Chemistry Central Journal

ChemistryCentral

Poster presentation

Open Access

PocketGraph: graph representation of binding site volumes

M Weisel*, J Kriegl and G Schneider

Address: Johann Wolfgang Goethe-University, Beilstein Endowed Chair for Cheminformatics, Siesmayerstraße 70, D-60323 Frankfurt/Main, 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):P66 doi:10.1186/1752-153X-3-S1-P66

This abstract is available from: http://www.journal.chemistrycentral.com/content/3/S1/P66

The representation of small molecules as molecular graphs [1] is a common technique in various fields of cheminformatics. This approach employs abstract descriptions of topology and properties for rapid analyses and comparison. Receptor-based methods in contrast mostly depend on more complex representations impeding simplified analysis and limiting the possibilities of property assignment. In this study we demonstrate that ligand-based methods can be applied to receptor-derived binding site analysis.

We introduce the new method PocketGraph that translates representations of binding site volumes into linear graphs and enables the application of graph-based methods to the world of protein pockets. The method uses the PocketPicker [2] algorithm for characterization of binding site volumes and employs a Growing Neural Gas [3] procedure to derive graph representations of pocket topologies.

Self-organizing map (SOM) projections revealed a limited number of pocket topologies. We argue that there is only a small set of pocket shapes realized in the known ligand-receptor complexes.

References

1. Balaban AT: **Applications of Graph Theory in Chemistry.** *J Chem Inf Comput Sci* 1985, **25:**334-343.
2. Weisel M, Proschak E, Schneider G: **PocketPicker: Analysis of Ligand Binding-Sites with Shape Descriptors.** *Chem Cent J* 2007, **1:**7.
3. Fritzke B: **Growing cell structures – a selforganizing network for unsupervised and supervised learning.** *Neural Networks* 1994, **7:**1441-1460.