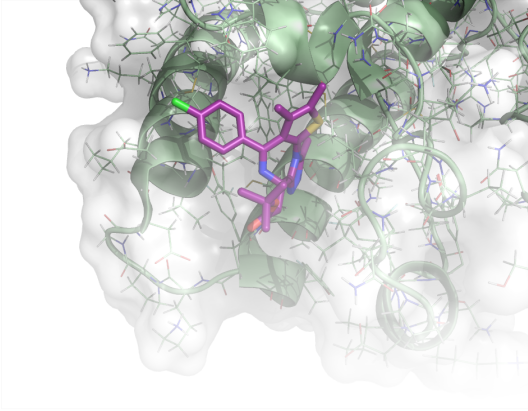
SELENE



Receptor-based virtual screening solution

SELENE is a computational tool which identifies active molecules with the ability to bind a receptor.

Working with SELENE

- We need a target and a data base containing molecules of interest. The data base can either be your proper one,provided by Intelligent Pharma or newly created inrespect to your needs.

How does SELENE works?

- SELENE fits molecules into pockets, which are in most of the projects the active site of the protein.
- SELENE considers different physicochemical properties during the fitting of a molecule into the pocket, resulting in the simulation of a molecular interaction.
- SELENE can treat the molecules and the target as flexible
- SELENE yields a list of ranked compounds according to the binding free energy of each compound with the receptor.
- SELENE gives structural data as the binding mode of the compound in the target pocket which can be used for improving the activity of small molecules
- SELENE uses Docking algorithims based on Vina[1] and Autodock 4.2[2].

1 O Trott, AJ Olson J Comput Chem. 2010, 31, 455-461.
2 G Morris, D Goodsell, R Halliday, R Huey, W Hart, R Belew, A Olson J ComputChem. 1998, 19, 1639-62

SELENE's applications

- Determination of new active molecules
- Determination of inhibitors
- Hit to Lead optimization
- Design of more potent ligands
- Drug reproofiling
- Prediction of toxicology properties
- Prediction of mechanisms of action
- Determination of the binding energy and binding constants Kd (mM, μM, nM)

Competitive Advanges

- SELENE uses Autodock and Vina as docking engine.
- Molecules and the target can be treated as flexible, a feature which increases the accuracy of the method.
- SELENE is run by Intelligent Pharma's experts so you do not need to be trained and we provide the supercomputational resources

Visit us!

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