Accepted Manuscript

Application of singular value decomposition to the inter-fragment interaction energy analysis for ligand screening

Keiya Maruyama, Yinglei Sheng, Hirofumi Watanabe, Kaori Fukuzawa, Shigenori Tanaka

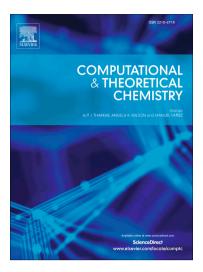
PII: S2210-271X(18)30122-1

DOI: https://doi.org/10.1016/j.comptc.2018.04.001

Reference: COMPTC 2768

To appear in: Computational & Theoretical Chemistry

Received Date: 28 February 2018
Revised Date: 31 March 2018
Accepted Date: 2 April 2018



Please cite this article as: K. Maruyama, Y. Sheng, H. Watanabe, K. Fukuzawa, S. Tanaka, Application of singular value decomposition to the inter-fragment interaction energy analysis for ligand screening, *Computational & Theoretical Chemistry* (2018), doi: https://doi.org/10.1016/j.comptc.2018.04.001

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

ACCEPTED MANUSCRIPT

Application of singular value decomposition to the inter-fragment interaction energy analysis for ligand screening

Keiya Maruyama¹, Yinglei Sheng¹, Hirofumi Watanabe², Kaori Fukuzawa³, Shigenori Tanaka^{1*}

- Department of Computational Science, Graduate School of System Informatics, Kobe University, 1-1 Rokkodai, Nada-ku, Kobe, Hyogo 657-8501, Japan
- 2 Education Center on Computational Science and Engineering, Kobe University, 7-1-48 Minatojima-minamimachi, Chuo-ku, Kobe 650-0047, Japan
- Department of Physical Chemistry, School of Pharmacy and Pharmaceutical Sciences, Hoshi University, 2-4-41 Ebara, Shinagawa-ku, Tokyo 142-8501, Japan *email: tanaka2@kobe-u.ac.jp

Keywords: p38 MAP kinase; Ligand binding; Fragment Molecular Orbital (FMO) method; Inter-Fragment Interaction Energy (IFIE); Singular Value Decomposition (SVD)

Download English Version:

https://daneshyari.com/en/article/7838831

Download Persian Version:

https://daneshyari.com/article/7838831

<u>Daneshyari.com</u>