



ONE AND TWO DIMENSIONAL NMR SPECTROSCOPY FOR CHEMISTS

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INTENDED AUDIENCE : It is for chemistry students, pharmaceutical students, biology students

INDUSTRIES APPLICABLE TO : The pharma industries, such as, sun pharma, syngine, Biocon, Bal pharma, Aurigine, etc..

COURSE OUTLINE :

In this course, I will discuss fundamental concepts of NMR spectroscopy, experimental determination of NMR spectral parameters, their interpretation, selective and broadband homo and Heteronuclear spin decoupling, numerous examples of the analysis of NMR spectra of ^1H , ^{13}C and other heteronuclei will be given. The relaxation processes, their measurement and utility in understanding molecular dynamics, the polarization transfer mechanism, the spectral editing techniques, such as, APT, DEPT, INEPT will also be discussed. Two dimensional NMR and the commonly employed experiments, viz., COSY, TOCSY, HSQC, HMQC, HMBC, NOESY, etc will be discussed with number of examples. The practical aspects of one and two dimensional NMR data acquisition and processing will also be highlighted. The solid state NMR, magic angle spinning and cross polarization will also be discussed.

ABOUT INSTRUCTOR :

Prof. N. Suryaprakash is currently a CSIR Emeritus Scientist at the Solid State and Structural Chemistry Unit, Indian Institute of Science. Previously he held various positions at IISc including Tatachem Chair Professor, before superannuation as a Professor and Chairman of NMR Research Centre. His academic career has proven to be nothing but exceptional in all aspects and his research achievements have received worldwide recognition, appearing in more than 155 publications in peer-reviewed journals of National and International repute, which include several invited book chapters. His research work is focused on diverse wings of NMR spectroscopy, with a major focus on the manipulation of spin dynamics to design novel experimental techniques to combat inherent challenges encountered in NMR spectroscopy, viz., weak sensitivity, poor resolution, and spectral crowding. He has also designed methods for the rapid acquisition of data, discerning degenerate transitions, and facile extraction of spectral parameters. His designed single and multiple quantum methodologies significantly transformed the chiral analysis of molecules in weakly aligned liquid crystalline media using ^1H NMR, a field that remained unchallenged for decades. His research work led to the discovery of three novel water-compatible weak chiral aligning media that surpassed many inherent limitations of enantiomeric differentiation. His group has introduced a number of novel chiral auxiliaries, for enantiodiscrimination of molecules with diverse functionalities, accurate determination of enantiomeric contents, and also for the assignment of their absolute configurations, an area of very high significance in pharmaceutical industries. His innovative NMR approaches for the investigation of hydrogen bonds involving organic fluorine pave the way for the artificial architectural design of macromolecules. His seminal contributions have catapulted the research activities in NMR spectroscopy, structural chemistry, chiral chemistry, and in the area of weak molecular interactions.

COURSE PLAN :

Week 1: Conceptual Understanding of NMR Spectroscopy

Week 2: NMR Spectral Parameters I (Chemical Shifts)

Week 3: NMR Spectral Parameters II (Scalar and Dipolar Couplings)

Week 4: Analysis of ^1H NMR spectra with numerous examples

Week 5: Selective and Broadband, Homo and Heteronuclear Decoupling, with examples

Week 6: Analysis of NMR spectra of ^{13}C and many other Heteronuclei

Week 7: Polarization transfer and spectral editing techniques, APT, DEPT and INEPT

Week 8: Introduction to Multi-Dimensional NMR

Week 9: Analysis of 2D COSY, TOCSY, HSQC, NOESY spectra with examples

Week 10: Practical Aspects of obtaining high resolution NMR spectra

Week 11: Relaxation processes, their measurement and utility in understanding molecular dynamics

Week 12: NMR in solid state, Magic Angle Spinning and Cross polarization