

CHEM 6271: Analytical Chemistry I

Professor: Facundo M. Fernandez (facundo.fernandez@chemistry.gatech.edu, Office: ES&T Ford Building room L1-244 (lower level one).

Lectures: MWF 11:05am~11:55 am. Molecular Science and Engineering (MoSE) room 1224.

Textbook:

Various textbooks can be used for this class

- “Getting Started with Matlab. A quick introduction for Scientists and Engineers” Rudra Pratap, Oxford University Press. ISBN: 978-0-19-973124-4.
- “Statistics and Chemometrics for Analytical Chemistry”, 4th or newer Edition, J. Miller & J. Miller, Prentice Hall/Pearson. ISBN-13: 978-0273730422.
- “Design of Experiments for Engineers and Scientists”, Jiju Anthony, Elsevier, ISBN-13: 978-0750647090. (pdf available in GT library)
- “Chemometric Techniques for Quantitative Analysis”, Richard Kramer, Marcel Dekker, ISBN-13: 978-0824701987. (pdf available in GT library)
- “Handbook of Chemometrics and Qualimetrics”, (Data Handling in Science and Technology, V. 20), Elsevier, ISBN-13: 978-0444897244. To be used only as reference. (available in GT library)

Requirements:

- All the students enrolled in CHEM 6271 are expected to conform to the Honor Code.
- Matlab (The Mathworks). You should have a working version of this software installed on your computer and bring that to class. Student licenses start at \$99. The statistics toolbox will be used.
- A laptop computer that can run Matlab.
- PLS Toolbox for Matlab: Please create a user account at <http://software.eigenvector.com/toolbox/download/index.php> and download a student demo license of PLS_Toolbox. The license will function for 6 months for free.
- Download and install mzm2: <http://mzm2.sourceforge.net/>.

Course Description/Learning Objectives:

Students attending this course will learn about the basic statistic and data analysis tools used in classical and advanced analytical chemistry experiments. The class will consist of three modules.

Module 1: Introduction to Matlab. Brief review of linear matrix algebra. Design of Experiments. Optimization. **Experiment:** Optimization of Electrospray Ionization via DOE Techniques.

Module 2: Univariate calibration. Comparing analytical methods. Direct and inverse multivariate calibration (ILS, PCR, PLS)-Discussion of literature papers. **Experiment:** Univariate Calibration Statistics Involved in the Determination of Endogenous Metabolites by Liquid Chromatography-Tandem Mass Spectrometry.

Module 3: Multivariate pattern recognition and classification with applications to LC-MS and NMR data from metabolomics experiments. PCA, PLS-DA etc. **Experiment:** Investigation of Storage-induced Changes in the Beer Metabolome.

Grading system:

Students will be given one take-home midterm and one take-home final exam. Each exam will be graded in a 100-point scale and will account for 1/2 of the grade.

The final grade will be converted to a letter grade, based on the mean point grade, according to the following scale:

A (100 – 81 points); B (80 – 61 points); C (60 – 40 points); D (39 – 21 points); F (below 20 points).

Tentative Lecture Timeline:

August 20, 22, 24	Introduction to Matlab. Start beer storage for metabolomics experiment.
August 27, 29, 31	Intro to Design of Experiments and associated software (Statistics Toolbox). August 31st: Create experimental design for ESI optimization.
Sept 3, 5, 7	Sept 3rd-5th: Collect ESI Data using DOE. Response surface analysis.
Sept 10, 12, 14	Univariate Calibration. No class Sept 14th: prepare DOE experiment report.
Sept 17, 19, 21	Collect UPLC-MS data on EBC.
Sept 24, 26, 29	Univariate Calibration. Comparing Analytical Methods. Method Validation
October 1, 3, 5	Collect UPLC-MS Beer data
October 8, 10, 12	October 8th: Q&A. No class October 10th. Take home exam available on October 10 th , due back 1 week after. October 12 th : Introduction to mzmne.
October 15, 17, 19	Multivariate calibration. Data pre-processing
October 22, 24, 26	Hands on examples of multivariate calibration on multi-analyte datasets.
October 29, 31, Nov 2	Pattern recognition and classification. PCA and PLS-DA.
Nov 5, 7, 9	Hands on pattern recognition on DART MS cancer data
Nov 12, 14, 16	Hands on pattern recognition on SELDI cancer data
Nov 19, 21, 23	Hands on pattern recognition on UPLC-MS beer metabolomics data.
Nov 26, 28, 30	Pattern recognition on NMR plankton data.

	No class Nov 26th.
Dec 3, 5, 7	Pre-final review.
Final Exam	Turn in by December 12th.