

## Preface

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Cancer is a major human health problem worldwide and is the leading cause of death. Over the past 3 decades, significant progress has been done in understanding the molecular basis of cancer. The accumulation of this basic knowledge has established that cancer is a variety of distinct diseases and that defective genes cause these diseases. These gene defects are diverse in nature and can involve either loss or gain of gene functions. While cancer is clearly associated with an uncontrolled increase in cell number, alterations in mechanisms regulating new cell birth, or cell proliferation, are only one facet of the mechanisms of cancer. Decreased rates of cell death, or apoptosis, are now known to contribute to certain types of cancer.

Flavonoids belong to a group of polyphenolic compounds, which are classified as flavonols, flavonones, flavones, flavanols, flavan-3-ols and isoflavones according to the positions of the substitutes present on the parent molecule. Flavonoids of different classes have several pharmacological activities. Flavonoids have also been known to possess biochemical effects, which inhibit a number of enzymes such as aldose reductase, xanthine oxidase, phosphodiesterase,  $\text{Ca}^{+2}$ -ATPase, lipoxygenase, cyclooxygenase, etc. They also have a regulatory role on different hormones like estrogens, androgens and thyroid hormone. In view of their wide pharmacological and biological actions, they seem to be having a great therapeutic potential.

The aim of present research work is to explore the potential of quercetin and taxifolin towards the inhibition of enzymes, receptors, protein-protein complex etc which play crucial role in cancer progression by using in-silico approach such as molecular docking and molecular dynamics simulation along with in-vitro effect of quercetin and taxifolin on the cancer cell line.

The resulting subject matter, presented in this volume has been arranged in five chapters. Chapter 1 gives a brief idea introduction to different capabilities of cancer cells, potential of polyphenols and objectives of the present investigation. Chapter 2 critically access the available literature published on different molecular targets, quercetin, taxifolin and in-silico techniques. Details of methodology for the experimentation are given in Chapter 3. Results obtained are presented and discussed in Chapter 4 and finally Chapter 5 concludes the results. The references are given at the end of the thesis.