

Contents

PARTICULARS	Page No.
Contents	i-iii
List of Abbreviation	iv
List of tables and figures	v-xi
Preface	xii-xiii
1. Introduction	1-6
2. Literature review	7-25
2.1 Molecular targets of dietary polyphenols for prevention and therapy of cancer	7-14
2.1.1 B-cell lymphoma 2 (Bcl-2)	7-8
2.1.2 Heat shock protein-90 (Hsp90)	8-10
2.1.3 Mouse double minute 2 (MDM2)	11-13
2.1.4 Vascular epithelial growth factor receptor 2 (VEGFR-2) kinase	13-14
2.2 Quercetin	14-16
2.2.1 Ethnopharmacological relevance of quercetin	15-16
2.2.2 Quercetin and anticancer effects	16
2.3 Taxifolin	16-18
2.4 Molecular Docking	18-22
2.4.1 Lock and key analogy	18
2.4.2 Rigid-body docking vs. flexible docking	18-19
2.4.3 Search algorithms	19-20
2.4.4 Genetic algorithms	20
2.4.5 Lamarckian Genetic Algorithm	20-21
2.4.6 Scoring function	21-22
2.5 Molecular dynamics simulation	22-25
2.5.1 Energy minimization	24
2.5.2 Molecular dynamics	25

4.2.3 Effect of quercetin on markers of intrinsic apoptosis	87-88
5. Conclusions	89-93
5.1 In-silico studies	89-92
5.1.1 B-cell lymphoma 2 (Bcl-2)	89-90
5.1.2 Heat shock protein-90 (Hsp90)	90-91
5.1.3 Mouse double minute 2 (MDM2)	91-92
5.1.4 Vascular epithelial growth factor receptor 2 (VEGFR-2) kinase	92
5.2 In-vitro studies	92-93
References	94-125