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Editorial Note

Development Editor Note: Bio NMR Research

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The physical and chemical properties of atoms or the molecules in which they are found are determined. It is based on the nuclear magnetic resonance phenomenon and can provide detailed details about the structure, dynamics, reaction state, and chemical environment of molecules. The ability to investigate both the structure and dynamics of biomolecules with high resolution is unique to NMR spectroscopy. As a result, it has become a valuable structural biology tool. An summary of the process of structure determination is defined in this article. The appropriate sample and experiments are briefly discussed.

Every cell in a living organism consists of a number of macromolecules that are needed for different cellular functions and metabolism (called 'biomolecules'). The biological activity of these biomolecules is regulated by their interactions within the cell with other molecules. These interactions are governed by their three-dimensional (3D) spatial structures. Awareness of a biomolecule's 3D structure is thus important for a full understanding of its function. 'Structural biology' is a scientific discipline concerned with the study of the relationship between the 3D structure, function and interaction of biomolecules. Structural biology is a hotly sought field of study today, and it has aided in our understanding of the causes and treatments for a variety of human diseases. To evaluate the 3D structure of biomolecules at high resolution, there are several well-established experimental techniques. The most famous are X-ray crystallography and nuclear magnetic resonance (NMR) spectroscopy. The former includes high purity crystals, while the latter is used in an aqueous solution or solid state to establish biomolecular structures.

NMR offers knowledge complementary to that obtained from X-ray crystallography on 3D structures. NMR has an advantage over the X-ray approach as it can be used under physiological conditions or, as in the case of proteins, also in a molten globule or a denatured state to research biomolecules in their native state (i.e. in solution). In addition, the freedom of motion in the solution makes NMR more fitting for the dynamic behaviour of macromolecules to be studied. In the mid-1980s, NMR spectroscopy was used to determine the first high-resolution protein structure.

Access to fast computing facilities and the development of modern computational methods have been one of the significant contributions to speeding up the biomolecular structure determination process. This has arisen in the age of 'structural genomics' as a topic of pivotal interest, where the goal is to unravel tens of thousands of protein structures within this decade. In turn, the availability of a large number of 3D structures has contributed to our knowledge of NMR spectral data vis-à-vis protein structures, thus helping to refine these instruments. Two major public domain databases, the BioMagResBank(BMRB) and the protein data bank(PDB), which have become integral parts of NMR-based structural biology research, make such a wealth of data accessible to the NMR group. A variety of computer tools are being built that use this knowledge from BMRB and PDB at different stages of the procurement of structure determination process. NMR spectroscopy is currently being used in new research areas such as 'metabolomics' and 'biology of structures'. With the increased availability of high field NMR spectrometers with cryogenic probes, a greater focus will be put on reducing structure determination time. As a result, fast NMR spectroscopy will continue to advance in the future.

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