

## CHEM 528: Chemical and Biochemical Characterization Methods II Fall 2015

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Office hours: Tuesday, Wednesday and Thursday: 9:30-11:30am or by email

**Required Textbook:** Spectrometric Identification of Organic Compounds, 7<sup>th</sup> 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", 2<sup>nd</sup> 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 and inorganic 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 <sup>1</sup>H-, <sup>13</sup>C-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 independently. 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 MS.

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

1. Use different modern nuclear magnetic resonance (NMR), infrared spectrometry (IR), and mass spectroscopy (MS) 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 throughout the semester that will constitute 20 points of the grade. One midterm exam and final comprehensive exam will carry 30 and 40 points, for a total of 70. Unknown sample analysis and identification will be 10 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.

**Students with Disabilities:**

*The Americans with Disabilities Act (ADA) is a federal anti-discrimination statute that provides comprehensive civil rights protection for persons with disabilities. Among other things, this legislation requires that all students with disabilities be guaranteed a learning environment that provides for reasonable accommodation of their disabilities. If you have a disability requiring an accommodation, please contact: Office of Student Disability Resources and Services  
Texas A&M University-Commerce, Gee Library, Room 132  
Phone (903) 886-5150 or (903) 886-5835, Fax (903) 468-8148  
[StudentDisabilityServices@tamu-commerce.edu](mailto:StudentDisabilityServices@tamu-commerce.edu)*

**Tentative Schedule**

Week 1 – NMR spectroscopy (chemical shift, splitting pattern, integration)

Week 2 –  $^1\text{H}$ -NMR spectroscopy (interpretation of  $^1\text{H}$ -NMR)

Week 3 –  $^1\text{H}$ -NMR spectroscopy ( $^1\text{H}$ -NMR of alcohols, amine, reading correlation tables)

Week 4 –  $^{13}\text{C}$ -NMR Spectroscopy (interpretation and correlation tables)

Week 5 – 2-D NMR Spectroscopy

Week 6 – Hetero atoms  $^{19}\text{F}$  and  $^{31}\text{P}$  NMR spectroscopy

**Week 7 – Midterm Exam**

Week 8 – Mass spectroscopy

Week 9 – Mass spectroscopy

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 (Instruments training on commerce campus)

Week 14 - Unknown samples' analysis and identification (Instruments training on commerce campus)

Week 15 - **Final Exam** (MS, IR, and NMR)

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