



Oral Presentations – Afternoon Session 1

Location: NC 231

Time: 12:00 PM – 3:00 PM

Proton Permeability of Lipid Membranes Determined by Pyranine

Michelle Ireland

Biochemistry

Advisor: Dr. Sarah Maurer

Membranes are essential for cellular energy conversion, maintaining proton gradients that power processes such as ATP synthesis. Understanding how membrane composition affects proton permeability is key to explaining both cellular energy processes and environmental impacts on membrane stability. While fluorescence-based methods have been used to study proton transport, traditional techniques are often slow and limited. We are developing a pyranine-based fluorescence assay designed to measure proton permeability across different membranes using fluorescence kinetics. Encapsulating the pH-sensitive dye pyranine within vesicles and tracking fluorescence under controlled proton gradients allows rapid and quantitative measurement of membrane permeability. Preliminary data show fluorescence responses consistent with proton flux. Future work will apply this approach to a range of membranes, including model systems of prebiotic relevance and glycerophospholipid membranes affected by per- and polyfluoroalkyl substances (PFAS). This high-throughput method provides a platform for probing how membrane composition and environmental stressors influence proton transport and energy processes.



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Resolution of racemic aldehydes and ketones with a chiral amine via diastereomeric imine formation

Keira Guarco

Chemistry

Advisor: Dr. Neil Glagovich

Enantiomers are mirror-image compounds that have identical physical properties and cannot be separated by standard purification techniques. Most drugs are marketed as enantiomerically pure because the racemates may have unknown effects on the body. It is crucial to resolve racemates using more involved purification techniques such as chiral chromatography or diastereomeric formation with a resolving agent. Diastereomers are non-superimposable, non-mirror image compounds that do not share physical properties and can be separated via recrystallization or column chromatography. Enantiomers of aldehydes and ketones can be reacted with chiral amines to form diastereomeric imines, which once separated, can be hydrolyzed to recover the resolving agent and individual enantiomers. In this work, a chiral amine derived from camphor was used as a resolving agent for racemic aldehydes and ketones by forming diastereomeric imine derivatives. As a proof of concept, a simple aldehyde, 2,4-dichlorobenzaldehyde, was refluxed with the chiral amine and a catalytic amount of p-toluenesulfonic acid in 15 mL of toluene for 4 days to yield 41% of the imine product. The imine was recrystallized in ethyl acetate and characterized via MP, IR, ^1H NMR, and ^{13}C NMR. With this synthesis method verified, future directions involve reactions with chiral, sterically hindered aldehydes and ketones such as 3-methylcyclohexanone, citronellal, and menthone.



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Structural Studies of T-cell Protein Tyrosine Phosphatase or Structural Basis for the Inhibition of T-cell Protein Tyrosine Phosphatase

Cassandra Marshall

Chemistry

Advisor: Dr. Nilda Alicea-Velazquez

T-cell Protein Tyrosine Phosphatase (TCPTP) is a cytoplasmic enzyme that regulates cellular signaling by dephosphorylating tyrosine residues on various target proteins. It is associated in controlling immune responses and regulating cell propagation. In a recent study it was reported that the removal of TCPTP, rendered melanoma cells susceptible to immunotherapy. This implies that the inhibition of TCPTP could be used to promote anti-tumor immunity in this form of cancer. However, the possible negative consequences resulting from cross reactivity with other phosphatases (PTPs) can make the design of protein tyrosine phosphatase inhibitors difficult. This project targets a co-crystal structure of TCPTP and PTP-targeted inhibitors to identify distinctive intermolecular interactions that can be used to improve TCPTP-targeted drug design. Here, we present the purification of recombinant TCPTP from a bacterial source. In summation, the 6xHis-tagged recombinant protein was isolated from bacterial proteins using Ni-NTA affinity chromatography. The affinity tag was excised, and the tag-free protein was further purified by Ni-NTA affinity and size exclusion chromatography. The purified TCPTP will be used for crystallization screening and additional structural analysis.



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Structural Studies of SHP-1 C-SH2 Domain Recognition of a Phosphorylated Binding Partner

Jenna Villanueva
Biochemistry

Advisor: Dr. Nilda Alicea-Velazquez

Src homology region 2 (SH2) domain-containing phosphatase-1 (SHP-1), also known as tyrosine-protein phosphatase non-receptor type 6 (PTPN6), is a protein that contains two tandem SH2 domains at its N-terminus. These SH2 domains bind phosphotyrosine (pTyr) residues using two binding pockets, one of which carries a positively charged arginine residue that binds directly to the negatively charged phosphate group. Previous studies with p120-RasGAP (Ras GTPase activating protein), a protein also containing two SH2 domains, identified that the canonical binding mechanism was used by the N-SH2 domain, but not the C-SH2 domain. Carrying out structural studies of N-SH2 and C-SH2 domains with previously identified binding partners will allow for better understanding of how the SH2 domains in SHP-1 recognize their targets. This project aims to determine the crystal structure of SHP-1 C-SH2 domain in complex with a peptide derived from FcγRIIB1, a known binding partner. Presented here are the expression and purification of recombinant SHP-1 C-SH2 domain, the preliminary binding assays using Native Gel Electrophoresis to confirm the C-SH2/FcγRIIB1 interaction, and screening of crystallization conditions.



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Functionalization of Cyclic Peptoids for Use as Inhibitors of Human β -tryptase

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Chemistry

Advisor: Dr. Dilani C. Dehigaspitiya

Human β -tryptase is found in mast cells and plays a key role in triggering asthma, as well as various allergic and inflammatory conditions. Due to its central role in these disorders, it represents a promising target for therapeutic intervention. Human β -tryptase is a homo tetrameric serine protease with four identical active sites directed toward a central pore. A key factor that differentiates β -tryptase and other tryptases is that the former is active as a tetramer and the latter is active as a monomer. The arrangement of β -tryptase provides an ideal platform to be targeted by a multivalent construct based on a small scaffold. Herein we describe the synthesis of cyclic peptoid constructs bearing multiple low-affinity pharmacophores. While these individual pharmacophores are expected to exhibit minimal binding to monomeric forms of tryptase, their spatial organization within a multivalent framework is designed to exploit the cooperative binding effects afforded by multivalency. Through this strategy, we anticipate a significant increase in binding affinity and selectivity toward the tetrameric form of human β -tryptase, while minimizing off-target interactions with monomeric tryptases.



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Amino Acids as Small Molecule Catalysts for adenosine-5'-monophosphate Polymerization

Amoy King

Biochemistry

Advisor: Dr. Sarah Maurer

Formation of nucleotide polymers was important to the origins of life on Earth. The role that wet-dry cycling plays in driving condensation reactions necessary for oligomerization in adenosine monophosphate (AMP) has been evaluated, however, the role that proteinogenic amino acids have on these processes has been little studied. To investigate the potential role amino acids play as small molecule catalysts for nucleotide polymerization, solutions of amino acids and AMP were combined and subjected to varying rounds of wet-dry cycling. To test for formation of dimer and trimer, LC-MS analysis and UV-Vis spectroscopy were utilized. In this study, we evaluate and quantify evidence of AMP polymerization when wet-dry cycled with different amino acids.



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Mineral Effects on Nonenzymatic Adenosine Monophosphate Polymerization Under Variable Hydration Conditions

Allison Gonzalez Fernandez

Chemistry

Advisor: Dr. Sarah Maurer

Various minerals have been studied for their potential role in the origins of life. Montmorillonite, specifically, has been shown to catalyze nucleotide polymerization under simulated prebiotic conditions. However, the influence of other minerals on abiogenesis remains poorly understood.

This study quantifies the extent of adenosine monophosphate (AMP) polymerization in the presence of varying minerals, acids, salts, and lipids under variable hydration conditions. The yields were determined using liquid chromatography–mass spectrometry (LC-MS). The results contribute to our understanding of how mineral chemistry and environmental factors affect nonenzymatic polymerization processes.



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From Radio Waves to Stellar Properties: Using Circumstellar Carbon Monoxide to Understand Nearby Pre-Main Sequence Stars

Caroline Kilian

Physics

Advisor: Dr. Kristine Larsen

To infer the masses of stars, astronomers typically rely on measurements of luminosity and temperature, interpreted through stellar evolution models. However, with the unprecedented accuracy and precision of distance measurements provided by the Gaia mission, combined with the angular resolution of the Atacama Large Millimeter/submillimeter Array (ALMA), a radio telescope located in Chile, it is now possible to make dynamical (i.e. direct) mass measurements of stars that host circumstellar gas disks. These dynamical mass measurements use Kepler's third law of planetary motion to derive the stellar mass based on the measured orbital velocity of gas as a function of distance from the host star. The dynamical mass can then be compared with the output of stellar evolution models to test if the models can reproduce our measurements. This serves as an important benchmark for the success of these stellar evolution models, especially as the fifteen star sample in this project represents both early main-sequence and pre-main sequence (i.e. young) stars where the astrophysical processes in this epoch are the least understood. This project uses carbon monoxide emission in gas-bearing debris disks (disks of dust and rock circling stars, analogous to the Kuiper Belt of our solar system) to measure stellar mass and identify possible non-Keplerian features of the disks. Our results show that stellar evolution models consistently overpredict the stellar masses of the stars in our sample.



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Anatomical Analysis of *Hamamelis virginiana* Leaf Venation in Relation to Spatial Distribution of *Hormaphis hamamelidis* Galls

Jessica Rustico

Biology

Advisor: Dr. Alicia Bray

Insect herbivory is a form of predation in which insects feed on a variety of plant tissues. In the case of galling insects, the interaction goes beyond the insect just feeding on plant tissue. Galling insects are specialized parasites that chemically manipulate plant tissue to form gall structures, which provide the insect with food and shelter. The process begins with the insect secreting a “cecidogen” during feeding that alters cell division in the plant, resulting in gall growth. For aphid species *Hormaphis hamamelidis*, the cecidogen enters plant cells during aphid feeding when a first instar fundatrix inserts a stylet into plant tissue. The location of feeding for this insect is typically near a plant vein, since aphids feed on nutrients in the phloem of plant vascular tissue. This would explain why gall structures are all located very close to veins of the insect's host plant, *Hamamelis virginiana*. However, this does not answer the question as to why significantly more galls were located specifically on secondary leaf veins as opposed to midrib veins or tertiary veins. This study aims to identify anatomical differences between different vein types and between galled and non-galled veins by measuring the distance of the phloem to the surface of each vein. To do this, veins will be cross-sectioned and analyzed under a compound microscope. It is predicted that phloem in galled veins and secondary veins will be closer to the surface, making access easier for aphids.