

# Biomolecular NMR Spectroscopy

(\*syllabus version 2.03, 18 January, 2022)

*\*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 (lectures): 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 (lectures): The lecture component of 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.

For the discussion session, students at each participant institution will meet together, in person, with communication between institutions using 'Zoom' (see below). The time, day of the week, and location of these discussion sessions will be decided by the students in the class during the organizational meeting at the beginning of the semester. These discussion sessions 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 discussion. In theory, it could be held any time, and it does not have to be held on Wednesday. For example, if all the students at one institution prefer to have the discussion at 7:00 pm on Thursday evening, that can be arranged.

*Past Course Organization (lab sessions):* In the past, on Fridays, students at each institution participated in computer lab exercises, common to all institutions, at times and locations specific for their institutions. At each institution, students and instructors met together in person in dedicated university computer labs to perform the tutorials using university computers with pre-installed software packages.

That model suffered some significant drawbacks. The lab sessions were mostly limited to the 50 minute timeslot allotted for the course, and often the tutorials would take longer than that time. It was difficult to access the computer labs at other times due to use by other courses. Sometimes, the software or computers would fail in some way, and often only authorized IT personnel were allowed to make the necessary fixes. There were other issues related to software installation and computer access as well.

The most significant advantage of the previous model was the direct weekly interactions with other students and instructors in the context of the computer lab.

*Current Course Organization (lab sessions):* The lab component of the course has been reorganized in an attempt to keep the positive aspects of the previous design, and to minimize the drawbacks. Instead of university computer labs and resources, students are encouraged to use their own computers or computers in their research labs that they have permissions to install software on. This eliminates the time restrictions of dedicated university computer labs and it eliminates the inherent limitations of requiring IT personnel. Furthermore, most of the software that will be used is accessed via the NMRBox resource, and it is free. Students get all of the advantages of the NMRBox resource, which are significant, and which may prove beneficial for their research efforts. Detailed tutorials both for software installation, NMRBox account setup, and software use have been written and tested. Students can work on these alone or in groups, and they can get assistance from instructors as needed, both in person and virtual.

#### **Instructors:**

UGA Instructors: Jeffrey Urbauer ([urbauer@uga.edu](mailto:urbauer@uga.edu), 706 542 7922)

GA Tech Instructors: Les Gelbaum (Emeritus)

GSU Instructors: Markus Germann, Jenny Yang

#### **Enquiries:**

All enquiries to Professor Urbauer ([urbauer@uga.edu](mailto: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 at the number listed above.

## 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 to lecture notes and recorded lectures. Typically there are two lectures per week. 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 is also a link to the course syllabus (this document).

On the 'Problem Sets' page there are problem sets posted, as well as answers to the problems. Students are advised to attempt the problems without the answers, and only consult the answers when necessary and to check their answers.

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

The 'Links' section currently only includes a few links, one 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.

## Class Discussions:

We anticipate that, as in years past, students and instructors at each participant institution will convene in person for class. Communication between institutions will use 'Zoom' as the platform for these communications and online discussions. In the past, we used the Blackboard Collaborate Ultra Classroom real-time video conferencing tool, which was freely available through UGA, but now no longer exists. A permanent 'Zoom' link will be generated for the course and will be distributed via email (will NOT be posted on the website for security purposes). Please keep in mind that the preferred browser is the Chrome browser, and, in fact, other browsers are not necessarily supported and may not work properly or at all.

## Texts:

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

- "Spin Dynamics - Basics of Nuclear Magnetic Resonance, 2<sup>nd</sup> edition"  
M. H. Levitt
- "Protein NMR Spectroscopy, Principles & Practice, 2<sup>nd</sup> edition"  
J. Cavanagh, W. J. Fairbrother, A. G. Palmer III, N. J. Skelton.
- "Understanding NMR Spectroscopy, 2<sup>nd</sup> 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
- product operator manipulations with Maple
- NMR assignments with NMRFAM-Sparky
- 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 (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.

**GENERAL POLICIES:**

The following policies, although written for UGA students, apply to all students, with adjustments specific for the students' institutions.

**ACADEMIC HONESTY POLICY:**

As a University of Georgia student, you have agreed to abide by the University's academic honesty policy, "A Culture of Honesty," and the Student Honor Code. All academic work must meet the standards described in "A Culture of Honesty" found at:

[https://honesty.uga.edu/resources/documents/academic\\_honesty\\_policy\\_2017.pdf](https://honesty.uga.edu/resources/documents/academic_honesty_policy_2017.pdf)

Lack of knowledge of the academic honesty policy is not a reasonable explanation for a violation. Questions related to course assignments and the academic honesty policy should be directed to the instructor.

*UGA Student Honor Code: "I will be academically honest in all of my academic work and will not tolerate academic dishonesty of others." A Culture of Honesty, the University's policy and procedures for handling cases of suspected dishonesty, can be found at [www.uga.edu/ovpi](http://www.uga.edu/ovpi). Every course syllabus should include the instructor's expectations related to academic honesty.*

**ACCESSIBILITY STATEMENT:**

*If you anticipate issues related to the format or requirements of this course, please meet with Professor Urbauer, who will discuss with you ways to ensure your full participation in the course. If formal, disability-related accommodations are necessary, it is very important that you be registered with the Disability Resource Center (Voice: 706-542-8719 or TTY: 706-542-8778) and notify Professor Urbauer of your eligibility for reasonable accommodations. A plan to best coordinate your accommodations can then be developed. The website for the disability resource center can be found at: <https://drc.uga.edu>*

**FERPA NOTICE:**

The Federal Family Educational Rights and Privacy Act (FERPA) grants students certain information privacy rights. See the registrar's explanation at: <https://apps.reg.uga.edu/FERPA/>

**UGA NON-DISCRIMINATION AND ANTI-HARASSMENT POLICY:**

The University of Georgia ("the University") is committed to maintaining a fair and respectful environment for living, work and study. To that end, and in accordance with federal and state law, University System of Georgia policy, and University policy, the University prohibits harassment of or discrimination against any person because of race, color, sex (including sexual harassment and pregnancy), sexual orientation, gender identity, ethnicity or national origin, religion, age, genetic information, disability, or veteran status by any member of the University Community (as defined below) on campus, in connection with a University program or activity, or in a manner that creates a hostile environment for any member of the University Community. Incidents of harassment and discrimination will be met with appropriate disciplinary action, up to and including dismissal or expulsion from the University. The full policy can be found at: <https://eoo.uga.edu/policies/non-discrimination-anti-harassment-policy>

**CAMPUS CARRY (HOUSE BILL 280, "HB280"):**

For information about House Bill 280, commonly known as the "campus carry" legislation, which became effective July 1, 2017, please refer to information and guidance provided by the University System of Georgia at: <http://www.usg.edu/hb280>

Students are free to contact the UGA Police Department concerning the enforcement of HB280.

**MENTAL HEALTH AND WELLNESS RESOURCES:**

- *If you or someone you know needs assistance, you are encouraged to contact Student Care and Outreach in the Division of Student Affairs at 706-542-7774 or visit <https://sco.uga.edu>. They will help you navigate any difficult circumstances you may be facing by connecting you with the appropriate resources or services.*
- *UGA has several resources for a student seeking mental health services (<https://www.uhs.uga.edu/bewelluga/bewelluga>) or crisis support (<https://www.uhs.uga.edu/info/emergencies>).*
- *If you need help managing stress anxiety, relationships, etc., please visit BeWellUGA (<https://www.uhs.uga.edu/bewelluga/bewelluga>) for a list of FREE workshops, classes,*

*mentoring, and health coaching led by licensed clinicians and health educators in the University Health Center.*

- *Additional resources can be accessed through the UGA App.*

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## **CORONAVIRUS INFORMATION FOR STUDENTS**

**UGA adheres to guidance from the University System of Georgia and the recommendations from Georgia Department of Public Health (DPH) related to quarantine and isolation. Since this may be updated periodically, we encourage you to review the latest guidance [here](#). The following information is based on guidance last updated on December 29, 2021.**

### **Face coverings:**

Following guidance from the University System of Georgia, face coverings are recommended for all individuals while inside campus facilities.

### **How can I obtain the COVID-19 vaccine?**

University Health Center is scheduling appointments for students through the UHC Patient Portal ([https://patientportal.uhs.uga.edu/login\\_dualauthentication.aspx](https://patientportal.uhs.uga.edu/login_dualauthentication.aspx)). Learn more here – <https://www.uhs.uga.edu/healthtopics/covid-vaccine>.

The Georgia Department of Health, pharmacy chains and local providers also offer the COVID-19 vaccine at no cost to you. To find a COVID-19 vaccination location near you, please go to: <https://georgia.gov/covid-vaccine>.

In addition, the University System of Georgia has made COVID-19 vaccines available at 15 campuses statewide and you can locate one here: <https://www.usg.edu/vaccination>

### **What do I do if I have COVID-19 symptoms?**

Students showing COVID-19 symptoms should self-isolate and get tested. You can schedule an appointment with the University Health Center by calling 706-542-1162 (Monday-Friday, 8 a.m.-5p.m.). Please DO NOT walk-in. For emergencies and after-hours care, see <https://www.uhs.uga.edu/info/emergencies>.

### **What do I do if I test positive for COVID-19? (Isolation guidance)**

If you test positive for COVID-19 at any time, either through a PCR test, an Antigen test, or a home test kit, you are **required to report it** through the [DawgCheck Test Reporting Survey](#). Follow the instructions provided to you when you report your positive test result in DawgCheck.

As of December 29, 2021, when an individual receive a positive COVID-19 test: Everyone, **regardless of vaccination status**, should:

- Stay home for 5 days.
- If you have symptoms or your symptoms are resolving after 5 days, you can leave your house and return to class.
- Continue to wear a mask around others for 5 additional days.

### **What do I do if I have been exposed to COVID-19? (Quarantine guidance)**

If you have been exposed (within 6 feet for a cumulative total of 15 minutes or more over a 24-hour period – unmasked\*\*) to someone with COVID-19 or to someone with a positive COVID-19 test and you are:

- Boosted, or have become fully vaccinated within the last 6 months (Moderna or Pfizer vaccine) or within the last 2 months (J&J vaccine)
  - You do not need to quarantine at home and may come to class.
  - You should wear a mask around others for 10 days.
  - If possible, get tested on day 5.
  - If you develop symptoms, get tested and isolate at home until test results are received, then proceed in accordance with the test results.
- Unvaccinated, or became fully vaccinated more than 6 months ago (Moderna or Pfizer vaccine) or more than 2 months ago (J&J vaccine) and have not received a booster:
  - You must quarantine at home for 5 days. After that you may return to class but continue to wear a mask around others for 5 additional days.
  - If possible, get tested on day 5.
  - If you develop symptoms, get tested and isolate at home until test results are received, then proceed in accordance with the test results.

\*\* “Masked-to-masked” encounters are not currently considered an exposure; this type of interaction would not warrant quarantine.

You should report the need to quarantine on [DawgCheck](https://dawgcheck.uga.edu/) (<https://dawgcheck.uga.edu/>), and communicate directly with your faculty to coordinate your coursework while in quarantine. If you need additional help, reach out to Student Care and Outreach ([sco@uga.edu](mailto:sco@uga.edu)) for assistance.

### **Well-being, mental health, and student support**

If you or someone you know needs assistance, you are encouraged to contact Student Care & Outreach in the Division of Student Affairs at 706-542-7774 or visit <https://sco.uga.edu/>. They will help you navigate any difficult circumstances you may be facing by connecting you with the appropriate resources or services. UGA has several resources to support your well-being and mental health: <https://well-being.uga.edu/>

Counseling and Psychiatric Services (CAPS) is your go-to, on-campus resource for emotional, social and behavioral-health support: <https://caps.uga.edu/>, TAO Online Support (<https://caps.uga.edu/tao/>), 24/7 support at 706-542-2273. For crisis support: <https://healthcenter.uga.edu/emergencies/>.

The University Health Center offers FREE workshops, classes, mentoring and health coaching led by licensed clinicians or health educators: <https://healthcenter.uga.edu/bewelluga/>

### **Monitoring conditions:**

Note that the guidance referenced in this syllabus is subject to change based on recommendations from the Georgia Department of Public Health, the University System of Georgia, or the Governor’s Office. For the latest on UGA policy, you can visit [coronavirus.uga.edu](https://coronavirus.uga.edu).