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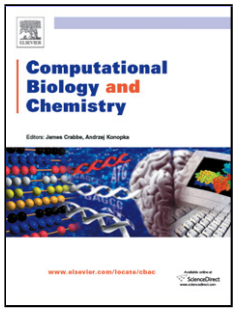

Title: Experimental and density functional theory studies on benzalkonium ibuprofenate, a double active pharmaceutical ingredient

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PII: S1476-9271(17)30667-9
DOI: https://doi.org/10.1016/j.compbiolchem.2017.12.004
Reference: CBAC 6762

To appear in: *Computational Biology and Chemistry*

Received date: 21-9-2017
Revised date: 21-11-2017
Accepted date: 8-12-2017

Please cite this article as: Safna Hussan, K.P., Thayyil, M.Shahin, Rajan, Vijisha K., Muraleedharan, K., Experimental and density functional theory studies on benzalkonium ibuprofenate, a double active pharmaceutical ingredient.Computational Biology and Chemistry https://doi.org/10.1016/j.compbiolchem.2017.12.004

Experimental and density functional theory studies on benzalkonium ibuprofenate, a double active pharmaceutical ingredient

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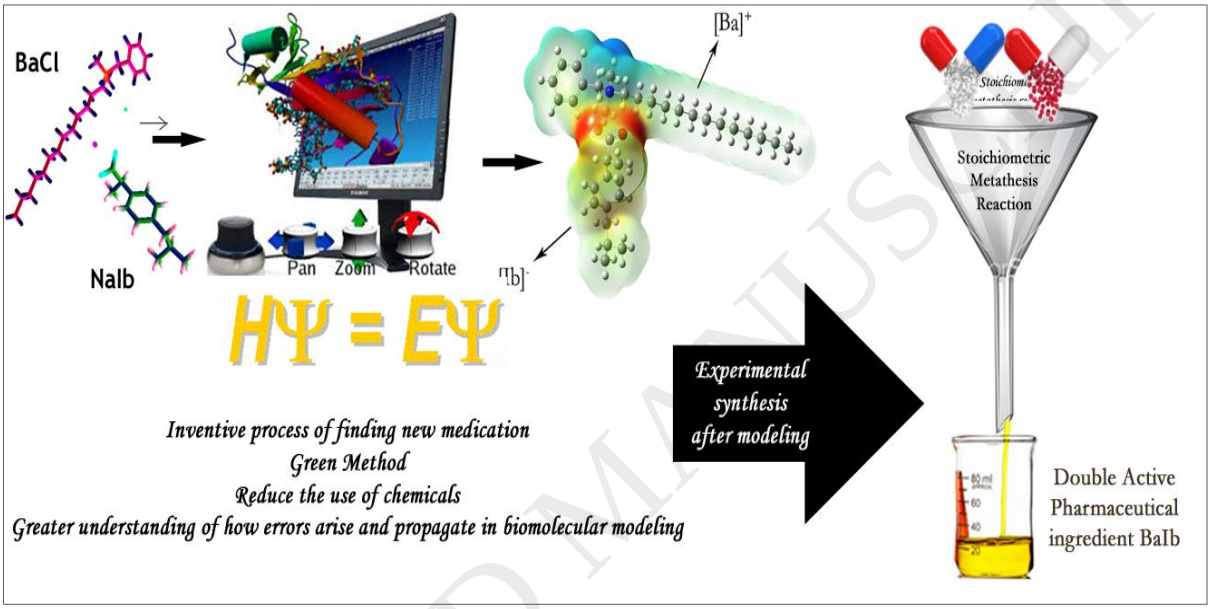
Graphical Abstract



Highlights

- ♦ Studies on a double active pharmaceutical ingredient benzalkonium ibuprofenate
- ♦ Predicted aromaticity, delocalization effects & stabilization energy *via* NBO analysis
- ♦ BaIb is stable with better biological activity than its parent drugs.
- ♦ Ib^- is an excellent precursor for the synthesis of double active pharmaceutical ingredient

ABSTRACT

Molecular aspects of a double active pharmaceutical ingredient in ionic liquid form, benzalkonium ibuprofenate (BaIb), were studied using density functional theory (DFT/B3LYP/6-31+G (d, p)). A detailed discussion on optimized geometry, energy, heat and the enthalpy of BaIb was carried out. The computed vibrational results agree well with the experimental results. The stability and biological activity were compared to the parent drugs on the basis of global descriptive parameters. The electrophilic and nucleophilic sites were pointed out in the MESP structures well evidently. NBO analysis was also done to predict the