# CHAPTER II

## REVIEW OF LITERATURE

### 2.1 REVIEW OF LITERATURE ON SPECTROSCOPY AND BIOACTIVITY OF CHALCONE COMPOUNDS

Literature review is a basis for research in nearly every academic field [5]. The process of reviewing the literature requires different kinds of activities and ways of thinking.The literature review plays an extremely important role in shaping the research problem because the process of reviewing the literature helps to understand the subject area better and thus helps to conceptualize the research problem clearly and precisely and makes it more relevant and pertinent to the field of enquiry. If ample amount of literature is not available for reference in the field of research then pursuing research will be difficult. Modern developments in structure-activity relationship and bioactivity studies have made greater evolution in spectroscopic techniques.

FT-IR and FT-Raman spectroscopy combined with *ab initio*/DFT is becoming a powerful tool for vibrational assignment, structure and property study of organic molecules. Abundant work on structure activity relation based on FT-IR and FT-Raman spectra on number of biologically active compounds have been reported. Vibrational spectra and DFT calculations on chalcone like, (2E)-1-(5-Chlorothiophen-2-yl)-3-4-[(E)-2-phenylethenyl] phenyl prop-2-en-1-one [6], (2E)-1-(5-Chlorothiopene-2-yl)-3-(2,3,4-trimethoxyphenyl)prop-2-en-1-one[7], 3-(2-Chloro-6-flurophenyl)-1-(2-thienyl) prop-2-en-1-one [8], 2-Mercaptoimidazole [9], 1,3-bis (4-methoxyphenyl) prop-2-en-1-one was carried out [10].

DFT explains the interaction system of electrons approximated by using a function to describe the electron density rather than individual wave functions for each of the electron. DFT relies on the total electron density, with the electron placed in non-interacting Kohn-Sham (KS) orbital. There are some results indicating that the vibrational frequencies and intensities from DFT calculations are better than those obtained from second order Mooler-Plesset (MP2) perturbation theory [11]. DFT computations with different basis sets have been performed by many researchers to investigate the structural stability of bioactive compounds like, 5-(2,5-dimethylphenoxy)-2,2-dimethylpentanoicacid (Gemfibrozil) [12], DFT and MD approaches and Molecular Docking Study of a novel chalcone derivative [13], 7-hydroxy-4-methyl-8-(arylazo)-2H-1-benzopyran-2-one [14], (2E)-3-(2-chloro-4-fluoropheyl)-1-(3,4-dimethoxyphenyl)prop-2-en-1-one [15], Experimental and quantum chemical studies of a novel synthetic prenylated chalcone [16]. The DFT methods are nowadays more and more in use and predictable as good choice to study larger molecular systems with biological interest.

Hirshfeld-surface (HS) analysis and 2-D finger print plot has recently become popular method for the analysis of X-ray structures and the interactions present in the molecules. Crystal design and crystal engineering, prediction and computation of molecular crystal structure through intermolecular interactions also aroused attention [17, 18, 19]. The Crystal Explorer package version 3.1 uses crystal information file (CIF) as input gives complete details about various interactions present and also the percentage of contribution. Several works has been done to understand the types of interactions present, (2E)-2-(ethoxycarbonyl)-3-[(1-methoxy-1-oxo-3-phenylpropan-2-yl) amino] prop-2-enoic acid [20].

Certain chalcone derivatives are reported to inhibit the polymerization of tubulin to form microtubules and can be used as antimitotic agents [21]. Chalcone derivatives are also known to inhibit the destruction of myelin sheath in the central nervous system of multiple sclerosis patients and are thus useful in controlling the progressive nature of the disease. Molecular docking studies of (2E)-3-(3-nitrophenyl)-1-[4-piperidin-1-yl] prop-2-en-1-one [22] and (2E)-1-(4-Chlorophenyl)-3-[4-(propan-2-yl) phenyl] prop-2-en-1-one [23] have been carried out. Among many organic compounds, chalcone derivatives have excellent pharmacological properties. They show preference to crystallize as non centro symmetric structures. Due to this fact they have been the objective of several experimental and theoretical studies. Lynnette Joseph *et al* [24] have reported the FT-IR, FT-Raman and UV-visible spectral and thermal analysis of 1-(4-Aminophenol)-3-(3, 4-dimethoxyphenyl)-prop-2-en-1-one. Jasinski *et al* have grown 1- 4-Bromophenyl -3-(2-methoxyphenyl) prop-2-en-1-one and [25], (2E)-1-(3Chlorophenyl)-3-(4-chlorophenyl) prop-2-en-1-one and carried out X-ray diffraction studies [26].

## 2.2 SCOPE OF THE PRESENT WORK

Modern style of food habits attracts the chemist to think about varieties of organic food preservatives to keep the foods free from contamination for a long period of time. Synthesis and development of new organic food preservatives without affecting the human system and at the same time useful as a medicine for certain type of diseases has become the foremost mission of the food industry. Chalcone, the synthetic precursor of many plant derived metabolites, is a privileged

structure with varied biological and synthetic utilities. With the replacement of homogeneously catalyzed classical yield oriented methods of their synthesis with environmentally benevolent methods and with advanced techniques of biological studies, chalcone based research is gaining momentum. It is clear that chalcone will continue to be a major source of food preservative and drugs. A deeper insight of the spectra of complex molecules can be obtained from the theoretical simulations and molecular modeling approach. Quantitative structure-activity relationship (QSAR) model describes the mathematical relation between structural attributes and target response to identify the relationship between those descriptors in maximizing the predictive power of the food preservative chalcone molecule. The results of various quantum chemical calculations and spectroscopic simulations carried out on the chalcones are presented as summary in the thesis. New varieties of chalcone based food preservatives are manufactured in the industry from the idea evolved from the current research work.