CHEM4710

Honours Project in Chemistry or Biochemistry

2025/2026 Projects

Table of Content:

Welcome!

Welcome to the 'Honours Project in Chemistry or Biochemistry' (CHEM4710) for the 2025/26 academic year. This course offers you an opportunity to follow your research passions by trying your hands on original research in chemistry or biochemistry as part of an active research group in the chemistry department.

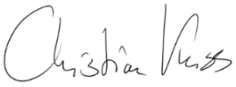
This course gives you an opportunity to contribute to research at one of Canada's top 15 research intensive universities (U15). We have highly competitive research groups in our department that are well-recognized in their respective fields. Through your research project, you may interact with some of our world-class research facilities, such as the Manitoba Institute for Materials. Most research groups maintain national and international collaborations and are part of research endeavours all around the world. Yet, the size of our department allows you to interact closely with senior group members and project advisors.

To find a project that aligns with your goals, you will need to review the projects in this booklet and interview with at least three potential advisors. You will provide a prioritized list of projects through an online form and I will base project assignments on those prioritizations. Each project extends over two terms (Fall 2025 and Winter 2026) and can only have one student assigned to it. During your research, your advisor and their research group members will provide guidance and supervision. Some of you might have already research experience, but you should note that every research group functions a little differently. Your potential advisor can provide more information on how their group operates during the interview.

It should be noted that biochemistry students can choose to take MBIO4530 instead of CHEM4710 for credit for their program.

I sincerely hope that you will explore the opportunities accessible in the Department of Chemistry by looking at the project descriptions in this booklet and that you will take the opportunity to meet with faculty members and discuss their projects within the framework of CHEM4710.

I am looking forward to exciting research discussions and discoveries,



Dr. Christian Kuss

Course coordinator for CHEM4710 2025/26

More about this course

Registering for this course

This course is designed and initially reserved for Chemistry and Biochemistry Honours students in their fourth year. However, students may choose to take this course earlier or outside the honours program, if space permits. To register, please fill in the following online form by **July 18th, 2025** to ensure your timely registration:

https://forms.microsoft.com/r/zwdzKwsgnn

Project selection

Students interested in taking CHEM4710 should review the projects in this booklet. Students need to contact and interview with at least three project advisors and discuss projects listed in this booklet. During those meetings, some of the aspects you may wish to inquire about include:

- Needed background knowledge
- Relevance and impact of the project
- Methods that you might use
- What are the objectives, and can you contribute to shaping the direction of the project
- What safety risks you might encounter
- Who you will interact with mostly during the project
- Expectations about time management, group interactions, etc
- Expected outcomes of the project

Project advisors are usually more than happy to meet with you to discuss their research projects. Once you have ranked your preferred projects, you will submit this filled form together with your project priorities in this online form: https://forms.microsoft.com/r/YVBgHDimi8

A minimum of 3 choices should be submitted and comments can be added in the provided comment field. To be considered for the entire set of advertised projects you are asked to submit this form by **August 8th, 2025**. Matching of students with research projects will only occur after. If you are late to the party, you may still submit your project choices after that date. However, the number of available projects might be limited by then. Students that have submitted their project choice on time will be informed about their project assignment by August 22nd, 2025.

Course progress

The research projects will start during the first week of the 2025 Fall term. For each project the student and project advisor must submit a completed and signed Student – Advisor Agreement (form to follow) no later than September 13th, 2025. Please note that this agreement clearly describes the obligations of both parties. In addition to the research conducted in the individual research groups there will be mandatory class meetings for CHEM4710. Those meetings will cover general topics relevant to your research activities and will provide you with important skills related to the project course. The class meetings will also help in getting to know all research project students. Students should reserve the Friday time slot from 1:30 pm till 2:20 pm for CHEM4710 meetings for the Fall 2025 and Winter 2026 terms. It is important for students to communicate regularly with their project advisors, share information about research progress, research needs, administrative needs and talk about upcoming deadlines.

The progress report is due in November 2025. The research projects should be concluded by the end of the 2025 Winter term. On Saturday March 28th, 2026 each student will present a 15-minute talk followed by 5 minutes of questions during a conference style presentation day. Students and advisors should reserve this day for the presentations. This will be a public event and faculty members, students, friends, family and other guests are welcome to attend. The final written reports will be due beginning of April, 2026. More information on interim and final reports, the final presentation, marking, deadlines, etc. will be provided in the course syllabus closer to the start of the fall term.

Important dates and deadlines to get started

July 18th, 2025: Registration form – ensure you are registered to be included in faculty scholarship selections at the beginning of August

August 8th, 2025: Submit your project selection to be included in the first round of project assignments

September 3rd, 2025: First day of classes in the fall term – your project officially begins

September 5th, 2025: CHEM 4710 orientation class

September 13th, 2025: Student – Advisor Agreement is due

Projects

Project # 1

Preparation of Novel Quantum Magnets

Dr. Mario Bieringer (Mario.Bieringer@UManitoba.ca, (204) 474 6258)

INTRODUCTION:

Materials science is largely based on solid state materials. Magnetic materials that do not show classical long range magnetic order at low temperatures are particularly intriguing. Magnetic ordering can be manipulated by structural disorder and competing magnetic exchange paths. E.g. a triangle of paramagnetic cations (e.g. V^{4+} or Ti^{3+}) with antiferromagnetic coupling results in magnetic frustration, i.e. at least one of the magnetic moments is unable to satisfy all interactions simultaneously, see figure 1A). For large magnetic moments a 120° compromise structure may be observed, figure 1B). In contrast small magnetic moments (e.g. d^1 ➔ S= ½) may form exotic magnetic ground states enhancing our fundamental understanding of magnetic interactions. This concept can be further expanded to tetrahedral motifs, see fig. 2. Quantum magnets fall into this category and are under intense investigation for quantum computing applications.

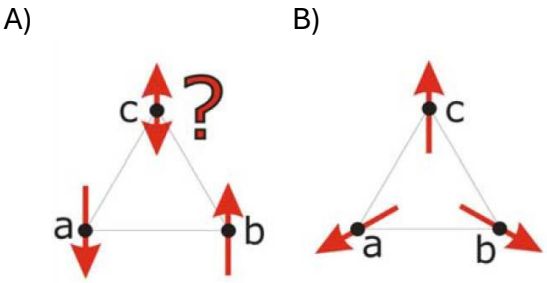


Figure 1: *A) Geometric magnetic frustration. Three spins on a triangular lattice cannot all align antiparallely with respect to all neighbours. B) 120° magnetic structure.*

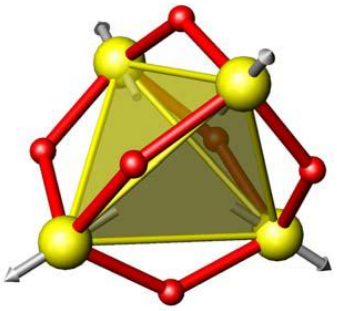


Figure 2: *Tetrahedral spin arrangement on metals (yellow) with oxide (red) bridges.*

PROJECT:

In this project novel materials with triangular and tetrahedral magnetic lattices will be synthesized and the transition metal oxidation states will be fine-tuned to enable quantum behaviour. The work will be based on ABO_3 and ABO_4 structures where A^{n+} is a diamagnetic cation (Ca, Sr, La, Y, Lu etc.) and B is a redox active paramagnetic cation such as Ti^{m+}, V^{m+}, Cr^{m+}, Mn^{m+} or Fe^{m+} etc. Notably the ABO_3 and ABO_4 samples are chosen to further reduce or oxidize the parent compounds under mild conditions (use of buffer gases and solid state hydrides in particular). This project consists of a synthetic component, a structure determination (diffraction) part in order to understand the newly generated phases and advanced property measurements. The advanced characterization will potentially include magnetic measurements, neutron scattering (NPD), X-ray photoelectron spectroscopy (XPS) and related EXAFS and XANES experiments. This project will provide students with a strong background in materials chemistry coupled with materials characterization skills.

REFERENCES:

[1] S. Nishimoto et al., Nature Communications. (2016) 7, 10273
[2] B. Hernden, J.A. Lussier, M. Bieringer, Inorg. Chem. (2015), 54, 4249−4256
[3] D. Vrublevskiy et al., Inorg. Chem. (2021) 60, 872-882

Project # 2

Designing Next Generation Thermal Expansion Materials

Dr. Mario Bieringer (Mario.Bieringer@UManitoba.ca, (204) 474 6258)

INTRODUCTION:

Solid state materials are dominating the majority of communication, energy, sensing, electronic and optical technologies. Solid state oxides are particularly enticing due to their large density of functional metal cations and their diverse structures. Surprisingly the formation pathways and mechanisms are only very poorly understood. In order to advance materials chemistry such as switching from environmentally concerning and toxic materials to the preparation of high-performance benign materials the synthesis of those materials need to be understood.

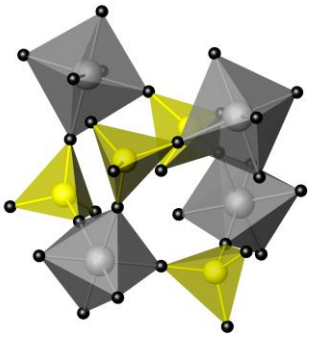


Figure 1: *Fragment of the ZrW_2O_8 structure. Yellow = W^{6+}, grey = Zr^{4+} and black = O^{2-}. Note that all polyhedra are corner connected.*

Thermal expansion describes the volume change of a material as a function of temperature. While the majority of structures expand upon heating there are also negative thermal expansion materials known that undergo volume contraction upon heating. Particularly important are isotropic materials that show identical properties along all 3 principal directions. A key structural component for negative thermal expansion materials is a network of corner connected polyhedra. ZrW_2O_8 is a good structural example with corner connected ZrO_6 octahedra and WO_4 tetrahedra acting as 3-dimensional hinges permitting volume reduction upon heating.

PROJECT:

In this project novel materials with corner sharing octahedra based on the ReO_3 structure will be developed. Notable $CaSnF_6$ is a superstructure of the ReO_3 structure type. The structure of $CaSnF_6$ is shown in figure 2 forming a network of corner sharing octahedra. Using fluoride anions permits to use an average cation oxidation state of 3+, thus permitting the combination 2+ and 4+ cations and in case of transition metals those can oxidation states can be fine tuned using redox chemistry. It is proposed to form $A^{4+}B^{2+}F_6$ and $A^{3+}B^{3+}F_6$. The structures of those new compounds will be solved using powder X-ray diffraction and thermal expansion measurements will be conducted using high-temperature *in-situ* powder X-ray diffraction. The structures can be fine tuned via redox chemistry generating systems such as $A^{4+}B^{2+}{}_{1-x/2}B^{3+}{}_{x/2}F_{6-x}O_x$. This project will provide students with a strong background in materials chemistry coupled with materials characterization.

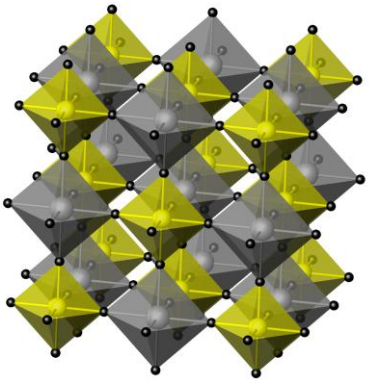


Figure 2: *Cubic $CaSnF_6$ structure. Yellow = Sn^{4+}, grey = Ca^{2+} and black = F^-. All polyhedra are corner sharing.*

References:

[1] J.S.O. Evans et al., Chem. Mater. (1996), 8, 2809−2823
[2] Q. Gao et al. Nano Research, 2023, 16(4): 5964−5972

Project # 3

Preparation and Reactivity of ZrO_2 based Oxide Ion Conducting Materials for Solid Oxide Fuel Cell Applications

Dr. Mario Bieringer (Mario.Bieringer@UManitoba.ca, (204) 474 6258)

INTRODUCTION:

Solid Oxide Fuel Cells (SOFCs) are highly efficient and fuel tolerant devices for the conversion of chemical energy directly to electrical energy. Fuel cells are compact and virtually maintenance free if exclusively designed with solid state materials. Currently the major drawback of SOFCs is the high operating temperature of almost 1000°C. In an effort to lower the operating temperature of SOFCs oxide defect structures based on ZrO_2 are being synthesized and the formation of the oxide defects are investigated systematically, fig. 1.

PROJECT:

Yttria stabilized zirconia, $Zr_{1-x}Y_xO_{(2-x/2)}\square_{x/2}$ (where $\square$ denotes oxide defects, i.e. missing O^{2-} anions) are cubic fluorite structures with randomized oxide defects.

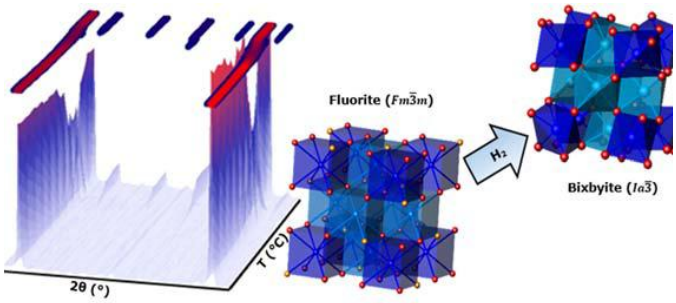


Figure 1: Real time *in-situ* X-ray diffraction experiments illustrating the selected oxide removal from the disordered fluorite structure (right structural diagram) during $Y_{(1-x)}Pr_xO_{3.5}$ reduction.

In order to investigate the creation and annihilation of these oxide defects it is proposed to replace Y^{3+} with $Pr^{3+/4+}$ cations. With the addition of Pr^{4+} to ZrO_2 a redox active cation allows the reversible removal of oxide anions during reduction and repopulation of the oxide defects with actual oxide ions during oxidation. In this project $Zr_{1-x}Pr_xO_2$ will be prepared using high temperature reactions. The reversible oxide uptake and removal will be investigated using in-situ powder X-ray diffraction experiments and thermogravimetric analysis in order to determine structural details and oxygen stoichiometries as a function of reaction conditions. Ion conductivities will be measured for this system under redox conditions. Students carrying out this project should be familiar with inorganic chemistry and willing to learn structure determination techniques for crystalline solids and be interested in characterization of physical properties. Laboratory skills and data analysis will be one of the many potential learning outcomes of this project.

REFERENCES:

[1] J.A. Lussier, G. Devitt, K.M. Szkop, M. Bieringer, *J. Solid State Chem.*, (2016) **242**, 126–132
[2] J.A. Lussier, K.M. Szkop, A.Z. Sharma, C.R. Wiebe, M. Bieringer, *Inorg. Chem.*, (2016) **55**, 2381−2389
[3] J.A. Lussier, D.H.P. Souza, P.S. Whitfield, M. Bieringer, *Inorg. Chem.* (2018) **57**, 14106−14115

Project # 4

Assessment of possible repair mechanisms of ancient parchment Infrared vibrational spectroscopy

Dr. Kathleen M. Gough (kathleen.gough@umanitoba.ca, (204) 474-6262)

INTRODUCTION:

Parchment, a complex biological material made from processed animal skins, was widely used as a writing medium across Europe, the Mediterranean, and the Horn of Africa from the 2nd century BC. Historically significant documents, e.g: the Magna Carta[1], are kept under strict environmental control to preserve these precious, unique cultural and historical artifacts from our past. Despite its longevity, parchment is susceptible to collagen-specific degradation mechanisms. Our 5-year NSERC Discovery Horizons project "Archival Parchments Rejuvenation: Re-engineering native collagen crosslinks for the test of time", led by Prof. Laurent Bozec (UToronto) was funded in spring 2023. Our proposal focuses on re-engineering natural glycation crosslinks in collagen in parchment using methods translated from Tissue Engineering, in the Bozec lab. As a co-investigator, Kathy Gough is using her expertise in infrared spectroscopy of collagenous materials to evaluate the damaged parchments and the novel chemical treatments that are being developed in the Bozec lab, with the long-term goal of designing a process for repair of model parchments.

PROJECT:

Parchment samples to be studied include new parchment materials (full hide calf skin; Pergamena, USA) and a collection of historical parchments originating from the EU-funded Improved Damage Assessment of Parchment (IDAP) project. The unique triple helical structure of collagen at the molecular level results in an unusual, characteristic IR spectrum that is conformation- and orientation-dependent in normal tissues and measurable at the micro-[2] to nano-scale[3]. You will prepare collagen extracts from parchments supplied by the Bozec lab and examine them with our Agilent IR microscope [spatial resolution: 1-5 micron] the newly installed multimodal microscopy instrument: the mIRage-LS. Its Quantum Cascade Lasers (QCL) enable analysis at the sub-micron scale with simultaneous IR, Raman and super-resolution fluorescence-detected IR.[3] You will use near-field nanoscale-IR spectroscopy through remote access to the IR beamlines at the Advanced Light Source, Berkeley, USA.[2] You will participate in a collaborative, multi-team, cross-disciplinary study that is significant in that it addresses the urgent need of museum curators and conservators for long-term solutions to preserve parchment as a cultural heritage. You will learn the technical aspects of polarized IR spectroscopy and imaging, a technique used in research and applications from industry to health care.

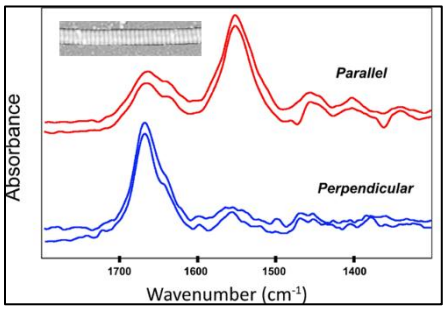


Fig. 1: Spectra of collagen fibrils under polarized IR light.[2]

REFERENCES:

1. Library, B. Magna Carta 1215
2. G Bakir, BE Girouard, R Wiens, S Mastel, E Dillon, M Kansiz, K Gough," Orientation Matters: Polarization Dependent IR Spectroscopy of Collagen from Intact Tendon Down to the Single Fibril Level" *Molecules* 25:4295 (2020); R Wiens, CR Findlay, SG Baldwin, L Keplak, J Lee, S Veres, KM Gough, *Farad Discuss* 187:555-573 (2016)
3. Prater C, ….Gough KM; "Widefield Super-Resolution Infrared Spectroscopy" Appl Spectrosc, 78:1208-1219

Project # 5

Polarized infrared spectrochemical imaging and Two-Dimensional Correlation spectral analysis of polylactic acid (PLA) biodegradation

Dr. Kathleen M. Gough (kathleen.gough@umanitoba.ca, (204) 474-6262)

INTRODUCTION:

Pollution caused by fossil fuel-based plastics is a major environmental concern.[1] Polylactic acid (PLA), a bio-based polymer, is often viewed as an environmentally friendly, practical alternative to petrochemical plastics,[2] as it possesses many of the desirable physical and mechanical characteristics, is bio-synthesized, and can be degraded by hydrolysis and microbial action. Unfortunately, complete biodegradation of PLA is still very challenging at best. Specific controlled conditions of temperature, humidity, pH and bio-organisms are required. Even then, the process is slow and incomplete as the crystalline phase is less susceptible to chemical and biochemical attack. Infrared vibrational spectroscopy,[2,3] offers a direct window into the state of PLA films, letting us evaluate of the efficacy of modified and novel treatments, *in vitro* and in composting systems in the field,[4] with the goal of enhancing the biodegradation rate of PLA.

PROJECT:

Commercial PLA-containing products have variable characteristics and composition. For this controlled study, you will prepare pure spin-cast PLA films. Infrared (IR) vibrational spectroscopy is widely used on polymer films such as PLA.[2] In the past year, we have optimized methods for cold crystallization of amorphous spin-cast PLA flims.[3a] You will focus on creating films annealed at higher temperatures to achieve maximum crystallinity. These films will be directly assessed with a combination of advanced IR techniques, including imaging, polarized IR, and 2D-COS analysis.[3b] Our lab has just completed installation of a CFI-funded, multimodal microscopy instrument: the mIRage-LS, enabling analysis at the sub-micron scale. With the 2DCOS software, you will plot the correlated spectral changes as a function of treatment and time sequence. You will be able to monitor the effect pre- and post-treatments[4] by examining the pre- and post-treated films using the same IR techniques. You will be part of an interactive team, working directly with students in my group, as well as interacting with students and professors who are involved in the campus-wide Prairie iGEM (International Genetically Engineered Machine) team. This project will give you a chance to work on problems of global environmental significance, and to gain experience state-of-the-art instruments and in experimental techniques that are widely used in research and industry.

REFERENCES:

1. Chatziparaskeva G; Papamichael I; Voukkali I; Loizia P; Sourkouni G; Argirusis C; Zorpas AA. End-of-Life of Composite Materials in the Framework of the Circular Economy. (2022) *Microplastics* 1:377–392.
2. Yan, J. et al. 2023. Application of infrared spectroscopy in the multiscale structure characterization of poly (L-lactic acid), *Polymer* 278 (2023) 125985.z
3. Popoff, Jamshidzadeh, Hartry, Levin, Gough, MS in preparation, July 2025; Park Y, Noda I and Jung YM (2015) Two-dimensional correlation spectroscopy in polymer study. *Front. Chem*. 3:14.
4. Mohanan N; Wong N C-H; Budisa N; Levin DB (2023) Polymer-degrading enzymes of *Pseudomonas chloroaphis* PA23 display broad substrate preferences. *Int J Mol Sci* 24:4501.

Project # 6

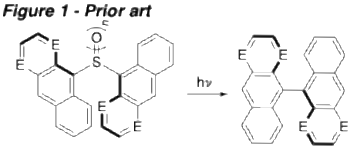
Let There Be Light! Accessing Functional Biphenanthridine Luminophores Through {S=O} Extrusion Chemistry

David Herbert (david.herbert@UManitoba.ca, (204) 474-7535)

INTRODUCTION:

Light-responsive materials are ubiquitous in modern life, from biology to chemistry to materials science. In one notable example, aromatic systems with bridging sulfur units with different degrees of oxidation have been shown to enable remarkable photoresponsive properties, with applications in anticounterfeiting and supramolecular assembly. Photoinduced sulfur extrusion leads to **drastic** photophysical changes that render such species useful as stimuli-responsive materials (Figure 1, ***Prior Art***).[1-2]

Figure 1 - Prior art



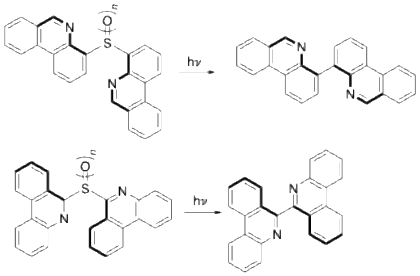
E = CH → Wolf *Angew. Chem., Int. Ed.* **2013**, *52*, 12946-12950
E = N → Wolf, Hudson *J. Org. Chem.* **2025**, *90*, 5788–5794

PROJECT:

In the Herbert Group, we have become, over the years, *very* interested in materials based on the tricyclic **phenanthridine** core.[3] These molecules can be highly fluorescent, can bind transition metal ions to generate coordination complexes with fascinating properties, and can be reversibly hydrogenated. **A recent 4710 project** (2023-2024) studied the formation of **dimers** of phenanthridines ('biphenanthridines', or 'biphe') showing they are highly promising materials for solar cell applications, leading to a publication with the 4710 student as the lead author.[4]

In this project, a motivated student will explore a **photo-activated** route to biphe materials via light-induced sulfur extrusion. The project will involve **organic synthesis** and both **molecular characterization** using solution-phase NMR spectroscopy and single-crystal X-ray diffraction, and **electronic structure** using UV-Vis absorption and luminescence spectroscopy. The student will build sulfur-bridged phenanthridine dimers substituted in the 4- (Figure 2, top) and 6-positions (Figure 2, bottom). Oxidation using *m*-CPBA will be used to generate sulfoxide (n = 1) and sulfone (n = 2) dimers from the sulfide (n = 0). Absorption spectroscopy will evaluate how these species absorb light, then photoirradiation using appropriate wavelength LED light will used in an attempt to produce 6,6'-biphenanthridines and 4,4'-biphenanthridines. This project will provide meaningful experience in light-activated chemistry, synthesis and molecular characterization with potential applications in novel light-emitting materials and anti-counterfeiting dyes.

Figure 2 - This work



REFERENCES:

1. P.R. Christensen, B.O. Patrick, E. Caron, M.O. Wolf* *Angew. Chem., Int. Ed.* **2013**, *52*, 12946-12950
2. R. Hojo, H. Noguchi, J. Toigo, M.O. Wolf*, Z.M. Hudson* *J. Org. Chem.* **2025**, *90*, 5788–5794
3. D.E. Herbert *Can. J. Chem.* **2023**, *101*, 892-902
4. K.A. Veilleux, G. Schreckenbach, D.E. Herbert* *Molecular Systems Design & Engineering* **2024**, *9*, 423-435

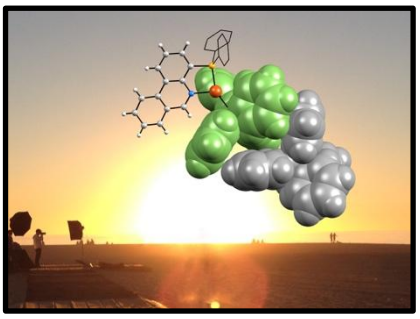
Project # 7

PHOTOCATALYSIS USING DESIGNER SUSTAINABLE CHROMOPHORES

David Herbert (david.herbert@umanitoba.ca, (204)474-7535)

Group Website: http://home.cc.umanitoba.ca/~dherbert/

INTRODUCTION: As the world's population grows, so too does the global demand for materials and energy. The ability to harvest solar energy (solar cells) and manipulate light output (display technologies and low-cost/energy usage lighting) using *abundant* materials will be key to providing a high global quality of life to as many people as possible, while limiting the impact of making and using these materials on our climate and environment. A very promising additional application is to use molecules to ***catalyze*** reactions leveraging sunlight in place of thermal energy ("photocatalysis").



PROJECT: As part of our group's broader efforts to target new dyes to harvest solar energy based on abundant elements such as iron (Fe), and new emissive materials based on copper (Cu) and zinc (Zn), we are designing ligand motifs for transition metals and constructing their transition metal coordination complexes, where we modify the molecular structure of **ligands** through **chemical synthesis** in order to tune the photophysical and electrochemical properties of complexes. In doing so, we target molecules that can absorb a broad range of the electromagnetic spectrum across the visible and, ideally, into the near-IR, and allow for tuneable emission from complexes of abundant metals.

This project takes our work to the **next level** by evaluating some of our molecules in **photocatalytic reactions.** A 4710 student will work directly alongside Dr. Herbert and a graduate student mentor to construct chromophores and using our photoreactor, examine their utility in photocatalysis.

REFERENCES:

R.J. Ortiz, R. Mondal, J.K. McCusker, D.E. Herbert *J. Am. Chem. Soc.* **2025**, *147*, 1694–1708

Project # 8

Chemical Vapor Transport to Discover New Optical Materials

Dr. Abishek Iyer (abishek.iyer@umanitoba.ca, https://www.iyerlab.ca/
(204) 474 7346)

INTRODUCTION:

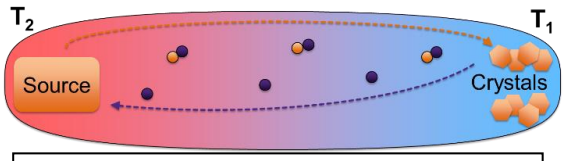


Figure 1: A Schematic of a CVT reaction showing the source at T2 (hot-zone) and the crystals at T1 (cold-

High-quality crystal growth of inorganic compounds has significantly advanced technologies in optics, electronics, and radiation detection. Chemical Vapor Transport (CVT) is a widely used method for growing bulk single crystals, including those that are otherwise difficult to synthesize by conventional means. The process involves a multi-zone furnace that establishes a temperature gradient to facilitate crystal growth. CVT typically proceeds through three key stages: solid dissolution, vapor-phase transport, and subsequent deposition. A critical factor in the success of CVT is the choice of an appropriate transport agent.[1] Halogens and halide compounds are commonly employed due to their high volatility and effectiveness in enabling mass transport. Recently, a new two-dimensional inorganic material, SnP_2Se_6, was discovered through the CVT method, which has shown promise in optoelectronics.[2]

PROJECT:

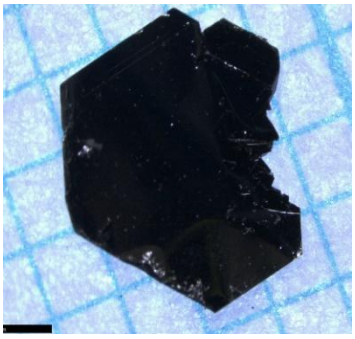


Figure 2: CVT grown crystal of MoS_2

This project aims to discover new semiconducting materials using the chemical vapor transport (CVT) method by exploring various transport agents, including iodine (I_2) and tin tetrabromide ($SnBr_4$). We will utilize CVT to access new phases that are stable at specific temperatures or metastable structures. The focus will be on the V–Sn–P–S and Sn–Bi–Se–I phase spaces, where precursor compounds synthesized via solid-state reactions will be used for bulk crystal growth. The materials will be characterized using X-ray diffraction (powder: phase identification; single: crystal structure determination), diffuse reflectance (band gap determination), and differential scanning calorimetry (DSC: melting behavior). Once the single crystal structure is obtained, we will test these materials for specific applications, such as nonlinear optics and radiation detectors. The project will combine the principles of synthesis from inorganic materials chemistry with those of physical chemistry to discover new materials.

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(2) Nag, J.; Sarker, S.; Imam, S.; Iyer, A.; Waters, M. J.; Suceava, A.; Rondinelli, J. M.; Kanatzidis, M. G.; Gopalan, V. Large Non-Resonant Infrared Optical Second Harmonic Generation in Bulk Crystals of Van der Waals Semiconductor, SnP_2Se_6. *Advanced Optical Materials* **2025**, *13* (9), 2402649. DOI: https://doi.org/10.1002/adom.202402649.

Project # 9

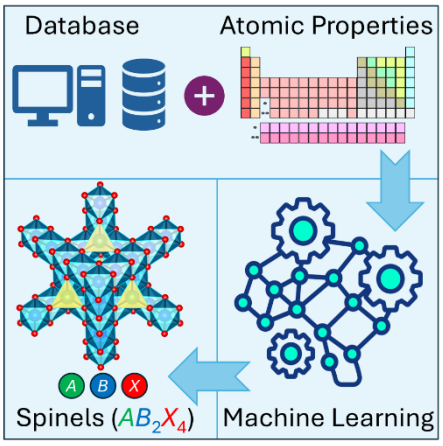
Accelerating the Discovery of New Spinels for Photovoltaics

Dr. Abishek Iyer (abishek.iyer@umanitoba.ca, https://www.iyerlab.ca/
(204) 474 7346)

INTRODUCTION:

Among many naturally occurring minerals, a broad class of compounds with the general formula AB_2X_4 is known as spinel compounds (where *A* and *B* are typically metal cations and *X* is an anion including O, S, Se, Te, or a halogen). Due to their structural tunability and functional versatility, spinels find applications in various areas, including redox catalysis, energy storage, dielectric devices, and water splitting.[1] Owing to the natural abundance of oxides, most spinels studied to date are oxides. While those containing alternative anions remain largely unexplored, their full potential applications remain untapped. It is probably because traditional approaches to discovering materials through laboratory synthesis are tedious and require years to identify new spinels.[2] Hence, an efficient and reliable screening method is essential to evaluate whether new arbitrary AB_2X_4 elemental combinations form spinels.

PROJECT:



During this project, various machine learning algorithms, including supervised, unsupervised, and semi-supervised methods, will be employed. As a starting point, a library of known spinel compounds comprising three unique elements will be prepared through a literature search. Once a list of compounds is ready, they will be cleaned and transformed into machine-interpretable data, which is a part of the data sanitization step. It is worthwhile noting that this step is the most time-consuming and requires considerable effort. The prepared data will be split into train, test, and validation sets to screen various ML models.[3] Once a reliable model is ready and new predictions are made, top-performing candidates will be synthesized on a laboratory scale to validate the model prediction and accuracy. High-temperature solid-state reactions for chalcogen-based spinels and solvothermal reactions for halogen-containing spinels will be employed. Upon the successful preparation of new candidates, their crystal structure will be evaluated using X-ray diffraction methods, including both single-crystal and powder techniques. Chalcogen-based spinels will be tested for their band gap, and their potential applications in photovoltaic cells will be explored.

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Project # 10

Magnetic organic-inorganic hybrid two-dimensional materials

Dr. Abishek Iyer (abishek.iyer@umanitoba.ca, https://www.iyerlab.ca/
(204) 474 7346)

INTRODUCTION:

Spintronics is a rapidly developing field that leverages the intrinsic spin of the electron to create next-generation, efficient electronics, for quantum information science. Traditional electronics are approaching their physical limitations, where further size reductions could lead to extreme heat generation, rendering them inoperable. Spintronics utilizes the concept of spin polarization, where spontaneous ferromagnetism is retained in the absence of an external magnetic field. Efficient computing requires electronics made up of materials where electron spins can be used for data storage and exchange at room temperature. Mn-GaAs, Si, and InMnAs have traditionally dominated semiconductor spintronics. However, these devices are typically prepared using expensive techniques like molecular beam epitaxy and face challenges in controlling structural defects, which can impede spin mobility.

PROJECT:

The project to study the effect of the intercalation of 2D materials with organic cations on magnetic ordering and the effect of interplanar spacing on the crystal structure. The bulk material will be synthesized using P_2S_5 flux as reported in literature.[2] The organic cation intercalation will be achieved via hydrothermal synthesis and/or electrochemical synthesis. We will start with the effect of intercalation due to length of organic cation like methyl (MA), formamidium (FA) and tert-butyl ammonium (TBA) cations and study the change in structure using X-ray diffraction and electron diffraction (ED). Powder x-ray refinements will provide structural information where the (00*l*) reflections will be compared with the pristine sample for any shifts to confirm the intercalation has worked. Once the organic cation intercalation is confirmed then their bulk magnetic properties will be measured to confirm their magnetic ordering. The project will combine the fields of molecular and semiconductor spintronics to create the next generation of hybrid materials for quantum computing. Solution processible thin films are expected to reduce the cost of chips as well as create efficient quantum computing devices.

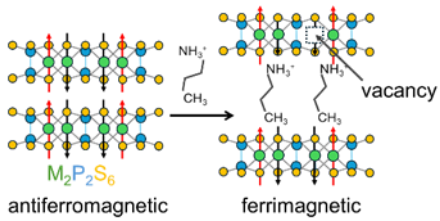

Figure 1: Effect of organic cation intercalation on magnetic ordering in 2D chalcogenides. is the vacancy created in the inorganic slab.

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Project # 11

Investigating Ion-specific Effects on Collagen Melting

Dr. Mazdak Khajehpour (Mazdak.Khajehpour@UManitoba.ca, (204) 272 1546)

INTRODUCTION:

Collagen is the building block protein for connective tissue. The assembly of this protein into fibrils leads to the formation of tendons. Collagen structures are held together through hydrogen bonding and electrostatic interactions. In this project we intend to investigate the nature of these electrostatic interactions through modulating them via salt addition.

PROJECT:

In this work we will investigate how salt addition affects the melting of type-I rat tail collagen. These effects will be characterized using differential scanning calorimetry (DSC) and circular dichroism spectroscopy (CD). Because ions interact specifically with protein moieties (the Hofmeister effect) through non-electrostatic interactions, measuring and characterizing how different salts affect collagen melting will allow us to understand the role of electrostatic interactions in forming the collagen triple helix.

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Project # 12

Investigating the effects of co-solutes upon folding of paratox

Dr. Mazdak Khajehpour (Mazdak.Khajehpour@UManitoba.ca, (204) 272 1546)

INTRODUCTION:

Paratox is a small protein that acts as an inhibitor of new DNA acquisition by streptococci bacteria. In this project we plan to study the effects of osmolytes (small molecules that stabilize proteins) upon the folding thermodynamic and kinetic properties of paratox in order to understand the folding mechanism of this protein. The purpose of this project is to determine if osmolytes effect the stability of paratox through modulating the enthalpy or entropy of the folding process

PROJECT:

In this project the student will learn how to over-express and purify paratox. They would then determine the thermodynamic parameters of the protein folding process using differential scanning calorimetry (DSC) and chemical denaturation methods. From these measurements the ΔH, ΔS, ΔG and ΔC_p of the protein will be determined. The folding mechanism of paratox will be studied through fast denaturation methods using stopped flow kinetics. These measurements will determine the number of intermediate steps involved in the protein folding process and the folding and unfolding rate constants. The effects of co-solutes on the kinetics and thermodynamics of the paratox folding process will also be determined. In addition to DSC and stopped flow the student in this project will also learn how to use and interpret steady-state and time-resolved fluorescence spectroscopy, as well as circular dichroism spectroscopy.

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1) *Khajehpour et al., J Biol Chem. 2021 Sep; 297(3): 100992.T*
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Project # 13

How small snoRNAs help making a large RNA machine - the ribosome

Dr. Ute Kothe (ute.kothe@UManitoba.ca, (431) 371 0878)

INTRODUCTION:

Ribosomes are large RNA-protein machines that synthesize all cellular proteins. While much is known about protein synthesis, we know comparably little about how ribosomes are assembled around the scaffold of long ribosomal RNA (rRNA). However, knowledge about ribosome assembly is critical to understand genetic diseases resulting in bone marrow failure and to inhibit the overproduction of ribosomes in cancer cells. The Kothe lab is focussed on understanding the role of small nucleolar RNAs (snoRNAs) during the early stages of ribosome assembly. Two types of snoRNAs are responsible for modifying rRNA by introducing pseudouridines and 2'-O-methylations, respectively, and some snoRNAs facilitate processing of rRNA from long precursors into the mature form.

PROJECT:

Current research in the Kothe lab investigates when, how and where snoRNAs interact with rRNA during the early stages of ribosome assembly. We are also interested to understand which role proteins called RNA helicases play in removing snoRNAs from rRNA after their action.

To address these questions, we isolate snoRNA complexes and early ribosome precursors from baker's yeast, and analyze their composition, RNA-RNA and RNA-protein interactions in the ribosome precursor as well as the modification status of rRNA. The purification strategies include tagging snoRNAs or rRNA precursors with RNA aptamers which allow for highly specific affinity chromatography. As a complementary approach, we tag RNA helicases and other protein factors aiding in ribosome assembly with inducible degradation tags to assess ribosome assembly in their absence. In this project, the honor thesis student will tag new snoRNAs or ribosome assembly factors and investigate their role during ribosome assembly. Thereby, the student will gain experience in molecular biology, yeast genetics, RNA purifications and analysis of ribosome assembly. Overall, this project will help determine whether snoRNA-rRNA interactions are suitable targets for future drugs.

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Project # 14

Structure-Property Relationships in Biologically Active Glasses for Soft-Tissue Wound Healing

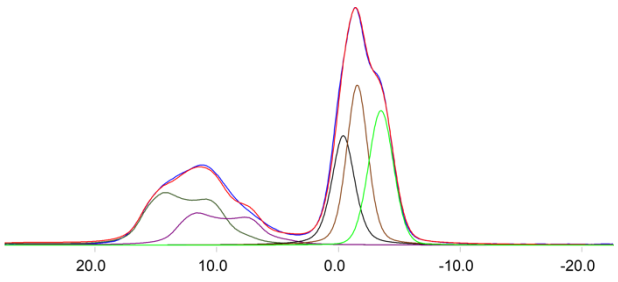
Dr. Scott Kroeker (Scott.Kroeker@UManitoba.ca, (204) 474 9335)

INTRODUCTION:

Phosphate glasses are emerging biomaterials for bone reconstruction and soft-tissue wound healing. Biologically active glasses dissolve in physiological fluids and redeposit bone minerals for increased mechanical strength, or release therapeutic ions to wound sites to enhance tissue formation. The dissolution properties of the glass determine which of these functions predominates, which in turn depends on the glass composition and structure. While silicophosphate glasses have been commercialized for some biomedical applications, borophosphate glasses hold promise for others. This *inorganic materials* project uses nuclear magnetic resonance (NMR) spectroscopy to study the structure of novel borophosphate glasses to determine the key compositional and structural parameters governing the dissolution of bioactive glasses.

PROJECT:

Borophosphate glasses doped with alkaline earths such as Ca, Mg or Sr, or transition metals such as Zn, Ag or Cu, will be prepared by high-temperature synthesis. The influence of dopants on the glass network structure will be studied by solid-state ^{11}B and ^{31}P magic-angle-spinning NMR spectroscopy. The chemical durability of these glasses in simulated body fluid will be evaluated in dissolution trials, with elemental release measured by ICP-OES as a function of time. The transformation of the materials during exposure to the aqueous environment will be characterized by NMR spectroscopy and complementary methods such as scanning-electron microscopy. Correlating structural changes with dissolution behaviour will provide a deeper understanding of how properties depend on glass composition, thereby guiding the design of bioactive glasses which release therapeutic ions at the wound site for optimal healing. This project can be tailored to student interests and strengths to emphasize inorganic, analytical or physical aspects.



^{11}B magic-angle spinning NMR of a borophosphate glass with two types of BO_3 and three types of BO_4

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Project # 15

Raindrops On A Window Pane: How Are Glass Surfaces Altered By Exposure To Water?

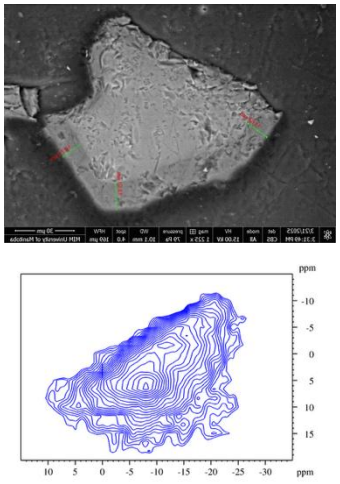
Dr. Scott Kroeker (Scott.Kroeker@UManitoba.ca, (204) 474 9335)

INTRODUCTION:

Many commercial applications of glass involve prolonged contact with aqueous solutions. From pharmaceutical vials to smartphone screens to nuclear waste disposal, the chemistry at the glass-water interface determines the suitability of a material for a given application. In silicate glasses, exposure to aqueous environments corrodes the surface, altering the local composition, molecular structure and properties. However, the characterization of glass surfaces is complicated by its amorphous structure, dynamics, and inherently low volume. Nuclear magnetic resonance (NMR) spectroscopy is uniquely capable of selectively observing nuclei in hydrated layers, making it ideal for studying the aqueous corrosion of glasses. This *inorganic materials* project uses NMR methods to understand molecular reorganization at the surface of glasses used for nuclear waste disposal.

PROJECT:

Boroaluminosilicate glasses will be prepared by high-temperature synthesis and exposed to aqueous solutions. Elemental release will be measured by ICP-OES as a function of time to quantify how dissolution properties change with glass corrosion. The morphology of the altered surface will be characterized scanning-electron microscopy. Surface-sensitive solid-state NMR methods will be used to selectively probe the structure of the layer, spectroscopically observing ^{1}H, ^{17}O, ^{11}B, ^{29}Si, ^{23}Na and ^{27}Al. By comparison with the unaltered glass structure, the mechanism of alteration may be inferred, providing valuable information about the long-term performance of glasses exposed to solution. Learning more about the formation, structure and properties of glass corrosion will aid the prediction of long-term behaviour of materials for radioactive immobilization, and the design of better glasses for environmental sustainability. This project can be tailored to student interests and strengths to emphasize inorganic, analytical or physical aspects.



SEM image of corrosion layer on glass particle, and ^{23}Na multiple-quantum magic-angle spinning NMR of altered

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Project # 16

Mechanochemical Preparation of Battery Materials

Dr. Christian Kuss (Christian.Kuss@UManitoba.ca, (204) 480-1823, kussmaterials.com)

INTRODUCTION:

As we transition away from fossil fuels, it's essential to ensure that the renewable energy technologies we adopt are truly sustainable. For instance, the production of battery materials can involve environmentally intensive processes, such as mining practices with adverse ecological and social consequences, high-energy synthesis methods, and the generation of chemical waste. My group investigates methods to reduce the environmental impact of batteries. In this project, we focus on mechanochemical methods that can convert some of the most abundant minerals into advanced battery materials.

Mechanochemistry offers a sustainable alternative by using mechanical force, such as grinding or shearing, to activate materials[1]. This approach can alter structure, surface chemistry, and reactivity, enabling greener pathways to functional materials.

PROJECT:

You will dive into the emerging field of mechanochemistry to explore how ball milling transforms a locally sourced, abundant mineral oxide into a high-performance material for lithium-ion batteries. While early results show remarkable potential, the fundamental chemistry behind these transformations remains a mystery. Your mission will be to uncover the reaction mechanisms, kinetics, and material performance. Specifically, you will:

1. Drive mechanochemical reactions under varied conditions to reveal how process parameters influence material transformation.
2. Explore purification strategies for better material performance.
3. Evaluate electrochemical performance by building and testing lithium-ion battery cells with the milled materials.

You will gain hands-on experience with ball milling, scanning electron microscopy (SEM), X-ray diffraction (XRD), and battery testing in an inert-atmosphere glovebox. This project is ideal for students excited about green chemistry, energy storage, and solid-state materials, and offers a chance to contribute to the development of sustainable technologies from local resources.

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Project # 17

Watching Materials at Work: Operando Spectroscopy for Batteries

Dr. Christian Kuss (christian.kuss@umanitoba.ca, (204) 480-1823, kussmaterials.com)

INTRODUCTION:

Battery materials undergo continuous structural and chemical changes during operation, directly affecting performance and degradation. Conventional ex situ characterization investigates material properties after extraction from the battery and captures only static states, often missing key transient phenomena. Operando techniques address this gap by enabling real-time observation of materials under realistic cycling conditions[1]. In this project, you will develop and apply operando infrared spectroscopy to track chemical changes in battery materials as they occur, providing new insights into reaction mechanisms and interfacial processes.

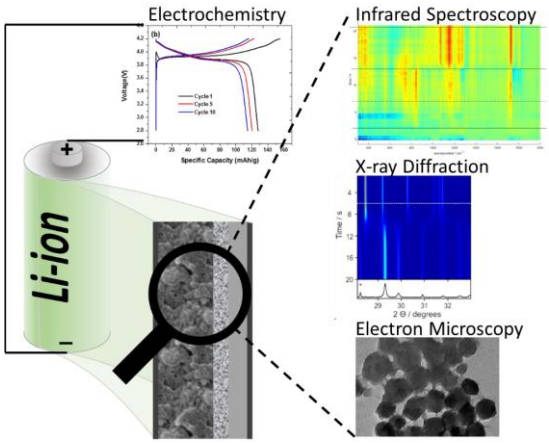

Figure 1. A combination of operando and ex-situ methods is needed to understand the performance-relevant properties of battery materials.

PROJECT:

Binders are crucial materials in batteries that adhere the charge-storing active materials to the electrode. Battery failures are often associated with binding problems. In 2019, the Kuss group developed a new conductive binder material for use in next-generation batteries that is more adhesive, can be processed in water (rather than toxic solvents), and is electronically conductive, improving the fast-charging performance of batteries[2]. To support the characterization of these binders and to understand their performance and limitations, recent funding from the Canada Foundation for Innovation has brought new operando characterization equipment to the Kuss group. You will choose whether to explore these new battery materials using operando infrared, Raman, or UV/Vis spectroscopy. The results will yield information on the dynamic behavior of these binders and their chemical environment, as well as their chemical stability and performance. The resulting data will inform the selection of the most appropriate next-generation battery technologies for the application of the Kuss group's novel conductive binders and underpin the development of new binders.

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Project # 18

Detection of Key Tryptophan Metabolites in the Gut-Brain Axis

Dr. S.Kuss (Sabine.Kuss@UManitoba.ca, (204) 474-9265)

INTRODUCTION:

The gut-brain axis refers to a fascinating and complex two-way relationship between the gut microbiome and the central nervous system.[1] Various tryptophan metabolites produced in the gut have been correlated to neurological conditions such as Parkinson's and Autism.[2,3] Detecting these molecules is therefore extremely important, however, there are many species for which rigorous analytical techniques have not yet been established. This project aims to establish electrochemical detection techniques for numerous tryptophan metabolites in biological samples.

PROJECT:

This project will focus on the electrochemical detection of four tryptophan metabolites; picolinic acid, xanthurenic acid, indole acetaldehyde, and 6-Formylindolo[3,2-b]carbazole. All of these molecules are related to key neurological processes or disorders, however the details of their redox behaviour and electrochemical detection are not well understood. For each molecule the electrochemical oxidation mechanism will be studied in detail utilizing voltammetric and coulometric techniques such as cyclic voltammetry, differential pulse voltammetry, and electrolysis. Lastly, the devised method will be applied to real biological samples in order to detect the key tryptophan metabolites. This project aims to better understand the electrochemical detection of these molecules, which in turn will help elucidate their role in neurological disorders and the gut-brain axis.

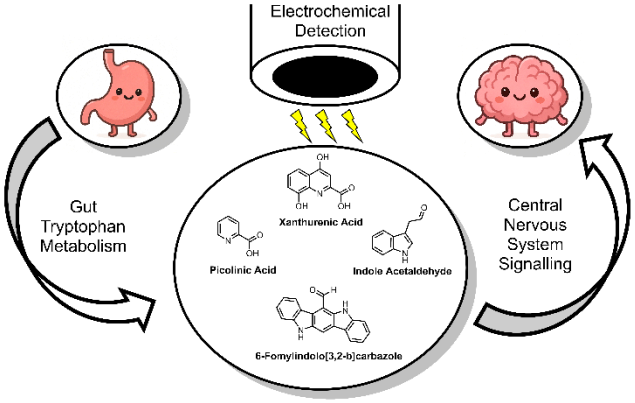

Figure 1 – Molecular structures of several tryptophan metabolites that have been correlated to the neurological conditions.

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Project # 19

Investigating Cancer Through the Lens of Tryptophan Metabolism

Dr. S.Kuss (Sabine.Kuss@UManitoba.ca, (204) 474-9265)

INTRODUCTION:

The depletion of tryptophan by various enzymes which are overexpressed in cancer cells effectively disguise and shield it from the immune system.[1] Recent medical studies have sought to inhibit these enzymes thereby removing the disguise and invoking an immune response. Unfortunately, clinical trials of such inhibitors have underperformed.[2] This project will investigate the relationship between tryptophan metabolism and cancer to help develop improved chemotherapy techniques.

PROJECT:

Scanning electrochemical microscopy (SECM) of live cells is a powerful technique that can reveal important information about cellular processes at the molecular level.[3,4] In this project SECM is applied to investigate tryptophan depletion in the environment surrounding cancer cells. The cells will then be treated with various inhibitors of tryptophan consuming enzymes (i.e. IDO1, IDO2, TDO2) and the changes in tryptophan consumption will be measured. These inhibitors will be evaluated individually and in combination with one another. By doing so, this project aims to develop techniques to halt tryptophan depeletion in the environment around cancer cells and remove their "disguise". If successful, this study would provide critical insight for the development of combination chemotherapeutics for cancer treatment.[5]

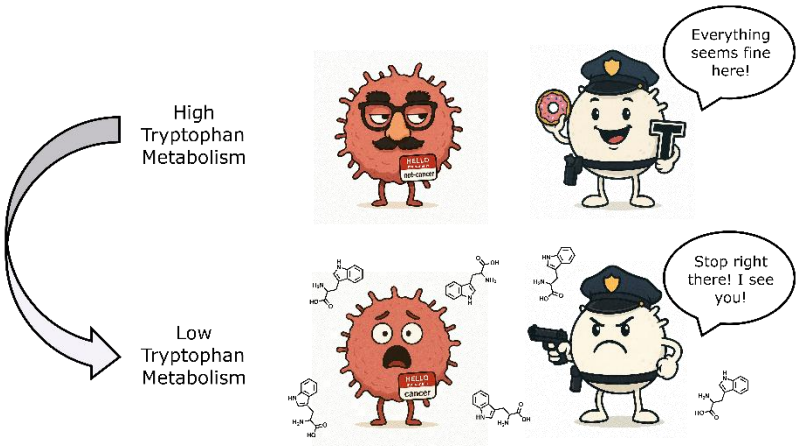

Figure 1 – Cancer cells are not 'visible' to T cells when high tryptophan metabolism takes place. When the metabolism is reduced the cell becomes 'visible' to the T cells.

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Project # 20

Chemistry Outreach in Manitoba: Life Beyond the Perimeter

Dr. Joey Lussier (Joey.Lussier@UManitoba.ca, (204) 474-7652)

INTRODUCTION:

Chemical literacy is becoming progressively more important as environmental consequences of resource management and sustainable energy development have increasing impacts on society. Unfortunately, students from rural and Indigenous communities often are disadvantaged because of a lack of laboratory infrastructure and may not be taught by experts (e.g. trained chemists). Furthermore, it becomes more difficult to effectively educate students in the hands-on techniques required in chemistry when resources and services found in large cities are not easily accessible. Consequently, students entering university from communities outside of larger cities/centers often struggle with their first years in chemistry. The goal of this chemical education project is to identify and address some of these issues both in the communities, and in the university curriculum.

PROJECT:

In this project a chemistry outreach program will be developed with a focus on rural and Indigenous communities in Manitoba. The goal of this project is twofold; a) to spark an interest in chemistry and engage Indigenous students and b) integrate Indigenous Knowledge into university chemistry.

Step one involves building partnerships with rural and Indigenous communities and working together with champions in the community (Elders, teachers, or other community members). Concerns of access to chemistry resources will be identified using qualitative and quantitative methods. This project will use an approach of two-eyed seeing[1] to blend Indigenous Ways of Knowing with western science to decolonize the current approach to scientific education. The project may include the development of new experiments, alternative lessons or lectures, and new tutorial formats. Consequently, this will spark an interest in chemistry in more students from diverse backgrounds. The knowledge gained will also flow into introductory university chemistry courses. The material will be a resource to the department of chemistry and will be included in new course development. The project student will gain many skills in the scholarship of teaching and learning, with a strong emphasis on chemical education beyond the traditional university approach.

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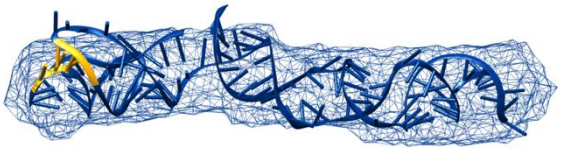
Project # 21

CHARACTERIZATION OF AN ENDOGENOUS RNA-PROTEIN COMPLEX THAT REGULATES TRANSLATIONAL CONTROL

Dr. Sean McKenna (Sean.McKenna@umanitoba.ca)

INTRODUCTION: Brain Cytoplasmic RNA 1 (BC200) is a 200 nucleotide long non-coding RNA that is hypothesized to regulate protein translation and play a key role in regulating carcinogenesis. We have begun to define the BC200-containing protein complexes that mediate BC200 function through immunoprecipitations of the RNA coupled with mass spectrometry analysis of bound proteins. From hundreds of potential hits, we have cross-validated a small subset of proteins that we suspect directly interact with BC200. We have recently discovered that the last 80 nucleotides of BC200 can be truncated in human cells, and that this truncation may be the key event regulating carcinogenesis. Our current hypothesis is that BC200 acts as a scaffold for a protein regulatory complex that interacts with messenger RNAs to regulate translation, with a different subset of proteins interacting with the RNA when truncated.

PROJECT: The proposed research project will use a combination of biochemistry, structural biology, and molecular biology to characterize the direct interactions between BC200 and target proteins identified from our screen. Intact protein-RNA complex will be endogenously purified using sequential co-immunoprecipitation from human cells. Protein components will be identified by Western blotting/mass spectrometry approaches. Structural biology approaches will be used to characterize the complex at low resolution (light scattering, x-ray scattering) and high resolution (cryo-EM).



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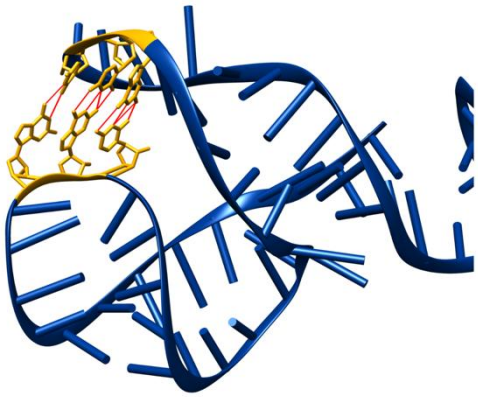

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Project # 22

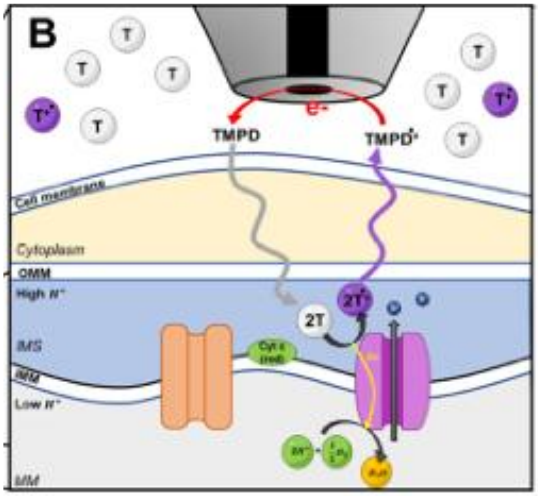
IMPACT OF A NON-CODING RNA ON MITOCHONDRIAL ENERGY PRODUCTION

Dr. Sean McKenna (Sean.McKenna@Umanitoba.ca)

Dr. Sabine Kuss (Sabine.Kuss@umanitoba.ca)

INTRODUCTION: Brain Cytoplasmic RNA 1 (BC200) is a 200 nucleotide long non-coding RNA that is hypothesized to regulate protein translation and play a key role in regulating carcinogenesis. We have recently developed a methodology that specifically immunoprecipitates BC200-contianing RNA-protein complexes in human cells. This approach has enabled comprehensive detection of all mRNAs interacting with the complex (via sequencing) as a first estimation of the specific mRNAs regulated. Surprisingly, many of the top hits are mitochondrial mRNAs that code for the proteins of the electron transport chain in the inner mitochondrial membrane. We hypothesize that BC200 acts as a scaffold for a protein regulatory complex that interacts with messenger RNAs to regulate translation of the electron transport chain in mitochondria, thereby enabling increased energy production required for rapidly dividing cancer cells.

PROJECT: The proposed research project will use a combination of molecular biology (in the McKenna lab) and electrochemistry (in the Kuss lab) test the hypothesis that BC200 is central to energy metabolism in cancer cells. Using established RNA interference approaches in the McKenna lab, the impact of BC200 knockdown on interaction with and expression of mitochondrial mRNA will be evaluated, as will cellular localization of the intact BC200 complex. Preliminary measures of electron transport chain function will be performed in parallel. With the Kuss lab, the impact of BC200 knockdown on electron transport chain function in individual human cells will be determined using scanning electrochemical microscopy. Together the project will assess the overall impact of BC200 on energy metabolism.



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Project # 23

REGULATION OF BC200 FUNCTION VIA INTERACTION OF THE POLY(C) BINDING PROTEIN AT ITS 3'-END

Dr. Sean McKenna (Sean.McKenna@umanitoba.ca)

INTRODUCTION: Brain Cytoplasmic RNA 1 (BC200) is a 200 nucleotide long non-coding RNA that is hypothesized to regulate protein translation and play a key role in regulating carcinogenesis. We have begun to define the BC200-containing protein complexes that mediate BC200 function through immunoprecipitations of the RNA coupled with mass spectrometry analysis of bound proteins. From hundreds of potential hits, we have cross-validated a small subset of proteins that we suspect directly interact with BC200. We have recently discovered that a cytosine-rich region at the 3'-end of BC200 interacts with the poly(C) binding protein (PCBP), and that this interaction protects the RNA from rapid degradation in human cells.

PROJECT: The proposed research project will use a combination of molecular biology and biochemistry to define the specific interaction between the PCBP and BC200, both in human cells and with purified components. In human cells, using a series of BC200 truncations that reduce the length of the cytosine tract (from 0-12), the minimal interaction site will be defined as will the impact on RNA stability. The impact of the PCBP-BC200 interaction on protein translation will be examined. Using purified *in vitro* transcribed BC200 truncations in the cytosine tract, the minimum binding site for purified PCBP will be determined and correlated with the cellular results. Time permitting, biophysical and low-resolution structural biology approaches will be used to characterize the complex at low resolution (light scattering, x-ray scattering).

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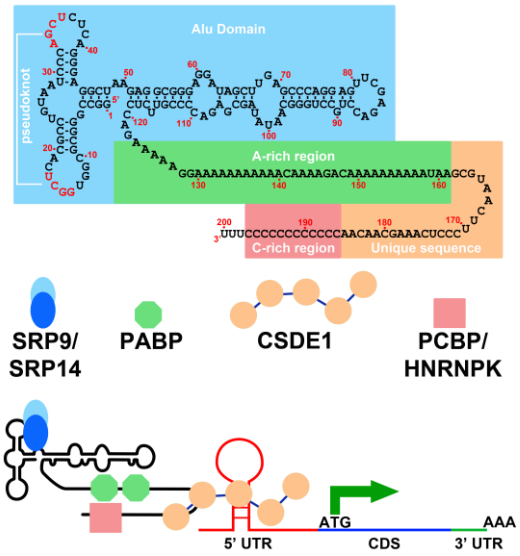
Booy E.P., *et. al.* (2018) " Comprehensive analysis of the BC200 ribonucleoprotein reveals a reciprocal regulatory function with CSDE1/UNR." ***Nucleic Acids Research.*** 46(21): 11575-11591.



Project # 24

Mapping the Protein Hydration Layer

Dr. Katie Mitchell-Koch (katie.mitchellkoch@UManitoba.ca, (204) 474 6053)

INTRODUCTION:

The Mitchell-Koch group focuses on the solvation layer surrounding proteins, as these intimately-related molecules are integral to protein structure, dynamics, and function, yet are often ignored in drug design and studies of biomolecular function. At the protein surface, water molecules exhibit altered dynamics- namely, diffusion, reorientation, and hydrogen bond lifetimes. The extent to which the dynamical properties of water are altered relative to bulk water varies around different regions of the protein. Using computational methods, we can map the water dynamics regionally at the protein surface, and characterize how water molecules are arranged around the protein surface (*i.e.* describe the local water structure). We found previously that the structure and dynamics of water in the solvation layer is connected by an excess entropy relationship[1] and we continue to explore relationships among water structure & dynamics and protein structure & dynamics.

PROJECT:

Our work uses molecular dynamics simulations to simulate proteins in water, and then we carry out specialized analysis to characterize the solvation layer around the proteins. Systems to be studied include a series of homologous proteins, starting with alcohol dehydrogenases. Our work will compare properties of the hydration layer across these enzymes with similar function, to see to what extent the solvation layer properties are similar or different at regions of the protein with similar function (for example, at the cofactor binding cleft). Our data will contribute to the creation of a data set in which the relationship between protein structure and hydration layer properties can be examined.

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1. J.N. Dahanayake and K.R. Mitchell-Koch "Entropy Connects Water Structure and Dynamics in Protein Hydration Layer" *Phys. Chem. Chem. Phys.* **2018**, *20 (21),* 14765-14777
2. Doan, L. C.; Dahanayake, J. N.; Mitchell-Koch, K. R.; Singh, A.; Nguyen, V. Q., "Probing Adaptation of Hydration and Protein Dynamics to Temperature" *ACS Omega,* **2022**, *7*(25)*,* 22020-22031.
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Project # 25

Toward Improved Non-Aqueous Biocatalysis: Enzyme Structure-Dynamics in Ionic Liquids

Dr. Katie Mitchell-Koch (katie.mitchellkoch@UManitoba.ca, (204) 474 6053)

INTRODUCTION:

Enzyme catalysis is an area for the development of green chemistry, offering mild conditions, atom efficiency, and reducing the use of harsh chemicals required for chemical transformations such as oxidation. Enzyme catalysis can be a crucial tool for the efficient production of commodity and fine chemicals from carbon precursors, including biomass. However, many organic compounds are sparsely soluble in water, the native solvent of enzymes. This can be overcome by the use of organic solvents and ionic liquids,[1] which solubilize hydrocarbons and expand enzyme function. Several lipases have been shown to retain their structure and catalytic function in organic solvents and ionic liquids. We have developed methods to simulate enzymes in organic solvent and ionic liquids.[2]

PROJECT:

Our work will use molecular dynamics simulations to model enzymes in newly-developed ionic liquids that are designed, synthesized, and characterized by our collaborators. We will characterize solvent-protein interactions in novel ionic liquids and monitor variations in enzyme structure and dynamics due to solvent.[2 3] Comparing results to experimental data from our collaborator, we will correlate simulations data with enzymatic activity to guide the design of new ionic liquids and biocatalysis strategies.

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Project # 26

Understanding Fluorine NMR Chemical Shifts

Dr. Katie Mitchell-Koch (katie.mitchellkoch@UManitoba.ca, (204) 474 6053)

INTRODUCTION:

Fluorine NMR spectroscopy is a valuable tool for studies of small molecules, as well as protein structure-function through the incorporation of fluorinated amino acids. The fluorine nucleus is highly sensitive to environment and bonding, displaying a broad range of chemical shifts (~800 ppm). It is generally understood that multiple factors influence fluorine chemical shifts in proteins, including local dielectric environment, hydrogen bonds, and solvation waters. However, the scientific community does not have a framework for interpreting what, exactly, the nucleus is reporting on. Our goal is to address these drawbacks through computationally-assisted assignment, interpretation, and prediction of fluorine nuclear resonances in different environments.

PROJECT:

Our work will use computational methods, primarily density functional theory (DFT) calculations to calculate fluorine chemical shifts with different models. We will compare the calculations with published values of fluorine chemical shifts in molecules that have been studied by systematically varying electronic structure or solvent environment. The contributions of different orbitals to the ^{19}F chemical shifts will be calculated using Natural Chemical Shielding Analysis, in order to understand the origins of differences in fluorine chemical shifts. We will also examine the influence of specific solvent interactions on fluorine chemical shifts in a series of fluorinated aromatic compounds.

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2. J.N. Dahanayake, C. Kasireddy, J.P. Karnes, R. Verma, R.M. Steinert, D. Hildebrandt, O.A. Hull, J.M. Ellis, and K.R. Mitchell-Koch. "Progress in Our Understanding of 19F Chemical Shifts." Annual Reports on NMR Spectroscopy, Vol. 93 , Graham A. Webb, *editor*, **2018**, 282-374.
3. J.N. Dahanayake, C. Kasireddy, J.M. Ellis, D. Hildebrandt, O.A. Hull, J.P. Karnes, D. Morlan, and K.R. Mitchell-Koch. "Evaluating Electronic Structure Methods for Accurate Calculation of ^{19}F Chemical Shifts in Fluorinated Amino Acids" *J. Comp. Chem.* **2017,** *38 (30)*, 2605-2617.

Project # 27

Design and development of protein reporters for CART-cell populations

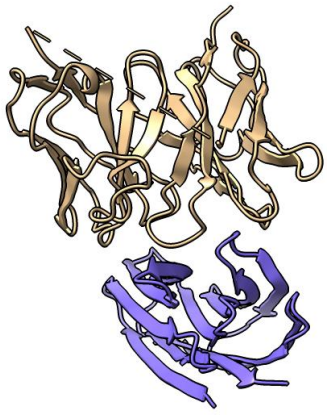
Dr. Zev Ripstein (Zev.Ripstein@UManitoba.ca, (204) 474-8504)

INTRODUCTION:

Induced pluripotent stem cells represent an emerging therapeutic technology with extensive applications in studying and treating autoimmune diseases and cancers. One major use is Chimeric Antigen Receptor (CAR) T-cell therapy which involves extracting blood samples from a patient through a procedure called leukapheresis, which collects lymphocytes, or white blood cells. By using T-cell engineering, scientists enhance the T-cell receptors in these white blood cell samples before reinfusing them into the patient. This process increases the recognition of antigens associated with B-cell cancers, aiding in their elimination.

PROJECT:

This project builds on the development of a novel CD19 mimic designed to bind to and report on the presence of chimeric antigen receptors (CARs) on T cells. The objective is to engineer and improve upon the design of a synthetic protein molecule that is stable, easily expressed and emulates the natural binding interaction of CD19 with its T-cell receptors, specifically targeting CARs incorporating CD19 co-stimulatory domains. The proposed CD19 mimic will be equipped with a detectable marker, allowing for real-time monitoring and quantification of CAR expression on the cell surface. This project aims to facilitate the assessment of CAR-T cell populations and their functional status, ultimately optimizing CAR-T cell therapies.



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Project # 28

Using Computational Chemistry to Predict the Properties of Biphenanthridines: New Frontiers

Dr. Georg Schreckenbach (georg.schreckenbach@umanitoba.ca, (204) 474 6261)
Dr. David Herbert (david.herbert@UManitoba.ca, (204) 474-7535)

INTRODUCTION:

Aromatic compounds in general, and substituted aromatics such as N-heterocycles in particular, are of great interest for applications from medicines to materials. One prominent example is as "singlet fission materials" which can effectively double the current obtainable from solar energy harvesting. [1] Recently, the Herbert group has developed synthetic methods to coupled benzannulated N-heterocycles such as "biphe" (6,6'-biphenanthridine). [2] Collaborative work between the Schreckenbach and Herbert groups have subsequently used computational methodologies developed here at UM [3] to computationally screen biphe analogs for use as singlet fission materials, leading to a peer-reviewed publication derived from a past undergraduate project. [4]

PROJECT:

The goal of this project is to extend this protocol using computational chemistry to predict the structural and optical properties of biphe and its analogs, as both neutral complexes and in their (di)anionic forms. The interested student would work primarily in the Schreckenbach group, but in close contact with the Herbert group, to simulate the absorption spectra of these compounds and evaluate their lowest lying singlet and triplet state structures and energies for potential application in singlet fission and related applications.

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[1] M. Smith, J. Michl *Chem. Rev.* **2010**, *110*, 6891-6936

[2] D.B. Nemez, I.B. Lozada, J.D. Braun, J.A.G. Williams, D.E. Herbert *Inorg. Chem.* **2022**, *61*, 13386-13398

[3] C. Match, J. Perkins, G. Schreckenbach *Theor. Chem. Acc.* **2018**, *137*, 109

[4] K.A. Veilleux, G. Schreckenbach, D.E. Herbert *Mol. Sys. Des. Eng.* **2024**, *9*, 423-435

Project # 29

Redox Chemistry of Lanthanide and Actinide Coordination Complexes using Computational Chemistry

Dr. Georg Schreckenbach (georg.schreckenbach@umanitoba.ca, (204) 474 6261)

INTRODUCTION:

The physical properties of lanthanides and actinides, especially uranium, neptunium, and plutonium are interesting because of their multiple oxidation states. Chelating organic ligands such as *acac* (acetyl acetonato) cannot stabilize different oxidation states of lanthanides and actinides, Recently, a phosphorus analogue of *acac*, known as bis(acyl)phosphide (BAP),**(1)** was found to react and stabilize uranium in its +3 and +4 oxidation states. The BAP ligand further demonstrated redox noninnocence. That is, it accepts unpaired electrons from uranium upon reacting with it. This pseudo-conservation of the oxidation state of the uranium as U(IV) instead of U(III) was not obvious from NMR, EPR and UV-Vis spectra. Density functional theory (DFT) calculations from the Schreckenbach group provided evidence for redox noninnocence in $U(BAP)_4$.**(2)** Similar reactivity was observed between the BAP^- ligand and Pu^{3+}, whereas Th^{4+} and Ce^{3+} are redox inactive metal centers.**(3)** However, Np^{3+} exhibited unusual chemistry and an "*ate*" complex was reported: $Np(BAP)_4^-$. U, Ce, Th, Np exhibited 2-electron redox events in cyclic voltammetry (CV) scans, whereas Pu exhibited 4-electron redox events.

PROJECT:

The goal of this project is to understand the redox noninnocence of BAP^- ligands in coordination complexes of U, Np, Pu, Ce and Th. The interested student will employ computational chemistry (DFT) **(4)** to construct model reactions to (i) elucidate reaction thermodynamics, (ii) compute redox potentials to reproduce the CV results, (iii) examine the intermediates in the CV from oxidation-reduction events, and (iv) probe the metal-ligand bonding for presence of covalency between the bonding atoms.

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(1) Carpenter et al., Inorg. Chem. **2022**, 61 (32), 12508-12517.

(2) DS Michael and G. Schreckenbach Inorg. Chem, **2024**, 63 (21), 9711-9714

(3) Carpenter et al., Inorg. Chem. **2025**, 64, 15, 7263-7272.

(4) Gao et al., Inorg. Chem. **2021**, 60, 10, 6971-6975.

Project # 30

Synthesis and *In Vitro* Evaluation of Amino Sugar-Monobactam Hybrids Against Gram-negative Bacteria

Dr. Schweizer (frank.schweizer@umanitoba.ca, (204) 474 7012)

INTRODUCTION:

The World Health Organization has identified several bacterial pathogens as critical contributors to a subtle but ever growing global antimicrobial resistance crisis.[1] Among these, Gram-negative bacilli present a challenge due to their low outer membrane permeability, which significantly impedes antibiotic entry. However, certain antimicrobial agents are designed to bypass this barrier. One mechanism to bypass the barrier is *self-promoted uptake*, wherein compounds exploit the amphiphilic nature of the outer membrane—interacting with both its hydrophilic and hydrophobic components—to facilitate penetration.[2] This project aims to leverage this phenomenon by enhancing bacterial uptake of β-lactam antibiotics through rational molecular design, ultimately enabling access to the periplasmic space where these agents exert their bactericidal activity.

PROJECT:

This project focuses on the synthesis and evaluation of novel hybrid antibiotics through the conjugation of amino sugars to the monobactam scaffold of aztreonam. The synthetic strategy involves selective protection of functional groups on the amino sugar to enable the regioselective installation of an azide moiety. In parallel, an alkyne functional group will be introduced onto aztreonam via amide coupling. The two components will then be joined using copper(I)-catalyzed azide–alkyne cycloaddition (CuAAC), forming a stable 1,4-disubstituted triazole linker. The resulting amino sugar–aztreonam hybrids will be purified and fully characterized by ^{1}H, ^{13}C, and 2D NMR spectroscopy, along with mass spectrometry (MALDI-TOF or ESI-MS). Antibacterial activity will be assessed via minimum inhibitory concentration (MIC) determination using broth microdilution against both wild-type and clinical multidrug-resistant Gram-negative isolates. Time-kill kinetics will be performed to evaluate bactericidal activity as a function of time.

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1. Geneva: *WHO Bacterial Priority Pathogens List,* (2024).

2. Hancock, R. E. W.; Wong, P. G. W., Compounds which increase the permeability of the *Pseudomonas aeruginosa* outer membrane, *Antimicrob. Agents Chemother.*, **26** (1984), 48–52.

Project # 31

The discovery of new drugs from lichen fungi

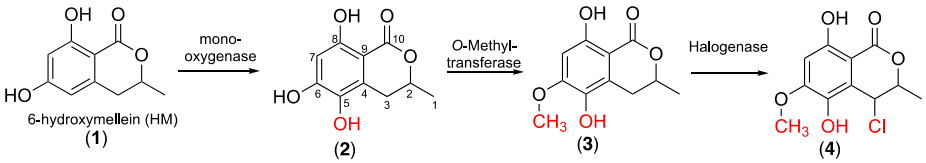
Dr. John Sorensen (John.Sorensen@umanitoba.ca, (204) 474 9504)

INTRODUCTION:

The Sorensen lab is working at the interface between chemistry and biology by exploring the biosynthesis of biologically active organic molecules produced by lichen and other fungi.[1,2] We have discovered over 40 biosynthetic gene clusters in a *single* strain of the lichen *Cladonia unicalis.*[3] These clusters, comprising of anywhere from 2 to 10 (*or more*) genes appears to each code for a unique natural product.[4] Our focus is now on assigning function to each of these gene clusters by expressing individual genes in a heterologous host. Our overarching goal is to discover new biologically active molecules that can be used as lead compounds for the design of new pharmaceuticals.

PROJECT:

This project will offer a student a unique opportunity to combine molecular biology with synthetic chemistry in a way that will allow us to probe individual chemical steps in natural products biosynthesis in fungi. One of the pathways that we have discovered in the lichen fungi appear to involve the conversion of 6-hydroxymellinin (**1**) to a halogenated isocoumarin (**4**). However, this pathway is a speculative assignment of function based on homology of the individual genes in the identified cluster. This project will aim to assign function to each of the individual genes that we have identified. Our initial focus will be on the gene that codes for a cytochrome P_{450} monooxengase that we suspect is involved in the conversion of (**1**) to (**2**). In order to accomplish this a polymerase chain reaction (PCR) method will be used to amplify and clone this gene in to an appropriate vector that will allow for expression in *E. coli* bacteria (*or some other suitable host*) in a manner that allows for the production of functional enzyme. In addition, the project will also focus on the expression of enzymes that convert (**2**) to (**3**) (*likely an O-methyltransferase*) and (**3**) to (**4**) which is a halongenase. This project will also require the chemical synthesis of molecules that can be used as substrates to test the biochemical function of the purified enzyme. For example, a chemical synthesis of compound (**2**, **3** and **4**) will be required in order to test if it is indeed a substrate for the *O*-methyltransferase. Successful competition of this project would then set the foundation for the investigation of the other genes that we have discovered in *C. uncialis*.



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3. Bertrand, R. L.; Abdel-Hameed, M.; **Sorensen J. L**. *J. of Nat. Prod.* **2018,** *81,* 723–731.
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Project # 32

Structure-Property Relationship of AhR

Dr. Stetefeld (jorg.stetefeld@umanitoba.ca, (204) 474 9731)

INTRODUCTION:

The Aryl Hydrocarbon Receptor (AhR) is a ligand-activated transcription factor that plays a crucial role in mediating responses to environmental toxins. It regulates gene expression involved in detoxification, immune response, and cell proliferation. Understanding AhR's function is vital for insights into its implications in health and disease. This project aims to investigate the molecular mechanisms governing AhR activation and signaling pathways. The findings could contribute to developing novel strategies for toxicology and therapeutic interventions.

PROJECT:

CHEM4710 candidates will continue to develop an integrated research program that combines high-resolution structural biology techniques with various biophysical and functional approaches. The project involves expressing AhR in a baculovirus/insect cell expression system and its structural elucidation via cryo-EM.

To gain a deeper understanding of the structure and function of AhR structural data will be compared with predicted models generated by AlphaFold. The study will focus on identifying key binding sites and amino acids and depicting various effects as a function of respective PAH-uptake.

The student will engage in an intensive research program aimed at elucidating the structure-property relationships of AhR with several highly relevant PAH-ligands involved in the formation of dynamic signaling complexes related to human disease. This will include recombinant protein expression, biochemical and biophysical characterization, and structural analysis of protein-ligand interactions.

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2. Dalei Wu et al.. Structural characterization of mammalian bHLH-PAS, COSB, 2016

Project # 33

Structure-Property Relationship of H5N1 Nucleoprotein

Dr. Stetefeld (jorg.stetefeld@umanitoba.ca, (204) 474 9731)

INTRODUCTION:

H5N1 nucleoprotein (NP) plays a crucial role in the replication and transcription of the influenza A virus, serving as a key component of the viral ribonucleoprotein complex. Its interactions with viral RNA and host cellular machinery make it a significant target for understanding viral pathogenicity and developing antiviral strategies. This project aims to explore the structural and functional characteristics of the H5N1 nucleoprotein to contribute to the broader understanding of influenza virus biology.

PROJECT:

CHEM4710 candidates will continue to develop an integrated research program that combines high-resolution structural biology techniques with various biophysical and functional approaches. The project involves expressing H5N1 in *E. coli*, including wild type and CPP-targeted variants of H5N1 nucleoprotein (NP), which will be thoroughly characterized.

To gain a deeper understanding of the structure and function of H5N1 nucleoprotein, high-resolution X-ray crystallography will be employed to determine its 3D structure. These structural data will be compared with predicted models generated by AlphaFold. The study will focus on identifying key binding sites and amino acids, analyzing structural environments, and exploring what differentiates various avian influenza strains. Particular attention will be given to why certain strains are more prevalent in human infections.

The overarching goal is to advance structure-based applications in biomedicine and biotechnology. The student will engage in an intensive research program aimed at elucidating the structure-property relationships of NP's involved in the formation of dynamic RNA-signaling complexes related to human disease. This will include recombinant protein expression, biochemical and biophysical characterization, and structural analysis of protein-protein and protein-ligand interactions.

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NATURE 2006

Project # 34

MULTI-COMPARTMENT DISTRIBUTION OF POLYCYCLIC AROMATIC COMPOUNDS IN ARCTIC SEABIRDS

Dr. Gregg Tomy (Gregg.tomy@UManitoba.ca, (204) 474-8127)

INTRODUCTION:

Polycyclic aromatic compounds (PACs) are environmentally persistent pollutants that can bioaccumulate in wildlife. Because of their high trophic position, seabirds are useful sentinels for monitoring environmental contamination in Arctic ecosystems. Assessing PAC burdens in different tissues allows for insights into chemical partitioning, metabolism, and potential toxicity. This project focuses on tissue-specific PAC distribution in Arctic seabirds to better understand exposure and bioaccumulation patterns.

PROJECT:

This project explores the multi-compartment distribution of PACs in two Arctic seabird species, black guillemots (*Cepphus grille*) and common Eider (*Somateria mollissima*), to evaluate exposure, tissue partitioning, and bioaccumulation dynamics. Polycyclic aromatic compounds are generated primarily through the incomplete combustion of organic material and can be transported long distances *via* atmospheric and oceanic currents, making remote regions like the Canadian Arctic vulnerable to contamination despite limited local sources. In 2023, ten individuals from each of two seabird species were collected from Postville (northern Labrador) as part of Environment and Climate Change long-term monitoring program. From each bird, five tissue types were collected: liver, kidney, heart, whole blood, and feathers. These tissues differ in metabolic activity, excretion potential, and lipid content, making them useful for assessing PAC distribution and potential routes of elimination or storage. Tissue samples will be extracted and analyzed using gas chromatography-tandem mass spectrometry (GC-MS/MS) to quantify a broad suite of PACs. The study aims to identify patterns of accumulation across tissues and between species and to evaluate potential biomarkers of contaminant exposure (e.g., feather concentrations).

Project # 35

Shear Logic: Designing Molecules That Compute Under Stress

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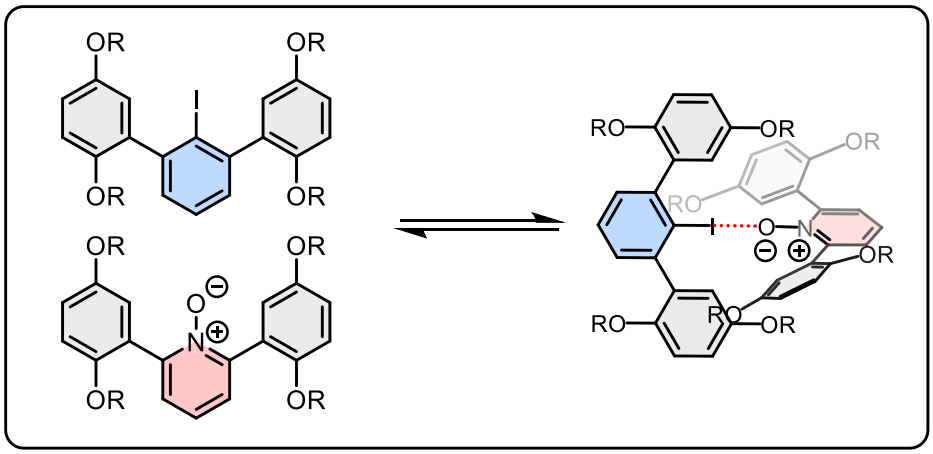
INTRODUCTION:

Shear-responsive fluids change viscosity under mechanical stress, transitioning between Newtonian, shear-thinning, or shear-thickening behavior. Embedding this functionality at the molecular level creates molecular logic gates[1], in this case, molecules that perform logic-like responses to shear. This project explores the design of such materials using halogen bonding[2], a reversible noncovalent interaction that can modulate molecular assembly under flow. By controlling structure and interaction sites, it may be possible to design molecules that exhibit distinct, shear-triggered viscosity states.

PROJECT:

This project involves synthesizing 1,2,3-trisubstituted benzenes and pyridines capable of forming halogen-bonded assemblies. The goal is to create a first-generation of two-state shear-responsive molecules that switch from Newtonian to non-Newtonian flow behavior under stress. Insights from this series will guide the future design of three-state molecular systems. The student will carry out synthesis and materials characterization using NMR, mass spectrometry, FTIR, UV-Vis absorption and emission spectroscopy, and rheology to link structure to shear behavior.



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Project # 36

Studying Molecules at the Edge of Order and Chaos

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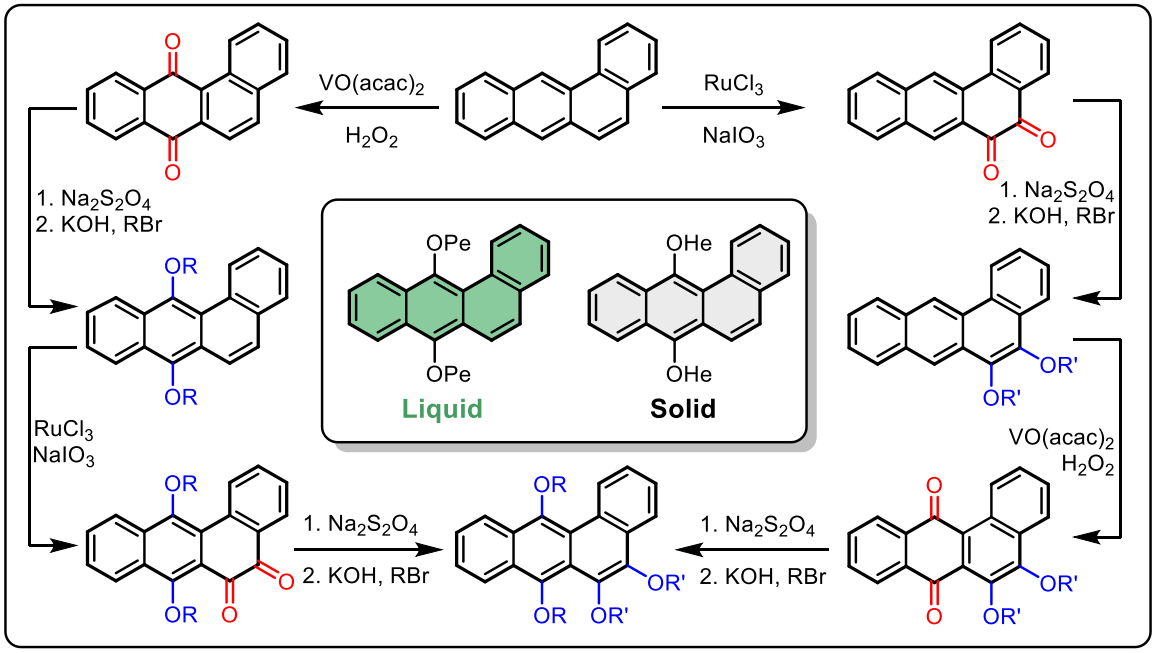
INTRODUCTION:

Organic chromophores that function in the liquid state are essential for emerging technologies like flexible displays and printable electronics.[1] Yet, the molecular rules that govern how structure affects fluidity and photophysical properties remain underdeveloped.[2] Benz[a]anthracene (BaA), with its low symmetry and tunable quinone chemistry, offers a powerful scaffold to study molecules at the boundary of order and disorder.

PROJECT: Building on a recently synthesized series of 7,12-dialkoxy BaA derivatives, this project will focus on two new classes: 5,6-dialkoxy and tetraalkoxy BaA derivatives. These systems are designed to access new regions of phase space and deepen understanding of how substitution patterns affect viscosity, emission, and aggregation. Characterization will include NMR, mass spectrometry, UV-Vis, fluorescence spectroscopy, and rheology. The goal is to uncover design rules for functional liquid chromophores with tunable optical properties.



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Project # 37

The Ratio of Tryptophan and Kynurenine in Saliva at Three Exercise Intensities

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INTRODUCTION:

Anxiety and depression are conditions that effect more than one in ten Canadians.[1] Physical exercise is used as a natural remedy for many patients, but the exact mechanisms and pathways remain undiscovered.[2] Tryptophan is an essential amino acid that can be broken down to kynurenine or serotonin through two separate biological pathways. The ratio of tryptophan to kynurenine has been linked both to mental illnesses and physical activity.[3][4] To date the effect of the intensity of exercise on the tryptophan and kynurenine ratio has not been properly explored. The objective of this project is to determine the effect on tryptophan to kynurenine ratio for three common exercise intensities, so that exercise can be more accurately prescribed as a natural remedy for anxiety and depression.

PROJECT:

This project will involve subjecting individuals to various intensities of activity and measuring the tryptophan to kynurenine ratio in their saliva using high performance liquid chromatography tandem mass spectrometry. 5+ subjects will perform VO_2 Max tests to obtain a personal associated lactate level with three common exercise intensities: maximum fat oxidation, lactate threshold and VO_2 max. Subjects will complete training sessions at the target intensities, taking saliva samples once before, four times during and three times post training. Subjects will also take lactate readings four times during the sessions to ensure that they are working within the proper intensity. Samples will be analyzed for tryptophan and kynurenine using HPLC-MS/MS.

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Project # 38

ADAPTIVE LABORATORY EVOLUTION OF *Escherichia coli*: SYNTHETIC LIFE MICROBES THAT THRIVE ON PLASTIC OR SYNTHETIC SUBSTANCES

Dr. Nediljko Budisa (nediljko.budisa@umanitoba.ca, (204) 474 9178)

INTRODUCTION:

We aim to create synthetic cells through top-down synthetic biology, focusing on engineering *Escherichia coli* to metabolically adapt to synthetic amino acids and materials like plastics as their sole carbon source. These biosafe cells will produce protein-based biomaterials crucial for tissue engineering, materials science, and environmental remediation. Our research environment prioritizes student learning in synthetic biology and organism-directed evolution.

PROJECT:

Our first experiment involves performing adaptive laboratory evolution (ALE) of *E. coli* cells in a medium containing fluorinated amino acids or plastics such as PET as the sole carbon source. Students will participate in the development of experiments with evolving microbial cultures with synthetic substances. The ALE experiments will focus on the creation of auxotrophic *E. coli* strains capable of metabolising halogenated amino acids or plastic. In ALE, several lines (at least 4) are used to distinguish adaptive mutations from hitchhiker mutations, supported by control experiments. Analysing the ALE process will provide insights into cellular functions, genetics, proteomics, and morphology, thus advancing synthetic biology for the development of innovative technologies.

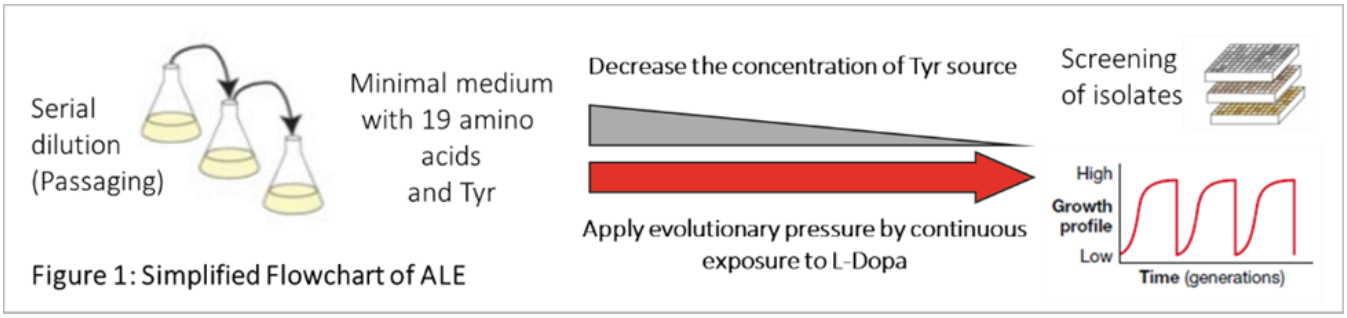

Figure 1: Simplified Flowchart of ALE

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Project # 39

EXPANDING THE GENETIC CODE BY DIRECTED ENZYME EVOLUTION

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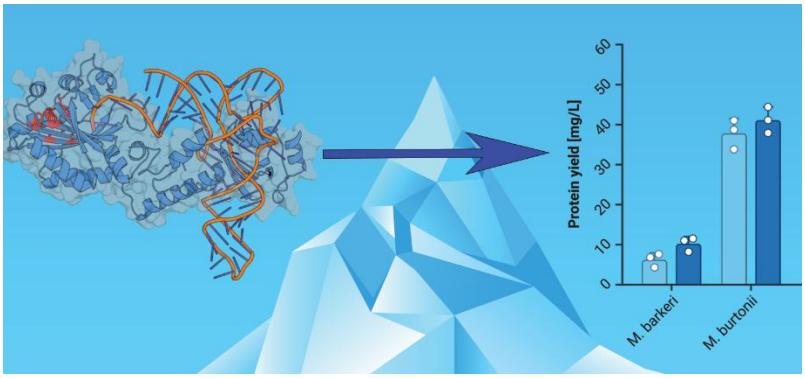
INTRODUCTION:

Aminoacyl-tRNA synthetases (aaRSs) are vital enzymes that ensure precision in translating the genetic code by attaching specific amino acids to their corresponding tRNAs. The natural genetic code limits the range of canonical amino acids permitted for ribosomal translation. Expanding this repertoire beyond the standard 20 necessitates altering the substrate specificity of aaRSs, as they play a fundamental role in interpreting the genetic code.

PROJECT:

Over 200 non-canonical amino acids (ncAAs) have been incorporated into proteins using diverse genetic code expansion methods, including selective pressure incorporation, stop codon suppression, fragment condensation, protein semisynthesis, and peptidomimetics. These ncAAs, with non-proteinogenic functional groups, offer tools to manipulate and explore various aspects of protein biology, including structure, dynamics, function, interactions, catalysis, folding, synthesis, trafficking, degradation, and aggregation.

The proposed research will establish a cutting-edge learning environment for students to delve into directed enzyme evolution. This will involve testing and enhancing existing enzymes, as well as screening orthogonal pairs of aminoacyl-tRNA synthetase (aaRS) and tRNA from available sources for beginners. Advanced students will design enzyme and tRNA libraries to further expand their understanding and skill set in this field. technologies.



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Project # 40

Photoaminocatalysis Design and Development

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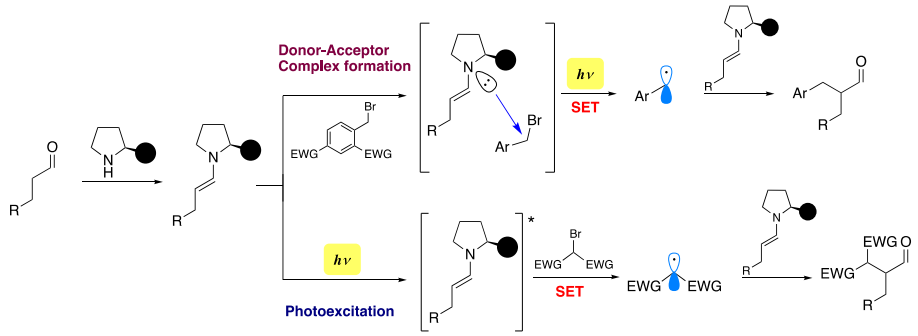
INTRODUCTION:

Photo-organocatalysis is set to be the next major advancement in the field of asymmetric synthesis and provide access to previously unachievable transformations. Recently it has been demonstrated that organocatalytic enamine intermediates can interact with visible light to directly activate substrates via single electron transfer (SET). The photocatalytic activity of these enamines holds great promise for the development of new asymmetric, regioselective reactions.

PROJECT:

The proposed work aims to determine the influence of the catalyst scaffold on promoting SET processes and identify what features should be considered when designing a photocatalyst or a photocatalytic reaction. Employing a combination of spectroscopic studies and theoretical calculations on the reactive enamine intermediates, formed from a range of chiral secondary amines, we will be able to establish which features of the catalysts are responsible for the absorption properties of the enamines. The results provided by these studies will serve to guide our reaction and catalyst design efforts and aid in the application of this methodology in new stereoselective γ- and ε-addition reactions. The student involved in this project will begin by using DFT methods to understand the interactions of the catalysts and substrates they will later move into the lab to study these interactions using state of the art spectroscopic methods including in situ IR and NMR flash photolysis.



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Project # 41

Decoding Protein Conformation Sensitivity in Molecular Docking: A Structure-Performance Analysis

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INTRODUCTION:

Computational docking is a cornerstone of structure-based drug design, but its predictive accuracy is highly dependent on protein conformation. Identifying which features of protein-ligand complexes yield reliable docking outcomes is essential for improving both methodology and drug discovery success rates. This project focuses on understanding the structural and physicochemical determinants of docking performance across different protein targets.

PROJECT:

This project aims to evaluate how variations in protein structure impact molecular docking outcomes, with a focus on identifying features that correlate with consistently high predictive performance. Using pre-curated ensembles of protein structures, the student will rank protein conformations based on docking accuracy metrics (e.g., AUC, EF1%) and analyze differences in binding pocket properties—such as volume, shape, and electrostatics. Advanced statistical and machine learning techniques (e.g., PCA, t-SNE, and random forest classifiers) will be used to identify predictive structural features. The student will also compare patterns across protein families to determine whether determinants of docking success are target-specific or universal. The final outcome will be a structural-performance map to guide future docking workflows.