P-46

Comparison of FlexX and Surflex Docking Algorithms Based on Astex Diverse Set.

Rafał Kurczab, Mateusz Nowak, Andrzej J. Bojarski

Department of Medicinal Chemistry, Institute of Pharmacology Polish Academy of Sciences, Smętna 12, 31-343 Kraków

e-mail:

Molecular docking is routinely used in lead finding and compound optimization, both for targets with experimental 3D coordinates and for homology-based models. Our study concentrates on comparison of two commercial docking programs: FlexX (BioSolveIT) and Surflex-Dock (Tripos). Their performance was explored using Astex Diverse Set that contains crystal structures of 85 protein-ligand complexes from different drug discovery or agrochemical targets [1]. Docking results were analyzed based on the success rate of producing near-native ligand binding geometries (rmsd < 2.0Å) and usage of different scoring functions (G_Score, D_Score, F_Score, Chem-Score, PMF, C_Score) are discussed. In addition, a number of technical issues and software limitations are described.

References:

[1] Hartshorn M. J., Verdonk M. L., Mortenson P. L., Murray C. W.: *J. Med. Chem. 2007, 50, 726-741*.