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Computational method for calculating ligand binding affinities

リガンド結合親和性の計算科学的手法

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Recentry, drugs which bind to a target protein and then inhibit protein-protein interaction or enzyme reactions have become of a subject of interest. The candidates of these drugs should strongly and specifically bind to the target proteins, thus the accurate rediction of the binding affinity of a ligand for a protein is a critical element in computer-aided drug discovery. Here, we will review different computational currently available to calculate ligand binding affinitis, and introduce an efficient method that we developed.

Keywords: binding free energy, mleular simulation, computer-aided drug design