University of Texas at San Antonio

Department of Physics & Astronomy

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Time: 3:00 p.m.-4:00 p.m.

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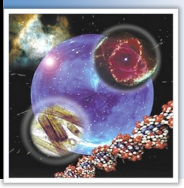
In Silico Characterization of Molecular Interactions in Biological Systems

Today, computational simulation is an invaluable tool to study macromolecular association, enzymatic reactions, and to understand at a molecular level the relationship between structure, dynamics and function. Thus, it provides an efficient and insightful complement to experimental evaluation. At the core of these calculations lies the potential energy function, which describes the intermolecular interactions in the system. I will present the latest developments in my research group focusing on the application of *in silico* methods to problems in the areas of structural biology, drug lead discovery, and binding free energy calculation, namely: i) the ligand-steered homology modelling method, where the interaction of known ligands with the receptor is used to shape and optimize the binding site through a stochastic global energy minimization, with the final goal of using the modelled structures in structure-based drug discovery; ii) the discovery of novel modulators of GPCRs and nuclear receptors through coarse-grained high-throughput docking followed by experimental evaluation; iii) the use of quantum mechanical (QM) methods to study biomacromolecular interaction; as a case study, the QM calculation of absolute and relative binding free energy of tetra-phosphopeptides to the SH2 domain of human LCK will be presented and compared to the failure of classical methods. Current limitations of computational methods and future trends will be also discussed.



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