CHEM4710

Honours Project in Chemistry or Biochemistry

2023/2024 Projects

University of Manitoba

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1. WELCOME

Welcome to the 'Honours Project in Chemistry or Biochemistry' (CHEM4710) for the 2023/24 academic year. The 'Honours Project in Chemistry or Biochemistry' is a research project based course providing undergraduate chemistry and biochemistry students with the opportunity to conduct original research as part of an active research group. The research project extends over a duration of 2 consecutive terms (Sep. 2023 – Apr. 2024). Students can request projects based on the list of projects provided in this booklet. Throughout the research projects students will receive guidance and support from their research advisors and other research group members. Notably research environments are very diverse in the Department of Chemistry and naturally individual research groups may operate differently and have varying foci. Specifics need to be discussed with the project advisors. The Department of Chemistry at the University of Manitoba is a medium size department and is well situated within the top 15 Canadian Universities (U15). In general the research groups in the Department of Chemistry are highly competitive, recognized in their respective fields and contribute to the large fields of chemistry and biochemistry. The experimental and theoretical opportunities offered in the Department of Chemistry are excellent with well equipped laboratories, state-of-the art instrumentation and outstanding expertise. The majority of the research is being conducted in the Parker Building and additionally many groups collaborate with other departments, faculties/schools and institutes within the University of Manitoba. The majority of research groups maintain national and international collaborations and are part of large scale facilities such as national laboratories and institutes all around the world.

I 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 a research-filled year of CHEM4710 projects for 2023/24.

Dr. Mario Bieringer
Course coordinator for CHEM4710 2023/24

2. INTRODUCTORY COMMENTS:

Students interested in taking CHEM4710 should look at all offered projects provided in this booklet and need to contact project supervisors and discuss any of the projects listed in this booklet. During those meetings the nature of the projects should be discussed and expectations should be made clear. Please note that project advisors are happy to meet with you to discuss their research projects. Students are expected to meet with at least 3 faculty members and are required to complete the 'Student – Faculty Interviews' page (Appendix A). Please prioritize your project choices on the attached 'Student Project Choices' page (Appendix- B). A minimum of 3 choices should be submitted and comments can be added in the provided comment field. In order to be considered for the entire set of advertised projects you are asked to submit the 'Student – Faculty Interviews' page and 'Student Project Choices' page with your project choices to Dr. Mario Bieringer (Mario.Bieringer@UManitoba.ca) by July 17th, 2023. Matching of students with research projects will only occur after July 17th, 2023. Students can submit your project choices after that date as well, however the number of available projects might be limited by then. Students will be informed about their projects by August 1st, 2023.
The research projects will start during the first week of the 2023 Fall term. For each project the student and project advisor must submit a completed and signed 'Student – Advisor Agreement' (Appendix-C) no later than September 22nd, 2023. 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 dates for the class meetings are tentative. Students should reserve Fridays the time slot from 1:30 pm till 2:20 pm for CHEM4710 meetings for the Fall 2023 and Winter 2024 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 on December 8th, 2023. The expectations for the progress report are clearly stated in the course syllabus. The research projects should be concluded by the end of the 2024 Winter term. On Saturday March 23rd, 2024 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 on April 9th, 2024. The final report will be graded by an expert reader who is familiar with the research subdiscipline and another faculty member as a non-expert reader whose research is in a different subdiscipline.

3. IMPORTANT DATES & DEADLINES

Jul. 17th, 2023	Students **submit project choices** to the course coordinator
Aug. 1st, 2023	Students receive **project assignments**
Sep. 6th, 2023	Students **begin** research projects (first day of classes)
Sep. 8th, 2023	**Class meeting #1** - Orientation meeting (all students and supervisors)
Sep. 22nd, 2023	**Signed contracts** (Student – Advisor Agreement) due
Sep. 22nd, 2023	**Class meeting #2** (Library resources and literature search)
Oct. 13th, 2023	**Class meeting #3** (Academic integrity)
Oct. 27th, 2023	**Class meeting #4 (**3 minute project presentations)
Nov. 10th, 2023	**Class meeting #5** (Report writing and proposal development)
Dec. 8th, 2023	Written progress report **due**
Jan. 12th, 2024	**Class meeting #6** (Career choices in chemistry and biochemistry)
Feb. 9th, 2024	**Class meeting #7** (Academic writing & peer review process)
Feb. 2nd, 2024	**Last day** for students to meet with course coordinator for proposal discussion.
Feb. 26th, 2024	Proposals **due**
Mar. 1st, 2024	**Class meeting #8** (Effective oral presentations)
Mar. 4th, 2024	Student evaluations of proposals **due**
Mar. 19th, 2024	Title and abstracts for oral presentations **due**
Mar. 23rd, 2024	**Oral research project presentation day**
Apr. 9th, 2023	Final written reports **due**

4. COURSE SYLLABUS

GENERAL COURSE DESCRIPTION:

CHEM4710 is a 6 credit hour research project course. Students will carry out research as a member of a research group in the Department of Chemistry. The course counts for 6 credit hours, and it extends over both the fall and winter terms. Students in CHEM4710 are expected to begin work on their research project at the beginning of September 2023 and to maintain a steady level of work during the entire academic year.

All available course projects will be made available to all students interested in or considering in taking CHEM4710 in Fall 2023/Winter 2024. Each project will consist of a brief 1 page description. Students are encouraged to read all projects and arrange appointments with supervisors for a brief interview/discussion. Each student needs to meet with 3 potential supervisors. Following those meetings students should submit their preferred project choices to the course coordinator in order of preference (e.g. 1st choice: "The investigation of ….", 2nd choice: "Synthesis of …", etc.). Project matching will commence after Jul. 10th, 2023 and the project assignments will be e-mailed to the students and supervisors on August 1st, 2023.

Throughout the project students are expected to consult regularly with their advising professor to ensure that adequate progress is being made. Each student in CHEM4710 is expected to conform to university standards of laboratory safety at all times and will also meet the standards of the research group that they are working in with regard to experimental procedures, notebook keeping, and general laboratory behavior.

The role of the student is to be an active and productive member of the hosting research group. CHEM4710 students will work on their own specific projects that are assigned. However, this project is likely integrated into the larger research program underway in the research group. Therefore, communication with group members and the research advisor is extremely important. The CHEM4710 project is an excellent opportunity to participate in the "life" of the research group and to learn from the senior members. Your active participation in the group as part of the CHEM4710 experience can also give you a good impression of what graduate studies would be like. More importantly, a good performance in the group will also earn you a positive reference from your advisor for any future applications for graduate studies, other degrees or for entry into the workforce.

The role of your advisor is to help guide your entry into the world of research. This quite often is a markedly different experience than what you have experienced in typical teaching laboratories. The transition into independent research can be challenging in some cases. The role of the advisor is to help you, point you at relevant literature, describe the opportunities and pitfalls, while at the same time avoiding guiding you in minute detail. The success of your research project lies with your ability to work in the research lab in a self-motivated manner and to develop a measure of independence in your abilities. Although your advisor is available to provide guidance on the preparation of your research proposal, reports, and presentations, the responsibility for the completeness of these course requirements rests solely with the student.

CHEM4710 projects provide the opportunity to develop practical lab skills beyond those that are usually taught in a 1st, 2nd or 3rd year laboratory course. The CHEM4710 course also provides the opportunity to develop other essential skills such as self-motivation and time management that allow you to be organized in your research. You will also be required to describe your results in a format that is more than a simple 'lab report' in both the written and oral presentation. A major part of the evaluation of your performance is on how well you develop these skills and not necessarily on the perceived success of your project. One meaningful result, generated in September, poorly reported on and described in a rambling talk will not rank the same as a series of carefully recorded experiments repeated several times and described in detail that nonetheless failed to work in the expected manner or at all.

I) INSTRUCTOR INFORMATION:

Course Coordinator:

Name: Dr. Mario Bieringer

Office: 520c Parker Building

E-mail: Mario.Bieringer@UManitoba.ca

Phone: (204) 474 6258

II) EVALUATION:

3 minute presentation	**3%**
Written Progress Report	**14%**
Proposal	**8%**
Oral Presentation	**20%**
Research Effort (Evaluated by the research advisor(s))	**20%**
Written Final Report (Evaluated by 2 readers)	**35%**

Final numerical scores will be converted to letter grades. As this is a senior level course, the marking scale will assume that F = less than 50%. Other scores will be scaled appropriately between D and A+ as described below. Ins

Percentage Score	Letter Grade	Grade Point Value
90.0 -100.0	A+	4.5
80.0 - 89.9	A	4.0
75.0 - 79.9	B+	3.5
70.0 - 74.9	B	3.0
65.0 - 69.9	C+	2.5
55.0 - 64.9	C	2.0
50.0 - 54.9	D	1.0
0.0 - 49.9	F	0.0

III) COURSE PARTICIPATION:

- Students are encouraged to attend the Departmental Seminars.
- Attendance of all Friday CHEM4710 class meetings (listed in the table below) is **mandatory**.

Date	Time	Location	CHEM4710 Class Meetings	Presenters
Sep. 8th, 2023	3:00–4:00pm	t.b.d.	Orientation Meeting	Mario Bieringer
Sep. 22nd, 2023	1:30-2:20pm	t.b.d.	Library and literature searches	
Oct. 13th, 2023	1:30–2:20pm	t.b.d.	Academic Integrity	
Oct. 27th, 2023	**1:30–3:20pm**	t.b.d.	3 min presentations	Students
Nov. 10th, 2023	1:30–2:20pm	t.b.d.	Report and proposal writing	Mario Bieringer
Jan. 12th, 2024	1:30–2:20pm	t.b.d.	Career choices	Mario Bieringer
Feb. 9th, 2024	1:30–2:20pm	t.b.d.	Academic writing & peer review	Mario Bieringer
Mar. 1st, 2024	1:30–2:20pm	t.b.d.	Oral presentations	Mario Bieringer

IV) IMPORTANT DATES:

The dates below are fixed and no extensions are possible.

Date	Milestone
Jul. 17th, 2023 (Monday)	Students submit project preferences to the course coordinator
Aug. 1st, 2023 (Tuesday)	Students receive project assignments
Sep. 22nd, 2023 (Friday)	Signed research contract **due**
Dec. 8th, 2023 (Friday)	Written progress report **due**
Feb. 2nd, 2024 (Friday)	**Last day** for students to meet course coordinator for proposal discussion
Feb. 26th, 2024 (Monday)	Proposals **due**
Mar. 4th, 2024 (Monday)	Student evaluations of proposals **due**
Mar. 19th, 2024 (Tuesday)	Title and abstract for oral presentations **due**
Mar. 23rd, 2024 **(Saturday)**	Oral presentation day
Apr. 9th, 2024 (Tuesday)	Written final report **due**

V) DESCRIPTIONS OF COURSE COMPONENTS:

- **Project Descriptions**
  Students should read all project descriptions and arrange for a minimum of 3 meetings with potential project supervisors. Supervisors must be full time faculty members in the Department of Chemistry. Please note that potential supervisors cannot promise projects to students.

- **Project Preferences**
  Due Monday July 17th, 2023 for the first project selection round. Students should submit their project preferences by that date by e-mail to the course coordinator (Mario.Bieringer@UManitoba.ca). The forms for this submission are part of the project description booklet. Students submitting their project requests after July 17th, 2023 may only be able to choose from a smaller (i.e. remaining) set of available projects.

- **Project Assignments** – Available Tuesday August 1st, 2023
  Students and supervisors will be informed regarding their projects on August 1st, 2023. It should be noted that every effort will be made to match students with their highest priority choices. However, this will not always be possible because multiple students may apply for the same project. Students applying for projects after August 1st, 2023 may do this up to the late registration deadline, however it is strongly encouraged that students start meeting with supervisors early on and submit their preferences as early as possible.

- **Written Progress Report** – Due Friday December 8th, 2023 (submit to Mario Bieringer)
  The Progress Report will be handed in to the course coordinator by e-mail (Mario.Bieringer@UManitoba.ca) for marking.

  The report should consist of:

  - a description of the goal(s) of the research project,
  - a detailed survey of the relevant literature that puts the project in context,
  - a description of the planned methods for the research project,
  - a summary of your research results during the Fall term including experimental data.

  The progress report should be about 2000 – 3000 words in length with **double-spaced pages** and will include any relevant figures and references (which are not included in the word count). It should conform to one of the formats described below for the Final Report. Students should have their research supervisor review and approve their report before handing it in to the course coordinator. It is important that the report makes the project **clear to a scientifically literate but non-expert reader**.
  The Progress Report is a crucial document that makes sure that projects are progressing, that there are no misunderstandings in terms of expectations and that the relevant literature has been digested. The graded progress reports will be returned to the students with comments and suggestions. The comments will be important for preparing the final report and for the oral presentation. It is well worth the effort to ensure that the progress report is as complete as possible as this effort will pay off at the end of the course. Electronic progress reports must be received by e-mail by the end of day on Dec 8th, 2023 to be considered for credit in the course.

- **Proposal** - Due Wednesday February 26th, 2024
  The proposal is a 2 to 3 page document with additional figures and references based on the students research project. The purpose of the proposal is that based on the critical evaluation of the students research (results, difficulties, challenges etc.) a concise request for follow up research will be written. Students are not supposed to propose new research, instead the request should enable the student to further or complete their current research. The following cases highlight possible proposal requests:

- If a student has experienced challenges that cannot be addressed in the current research group, the student may choose to write a proposal for access to an external research facility or a request for a collaboration.
- A proposal could also focus on obtaining specific materials (e.g. isotopes, starting materials, experimental probes). Alternatively, the proposal may focus on developing the current emphasis of the project towards a new direction (but not a new project)
- etc.

Proposals should be discussed with and approved by the course coordinator no later than Feb. 2nd, 2024. Every student will have to prepare a brief outline of the proposal before that meeting, a couple of sentences are sufficient. The course coordinator needs to be given the chance to at least identify the overall direction of the proposal before meeting with the student. The coordinator will comment and advise on the proposal during the meeting.

The final proposal will be peer reviewed by 2 CHEM4710 students and the course coordinator. The students need to submit their evaluations to the course coordinator by March 4th, 2024. Students will receive grades for their evaluations. The total proposal mark will be based on the quality of the student proposal and the 2 evaluations each student has submitted.

- **Title and Abstract for oral presentations** - Due Tuesday March 19th, 2024
  The Title and Abstract must be e-mailed to Mario Bieringer (Mario.Bieringer@UManitoba.ca) by Thursday March 19th, 2024. It is important to meet this deadline in order to create a presentation schedule on time for the oral presentation day.

- **Oral Presentations** - Saturday March 23rd, 2024
  You will be required to give a 15 minute oral presentation summarizing your research project. The presentation will be followed by 5 minutes for questions. The presentations will be moderated by the course coordinator who will strictly follow the time limits. An oral presentation normally consists of an introduction, a brief description of relevant methods, results and discussion, and conclusions; the last slide is typically an acknowledgment of the advisor and assistance provided by others during the project. It is essential that students prepare and practice their presentations to effectively communicate their project within these time limits. There will be a scoring penalty for exceeding the 15 minute time limit on the presentation.

  Please note that the final presentations are open to all members of the university community as well as the public and will be advertised on campus. Partners, family members and friends are particularly welcome to attend. Recording of any of the presentations will NOT be permitted.

  The use of PowerPoint (or equivalent software) is the standard for scientific presentations. You should plan to give your oral presentation using the computer that is provided in the room – or with your own laptop if you choose.

  This is a full day public event resembling a small conference. The audience usually consist of faculty members, research associates, postdocs, graduate students, undergraduate students and visitors such as friends and family members. All members of the audience will be allowed to ask questions. All CHEM4710 students are required to grade all (except their own) presentation, in addition all other audience members are encouraged to grade the presentations.

- **Final Report** - Due Tuesday April 9th, 2024 (17 days after the oral presentations)

  The final report is a major part of the evaluation for the project course. It will be marked by two readers. One reader will be close to your research sub-discipline, the second reader will be a faculty member from the Department of Chemistry who is not an expert in your sub-discipline.

  You need to submit the final report as a properly formatted PDF document to the course coordinator (Mario.Bieringer@UManitoba.ca). The course coordinator will distribute the reports to the two readers.

  Each reader will grade your report, both reviews together will be worth 35% of the course grade. It must be emphasized that the report has to be comprehensible to the general scientifically literate reader, and this will be taken into account when marking it. The report must show that you understand the context of the project as well as the actual experiments that you have done. The typical length for the final report is 6000 – 8000 words with double-spaced pages and including figures and references (which are not included in the word count). The exact length will depend on the style of reporting that is specific to the sub-discipline that your project falls in.

  The final report must be a formal piece of scientific writing, with Introduction, Results, Discussion, Conclusion and Experimental (Methods) sections. You may find it more effective if the Results and Discussion sections are combined. The report should also include the relevant figures and references as

  needed to make the report complete and clear. It should follow the style conventions of an appropriate scientific journal, the American Chemical Society (ACS) journals provide good templates to follow. Stylistic rules are found on journal Web pages and students are encouraged to consult the journal (i.e. J. Am. Chem. Soc.; J. Org. Chem. or J. Phys. Chem., Biochemistry) most appropriate to their project. Another useful resource is the ACS Style Guide which is available online and in the library and can offer useful information on formatting and referencing. Consult your advisor before beginning to write, to determine an appropriate approach. Students should have a draft of the report completed by early-March. Advisors are urged to provide constructive comments on their students' draft reports before the final version is submitted.

  Written reports should be reasonably free of typographical errors and be checked thoroughly for spelling and grammar. Frequent spelling or grammatical errors detract from the readability of your proposal,

  report or presentation, generate an impression of sloppiness with the audience, and will often result in a lower grade. The same applies to inconsistent formatting of text and figures in the report and references. Therefore, you are strongly advised to use the spelling and grammar checking functions on your word processing software. In addition, you will find the formatting and document handling features of the word processing software very useful. You are also strongly encouraged to use the "ACS 1996" template for formatting your ChemDraw structures. You should consider asking other members of your research group or another student in the project course to help proofread your documents. Your supervisor will be very willing to provide feedback on the content of your report, and this will be more meaningful on a report free of errors.

  The target audience, for your proposal, oral presentation and formal reports, is a student at approximately your stage in the Chemistry or Biochemistry program who may not be familiar with the specifics of your research project. The use of acronyms and shorthand notations should be kept to a minimum or fully explained. The formal report should attempt to describe in as much detail as possible all of the work you have done during the course of the project. However, in your oral presentation - where you have limited time - you may wish to provide a summary of the most significant results that you generated.

VI) ADDITIONAL INFORMATION:

Conference Opportunities

- **The 2024 Western Canadian Undergraduate Chemistry Conference (WCUCC – 2024)**
  It is highly recommended for all CHEM4710 students to consider presenting their research at the 2024 'Western Canadian Undergraduate Chemistry Conference' (WCUCC). This annual conference usually takes place in May in one of the universities west of Ontario. Date and place will be communicated at a later point in time. The format of oral presentations is identical to that used in CHEM4710, so you will already have a talk prepared by the time the course is complete. It is a superb opportunity for you to start some professional networking, and there are cash prizes for outstanding presentations. Interested students need to pre-register in January or February for this conference. There are some travel funds available for students (or groups of students) that intend to present at this conference.

- **Canadian Chemistry Conference and Exhibition (CCCE-2024)**
  The Canadian Chemistry Conference and Exhibition 2024 (CCCE-2024) is the national conference for chemists in Canada with up to 2000 delegates from all over Canada and a significant number of international speakers. The conference will be held in Winnipeg from June 2nd till June 6th, 2024 and will provide an excellent opportunity to highlight your research and to network with globally leading researchers. CHEM4710 students are encouraged to present their research at the CCCE-2024. The CHEM4710 project provides an excellent base for presenting a poster at that event. Note that conference registration is expected between the 1st week of January and mid February 2024.

VII) ACADEMIC INTEGRITY POLICIES:

Academic Dishonesty:

The University of Manitoba treats plagiarism and cheating as serious academic offenses.

- **The complete documentation regarding cheating, plagiarism and fraud be accessed in the calendar at:**
  http://umanitoba.ca/student/resource/student_advocacy/cheating_plagiarism_fraud.html
- **Additional documentation is available on the Faculty of Science website**
  https://sci.umanitoba.ca/statement-on-academic-dishonesty/

END OF SYLLABUS

5. PROJECTS

The following projects are being offered under the course number CHEM4710.

It should be noted that biochemistry students can choose to take **MBIO4530** instead of CHEM4710 for credit for their program. The following Professors from the Microbiology department have indicated to offer biochemistry related research projects as part of MBIO 4530.

- **S. CARDONA** Molecular mechanisms that control bacterial growth in different settings, such as during infection or biotechnological processes. Methods: functional genomics, synthetic biology tools, CRISPRi. Current projects: antibiotic discovery and degradation of bioplastics. Contact: Silvia.Cardona@umanitoba.ca

- **G. PREHNA** Molecular mechanisms of bacterial communication, inter-bacterial competition, and host-adaptation by *Streptococcus* (e.g. Strep throat) and by *Salmonella* (e.g. food poisoning). Our research is multidisciplinary combining biochemistry, molecular biophysics, microbiology, and structural biology. Contact: Gerd.Prehna@umanitoba.ca

- **H. J. WIEDEN** The design of molecular machines (ribosomes) involved in bacterial translation with a particular focus on antibiotic function and the rational construction of novel biological nanomachines and devices. We use a multidisciplinary approach based on advanced biophysical, computational and synthetic biology methods to development novel antimicrobial strategies. Hans-joachim.wieden@umanitoba.ca

Project #1

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.
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.

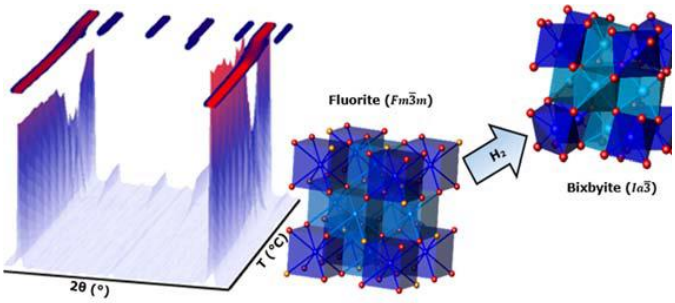

Figure 1: Real time *in-situ* X-ray diffraction experiments illustrating the selected oxide removal from the disordered fluorite structure (right structural diagram) during reduction of $Y_{(1-x)}Pr_xO_{3.5}$.

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 #2

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. Among magnetic materials particularly interesting are examples that do not show classical long range magnetic ordering at low temperatures. Magnetic ordering can be manipulated by 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 not able to satisfy all interactions simultaneously, see figure 1. For large magnetic moments a 120° compromise structure may be observed. In contrast small magnetic moments (e.g. d^1 ➔ S=1/2) 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.

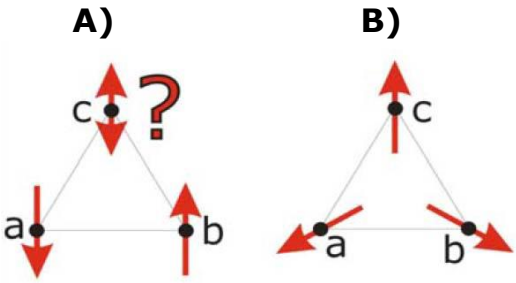

Figure 1: *A) Geometric magnetic frustration. 3 spins on a triangular lattice cannot align antiparallely with respect to each other. B) 120° magnetic structure for*

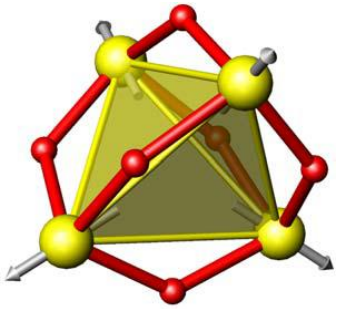

Figure 2: *Tetrahedral spin arrangement on metals (yellow) with oxide (red) bridges responsible for magnetic exchange.*

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 in order to realize quantum behaviour. The work will be based on ABO_3 and ABO_4 structures where A is a diamagnetic cation (Ca, Sr, La, Y, Lu etc.) and B is a redox active cation such as Ti, V, Cr, Mn or Fe etc. Notably the ABO_3 and ABO_4 samples are chosen in order 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 establish the newly generated phases and advanced physical 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.

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[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 #3

Adaptive laboratory evolution (ALE) of *Escherichia coli* and other microbes relevant to synthetic life and related technologies

Prof. Dr. Nediljko Budisa (nediljko.budisa@umanitoba.ca, http://chemsynbio.com)

INTRODUCTION:

Organofluorine and organohalogens compounds, which are used massively in industry, agriculture and human households, are also known as "inert" substances that have a strong tendency to accumulate and persist in soil and water, and are therefore extremely difficult to remediate. Microorganisms, and in particular bacteria, which have an exceptional ability to develop rapid metabolic or genetic responses to chemical stresses (such as *Escherichia coli* and *Pseudomonas putida*), are the most attractive research vehicles to develop new solutions to detoxify halogenated compounds, for example, by acquiring them as substrates for cellular biotransformations and growth. Our methodology can be broadly regarded as a framework for developing synthetic cells and associated technologies, drawing inspiration from natural structures and processes. These cells are biosafe, including a built-in genetic firewall, and can be applied in diverse fields, such as human health, smart biomaterials and devices, and environmental remediation.

The planned research should create a state-of-the-art environment for students and trainees to learn the discipline of synthetic biology and to provide the necessary infrastructure to supplement the existing faculty.

PROJECT:

As the simplest experiment, we will set up adaptive laboratory evolution of *E. coli* cells thriving in an artificial medium containing fluorinated amino acids (e.g., fluoroprolines or fluorotyrosines) or any other amino acid analogs (e.g., methionine analogue ethionine) as an example of currently widely used aromatic and aliphatic organofluorine compounds. We will develop microbial cultures that are fully adapted to defined media containing fluorinated amino acids as environmental stressors in relatively short periods of time.

ALE experiments will be set up to evolve suitable auxotrophic *E. coli* strains to incorporate halogenated amino acids (Fig. 1). We will exert increasing selection pressure by reducing the availability of canonical to full exhaustion. ALE experiments will be performed with multiple lineages (at least 4) so that adaptive mutations can be distinguished from hitchhiker mutations with properly designed control experiment. The analysis genomic mutations (UofM DNA Sequencing Services), dynamics of proteome (SILAC/TMT, in collaboration with Manitoba Centre for Proteomics and Systems Biology) and metabolomes of the adapted strains will enable us to set forward working hypotheses that need to be tested experimentally. For example, mutated enzymes or proteins involved in tyrosine uptake, metabolism and translation will be isolated and separately measured in order to address their role in adaptation.

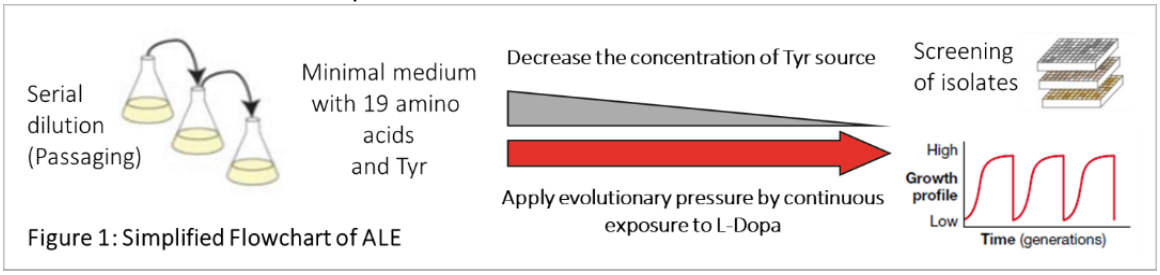


Figure 1: Simplified Flowchart of ALE

Reading:

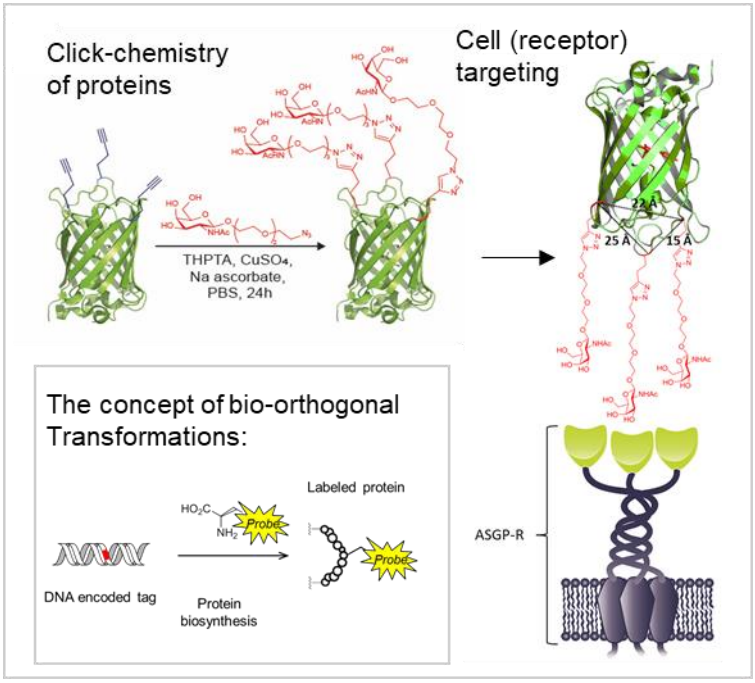
M.G. Hoesl, S. Oehm, P. Durkin, E. Darmon, L. Peil, H-R. Aerni, J. Rappsilber, J. Rinehart, D. Leach, D. Söll, N. Budisa, *Chemical Evolution of a Bacterial Proteome, Angew. Chem. Int. Ed. Engl.* **2015**, *54*, 10030–10034.F. Agostini, L. Sinn, D. Petras, C.J. Schipp, V. Kubyshkin, A. A. Berger, J. Rappsilber, P.C. Dorrestein, N. Budisa, B. Koksch, Multi-omics analysis provides insight into the laboratory evolution of Escherichia coli towards the metabolic usage of fluorinated indoles. *ACS Cent. Sci*. **2021**, 7, 1, 81–92.

Project #4

An expanded genetic code for the design of therapeutic proteins by site directed modifications and bioorthogonal conjugations.

Prof. Dr. Ned Budisa (nediljko.budisa@umanitoba.ca, http://chemsynbio.com)

INTRODUCTION:



Budisa' s team actively contributed during the formative stages of the ground-breaking research in the Genetic Code Expansion and Bioorthogonal Chemistries, recognized by the recent awarding of the 2022 Nobel Prizes to Bertozzi, Medal, and Sharpless. These emerging fields hold immense potential, particularly in the realm of protein engineering and design, leveraging non-canonical amino acids to create a diverse array of target proteins and protein complexes.

Our work is highly innovative, as we pioneer technologies that enable the mimicking of posttranslational modifications (PTMs), with a particular focus on glycosylations and halogenations and other modifications. Our research yields homogeneous preparations of viral and bacterial proteins, possessing a precisely defined chemical composition, thereby rendering them suitable for therapeutic applications.

Our students will gain core competencies in both protein production and protein engineering and design with an expanded genetic code, enabling us to design various proteins, protein-complexes, and particles. The work will be performed mainly with Green Fluorescent Protein (GFP) and other proteins relevant for human therapeutic use.

PROJECT:

We will synthesize protein-based therapeutic agents with protein scaffolds genetically competent for bioorthogonal ("clickable") conjugations. To establish the overall methodology, "clickable" green fluorescent protein (GFP) scaffolds will first be decorated with various ligands (e.g., commercially available glycopeptide moieties) by genetically encoded click chemistry, and their activities will be monitored by flow cytometry and fluorescence microscopy. In the second stage (in collaboration with various groups from campus), we will use this technology to incorporate unnatural residues into the sequences of the target protein (e.g., GFP, bioadhesives, collagens, etc.) that would allow ligation of external components via click chemistry.

Reading:

Sun, H., Jia, H., Kendall, O. et al. & N. Budisa, Halogenation of tyrosine perturbs large-scale protein self-organization. *Nature Communications* **2022**, 13, 4843 (https://doi.org/10.1038/s41467-022-32535-2)

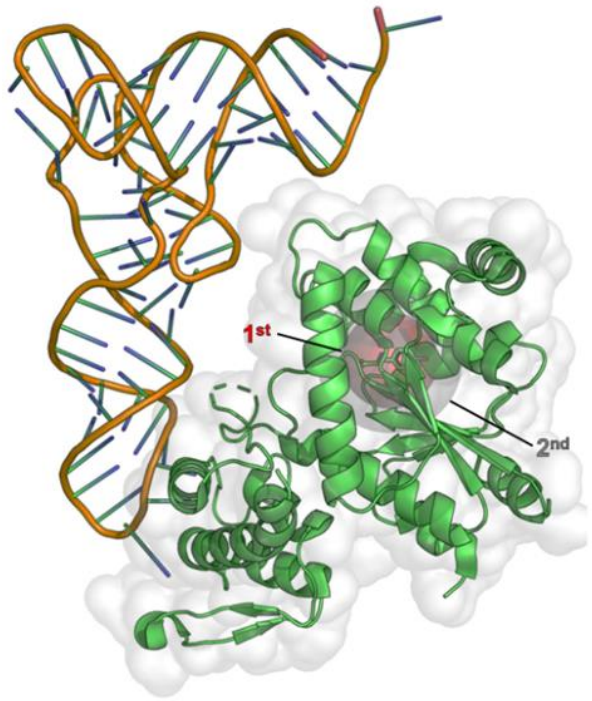
D. Lauster, S. Klenk, K. Ludwig et. Al & N. Budisa, R. Netz, C. Böttcher, S. Liese, A. Herrmann, C.P. Hackenberger, *Phage capsid nanoparticles with defined ligand arrangement block influenza virus entry - an antiviral strategy*. *Nature Nanotechnology*, **2021**, 15, 373–379 (https://doi.org/10.1038/s41565-020-0660-2)

Project #5

Engineering of orthogonal aminoacyl-tRNA ligases (synthetases) - crucial enzymes for expanding the genetic code

Prof. Dr. Ned Budisa (nediljko.budisa@umanitoba.ca, http://chemsynbio.com)

INTRODUCTION:



Aminoacyl-tRNA synthetases (aaRSs) are an important class of enzymes crucial for maintaining accuracy during translation of the genetic code (i.e. they are responsible for the attachment of specific amino acids to their cognate tRNAs). The natural genetic code dictates which canonical amino acids are allowed for ribosomal translation. The expansion of their number beyond the canonical 20 requires a change in the substrate specificity of an aaRS, since they are crucial interpretators of the genetic code.

More than 200 non-canonical amino acids (ncAAs) were introduced into proteins via various genetic code expansion routes: Selective pressure incorporation, stop codon suppression, fragment condensation, protein semisynthesis, and peptidomimetics. The ncAAs with non-proteinogenic functional groups can be used to manipulate, design, and elucidate protein structure, dynamics, function, allosterism, interactions, catalysis, folding, synthesis, trafficking, degradation, and aggregation.

The proposed research will provide a state-of-the-art environment for students and trainees to learn directed enzyme evolution: testing and improving existing enzymes and screening aaRS/tRNA orthogonal pairs from existing sources (beginners) and designing enzyme and tRNA libraries (advanced students).

PROJECT:

To determine the efficiency of such an unnatural translation, we need to know parameters related to the recognition and activation of unnatural amino acid substrates. We will take advantage of the fact that most aaRS enzymes can activate their amino acid substrate in the absence of tRNA. In particular, we will first express, purify and analytically characterize these enzymes. Next, we will determine the thermodynamic parameters of substrate binding by isothermal titration calorimetry and resolve high-resolution crystal structures of mutants. With these data in hand, we will gain important insights into how these molecular machines work. Finally, these parameters are also used to design optimally engineered, unnatural enzymes with good efficiency and improved accuracy.

Reading:

T. Baumann, M. Hauf, F. Schildhauer, K.B. Eberl, P.M. Durkin, E. Deniz, J.G. Löffler, C.G. Acevedo-Rocha, J. Jaric, B.M. Martins, H. Dobbek, J. Bredenbeck, N. Budisa. "Observation of Site-Resolved Vibrational Energy Transfer Using a Genetically Encoded Ultrafast Heater." *Angewandte Chemie International Edition (English),* **2019**, *58* (9), 2899-2903. doi: 10.1002/anie.201812995.

Koch NG, Goettig P, Rappsilber J, Budisa N. "Engineering Pyrrolysyl-tRNA Synthetase for the Incorporation of Non-Canonical Amino Acids with Smaller Side Chains." *International Journal of Molecular Sciences*. **2021**; 22(20):11194. https://doi.org/10.3390/ijms222011194.

Project #6

Photochemical Flow in Development of New Carbon-Halogen bond Forming Reactions

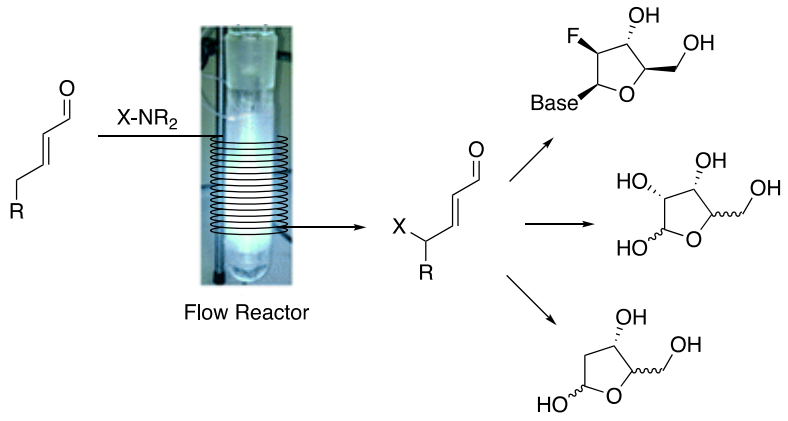
Dr. Rebecca Davis (Rebecca.Davis@umanitoba.ca)

INTRODUCTION:

Facile functionalization of five-membered heterocycles has long been a challenging task for organic synthesis. Asymmetric organocatalysis has emerged as a powerful synthetic methodology that has provided access to a variety of previously unachievable stereoselective transformations, resulting in a diverse array of chiral molecules. Currently, remote functionalization using dieneamine and trienamine activation are state-of-the-art in aminocatalysis, with a great deal of effort being devoted to the expansion of the scope of substrates avalible.[1] Using a combination of the a recently developed regioselective Wohl-Ziegler reaction and aminocatalytisis we have devised a method for achieving functionalized five-membered heterocycles. This methodology will allow for rapid, scalable access to pharmaceutically relaven carbohydrates/nucleosides from cheap starting materials.

PROJECT:

The Davis lab recently developed a methodology for γ-functionalization of conjugated aldehydes (enals) that has brought forth a new route to create enantioselectively substituted heterocycles. Using these γ-functionalized aldehydes along with robust asymmetric aminocatalysis to add substituents to the α- and γ- positions, cyclization of these compounds will allow us to create a simple method for production of enantioselectively substituted heterocycles. This work will provide efficient new routes to a wide range of natural product and has the potential to produce novel small molecule pharmaceuticals. The student involved in this project will learn advanced synthetic techniques as well as small molecule characterization techniques including HPLC-MS, GC, polarimetry, and NMR spectroscopy.



REFERENCES:

1 a) Kiler, L.; Tur, F.; Poulsen, P. H.; Jorgensen, K. A. *Chem. Soc. Rev.* **2017**, *46*, 1080. b) Reboredo, S.; Parra, A.; Aleman, J. *Asymm. Cat.* **2014**, *1*, 24.

Project #7

Photoaminocatalysis Design and Development

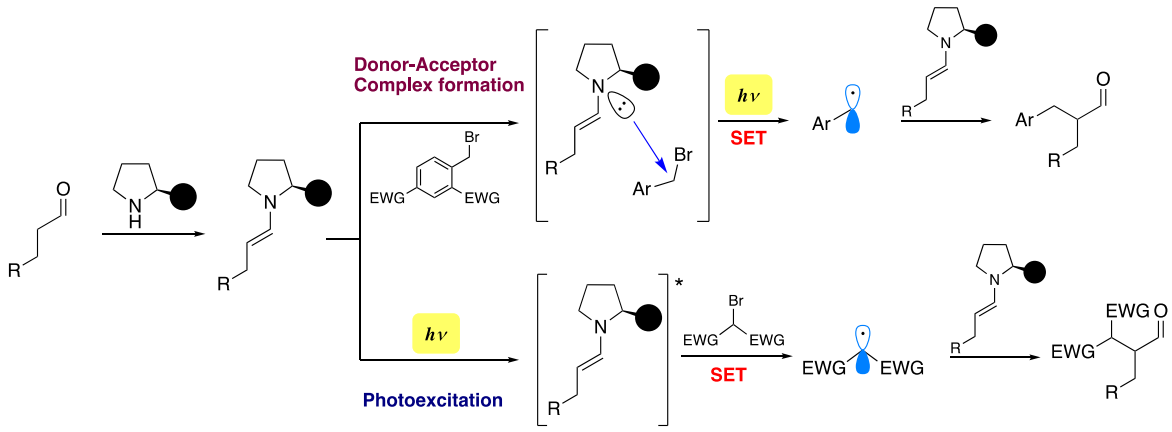
Dr. Rebecca Davis (Rebecca.Davis@umanitoba.ca)

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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1) Silvi, M., and Melchiorre, P. Enhancing the potential of enantioselective organocatalysis with light *Nature,* **2018***, 554*, 41-49.

2) Lima, C. G. S., Lima, T. de M., Duarte, M., Jurberg, I. D., Paixao, M. W. Enabled by Light-Irradiation of EDA Complexes: Theoretical Background and Synthetic Applications, *ACS Catal.* **2016**, Volume 6, 1389-1407.

Project #8

FTIR OF COLLAGEN IN ARCHIVAL PARCHMENTS

Dr. Gough (Kathleen.Gough@UManitoba.ca, (204) 474-6262)

INTRODUCTION:

Parchment was widely used as a writing medium, across Europe to the Horn of Africa, from the 2nd century BC until the 17th CE. Parchment is a complex biological material from processed animal skins (calf, sheep, or goats), primarily composed of collagen. All collagens are susceptible to collagen-specific degradation mechanisms; in the case of archival parchment, degradation leads to the disintegration of these important historical records. This project is part of an international study on possible restoration methods.

PROJECT:

The functional properties of collagen-based mammalian tissues are determined by their complex hierarchical structures, chemical cross linking and post-translational modifications. Members of the Gough lab have been studying collagen in scar tissue and in tendon for many years. Collagen's unique triple helical structure at the molecular level results in an unusual and very characteristic IR spectrum [1] that is conformation- and orientation-dependent in normal tissue and measurable in fibrils at the micro- and nano-scale (Figure 1). Research on archival parchments is a part of a new collaborative study led by Prof. L. Bozec at the University of Toronto. An important question that we aim to answer is how the aging process and the formation of advanced glycation end products affect inter-fibrillar cross-linking and the mechanical properties of these materials; see e.g.: [2].

The student will conduct experiments in spectrochemical imaging of archival parchments with polarized IR using the Agilent FTIR microscope in Dr. Gough's lab, and correlate results with students conducting AFM and other experiments here and in our collaborator's group. Where possible, some nanoFTIR experiments will be conducted remotely at the Advanced Light Source, Berkeley CA, USA.

The student will gain hands-on experience with IR imaging and analysis, as a member of a collaborative, interdisciplinary, international team. They will be a co-author on publication(s) that include their results and have opportunities to present their work in public.

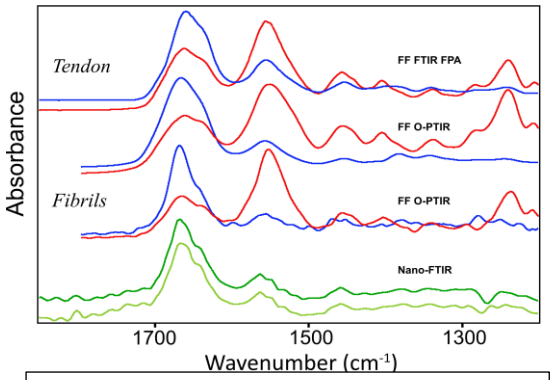


Fig.1: Representative polarized IR spectra from Agilent Far-field IR microscope (top), Optical-PhotoThermal IR (middle) and near field nanoIR (bottom) offset for clarity, illustrate the power of polarized IR studies to characterize collagen. Fig. 5 in *Molecules* 2020. [Ref.1]

REFERENCES:

1. 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).
2. M Vaez, M Asgari, L Hirvonen, G Bakir, E Khattignavong, M Ezzo, S Aguayo, C Schuh, K Gough, L Bozec "Modulation of the biophysical and biochemical properties of collagen by glycation for tissue engineering applications" Acta Biomaterialia 155:182-198 (2023)

Project #9

Correlative FTIR and Fluorescent imaging analysis of cells

Dr. Gough (Kathleen.Gough@UManitoba.ca, (204) 474-6262)

INTRODUCTION:

The long-term goal of this collaborative project is to correlate fluorescence and infrared image analyses of human buccal cells obtained via standard cheek swabs, to improve our understanding of genomic instability and changes in nuclear architecture related to ageing and Alzheimer's disease (AD). This project is a continuation of on-going international collaborative efforts. Fundamental research is required to develop, optimize, and confirm these correlative methods.

PROJECT:

The student will conduct FTIR spectroscopic imaging experiments on fibroblasts and subsequently obtain correlative fluorescence images of the same cells. GL 51/92 cells are chosen as they can be maintained and grown through >20 passages without aging. The student will be trained in cell culture and sample preparation with Dr. Sabine Mai (Physiology and Pathophysiology). FTIR spectrochemical imaging will be done in Dr. Gough's laboratory. Hyperspectral images will be analyzed for known biomarkers to identify spectra characteristic of organelles. With training in immunostaining for Fluorescent In Situ Hybridization (FISH) techniques in Dr. Mai's lab, they will seek correlation between FTIR spectral markers and FISH images. The student will participate in analysis of some O-PTIR data acquired in spring 2023, by Dr. Gough in collaboration with Dr. Rohith Reddy (U Houston). Dr. Mai has shown differences between cells as AD progresses (Fig 1.) with superresolution imaging of buccal cells.[1] Drs. Gough, Mai and Reddy have demonstrated proof of principle feasibility of correlative O-PTIR and fluorescence imaging (Fig. 2).[2]

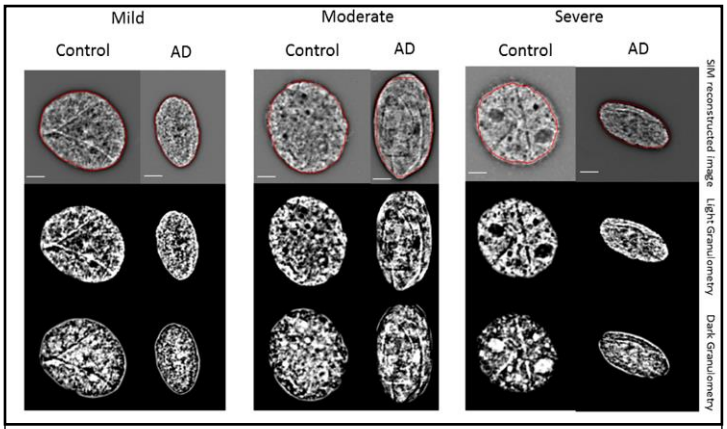


Figure 1.Superresolution fluorescence imaging of buccal cell nuclei show ellipsoidal shape and increased DNA-Free and DNA-poor space with AD.[1]

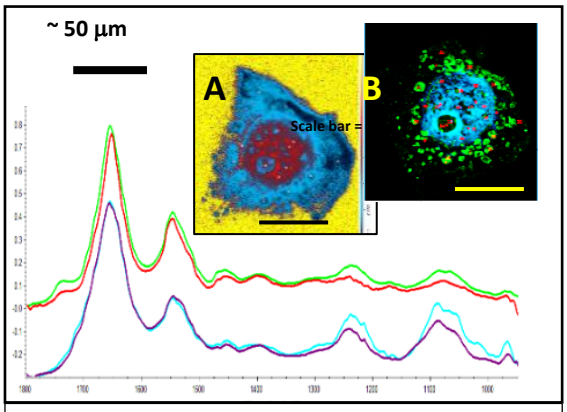


Figure 2. IR spectra obtained with O-PTIR exhibit organelle-specific features that may be correlated with (a) single λ and (b) fluorescent images.[2]

REFERENCES:

1. Garcia et al, 2017 J. Cellular Physiology 232:2387-2395
2. Gajella, C; Fabiao de Lima, M; Dyck, D. Reddy, R; Mai, S; Gough KM; *manuscript in preparation*

Project #10

Scaffold Hopping by Photochemical Carbon Deletion from Benzannulated Azaarenes

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

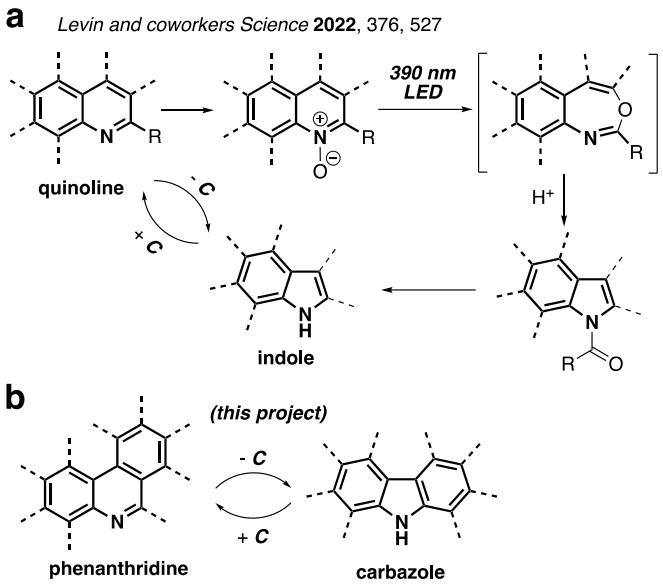
Group Website: http://home.cc.umanitoba.ca/~dherbert/

INTRODUCTION:

Chemists often identify molecular structures that show promise for a specific application, for example, as chemotherapeutics, molecular electronics, or solar materials. The preparation of each new candidate molecule in a series can often require a completely new synthetic approach if the **core** of the molecule needs to be altered. Synthetic methodologies that can easily and directly interconvert between molecular cores are tantalizingly attractive ways to streamline molecular discovery.

PROJECT:

Very recently, chemists at the University of Chicago reported[1] an exciting new approach to 'hop' directly between chemically distinct heteroaromatic scaffolds, namely quinoline *N*-oxides and *N*-acylindoles (**a**). We have developed synthetic routes to functionalized phenanthridines, also known as benzo[c]quinolines,[2] and demonstrated their use in diverse applications including as emissive materials.[3] This project will involve applying this scaffold hopping protocol to convert **phenanthridine *N*-oxides** to **carbazoles** to investigate the extension of this exciting work to *benzannulated* azaarenes (**b**).



This project requires an enthusiastic and engaged student interested in **sustainable chemistry** and learning about **synthetic organic chemistry**, in particular the use of **photochemistry**. A 4710 student will work directly alongside Dr. Herbert and a graduate student mentor to develop an **optimized protocol** for ring-contraction starting with 6-methyl phenanthridine *N*-oxide. The starting materials will be characterized using multinuclear NMR and UV-Vis absorption spectroscopy. A photochemical protocol using an LED photoreactor will be developed, and products isolated and analyzed chemically. Once an optimized procedure is established, the 4710 project will then look to establish a **substrate scope** for this transformation using a library of phenanthridine *N*-oxides prepared using our pre-existing library of available substituted phenanthridines.

REFERENCES:

[1] J. Woo, A.H. Christian, S.A. Burgees, Y. Jiang, U.F. Mansoor, M.D. Levin *Science* **2022**, *376*, 527

[2] P. Mandapati, J.D. Braun, I.B. Lozada, J.A.G. Williams, D.E. Herbert *Inorg. Chem.* **2020**, *59*, 12504

[3] I.B. Lozada, R.J. Ortiz, J.D. Braun, J.A.G. Williams, D.E. Herbert *J. Org. Chem.* **2022**, *87*, 184

Project #11

Designer Molecules for Sustainable Energy Capture and Conversion

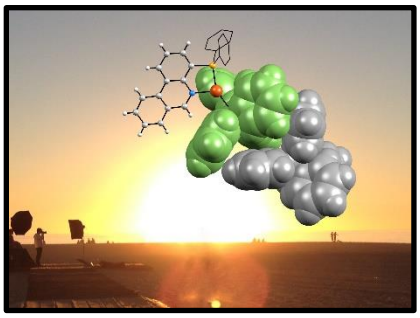
Dr. David Herbert (david.herbert@umanitoba.ca, (204)474-7535)
Group Website: http://home.cc.umanitoba.ca/~dherbert/

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.

PROJECT:

Designing emissive molecules and materials for solar energy capture and conversion



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 requires an enthusiastic and engaged student interested in **sustainable chemistry** and learning about **synthesis**, how to manipulate air- and moisture-sensitive reagents, and characterization techniques including single-crystal X-ray diffraction, cyclic voltammetry, multi-nuclear NMR and absorption/emission spectroscopy. A 4710 student will work directly alongside Dr. Herbert and a graduate student mentor to construct their own novel ligand and form coordination complexes. Working as part of this team, the student will evaluate their complexes' properties to examine their suitability in energy and sustainable chemistry applications.

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I.B. Lozada, J.A.G. Williams, D.E. Herbert *Inorg. Chem. Front.* **2022**, *9*, 10-22

C.B. Larsen, J.D. Braun, I.B. Lozada, K. Kunnus, E. Biasin, C. Kolodziej, C. Burda, A. Cordones, K. Gaffney, D.E. Herbert *J. Am. Chem. Soc.* **2021**, *143*, 20645

R.J. Ortiz, J.D. Braun, J.A.G. Williams, D.E. Herbert *Inorg. Chem.* **2021**, *60*, 16881

Project #12

Computational Study of Singlet-Triplet Excitations in Aromatic Heterocyclic Compounds

Dr. H. Georg Schreckenbach (schrecke@cc.umanitoba.ca, 204-474-6261)
Dr. David E. 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 in their own right. Extended aromatic systems are of interest as singlet fission materials for solar energy harvesting.[1, 2] In addition, they can serve as ligands in transition metal complexes. Recently, some intriguing trends have been observed in phosphorescence of transition metal complexes with *N*-heterocyclic ligands.[3] It has been speculated that, while singlet-triplet excitation (S_1-T_1) in these aromatics goes along with significant structural distortion (e.g., T_1 of benzene has two significantly elongated C–C bonds), this distortion may be hindered upon metal complexation.

PROJECT:

The goal of this project is to use computational chemistry for the systematic study of the S1-T1 excitations in simple aromatic compounds such as pyridine, quinoline, isoquinoline, phenanthridine, and acridine, amongst others. The research is based on the hypothesis that changes in geometry can at least partly explain trends in excited state energies. This will be achieved through comparing vertical excitations (no change in geometry) with emission (relaxed geometries). The student will be based primarily in the Schreckenbach group.

REFERENCES:

[1] Smith, M. B.; Michl, J.: Singlet Fission. *Chem. Rev.* **2010**, *110*, 6891-6936.

[2] Match, C.; Perkins, J.; Schreckenbach, G.: Simple computational screening of potential singlet fission molecules. *Theor. Chem. Acc.* **2018**, *137*.

[3] Mondal, R.; Lozada, I. B.; Davis, R. L.; Williams, J. A. G.; Herbert, D. E.: Site-Selective Benzannulation of Heterocycles in Bidentate Ligands Leads to Blue-Shifted Emission from Dimers. *Inorg. Chem.* **2018**, *57*, 4966-4978.

Project #13

Investigating the folding of paratox

Dr. Khajehpour (Mazdak.Khajehpour@UManitoba.ca, (204) 2721546)

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 folding thermodynamic and kinetic properties of paradox in order to understand the folding mechanism of this protein.

PROJECT DESCRIPTION:

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 salts, osmolytes and pH 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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Project #14

tRNA maturation – how specific modifications are introduced

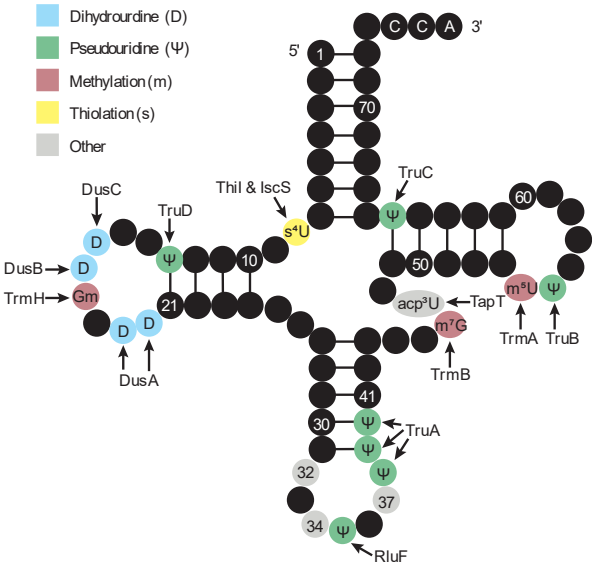
Dr. Ute Kothe (Ute.Kothe@UManitoba.ca, (204) 474 9265)

INTRODUCTION:

Transfer RNAs (tRNAs) are central molecules mediating gene expression in all cells by reading the genetic code on the mRNA and specifying the amino acid encoded by each codon. For optimal function and stability, all tRNAs are heavily chemically modified such that they contain about 10% modified nucleotides in addition to the four standard nucleotides (U, C, G, and A). tRNA modifications in the anticodon arm can modulate how tRNAs base-pair to mRNA codons whereas modifications in the D- and T-arm affect tRNA folding and stability. Many diseases are linked to mutations in tRNA modifying enzymes.

PROJECT:

This project is aimed at understanding how specific tRNA modifying enzymes recognize their tRNA target, how they distinguish it from other tRNAs and how they influence tRNA folding and stability. In several proof-of-concept studies, we have identified novel roles and mechanisms of enzymes targeting the variable and the T-arm of tRNA (see references). With your help, we would like to expand these studies to enzymes modifying the D- and the anticodon-arm (e.g., Dus A modifying position 19/20, and MnmE-MnmG modifying position 34).



This project will use technique in biochemistry, molecular biology, and biophysics. Specifically, you will gain experience in protein and RNA purification. To study the interaction of an enzyme with tRNA, we apply a variety of techniques including fluorescence studies, size-exclusion chromatography, and isothermal titration calorimetry. We also aim to determine structures of enzymes bound to tRNA using cryo-electron microscopy.

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Project #15
The function of H/ACA small nucleolar Ribonucleoproteins during ribosome assembly

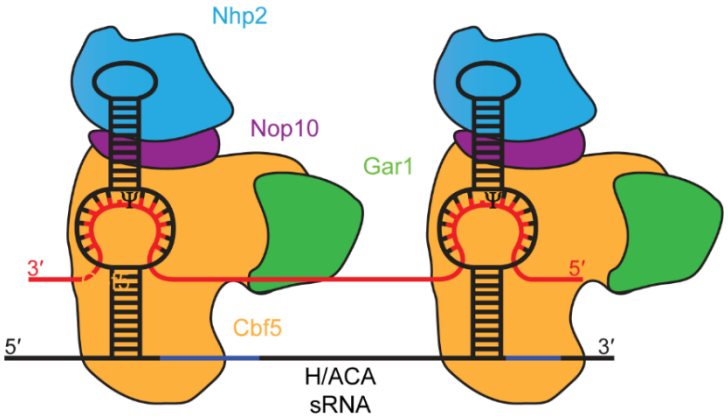
Dr. Ute Kothe (Ute.Kothe@UManitoba.ca, (204) 474 9265)

INTRODUCTION:
Ribosome assembly is a multistep process that generates the cell's protein synthesis machinery called ribosome which is composed of both large ribosomal RNAs (rRNA) and many proteins. In addition to rRNA and ribosomal proteins, hundreds of additional proteins and small nucleolar RNAs (snoRNAs) assist with ribosome biogenesis by transiently interacting with ribosome precursors. The Kothe group aims to understand the molecular mechanisms how these proteins and snoRNAs facilitate ribosome assembly with the long-term goal of identifying strategies to inhibit ribosome formation in rapidly growing cancer cells.

H/ACA snoRNPs are versatile molecular machines that are composed of an H/ACA snoRNA and a core set of four H/ACA proteins. The snoRNA facilitates base-pairing with ribosomal RNA whereas the H/ACA protein called Cbf5 in yeast (dyskerin in humans) is responsible for site-specifically modifying a uridine in ribosomal RNA to pseudouridine.

PROJECT:
The objective of this project is to investigate how H/ACA small nucleolar Ribonucleoproteins (snoRNPs) interact with ribosomal RNA. In addition to base-pairing with the target site for pseudouridine formation, the Kothe lab has recently shown that H/ACA snoRNPs can also bind to other regions of ribosomal RNA. Moreover, H/ACA snoRNPs have the ability to unfold structures in ribosomal RNA.

In order to dissect the function and the mechanism of H/ACA snoRNP interactions with ribosomal RNA, you will acquire expertise in generating and purifying both proteins and RNAs.



snR30 RNA and its potential protein interactions

This project is based on previous work in the Kothe lab where we have identified mutations in the internal hairpin of snR30 that cause temperature sensitivity suggestion that this region is functionally important. Here, we will take a predominantly biochemical approach to identify the interactions of the internal hairpin in snR30 with purified proteins [2, 3]. Towards this goal, you will in vitro transcribe and purify snR30 variants harboring mutations, and you will also purify selected proteins such as Utp23. RNA-protein interaction assays will be completed together with an experienced lab member. If time permits, we may also assess snR30-protein interactions in baker's yeast through co-purification.

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Project #16

Solid-State NMR of Biologically Active Glasses

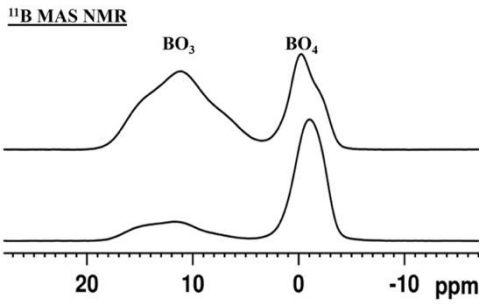
Dr. Scott Kroeker (Scott.Kroeker@UManitoba.ca, (204) 474 9335)

INTRODUCTION:

Glasses are becoming widely used for bone reconstruction and soft-tissue wound healing. Biologically active glasses can convert to bone minerals in the body, or deliver therapeutic ions to wound sites. Both of these applications depend on the ability of the glass to dissolve at an appropriate rate under physiological conditions, however every compositional modification alters the dissolution properties. Without a comprehensive understanding of how the glass composition and structure influence dissolution, biomedical engineers must rely on trial-and-error to develop viable materials. Nuclear magnetic resonance (NMR) spectroscopy is uniquely suited for studying the glass network and determining the key structural parameters which govern the dissolution of bioactive glasses.

PROJECT:

Borophosphate glasses will be prepared by high-temperature synthesis or sol-gel chemistry, followed by analysis using ^{11}B, ^{23}Na, ^{31}P, ^{29}Si and ^{27}Al NMR spectroscopy. Spectral interpretation yields the identities and quantities of different cationic environments, which are used to define the connectivity patterns that make up the glass network. The chemical durability of these glasses will be evaluated in dissolution trials, and elemental release measured as a function of time. The transformation of the materials will be characterized by NMR spectroscopy and complementary methods such as scanning-electron microscopy. By correlating structural changes with properties such as dissolution behaviour and crystallization, a deeper understanding of how properties depend on glass composition can be established to aid the design of bioactive glasses which require the smooth release of therapeutic ions near the injury site for soft-tissue wound healing. The same principle is used in environmental applications such as the design of glasses for the safe disposal of nuclear waste: selecting a composition in which bonding supports maximum chemical durability is essential to prepare materials which will protect the environment from radioactivity for thousands of years. Projects can be tailored to student interests and strengths to emphasize synthetic, analytical or physical aspects of these projects.



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Project #17

Solid-State NMR of Metal-Organic Frameworks

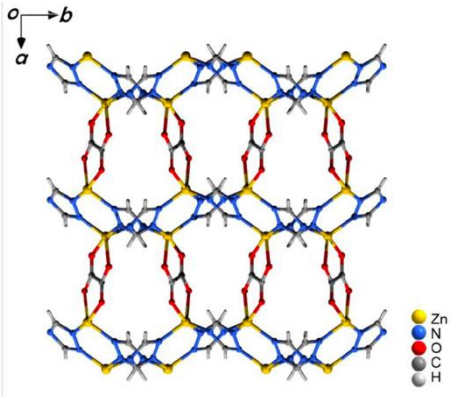
Dr. Scott Kroeker (Scott.Kroeker@UManitoba.ca, (204) 474 9335)

INTRODUCTION:

The growing importance of metal-organic frameworks (MOFs) in applications such as drug delivery, carbon capture and catalysis demands reliable characterization of their structure and dynamics. The disordered nature and flexibility of many MOFs renders them difficult to study by x-ray crystallography. Whereas solid-state NMR should be a natural choice for such materials, the development of methods to address the specific challenges of these highly porous, dynamically disordered systems demands careful consideration of their electronic structure and unique bonding characteristics.

PROJECT:

The analysis of ^{13}C and ^{1}H magic-angle spinning (MAS) nuclear magnetic resonance (NMR) spectra of MOFs supplied by collaborators will be used to determine essential structural motifs such as the connectivity of metal nodes to organic linkers, or the adsorption of small molecules to specific sites within the MOF pores. The latter may involve *in situ* experiments at variable temperatures and pressures to provide a structural explanation for the observed uptake properties of MOFs designed for carbon capture. The former will require theoretical modeling of paramagnetic chemical shifts to generate contour maps of the unpaired-electron spin density. Our recent success in predicting extreme ^{13}C chemical shifts in metal complexes with acetylacetonate and oxalate ligands has prompted us to examine node-linker connectivity in paramagnetic hydrogen-bonded organic frameworks (HOFs), where the porosity depends on hydogen-bonded scaffolds of phosphonate ligands coordinated to transition metals. Experimental ^{31}P MAS NMR spectra will be compared with computed spin-density maps to gain information about the role of H-bonding in MOF stability. The ultimate goal of such studies is to develop tools for the effective use of NMR in studying structure and dynamics in MOFs for a variety of applications. Projects may be adapted to emphasize inorganic, physical or analytical interests.



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Project #18

Sustainable dry battery electrode process

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

INTRODUCTION:

Batteries are a key technology for the sustainable energy transition as they store and release renewable energy for intermittent use and transportation. Massive investments into renewable energy harvesting and storage are currently transforming our energy economy. Impacts of this paradigm shift will be felt over decades and maybe centuries. In this rush to a green energy economy, it is important that we consider the sustainability of the replacing technologies as well. Battery electrode manufacturing requires large amounts of space and energy due to the toxic and environmentally hazardous solvent N-Methyl Pyrrolidone used in the casting of electrode slurries. Recent research has shown that dry electrode processing reduces energy and space requirements by more than 50% and avoids the use of toxic solvents[1]. This can currently only be achieved in conjunction with the use of the perfluorinated forever chemical poly(tetrafluoroethylene) (PTFE) as electrode binder.

PROJECT:

Over the last years, my research group has developed a novel composite binder, based on an intrinsically conductive polymer and a cellulose-based polyanion (patent pending, figure 1)[2,3]. The intrinsic fibrillar nature of natural cellulosic polymers may allow for fibrilization of the dry polymer upon application of shear forces, similar to that observed with PTFE[4,5]. Initial experiments have shown promising mechanical properties. As such, the new binder offers a unique opportunity to explore dry processing.

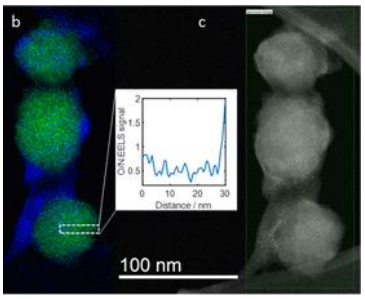

Figure 1. Composite binder nano-structure (STEM).

This project will start from the synthesis of the composite binder. The impact of polymer molecular weight, synthesis conditions, and use of plasticizing additives on mechanical properties will be explored to understand the promise of these novel binders for dry processing. Battery electrodes will be prepared through traditional slurry casting and dry processing methods. The resulting electrodes will be tested in button-cell batteries and characterized through electron microscopy imaging and spectroscopic methods.

The successful processing of these binders in dry state would constitute a major milestone in the development of more environmentally friendly battery fabrication methods.

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4. Bresser, D., Buchholz, D., Moretti, A., Varzi, A. & Passerini, S. *Energy Environ. Sci.* **11**, 3096–3127 (2018).
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Project #19

Detection of Drug Resistance in Yeast by Electrochemistry

Dr. Sabine Kuss (sabine.kuss@UManitoba.ca, (204) 272 1693)

INTRODUCTION:

Drug resistance is a growing problem that severely increases the number of deaths from bacterial infections and cancer.[1] Cellular resistance mechanisms are at the root of drug resistance, which include cell membrane protein modifications, intracellular drug target alterations, and the over-expression of efflux pumps.[2] To investigate resistance mechanisms towards specific antimicrobial agents, such as chloramphenicol, yeast cells are ideal model systems because they are easy to grow, low-risk, and extensive libraries of mutants are available. This project will explore the resistance mechanism of chloramphenicol in living yeast cells and isolated mitochondria.

PROJECT:

Chloramphenicol is an antibiotic substance administered against bacterial infections.[3] Electrochemical studies will characterize the electrochemical fingerprint of chloramphenicol using voltammetry. Yeast cells will be positioned in Petri dishes and imaged electrochemically by scanning electrochemical microscopy (SECM). By positioning an utramicroelectrode close to target cells, electrochemistry can quantify the efflux of molecules from cells. This project aims to detect the cellular efflux of chloramphenicol across the cell membrane. Molecules diffusing towards the electrode will be oxidized or reduced, enabling the quantification of drug resistance in living cells. In collaboration with the laboratory of Dr Deborah Court, mitochondria will be extracted from yeast. By comparing electrochemical signals between mitochondria and whole yeast cells in the presence of chloramphenicol, conclusions will be drawn about chloramphenicol resistance mechanisms in *Saccharomyces cerevisiae* and *Neurospora crassa*.

Figure 1: *Saccharomyces cerevisiae* seen in a false color electron microscopy image.[4]

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Project #20

Single-Entity Electrochemistry

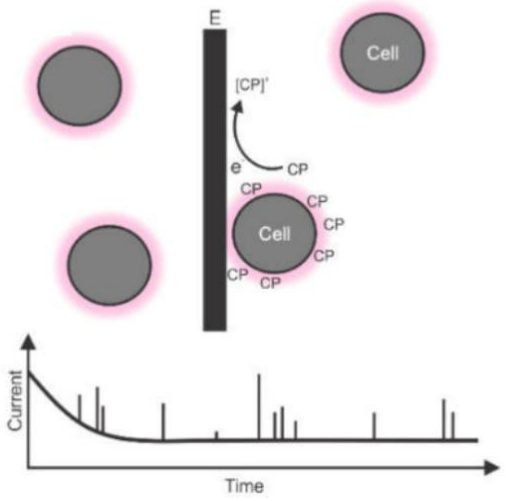
Dr. Sabine Kuss (sabine.kuss@UManitoba.ca, (204) 272 1693)

INTRODUCTION:

Impact electrochemistry is a powerful technique for the detection of single entities.[1,2] In the literature, its main application is related to the detection and characterization of nanoparticles in solution.[3] This project explores the application of impact electrochemistry to biological organisms to detect pathogens in aqueous solutions, but also to quantitatively assess cellular features, such as molecule efflux across cell membranes. If successful, this study will demonstrate the immense potential of single-entity electrochemistry as a revolutionary tool in biosensing.

PROJECT:

Impact electrochemistry is based on the faradaic charge transfer, following the collision of redox-active entities with an electrode. Governed by diffusional Brownian motion, single particles collide with an electrode, which is held at an oxidizing or reducing potential of a redox species. Thereby, entity impacts at the electrode result in short current bursts ("spikes"). To date, no redox active cell metabolite has been reported for the application to impact electrochemistry, but methodologies involving nanoparticle-labeled bacteria and their detection through an electrochemical "off"-signal have been proposed.[4,5] In this project, the cell metabolite glutathione, the efflux of antibiotics from bacteria, and the efflux of chemotherapeutics from living cancer cells will be studied (scheme 1). All of these three cellular events are intrinsically connected to drug resistance mechanisms of cells, as drugs are commonly expelled from the cell interior through active pumps, either in conjugation with glutathione or on their own. If successful, this methodology will not only detect pathogens in aqueous solutions at high throughput rates, but will also enable the quantification of drug resistance phenotypes in bacteria and cancer.



Scheme 1: Living cells collide with an electrode during impact electrochemistry. The efflux of the chemotherapeutic carboplatin (CP) results in current spikes.

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Project #21

Electrochemical Detection of Mycotoxins in Canadian Grain

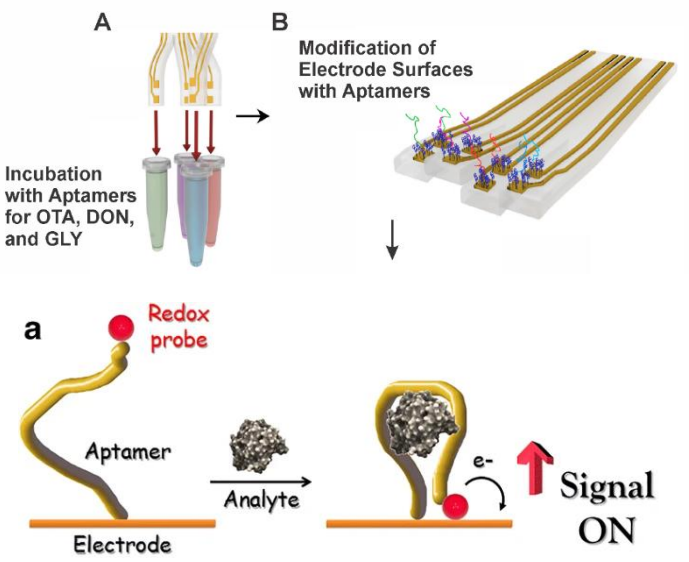
Dr. Sabine Kuss (sabine.kuss@UManitoba.ca, (204) 272 1693)

INTRODUCTION:

Mycotoxins, such as ochratoxin A (OTA) and deoxynivalenol (DON) are prevalent contaminants in Canadian grain and cause devastating losses for grain producers across Canada.[1] Grain that is intended for human consumption, but also animal feed is susceptible to contamination with mycotoxins. Current multi-analyte tests require costly scientific instrumentation, laboratory equipment, and expertise. Electrochemistry can offer portable, inexpensive, and fast alternative methods. The aim of this project is to detect at least two grain contaminants simultaneously using disposable screen-printed electrodes that can be implemented into a micro-fluidic device for the detection of mycotoxins in Canadian grain.

PROJECT:

As shown in scheme 1, this project involves structure-switching electrochemical aptamer sensors. Individual electrode arrays are incubated with aptamers specific for relevant grain contaminants. A DNA or RNA aptamer structure is bound to a gold electrode surface and tagged with the redox probe methylene blue. The aptamer-modified electrodes will be exposed to solutions of OTA and DON. Upon binding of target analytes, folding of the aptamer structure brings the redox tag in close proximity to the gold, enabling faster electron transfer and an increase in electrochemical current during voltammetric measurements. Upon successful detection of OTA and DON in a buffer, real grain samples will be analyzed in collaboration with the Canadian Grain Commission. Mycotoxins will be extracted from grain matrices by washing and the design of a microfluidic flow-through chamber for high throughput analysis will be explored.



Scheme 1: (A) Mycotoxin-specific aptamers will bind to gold coated electrochemical arrays (B).[2] A redox probe is attached to the aptamer (a), and upon binding of OTA or DON, folding of the aptamer structure brings the redox tag near the gold, enabling faster electron transfer.[3]

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Project #22

Bioelectrochemical Quantification of Reactive Oxygen Species in Living Cancer Cells

Dr. Sabine Kuss (sabine.kuss@UManitoba.ca, (204) 272 1693)

INTRODUCTION:

Bioelectrochemistry is an emerging field in bioanalytical chemistry and recent applications of electrochemistry to biology include studies on tissue and cancer cells.[1] Scanning electrochemical Microscopy (SECM) is an electroanalytical technique that enables the quantification of molecule exchange between living cells and their environment. This project aims to detect, quantify, and compare the production of reactive oxygen species (ROS) in cancer cells and healthy cell tissue.

PROJECT:

Electrochemical studies of living cells will be conducted using the techniques cyclic voltammetry, chronoamperometry and SECM. By positioning an electrode close to target cells, electrochemistry can quantify the efflux of molecules from cells in real-time as shown in figure 1.[2], Living keratinocytes, ovarian cancer and skin melanoma cells will be investigated for ROS production. Because ROS are highly reactive molecules that diffuse and disappear quickly, a microscopic tool is needed that can be positioned close to the cell membrane. Ultramicroelectrodes can detect and compare the amounts of ROS naturally produced by different cell lines. Strategies will be explored to induce ROS production through chemical stimulation and UV irradiation. Depending on ROS levels, this project will attempt to differentiate between different ROS species. This study is recommended to students who already have a basic understanding of electrochemical methods.

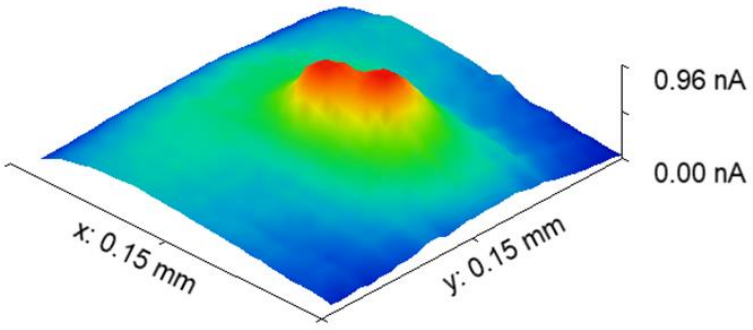

Figure 1: Electrochemical detection of molecule efflux from living ovarian cancer cells by SECM.

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Project #23

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 #24

Structural Characterization of RNA-Protein Complexes that Regulate Translational Control

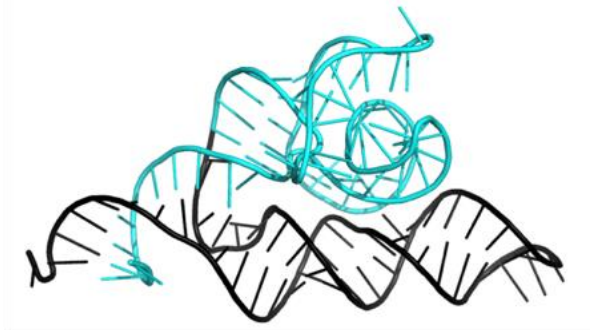
Dr. Sean McKenna (Sean.McKenna@UManitoba.ca)

INTRODUCTION:

Brain Cytoplasmic RNA 1 (BC200) is a 200 nucleotide long non-coding RNA that is hypothesized to regulate protein translation. 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. Our current hypothesis is that BC200 acts as a scaffold for a protein regulatory complex that interacts with messenger RNAs to regulate translation.

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. Molecular biology approaches coupled with bacterial/eukaryotic expression systems will be used to produce the BC200 binding partners (starting with one initially and building to more as time permits). Expression/purification protocols will need to be individually developed for each protein. BC200 will be produced (using an established protocol) using *in vitro* transcription, as will a series of BC200 truncations (to probe the specific regions responsible for binding). RNA-protein binding affinity and complex stability will be evaluated. Promising complexes will be structurally characterized using cryo-electron microscopy approaches.



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Project #25

Probing the Structure-Function Relationship of Dynamic Bacterial Proteases

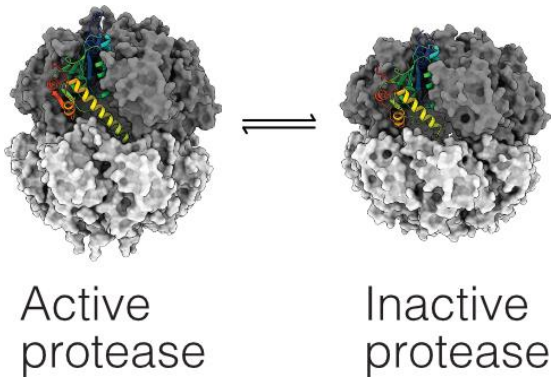
Dr. Zev Ripstein [Zev.Ripstein@UManitoba.ca, 204-474-8504]

INTRODUCTION:

Macromolecular protein degradation machinery assumes a central role in cellular physiology, from the timing of cell division, to stress responses, and the removal of damaged or aberrantly folded proteins. As such the protease machinery responsible for these functions are critical factors in the virulence pathways of many pathogenic organisms. ClpPs are a conserved family of serine proteases that collaborate with ATP-dependent translocases to degrade protein substrates.

PROJECT:

Understanding the protein-protein interaction rules governing the targeting of proteins for degradation represents an opportunity to leverage these systems for targeted proteolysis. As such, there is significant interest in understanding structure−function relationships for this protein family. Utilizing new tools in **protein and peptide design**, this research project will focus on producing and characterizing small peptides that interact with the ClpP machinery. This project will complement my lab's ongoing work using structural information from **cryoEM**, coupled with other biochemical and biophysical tools to engineer new peptides capable of leveraging the Clp proteostasis machinery with therapeutic and biotechnology potential.



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Project #26

Computational Studies of Uranium-Vanadium Separations

Dr. H. Georg Schreckenbach (schrecke@cc.umanitoba.ca, 204-474-6261)

INTRODUCTION:

Separations– of different compounds in a mixture, of different elements, and so on – are central to various areas of chemistry. This includes actinide chemistry where one needs to, among others, separate different parts of nuclear waste (e.g. the later actinides such as Am from the chemically very similar lanthanides). Computational chemistry is of particular utility in the field of actinide chemistry (5f elements) [1] as it reduces the need for difficult and expensive experiments involving the radioactive actinide elements.

PROJECT:

We have recently [2, 3] shown that certain N-donor ligands (see Figure 1) can be used to separate actinyls (UO_2^{2+}, NpO_2^{2+}, PuO_2^{2+}), as well as Am^{3+} from Eu^{3+}. Ligand geometry (preorganization into a shape that is conducive to metal bonding) and electronic effects including f-orbital contributions are of particular importance. In this project, we will use similar computational tools (chiefly relativistic density functional theory, DFT, combined with models for solvation; appropriate model reactions; analysis tools; as well as, potentially, accurate high-level ab initio methods) to investigate whether these same ligands also allow for separation between aqueous uranium and vanadium, a d-block element. This choice of metals is motivated by the fact that Earth's oceans contain large amounts of uranium (though in a very diluted form), requiring selective extraction based on preferential ligand binding of U over V and other metals.

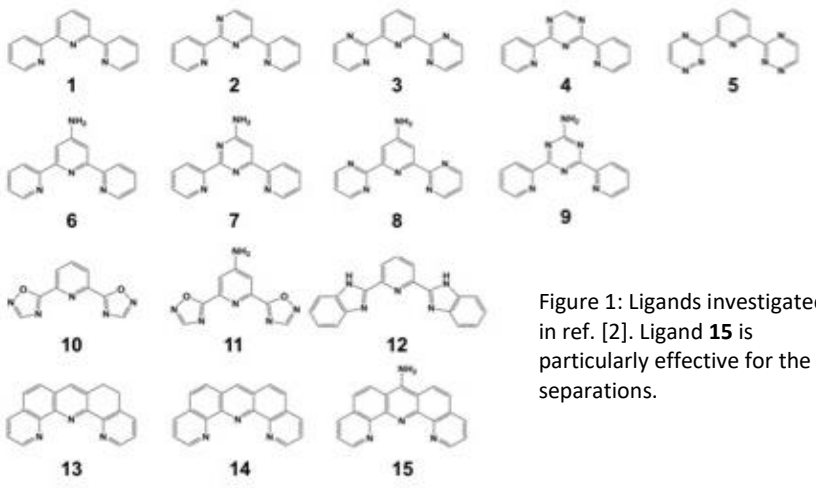


Figure 1: Ligands investigated in ref. [2]. Ligand **15** is particularly effective for the separations.

REFERENCES:

[1] G. Schreckenbach, G. A. Shamov "Theoretical Actinide Molecular Science", *Acc. Chem. Res.* **43** (2010), 19.

[2] X. Zhang *et al*. "Advancing the Am Extractant Design through the Interplay among Planarity, Preorganization, and Substitution Effects", *Inorg. Chem*. **61** (2022), 11570.

[3] X. Zhang *et al*., *to be published*.

Project #27

Theoretical Prediction of Singlet-Triplet Gaps in Organic Emitters for Thermally Activated Delayed Fluorescence (TADF)

Dr. H. Georg Schreckenbach (schrecke@cc.umanitoba.ca, 204-474-6261)

INTRODUCTION:

Organic π-conjugated molecules with substituted donor (D) and acceptor (A) units are known to exhibit excitations in the ultraviolet-visible (UV-Vis) spectrum with strong charge-transfer characteristics. As a result, they exhibit interesting optoelectronic properties and find applications in organic non-linear optics, organic field-effect transistors, and organic photovoltaic cells. Recently, appropriate D-A substituted chromophores have been employed to design thermally activated delayed fluorescence (TADF) materials. [1] These molecules can be used in organic light-emitting diodes (OLEDs) and are third-generation materials. They require a "bright" radiative singlet excited state (S_1) whose efficiency is governed by the internal quantum efficiency (IQE) of the S_1 state, which, in most cases, is relatively low (S_1< 25% while the rest is in the triplet state). However, TADF provides an option to increase excitons (excited electrons) by an up-conversion process from the non-radiative "dark" triplet state (T_1) back to S_1. The up-conversion from T_1 to S_1 is possible by thermal energy if the energy difference (ΔE_{ST}) between S_1 and T_1 is less than 0.30 eV. This involves reverse intersystem crossing (RISC). The ΔE_{ST} is the governing factor for designing TADF materials and arises from a spatial separation between the highest occupied and lowest unoccupied molecular orbitals (HOMO and LUMO).

PROJECT:

In this project, a benchmark [2] set of molecules from STGABS27 will be used to study their electronic structure and TADF properties in comparison with experimental results. A recently proposed time-independent density functional theory (DFT) method – the constricted variational method based on DFT, the CV-ΔSCF method after Park et al. [3] – will be used to study vertical ΔE_{ST} gaps. Adiabatic ΔE_{ST} gaps will also be calculated from CV-ΔSCF method from the TD-DFT (time-dependent DFT) optimized excited state geometries. Kinetics of RISC will also be studied to understand the rates of the photophysical processes.

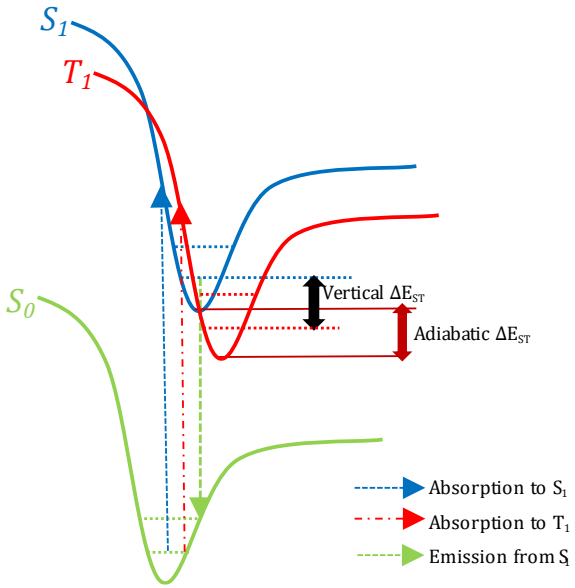


Figure 1: Potential Energy surfaces of the photophysical processes in TADF compounds.

REFERENCES:

[1] *J. Am. Chem. Soc.* 2017, 139, 11, 4042–4051

[2] *J. Phys. Chem. Lett.* 2021, 12, 35, 8470–8480

[3] *J. Chem. Theory Comput.* 2016, 12, 11, 5438–5452

Project #28

Design, synthesis and biological properties of amphiphilic nebramines: Rescuing antibiotics from resistance against Gram-negative pathogens

Dr. Frank Schweizer (Frank.Schweizer@UManitoba.ca, 204-474-7012)

Antimicrobial resistance is one of the largest threats to public health and economic growth [1]. Despite significant investments into antibiotic discovery in the past, no new antibiotic class against Gram-negative bacteria (GNB) has been approved in half a century. The reasons for this failure are due to low outer membrane (OM) permeability and extensive efflux generally referred to as the "Achilles Heel" in antibacterial drug discovery (FIG. 1) [2]. To overcome this bottleneck, the project plans to develop small molecules (***adjuvants***) with little or no antibacterial activity that will enhance OM permeability and/or increase inner membrane (IM) uptake of antibiotics against priority GNB [3]. The adjuvants are derived from the aminoglycoside nebramine, a fragment derived from the antibiotic tobramycin. Recent results in the Schweizer group have shown that amphiphilic nebramine is capable of increasing OM permeability of antibiotics by self-promoted uptake (SPU). SPU is a process by which cationic molecules displace the divalent cations (Ca^{++} or Mg^{++}) which are stabilizing counterions for the phosphate groups of lipid A and the phosphorylated core sugars located in the outer membrane. Displacement of the divalent counterions is thought to induce localized disruption of the lipopolysaccharide (LPS) layer of the outer membrane, allowing passage of the promoting molecules into the periplasm (FIG. 2). The project will involve design and synthesis of two amphiphilic nebramine analogs and biological evaluation of the antibacterial effect of the adjuvants (alone) and in combination with existing antibiotics.

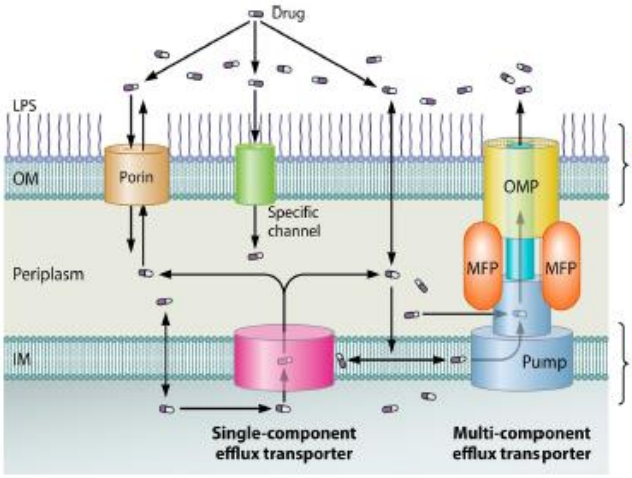


FIG. 1

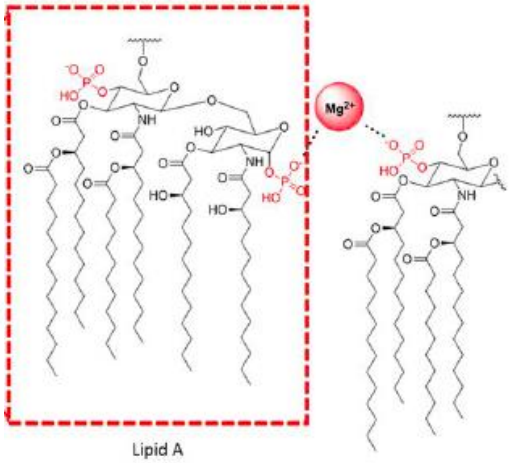


FIG. 2

References:

1. taken from the Lancet https://doi.org/10.1016/S0140-6736(21)02724-0 , January 20, 2022
2. *Nature.* **2016**, *529*, 336-343.
3. *Clin. Microbiol. Rev.* **2018**, *2*, 2018, e00077-17

Project #29

The discovery of new drugs from lichen fungi

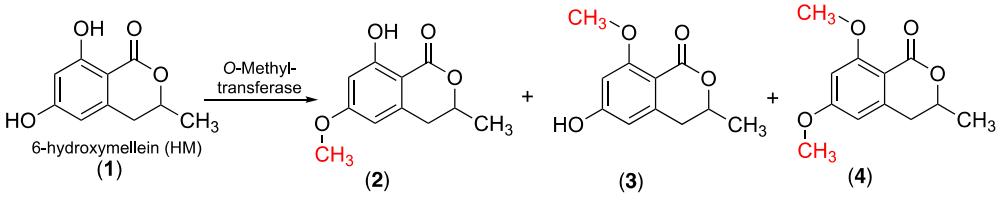
Dr. John Sorensen John.Sorensen@umanitoba.ca, (204) 474 9504

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 genes that we have discovered in the lichen fungi appear to code for an O-methyltransferase. This enzyme catalyzes the conversion of 6-hydroxymellinin (**1**) to an O-methylated analogue however the identity of the chemical product of this conversion is still undetermined. There are two possible sites of methylation on (**1**) and this can result in two different mono-methylation products (**2**) or (**3**) or a permethylated product (**4**). This project will determine the product distribution from this enzyme. The Sorensen lab has successfully expressed this enzyme in a heterologous host, *Aspergillus oryzae*, and this construct will be used in these biotransformation experiments. Current efforts in the Sorensen lab are focused on the expression of this enzyme in *E. coli* which would allow the production of pure protein, which will greatly aid this project.



The substrate scope of this enzyme will also be examined by the biotransformation of analogues of **1**, where the terminal methyl ($-CH_3$) group has been replaced with other substituents. Some of these analogues are already in hand in the Sorensen lab, while others will have to be synthesized as part of this project. These synthetic analogues of **1**, will then incubated with pure O-methyltransferase and S-adenosylmethionine (SAM), the methyl group donor, to determine if any conversion to product can be observed.

REFERENCES:

1. Abdel-Hameed, M.; Bertrand, R.; Piercey-Normore, M.; Sorensen J. L. *Fung. Biol.* **2016**, *120*, 306-316.
2. Abdel-Hameed, M.; Bertrand, R.; Piercey-Normore, M.; Sorensen J. L. *J. Nat. Prod.* **2016**, *79*, 1645-1650.
3. Bertrand, R. L.; Abdel-Hameed, M.; Sorensen J. L. *J. of Nat. Prod.* **2018,** *81,* 723–731**.**
4. Bertrand, R. L.; Abdel-Hameed, M.; Sorensen J. L. *J. of Nat. Prod.* **2018,** *81,* 732–748.

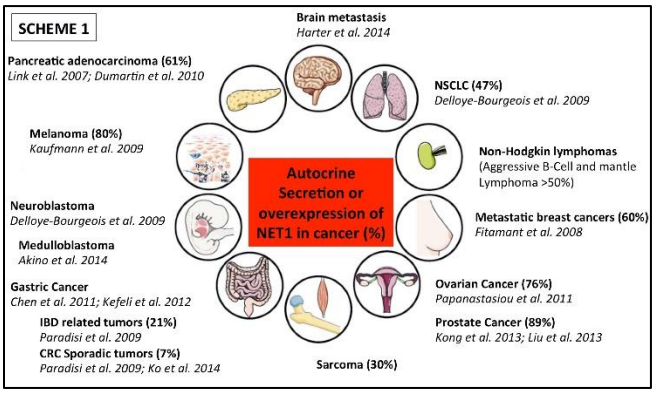
Project #30

To develop a mechanistic understanding of higher-order extracellular signaling clusters in human disease and develop targeted inhibitors for therapeutic application.

Dr. Jörg Stetefeld Jorg.Stetefeld@umanitoba.ca, (204) 474 9731

INTRODUCTION:

Netrins (which means "one who guides") are a family of extracellular morphogens that act as chemotropic guidance cues for migrating cells. Known functions of netrin 1 (NET1) include the attraction and repulsion of cells, cell adhesion, the regulation of cell survival, the epithelial cell homeostasis and tumorigenesis. NET1 can bind several dependence receptors and mediates as bifunctional guidance molecule attraction and repulsion of growth cones. Importantly, these cell surface receptors determine cell fate dependent on NET1 availability ("dependence receptor hypothesis".



It has been shown that NET1 is up – regulated in a large fraction of human tumors (see **SCHEME 1**) and that interference with NET1-dependence receptor interactions is associated with inhibition of tumor growth and metastasis in various preclinical model. **Therefore, NET1 and its dependence receptors define a powerful mechanism for both the induction and suppression of apoptosis.**

PROJECT:

CHEM4710 student candidates will continue to apply and develop further an integrated research program combining high-resolution structural biology techniques, with various biophysical and functional approaches. The overarching goal is to continue to develop structure-based applications in the fields of biomedicine and biotechnology. The student will be performing an integrated research program with the final goal to understand in detail the structure-property relationships of extracellular proteins involved in the formation of dynamic high-order signaling complexes related to human disease. The student will be explored to recombinant cell expression, biochemical and biophysical charaterisation of protein targets and structural elucidation of potential target complexes, incl. protein-protein and protein-ligand systems.

References

Gabir H et al. Investigation of dynamic solution interactions between NET-1 and UNC-5B by multi-wavelength analytical ultracentrifugation. *Eur Biophys J*. (2023) Mar 20

Meier M, et al. The dynamic nature of netrin-1 and the structural basis for glycosaminoglycan fragment-induced filament formation. *Nat Commun*. (2023) Mar 3;14(1):1226.

Reuten R et al.. Structural decoding of netrin-4 reveals unique non-enzymatic disruptive forces towards mature basement membranes. *Nature Communications* (2016) Nov 30;7:13515.

Grandin M, et al. . Structural decoding of the Netrin-1-UNC5 interaction and its therapeutical implications in Netrin-1 expressing cancers. *Cancer Cell* (2016) Feb 8; 29(2):173-85

Project #31

Migration of Petroleum-Based Chemicals from Food Storage Containers to Foods: Estimation of Human Dietary Exposure

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

INTRODUCTION:

Plastics have become a necessity of modern-day life with a range of uses from medical supplies, children's toys, and food packaging. Production of plastics fall into two types: synthetic- or bio-based. Synthetic based plastics are derived from petrochemicals while bio-based plastics are made from renewable products. Overwhelmingly, the vast majority of plastics in consumer use are synthetic-based. It has been shown that some chemicals (i.e., bisphenol-A) can partition out of plastics into the surrounding media. Here, we hypothesize that petroleum-based chemicals migrate from consumer-based plastics into food-based media and represent a significant source of exposure to humans.

PROJECT:

The research will test the hypothesis that commercial food storage plastic containers are a source of petroleum-based chemicals. The experiments we will use to test this hypothesis will be based on the guidance document from the US-Food and Drug Administration[1]. Food storage containers will be exposed to a variety of food simulants for a prescribed period of time and we will identify and quantify chemicals in the simulants using gas chromatography tandem mass spectrometry. The amount of chemicals in the simulants will then be used to calculate the daily exposure of humans to these compounds.

REFERENCES:

1. https://www.fda.gov/regulatory-information/search-fda-guidance-documents/guidance-industry-preparation-premarket-submissions-food-contact-substances-chemistry

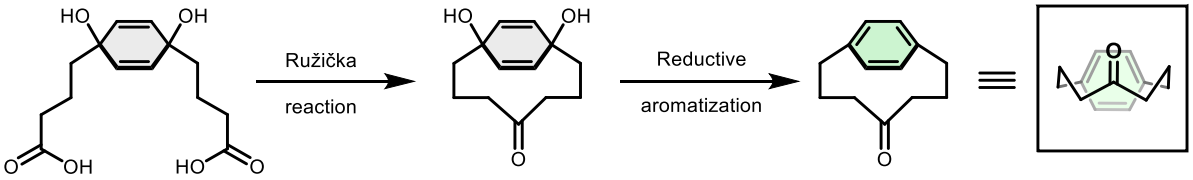
Project #32

Bridge Functionalized Cyclophanes: The Ružička Reaction

Dr. Joshua C. Walsh (Joshua.Walsh@UManitoba.ca, (204) 474 6605)

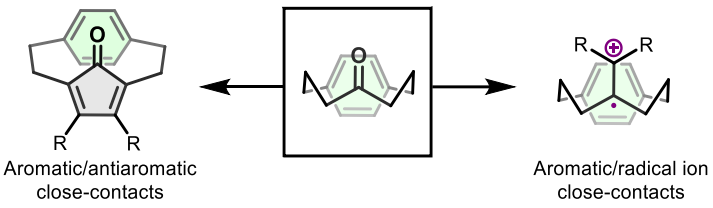
INTRODUCTION:

Cyclophanes have attracted the attention of organic chemists for more than 70 years.[1][2] Cyclophane research over the past decades has focused on aromatic-aromatic interactions[3] and contesting the textbook definition of aromaticity.[4] Close contacts of aromatic surfaces with isolated functional groups has largely been overlooked. This is a result of the state of the art in cyclophane synthesis which has remained nearly unchanged since its early days.



PROJECT:

This project is focused on building a new synthetic methodology to access bridge-functionalized cyclophanes through a short and high-yielding sequence of reactions. This will allow us to answer fundamental questions about what happens when unpaired electrons and antiaromatic systems are crammed into the ring current of aromatics. Additionally, a synthetic handle on the bridge will enable the exploration of the chemical space that is opened when cyclophanes move from being the end of the synthetic road to the starting point for more complex structures. The student working on this project will be mainly involved in organic synthesis as well as characterization including NMR, mass spectrometry, FT-IR, UV-vis and fluorescence spectroscopy.



REFERENCES:

[1] C. J. Brown, A. C. Farthing, *Nature* **1949**, 164, 915.

[2] I. Roy, A. H. G. David, P. J. Das, D. J. Pe, J. F. Stoddart *Chem. Soc. Rev.* **2022**, *51*, 5557.

[3] J. L. Zafra et al., *J. Am. Chem. Soc.* **2017**, *139*, 3095.

[4] T. Tsuji, M. Okuyama, M. Ohkita, H. Kawai, T. Suzuki, *J. Am. Chem. Soc*. **2003**, *125*, 951.

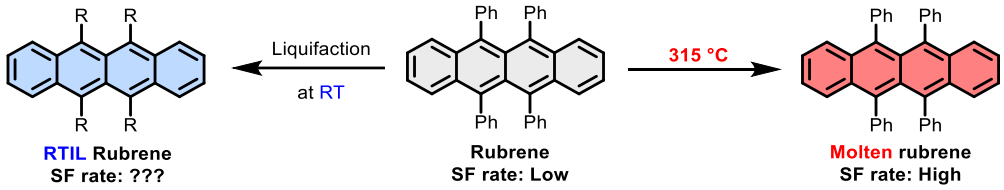
Project #33

Singlet Fission in Room Temperature Liquids

Dr. Joshua C. Walsh (Joshua.Walsh@UManitoba.ca, (204) 474 6605)

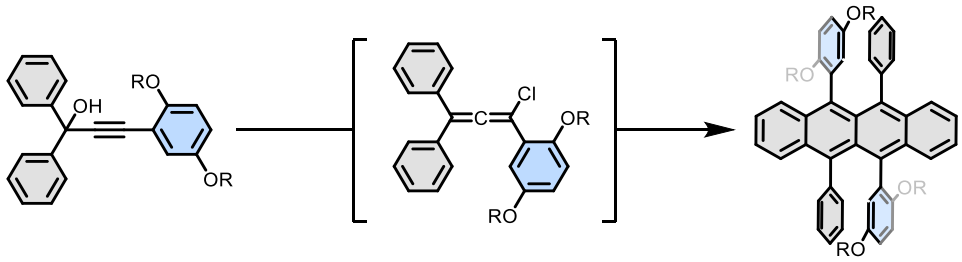
INTRODUCTION:

Singlet fission (SF) is a spin-allowed photophysical phenomenon charged with the potential to bypass an upper limit in solar cell efficiency, known as the Shockley–Queisser limit.[1] Through the conversion of a singlet excited state to two triplet excited states, SF can generate two lower-energy excitons from a single photon, negating some thermal losses.[2] SF has been observed in rubrene in both the solid and molten liquid phases.[3] While SF is maintained over the temperature range, triplet dynamics differ dramatically upon melting.



PROJECT:

This project is focused on gaining synthetic access to room-temperature isotropic liquid (RTIL) rubrene derivatives to investigate whether the intriguing changes in SF dynamics can be observed at realistic device temperatures. Sterically demanding alkyl chains will be introduced to the rubrene core to render the chromophore an RTIL[4] and the potential for its use as a singlet fission dye will be investigated. The student working on this project will be mainly involved in organic synthesis as well as characterization including NMR, mass spectrometry, FT-IR, UV-vis and fluorescence spectroscopy.



REFERENCES:

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[2] A. Rao, R. H. Friend, *Nat. Rev. Mater*. **2017**, *2*, 17063.

[3] G. B. Piland, C. J. Bardeen, *Chem. Phys. Lett*. **2017**, *669*, 99.

[4] F. Lu et al., *Sci. Rep*. **2017**, *7*, 3416.

6. Appendix A

Signature Sheet for Student – Faculty Interviews

Student: _____ _____
(print name) (student #)

e-mail: _____
(University of Manitoba e-mail address)

Program: _____ _____
(e.g Honours Chemistry) (year in program on Sep. 8, 2023)

Interview #1:

Faculty member: _____
(print name)

_____ _____
(signature) (date)

Interview #2:

Faculty member: _____
(print name)

_____ _____
(signature) (date)

Interview #3:

Faculty member: _____
(print name)

_____ _____
(signature) (date)

Notes:
1. Each student should interview at least 3 faculty members willing to offer CHEM4710 projects. During the meeting the nature of the project should be explored and expectations of the student and advisor should be discussed. You can interview as many faculty members as you wish.

2. Students should prioritize their project choices, a minimum of 3 projects are required. Note that every student can apply for any project. Students are strongly discouraged from only choosing projects from a single advisor.

7. Appendix B

Student Project Choices

Student: _____ _____
(print student name) (student #)

_____ _____
(student signature) (date)

Project choices (1 = highest priority, 2, 3,…)

Choice 1: Project title: _____ Project #_____

Supervisor: _____

I, the student, have carried out research with this research group before. YES___ NO___

Choice 2: Project title: _____ Project #_____

Supervisor: _____

I, the student, have carried out research with this research group before. YES___ NO___

Choice 3: Project title: _____ Project #_____

Supervisor: _____

I, the student, have carried out research with this research group before. YES___ NO___

Choice 4: Project title: _____ Project #_____

Supervisor: _____

I, the student, have carried out research with this research group before. YES___ NO___

Choice 5: Project title: _____ Project #_____

Supervisor: _____

I, the student, have carried out research with this research group before. YES___ NO___

Student comments:

8. Appendix C
CHEM 4710 - Research Project in Chemistry or Biochemistry - 2023/24

Course Coordinators:	Mario Bieringer
Office:	520c Parker Building
Email:	Mario.Bieringer@UManitoba.ca
Phone:	204-474-6258

Student - Advisor Agreement

This agreement is between

1. _____

*a **student** registered in CHEM 4710 "Research Project in Chemistry or Biochemistry", hereafter called "the Student"*

2. _____

*a **professor** at the University of Manitoba, and an advisor of a CHEM 4710 student, hereafter called "the Advisor"*

The Student agrees to carry out a research project, as described in the attached research proposal, under the direction of the Advisor. The student agrees to meet the goals and expectations that have been set out by the advisor. These goals and expectations will include not only the scientific aims of the project, but also the time commitment that is required of the student to achieve these goals. The student agrees to a schedule of attendance at regular meetings with the advisor and the research group. The student is expected to become an active member of the research group and will assume responsibility for maintaining a safe work environment in the laboratory. The student may also be expected to assume various duties in addition to those directly associated with the project in order to maintain the safe laboratory environment. The student understands that the main goal of the Research Project is to gain experience in the process of scientific research and that effort is evaluated as much as obtaining research results. The student agrees to meet the deadlines for reporting for both written reports and the oral presentation as set out in the course outline.

The Advisor pledges to support the student in the research project by making available to the student the full resources of the research group and department. In addition the advisor will provide the scientific and intellectual guidance to ensure the success of the project. The advisor agrees to hold regular meetings with the student to discuss the current progress and results. The advisor will encourage the student to develop skills in critical thinking and help to develop a sense of scientific independence. The advisor will provide the necessary training in lab techniques and ensure that the student has received adequate safety training relating to the project. The advisor will also provide the student with timely advice on the content and style of both written reports and oral presentations. The advisor also agrees to give the student appropriate credit for the results generated during the project. This may also include authorship on publications that are generated from the results of the project.

The Student:	The Advisor:
_____	_____
Date:_____	Date:_____

Please sign this form and submit to the course co-ordinator by September 22nd, 2023.