CHM410-1410 Analytical Environmental Chemistry
Fall 2017

Schedule
Lecture: Tuesdays and Thursdays 4-5 Lash Miller 155
Lab: Friday 9:00-12:30 or 1:15-4:45 LM 9 (ANALEST)
Office Hours: TBD

Contact Information
Prof. Jessica D'eon, LM 119, (416) 978-7283, jessica.deon@utoronto.ca
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Course Goals
The goals of CHM410-1410 are to introduce and apply concepts and techniques of sample collection, preparation, and analysis of trace level concentrations of both organic and inorganic environmental pollutants. This course seeks to produce analysts with a basic conceptual understanding of a broad range of modern analytical equipment relevant to trace environmental analysis. The lab component is designed to provide practical knowledge of sample collection and analysis, as well as data interpretation and visualization involved in environmental analysis.

Learning Objectives
Upon completing CHM410-1410 students will be able to design an environmental analysis starting with a literature search through experimental design and data analysis.

To complete this task student must be able to:

1. Search the scientific literature for relevant background information and methodologies.
2. Make educated decisions related to analytical methodology and instrumentation.
3. Analyze, interpret, and effectively visualize analytical data.
4. Confidently ask for help or advice.

Discussion Topics
U1: Chemical Partitioning – We will discuss chemical partitioning as it applies to where you expect to find chemicals in the environment as well as sample preparation techniques in the lab.
U2: Quality Control – These techniques ensure the concentrations we observe in the lab reflect the concentrations present in the environment.
U3: Chromatography – Chromatography is relevant both as a separation technique to separate chemicals of interest from each other and possible interferences, as well as an effective means of delivering the compound of interest to the chosen detector.
U4: Detectors – We will discuss the general process by which a compound creates a signal in a detector and discuss the workings of non-mass spectral detectors.
U5: Metal Analysis – A specific discussion of how metals are detected in environmental samples.
U6: Analyte Ionization – Mass spectral analysis requires gas phase ions. We will discuss various processes to produce gas phase ions and how these processes are optimized for environmental applications.
U7: Mass Spectrometry – We will discuss different techniques to control the movement of gas phase ions and the types of datasets that can be generated using these instruments.
U8: Identification of Unknown Compounds – Most of the term is dedicated to quantifying concentrations of known analytes, however environmental issues are complex and sometimes it's not clear which compounds are most important. In the final unit we will explore techniques researchers use to identify compounds without *a priori* knowledge.

Lecture Schedule

September	7	R	Class Introduction	*D'eon/Peng*
	12	T	Lab Format and Discussion	*D'eon*
	14	R	U1: Chemical Partitioning	*D'eon*
	19	T	U1: Sample Extraction	*D'eon*
	21	R	U2: Quality Control	*D'eon*
	26	T	U3: Introduction to Chromatography	*D'eon*
	28	R	**Field Trip Discussion**	*Joudan*
October	3	T	U3: Van Deemter Equation	*D'eon*
	5	R	U3: Gas and Liquid Chromatography	*D'eon*
	10	T	U4: GC Non-MS Detectors (FID and ECD)	*D'eon*
	12	R	U4: LC Non-MS Detectors (UV and fluorescence)	*D'eon*
	17	T	U5: Metal Analysis	*D'eon*
	19	R	U6: Introduction to Ionization	*Peng*
	24	T	**Midterm Test**	
	26	R	U6: GC-MS Ionization interfaces	*Peng*
	31	T	U6: LC-MS Ionization Interfaces	*Peng*
November	2	R	U6: Matrix effects and Derivatization	*Peng*
	7	T	**Study Break**	
	9	R	**Study Break**	
	14	T	U7: Introduction to Mass Spectrometry	*Peng*
	16	R	U7: Mass Spectrometry Instrumentation	*Peng*
	21	T	U7: Mass Spectrometry Applications	*Peng*
	23	R	U8: Isotopes and Fragmentation Patterns	*Peng*
	28	T	U8: Untargeted chemical analysis	*Peng*
	30	R	U8: Environmental omics	*Peng*
December	5	T	Review	*D'eon/Peng*

Grading Scheme

Laboratory Grade **50%**

- **Introductory Labs 1-3** **12%**
  (Due one week after the lab is completed)
  - Lab 1 – Short report 2%
  - Labs 2 and 3 – Full lab reports 2 x 5%
- **Field Trip and Analysis** **12%**
  (Trip: *Fri Oct 6*, Analysis: *Fri Oct 13* & *Fri Oct 20*)
  - Report outline (*Tues Oct 31*) 2%
  - Report (*Tues Nov 14*) 10%
- **Student-Directed Group Project** **26%**
  - Proposal (*Thurs Oct 12*) 3%
  - Preparation and participation 3%
  - Final presentation and defense (*Fri Dec 1*) 10%
  - Final report (*Tues Dec 5*) 10%

Midterm (*Tues Oct 24 in class*) **15%**

Final Exam **35%**

Website
All material including presentation slides and literature resources, when provided, and the lab manual will be available on Blackboard. You are responsible for checking this site regularly.

Textbook
There is no textbook requirement for CHM410-1410. As this course aims to present current topics in environmental analytical chemistry primary scientific literature resources are provided when appropriate and can be accessed via Blackboard. Although students are encouraged to use additional resources these are not mandatory and testing will only include the specific material discussed in class.

The ChromAcamdemy is a web-based tutorial series offered jointly by LCGC online magazine and Agilent Technologies. This resource is available free of charge to those with an academic email. Relevant sections will be provided for review throughout the term. Depending on your analytical chemistry background this may or may not be a useful resource.

Instructions for creating a CHROMacademy account:

1. Go to http://www.chromacademy.com
2. Click 'Subscribe / Login' on the top right of the website
3. Choose 'Get an Agilent Sponsored Academic License' option on the pop-up menu
4. Click 'FREE university membership'
5. A window will appear where you have to input relevant details to create an account.

Note: You must use an academic email address to receive a free account. The account itself isn't created immediately, but you are sent a confirmation email for full registration.

If necessary students are encouraged to use any introductory analytical chemistry textbook to review relevant topics discussed in class. Two excellent textbooks are: *Quantitative Chemical Analysis* by Daniel Harris and *Fundamentals of Analytical Chemistry* by Douglas Skoog. A large portion of the latter half of this course is dedicated to mass spectrometry and ionization processes; two excellent textbooks on these topics are *Mass Spectrometry: Principles and Applications* by Edmond de Hoffmann and Vincent Stroobant and *Chemical Ionization Mass Spectrometry* by Alex Harrison. All of these textbooks are available from the University of Toronto libraries.

Academic Integrity
While peer discussions are encouraged, laboratory reports MUST represent your own independent work and comprehension. Information about academic integrity can be found here: http://www.artsci.utoronto.ca/osai/, and a copy of the University of Toronto's Code of Behavior can be found here: http://www.governingcouncil.utoronto.ca/AssetFactory.aspx?did=4871

Accommodations
All students are welcome in this course. If you have a disability/health consideration that may require accommodations, please feel free to approach Prof. Jessica D'eon and/or Accessibility Services at (416) 978 8060; http://accessibility.utoronto.ca

Late Materials
Unless otherwise explicitly stated, lab reports are due the following week at the beginning of the lab period. Anything handed in late will be docked 10% per day including the weekend. If the material is completed over the weekend it should be emailed to Prof. D'eon or the relevant TA and a hardcopy delivered at the beginning of the workweek.

Absences

Students who miss labs or tests for legitimate reasons should contact Dr. D'eon as soon as possible, and no later than one week after returning to class. A legitimate reason for an absence or missed deadline due to medical, personal, or family reasons should be documented by one of the following:

1) U of T Student Medical Certificate
2) Student Health or Disability Related Certificate
3) College Registrar's Letter
4) Accessibility Services Letter

Lab Schedule

Date	**Lab 1** *NMR as a Tool for Quality Control in the Food Industry*		**Lab 2** *Markers of Polluted Air*		**Lab 3** *Analysis of Organophosphate Flame Retardants in Dust*	
	9:00 – 12:30	1:15 – 4:45	9:00 – 12:30	1:15 – 4:45	9:00 – 12:30	1:15 – 4:45
Sept 15	A	D	B	E	C	F
Sept 22	C	F	A	D	B	E
Sept 29	B	E	C	F	A	D
Oct 6	**Field Sampling at Lake Niapenco near Hamilton** All groups working together					
Oct 13	**Water, Sediment, and Invertebrate Analysis** All groups working together					
Oct 20	All groups working together					
Oct 27	**Student-Driven Group Projects** All groups working on separate projects					
Nov 3	All groups working on separate projects					
Nov 10	*Study Break*					
Nov 17	All groups working on separate projects					
Nov 24	All groups working on separate projects					
Dec 1	Group Presentations and Defense					

Lab Preparation

Laboratory experiments are designed with the intention of being completed during the allotted classroom time, however, some may require more or less time depending on the pace at which you work. In order to expedite things it is mandatory that you be prepared prior to coming to the lab. **Your overall grade contains a 3% *preparation and participation* component.**

Lab Notebook

You are required to maintain a lab notebook. This must be a **bound** notebook with numbered pages, like the type used in other chemistry labs – **loose-leaf and spiral notebooks are not appropriate**. It is very important to get in the habit of writing in a lab notebook. Every good lab researcher can tell you stories about being "saved" by having kept a good notebook. It is suggested that you write an outline of each lab in your notebook before you start, that way you have a good overall picture of the experiment before starting. Your notebook should be a concise record of all your results including typical

chromatograms/spectra, tables of data, calculations, etc. In other words your notebook should be the source of your lab report. As well the TA should be able to "read" what you did and the results obtained.

Lab Groups

During the first week of class you will be assigned to a lab group. These groups will work together the entire semester. It is suggested that you work with your group as much as possible in terms of understanding the labs. You may work cooperatively on the labs to the extent of sharing information on the different sections that were performed by different people, but you must do your own write-up. With the exception of the independent project proposal there are no group lab reports.

Lab Safety

Please remain aware that you are working with "toxicants" in all your experiments! If handled correctly, these compounds pose little or no danger in a laboratory setting. However, carelessness could lead to serious problems for yourself or someone else. With this in mind, absolutely no food or beverages will be permitted in the lab. **EYE PROTECTION MUST BE WORN BY ALL PERSONS AT ALL TIMES IN THE LAB!!!** Long pants and shoes (no sandals) are required laboratory attire. A lab coat is highly recommended. In addition, disposable gloves are provided for your safety during procedures when exposure might happen. Clean up any spills immediately and thoroughly; if you are not sure how, **ASK SOMEONE**! Be considerate of the person using the scale, bench, or instrument after you. Keep the lab benches clear of non-essential items. Backpacks, etc., should be kept somewhere out of the way. Do not leave them on the floor or in the aisles.

Waste Handling

Chemical and solvent wastes are divided into several categories: you will be directed by the TAs where to put your waste. Make sure you dispose of all your solutions and samples at the end of your experiments. Also, **thoroughly clean up your bench area at the completion of your work**. You have the option of analyzing samples that pose a biosafety risk (i.e. human urine), when performing this analysis the student who provides the sample is the only group member who can handle that sample. All relevant TAs have biosafety training and will be present to guide you through the safe handling of biological samples.

Lab Report Grading

You are required to write full-length lab reports for Labs 2 and 3, as well as the field trip and the final student directed group project. Formal lab reports will be graded out of 100 using grading schemes posted on Blackboard. ***Use the marking scheme as a guide to ensure your report is properly structured and includes all relevant material.*** Please strive to draw connections throughout your report between the experimental data you generated and the larger principles/concepts in environmental chemistry.

Field Trip to Lake Niapenco in Hamilton

In 2012 researchers from Environment and Climate Change Canada, Shane de Solla and Amila De Silva, were part of a team that discovered Lake Niapenco in Hamilton had been contaminated with fluorinated surfactants from firefighting activities at the nearby Hamilton airport (*Environ. Int.* **2012**, *39*, 19-26). We will be visiting this site with Shane and Amila on Friday October 6th to collect water, sediment, and invertebrates to bring back to the lab for analysis.

Field Trip Report Outline

The field trip will result in a large dataset that can be overwhelming to analyze. To help you collect your thoughts you will submit a report outline in class on Tuesday October 31 that includes the following details:

- Descriptive Title

- Purpose of the analysis
- Figure/tables to be included in the body of your final report. Maximum 3 total and they should be publication quality with proper axes and labels.
- 3-4 discussion points. These should be bullet point only, not full sentences, and are the discussion topics for the paragraphs that will appear in your final report. These discussion points should refer to and/or use the figures/tables included. At least one discussion point should deal with quality control.
- Overall Conclusion

This outline will be graded and returned to you on Tuesday November 7th. You are expected to review the comments from the outline and incorporate the suggestions into your final report that is due in class on Tuesday November 14th.

Student-Directed Group Project

CHM410/1410 laboratory includes a final project where each lab group develops a testable hypothesis and carries out an entirely student-driven analysis in the final three lab periods.

Student-Directed Group Project Timeline

Date	Week	Lab Session	Milestone
Sept 7-8	1	-	
Sept 11-15	2	1	Lab groups chosen, TAs assigned (*in class, Tues Sept 12*)
Sept 18-22	3	2	
Sept 25-29	4	3	Meeting with TA mentor
Oct 2-6	5	4	Meeting with TA mentor
Oct 9-13	6	5	Proposal due (*in class, Thurs Oct 12*)
Oct 16-20	7	6	Proposals reviewed and returned (*in class, Thurs Oct 19*)
Oct 23-27	8	7	Student-directed project week 1 (*in lab*)
Oct 30 - Nov 3	9	8	Student-directed project week 2 (*in lab*)
Nov 6-11	-	-	**Study Break**
Nov 13-17	10	9	Student-directed project week 3 (*in lab*)
Nov 20-24	11	10	Student-directed project week 4 (*in lab*)
Nov 27 - Dec 1	12	-	Presentation of final results (*Fri Dec 1*)
Dec 5-7	13	-	Lab report due (*in class, Tues Dec 5*)

Some Examples of Past Projects

- The Effectiveness of the Corktown Common Urban Marsh as a Water Treatment and Quality
- Analysis of Bisphenol-A (BPA) in Thermal Paper
- Caffeine in Coffees and Teas using GC-MS and Isotope Dilution
- Analysis of the Relationship Between Metal Content in Paint and Nearby Soils
- Fish: Friend or Food? Nutritive Analysis of Fish for Consumption
- Is Your Cooking Killing You? Determination of Aldehyde Emissions from Heat-Stressed Cooking Oils by LC-MS/MS and LC-UV
- Observation of Common Pharmaceuticals in Wastewater and Drinking Water Samples

Student-Driven Group Project Proposal (Due in class on Thursday October 12th)
The purpose of this proposal is twofold. To help you organize your project and think through its execution, and also to allow us (myself and the TAs) to evaluate the feasibility of the project and coordinate all the necessary instrumentation and consumables. You will only submit ONE proposal per group, please work on this proposal together either in person or online. The components of the proposal are outlined below.

Hypothesis
The hypothesis can take the form of a question you are trying to answer, or can describe a situation you are interested in characterizing.

Experimental Plan
A step-by-step experimental approach that includes tasks that need to be completed, a person or people who will be in charge of this task and an estimated amount of time it will take to complete it. This plan can take many forms, such as a flow scheme or simply a list, and should be organized by lab period (i.e. week 1, 2, 3, and 4). It is possible you will be unsure as to how to proceed experimentally in weeks 2 and 3 of the project as this may be dictated by the results obtained in week 1. If this is the case, please indicate this expectation, but also outline some potential expected results and how you would proceed given a specific scenario.

Implicit in the exercise of creating this plan is the understanding that you will likely deviate from it. This plan will be used to give you direction at the outset of the project, not so that you feel constrained to stick with it even if it's not working. It could also happen that by the time the project begins you have abandoned or revised this plan significantly. This is also not a problem, as the experimental plan presented here is meant to act as a starting point only and changes can take place anytime, even before the project begins.

Quality Control
Outline the measures you are going to take to ensure the numbers you present at the end of your project represent the actual concentrations in the materials you analyzed.

Greenness
Green chemistry is all the rage these days, and rightly so. Please include a couple of sentences about whether you believe your project as outlined is 'green'. To make this decision consider the waste you are generating from the project (i.e. consumables and the amount and type of solvents). Could the project be greener, or are you already using a relatively green technique? The point of this exercise is to create awareness about green chemistry as opposed to trying to implement only green techniques, and so grades will be awarded based not on the greenness of the method, but on your awareness of whether your method is a green alternative.

References
I would like to see at least 3 references. Your experimental method can be built predominantly on one reference, but I would like you to have read more than that one paper. For each reference add one sentence that describes how this reference was used.

Budget
Please outline any chemicals or consumables (i.e. SPE cartridges) you will need to purchase. Your budget should remain under $100, however there's a (good) chance some of the items are already present in the department and so you can submit higher budgets that may be reduced once we look around.