**Structural, Spectroscopic on structure vibrational spectroscopic, and RDG analysis Molecular docking of biological active 4-(2,3-Dichlorophenyl)piperazin-1-ium picrate**

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This study aims to investigate the structural and vibrational features of 4-(2,3-Dichlorophenyl) piperazin-1-ium picrate based on spectroscopic theoretical quantum chemical approach. The fundamental structural aspects of 4-(2,3-Dichlorophenyl) piperazin-1-ium picrate have been examined based on optimized geometry, spectroscopic behaviour, intermolecular interaction, chemical reactivity, intramolecular hydrogen bonding, and molecular docking analysis. The chemical reactivity and stability were estimated based on the HOMO-LUMO energy gap and NBO approach. The overall picture of accumulation of charges on individual atoms of the molecule was predicted by molecular electrostatic potential (MEP) surface map which in turn identifies the nucleophilic and electrophilic region or sites. The quantitative analysis of electrophilicity and nucleophilicity indices were done by Hirshfeld surface analysis. Molecular docking studies were performed to examine the active binding residues of the target protein.