


NMR SPECTROSCOPY FOR CHEMISTS AND BIOLOGISTS

PROF. ASHUTOSH KUMAR
Department of Biosciences and Bioengineering
IIT Bombay
PROF. R. V HOSUR
Department of Biosciences and Bioengineering
IIT Bombay

PRE-REQUISITES : Under graduate level understanding of Physics and Mathematics

INTENDED AUDIENCE : M. Sc./ PhD and Scientists working in Pharma and Biopharma Industries

INDUSTRIES APPLICABLE TO : Biocon, Wockhardt, Aurobindo Biopharma etc

COURSE OUTLINE :

This course starts with Basic principles of NMR, walks through the analysis of spectra and demonstrates the application of multidimensional NMR spectroscopy in Chemistry and structural Biology.

ABOUT INSTRUCTOR :

Prof. Kumar is an Associate Professor in the Department of Biosciences and Bioengineering. His area of research is NMR based structural biology. Prof. Kumar develop and apply NMR methods to understand protein structure and dynamics.

Prof. Hosur is Distinguished Visiting Professor in the Department of Biosciences and Bioengineering, IIT Bombay. Prior to this, he was senior Professor in Tata Institute of Fundamental Reseach, Mumbai

COURSE PLAN :

Week 1 :
Nuclear Spin and Magnetic Moments
Nuclear Spins in a Magnetic Field Spin
Lattice Relaxation Spin temperature Resonance
Absorption of Energy and The NMR Experiment Resonance
Absorption of Energy and The NMR Experiment Kinetics of Resonance Absorption

Week 2 :
Selection Rules and Line widths
Bloch equations
More about relaxation
More about relaxation Sensitivity

Week 3 :
Instruction to operator Algebra
Chemical Shift
Anisotropy of chemical shifts Learning spectral simulation

Week 4 :
Factors Influencing Isotropic Chemical shifts: Spin Spin Coupling
Analysis of NMR spectra of molecules
Learning spectral simulation

Week 5 :
Dynamic Effects in the NMR spectra : Two site exchange
Collapse of spin multiplets
Conformational Averaging of J- values
Analysis of NMR spectra of molecules with J Values

Week 6 :
Principles of Fourier transform
NMR Theorems on Fourier transforms
Practical aspects of recording FTNMR spectra
Free Induction Decay (FID) and the spectrum
Pulse repetition rate
Folding of signals
Acquisition time and the resolution
Data processing in FT
NMR Learning of Data processing

Week 7 :
Dynamic range in FTNMR and solvent suppression
The Nuclear Overhauser Effect - Experimental Schemes,Advanced Treatment
Steady state NOE and Transient NOE

Week 8 :
Spin Echo Uncoupled spins
Spin Echo Coupled spins
Spin-lattice relaxation
Spin-spin relaxation
Polarization transfer SPT and INEPT spectral simulation

Week 9 :
Density matrix, Elements of Density Matrix, Time evolution of density operator
Time evolution of density operator
Product operator formalism

Week 10 :
Segmentation of the time axis
Two dimensional NMR 2D
Fourier Transformation in NMR
Peak shapes in 2D spectrum
Quadrature detection in two-dimensional NMR

Week 11 :
2D- resolution/ separation experiments
Two-dimensional correlation experiments COSY, TDQ-COSY etc TOCSY

Week 12 :
2D NOESY, 2D ROESY, Heteronuclear COSY,
The HETCOR pulse sequence HSQC