**Computational and Spectroscopic analysis of L-Histidinium iodide: an antimicrobial analysis**

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**Abstract**

Theoretical study of FT-IR and FT-Raman has been performed utilising vibrational spectroscopy with the DFT method and the basis set 6-311++G. (d, p). The DFT approach was employed in the HOMO-LUMO investigations and MEP studies. UV-Vis spectra have been studied using the TD-SCF method. To understand electron delocalization caused by hyperconjugation, the NBO method was used. The molecule's reactive sites were identified using Fukui functions. The non-bonding interactions were discovered through an NCI study. To investigate the compound's antimicrobial property, a molecular docking analysis was performed. To obtain drug-like properties, the Swiss-ADME mechanism was used.