

## LIST OF CONTENT

<b>UNDERGRADUATE THESIS</b>	i
<b>RATIFICATION PAGE</b>	i
<b>STATEMENT LETTER</b>	iii
<b>FOREWORD</b>	iv
<b>LIST OF CONTENT</b>	v
<b>LIST OF FIGURES</b>	vii
<b>SYMBOLS AND ABBREVIATION LIST</b>	viii
<b>ABSTRACT</b>	ix
<b>INTISARI</b>	x
<b>CHAPTER I INTRODUCTION</b>	1
I.1 Background	1
I.2 Research Purpose	3
I.3 Research Benefit	3
<b>CHAPTER II LITERATURE REVIEW &amp; HYPOTHESIS FORMULATION</b>	4
II.1 Literature Review	4
II.1.1 Acne	4
II.1.2 PaNA enzyme (Propionibacterium acnes neuraminidase)	4
II.1.3 Kaempferol	6
II.1.4 Computational Chemistry Calculation	8
II.1.5 Molecular Docking	9
II.1.6 Molecular Dynamic Simulation	11
II.2 Hypothesis Formulation and Research Plan	15
II.2.1 Hypothesis Formulation 1	15
II.2.2 Hypothesis Formulation 2	15
II.2.3 Research Planning	16
<b>CHAPTER III RESEARCH METHODS</b>	18
III.1 Equipment	18
III.2 Materials	18
III.3 Procedure	20

III.3.1 Ligand Preparation	20
III.3.2 Molecular Docking	20
III.3.3 Molecular Dynamic Simulation	21
<b>CHAPTER IV RESULT &amp; DISCUSSION</b>	22
IV.1 Energy Minimization	22
IV.2 Molecular Docking	25
IV.2.1 Redocking	26
IV.2.2 Molecular Docking of Kaempferol	27
IV.2.3 Molecular Docking of Derivative A	28
IV.2.4 Molecular Docking of Derivative B	29
IV.2.5 Molecular Docking of Derivative C	30
IV.2.6 Molecular Docking of Derivative D	31
IV.2.7 Molecular Docking of Derivative E	31
IV.2.8 Molecular Docking of Derivative F	32
IV.2.9 Molecular Docking of Derivative G	33
IV.2.10 Molecular Docking of Derivative H	33
IV.2.11 Molecular Docking Results Comparison	34
IV.3 Molecular Dynamic Simulation	38
IV.3.1 Root Mean Square Deviation (RMSD)	40
IV.3.2 Root Mean Square Fluctuation (RMSF)	41
IV.3.3 Radius of Gyration (Rg)	41
IV.4 Retrosynthesis Analysis	42
<b>CHAPTER V CONCLUSION &amp; SUGGESTION</b>	49
V.1 Conclusion	49
V.2 Suggestion	49
<b>REFERENCES</b>	50