Molecular Simulations on Biological Systems

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Biological systems are sets of molecules from living organisms whose astounding properties have been developed by eons of evolution. These characteristics include not only high affinity for their natural ligands but also strong selectivity; also, regulation of their functions, efficient catalysis and addressing their proper folding to the functional conformation. Molecular simulations on these systems have attempted during more than three decades, with the aim to identify the molecular basis of their biological function and also to predict the effect of mutations or modifications in their structure or the changes required to appropriate tuning of their function. Three main difficulties have arisen from them: their huge number of atoms, the delicate balance between attractive and repulsive interactions among their parts, and the solvent and entropic effects. In the recent years the technological improvement has produced both unbelievable computing power, and also trillions of bites of biological data. In this talk a comparison between those progresses will be compared and discussed. Also, other computational challenges from the biological ambit will be discussed in terms of their molecular representation and simulation focusing on whole genome analysis, omics sciences, drug design, stability prediction, and medical purposes.