Biomolecular NMR Spectroscopy

(*syllabus version 1.04, 6 January, 2020)

**subject to change at any time*

Offered cooperatively by the Georgia State University, the Georgia Institute of Technology, and the University of Georgia

course website: https://urbauerlab.uga.edu/8190

GRADUATE COURSE OFFERING IN NUCLEAR MAGNETIC RESONANCE

"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 material will focus on methods and experiments to address biomolecule structure and function. 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 4190/8189 (UGA course). Some previous exposure to elementary quantum mechanics and its applications in spectroscopy would also be useful, but not required, as we will attempt to provide sufficient background material to aid those who have not had this exposure.

Participating Institutions:

This course is taught with the cooperation of faculty at the Georgia State University (GSU), the Georgia Institute of Technology (Ga Tech), and the University of Georgia (UGA).

Course Reorganization: Rationale:

Past Course Organization: In past semesters, lectures, delivered via the internet, were broadcast to all participating students at all three institutions on Mondays and Wednesdays at 10:05 – 10:55 am (this time was a compromise given the different standard class start times at the three institutions). On Fridays, students at each institution participated in computer lab exercises, common to all institutions, at times and locations specific for their institutions. Lectures were recorded so that students could access them at any time on the website so that they could listen to them again, and the recordings could also be downloaded, then subsequently replayed without internet access.

That model suffered some significant drawbacks. First, despite the fact that the internet delivery of the lectures offered two-way communication between lecturers and the audience, which allowed students to ask questions in real time, the process of asking questions was cumbersome, and, due to instructors (lecturers) striving to cover as much material as completely as possible during the lectures, often there was no time for questions at the end. All too often, the lectures went over the allotted time. So, the opportunity to ask questions in real-time was thwarted. Finally, and as a result, that meant there was very little real interaction between students and lecturers.

That model did have some important advantages. Specifically, recording the lectures allowed students to listen to them as many times as they wanted, both online and offline, as pointed out above. This is a significant advantage to students.

Current Course Organization: The course has been reorganized in an attempt to keep the positive aspects of the previous design, and to minimize the drawbacks. Specifically, lectures will no longer be delivered “live”, but will only be delivered as pre-recorded videos. There will be no formal meeting of the class on Mondays, in recognition of the fact that students will be using this, or some equivalent time, to listen and study the video lectures assigned for the week. The video lectures assigned for each week will be approximately equal in time to two 50 minute lectures. Students will be expected to listen and study these lectures before the discussion session.

The discussion session will be held online, in much the same way that previous lectures were delivered. Initially, these will be held during the Wednesday time slot allotted for the course (10:05 – 10:55 am). These will not be lectures. These will be times for students to interact in real time with instructors or lecturers, to ask questions and get answers, to review material or concepts, and to exchange ideas. Once the semester gets going, it may be reasonable to reschedule this online discussion. In theory, it could be held any time, and it does not have to be held on Wednesday. For instance, if all the students at one institution prefer to have the discussion at 7:00 pm on Thursday evening, that can be arranged.

The Friday computer lab will remain unchanged.

Instructors:

UGA Instructors: Jeffrey Urbauer (urbauer@uga.edu, 706 542 7922)
GA Tech Instructors: Les Gelbaum
GSU Instructors: Jenny Yang, Markus Germann

Inquiries:

All inquiries to Professor Urbauer – urbauer@uga.edu, 706 542 7922)

Email Communication with Dr. Urbauer:

Dr. Urbauer encourages students to email or call him whenever there are questions or concerns. **All email communications should use only official GSU/GT/UGA email addresses/accounts**. Do not use Gmail, Yahoo mail, or any other unofficial accounts. If you do not receive a response within 24 hours, please try a reminder email. If you have an emergency, in addition to sending an email you should try to phone Dr. Urbauer or drop by his office.

Course Materials:

All lecture notes, pre-recorded lectures, lab tutorials and data will be available via the course website (link shown at the beginning of this document). These materials are for the sole use of the students enrolled in the course. They are not to be distributed in any way. Copies of notes and recordings may be downloaded to devices used by students enrolled in the course, but duplicates cannot be made or distributed in any way. The only exception regarding duplication is that students may print a copy of lecture notes for their personal use (and students may want to do this for exams, see below). Not abiding by these policies will constitute a breach of academic honesty policies.

Course Website:

The course website can be found at https://urbauerlab.uga.edu/8190 .

The main page gives information about the institutions and instructors. It also lists the recommended (but not required) text books. These books generally are expensive, so it is not recommended to purchase them all. However, the Levitt book (second edition, all are second editions) is offered as a softcover paperback, as is the Keeler book. The Cavanagh book can be viewed online by UGA students through the UGA libraries.

The ‘Lectures’ page shows the tentative course schedule, and includes links (all active) to lecture notes. As recorded lectures become available, the recordings will also be posted. The lectures that will be covered each week are indicated at the left. For instance, there is only one lecture for week one (week of 1/6), but two for week two (week of 1/13). Week three is a short week due to the Martin Luther King Jr. Holiday, so there is only one lecture (week of 1/20) for that week, but two for most of the remaining weeks of the semester. Suggested readings from the books that coincide with the lectures are noted on the right (the ‘L’, ‘C’, and ‘K’ letters correspond to the Levitt, Cavanagh, and Keeler texts). At the top of the ‘Lectures’ page are also links to the Blackboard Collaborate Ultra Classroom login link (see below), and to the course syllabus (this document).

On the ‘Problem Sets’ page there are problem sets posted, but not answers. Students can begin to attempt to work the problems without the answers, then the answers will be posted so students can check their answers. Answers will be posted regularly.

The ‘Notices’ tab will ordinarily not be used. Most communication will be via email.

The ‘Links’ section currently includes a single link to an interesting ‘NMR Periodic Table’, which is useful as a reference for the NMR/magnetic properties of NMR active nuclei.

The ‘Labs’ link shows the timing of the individual labs, and the tutorials and data for the exercises are posted there and can be downloaded. The date of the midterm exam is also posted there.

Blackboard Collaborate Ultra Classroom:

For the online discussions, the Blackboard Collaborate Ultra Classroom real-time video conferencing tool will be used, as it was the last time the course was held. The link to the ‘Guest’ login, which all students will use to log into the session, is shown at the top of the page under the ‘Lectures’ page of the course website. The actual link is shown here:

https://us.bbcollab.com/collab/ui/session/guest/fa209a294fd04d4498d5d9c872e98075

This will allow users to join the ‘biomolecular-nmr-2020’ session, which will be used for the online discussions. ***For best results use the Chrome Browser***. Other browsers are not necessarily supported.

Texts:

There are no required texts. Readings will be suggested from the following texts:

- "Spin Dynamics - Basics of Nuclear Magnetic Resonance, 2nd edition"
  M. H. Levitt

- "Protein NMR Spectroscopy, Principles & Practice, 2nd edition"
  J. Cavanagh, W. J. Fairbrother, A. G. Palmer III, N. J. Skelton.

- “Understanding NMR Spectroscopy, 2nd edition”
  James Keeler

Lectures:

The first part of the course will focus on fundamentals of NMR. Topics will include:

- magnetic properties of nuclei and electrons
- instrumental considerations
- scalar couplings and chemical shifts
- second order spectra
- heteronuclear/homonuclear correlation
- triple resonance methods for proteins
- spin relaxation and NOE
- rf pulses and spin relaxation
- Fourier transform methods / data processing
- quantum mechanical description of NMR
- density matrix and product operators
- pulsed field gradients
- sequential assignments for proteins
- residual dipolar couplings

The second part of the course will focus on applications. Potential topics will include:

- spin relaxation in proteins
- chemical exchange and diffusion
- structure determination protocols
- *in vivo* spectroscopy (MRS)
- drug discovery
- solids NMR
- NMR of RNA and DNA
- protein folding and amide exchange
- imaging (MRI)
- sensitivity enhancement / polarization transfer
- paramagnetic effects

Labs:

Lab exercises will include the following:

- using UNIX/LINUX
- data processing/analysis with MNova
- data display with NMR Draw
- productor operator manipulations with Maple
- NMR assignments with NMRView
- ligand docking with HADDOCK
- NMR simulations with PjNMR
- data processing/analysis with NMR Pipe
- introduction to Maple, a general analysis tool
- REDCAT analysis of residual dipolar couplings
- structure calculations with CNS

Grading:

There will be a midterm exam on Friday, February 28 (this date is also posted on the 'Labs' page of the website). Students will have a normal class period (50 minutes) to answer this exam.

There will be a comprehensive final exam. Students will have three hours to answer the exam. The time and location of the exam will be dictated by the standard final exam schedules at the individual institutions.

The midterm will count 25% towards the overall course grade. The final exam will count 75% towards the overall course grade.

All exams are open-book, open-note. Students can bring whatever books or notes they wish to exams. Each student should also bring a hand-held calculator to the exam periods, as a calculator will be necessary for answering some of the questions. Otherwise, NO other electronic devices are allowed during the exam (no laptops, no phones, no iWatches or equivalent, no iPads or equivalent, etcetera). Students can bring hard copies of lecture notes, but will not have access to electronic copies during the exam. Students will NOT have access to the internet during exams.