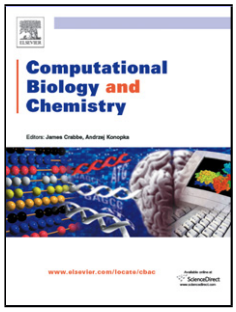

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Author: Keisuke Yanagisawa Shunta Komine Rikuto Kubota Masahito Ohue Yutaka Akiyama

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

Keisuke Yanagisawa[a,b], Shunta Komine[a,b], Rikuto Kubota[a], Masahito Ohue[a,c], Yutaka Akiyama[a,b,c,*]

[a] *Department of Computer Science, School of Computing, Tokyo Institute of Technology, W8-76 2-12-1, Ookayama, Meguro-ku, Tokyo 152-8550, Japan*
[b] *Education Academy of Computational Life Sciences (ACLS), Tokyo Institute of Technology, J3-141 4259, Nagatsutacho, Midori-ku, Yokohama City, Kanagawa 226-8501, Japan*
[c] *Advanced Computational Drug Discovery Unit (ACDD), Institute of Innovative Research, Tokyo Institute of Technology, 4259 Nagatsutacho, Midori-ku, Yokohama City, Kanagawa 226-8501, Japan*

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

*Corresponding author
Email address: akiyama@c.titech.ac.jp (Yutaka Akiyama)