“Biomolecular Simulations as a Toolkit: From Folding Dynamics to Structure Prediction and Beyond”

Exploring the interrelationship of structure and function is crucial for the understanding of molecular life. Yet despite significant progress of experimental methods, full characterization of functional cycles for proteins and RNA remains an ongoing challenge. Biomolecular simulations offer a complementary option to experiments. One can use such simulations akin to an atomically resolved microscope to gain insight into the dynamical motion of biomolecules, such as during protein folding [1].

It is also possible to include additional information as constraints into such simulations. The increasingly ubiquitous availability of sequential information and novel statistical analysis has allowed to trace the co-evolution of residues [2], which can be exploited in structure prediction tools and is, e.g., sufficient for the blind prediction of protein complexes and their active conformations [3] or RNA structure prediction [4]. Similarly, one can use low-resolution experimental information such as SAXS data to model suitable biomolecular conformations [unpublished data] or compare data from simulations directly against experimental measurements such as smFRET data [unpublished data].

References

Date & time: Tuesday, April 12, 2016 at 05:00 pm
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