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Research Articles

Validation of crystal structure of 2-acetamidophenyl acetate: an experimental and theoretical study

S. M. Shankar, **A. David Stephen**, C. Pitchumani Violet Mary, Hemamalini Madhukar, Necmi Dege, Nermin Kahveci Yagcl, ...show all

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Abstract

In this present study, we have determined the crystal structure of 2-acetamidophenyl acetate (2-AAPA) commonly used as influenza neuraminidase inhibitor, to analyze the polymorphism. Molecular docking and molecular dynamics have been performed for the 2-AAPA-neuraminidase complex as the ester-derived benzoic group shows several biological properties. The X-ray diffraction studies confirmed that the 2-AAPA crystals are stabilized by N–H···O type of intermolecular interactions. Possible conformers of 2-AAPA crystal structures were computationally predicted by *ab initio* methods and the stable crystal structure was identified. Hirshfeld surface analysis of both experimental and predicted crystal structure exhibits the intermolecular interactions associated with 2D fingerprint plots. The lowest docking score and intermolecular interactions of 2-AAPA molecule against influenza neuraminidase confirm the binding affinity of the 2-AAPA crystals. The quantum theory of atoms in molecules analysis of these intermolecular interactions was implemented to understand the charge density redistribution of the molecule in the active site of influenza neuraminidase to validate the strength of the interactions.

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