Chem 511: Advanced Analytical Chemistry

Fall Semester 2022 MWF 7:45-8:35 Room: Hach 1221

Instructor

Alexander Gundlach-Graham

Office: Hach 3101C

Email: alexgg@iastate.edu Phone: 515-294-7853

Office Hours: Monday 4-5:00 p.m. and by appointment

Course Description

This course aims to provide an overview of several topics essential to analytical chemistry. In the first portion of the course, we will discuss the "analytical process," which is the series of steps employed in the development and implementation of any analytical measurement scheme: from 1. defining an analyte, to 2. collecting and preparing a sample, to 3. performing a measurement to 4. data analysis and reporting. We will discuss basic statistics, representative sampling, calibration approaches, and data analysis approaches. Students will gain practical experience with scientific programming in R. We will also discuss details of the measurement process itself, including aspects of detection, signal transduction, and analog-to-digital conversion. In the second portion of the semester, we will discuss trace-element analysis. In addition to lecture material, students will research a type of analytical instrumentation or an analytical method. Students will each prepare a report (details provided below) describing the analytical instrumentation or method, as well as deliver a 15 minute in-class presentation. The aim of this research paper and presentation is to promote communication skills essential to a successful scientific career.

Required Readings

Readings will be posted to Canvas as files associated with each course week. For best learning outcomes, it is recommended that students complete pertinent readings prior to class sessions. Introduction to chemometrics text:

https://chem.libretexts.org/Bookshelves/Analytical Chemistry/Chemometrics Using R (Harvey)

Recommended Readings (Not Required):

Skoog D.; Holler, F.; Crouch, S.R. Principles of Instrumental Analysis, 7th Ed.

Student-Led Paper Discussions

Each student will lead a class discussion about a scientific paper. These student-led discussions will occur most Fridays throughout the semester. Details about the organization and requirements of student-led discussion sessions will be provided in a stand-alone document.

Research Paper and Presentation Requirements

The research paper should cover a topic of interest in analytical chemistry such as a type of analytical instrumentation or a specific analytical method; it may or may not directly pertain to the student's research at ISU. A list of potential analytical topics of interest will be provided; however, students should not feel constrained to this topic list. All topics should be approved by the instructor by **Sept. 30**. Research papers will have a maximum length of eight pages (single-spaced, 12-point Times New Roman) including figures, but not including citations. The formatting of the paper is up to each author; however, generally, the following aspects should be addressed:

description of the analytical instrumentation or method, comparison with other approaches (i.e. how topic of interest compares to the state of the art), description of the benefits and limitations of the approach (i.e. figures of merit, areas of application, etc.), and an outlook or conclusion section. Warning: Composing an effective description of your analytical chemistry topic is going to be a challenge; an effective paper will be written in a concise and information-rich style typical of a scientific paper.

Important Dates

Exam 1	Monday, Sept. 26
Exam 2	Friday, Oct. 21
Exam 3	Friday, Dec. 2
Report	Friday, Dec. 9

Grading

The final course grade is based on the percentage scores in each graded category, as listed in the table below. The point value obtained in any of the grade categories only contributes to the percentage obtained in that category. Class participation is based on reading quizzes, attendance, and participation in class discussion. Homework and assigned exercises will be graded based on completion and correct answers for selected problems. Three exams each make up 1/5th of the overall course grade; there is no cumulative final exam. All grades will be recorded in Canyas

Category	Grade Percentage
Participation / Attendance	10%
Exercises / HW	5%
Student Presentation	10%
Term Paper	15%
Exam 1	20%
Exam 2	20%
Exam 3	20%
Total	100%

Course Learning Objectives

By the end of this course, the student should:

- have deeper understanding of the analytical method including strategies for sampling, calibration and data analysis
- be familiar with scientific programming in R
- be familiar with basics of signal detection, transduction, and digitization in analytical measurements
- have a detailed understanding of ICP-MS and other trace-element analytical approaches

Tentative Schedule

<u>D</u>	ate	<u>Topic</u>
8/22	(M)	Course Introduction, What is the Analytical Process?
8/24	(W)	Statistics: Normal (Gaussian)
8/26	(F)	Introduction to R (Complete Ch. 1 of Chemometrics Using R)
8/29	(M)	Poisson Statistics and Log-Normal Distribution
8/31	(W)	Sampling Theory – Part I

9/2	(F)	Student-Led Paper Discussion, Sampling Theory – Part II
9/5	(M)	No Class – Labor Day
9/7	(W)	Calibration – Zero Order, External Calibration
9/9	(F)	Student-Led Paper Discussion, Calibration – Internal Standardization
9/12	(M)	Calibration – Standard Addition
9/14	(W)	Figures of Merit
9/16	(F)	Student-Led Paper Discussion, Detection Limits
9/19	(M)	Chemometrics I
9/21	(W)	Chemometrics II
9/23	(F)	Student-Led Paper Discussion, Chemometrics III
9/26	(M)	EXAM I
9/28	(W)	What is detection? Signals and Noise
9/30	(F)	Student-Led Paper Discussion, Signal Transduction
10/3	(M)	Exercises with R: Calibration
10/5	(W)	Exercises with R: PCA and Clustering
10/7	(F)	Exercises with R: Discriminant Analysis
10/10	(M)	Amplification
10/12	(W)	Analog-to-Digital Conversion, Part I
10/14	(F)	Student-Led Paper Discussion, Analog-to-Digital Conversion, Part II
10/17	(M)	Intro to Trace-Elemental Analysis
10/19	(W)	Inductively Coupled Plasma (ICP)
10/21	(F)	EXAM 2
10/24	(M)	ICP-MS, Part I
10/26	(W)	ICP-MS, Part II
10/28	(F)	Student-Led Paper Discussion, Interferences and Matrix Effects
10/31	(M)	Isotope Dilution Analysis, Part I
11/2	(W)	Isotope Dilution Analysis, Part II
11/4	(F)	Student-Led Paper Discussion, Laser Ablation ICP-MS, Part I
11/7	(M)	Laser Ablation ICP-MS, Part II
11/9	(W)	Speciation Analysis
11/11	(F)	Student-Led Paper Discussion, XRF Analysis, Part I
11/14	(M)	XRF Analysis, Part II
11/16	(W)	Carbon-14 Dating, Part I
11/18	(F)	Student-Led Paper Discussion, Carbon-14 Dating, Part II
11/21	(M)	No Class – Thanksgiving Break (All week)
11/23	(W)	
11/25	(F)	
11/28	(M)	Special Topics in Trace-Element Analysis
		•

11/31	(W)	Review Day
12/2	(F)	EXAM 3
12/5	(M)	Student Presentations
12/7	(W)	Student Presentations
12/9	(F)	Student Presentations, Report Due

Public Health

If you are not feeling well, you should stay home and focus on your health. Should you miss class due to illness, it is your responsibility to work with your instructor to arrange for accommodations and to make up coursework, as consistent with the instructor's attendance policy.

You may choose to wear a face mask and/or receive the COVID-19 vaccine and boosters, as well as other vaccines such as influenza, but those options are not required. Thielen Student Health Center will continue to provide COVID-19 vaccinations free-of-charge to students. The university will continue to offer free masks and COVID-19 test kits during the fall 2022 semester. Other wellbeing resources for students are available at: https://www.cyclonehealth.iastate.edu/wellbeing-resources/

Public health information for the campus community continues to be available on Iowa State's <u>public health website</u>. All public health questions should be directed to <u>publichealthteam@iastate.edu</u>.

Academic Dishonesty

Academic dishonesty in any form is unacceptable and will result in a grade of "F" for the course. Academic dishonesty includes plagiarism, cheating on any assignment, or otherwise seeking to earn credit for the work of others. Furthermore, the offense will be reported to the university and could result in more serious consequences. The class will follow lowa State University's policy on academic dishonesty. Anyone suspected of academic dishonesty will be reported to the Dean of Students Office.

Accessibility Statement

lowa State University is committed to assuring that all educational activities are free from discrimination and harassment based on disability status. Students requesting accommodations for a documented disability are required to work directly with staff in Student Accessibility Services (SAS) to establish eligibility and learn about related processes before accommodations will be identified. After eligibility is established, SAS staff will create and issue a Notification Letter for each course listing approved reasonable accommodations. This document will be made available to the student and instructor either electronically or in hard-copy every semester. Students and instructors are encouraged to review contents of the Notification Letters as early in the semester as possible to identify a specific, timely plan to deliver/receive the indicated accommodations. Reasonable accommodations are not retroactive in nature and are not intended to be an unfair advantage. Additional information or assistance is available online at www.sas.dso.iastate.edu, by contacting SAS staff by email at accessibility@iastate.edu, or by calling 515-294-7220. Student Accessibility Services is a unit in the Dean of Students Office located at 1076 Student Services Building.

Discrimination and Harassment

lowa State University does not discriminate on the basis of race, color, age, ethnicity, religion, national origin, pregnancy, sexual orientation, gender identity, genetic information, sex, marital status, disability, or status as a U.S. Veteran. Inquiries regarding non-discrimination policies may be directed to Office of Equal Opportunity, 3410 Beardshear Hall, 515 Morrill Road, Ames, Iowa 50011

Telephone: 515-294-7612, Hotline: 515-294-1222, email: eooffice@iastate.edu

Religious Accommodation

lowa State University welcomes diversity of religious beliefs and practices, recognizing the contributions that differing experiences and viewpoints can bring to the community. There may be times when an academic requirement conflicts with religious observances and practices. If that happens, students may request the reasonable accommodation for religious practices. In all cases, you must put your request in writing. The instructor will review the situation in an effort to provide a reasonable accommodation when possible to do so without fundamentally altering a course. For students, you should first discuss the conflict and your requested accommodation with your professor at the earliest possible time. You or your instructor may also seek assistance from the Dean of Students Office at 515-294-1020 or the Office of Equal Opportunity at 515-294-7612.

Free Expression

lowa State University supports and upholds the First Amendment protection of <u>freedom of speech</u> and the principle of <u>academic freedom</u> in order to foster a learning environment where open inquiry and the vigorous debate of a diversity of ideas are encouraged. Students will not be penalized for the content or viewpoints of their speech as long as student expression in a class context is germane to the subject matter of the class and conveyed in an appropriate manner.