Master's Thesis

Title of project / Master's thesis	Molecular Modelling
Track	Active molecule-oriented ACLS
Topic / Key words	Molecular Docking, Molecular Modelling, (KNIME)
Supervisor	Prof. Dr. Rainer Riedl / Dr. Stefan Höck
Co-Supervisor	Prof. Dr. Rainer Riedl / Dr. Stefan Höck
External partners	Depends on topic
Place(s) of work	Wädenswil
Abstract	Molecular docking, the technique of fitting ligands into the active sites of target proteins, plays an important role in modern drug design. A master thesis in this topic can involve one or several of the following areas of interest: • Validation of docking methods: Statistical analysis of the performance and quality of docking results when compared to published activity data, depending on the set of parameters chosen for the docking experiment; • Combining different modeling techniques (molecular mechanics, quantum mechanical calculations) to improve the quality of the generated poses and docking scores; • Mining protein-ligand databases for interesting targets and possible candidate ligands; • Designing and implementing typical workflows of the drug discovery process using tools such as KNIME or suitable scripting languages. We certainly wish to validate the results generated in these modeling experiments by synthesizing and testing potential candidates in our laboratories. It is possible (but not necessary) for interested master students to carry out these syntheses themselves.
Requirements	What competences are required from the student? ⇨ Background in chemistry or biological chemistry ⇨ Fluency in at least one programming language (as taught in the Algorithms and Programming core module)
Comments	Molecular Modelling is a central methodology within the Center of Organic and Medicinal Chemistry. Scaffold replacement experiments as well as virtual screening campaigns are executed on a variety of therapeutically relevant target proteins. The improvement of these processes is critical for successful drug discovery projects.
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