

Preface

The work in the thesis has been published, and most of the chapters are reworking of these published work. The entire Thesis work has been divided into 11 chapters: Chapter 1 deals with a general introduction about Gedunin($C_{28}H_{34}O_7$) and its relation with cancer, Diabetes mellitus, and snake anti-venom. It also highlights the motivations and significance of the research work. Chapter 2 presents the literature survey covering the uses and applications of gedunin against snake venom, diabetes, liver, prostate, and ovarian cancer. Chapter 3 describes the ripen fruit materials, various techniques (polarity-based extraction using soxhlet, HPLC, HRLCMS, and Column chromatography) involved in the Extraction, purification, and characterization of gedunin from *Azadirachta indica* and their results and discussion. Chapter 4 presents the methods of computational analysis including docking, simulation, and pharmacokinetics analysis of gedunin against snake venom enzymes and their results and discussion. Chapter 5 deals with *insilico* analysis of modified gedunin derivative $C_{26}H_{31}N_2O_6F$ with their methods, results, and discussion. Chapter 6 deals with methods, results, and discussion of QSAR and Retrosynthesis of $C_{26}H_{31}N_2O_6F$. Chapter 7 deals with methods, results, and discussion of molecular property prediction of $C_{26}H_{31}N_2O_6F$ (modified gedunin derivative) using LSTM, CNN, VGGNET, and k-means clustering. Chapter 8 deals with the method, results, and discussion of the antidiabetic potential of gedunin using alpha-glucosidase and alpha-amylase enzymes. Chapter 9 covers the materials, methods, results, and discussion of the anti-cancer activity of gedunin using liver cancer cell HepG2, PA1, and PC3 where ROS activity, Apoptosis activity, scratch assay/migration assay and colony

formation assay/proliferation assay has been shown. Chapter 10 deals with Transcriptomics studies of gedunin using the HeLa cell line with methods, results, and discussion. Chapter 11 presents a brief summary and conclusions of experimental findings.