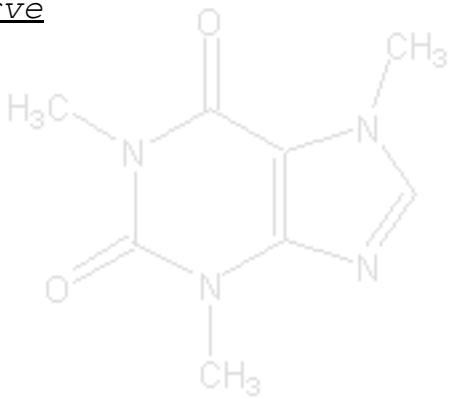


## 1/14 Instrument Calibration I: 1<sup>st</sup> Order Calibration Curve

### 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 ( $SS_{\text{tot}}$ ), Regression SS ( $SS_{\text{regr}}$ ), Residual SS ( $SS_{\text{res}}$ ), and Coefficient of Determination ( $R^2$ )
- Replicate Sum of Squares ( $SS_{\text{repl}}$ ) and Lack of Fit Sum of Squares ( $SS_{\text{l/of}}$ )
- 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 Exam

- Limits of detection
- Method of standard additions
- Problem Set 3



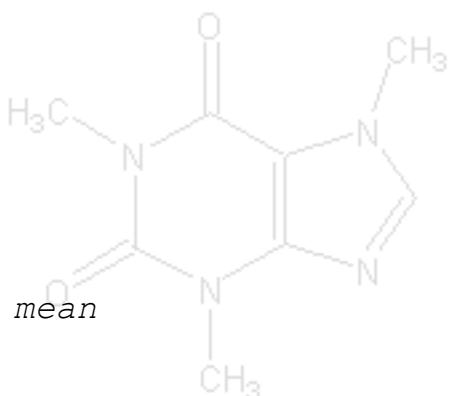
## 2/4 Instrument Calibration IV: Internal Standard Methods of Quantitation Class Example

- 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



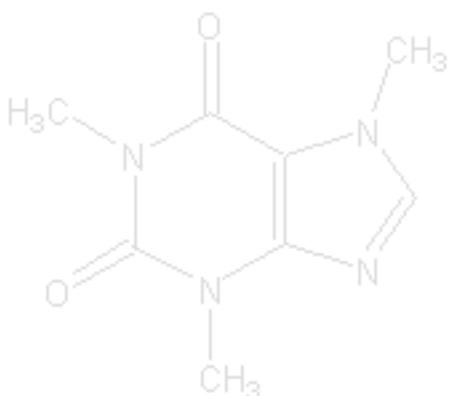
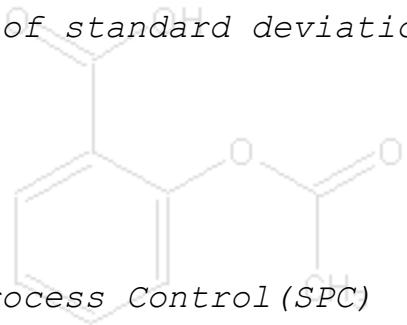
## 2/25 Inferential Statistics: Class Example Spreadsheet,

- 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

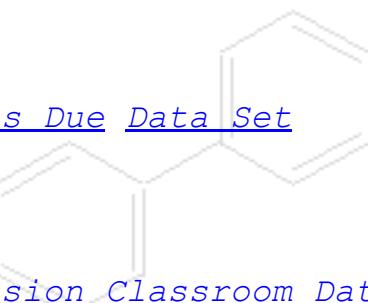


- Overview of Statistical Process Control (SPC)
- Shewhart Control Charts for mean values and ranges

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

