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Efficient ant colony optimization algorithms for structure- and ligand-based drug design

O Korb

Address: Theoretische Chemische Dynamik, Fachbereich Chemie, Universität Konstanz, D-78457 Konstanz, Germany
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In this work the hybrid Ant Colony Optimization (ACO) [1] algorithm PLANTS [2][3][4] (Protein-Ligand ANT System) for the task of structure- and ligand-based drug design is introduced. Like other ACO-based approaches it is inspired by the behaviour of real ants finding a shortest path between their nest and a food source. The ants use indirect communication in the form of pheromone trails, which mark paths between the nest and a food source. In the case of protein-ligand docking, an artificial ant colony is employed to find a minimum energy conformation of the ligand in the binding site. The artificial ants are used to mimic the behaviour of real ants and mark low energy ligand conformations with pheromone trails. The artificial pheromone trail information is modified at computation time to bias the search towards low energy conformations.

The problem representation and the scoring functions employed in PLANTS are described, followed by pose prediction results obtained for publicly available benchmark data sets. Besides pose prediction, also virtual screening results considering additional degrees of freedom like explicit water molecules or flexible side-chains in the protein structure are presented. Furthermore, a graphics card accelerated version of the PLANTS approach capable of exploiting the enormous floating point computation power of modern graphics processing units (GPU) for the structure transformation and scoring function evaluation step is highlighted. Finally, a short overview of the multiple flexible ligand alignment module is given.

References

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