

POSTER PRESENTATION

Open Access

# DecoyFinder, a tool for finding decoy molecules

Cereto Massagué Adrià\*, S Garcia-Vallvé, G Pujadas

From 7th German Conference on Chemoinformatics: 25 CIC-Workshop  
Goslar, Germany. 6-8 November 2011

DecoyFinder is a graphical tool which helps finding sets of decoy molecules for a given group of active ligands. It does so by finding molecules which have a similar number of rotational bonds, hydrogen bond acceptors, hydrogen bond donors, logP value and molecular weight, but are chemically different, which is defined by a maximum Tanimoto value threshold between active ligand and decoy molecule MACCS fingerprints. Optionally, a maximum Tanimoto value threshold can be set between decoys in order assure chemical diversity in the decoy set.

During the talk, the algorithm used by DecoyFinder in order to look for decoys sets will be described in detail and some examples of its application will be described and discussed.

Published: 1 May 2012

doi:10.1186/1758-2946-4-S1-P2

**Cite this article as:** Adrià et al.: DecoyFinder, a tool for finding decoy molecules. *Journal of Cheminformatics* 2012 **4**(Suppl 1):P2.

Publish with **ChemistryCentral** and every scientist can read your work free of charge

*“Open access provides opportunities to our colleagues in other parts of the globe, by allowing anyone to view the content free of charge.”*

W. Jeffery Hurst, The Hershey Company.

- available free of charge to the entire scientific community
- peer reviewed and published immediately upon acceptance
- cited in PubMed and archived on PubMed Central
- yours — you keep the copyright

Submit your manuscript here:  
<http://www.chemistrycentral.com/manuscript/>



**ChemistryCentral**

Tarragona, Spain