Journal of Cheminformatics

POSTER PRESENTATION Open Access

PoseView – molecular interaction patterns at a glance

Katrin Stierand*, Matthias Rarey

From 5th German Conference on Cheminformatics: 23. CIC-Workshop
Goslar, Germany. 8-10 November 2009

Chemists are well trained in perceiving 2D molecular sketches. On the side of computer assistance, the automated generation of such sketches becomes very difficult when it comes to multi-molecular arrangements such as protein-ligand complexes in a drug design context. Existing solutions to date suffer from drawbacks such as missing important interaction types, inappropriate levels of abstraction and layout quality.

During the last few years we have developed PoseView [1,2], a tool which displays molecular complexes incorporating a simple, easy-to-perceive arrangement of the ligand and the amino acids towards which it forms interactions. Resulting in atomic resolution diagrams, PoseView operates on a fast tree re-arrangement algorithm to minimize crossing lines in the sketches. Due to a de-coupling of interaction perception and the drawing engine, PoseView can draw any interactions determined by either distance-based rules or the FlexX interaction model (which itself is user accessible). Owing to the small molecule drawing engine 2Ddraw [3], molecules are drawn in a textbook-like manner following the IUPAC regulations.

The tool has a generic file interface for other complexes than protein-ligand arrangements. It can therefore be used as well for the display of, e.g., RNA/DNA complexes with small molecules. For batch processing, an additional command line interface is available; output can be provided in various formats, amongst them gif, ps, svg and pdf.

Besides the underlying interaction models, we will present new algorithmic approaches, assess usability issues and a large-scale validation study on the PDB.

Published: 4 May 2010

Center for Bioinformatics (ZBH), University of Hamburg, Bundesstrasse 43, 20146 Hamburg, Germany

References

1. Stierand K, Rarey M: *ChemMedChem* 2007, **2**:853.
2. Stierand K, Maaß P, Rarey M: *Bioinformatics* 2006, **22**:1710.
3. Fricker PC, Gastreich M, Rarey M: *J Chem Inf Comput Sci* 2004, **44(3)**:1065.

doi:10.1186/1758-2946-2-S1-P50
Cite this article as: Stierand and Rarey: PoseView – molecular interaction patterns at a glance. *Journal of Cheminformatics* 2010 **2**(Suppl 1):P50.