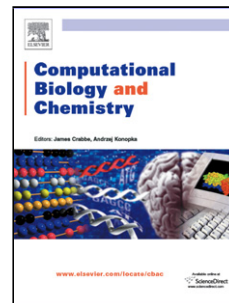


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Optimization of memory use of fragment extension-based protein-ligand docking with an original fast minimum cost flow algorithm

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Abstract

The need to accelerate large-scale protein-ligand docking in virtual screening against a huge compound database led researchers to propose a strategy that entails memorizing the evaluation result of the partial structure of a compound and reusing it to evaluate other compounds. However, the previous method required frequent disk accesses, resulting in insufficient acceleration. Thus, more efficient memory usage can be expected to lead to further acceleration, and optimal memory usage could be achieved by solving the minimum cost flow problem. In this research, we propose a fast algorithm for the minimum cost flow problem utilizing the characteristics of the graph generated for this problem as constraints. The proposed algorithm, which optimized memory usage, was approximately seven times faster compared to existing minimum cost flow algorithms.

Keywords: virtual screening, protein-ligand docking, weighted offline cache problem, minimum cost flow problem

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