Protein-Ligand Docking

Date: 2022-07-01
Tags: *1_Drylab 3_Protein-Ligand Docking*
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The proteins were aligned on their respective {binding pocket|docking target}.

The proteins were protonated with {Maestro|Modeling tool} at a pH of {7.4|pH}, with protonation states as determined by {PROPKA|pKa method}.

For the molecular docking, ligands {PP, 5BFA, 6MSA, 4HCA, 4HBA, CA|ligand} were drawn and converted into a 3D structure with {Maestro|Modeling tool}.

The protonation state of the ligand was determined using {Epik|ligand protonation program}.

The ligands were made using all possible combinations of stereocenter configurations and docked individually.

The ligands were placed into the {binding pocket|docking target} using {Maestro|Modeling tool}.

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The ligands were subsequently docked into the binding pockets of the respective sensors utilizing a combination of {AutoDock|docking engine} as a docking engine and the {DrugScore2018|docking potentials} distance-dependent pair-potentials as an objective function. The pair potentials were generated for at least {8.0 Å|map size} in each direction around the {largest ligand|map center}.

During docking, default parameters were used, except for the clustering RMSD cutoff, which was set to {2.0 Å|clustering RMSD cutoff}.

Binding modes were considered valid if they were located in the {binding pocket|docking target} and contained in the {largest cluster|success criterion}, which comprised at least {20%|valid cluster criterion} of all docking poses.