Chemistry Central Journal

Oral presentation

Open Access

Natural product-likeness score and its applications in the drug discovery process

Peter Ertl*, S Roggo and A Schuffenhauer

Address: Novartis Institutes for BioMedical Research, Basel, Switzerland

Email: Peter Ertl* - peter.ertl@novartis.com

* Corresponding author

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

Published: 26 March 2008

Chemistry Central Journal 2008, **2**(Suppl 1):S2 doi:10.1186/1752-153X-2-S1-S2

This abstract is available from: http://www.journal.chemistrycentral.com/content/2/S1/S2

Natural products (NPs) – i.e. secondary metabolites of plants or lower organisms - have been optimized in a very long natural selection process for optimal interactions with biological macromolecules. NPs are therefore an excellent source of validated substructures for the design of novel bioactive molecules. Indeed, many drugs in the current pharmacopeias are NPs, NP derivatives, or are of NP origin.

Various cheminformatics techniques can provide useful help in design of new bioactive molecules by taking into account information extracted from structures of NPs. In this presentation we describe a method to calculate natural product-likeness score - a Bayesian measure that characterizes similarity of molecules to the structural space covered by natural products. This score is shown to efficiently separate NPs from synthetic molecules in a cross-validation experiment. Possible applications of the NP-likeness score in drug discovery process are discussed, including virtual screening, prioritization of compound libraries towards NP-likeness and design of building blocks for the synthesis of NP-like combinatorial libraries.

References

1. Ertl P, Roggo S, Schuffenhauer A: **Natural product-likeness score and its application for prioritization of compound libraries.** *J Chem Inf Model* . ASAP Article 10.1021/ci700286x. Accepted for publication.