

Accepted Manuscript

A combined experimental and *in silico* characterization to highlight additional structural features and properties of a potentially new drug

Isadora T.S. Bastos, Fanny N. Costa, Tiago F. Silva, Eliezer J. Barreiro, Lídia M. Lima, Delson Braz, Giuseppe M. Lombardo, Francesco Punzo, Fabio F. Ferreira, Regina C. Barroso

PII: S0022-2860(17)30841-4

DOI: [10.1016/j.molstruc.2017.06.061](https://doi.org/10.1016/j.molstruc.2017.06.061)

Reference: MOLSTR 23947

To appear in: *Journal of Molecular Structure*

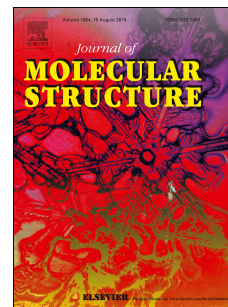
Received Date: 21 February 2017

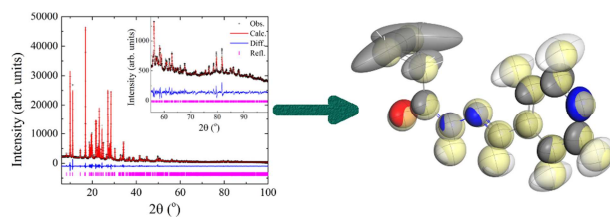
Revised Date: 13 June 2017

Accepted Date: 14 June 2017

Please cite this article as: I.T.S. Bastos, F.N. Costa, T.F. Silva, E.J. Barreiro, Lí.M. Lima, D. Braz, G.M. Lombardo, F. Punzo, F.F. Ferreira, R.C. Barroso, A combined experimental and *in silico* characterization to highlight additional structural features and properties of a potentially new drug, *Journal of Molecular Structure* (2017), doi: 10.1016/j.molstruc.2017.06.061.

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.





Inference of anisotropic atomic displacement parameters by integrating X-ray powder diffraction data and a molecular dynamics calculation.

ACCEPTED MANUSCRIPT

Download English Version:

<https://daneshyari.com/en/article/5160310>

Download Persian Version:

<https://daneshyari.com/article/5160310>

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