

RMRM 1

Ethnoscience strategies to indigenize science at tribal colleges: Connecting chemistry to the tribal community

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The importance of engaging students through hands-on laboratory experiments and connecting to their personal experiences cannot be overstated. Including students' cultural backgrounds as a component of the class is often called Ethnoscience. Ethnoscience, its foundations and principals, in terms of American Indians and Alaska Natives was described in the 1990s. Building on this model, Turtle Mountain Community College revised their chemistry labs in the early 2000s. We have developed a two-semester chemistry lab manual for a general, organic, and biochemistry introductory course. Each lab has a tribal community connection to increase authenticity and relevancy of the chemistry concepts. Specific community connection information has been provided in the background of each lab, but each lab report provides students the opportunity to share their own personal connection. Why community connections? Connecting chemistry content to students' a prior knowledge, authentic phenomenon, and culturally-relevant topics increases the learning of new content. The community connection section of each lab only scratches the surface of the tribal community connections. Students sharing their own connections will enrich the authenticity of the chemistry as well as the instructor's and classmates own knowledge. We have incorporated some of these stories into the lab manual, but each instructor and time the course meets, students will bring their own connections that will enhance learning and understanding of content. In fact, while the lab is static, the indigenization is a dynamic work in progress. This increases the sustainability of the chemistry course as well.



RMRM 2

Regenerable single atom catalysts for alkane conversions

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Single atom catalysts are currently of great interest due to high selectivity, reactivity and excellent atom efficiency. Here we have explored the use of single atom catalysts for high temperature reactions involving alkane conversions. The work is motivated by the availability of natural gas due to advancements in fracking and drilling technologies. The increased production has led to lower costs, which are beneficial in lowering the carbon footprint of fuels when methane is used to replace coal for electricity production. Ethane and other natural gas liquids (NGLs) recovered from shale with methane, however, have limited markets resulting in export of US produced ethane to Europe starting in 2016. Platinum based catalysts require regeneration which requires significant catalyst handling and the use of corrosive, halogen based treatments. The use of single atom catalysts provides an alternative approach which also alleviates the problem of coke formation which is less likely on single sites.

In previous work we have demonstrated the ease of synthesis of single atom Pt catalysts via vapor phase synthesis on industrial catalyst supports. These single atom catalysts are regenerable using oxidizing conditions at modest temperatures. The focus of the present work is the use of single atom dopants as modifiers to improve the selectivity and stability of the single atom catalysts for alkane conversions, and gaining insight into the deactivation mechanism of these catalysts. Characterization via X-ray absorption spectroscopy helps us advance the applications of SACs to industrially relevant reactions.

RMRM 3

LigandNet: Machine-learning based toolkit for predicting ligand activity to proteins

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LigandNet is a Machine Learning (ML) toolbox that combines different models into an open source platform that can predict if a ligand may have activity to a specific protein. Finding a ligand that will bind to a human protein and have a significant signaling effect through the cell can be an expensive task. Nowadays, ML models are being employed throughout many scientific fields and are being successfully applied to drug discovery research. In this project, we have applied advanced ML approaches such as Random Forest (RF), Support Vector Machine (SVM), Linear Regression (LR), Extra Tree

Classifier (ETC) and Deep Learning (DL) to classify the ligands as actives/binders or inactives/nonbinders (labeled as decoys). We obtained the known active ligands for each of 1704 proteins from Pharos (pharos.nih.gov) database. For each of the known active ligands, decoys were generated using DecoyFinder (<http://urvnutrigenomics-ctns.github.io/DecoyFinder/>) and Zinc database (<http://zinc.docking.org/>). ML models were developed for each of the protein-ligand sets by using known actives and generated decoys. ECFP6 fingerprints and Topological Pharmacophore Atomic Triplet Fingerprint (TPATF) from MayaChemTools (<http://www.mayachemtools.org/>) were employed as feature generators in developing the models. Models were validated using highest positive predictive value (PPV), sensitivity, and area under the curve of receiver operating characteristic plots (ROC-AUC) to determine which model works best with each datasets of the proteins, determining the accuracy and precision of each ML approach. The developed models are available on github (<https://github.com/sirimullalab/LigandNet>).

RMRM 4

Crowding effect on electron transfer in inducible nitric oxide synthase

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Crowding reagents (Ficoll 70 and Dextran 70) were used to study the crowding effect on the FMN-heme interdomain electron transfer (IET) in NO synthase, the rate-limiting step in NO production. The IET kinetics in holoenzyme and oxygenase/FMN (oxyFMN) construct of human iNOS were determined in the presence of Ficoll 70 over the concentrations range from 0%-14% w/v. A notable increase in the IET rate was observed, which is not saturable, a hallmark of crowding effect. The docked FMN-heme state population in human iNOS oxyFMN was also increased continuously upon addition of the crowder. The magnitude of IET enhancement for the holoenzyme (25%-76%) is much higher than that of the oxyFMN construct (10%-25%). This can be attributed to the larger fractional excluded solvent volume of holoenzyme. To determine whether non-specific soft interactions may contribute to the effect, the influence of Dextran 70 on the IET rate was also investigated. Moreover, fluorescence lifetime measurements show that the population of the output state in human iNOS was increased from 10% to 33% upon addition of 14% Ficoll 70. NO production activity of human iNOS holoenzyme is also enhanced by Ficoll. These results together provide the strong evidence that the FMN-heme IET can be significantly enhanced by crowders through shifting the conformational equilibrium toward formation of the output state for NO production. This is a significant finding because biochemical studies of NOS proteins have been conducted in diluted solutions, which is not a good proxy to the proteins functioning in crowded cellular environments.

RMRM 5

Synthesis and characterization of lanthanide-silica based core/shell nanoparticles for scintillator applications

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Scintillators, such as the commercial standard NaI(Tl), are materials that fluoresce when exposed to high energy particles. This property has been important in the development of instruments such as the medical CT scan, X-rays in airport security systems, and even nuclear detection systems. There are a wide range of materials that scintillate, ranging from organic to inorganic to plastic scintillator materials. Inorganic crystal scintillators consist of a wide range of materials, including alkali metal halides, lanthanum halides, metal oxides, and metal-silicates ($MSiO_x$). For the M-SiO₂ optimized inorganic scintillators their fluorescent properties can be further improved through the doping with lanthanide cations.

Original synthetic pathways using metal siloxide [$M(OSi(OR)_3)_x$] precursors have had varying success in converting to the $MSiO_x$ -based materials. Interest in alternative ligands lead to us to studying tris(trimethylsilyl)silanol (or H-SST). The H-SST ligand was of interest due to its potential favorable decomposition properties, therefore, upon processing it might be possible to generate the $MSiO_x$ fluorescent materials of interest. Metal alkoxides ($[M(OR)_x]$) are excellent precursors to ceramic materials and can be easily modified by altering their ligand set. Consequently, it was reasoned that the combination of H-SST and $[M(OR)_x]$ precursors increases the potential for producing a single-source precursor to $MSiO_x$ scintillators.

In previous research performed in the Boyle group at Sandia National Laboratories, a series of Group 4 $[M(OR)_4]$ were modified with the H-SST ligand and processed by thermally heating them in air. The product formed was a core/shell nanomaterial, in which the metal core was surrounded by a silica based matrix or a silica core was surrounded by a metal-based matrix. Even though the SST successfully bound to the metals, when exposed to radiation the molecules and the final products did not luminesce. In order to synthesize scintillators with higher sensitivity different metal options must be considered. Due to the previous success with the lanthanide metals in the production of scintillators, combining these metals with the H-SST ligand could prove an interesting alternative to producing metal silica based scintillators. This work will present the synthesis, characterization, and materials properties of a series of $[Ln(SST)_3(solvent)_2]$ molecules that were generated.

RMRM 6

Synthesis of manganese-based precursors and nanoparticles for electronic printing applications

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Manganese makes up 0.11% of the earth's crust and is an important element in stainless steel manufacturing due to its low cost, malleability, ease of alloying, and ability to remove impurities. Manganese oxide is also desirable due to its magnetic properties, catalytic activity and high energy density. As instrumentation get smaller and smaller, the electronics that control them will also have to be reduced in size. Direct write manufacturing is a method that provides precision when printing for products in computer electronics. These technologies require high quality nanoinks composed of nanoparticles suspended in organic solvents. Manganese-based inks are of interest due to their potential applications noted above but little work has been proffered concerning their development. This fundamental study focuses on the impact the ligand has on the properties (size, morphology, phase, etc.) of the final nanoparticles generated and was investigated using commercial (Mn-nitrates, chlorides, and acetates) and tailor-made precursors. In particular, the various Mn-L bonds (i.e., Mn-O, Mn-C, Mn-N) were investigated using alkoxides, mesityl, and amide derivatives synthesized in-house. Additionally, the commercially available were evaluated.

Manganese mesityl was synthesized from the metathesis reaction of manganese bromide and mesityl magnesium bromide. Manganese alkoxide precursors were synthesized from manganese mesityl and various aryl alcohols in coordinating solvents. Inorganic crystals were characterized with single crystal X-ray diffraction (SCXRD) and Fourier Transform Infrared Spectroscopy (FTIR). Nanoparticles were synthesized from this family of precursors using solution precipitation and solvothermal syntheses techniques. To examine the influence of various precursor choice on morphology of nanoparticles, Transmission Electron Microscopy (TEM) and Powder X-ray Diffraction (PXRD) were conducted. This presentation will report on the synthesis of the compounds, the nanomaterials generated, and try to reestablish how the variables of synthesis (e.g., precursors, coordinating solvents, time and temperature) affected the final size, shape and phase of the final nanomaterials product.

RMRM 7

New model systems for periplasmic nitrate reductase (Nap) and formate dehydrogenase (Fdh) catalytic intermediates

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Formate dehydrogenase (Fdh) and periplasmic nitrate reductase (Nap) belong to the DMSOr enzyme family and are very important contributors to the global nitrogen and carbon cycles. Fdh is found important in recent efforts to convert CO₂ into formate as alternate source of energy. All enzymes of the DMSOr family have a common structural motif with four sulfur donors originating from two pyranopterin dithiolene (PDT) chelating ligands bound to Mo. DMSOr family enzymes are grouped into different subfamilies based on the type of ancillary ligands present. There are limited spectroscopic studies that have focused on determining the type and role of ancillary ligands in Nap and Fdh. These enzymes possess other strongly absorbing chromophores (e.g. Fe-S clusters),

which effectively prohibit probing their electronic structure using optical spectroscopies. This limits our ability to understand electronic structure contributions to reactivity. In an effort to better understand their catalytic mechanisms, it is important to understand the geometric and electronic structure of the key catalytic intermediates. To address this problem, we have synthesized new biomimetic model complexes of paramagnetic Nap and Fdh enzyme intermediates. In this study, we have compared enzyme g-anisotropies with those synthetic model complexes. The geometric and electronic structures of the models have also been studied using electronic and x-ray absorption spectroscopies coupled with electronic structure computations to assess potential roles for the ancillary ligand set and PDTs in the electron transfer half reaction.

RMRM 8

Insights into molecular rectification using donor-acceptor molecules

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Fundamental advances in our ability to design and construct electronic components at the nanoscale will require new design paradigms. One proposed nanoscale electronic component is the molecular rectifier. The original concept of a molecular rectifier was proposed by Aviram and Ratner in 1974 by using a donor-insulator-acceptor (D- σ -A) type molecular construct. Molecular and molecule-based electronic components are advantageous due to their ease of synthetic manipulation, and the fact that the size dimensions of molecules are inherently at the nanoscale (0.5 - 3nm). Our group has shown how the Donor-Bridge-Acceptor biradical approach can be used to derive key structure-property relationships that allow insight into the choice of bridge fragments for molecular rectification by using constitutional isomers of the donor-bridge-acceptor biradical (NN-Th-Py-SQ) (S=1/2 *ortho*-semiquinonate, **SQ**; A: S=1/2 nitronyl nitroxide, **NN**; Th = thiophene; Py = pyridine). These NN-bridge-SQ complexes serve as constant bias analogs for molecular current rectifying devices. The efficiency of rectification is given by the rectification ratio ($RR = g_{forward}/g_{reverse}$; where g = conductance). The experimental and calculated RR for (NN-Th-Py-SQ) isomers is 1.58 and 1.24 respectively at $\pm 2.56V$ applied bias. Low RRs are obtained for this system since the Py and Th π -systems have not been effectively decoupled. A new idea for decoupling the donor and acceptor π -systems in a molecular rectifier is to employ a transition metal. Here, we describe square planar complexes of Nickel(II), Palladium(II), and Platinum(II) using dioxolane donor and a bipyridine acceptor ligands, which are localized on the HOMO and LUMO, respectively. The RRs are observed to be markedly higher (RR as high as 16) using this motif. Electronic structure contributions to rectification will be discussed.

RMRM 9

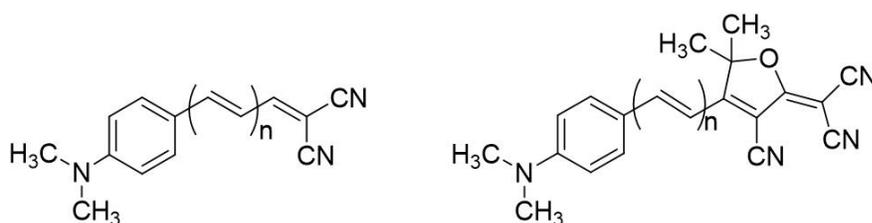
Structure and properties of new push-pull molecules

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For several decades attention to structures and properties of push-pull systems with donor and acceptor groups connected with pi-conjugated bridge was attracted due to their potential nonlinear optical properties [1-3] and corresponding applications such as terahertz (THz) generation and detection [4] and microresonator filters and modulators [5]. Relatively recently emerged are several publications devoted to biological applications of push-pull molecules as near infrared (NIR) probes for non-invasive detection of accumulation of beta-amyloid plaques in the brain related to Alzheimer disease [6].

Here we present structural studies of two series of push-pull molecules: homologues of 4-(4-dimethylamino)-dicyanovinylbenzene and organic chromophores with (3-cyano-5,5-dimethyl-2(5H)-furylidene)malononitrile (so called tricyanofuran, TCF) as an acceptor group with the polyene bridges containing 1-5 -C=C- bonds (**Scheme 1**).

Properties of these materials are discussed based on information obtained on their structures, results of quantum chemical computations and spectroscopic data.



Scheme 1

RMRM 10

Design, synthesis, and evaluation of cystargolide-based β -lactones as potent proteasome inhibitors and anti-cancer agents

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The inhibition of proteasome function is a clinically validated strategy for the treatment of certain forms of cancer and related diseases. Despite the clinical availability of FDA approved drugs including bortezomib and carfilzomib, these compounds are associated with several side effects diminishing their efficacy. There is an unmet need for more potent anti-cancer drugs that could address these limitations. As a part of our drug discovery efforts, the total synthesis and absolute stereochemistry of β -lactone

proteasome inhibitors cystargolides A and B was accomplished, and the same scaffold was used to conduct structure-activity relationship (SAR) studies in order to assess their anticancer potential. A wide variety of analogs was designed, synthesized and evaluated for proteasome inhibition, for cytotoxicity towards several cancer cell lines, and for their ability to enter intact cells. The cystargolide derivative **5k**, structurally unique at both P_γ and P₁, exhibited the most promising inhibitory activity for the β5 subunit of human proteasomes (IC₅₀ = 3.1 nM) and significant cytotoxicity towards MCF-7 (EC₅₀ = 416 nM), MDA-MB-231 (EC₅₀ = 74 nM) and RPMI 8226 (EC₅₀ = 41 nM) cancer cell lines. Cellular infiltration assays revealed that minor structural modifications have significant effects on internalization. We identified **5k** as a promising candidate for continued therapeutic studies. Our novel drug lead **5k** is a more potent proteasome inhibitor than carfilzomib with low nanomolar IC₅₀ measurements and it displays promising potency against multiple cancer cell lines. Although β-lactones were identified as the first natural ligands for the proteasome, these compounds have not been developed yet as commercial drugs. This work provides useful insights into the design of novel peptidic β-lactone proteasome inhibitors for future therapeutic applications.

RMRM 11

Concepts important for proficiency in organic reaction mechanisms

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Reaction mechanisms in organic chemistry present challenges for many undergraduate and graduate students. It is an important skill required for developing a good understanding of chemical reactions and syntheses in organic chemistry. In the first phase of a multi-step study, organic chemistry instructors (N=10) were interviewed to elicit their opinions on important topics required for the development of the ability to write mechanisms of reactions. The instructors identified 10 important topics. Additionally, the instructors were interviewed regarding their opinions and awareness of students' strategies and difficulties with the concept. In the second phase of this study, a survey was sent out to organic chemistry instructors across the country (N=1500), to find out if there is consensus at the national level regarding these topics perceived to be relevant by experts. The results show that there is strong agreement among experts from multiple universities regarding the importance of these topics. The goal of this project is to design and develop a two-tier inventory that will assist instructors in assessing their students' understanding of key concepts required for developing proficiency in organic reaction mechanisms.

RMRM 12

Progress report on the design of a flow-based ATR-FTIR Spectrometer

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α -Acetolactate, produced by yeast during the fermentation process in beer production, decarboxylates to give diacetyl (2,3-butanedione) and carbon dioxide. Current analytical methods to detect diacetyl, an off-flavor in beer, include spectrophotometry or gas chromatography. These methods are time consuming and expensive; however, measurements of carbon dioxide can be rapid and inexpensive. Attenuated total reflectance–Fourier transform infrared spectroscopy (ATR-FTIR) utilizing a flow cell and mid-range infrared light (400cm^{-1} – 4000cm^{-1}) is capable of this analysis. Samples containing dissolved CO_2 are pumped through a pressurized flow cell, as infrared light passed through the device. Dissolved CO_2 absorption values can be directly related to diacetyl concentration, increasing a brewery's efficiency. The design and construction of the instrument, with associated data on dissolved CO_2 concentrations, will be presented.

RMRM 13

Fluorescent bead-based method to study the phospholipase A2 -lipid membrane interaction

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The phospholipase A2 (PLA2) is a large group of biologically active enzymes that can hydrolyze lipid membranes. PLA2 is overexpressed in some disease conditions including colon, breast, lung, pancreatic and prostate cancer. Moreover, some cancer biomarkers can inhibit the reactivity of PLA2. It is thus important to study the PLA2 interaction with lipid membranes in order to develop new sensitive diagnostic tools and drug delivery methods for diseases like cancer. Currently, liposomes are utilized to study the membrane-enzyme interaction. However, liposomes lack long-term stability, defined shape and size, and robustness. One attractive alternative for the liposomal assay is to use lipid membranes supported on spherical solid microspheres. In this work, we demonstrate the use of lipid-coated microspheres to study the PLA2-lipid membrane interaction. In our approach, we utilize a sensor dye encapsulated silica microparticles and the enzyme-membrane interaction is detected by flow cytometry. In the presence of PLA2, lipid membranes are hydrolyzed thus released the encapsulated dye. The extent of dye release is measured via flow cytometry and it is used to investigate the degree of enzyme-membrane interaction.

RMRM 14

Method development: Transition characterization of poly(ester urethane) block copolymer elastomer via thermal and mechanical analyses

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A systematic series of thermal and mechanical experiments are presented to resolve thermal transitions of Estane[®]5703 poly(ester urethane) block copolymer elastomer. Using conventional Differential Scanning Calorimetry (DSC) the low temperature melt peaks overlap, resolving these peaks is valuable in that it can give indication of acid catalyzed hydrolytic chain scission. Chain scission is directly related to polymer chain length and mechanical properties. To resolve the overlapping peaks we developed an experimental methodology. First, utilizing Thermogravimetric Analysis (TGA) degradative limits are established. Second, Heat-only Modulated Differential Scanning Calorimetry (MDSC) is used to resolve the overlapping lower temperature melt peaks. Finally, Dynamic Mechanical Analysis (DMA) is used to verify the melt temperature using thermal-step-wise, creep analysis and extrapolating temperature dependent moduli to zero. In all experimental sets, method parameters are optimized through various diagnostic procedures, leading to method parameters tailored to the polymer. The take away from this work is the value of the method development process. Further than resolving thermal transitions for Estane[®]5703, the work defined a methodology which can be applied to any block copolymer, particularly those with difficult to resolve thermal transitions.

RMRM 15

Effects of encapsulated cells on the physical-mechanical properties and microstructure of gelatin methacrylate with high degree of functionalization

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Gelatin methacrylate (GelMA) is gaining more and more attention in a variety of bioprinting and tissue engineering applications due to its good biocompatibility to allow cell adhesion. Cells are encapsulated within the GelMA hydrogels, which significantly affects the physical-mechanical properties and microstructure of the GelMA. This study systematically investigates the effects of encapsulated cells on the physical-mechanical properties and microstructure of GelMA. GelMA is synthesized by the grafting of methacrylamide groups on gelatin. The GelMA degree of functionalization (DoF) is characterized using the ¹H NMR spectroscopy, and a primary amine-reactive fluorescent detection reagent. The effects of encapsulated cells are investigated on the physical properties (swelling and degradation), the mechanical properties (elastic modulus, tensile strain and strength), the microstructure (pore size), and the cell viability.

RMRM 16

Micromachined aluminum microfluidic devices: Miniaturized tool for biomedical applications

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Microfluidics is evolving as a new platform for the development of miniaturized techniques that are advantageous for wide ranges of clinical and bio-analytical applications. A typical microfluidic device is comprised of single to multiple fluid channels with the width of few hundred micrometers and many laboratory functions are performed in these channels. The ability to integrate sound waves into these channels has further enabled the development of a new array of bio-analytical devices with unique capabilities that are not possible in macroscale. The integration of sound waves in microfluidics, known as acoustofluidics, forms a non-contact, gentle new method of particle manipulation that can be utilized to purify, separate, concentrate and analyze cells. To date, silicon and glass have been the materials of choice for acoustofluidic device fabrication. The need of hazardous chemicals, specialized equipment and facilities, and lengthy processes have hindered the widespread use of the technique, especially in biomedical and bioanalytical analyses. To address some of these limitations, we have developed a new acoustofluidic device fabrication method using aluminum sheets. In this presentation, we present the simple construction of aluminum acoustofluidic devices using common metal micromachining techniques. The usefulness of these devices in biomedical and bioanalytical applications is demonstrated by isolation of labeled particles, bovine red blood cells, and Jurkat cells. Further, the high-throughput analytical capability of the device is demonstrated by generating multiple streams of particles and cells in a flow-through manner. Our experimental results indicate that these devices can be used to separate and concentrate microspheres as well as biological samples rapidly and efficiently. In addition, we also demonstrate that these devices can be used to purify samples in a high flow through manner.

RMRM 17

Microsphere-supported lipid bilayers with fluorescent lipid probes for the detection of phospholipase D activity

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Abnormal Phospholipase D (PLD) enzyme levels have been associated with various disease conditions including cancer and Alzheimer's. Thus, PLD can be a potential biomarker for the early detection of these conditions. To detect low quantities of the enzyme, an analytical method with high sensitivity and high selectivity for PLD is

essential. In this work, we investigate the development of lipid coated microspheres and flow cytometry based bio-analytical technique to determine PLD in bio-fluids and cell extracts. Microspheres provide a high surface area to volume ratio medium, thereby allowing us to create reactive surfaces with high lipid concentrations. Additionally, these microsphere-based biomimetic model systems can be easily analyzed using sensitive and high-throughput bioanalytical technique like flow cytometry. PLD hydrolyzes the phosphodiester bond of the glycerophospholipids and generate phosphatidic acid and their respective head groups, thus the presence of the enzyme can be monitored by the lipid-enzyme interaction. The surface of the silica microspheres modified with specific lipid membrane containing fluorescent tags in the head group provides the substrate for the enzymatic interaction. The fluorescent label will be cleaved in the presence of PLD, thereby allowing us to quantify the PLD enzyme through the extent of loss in fluorescence signal. Preliminary experiments with phospholipid model membranes have successfully demonstrated that the proposed biosensor can detect the enzyme at concentrations as low as 1.5 nM in laboratory prepared samples. We are currently investigating its application as a biosensor in measuring PLD activity in biological samples using non-cancerous human breast epithelial cell line (MCF-10A) and breast cancer cell lines (MCF-7 and MDA-MB-231).

RMRM 18

Kinetics of peroxytaurine reactions

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Taurine (2-aminoethanesulfonic acid) is an abundant, biologically-relevant amino acid-derivative found in many Eukaryotes. Peroxytaurine (2-aminoethanesulfonoperoxoic acid) is a recently-discovered molecule involved in the synthesis of taurine. Chemical parameters of peroxytaurine reactions have not been investigated previously. UV-Vis spectrophotometry is used to measure kinetic values for the spontaneous hydrolysis of peroxytaurine, which yields taurine and hydrogen peroxide. Changes in peroxytaurine concentration also are measured through spectroscopy of oxidation reaction products. Kinetic values, as determined *in vitro*, can inform how often peroxytaurine synthesis occurs biologically.

RMRM 19

Normalized Timescale Method for the determination of order in catalyst for electrocatalytic reactions

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A modified version of the Normalized Timescale Method (NTM) has been used to determine order in catalyst in electrocatalytic reactions. This method directly plots cyclic voltammogram (CV) data as current on the y-axis against the time of the CV scan on the x-axis at different catalyst concentrations. The determination of kinetic order from the NTM can provide meaningful information about the mechanism of the catalytic reaction, specifically, the catalyst resting state during turnover. From this analysis, parasitic processes and undesired catalytic pathways may be identified and prevented from occurring. We discuss the application of the NTM to two key electrocatalytic reactions in molecular catalysis for solar fuel conversion, $\text{Mn}^{\text{(Mes)ppy}}(\text{CO})_3\text{Br}$ and $\text{Re}^{\text{(tBu-ppy)}}(\text{CO})_3\text{Cl}$, and highlight the two distinct mechanisms.

RMRM 20

Manganese N-heterocyclic carbene pincers for the electrocatalytic reduction of carbon dioxide

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Two complexes, $[\text{MnCNC}^{\text{Me}}]\text{Br}$ **1** and $[\text{MnCNC}^{\text{Bn}}]\text{Br}$ **2**, were synthesized using $\text{Mn}(\text{CO})_5\text{Br}$ and N-heterocyclic carbene pincer ligands then characterized and tested for CO_2 reduction catalysis. Both compounds catalyze the reduction of CO_2 to CO in the presence and absence of 2,2,2-trifluoroethanol, a proton source. Although **2** operates at a potential 100 mV more positive than **1**, both show similar current densities. A 1 e⁻ reduction per manganese center was calculated using a combination of Normal Pulse Voltammetry (NPV) and Diffusion Ordered Spectroscopy (DOSY). A variant of the Normalized Timescale Method (NTM) was used to determine the order in catalyst of the reaction.

RMRM 21

Hierarchical zinc oxide nanostructures for the photochemical reduction of bicarbonate to solar fuels

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Zinc oxide (ZnO) is an earth abundant, non-toxic, and low-cost material that has been used widely for photocatalytic water splitting, gas sensing, and dye degradation. In this study, several ZnO structures were synthesized, characterized, and tested for the photocatalytic reduction of bicarbonate to formic acid, an intermediate to methanol, a high-octane fuel. The different ZnO morphologies studied included micron- and nano-particulate ZnO, rods, wires, belts, and flowers. ZnO was also synthesized from the direct calcination of zinc acetate, which provided a cheap and large-scale synthesis method to produce ZnO. The photocatalytic efficiency of the synthesized ZnO was compared to commercial micron- and nano-particulate ZnO, and was proven to be just as efficient. ZnO flowers, possessing the largest surface area of 12.9 m²/g, were found to be the most efficient reaching an apparent quantum efficiency (AQE) of 10.04±0.09%, with a superior performance over commercial TiO₂ (P25), a benchmark photocatalyst. Green chemistry solvent, glycerol, proved to be a far superior hole scavenge in comparison to 2-propanol, which is derived from petroleum sources. This is the first study to compare different shapes and sizes of ZnO for bicarbonate reduction in an aqueous system with excellent photocatalytic performance.

RMRM 22

Molecular rectification behavior of the pyranopterin ligand of molybdoenzymes

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Molybdenum plays an indispensable role in human metabolism, global nitrogen and sulfur cycles, greenhouse gas formation, bacterial detoxification pathways, and anaerobic respiration. These processes are critical for maintaining human health and ecological balance. To become catalytically active, the Mo ion must be incorporated into a molecular scaffold by complexation with a singular ligand known as the pyranopterin dithiolene. The resulting molybdenum cofactor, or Moco, is found in molybdoenzymes with the sole exception of nitrogenase. Molybdoenzymes typically catalyze the two-electron oxidation or reduction of a substrate coupled to formal oxygen atom transfer. The pyranopterin dithiolene (PDT) ligand can adopt several distinct geometries that may correspond to different oxidation and tautomeric states, which we hypothesize will contribute to its suspected role as an electron transfer conduit during catalysis. Interestingly, the fully reduced tetrahydro and the oxidized quinoid dihydro PDT both exemplify the Van Dyke/Ratner design rules for synthetic molecular rectifiers, indicating that nature may utilize molecular rectification in catalytic processes involving vectorial electron transfer. The rectification ratio (RR) is the ratio of current that can flow at forward and reverse biases. High RRs are an indicator of the efficiency of vectorial electron transfer. In this study, we computationally demonstrate how the RR can be modulated with changes in oxidation and tautomeric state of the PDT. Furthermore, we analyze this rectification behavior by identifying the frontier molecular orbitals responsible for transmission. This provides a basis for understanding how electron

transfer processes occur in molybdoenzymes as well as informing further design criteria for novel biologically inspired synthetic molecular rectifiers.

RMRM 23

Charge effect on oxygen atom transfer reactivity related to molybdoenzymes

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The effect of a unit charge difference on the electronic structure and OAT reactivity of *cis* dioxo-Mo(VI) complexes has been explored using kinetic and computational methods. A comparative study on isoelectronic and isosteric [Tpm*MoO₂Cl]⁺ and Tp*MoO₂Cl complexes [where Tpm* = (tris(3,5-dimethyl-1-pyrazolyl)methane, Tp* = hydrotris(3,5-dimethyl-1-pyrazolyl)borate)] provides insight into how charge affects electronic structure, and how this is manifested in remarkable differences in their oxygen atom transfer rates toward the same substrate. Based on our computational results, the primary difference in oxygen atom transfer reactivity is attributed to a lowering of LUMO energy in cationic [Tpm*MoO₂Cl]⁺ compared to charge neutral Tp*MoO₂Cl. This leads to a significant lowering of the activation barrier with concomitant rate enhancement. The lowering of the LUMO energy in [Tpm*MoO₂Cl]⁺ leads to an early transition state coupled to a greater thermodynamic driving force for oxygen atom transfer reactivity.

RMRM 24

Generation and characterization of functional phosphoserine incorporated neuronal nitric oxide synthase holoenzyme

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Protein phosphorylation is an important mechanism for regulation of nitric oxide synthase (NOS) at the posttranslational level. Utilizing phosphomimetic residues, a common method for studying protein phosphorylation, fails to recapitulate the charge and steric nature of the phosphorylation modification. Herein, we have established a system in which recombinant rat nNOS holoprotein can be produced with site-specific incorporation of phosphoserine (pSer) using expanded genetic codon. Our analyses of

purified wild type (wt, the terms 'wt' and 'nonphosphorylated' can be used interchangeably) and pSer nNOSs showed that the amber suppressed nNOS, pSer nNOS, has been successfully overexpressed. Purified wt and pSer nNOS showed identical spectra properties and perform normal enzymatic activity. Conversely, the rate of interdomain electron transfer (IET), the rate limiting step in NOS catalysis, in pSer nNOS significantly decreased compared to the wt, whereas the phosphomimetic mutant showed similar electron transfer rate to that of wt protein. These results clearly demonstrate that it is highly advantageous to utilize pSer-incorporated NOS, a true phosphorylated NOS form, in future biochemical and mechanistic studies. The new pSer-incorporation system will be extremely useful for robust preparation of large amounts of active phosphorylated nNOS for use in mechanistic and structure/function studies.

RMRM 25

Implications of pyran cyclization and pterin conformation on oxidized forms of the molybdenum cofactor

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ABSTRACT: The large family of mononuclear molybdenum and tungsten enzymes all possess the special ligand molybdopterin (MPT), which consists of a metal-binding dithiolene chelate covalently bound to a pyranopterin group. These molybdoenzymes catalyze a variety of oxygen atom transfer (OAT) and hydroxylation reactions on a broad range of substrates. MPT pyran cyclization/scission processes have been proposed to modulate the reactivity of the metal center during the course of catalysis. However, the role of MPT and its participation in the catalytic reaction is still under considerable debate and is a focus of this study. We have designed several small molecule models for the Mo-MPT cofactor that allow detailed investigation into how pyran cyclization modulates electronic communication between the dithiolene and pterin moieties, and how this cyclization alters the electronic environment of the molybdenum catalytic site. Using a combination of cyclic voltammetry (CV), vibrational spectroscopy (FT-IR and rR), electronic absorption spectroscopy, and x-ray absorption spectroscopy (XAS), distinct changes in the Mo \equiv O stretching frequency, Mo(V/IV) reduction potential, and electronic structure across the pterin-dithiolene ligand are observed as a function of pyran ring closure. The results are significant for they reveal that a dihydropyranopterin is electronically coupled into the Mo-dithiolene group due to a coplanar conformation of the pterin and dithiolene units. This coplanarity creates extended π conjugation from the Mo-dithiolene unit through the pterin, providing a mechanism for the electron-deficient pterin to modulate the Mo environment. A spectroscopic signature identified for the pyranodihydropterin-dithiolene ligand on Mo is a strong dithiolene \rightarrow pterin charge transfer

transition. In the absence of a pyran group bridge between pterin and dithiolene, the pterin rotates out of plane, largely decoupling the system. The results support a hypothesis that pyran cyclization/scission processes in MPT may function as a molecular switch to electronically couple and decouple the pterin and dithiolene to adjust the redox properties in certain pyranopterin molybdenum enzymes.

RMRM 26

Synthesis of nitrile-functionalized ladder-type oligo(*p*-phenylene)s for probing electron delocalization

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Phenylene-based conjugated oligomers and polymers (e.g., fluorenes) are promising candidates for organic electronics and solar cells, due to their great electrochemical and thermal stability, high photoluminescence quantum efficiency, prominent charge-carrier mobility, and highly tunable electronic properties through molecular design and organic synthesis. To probe electron delocalization, the key in controlling the energetics and dynamics of electrons, we have selected time-resolved Infrared spectroscopy coupled with pulse radiolysis for a series of newly designed ladder-type oligo(*p*-phenylene)s. Such oligo(*p*-phenylene)s are rigidified with two to five bridges for maximizing *p*-conjugation. They bear an electron-withdrawing nitrile group as an infrared reporter group and hexyl side chains for increasing their solubility. Compared to the oligofluorene counterparts, they have conformational rigidity and planarity and are expected to exhibit sharper infrared peaks and faster electron transfer rates. In this presentation, we will talk about our organic synthesis of the title oligo(*p*-phenylene)s, and characterizations of several important intermediate molecules by ¹H-, ¹³C-NMR spectroscopy, X-ray single crystal diffraction, and pulse radiolysis using the laser-electron accelerator facility at Brookhaven National Laboratory. Our focus will be on their optical signatures of the charged and triplet states.

RMRM 27

Discrete stochastic solution to lipid bilayer permeation model

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Molecular dynamics (MD) simulations of diffusion/permeation of small molecules/oxygen are able to measure the permeation of oxygen through lipid bilayers at equilibrium conditions. MD does not simulate steady-state flux of molecules. To

circumvent that limitation MD results were used to create a stochastic Markov chain. The probability matrix features a collection of normal distributions comingled with a drift term/probability. Depth-dependent diffusions are calculated and equilibrium distribution of molecules agree with previously simulated results benchmarked by EPR oximetry. Steady state results can be obtained by perturbation of the equilibrium state on the outflux end of the system thus generating a chemical potential drop. The solution can easily be adapted to different models that are beyond the limitations of long simulations. Moreover, it features fast and easy calculations that reduce computational time by three degrees of magnitude.

RMRM 28

Counting triplets on single polymer chains for solar cells

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Current power conversion efficiencies for organic solar cells (OPVs) has hit a wall with only incremental improvement in the last five years. Optimizing OPVs using conjugated polymers is advantageous due to the ease of processing and low cost of production. Yet limited understanding of the structure-function relationship of conjugated polymers hinders progress towards increasing power conversion efficiencies. New molecular design strategies promising increase performance attempt to utilize multiple exciton generation (MEG), but without proper tools to assess consequences of the approach results in a zero-sum. Understanding multiple singlet and triplet exciton generation at the single polymer chain level is essential for assessing the prospect of current design strategies. Our approach uses single molecule photomodulation spectroscopy to resolve interactions of singlet and triplet populations. This technique ascertains the pulse-induced kinetics of triplet formation through synchronously averaging of the fluorescence emission. Thus, allowing to measure singlet-triplet dynamics intrinsic to the conjugated polymer. In parallel, we utilized the solutions to the probabilistic master equation describing the time-dependent kinetics of triplet formation. Using measured rates from our experiments and numerical simulations from our model we can now count the most likely number of triplets on the single polymer chain. Measuring both poly-3-hexylthiophene (P3HT) and poly-3-hexylselenophene (P3HS) we observe that heavy atom substitution increases the rate of triplet formation yet leads to smaller steady-state triplet population on P3HS compared to P3HT. These result highlights the seemingly un-intuitive consequences of a molecular design to increase triplet formation resulting in less, not more, triplet population for the conjugated polymer.

RMRM 29

Non-reactive binding sites and their role in the $\text{AlVO}_4^+ + \text{CO}/\text{AlVO}_3^+ + \text{N}_2\text{O}$ catalytic cycle

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The mechanisms involved in catalytic oxidation of CO by N₂O promoted by the AlVO₃⁺ and AlVO₄⁺ ions are evaluated using temperature-dependent rate constants and statistical modeling. Reactions were studied from 300 to 600 K using a selected ion flow tube (SIFT) apparatus, and the data compared to statistical modeling of proposed mechanisms previously identified by density functional theory (DFT) calculations. Reduction of N₂O by AlVO₃⁺ was found to take place only by complexation to the Al site; however, attack on the V site also occurred and led to stable association complexes, reducing the overall efficiency of the reaction. As the AlVO₃⁺(N₂O) complex resulted from approach on the V site, it did not block the reactive Al site and was observed to further react with N₂O to form AlVO₄⁺(N₂O). The oxidation of CO by AlVO₄⁺ was found to proceed solely by activation on the Al–O site; however, isomerization of complexes formed with CO initially complexed to the V site were found to add to the reactivity, especially at lower temperatures.

RMRM 30

How cerium oxide traps high concentrations of thermally stable platinum single atoms

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Single atom catalysts have attracted attention because of improved atom efficiency, higher reactivity and better selectivity for a range of catalytic reactions. A major challenge is to prevent these atoms from agglomeration while maximizing their density,

especially when catalysts are subjected to elevated temperatures. Here we investigate the factors responsible for the strong binding of Pt to ceria. We used a combination of surface sensitive techniques, density functional theory, x-ray absorption spectroscopy and electron microscopy to demonstrate that ceria can support Pt single atoms at high concentrations (3 wt% Pt), without forming any clusters or 3D aggregates. The mechanism of trapping involves a reaction of the mobile PtO₂ with under-coordinated cerium cations present at step edges, allowing Pt to achieve a stable square planar configuration. This finding paves the way for a better understanding of catalyst sintering and regeneration which occurs through the emission and capture of mobile single atom species.

RMRM 31

Infrared photodissociation spectroscopy of the H₆⁺ cation in the gas phase

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H₆⁺ is generated in a supersonic expansion via pulsed electrical discharge of hydrogen. H_n⁺ clusters are extracted into a reflectron time-of-flight mass spectrometer and probed with infrared photodissociation spectroscopy (IRPD) in the 2050 – 4600 cm⁻¹ region. H₆⁺ was mass selected and found to have three distinct photodissociation channels by loss of one hydrogen atom, one hydrogen molecule or both. Each channel results in different spectra as a result of mode specific dissociation channels. The ground ²D_{2d} state is 4 kcal/mol lower in energy than the ²C_s state with a 7 kcal/mol barrier. The three H_m⁺ (m=3,4,5) fragment channels may be a result of rapid interconversion between the two states with a small barrier, after IR photon absorption.

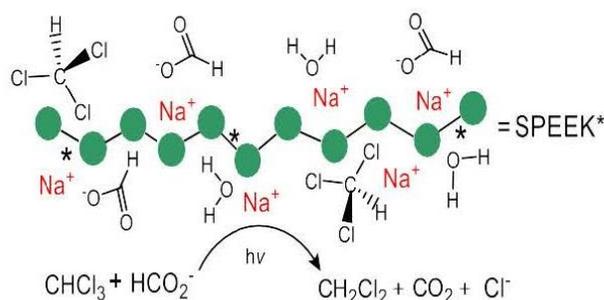
RMRM 32

Photoreduction of CHCl₃ in aqueous SPEEK/HCO₂⁻ solution involving free radicals

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Exposure of sulfonated poly(ether etherketone), SPEEK, in aqueous solutions to 350 nm photons induced reduction of CHCl₃ to CH₂Cl₂ and chloride ions in the presence of HCO₂H/HCO₂⁻ buffers, or poly(vinyl alcohol), PVA. The kinetics of the SPEEK-sensitized photoreaction was characterized by quantum yields of halide ion formation, $\phi(\text{Cl}^-)$, evaluated from *in situ* determinations of [Cl⁻]. Particularly efficient reductions took place when formate buffers serve as H-atom donors in the absence of air and with excess CHCl₃. The linear dependence of $\phi(\text{Cl}^-)$ on the inverse square root of the light intensity together with a post-irradiation formation of Cl⁻ in the dark indicated that the

CHCl₃ photoreduction occurred via a chain process. EPR determinations identified the α-hydroxyl radical of the SPEEK and CHCl₂ as chain carriers. Most of the kinetic findings were rationalized in terms of a free radical mechanism where CHCl₂ radical dimerization acted as termination step. Photoreduction of CHCl₃ was also detected in the presence of air albeit with lower quantum efficiencies. Observations made during post-irradiation experiments indicated that a chain process was also operative under such conditions.



RMRM 33

Size effect of gold nanoparticles on graphene quantum dots fluorescence intensity

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Graphene quantum dot (GQD) is a new type of nanomaterials, which has gained great attention in many application fields, such as biological, optoelectronic, and energy-related fields. They have some unique properties, such as strong and stable fluorescence emission, good chemical inertness, outstanding biocompatibility, low toxicity, and low-cost preparation; Therefore, they have been applied in various biosensors as “fluorophores” Gold nanoparticles (AuNPs) are good quenchers to many organic fluorophores as well as GQDs. However, very limited studies have been focused on the mechanism of the AuNPs quenching on GQDs. This study will broaden the application fields of GQDs, especially in bioanalytical field and biosensor design.

RMRM 34

Facile synthesis of graphene quantum dots and their applications in bioimaging

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Graphene Quantum Dots (GQDs) are a kind of 0D materials that have been attracting tremendous interests in biomedical and bioanalytical fields due to their excellent properties such as high photostability, tunable emission, great biocompatibility, etc. In this work, we have successfully synthesized nitrogen-sulfur modified GQDs using a one-pot hydrothermal reaction. The reaction is simple and fast and the synthesized GQDs showed a lattice spacing of 0.286 nm with an average size of 3.26 ± 1.30 nm. Meanwhile, GQDs showed excellent photostability, thermo-stability and chemical stability under different temperatures and metal ions. Finally, two implementations, cell imaging and gold nanoparticle detection, demonstrated the applications of the GQDs. It is anticipated that the GQDs would have promising applications in the field of biosensing and bioimaging.

RMRM 35

Efficiency enhancement of anaerobic digester in microbial fuel cell through use of *R. Albus*

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The current study has been undertaken to examine the beneficial effect in the power output of a microbial fuel cell (MFC) by adding cellulolytic bacteria *Ruminococcus albus* (*R. albus*) into the anodic chamber. Mediator-less H-type MFCs were set up where the anode chamber contained anaerobic digester microorganisms as inocula on finely ground pine tree (Avicel) at 2% (w/v) and the cathode chamber of 10 mM phosphate buffered saline conductive solution, both separated by a cation exchange membrane. The functioning of the MFCs for generation of electrical power and the amounts of gaseous byproducts was monitored over a 9 day period. The addition of cellulolytic bacteria caused an increase of average power density from 7.9 mW/m² to 19.5 mW/m², about 245% increase over a 9 day period. For both groups of MFCs; with *R. albus* and the control, the head space gases collected were methane and CO₂. While the methane:CO₂ ratios were found unchanged at 1.7:1 throughout the 9 days of observation, the total gas production increased from 248 mL to 319 mL due to the presence of *R. albus* addition. This study confirms that whereas the biocatalytic activity of anode microbial population determines the energy production, the addition of external cellulolytic bacteria into anode microbial population can improve and extend the biomass utilization.

RMRM 36

Silver nanoparticles synthesis in ionic liquids

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Silver nanoparticles, known to display broad-spectrum antimicrobial properties, have now been incorporated in a wide range of household items. Silver nanoparticles also display strong optical sensitivity through surface plasmon resonance, which has been used towards the development of biosensing applications. Here, silver nanoparticles were prepared from the reduction of silver nitrate with sodium borohydride in ionic liquids (ILs), with citrate ion as the stabilizer. The effect of IL structure and concentration on the formation and stability of silver nanoparticles was studied.

RMRM 37

Progress report on the use of viscometry in DNA-drug interactions

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It has been shown that aminoacridines intercalate double-stranded DNA forming a ternary complex with topoisomerase II. The result inhibits the reannealing process during supercoiling. Because of this, we explored different aminoacridine derivatives. O-Benzyl-N-(9'-acridinyl)hydroxylamine, for example, can be synthesized in high yields using three reactions starting from commercially available N-hydroxyphthalimide. The viscosity of the DNA drug solution was tested using a 1:1 molar ratio of DNA:O-benzyl-N-(9'-acridinyl)-hydroxylamine at pH 6. The viscosity was compared to the initial viscosity of the DNA, the ΔT_m values, and MTT assay.

RMRM 38

Microwave assisted synthesis of 3,6-disubstituted pyrazolo[1,5-a]pyrimidines and progress toward discovery of anticancer activities

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Research in our group has focused on the synthesis of several different types of protein kinase inhibitors. A recent emphasis has been synthesis of 3,6-disubstituted pyrazolo[1,5-a]pyrimidines a molecular scaffold known to inhibit VEGFR2, a receptor tyrosine kinase (RTK) overexpressed in a variety of cancers. We have prepared several 3,6-disubstituted pyrazolo[1,5-a]pyrimidines using a microwave assisted approach that greatly streamlines the previously published synthesis. We will present background information relative to the known antiangiogenic activity of this class of compounds together with an overview of the progress we have made in preparing new analogues. Two of our analogues selectively inhibited melanoma cell line MDS-MB-435 and leukemia cell lines K-562 and SR by 50-70% at 10 μ M concentration.

RMRM 39

Efficient microwave assisted synthesis of N'-aryl/(alkyl)-substituted N-(4-hydroxy-6-phenylpyrimidin-2-yl)guanidines: Scope and limitations

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Treatment of N-[(4-hydroxy-6-phenyl)pyrimidin-2-yl]cyanamide with 1° alkyl or arylamines in isopropyl alcohol for only 10 minutes at 110–120 °C under microwave conditions gave the corresponding N'-alkyl(aryl)guanidine derivatives in excellent yields (65–84%). Isolated yields were greatest when > 1.0 equiv. of amines were employed, but excellent results were also obtained when aryl and alkylamines were reacted with a more atom-economical loading (1.0 equiv.; 70% and 72% ave. yields, respectively). Arylamines with either highly electron withdrawing substituents (e.g. CO₂H) or pi-deficient heterocycles (e.g. variously substituted aminopyridines) did not work well under these conditions, and reaction with ureas and/or amino acids did not give detectable products. Work-up was exceedingly simple, and involved simple collection and washing of product on a sintered glass funnel. Products were obtained in analytically pure form and required approximately 1 h to prepare, start to finish.

RMRM 40

Synthesis and characterization of high mobility, side-strapped phthalocyanines for organic photovoltaics

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Phthalocyanines are a class of dyes that have been extensively studied as semiconductor materials for organic photovoltaics (OPVs). They are primarily attractive as the p-type semiconductor in heterojunction OPVs due to their relatively high lying HOMO energy level. Furthermore, their strong Q-band absorbance (680 nm) renders them as promising materials for near infrared absorbing OPVs. Two major limitations of Pcs as active layer components in OPVs include: 1. their limited solubility in common organic solvents necessary for the formation of thin films and 2. the low charge mobility due to weak pi-pi interactions. New two-fold symmetric, "side-strapped" Pcs have been developed with extended conjugation that allows for greater pi-pi interactions and substituents along one axis to minimize pi blocking while ensuring solubility. Using conductive mode atomic force microscopy measurements we have found that these side-strapped Pcs exhibit hole mobility up to 0.97 cm²V⁻¹s⁻¹, which is among the highest values recorded for solution processable Pcs. This research aims to further improve the hole mobility via the synthesis of more side-strapped Pcs with various "straps" and solubilizing groups.

RMRM 41

On the reduction chemistry of imidazolium salts

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This work discusses the redox properties of several pyridine-based imidazolium salts widely used as N-heterocyclic carbene (NHC) precursors in catalytic frameworks. Although various quinone-annulated redox-active NHCs have been metallated and previously reported in catalytic contexts, no study has yet described the redox properties of the more common imidazolium-based precursors. Our study shows that the ligand framework itself can harbor electron equivalents, thus raising the possibility of the use of electrochemical methods for the generation of free-N-heterocyclic carbenes from their imidazolium salts. We use Diffusion Ordered Spectroscopy (DOSY) and Normal Pulse Voltammetry to determine a 1e⁻ reduction associated with each of the N-heterocyclic imidazolium precursor cores. We further discuss our efforts in the generation and capture of free NHCs through electrochemical methods.

RMRM 42

Olfactory receptor mediated repellency of linalool, geranyl acetate, and EBF in two drosophila species

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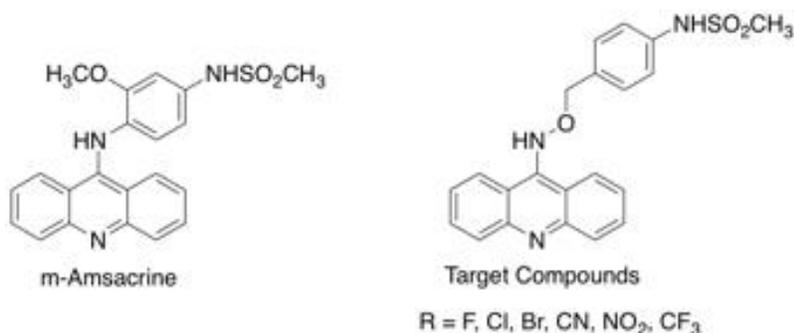
Spotted winged drosophila (*Drosophila suzukii*, also known as SWD) is a serious pest that consumes various fruit crops for its own species nourishment. These insects are able to smell various chemicals in the environment. Some of these chemicals are attractive to SDW, and others are repellents. It is critical to identify strong repellents in order to dissuade these pests from inflicting damage on agro systems. Plant essential oils have been shown to exhibit high repellency against arthropod species. To identify repellents against SWD, plant essential oils will be tested in T-maze trap assay. Using single sensillum recording, we recorded responses to plant essential oils from basiconic sensillum (ab7) on the antennae. The chemicals utilized in this study include E-β-Farnesene (EBF), Linalool, and Geranyl acetate (GA). A series of concentrations of the tested compounds will be used in the behavioral assays to generate dose-response curves. The control chemical is DMSO. These experiments will allow us to determine whether these compounds elicit repellency and the potency of repellency. Our findings will further increase the knowledge of *Drosophila suzukii* preference.

RMRM 43

Progress report on the preparation of O-benzyl-N-(9'-acridinyl)hydroxylamines

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Leukemia is a devastating disease common in children and teens that can be treated with the chemotherapy drug amsacrine (m-AMSA). This compound intercalates DNA, and upon binding of Topoisomerase II, creates a ternary complex. Although m-AMSA has proven to be an effective pharmaceutical agent, it has a short half-life in the human body limiting the molecule's effectiveness as an anti-cancer agent. In addition, because this molecule denatures quickly after entering the human body, larger dosages are required with subsequent worsening of harmful side effects that the patient endures over the course of treatment. However, if the molecule were stabilized and its half-life extended, such harmful effects of chemotherapy treatment could be mitigated, improving the patient's quality of life. This short life is due to the rapid hydrolysis of the C9-N bond. We envisioned the insertion of an oxygen atom adjacent to the nitrogen atom in an effort to extend the compound's half-life. Herein, we report the preparation of a series of O-benzyl-N-(9'-acridinyl)hydroxylamines that address this concern. Electron-withdrawing groups are particularly useful in that they draw electron density away from the oxygen and force the formation of an imine in the molecule that resists hydrolysis. The effectiveness of the specific groups will be measured by thermal denaturation and MTT assays.



RMRM 44

Aldol approach to efficient, stereoselective synthesis of structurally diverse beta-lactones

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Proteasomes are protein complexes that can be found in the nucleus and the cytoplasm of all eukaryotic organisms and some bacteria. These cellular structures are responsible for degrading damaged or unneeded proteins. The inhibition of proteasome activity is a

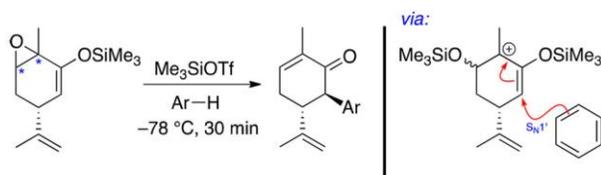
powerful strategy for the treatment of multiple myeloma, a cancer of plasma cells. Several classes of proteasome inhibitors (PI's) consist of short peptides bearing electrophilic pharmacophores. Although, there are currently three clinically approved proteasome inhibitors (Bortezomib, Carfilzomib, and Ixazomib) for the treatment of multiple myeloma, the development of a potent inhibitor with minimal side effects associated with non-specificity remains a challenge. Beta-lactone-PI's are interesting and potentially useful drugs that act by competitively acylating the active site of the enzyme. The efficient synthesis of structurally diverse beta-lactones is important for structure-activity relationship studies. Our currently used method for the synthesis of beta-lactones involves a chiral auxiliary-controlled asymmetric alkylation, diastereoselective chlorination, and lactonization as key steps. Despite its usefulness, this method has some limitations such as narrow substrate scope, potential low yields and reproducibility, etc. An alternative synthetic approach for the stereoselective construction of beta-lactones will be developed. The key step of the proposed synthetic route will control the stereochemistry of the beta-lactone using an asymmetric aldol condensation reaction mediated by a thiazolidinethione chiral auxiliary. The obtained asymmetric aldol products will be transformed into beta-hydroxy acids and elaborated into the target beta-lactones via cyclization reactions. This study will contribute to the study of proteasome inhibition activity and its potential applications in anti-cancer drug development.

RMRM 45

Lewis-acid-mediated union of epoxy-carvone diastereomers with anisole derivatives: Mechanistic insight and application to the synthesis of non-natural CBD analogues

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The use of trimethylsilyl trifluoromethanesulfonate as a mild means to unite epoxy-carvone silyl ethers with anisole derivatives to yield products that are structurally similar to the CBD scaffold is reported. Importantly, unlike related methods, this process can utilize both epoxy-carvone diastereomers and does not require the use of air/moisture-sensitive organometallic reagents. Several examples of aryl nucleophiles as well as mechanistic insight based on *in silico* computational analysis are presented.



RMRM 46

Mechanism of hop oil isomerization

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In the beer industry, one of the most essential ingredients is hops. Hop oils contain lupulones and humulones, commonly known as hop β -acids and α -acids. Since humulone is the main contributor to the bitterness in beer, we decided to focus solely on humulone. Humulone undergoes an isomerization during the brewing process to form the bitter bacteriostatic compound found in beer. We have explored this reaction using UV-vis spectroscopy and polarimetry at various temperatures and pH's to elucidate the mechanism of the process. Our results indicate that Mg^{2+} binds to humulone resulting in structural changes that promote the isomerization via an acyloin-type ring contraction. The kinetics, thermodynamics, and a proposed mechanism of the reaction will be presented.

RMRM 47

Oximation of benzalacetone

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More than 100 million adults in the U.S. live with diabetes or prediabetes according to the Centers for Disease Control and Prevention (CDC). To put this number in perspective, nearly 1 in 4 adults lives with diabetes. The CDC research found that the majority of people diagnosed with diabetes are minorities. A more efficient and cost-effective method to produce derivatives of isoxazolines used in antidiabetogenic drug research can involve a simple oximation-cyclization reaction. The results afford the 3,5-disubstituted isoxazoline ring system found in ISO-1, a known antidiabetogenic compound. Herein, we report the synthesis of benzalacetone oxime, the precursor to this cyclization. The method and mechanism will be discussed.

RMRM 48

Synthesis and characterization of Iron containing MOFs for environmental remediation

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Metal Organic Frameworks (MOFs) are hybrid inorganic porous materials made up of an organic ligand called a linker and cluster of metal atoms/ions called secondary building unit. Due to their high surface area and controllable structure including porosity, MOFs have received the attention of many researchers for a wide range of applications such as catalysis, proton conductivity, drug delivery, waste water treatment, CO₂ capture, sensing, gas storage and separation, etc.

Wastewater treatment, CO₂ reduction is a focus of the research community worldwide for the serious impact on the environment (for example, global warming) as well as on the health of living organisms, including humans. There are several methods developed already but most of them are cost prohibitive, time consuming and inconvenient on plant scale. So, it is necessary to solve this issue on an urgent basis, which must be cost effective, and easy to implant on industrial scale. It is well known that, MOFs structure, properties and porosity can be tailored using various parameters such as type of metal and ligand, pH, temperature, solvent etc. Due to its controlled features and high surface area, MOFs showed promising efficiency for both water purification and CO₂ capture applications. However, there is still wide space for optimization in efficiency and development of methods to use the MOFs more efficiently.

In the current study, we focused on the synthesis and development of iron containing MOFs for environmental remediation. In this regards, we have synthesized several Fe-containing MOFs under solvothermal conditions in DMF, H₂O and EtOH at different temperatures for 72hrs. The obtained MOFs were investigated by powder X-ray diffractometer (PXRD), Scanning Electron Microscopy (SEM), IR, Thermal Gravimetric Analysis (TGA) etc.

The characterization result shows that, the prepared samples are crystalline in nature with good thermal stability; the other characterization results are in progress. We have also planned to measure the magnetic study, which will be potentially applicable in the method development for water purification.

RMRM 49

X-ray and DFT studies of novel thiobarbituric chromophores with nonlinear optical properties

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The search for new materials with non-linear optical properties is of great interest for photonics and optoelectronics. The large variety of organic chromophore compounds offers exceptional versatility upon design of new materials for non-linear optics applications. Organic chromophores should not only have high optical nonlinearities but also possess good thermal and chemical stability and low optical loss (high transparency). Thiobarbiturate groups are strong electron acceptors because they gain

aromatic stabilization upon reduction. They can be used along with amine group donors for synthesis of molecules with high nonlinear optical activity. Single crystal X-ray diffraction study of series of thiobarbituric acid derivative chromophores is presented. DFT calculations were performed to determine thermal stability on structure and energy dependence for these molecules.

RMRM 50

Evaluation of amyloid- β protein as an antimicrobial peptide in Alzheimer's disease

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Alzheimer's disease (AD) affects more than five million Americans, and the main pathological hallmark of the disease is plaques composed of amyloid- β (A β) fibrils. Currently, the cause of AD is unknown and no treatment is available. However, evidence suggests that AD involves an infectious component. Observations that bacteria and viruses are present within the brain and that pathogenic signatures tend to co-localize with AD pathology have led to a novel hypothesis that A β expression and deposition may be due to its function as an antimicrobial peptide (AMP).

Our research seeks to determine how A β functions as an AMP by investigating the peptide's toxicity toward bacteria using a live/dead assay of membrane permeation via flow cytometry, a metabolic assay of cell viability, and turbidity measurements to quantify the effects of A β on bacterial growth. This will be followed by transmission electron microscopy to examine how bacteria influence fibril formation. Further, studies of the gut microbiome of those with AD have led some to hypothesize that AD may be caused by translocation of pro-inflammatory bacterial components, such as the lipopolysaccharides (LPS) that make up some bacterial membranes. To determine if LPS elicits A β fibril formation, we are going to be creating LPS-containing lipid vesicles to model interactions between gram-negative bacteria and A β .

The role that infection plays in AD is an exciting new approach to investigate the cause of the disease. Studying the interactions between bacteria and proteins involved in the mediation of AD pathology will provide a stronger understanding of the context within which neurodegenerative diseases develop, and this has the potential to lead to better detection and treatments for not just AD, but a wide array of neurodegenerative diseases.

RMRM 51

DLSCORE: Deep Learning model for predicting protein-ligand binding affinities

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The prediction of protein-ligand binding affinities is very crucial for drug discovery research. Molecular docking is widely used in finding initial hits in the early drug discovery stage. Though docking programs have successfully been used for years, they are still not fully reliable. Many physics-based scoring functions are developed over the years. However, machine learning based scoring functions are proved to outperform the traditional scoring functions.

In this study, the performance of an ensemble of the neural networks, trained on the recent release of PDBBind data using Binding Analyzer (BINANA) descriptors, will be presented. The neural networks consist of a varied number of hidden layers with a different choice of network parameters (dropout rate, regularization method, activation function etc.) and were trained using 348 descriptors generated by the BINANA code. We have achieved an R2 of 0.96 for training and 0.79 for our test.

RMRM 52

New Mexico Highlands University Chemistry Club

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The New Mexico Highlands University Chemistry Club is an active club that is certified through the American Chemical Society. The mission of the club is to engage, expose, and draw students toward STEM degrees especially through Chemistry. The club has even received recognition on the NMHU campus by being named "Club of the Year" in 2017. Throughout the years, one of the main focuses of the club is to plant the idea of science and chemistry into the Las Vegas youth. The club has done multiple outreach projects with children ranging from 4 years of age all the way to high school students. By exposing the students to new ideas of thinking and giving them visual experiments, though small, leaves them with the impression that science is both interesting and informative. The club has collaborated with organizations such as MESA, Bright Beginnings Child Development Center, Memorial Middle School, West Las Vegas High School and Middle School, and the Mora Independent School District. Another aspect of the club is to expose members to all types of careers in chemistry. The club has been on field trips to Sandia National Lab and Los Alamos National Labs. These trips allowed students to see all of the possibilities that a Chemistry or STEM degree can offer. The club will be traveling in the 2019 Spring Semester to Los Alamos to give some of the new members an opportunity that they could have never experienced.

In the future the club plans on doing outreach to local high schools to raise the

importance of attending college and to even show students all of the job and life opportunities that are available with a STEM degree.



The 2018-2019 Chemistry Club Members and Advisors

RMRM 53

Lobo Chemistry Club: American Chemical Society student chapter at University of New Mexico

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The Lobo Chemistry Club, located at the University of New Mexico Albuquerque Main Campus, is an active and thriving Student Chapter of the American Chemical Society. Currently, there are 20 active members with majors in Biology, Biochemistry, Chemistry and Chemical Engineering. Members participate in a variety of outreach activities, including magic shows, chemical demonstrations and educational outreach, on the UNM campus and in the Albuquerque area. The target audience of these outreach activities consists mainly of elementary and high school students. From this, they are exposed to basic chemistry concepts and the scientific method in the hopes of generating interest towards the scientific community. Members are also able to network with other undergraduate students and become involved in current research opportunities occurring at the University of New Mexico. Lobo Chemistry Club provides chemistry students an enriching experience for their undergraduate careers through involvement with the local and STEM communities at the University of New Mexico.

RMRM 54

Get involved with the ACS Division of Chemical Education

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Want to know more about the Division of Chemical Education, learn how you can get more involved with DivCHED, learn about educational resources for chemistry, find out how to apply for travel awards, or meet and network with people from your region, nationally, and around the world who have similar interests? The Division of Chemical Education aims to serve as a means of focusing and enhancing the interest and efforts of all constituencies involved in the teaching and learning of chemistry at every level. If you have an interest in chemistry education, we want you involved in DivCHED. Come visit our poster to learn more about the Division and all we have to offer, meet representatives from the Division, and let us know what you think the Division can do to better meet the needs of our members.

