

Accepted Manuscript

The electronic density obtained from a QTAIM analysis used as molecular descriptor.
A study performed in a new series of DHFR inhibitors

Rodrigo D. Tosso, Marcela Vettorazzi, Sebastian A. Andujar, Lucas J. Gutierrez,
Juan C. Garro, Emilio Angelina, Ricaurte Rodríguez, Fernando D. Suvire, Manuel
Nogueras, Justo Cobo, Ricardo D. Enriz

PII: S0022-2860(16)31379-5

DOI: [10.1016/j.molstruc.2016.12.060](https://doi.org/10.1016/j.molstruc.2016.12.060)

Reference: MOLSTR 23258

To appear in: *Journal of Molecular Structure*

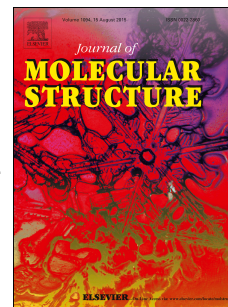
Received Date: 13 September 2016

Revised Date: 20 December 2016

Accepted Date: 22 December 2016

Please cite this article as: R.D. Tosso, M. Vettorazzi, S.A. Andujar, L.J. Gutierrez, J.C. Garro, E. Angelina, R. Rodríguez, F.D. Suvire, M. Nogueras, J. Cobo, R.D. Enriz, The electronic density obtained from a QTAIM analysis used as molecular descriptor. A study performed in a new series of DHFR inhibitors, *Journal of Molecular Structure* (2017), doi: 10.1016/j.molstruc.2016.12.060.

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.

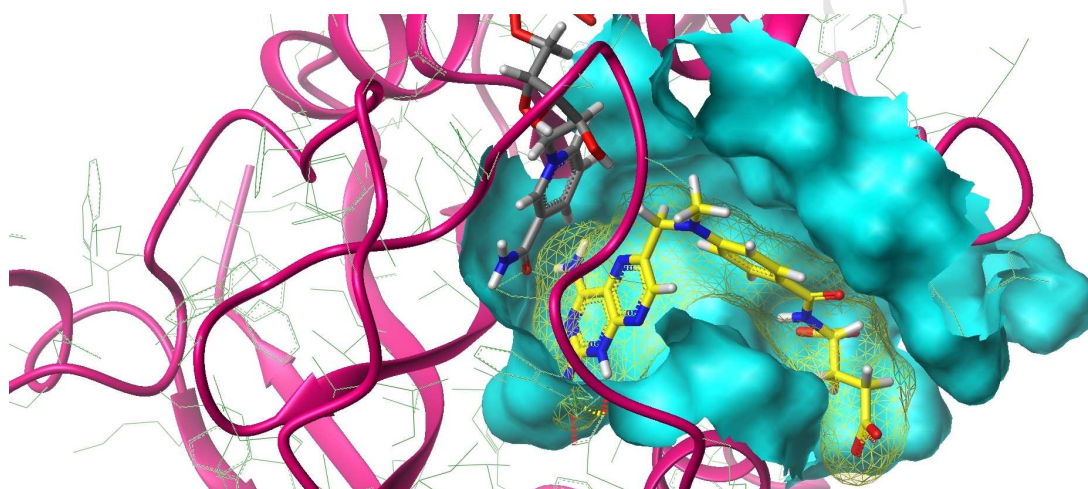


Graphical Abstract

The electronic density obtained from a QTAIM analysis used as molecular descriptor. A study performed in a new series of DHFR inhibitors

Rodrigo D. Tosso, Marcela Vettorazzi, Sebastian A. Andujar, Lucas J. Gutierrez, Juan C. Garro, Emilio Angelina, Ricaurte Rodríguez, Fernando D. Suvire, Manuel Nogueras, Justo Cobo and Ricardo D. Enriz

Departamento de Química, Facultad de Química, Bioquímica y Farmacia, Universidad Nacional de San Luis, Chacabuco 915, 5700 San Luis, Argentina



Download English Version:

<https://daneshyari.com/en/article/5160729>

Download Persian Version:

<https://daneshyari.com/article/5160729>

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