Phcg 631: ANALYSIS OF NATURAL PRODUCT DRUGS I
(NMR Structure Elucidation)
Fall Semester 2018

Graduate course offering in Structure Characterization by Nuclear Magnetic Resonance (NMR)

Course Instructor: Dr. Vitor H. Pomin, 317A Faser Hall
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Time/Days: 3:30-4:45 PM/ Tuesdays & Thursdays
Location: TCRC 3054
Starting/Ending Dates: 08-21-2018/12-06-2018

Course description: This is an introductory course in nuclear magnetic resonance (NMR) spectroscopy as a tool for assessing or confirming simple and/or complex organic structures.

Course description: This course is designed as an NMR introduction for graduate students in *medicinal chemistry, pharmacognosy, chemistry and biochemistry*. This course illustrates conventional 1D and 2D NMR experiments routinely used in structure determination. Emphasis is placed on learning NMR cross-peak assignments and assessment of structural characteristics through NMR spectra. The ability of the student (a) to absorb the background, (b) to solve related problems and (c) make judicious decisions regarding the use of NMR in structure identification will be evaluated. This course is not designed to assist you in operating the NMR instrument. But it can certainly help in data acquisition, result interpretation and structural assignment.

Prerequisites: There are no prerequisites for this course

Learning Goals: Upon successful completion of this course, the student should be able to:

1) Recognize the importance in the application of NMR spectroscopy mainly in structure elucidation but also in structural biology and biochemistry;
2) Understand the nuclear magnetic properties of certain nuclei that lead to signals in NMR spectra;
3) Understand basic methodological parameters employed in NMR experiments (pulse sequences) that will yield specific chemical or structural information;
4) Critically evaluate and interpret NMR spectra from both 1D and 2D experiments to elucidate and confirm structures;
5) Effectively communicate the "*language*" (jargon) used in NMR, both in oral and written contexts.

Grading and Evaluation Process:

Problem Sets (6), take home (2.5% each)	15%
Exam 1, in class (100 Pts)	20%
Exam 2, in class (100 Pts)	20%
Exam 3, take home (100 Pts)	15%
Presentation	15%
Final Exam, take home (100 Pts)	15%
Total:	100%

Problem Sets: After some lessons, the students will receive a problem set at the end of some Thursday's classes. The problem sets are due on at the beginning of the following Tuesday class. Work will be not accepted late unless with a reasonable justification for the excuse. The problem sets will not be graded for correctness; rather, they will be evaluated in class to ensure that the students have attempted to make them with effort. *The student who failure to attempt in solving the problem sets will lose the pts of that specific problem set*. Problems will be reviewed and discussed with audience participation during the classes named "*Problem set discussion*". The problem sets 1, 3 and 5 will be retained with the course instructor and given back to the student on the day of discussion. The work on problem sets 2, 4 and 6 will be checked in on the beginning of the day "*Problem set discussion*".

Class Presentation: Each graduate student will be required to present a paper from the literature about the current topics covered in the area of NMR suggested by course instructor. Reviews won't be accepted. Articles discussing structure elucidation, structural modifications for NMR analysis, NMR methods and its combination with other analytical techniques are welcome. The oral power point presentation should be between 20-25 min in length, with 5 minutes reserved for questions and discussion with the audience. The instructor will assist the students with the assignments of topics. The student MUST provide the instructor with his/her power point slide set at least one week in advance to the presentation. Your presentation will be judged by your organization of the concepts from the paper as well as by your peers. A peer-evaluation form will provided.

EXAMS: The three exams will cover materials of the lectures, assigned readings, and problem sets respectively from the first, middle and last segments of the course. The exams will be administered during a Thursday class period, right after a "*Problem set discussion*" class. The graduate students will have the time from 2:30 to 4:30 PM to complete the exam. All non-digital material (lecture prints, handouts, personal notes, textbooks) can be used during the examination. No computer/electronic devices, with exception to the calculator, will be allowed during the exams. Each individual MUST bring their OWN materials. There will be no sharing of materials during the examination. Exam 3 and Final Exam (covering the content of the entire course) will be administered as a take-home examination. The students must bring the solutions of the questions of both Exams after one week - Exam 3 to TCRC 3054 Nov 15th and Final Exam to the office of the instructor (Faser Hall 417A) any time before the end of the course (Tuesday, Dec 4, 5 PM).

Letter Grades of A, B, C, D and F will be assigned based on the following scale:
A = ≥ 92.5, A- = ≥ 90.0, B+ = ≥ 87.5, B = ≥ 82.5, B- = ≥ 80.0, C+ = ≥ 77.5, C = ≥ 72.5, C- = ≥ 70.0, D+ = ≥ 67.5, D = ≥ 62.5, D- = ≥ 60.0, F = < 60

Credits and Grades Policy: This course will abide by the university's Credits and Grades Policy, found at: https://policies.olemiss.edu/ShowDetails.jsp?istatPara=1&policyObjidPara=10647554

Examinations and Last Week of Class Policy: This course will abide by the university's Examinations and Last Week of Class Policy, found at: https://policies.olemiss.edu/ShowDetails.jsp?istatPara=1&policyObjidPara=10647552

Recommended literature: (1) Timothy D.W. Claridge, "High-Resolution NMR Technique in Organic Chemistry", 3rd edition, Elsevier, 2016. ISBN: 978-0-08-099986-9. (2) P.J. Hore, "Nuclear Magnetic Resonance" 2nd edition, Oxford, 2015. ISBN: 978-0-19-870341-9. (3) David P. Goldberg, "Principles of NMR Spectroscopy – An Illustrated Guide", 1st edition, University Science Books, 2016. ISBN: 978-1-891389-88-7. (4) Horst Friebolin, "Basic One- and Two-Dimensional NMR Spectroscopy" 4th edition, Wiley-VCH, 2005. ISBN: 3-527-31233-1. (5) J.W. Akitt & B.E. Mann, "NMR and Chemistry – An

Introduction to Modern NMR Spectroscopy", 4th edition, CRC Taylors & Francis, 2000. ISBN: 0-7487-4344-8. (6) Harald Günther, "NMR Spectroscopy – Basic Principles, Concepts, and Applications in Chemistry" 3rd edition, Wiley-VCH, 2013. ISBN: 978-3-527-33000-3. (7) S. Braun, H.-O. Kalinowski, S. Berger, "150 and More Basic NMR Experiments" 2nd edition, 1998. ISBN: 3-527-29512-7.

Academic Dishonesty and Plagiarism Policy: Academic dishonesty includes cheating, fabricating or falsifying information or sources, improper collaboration, submitting the same paper for different classes without permission, and plagiarism. Plagiarism occurs when writers deliberately or unintentionally use another person's language, ideas, or materials and present them as their own without properly acknowledging and citing the source. This includes, but is not limited to, turning in all or part of an essay written by someone other than yourself (a friend, an internet source, etc.), and claiming it as your own, including information or ideas from research material without citing the source. Familiarize yourself with UM's Student Code of Conduct and UM's policies on academic dishonesty. The University of Mississippi considers plagiarism a serious form of academic dishonesty. Avoid plagiarism by carefully and correctly citing your sources whenever you use someone else's words, equations, graphics, or ideas. If you are unsure of something and are worried you may be plagiarizing, come see me. Plagiarism in this course results in one or more of the following consequences: failure of the assignment, failure of the course, and/or disciplinary action by the University.

Academic Conduct and Discipline: Students are expected to adhere to the University of Mississippi Creed and the Standards of Honesty as described in Policy Code ACA.AR.600.001 (https://secure4.olemiss.edu/umpolicyopen/ShowDetails.jsp?istatPara=1&policyObjidPara=10817696) and written in the M Book. If you violate the Standards of Honesty, you will be reported and subject to the appropriate sanction which may include expulsion from the University. The School of Pharmacy has an additional of Professional and Ethical Conduct, which students are expected to uphold. Consequences of violating the Code of Conduct are outlined in the SOP Student Handbook (Section 3).

Disability Access Statement: It is University policy to provide, on a flexible and individual basis, reasonable classroom accommodations to students who have verified disabilities that may affect their ability to participate in course activities or meet course requirements (cf. https://secure4.olemiss.edu/umpolicyopen/ShowDetails.jsp?istatPara=1&policyObjidPara=10868401). It is the responsibility of any student who requests accommodations to contact the Office of Student Disability Services (SDS, 915-7128) to discuss their individual needs for accommodations. SDS will provide eligible students with an Instructor Notification form that details approved accommodations, which the student will share with the instructor. The instructor will then work with the student so that reasonable accommodations can be provided. Students should be aware that accommodations are not provided retroactively, so it is important to request accommodations as early in the semester as possible.

Sexual Misconduct Policy Statement: It is the position of the University that sexual misconduct in any form will not be excused or tolerated. Criminal, civil and University disciplinary processes are available to a student with a complaint. The University is committed to prompt, effective and fair procedures to investigate and adjudicate reports of sexual misconduct and to the education of the University community about the importance of responding to all forms of sexual misconduct. Special emphasis is placed on the rights, needs, and privacy of the student with the complaint, as well as the needs and privacy of the respondent. At the same time, the University adheres to all federal, state, and local requirements for intervention and crime reporting related to sexual misconduct. This policy can be found at: https://secure4.olemiss.edu/umpolicyopen/ShowDetails.jsp?istatPara=1&policyObjidPara=11079479

Course calendar:

Week	Date	Topic	Assignment deployed	Due date
1	Aug 21 (T)	Introduction to Phcg 631 and NMR		
	Aug 23 (Th)	History of NMR Spectroscopy		
2	Aug 28 (T)	Instrumental and experimental aspects		
	Aug 30 (Th)	NMR Basics 1	PS 1 (take home)	Sep 04
3	Sep 4 (T)	Chemical shift (δ)		
	Sep 6 (Th)	Scalar coupling (*J*)	PS 2 (take home)	Sep 11
4	Sep 11 (T)	Problem set discussion		
	Sep 13 (Th)	EXAM 1 (in class 3:30-5:30 PM)		
5	Sep 18 (T)	Introduction to homonuclear 2D		
	Sep 20 (Th)	Spin evolution (COSY)		
6	Sep 25 (T)	COSY		
	Sep 27 (Th)	TOCSY	PS 3 (take home)	Oct 2
7	Oct 2 (T)	NOESY		
	Oct 4 (Th)	ROESY/HOESY	PS 4 (take home)	Oct 9
8	Oct 9 (T)	Problem set discussion		
	Oct 11 (Th)	EXAM 2 (in class 3:30-5:30 PM)		
9	Oct 16 (T)	Introduction to heteronuclear 2D (HMQC/HSQC)		
	Oct 18 (Th)	HMQC/HSQC		
10	Oct 23 (T)	HMBC		
	Oct 25 (Th)	HMBC	PS 5 (take home)	Oct 30
11	Oct 30 (T)	Structural conformation (NOE and J)		
	Nov 1 (Th)	Molecular motion (spin relaxation rates)	PS 6 (take home)	Nov 6
12	Nov 6 (T)	Problem set discussion		
	Nov 8 (Th)	EXAM 3	Take home	
13	Nov 13 (T)	Student(s) presentation(s)		
	Nov 15 (Th)	Student(s) presentation(s)	Answers of Exam 3	
14	Nov 20 (T)	No Class – Thanksgiving		
	Nov 22 (Th)	No Class – Thanksgiving		
15	Nov 27 (T)	Students(s) presentation(s)	Final Exam (Take Home)	Dec 4
	Nov 29 (Th)	Students(s) presentation(s)		
16	Dec 4 (T)	FINAL EXAM Due 5 PM (Faser Hall 417A)		
	Dec 6 (Th)	Grades of students		