UCI Chem-SURF Research Projects

Selected profiles of Faculty Mentors are included below. These Faculty Mentors have been very successful in mentoring undergraduate researchers, including Chem-SURF students, in recent past. The references cited at the end have been specifically chosen to highlight accomplishments by undergraduate student researchers, including previous Chem-SURF participants.

Ioan Andricioaei, Professor, Chemistry: ***1) Enhanced Sampling in Trajectory Space.*** Many important equilibrium and kinetic properties of chemical systems (including proteins and nucleic acids) can be cast in terms of paths in multi-dimensional spaces. We see fertile ground for theoretical and computational work on several categories of paths, from chemical-reaction paths to paths in the sequence space of evolving proteins. We have developed a set of trajectory reweighting techniques based on a stochastic path integral formalism that is particularly useful to treat both computer simulations and single-molecule experimental traces. ***2) Computer Simulations of DNA-Binding Machines.*** Protein-DNA interactions are essential in such crucial cellular functions as replication, repair, transcription or recombination. Many enzymes at and ahead of the replication fork affect large DNA fragments. For instance, topoisomerases undo DNA knotting. Others, like helicases and polymerases, are biomolecular motors: they use the energy of binding and/or hydrolysis of nucleotides to do mechanical work on the DNA fragments to which they bind. Another example is the machinery that compacts DNA inside the capsid of viruses. We have an avid interest in the theoretical description of these fundamental genetic processes through massively parallel computer simulations. ***3) Dynamics-Function Relationships.*** An accurate measure of free energy, important for protein/RNA stability or ligand binding, has to include the entropy manifested in molecular flexibility. On the experimental side, this dynamic aspect is brought in by developments in solution NMR spectroscopy, which measures motion by relaxation experiments. Molecular dynamics simulation is an important tool to complement these measurements and to connect dynamics to entropy. Undergraduate research involves running molecular dynamics simulations of DNA, RNA, and/or proteins, visualizing (e.g., making movies of the molecules in motion) and analyzing the simulation data.

Shane Ardo, Assistant Professor, Chemistry, and Chemical Engineering and Materials Science (1,2): ***The Molecular Science of Materials for Solar Energy Conversion***. The central theme of the Ardo Group's research program is to understand and control molecular-level reaction mechanisms at materials interfaces, with the goal of maximizing energy-conversion efficiency for realistic applications, including solar cells, solar seawater desalination, solar fuels devices, redox flow batteries, and fuel cells. Several REU positions are available in the group on projects ranging from *(i)* hybrid organic–inorganic halide perovskite materials containing organic dications as light absorbers in next-generation solar cells to *(ii)* ion-conducting polymers containing bound photoacid dye molecules for use in light-driven ion pumps and direct solar desalination of salt water to *(iii)* doped metal-oxide perovskite photocatalyst nanoparticles for solar water splitting in cost-effective particle suspension reactors to *(iv)* studies of intermolecular charge transfer between dye molecules anchored to metal-oxide nanoparticles for use in next-generation dye-sensitized solar cells. In the < 3.5 years since the inception of the Ardo Group Laboratories, 17 undergraduate and high school students have worked on these projects and others. Collectively, this work includes opportunities in materials synthesis (inorganic, hybrid, and polymer materials), synthesis of molecules (photoacid and traditional dye molecules), advanced characterization (spectroscopic and (photo)electrochemical), and device fabrication and evaluation (solar cells, solar desalination constructs, benchtop particle suspension reactors). From this work, two undergraduate co-author publications are currently under review, with several more publications in the pipeline.

Kieron Burke, Chancellor's Professor, Chemistry & Physics (3,4): ***Machine learning in Density Functional Theory***. We have an ongoing NSF-funded project to find density functionals using machine learning methods. We currently use kernel ridge regression to develop highly non-local functional approximations that can be made arbitrarily accurate with sufficient training. Recent undergraduates

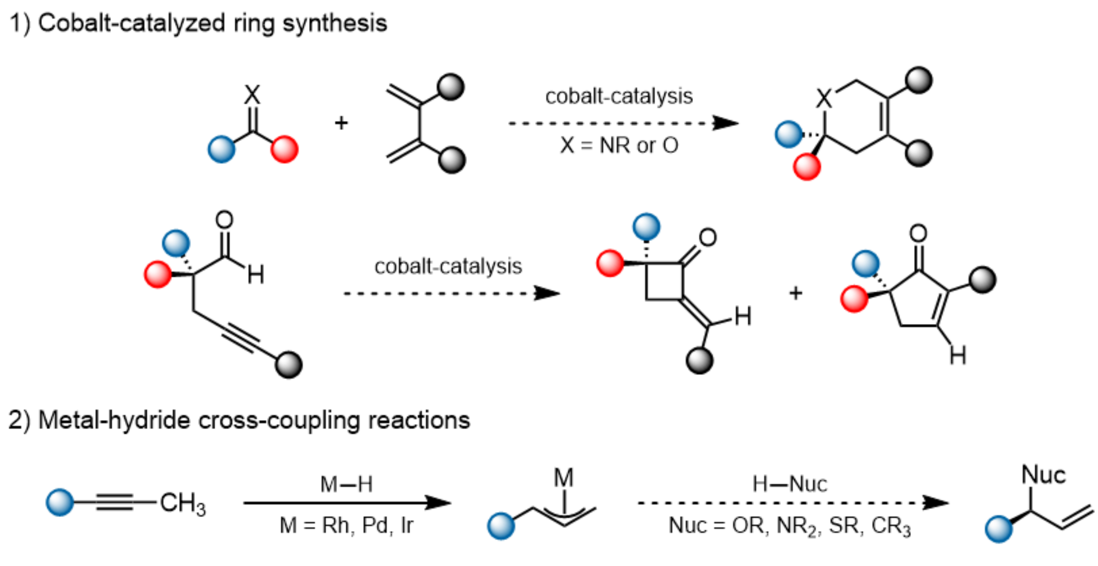
(Isabelle Pelaschier, Kevin Vu) have published papers (3,4). Undergraduates should have taken a basic course in quantum mechanics (either physical chemistry or modern physics) and should having a working knowledge of Mathematica or Python. Professor Burke has a long history of involving many undergraduates from different fields in his research and most continue to excellent graduate programs in their subjects.

Annmarie Carlton, Associate Professor, Chemistry (5-7): ***Atmospheric Multiphase Chemistry***. Most particles in the atmosphere are not directly emitted; rather precursor gases undergo chemical transformation during transport. Untangling the physicochemical complexities to understand sources, chemical pathways, fate and transport requires knowledge and application of field, laboratory and modeling experiments. Undergraduate students are sometimes paired with a graduate student and repeat their experiments for quality assurance. Some undergraduates lead their own research, typically in groups, and this has led to publications in peer-reviewed literature and presentations at national and international meetings. Undergraduates should be comfortable coding and writing scripts in R or Python. Dr. Carlton has involved 10 undergraduates from different majors (chemistry, meteorology, environmental science, physics, engineering, computer science and business) in her research and contributed to publications and in public outreach to create air quality aware communities. Carlton group alum undergraduate researchers now excel in professional and academic graduate positions.

Robert M. Corn, Professor, Chemistry: ***On-Chip Biosynthesis and Self Assembly of Protein Microarrays for Biosensing and Biotechnology***. The multiplexed detection of protein and microRNA biomarkers with microarrays has exploded onto the biosensor scene over the past decade. Label-free multiplexed detection methods such as surface plasmon resonance imaging (SPRI) have achieved sufficient sensitivity (picomolar or femtomolar concentrations); however, all of these methods typically require the fabrication of high fidelity microarrays of purified proteins or antibodies. Our research group has been developing on-chip fabrication strategies for the creation of protein microarrays that utilize a combination of templated biosynthesis (cell-free in vitro translation and transcription, IVTT) and subsequent self-assembly of the protein microarray on the SPRI chip for immediate use in SPRI surface bioaffinity measurements. As part of the proposed REU project, the Chem-SURF Fellow will create and verify novel surface attachment strategies for protein microarrays using Zinc finger fusion protein tags. In addition to learning the IVTT and other biochemical methods, the fellow will acquire knowledge in FTIR, XPS and SPRI surface analysis.

Vy Dong, Professor, Chemistry (8-10): ***Development of Transition Metal-Catalyzed Transformations***. Transition metal-catalysis has become a powerful tool in synthetic organic chemistry for the discovery of new medicines and their preparation on large scale. The Dong research laboratory is interested in developing new catalysts to enable more green and sustainable organic chemistry. We aim to address various challenges, (e.g., strained ring synthesis, enantioselective bond formations, and functionalization of simple precursors). 1) The development of cobalt-catalyzed transformations in the synthesis of strained rings. Proof of principle experiments have already been demonstrated and REU fellows will assist in the synthesis of starting material precursors as well as running Co-catalyzed reactions inside of an air-free glove box to achieve enantioselective synthesis of 4-, 5-, and 6-membered rings (8). 2) The development of metal-hydride chemistry turning feedstock alkynes into pi-allyl electrophiles. Fellows will run Rh-, Pd-, and Ir-catalyzed reactions to determine nucleophilic partners for cross-coupling reactions. In these projects, the REU student will work closely with a postdoctoral fellow or graduate student to identify and characterize new catalysts to synthesize new C–C, C–N, C–O, and C–S bonds (9,10). Undergraduate researchers have been able to make significant impact in research projects, which has resulted in authorship in peer-reviewed journals. Additionally, undergraduates have been successful in winning prestigious awards and have been well-trained to continue on in both professional and graduate schools. Along the way, REU fellows will participate by developing new methods to tackle synthetic challenges, characterize new organic compounds, and become familiar with synthetic techniques and instrumentation.

Students will be exposed to a variety of organic and inorganic literature, as well as participating in lively discussions, weekly research meetings, and learning fundamental principles.



William Evans, Professor, Chemistry: ***Synthetic f Element Chemistry: Learning to Handle Air-Sensitive Materials***.Tradition has held that the f orbital metals (lanthanides and actinides) had a limited chemistry because their f valence orbitals lacked the necessary radial extension of d orbital metals. Although the chemistry of these metals is now recognized as extensive, experimental difficulty in handling these air-sensitive compounds has limited their investigation. This project will introduce undergraduates to f orbital chemistry and to the special lab methods needed to handle complexes highly reactive with oxygen and water. The f elements will also be with us for thousands of years in the form of radioactive waste products; so, it is important to interest students in this area and train them in the necessary techniques, using nonradioactive model systems. Given the difficulty of working with these elements, this project is narrowly focused to foster publishable results in the time available. In this project, the students will synthesize a series of (C5R5)3M complexes (R = H, alkyl, phenyl, silyl) as potential precursors to [(C5R5)3M]1- compounds containing new Ln2+ ions recently discovered in our lab. We will evaluate the stability of the Ln2+ complexes as a function of the R5 substituent set. The most stable complexes will be studied further in terms of their physical properties and particularly their magnetism. The Evans laboratory has trained a large number of outstanding undergraduate researchers, who have continued their studies at the Ph.D. level.

Fillmore Freeman, Professor, Chemistry (11,12): ***Computational Quantum Chemistry Investigations of Structures, Reaction Mechanisms, and Molecular Rearrangements***. High levels of modern electronic theory are used to increase our understanding of structures, reaction mechanisms, molecular rearrangements, and solvation in the areas of bioorganic, inorganic, medicinal, organic, and organometallic chemistry. The REU student will be introduced to the fundamental concepts and principles of computational organic quantum chemical calculations in order to elucidate the mechanisms of 1,3-dipolar cycloadditions, 1,2- and 1,4-additions to 1,3-dicarbonyl compounds, cyclocondensations, and the chemistry of amino acids, peptides, sulfenic acids, and selenenic acids. Professor Freeman has mentored more than 200 undergraduate researchers. Many of them are coauthors, made presentations at local, regional, and national scientific meetings, won prestigious research awards, and attended graduate schools and professional schools.

Filipp Furche, Professor, Chemistry (13-17): ***Theoretical and computational method development and chemical applications***. While electronic structure calculations have become widespread in chemistry, very few students have the opportunity to look behind the scenes and understand the inner workings of electronic structure codes. Undergraduate students in the Furche group have the opportunity to explore the connection between quantum theory, high-performance computing, and chemistry in a supportive and collaborative environment. From the very beginning of their REU project, students will be immersed into research projects currently pursued by the Furche group in a team together with other undergraduates, graduate students, and postdocs. Current research directions include the development of new methods to solve the electronic Schrödinger Equation from first principles efficient and general enough for wide application to chemistry, nonadiabatic molecular dynamics methods, as well as applications in collaboration with experimental chemistry groups at UCI. Students will work in a UNIX environment and be introduced to scientific computing techniques, including programming, use of high-performance computers, and scientific software. The Furche group currently has four permanent undergraduate members. In the past two years, four undergraduates, including one former REU student, have co-authored publications (13-17) in journals such as JACS or JPC Letters, and three have been accepted to renowned graduate programs in theoretical and computational chemistry.

Alon Gorodetsky, Assistant Professor, Chemistry; Chemical Engineering and Materials Science: ***Cephalopod Proteins***. Cephalopods are known as the chameleons of the sea – they can alter their skin's coloration, patterning, and texture to blend into the surrounding environment. These capabilities are enabled by unique proteins and self-assembled nanostructures found within cephalopod skin. Our group is exploring new types of photonic and protonic devices from naturally occurring materials found in cephalopods. Our findings hold implications for the next generation of camouflage and renewable energy technologies. The Gorodetsky Group has an extensive track record of mentoring undergraduate student researchers. A total of 12 students from various majors have worked in the lab between 2011 and 2013 The Gorodetsky Group has specifically focused on the recruitment of individuals from disadvantaged and STEM underrepresented groups; the twelve students include 3 females and 4 Hispanic students, as well as 3 economically disadvantaged transfer students from community colleges. These undergraduate researchers have been supervised by senior graduate students and postdocs, but have also been granted quite a bit of independence. Indeed, the students develop and evaluate their own experimental strategies, participate in group meetings, present at local conferences, contribute to published work, and prepare proposals for fellowships. The success of our internal undergraduate research and training program is supported by several pieces of evidence: 1) 10 of the 12 students have received either Undergraduate Research Opportunity Program (UROP) or Research Experience for Undergraduates-like fellowships based on independently written and conceptualized proposals. 2) 2 of the 12 students are listed as co-authors on journal articles, and 4 other students are co-authors on manuscripts in the early stages of preparation; 3) 5 of the 12 students have already applied to graduate school, with two receiving acceptance notices.

Zhibin Guan, Professor, Chemistry: ***Biomimetic Modular Polymers for Advanced Biomaterials***. To mimic the modular domain structure of structural biopolymers such as the muscle protein, titin, our lab is developing polymers with a linear array of modules held together by programmed intramolecular weak interactions. Single-molecule nanomechanical studies demonstrate our biomimetic concept's feasibility: introducing modular structures held by sacrificial weak bonds into a polymer chain can combine in one polymer the three fundamental mechanical properties: high tensile strength, toughness and elasticity. We will investigate these polymers at single-molecule and macroscopic scales for their strength, toughness, and elasticity. An REU Fellow will participate in the synthesis of intermediates for the modules and gain experience in organic and polymer synthesis, molecular characterization, single molecule studies using Atomic Force Microscopy (AFM), and bulk physical property studies by MTS and DMAT. The Guan laboratory includes a number of undergraduates, and former students from his laboratory have pursued successful graduate and scientific careers; he currently has three undergraduates working in his group.

Alan Heyduk, Professor, Chemistry: ***Electronic Structure of Redox-Active-Ligand Transition-Metal Complexes***. The Heyduk group is developing new transition metal complexes of redox-active phenylenediamine and aminophenol ligands to apply their electron reservoir capabilities in new stoichiometric bond cleavage and formation reactions to challenging catalytic processes such as C–H bond functionalization. Our lab recently developed new transition-metal complexes capable of promoting multi-electron reactions, which suggests that a strategy for catalytic alkane functionalization may be attainable. REU Fellows will explore two disparate areas, non-innocent ligands and organometallic chemistry, now being synthesized to develop new catalytic complexes. To incorporate stereo-electronic factors governing reactivity in reaction design, the program interrogates electronic structure using physical-inorganic techniques. Intermingling synthetic and physical methods is central to the program and to training students. REU Fellows will gain exposure to widely-varied techniques for synthesis and characterization of air- and moisture-sensitive transition metal complexes, including NMR and EPR spectroscopies and X-ray crystallography, and to physical methods for elaborating electronic structure, including magnetic susceptibility and electronic spectroscopy. Although relatively nascent, the Heyduk laboratory can count several former undergraduates in the ranks of Ph.D. programs, and typically includes 2-3 undergraduate researchers.

Wilson Ho, Donald Bren Professor, Chemistry, Physics & Astronomy: ***Surface Chemistry***. Probing single molecules on solid surfaces, a new approach to understanding chemical interactions, uses a low-temperature scanning tunneling microscope to image, spectroscopically characterize, manipulate, and chemically modify individual molecules and their interactions with surrounding molecules and environment. Changes in the electronic, vibrational, and spin-dependent spectra reveal the spatial dependence in three dimensions of the chemical interactions between two reactants, providing understanding and control of chemistry at the nanoscale. Using ultrahigh vacuum conditions and surface science methodologies to probe organic and inorganic molecules on metal and oxide surfaces, students will be exposed to both physical and chemical techniques. Collaboration will be sought with other REU program chemists to synthesize molecules tailored to specific functions. These studies are expected to lead to technological innovations in molecular electronics, catalysis, solar energy conversion, corrosion, and materials of interest to the DOD. Professor Ho has mentored one REU student during the summer and the past academic year.

Allon Hochbaum, Assistant Professor, Chemistry; Chemical Engineering and Materials Science: ***High Performance Thermoelectric Materials from Nanoscale Building Blocks***. Thermoelectric materials are promising targets for converting waste heat to useful electrical energy in applications ranging from cars to heavy industry to wearable power sources. Nanostructured materials have exhibiting substantial improvements over conventional bulk thermoelectric materials. As part of the proposed REU project, the Chem-SURF Fellow will develop nanocrystal building blocks for solution processed thermoelectric materials. The Fellow will participate in the synthesis of unique nanocrystals, their surface functionalization, and processing them into thin film. The films will be characterized for their electrical and thermal transport properties to benchmark their promise as advanced thermoelectric materials. Experiments will focus on assessing the roles of inter-particle ligand chemistry in determining thermoelectric properties. Over the past two years, 11 undergraduate researchers have worked or are still working in the Hochbaum lab. Of the 5 that have graduated, two are attending graduate school (Caltech and UCI), and one received a Fulbright Scholarship.

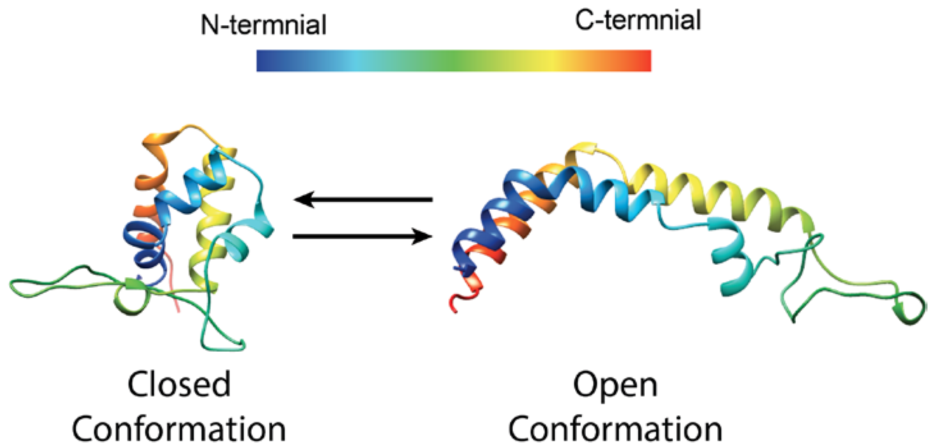
Elizabeth Jarvo, Associate Professor, Chemistry (18,19): ***Stereoselective Cross-Coupling Reactions for Synthesis of Anti-Cancer Compounds***. The Jarvo lab is developing nickel-catalyzed cross-coupling reactions of alkyl ethers and esters as a new method for enantioselective synthesis. Alkyl ethers are typically not considered reactive electrophiles, however, in the presence of the appropriate catalyst, they undergo coupling with Grignard and organozinc reagents. Reactions are typically highly stereospecific, where enantioenriched starting material is transformed to enantioenriched product with inversion at the reactive center and high stereochemical fidelity. This method is a particularly effective method for synthesis of 1,1-diarylalkanes, a pharmacophore that is present in compounds with anti-cancer, anti-diabetes, and anti-viral activity. NSF REU fellows will participate by synthesizing new enantioenriched ethers and esters, developing methods for cross-coupling reactions, synthesizing known anti-cancer agents, and evaluation of the compounds prepared for selective activity against breast cancer cell lines.

Matthew Law, Professor, Chemistry: ***New Materials for Making Green Hydrogen from Water and Sunlight***. In this project, the REU student will team with a postdoctoral and a graduate student to synthesize and characterize new hole-conducting mesoporous materials for a water oxidation half-cell (the side of a water splitting photocell that produces oxygen). Hydrothermal and polymeric precursor synthetic techniques will be used to make a variety of complex oxide nanocrystals. Spectroelectrochemistry, impedance measurements, and time-resolved spectroscopy are then applied to determine the band edge energies and flatband potentials of these nanocrystals in the solid state and to study hole injection and transport in nanocrystalline films. Insights from these fundamental spectroscopic and electronic investigations will be leveraged to build the first efficient, stable, and economical p-type dye photocell that produces O2 from sunlight. This cell will then be paired with an H2-evolving cell to split water. Students interested in this project should have mastered Physical Chemistry. Experience with Inorganic Chemistry and Materials Chemistry is also a plus. In two years, Professor Law has worked with five undergraduate researchers, including 3 UROP students and a CAMP Summer Scholar. Two of these students have been members of the Law Group for over a year and one of them has a first-author publication in ACS Nano.

Stephen Mang, Assistant Professor, Chemistry: ***Incorporating research experiences into the undergraduate curriculum***. Since the main focus of my career has been teaching upper-division chemistry laboratory classes, my research interests have evolved to support that focus by developing new experiments and modifying or creating courses (20,21). I have adapted the curricula of several lab classes over the course of my career to incorporate more research-like experiences, including instrument construction, student-proposed projects, and presentation skills. I have also mentored undergraduates as they developed experiments to be incorporated into the chemistry lab curriculum, in their own classes and in lower-division classes. During the most recent school year there were three undergraduate students working with me, and I anticipate similar levels of participation in the future.

Craig Martens, Professor, Chemistry: ***Molecular Dynamics Simulations of Separation and Purification of Aqueous Solutions***. Students use NAMD software for molecular dynamics simulation to investigate the properties of water around solute species and in nanoenvironments, in systems including aqueous salt solutions in nanopores and clathrate hydrates. The influence of nanometer-scale structure on the solution's boundaries and properties is evaluated by calculating structural and dynamical quantities, such as hydrogen bond lifetimes and correlation functions, versus those of bulk solutions. The free, user-friendly and well supported, NAMD software offers undergraduate students a relatively painless entrée into computational chemistry. A significant UCI NAMD user community of chemists, physicists, and biologists is available for interaction with the student researcher. In addition, close connection with experimental groups at UCI studying the chemistry and physics of water is possible. This fundamental research on water at the nanoscale has applications to nanotechnological approaches to separation and transport of species in aqueous solutions, and to desalination and purification of water. The Martens laboratory has trained a large number of undergraduate researchers.

Rachel Martin, Professor, Chemistry and Molecular Biology & Biochemistry (22-25): ***From Genomic Source Code to Enzyme Discovery in Carnivorous Plants***. With the advent of inexpensive gene sequencing, genomic data proliferates at a pace that far outstrips experimental resources for protein characterization. The overall goal of this project is to provide a road map for approaching complex systems of biomolecules in which many similar isoforms are employed simultaneously. The first target is *Drosera capensis*, a carnivorous plant that catches its prey using flypaper traps. Carnivorous plants face unique proteomic challenges and are thus a potentially valuable resource for the discovery of enzymes with improved or novel functional characteristics. Participating students will be introduced to bioinformatics tools, molecular modeling, protein expression and purification, and/or functional enzyme characterization. In the Martin lab, undergraduates are assigned a graduate student mentor who trains them in the relevant laboratory and computational methods. They also attend project subgroup meetings where the underlying chemical and physical principles are discussed. Undergraduates start by preparing proteins and performing bioinformatics analyses under close supervision from their graduate student mentors and gradually become more independent as they build their skills. By the time they graduate our most motivated undergraduates are already performing at the level expected of first-year Ph.D. students. Professor Martin has mentored more than 30 undergraduates from chemistry, biology, and engineering in her research group. Several recent alumni have moved on to Ph.D. programs in chemistry and biology; two received NSF GRFP fellowships in 2016 and 2017.



David Mobley, Associate Professor, Chemistry and Pharmaceutical Sciences (26-29): ***Protein-ligand interactions, solvation, and solubility***. The group works on developing, testing, and applying computational techniques to help aid pharmaceutical drug discovery. We have major interests in predicting protein-ligand binding, as well as solvation properties and solubilities of small drug-like molecules. Students in the group work on a range of projects, including high-throughput studies of binding (such as with docking techniques), detailed binding free energy calculations using molecular dynamics simulations, and studies of solvation or energetics of small molecules in the gas phase or in solution. In some cases students are involved with projects like the SAMPL series of challenges, where we run community blind prediction challenges to test the state of computational methods in the field. Usually projects have implications relating to pharmaceutical drug discovery, either directly or by helping to improve the predictive power of our tools. The work is entirely computational, but we often collaborate with experimental groups. Professor Mobley has mentored roughly a dozen undergraduate students, and most students have published work done in the group. Selected publications include Refs. (26-29).

James Nowick, Professor, Chemistry (30-33)*: **Supramolecular chemistry of amyloidogenic peptides***. This project seeks to learn more about the structures of amyloid oligomers through the use of chemical models systems. Amyloid oligomers appear to be the toxic agents responsible for neurodegeneration and cellular death in amyloid diseases such as Alzheimer's disease, frontotemporal dementias, Parkinson's disease, and type 2 diabetes. Relatively little is known about the structures of amyloid oligomers, and only a few studies have provided glimpses of amyloid oligomers at atomic resolution. Dr. Nowick and his students have developed an effective strategy to elucidate the structures of oligomers formed by amyloidogenic peptides: incorporating the peptides into macrocycles and using a single N-methyl group to prevent uncontrolled aggregation to fibrils. The resulting macrocyclic beta-sheet peptides assemble to form well-defined oligomers, and a good fraction of the peptides form crystals suitable for X-ray crystallography. Students in the group are using this approach to elucidate the structures of oligomers from amyloidogenic peptides derived from the protein tau, the protein alpha-synuclein, and the islet amyloid polypeptide (IAPP, amylin). The structures of the oligomers that form are determined at atomic resolution by X-ray crystallography, and the crystallographic structures of the oligomers are correlated with the solution state biological and biophysical properties. Six undergraduate students are currently working on this project and related projects involving the structure and biological properties of peptides. Since 2013, eight undergraduates have coauthored papers that have been published or submitted, and two undergraduates have gone on to graduate school in Chemistry.

Sergey Nizkorodov, Professor, Chemistry (34-40): ***Characterization of optical properties of particulate air pollutants***. A significant fraction of volatile organic air pollutants emitted by traffic and industrial sources are converted into fine particles. This organic aerosol contributes to visibility degradation, reduces the air quality in urban areas, and affects regional climate. Light-absorbing “black” and “brown” particles are of particular concern as they heat up the air by absorbing solar radiation. To determine what compounds are responsible for the brown aerosol in urban air, we investigate detailed composition and chemical properties of organic aerosols produced from various anthropogenic air pollutants. The aerosols are generated by photochemical oxidation of selected biogenic and anthropogenic volatile organic precursors in the UCI smog chamber or flow tubes equipped with a host of state-of-the art instruments. The REU participant will be given a crash course in atmospheric and aerosol chemistry, and standard atmospheric chemistry measurement methods. The REU participant will learn to prepare various types of aerosols using smog chamber and flow tube methods, characterize optical properties of the aerosol, and analyze aerosol composition by mass spectrometry and other analytical methods. More than 40 students, including REU participants, have done research in the Aerosol Photochemistry Lab, and many won prestigious awards, contributed to writing peer-reviewed publications (34-39), and went to graduate or professional schools after that.

Reginald Penner, Chancellor’s Professor, Chemistry: ***Polymer Nanowire Growth Using Electrochemical Step Edge***. Lithographically patterned Nanowire Electrodeposition (LPNE) is a new method for the patterning ultra-long (millimeters) nanowires of metals and semiconductors on dielectrics like glass and plastics. We are studying the application of the nanowire obtained using the LPNE method to the preparation of new types of chemical sensors, optical detectors, and a variety of other devices. Professor Penner has supervised 10 local Irvine high school students over the last six years: eight have gone on to graduate schools (UC Berkeley, MIT, Dartmouth College, Caltech, Harvard,), and two are presently in the group. In addition, a large number of undergraduates have trainedin the Penner laboratory.

Eric Potma, Professor, Chemistry (41-43): ***Molecular orientation and crosslinking in collagen fibers***. Research in our lab focuses on investigating molecular distribution and molecular orientation in complex natural materials such as cellulose fibers, keratin fibers and collagen. Our research tools consists of a suite of spectroscopic imaging techniques based on vibrational contrast, including Fourier-transform infrared (FTIR) absorption spectroscopy, Raman microscopy and sum-frequency generation (SFG) microscopy. The current REU project in our laboratory focuses on the molecular orientation of collagen fibrils in tissues. The student will perform SFG microscopy of several collagen-rich samples and help determine the orientation and crosslinking of the fibers. This project will be coordinated by Professor Potma. Hands-on training and daily supervision will be provided by a graduate student, Adam Hanninen, who has extensive experience with vibrational spectroscopy and imaging of biopolymers. Adam has already trained five undergraduate students in our laboratory and exhibits excellent teaching skills. The SFG instrumentation is considered rather challenging for most undergraduate students. Our experience indicates, however, that once students have received an extensive training on this instrument, most trainees feel empowered and confident to take on challenging imaging experiments. After the student has acquired sufficient training to operate the instruments, the student will have the opportunity to independently design and schedule measurements. The graduate student will be available for daily help with the direction of the project. Weekly meetings between the REU student, the graduate student and Professor Potma will be held to facilitate the success of the project.

Jennifer Prescher, Associate Professor, Chemistry, Molecular Biology & Biochemistry, and Pharmaceutical Sciences (13,44-47): ***Generating orthogonal bioluminescent probes for multi-cellular imaging in vivo***. Bioluminescence imaging is among the most powerful techniques for visualizing cells in complex tissues and organisms. At the core of this technology are enzymes (luciferases) that catalyze the oxidation of small molecule substrates (luciferins) to release visible light. Several luciferase-luciferin pairs exist in nature, and many have been adapted for tracking cells and gene expression patterns in whole animals. Unfortunately, the optimal luciferases for *in vivo* imaging utilize the same substrate, and therefore cannot be used to distinguish multiple cell types in a single subject. We are expanding the bioluminescence toolkit by creating new luciferases that are responsive to unique luciferin substrates (i.e., “orthogonal” pairs). Our approach involves re-engineering firefly luciferase, generating a panel of mutant enzymes that accept chemically distinct luciferin analogs. When the mutants and analogs are mixed together, light is produced when complementary enzyme-substrate partners interact. NSF REU fellows will be involved in diverse aspects of this project, including chemical syntheses and enzyme engineering. The probes identified from our research will enable the direct interrogation of cell systems not currently possible with existing toolsets. Such studies will provide some of the first macroscopic images of tumor heterogeneity, immune function, and other complex networks, and may fundamentally change existing views on human health and disease. Additionally, similar to other imaging technologies, the bioluminescent probes will likely inspire new discoveries in a broad spectrum of fields. More than 10 undergraduates, including REU participants, have contributed to our ongoing research program. Many have contributed to publications from the group and been recognized by external awards. Several have also continued on to graduate or other professional training.

Scott Rychnovsky, Professor, Chemistry (48-54): ***Competing Enantioselective Conversion Method to Assign Absolute Configuration***. Chirality is a property of many three-dimensional objects, and most organic molecules are chiral. For convenience, we label one molecule “right-handed” and the other “left-handed”, but how do we determine which is which? My group is exploring a new strategy based on the reactivity of the chiral molecule with mirror-image (enantiomeric) reagents or catalysts. The fast-reacting reagent complements the structure of the chiral molecule, and from this relationship we can assign the absolute handiness (configuration) of the molecule in question. An analogy is a handshake between the molecule and the reagent; only complementary chirality between the two leads to a good fit and a fast reaction. The REU student will learn about organic synthesis, catalysis, physical organic chemistry and analytical methods. Over the past ten years I have worked with 28 undergraduate students in my lab. Eleven of them have gone on to graduate school in chemistry, with several more attending professional schools and six of them going directly into chemistry careers. A number of them are coauthors on papers, and many have presented their work at professional meetings.

Kenneth Shea, Professor, Chemistry, Chemical Engineering and Material Science: ***Tunable Optical and Mechanical Properties of Polymers and Materials***. Polymers and materials, many of which are "one of a kind," enable the researcher to acquire a broad range of characterization skills. One project involves polymers and materials with "tunable" optical and mechanical properties and would expose the student to small-molecule, polymer, and materials synthesis, and a variety of characterization techniques.

Historically, undergraduate students on these summer projects wind up as coauthors on publications. Bridged polysilsesquioxanes are fabricated from molecular building blocks composed of a variable organic component and two or more sol-gel polymerizable trialkoxy silanes. Important physical characteristics include high surface area, pore volume, and functional group loading. One project, involving photo-responsive materials, is synthesizing bifunctional coumarin photodimers, monomers incorporated into the backbone of materials ranging from elastermers to thermosets, which include silicone linear polymers and networks and bridged polysilsesquioxanes. We are evaluating these materials' optical and mechanical properties before and after short wavelength and UV irradiation using fluorescence microscopy, AFM, imaging ellipisometry, gas absorption (SA analysis), and solid-state NMR. The materials have applications in waveguide fabrication and secure encryption, and as UV dosimeters. Professor Shea has served as mentor for over 60 undergraduates. Almost all of these students have gone on to graduate or professional school. These students now occupy positions in academics government laboratories and industry. In addition a significant number have gone on to medical school to become doctors. Over the span of his career they have been coauthors of over sixteen manuscripts and they have presented numerous papers at scientific meetings and conferences.

Manabu Shiraiwa, Assistant Professor, Chemistry: ***Quantifying reactive oxygen species (ROS) and radicals in atmospheric fine particulate matter***. ROS play a central role in the adverse health effects of air pollution, as they can cause oxidative stress. Fine air particulate matter contains stable radicals and redox-active components including transition metals, quinones and other organic compounds, which can induce chemical reactions producing ROS in lung lining fluid upon inhalation and deposition in the human respiratory tract. The REU participant will collect atmospheric particles using a cascade impactor or generate particles using a reaction chamber, and then detect and quantify ROS and radicals associated with particles using an electron paramagnetic resonance (EPR) spectrometer. Participants will work with the PI, graduate students or postdoctoral fellows in the group, and participate in weekly group meetings.

Zuzanna Siwy, Professor, Physics and Chemistry (55-58): ***Preparation of biomimetic nanopores and ionic circuits***. Ion transport through channels and pores embedded in a cell membrane is the basis of all physiological processes of a living organism. In this project, the REU participant will learn fabrication of single nanopores whose transport properties resemble these of biological channels. For example, voltage gated channels open and close in response to electric field. The project will also involve chemical modification of the pore walls, microscopy and electrochemical characterization. The REU participant will also create an ionic circuit consisting of two pores with different functionalities.

Jim Smith, Professor, Chemistry: ***Investigations of atmospheric new particle formation and growth***. In this project, the REU participant will team with graduate students on laboratory and field measurements focusing on the formation and growth of atmospheric aerosol particles. Our laboratory has developed novel instruments to study of the composition of the smallest particles in the atmosphere, with diameters as small as 5 nm, as well as the gases that are responsible for the new particle formation and growth. Our current lab studies address questions such as "What possible roles do organic compounds play in the formation of the stable clusters and for the growth of these clusters into new particles?" and "Are the compounds responsible for the birth and growth of atmospheric aerosol particles formed in the atmosphere or within the particles themselves? Prof. Smith recently arrived at UC Irvine, and is anxious to establish a vibrant undergraduate research program in his laboratory. In the past year he has already hosted two undergraduate students, one of whom was from the California Alliance for Minority Participation (CAMP) summer scholars program.

Douglas Tobias, Professor, Chemistry (25): ***Toward Molecular-Scale Models of Congenital and Age-Related Cataract: Molecular Modeling Studies of Structural Proteins in the Eye Lens***. The elongated fiber cells making up the eye lens contain a high-concentration solution of crystallin proteins. To maintain proper transparency and refractive properties of the lens, because of very low protein turnover the crystallins must remain in solution for the lifetime of the organism. Precipitation of crystallins leads to cataract, a major cause of blindness worldwide. Altered protein-protein interactions, resulting from mutations in the case of congenital cataracts, or post-translational modifications in age-related cataract, leads to protein aggregation and, ultimately, loss of lens transparency. The REU participant will carry out atomistic molecular dynamics (MD) simulations that will elucidate protein-protein interactions in solutions of wild-type crystallins and their cataract-related variants that will contribute to the development of atomically detailed structural models of individual crystallin molecules and their organization in soluble and aggregated states. Specifically, MD simulations of single molecules of wild type, congenital cataract-related mutants, and de-amidated variants of S-crystallin will be used to gain insight into the changes in structural dynamics and hydration that result from modifications of the protein sequence, and validated by comparison with experimental data, in collaboration with Prof. Rachel Martin in the Department of Chemistry at UC Irvine. Configurations from the MD simulations will be used as input into Monte Carlo simulations of concentrated solutions of wild-type and cataract-prone crystallins that will provide molecular-scale insight into the role of altered protein-protein interactions in crystallin aggregation. By participating in this project, the REU participant will be trained in state-of-the-art computer simulation techniques, computer programming, and molecular graphics, and s/he will have the opportunity to work in close collaboration with experimental biophysicists and structural biologists. The Tobias group has trained numerous undergraduate students, including four REU students during 2011-2014. Most of the Tobias group undergraduate alumni have gone on to graduate or professional schools, and many have won prestigious fellowships.

Shiou-Chuan (Sheryl) Tsai, Professor, Chemistry; Molecular Biology and Biochemistry; Pharmaceutical Sciences: ***Chemical Biology and Structural Enzymology of Natural Product Biosynthesis***. The Tsai lab investigates the chemical biology and structural biology of enzymes that biosynthesize natural products, which include many pharmaceutically important compounds. This project aims to determine the molecular basis of substrate specificity of three enzyme complexes that biosynthesize pharmaceutically active polyketides: acyl-CoA carboxylase (ACCase), polyketide synthase (PKS), and deoxysugar-synthesizing enzymes. The long-term goal is to biosynthesize new "unnatural" natural products and screen them for pharmaceutical activity. The central hypothesis is that the product from these three complexes can be changed by mutating active site residues of ACCase, PKS, and sugar-synthesizing enzymes. REU Fellows will be exposed to such techniques as identification of active site residues by site-directed mutagenesis; probes of the PKS active site by solving PKS crystal structures, and probes of enzyme active sites by biophysical methods. Problem-based learning will emphasize strategic polyketide metabolism concepts and structure-function relationships across genomes of organisms that produce polyketides. Professor Tsai has mentored 60+ undergraduates during the past seven years. Many of these students are now in graduate school or have completed graduate school.

Christopher Vanderwal, Professor, Chemistry: ***Synthesis of Diverse Heterocycles Starting from Pyridines***. Heterocycles form the core of a significant proportion of biologically active natural products and man-made pharmaceutical agents. As a result, new technologies for the synthesis of heterocyclic scaffolds are of tremendous value for medicine as well as basic understanding. The proposed REU project involves the development of a method for the synthesis of diverse heterocycles, using the vast array of commercially available substituted pyridines as a feedstock. The goal of the project is to use the century old Zincke reaction, which leads to the ring opening of pyridines, as the basis for heterocycle construction. Our research group has already demonstrated proof of principle for this chemistry, as we have synthesized a variety of nitrogen heterocycles according to this plan. The further development of this chemistry and its application to oxygen and sulfur heterocycles, and possibly to carbocycles, is the specific aim of the REU project. This project is ideal for an undergraduate research participant, as he/she will be exposed to a variety of organic chemical reactions and related techniques. Weekly research and literature group meetings, in addition to formal and informal mentoring sessions with the advisor, will greatly enhance the REU experience.

David Van Vranken, Professor, Chemistry (59-62): ***Integration of Machine Learning with Organic Synthesis***. Organic chemists design and synthesize the types of molecules that drive modern society like powerful new medicines, functional materials, and biological probes. The reactions that are developed and used by synthetic organic chemists imprecise, generating mixtures of the anticipated products and inscrutable side products. The Van Vranken group is exploiting machine learning to identify the molecular debris that is omnipresent in synthetic organic reactions, drug degradation processes, and other chemical processes. The group develops novel palladium-catalyzed reactions of carbene groups to assemble structurally complex organic molecules. REU students will learn traditional techniques of organic synthesis including inert atmosphere reaction techniques, chromatographic purification of products and spectroscopic characterization. The Van Vranken group has mentored over 13 undergraduate researchers (5 current).

Gregory Weiss, Professor, Chemistry, Molecular Biology and Biochemistry: ***Listening to Individual Molecules and Cancer Biomarkers with Nanotechnology***. Dr. Weiss' lab develops new tools to dissect the relationship between protein structure and function. Many projects apply phage display to access vast libraries of bacteriophage-presented peptides and proteins. Dr. Weiss has identified binding partners to cancer-associated biomarkers, including prostate tumor antigens (PSMA and PSA). The resultant phage with the cancer-binders have been wired into nanometer-scale electrical circuits for direct measurement of cancer marker levels in the early diagnosis of cancer (63). He has extended a similar bioelectronic system to an individual enzyme molecule wired into electronic circuits based on carbon nanotubes; recent studies focus on two cancer-associated enzymes and therapeutic targets, cAMP-dependent Protein Kinase A and DNA polymerase (64). Awarded the School of Physical Sciences Award for Contributions to Undergraduate Education in 2004, Professor Weiss has trained more than 45 undergraduate researchers, including 4-6 undergraduates every quarter for the last three years. Seven undergraduates have co-authored four publications from the lab during this period (63-66), and two undergraduates were part of the team awarded an Ig Nobel Prize for "partially unboiling an egg" (66). The vast majority of undergraduates who have graduated from the Weiss laboratory have pursued science careers, including PhD programs at UCSF, U. Wisconsin, U. North Carolina, City of Hope, and other institutions.

Jenny Yang, Assistant Professor, Chemistry (67-70): ***Inorganic Synthesis, Small Molecule Catalysis, Solar Fuels***. My research efforts are focused on the development of catalysts for the production and utilization of carbon-neutral chemical fuels from renewable energy sources. Undergraduate researchers will learn how to synthesize and characterize new ligands and metal complexes using air-sensitive techniques. They will also learn how to characterize catalytic activity using electrochemical methods. Detailed mechanistic and kinetic studies will complement the electrochemical studies to achieve insights into improving catalyst design. REU Fellows will work on independent projects with the goal of publishing their work. They will work with the PI and with other graduate students or postdoctoral fellows in the group, and participate in weekly sub-group and super-group meetings, as well as literature reviews. Since 2013, Professor Yang has mentored over 14 undergraduate researchers, most of whom have gone on to graduate programs and industrial positions. 4 have been co-authors in peer-reviewed publications, for example Refs. (67-70).

References

(1) Tkacz, K.; Nitz, S. T. E.; White, W.; Ardo, S. Activity on saltwater desalination by electrodialysis and accompanying curriculum to introduce students to the chemical physics of polymeric ion-exchange membranes. *J. Chem. Educ.* **2017**, *in revision*.

(2) Krueper, G.; Angsono, J.; Macedonio, V.; Cardon, J. C.; Logan, J. G.; Tkacz, K.; Chen, H.-Y.; Ardo, S. Synergistic effect of electrolyte cations on the rate of intermolecular electron transfer between dye molecules anchored to TiO2 nanocrystallites cast as mesoporous thin films. *ACS Energy Lett.* **2017**, *submitted*.
(3) Li, L.; Snyder, J. C.; Pelaschier, I. M.; Huang, J.; Niranjan, U. N.; Duncan, P.; Rupp, M.; Muller, K. R.; Burke, K. Understanding machine-learned density functionals. *International Journal of Quantum Chemistry* **2016**, *116*, 819-833.
(4) Vu, K.; Snyder, J. C.; Li, L.; Rupp, M.; Chen, B. F.; Khelif, T.; Mueller, K. R.; Burke, K. Understanding kernel ridge regression: Common behaviors from simple functions to density functionals. *International Journal of Quantum Chemistry* **2015**, *115*, 1115-1128.
(5) Farkas, C. M.; Moeller, M. D.; Felder, F. A.; Henderson, B. H.; Carlton, A. G. High Electricity Demand in the Northeast US: PJM Reliability Network and Peaking Unit Impacts on Air Quality. *Environ. Sci. Technol.* **2016**, *50*, 8375-8384.
(6) Farkas, C. M.; Moeller, M. D.; Felder, F. A.; Baker, K. R.; Rodgers, M.; Carlton, A. G. Temporalization of Peak Electric Generation Particulate Matter Emissions during High Energy Demand Days. *Environ. Sci. Technol.* **2015**, *49*, 4696-4704.
(7) Carlton, A. G.; Little, E.; Moeller, M.; Odoyo, S.; Shepson, P. B. The Data Gap: Can a Lack of Monitors Obscure Loss of Clean Air Act Benefits in Fracking Areas? *Environ. Sci. Technol.* **2014**, *48*, 893-894.
(8) Kim, D. K.; Riedel, J.; Kim, R. S.; Dong, V. M. Cobalt Catalysis for Enantioselective Cyclobutanone Construction. *J. Amer. Chem. Soc.* **2017**, *139*, 10208-10211.
(9) Cruz, F. A.; Zhu, Y.; Tercenio, Q. D.; Shen, Z.; Dong, V. M. Alkyne Hydroheteroarylation: Enantioselective Coupling of Indoles and Alkynes via Rh-Hydride Catalysis. *J. Amer. Chem. Soc.* **2017**, *139*, 10641-10644.
(10) Cruz, F. A.; Chen, Z. W.; Kurtoic, S. I.; Dong, V. M. Tandem Rh-catalysis: decarboxylative beta-keto acid and alkyne cross-coupling. *Chemical Communications* **2016**, *52*, 5836-5839.
(11) Freeman, F.; Adesina, I. T.; Le La, J.; Lee, J. Y.; Poplawski, A. A. Conformers of Cysteine and Cysteine Sulfenic Acid and Mechanisms of the Reaction of Cysteine Sulfenic Acid with 5,5-Dimethyl-1,3-cyclohexanedione (Dimedone). *J. Phys. Chem. B* **2013**, *117*, 16000-16012.
(12) Freeman, F.; Bui, A.; Dinh, L.; Hehre, W. J. Dehydrative Cyclocondensation Mechanisms of Hydrogen Thioperoxide and of Alkanesulfenic Acids. *J. Phys. Chem. A* **2012**, *116*, 8031-8039.
(13) Steinhardt, R. C.; Rathbun, C. M.; Krull, B. T.; Yu, J. M.; Yang, Y. H.; Nguyen, B. D.; Kwon, J.; McCutcheon, D. C.; Jones, K. A.; Furche, F.; Prescher, J. A. Brominated Luciferins Are Versatile Bioluminescent Probes. *Chembiochem* **2017**, *18*, 96-100.
(14) Langeslay, R. R.; Chen, G. P.; Windorff, C. J.; Chan, A. K.; Ziller, J. W.; Furche, F.; Evans, W. J. Synthesis, Structure, and Reactivity of the Sterically Crowded Th3+ Complex (C5Me5)(3)Th Including Formation of the Thorium Carbonyl, (C5Me5)(3)Th(CO) BPh4. *J. Amer. Chem. Soc.* **2017**, *139*, 3387-3398.
(15) Vincent, J. C.; Muuronen, M.; Pearce, K. C.; Mohanam, L. N.; Tapavicza, E.; Furche, F. That Little Extra Kick: Nonadiabatic Effects in Acetaldehyde Photodissociation. *Journal of Physical Chemistry Letters* **2016**, *7*, 4185-4190.
(16) Furche, F.; Krull, B. T.; Nguyen, B. D.; Kwon, J. Accelerating molecular property calculations with nonorthonormal Krylov space methods. *J. Chem. Phys.* **2016**, *144*.
(17) Johansson, M. P.; Warnke, I.; Le, A.; Furche, F. At What Size Do Neutral Gold Clusters Turn Three-Dimensional? *Journal of Physical Chemistry C* **2014**, *118*, 29370-29377.
(18) Johnson, A. G.; Tranquilli, M. M.; Harris, M. R.; Jarvo, E. R. Selective synthesis of either enantiomer of an anti-breast cancer agent via a common enantioenriched intermediate. *Tetrahedron Lett.* **2015**, *56*, 3486-3488.
(19) Kohn, B. L.; Ichiishi, N.; Jarvo, E. R. Silver-Catalyzed Allenylation and Enantioselective Propargylation Reactions of Ketones. *Angewandte Chemie-International Edition* **2013**, *52*, 4414-4417.
(20) Harmon, C. W.; Mang, S. A.; Greaves, J.; Finlayson-Pitts, B. J. Identification of fatty acids, phospholipids, and their oxidation products using matrix-assisted laser desorption ionization mass spectrometry and electrospray ionization mass spectrometry. *Journal of Chemical Education* **2010**, *87*, 186-189.
(21) Mang, S. A.; Walser, M. L.; Nizkorodov, S. A.; Laux, J. M. Measurement of Ozone Emission and Particle Removal Rates from Portable Air Purifiers. *Journal of Chemical Education* **2009**, *86*, 219-221.
(22) Butts, C. T.; Bierma, J. C.; Martin, R. W. Novel proteases from the genome of the carnivorous plant Drosera capensis: Structural prediction and comparative analysis. *Proteins-Structure Function and Bioinformatics* **2016**, *84*, 1517-1533.
(23) Butts, C. T.; Zhang, X. H.; Kelly, J. E.; Roskamp, K. W.; Unhelkar, M. H.; Freites, J. A.; Tahir, S.; Martin, R. W. Sequence comparison, molecular modeling, and network analysis predict structural diversity in cysteine

proteases from the Cape sundew, Drosera capensis. *Computational and Structural Biotechnology Journal* **2016**, *14*, 271-282.
(24) Unhelkar, M. H.; Duong, V. T.; Enendu, K. N.; Kelly, J. E.; Tahir, S.; Butts, C. T.; Martin, R. W. Structure prediction and network analysis of chitinases from the Cape sundew, Drosera capensis. *Biochimica Et Biophysica Acta-General Subjects* **2017**, *1861*, 636-643.
(25) Brubaker, W. D.; Freites, J. A.; Golchert, K. J.; Shapiro, R. A.; Morikis, V.; Tobias, D. J.; Martin, R. W. Separating Instability from Aggregation Propensity in gamma S-Crystallin Variants. *Biophysical Journal* **2011**, *100*, 498-506.
(26) Liu, S.; Cao, S.; Hoang, K.; Young, K. L.; Paluch, A. S.; Mobley, D. L. Using MD Simulations To Calculate How Solvents Modulate Solubility. *Journal of Chemical Theory and Computation* **2016**, *12*, 1930-1941.
(27) Bannan, C. C.; Calabro, G.; Kyu, D. Y.; Mobley, D. L. Calculating Partition Coefficients of Small Molecules in Octanol/Water and Cyclohexane/Water. *Journal of Chemical Theory and Computation* **2016**, *12*, 4015-4024.
(28) Mobley, D. L.; Liu, S.; Lim, N. M.; Wymer, K. L.; Perryman, A. L.; Forli, S.; Deng, N. J.; Su, J.; Branson, K.; Olson, A. J. Blind prediction of HIV integrase binding from the SAMPL4 challenge. *Journal of Computer-Aided Molecular Design* **2014**, *28*, 327-345.
(29) Duarte Ramos Matos, G.; Kyu, D. Y.; Loeffler, H. H.; Chodera, J. D.; Shirts, M. R.; Mobley, D. L. Approaches for Calculating Solvation Free Energies and Enthalpies Demonstrated with an Update of the FreeSolv Database. *Journal of Chemical & Engineering Data* **2017**, *62*, 1559-1569.
(30) Yang, H.; Du Bois, D. R.; Ziller, J. W.; Nowick, J. S. X-ray crystallographic structure of a teixobactin analogue reveals key interactions of the teixobactin pharmacophore. *Chemical Communications* **2017**, *53*, 2772-2775.
(31) Chen, K. H.; Corro, K. A.; Le, S. P.; Nowick, J. S. X-ray Crystallographic Structure of a Giant Double-Walled Peptide Nanotube Formed by a Macrocyclic beta-Sheet Containing A beta(16-22). *J. Amer. Chem. Soc.* **2017**, *139*, 8102-8105.
(32) Kreutzer, A. G.; Harnza, I. L.; Spencer, R. K.; Nowick, J. S. X-ray Crystallographic Structures of a Trimer, Dodecamer, and Annular Pore Formed by an Ab(17)_(36) beta-Hairpin. *J. Amer. Chem. Soc.* **2016**, *138*, 4634-4642.
(33) Zheng, J.; Baghkhanian, A. M.; Nowick, J. S. A Hydrophobic Surface Is Essential To Inhibit the Aggregation of a Tau-Protein-Derived Hexapeptide. *J. Amer. Chem. Soc.* **2013**, *135*, 6846-6852.
(34) Romonosky, D. E.; Ali, N. N.; Saiduddin, M. N.; Wu, M.; Lee, H. J.; Aiona, P. K.; Nizkorodov, S. A. Effective absorption cross sections and photolysis rates of anthropogenic and biogenic secondary organic aerosols. *Atm. Environ.* **2016**, *130*, 172-179.
(35) Hinks, M. L.; Brady, M. V.; Lignell, H.; Song, M. J.; Grayson, J. W.; Bertram, A. K.; Lin, P.; Laskin, A.; Laskin, J.; Nizkorodov, S. A. Effect of viscosity on photodegradation rates in complex secondary organic aerosol materials. *Phys. Chem. Chem. Phys.* **2016**, *18*, 8785-8793.
(36) Romonosky, D. E.; Nguyen, L. Q.; Shemesh, D.; Nguyen, T. B.; Epstein, S. A.; Martin, D. B. C.; Vanderwal, C. D.; Gerber, R. B.; Nizkorodov, S. A. Absorption spectra and aqueous photochemistry of beta-hydroxyalkyl nitrates of atmospheric interest. *Molecular Physics* **2015**, *113*, 2179-2190.
(37) Lignell, H.; Epstein, S. A.; Marvin, M. R.; Shemesh, D.; Gerber, R. B.; Nizkorodov, S. Experimental and Theoretical Study of Aqueous cis-Pinonic Acid Photolysis. *J. Phys. Chem. A* **2013**, *117*, 12930-12945.
(38) Updyke, K. M.; Nguyen, T. B.; Nizkorodov, S. A. Formation of brown carbon via reactions of ammonia with secondary organic aerosols from biogenic and anthropogenic precursors. *Atm. Environ.* **2012**, *63*, 22-31.
(39) Bones, D. L.; Henricksen, D. K.; Mang, S. A.; Gonsior, M.; Bateman, A. P.; Nguyen, T. B.; Cooper, W. J.; Nizkorodov, S. A. Appearance of strong absorbers and fluorophores in limonene-O_3 secondary organic aerosol due to NH_4^+-mediated chemical aging over long time scales. *Journal of Geophysical Research-Atmospheres* **2010**, *115*, D05203, doi:05210.01029/02009JD012864.
(40) Aiona, P. K.; Lee, H. J. J.; Leslie, R.; Lin, P.; Laskin, A.; Laskin, J.; Nizkorodov, S. A. Photochemistry of products of the aqueous reaction of methylglyoxal with ammonium sulfate. *ACS Earth and Space Chemistry* **2017**, *submitted*.
(41) Gallagher, K. L.; Alfonso-Garcia, A.; Sanchez, J.; Potma, E. O.; Santos, G. M. Plant growth conditions alter phytolith carbon. *Frontiers in Plant Science* **2015**, *6*.
(42) Hanninen, A.; Shu, M. W.; Potma, E. O. Hyperspectral imaging with laser-scanning sum-frequency generation microscopy. *Biomed. Opt. Express* **2017**, *8*, 4230-4242.
(43) Kenison, J. P.; Fast, A.; Guo, F.; LeBon, A.; Jiang, W.; Potma, E. O. Imaging properties of surface-enhanced coherent anti-Stokes Raman scattering microscopy on thin gold films. *J. Opt. Soc. Am. B* **2017**, *in press*.

(44) Row, R. D.; Shih, H. W.; Alexander, A. T.; Mehl, R. A.; Prescher, J. A. Cyclopropenones for Metabolic Targeting and Sequential Bioorthogonal Labeling. *J. Amer. Chem. Soc.* **2017**, *139*, 7370-7375.
(45) Kamber, D. N.; Liang, Y.; Patterson, D. M.; Briggs, J. S.; Shih, H.-W.; Houk, K. N.; Prescher, J. A. 1,2,4-Triazines can be tuned to access unique bioorthogonal cycloadditions. **2017**, *in revision*.
(46) Jones, K. A.; Porterfield, W. B.; Rathbun, C. M.; Hua, C. T.; Reyes, M. A.; Sagoe, M.; Prescher, J. A. Rapid production of orthogonal luciferase-luciferin pairs. **2017**, *submitted*.
(47) Patterson, D. M.; Nazarova, L. A.; Xie, B.; Kamber, D. N.; Prescher, J. A. Functionalized Cyclopropenes As Bioorthogonal Chemical Reporters. *J. Amer. Chem. Soc.* **2012**, *134*, 18638-18643.
(48) Burns, A. S.; Wagner, A. J.; Fulton, J. L.; Young, K.; Zakarian, A.; Rychnovsky, S. D. Determination of the Absolute Configuration of β-Chiral Primary Alcohols Using the Competing Enantioselective Conversion Method. *Organic Letters* **2017**, *19*, 2953-2956.
(49) Wagner, A. J.; Miller, S. M.; King, R. P.; Rychnovsky, S. D. Nanomole-Scale Assignment and One-Use Kits for Determining the Absolute Configuration of Secondary Alcohols. *Journal of Organic Chemistry* **2016**, *81*, 6253-6265.
(50) Samame, R. A.; Owens, C. M.; Rychnovsky, S. D. Concise synthesis of (+)-fastigiatine. *Chem. Sci.* **2016**, *7*, 188-190.
(51) Wagner, A. J.; Miller, S. M.; Nguyen, S.; Lee, G. Y.; Rychnovsky, S. D.; Link, R. D. Undergraduate Laboratory Experiment To Determine Absolute Configuration Using Thin-Layer Chromatography. *Journal of Chemical Education* **2014**, *91*, 716-721.
(52) Tay, G. C.; Huang, C. Y.; Rychnovsky, S. D. Silyl Enol Ether Prins Cyclization: Diastereoselective Formation of Substituted Tetrahydropyran-4-ones. *Journal of Organic Chemistry* **2014**, *79*, 8733-8749.
(53) Miller, S. M.; Samame, R. A.; Rychnovsky, S. D. Nanomole-Scale Assignment of Configuration for Primary Amines Using a Kinetic Resolution Strategy. *J. Amer. Chem. Soc.* **2012**, *134*, 20318-20321.
(54) Wagner, A. J.; David, J. G.; Rychnovsky, S. D. Determination of Absolute Configuration Using Kinetic Resolution Catalysts. *Organic Letters* **2011**, *13*, 4470-4473.
(55) Qiu, Y. H.; Hinkle, P.; Yang, C.; Bakker, H. E.; Schiel, M.; Wang, H.; Melnikov, D.; Gracheva, M.; Toimil-Molares, M. E.; Imhof, A.; Siwy, Z. S. Pores with Longitudinal Irregularities Distinguish Objects by Shape. *Acs Nano* **2015**, *9*, 4390-4397.
(56) Powell, M. R.; Sullivan, M.; Vlassiouk, I.; Constantin, D.; Sudre, O.; Martens, C. C.; Eisenberg, R. S.; Siwy, Z. S. Nanoprecipitation-assisted ion current oscillations. *Nature Nanotechnology* **2008**, *3*, 51-57.
(57) Pevarnik, M.; Healy, K.; Davenport, M.; Yen, J.; Siwy, Z. S. A hydrophobic entrance enhances ion current rectification and induces dewetting in asymmetric nanopores. *Analyst* **2012**, *137*, 2944-2950.
(58) Innes, L.; Powell, M. R.; Vlassiouk, I.; Martens, C.; Siwy, Z. S. Precipitation-Induced Voltage-Dependent Ion Current Fluctuations in Conical Nanopores. *Journal of Physical Chemistry C* **2010**, *114*, 8126-8134.
(59) Arredondo, V.; Hiew, S. C.; Gutman, E. S.; Premachandra, I.; Van Vranken, D. L. Enantioselective Palladium-Catalyzed Carbene Insertion into the N-H Bonds of Aromatic Heterocycles. *Angewandte Chemie-International Edition* **2017**, *56*, 4156-4159.
(60) Gutman, E. S.; Arredondo, V.; Van Vranken, D. L. Cyclization of eta(3)-Benzylpalladium Intermediates Derived from Carbene Insertion. *Organic Letters* **2014**, *16*, 5498-5501.
(61) Kitamura, M.; Yuasa, R.; Van Vranken, D. L. Synthesis of the cyclic prenylguanidine nitensidine E using a palladium-catalyzed carbenylative amination. *Tetrahedron Lett.* **2015**, *56*, 3027-3031.
(62) Premachandra, I.; Nguyen, T. A.; Shen, C. T.; Gutman, E. S.; Van Vranken, D. L. Carbenylative Amination and Alkylation of Vinyl Iodides via Palladium Alkylidene Intermediates. *Organic Letters* **2015**, *17*, 5464-5467.
(63) Ogata, A. F.; Edgar, J. M.; Majumdar, S.; Briggs, J. S.; Patterson, S. V.; Tan, M. X.; Kudlacek, S. T.; Schneider, C. A.; Weiss, G. A.; Penner, R. M. Virus-Enabled Biosensor for Human Serum Albumin. *Analyt. Chem.* **2017**, *89*, 1373-1381.
(64) Choi, Y.; Olsen, T. J.; Sims, P. C.; Moody, I. S.; Corso, B. L.; Dang, M. N.; Weiss, G. A.; Collins, P. G. Dissecting Single-Molecule Signal Transduction in Carbon Nanotube Circuits with Protein Engineering. *Nano Letters* **2013**, *13*, 625-631.
(65) Gilliam, A. J. H.; Smith, J. N.; Flather, D.; Johnston, K. M.; Gansmiller, A. M.; Fishman, D. A.; Edgar, J. M.; Balk, M.; Majumdar, S.; Weiss, G. A. Affinity-Guided Design of Caveolin-1 Ligands for Deoligomerization. *Journal of Medicinal Chemistry* **2016**, *59*, 4019-4025.
(66) Yuan, T. Z.; Ormonde, C. F. G.; Kudlacek, S. T.; Kunche, S.; Smith, J. N.; Brown, W. A.; Pugliese, K. M.; Olsen, T. J.; Iftikhar, M.; Raston, C. L.; Weiss, G. A. Shear-Stress-Mediated Refolding of Proteins from Aggregates and Inclusion Bodies. *Chembiochem* **2015**, *16*, 393-396.

(67) Lydon, B. R.; Germann, A.; Yang, J. Y. Chemical modification of gold electrodes via non-covalent interactions. *Inorganic Chemistry Frontiers* **2016**, *3*, 836-841.
(68) Tsay, C.; Livesay, B. N.; Ruelas, S.; Yang, J. Y. Solvation Effects on Transition Metal Hydricity. *J. Amer. Chem. Soc.* **2015**, *137*, 14114-14121.
(69) Shaffer, D. W.; Bhowmick, I.; Rheingold, A. L.; Tsay, C.; Livesay, B. N.; Shores, M. P.; Yang, J. Y. Spin-state diversity in a series of Co(II) PNP pincer bromide complexes. *Dalton Transactions* **2016**, *45*, 17910-17917.
(70) Thammavongsy, Z.; Kha, I. M.; Ziller, J. W.; Yang, J. Y. Electronic and steric Tolman parameters for proazaphosphatranes, the superbase core of the tri(pyridylmethyl)azaphosphatrane (TPAP) ligand. *Dalton Transactions* **2016**, *45*, 9853-9859.