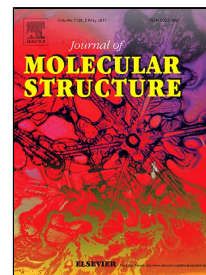


Accepted Manuscript



Combined 3D-QSAR and Molecular Docking Study on 7,8-dialkyl-1,3-diaminopyrrolo-[3,2-f] Quinazoline Series Compounds to understand the binding mechanism of DHFR Inhibitors

Adnane Aouidate, Adib Ghaleb, Mounir Ghamali, Samir Chtita, M'barek Choukrad, Abdelouahid Sbai, Mohammed Bouachrine, Tahar Lakhliifi

PII: S0022-2860(17)30300-9

DOI: 10.1016/j.molstruc.2017.03.039

Reference: MOLSTR 23535

To appear in: *Combined 3D-QSAR and Molecular Docking Study on 7,8 dialkyl-1,3-diaminopyrrolo-(3,2-f) Quinazoline Series Compounds to understand the binding mechanism of DHFR Inhibitors*

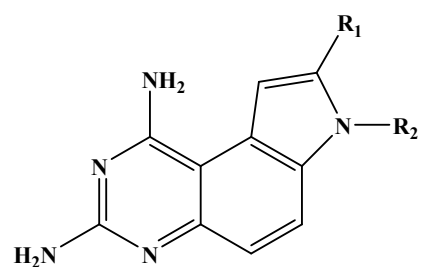
Received Date: 18 January 2017

Revised Date: 06 March 2017

Accepted Date: 08 March 2017

Please cite this article as: Adnane Aouidate, Adib Ghaleb, Mounir Ghamali, Samir Chtita, M'barek Choukrad, Abdelouahid Sbai, Mohammed Bouachrine, Tahar Lakhliifi, Combined 3D-QSAR and Molecular Docking Study on 7,8-dialkyl-1,3-diaminopyrrolo-[3,2-f] Quinazoline Series Compounds to understand the binding mechanism of DHFR Inhibitors, *Combined 3D-QSAR and Molecular Docking Study on 7,8 dialkyl-1,3-diaminopyrrolo-(3,2-f) Quinazoline Series Compounds to understand the binding mechanism of DHFR Inhibitors* (2017), doi: 10.1016/j.molstruc.2017.03.039

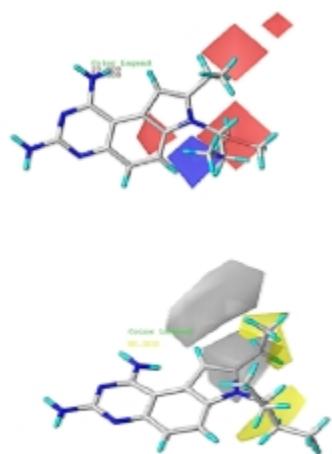
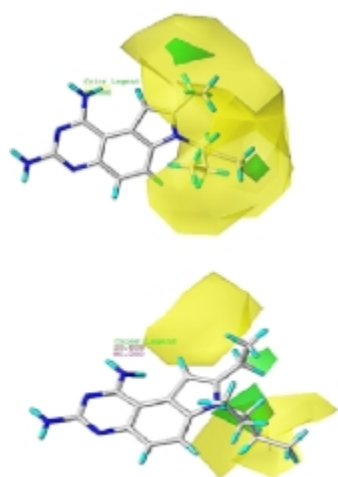
This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please 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.



7,8-dialkyl-1,3-diaminopyrrolo-[3,2-f] Quinazoline derivatives

3D-QSAR (CoMFA and CoMSIA)

Molecular Docking



Quantitative structure activity relationship

The binding mechanism between ligand and protein

Leads DHFR drug candidates

Download English Version:

<https://daneshyari.com/en/article/5161277>

Download Persian Version:

<https://daneshyari.com/article/5161277>

[Daneshyari.com](https://daneshyari.com)