

***IN SILICO* DOCKING ANALYSIS OF *PHALERIA MACROCARPA* FRUIT
PHYTOCHEMICALS IN INHIBITING SARS-COV-2**

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ABSTRACT

***IN SILICO* DOCKING ANALYSIS OF *PHALERIA MACROCARPA* FRUIT PHYTOCHEMICALS IN INHIBITING SARS-COV-2**

SARS-CoV-2, which has struck the world, has shocked society with its devastating death toll. Synthetic antivirals are commonly used but have the potential to cause serious side effects and long-term health problems. Consequently, there's a rising demand for natural antivirals due to their potential for fewer side effects and their promise of more sustainable treatments. *Phaleria macrocarpa* was reported to possess high antiviral properties due to the presence of the flavonoid compound such as quercetin, kaempferol, myricetin and naringenin. However, the antiviral properties of these compounds against SARS-CoV-2 have not yet been fully elucidated. Thus, the objectives of this study are to determine the phytochemicals of *P. macrocarpa* fruit using GC-MS analysis and phytochemical screening test, to evaluate the potential of the phytochemical in inhibiting SARS-CoV-2 via *in silico* docking analysis and also to determine the pharmacokinetics properties of its phytochemical using SWISSADME. In this study, the fruit of the *P. macrocarpa* was subjected to extraction using maceration method. Then, the phytochemical constituents in the fruit extract were identified using phytochemical screening and GC-MS analysis. The result obtained is positive for phytochemical screening test, however the GC-MS analysis showed less favorable results, whereby it just produced 7 peaks that have 90% of a quality. Among the 7, there's only one compound which is squalene that has antiviral properties. Thirteen phytochemical constituents were chosen from databases based on their potential in exhibiting the antiviral properties and were analyzed for their pharmacokinetic properties using SwissADME, which were aligned with the docking score obtained from PyRx. It was found that the potential compounds to inhibit SARS-CoV-2 were sesamin, Mahkoside A and Mahkoside B with docking score of -7.8, -7.4 and -7.5 respectively. This discovery of phytochemical constituents derived from *P. macrocarpa* fruit extract could potentially be developed as a natural alternative to existing medicines and vaccines currently available in the market.

TABLE OF CONTENTS

	Page
ACKNOWLEDGEMENT	v
TABLE OF CONTENTS	vi
LIST OF TABLES	viii
LIST OF FIGURES	ix
LIST OF SYMBOLS	xi
LIST OF ABBREVIATIONS	xii
ABSTRACT	iii
ABSTRAK	iv
CHAPTER 1 INTROUCTION	1
1.1 Background of study	1
1.2 Problem Statement	3
1.3 Significance of study	4
1.4 Objectives	4
CHAPTER 2 LITERATURE REVIEW	5
2.1 Botanical description of <i>Phaleria macrocarpa</i>	5
2.2 Traditional Uses of <i>Phaleria macrocarpa</i>	6
2.3 Phytochemical composition of <i>Phaleria macrocarpa</i>	8
2.4 Viruses and Antiviral Strategies	12
2.5 Overview of SARS-CoV-2	13
2.6 SARS-CoV-2 life cycle	14
2.7 Phytochemical compounds potential against COVID-19	16
2.8 Pharmacokinetic properties using SWISSADME	17
2.9 <i>In silico</i> docking analysis	18
2.10 Phytochemical screening test	19
CHAPTER 3 METHODOLOGY	20
3.1 Materials, chemicals, apparatus and instrument	20
3.1.1 Materials	20
3.1.2 Chemicals	20
3.1.3 Apparatus	20
3.1.4 Instrument	20
3.2 Sample collection and preparation	21
3.3 Phytochemical screening	21
3.3.1 Test for Flavonoid (alkaline reagent test)	21
3.3.2 Test for Phenolic (Ferric (III) chloride test)	22
3.3.3 Test for Sterol	22
3.3.4 Test for Terpenoid	22
3.3.5 Test for glycoside	22
3.4 GCMS Analysis	23
3.5 <i>In silico</i> docking analysis	23

3.5.1 ADME and other pharmacokinetic properties	23
3.5.2 Preparation of ligands and target proteins	24
3.5.3 Antiviral probability prediction	25
3.5.4 Active site prediction and molecular docking	25
3.5.5 Flowchart	26
 CHAPTER 4 RESULTS AND DISCUSSIONS	 28
4.1 Confirmation Species and GC-MS Analysis	28
4.2 Phytochemical Screening Test	31
4.3 Physicochemical and drug-likeness properties	35
4.4 <i>In silico</i> docking analysis	41
4.5 Structure activity relationship	51
 CHAPTER 5 CONCLUSIONS AND RECOMMENDATION	 54
5.1 Conclusion	54
5.2 Recommendation	54
 CITED REFERENCES	 56
APPENDICES	64
<i>CURRICULUM VITAE</i>	65