1. INTRODUCTION

Vegetables fulfil one of the basic needs as food by providing appetizing colour, flavour, taste and ultimately nutrition. All these characteristics of vegetables are attributed to the phytochemicals present in them. A variety of phytochemicals are reported to be present in vegetables that are categorized as nutritive and non-nutritive. As nutritive phytochemicals provide nutrition, the non-nutritive phytochemicals are said to provide various biological activities to plant as well as medicinal properties to human. When man ingests these plant foods to meet his nutritional needs, he also ingests a wide variety of these non-nutrient phytochemicals. These phytochemicals are normally non-toxic and possibly would have the potential for preventing chronic diseases. Therefore studies to coordinate the chemical and biological activities of these phytochemicals to identify their disease-preventing potential, is in need (Narasinga, 2003).

In the last decade, the scientific field that combines knowledge about crops and human health is termed as functional foods. Functional foods are so-called because they deliver some physiological benefit beyond nutrition. Carrot (Daucus carota) was reported as an excellent example of a functional food, which contains carotenoids that deliver antioxidant activity in addition to their provitamin-A activity. This multifunctionality of the molecule endorsed, carrot and possibly other foods containing carotenoids, as functional for health (Sloan, 2000). So it is certainly possible that all foods are functional.

On the other hand, the spread of communicable and occurrence of non-communicable diseases are posing serious threats in the well being of human. This is due to biased knowledge on the usage of antibiotics and nutritive values of native food. Communicable diseases (CDs) that are especially caused by drug resistant bacterial (Fred, 2006), mycobacterial (Pushpendra and Katoch, 2006) and fungal (Zeina and John, 2008) pathogens are at high risk due to lack of effective drugs, in the dawn of post antibiotic era. Extensive use and misuse of antibiotics have resulted in worldwide spread of resistant pathogens. Therefore potential drugs are in demand to combat against day-to-day evolving drug resistant pathogens.
Non-communicable diseases (NCDs) are diet related chronic diseases that are caused by behavioural changes from traditional to modern life style. It has been calculated that in 2001, NCDs contributed about 46% of the global disease rate and is expected to increase to 57% by the year 2020 (Murray and Lopez, 1996; Jordan et al., 2001 and WHO, 2002). In developing countries 79% of deaths were attributable to chronic NCDs (WHO, 2002).

NCDs are, themselves, a series of overlapping and complicated disease entities, some of which markedly amplify the likelihood of developing a further disease, and in that sense become risk factors themselves, e.g. obesity and diabetes (Darnton et al., 2004). Diabetes, a metabolic syndrome known as clustering of risk factors including hyperglycaemia, hypertension, dyslipemia, mediated by insulin resistance and resulting in a range of end-point diseases beginning with type 2 diabetes. The global prevalence of diabetes is projected to rise from 171 million in 2000 to 366 million in 2030 (Wild et al., 2004).

Rational drug discovery through computational (in silico) method rather than empirical method is a recent approach to find out new potential leads for drug development. Computational methods have been developed and widely applied to pharmacology related hypothesis development and testing, which include - databases, data mining, Quantitative Structure Activity Relationship (QSAR), similarity searching, pharmacophore analysis molecular modeling, docking and toxicity prediction. Such methods have seen frequent use in the discovery and optimization of novel molecules (Ekins et al., 2007).

The completion of the human genome project; the dawn of proteomics, genomics, metabolomics and the development in information technology have fuelled an even greater application of structure based drug design by rational approach.

Here, vegetables are taken into consideration to screen drug leads, because of their strong domestication and easy availability instead of endangered plant sources. Even though vegetables used in India were widely studied for their nutritive and medicinal values, most of the reports are either on their effect on particular biological activity tested with crude extract or on isolation and structure
elucidation of the particular phytochemical present in the vegetable. Only a few vegetables studied for their phytochemical characterisation and its role in disease prevention by trial and error method.

The present study is aimed to identify new lead molecules from commonly consumed vegetables in India, by applying structure based drug discovery method. The phytochemicals present in vegetables are screened for pharmacophore similarity with respective classes of commercial drugs for communicable (bacterial, fungal and mycobacterial human pathogens) and non-communicable (diabetes) diseases.

Main objectives are:

- To find out lead molecules from vegetables for antimicrobial and antidiabetic treatment.
- To collect data on commonly consumed vegetables and their phytochemicals. To predict possible biological activity of phytochemicals and develop a database for easy and effective data mining.
- To find out structural analogues from vegetable phytochemicals for commercial antibacterial, antifungal, antimycobacterial and antidiabetic drugs by quantitative structure activity relationship and molecular docking methods.
- To extract the phytochemicals and confirm their presence by qualitative analysis.
- To test the antimicrobial effect of the phytochemicals in partially purified extracts on standard and clinical isolates of the bacterial, fungal and mycobacterial pathogens under in vitro conditions.
- To study the antidiabetic effect of phytochemicals in partially purified extracts in test animals.