BCMB / CHEM 8190 Biomolecular NMR

GRADUATE COURSE OFFERING IN NUCLEAR MAGNETIC RESONANCE (Spring 2012)

"Biomolecular Nuclear Magnetic Resonance" is a course intended for all graduate students with an interest in applications of nuclear magnetic resonance (NMR) to problems in molecular and structural biology. It will begin with a treatment of the fundamentals that underlie magnetic resonance phenomena and develop this into a basis for experimental design, interpretation of data, and critical reading of the literature. The course will assume students have had some introduction to NMR through a basic course in spectroscopy or an introductory NMR course such as CHEM/BCMB 6190 (UGA course). Some previous exposure to elementary quantum mechanics and its applications in spectroscopy would also be useful, but we will attempt to provide sufficient background material to aid those who have not had this exposure.

There will be problem sets; the sets will not be graded, but they will serve as important preparation for the midterm and the final. The sets will be initially posted on the website and answers will appear approximately a week later. Grades will be based on performance on the midterm and the final exam. A complete syllabus and additional information are available through the course website:

http://tesla.ccrc.uga.edu/courses/bionmr/

Class Time: M, W, F 10:05 - 11:00

Location: This course is being taught with the cooperation of faculty at the University of Georgia (UGA), Georgia State University (GSU), and the Georgia Institute of Technology (GA Tech). On Monday and Wednesday of each week lectures will be given via a teleconferencing network. At UGA the class will be held in the Life Sciences Building, B116. The rooms at Georgia Tech, and Georgia State will be posted as soon as they are available (see Dr. Gelbaum (GA Tech), or Drs. Yang or Germann (GSU)). On Fridays students will participate in an interactive problem solving session and software demonstrations at their local sites (The C122 in the Life Sciences building for UGA students).

Instructors:
UGA Instructors: James Prestegard, Jeffrey Urbauer
GA Tech Instructors: Les Gelbaum
GSU Instructors: Jenny Yang, Markus Germann

Inquiries to Professor Prestegard - jpresteg@ccrc.uga.edu

Text: "Spin Dynamics - Basics of Nuclear Magnetic Resonance", M. H. Levitt (L)

Supplementary Text: "Protein NMR Spectroscopy, Principles & Practice"
J. Cavanagh, W. J. Fairbrother, A. G. Palmer III, N. J. Skelton. (C)

Friday Labs: The laboratory schedule on the following pages contains Friday laboratory session information specific to UGA. Check with the lead instructor at your university for information regarding your Friday lab sessions.

Final Exam: The exact date and time you take the final exam is determined by your university. The date and time given in the lecture schedule is for UGA only. Check with the instructor at your university for the date and time of your final exam.

Lecture Schedule

Date	Instructor	Topic	Suggested Reading
I. Introduction			
M 1/9	Prestegard	A. Magnetic properties of nuclei and electrons - precession	5-38 L*
W 1/11	Prestegard	B. RF pulses and spin relaxation - Bloch equations	39-50 L*, 653 L*
II. Instrumentation			
M 1/16		MLK Jr. Holiday (no class)	
W 1/18	Prestegard	A. Instrumental considerations - a look at probes	65-76L*
M 1/23	Prestegard	B. Fourier transform methods and data Processing	85-102 L*
III. NMR observables – Classical and Quantum Descriptions			
W 1/25	Prestegard	A. Scalar Couplings	217-223 L*
M 1/30	Prestegard	B. Chemical Shifts	195-206 L*
W 2/1	Prestegard	C. Introduction to a QM description of NMR	171 – 194 L*
M 2/6	Prestegard	D. Applications to second order spectra	615-623 L*
IV. Density Matrices and Product Operator Formalism			
W 2/8	Prestegard	A. Density Matrix – Evolution and interpretation	259-289 L*, 369-381 L*
M 2/13	Prestegard	B. Density matrix in Product Operator Form	381 – 405 L*
W 2/15	Prestegard	C. 2D Heteronuclear Correlation	105-113 L*, 436-443 L*, 410-447 C
M 2/20	Prestegard	D. COSY, TOCSY	409-418 L*, 492-506 L*
V. Basic Pulse Sequences			
W 2/22	Prestegard	A. Pulsed field gradients and extensions to 3D	649-652 L*, 114 L*
M 2/27	Urbauer	B. Triple resonance experiments for proteins	468-530 C
W 2/29	Urbauer	C. Sequential assignment strategies in proteins	533-543 C
M 3/5	Prestegard	D. Spin relaxation and NOEs	543-576 L*
W 3/7	Prestegard	E. Spin relaxation and TROSY	584-593 L*, 306-308 L*
VI. Assignment Strategies and Structure determination: proteins and nucleic acids			
M 3/12		Spring break – no class	
W 3/14		Spring break – no class	
M 3/19	Urbauer	C. Structure determination protocols	543-554 C
W 3/21	Germann	D. Homonuclear strategies for RNA and DNA	

M 3/26	Germann	E. Heteronuclear strategies for RNA and DNA	

VII. Advanced techniques for Structure and Dynamics

W 3/28	Prestegard	A. Dipolar Coupling and Solids NMR	211-217 L*
M 4/2	Prestegard	B. Residual Dipolar Coupling	443-454 L*
W 4/4	Prestegard	C. Paramagnetic effects	
M 4/9	Prestegard	D. Sensitivity enhancement by polarization transfer	
W 4/11	Prestegard	E. metabolomics and *in vivo* spectroscopy (MRS)	

VIII. Other Applications

M 4/16	Yang	A. Chemical Exchange and diffusion	515 – 524 L*
W 4/18	Yang	B. Protein folding and amide exchange	
M 4/23	Prestegard	C. A. A. Drug discovery, SAR by NMR, STD, Tr-NOEs	309-315 L*
W 4/25	Zhao	D. Imaging (MRI)	
M 4/30	Prestegard	E. Review and Misc. Topics	
W 5/2		**FINAL EXAM (8:00 – 11:00) UGA**	

Laboratory Schedule

Date	Instructor	Topic
F 1/13	Prestegard	Class Introduction and Computer set-up
F 1/20	Prestegard	Introduction to Computer Resources – LINUX Tutorial
F 1/27	Prestegard	Classical Simulations of NMR Experiments with PjNMR
F 2/3	Urbauer	Intro to data processing, weighting functions – MNova
F 2/10	Urbauer	Advanced data processing NMR PIPE Intro to Macros
F 2/17	Urbauer	Data display using NMR Draw
F 2/24	Prestegard	Simulation of second order spectra
F 3/2		**----- midterm exam - no lab session -------**
F 3/9	Prestegard	Introduction to a general analysis tool: Maple
F 3/16		Spring break – (no class)
F 3/23	Prestegard	Product Operator manipulations using Maple
F 3/30	Urbauer	Assignments using NMR View
F 4/6	Urbauer	Assignments using NMR View II
F 4/13	Prestegard	Analysis of RDCs - REDCAT
F 4/20	Urbauer	Structure Calculation with CNS
F 4/27	Urbauer	Structure Calculation with CNS II