Physical & Environmental Sciences
UNIVERSITY OF TORONTO
SCARBOROUGH

DIRECTED RESEARCH IN CHEMISTRY

CHMD90/91

Syllabus

2023 Fall – 2024 Winter

CHMD90Y3 & CHMD91H3
DIRECTED RESEARCH IN CHEMISTRY

***Course Coordinator*: Prof. Xiao-an Zhang** (xiaoan.zhang@utoronto.ca)

Admittance requirements:

- A Cumulative Grade Point Average of at least **2.5 (or a project-specific GPA that will be advised upon the agreement of the research supervisor)**. Students who do not meet this requirement are encouraged to enroll in CHMD92H3 instead.
- Completion of at least 15 full credits
- Completion of at least 1.0 full credits of C-level CHM courses containing a lab component (i.e. CHMC16H3, CHMC31Y3, CHMC41H3 or CHMC42H3, CHMC47H3, BIOC23H3)

Plan of action for students planning to register in CHMD90Y3/D91H3

1. Look through the projects included in this document (project booklet), which are listed in alphabetical order of the supervisor's family name.
2. **Contact a research supervisor** who will take you to do a project of your choice (to expedite the process email your prospective supervisor your unofficial transcript, your CV along with a letter of intent).
3. Once you've reached agreement with the prospective supervisor, request the course on ACORN and contact the course Coordinator (listed in the timetable as the instructor) to inform of your intent to take the course. Your status will be INT. You will not be officially enrolled until you complete the remaining steps (below)
4. Obtain the D90/91 Supervised Study form, which is available online at https://www.utsc.utoronto.ca/registrar/supervised-study-form or at the Office of the Registrar (Highland Hall, Main Floor).
5. Meet with your Supervisor and obtain their signature on a 'Supervised Study form'. Make sure the course code, supervisor name, and the title of the project are **clearly** printed on the form as this information will appear on your transcript. Your supervisor will also complete information regarding the grading structure of the project.
6. Collect the two required signatures under the Physical and Environmental Sciences section. The course coordinator, Professor Xiao-an Zhang (xiaoan.zhang@utoronto.ca) can sign under the 'Secretary' section; the Department Chair or the Associate Chair Undergraduate can sign under the 'Chair' section.
7. Once the above steps are complete, please email the form to the Assistant to the Chair, Rose Jones (rosa.jones@utoronto.ca, Room EV241).
8. The completed forms will be collected and forwarded to the Registrar's Office to process enrolment. Once finalized, your course status on ACORN from interim (INT) to approved (APP). Students are advised to complete this process early so that the required forms can be submitted and processed by the last day to add courses for the session**.**

Note, it will be impossible to enroll without finding the research supervisor, thus this search is crucial. You could diversify your search by initiate conversations with more than one faculty members offering projects.

Course description:

These courses involve participation in an original research project under the direction of a faculty supervisor. Approximately 260 hours of work are expected in CHMD90Y3 and 130 hours in CHMD91H3. Topics will be selected in conference with the course coordinator who will provide project descriptions from potential faculty supervisors. Progress will be monitored through periodic consultation with the faculty supervisor as well as the submission of written reports. The final results of the project will be presented in a written thesis as well as an oral, poster or online presentation at the end of the term.

Prerequisite: Permission of a course coordinator.

Exclusion: Students may take either CHMD90Y3 or CHMD91H3 but not both. Note that CHMD92H3 is an exclusion to both CHMD90Y3 and CHMD91H3.

EVALUATION OF CHMD90 and CHMD91:

Grade distribution:
Thesis report: 80% (Supervisor: 40%; reader A: 20%; reader B: 20%)
Presentation: 20% (Presentation will be assessed by two or more evaluators, not including your supervisor/co-supervisor. Each evaluation will be weighed equally).

Important Dates for CHMD91-Fall

- **Submission deadline for the 1st draft of your thesis to your supervisor: November 24, 2023**. Find two external readers and presentation evaluators among faculty, research associates, and postdoctoral fellows.
- After completing the revisions requested by the supervisor, the student will submit the final version of thesis to the supervisor and two readers. **The submission deadline of the final thesis is December 01, 2023.**
- **Final oral, poster or online (TBD) presentation** 20% (Tentative date: **December 06, 2023**)
- **All marks due December 10, 2023.**

Important Dates for CHMD90 and CHMD91-Winter

- **Submission deadline for the 1st draft of your thesis to your supervisor: March 29, 2024.** Find two external readers presentation evaluators among faculty or postdoctoral fellows.
- After completing the revisions requested by the supervisor, the student will submit the final version of thesis to the supervisor and two readers. **The submission deadline of the final thesis is April 05, 2024.**
- **Final oral, poster or online (TBD) presentation** 20% (Tentative date: **April 09, 2024**)
- **All marks due April 12, 2024**

Guidelines regarding the thesis reports: The thesis reports should be prepared in max. 20 pages of text with balanced images, illustrations, figures, reaction schemes, and tables, when needed, single-spaced using Times New Roman font-12 including the following sections.

1. **Title page** with the title of your project, your name and number, your supervisor(s) name, the course code, and the date of submission. **(1-page)**
2. **Table of Contents (1-page)**
3. **Abbreviations (if necessary, 1-page)**
4. **Abstract (1-page,** short summary of your thesis highlighting the most important results and conclusions, max. 300 words**)**
5. **Introduction (max. 4 pages)**
6. **Experimental** with subsections such as reagents and chemicals, instruments, procedure and methods.
7. **Results and Discussion**
8. **Conclusions & Future Perspectives**
9. **Acknowledgments**
10. **References (**References should be prepared using the *Journal of American Chemical Society* guidelines**)**

Appendices can be attached as Supporting Information file to your thesis with unlimited number of pages displaying additional figures, tables, images, illustrations and raw experimental results such as MS, NMR, and IR data.

Lab Safety & Onboarding Training Requirements

The Department of Physical and Environmental Sciences has recently introduced new safety and on-boarding training requirements, for all new laboratory personnel, including CHMD90/91 students whose research projects include "wet-lab" components:
https://www.utsc.utoronto.ca/physsci/onboarding-and-training

Please carefully review the webpage. It covers guidelines for both safety training and registration requirements to gain access to the research building.

Safety Training: The EHS courses listed in the webpage above are required for wet-lab experiments. Please discuss this with your supervisor. Students are recommended to complete the online training courses on time, so there will be no delay to gain the access to the lab. Specific instructions also could be found in the Department Personnel Registration and Emergency Preparedness (PREP) document:
https://www.utsc.utoronto.ca/physsci/sites/utsc.utoronto.ca.physsci/files/docs/DPES%20PREP%20Form%20-%20Jan%2014%2C%202022.pdf
You can enroll into the required online EHS courses, including the WHMIS training via the link: https://ehs.utoronto.ca/training/my-ehs-training/

Training certification submission: After finishing the online training successfully, you should give/email a copy of your certificate to your supervisor.

Biosafety course: Please, consult with your supervisor whether a Biosafety Certificate is required for your project. The course can be found from the following link:
https://ehs.utoronto.ca/our-services/biosafety/biosafety-training/

(You should give a copy of your certificate to your supervisor)

***Note: Please, consult your supervisor about the attached NSERC Consent Form on the next page. You can give the signed form to your supervisor if you wish to give them your consent to include your name in their grant applications.**

Na:uralSciencesandEngineering ResearchCouncil ofCanada
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Consent to Provide Limited Personal Infom,ation About Highly Qualified Personnel (HQP) to **NSERC**

NSERC applicants al'c! requiied to @scribe theiroontributionsto the trainingor supQrviSion of highly qualifiQd personnel (HQP) by providing autain detailSabout the individualS they haw traiOQd or supervised duringthe siXyQarS priOrto their current applicatiOn. HQP infonnatiOn must be entered on the Personal Data Fonn (Fonn 100). This infonnatiOn includes the trainee's name, type of HQP training (e.g., undergraduate,master's, technicaletc.)andstatus (oornplQted, in-progress, inoornplQte), Y'!arSsupQrviSed oroo-superviSed, titleof the project or thQsis, and the individuars p s-Qnt position.

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Consent Not Obtained from Marie Ro)'				
(name withheld)	Undergraduate (Completed)	Supervised 1994 - 1997	Isotope geochemistry	research executive in petroleum indus1ry - western Canada

Consent Form

Nameof Trainee

Applicant Infonn ion

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Canada

Physical & Environmental Sciences
UNIVERSITY OF TORONTO
SCARBOROUGH

DIRECTED RESEARCH IN CHEMISTRY

CHMD90/91

Project Booklet

2023 Fall –

2024 Winter

The projects are listed in the alphabetical order of the family names of the supervisors.

Supervisor: Artur Izmaylov

Co-supervisor (if any):

Office: EV356

Sub-discipline: Theory

Laboratory: EV327

Course code: CHMD90/91

e-mail: see the webpage below

# of students: 2

Web: https://www.utsc.utoronto.ca/~aizmaylov/index.html

Quantum Computing for Quantum Chemistry

The electronic structure problem is the key for material and drug designs. Solving it accurately using quantum mechanical methods on regular classical computers leads to algorithms whose execution time grows exponentially with the system size. Emerging technology of quantum computing recently provided a new hope to solve this problem efficiently. Yet, the new quantum hardware requires new algorithms. Currently, there are two main algorithmic frameworks for solving the electronic structure problem on a quantum computer: 1) quantum phase estimation (QPE) and 2) variational quantum eigensolver (VQE). None of these approaches have provided a solution to the problem that is competitive with well-developed numerical techniques on a classical computer. Thus, none of them has yet demonstrated quantum advantage (superiority of quantum computing over its classical counterpart) for the electronic structure problem. In this project we will be developing new alternative frameworks for solving the problem on a quantum computer that will address main deficiencies of the previous techniques. The main goal is to develop a framework demonstrating quantum advantage in quantum chemistry problems.

- Learning outcomes: You will learn the basics of the scientific approach and methods of quantum computing for theoretical chemistry
- Required training certificates: None
- Our expectations from students: Will be communicated in person

References:

[1] See our most recent publications on Google Scholar
[2] Also, here are videos highlighting our research on YouTube

Supervisor: Dr Shadi Dalili
Co-supervisor (if any): Dr Kagan Kerman
Dr Meissam Noroozifar
Office: EV 562
Sub-discipline: Organic/Materials
Laboratory: EV 261
Course code: CHMD90Y

Web: https://www.utsc.utoronto.ca/physsci/shadi-dalili

e-mail: sh.dalili@utoronto.ca
# of students: 1-2

Application of COFs and MOFs in solar cells

The main goal of this project is development of covalent organic frameworks (COFs) and/or metal organic frameworks (MOFs) as a new generation of materials for solar cells (SC). One of the major issues in current solar cells is that they are not stable with a light simulator (SUN), due to unstable sensitizers, whose role is to allow for absorption of the light and injection of photoexcited electrons into the conduction band of TiO2 as semiconductor. Generally, the sensitizers decompose with the SUN.

COFs and MOFs composed of a high number of C-C, C-O, C-H, and M-O bonds have shown to create high thermal stability between 300-500°C. Along with this high thermal stability, high chemical stability, tunability in pore or channel architecture, and the ability to change chemical properties after synthesis via post-synthetic techniques are the most attractive properties in these materials.

Our hypothesis is that based on this heterojunction between MOF with the TiO2 and other elements in SC, the efficiency of SC can be increased.

The successful candidate(s) for the project will conduct a comprehensive literature research on the different types, applications and syntheses of COFs and MOFs and use this information to propose and design novel COFs and MOFs that could show high stability with high molar absorptivity by varying the different organic moieties in the structures. The 2nd stage of the project will be the synthesis and characterization of the proposed structure(s) and subsequent building of the solar cells and testing of compounds in the SC in Dr. Kerman's lab under co-supervision and conceptualization by Dr. Meissam Noroozifar.

Supervisor: **Kagan Kerman**

Office: **EV548** **Sub-discipline: Bioelectrochemistry**

Laboratory: **EV506** **Course code:** **CHMD90**

e-mail: **kagan.kerman@utoronto.ca** **# of students: 1**

Web: **https://bioelectrochemistry.utoronto.ca/**

IMMUNOCHIPS FOR AMYLOID-BETA USING ELECTROCHEMICAL IMPEDANCE SPECTROSCOPY

Alzheimer's disease (AD) is a progressive and irreversible neurodegenerative dementia marked by substantial impairments to episodic memory and cognitive functions. Approximately 60% of all late-onset cases of dementia are attributed to AD, which is estimated to afflict more than 500,000 Canadians. The amyloid cascade hypothesis attributes AD pathogenesis to an imbalance in amyloid-beta (Abeta), a small 4 kDa peptide capable of undergoing spontaneous self-association to form neurotoxic supramolecular assemblies. Notably, soluble oligomers have been identified as the more relevant toxic species of Abeta relative to later stage fibrillar aggregates and has since become a critical target for future drug therapy development.

We will be developing a rapid, disposable electrochemical immunosensor for determination fibril and oligomer distribution over the course of Abeta aggregation [1]. To this effect, conformation-specific antibodies will be immobilized onto the surface of a gold electrode to monitor the inhibition of distinct aggregate states. Surface binding events will be determined by impedance spectroscopy, in which antigen-antibody interactions are quantified as a function of charge transfer resistance across the electrode interface. The results are expected to demonstrate the utility of impedimetric immunosensing for comprehensive identification of effective Abeta aggregation modulators.

Ø A student working on this project will gain experience in biosensor development using electroanalytical and biological techniques.

Ø Student is expected to present the research results in weekly group meetings (Friday afternoons).

References: **[1]** Electrochemical immunosensors for effective evaluation of amyloid-beta modulators on oligomeric and fibrillar aggregation processes. Veloso AJ, Chow AM, Ganesh HV, Li N, Dhar D, Wu DC, Mikhaylichenko S, Brown IR, **Kerman K.** Anal Chem. 2014 May 20;86(10):4901-9. doi: 10.1021/ac500424t. Epub 2014 Apr 30.

Supervisor: Bernie Kraatz Co-supervisors:

Office: ESCB 5th floor Sub-discipline: Inorganic/ Biological

Laboratory: ESCB 5th floor Course code: CHMD90

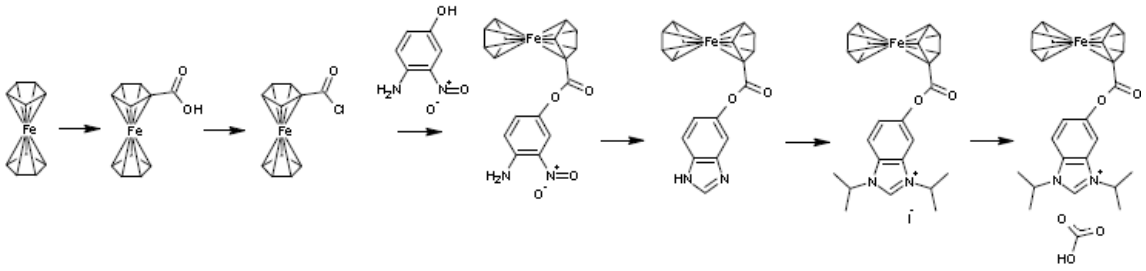
e-mail: bernie.kraatz@utoronto.ca # of students: 1

Web: http://www.utsc.utoronto.ca/~bkraatz/

Ferrocene-terminated benzimidazole and its derivatives

Carbenes, a class of compounds that have one of the carbon atoms in an oxidation state of two, are known to react with variety of metals forming stable self-assembled monolayers (SAMs) on surfaces. In situ carbene formation from air-stable precursors followed by a reaction with a metal surface may lead to an analogous coat formation. This organic layer covalently bound to a metal may be potentially used as a corrosion protection coat.

The ferrocene is a redox active moiety; as a result, ferrocene based building blocks have already been used successfully in fabrication of various SAMs. Analysis of cyclic voltammograms of ferrocene-terminated SAMs allows determination of the charge involved in the redox process, and thus to calculate actual surface coverage of the ferrocene units.



Ø Learning outcomes: In this project, the student will be involved in the synthesis of various ferrocene-terminated benzimidazole derivatives by solution phase methods, their isolation and characterization by spectroscopic methods (NMR, IR, MS) thus gaining invaluable experience in advanced synthetic and analytical techniques.

Ø Required training certificates WHMIS

Ø Our expectations from students: I expect students to work effectively and collaboratively with graduate students and postdoctoral fellows and fully participate in all group activities and meetings. I expect monthly written updates on progress. Weekly meetings with the supervisor will be arranged. Day-to-day interactions with Drs. Iralkii Ebralidze and Zhe She and graduate students.

Supervisor: Bernie Kraatz Co-supervisors:

Office: ESCB 5th floor Sub-discipline: Inorganic/ Biological

Laboratory: ESCB 5th floor Course code: CHMD90

e-mail: bernie.kraatz@utoronto.ca # of students: 1 -2

Web: http://www.utsc.utoronto.ca/~bkraatz/

Development of Peptide Co-Gels

Peptide molecules can interact via hydrogen bonding and π-stacking interactions to generate materials that allow the inclusion of large quantities of solvent molecules. In these gels, peptides engage in interactions that exhibit some level of order but lack crystallinity. Our group has studied a series of stimuli-responsive gels in which the gel can react to external stimuli (see references).

This project focuses on co-gels, in which two peptide gelators can interact with each other and generate a wide range of gel properties. This project will explore issues related to co-assembly and to self-sorting. We have reported before the self-sorting behavior of a series of gels that carry a fluorescent label (see references). Here, the gel forming properties of the ferrocene-peptide conjugate Fc-CO-FFL-OMe will be probed. The investigation will involve various diasteromers of this peptide and the gel and co-gelation will be studied using a range of experimental techniques, including circular dichroism, 1H-NMR, and IR spectroscopies. In addition, variable temperature NMR spectroscopy is ideal for the study of intermolecular H-bonding interations. Morphologies of the gels will be studied by electron microscopy.

R. Afrasiabi, H.B. Kraatz, *Chem. Eur. J.* **2015**, *21*, 7695-7700; B. Adhikari, H.-B. Kraatz, *Chem. Commun.* **2014**, *50*, 5551-5553 and references therein.

Ø Learning outcomes: In this project, the student will be involved in the synthesis of various ferrocene-peptide derivatives by solution peptide coupling methods, their isolation by column chromatography and characterization by spectroscopic methods (CD, NMR, IR, MS) thus gaining invaluable experience in advanced synthetic and analytical techniques.

Ø Required training certificates WHMIS

Ø Our expectations from students: I expect students to work effectively and collaboratively with graduate students and postdoctoral fellows and fully participate in all group activities and meetings. I expect monthly written updates on progress. Weekly meetings with the supervisor will be arranged. Day-to-day interactions with Drs. Iralkii Ebralidze and Zhe She and graduate students.

Supervisor: Bernie Kraatz | Co-supervisors:

Office: ESCB 5th floor | Sub-discipline: Inorganic/ Biological

Laboratory: ECSB 5th floor | Course code: CHMD90

e-mail: bernie.kraatz@utoronto.ca | # of students: 1

The influence of benzimidazolium hydrogen carbonates on formation of nanostructured silver surfaces

Carbenes, molecules containing a neutral carbon atom with a valence of two and two unshared valence electrons, are known to react with variety of metal ions and metals forming stable metal complexes or self-assembled monolayers (SAMs) on metal surfaces. However anhydrous conditions and inert atmosphere are required for carbenes in their so called "free carbene" form. Alternatively air-stable carbene precursors could be utilized for the same purposes. We plan to elaborate and optimize a method for the formation of stable carbene based SAMs at ambient conditions.

This project will start with synthesis of several benzimidazolium based carbene precursors and formation of SAMs on silver surfaces. Electrochemical cycling of these SAM-covered silver surfaces in aqueous solutions will be performed to get an idea of stability of the SAMs. Further electrochemical cycling of SAM- functionalized silver surfaces in solutions of carbene precursors in organic solvents will be performed to track changes in the electrochemical response due to either disruption of the original SAM layer, or due to the formation of silver nanostructures. Since carbene precursors may form either homogeneous silver complexes or react directly with a surface of a metal cluster, electrochemical cycling may result in silver leaching from the surface followed by the formation of silver complexes in solution. Alternatively, it may result in the formation of metal clusters followed by their deposition on the surface. These clusters on silver surfaces may be potentially useful for sensing applications in biomedical sciences or pollution monitoring.

Ø Learning outcomes: Student participating in this project will be involved in the synthesis of various benzimidazole derivatives by solution phase methods, their isolation and characterization by spectroscopic methods (NMR, IR, MS) thus gaining invaluable experience in advanced synthetic and analytical techniques. In addition, the student will get valuable experience in the formation of SAMs, their characterization (XPS and e-chem stripping), and surface modification by e-chem cycling.

Ø Required training certificates: WHMIS

Ø Our expectations from students: I expect students to work effectively and collaboratively with graduate students and postdoctoral fellows and fully participate in all group activities and meetings. I expect monthly written updates on progress. Weekly meetings with the supervisor will be arranged. Day-to-day interactions with Drs. Iralkii Ebralidze and Zhe She and graduate students.

Supervisor: Bernie Kraatz Co-supervisors:

Office: ESCB 5th floor Sub-discipline: Inorganic/ Biological

Laboratory: ECSB 5th floor Course code: CHMD90

e-mail: bernie.kraatz@utoronto.ca # of students: 1

Pathogen detection by electrochemical methods

The objective of this project is to study the electrochemical behaviour of modified surfaces and their interactions with pathogenic agents. My group has studied biosensing surfaces for a wide range of bioanalytes, including DNA. In previous studies, electrochemical studies of DNA-modified gold micro-electrodes allowed us to distinguish mismatched positions and mismatch pairs of DNA, as well as being able to distinguish between mitochondrial DNA fragments in the cytochrome C1 oxidase gene (see references).

In this study, different bio-recognition elements, such as DNA and antibody proteins, will be investigated towards detection whole bacteria and pathogen-associated molecular patterns, such as for Escherichia coli and Salmonella, which are commonly found in our lake water and in contaminated meats.

The approach will be carried out in this project is to combine surface chemistry with electrochemistry. Bio-recognition elements will be immobilized onto gold surfaces and their bindings to the targets will be monitored using Cyclic Voltammetry, Square Wave Voltammetry and Electrochemical Impedance Spectroscopy. The aim is to develop biosensors that are able to convert biological responses into sensitive quantifiable electric signals and construct calibration curves for the biological targets

Diakowski, P. M.; Kraatz, H.-B. *Chem. Commun.* **2009**, 1189; Shamsi, M. H.; Kraatz, H.-B. *Analyst* **2010**, *135*, 2280; Shamsi, M. H.; Kraatz, H. B. *Analyst* **2011**, *136*, 4724; 3107; Diakowski, P. M.; Kraatz, H. B. *Chem. Commun.* **2011**, *47*, 1431.

Ø Learning outcomes: Student will be involved in the modification of surfaces, their characterization by spectroscopic and electrochemical methods and their interactions with bioanalytes and the construction of response curves.

Ø Required training certificates: WHMIS

Ø Our expectations from students: I expect students to work effectively and collaboratively with graduate students and postdoctoral fellows and fully participate in all group activities and meetings. I expect monthly written updates on progress. Weekly meetings with the supervisor will be arranged. Day-to-day interactions with Drs. Iralkii Ebralidze and Zhe She and graduate students.

Supervisor: Bernie Kraatz Co-supervisors:

Office: ESCB 5th floor Sub-discipline: Inorganic/ Biological

Laboratory: ECSB 5th floor Course code: CHMD90

e-mail: bernie.kraatz@utoronto.ca # of students: 1

Study of metal ion interactions with peptides.

The protein Tau is responsible for microtubule stabilization in neuronal cells and their activity is regulated by kinase-catalyzed phosphorylations. Hyperphosphorylation of Tau causes catastrophic destabilization of the microtubules, followed by assembly of phosphorylated Tau into neurofibrillar tangles on the interior of the neuronal cells causing cell death. Metal ions are found to be associated with these neurofibrillary protein tangles.

This project focuses of the study of a range of metal ions (Fe^{3+}, Cu^{2+} etc) with peptide fragments of Tau. We have evaluated phosphorylations and Cu^{2+} binding to full length Tau before and studied its behavior by electrochemical and spectroscopic means (see references). This project will focus on solution studies involving Tau peptides and metal ions. The interactions will be monitored by calorimetry, which will allow the evaluation of the thermodynamics of the interaction, and by circular dichroism spectroscopy, which will allow probing structural changes as a result of the interaction.

S. Martić, M.K. Rains, H.-B. Kraatz, *Anal. Biochem.* **2013**, *442*, 130-137; S. Martić, S. Beheshti, M. K. Rains, H.-B. Kraatz, *Analyst* **2012** *137*, 2042-2046.

Ø Learning outcomes: Student will be involved in the calorimetric and CD spectroscopic studies and their evaluation and learn basic bioinorganic techniques.

Ø Required training certificates: WHMIS

Ø Our expectations from students: I expect students to work effectively and collaboratively with graduate students and postdoctoral fellows and fully participate in all group activities and meetings. I expect monthly written updates on progress. Weekly meetings with the supervisor will be arranged. Day-to-day interactions with Soha Ahmadi.

Joint Supervisor: **Andre Simpson** Joint Supervisor: **Xiao-an Zhang**

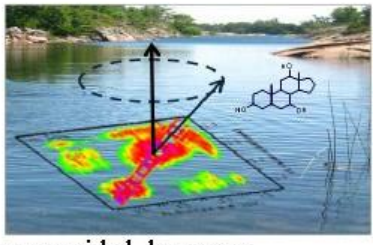
Office: **SY324** Sub-discipline: **Organic/Analytical/Environmental**

Laboratory: **SY050** Email: andre.simpson@utoronto.ca and xazhang@utsc.utoronto.ca

NMR Anion Sensors, Functional Group Capping and Mass Spectrometry: A multidisciplinary approach to address the world's most complex mixture.

Dissolved Organic Matter (DOM) is ubiquitous in all natural waters and known to play important roles in the global carbon and nitrogen cycles, the fate, transport and transformation of contaminants and nutrients and the health and biodiversity of aquatic species. DOM, however, is not just important due to its key role in environmental processes but its structural signatures themselves of immense interest. This is probably best summarized by John Hedges, arguably one of the greatest oceanographers of the modern era, he stated, "*The 10^{12} diverse organic molecules dissolved in every milliliter of seawater are the only constituents whose stored information approaches the richness needed to understand where the water has been and what has happened within it over time. The future of oceanographic research belongs in part to those who can learn to read these molecular messages.*"

Recently the A. Simpson group through hyphenation of 2D HPLC and 3D NMR has discovered the main constituents of DOM are highly oxygenation terpenoids. However, the analysis took 2 years making it impractical for routine applications. Theoretically if the material could be derivatized such that it can be dissolved it non-polar solvents, high resolution GC-MS methods should be ideal for rapid routine screening of the material. Simple derivatization is not easy as there are many acid and alcohol groups per terpenoids structure and steric hindrance may be problematic when trying to cap all of them. The Zhang group have developed a unique NMR based anion sensor. The sensor works in organic solvents and provides a simple and rapid indicator as to how many unexposed polar groups remain after derivatization.



The project with be a 50:50 collaboration between the A. Simpson and Zhang research groups. The student will attempt various derivatizations (mainly methylations) in the Zhang group and then compare the effectiveness of each approach using the NMR sensor with the A. Simpson group. Finally GC-MS analysis will be performed to assess the additional information provided by more complete derivatization of the materials.

Learning outcomes

(**1**) Various organic reactions and derivatization.
(**2**) Advanced NMR and NMR sensors.
(**3**) Gas Chromatography – Mass Spectrometry Analysis.

Required Training: WHMIS

Our expectation from students: Hard working, open minded student, with interests in more than one area of chemistry. It is highly likely the work will lead to a scientific publication, we expect the student to be highly involved and lead this process.

Supervisor: **Andre Simpson** co-supervisor: **Ronald Soong**

Office: **SY324** Sub-discipline: **Analytical/Biological**

Laboratory: **SY050** Course code: **CHMD90**

Email: andre.simpson@utoronto.ca and ronald.soong@utoronto.ca

Investigating ^{15}N as an important nucleus to better understand biochemical processes through *in-vivo* NMR

D. magna are the standard organism used globally for aquatic toxicity testing. The present method used by regulatory bodies to assess aquatic toxicity of a compound is the "21 day reproducibility test". If no perturbations are noted in reproducibility then the chemical is deemed to be safe at that concentration. However, the literature has repeatedly reported more subtle effects such as DNA damage, changes to metabolic pathways, bioaccumulation, permanent binding can be missed using this standard approach as such there is great need to develop more informative, sensitive and rapid methods to truly evaluate aquatic toxicity.

In-vivo NMR, has the potential to monitor not only the entire molecular fingerprint of an organism in real time but also relates changes in the molecular profile to uptake, transformation, binding, bio-concentration and secretion of a contaminant species. As such *in-vivo* NMR provides the technical framework required to understand "how" and "why" certainly chemicals are toxic, information desperately needed by regulators to set more meaningful standards. Despite its considerable potential *in-vivo* NMR has not yet been applied to evaluate toxicity in an environmental context.

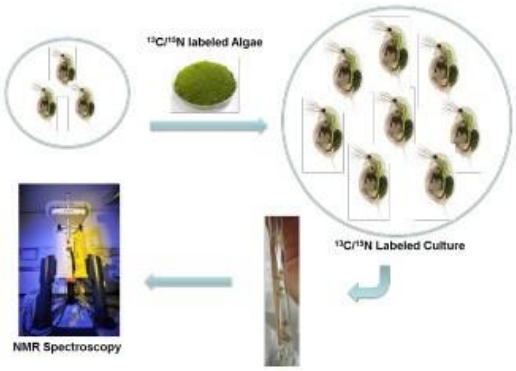
Optimizing the depth and variety of information that can be obtained via *in-vivo* NMR will be critical to comprehensively evaluate toxic pathways. With this in mind ^{15}N NMR (1D and multidimensional) will be explored as a potentially powerful tool to study metabolites, proteins and other biomolecules *in-vivo*. Organisms will be fed a diet of ^{15}N labelled algae and various NMR schemes will be developed to observe and differentiate metabolites and macromolecules *in-vivo*. It is anticipated ^{15}N labelling will provide a wealth of novel information complimentary to common NMR studies focusing on ^{1}H and ^{13}C.

Learning outcome

(1) The student will receive hands-on training on culturing and isotopic labelling *D. Magna*

(2) The student will receive training on using advanced NMR spectroscopy required for *in-vivo* studies.

(3) The student will learn about different statistical methods for data analysis and interpretation.



Required Training: WHMIS

Our expectation from students: Hard working, open minded student, with interests in more than one area of chemistry. It is highly likely the work will lead to a co-authored scientific publication, we expect the student to be involved in this process as required.

Supervisor: **Andre Simpson** co-supervisor: **Ronald Soong**

Office: **SY324** Sub-discipline: **Analytical/Biological**

Laboratory: **SY050** Course code: **CHMD90**

Email: andre.simpson@utoronto.ca and ronald.soong@utoronto.ca

Investigating ^{31}P as an important nucleus to better understand energetic processes through *in-vivo* NMR

D. magna are the standard organism used globally for aquatic toxicity testing. The present method used by regulatory bodies to assess aquatic toxicity of a compound is the "21 day reproducibility test". If no perturbations are noted in reproducibility then the chemical is deemed to be safe at that concentration. However, the literature has repeatedly reported more subtle effects such as DNA damage, changes to metabolic pathways, bioaccumulation, permanent binding can be missed using this standard approach as such there is great need to develop more informative, sensitive and rapid methods to truly evaluate aquatic toxicity.

In-vivo NMR, has the potential to monitor not only the entire molecular fingerprint of an organism in real time but also relates changes in the molecular profile to uptake, transformation, binding, bio-concentration and secretion of a contaminant species. As such *in-vivo* NMR provides the technical framework required to understand "how" and "why" certainly chemicals are toxic, information desperately needed by regulators to set more meaningful standards. Despite its considerable potential *in-vivo* NMR has not yet been applied to evaluate toxicity in an environmental context.

Optimizing the depth and variety of information that can be obtained via *in-vivo* NMR will be critical to comprehensively evaluate toxic pathways. With this in mind ^{31}P NMR (1D and multidimensional) will be explored as a potentially powerful tool to study metabolites (such as ADP, ATP, phospholipids etc.) and biomolecules RNA/DNA *in-vivo*. Organisms will studies *in-vivo* and *in-vitro* after chemical extraction. High resolution NMR from extracts will be useful for assignments of broader signal in ^{31}P *in-vivo* NMR. It is anticipated ^{31}P NMR provide a wealth of novel information complimentary to common NMR studies focusing on ^{1}H and ^{13}C.

Learning outcome

(1) The student will receive hands-on training on culturing *D. Magna*

(2) The student will learn various extraction approaches.

(3) The student will receive training on using advanced NMR spectroscopy required for *in-vivo* studies.

(4) The student will learn about different statistical methods for data analysis and interpretation.

Required Training: WHMIS

Our expectation from students: Hard working, open minded student, with interests in more than one area of chemistry. It is highly likely the work will lead to a co-authored scientific publication, we expect the student to be involved in this process as required.

Supervisor: **Andre Simpson** co-supervisor: **Ronald Soong**

Office: **SY324** Sub-discipline: **Analytical/Biological**

Laboratory: **SY050** Course code: **CHMD90**

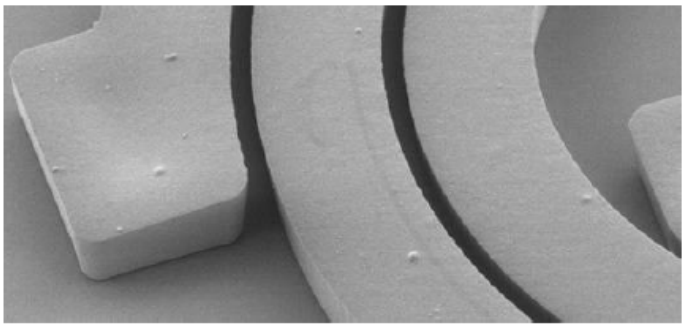
Email: andre.simpson@utoronto.ca and ronald.soong@utoronto.ca

The Application and Development of Micro Surface Coil NMR.

NMR spectroscopy is arguably the most powerful tool in modern research with the ability to provide unprecedented levels of information regarding molecular structure and interactions. However, the relatively low sensitivity of NMR is it's main drawback. Recently, new nanolithography techniques allow the "printing" of NMR coils as small as individual cells. Such coils provide theoretical mass sensitivities ~50 times higher or time savings of ~2500 times in comparison to conventional NMR technology.

However, when moving to such small samples questions become: "how do we handle such samples?", "how do we retain the sample on the coil?", "how do we prevent evaporation?", "can organisms be kept alive on these coils?", "how small can we go?", and "what are applications of coils of varying diameter?"

The D90 student with work alongside graduate students and PI's to assist in answering these questions. The student will be immersed in all areas of the project and will learn a diverse array of techniques, application and theory. The student will test various applications that include plants, cells, organisms, tissue, small fruits/seeds. In both static and flow orientations.



Learning outcome

(1) The student will receive hands-on training on handling tiny samples using microscopes.

(2) The student will receive training on using advanced NMR spectroscopy, including advanced water suppression, advanced acquisition and spectral interpretation approaches.

(3) The student will learn about theory and application of cutting edge, globally unique, micro-coil NMR technology.

(4) The student will work with a diverse range of chemical, environmental and biological samples.

Required Training: WHMIS

Our expectation from students: Hard working, open minded student, with interests in more than one area of chemistry. It is highly likely the work will lead to a co-authored scientific publication, we expect the student to be involved in this process.

Supervisor: **Andre Simpson** co-supervisor: **Ronald Soong**

Office: **SY324** Sub-discipline: **Analytical/Biological**

Laboratory: **SY050** Course code: **CHMD90**

Email: andre.simpson@utoronto.ca and ronald.soong@utoronto.ca

Understanding real-time bioaccumulation and transformation of perfluorinated contaminants in *Daphnia magna* using *in-vivo* NMR

D. magna are the standard organism used globally for aquatic toxicity testing. The present method used by regulatory bodies to assess aquatic toxicity of a compound is the "21 day reproducibility test". If no perturbations are noted in reproducibility then the chemical is deemed to be safe at that concentration. However, the literature has repeatedly reported more subtle effects such as DNA damage, changes to metabolic pathways, bioaccumulation, permanent binding can be missed using this standard approach as such there is great need to develop more informative, sensitive and rapid methods to truly evaluate aquatic toxicity.

In-vivo NMR, has the potential to monitor not only the entire molecular fingerprint of an organism in real time but also relates changes in the molecular profile to uptake, transformation, binding, bio-concentration and secretion of a contaminant species. As such *in-vivo* NMR provides the technical framework required to understand "how" and "why" certainly chemicals are toxic, information desperately needed by regulators to set more meaningful standards. Despite its considerable potential *in-vivo* NMR has not yet been applied to evaluate toxicity in an environmental context.

In this project *in-vivo* NMR will be used to monitor the real time uptake, biotransformation and binding of perfluorinated contaminants which are now found ubiquitously in our environment. Perfluorinated hydrocarbons are present in human blood in the ppb range (50 ppb average in the public) to ppm range (3M workers). The chemicals exhibit complex toxicity that is not well understood. NMR has a key role to play in understanding the toxicity of PFC's for example our group showed that PFOA and PFOS interact preferentially and irreversibly with Sudlow's site I and II on human serum albumin when introduced to human blood. However, at present there have been no studies of PFC's *in-vivo*. The chemicals themselves will be monitored by a range of NMR approaches to understand and explain their biological uptake, accumulation, transformation and secretion. *In-vivo* NMR holds great potential to understand the impact of chemicals prior to mass release into the environment.

Learning outcome

(1) The student will receive hands-on training on culturing *D. Magna*

(2) The student will receive training on using advanced NMR spectroscopy required for in-vivo studies.

(3) The student will learn about different statistical methods for data analysis and interpretation.

Required Training: WHMIS

Our expectation from students: Hard working, open minded student, with interests in more than one area of chemistry.

Supervisor: **Prof. Myrna Simpson** **Co-supervisor (if any):**

Office: **SY322** **Sub-discipline(s): Environmental, Analytical, Organic**

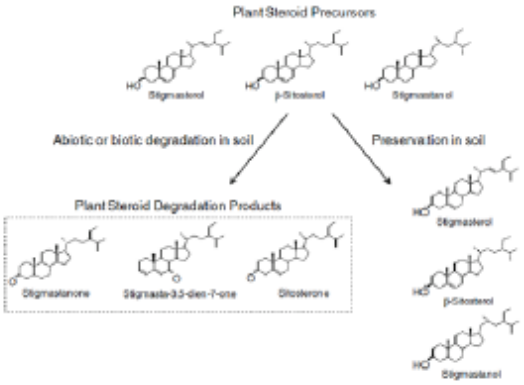
Laboratory: **SY315** **Course code: CHMB42, CHMB55, CHMC11**

e-mail: **myrna.simpson@utoronto.ca** **# of students: 1**

Web: www.utsc.utoronto.ca/~msimpson

Antimicrobial properties of plant steroids in soil

Several plant steroids (β-sitosterol, stigmasterol, sitosterone, stigmasta-3,5-dien-7-one, and campesterol) are deposited into soil environments after cell death. Some of these steroids are degraded by bacteria and fungi and some are preserved through binding to the inorganic portion of the soil. Recently, it has been found that when the concentrations of these steroids increase, they exhibit anti-microbial properties and impact the natural process of soil carbon cycling (biogeochemistry) [1]. This project will test how the addition of plant steroids may alter soil biogeochemistry in laboratory incubations.



- Learning outcomes: The student will learn about environmental chemistry processes in soil. They will also apply organic chemistry skills to isolate and purify plant-steroids. Laboratory incubations will be monitored using headspace CO_2 analysis and monitor degradation products using GC-MS. The student on this project will be able to apply knowledge in organic, environmental and analytical chemistry to this research.

- Required training certificates: EHS005 WHMIS; EHS002 Basic Health and Safety Awareness

- Student expectations: The student on this project will be encouraged to attend and participate in Group meetings. The student will meet with the supervisor every 2-3 weeks to discuss project logistics and progress.

References:

[1] Wang, J. et al. *Biogeochemistry* 142, 299–313 (2019)

Supervisor: **Prof. Myrna Simpson** **Co-supervisor (if any):**

Office: **SY322** **Sub-discipline(s): Environmental, Analytical, Organic**

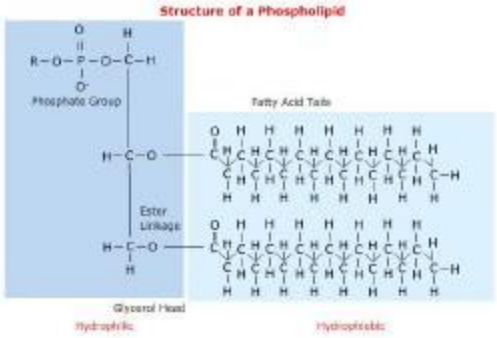
Laboratory: **SY315** **Course code: CHMB42, CHMB55, CHMC11**

e-mail: **myrna.simpson@utoronto.ca** **# of students: 1**

Web: www.utsc.utoronto.ca/~msimpson

Can we use ^{31}P NMR to quantify isolated phospholipid fatty acids from soil?

Phospholipid fatty acid (PLFA) profiling is commonly used to measure the total microbial biomass and community structure in soils and sediments. The most common method involves using a Bligh and Dyer extraction followed by several purification and isolation steps to isolate the hydrophobic fatty acid "tails" [1]. Once the extract has been isolated, the lipids are derivatized for GC-MS analysis. The entire process requires 2-3 days of lab work but yields quantitative information about different PLFA types that are indicative of microbial community (actinomycetes, bacteria and fungi). This project will compare quantification of PLFAs using the standard GC-MS method and solution-state ^{31}P NMR of the total lipid extract. The ^{31}P NMR requires less sample preparation steps and could serve as a rapid measure of total microbial biomass. The aim of this project is to compare the two methods and determine the benefits and limitations of each method.



- Learning outcomes: The student will learn about organic extraction and purification methods. The student will learn and use GC-MS and NMR for quantification of PLFA fractions. The student on this project will be able to apply knowledge in organic, environmental and analytical chemistry to this research.

- Required training certificates: EHS005 WHMIS; EHS002 Basic Health and Safety Awareness

- Student expectations: The student on this project will be encouraged to attend and participate in Group meetings. The student will meet with the supervisor every 2-3 weeks to discuss project logistics and progress.

References:

[1] Frostegård, A. & Bååth, E. *Biol. Fertil. Soils* 22, 59–65 (1996)
[2] Watts, E. E. & Dean, P. *Can. J. Anal. Sci. Spectrosc.* 47, 127-133 (2002)

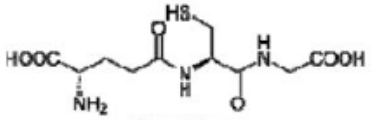
Supervisor: Ronald Soong **Co-supervisor (if any): Andre Simpson**
Office: SY324 **Sub-discipline: Analytical/Biological**
Laboratory: SY050 **Course code: CHMD90**
e-mail: ronald.soong@utoronto.ca **# of students: 1**
Web: http://www.utsc.utoronto.ca/~asimpson/

^{19}F TAGGING OF THIOLS AS AN APPROACH FOR THE NMR DETECTION AND QUANTIFICATION OF GLUTATHIONE AND ITS DERIVATIVES IN BIOFLUIDS

Glutathione and its derivatives are important biomarkers in the measurement of oxidative stress in an organism. Therefore, significant amount of work has been done for the detection and qualification of glutathiones in various biofluids, such as blood, urine and tissue extracts. Nuclear Magnetic Resonance (NMR) NMR spectroscopy is one of the most powerful tools for studying metabolite fluxes in intact biofluids. However, for most complex biological fluids the ^{1}H NMR resonances of glutahiones are often indistinguishable from other metabolites due to serve spectral overlap. However, the thiol (SH) group can be activated to form disulfide bonds, allowing us to add NMR observable ^{19}F tag for detection. ^{19}F tag offers several advantages, including 100% natural abundance and highly sensitive to its chemical environment. The goal of this D90 project is to investigate various strategies in incorporating different ^{19}F tag through disulfide bond linkage in standard Glutathiones and in biological tissue extracts.

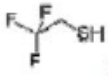
Learning outcomes :

- Hands-on-experience and training with state-of-art NMR spectroscopy. Experience with the derivatization of biological molecules. Experience in metabolomics (one of the most powerful approaches to understand biological response).
- Required training certificates : WHMIS
- Our expectations from students. Hard working, open minded student, with interests in more than one area of chemistry. Ambition to publish results in a top international journal.

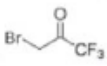


Glutathione

Possible ^{19}F Tag



2,2,2-Trifloroethanethiol



3-bromo-1,1,1-trifluoroacetone

References

Potapenko, D.I. et al. *Magn. Reson. Chem.*, **43** (2005) 902–909

Loewen. M.C. et. al. *Proc. Natl. Acad. Sci. USA*, **98** (2001) 4888-4892.

Supervisor: **Ronald Soong**

Co-advisor: **Artur Izmaylov**

Office: **SW155B**

Sub-discipline: **Instruments**

Laboratory:

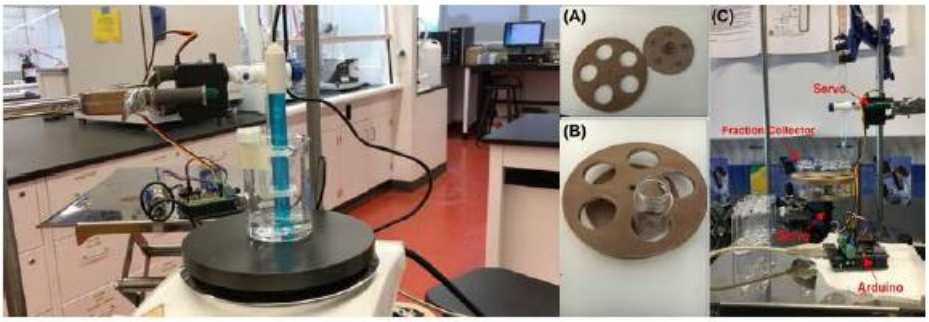
Course code: **CHMD90/91**

e-mail: ronald.soong@utoronto.ca

# of students: **1**

Construction and Evaluation of Portable Analytical Instruments Based on the Arduino Microcontroller

A microcontroller is a micro-computer that is small and generally inexpensive. They are low-powered and can be powered through a variety of ways, including a USB connection, a wall socket, and a 9V battery[1]. Several types of microcontrollers are commercially available; the specific microcontroller studied here is called the Arduino. In this project, the student will be tasked with designing and making analytical instruments for undergraduate experiments. The goal is to create these low cost instruments such that they are affordable. The student is encourage to be creative while applying their knowledge in chemistry. The instruments that the student will be building will be 1) An auto-titrator 2) A cellphone spectrophotometer 3) auto-pipeter. Through designing and making these instruments, the student will gain hand-on experience with microelectronics and engineering in addition to basic analytical chemistry.



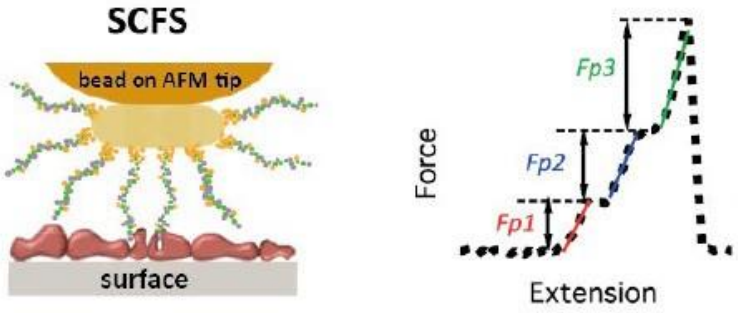
Supervisor: Ruby Sullan
Office: EV566
Laboratory: EV 506-523
e-mail: ruby.sullan@utoronto.ca
Web: http://www.utsc.utoronto.ca/physsci/ruby-sullan

Co-supervisor (if any): NA
Sub-discipline: Biophysical Chemistry
Course code: CHMD90/91
# of students: 1

Interaction forces between *E. coli* and PDMS substrates of varying stiffness: Single cell force spectroscopy

Central to the initiation and maturation of biofilms are the bacterial cell surface adhesion molecules (adhesins) that mediate initial attachment between the cell and a wide range of surfaces. The chemical nature of these surfaces as well as the biochemical characteristics of the adhesins has been a focus of numerous studies. An important gap that remains to be filled is how bacterial adhesion depends on the stiffness of the underlying substrate. Nothing is currently known about the underlying molecular mechanisms and mechanical forces that govern this substrate-stiffness dependent bacterial adhesion. The goal of this CHMD90/91 research project is to quantify the interaction forces between *E. coli* (wild-type and knockout mutants) and polydimethylsiloxane (PDMS) substrates of varying stiffness using atomic force microscopy (AFM)-based single cell force spectroscopy (SCFS). This will quantify the degree of contribution of the key adhesins that mediate the initial attachment and growth of bacteria to substrates of varying stiffness, at the single-cell level.

- In this project, the student will learn to grow and manipulate bacteria, and measure forces of interactions with substrates using the AFM. The student will acquire and analyze force-extension curves to quantitatively characterize bacterial adhesion.
- The student is required to take WHMIS and Biosafety trainings prior to lab work.
- The student is expected to carry out experiments and analyze data as pre-discussed with the supervisor, meet weekly with the supervisor to track research progress, and write a final thesis report at the end of the project.



References:

[1] Friedrichs, J, et al. A practical guide to quantify cell adhesion using single-cell force spectroscopy. *Methods*, **2013**, 60, 169-178.

[2] Sullan RM, et al. Single-cell force spectroscopy of pili-mediated adhesion. *Nanoscale*, **2014**, 6, 1134-43.

Supervisor: Prof. N. Thavarajah **Co-supervisor (if any): N/A**

Office: ESB544 **Sub-discipline: Medicinal Chemistry**

Laboratory: N/A **Course code: CHMD90H3**

e-mail: nirusha.thavarajah@utoronto.ca **# of students: 1**

Web: nirusha.thavarajah@utoronto.ca
https://www.utsc.utoronto.ca/people/thavarajah/

Project Title: Isolation and Characterization of Potential Botanical Bio-pesticides

Abstract:

Essential oils are considered effective botanical bio-pesticides that can be considered an effective and environmentally friendly alternative to synthetic pesticides. Essential oils contain volatile molecules that are primarily composed of terpenes, monoterpenes and sesquiterpenes. Many essential oils have non-terpenic compounds such as eugenol, cinnamaldehyde and safrole. Essential oils can be taken up by insects via inhalation, ingestion or through skin absorption. In this research study students will extract various essential oils from various plant biomass, purify and characterize them using analytical techniques and explore their potential as bio-pesticides.

Learning outcomes:
By the end of this course, students will be able to:

i. Critically analyze research literature
ii. Synthesize new knowledge using the information in the literature
iii. Explain the applications of green chemistry principles
iv. Improve their lab techniques.
v. Write publishable quality scientific articles.

Required training certificates: N/A

Our expectations from students:

- Passion for research
- Ability to work independently
- Good time management skills

References:

Maia M.F., Moore S.J. Plant-based insect repellents: A review of their efficacy, development and testing. *Malar. J.* 2011;10(Suppl. 1) doi: 10.1186/1475-2875-10-S1-S11

Supervisor: Prof. N. Thavarajah **Co-supervisor (if any): N/A**

Office: ESB544 **Sub-discipline: Medicinal Chemistry**

Laboratory: N/A **Course code: CHMD90H3**

e-mail: nirusha.thavarajah@utoronto.ca **# of students: 1**

Web: nirusha.thavarajah@utoronto.ca
https://www.utsc.utoronto.ca/people/thavarajah/

Project Title: Synthesis & Characterization of Eco-Friendly Aerogels

Abstract:

Aerogels are highly porous materials that have versatile applications including wastewater treatment, catalysis, and energy storage. In this research, students will explore the synthesis and characterization of aerogels from agricultural waste. Students will characterize the morphology of the beads and assess their physical and chemical properties using Gass Chromatography-Mass Spectrometry (GC-MS), Fourier Transform Infrared Spectroscopy (FTIR) and Scanning Electron Microscopy (SEM).

Learning outcomes:
By the end of this course, students will be able to:

vi. Critically analyze research literature
vii. Synthesize new knowledge using the information in the literature
viii. Explain the applications of green chemistry principles
ix. Improve their lab techniques.
x. Write publishable quality scientific articles.

Required training certificates: N/A

Our expectations from students:

- Passion for research
- Ability to work independently.
- Good time management skills

Reference:

Sundarraj, A.A., Ranganathan, T.V.: A review on cellulose and its utilization from agro-industrial waste. Drug Invent. Today. 10, 89–94 (2018)

Supervisor: **O.Voznyy** **Co-supervisor (if any):**

Office: **EV564** **Sub-discipline: Materials / Electrochem**

Laboratory: **EV306** **Course code: CHMD90/91**

e-mail: **o.voznyy@utoronto.ca** **# of students: 1**

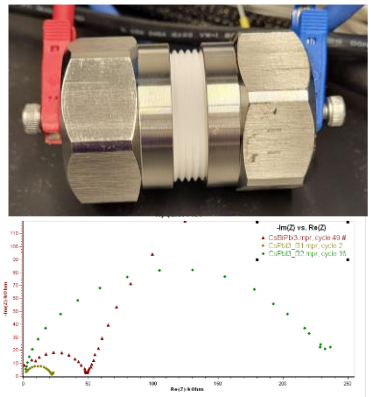
Web: **http://cleanenergy.utoronto.ca**

Synthesis and Method Development for Investigating Ionic Conductivity of Inorganic Solid-State Battery Materials

All-solid-state batteries, a technology that relies on entirely solid materials for energy storage, are defined as key research steps to advance our technologies. A core component of all-solid-state batteries is the solid-state electrolyte, which defines the medium for ion transport. While there are plenty of established methods for determining ionic conductivity of solid electrolytes, the involved measurement parameters are difficult to control without performing complex surface modifications and treatment. The main goal of this CHMD90/91 project is to develop a robust and reliable method to characterize solid-state electrolyte materials by solid electrochemical methods. The student will work alongside a graduate student to synthesize solid lithium electrolytes and develop an electrochemical setup to measure the ionic conductivities.

Learning outcomes:

- The student will gain experience working independently for a research project with an unknown outcome.
- The student will receive training on glovebox operation and perform advanced crystal growth/solid-state methods used in inorganic syntheses.
- The student will learn unique characterization methods, including electrochemical impedance spectroscopy, and Powder X-Ray Diffraction (if time is permitted).
- The student will develop data analysis and interpretation skills from characterization.



Required Training and Qualifications:

- WHMIS Training Certificate
- X-Ray Safety Training (As needed) and instrument training at TRACES.
- Previous lab experience in inorganic synthesis (i.e. CHMC31) is highly preferred.

Our Expectations from Students:

- Be passionate in multiple areas of chemistry, hard-working, open-minded, and creative.
- Work effectively and collaboratively with graduate students and postdoc fellows in lab.
- Be present and report progress at weekly lab meetings.

References:

[1] Chang, H. et al**.** ***Chem. Sci.*****, 2023.** doi: 10.1039/D3SC02093B and references therein.

Supervisor: Frank Wania
Office: EV448 **Sub-discipline: Chemistry/Environmental Science**
Laboratory: EV427 **Course code: CHMD90/91**
e-mail: frank.wania@utoronto.ca **# of students: 1**
Web: https://www.utsc.utoronto.ca/labs/wania/

Transboundary Flows of Trade-Embodied Emissions of Commercial Chemicals

In an increasingly global world, chemical production, product manufacturing, product use and product disposal may all occur in different countries. This global division of labor can lead to an ecologically unequal exchange, as the emissions of a chemical often no longer occur only or largely in the country in which the benefit of the chemical's use is enjoyed. Emissions associated with production, manufacturing and waste disposal occur increasingly in "peripheral" and "semi-core" countries with manufacturing economies, whereas emissions in "core" countries with service-dominated economies are more and more restricted to those occurring during product use. This not only leads to much reduced occupational exposure in core countries, but also to lower emissions to the environment and therefore reduced exposure to the general population. Conversely, manufacturing countries and those involved in the handling of waste are "importing" emissions and, accordingly, are also suffering increased contaminant exposure. We seek to quantify this unequal exchange embedded in the international trade of chemicals and of the products, wastes and foods containing such chemicals. In doing so, we rely on a toolbox of simulation models that describe contaminant behaviour in the technosphere, the natural environment, in aquatic and terrestrial food chains, in the human residential environment, and in human individuals and populations. EUE is likely very pronounced with respect to pesticides in the context of the international trade in food and feed. Demonstrating the shared responsibility for contamination between consumers and producers is an essential element for making progress in efforts towards improved chemicals and waste management globally.

We will seek to quantify the exchange of the pesticide chlorothalonil (CT) between different parts of the world as facilitated by (i) environmental long-range transport, (ii) internationally traded food containing residues, and (iii) the virtual transfer of pesticide exposure embodied in international trade. The student will review what is known about (i) the production and use of CT around the world, (ii) its environmental fate, and (iii) the human exposure to CT.

Learning Outcomes
- literature searching and information synthesis
- data "hunting" skills
- knowledge on environmental fate of, and human exposure to, organic contaminants

Reference:

[1] Tong, K., L. Li, K. Breivik, F. Wania. Ecological unequal exchange: quantifying emissions of toxic chemicals embodied in the global trade of chemicals, products, and waste. *Environ. Res. Lett.* 2022, *17*, 044054 https://doi.org/10.1088/1748-9326/ac5f95

Supervisor:	**Xiao-an Zhang**	Co-supervisor (if any):	**N/A**
Office:	**SW511**	Sub-discipline:	**Organic & Biological Chemistry**
Lab:	**SW332**	Course code:	**CHMD90**
e-mail:	**xazhang@utsc.utoronto.ca**	# of students:	**1~2**
Web:	http://www.utsc.utoronto.ca/~xazhang/		

DEVELOPMENT OF Gd-FREE HIGH RELAXIVITY MRI CONTRAST AGENT

Magnetic resonance imaging (MRI) is a powerful and versatile biomedical imaging modality that is increasingly applied for clinical diagnosis, owing to its noninvasiveness, high resolution, deep penetration and capability of 3-dimetional real-time scans. Conventional MRI relies on the ^{1}H-NMR signal of water, the most abundant molecule *in vivo*. MRI contrast agent (CA) is a new class of pharmaceuticals that can improve contrast and sensitivity of MRI. Current FDA-approved clinical MRI CAs are predominantly based on low-molecular-weight Gd(III)-complexes, which can enhance the MRI contrast via shortening the longitudinal relaxation time ($T1$) of water proton. These Gd $T1$ agents, however, typically exhibit relatively low relaxivity (the efficiency of relaxation enhancement), in particular at high magnetic field. Grams-quantities of Gd-agents are required *in vivo* in order to obtain satisfactory imaging effect. Higher dose is unavoidably associated with higher risk of side effects. Recently, several Gd CAs have been implicated in nephrogenic systemic fibrosis (NSF), a severe side effect related to Gd toxicity in patients with renal dysfunction. Therefore, safer and more efficient MRI CAs are highly desirable. This D90 project will be part of our research program in developing next generation MRI $T1$ CAs with high relaxivity and low toxicity. The primary goal is to design, synthesize and characterize novel Gd-free agents.

Learning outcomes

- Students will receive hands-on trainings on advanced organic and inorganic synthesis, and are expected to do chemical synthesis independently after training;
- Students will receive trainings on how to use modern spectroscopy techniques, including NMR, ESI-MS, UV-vis, etc to characterize the synthetic intermediates and final product;
- Students will learn background knowledge on MRI contrast agents and explore theory about relaxivity.
- Students are expected to present their research results in group meetings.

Required training certificates

(1) WHMIS training; (2) Chemical Safety Training; Our expectations from students…

(1) Successfully completed CHMC41 or 42; (2) Previous experience in organic synthesis is preferred.

References: **[1]** Merbach, A. E.; Tóth, É., *The chemistry of contrast agents in medical magnetic resonance imaging*. Wiley: Chichester ; New York, 2001 **[2]** Zhang, X.-a.; Lovejoy, K. S.; Jasanoff, A.; Lippard, S. J, *Proc. Natl. Acad. Sci. USA* 2007, 104 (26), 10780.

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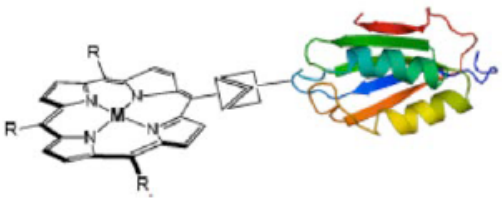
DESIGN AND SYNTHESIS OF MRI CONTRAST AGENT FOR COVALENT PROTEIN LABELING

Molecular imaging probes, including fluorophores, radioactive tracers, or magnetic resonance imaging (MRI) contrast agents (CAs) that can be selectively attached to specific bio-macromolecules, such as proteins, are powerful and versatile research tools for molecular biology as well as for medical diagnosis. These biomedical imaging probes can be used to label and track the selected protein targets inside the biological system to provide their distribution kinetics and functional information. On the other hand, certain proteins, such as antibody, can be used as a cargo to deliver imaging probes to specific sites, such as surface of tumor cells.

This project aims to develop novel MRI contrast agents based on water-soluble porphyrins for protein labeling. MRI is one of the major medical imaging modalities that is increasingly used for clinical diagnosis. The immediate goal of current project is to establish a synthetic strategy with reasonable yield and to structurally characterize the final product.

Learning outcomes

- Students will be systematically trained on organic and inorganic synthesis, in particular on porphyrin synthesis;
- Students will receive hands-on trainings on how to use modern spectroscopy techniques, including NMR, ESI-MS, UV-vis, etc to characterize the synthetic intermediates and final product;
- Students will learn background knowledge on MRI contrast agents, molecular imaging and molecular design.
- Student is expected to present the research results in group meetings.
- Required training certificates: (1) WHMIS training; (2) Chemical Safety Training; Our expectations from students…
- Successfully completed CHMC41 or 42; (2) Previous experience in organic synthesis is preferred.



References: **[1]** Merbach, A. E.; Tóth, É., *The chemistry of contrast agents in medical magnetic resonance imaging*. Wiley: Chichester ; New York, 2001 **[2]** Zhang, X.-a.; Lovejoy, K. S.; Jasanoff, A.; Lippard, S. J, *Proc. Natl. Acad. Sci. USA* 2007, 104 (26), 10780.