CHE 512B: NMR in Life Sciences (Spring 2018)

Monday, Wednesday, Friday 11.00 AM - 11.50 AM, Talbert Hall 112

Instructor: Prof. Thomas Szyperski, 816 NSC
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Office hours: Thursday 2-3 PM and by appointment

Course Description:

***Objectives*:**

A one semester (three credit hours) advanced physical chemistry lecture course focusing on NMR spectroscopy and biophysical techniques in life science.

***Learning outcomes*:**

Upon completion of this course, students will

1) have an understanding of basic and advanced theory of Fourier Transform NMR spectroscopy and related data processing;

2) will be familiar with the concepts of multi-dimensional NMR experiments and their applications;

3) have an understanding of various important biophysical techniques in life science;

4) be acquainted with principles governing protein folding.

Course requirements:

CHE 512 is a *controlled enrollment course* and is restricted by the available student positions.

***Academic content*:**

Lectures, Reading, Homework

Presentation of course material:

The instructor will mostly use the black board / overhead projector to present the course material using his own notes. This shall ensure that the students can follow how equations are derived and have sufficient time to take their own notes while the material is presented. The lecture notes will define the scope of the exams: all questions can be answered with the knowledge and understanding of the material presented by the instructor. Students are expected to study the corresponding textbook chapters / material provided not only in preparation of each lecture but also after each lecture to further improve understanding of the material.

***Grading and academic policies*:**

Grading. Two in class exams of 90 minutes duration (each contributing 33% to the total score) and a student's presentation of a scientific publication (20 minutes duration; 33% of total score) will be the basis for grading. Each of the two exams covers the material indicated in the schedule below. The scientific publication chosen for the presentation needs to be (i) related to the topics covered in this class and (ii) approved by the instructor.

There is *no final exam* after the last day of classes.

For each exam, you are allowed to bring one *hand-written* U.S. letter sized 'equation sheet' and a pocket calculator (calculators of cell phones are not permitted). The equation sheet must not contain sentences or graphs. You will have to hand in the page with your notes along with the exam. If any sentences or graphs are on the sheet, questions related to these notes will receive no points. The equation sheet must *not* contain labels, words, sentences, explanations, pictures, diagrams, or graphs. You will have to hand in the page with your notes along with the exam. If any labels, words, sentences, explanations, pictures, diagrams, or graphs are found on the sheet, questions related to these notes will receive no points

Make–up exams may be taken only in cases of exceptional urgency (medical emergencies, car accidents on the way to the campus, etc.) and you need to provide proper documentation (letter from your physician, police report, etc.). Otherwise do not ask to take a make–up exam — we cannot make any exceptions out of fairness to the other students.

Homework Assignments: Homework will be selected by the lecturer and emailed after to students once a week. Homework will ne be graded. However, homework will be briefly discussed in class and the lecturer will select students to present / comment on the solutions of the homework exercises.

For *incomplete grade* policies, see
http://undergrad-catalog.buffalo.edu/policies/grading/explanation.shtml#incomplete

Academic integrity as defined in UB's guidelines will be strictly enforced. Make sure you know what is meant by "academic integrity" according to these guidelines. See
http://undergradcatalog.buffalo.edu/policies/course/integrity.shtml

Accessibility Resources. See http://www.buffalo.edu/accessibility/resources.php for information about UB's Accessibility Resource Office.

Intellectual property: Course materials that I (Prof. Thomas Szyperski) have prepared, together with the content of all lectures and materials presented and prepared by me in this course, are my intellectual property. **Video, audio, and photographic recording of lectures is prohibited without my explicit permission**. Use of handouts (and all other material) for any purpose other than studying for this course without first obtaining my consent is prohibited. The selling or dissemination of any exams, quizzes, study guides, homework assignments, and notes presented in this course or derived from my lectures is also prohibited without my explicit permission.

Materials needed:

Required are:

Textbook*.* James Keeler (2010) *Understanding NMR Spectroscopy.* Wiley, 2nd edition. eBook (currently $49): *https://www.wiley.com/en-us/Understanding+NMR+Spectroscopy%2C+2nd+Edition-p-9781119964933*

Biophysical techniques. Material will be provided by the lecturer.

Recommended additional resources:

1. J. Cavanagh et al. "Protein NMR Spectroscopy", 2nd Edition, Academic Press, New York, 2007.
2. http://www-keeler.ch.cam.ac.uk/lectures/Irvine/
3. http://spindynamics.org/support.php
4. B. A. Shirley (Ed.) "Protein Stability and Folding. Theory and Practice", Methods in Molecular Biology, Humana Press, Totova, 1995.
5. Atta-ur-Rahman "Solving Problems with NMR Spectroscopy", Academic Press, San Diego, 1996.
6. Student Resource: A. Ben Wagner, Chemistry Librarian, 118 Lockwood Library, Phone: 645-1333. Email: abwagner@buffalo.edu. Info: http://library.buffalo.edu/bwagner

Additional course documents*:* The UBLearns (https://ublearns.buffalo.edu) web site of CHE 349 will provide additional documents such as the syllabus and announcements regarding the course, unless they are send by email to the enrolled students.

Homework:

Homework is assigned on a weekly basis according to the schedule below and can be returned voluntarily. The homework will be concisely presented during the lecture and can be discussed in detail with the instructor during office hours. It is stressed that everyone is responsible for their own homework.

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Schedule:

Part 1: NMR Spectroscopy

Week 1 of Jan 29	Organizational issues, General Introduction: scope of the course, Fundamentals of NMR, Chapters 1 and 2 of Keeler textbook
Week 2 of Feb 5	Chapter 3 (Energy levels and NMR spectra), Chapter 4 (The vector model)
Week 3 of Feb 12	Chapter 5 (Fourier transformation and data processing) Chapter 6 (The quantum mechanics of one spin)
Week 4 of Feb 19	Chapter 7 (Product operators), Chapter 8 (Two-dimensional NMR)
Week 5 of Feb 26	Chapter 9 (Relaxation and the NOE)
Week 6 of March 5	Chapter 10 (Advanced topics in two-dimensional NMR)
Week 7 of March 12	Chapter 11 (Coherence selection), Chapter 12 (Equivalent spins)
Week 8 of March 19	*Spring Recess*
Week 9 of March 26	First Exam, Advanced NMR topics: Chemical exchange saturation transfer (CEST), Transverse relaxation optimized spectroscopy (TROSY)
Week 10 of April 2	Fluorescence and circular dichroism (CD) spectroscopy of biological macromolecules
Week 11 of April 9	Molecular dynamics (MD) simulations of proteins
Week 12 of April 16	Differential scanning and isothermal titration Calorimetry (DSC and ITC)
Week 13 of April 23	Protein folding: thermodynamics and kinetics; Enzyme kinetics and enzyme reaction mechanisms
Week 14 of April 30	Small angle X-ray scattering (SAXS) and free electron lasers (FEL)
Week 15 of May 7	**Student presentations**, summary and outlook, **second exam**