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Multi-Scale Computational Biology

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Cellular functions such as growth, programmed cell death, sensing, and metabolism, as well as the pathological processes underlying protein malfunctioning, involve molecular interactions that span from single protein to multi-protein complexes. Indeed, huge protein complexes are regulated through complex networks of transient molecular interactions. Consequently, the behaviour of a biological system is determined by inter-relationships between molecules, rather than by its individual components. The key technique for this kind of characterization, i.e. considering complete cellular pathways, is 'systems biology'. This approach is mainly devoted to the unravelling at a mathematical level the functioning of cellular pathways or gene-regulatory networks. But, in the other hand, systems biology needs to be accompanied by a quantitative molecular description of pathways, so far most lacking. The characterization of these phenomena needs to be performed computationally and it is highly challenging as it requires bridging many orders of magnitude in spatial and temporal dimensions, as well as advanced techniques in data-mining. This calls for the development of computational approaches, able to deeply characterize complex molecular systems into their individual players. For each individual level many simulation methods and strategies exist: bioinformatics uses the information encoded in the protein sequences to predict structure and function, molecular dynamics (MD) simulations predicts structural, dynamical, and energetic (bio)molecular properties, quantum mechanics simulations allow the characterization of bond-forming and bond -breaking phenomena, the prediction of spectroscopic and vibration properties of drugs bound to their targets and the study of enzyme reaction. Finally, hybrid methods, i.e. quantum mechanics/molecular mechanics (QM/MM) and molecular mechanics/coarse-grained (MM/CG) simulations, allow the characterization of events occurring at different temporal and spatial scales. The ultimate goal of computational biology is thus the development of multi-scale computational methods, able to extract properties computed from protein structures (such as kinetic parameters, affinities and binding energies) into macroscopic biochemical network models. This novel area of investigation will impact strongly on pharmaceutical sciences and toxicology, as drugs target (and mutations affect) pathways, rather than a single bio molecule.

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