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12th May 2022

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VIBRATIONAL, ELECTRONIC AND AUTOMATED DOCKING ANALYSIS OF BUTANEDIOL METHANESULFONATE

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Abstract

In this work, Butanediol methanesulfonate (BMS) was characterized by multi-spectroscopic investigations (FT-IR, FT-Raman, UV-vis) and quantum chemical computations employing Density functional theory with cam-B3LYP basis functional. Electronic Chemical stability of the BMS arising from hyper conjugative interactions and charge delocalization was analyzed using natural bond orbital analysis. The assignments of vibrational spectral features were made with the help of Gar2ped which incorporates scaled quantum mechanical force field (SQMFF) methodology. The absolute energy gap between the frontier molecular orbitals (HOMO and LUMO) at room temperature and reactivity descriptors confirm that the molecule BMS is chemically active and the atomic sites prone to electrophilic/nucleophilic attack were recognized form molecular electrostatic potential (MEP) surface and Fukui function analysis. Molecular docking studies, the inhibition activity of BMS against the selected targets.

Keywords: BMS, SQMFF, HOMO, LUMO, MEP