

CHM 6165
INTRODUCTION TO CHEMOMETRICS
Spring Semester 2025, 3 Credits
LEIGH 242

- Instructor:** John Bowden, Vet Academic Bldg (VAB) 2-167
Phone: 352-294-4063, Email: john.bowden@ufl.edu
- Lectures:** Tuesday, 11:45AM-1:40PM (Periods 5 and 6)
Thursday, 12:50-1:40PM (Period 6)
- Office hours:** After class periods or by appointment.
- Course objectives:** To provide students with an introductory foundation in statistical and data management methods/tools often used by analytical chemists, using the programming language R as the teaching platform. Students will learn how to select the appropriate method, handle data, and effectively disseminate results.
- Textbooks:** Txt1 – "R in Action," 2nd Edition, Robert I. Kabacoff; \$31.65 (Amazon, new), \$11.82 (Amazon, used) AND Txt2 – "Practical Statistics for the Analytical Scientist", 2nd Edition, Stephen Ellison, Vicki Barwick, Trevor Farrant, \$41.13 (Amazon new) or \$36.00 (Amazon used). Both books are not required, but strongly suggested and may serve as useful references. Amazon has the option to rent these books as well, I believe.
- Grading:** Grades will be based out of 500 points:
150 points for midterm exam (take home)
200 points for final exam (in class)
60 points for in class quizzes – 6 of them at 10 pt. each
90 points for in class presentation (30 pt. each)
- Grade scale: Course grades will be assigned based on the following grading scheme: A (100 – 94), A- (93.99-90), B+ (89.99 – 87), B (86.99 – 84), B- (83.99 – 80), C+ (79.99 – 77), C (76.99 – 74), C- (73.99 – 70), D+ (69.99 – 76), D (66.99 – 64), D- (63.99 – 61), E (60.99 – 0).
- Class Presentations: In an effort to provide an interactive element, there will be 3 class presentations.
- Presentation #1 – Students will select a case study on a manuscript that was retracted and will give a 10 min

presentation to the class. Grading will be focused on presentation quality, description of specifics (study, retraction reasons), and each student's own personal opinion of the retraction and possible big picture impact.

Presentation #2 – Students will select an R code not presented in class (in consultation with Dr. Bowden) and will present the code to the class. 10-minute presentations. Grading will be focused on presentation quality, description of code, example of code being used, and any tips or tricks associated with using the code.

Presentation #3 – Students will provide a journal review/critique of the paper to the class (Dr. Bowden will distribute papers). 10-minute presentations. Grading will be focused on presentation quality, depth of review, and overall quality of review assessment.

Quizzes: There will be 6 quizzes (no notes allowed) throughout the semester that will cover basic concepts covered prior to the quiz date.

Mid-term: The mid-term exam will be take-home and will be handed out **March 4 and will be due March 13 at the beginning of class.**

Final exam: The cumulative final exam will be on **May 1, 10am to 12 pm, LEIGH 242.**

Information on current UF grading policies is online: (<https://catalog.ufl.edu/ugrad/current/regulations/info/grades.aspx>).

Course policies:

Attendance will not be recorded, but participation in lectures and demonstration periods is important for assimilating the course material. Any request for make-up exams or quizzes should be made to Dr. Bowden as far in advance as possible.

Students with disabilities requesting accommodations should first register with the Disability Resource Center (352-392-8565, www.dso.ufl.edu/drc/) by providing appropriate documentation. Once registered, students will receive an accommodation letter which must be presented to the instructor when requesting accommodation. Students with disabilities should follow this procedure as early as possible in the semester.

UF students are bound by The Honor Pledge which states: "We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honor and integrity by abiding by the Honor Code. On all work submitted for credit by students at the University of Florida, the following pledge is either required or implied: "On my honor, I have neither given nor received unauthorized aid in doing this assignment." The Honor Code (<http://www.dso.ufl.edu/sccr/process/student-conduct-honorcode/>) specifies a number of behaviors that are in violation of this code and the possible sanctions. Furthermore, you are obligated to report any condition that facilitates academic misconduct to appropriate personnel. If you have any questions or concerns, please consult with the instructor or TAs in this class."

Students are expected to provide feedback on the quality of instruction in this course by completing online evaluations at <https://evaluations.ufl.edu>. Evaluations are typically open during the last two or three weeks of the semester, but students will be given specific times when they are open. Summary results of these assessments are available to students at <https://evaluations.ufl.edu/results/>.

For counseling the following resources are available to students: **U Matter, We Care:** If you or a friend is in distress, please contact umatter@ufl.edu or 352-392- 1575. **Counseling and Wellness Center:** <http://www.counseling.ufl.edu/cwc/Default.aspx>, 352-392-1575; the University Police Department: 352-392-1111 or 911 for emergencies. **Sexual Assault Recovery Services (SARS):** Student Health Care Center, 352-392-1161.

In order to ensure student privacy, communication concerning grades will only be conducted through Canvas or in a personal meeting (zoom or face to face).

Tuesday	1/14/2025	1 - Introduction to Chemometrics	
Tuesday	1/14/2025	2 - R Data Structures and Functions	
Thursday	No class	No Class (Instructor Travel)	
Tuesday	1/21/2025	3 - Data Organization in R: Tidyverse and Dplyr	
Tuesday	1/21/2025	4 - Graphing in R I	
Thursday	1/23/2025	5 - Graphing in R II	Quiz 1 (L1-3)
Tuesday	1/28/2025	6 - Graphing in R III	
Tuesday	1/28/2025	7 - Distribution and Normality Tests	
Thursday	1/30/2025	8 - Basic Statistics	
Tuesday	2/4/2025	Student Presentation 1: Paper Retractions	
Tuesday	2/4/2025	Student Presentation 1: Paper Retractions	
Thursday	2/6/2025	9 - Analysis of Variance (ANOVA) I	
Tuesday	2/11/2025	10 - Analysis of Variance (ANOVA) II	Quiz 2 (L7-9)
Tuesday	2/11/2025	11 - Analysis of Variance (ANOVA) III	
Thursday	2/13/2025	12 - Analysis of Variance (ANOVA) IV	
Tuesday	2/18/2025	13 - Bivariate Relationships	
Tuesday	2/18/2025	14 - Regression	
Thursday	2/20/2025	15 - Regression II	
Tuesday	2/25/2025	16 - Nonparametric Tests	Quiz 3 (L10-15)
Tuesday	2/25/2025	17 - Outliers and Robust Methods	
Thursday	2/27/2025	18 - Categorical Methods	
Tuesday	3/4/2025	Student Presentation 2: Teach an R code	Mid Term Out
Tuesday	3/4/2025	Student Presentation 2: Teach an R code	
Thursday	3/6/2025	19 - Principal Component Analysis (PCA) I	
Tuesday	3/11/2025	20 - Principal Component Analysis (PCA) II	
Tuesday	3/11/2025	21 - MetaboAnalyst	
Thursday	3/13/2025	22 - PLSDA and Clustering	Mid Term Due, Quiz 4 (L16-19)
Tuesday	3/18/2025	Spring Break	
Thursday	3/20/2025	Spring Break	
Tuesday	3/25/2025	23 - Machine Learning and Supervised Methods	
Tuesday	3/25/2025	24 - Time Series and Resampling	
Thursday	3/27/2025	25 - Experimental Design, Sampling, and Power	
Tuesday	4/1/2025	26 - Instrumental Analysis: Calibration Curves	Quiz 5 (L22-25)
Tuesday	4/1/2025	27 - Quality Assurance, Quality Control, and Proficiency	
Thursday	4/3/2025	28 - Method Performance/Evaluation I	
Tuesday	4/8/2025	29 - Method Performance/Evaluation II	
Tuesday	4/8/2025	30 – Real World Examples using R	
Thursday	4/10/2025	31 - Advanced Graphing in R - IV	
Tuesday	4/15/2025	32 - Scientific Publishing	Quiz 6 (L26-31)
Tuesday	4/15/2025	33 - The Peer-Review Process and Career Metrics	
Thursday	4/17/2025	34 - R Shiny, Data Management and Data Ethics	
Tuesday	4/22/2025	Student Presentations 3: Review a Manuscript	
Tuesday	4/22/2025	Student Presentations 3: Review a Manuscript	
Thursday	5/1/2025	Final Exam (Lei 242, 10 am - 12 pm)	Final Exam