Chemistry 5235/4230 (Section O535/O430) Organic Spectroscopy

Instructor: Prof. Sandra Loesgen Office: Whitney Laboratory, St Augustine FL e-mail: sandra.loesgen@whitney.ufl.edu phone: 904-201-8437 TA: Joe Mangun (mangun.joseph@whitney.ufl.edu)

Lectures are on Tuesdays 11:45am to 1:40pm in Leigh 207

Problem Sessions on selected Thursdays 12:50-1:40pm: 09/12; 10/03; 10/17; 11/07, 11/21; 12/05 via Zoom: https://ufl.zoom.us/j/99250346269?pwd=zBXX8b7GpIYgHm0pB8SA5z3NwXX4Jr.1

The problem session is <u>mandatory</u> for CHM 5235 students and participation will be graded. CHM 4230 students are <u>highly</u> encouraged to attend the problem session to practice for the exams.

JM's Office Hours on selected Thursdays 12:50-1:40pm: 8/29, 9/5, 9/19, 9/26, 10/10, 10/24, 10/31, 11/14 via Zoom: https://ufl.zoom.us/j/99250346269?pwd=zBXX8b7GpIYgHm0pB8SA5z3NwXX4Jr.1

SL's Office Hours on selected Tuesdays 2-2:50pm in Leigh Hall 400 (9/10, 10/1, 10/15, 11/5, 11/19, 12/3)

Course texts:

- 1. Spectrometric Identification of Organic Compounds (Silverstein, 8th or 7th ed.)
- 2. Structure Determination of Organic Compounds: Tables of Spectral Data (E. Pretsch, 4th ed.)

E-Learning: We will use a Canvas site: <u>https://lss.at.ufl.edu/</u> (check regularly to find announcements, lecture notes and handouts, exam scores, and other information related to this class). From this webpage, click on the Canvas login button and then use your Gatorlink ID to log in.

Prerequisites: One year of organic chemistry (CHM 2210/2211) is necessary.

Course description and objectives: Survey of spectroscopic techniques used to elucidate the structures of unknown organic compounds. These topics will include mass spectrometry, infrared and ultraviolet spectroscopy, 1- and 2- dimensional NMR applications. Beside theory and fundamentals of these techniques, the major emphasis is to enable students to elucidate structures of various complexities by illustrated examples, guided in-class exercises, and working on weekly problem sets.

Course learning outcomes

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

- 1. Distinguish spectroscopic techniques (UV, IR, NMR, MS) and plan hands-on experiments.
- 2. Use different modern NMR, IR, and mass spectrometry techniques to determine the structure of a complex, unknown organic compound.
- 3. Understand and be able to optimize modern multi-dimensional NMR techniques such as COSY and 2D heteronuclear experiments.
- 4. Design their own multi-dimensional NMR experiments for specific purposes.
- 5. Be able to critically evaluate and discuss techniques used in the literature.

Evaluation	CHM 5235	CHM 4230
Exam 1 (in class)	30%	45%
Exam 2 (in class)	30%	35%
Exam 3 (take home)	20%	25%
Problem Sets (5 sets)	20%	-

Here is a <u>link to the university grades and grading policies</u>. This is a problem-solving class; thus, your grade will be largely determined by how well you interpret the various types of spectral problems. I will introduce each spectroscopic technique with 1-3 lectures including demonstrations and problem sets (5) will follow each paragraph. Problem sets are take-home assignments; the due date will be announced in class. Midterm and Final are in-class exams and will be mostly on determining the connectivity and stereochemistry of organic compounds from spectral data provided. You will be able to use your notes and the textbooks.

It is **critical** that you attend every lecture session or watch the recording/notes timely, as we will be covering significant amounts of material daily and demonstrating problem-solving techniques. There are no make-up quizzes (if an exam/problem set is missed with approved absence, the final grade will replace it. Requirements for class attendance and make-up exams, assignments, and other work in this course are consistent with university policies. <u>Click here to read the university attendance policies</u>.

Classroom Policies

Students are expected to behave in a professional manner at all times. Positive contributions to the learning environment and participation in classroom learning activities are expected. Students should demonstrate courtesy to the instructor, as well as to their fellow classmates. Focusing your attention on anything other than pertinent classroom material could be considered discourteous.

Our class sessions may be audio visually recorded for students in the class to refer back and for enrolled students who are unable to attend live. Students who participate with their camera engaged or utilize a profile image are agreeing to have their video or image recorded. If you are unwilling to consent to have your profile or video image recorded, be sure to keep your camera off and do not use a profile image. Likewise, students who un-mute during class and participate orally are agreeing to have their voices recorded. If you are not willing to consent to have your voice recorded during class, you will need to keep your mute button activated and communicate exclusively using the "chat" feature, which allows students to type questions and comments live. The chat will not be recorded or shared. As in all courses, unauthorized recording and unauthorized sharing of recorded materials is prohibited.

Student Honor Code

The UF Student Honor Code (see https://policy.ufl.edu/regulation/4-040/ for details): We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honesty and integrity. 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." Honor Code violations include copying on an exam (or helping another student to copy) and/or turning in an exam for regrading that has been changed since it was graded by the instructor.

Any student found responsible for an academic honesty violation in this course will be recommended sanctions consistent with the offense.

Other Important Information

- Disability Resources: Students with disabilities who experience learning barriers and would like to request academic accommodations should connect with the disability Resource Center. <u>Click here to get started with the Disability Resource Center</u>. It is important for students to share their accommodation letter with their instructor and discuss their access needs, as early as possible in the semester.
- Division of Student Affairs (Counseling, Dean of Students Office): <u>http://www.ufsa.ufl.edu/</u>.
- Need help dropping this class? Contact a Chemistry undergraduate advisor here: https://www.chem.ufl.edu/undergraduate/advising/
- Your well-being is important to the University of Florida. The U Matter, We Care initiative

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(http://www.umatter.ufl.edu/is committed to creating a culture of care on our campus by encouraging members of our community to look out for one another and to reach out for help if a member of our community is in need. If you or a friend is in distress, please contact umatter@ufl.edu so that the U Matter, We Care Team can reach out to the student in distress. A nighttime and weekend crisis counselor is available by phone at 352-392-1575. The U Matter, We Care Team can help connect students to the many other helping resources available including, but not limited to, Victim Advocates, Housing staff, and the Counseling and Wellness Center. Please remember that asking for help is a sign of strength. In case of emergency, call 9-1-1.

• Online course evaluation: Students are expected to provide professional and respectful feedback on the quality of instruction in this course by completing course evaluations online via GatorEvals. <u>Click here for guidance on how to give feedback in a professional and respectful manner</u>. Students will be notified when the evaluation period opens, and can complete evaluations through the email they receive from GatorEvals, in their Canvas course menu under GatorEvals. <u>Summaries of course evaluation results are available to students here</u>.

PS Date Theme Topics (textbook chapters) 8/27/24 A Syllabus, Intro MS, CH1 Intro CH1 [theory, EI, CI ionization] 8/27/24 B MS 1 9/03/24 A MS₂ CH1 [EI, ESI] 9/03/24 B MS 3 CH1 [MALDI, FAB] PS1 out 9/10/24 A MS₄ CH1 [mass detectors] 9/10/24 B MS 5 CH1 [mass detectors, halogens, degree of unsaturation, fragmentation] 9/17/24 A MS 6 & IR 1 CH1 [MS summary slides], CH2 PS1 due 9/17/24 B IR 2 CH2 IR 9/24/24 A UV vis NOTE: Extra hand out (not in Silverstein book) CH3 [theory: nuclear spin, resonance, NMR spectrometer, 9/24/24 B NMR 1 magnetization, relaxation] CH3 [chemical shift, Integration, coupling, coupling constant J] 10/01/24 A NMR 2 PS2 out 10/01/24 B NMR 3 CH3 [chemical and magnetic equivalence, examples, first order, higher order spectra, Pople notation, multiplets] 10/08/24 A NMR 4 PS2 due CH3 [chemical and magnetic equivalence, examples, first order, higher order spectra, Pople notation, multiplets] 10/08/24 B NMR 5 CH3 [multiplet analysis, Hoye, second order spectra] 10/15/24 A NMR 6 CH3 [multiplet analysis, calculating shifts, chemdraw, solvents, data reporting] 10/15/24 B NMR 7 PS3 out CH4 [13C NMR theory, decoupling, chemical shift range]

ALL DATES AND ASSIGNMENTS ARE TENTATIVE AND SUBJECT TO CHANGE.

CHM 4230/5235			Fal
10/22/24	Exam 1 11:45am - 1:40pm in Leigh 207		
10/29/24	NMR 8	PS3 due	CH4 [DEPT, examples for better 13C]
10/29/24	NMR 9		CH3 [dynamic NMR line width, coalescence, Erying equation, proton exchange]
11/05/24_A	NMR 2D 1	PS4 out	CH5 [Intro 2D NMR, COSY, TOCSY, 2D COSY, selective TOCSY]
11/05/24_B	NMR 2D 2		CH5 [Types of C-H exp, HMQC, HMBC, inadequate]
11/12/24_A	NMR 2D 3	PS4 due	CH5 [NOE, difference NOE, 2D NOESY]
11/12/24_B	NMR 2D 4		CH5 [through space correlations, examples Ipsenol, 8.27, NMR history]
11/19/24_A	Stereochemistry 1	PS5 out	Stereochemistry start, acetonide, Kishi's database, Mosher's Ester
11/19/24_B	Stereochemistry 2		Stereochemistry: Murata's J-based, NMR calculations, Marfey's analysis, optical rotation, ECD, hexacyclinol story
11/26/24			No class - Thanksgiving
12/03/24_A	Other Nuclei	PS5 due	CH6 [15N, protein NMR, STD NMR, 2H, 19F, 29Si, 31P, 119Sn]
12/03/24_B	Other Nuclei		Finish other nuclei, PS5, exam practice
12/12/2024 12/09 - 12/11	24Exam 2: 7:30 - 9:30am room TBD2/11Exam 3: 48h take-home assignment (Dec 9 1pm - Dec 11 1pm)		