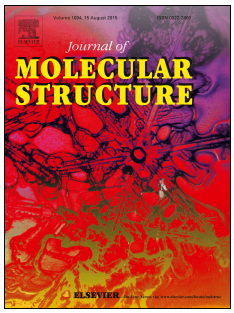
Accepted Manuscript



The vibrational spectroscopic studies and molecular property analysis of Estradiol, Tamoxifen and their interaction by density functional theory

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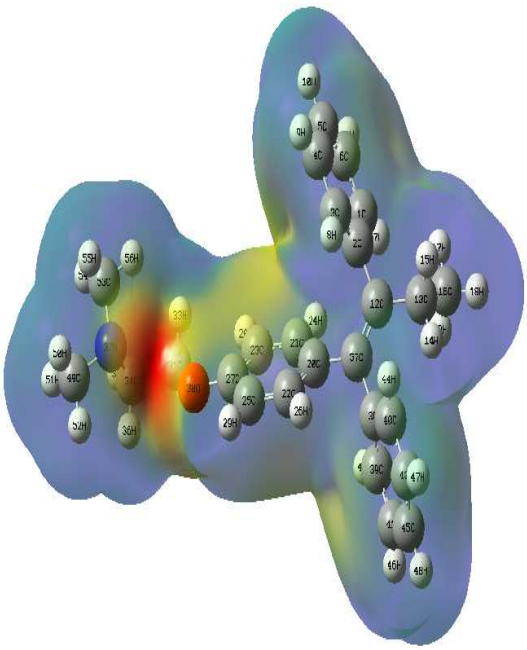
Raman and IR technique have been used to study the vibrational wave numbers. All the normal modes have been assigned and the scaled theoretical results found to be in a good agreement with the experimental findings. The molecular parameters, i.e. the bond lengths and bond angles have been calculated to gain more insights of this molecule. HOMO-LUMO energy gap is also calculated in order to study the electrical properties of the biomolecule. The study is extended to calculate the Natural Bond Orbital and different thermo-dynamical parameters.



Molecular Electrostatic Potential (MEP) surface of Tamoxifen

The Vibrational Spectroscopic studies and molecular property analysis of Estradiol, Tamoxifen and their interaction by Density functional theory

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