Chemistry Central Journal

Poster presentation

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A new method in docking for rotatable OH bonds of amino acids in active sites

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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):P45 doi:10.1186/1752-153X-2-S1-P45

This abstract is available from: http://www.journal.chemistrycentral.com/content/2/S1/P45

We present a new concept in FlexX that determines torsion angles for OH-groups on the receptor side. For the affected amino acids SER, THR, and TYR, hydrogen bonds to neighbouring residues and the ligand are taken into account, providing a more realistic representation of the binding site. This is done irrespective of the ligand type, and without the user's interaction.

We present the concept itself as well as some case studies as early proof-of-concept.