

POSTER PRESENTATION

Open Access

PriaXplore[®] - a novel technology platform for the identification of small molecule modulators of protein-protein interactions

Susanne Eyrisch^{*}, Tobias Girschick, Günter Ross, Cédric Kalinski, Vladimir Khazak, Lutz Weber

From 8th German Conference on Chemoinformatics: 26 CIC-Workshop
Goslar, Germany. 11-13 November 2012

Protein-protein interactions (PPIs) are broadly recognized as an emerging target class for a whole new era in drug discovery. They show significant differences to classical target classes and have been regarded as “undruggable” for a long time. Priaxon AG has developed a unique, proprietary technology platform for PPI drug discovery. PriaXplore[®] employs novel computational and synthetic approaches to address PPIs with small molecule modulators. PriaXplore[®] utilizes Multicomponent Reactions (MCRs) to create an *in silico* search space of 200 million compounds pre-selected for PPI relevance. The PriaXplore[®] *in silico* screening process combines independent descriptor systems to search the MCR product space with maximum speed and accuracy. This combination of independent description methods enables a highly efficient selection of potential hit compounds that are further filter by our in-house docking protocol PriaDock. As protein-protein interaction sites are known to be very flexible and binding pockets of small molecule modulators may not be (fully) accessible in all protein structures, PriaDock uses multiple protein conformations derived from crystal/NMR structures or molecular dynamics simulations to account for this flexibility. Thus, smaller sets of compounds have to be synthesized and tested, lab resources are saved.

PriaXplore[®] has been validated by a successfully out-licensed Mdm2/p53 PPI inhibitor program. Currently PriaXplore[®] is applied in several drug discovery projects which are run either as Priaxon in-house projects or as cooperations with Pharma partners.

Published: 22 March 2013

^{*} Correspondence: eyrisch@priaxon.com
Priaxon AG, Munich, 81379, Germany

doi:10.1186/1758-2946-5-S1-P35

Cite this article as: Eyrisch et al.: PriaXplore[®] - a novel technology platform for the identification of small molecule modulators of protein-protein interactions. *Journal of Cheminformatics* 2013 **5**(Suppl 1):P35.

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