SYNTHESIS, CHARACTERIZATION, HIRSHFELD AND ADMET ESTIMATION STUDIES OF A NOVEL OF 3-(2,4,6-TRIMETHYL-PHENYLAMINO)-BUT-2-ENOIC ACID ETHYL ESTER

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Abstract. The title compound 3-(2,4,6-timethyl-phenylamino)-but-2-enoic acid ethyl ester (**3**) was obtained by condensation reaction of ethyl acetoacetate and 2,4,6-trimethyl-phenylamine, in the presence of $CoCl_2$.The structure of the synthesized enaminoester was identified thanks to NMR spectroscopy, and stabilized by intramolecular interactions. The intermolecular contacts were further analyzed by the mapping of contacts descriptors d_{norm}, d_e, d_i, the shape-by-Shape index and surface property by electrostatic potential mapped on the Hirshfeld surface (HS). Data from density functional theory (DFT) was compared to experimental results for this process. Global reactivity factors such electronegativity, chemical hardness, potential, and softness were calculated using DFT. The effects of the molecular environment were accessed by analyzing the electrostatic potentials surface mapped over the HS and the 3D-topology of energy frameworks. As a potential bioactive molecule, the physicochemical and ADME-Tox predictions were performed suggesting that compound **3** could be considered as promising drug candidate.

Keywords: β-enaminoester; X-ray diffraction, monoclinic space, Hirshfeld surface, ADME-Tox.