domain. Cross-referencing ensured that the TAD contained the predicted disorder. The BLAST search engine was used to confirm the identity of each transcription factor. Of the 65% predicted disordered TAD, 35% of them have a predicted disorder TAD with sequence size larger than 100 amino acids. Future expansion of the database will entail analyzing the rest of the Homo sapiens transcription factor database.

Biochemistry #7
A natural nanotechnological marvel, self-assembling protein structures might be useful as templates in the manufacturing of intricate structures not currently possible with lithographic methods. As a step towards producing such ordered protein templates, we aim to construct a new type of two-dimensional protein lattice linked by cysteine disulfide bridges which features configurable symmetry. The building block for these assemblies is dihydroneopterin aldolase (FolB) from Mycobacterium tuberculosis. The tetrameric protein is an attractive base material due to its C₄ symmetric, square shape and the proximity of the C and N termini of its subunits. This structure allows the protein’s monomers to be genetically fused, yielding C₂ symmetric or asymmetric building blocks. As a first step towards producing this unprecedented configurable material, FolB was engineered to present a cysteine on each of its four sides. Under gradually oxidizing conditions, uM scale FolB sheets were formed in solution, as visualized in TEM. We are currently working to optimize the size and order of these assemblies. To this end, the structure assembly’s protein-protein interfaces will be investigated using X-ray crystallography. Furthermore, we will assess the impact of tetramer-tetramer interactions on the order and size of the sheets by disrupting hydrogen bonding between tetramers through mutagenesis. The information gathered will help us rationally design further refinements to the protein building block to improve assembly quality. If successful, we will proceed by designing C₂ and asymmetric FolB variants, which will enable us to vary the interactions at each face of the protein in the pursuit of patterned 2-D assemblies.
The Tor Lab focuses on the synthesis and biophysical evaluation of fluorescent nucleoside analogues. Our lab has developed two libraries of fluorescent nucleosides that are remarkably similar to the native molecules in structure relative to other commonly used nucleoside analogues. Though our molecules are structurally similar to the native, we also want to know if they are functionally similar. To evaluate iso-functionality we incorporate our nucleosides into biomolecules and perform enzymatic reactions with them.

During my time in the Tor lab I successfully synthesized both analogues of guanosine. I am currently working on converting our guanosine analogues into cyclic guanosine monophosphate (cGMP). Once achieved, I will use cGMP-Specific Phosphodiesterase 5 to see if it will convert our analogues of cGMP to GMP as it does with the native guanosine nucleoside. This enzymatic reaction will be monitored using HPLC. Since enzymes are highly sensitive to changes in the structure of their substrates, this experiment will tell how the functionality our analogues of cGMP compare to that of the native cGMP.
Domoic acid (DA) is a metabolite synthesized by marine *Pseudo-nitzschia* spps. diatoms, and is a known mammalian neurotoxin. Eating DA-contaminated shellfish could cause amnesic shellfish poisoning (ASP), a disease associated with brain damage, memory loss, and possibly death. Recently, the Moore lab discovered the DA biosynthetic (Dab) pathway using *in vitro* assays with heterologously expressed Dab proteins; however, no identified enzymes catalyzed the isomerization of isodomoic acid A (isoDA-A) to the mature DA toxin. To further validate the Dab pathway *in vivo* and understand when isomerization occurs, we designed syntheses of five DA intermediates that incorporate heavy isotopes $^2$H (D) and $^{15}$N into their chemical structures. Three different doubly labeled linear N-prenylated molecules were chemically synthesized via a reductive amination strategy using $^{15}$N-labeled L-glutamate ($^{15}$N-L-Glu) and variable monoterpene-derived aldehydes in the presence of NaBD$_4$. We next heterologously expressed and purified DabC, a novel dioxygenase enzyme in the Dab pathway, from *E. coli*. DabC was then used to biochemically transform two of these linear molecules to their cyclic counterparts, including a synthetically challenging $[^{15}$N, D]-labeled isoDA-A. Milligram quantities of all intermediates were purified by HPLC and characterized by high-resolution mass spectrometry and NMR. Our next plan to incubate these labeled molecules with live cultures of DA-producing and non-producing *Pseudo-nitzschia* diatoms to assess *in vivo* conversion to DA. This experiment will give better insight into understanding DA biosynthesis and help us to understand the final isomerization unobserved through *in vitro* Dab assays.
Thrombin is the serine protease responsible for cleaving fibrinogen and Protease Activated Receptors (PAR) on the surface of platelets in the blood, which initiates the formation of a blood clot. However, binding of thrombomodulin (TM) to thrombin switches the specificity of thrombin away from these procoagulative substrates, and toward protein C, triggering an anticoagulative response. Excessive clot formation can be life threatening, highlight the important regulatory role TM plays in maintaining a healthy degree of clotting. Interestingly, the double mutant W215A/E217A has been show to exhibit poor activity towards procoagulative substrates, yet retains much of its activity towards anticoagulative substrates. In fact, this thrombin mutant has already been included in clinical studies for its potential application as an anticoagulative agent in a medical setting. Previous studies from the Komives lab have identified protein dynamics as a key in describing the allosteric communication between the Anion Binding Exosite 1 (ABE1), where TM binds, and the thrombin active site. In order to understand whether the W215A/E217A thrombin mutations alter thrombin specificity in a way similar to TM binding, Hydrogen-Deuterium Exchange Mass Spectrometry (HDX-MS) were conducted on the W215A/E217A thrombin mutant and on wild type (WT) thrombin with and without thrombomodulin present. HDX-MS measures the changes in solvent accessibility of the peptide backbone of a protein, informing us on how protein confirmation changes over time. If the effect of the W215A/E217A mutations induce an allosteric effect on thrombin similar to that of TM binding, then we should observe similar dynamics when comparing the HDX-MS results of TM-bound WT thrombin to the W215A/E217A thrombin mutant when TM is absent.

Biochemistry #11
G protein-coupled receptors (GPCRs) are 7-transmembrane helical proteins that are embedded in the plasma membrane. They recognize various extracellular signals and transduce them to intracellular heterotrimeric G proteins, which further activate cellular responses. Neurotensin receptor 1 (NTR1) interacts with neurotensin, a 13-residue peptide, which plays important roles in the pathogenesis of neurological disorders such as Parkinson’s disease and schizophrenia, and in lung cancer progression. To characterize the structure and dynamics of NTR1 in phospholipid bilayers by solid-state NMR spectroscopy, we prepared isotopically labeled receptors using glutathione S-transferase-fusion expression system in *E. coli*. Optimization of the sample preparation and preliminary NMR results of the receptor in lipid bilayers will be presented.
The Impact of Concentration on the Surface Adsorption of Fatty Acids at the Air-Water Interface

Meishi Song, Man Luo, and Vicki H. Grassian

Principal Investigator: Dr. Vicki H. Grassian

Organic coatings, such as fatty acid surfactants, on sea spray aerosol (SSA) can determine the lifetime, reactivity, and properties such as light scattering and ice nucleation of the aerosol in the atmosphere. Moreover, the change in the protonation state of the surfactant can lead to the change in surface activity and affect those properties. Studies have revealed that there is a difference between the surface and bulk pKa values for medium- and long-chain acids and used it to explain the relationship between surface activity and the protonation state of fatty acids. However, in our experiment, we found that instead of approaching the value of bulk pKa, the measured values of “surface pKa” can be higher or lower than it. This observation led to a search on a more suitable concept for data explanation, which has been determined to be surface adsorption. The effects of fatty acid concentration on the surface adsorption are not well understood. Surface adsorption does depend on concentration due to the unique environment of the interface that can concentrate the fatty acid and can increase the intermolecular interaction. It is interesting to find that surface lowers with decreasing concentration of the fatty acid. In future studies, we will probe the change in surface adsorption of various fatty acids at different concentrations of salt solutions. These experiments with the addition of salts can mimic marine-relevant conditions. Overall, this study provides insights into the properties of sea spray aerosol while predicting its compositional and structural change due its environment.

Biochemistry #13
Inhibitions of rPhosphofructokinase-1 (rPFK-1) Enzyme Activity By Fatty Acid Derivatives of Vitamin C
Dagoberto Valdes, Ami Abbott, and Eduardo Fricovsky
Principal Investigator: Dr. Eduardo Fricovsky

Multiple research studies on fatty acid derivatives of Ascorbic Acid (AA) have been of major interest due to their applications in areas such as: anti-metastatic action of certain cancers, and the demonstrated inhibitory effects on the glycolytic enzyme phosphofructokinase-1 from rabbit muscle (rmPFK-1), which is used in the metabolism of glucose and aids in the regulation of glycolysis. Studies have shown that cancer cells demonstrated a greater need for glucose than normal cells for survival. Based on the activity of ascorbate on phosphofructokinase-1 (PFK-1), we developed a working hypothesis that derivatives of Ascorbic Acid (AA), specifically, ascorbic acid-6-palminate (AAP) and ascorbic acid-6-sterate (AAS), reduce rmPFK-1 enzyme activity by orders of magnitude. To achieve the study, we synthesized ascorbic acid-6-palminate (AAP) and ascorbic acid-6-sterate (AAS) and tested the inhibition on PFK-1 at varying concentrations using a buffered solution of 95% ethanol. The results along with IC50 levels of PFK-1 encourages further research, into various differing Ascorbic Acid (AA) derivatives.

Biochemistry #14
Importance of DOM34 in Regulating Translation of Polyproline-harboring Mitochondrial Proteins

Fan Xu, Tatsuhisa Tsuboi, and Brian Zid
Principal Investigator: Dr. Brian Zid

Translational quality control system is important to maintain protein production. During translation in ORF, ribosome can be stalled by polyproline, a sequence of repeating proline residues that lead to destabilization of peptidyl-tRNA. Recently, our lab found that polyproline also accelerates mitochondria targeting signal-dependent mRNA localization to mitochondria. To further evaluate functional consequence of this localization, we analyzed protein production from polyproline-harboring mRNA and found that its protein production was diminished. It is known that translational quality control system regulates polyproline-harboring protein production. Therefore, we decided to analyze the involvement of translation quality control factors in regulating polyproline-harboring protein production. We deleted Vms1, Pim1, Not4, and Dom34 from yeast wildtype strains expressing polyproline-harboring proteins. Surprisingly, in Dom34 deletion strains, we observed recovery of polyproline-harboring protein production. Furthermore, we observed defective growth of Dom34 deletion strains that express polyproline-harboring protein in respiratory condition. These suggest that Dom34 is essential for downregulating polyproline-harboring mitochondrial protein production and maintaining cell viability.

Biochemistry #15
Method of Determining Molybdenum Iron Protein Concentration in Cell Lysate

Robin Yu, Hannah Rutledge, and Akif Tezcan
Principle Investigator: Dr. Akif Tezcan

The nitrogenase enzyme is a vital catalyst that reduces dinitrogen into ammonia at ambient temperature and pressure described by the equation:

\[ \text{N}_2 + 8\text{H}^+ + 8\text{e}^- + 16\text{MgATP} \rightarrow 2\text{NH}_3 + \text{H}_2 + 16\text{MgADP} + 16\text{Pi} \]

Nitrogenase consists of two proteins: a homo-dimeric iron protein and a hetero-tetrameric molybdenum iron protein (MoFeP). Assays that study the catalytic efficiency of nitrogenase are typically done with varying concentrations of MoFeP, and thus, the accurate quantification of MoFeP is critical. Currently, the quantification of impure MoFeP from whole-cells is done with a Western blot, which is an expensive and time-consuming method. Therefore, we’ve developed a cheaper and more efficient process whereby the concentration of MoFeP \textit{in vivo} can be determined through a MoFeP standard curve on a protein gel. In our experiments, MoFeP samples are partially and quickly purified and then quantified relative to the standard by using a linear model obtained from ImageJ analysis. Of an amiconed cell lysate sample of \textit{Azotobacter Vinelandii}, we found the average MoFeP concentration to be 4.6 mg/mL with a standard deviation of 0.5 mg/mL. These results show that this protocol provides an inexpensive, reproducible and efficient method of quantifying intracellular MoFeP and is a viable solution for \textit{in vivo} assay procedures.

Biochemistry #16
Inorganic Division

1. Riddhi Ananth
2. Jerika Chiong
3. Polin P. Ivanova
4. Jerry Li
5. Nicholas Tu
Facile bench-top stabilization of porous silicon surfaces using heterocyclic silane grafting chemistry

Riddhi Ananth, Lorenzo J. Calvano, Anushree Chaudhuri, Hsuan Chang, Chinglin Chan, Tiffany K. Chen, and Michael J. Sailor

Principal Investigator: Dr. Michael J. Sailor

Porous silicon is a nanomaterial of interest for a range of sensing, energy, and biomaterials applications. For these applications it is often necessary to impart functionality to the surface. This work presents a new means of generating a functional porous silicon surface by grafting of the 5-membered heterocyclic silane, 2,2,5,5-tetramethyl-2,5-disila-1-oxopentane onto mildly oxidized porous silicon surfaces. The grafting reaction was carried out at room temperature, in a sealed glass vial by immersing the porous silicon sample in a reaction mixture consisting of the liquid reagent and chloroform. The resulting functional surface was characterized by ATR FT-IR, and the open porosity of the material was determined by the Spectroscopic Liquid Infiltration Method (SLIM). Scanning Electron Microscope (SEM) imaging was used to obtain plan- and cross-sectional views of the nanostructures. We conclude that the reaction reaches completion in under 10 minutes while retaining the open pore structure of the original porous silicon substrate, although the porosity is reduced due to partial filling of the pores by the silane polymer product. The extent of grafting can be modulated by varying the concentration of silane in chloroform solvent. In hydroxylated porous silicon rugate filters, starting porosities of 50.3 ± 0.5% were observed to have fractional decreases between 20% and 90% after the grafting reaction. The modified surface was highly hydrophobic, with a water contact angle of ~130°. This chemistry also prevented degradation of the nanostructure in alkaline media. Repeated heating and cooling of the modified samples from room temperature to 120 °C produced no appreciable change in the nanostructures. Therefore, this chemistry is a convenient means to generate stable and highly hydrophobic porous silicon.

Inorganic #1
Rational design of metal-organic frameworks from discrete synthetic clusters

Jerika Chiong, Jake Bailey, Jie Zhu, Rohit Subramanian, Wenqian Xu, Seth Cohen, and Akif Tezcan
Principal Investigator: Dr. Akif Tezcan

Metal-organic frameworks (MOFs) are porous coordination polymers comprised of metal ions/clusters (nodes) and metal-coordinating organic ligands (struts). The metal-ligand interactions of these nodes and struts promote self-assembly into organized supramolecular architectures in which the struts control the spatial geometry of the nodes through their size and number of coordination sites. The discrete components of these frameworks can be systematically altered in a predictable manner to produce desired functionalities such as gas storage, catalysis, drug delivery, and molecular recognition. We aim to rationally design highly stable MOFs based on a previously synthesized symmetric cluster. We selected a robust M₄L₆ cluster with dihydroxamate chelating ligands to act as the node. Replacing this ligand with a symmetric tetrahydroxamate bridging ligand would allow multiple clusters to be chemically linked, leading to the formation of an ordered 3D network instead of a discrete cluster. To this end, we synthesized multiple tetrahydroxamate ligands for MOF assembly. Solvothermal synthesis was employed to facilitate the formation of crystalline frameworks. We used both single-crystal and powder X-ray diffraction to determine the structures of the materials that formed. Gas sorption experiments, thermogravimetric analysis, and stability tests were conducted to characterize the MOFs. The development of these cluster-based MOFs ultimately represents an organized architecture where metal-ligand interactions form highly stable clusters, and the symmetry of the ligands dictates the crystallographic organization of the clusters. The formation of the proposed MOFs allows for precise tuning of the lattice pores while retaining the functionality of the individual clusters.

Inorganic #2
Photodynamic Anticancer Benzoyl-Ferrocene Compounds
Polin P. Ivanova, Pauline M. Olsen, and Joseph M. O’Connor
Principal Investigator: Dr. Joseph M. O’Connor

Ferrocene derivatives have been employed as substituents in a number of bioactive compounds, such as Hydroxyferrocin, which is a ferrocene derivative of the antitumor compound Tamoxifen, and Ferroquine, which is currently in late-stage of clinical trials as an antimalarial drug candidate. Ferrocene has been used as a structural scaffold due to its’ biological stability, cost effectiveness, and high membrane permeability. In the O’Connor group, we focus on benzoyl-ferrocene derivatives due to their ability to release iron (II) into a cell upon photolysis with visible light. We have observed photo-induced cytotoxicity with these compounds, and we hypothesize that cell death is due to an increased concentration of radicals due to the iron catalyzed Fenton reaction and Haber-Weiss catalytic cycle. Recent results on the synthesis and study of a new benzoyl-ferrocene derivatives conjugated to triphenylphosphine will be presented.
Examining the extent that high symmetry can influence the magnetic anisotropy in hexasolvento metal complexes

Jerry Li, Alex Mantanona, and Jeffery D. Rinehart

Principal Investigator: Dr. Jeffrey D. Rinehart

Slow magnetic relaxations of mononuclear single molecule magnets (SMM) can be generated by inducing anisotropy. Magnetic anisotropy is closely influenced by the strength and symmetry of the crystal field, and, in general, systems with better axial symmetry tend to have better anisotropy. Although axial coordination is the most common way to generate anisotropy, highly symmetric systems have shown slow relaxation as well. While, it is understood that symmetry plays an important role in generating anisotropy, current theoretical models fail to provide meaningful analysis of highly symmetric systems with slow magnetic relaxation. Therefore, a large interest is placed onto octahedral homoleptic six-coordinate metal complexes. To examine the extent symmetry can influence slow relaxations, several hexasolvento complexes with non-coordinating ligands were prepared, such as [Co(DMSO)₆](BPh₄)₂ and [Fe(DMSO)₆](BPh₄)₂. [Co(DMSO)₆](BPh₄)₂ was examined with UV-Vis and SQUID magnetometry, and it was shown to be a SMM. Herein we describe the synthesis of additional analogs with different ligands, such as DMF and NMF, to see if those analogs are also SMMs. These complexes will help build new theoretical models to describe systems that have slow magnetic relaxation where traditional models fail.

Inorganic #4
Tuning synthesis of polydopamine nanoparticles for variable morphological properties
Nicholas Tu, Yijun Xie, and Jeffrey Rinehart
Principal Investigator: Dr. Jeffrey Rinehart

Polydopamine (PDA) nanoparticles have been of interest for drug delivery and also as an ultrasound contrasting agent with post-synthetic modifications enabling gas microbubble activity. Examining the syntheses of the nanoparticles, a number of protocols enable a variety of morphological states to be achieved, such as solid, hollow, and mesoporous states.

We aimed to change the parameters of different synthetic methods to study their effects on PDA nanoparticles’ morphologies, both intrinsic and inter-nanoparticle properties. Parameters included the identity and amount of solvent(s), metal catalyst, and monomer. Nanoparticles were characterized primarily by transmission electron microscopy (TEM) and scanning electron microscopy (SEM) to observe morphologies, inconsistencies, and crosslinking of nanoparticles. In addition, dynamic light scattering (DLS) was used to identify size and distribution quantitatively and contact-angle analysis was used to infer hydrophobicity. By the parameterized changes, we obtained solid PDA nanoparticles, hollow PDA nanoparticles, and mesoporous PDA and poly-L-DOPA nanoparticles, each monodisperse. These results allow for precise tuning of each type of nanoparticle and enable post-synthetic treatment of hollow PDA nanoparticles with perfluoroalkyl groups to be used for ultrasound imaging.
Organic Division

1. Kaitlyn Freiberg, Seth Vigneron
2. Michelle Kinney
3. Christine Lee
4. Kristine Luong
5. Anton Samoylov
Synthesis of Aryl Substituted 2-Pyrazolines
Kaitlyn M. Freiberg, Seth F. Vigneron (co-presenter), Tiffany L. Hamilton, Melinda Chan, and Dionicio Siegel
Principal Investigator: Dr. Dionicio Siegel

Malaria remains a persistent target for new pharmaceuticals as despite best efforts by researchers 214 million people became infected leading to an estimated 438,000 deaths globally in 2015.1 Current treatments in use have depreciated in effectiveness as the P. falciparum parasite continues to develop resistance to combination therapies.2 These issues have sparked new interest in combating the parasite in its larval liver stage using a new class of compounds. Synthesized small molecule inhibitors are given to isogenic clones of the parasite for testing. This study aimed to measure the effectiveness of differing substituted aryl rings bound to a central 2-pyrazoline through a two-step modular synthesis and subsequent IC50 analysis.

Organic #1
Viruses—the most abundant biological entities in the world’s oceans—affect all marine lifeforms, from bacteria to protists, crustaceans, fish and mammals. Viruses especially influence marine microbial populations and community composition as they lyse an estimated 10-50% of all marine microbes every single day. Unsurprisingly, cellular organisms like phytoplankton have evolved numerous antiviral defense mechanisms, including well-known proteogenic response systems such as CRISPR-Cas, restriction-modification, and abortive infection. A small molecule chemical response to viral infection, however, is not yet known. In this investigation, secondary metabolites of control and virally infected phytoplankton were analyzed for bioactivity and novelty. Several active viruses against the diatoms *Pseudonitzschia* and *Cylindrotheca* were first identified. Cultures of each diatom were then subjected to viral lysis and then compared against control cultures. The extracts of the biomass generated for each diatom were then analyzed by liquid chromatography mass spectrometry (LCMS) for qualitative and quantitative profiling of secondary metabolites. LCMS was also coupled with a bioassay-guided fractionation and Global Natural Products Social Molecular Networking database to identify the presence of novel lead compounds, which were purified and isolated for further bioactivity studies and structure elucidation.
Copper Mediated Photocyclic Addition for Synthesis of Small Heterocycles

Christine Lee, Daniel Flores, and Valerie Schmidt
Principal Investigator: Dr. Valerie Schmidt

Azetidines are four-membered nitrogen containing heterocycles that are prevalent in biological active molecules, but there is a dearth of practical synthetic methodology to synthesize them. To expand this chemical space, we developed a copper-based catalytic system to facilitate the 2+2 photochemical cycloaddition of simple imines and olefins. Mechanistically, this allows for selective activation of one pi component via coordination. The method described leads to the formation of azetidines in high yields with broad functional group tolerance.

Organic #3
A Radical Mediated Approach to Smiles Rearrangement with Hydroxamic Acids for Aniline Synthesis

Kristine Luong, Samuel Lardy, and Valerie Schmidt

Principal Investigator: Dr. Valerie Schmidt

Nitrogen-containing aromatic compounds are prevalent in pharmaceuticals and natural products and a great deal of effort has been expended to produce chemicals of this type using the most cost-effective and efficient means possible. However, a vast majority require the use of harsh conditions or costly transition metal catalysts, thereby hampering the synthetic utility of such methods. Preliminary data in the Schmidt Lab at UCSD suggests that there is a way to synthesize aromatic nitrogen-containing compounds using a novel approach that employs exceptionally mild reaction conditions and circumvents the need for transition metal catalysts.

This new strategy that we are developing relies on the production of nitrogen-centered radicals from molecules containing weak nitrogen-oxygen bonds, specifically those with hydroxamic acid groups. These molecules are activated in the presence of radical initiators and phosphorous (III) reagents, which homolytically cleaves the nitrogen-oxygen bond, generating a reactive nitrogen center that undergoes a substitution reaction to generate an aryl migration and forge a new carbon-nitrogen bond.

Organic #4
Over the past decade the polyurethane market has been steadily growing, particularly within the flexible and rigid foam products sector. However, the majority of existing polyurethane products use petroleum formulations which do not biodegrade, instead breaking down into microplastics which infiltrate ecosystems. Bioplastics offer an environmentally friendly and economically viable alternative, with the market expected to grow about 21% compounded annually throughout 2025. Botryococcene is one such alternative to petroleum polyols. Botryococcene is a terpenoid originating from the microalgae *Botryococcus braunii*, which contains five primary alkenes that can be converted into hydroxyl groups, making it a contender for use in rigid foam formulations. The method used in this project involved hydroboration-oxidation using borane in THF to target the five terminal alkenes for conversion into hydroxyl groups to produce a polyol, an ingredient which composes a significant portion of polyurethane formulas. The resulting product was analysed using LCMS and FTIR to determine its characteristics.
Physical/Analytical Division

1. Danielle Bisbee
2. Brandon Bizzarro
3. Heidi Busse
4. Isaac Canada
5. Ivan Cruse
6. Jiayin Dai, Ruochen Cao
7. Tongshan Liu
8. Michael Mundo, Connie Li
9. Ngoc Hung Nguyen
10. Debbie Zhuang
Extraction of succinic acid from cyanobacteria

Danielle Bisbee, Marissa Tessman, Enid Partika, Graham Griffin, and Robert Pomeroy

Principal Investigator: Dr. Robert Pomeroy

A comprehensive extraction of succinic acid from cyanobacteria is in the process of being developed at the microscale and processing scale to maximize yield as a proof of concept. Microscale tests on raw, centrifuged, and centrifuged and filtered media determined that raw media had the highest yield of succinic acid – 93.1% – and that therefore centrifugation and filtering was not necessary. Separate solutions of succinic acid in media (~pH 3) were subjected to acetone extractions to remove the salts, followed by barium succinate precipitation and conversion back to succinic acid via barium sulfate precipitation, with yields of 73.2% to 84.3% by the completion of the barium succinate precipitation. The resulting succinic was tested for purity via HPLC, with results confirming the presence of succinic acid and reduced impurities. When done at scale, removing the cyanobacteria cells proved to be necessary, and can be accomplished via flocculation and centrifugation, with the resultant supernatant containing the succinic acid evaporated and dried product beginning the extraction procedure with the dissolution via acetone.

Physical/Analytical #1
Ion solvation plays an important role in a number of environmental processes, but detailed explorations of these chemical phenomena are often experimentally untenable. Molecular dynamics (MD) simulations offer one method to circumvent this issue using some representation of the potential energy surface (PES) for the given molecular configuration. In this study, a number of computational models capable of describing these PESs are employed to assess the energetics of solvated halide ions in simple water systems, from many-body potential energy functions (PEFs) and force fields (FFs) to exchange-correlation functionals culled from the hierarchy of density functional theory (DFT) approximations. A comprehensive analysis of the many-body models in the description of the interaction energy for these systems reveals that insufficiently representing close-range intermolecular interactions, like charge transfer and charge penetration, results in significant disagreements with reference data from high-level electronic structure calculations. Additionally, energy decompositions of the total interaction energy allow for a thorough comparison of the theoretical design underlying various classes of XC functionals, as well as FFs and PEFs and uncover important features governing the behavior of halide-water interactions.
Aerosols in the atmosphere nucleate ice clouds through two major pathways, deposition and immersion freezing. On the single particle level, depositional freezing has been extensively studied using spectroscopic methods while immersion freezing has been largely studied through optical imaging or in bulk aqueous solutions. These aerosols can also undergo heterogeneous reactions with reactive atmospheric gases during their lifetime thus changing the composition of the aerosol. Therefore, there is a need for a method that allows for the spectroscopic study of single particle immersion freezing and the impact that heterogeneous reactions with atmospheric gases have on the freezing process. We have developed a method that permits for the spectroscopic study of single particle immersion freezing and the impact of in situ heterogeneous reactions by coupling a confocal Raman spectrometer to an environmental cell. This system can control relative humidity and temperature so that low temperature water uptake and ice nucleation of atmospheric aerosols can be explored while information about the chemical composition and phase state of ice nuclei is provided via Raman spectroscopy. This provides insight into how ice nuclei and their heterogeneous reactions with atmospheric gases impact cloud formation in the atmosphere.
Modeling Studies of Isoprene- and Monoterpene-Derived Organic Nitrates in a Mixed Forest Environment and the Role of Deposition and Aerosol Multiphase Chemistry

Isaac Canada, Paul B. Shepson*, and Jonathan Slade

*Stony Brook University, New York

Principal Investigator: Dr. Jonathan Slade

Organic nitrates (RONO$_2$) produced during the oxidation of VOCs in the presence of nitrogen oxides (NO$_x$=NO+NO$_2$) limit ozone production by sequestering NO$_x$ and contribute to secondary organic aerosol (SOA) formation. While forested environments represent the largest source of biogenic VOC emissions, and biogenic SOA is the most abundant source of OA in the atmosphere, the formation of biogenic-derived RONO$_2$ is poorly understood with sparse measurements. Here, we present modeling results of RONO$_2$ and compare to measured RONO$_2$ sampled in a mixed deciduous/coniferous forest in northern Michigan during the summer of 2016. During that study, concentrations of hydroxylated RONO$_2$ (HORONO$_2$) resulting from the oxidation of isoprene (IN) and monoterpenes (MTN) were quantified over multiple daily cycles. We apply a 0-D chemical kinetics box model using the Master Chemical Mechanism constrained by measured species and compare our results to those measured. Our results demonstrate the importance of deposition processes, including HORONO$_2$ uptake and loss to the aerosol phase. The results indicate that without aerosol mass, the model overpredicts daytime IN and MTN by close to a factor of two, especially in the early afternoon when aerosol number concentrations are highest. Including depositional loss of IN and MTN to the available aerosol mass as a function of time results in better agreement between the modeled and measured concentrations. These results emphasize the importance of RONO$_2$ multiphase chemistry and likely hydrolysis of HORONO$_2$ in biogenic SOA particles in controlling the NO$_x$ and thus ozone budgets in forested environments.

Physical/Analytical #4
The polydispersity index, PDI, is a metric used in the polymer industry to characterize the distribution of molecular weights associated with a polymer sample. PDI is commonly determined by size exclusion chromatography, SEC. While useful, SEC has its drawbacks as it is not only a slow and pricy technique, but also one which has difficulty resolving a 10% difference in mass between components. This project seeks to rectify these shortcomings by using direct insertion mass spectrometry via a high resolution Thermo Fisher Fusion equipped with an Orbitrap which cuts down both the time and cost of analysis while also allowing for differentiation of components with a 5ppm margin of error. A calculator has been developed to compute the PDI from the MS data. The PDI was calculated for four different polyols used in the synthesis of polyurethane foams and is compared to the findings utilizing the industry standard SEC. The comparison will examine figures of merit such as: instrument cost, sample cost, sample run time, and resolution.
Carbon content and speciation are major factors affecting climate-relevant properties of sea spray aerosols (SSA). Field studies attempting to constrain SSA carbon speciation under various oceanic conditions (e.g. high biological activity) are hindered by inadequately understood carbon transfer processes and chemical transformations during atmospheric transport. In this study, carbon isotopic compositions ($^{13}$C) were measured to track changes in carbon transfer and speciation between the bulk seawater, sea-surface microlayer (SSML) and SSA during two laboratory-controlled phytoplankton blooms. Higher $^{13}$C values and phytoplankton fatty acid biomarker concentrations measured in SSA immediately following the bloom peak indicate significant contributions of biologically-produced, “fresh” carbon to SSA. Isotopic differences between the bulk, SSML and SSA also suggest increased surfactant concentrations in biologically active waters may prolong bubble persistence and drainage time resulting in enrichment of insoluble, “fresh” carbon species in SSA. Additionally, differences between $^{13}$C for marine carbon and SSA ($^{13}$C$_{SSA}$) observed during periods of high biological activity in these experiments, challenge the long-held assumption that nascent $^{13}$C$_{SSA}$ in marine environments is equivalent to $^{13}$C for marine carbon. Instead our results suggest that $^{13}$C$_{SSA}$ reflects specific changes in carbon speciation during ocean-aerosol transfer.

Physical/Analytical #6
Heterogeneous Interactions of Limonene on Hydrophobic and Hydrophilic Silica Surface

Tongshan Liu, Liubin Huang, Mona Shrestha, and Vicki Grassian

Principal Investigator: Dr. Vicki Grassian

Indoor surfaces are commonly coated with organic compounds. Limonene is one of the most abundant monoterpenes found in the indoor environment. However, the detailed chemistry between limonene and indoor relevant surfaces is poorly understood. In this study, we have investigated the heterogeneous reactions of limonene on silica (SiO$_2$), a prevalent surface in the indoor environments, using transmission-Fourier transform infrared (T-FTIR) spectroscopy. Since limonene uptake by SiO$_2$ particles is a reversible process via hydrogen bonding with surface hydroxyl groups (Si-OH) of SiO$_2$, the adsorption of limonene is inhibited on hydrophobic SiO$_2$ surface in which Si-OH is replaced by Si-OCH$_3$. The adsorption of limonene is also affected by the presence of water vapor. In addition to kinetics, adsorbed water seems to interact with limonene to form oxidized species as suggested by the appearance of a new band at 1700 cm$^{-1}$. These experimental results that combined with theoretical analyses provide molecular level insights into the interaction of organic compounds with indoor relevant surfaces and deepen the understanding of indoor air chemistry.
Isotope Analysis of Sulfate Aerosols and its Implications for Pollutant Transport

Michael Mundo, Connie Li (co-presenter), Robina Shaheen, Justin Vu, Christopher Cheng, Terri Jackson, and Mark Thiemens
Principal Investigator: Dr. Mark Thiemens

Sulfate aerosols play an important role in the atmospheric energy budget, such as the planet’s albedo and cloud formation. Furthermore, exposure to sulfate aerosols has implications on human health, such as respiratory and cardiovascular diseases. The measurement of stable sulfur and oxygen isotopes can provide critical information about the sources of sulfate aerosols. Major sources include the combustion of coal, biomass burning, and sea spray. In this study, aerosol samples were collected at the Hanimaadhoo Observatory through a NASA and NSF-funded study called SAPOEX-18. The Maldives is an ideal site for the study of transport and transformation of aerosols because air intercepts from Africa, the Middle East, India, and parts of Asia based on the seasons. The samples were dissolved in Millipore water, and sulfate was extracted using analytical IC and processed for pyrolysis. The radioactivity of Sulfur-35 was measured with a scintillation counter by monitoring the beta decay emissions. Oxygen triple isotopes of sulfate aerosols were analyzed using Isotope Ratio Mass Spectrometer. Tracking the concentration of Sulfur-35 between the tropospheric and stratospheric boundary layers allows us to quantify the vertical transport of air-masses as it moves through the atmosphere. The source of air masses collected and the contribution from other sources were determined and evaluated using the NOAA-HYSPLIT Trajectory method. The oxygen triple isotope data indicates that ozone and hydrogen peroxide were the major oxidants during the oxidation process. The analysis of the origin of the air masses demonstrates that some oceanic aerosols were mixed with anthropogenic sulfates. Sulfur-35 analysis indicates transport of stratospheric air mass during the winter months at the sampling site.

Physical/Analytical #8
Climate change is bringing many challenges to humanity, including a massive impact on the agriculture sector, with a worldwide increase in the frequency of prolonged drought. While the importance of plant-microbe interactions is well established for the assimilation of soil nutrients for plant physiology, little is known about the role of microbes in abiotic stresses such as drought, saltwater invasion, etc. To better understand the role of symbiotic microbes during these stressful events, we are looking for bio-inspiration in microbes found within extreme natural environments. Fungi and bacteria associated with plants collected in desertic area of West-Alabama were isolated and evaluated for their effect on plant resilience using tomato seedlings exposed to abiotic stresses. Two species (Penicillium sp. and Ampelomyces sp.) were found to improve plant resilience and were further investigated to understand the plant metabolic differences between colonized and non-colonized plants. Plant samples were collected and processed for mass-spectrometry based metabolomics analysis and analyzed using GNPS (Global Natural Products Social Molecular Networking). Pathway enrichment analysis showed that four metabolic pathways were impacted: 1) flavone and flavanol metabolism, 2) vitamin B6 metabolism, 3) phenylalanine metabolism, and 4) alanine, aspartate, and glutamate metabolism. We are currently analyzing the specialized metabolites produced by the fungal species using genome mining of biosynthetic gene clusters and computational mass spectrometry methods. The study has the potential to expand our fundamental understanding of plant-microbe interaction and potentially provide bioinspired microbiome tools that could be used to adapt agricultural practices to a changing climate.
Many-Body Effects Determine the Local Hydration Structure of Cs+ in Solution

Debbie Zhuang, Marc Riera, and Francesco Paesani
Principal Investigator: Dr. Francesco Paesani

A systematic analysis of the hydration structure of Cs+ ions in solution is derived from simulations carried out using a series of molecular models built upon a hierarchy of approximate representations of many-body effects in ion–water interactions. It is found that a pairwise-additive model, commonly used in biomolecular simulations, provides poor agreement with experimental X-ray spectra, indicating an incorrect description of the underlying hydration structure. Although the agreement with experiment improves in simulations with a polarizable model, the predicted hydration structure is found to lack the correct sequence of water shells. Progressive inclusion of explicit many-body effects in the representation of Cs+ –water interactions as well as accounting for nuclear quantum effects is shown to be necessary for quantitatively reproducing the experimental X-ray spectra. Besides emphasizing the importance of many-body effects, these results suggest that molecular models rigorously derived from many-body expansions hold promise for realistic simulations of aqueous solutions.

Physical/Analytical #10
Chemical Education Division

1. David Callahan
2. Hannah Martin
3. Jeffrey Lampert
Developing a teaching identity as a graduate teaching assistant in chemistry

*David Callahan, Skylar Holewinski, Carly Schnoebelen, Stacy Brydges, and Thomas Bussey*

Principal Investigator: Dr. Thomas Bussey

In most institutions, graduate students are required to gain experience teaching as part of a PhD or Master’s program. Many studies have looked at the factors and perceptions of students who are developing a teaching identity, but few have captured the longitudinal progression of how graduate students develop a teaching identity. In this case study, we followed one first-year graduate student who taught an undergraduate chemistry laboratory course over the course of a year to see how their perceptions of teaching changed and what factors affected their practice. We analyzed interview transcripts taken throughout the year and observed several classroom teaching events using the Laboratory Observation Protocol for Undergraduate STEM. In this poster, we will present preliminary analysis using phenomenography as a lens, looking at alignment of teaching beliefs with enacted teaching practice.

Chemical Education #1
Strategies for multicolor 3D printed molecular models to enable student representational literacy

*Hannah Martin, Scott McAvoy, and Jeremy Klosterman*

Principal Investigator: Dr. Jeremy Klosterman

Ball and stick (BS) molecular models are widely used in organic chemistry for teaching connectivity, bond angles, and the stereochemistry of organic molecules. However, BS models do not accurately convey the reality of atomic radii or bond lengths, yet understanding the steric size and shape of molecules essential for predicting the reactivity and selectivity in organic reactions. The goal of this project was to create inexpensive and accessible space-filling molecular models with accurate atomic radii to physically represent the sterics of any molecule for organic chemistry students use while predicting reactivity. 3D printing has become increasingly accessible and has enabled a widespread access to custom 3D printed models. Here we first obtained atomic coordinates from crystallographic or computational structures, which were converted to space-filling spheres for common organic molecules. The individual atomic spheres were separated and trimmed in blender for 3D printing in separate colors. We also report progress in the development of fully 3D printed versions of the original Corey Pauling Kolton (CPK) molecular models, where atoms are designed from cropped spheres and connected via flexible connectors that allow bond rotation. Students can hold and interact with these models to tangibly experience molecular sterics and its effects when examining the conformations and reactivity of organic molecules. Furthermore, these 3D printed molecular models can be printed at large scale for supplemental lecture demonstrations.

Chemical Education #2
Laboratory classes are viewed as an important part of learning sciences. However, students often do not achieve the standards set for them in regard to science practices. In order to gain an understanding of students’ perceptions and experiences in lab, we surveyed students in chemistry laboratory courses regarding their background and prior experiences in lab. We then interviewed a sub-set of students with varying levels of prior lab experience, asking them to bring in a recently-completed lab report. In the interviews, we asked students about the purpose of various components of the lab, using their lab report as a guide. We analyzed interview transcripts through the lens of phenomenography to determine which science practices students recognized and valued in lab. In this poster, we will discuss the results from analysis of student interviews from the general chemistry lab, as part of a larger study of the undergraduate laboratory experience.

Chemical Education #3
We are grateful for the time, expertise, and encouragement from our industry and visiting judges from Molecular Assemblies, Inc., Pfizer Inc., Southwestern College, and Vertex Pharmaceuticals, and our faculty, postdoc, and graduate student judges from the UC San Diego Department of Chemistry and Biochemistry.

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