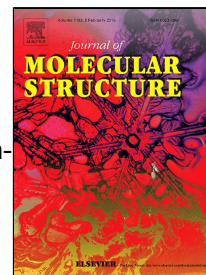


Accepted Manuscript



Carbonic anhydrase inhibition of Schiff base derivative of imino-methyl-naphthalen-2-ol: Synthesis, structure elucidation, molecular docking, dynamic simulation and density functional theory calculations

Saghir Abbas, Hafiza Huma Nasir, Sumera Zaib, Saqib Ali, Tariq Mahmood, Khurshid Ayub, Muhammad Nawaz Tahir, Jamshed Iqbal

PII: S0022-2860(17)31574-0
DOI: 10.1016/j.molstruc.2017.11.086
Reference: MOLSTR 24573
To appear in: *Journal of Molecular Structure*
Received Date: 16 October 2017
Revised Date: 19 November 2017
Accepted Date: 20 November 2017

Please cite this article as: Saghir Abbas, Hafiza Huma Nasir, Sumera Zaib, Saqib Ali, Tariq Mahmood, Khurshid Ayub, Muhammad Nawaz Tahir, Jamshed Iqbal, Carbonic anhydrase inhibition of Schiff base derivative of imino-methyl-naphthalen-2-ol: Synthesis, structure elucidation, molecular docking, dynamic simulation and density functional theory calculations, *Journal of Molecular Structure* (2017), doi: 10.1016/j.molstruc.2017.11.086

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.

Highlights

- Design and synthesis of Schiff base derivative
- Characterization by FT-IR, ^1H and ^{13}C NMR spectroscopy.
- Single crystal X-ray diffraction and NMR studies were performed.
- The synthetic compound was active against carbonic anhydrase II.
- Molecular docking and dynamic simulations studies were carried out.

Download English Version:

<https://daneshyari.com/en/article/7808474>

Download Persian Version:

<https://daneshyari.com/article/7808474>

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