Chemistry Central Journal

Poster presentation

Further adventures in shape space

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from 3rd German Conference on Chemoinformatics
Goslar, Germany. 11-13 November 2007

Published: 26 March 2008

Chemistry Central Journal 2008, **2**(Suppl 1):P41 doi:10.1186/1752-153X-2-S1-P41

This abstract is available from: http://www.journal.chemistrycentral.com/content/2/S1/P41

It has been a long-held assumption in ligand-based virtual screening that the bioactive conformation of a molecule is privileged. The assumption is that superior performance in 3D searching (pharmacophores, shape similarity) should be obtained when using the bioactive conformation of a query molecule for searching for other active molecules. A parallel assumption has been that extensive sampling of the conformational space of database molecules is necessary to obtain optimal performance for 3D ligand-based screening. Both of these assumptions will be critically assessed for ligand-based virtual screening carried out in shape space.