Spectroscopic studies and theoretical calculations have been performed on some pharmaceutically and biologically important four enamide derivative molecules. The compounds employed for investigation are (2E)-3-(2H-1,3-benzodioxol-5-yl)-N-phenylprop-2-enamide (2BNP2E), (2E)-3-(2H-1,3-benzodioxol-5-yl)-N-(4-chlorophenyl)prop-2-enamide (3B5NCE), (2E)-N-phenyl-3-(4H-pyran-4-yl)prop-2-enamide (P3P2E), (2E)-3-(1H-indol-2-yl)-N-phenylprop-2-enamide (2INP).

FT-IR and FT-Raman spectra have been obtained for the investigated compounds. Theoretical calculations were undertaken at the density functional theory (DFT)/B3LYP method with 6-311++G(d,p) basis sets. The above mentioned calculations allowed FT-IR and FT-Raman spectra to be computed at the optimized molecular geometry and the results were compared with the experiments. The molecular geometry of investigated compounds has been provided with the computed bond lengths, bond angles as well as calculated vibrational wavenumbers. The calculated vibrational wavenumbers and chemical shifts were obtained and are found to be in a good agreement with experimental data. The enamide derivative molecules have been screened for their antimicrobial activity and found to exhibit antifungal and antibacterial effects. In addition, the Molecular docking was also performed for the different antimicrobial receptors.

In this present work, the investigation on different structural parameters such as geometrical parameters, structure conformation, energy, NLO, NBO, MEP, Fukui function, antimicrobial and Molecular docking and other molecular properties based on the structure and substitution were elaborately discussed and reported separately. The entire results obtained by this research work on the basis of substitutions in enamide derivatives, theoretical methods etc., the comparative conclusions are listed below.
The four enamide derivative compounds (2BNP2E, 3B5NCE, P3P2E and 2INP) were successfully synthesized and characterized. All the molecules characterized by FT-IR, FT-Raman and tools derived from the density functional theory. In all the molecules, the theoretically calculated optimized bond lengths are comparatively larger than the experimental values. These indicate that the theoretical calculation refer to isolated molecules in the gas phase while the experimental results belong to solid phase.

The energy gap was calculated. In the entire enamide molecules lower band gap energy is indentified. The lower band gap energy explains the eventual charge transfer interactions taking place within the molecule. The nonlinear optical (NLO) response was noticed in the 2BNP2E, 3B5NCE, P3P2E and 2INP molecules. The computed first order hyperpolarizability of all the molecules were 13.586, 16.4610, 10.2210 and 2.6366X 10\(^{-30}\) esu respectively suggest that the investigated molecules have potential for future NLO applications. Reactive sites for the all semicarbazide derivative compounds were identified from MEP analysis. Stability of the entire molecules arising from hyperconjugative interactions and charge delocalization has been analyzed using NBO analysis. The antimicrobial activity of all the molecules 2BNP2E, 3B5NCE, P3P2E and 2INP are found to be high. However the molecular docking results of enamide derivative molecules suggest that 2BNP2E and 3B5NCE molecule has higher antimicrobial activity when compared to all other molecules.

Theoretical calculations gave the thermodynamic properties (heat capacity, entropy and enthalpy) for the compounds. From these it is observed that these thermodynamic functions were found to increase with temperatures ranging from 100 to 1000 K. This can be attributed as due to the fact that the molecular vibrational intensities increase with temperature. By analyzing the overall
results obtained in this research on different parameters, among DFT/B3LYP method, the results obtained by 6-311++G(d,p) basis set show a pleasing, accurate and precise qualitative agreement with the experimental findings by applying suitable scaling factors.

We hope our results will be of assistance in the quest of the experimental and theoretical evidence for the investigated compounds in reaction intermediates, nonlinear optical and antimicrobial materials and will also be helpful for the design and synthesis of new enamide materials.