Optimization function and modeling of the structure-activity relationships

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Molecular docking algorithms predict the binding of a macromolecule (receptor) and a small molecule (ligand). Molecular binding is an optimization problem where the most appropriate location is determined by a well defined evaluation function. The docking problem includes a method of generating and evaluating of structures of the obtained ligand-receptor (LR) complexes. These methods consists of interconnected parts - a formation of conformational space and calculation of LR complexes. The main purpose is to determine the correct way of ligand binding to the receptor in order to find a complex with a minimal energy. In this paper we examine some various optimization functions which can be used in the docking algorithms in order to determine the binding strength of a given ligand to a receptor in the formation of a LR complex. Predicting the protein-ligand binding models we can contribute a study of a structure-activity relationship which can be useful in drug discovery.

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