DrugPoint – a retrieval software and databank to connect proteins, drugs and targets.

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Some years before, it seemed that bioinformatics had struck a gold-mine for pharmacology by predicting many potential new drug targets. The situation has changed to a more sobering perspective now- the long way to identify valuable targets becomes only all too clear.

The software and database DrugPoint combines several types of software and data to help to better understand the relation between proteins, drugs and potential drug targets. This combination allows specific advantages over single software and data sources. In particular, each prediction is double checked by alternative algorithms. Furthermore, the DrugPoint software allows pre-screening of chemical compounds and first insights between the correlations of antibiotic activities against various organisms.

The user can query the database either for known drugs, for new compounds (in fact, any compound that can be drawn in or converted into smiles notation), for proteins or even for clusters of orthologous genes.

The database relies on publicly available data such as DrugBank. It allows to elucidate predicted drug-protein interactions, protein-protein interactions as well as organism variations of the different protein-protein interaction networks. Furthermore, the different drug candidates are screened for their properties according to Lipinski´s rule as well as a number of other chemical properties.

The database proved to be quite useful in different drug design steps in the context of the SFB630 in Würzburg already (e.g. Cecil et al., 2011), and will also be updated and refined in a public version.

References:
Cecil A, Rikanovic C, Ohlsen K, Liang C, Bernhardt J, Oelschlaeger TA, Gulder T, Bringmann G, Holzgrabe U, Unger M, Dandekar T. Modeling antibiotic and cytotoxic effects of the dimeric isoquinoline IQ-143 on metabolism and its regulation in Staphylococcus aureus, Staphylococcus epidermidis and human cells. Genome Biol. 2011, 21;12(3):R24.