Expert system to identify promising drug candidates

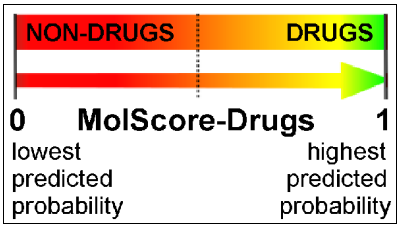
==> Lead selection

==> Prioritisation of drug candidates

MolScore-Drugs identifies and prioritises promising drug candidates with the maximum possibility of success in clinical trials in humans.

The expert system is based on a variety of reliable models. Extremely large structure-activity relationships (SAR) with up to hundreds of thousands compounds allow the estimation of useful drug-like chemical space. Structure-property relationships (SPR) which are derived from PharmaInformatic´s large in-house ADME/Tox-database have been applied to identify potential risks in order to reduce failures in clinical trials.

MolScore-Drugs calculates a value between 0 and 1 for each substance. This value correlates with the predicted probability of a substance becoming a successful drug.

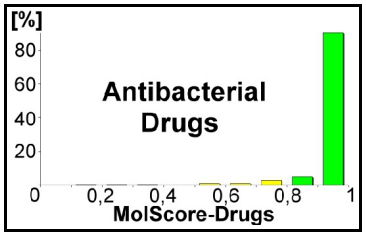


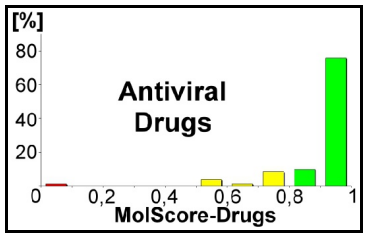
The expert system evaluates drug-candidates at an early state in order to reduce the costs and time for the development of novel drugs.

Application & Advantages

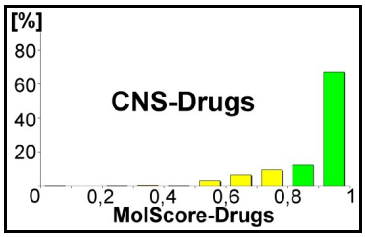
- Selects and prioritises promising drug candidates for further development
- Prioritises derivatives even of different lead structures
- Simple usage and integration of results
- Reduces clinical failures

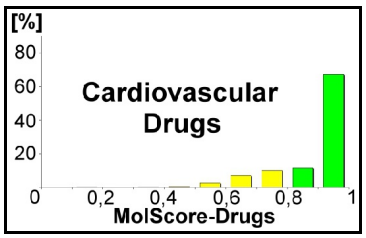
MolScore-Drugs prioritises drugs in multiple therapeutic areas correctly. The following figures show the prediction results of MolScore-Drugs on approved drugs in different therapeutic areas.



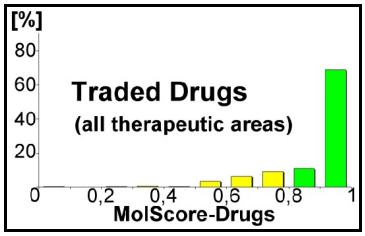


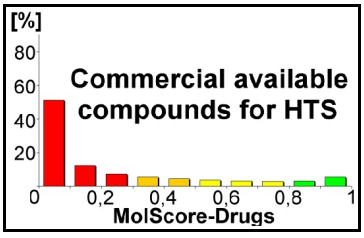
Despite the high variability of structures from marketed drugs, they have certain features in common. The expert system identifies general molecular patterns and properties of save and successful drugs.





MolScore-Drugs detects promising drug candidates in multiple therapeutic areas, including central nervous system diseases, infectious diseases, cardiovascular diseases, but is not limited to these.

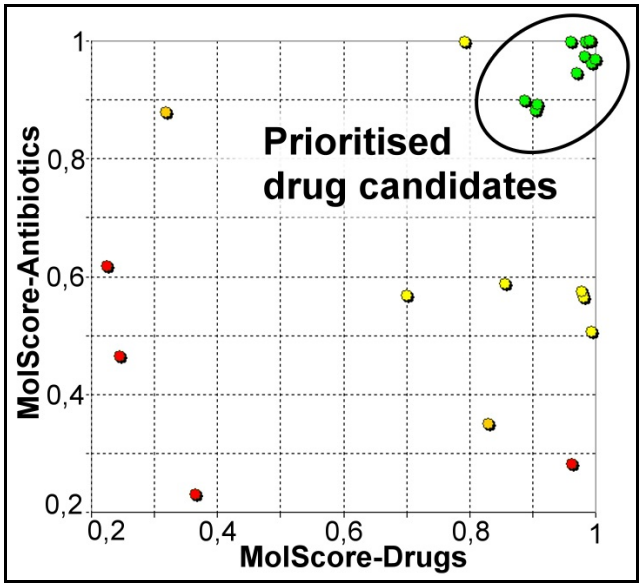




The examination of more than 500.000 commercial available compounds used for HTS showed that only a low amount of these compounds will satisfy the require-ments of becoming a promising drug.

Lead selection & prioritisation

MolScore-Drugs can be combined with other predictive tools to identify the most suitable drug candidates for further development. To provide an example we have used MolScore-Drugs and MolScore-Antibiotics to prioritise novel antibacterial lead structures.



Both expert systems are based on a variety of independent models which assess different molecular patterns and properties. Therefore a combination of both tools improves the drug candidate selection process.

MolScore-products are able to prioritise derivatives of lead structures. In practice the substitution of one functional group can have an important influence on biological activity & ADME-properties and this is reflected in the prediction result.

Application of customised tools derived from our ADME/Tox database will further improve the identification of potential risks in order to reduce clinical failures.

Oral bioavailability knowledge base and prediction

Oral bioavailability is one of the most important properties in drug development. Low oral bioavailability in clinical trials is a major reason for drug candidates failing to reach the market.

PharmaInformatic develops and licenses PACT-F, the largest knowledge base on bioavailability worldwide. PACT-F contains experimental bioavailability results of clinical trials in humans and preclinical trials in animals. The results and conditions of those trials have been taken manually from more than 5000 scientific research articles related to bioavailability.

The knowledge base has been used to develop the expert system IMPACT-F, which estimates oral bioavailability in humans much more precisely compared to animal trials. The expert system can forecast oral bioavailability of novel drugs reliable. Predictions of IMPACT-F were as accurate as the common deviation between individual humans taking part in the same clinical trial (inter-subject variability in humans).

About PharmaInformatic

PharmaInformatic is a German biotech company, which provides ADME/Tox knowledge bases and predictive tools (expert systems) to improve drug discovery and development. Expert systems help to discover and validate hits, followed by selection and prioritisation of suitable compounds for clinical trials in humans.

PharmaInformatic was founded in 2004 by Dr Wolfgang Boomgaarden. He has invented several drug design and virtual screening products, which have been successfully used in pharmaceutical research. Before he founded the company, he worked as a professor in bioinformatics at the University of Applied Science in Emden, Germany.

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