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SYNTHESIS, CHARACTERIZATION, HIRSHFELD AND ADMET ESTIMATION STUDIES OF NOVEL 3-(2,4,6-TRIMETHYL-PHENYLAMINO)-BUT-2-ENOATE

Mohamed Loughzail [a], Koffi Senam Etsè [b], Zaragoza Verez Guillermo [c], Rachid Touzani [d], Anna Moliterni [e], Abdessamad Tounsi [f], Mohamed Anouar Harrad [f,g*]

[a]*Molecular Chemistry Laboratory, Cadi Ayyad University, Marrakech 40000, Morocco*
[b]*Medicinal Chemistry Laboratory, Center for Interdisciplinary Research on Medicines (CIRM), University of Liège, B36 Av. Hippocrate 15 B-4000 Liege, Belgium*
[c]*X-Ray Diffraction Unit, RIAIDT, University of Santiago de Compostela, Campus VIDA, 15782 Santiago de Compostela, Spain*
[d]*Applied Chemistry and Environment Laboratory, University of Mohamed 1, Oujda, Morocco.*
[e]*Institute of Crystallography Via Amendola, 122/O, Bari 70126, Italy*
[f]*Environmental, Ecological, and Agro-Industrial Engineering Laboratory, Sultan Moulay Slimane University, Beni-mellal 23000, Morocco*
[g]*Regional center for Education training and formation, CRMEF 40000 Marrakech-Safi, Morocco*
[*]*e-mail: ma.harrad@yahoo.fr*

Abstract. The title compound 3-(2,4,6-timethyl-phenylamino)-but-2-enoate was obtained by condensation reaction of ethyl acetoacetate and 2,4,6-trimethyl-phenylamine. X-ray structural analysis identified the structure of the synthetized *β*-enaminoester, NMR spectroscopy complemented it, and the structure stabilized by intramolecular interactions. The intermolecular contacts were further analysed 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 analysing 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, ADMET-Tox.

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