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Study on Structure, Vibrational assignment, NBO- Analysis, HOMO-LUMO, and Molecular Docking of D-Pinitol

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Abstract : The plant source based on natural material products cover a major sector of the biomedical and medical field then the focus on plant research has been increased worldwide. We have performed a structural investigation and spectroscopic studies of a natural plant material product cyclitol: D-Pinitol. The spectroscopic properties of D-Pinitol were analyzed in the present study using FT-IR, FT-Raman spectra in the region of FT-IR (4000-400cm⁻¹ and FT-Raman cm⁻¹). The vibrational frequencies were obtained by DFT-B3LYP/-311++G(d,p) as a basis set. The optimized geometry of D-Pinitol has been elucidated using, vibrational assignment and calculation of potential energy distribution (PED). The charges of atoms and electronic structural system NBO/NLMO. The molecular electrostatic surface and reactivity of this natural molecule have been calculated. The UV-Vis spectrum has been recorded in methanol solvent (MeOH) and electronic properties such as frontier orbitals (FMOs) calculated HOMO-LUMO is measure by the TD-DFT approach. Docking simulation is powerful way to figure out the binding structure of a substrate in its receptor.

Key Words : PED, NBO, FMOs, Docking Study.

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