

1/14 Instrument Calibration I: 1<sup>st</sup> Order Calibration Curve

- [Calibration Curve Handout](#)
- [Excel Example Worksheet](#)
- Calibration graphs in instrumental analysis
- Product-moment correlation coefficient
- Regression of  $y$  on  $x$
- Calculation of concentration and its random error
- Linest Excel Function (Harris Section 4.7)
- [Problem Set 1: "Cadmium Calibration Problem"](#)

1/21 Instrument Calibration II: ANOVA, Regression Calculations, Curvilinear Regression Methods

- Variance, Sum of Squares ( $SS$ ), and Degrees of Freedom ( $DOF$ )
- Total Sum Squares ( $SS_{tot}$ ), Regression  $SS$  ( $SS_{regr}$ ), Residual  $SS$  ( $SS_{res}$ ), and Coefficient of Determination ( $R^2$ )
- Replicate Sum of Squares ( $SS_{repl}$ ) and Lack of Fit Sum of Squares ( $SS_{lof}$ )
- Curvilinear regression methods
- Calculation of unknown concentrations from nonlinear curves (Harris Box 4-2)
- [Problem Set 2: "Sum of Squares Calculation,"](#) [Sum of Squares Classroom Handout](#)

1/28 Instrument Calibration III: Limits of Detection, the Method of Standard Addition Class Examp

- Limits of detection
- Method of standard additions
- [Problem Set 3](#)

2/4 Instrument Calibration IV: Internal Standard Methods of Quantitation Class Example

- Internal standard ( $IS$ ) methodology (Harris 5-4)
- Response factor  $IS$  methods
- Response ratio  $IS$  methods
- [Problem Set 4](#)

2/11 Descriptive Statistics I:

- Mean and standard deviation
- Distribution of repeated measurements
- Log-normal distribution
- Sample definition and sampling distribution of the mean
- Confidence limits of the mean for large samples

2/18 [Calibration Quiz](#) in Sims 211

2/25 Inferential Statistics: [Class Example Spreadsheet](#),

- Comparison of experimental mean with known value
- Comparison of two experimental means
- Paired  $t$ -test
- One-sided and two-sided tests

- F-Test for the comparison of standard deviations
- Outliers
- [Problem Set 5](#)

### 3/3 Analytical Quality I

- Overview of Statistical Process Control (SPC)
- Shewhart Control Charts for mean values and ranges

### 3/10 ANOVA

- [PS6 Shewhart Control Charts Due Data Set](#)

### 3/24 Multivariate Regression

- [Multivariate Linear Regression Classroom Data](#)
- Mathematical models to describe experimental data
- Determining the model
- Predictions, root-mean-square errors of calibration and prediction
- Problem Set: [Predicting Daily Maximum Ozone Concentrations](#)

3/31 No Class Problem Set Due: [Predicting Daily Maximum Ozone Concentrations](#)

### 4/7 Quantitative Structure-Activity Relationships (QSAR)

4/14 No Class QSAR Problem Set Due; [QSAR Data Set](#)

### 4/21 Review

4/29 Cumulative Final Examination 3:00 PM