

Biochemistry 8990: Bio-Macromolecular NMR Spectroscopy

1.5 ch, Call # 24754

Autumn 2017, Tuesdays 12:45-2:05 pm, Biological Sciences 668

Instructor: Mark P Foster (foster.281)

Description: This course will meet once per week to provide an introduction to the application of NMR spectroscopy to problems in biochemistry, structural biology and drug discovery. The approach will emphasize an intuitive understanding of NMR spectroscopy, using the vector model and product operator formalism to describe evolution of magnetization; thus, no background in quantum mechanics or matrix algebra are required. The course will include hands-on tutorials in NMR data collection on high-field instruments in the CCIC, as well as off-line data processing and analysis. Grades will be assigned based on regular homework exercises and a presentation from the literature on an application of NMR to a biomolecular problem.

OSU has world-class facilities for biomolecular NMR (see <http://ccic.ohio-state.edu/nmr>); students will learn how these great resources can advance their research.

Topics (subject to change):

1. Spin $\frac{1}{2}$ nuclei, sensitivity, magnetic field strength, vector model, coupling, chemical shift, proteins, nucleic acids
2. FT NMR, the FID, discrete sampling, quadrature detection, spectral resolution, zero filling, apodization, spectral width, aliasing
3. Product operators: chemical shift, coupling, de-coupling
4. 2D homonuclear NMR (COSY, TOCSY, NOESY), quadrature detection – hypercomplex datasets
5. 2D heteronuclear NMR (HSQC, HMQC, HMBC)
6. 3D heteronuclear NMR (NOESY-HSQC, TOCSY-HSQC, triple-resonance)
7. NMR data processing (TOPSPIN, NMRPipe, NMRfX) and analysis (SPARKY, NMRView)
8. Resonance assignments (proteins, nucleic acids)
9. Structure calculation from NMR data (CYANA, CNS/XPLOR, CS-ROSETTA)
10. Practical aspects: volume, concentration, lock solvent, temperature control/calibration, pulse calibration, receiver phase, phase correction, water suppression
11. Relaxation, dynamics, exchange, relaxation dispersion, chemical exchange saturation transfer
12. Protein-ligand interactions (chemical shift perturbation, isotope filters, transferred NOE, saturation transfer difference, paramagnetic relaxation enhancement)
13. Special topics

Text: Rule & Hitchens, Fundamentals of Protein NMR Spectroscopy, 2006, Springer

Other texts:

Cavanagh *et al.*, Protein NMR Spectroscopy 2nd Ed. 2007, Elsevier/Academic Press

Keeler, Understanding NMR, 2005, Wiley

Hore *et al.*, NMR: The Toolkit (2000) [Oxford University Press]

Levitt, Spin Dynamics (2008) [Wiley]

Misconduct

All work submitted for this class is expected to be your sole effort. No form of academic misconduct will be tolerated. Suspected cases will be referred to the Committee on Academic Misconduct per OSU procedures. Any falsification or improper alteration of grades, marks, answers or University forms will be dealt with severely. You will also be held to a high standard of treating your instructor and peers with the utmost respect.

It is the responsibility of the Committee on Academic Misconduct to investigate or establish procedures for the investigation of all reported cases of student academic misconduct. The term “academic misconduct” includes all forms of student academic misconduct wherever committed; illustrated by, but not limited to, cases of plagiarism and dishonest practices in connection with examinations. Instructors shall report all instances of alleged academic misconduct to the committee (Faculty Rule 3335-5-487). For additional information, see the Code of Student Conduct <http://studentlife.osu.edu/csc/>.

Accessibility

Students with disabilities (including mental health, chronic or temporary medical conditions) that have been certified by the Office of Student Life Disability Services will be appropriately accommodated and should inform the instructor as soon as possible of their needs. The Office of Student Life Disability Services is located in 098 Baker Hall, 113 W. 12th Avenue; telephone 614- 292-3307, slds@osu.edu.