Summary: Molecular docking method plays an important role on the quest of potential drug candidates, which has been proven to be a valuable tool for virtual screening. Molecular docking is commonly referred to as a parameter optimization problem. During the last decade, some optimization algorithms have been introduced, such as Lamarckian genetic algorithm (LGA) and SODOCK embedded in the AutoDock program. On the basis of the latest docking software AutoDock4.2, we present a novel docking program ABCDock, which incorporates mutual artificial bee colony (MutualABC) into AutoDock. Computer simulation results demonstrate that ABCDock takes precedence over AutoDock and SODOCK, in terms of convergence performance, accuracy, and the lowest energy, especially for highly flexible ligands. It is noteworthy that ABCDock yields a higher success rate. Also, in comparison with the other state-of-the-art docking methods, namely GOLD, DOCK and FlexX, ABCDock provides the smallest RMSD in 27 of 37 cases.

Keywords: artificial bee colony; AutoDock; molecular docking

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