Discovering Unique, Low-Energy Transition States Using Evolutionary Molecular Memetic Computing - DTU Orbit (01/08/2017)

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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
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Pages: 54-63
Publication date: 2013
Main Research Area: Technical/natural sciences

Publication information
Journal: IEEE Computational Intelligence Magazine
Volume: 8
Issue number: 3
ISSN (Print): 1556-603x
Ratings:
Web of Science (2017): Indexed Yes
Scopus rating (2016): SJR 1.236 SNIP 3.164 CiteScore 2.96
Scopus rating (2015): SJR 0.784 SNIP 2.181 CiteScore 1.89
Scopus rating (2014): SJR 0.903 SNIP 2.327 CiteScore 1.99
Scopus rating (2013): SJR 1.445 SNIP 3.001 CiteScore 2.71
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 1.597 SNIP 4.047 CiteScore 3
ISI indexed (2012): ISI indexed yes
Scopus rating (2011): SJR 1.231 SNIP 2.417 CiteScore 2.39
ISI indexed (2011): ISI indexed yes
Scopus rating (2010): SJR 0.832 SNIP 2.171
Scopus rating (2009): SJR 0.954 SNIP 2.1
Scopus rating (2008): SJR 0.848 SNIP 2.888
Scopus rating (2007): SJR 0.389 SNIP 1.178
Original language: English
DOIs: 10.1109/MCI.2013.2264252
Source: dtu
Source-ID: n::oai:DTIC-ART:iel/389622202::30470
Publication: Research - peer-review > Journal article – Annual report year: 2013