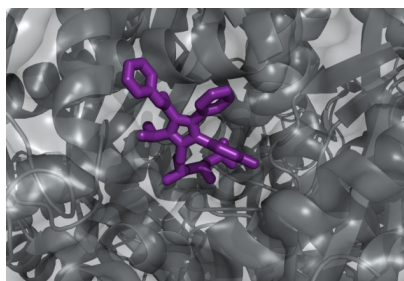


SELENE is a computational tool which identifies active molecules with the ability to bind a receptor.

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 in respect to your needs.

How does SELENE work?



- 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 algorithms based on Vina¹ & Autodock 4.2²

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 Comput Chem. 1998, 19, 1639-62.

Competitive Advantages

- 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.

SELENE's Applications






- Determination of new active molecules.
- Determination of inhibitors.
- Hit to lead optimization.
- Design of more potent ligands..
- Drug Reprofilling.
- Prediction of toxicologic properties.
- Prediction of mechanisms of action.
- Determination of the binding energy and binding constants K_d (mM, μ M and nM).

INTELLIGENT PHARMA

Intelligent Pharma offers different services in computation aided drug discovery. Our molecular modeling department carries out research projects to help your team in designing and developing new drugs using computational chemistry & biology expertise.

SELENE is a very fast and highly effective receptor-based virtual screening solution.

Other technologies

-  **HERCULES**
3D Ligand-based virtual screening solution
-  **PEGASUS**
2D Ligand-based virtual screening solution
-  **CHIRON**
Computer-aided hit to lead optimization
-  **MEDEA**
Data mining solution for medicinal chemistry
-  **HYPERION**
Allosteric site detector