PyBindE: Development of a Simple Python MM-PBSA Implementation for Estimating Protein-Protein and Protein-Ligand Binding Energies

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There are several approaches for calculating binding free energies, with single-trajectory MM-PBSA being particularly useful when the relative energy differences between configurations are most significant. These methods also become a very popular option since they can be applied to a vast variety of systems, including protein-protein, protein-ligand and even protein-membrane binding events. MM-PBSA can generate binding energies over time, with various force-fields, and can be used to investigate the impact of protonation changes in a complex stability.

With this in mind, we have just developed PyBindE, a single-trajectory MM-PBSA Python implementation designed to be easily inserted into existing MD protocols [1]. Although PyBindE is in its early stages of validation it has already been applied to a few different systems of protein-protein and protein-ligand. Here, we provide a detailed description of the PyBindE implementation, how it can be easily installed and inserted into MD simulations pipelines and some of the results from on-going and published projects [2].

1. João Vitorino, PR. PyBindE: Molecular Mechanics Poisson-Boltzmann Surface Area (MMPBSA) calculations in protein-protein and protein-ligand systems. Github; Available: https://github.com/mms-fcul/PyBindE

2. Oliveira NFB, Rodrigues FEP, Vitorino JNM, Loureiro RJS, Faísca PFN, Machuqueiro M. Predicting stable binding modes from simulated dimers of the D76N mutant of β 2-microglobulin. Comput Struct Biotechnol J. 2021;19: 5160–5169.