**SPECTROSCOPIC ANALYSIS, DFT CALCULATIONS AND DOCKING STUDIES OF 3-ACETYLQUINOLINE**

**Prabeena Jelin A. Pa,b, Jebalenet. Ja & T. F Abbs Fen Rejia\***

a Department of Chemistry & Research Centre, Nesamony Memorial Christian College, Marthandam, Tamilnadu, India

b Research Scholar, Reg. No : 23213112032005, Affiliated to Manonmaniam Sundaranar University, Tirunelveli, Tamilnadu, India

Quinolines and its derivatives are widely used in medicinal chemistry and are present in various natural products. In this work we report a combined experimental and theoretical study on molecular structure and vibrational analysis of 3-acetylquinoline. The electronic structure of 3-acetylquinoline has been computed theoretically using the Gaussian 09 W package of program using B3LYP\6-31G level of theory. The chemical descriptors such as Ionization potential, Electron affinity, total density, electrostatic potential, electronegativity, hardness, softness, bond angle, bond length, dihedral angle, and intensities of the titled compounds were investigated. The Mullikan population analysis on atomic charges also calculated. The HOMO – LUMO analysis was used to determine the charge transfer within the molecule. IR Spectra, obtained and assigned by vibrational analysis are compared with the experimental FT-IR results. The insilico docking studies were carried out using AutoDock 1.5.7 software. The docking energy of 3-acetylquinoline with 4I2P is -9.0 kcal\mol.

**Keywords:** Gaussian, quinoline, DFT, docking