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Title (English)

Evaluation of docking in ICM as a tool in structure-based drug design

Title (Swedish)

Abstract

The ICM docking algorithm was studied and evaluated as a tool in structure-based drug design. ICM VLS, v. 2.8 Molsoft L.L.C, was evaluated in terms of docking accuracy and scoring function performance. Different approaches to improve docking results were studied and generated conformations were analysed. The discriminative power of the implemented scoring functions i.e. the ability of distinguishing a small number of active compounds from a large compound database was studied. Existing methods of processing virtual screening results were applied and compared with other filtering method approaches. Consensus scoring and Bayesian classification based on the two scoring functions implemented in ICM were shown to be superior in discriminating active from inactive compounds compared to ranking based on single scoring function results.

Keywords

Docking, virtual screening, scoring functions, consensus scoring, Bayesian classification, conformational analysis

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