Poster presentation

New and improved features of the docking software PLANTS

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We will summarize the latest developments for our protein-ligand docking software PLANTS (Protein-Ligand ANT System) [1][2][3]. This will include the pre-processing of the ligands and the protein performed by the program SPORES (Structure PrOtonation and REcognition System), parameterization of a new scoring function, as well as the inclusion of additional degrees of freedom into the docking process like flexible side chains and essential water molecules. The use of constraints from experimental data for improving the docking poses will be presented. Finally, an outlook towards the possible usage of the PLANTS approach for the flexible alignment of multiple ligands will be given.

References

1. Korb O, Stützle T, Exner TE: **Empirical Scoring Functions for Advanced Protein-Ligand Docking with PLANTS.** *J Comp Chem* 2008 in press.
2. Korb O, Stützle T, Exner TE: **An ant colony optimization approach to flexible protein-ligand docking.** *Swarm Intell* 2007, **1:**115-134.
3. Korb O, Stützle T, Exner TE: **PLANTS: Application of Ant Colony Optimization to Structure-Based Drug Design.** *Lecture Notes in Computer Science 4150* 2006:247-258.