SYNTHESIS, MOLECULAR STRUCTURE, VIBRATIONAL CHARACTERISTICS, PROFILES OF OTHER MOLECULAR PROPERTIES AND ANTICANCER ACTIVITY OF 2-((2-AMINOPYRIDIN-3-YL)METHYLENE)-N-PHENYLHYDRAZINECARBOTHIOAMIDE AS PROVIDED BY SPECTROSCOPIC AND DFT INVESTIGATIONS

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Synthesis of 2-((2-aminopyridin-3-yl)methylene)-N-phenylhydrazinecarbothioamide (APHB) was attempted. Elemental analysis and NMR spectra were used to ascertain its formation. Torsional potential energy scans, for all the rotating bonds were made to get approximate initial values of dihedral angles. FT-IR, FT Raman, and UV-Vis spectra were measured for APHB. Their anticancer activity was determined experimentally, for human carcinoma cell lines pertaining to liver, colorectal, and lung. Barrier heights, around six rotating bonds in APHB were computed. Optimized structure parameters, general valence force field, harmonic vibrational fundamentals, potential energy distribution, infrared and Raman intensities, frontier molecular orbital (FMO) parameters, NLO behaviour, and NBO characteristics were determined using DFT/B3LYP/6-311++G(d,p) level of theory. TD-DFT was used to compute absorption maxima (λ_{max}) of electronic transitions for the molecule in DMSO-d_6 solvent. Frontier molecular orbitals were used to understand origin of UV-Vis spectrum and chemical reactivity of the molecule. Good agreement was found between measured and computed structure parameters, IR, Raman and UV-Vis spectra. The rms error between experimental and theoretical vibrational frequencies was 9.5 cm^{-1}, for APHB. All vibrational fundamentals were assigned unambiguously. The computations demonstrated that the molecule was good for NLO applications, which was substantiated by NBO analysis. Existence of bifurcated intramolecular hydrogen bond was predicted for APHB.