

CHEM 528: Chemical and Biochemical Characterization Methods II

Fall 2012

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Required Textbook: Spectrometric Identification of Organic Compounds, 7th Edition, Robert M. Silverstein and Francis X. Webster, and David J. Kiemle. ISBN: 978-0-471-39362-7

Additional Book for your study of this course:

"Organic Structure Analysis", 2nd Edition, Phillip Crews, Jaime Rodríguez, and Marcel Jaspars. ISBN: 978-0-19-533604-7.

Course Description: Our goal in this course is to develop skill in determining the structures of organic compounds from spectral information. This will require you to learn about each type of spectroscopy (basic principles of IR and mass spectroscopy, but will focus on ¹H-, ¹³C-NMR spectroscopy). The chiral HPLC and polarimeter will also be introduced in the class. It will require you to practice the type of reasoning by which information from divergent sources is reconciled to reach a logical conclusion. For you to improve, it is absolutely essential that you work all of the problems assigned. We will move fairly rapidly through each type of spectroscopy and then will gain a better understanding of them as we solve problems using a combination of information from all. Much of the problem solving will be "open-book" to reduce the memorization required for the course. However, a certain amount of information is essential for efficient interpretation of spectral data in terms of molecular structural characteristics. By the end of this course, you will be able to determine the structure of a complex unknown organic compound by the use of NMR, IR, and mass spectra.

Learning Outcome: By the end of this course, students will be able to:

1. Use different modern NMR, visible, IR, and mass spectroscopy techniques to determine the structure of a complex unknown organic compound.
2. Understand and be able to optimize modern multi-dimensional NMR techniques such as COSY and NOESY experiments.
3. Design their own multi-dimensional NMR experiments for specific purposes.
4. Be able to use the chiral HPLC and polarimeter to analyze the chiral compounds.
4. Be able to critically evaluate techniques used in the literature.

Grading

There will be some problem sets assigned and discussion throughout the semester that will constitute 15 points of the grade. Two partial exams and comprehensive final exam will carry 40 and 30 points, for a total of 70. Unknown sample analysis and identification will be 15 points. The final letter grade will be based on a standard scale 90-100% A, 80-89% B, 70-79% C, 60-69% D, and below 60% F. The grades may be curved, if warranted.

There will be absolutely no make-ups for exams. If you miss an examination, you will be assigned a zero for that assignment. Problem sets not submitted on time may receive a grade of zero.

Tentative Schedule

Week 1 – NMR spectroscopy (chemical shift, splitting pattern, integration)
Week 2 – ^1H -NMR spectroscopy (interpretation of ^1H -NMR)
Week 3 - ^1H -NMR spectroscopy (^1H -NMR of alcohols, amine, reading correlation tables)
Week 4- **Exam 1** and ^{13}C -NMR Spectroscopy (interpretation and correlation tables)
Week 5 – 2-D NMR Spectroscopy
Week 6 – Hetero atoms ^{19}F and ^{31}P NMR spectroscopy
Week 7 - Mass spectroscopy
Week 8 - Mass spectroscopy
Week 9 – **Exam 2**
Week 10 - IR spectroscopy (interpretation of IR spectrums)
Week 11 - IR spectroscopy – (interpretation and reading correlation tables)
Week 12 – Introduction of chiral HPLC and polarimeter for the chiral sample analysis
Week 13 - Unknown samples' analysis and identification
Week 14 - Unknown samples' analysis and identification
Week 15 - **Final Exam** (MS, IR, and NMR)

ADA ELIGIBLE STUDENTS: Students requesting accommodations for disabilities must make arrangements through the Disability Resources & Services office. For more information, please contact Office of Student Disability Resources and Services in Room 132 in the Gee Library, phone number (903) 886-5835, email address: StudentDisabilityServices@tamuc.edu. ADA eligible students should make arrangements with the instructor in the first week of the semester regarding special arrangements needed for classroom or testing facilities and procedures to accommodate the disability.

* Please note that this schedule and topics are subject to change