BBMB/CHEM 549X – Nuclear Magnetic Resonance Spectroscopy –SYLLABUS

Course Description: Advanced Nuclear Magnetic Resonance spectroscopy. Topics include theoretical principles of NMR, practical aspects of experimental NMR, solution and solid state NMR, methodologies for molecule characterization, protein structure determination, NMR relaxation, recent advances in NMR spectroscopy.

Prerequisites: CHEM324, CHEM325, CHEM572, BBMB461, BBMB561, or permission of the instructor.

Course Organizer: Vincenzo Venditti, 515 294 1044, 0219 Hach Hall, venditti@iastate.edu
Office Hours by appointment

Instructors: Julien Roche (BBMB), 4-6437, 4210 MBB, roche@iastate.edu
Aaron Rossini (CHEM), 4-8952, 0205 Hach Hall, arossini@iastate.edu
Vincenzo Venditti (CHEM), 4-1044, 0219 Hach Hall, venditti@iastate.edu

3 Credits, 2 lectures, Tue. & Thus. 11:00 AM – 12:20 PM
Room: Lagomarcino Hall 2485

Grading:		
	3 Assignments, 5% each	15%
	Exam I	20% (Venditti)
	Exam II	20% (Roche
	Exam II	20% (Rossini)
	Student Presentation	25%

Note: Exam II will not be strictly cumulative, but questions may probe concepts that build upon topics covered in Exam I.

Textbook: None required. Recommended: Understanding NMR Spectroscopy, Keeler, 2nd ed, (Wiley). Other Helpful Texts: Protein NMR Spectroscopy, Cavanagh et al. 2007, 2nd ed. (Academic Press); Spin Dynamics, Levitt, 2008, 2nd ed. (Wiley).; NMR: the Toolkit, Hore, Jones and Wimperis, 2nd ed. (Oxford); Solid-State NMR: Basic Principles and Practice, Apperley, Harris and Hodgkinson.

Student Presentations:
Students will choose from the list of topics below, or submit their own topic for instructor approval, and present a ca. 30 minute presentation regarding the technique to cover the theoretical and practical aspects. Topics are first-come first-served and will be managed by Prof. Rossini or other course instructors. For example, if a student chose the HNCA pulse sequence: a detailed explanation of how the pulse sequence selects specific coherences, what sort of molecules is this technique appropriate for, what do the data look like, how are the data analyzed, what questions does this answer, etc. Students will be required to meet with an instructor no less than three weeks before to the presentation date to review the material. Students must make an appointment with an instructor.

Potential (but not inclusive) List of Presentation Topics:

- TROSY
- Residual Dipolar Couplings
- Dissolution Dynamic Nuclear Polarization
- Solid State Dynamic Nuclear Polarization
- Quadrupolar Nuclei
- Ultrafast MAS (ssNMR)
- Measuring Hydrogen Bonds
- Transfer NOESY
- Saturation Transfer Difference Spectroscopy (STD-NMR)
- Nucleic Acid Residue Assignment
- Nucleic Acid Structure Calculation

Spatial Resolution/Magnetic Resonance Imaging
Measurements of Intermediate Exchange
Coupling Molecular Dynamics Simulations and NMR Measurements
Statistical TOCSY (sTOCSY)
Diffusion Measurements
CHESCA and CHESPA
Invisible states
Intrinsically disordered proteins
Protein folding

Lecture	Date	Topic	Instructor	Assignments/Exams
1	Tu. 01/18	Introduction and Basic Overview of NMR NMR signal, Chemical Shift, Couplings	Venditti	
2	Th. 01/20	Vector model RF pulses, Larmor frequency, the 1D experiment	Venditti	
3	Tu. 01/25	Data processing FT, apodization, zero filling, phase correction	Venditti	
4	Th. 01/27	Product Operator formalism and 2D NMR	Venditti	
5	Tu. 02/01	NMR Relaxation	Venditti	
6	Th. 02/03	Phase cycling and gradient pulses	Venditti	
7	Tu. 02/08	Intro to NMR Instrumentation	Venditti	
8	Th. 02/10	Review	Venditti	Assignment 1 due
-	Tu. 02/15	Exam I	Venditti	Exam I
9	Th. 02/17	Protein NMR I Overview and Assignment	Roche	
10	Tu. 02/22	Protein NMR II TROSY	Roche	
11	Th. 02/24	Protein NMR III Structure determination	Roche	
12	Tu. 03/01	Protein NMR IV Protein dynamics – part 1	Roche	
13	Th. 03/03	Protein NMR V Protein dynamics – part 2	Roche	
14	Tu. 03/08	Protein NMR VI Dark states – part 1	Roche	
15	Th. 03/10	Protein NMR VII Dark States – part 2	Roche	
16	03/14-18	Spring Break	-	No Class
17	Tu. 03/22	Review	Roche	Assignment 2 due
-	Th. 03/24	Exam II	Roche	Exam II
18	Tu. 03/29	Intro to Solid State NMR (CSA and dipolar couplings)	Rossini	
19	Th. 03/31	Intro to Solid State NMR – cont'd	Rossini	
20	Tu. 04/05	High Resolution Solid State NMR	Rossini	
21	Th. 04/07	High Resolution Solid State NMR	Rossini	
22	Tu. 04/12	High Resolution SSNMR of Quadrupoles	Rossini	
23	Th. 04/14	Advanced SSNMR Methods	Rossini	
24	Tu. 04/19	The density matrix formalism; numerical evaluation	Rossini	
25	Th. 04/21	Review	Rossini	Assignment 3 due
-	Tu. 04/26	Exam III	Rossini	Exam III
26	Th. 04/28	Student presentations	-	

27	Tu. 05/03	Student presentations	-	
28	Th. 05/05	Student presentations	-	

Academic Dishonesty
The class will follow Iowa State University's policy on academic dishonesty. Anyone suspected of academic dishonesty will be reported to the Dean of Students Office.
http://www.dso.iastate.edu/ja/academic/misconduct.html

Disability Accommodation
Iowa State University complies with the Americans with Disabilities Act and Sect 504 of the Rehabilitation Act. If you have a disability and anticipate needing accommodations in this course, please contact (instructor name) to set up a meeting within the first two weeks of the semester or as soon as you become aware of your need. Before meeting with (instructor name), you will need to obtain a SAAR form with recommendations for accommodations from the Disability Resources Office, located in Room 1076 on the main floor of the Student Services Building. Their telephone number is 515-294-7220 or email disabilityresources@iastate.edu . Retroactive requests for accommodations will not be honored.

Dead Week
This class follows the Iowa State University Dead Week policy as noted in section 10.6.4 of the Faculty Handbook http://www.provost.iastate.edu/resources/faculty-handbook .

Harassment and Discrimination
Iowa State University strives to maintain our campus as a place of work and study for faculty, staff, and students that is free of all forms of prohibited discrimination and harassment based upon race, ethnicity, sex (including sexual assault), pregnancy, color, religion, national origin, physical or mental disability, age, marital status, sexual orientation, gender identity, genetic information, or status as a U.S. veteran. Any student who has concerns about such behavior should contact his/her instructor, Student Assistance at 515-294-1020 or email dso-sas@iastate.edu, or the Office of Equal Opportunity and Compliance at 515-294-7612.

Religious Accommodation
If an academic or work requirement conflicts with your religious practices and/or observances, you may request reasonable accommodations. Your request must be in writing, and your instructor or supervisor will review the request. You or your instructor may also seek assistance from the Dean of Students Office or the Office of Equal Opportunity and Compliance.

Contact Information
If you are experiencing, or have experienced, a problem with any of the above issues, email academicissues@iastate.edu.

Learning outcomes
Understanding molecular structure and dynamics is critical to our understanding of chemical, physical and biological processes that underpin the basic and applied research advances in diverse fields such as biomedicine, agriculture and materials science. To this end, students in BBMB/CHEM550 will learn fundamental aspects of Nuclear Magnetic Resonance (NMR) spectroscopy, a widely used technique to view the three-dimensional structures of proteins, nucleic acids, carbohydrates, small molecules, pharmaceuticals and complex solid materials at the atomic level. Topics covered include: theoretical and practical aspects of modern biomolecular and solid-state NMR ranging from sample requirements to instrumentation, data collection, data processing and analysis; structure determination; introduction to advanced NMR techniques and independent, take home exercises accompanied by instructor analyzed, hands-on application of NMR theory to practical questions.

Free Expression
Iowa State University supports and upholds the First Amendment protection of freedom of speech and the principle of academic freedom in order to foster a learning environment where open inquiry and the vigorous debate of a diversity of ideas are encouraged. Students will not be penalized for the content or viewpoints of their speech as long as student expression in a class context is germane to the subject matter of the class and conveyed in an appropriate manner.

Face masks encouraged
Because of the continuing COVID-19 pandemic, all students are encouraged—but not required—to wear face masks, consistent with current recommendations from the Centers for Disease Control and Prevention. Further information on the proper use of face masks is available at: https://www.cdc.gov/coronavirus/2019-ncov/your-health/effective-masks.html

Vaccinations encouraged
All students are encouraged to receive a vaccination against COVID-19. Multiple locations are available on campus for *free*, convenient vaccination. Further information is available at: https://web.iastate.edu/safety/updates/covid19/vaccinations
Vaccinations may also be obtained from health care providers and pharmacies.

Physical distancing encouraged for unvaccinated individuals
Classrooms and other campus spaces are operating at normal capacities, and physical distancing by faculty, staff, students, and visitors to campus is not required. However, unvaccinated individuals are encouraged to continue to physically distance themselves from others when possible.