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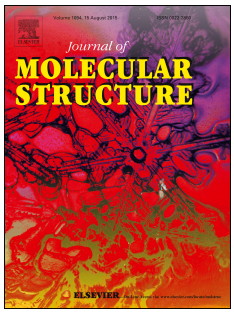

Structure-activity relationship of the ionic cocrystal: 5-amino-2-naphthalene sulfonate·ammonium ions for pharmaceutical applications

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Structure-activity relationship of the ionic cocrystal: 5-amino-2-naphthalene sulfonate· ammonium ions for pharmaceutical applications

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ABSTRACT

The ionic cocrystals of 5-amino-2-naphthalene sulfonate · ammonium ions ($ANSA^{-}\cdot NH4^{+}$) were grown under slow evaporation method and examined in detail for pharmaceutical applications. The crystal structure and intermolecular interactions were studied from the single X-ray diffraction analysis and the Hirshfeld surfaces. The 2D fingerprint plots displayed the inter-contacts possible in the ionic crystal. Computational DFT method was established to determine the structural, physical and chemical properties. The molecular geometries obtained from the X-ray studies were compared with the optimized geometrical parameters calculated using DFT/6-31+G(d,p) method. The band gap energy calculated from the UV-Visible spectral analysis and the HOMO-LUMO energy gap are compared. The theoretical UV-Visible calculations helped in determining the type of electronic transition taking place in the title molecule. The maximum absorption bands and transitions involved in the molecule represented the drug reaction possible. Non-linear optical properties were characterized from SHG efficiency measurements experimentally and the NLO parameters are also calculated from the optimized structure. The reactive sites within the molecule are detailed from the MEP surface maps. The molecular docking studies evident the structure-activity of the ionic cocrystal for anti-cancer drug property.

Keywords: Ionic Cocrystals; SCXRD; DFT; HOMO-LUMO energy gap; antioxidant activity; molecular docking

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