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Benzothiazole-derived Compound with Antitumor Activ?iy: Molecular Structure Determination Using Density Functional Theory (Dft) Method

The Gaussian computational chemistry software package was employed to investigate the molecular structure and energetics of benzothiazole, a compound known for its anti-tumor properties. Density functional theory (DFT) calculations were conducted using the Becke, 3-parameter, Lee-Yang-Parr (B3LYP) method, coupled with the LanL2DZ basis set. Molecular structure optimization was carried out to determine the most stable configurations of the benzothiazole compound. Furthermore, thorough analyses of molecular orbital energies, molecular properties, and molecular electrostatic potential surface maps were performed on the optimized molecular system. Our current research suggests that the compound 2-(4-aminophenyl) benzothiazole, containing benzothiazole, maybe a potential drug candidate for free radical species on cells due to its anti-cancer properties.