International Journal of ChemTech Research
CODEN (USA): IJCRGG, ISSN: 0974-4290, ISSN(Online):2455-9555
Vol.14 No.01, pp 214-223, 2021

Quantum Chemical Analysis, Biological Activity and *In-Silico* ADME Properties of N,N´ - Diphenylguanidinium Hydrogen (+) –L-Tartrate Monohydrate

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Abstract : Good quality single crystal of N,N´ -Diphenylguanidinium Hydrogen (+) – L-Tartrate Monohydrate (DPGTM) was grown by low temperature solution growth. The lattice parameters and crystal system were elucidated by single crystal X-ray diffraction analysis. The molecular structure of DPGTM was optimized by DFT/B3LYP level. The UV-vis spectral activity was computed from optimized molecular structure in order to understand the electronic properties. The HOMO-LUMO analysis was carried out in order to assess the charge transfer and various chemical factors. The thermodynamic properties were computed and examined. The biological activities of DPGTM were expounded. The pre-ADME and pharmacokinetics activities of DPGTM were evaluated through, absorption, distribution, metabolism, excretion (ADME) properties.
Key Words : Crystal growth, DFT, UV-vis spectral analysis, Biological activity, ADME.

DOI= http://dx.doi.org/10.20902/IJCTR.2021.140120

G. Saravana Kumar *et al* /International Journal of ChemTech Research, 2021,14(1): 214-223.

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