

Nuclear Magnetic Resonance (NMR) Spectroscopy



Prof. (Dr.) Ashutosh Kumar

Professor, Structural Biology

Department of Biosciences and Bioengineering

Indian Institute of Technology Bombay, Mumbai, 400 076, India

Phone: +91-22-25767762

Email: ashutoshk@iitb.ac.in

<https://www.bio.iitb.ac.in/~ashutoshk/>

Nuclear Magnetic Resonance (NMR) Spectroscopy is a potent analytical technique utilized extensively in science, medical science, and pharma industry. It gives precise information about the molecular structure, dynamics, and local environment of the material under investigation. There are many reasons NMR spectroscopy has attained a central stage among various analytical techniques. NMR spectroscopy is a highly effective method for determining the structure of organic compounds. It identifies the types and nature of nuclei (usually hydrogen and carbon) in a molecule. The chemical shift values, coupling constants, and integration of NMR signals reveal the atomic framework, allowing scientists to build a precise image of a compound's structure. Unlike other approaches, such as X-ray crystallography, NMR may be conducted in solution, making it excellent for examining molecules in their natural environment. NMR is uniquely capable of exploring the dynamics of molecules, revealing information about the mobility of atoms inside a molecule over different timescales. This is especially relevant in biochemistry, where understanding protein folding, ligand binding, and molecular interactions is critical. Relaxation times (T_1 and T_2) and techniques such as 2D NMR (NOESY and ROESY) enable researchers to investigate the dynamics and structural changes of massive macromolecules.

NMR spectroscopy is exceedingly versatile and may be used on a wide range of samples, including small chemical compounds and complex biological macromolecules such as proteins and nucleic acids. It is employed in a variety of sectors, including pharmaceuticals, where it aids in drug development and quality control and in food science to analyse complicated mixes. Furthermore, NMR is utilized in materials research to investigate polymers and nanomaterials, providing information on their molecular structure and behaviour. The approach gives a thorough picture of the chemical environment around the nuclei of interest. The chemical shift is determined by the electron density around the nucleus, which is then impacted by adjacent atoms and functional groups. NMR's sensitivity to the

local electrical environment makes it an essential tool for detecting functional groups and predicting chemical reactivity.

NMR spectroscopy yields exact quantitative data without substantial calibration. The area under each NMR signal is proportional to the number of nuclei that produce that signal. This makes NMR a great technique for assessing sample purity and detecting component ratios in combination. One key advantage of NMR spectroscopy is that it is non-destructive. NMR, unlike mass spectrometry, does not ionise or fragment the material. This capability is very useful for analysing delicate or important samples, as it allows for additional examination using alternative methods if necessary. Modern NMR techniques, such as 2D, 3D, and solid-state NMR, provide greater insight into complicated chemical structures and interactions. Multidimensional NMR techniques aid in the resolution of overlapping signals, making it possible to analyse larger and more complex molecules. Solid-state NMR, on the other hand, allows for the investigation of intractable and crystalline compounds, broadening the application of NMR beyond solution-state samples.

NMR spectroscopy's capacity to provide a thorough, quantitative, and non-destructive examination of molecular structures makes it a must-have tool in scientific research. Its use in a variety of sectors demonstrates its adaptability and usefulness in understanding the basic characteristics of molecules. As NMR technology advances, it promises even more insights into the molecular world, cementing its place as a foundation for modern analytical chemistry and molecular biology.