Discovering Unique, Low-Energy Transition States Using Evolutionary Molecular Memetic Computing - DTU Orbit (28/03/2019)

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In the last few decades, identification of transition states has experienced significant growth in research interests from various scientific communities. As per the transition states theory, reaction paths and landscape analysis as well as many thermodynamic properties of biochemical systems can be accurately identified through the transition states. Transition states describe the paths of molecular systems in transiting across stable states. In this article, we present the discovery of unique, low-energy transition states and showcase the efficacy of their identification using the memetic computing paradigm under a Molecular Memetic Computing (MMC) framework. In essence, the MMC is equipped with the tree-based representation of non-cyclic molecules and the covalent-bond-driven evolutionary operators, in addition to the typical backbone of memetic algorithms. Herein, we employ genetic algorithm for the global search, Berny algorithm for individual learning, and make use of the valley-adaptive clearing scheme as the niching strategy in the spirit of Lamarckian learning. Experiments with a number of small non-cyclic molecules demonstrated excellent efficacy of the MMC compared to recent advances of several state-of-the-art algorithms. Not only did the MMC uncover the largest number of transition states, but it also incurred the least amount of computational costs.

General information
State: Published
Organisations: Department of Systems Biology, Center for Systems Microbiology, Nanyang Technological University, Boston University
Contributors: Ellabaan, M. M. H., Ong, Y., Handoko, S., Kwoh, C., Man, H.
Pages: 54-63
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: IEEE Computational Intelligence Magazine
Volume: 8
Issue number: 3
ISSN (Print): 1556-603x
Ratings:
Web of Science (2019): Indexed yes
Web of Science (2018): Indexed yes
Scopus rating (2017): CiteScore 3.92 SJR 1.296 SNIP 3.631
Web of Science (2017): Impact factor 6.611
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 2.96 SJR 1.172 SNIP 3.269
Web of Science (2016): Impact factor 6.343
Scopus rating (2015): CiteScore 1.89 SJR 0.809 SNIP 2.109
Web of Science (2015): Impact factor 3.647
Scopus rating (2014): CiteScore 1.99 SJR 0.826 SNIP 2.349
Web of Science (2014): Impact factor 2.571
Scopus rating (2013): CiteScore 2.71 SJR 1.301 SNIP 2.9
Web of Science (2013): Impact factor 2.706
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): CiteScore 3 SJR 1.479 SNIP 4.029
Web of Science (2012): Impact factor 4.629
ISI indexed (2012): ISI indexed yes
Scopus rating (2011): CiteScore 2.39 SJR 1.182 SNIP 2.489
Web of Science (2011): Impact factor 3.368
ISI indexed (2011): ISI indexed yes
Scopus rating (2010): SJR 0.844 SNIP 2.382
Web of Science (2010): Impact factor 2.905
Scopus rating (2009): SJR 1.053 SNIP 2.51
Scopus rating (2008): SJR 0.895 SNIP 3.006
Scopus rating (2007): SJR 0.415 SNIP 2.08
Original language: English
DOIs: