9. SUMMARY AND CONCLUSIONS

The activity of certain food preservative chalcones has been experimentally probed by spectroscopic techniques with theoretical aid on quantum chemical computations. Spectroscopic techniques such as FT-IR, FT-Raman and electronic spectra aided by DFT methods, were implemented to predict the active site of the molecule and to get deeper insight into structural and bonding features of the molecules. A brief account of the important conclusion reported in this thesis is summarized as follows.

Structural and bonding features of 1-4-Bromophenyl-3-(2-methoxyphenyl) prop-2-en-1-one have been investigated using quantum chemical calculations and spectral studies. Peculiar blue shift was spectrally identified as an outcome of C–H…O hydrogen-bonding interaction, which was also substantiated by decreasing C–H bond length. Phenyl C–C stretching mode 8 is found to be simultaneously active as strong bands in both IR and Raman because of ICT through conjugated ring path leading to hyperpolarizability enhancement and thereby NLO activity. NPA shows that the highest energetic atomic orbital is located on Br. the conjugation of $C_{12}=O_{13}$ bond with $C_{14}=C_{16}$ increases its single-bond character resulting in red shifting of carbonyl stretching wave numbers. The 2-D finger print plot, shows that the H–H contact contributes a significant amount of (38.4%) to the Hirsfeld surface. It is obviously evident from molecular docking studies that the ligand binds to receptor by hydrogen and hydrophobic bond interactions.

The optimized molecular structure, natural bond orbital analysis, vibrational frequencies, and the corresponding vibrational assignments have been carried out using B3LYP/6-31G** method. The O_9-H_{10} distances involved in hydrogen bonding

are lengthened by 0.019 Å on two molecule modelling. The magnitude of charge transferred from lone pair n (O_{51}) of the hydrogen bonded O atom to the antibond σ* (O_9-H_{10}) significantly increased (0.06096e) upon two molecule modelling providing clear-cut substantiation about the weakening of bonds and their elongation. The red shifted broad and shallow O-H stretching mode offers a valid spectral evidence for O-H…O intermolecular interactions. The normal coordinate analysis envisages a good agreement between the observed and calculated frequencies. It is noted that the IR and Raman peaks in the experimental spectra are red shifted. In Hirsfeld surface analysis the O-H…O and C-H…O interactions show a red colour in the surface indicating the presence of intermolecular interaction. The BCPs located at H_{10}-O_{51}, O_9-H_{55}, H_{11}-O_{51} hydrogen bonds with positive Laplacian electron density confirms the presence of intermolecular interactions.

Theoretical modeling and vibrational spectroscopic studies of (2E)-1-(3-chlorophenyl)-3-(4-chlorophenyl) prop-2-en-1-one and its contributions were analyzed from the optimized structure and vibrational spectral analysis with the aid of density functional theory (DFT) methods. Red shifting of C=O spectral band provides the spectral evidence for the formation of weak intermolecular hydrogen bonding which contributes to the stability of the molecule. Transfer of energy between π antibonding of (C_{18}-C_{19}) with π antibonding of C=O weakens the respective bond. TD-DFT calculated electronic absorption spectra has been analyzed in comparison with the experimental UV-Vis spectrum and infers that the main contribution arises from π-π* bands. The optical band gap measurements show that the band gap energy is about 2.568 eV and the absorption coefficient changes with increasing values of optical band gap. The multi linear regression ratio shows that

the R and R^2 values are close to 1 and it implies good correlation between drug likeness and docking scores. The changing docking score confirms the relation between structure and activity.

Using DFT method the molecular structure of (2E)-3-(3-Bromo-4methoxyphenyl)-1-(pyridin-2-yl) prop-2-en-1-one was modeled and it agrees well with the experimental structure. Blue shifting of (36 cm^{-1}) C-H stretching mode provides the spectral evidence for the intermolecular interactions of C-H...Br. The lowering of stretching wave number of C=O vibration is due to the conjugation of carbonyl group with the neighbouring phenyl ring. Red shifting of C=O spectral band provides the spectral evidence for the formation of weak intermolecular hydrogen bonding which contributes to the stability of the molecule. Transfer of electron charge from π antibonding of C=O to the σ antibonding of C=O causes weakening of the bond and its elongation. Low value of HOMO-LUMO energy gap demonstrates an increasing level of biological activity.

With the aid of quantum chemical computations and vibrational spectral studies the structural and bonding features of the studied compound DINO have been investigated. The experimental vibrational spectra were analyzed and compared with the simulated spectra. The blue shifting of (~33 cm^{-1}) C_{14}-H_{19} stretching mode provides the spectral evidence for the existence of C-H…O intermolecular hydrogen bonding. The Hirsfeld surface analysis and the 2-D finger print plot shows that the O-H intermolecular interactions contribute 28.1% in the region of the fingerprint plot. Positive value of MLR values show that there is a relation between drug likeness and docking scores.