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Protein-Ligand Docking Using Artificial Bee Colony Algorithm

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Protein-ligand docking is one of the most significant issue in structure-based drug design (SBDD). Generally, this docking is considered as an optimization problem which specifies the energetically stable conformation of the ligand at the binding site. However, it is very difficult to identify the correct pose because of many optimization parameters with high correlation. In previous studies, it has been reported that popular docking programs (Glide[1], GOLD[2], FlexX[3], AutoDock[4], etc.) can identify the correct docking pose with an accuracy of only about 60%[5]. In this work, we attempted to apply Artificial Bee Colony algorithm[6] (ABC) to docking. ABC is an optimization algorithm based on the intelligent behavior of honey bee swarm, which has a higher global ability than other algorithms such as Simulated Annealing (SA), Genetic Algorithm (GA), Particle Swarm Optimization (PSO). The performance of the ABC for docking is evaluated for several protein-ligand complexes including some highly flexible ligands in comparison with other algorithms. The results reveal that the ABC might be more suitable for docking than others in particular for dealing with highly flexible ligands.

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