

TABLE OF CONTENTS

UNDERGRADUATE THESIS	i
RATIFICATION PAGE	ii
STATEMENT OF ORIGINALITY	iii
PREFACE	iv
TABLE OF CONTENTS	v
LIST OF FIGURES	vii
LIST OF APPENDICES	viii
SYMBOLS AND ABBREVIATIONS LIST	ix
ABSTRACT	x
INTISARI	xi
CHAPTER I INTRODUCTION	1
I.1 Theoretical Background	1
I.2 Purpose of Research	2
I.3 Benefits of Research	2
CHAPTER II LITERATURE REVIEW AND HYPOTHESIS FORMULATION	3
II.1 Literature Review	3
II.1.1 Molecular docking	3
II.1.2 Molecular dynamics	5
II.1.3 Breast cancer	7
II.1.4 Extracellular signal-regulated kinase 2	7
II.1.5 Tangeretin	10
II.2 Hypothesis Formulation and Research Design	11
II.2.1 Hypothesis formulation 1	11
II.2.2 Hypothesis formulation 2	13
II.2.3 Research design	14
CHAPTER III EXPERIMENTAL METHOD	16
III.1 Equipment	16
III.1.1 Hardware	16
III.1.2 Software	16
III.2 Materials	16
III.3 Procedure	18
III.3.1 Preparation of protein and ligands	18
III.3.2 Energy minimization and redocking	18
III.3.3 Molecular docking & molecular dynamics	19
CHAPTER IV RESULTS AND DISCUSSION	21
IV.1 ERK2 Structure and Energy Minimization	21
IV.2 Redocking	22
IV.3 Molecular docking	22
IV.3.1 Molecular docking of tangeretin	23
IV.3.2 Molecular docking of TGN-1 derivative	24
IV.3.3 Molecular docking of TGN-2 derivative	25
IV.3.4 Molecular docking of TGN-3 derivative	26
IV.3.5 Molecular docking of TGN-4 derivative	27

IV.3.6 Molecular docking of TGN-5 derivative	28
IV.3.7 Molecular docking of TGN-6 derivative	29
IV.4 Comparison of Docking Results	30
IV.5 Molecular Dynamics Simulations	31
IV.5.1 RMSD result	33
IV.5.2 RMSF result	34
IV.5.3 Radius of gyration result	35
IV.6 Synthesis and retrosynthesis of tangeretin derivative	36
CHAPTER V CONCLUSION AND SUGGESTION	40
V.1 Conclusion	40
V.2 Suggestion	40
BIBLIOGRAPHY	41
APPENDICES	46