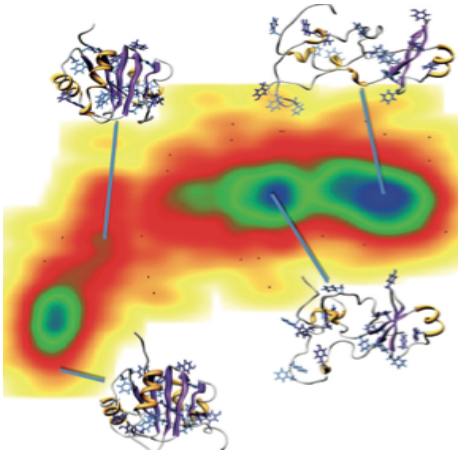
Biomolecular Structure and Dynamics through the Synergy of Experiment and Computation

Aleksandr B. Sahakyan
Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, United Kingdom.
as952@cam.ac.uk

The recent advances in biological chemistry and structural biology have much signified the importance of the high-quality structural information from bio-macro-molecules. Moreover, we are becoming increasingly convinced that the dynamics of such molecules plays an equally important role in defining the complex function of proteins and nucleic acids. In this regard, of the two major techniques for biomolecular structure determination, the nuclear magnetic resonance (NMR) spectroscopy does provide a number of measurable parameters that have temporal resolution in structural studies. However, those parameters are hard to measure and are mostly inaccessible for large systems, intrinsically disordered proteins and protein aggregates. Furthermore, the structure determination procedures that use the standard approaches in NMR spectroscopy may be insufficient to even resolve the correct structure of small dynamic proteins and most of the RNA molecules.

In this talk, I shall present the advances and ongoing steps towards the development of a unified platform that merges experiment and computation into a single methodology for direct structural and dynamical studies of biomolecules. The methodology, amongst other parameters, can utilise and fully rely on the most accessible NMR parameters, chemical shifts, thus substantially extending the applicability of the NMR spectroscopy in inferring atomic-scale structures and dynamics of the "over-sized" macromolecules, nucleic acids and their hidden low-populated states



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