NMR experiment-driven modeling of biological macromolecules

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Nuclear Magnetic Resonance Spectroscopy (NMR) is one of the more versatile experimental techniques that allow determining three-dimensional (3D) structures of biomacromolecules at atomic resolution, whether these are proteins, RNA, DNA, and their complexes. Knowledge of the 3D structure is vital for understanding functions and mechanisms of action of macromolecules, and for rationalizing the effect of mutations. 3D structures are also important as guides for the design of new experimental studies and as starting point for rational drug design.

Little more than ten years ago, protein NMR structure determination projects were framed in terms of months if not years of laborious, interactive work. Nowadays, owing to stunning advances in NMR experiments, instrumentation and notably computational data analysis, a relatively propitious protein candidate may be solved in a few weeks. Not surprisingly, around half of all protein structures solved in the Protein Data Bank using NMR have been thanks to automated, computational approaches.

Here we will discuss emerging methods at the intersection of experimental NMR and computational analysis and prediction. Special emphasis will be placed on the development of computational approaches that are able to handle large amount of experimental data efficiently and that integrate with data from other experimental techniques. The latter aspect is essential for applications of NMR to advanced and challenging problems in systems biology.