CHAPTER I

INTRODUCTION

Spectroscopy is the study of the interaction of electromagnetic radiation in all its forms with matter. The interaction might give rise to electronic excitations, such as UV, molecular vibrations like IR or nuclear spin orientations such as NMR. Vibrational spectroscopy is one of the most versatile tools to elucidate structure composition, hydrogen bonding, charge transfer interactions, intra and inter molecular interaction of bioactive molecules. Simulation studies on the preservative compounds give better understanding between the structure and spectroscopic characteristics. To examine the structural change occurring in biological active compounds, very sensitive analytical methods such as Fourier transform Raman scattering and infrared spectroscopy are used. Raman spectroscopy is one of those techniques which have immense potential in the analysis of structure of pharmaceuticals and bioactive molecules. It has been widely utilized in many other areas like food and dye stuff industry. In addition to vibrational analysis, quantum chemical methods have been developed in a successful way that they form an indispensable complement to experimental studies. The ultimate task in computational chemistry is the accurate and efficient prediction of molecular geometries, vibrational modes and energies of chemical reactions. Detailed information about reaction transition structures, excited states, hypothetical molecular arrangements and deformed molecules are obtained by these computations.

1.1 CHEMISTRY OF CHALCONES

The chemistry of chalcones has generated intensive scientific studies throughout the world. Especially interest has been focused on the synthesis and biodynamic activities of chalcone. The name chalcone was given by Kostanecki and Tambor [1]. In chalcones, two aromatic rings are linked by an aliphatic three carbon chain. Chalcone bears a very good synthon so that variety of novel heterocycles with good pharmaceutical profile can be designed. Chalcones are α, β-unsaturated ketone containing the reactive keto-ethylenic group –CO-CH=CH-. These are coloured compounds because of the presence of chromophore-CO-CH+CH-, which depends on the presence of other auxochromes. Chalcones or 1, 3- diaryl-2-propen-1-ones, belong to the flavonoid family. A vast number of naturally occurring chalcones are polyhydroxylated in the aryl rings and are used as drugs or food preservatives either as a compound or chalcone rich plant extract because of their radial quenching properties [2]. Chalcones abundantly present in nature from fern to higher plants display a number of interesting biological activities such as antimalarial, antimicrobial, anti angiogenic, antiviral, anti-HIV, anticancer, antioxidant, anti-inflammatory, antianalgesic, antipergly-cemic, anti tubercular and anti leishmananial activities. The presence of a reactive alpha, beta-unsaturated keto function in chalcones is found to be responsible for their antimicrobial activity.

Throughout the ages mankind depends on nature, particularly on plants as source of carbohydrates, proteins and fats for food and shelter. In addition, plants are valuable source for a wide range of secondary metabolites, which are used as pharmaceuticals, agrochemicals, flavours, fragrance, colours, bio pesticides and food preservatives. With the presence of a wide variety of secondary metabolites,

plants have formed the basis of the traditional medicine systems that have been in existence for thousands of years in many countries. The flavonoids and allied phenolic and poly-phenolic compounds including tannins and derived poly-phenols and their different derivatives form one major group of photochemical [3]. It has been found that many plant flavonoids protect them against their pathogenic bacteria and fungi [4]. The Homo sapience is the prime beneficiary of the dietary flavonoids knowingly or unknowingly they utilize them for prevention of diseases or cure. Their antioxidant properties, cytostatic effects in tumorigenesis and ability to inhibit a broad spectrum of enzymes have led researchers to regard these compounds as potential food preservatives and food additives. Chalcones (1, 3-diphenyl-2-prop-en-1-one,) are the biogenetic precursor of flavonoids abundant in edible plants in different chemical forms. Chalcone based compounds both natural and synthetic are very versatile as physiologically active compounds with a diverse array of biological activities associated with them.

The therapeutic potential of the chalcone based compounds is supported by their ease of preparation, potential of oral administration, safety and profound natural abundance. The last decade witnessed the devotion of tremendous effort around the world to elucidate the mechanism of these chalconoids for their unparallel array of biological activities. Consequently, a number of synthetic methods have also been developed for the synthesis of this very important class of molecules including the structural modification of the core chalcone moiety. Many plants used as traditional medicine for different ailments have been reported to contain a substantial amount of these chalconoids. In addition to their numerous biological activities, chalcones find a pronounced application in synthetic organic chemistry. Application

of chalcones in the synthesis of many heterocycles and as intermediate in the synthesis of many pharmaceuticals has been well documented. A number of naturally occurring chalcones as well as their derivatives have been isolated from various sources and identified with different biological activities.

1.2 FOOD PRESERVATIVES

Food safety refers to all hazards, whether chronic or acute, that makes food injurious to health. Negative attributes of food such as spoilage, contamination with filth, discoloration, and off-odors make a food waste. Most food contains enzymes or natural chemicals, such as acids or alcohols that cause them to begin to lose desirable characteristics almost immediately after harvest or preparation. In addition, a host of environmental factors, such as heat and the presence of microorganism, act to change food stuffs in ways that harm the food product. Food preservation has traditionally had three goals: the preservation of nutritional characteristics, the preservation of appearance, and a prolongation of the time that the food can be stored. Traditional methods of preservation usually aim to exclude air, moisture, and microorganisms, or to provide environments in which organisms that might because spoilage cannot survive. Factors which contribute to potential hazards in foods include poor hygiene at all stages of the food chain, lack of preventive controls in food processing and preparation, misuse of chemicals, contaminated raw materials etc.

The use of chemicals to prevent or delay the spoilage of food derives in part from the fact that such compounds are used with great success in the treatment of diseases of humans. This is not to imply that all chemotherapeutic compounds can

or should be used as food preservatives. Although a large number of chemicals have been described that show potential as food preservatives, only a relatively small number are allowed in food products. Food preservation is to prevent the growth of microorganism or other microorganisms as well as slowing the oxidation of fats that cause rancidity.

Chalcones (or 1, 3-diaryl-2-prop-en-1-ones) are natural compounds that are largely dispensed in plants, fruits, and vegetables. They are precursors in flavonoid biosynthesis and are responsible for the yellow color of many plant organs and play crucial role in their biosynthesis. Flavonoids and chalcones belong to the broad class of compounds present in terrestrial parts, roots, flakes and seeds of vascular plants. Some chalcones possess bacterial, antifungal and insecticidal activity and some of their derivatives are reported to be anti-mutagenic. Antifungal and antibacterial activities are augmented when the phenyl ring of the preservative compound is substituted with lipophilic electron- withdrawing groups.

1.3 METHODS

Simulation studies on the preservative compounds give better understanding between the structure and spectroscopic characteristics. To examine the structural changes occurring in biological active compounds, very sensitive analytical methods such as Fourier transform Raman scattering and infrared spectroscopy are used. We can use different analysis like Hirsfeld surface and 2-D finger print plot to examine various interactions present in the preservative compounds. QSAR, is used for quantitative correlation of physicochemical attributes of drug like molecules ligand. It has transformed into an extensively used tool, significantly contributing to the

drug discovery process. Multiple linear regression method was used to find and confirm the best regression relation that is capable of correlating the changes in biological activity of the compounds. Multi Linear Regression (MLR) is used as a chemo-metric method for variable selection and statistical fitting.

1.4 AIMS AND OBJECTIVES

Identifying the nature of interactions present and the structure activity relationships are vital for the study of food preservative chalcone. Probing the structural changes using vibrational spectroscopic methods with the aid of *ab initio* quantum chemical computations are significant in the field of food industry. The present work aimed at exploring the structural elucidation, various interactions and the docking sites present in the chalcone molecule. This work will document a more detailed insight of certain food preservative chalcone activities such as relative stability, bioactivity and geometry.