

CHEM 6271: Analytical Chemistry I

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 mzmime2: <http://mzmime.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:

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| 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 mzmine. |
| 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. |

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