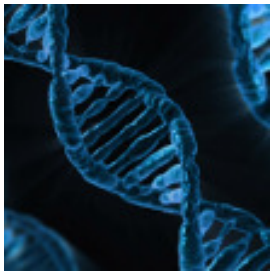

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KEYNOTE 4 - Comparing molecular simulations with NMR and SAXS measurements: A cautionary tale

Monday, 4 June 2018 16:25 (40)

The degree of compaction of the polypeptide chain is a property of key importance in intrinsically disordered proteins. Experimentally, compaction is often measured either by NMR (as the hydrodynamic radius) or SAXS (as the radius of gyration), and more detailed information may also be obtained by NMR paramagnetic relaxation enhancement measurements. A more detailed, atomic-level description of the structure, dynamics and compaction of IDPs, may however, be obtained from molecular simulations, but these need to be validated or generated by comparison with experiments. The comparison between computed conformational ensembles and NMR and SAXS experiments is, however, not trivial. I will discuss recent results that provide new insights into how we can compare atomic level structures of IDPs with NMR diffusion, NMR paramagnetic relaxation enhancement and SAXS experiments. Further, I will discuss recent theoretical and practical progress in using experimental NMR and SAXS data to refine computational models of biomolecules.

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