DFT calculation, biological activity, anion sensing application studies and crystal structure of (E)-4-methoxy-2-((4-methylbenzo[d]thiazol-2-ylimino)methyl)phenol

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Abstract: (E)-4-methoxy-2-((4-methylbenzo[d]thiazol-2-ylimino)methyl)phenol was synthesized from the reaction of 4-methylbenzo[d]thiazol-2-amine with 2-hydroxy-5-methoxybenzaldehyde. The structure of compound has been investigated by using FT-IR, UV-VIS, \textsuperscript{1}H-NMR, \textsuperscript{13}C-NMR spectroscopic and X-ray crystallographic techniques. The molecular structure, HOMO-LUMO analysis, molecular electrostatic potential (MEP) and nonlinear optical (NLO) effects of the compound were investigated by using DFT calculations. Additionally, the title compound was tested for its biological activity. UV-Vis spectroscopic studies of the interactions between the Schiff base and calf thymus DNA (CT-DNA) showed that the compound interacts with CT-DNA. The colorimetric response of the compound receptors was investigated before and after the addition of an equivalent amount of each anion to evaluate anion recognition properties.

Keywords: Biology activity; DFT calculations; Calf thymus DNA; Anion sensing; X-ray