

TABLE OF CONTENTS

| | |
|-------------------------------------------------------|------|
| PREFACE | iv |
| TABLE OF CONTENTS | v |
| LIST OF TABLES | vii |
| LIST OF FIGURES | viii |
| ABSTRACT | ix |
| INTISARI | x |
| CHAPTER I INTRODUCTION | 1 |
| I.1 Background | 1 |
| I.2 Research Objectives | 4 |
| I.3 Research Benefits | 4 |
| CHAPTER II LITERATURE REVIEW | 5 |
| II.1 Prostate Cancer | 5 |
| II.2 Curcumin | 6 |
| II.3 QSAR | 8 |
| II.4 Density Functional Theory (DFT) | 11 |
| II.5 Multiple Regression Analysis | 13 |
| II.6 Statistical Parameters | 13 |
| II.7 Hypothesis and Research Design | 16 |
| CHAPTER III IMPLEMENTATION METHOD | 18 |
| III.1 Tools | 18 |
| III.2 Materials | 18 |
| III.3 Method | 20 |
| CHAPTER IV RESULTS AND DISCUSSION | 22 |
| IV.1 Basis Set Selection and Validation Method | 22 |
| IV.2 Molecular and Electronic Descriptors Calculation | 27 |
| IV.3 Selecting QSAR Model | 28 |
| IV.4 Modelling of new compound | 32 |

| | |
|--------------------------------------------------|----|
| CHAPTER V CONCLUSION | 39 |
| REFERENCES | 40 |
| APPENDIX | 45 |
| APPENDIX 1 Compound of test set and training set | 45 |
| APPENDIX 2 Data View and Variable View on SPSS | 46 |