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A rhodanine derivative as a potential antibacterial and anticancer agent: Crystal structure, spectral characterization, DFT calculations, *Hirshfeld* surface analysis, *in silico* molecular docking and ADMET studies

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ABSTRACT

A novel rhodanine derivative, namely 5-(4-dimethylaminobenzylidene) rhodanine "$C_{12}H_{12}N_2OS_2$", was successfully crystallized from condensation route and characterized by NMR, FT-IR, UV–Vis spectral methods as well as single-crystal X-ray diffraction. This rhodanine derivate crystallizes in the monoclinic $P2_1/c$ space group, with the cell parameters: a = 3.93590(10), b = 11.2480(3), c = 26.6703(7) Å and β = 93.8530(10)°. The molecular structure displays intra- (C – S···H) and intermolecular ($N - H$···O) hydrogen-bonding interactions. Micro-spectroscopy performed on single-crystals of the studied compound revealed the first absorption transition at 2.25 eV, and a well-structured luminescence peaked at 2.01 eV (0.15 eV broad). Density functional theory (DFT) calculations allowed the structure optimization, the electronic properties, the IR-vibrational modes and frequencies as well as the ^{1}H and ^{13}C NMR chemical shifts' calculation. Furthermore, time-dependent DFT (TD-DFT) calculations were performed for the vertical transition energies. *Hirshfeld* surface analysis (**HSA**) showed the presence of non-conventional C–H···H–C, C–H···π and π···*lp* interactions and $\pi - \pi$ stacking. The anti-cancer and anti-bacterial activities of the studied compound towards the Polo-like kinase PLK1 and the *Escherichia coli* MurB enzymes were *in silico* evaluated by performing molecular docking simulations. The results suggest that the molecule can significantly inhibit the enzymes' active sites. Additionally, the physicochemical and pharmacokinetic characteristics of the molecule were evaluated through absorption, distribution, metabolism, excretion and toxicity (ADMET) analysis, and the results ensure its good drug-likeness properties.

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