

ORAL PRESENTATION

Open Access

Improvements in docking scoring functions: the physics-based perspective

Xavier Barril

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

Docking is possibly the most widely used technique in structure-based drug design. It is recognized as extremely useful to guide the development of active molecules as well as in virtual screening to identify new leads. But docking is also notoriously imperfect and many aspects need to improve. In this talk I will present our work on two different sources of errors in the docking predictions: protein-ligand interaction potentials and internal energy of the ligands. The use of higher-level calculations offers an opportunity to obtain better quality results and offers a glimpse of the full potential of the technique, but introducing this information back into fast and general scoring functions remains a challenge.

Published: 1 May 2012

doi:10.1186/1758-2946-4-S1-O22

Cite this article as: Barril: Improvements in docking scoring functions: the physics-based perspective. *Journal of Cheminformatics* 2012 **4**(Suppl 1):O22.

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

Correspondence: xbarril@ub.edu
Dept. Físicoquímica, Facultat de Farmàcia, Av. Joan XXIII, s/n 08028 -
Barcelona, Spain



© 2012 Barril; licensee BioMed Central Ltd. This is an Open Access article distributed under the terms of the Creative Commons Attribution License (<http://creativecommons.org/licenses/by/2.0>), which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.