سمینار هفتگی ماده چگال نرم

Computational model to predict protein binding sites of a luminescent ligand

Abstract

How ligands interact with proteins and affect protein-protein interactions (PPI) has become a topic of interest especially in the field of drug design. Specific supramolecular ligands can modulate, inhibit, or stabilize these PPIs. In experiment, the readout of binding event is usually done via indirect measurements or fluorescence emission. However, the binding positions cannot be specified experimentally and here computer simulations come to help.

Programs such as Autodock or Autodock vina have been developed to answer the question. These standard docking methods provide reasonable results only when the binding region is known. Therefore, for blind-docking or for large, highly flexible, and charged ligands, such standard docking tools are ill-equipped, and results are usually prone to error. On the other hand, the protein size and ligand flexibility make all-atom Molecular Dynamics (MD) simulation impractical and prone to under-sampling. Moreover, for such systems, deriving all-atom parameters for MD is a complex and time-consuming task.

The above-mentioned reasons explain why Epitopsy was developed in our group and why we have further developed a Simulated Annealing Monte Carlo method based on it.

In this presentation, I will introduce our method and present our results obtained from two recent applications:

1- A designed hybrid compound featuring aggregation-induced emission luminophores as a potential supramolecular ligand for 14-3-3ζ protein
2- A phosphate-based ligand (11d) for cancer-relevant protease **T**hreonine **asp**art**ase 1** (Taspase 1) protein

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