

## BCMB / CHEM 8190 Biomolecular NMR

### GRADUATE COURSE OFFERING IN NUCLEAR MAGNETIC RESONANCE (Spring 2005)

"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 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 weekly 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 posted on the website near the beginning of each week and answers will appear near the end of the week. 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/BioNMR2005>

**Class Time:** M, W, F 10:10 - 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 teleconferencing room is in the South OISD building on Hooper Street (teleconference room). 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 (C128 in Life Sciences for UGA students).

**Instructors:**

UGA Instructors: James Prestegard, Jeffrey Urbauer

GA Tech Instructors: Les Gelbaum, Nicholas Hud

GSU Instructors: Jenny Yang, Markus Germann

Inquiries to Professor Prestegard - [jpresteg@ccrc.uga.edu](mailto: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
<b>I. Introduction</b>			
M 1/10	Prestegard	A. Magnetic properties of nuclei and electrons - precession	5-32 L
W 1/12	Prestegard	B. RF pulses and spin relaxation - Bloch equations	32-46 L, 626-627 L
<b>II. Instrumentation</b>			
M 1/17		MLK Jr. Holiday (no class)	
W 1/19	Urbauer	A. Instrumental considerations - a look at probes	72-87 L
M 1/24	Prestegard	B. Fourier transform methods and data Processing	89-122 L
<b>III. NMR observables – Classical and Quantum Descriptions</b>			
W 1/26	Prestegard	A. Spin operators and their time dependence	169 – 184 L
M 1/31	Urbauer	B. Scalar Couplings	211-216 L
W 2/2	Urbauer	C. Spin Relaxation and NOEs	226-236, 588-594 L
M 2/7	Prestegard	D. Chemical Shifts	192-200 L
<b>IV. Density Matrices and Product Operator Formalism</b>			
W 2/9	Prestegard	A. Density Matrix – Evolution and interpretation	344 – 355 L
M 2/14	Prestegard	B. Density matrix in Product Operator Form	355 – 356 L
W 2/16	Prestegard	C. RF pulses and Evolution	357 – 384 L
<b>V. Basic Pulse Sequences</b>			
M 2/21	Prestegard	A. Coherence transfer in COSY	388 – 398 L
W 2/23	Prestegard	B. Basic heteronuclear experiments INEPT and HSQC	418-434 L, 410-447 C
M 2/28	Prestegard	C. TOCSY and NOESY	543 – 569 L
W 3/2	Prestegard	D. Extension to 3D	447 – 467 C
F 3/4		----- Midterm -----	
<b>VI. Assignment Strategies: proteins and nucleic acids</b>			
M 3/7	Urbauer	A. Triple resonance experiments for proteins	468-530 C
W 3/9	Urbauer	B. Sequential assignment strategies in proteins	533-543 C
M 3/14		Spring Break (no class)	
W 3/16		Spring Break (no class)	
M 3/21	Germann	C. Homonuclear assignment strategies for RNA and DNA	
W 3/23	Germann	D. Heteronuclear assignment strategies for RNA and DNA	

## Lecture Schedule

Date	Instructor	Topic	Suggested Reading
<b>VII. Applications to Structure and Dynamics</b>			
M 3/28	Prestegard	A. Molecular motions in nucleic acids and proteins	
W 3/30	Prestegard	B. Dipolar Coupling in Solids	203-210 L
M 4/4	Prestegard	C. Residual Dipolar Coupling	425-432 L
W 4/6	Prestegard	D. Structure determination protocols	543-554 C
<b>VIII. Other Applications</b>			
M 4/11	Prestegard	A. Drug discovery, SAR by NMR, STD, Tr-NOEs	
W 4/13	Hud	B. Ion binding sites in macromolecules	
M 4/18	Hud	C. Bound waters in macromolecules	
W 4/20	Yang	D. Chemical Exchange Rates	
M 4/25	Yang	E. Protein folding, amide exchange rates	488 – 504 L
<b>IX. Advanced Techniques</b>			
W 4/27	Prestegard	A. Gradients, Imaging and Diffusion	
M 5/2	Prestegard	B. TROSY, Paramagnetic Effects	
F 5/6		<b>FINAL EXAM (8:00 – 11:00) UGA</b>	

## Laboratory Schedule

<b>Date</b>	<b>Instructor</b>	<b>Topic</b>
F 1/14	Staff	Introduction to Computer Resources – LINUX Tutorial
F 1/21	Staff	Classical Simulations of NMR Experiments with PjNMR
F 1/28	Urbauer	Intro to data processing, weighting functions – MestRe-C
F 2/4	Urbauer	Advanced data processing NMR PIPE Intro to Macros
F 2/11	Prestegard	Simulation of second order spectra (GAMMA)
F 2/18	Prestegard	Product Operators and Maple
F 2/25	Urbauer	Multidimensional processing NMR PIPE
F 3/4		----- <b>Midterm</b> ----- (no lab session)
F 3/ 11	Urbauer	Data display using NMR Draw
F 3/18		<b>Spring Break</b> (no lab session)
F 3/25	Urbauer	Assignments using NMR View
F 4/1	Urbauer	Assignments using NMR View II
F 4/8	Prestegard	Analysis of RDCs - REDCAT
F 4/15	Urbauer	Structure Calculation with CNS
F 4/22	Prestegard	Docking of Proteins and Ligands
F 4/29		Make-up Lab Session