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DFT, wave function analyses of protocatechualdehyde, a natural product

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Protocatechualdehyde (3,4-dihydroxybenzaldehyde) is a structurally familiar molecule. In its structure, an electron-withdrawing moiety (–CHO) and two electron donor groups (–OH) are present at neighbouring positions. A bridge and π-linker (aromatic ring) interconnect them. As a consequence, electrons may travel from the donor to the acceptor through the bridge. Gaussian 16W has been employed for all investigations on the DFT/B3LYP/6-311++G(d,p) basis set. MEP analysis predicts that the molecule has electrophilic and nucleophilic domains. Frontier energy gap analysis implies that the molecule is hard and stable. The NBO analysis reports the same results. The IEFPCM solvation effect has been studied for MEP, Mulliken charge, FMO, and UV-Vis spectra. The shaded surface map, NCI, STM, and electron transport studies have been conducted using the Multiwfn 3.8 software. The electron transport analysis results reveal that charge transfer is possible in the S0 → S4, S9, and S10 excitation states. The molecular docking study has been conducted using PyRx. *In silico* toxicity analysis and activity predictions, along with comparisons, have been performed using EPA, DSS, TOX and PASS, respectively.

Keywords: Protocatechualdehyde, DFT, NBO, NCI, Hole-electron transport, Toxicity analysis