ACS Local Section
Portland

American Chemical Society

2022 Portland Section ACS Poster Symposium

Robertson Life Sciences Building
2730 S Moody Ave
Portland, OR 97201

Hosted by
the Portland Section
of the American Chemical Society

Saturday October 29, 2022
11 AM to 1 PM

Portland State
UNIVERSITY

The ACS Portland Local Section Poster Symposium

This year's Symposium takes place Sunday, October 29, 2022, in the Portland State University's waterfront Robertson Life Sciences Building from 11 AM-1:00 PM.

The Poster Symposium showcases high school, undergraduate, and graduate research projects in seven major divisions: Analytical, Biochemistry, Inorganic, Materials, Organic, Physical and Promoting Inclusion.

Free food and beverages will be provided for all present!

There will be prizes of $100 for best poster by grad students and others in each category.

Acknowledgments

The Portland Section ACS acknowledges the teachers, mentors, and students who have worked to bring these posters to this year's Poster Symposium, which shares its venue with the Linus Pauling Medal Symposium. The Pauling Medal Symposium follows the Poster Symposium at 1 PM.

About Us

The Portland Section of the American Chemical Society was chartered in 1961. It is a mix of industrial and academic chemists, committed to providing support for professional chemists as well as chemistry students throughout the Section area, which includes 13 counties in Southwest Washington and Northwest Oregon.

Sponsors

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Abstracts

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Undergraduate Students

Biochemistry

1. The Distinct Impact of Metal Ions in Beta-Amyloid Aggregation and Alzheimer's Disease Mechanisms

Schroeder, A. N. (**schralys@oregonstate.edu**, Oregon State University); Mackiewicz, M. R.

Faculty Mentor: Dr. Marilyn Rampersad Mackiewicz, Oregon State University, Department of Chemistry, Corvallis, OR

Alzheimer's Disease (AD) is the sixth leading cause of death in the US and the most common cause of dementia worldwide. Yet, no methods to cure nor reverse the neurodegenerative disease's effects exist due to AD pathology's elusiveness. The metal hypothesis of AD states that CuI/II, ZnII, and FeII/III ions bind to beta-amyloid peptides, forming aggregates that disrupt membranes or generate ROS through redox cycling in the presence of CuI/II or FeII/III and a reducing agent. These effects ultimately lead to weakened synaptic cell signaling or neuronal cell death. Though controversial, depending on the experimental conditions and beta-amyloid species, inhibitory effects are also reported. Namely, CuII ions are known to inhibit aggregation and fibrillation by ZnII, yet other studies have shown that ZnII aids in attenuating non-toxic plaque formation and is potentially neuroprotective. These contradictory results necessitate more controlled studies to uncover the driving mechanisms by which metals promote beta-amyloid aggregation and ROS production. Here we present studies using fluorescence anisotropy and UV-Vis spectroscopy to demonstrate the effects of exogenous metals on beta-amyloid and metallated-beta-amyloid These studies can be utilized to characterize the distinct roles of each metal species and identify significant therapeutic targets to promote AD drug discovery.

2. Predicted Three-Dimensional Structure of TAS2R50 Including Associated G-Protein and Agonists

Clancy, D. (**dclancy19@georgefox.edu,** George Fox University); Goddard, W.; Kim, S.; Park, A.

Faculty Mentor: William A. Goddard, Caltech

Bitter taste receptors (TAS2R) are a member of the expansive G-protein coupled receptor (GPCR) super family of proteins. There are 25 different TAS2Rs found dispersed around the human body in both smooth and cardiac muscle cells. This includes TAS2R50, which has been associated with cardiovascular diseases. So far, there is no known experimental structure for TAS2R50. However, the Goddard group has developed a complete sampling method (GEnSeMBLE) for predicting the 3-D structure of these GPCRs. Bitter taste receptors TAS2R4, TAS2R5, and TAS2R14 were used as templates for GEnSeMBLE because they have known experimental structures. There are two known ligands for TAS2R50, Amarogentin and Andrographolide, which were both prepared for docking. This study not only provides an atomistic understanding of the mechanism for the TAS2R50 bitter taste receptor, it also identifies new drug candidates to treat cardiovascular diseases. The best structures will be experimentally validated by collaborators at the University of Arizona and the University of Southern Florida. Future studies will optimize the binding to enable experimental investigations into its role in cardiovascular disease

3. Antibiotic activity by an unknown Streptomycete from an archeological site on Mallorca

Bright, H; (**brighth23@up.edu**, University of Portland); Hoffman, A.

Faculty Mentor: Professor Angela Hoffman, University of Portland, Chemistry Department, Portland, OR

The purpose of this study is to isolate new antibiotic and anti-pathogenic compounds from soil bacteria excavated from an archaeological site in the ancient Roman city of Pollentia on the island of Mallorca, Spain. Bacteria were collected from three to four feet underground, isolated and cultured onto yeast or potato dextrose media. Bacteria products were extracted from liquid cultures and activity was tested against Staphylococcus aureus, Escherichia coli, and Pythium ultimum, and fractionated on silica TLC and flash chromatography with hexane, ethyl acetate, and methanol. One promising culture (OIV-4d) had significant activity against S. aureus, E. coli, and P. ultimum. The second and third rounds of flash chromatography of the

sample had 10 of the 16 fractions were able to inhibit growth of bacteria and P. ultimum. The fractions with the greatest inhibition were further separated using an HPLC with a C-18 column. The bacterium's identification is being identified using DNA extraction and PCR sequencing of the 16s rRNA. Findings from this study suggest that many antibiotics are yet to be discovered.

4. Making Moves: Elucidating the Binding Region of the Dynein IC-2C and Dynactin p150Glued Interaction

Di Nicola, AJ (**ajdinicola@lclark.edu,** Lewis & Clark College); Ancheta, J.; Loening, N.M.

Faculty Mentor: Prof. Nikolaus Loening, Lewis & Clark College, Chemistry Department, Portland, OR

Dynein is a multi-subunit motor protein integral to the transport of molecular cargo throughout the cell. In mammals, dynein only exhibits movement when interacting with the protein dynactin. This interaction is regulated through the binding of the intrinsically disordered intermediate chain (IC) subunit of dynein with the p150Glued subunit of dynactin. Specifically, the single alpha helix (SAH) region of dynein IC (residues 1-44) interacts with the coiled-coil 1B (CC1B) region of p150Glued (residues 358-555). Previous research has only narrowed down the CC1B residues that directly interact with IC to residues 382-531. To further narrow down which CC1B residues play a significant role in dynein-dynactin binding, we used nuclear magnetic resonance (NMR) spectroscopy to measure the intermolecular paramagnetic relaxation enhancements (PREs) of 15N-labeled IC-2C when interacting with paramagnetically-labeled p150Glued CC1B single-cysteine mutants. Preliminary PRE NMR results suggest the IC-2C1-96 binding site on CC1B is close to residue 434. However, preliminary isothermal titration calorimetry (ITC) data indicate differences in IC-2C1-96 binding to p150Glued382-531 compared to paramagnetically-labeled p150Glued382-531 mutants. Additional research is needed to further constrain which residues on CC1B are essential for binding IC-2C and to determine the extent to which the single-cysteine mutations and paramagnetic label affect this binding interaction.

5. Varying doses of Ibuprofen induced differing effects on memory, cognitive flexibility, and GluN1 and C-terminal splice variants expression across sex and age

I. Abou-Seada (**abouseai@oregonstate.edu,** Oregon State University); M. Frischman; K. Kim; D. Kulkarni; E.; Sackinger; K. Magnusson

Faculty Mentor: Dr. Kathy Magnusson, Oregon State University, Department of Biomedical Sciences

Ibuprofen is a commonly used non-steroidal anti-inflammatory drug. Drugs like this reduce risk of Alzheimer's disease development, but interventional studies have neutral or negative impacts on disease progression. In the current study we tested the effects of varying ibuprofen doses on cognitive functions across aging in male mice and across sexes in young mice. To do this both male and female young mice (2 month; N=6) and male older mice (23-24 month; N=6-7) were administered NIH-31M chow with either 0, 375, or 1000ppm of ibuprofen. Memory and cognitive flexibility were tested with the use of the Morris water maze, and results were analyzed based on dosage and separately for age or sex. Results indicated that at high dosages (1000ppm or 5.8 pills/day for humans) ibuprofen impaired long-term memory in older males. Ibuprofen was found to improve cognitive flexibility and other functions in young males, but had little effect on females. Western blotting was then used to try to relate these behavioral results with the altered expression of all GluN1 subunits or C-terminal splice variants of the N-methyl-D-aspartate (NMDA) receptor in synaptic and extrasynaptic membranes of the frontal cortex and hippocampus. No significant differences in all GluN1 subunits or splice variants expression were seen in frontal cortex synaptic membranes. Frontal cortex extrasynaptic membranes: Young females expressed all GluN1 subunits at higher levels than young males when fed 0 ppm ($p=0.04$). For young males, 1000ppm ibuprofen increased GluN1 subunit expression compared to 0 ppm ($p=0.05$). In older males, we observed that 375 ppm of ibuprofen increased C1 ($p=0.02$) and C2 ($p=0.04$) splice cassette expressions compared to those fed 0 ppm. Hippocampal synaptic membranes: Young males fed 375 ppm ibuprofen had significantly increased C2 splice cassette expression when compared to both 0 ($p=0.03$) and 1000 ppm ($p=0.02$). This bell-shaped curve pattern was also evident in the GluN1 subunit expression for young males. Interestingly this bell-shaped pattern also appeared for the C1 and C2 splice cassettes in frontal cortex extrasynaptic membranes, but for older males not younger ones. The behavioral results indicated that ibuprofen use, especially in older males, can be detrimental to long term memory. These results further suggested that ibuprofen may impact cognition not only by affecting GluN1 subunit expression, but also by altering splicing and trafficking. It is important to determine the extent to which ibuprofen causes these NMDA receptor changes, specifically in older males, due to ibuprofen's use by so many of the elderly population.

6. In silico development of an agonist model for S1P2

Daszuta, Lela (**daszuta24@up.edu**, University of Portland); David Hoang; Alexis Hazim; Daniel Osborne

Faculty Mentor: Professor Daniel Osborne

S1P2 is a type A G protein-coupled receptor that is unregulated in a variety of tumors. Mouse knockout studies have demonstrated that activated S1P2 is positively correlated with the prevention of tumor cell migration, invasiveness and angiogenesis. We have utilized the crystal structure of S1P2 with its associated G protein to explore the putative binding pocket of S1P. We have compared the amino acid mutagenesis studies of Osborne and coworkers to our current model. We have identified a triad of amino acids that ultimately result in a strong ion paring interaction between R108 and the negatively charged phosphate moiety of S1P. We will present in silico mutagenesis results that will guide experiments in fully validating the S1P2 agonist binding pocket. Our model has also proven useful in proposing novel scaffolds that exhibit the proper conformation and charge properties for further development of anti tumor lead compounds.

7. In silico discovery of SIRT3 inhibitors as anti tumor lead compounds

Khoi Hoang, (**hoangk24@up.edu**, University of Portland); Lela Daszuta; Daniel Osborne

Faculty Mentor: Professor Daniel Osborne

SIRT3 is an NAD+ dependent deacetylase that is localized in the mitochondria. Numerous natural products and synthetic lead compounds have shown the ability to function as pan-inhibitors of SIRT1-3. Knockout studies have implicated selective and potent SIRT3 in the effective treatment of squamous cell carcinomas of the head and neck. We have built a computational model of SIRT3 based on different synthetic ligands and identified two major binding poses for 16 inhibitors. We have identified 12 residues for computational and experimental mutagenesis. Using a computer algorithm, we have used discovered and designed 5. novel scaffolds for synthetic efforts.

8. Hybrid lipid-coated Silver Nanoparticles are Sticky on Fabrics

Fischer, S. (**fischeso@oregonstate.edu**, Oregon State Univeristy)

Faculty Mentor: Marilyn Mackiewicz, Oregon State University, Chemistry Department, Corvallis, OR

Silver nanoparticles (AgNPs) have been widely used in over 1400 commercial applications because of their great antimicrobial properties and are found in everyday items such as food packing, UV-protectants, makeup, clothing, and medical devices such as stents, gauze, and surgical tools. AgNPs can eliminate body odor in clothing, as well as reduce biofilm formation on implants, making them a versatile and effective solution for unwanted bacterial growth. There is also a significant interest in harnessing the X-ray attenuation properties of AgNPs for use as X-ray imaging agents or tags on medical devices. Consequently, there is a critical need for the development of not only safe AgNPs, with minimal or no Ag+ ion release, but also effective deposition and retention on their applied surfaces. In this presentation, we will discuss the design of AgNPs with a hybrid lipid-coating with controlled Ag+ ion release, as well as their deposition and retention on surfaces for potential use as antimicrobial agents, X-ray tags, or conductive inks. We will discuss methods of deposition and adherence onto surfaces using UV-Vis spectroscopy and scanning electron microscopy after exposure to conditions that damage or remove of AgNPs from surfaces.

9. Mechanistic Investigation of an Ir-Ru catalyst for Formic Acid Dehydrogenation

E. Gregor (**begregor@reed.edu**, Reed College); C. Tong; M. Nguyen; I. Rettig; P. Truong; M. Bowring

Faculty Mentor: Prof. Mir Bowring, Reed College, Chemistry Department, Portland, OR

We are investigating the mechanism of a promising Ir-Ru bimetallic catalyst for formic acid dehydrogenation (FAD). The reported reaction has an unusually large kinetic isotope effect of 40, which has been attributed to proton tunneling during protonolysis of an Ir-H bond. We present preliminary mechanistic studies of this catalytic system. We have isolated proposed intermediates and tested their reactivity and observed kinetic profiles for catalysis. We have compared the properties of 7 related complexes computationally. Further, we have synthesized monometallic and Ir-Zn analogues of the original catalyst to

understand the role of Ru. Overall, our results suggest that the mechanism is more complex than previously believed.

Materials Chemistry

10. Enlighted: Silver Nanoparticles Undergo Shape Transformations in the Presence of Light EXCEPT when coated with Hybrid Lipid Membranes

Nieves Lira, C. (**nieveslc@oregonstate.edu**, Oregon State University); Mackiewicz M.

Faculty Mentor: Dr. Marilyn Mackiewicz, Oregon State University, Chemistry Department, Corvallis, OR

Silver nanoparticles (AgNPs) are extensively used for their antimicrobial properties in commercial products designed for UV-blocking or food packaging. They are also being explored for use in biomedical applications such as drug delivery, X-ray Computed Tomography Imaging, and optical imaging. Because of their high demand, over 500 tons of AgNPs are produced annually and there is a need for tuning and controlling the shape and size distribution, their rate of silver ion release, and the stability of the materials for intended applications. While there are many chemical, physical, and biochemical methods for producing AgNPs, there is still difficulty in producing samples of homogenous shape and size. Here we present an accessible, fast, and effective synthesis that guarantees the homogeneity of triangular plates with visible light. This technology can transform a variety of differently shaped nanoparticles, with citrate and PVP coatings, into sharp triangular plates. The only protection against this light-driven transformation is the presence of a hybrid-lipid membrane that shields the AgNPs from intense light and heat exposure without shape change or oxidation. We will present UV-Vis spectroscopy and transmission electron microscopy to characterize the shape transformation and the stability of the hybrid lipid-coated AgNPs. The light-resistant characteristics of AgNPs will also be presented to identify newfound features of AgNPs that allow for a broader range of applications. These studies will provide valuable information on the resistance of AgNPs to light from their surroundings while also providing a mechanistic understanding of factors governing shape transformation.

11. From Blue Pigment to Green Technology: Properties and Applications of Fungi-Derived Pigment Xylindein

M.J. Brodeur, (**brodeurm@oregonstate.edu**, Oregon State University); G. Giesbers; R.C. Van Court; S. Robinson; O. Ostroverkhova

Faculty Mentor: Dr. Oksana Ostroverkhova, Oregon State University, Physics Department, Corvallis, OR

Xylindein, a fungi-derived, organic blue pigment, has been shown to demonstrate remarkable charge carrier mobility despite only forming amorphous thin films during characterization. This unique property is something typically reserved for crystalline materials like indigo, and its derivatives. While performing current-voltage measurements of the material when it was used to manufacture transistor devices, redox activity was discovered. Subsequent experiments of xylindein for energy-storage applications resulted in the observation of a wide potential window, demonstrating its feasibility in future energy-storage devices.

12. Computational Analyses of Anthraquinone Isomers for Reversible CO2 Capture and Assessment of Anthraquinone Linkers Embedded in Covalent Organic Frameworks

C. Frederickson (**frederc4@wwu.edu**, Western Washington University); C. Defreest; T. Kowalczyk

Faculty Mentor: Dr. Tim Kowalczyk, Western Washington University, Department of Chemistry, Bellingham, WA

Anthraquinone (AQ) is a redox-active, aromatic organic compound with the potential to adsorb and release gaseous carbon dioxide upon the gain and removal of electrons. Previous research from other groups implemented the use of 9,10-anthraquinone (the common isomer) in CO2 adsorption and desorption mechanisms, while not touching on the use of other anthraquinone isomers. The goals of these computational analyses were to: 1) quantify the effects of charge and carbonyl placement in various AQ derivatives along the reaction pathways of CO2 adsorption and desorption reactions, 2) compare the results of those derivatives to that of anthraquinone, and 3) embed anthraquinones as linkers in covalent organic frameworks (COF)'s and analyze the molecular properties of those COFs to analyze the thermodynamic favorability of different anthraquinone linker groups. Results suggest that the CO2 adsorption/desorption mechanism is not limited to 9,10-AQ, and that other anthraquinone isomers could be more favorable, depending on how the anthraquinone linker is embedded into the COF.

13. Synthesis and Characterization of ZnuA Inhibitor

Agarwal, S. (sidagarwal@reed.edu, Reed College); Daryush GhaneaBassiri (daryushg@reed.edu); Truong, P.

Faculty Mentor: Prof. Phan Truong, Reed College, Chemistry Department, Portland, OR

Bacteria use a metal binding transport system called ATP-binding cassettes (ABC); which are integral for their metabolic and reproductive processes. ABC transport systems are used to transport various metals, such iron, zinc, magnesium, manganese etc., into the bacterial cell. This project uses air-free and water free techniques to synthesize an inhibitor for the ZnuABC complex. The ZnuABC complex is a three component, Zn import system for S. enterica; its components are ZnuA, ZnuB, and ZnuC. It has been shown that di-aryl pyrrole hydroxamic acids can inhibit the release of Zn in ZnuA subunit of ZnuABC complex. It is the objective of this project to synthesize di-aryl pyrrole hydroxamic acids for use in tryptophan fluorescence and saturation transfer difference (STD) NMR experiments to develop facile methods to monitor metal transport in ABC transport systems, such as ZnuABC.

14. An Exploration into Ideal Reaction Conditions for Rhenium-Catalyzed Olefin Metathesis

Palmateer, A. (palmatea@oregonstate.edu, Oregon State University); Moore, S.; Ellis, L.

Faculty Mentor: Dr. Lucas Ellis, Oregon State University, School of Chemical, Biological, and Environmental Engineering, Ph. D.

Polyethylene is the most abundant waste plastic globally, and new technologies are needed to monetize this waste. Tandem dehydrogenation and olefin metathesis is a new potential technology to convert waste polyethylene into olefinic products. This project focused on using olefin metathesis and isomerization to depolymerize simulated polymers to olefinic products. We utilized a heterogeneous rhenium catalyst to perform olefin metathesis and isomerization with the goal of optimizing the chemistry to produce small molecule olefins. To accomplish this, we utilized a high throughput reactor system. A rhenium supported on gamma-alumina catalyst was first pre-treated to produce the catalyst's active form. Reactor cups were loaded with 1-octene, dissolved in n-hexane solvent, which was pressurized with ethylene gas. Temperature, pressure, and time of reaction were varied. Following the

reaction, the liquid products were characterized using GC-FID with a DB-5 column. Conversion, along with selectivity to desired metathesis products, was calculated using area data acquired from the GC, which was converted to units of concentration using a calibration curve. Preliminary results determined we could optimize reaction conditions to increase the concentration of desired products, but further experimentation is needed to confidently define the full effect of reaction conditions on metathesis.

15. Computational and Experimental Analysis of Warfarin and Derivatives

Edward Danielyan (**Danielya23@up.edu**, University of Portland); Khoi Hoang; Edward Valente; David Magers; Daniel Osborne

Faculty Mentor: Professor Daniel Osborne, University of Portland, Department of Chemistry and Biochemistry

Warfarin is an anticoagulant drug that exists in over forty tautomeric forms. We have synthesized warfarin an associated derivatives and have used 400 MHz 1H NMR to determine the mole percents of the three major isomers: open chain, cis hemiketal and trans hemiketal. We have subjected each of these major isomers to DFT computations using the M962x functional and ccPDZ basis set to determine rank energies of various derivatives in different implicit solvating models. We present our theoretical and experimental results and describe the effect of steric bulk on hemiketal formation.

Physical Chemistry

16. Synthesis and Characterization of Copper Nanowires on Electrode Surfaces using Reduction Chemistry

Abdellatif, Malik (**abdel4@pdx.edu**, Portland State University)

Faculty Mentor: Dr. Shankar Rananavare

Copper nanowires are functional electrodes that exhibit superior electrical conductivity and mechanical flexibility. These nanowires play an important role in several scientific and engineering applications including solar cell production, LED, medical imaging, and renewable energy. Copper nanowires have been synthesized in an environmentally friendly way through the common reduction chemical reaction of copper (II) nitrate as a precursor, ethylenediamine as a growth directing agent, and hydrazine as a reducing agent. In this experiment, I observed and characterized the growth of copper nanowires on glass substrates aided by stannous chloride. The growth and presence of the CuNWs occurred

on the lower portion of the glass plate that was dipped in the stannous chloride solution, because stannous chloride acts as an excellent reductant.

Promoting Inclusion

17. Deficit and Anti-Deficit framing in Chemistry Education

J. Bicknell; (**jobicknell@reed.edu**, Reed College); K. Anachebe; H. Holleb

Faculty Mentor: Prof. Nicole James, Reed College, Chemistry Department, Portland, OR

A current barrier to inclusive and accessible higher science education is the deficit model, which implicitly or explicitly assumes that perceived deficits lie in students, rather than the systems and structures serving students. This can have damaging repercussions that add additional burdens on individuals who are already most poorly served and supported, thus perpetuating inequities. Deficit and anti-deficit approaches have been heavily studied by education researchers, but deficit modeling continues to be prevalent in chemistry education research and practice. Here, we conduct a systematic literature review to facilitate the awareness of deficit and anti-deficit approaches in STEM. This resource will enable chemistry practitioners and researchers to identify and reject the deficit model and consciously adopt anti-deficit approaches, which will broadly improve student outcomes and STEM equity.

18. Reinforcing Linguistic Accessibility in Chemistry: Developing More Equitable Assessment Items

Stephens, A. (**alst2@pdx.edu**, Portland State University); Pares Alicea, A. S.; Kim, A. E.; Lee, E. N.; Barbera, J.

Faculty Mentor: Dr. Jack Barbera, Portland State University, Chemistry Department, Portland, OR

As part of a larger NSF-funded research project with the goal of reducing the language barrier in chemistry assessments, we will be discussing how general chemistry assessments items can be modified to be more accessible and equitable for English language learners (ELLs). The purpose of this work is to investigate an effective method of adjusting chemistry assessment items to ensure that ELL students are given an equal opportunity to showcase their chemical content understanding without undue burden of unpacking the linguistic barriers of the problem. Existing general chemistry assessment items on the topics of limiting reagents and percent yield were systematically modified using the guidelines of the Equitable Framework for Classroom

Assessments (EFCA) (Siegel, 2007) to be more linguistically accessible without changing the items' inherent content level difficulty. Modifications such as replacing complicated vocabulary with more comprehensible words with similar meanings and simplifying sentence structures were implemented to create revised versions of each assessment item. Both revised and original items were presented to undergraduate general chemistry students in a preliminary study to understand how the items are perceived. Students' perceptions were qualitatively analyzed, and results will be discussed. The findings will provide beneficial insights about designing more equitable assessment items.

Graduate Students

Analytical Chemistry

19. Development of Electrochemical pH Microsensor for Biological and Dental Applications

Nguyen, AT. (**nguyean9@oregonstate.edu**, Oregon State University); Goswami, S.; Koley, D*.

Faculty Mentor: Prof. Dipankar Koley, Oregon State University, Corvallis, OR

Electrochemical sensors have been developed for the past decades with various applications, including biomedical and biomaterial applications. Bacterial-mediated local pH change plays a vital role in corrosion for material in dental and medical field. Herein, we have developed a potentiometry flexible microsensor capable of quantifying pH at the interface of microbiological biofilm and material in real-time for more than ten days. We used fluorinated poly(3,4-ethylenedioxythiophene) as the back contact in our newly developed pH sensor, along with a PVC-based ion-selective membrane and hydrophobic top coating. The developed sensor showed a sensitivity near-Nernstian response 58 mV/pH from pH 11 to 4 in universal buffer, 500 ms response time, and highly selective toward H+. We have measured the pH of multispecies derived oral biofilm growth on the resin substrate. We could observe the fluctuations in pH mediated by lactic acid production within the biofilm. The localized real-time monitoring of the pH within the biofilm showed that the pH shift underneath the biofilm could lead to damage to the underlying material and cannot be sensed external to the biofilm.

20. Probing Tertiary Structure and RNA-RNA Interactions in the SARS-CoV-2 Genome via Chemical Crosslinking

Kimmett, E. (**ekimmett@uoregon.edu**, University of Oregon); Willis, D.; DeRose, V.

Faculty Mentor: Prof. Victoria J. DeRose, University of Oregon, Department of Chemistry and Biochemistry, Eugene, OR

To improve understanding of the structure and function of the SARS-CoV2 virus, and to inform the development of therapeutics against COVID19, accurate 3D models of SARS-CoV2 RNA structures are essential. SARS-CoV2 RNAs are predicted to form extensive secondary structures, suggesting regions of complex three-dimensional structure, mediated by short- and long-range tertiary interactions that regulate viral replication and transcription. However, computational predictions of tertiary structure have been limited by lack of experimental constraints on global RNA-RNA contacts. Our work seeks to enable more accurate 3D modeling of SARS-CoV2 RNA structures through the identification of tertiary contact points by means of chemical crosslinking. The DeRose lab has previously shown that cisplatin and other similar platinum(II)-based reagents can act as robust, selectively reversible, cell-soluble crosslinkers, and can be functionalized with clickable handles for the efficient isolation of crosslinked samples. Recent work has focused on characterizing interactions involving the untranslated regions of the viral genome. Identified crosslinks will refine current models of SARS-CoV2 RNA structures and aid the development of small-molecule therapeutics against the virus. Additionally, the tools and methods developed will be applicable for the structural characterization of emerging SARS-CoV-2 variants and future novel RNA viruses.

21. 7-Deazaguanine-based bacterial restriction-modification system: Elucidation of a modification system that incorporates 7-cyano and 7-amido-7-deazaguanine into DNA

Herath Gedara, S. (**samanthi@pdx.edu**, Portland State University); Gustafson, A.; Wood, E.; Swairjo, M.; Crécy-Lagard, V.; Dedon, P.; Iwata-Reuyl, D.

Faculty Mentor: Prof. Dirk Iwata-Reuyl, Portland State University, Chemistry Department, Portland, OR

Restriction-modification (R-M) systems are common strategies bacteria use as anti-pathogen defense against bacteriophages. Typically, these systems

contain a methyltransferase (MTase) that modifies a particular sequence of the host DNA and a restriction endonuclease (REase) that cleaves pathogen DNA by identifying the unmodified recognition sequence. Recently we discovered a novel R-M system that introduces two 7- deazaguanine based modifications into the DNA, 2′ -deoxy-7-cyano-7-deazaguanine (dPreQ0) and 2′ -deoxy-7-amido-7-deazaguanine (dADG). 7-deazaguanine R-M systems are found across a diverse set of bacteria. The Salmonella montevideo R-M system comprises eleven different proteins exemplifying the complexity of 7-deazaguanine R-M systems. Three of these, DpdA, DpdB, and DpdC are responsible for the formation of structural modification to DNA, whereas the rest of the proteins are involved in restriction endonuclease activity. Radiochemical guanine-exchange assays, ATPase assays, restriction digestion experiments, LCMS, binding assays, and small angle scattering diffraction (SAXS) structural studies were used to investigate this modification machinery system. The project aims are to identify the relevant proteins involved in the formation of dPreQ0 and dADG in DNA, and to elucidate the molecular basis for their function. Another specific aim is to identify a target sequence of the bacterial modification apparatus associated with the preQ0 modification of DNA.

Inorganic Chemistry

22. The Effect of the Physicochemical Features of Nanomaterials on their Reflectance

Sihang.H (**huosi@oregonstate.edu**, Chemistry Department); Mackiewicz, Marilyn R.

Faculty Mentor: Prof. Marilyn Mackiewicz, Oregon State University, Chemistry Department, Corvallis, OR

Performing micron-scale imaging in complex biological environments is crucial for diagnostic imaging and visualization of stem cell-based therapies. By using existing techniques such as optical coherence tomography (OCT) and confocal reflection microscopy, targeted contrast agents can improve spatial resolution. OCT relies on high scattering and absorption for image contrast, so molecular contrast agents are not ideal due to their low scattering rates and low scattering rates. Due to this, contrast agents with high scattering, absorption, and backscattering efficiency are urgently needed. As a result of their high scattering rates and reflectivity properties, nanomaterials have gained great interest in OCT imaging in recent years. The size and composition of the metal core play an important role in high reflectivity, but there are also gaps that influence it. In this study, silver and gold nanoparticles (20 to 80

nm) in different physiological environments will be examined for reflectance spectra. By identifying new materials for high-resolution OCT contrast agents, these studies fill a knowledge gap and allow researchers to visually track the migration and survival of therapeutic stem cells.

Organic Chemistry

23. Orbital Analysis of Bonding in Diarylhalonium Salts and Relevance To Periodic Trends in Structure and Reactivity

Karandikar, S. (ssk3@pdx.edu, Portland State University); Bhattacharjee, A.; Metze, B.; Javaly, N.; Valente, E.; McCormick, T.; Stuart, D. R.

Faculty Mentor: Dr. David Stuart, Portland State University, Portland, Oregon.

Diarylhalonium compounds provide new opportunities as reagents and catalysts in the field of organic synthesis. The three center, four electron (3c–4e) bond is a center piece of their reactivity, but structural variation among the diarylhaloniums, and in comparison with other λ3-iodanes, indicates that the model needs refinement for broader applicability. We use a combination of Density Functional Theory (DFT); Natural Bond Orbital (NBO) Theory, and X-ray structure data to correlate bonding and structure for a λ3-iodane and a series of diarylchloronium, bromonium, and iodonium salts, and their isoelectronic diarylchalcogen counterparts. This analysis reveals that the s-orbital on the central halogen atom plays a greater role in the 3c–4e bond than previously considered. Finally, we show that our revised bonding model and associated structures account for both kinetic and thermodynamic reactivity for both acyclic phenyl(mesityl)halonium and cyclic dibenzohalolium salts.

24. Remote Formation of Arynes via Formal Dehydrogenation of Arenes

Riley Roberts (rar7@pdx.edu, Portland State University); Bryan E. Metze; Aleksandra Nilova†; David R. Stuart*

Faculty Mentor: David Stuart

Arynes offer immense potential for diversification of benezenoid cores, which occur in pharmaceuticals, agrochemicals, and liquid crystals. However, accessing these high-energy intermediates requires either harsh conditions or multistep syntheses of designer reagents, and alternative methods with simpler substrates and milder conditions remain underdeveloped. Here, we describe a two-step formal dehydrogenation of simple arenes to generate arynes at a remote position relative to traditionally reactive groups, i.e.,

halides. This approach is enabled by regioselective installation and ejection of an onium leaving group, and we demonstrate the compatibility of simple arenes and arynophiles. The mildness of this strategy is highlighted by formal dehydrogenation of clofibrate, an active pharmaceutical ingredient, and demonstrates that arynes are viable intermediates for late-stage functionalization. Finally, we show that aryne intermediates offer opportunities for orthogonal C-H amination relative to other methods.

25. Diaryl Halolium Compounds as Potential Organic Catalysts

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Faculty Mentor: Dr. David R. Stuart, Dr. Theresa M. McCormick

Hypervalent iodine-based compounds have been exploited extensively for their synthetic and catalytic versatility, but exploration of the analogous bromine and chlorine compounds has been limited by their synthetic inaccessibility. Diaryl cyclic iodolium compounds have shown strong potential for exploitation as tunable organic catalysts in Michael additions, Nazarov cyclizations, and other reactions. For these cyclic compounds, the bromine and chlorine based analogues are possible to synthesize, but are relatively under-explored.

This study employed synthetic, density functional theory, and natural bond orbital approaches to explore the impact of the central halogen on the structure, bonding, and catalytic activity of chlorolium, bromolium, and iodolium compounds. The potential impact of varying counterions was also investigated, as well as the interrelationship between the orbital composition of bonds formed by the hypervalent halogen and chemical structure.

Physical Chemistry

26. Empirical DFT Model to Predict Triplet Quantum Yield Through Singlet Oxygen Yields

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Triplet photosensitizers can be used for a variety of applications, including photocatalysis, OLEDs, and photodynamic therapy. Excited triplet states can be quenched by triplet oxygen to make singlet oxygen. Often the singlet oxygen quantum yield ($\Phi\Delta$) is used as a lower approximation for the triplet yield. Unpredictable effects of even minor structural changes can drastically alter

the ΦΔ and complicate the design of new triplet photosensitizers. The most common strategy to increase ΦΔ is to incorporate heavy atoms, promoting the heavy atom effect. However, the position and the identity of the heavy atom greatly influences the ΦΔ. We have created a predictive model that correlates calculated natural atomic orbital composition of the heavy atom(s) contributing to the frontier molecule orbitals of a photosensitizer with the experimental ΦΔ. I will be presenting on this model, derived from several fluorescein derivatives, which provides a calculated ΦΔ in agreement with the experimental values for a variety of well-known photosensitizers, including rhodamine dyes, fluorescein derivatives, and octahedral metal complexes.

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