

Biomolecular NMR (MCB 5076)

The course covers NMR (nuclear magnetic resonance) theory, with a particular emphasis on the applications of the technique to determining protein structure and dynamics. Starting from the principles of NMR spectroscopy, we move to the two- and three-dimensional NMR experiments used to assign resonances to specific atoms in proteins. Once NMR signals are assigned, interactions between spins and their environment provides the information needed for calculating NMR structures. Next, we focus on methods to obtain complementary information on protein dynamics. The last part of the course describes advanced applications of NMR such as studies of protein folding intermediates, amyloids, membrane proteins, and the use of NMR in drug discovery.

Open to graduate students and undergrads (by permission)

Credit hours: 2

<u>Month</u>	<u>Date</u>	<u>Lecture</u>
Aug	31	1 Overview of Nuclear Magnetic Resonance
Part I: NMR Basics		
Sept	7	2 Fundamentals of NMR (EM radiation, spin, coupling, NMR timescale)
Sept	14	3 NMR experiments (semi-classical formalism, FID, FT, 1D)
Sept	21***	4 Coupling: scalar, dipolar
Sept	28	5 2D-NMR spectroscopy (Fourier transforms, COSY, NOESY)
Part II: Multidimensional NMR experiments		
Oct	5***	6 Relaxation / measurements of protein dynamics
Oct	12	7 Sample considerations & protein expression for NMR
Oct	19***	8 Multidimensional NMR experiments & sequential assignments
Part III: Structure Determination		
Oct	26	9 Structure determination: Algorithms & protocols
Nov	2	10 Structure validation: Refinement and measures of quality
Part V: Advanced applications		
Nov	9***	11 Shift mapping, Drug screening, complex docking, SAR by NMR
Nov	16	12 NMR of oligomers and large complexes & membrane proteins
Nov	23	13 ~~~ T'giving recess: No Classes Nov 19-25 ~~~
Nov	30	14 Hydrogen exchange
Dec	7***	14 Protein Folding

NOTE : Dec 8 = Last day of classes

There will be a take home exam for the final (a report on an NMR paper from the scientific literature).

The Final Exam will be handed out November 2 and is due on our last class meeting Dec 10 at the latest (no exceptions).

Grading:

Quizzes ~ 50 pts.

Take home final ~ 50 pts

Total = 100 pts*

*Class participation will be considered for borderline grades.

*****Quizzes:**

Quiz 1 – NMR fundamentals (Sept 21)

Quiz 2 – Coupling & 2D-NMR (Oct 5)

Quiz 3 – Relaxation and isotope labeling (Oct 19)

Quiz 4 – Structure determination (Nov 9)

Quiz 5 – Advanced applications (Dec 7)