Incorporating quantum-mechanical methods in structure-based drug discovery

Claudio N. Cavasotto
Biomedicine Research Institute of Buenos Aires – CONICET –
Partner Institute of the Max Society (IBioBA-MPSP)

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. In this short presentation, I will focus on the use of quantum mechanical (QM) methods to study biomacromolecular interaction; as an example, the QM calculation of absolute and relative binding free energy of tetra-phosphopeptides to the SH2 domain of human LCK will be presented, and the results compared to classical methods.