Studying Induced-fit Effects in Protein Kinase Systems by a Flexible Ligand-Flexible Protein Docking Model

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Protein kinases are flexible proteins that adopt different conformations when different ligands are bound to them. Here, we describe a molecular dynamics-based flexible ligand-flexible protein docking model capable of describing induced-fit effects in protein kinase systems. The model used an efficient simulated annealing cycling protocol and an inexpensive distance-dependent dielectric model. To better compare docking result with experimental structure, we also calculated correlation coefficient of protein-ligand/protein-protein distances between docking and experimental structures, in addition to the commonly used Root-Mean-Square Deviation (RMSD) between docking pose and experimental structure.