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Role of vibrational spectroscopy in characterization of drug-ligand interaction

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Abstract

Vibrational spectroscopy plays an important role in characterization of drug-biomolecular complexes and aids in finding out potential compounds for new hybrid drugs of different kinds of diseases. Vibrational spectroscopy in combination with quantum chemical calculation and molecular modelling has revolutionised the field of spectroscopy in elucidating molecular fingerprint spectra, molecular parameters of the complexes, finding the best binding sites of the receptor and drug complexes. This in turns, assists in finding out the potential of the complexes to be a drug candidature. At this presentation, the interacting states of Estradiol-Tamoxifen drug, L-Threonine-Metformin drug shall be discussed.

Estradiol, a primary female sex hormone is associated with the development and progression of breast cancer, ovarian cancer and endometrial cancer. Tamoxifen is a drug used for the treatment of breast cancer. On the other hand, L-Threonine + Metformin drug (for diabetes) is studied to obtain structural skeleton as well as the characterization of drug-ligand interaction. The interacting environment of drug ligand interaction is studied using DFT method and FTIR and Raman techniques. The biomolecular complexes are optimized using B3LYP/6-31+G(d,p) level of theory. The theoretical spectral data of the drug-ligand interacting states are found correlated with the experimental vibrational spectra.

Fig. 1: The optimized geometrical structure of L-Threonine + Metformine

The molecular parameters such as HOMO-LUMO, NBO, hyperpolarizability, ionization energy, electrophilicity index are reported. The study shall bring new insights about the association states which provide molecular properties essential in finding new potential biomolecular complexes for the development of new hybrid drugs. Molecular docking study reveals the highest binding energy of the interaction of ligand with the chosen receptors.

Keywords: Raman, FTIR, SERS, Vibrational, Docking, DFT

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