Synthesis, Quantum Chemical Calculations, Molecular Docking Studies and Anion Sensor Properties of Vanillin Schiff Base

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In this study, the new a novel bidentate Schiff base has been synthesized by the reaction of 4-ethoxyaniline with 3-Methoxy-4-hydroxybenzaldehyde. The chemical structure was determined through spectroscopic and crystallographic methods. The compound crystallize in the monoclinic space group P21/c with a = 10.3120(1), b = 9.9950(1), c = 26.5762(4) Å, β= 92.276(1)°, V =2737.01(6) Å^3, D_x = 1.160 g.cm^{-3}, respectively. It was investigated for its ability selectively sense anions [1-2].

The molecular docking was also done to identify the interaction of the title compound with the DNA [3]. Moreover, theoretical and experimental structures were compared using quantum-mechanical calculations [4]. In addition, atomic charges, molecular electrostatic potential (MEP), nonlinear optical (NLO) effects and thermodynamic properties of the title compound was predicted using DFT [5].

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