

**Chemistry 6120**  
**Analytical Data Treatment - Statistical and Numerical Analysis**  
Autumn Semester 2012  
2002 Evans Lab  
M W F 1:50 PM - 2:45 PM

**Instructor:** Philip Grandinetti

**Office:** 1046 Smith Lab

**Office Hours:** Monday, Wednesday, Friday at 12:30-1:30 PM or by appointment

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**Objectives:** To familiarize advanced undergraduates and beginning graduate students with modern methods for the acquisition and treatment of information obtained from chemical systems.

**Suggested Texts:**

*Statistics*, R. J. Barlow

*Data Reduction and Error Analysis for the Physical Sciences*, Bevington and Robinson

*C, A Programming Language*, Kernighan and Ritchie

*Numerical Recipes, 2nd Ed.*, Press, Teukolsky, Vetterling, and Flannery

**Math Prerequisite:** Calculus and Linear Algebra

**Homework:** All Homework will be graded. Some homework will involve writing computer programs in C. Hard and soft copies of both the code and output must be turned in for grading. Computers and software are available via ID card access in Room 2105 Newman-Wolfrom.

**Syllabus:**

1. Statistical Descriptions of Data
  - Characterizing Experimental Distributions
  - Theoretical Distributions
  - Confidence Limits
  - Hypothesis testing
2. Modeling of Data
  - Maximum Likelihood Estimator
  - Linear Models
  - Non-Linear Models
  - $\chi^2$  minimization techniques - The Marquardt Method
  - Rejection of Data, Goodness of Fit, Confidence Intervals
3. Fourier transform techniques
  - Fourier Transform pairs
  - FT Theorems - Similarity, Addition, Shift, Convolution
  - Digital Fast Fourier Transform
4. Characteristics of analog and digital data acquisition
  - A/D conversion, Sampling theorem
  - Signal averaging
  - Filtering

**Grading:**

Midterm Exam	35%
Homework	30%
Final Exam	35%