QSAR

Chemspace Virtual Screening Services

CHEMSPACE
Delivering Discovery Solutions®

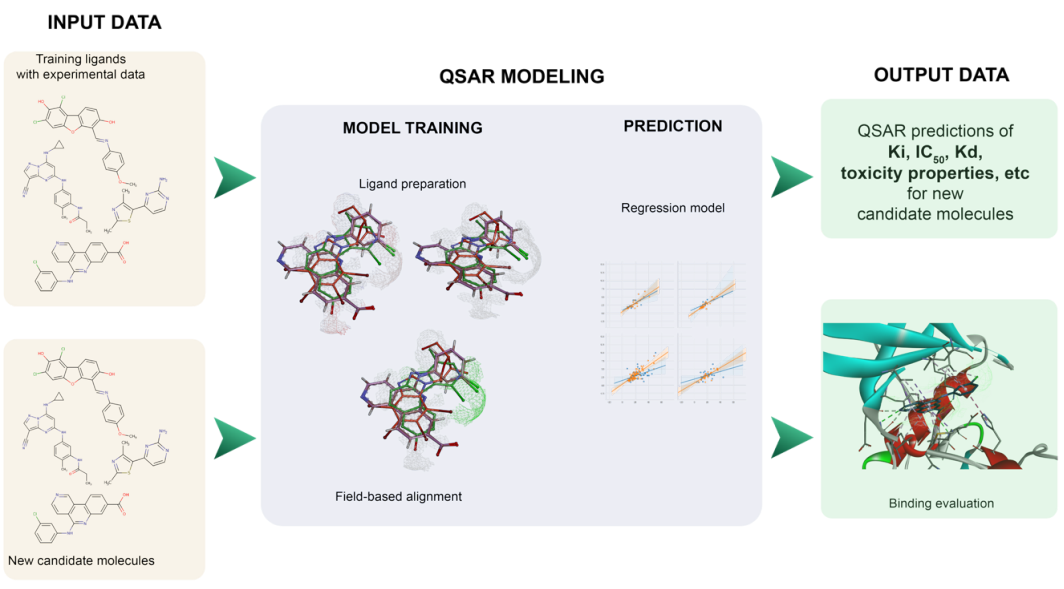
INPUT

What would we like to have as input?

- *In vitro* or *in vivo* data for training a relevant set of active molecules
- Any X-ray data is of great help
- Results of Molecular Docking and Molecular Dynamics is beneficial
- A wishlist of molecules for virtual screening (optional)

PIPELINE

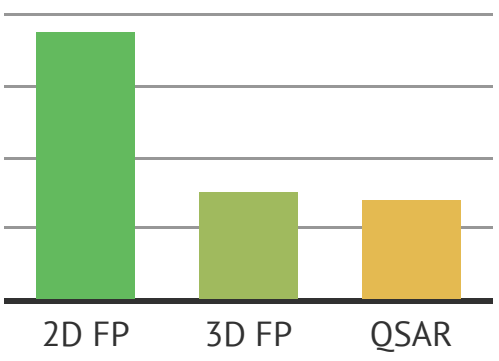
QSAR Pipeline



OUTPUT

What do we offer?

- Pharmacophore modeling of known ligands for a target of interest
- Refinement of candidate molecules by means of lead optimization procedure
- Identifying which areas of a given molecule should be altered and in what way



- A proposal of the most promising compounds based on predicted activities for the further drug development process
- Prediction of various important molecular properties of the new compounds
- Get a clear picture on what factors are of a certain impact on the activity of the putative lead compounds
- Improvement of your high throughput virtual screening searches in different ligand libraries

MISSION OF QSAR

- Estimation of physicochemical properties and biological activity of a compound
- Prediction of a full activity profile of a given compound against a panel of different biological targets, leading to the development of target profiling and target fishing applications.
- Establishment of structure-activity relationships (and therefore suggesting the way of compound modification to achieve maximum efficiency)