Accepted Manuscript

Title: A comprehensive conformational space analysis of N-formyl-L-Tryptophanamide system by using a genetic algorithm for multi-modal search

Authors: Anouar El Guerdaoui, Rachida Tijar, Brahim El Merbouh, Malika Bourjila, Rachid Drissi El Bouzaidi, Abderrahman El Gridani

PII: \$1093-3263(16)30451-X

DOI: http://dx.doi.org/doi:10.1016/j.jmgm.2017.05.008

Reference: JMG 6918

To appear in: Journal of Molecular Graphics and Modelling

Received date: 6-12-2016 Revised date: 28-4-2017 Accepted date: 15-5-2017

Please cite this article as: Anouar El Guerdaoui, Rachida Tijar, Brahim El Merbouh, Malika Bourjila, Rachid Drissi El Bouzaidi, Abderrahman El Gridani, A comprehensive conformational space analysis of N-formyl-L-Tryptophanamide system by using a genetic algorithm for multi-modal search, Journal of Molecular Graphics and Modellinghttp://dx.doi.org/10.1016/j.jmgm.2017.05.008

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.



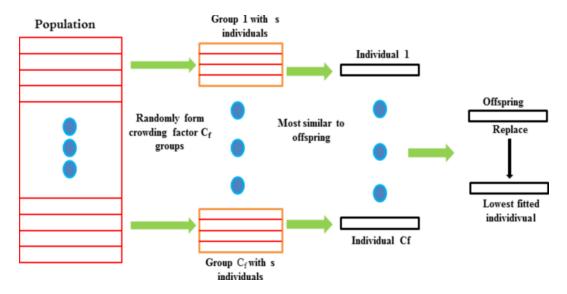
ACCEPTED MANUSCRIPT

A comprehensive conformational space analysis of N-formyl-L-Tryptophanamide system by using a genetic algorithm for multi-modal search

Anouar El Guerdaoui^{a*}, Rachida Tijar^a, Brahim El Merbouh^a, Malika Bourjila^a, Rachid Drissi El Bouzaidi^{a,b}, Abderrahman El Gridani^a

(*) to whom correspondence must be addressed: anouareguerdaoui@gmail.com; tel: ± 212610609070

Graphical abstract



Highlights:

- The potential energy surface of N-formyl-L-Tryptophanamide was explored using stochastic method combined with electronic structure calculations
- The electrostatic interactions induced by the indole ring side chain play a primordial role in the stability of the detected conformers.
- β_L and the γ_L are the most stable and populated building units among the the 9 legitimate areas predefined on the ramachandran map.

^a Equipe de Chimie Théorique, Electrochimie et Environnement CT2E, Faculté des Sciences, B.P. 8106, Université Ibn Zohr, 80000, Agadir, Maroc

^b Centre Régional des Métiers de l'Education et de la Formation (CRMEF), Souss Massa Daraa, Inezgane, Maroc

Download English Version:

https://daneshyari.com/en/article/4953056

Download Persian Version:

https://daneshyari.com/article/4953056

<u>Daneshyari.com</u>