

**CHEM 8853 - Special Topics in Biochemistry**  
**“Practical Biomolecular NMR Spectroscopy”**  
**Fall 2024**  
**Course Syllabus**

**COURSE MEETING TIME/PLACE**

Time: Monday/Wednesday/Friday (MWF) 8:25 - 9:15 am

Place: Cherry Emerson 320

Dates: August 19th, 2024 – December 12th, 2024

**COURSE DESCRIPTION**

This is a Special Topics in Biochemistry course where you will develop mastery in the nomenclature, theory, and practical application of Nuclear Magnetic Resonance (NMR) for small molecules, peptides, proteins, and other biomolecules (*i.e.*, with a biomolecular focus). You will learn state-of-the-art experimental techniques used in modern NMR research. The subject matter is intended to provide you with a foundational understanding of core NMR concepts as well as practical experience with analyzing NMR data. You will earn 3.0 credits from successful completion of this course. Learning objectives will be outlined at the start of each lecture. Lecture slides will be provided for each lecture (ideally before the lecture so you can take notes as needed).

NMR can be overwhelming since it applies fundamental concepts from several disciplines (chemistry, biology, physics). In addition, the material contains *a lot* of nomenclature in addition to practical problem solving. Don't panic! Come to lectures, take notes, review material often, complete practical labs, use the provided study guides, and use supplemental learning sources (*i.e.*, textbooks, YouTube videos). You might need to investigate different ways of studying (*i.e.*, flash cards). We are always available to help you and we will provide resources to help you succeed. Make friends and study in groups when possible. We aim to make learning NMR interesting, practical, and fun to help hold your attention in the material.

**PREREQUISITES**

It is recommended that you have taken college-level Chemistry, Biology, and Organic Chemistry courses previously. Note that these classes are not a strict prerequisite for CHEM 8853, but you may find yourself lost during some sections if you haven't taken them. We will do our best to provide refreshers and summary material related to these subjects, such that everyone is on the same page for learning biochemistry. If you have concerns about your past experiences or past courses taken, please talk to us. Most likely you will be fine. You will also need to know basic Unix/SHELL (bash, csh) but we can help if needed.

**INSTRUCTOR(S)**

**Primary Instructor:** Andrew McShan, Ph.D.

Pronouns: They/them

Assistant Professor

School of Chemistry and Biochemistry

E-mail: andrew.mcshan@chemistry.gatech.edu

Website: <http://mcshanlab.com/>

Office Location: Molecular Sciences and Engineering Building (MoSE) G022

901 Atlantic Dr NW, Atlanta, GA 30318

My office is located on the *ground floor of MoSE near the G021 lecture hall*

Office Hours: Upon e-mail request.

**Guest Instructor:** Anant Paravastu, Ph.D.

Pronouns: He/him

Associate Professor

School of Chemical and Biomolecular Engineering

E-mail: anant.paravastu@chbe.gatech.edu

**Guest Instructor:** Johannes (Hanno) Leisen, Ph.D.

Pronouns: He/him

Principal Research Scientist, Director for Solid-State NMR

School of Chemistry and Biochemistry

E-mail: johannes.leisen@chemistry.gatech.edu

**Guest Instructor:** Hongwei Wu, Ph.D.

Pronouns: He/him

Senior Research Scientist, Director for Solution NMR

School of Chemistry and Biochemistry

E-mail: hongwei.wu@chemistry.gatech.edu

### Teaching Assistants (TAs)

None for CHEM 8853

### COURSE MATERIALS

You will not need to purchase a textbook for this course. We will provide all material needed. However, a textbook might be a helpful supplement for you in which case we recommend:

#### Protein NMR Spectroscopy: Principles and Practice

Arthur G. Palmer III, Wayne J. Fairbrother, John Cavanagh, Nicholas J. Skelton, Mark Rance

ISBN-13 978-0121644918

<https://www.amazon.com/Protein-NMR-Spectroscopy-Principles-Practice/dp/012164491X>

#### Understanding NMR Spectroscopy

James Keeler

ISBN-13 978-0470746080

<https://www.amazon.com/Understanding-Spectroscopy-Second-James-Keeler/dp/0470746084>

#### Fundamentals of Protein NMR Spectroscopy

Gordon S. Rule, T. Kevin Hitchens

ISBN-13 978-1402034992

<https://www.amazon.com/Fundamentals-Protein-Spectroscopy-Structural-Biology/dp/1402034997>

#### Required Software:

NMRBox (free account)

<https://nmrbox.nmrhub.org/pages/getting-started>

VNCViewer (free, no account needed)

<https://www.realvnc.com/en/connect/download/viewer/>

+ other webservers mentioned in the practical labs.

### CANVAS PAGE (COURSE WEBSITE)

Canvas will include lecture slides, study guides, course materials, and relevant course updates. Check often!

### FINAL GRADES

A = 100 - 90%

B = 89.9 - 80%

C = 79.9 - 70%

D = 69.9 - 50%

F = < 50%

Assignments and grades *will not* be curved.

### EVALUATION CRITERIA

Item	Total Number of Points * 100	Percent of Final Grade (100%)
Attendance	42/42	55%
Practical Labs	800/800	45%

**I. Attendance – 42/42 points, 55% of final grade**

Lecture attendance is required for this course and will count towards your final grade. Each attended lecture is worth 1 point for a total of 42 points throughout the semester. Attendance will contribute to the final grade with the formula:  $42/42 * 100 * 0.55$ . If you cannot attend class for any reason (for example, illness, conference, research related meeting, etc.), please e-mail Dr. McShan for an excused absence ASAP *before* that class.

**II. Practical Lab – 800/800 points, 45% of final grade**

There will be eight (8) practical lab assignments given throughout the semester. Practical lab assignments will include a hands-on activity or worksheet to be completed using freely available software. Detailed descriptions of each practical lab assignments will be uploaded to Canvas, and you will receive guidance in class. You will also submit practical lab assignment answers via Canvas. Practical lab assignments will be graded for both accuracy and completeness. Each practical lab is worth 100 points each for a total of 800 throughout the semester. Practical labs will contribute to the final grade with the formula:  $800/800 * 100 * 0.45$ . Due dates will be noted on Canvas. You will be working in assigned groups for practical labs (just don't copy each other's answers or descriptions for submission).

**COURSE OUTLINE (SUBJECT TO CHANGE)**

Lecture	Date(s)	Topic(s)	Instructor
1	M Aug 19	Introduction to NMR Part 1 nuclear spin, magnetic properties of atomic nuclei, nuclear precession, Boltzmann distribution	McShan
2	W Aug 21	Introduction to NMR Part 2 radiofrequency fields, vector model, Larmor frequency, free induction decay	McShan
3	F Aug 23	Anatomy of modern NMR Spectrometer	McShan
4	M Aug 26	The chemical shift	McShan
5	W Aug 28	Dipolar interactions, Scalar couplings, Chemical shift anisotropy	McShan
6	F Aug 30	Relaxation (T1, T2); Solomon/Bloch Equations	McShan
	M Sept 2	NO CLASS - HOLIDAY	
7	W Sept 4	How to acquire NMR data TopSpin / NMR acquisition parameters	McShan
8	F Sept 6	NMR pulse sequence elements Part 1 hard pulse, soft/shape pulse, gradients, water suppression	McShan
9	M Sept 9	NMR pulse sequence elements Part 2 coherence transfer, coherence selection	McShan
10	W Sept 11	1D NMR <sup>1</sup> H, <sup>13</sup> C, Fourier transform	McShan
11	F Sept 13	2D NMR homonuclear; heteronuclear - COSY, HMBC, HMQC, TOCSY, NOESY, HSQC	McShan
12	M Sept 16	2D NMR homonuclear; heteronuclear - COSY, HMBC, HMQC, TOCSY, NOESY, HSQC	McShan
13	W Sept 18	NMR processing and analysis NMRBox, nmrPipe, SPARKY	McShan
14	F Sept 20	<b>Practical Lab 1: Determine the identity of small molecule X</b>	McShan/Wu
15	M Sept 23	Restraints for structure calculations Chemical shifts, NOEs, RDCs, PREs, PCSs	McShan
16	W Sept 25	Software for structure calculations CYANA, CS-Rosetta	McShan
17	F Sept 27	<b>Practical Lab 2: Assign peptide X</b>	McShan/Wu

18	M Sept 30	<b>Practical Lab 2:</b> Assign peptide X	McShan/Wu McShan/Wu
19	W Oct 2	<b>Practical Lab 3:</b> 3D structure calculation for peptide X	McShan/Wu
20	F Oct 4	<b>Practical Lab 3:</b> 3D structure calculation for peptide X	McShan/Wu
21	M Oct 7	Preparation of NMR labeled biomolecules - Isotopic labeling	McShan
22	W Oct 9	Preparation of NMR labeled biomolecules - Isotopic labeling	McShan
23	F Oct 11	nD NMR NUS, HNCA, HNCB, HNCB, etc	McShan
	M Oct 14	NO CLASS - HOLIDAY	
24	W Oct 16	nD NMR NUS, HNCA, HNCB, HNCB, etc	McShan
25	F Oct 18	<b>Practical Lab 4:</b> Assign a protein - Protein X	McShan/Wu
26	M Oct 21	<b>Practical Lab 4:</b> Assign a protein - Protein X	McShan/Wu
27	W Oct 23	<b>Practical Lab 5:</b> 3D structure calculations of Protein X	McShan/Wu
28	F Oct 25	<b>Practical Lab 5:</b> 3D structure calculations of Protein X	McShan/Wu
29	M Oct 28	Other biomolecules – Nucleic acids, lipids, carbohydrates	McShan
30	W Oct 30	Other biomolecules – Nucleic acids, lipids, carbohydrates	McShan
31	F Nov 1	NMR titrations	McShan
32	M Nov 4	Ligand binding WaterLOGSY, Saturation Transfer Difference	McShan
33	W Nov 6	<b>Practical Lab 6:</b> Determine dissociation constant/off-rates from NMR titration with TITAN	McShan/Wu
34	F Nov 8	Chemical exchange / Dynamics Timescales, T1/T2/HetNOE, Order parameter, CEST, CPMG	McShan
35	M Nov 11	<b>Practical Lab 7:</b> Analyze dynamics (order parameters, etc) of a protein	McShan/Wu
36	W Nov 13	Metabolomics	Leisen
37	F Nov 15	Diffusion Ordered Spectroscopy (DOSY)	Leisen
38	M Nov 18	Solid-state NMR Chemical shift anisotropy - Dipolar Interactions - Quadrupolar interactions - Magic angle spinning - Cross Polarization	Paravastu
39	W Nov 20	Solid-state NMR Chemical shift anisotropy - Dipolar Interactions - Quadrupolar interactions - Magic angle spinning - Cross Polarization	Paravastu
40	F Nov 22	<b>Practical Lab 8:</b> Analyze ssNMR data of a peptide	Leisen/Paravastu
41	M Nov 25	Magnetic Resonance Imaging Part 1	Leisen
	W Nov 27	NO CLASS - HOLIDAY	
	F Nov 29	NO CLASS - HOLIDAY	
42	M Dec 2	Magnetic Resonance Imaging Part 2	Leisen
		NO FINAL EXAM	

### STATEMENT OF INTENT FOR DIVERSITY, EQUITY, AND INCLUSIVITY

We are committed to creating a learning environment for students that supports a diversity of thoughts, perspectives and experiences that honors your cultural and social identities (including race, gender, class, sexuality, religion, or ability).

To help accomplish this:

- If you have a name and/or set of pronouns that differ from those that appear in your official Georgia Tech records, please let us know. If we pronounce your name wrong, please correct us (we want to do better).
- If you feel like your performance in the class is being impacted by your experiences outside of class, please don't hesitate to talk to us (if you feel comfortable doing so). We will do our best to point you in the direction to get help.
- If something was said by anyone in class (including the instructors) that made you feel uncomfortable, please feel free to bring it up. Anonymous feedback is always an option (see: <https://www.gatech.edu/accountability>).

Finally, in an ideal world, science would be objective and inclusive. However, much of science is subjective and is historically built on a small subset of privileged voices. We acknowledge that the readings and content for this course were primarily authored in the main by cisgendered white men. We will attempt to highlight the critical contributions and voices in science beyond this.

### ACADEMIC INTEGRITY

All course content is subject to the Georgia Institute of Technology's academic honor code: <https://policylibrary.gatech.edu/student-affairs/academic-honor-code>. Georgia Tech aims to cultivate a community based on trust, academic integrity, and honor. Students are expected to act according to the highest ethical standards. Any student suspected of cheating or plagiarizing an assignment or exam will be reported to the Office of Student Integrity, who will investigate the incident and identify the appropriate penalty for violations.

*The use of AI-powered language models (i.e., ChatGPT or related) is strictly prohibited in this course.*

### ACCOMMODATIONS FOR STUDENTS WITH DISABILITIES

If you are a student with disabilities that needs that require special accommodation, please contact me to discuss your needs. Also, contact the Office of Disability Services at (404) 894-2563 or <http://disabilityservices.gatech.edu/>, as soon as possible, to make an appointment to discuss your needs and to obtain an accommodation letter.

### CAMPUS RESOURCES FOR LEARNING

In your time at Georgia Tech, you may find yourself in need of support academic or emotional support. I am always available to you. However, a summary of additional resources for Georgia Tech students is available at <https://catalog.gatech.edu/academics/academic-resources/> and <https://grad.gatech.edu/resources>.

### CAMPUS RESOURCES FOR MENTAL HEALTH

The Center for Mental Health Care & Resources (<https://mentalhealth.gatech.edu/>) is here to offer confidential support and services to students in need of mental health care. During regular business hours, students who are not actively in counseling may **call 404-894-2575** or **walk-in to the office** located on the first floor, Suite 102B Smithgall Student Services Building, 353 Ferst DR NW Atlanta GA 30313 (Flag building next to the Student Center). Any time outside of business hours, students may **call 404-894-2575** and select the option to speak to the after-hours counselor.

### SPECIFIC RESOURCES

- Center for Academic Success <http://success.gatech.edu>
  - 1-to-1 tutoring <https://tutoring.gatech.edu/tutoring/>
  - Peer-Led Undergraduate Study (PLUS) <https://tutoring.gatech.edu/plus-sessions/>
  - Academic coaching <https://advising.gatech.edu/academic-coaching>
- OMED: Educational Services (<http://omed.gatech.edu/programs/academic-support>)
  - Group study sessions and tutoring programs
- Individualized help with writing and multimedia projects: Communication Center (<http://www.communicationcenter.gatech.edu>)
- Academic advisors for your major <http://advising.gatech.edu/>
- The Office of the Dean of Students: <https://studentlife.gatech.edu/content/get-help-now>; **404-894-6367**; Smithgall Student Services Building 2<sup>nd</sup> floor
  - You also may request assistance at [https://gatech-advocate.symplicity.com/care\\_report/index.php/pid383662?](https://gatech-advocate.symplicity.com/care_report/index.php/pid383662?)
- Center for Assessment, Referral and Education (CARE) **404-894-3498**; <https://care.gatech.edu/>
  - Smithgall Student Services Building 1<sup>st</sup> floor
  - A single point of entry through which students can access mental health resources and services on campus and in the community. Students seeking assistance from the Counseling Center or Stamps Psychiatry need to visit CARE first for a primary assessment and referral to on and off campus mental health and well-being resources.
  - *Students in crisis may walk in during business hours (8am-4pm, Monday through Friday) or contact the counselor on call after hours at 404-894-2575 or 404-894-3498. Other crisis resources: <https://counseling.gatech.edu/content/students-crisis>*

- Students' Temporary Assistance and Resources (STAR): <https://studentlife.gatech.edu/content/star-services>
  - Can assist with interview clothing, food, and housing needs.
- Stamps Health Services: <https://health.gatech.edu>; 404-894-1420
  - Primary care, pharmacy, women's health, psychiatry, immunization and allergy, health promotion, and nutrition
- OMED: Educational Services: <http://www.omed.gatech.edu>
- Women's Resource Center: <http://www.womenscenter.gatech.edu>; 404-385-0230
- LGBTQIA Resource Center: <http://lgbtqia.gatech.edu/>; 404-385-2679
- Veteran's Resource Center: <http://veterans.gatech.edu/>; 404-385-2067
- Georgia Tech Police: 404-894-2500; <http://www.police.gatech.edu>