Chemistry Central Journal

Poster presentation

Open Access

Evaluation of the performance of 3D virtual screening programs: docking vs. structure-based pharmacophore

G Erlenkamp*, R Heinke, R Meier and W Sippl

Address: Department of Pharmaceutical Chemistry, Martin-Luther-University, Halle-Wittenberg Wolfgang-Langenbeckstr. 4, 06120 Halle (Saale), Germany

* Corresponding author

from 4th German Conference on Chemoinformatics
Goslar, Germany. 9–11 November 2008

Published: 5 June 2009

Chemistry Central Journal 2009, **3**(Suppl 1):P56 doi:10.1186/1752-153X-3-S1-P56

This abstract is available from: http://www.journal.chemistrycentral.com/content/3/S1/P56

Virtual screening (VS) techniques are well established methods in the modern drug discovery process and an almost unmanageable number of different 3D VS techniques are available today. Beside protein-ligand docking approaches, pharmacophore search methods are applied to screen large compound libraries to identify potential hits. In recent years, structure-based pharmacophores became more and more popular for virtual screening when 3D information about the target protein is available. In the present work we have analyzed and compared the performance of two docking programs (GOLD and ParaDocks) and the pharmacophore-based procedure within the program LigandScout. For our evaluation study we choose the Astex Diverse Set including 85 protein-ligand structures and decoy sets derived from the NCI and the Derwent WDI database. Beside the reproducibility of the experimentally derived structures, a special focus was given to the discrimination between known actives and inactives. For this purpose we have analyzed in a retrospective way several real life examples from our laboratory.