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Computational Study of Telang Flower Extract (*Clitoria ternatea*) As an Anti-inflammantory Drug

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ABSTRACT

Telang Flower (*Clitoria ternatea)* is one of the plants rich in benefits for human health. Genistein is a natural bioactive compound derived from nuts and some plants with potential effects beneficial in some human degenerative diseases. The purpose of this research is to conduct bioinformatic studies of herbal compound in the plant *Clitoria ternatea*. The method used is modeling and computation using ChemDraw Pro 12.0 and Chem3D programs and analyze active compounds using website Dr. Duke's Phytochemical and Ethnobotanical databases, PubChem, and Swiss Target Prediction. The results obtained were extract *Clitoria ternatea* contains one active compound in it. Identified compound active in this plant, namely Genistein or 5,7-dihydroxy-3-(4-hydroxyphenyl) chromen-4-one. The total energy obtained from the compound Genistein after being optimized after 100steps and at a temperature of 300K which is 29,698 kcal/mol. Genistein is a soy-derived isoflavone and phytoestrogen with antinoplastick activity. Genistein exhibits antioxidant activity, antiangiogenic, and immunosuppressive. Genistein is a relative antioxidant bad. Genistein is currently being studied in clinical trials as a treatment for prostate cancer.

Keywords: Telang flower, Genistein, Antioxsidants

1. INTRODUCTION

Telang Flower (*Clitoria ternatea*) is one of the many traditional medicinal plants once contains benefits for human health.[1][21] Currently, people often make it this flower extract to be used as a drink.[2] Many have planted crops directly medicine in heir respective homes.[3][24] Even in a restaurant or café there are already those trading plants to be processed into drinks.[4] This is because it has many who do research that say that there are many benefits obtained from this plant.[5][28] This plant grows spread in various parts of the world in tropical and subtropical climates the continents of Asia and the Pacific, America and the Caribbean, Africa, and Australia.[6] This telang plant is a herbal plant that can be said to be very special in traditional medicine.[7] All parts are believed to have the effect of treating and strengthening the performance of organs ranging from root to flower.[8][27]

Several studies mention the benefits of this plant, among others to treat insomnia, rheumatism, asthma, ulcers, nourish the heart, reduce inflammation.[9][22] Healing wounds, even overcoming the symptoms of diabetes.[10] Various pharmacological activities of C. ternatea were reported in

literature such as antimicrobial, antipyretic, anti-inflammatory, analgesic, diuretic, local anaesthetic, antidiabetic, insecticidal, blood platelet aggregation inhibiting and vascular smooth muscle relaxant properties.[11] In 1954 there was who reported that there was fatty acid content in telang seeds and root has a diuretic effect.[12][26] Various secondary metabolites such as polyphenolic flavonoids, anthocyanin glycosides, pentacyclic triterpernoids and phytosterols have been reported from this plant.[13][23] The amount of total phenolic and flavonoids were estimated to be 358.99 ± 6.21 mg/g gallic acid equivalent and antioxidant activity of C. ternatea leaf extract was 67.85% at a concentration of 1 mg/mL.[14]

2. LITERATURE REVIEW

Telang flower is one of the plants that have relatively high source of polyphenols so that it has the potential to provide health benefits for humans.[15] The leaves and roots are used in the treatment of a number of ailments including body aches, infections, urinogenital disorders, and as anthelmentic and antidote to animal stings.[16] According to several studies that have been done, telang flowers contain compounds chemicals such as tannins, carbohydrates, saponins, phenols, flavonoids, proteins, alkaloids, anthraquinones, anthocyanins, cardiac gilcosides, essential oils and steroids.[17][30] Telang flower extract is also suspected can reduce serum glucose and hemoglobin glycosylation, and increase insulin serum, liver muscle glycogen and bone.[18][29] The methanol extract of Clitoria ternatea showed a significant antipyretic activity. The root methanol extract when given by oral route to rats was found to inhibit both the rat paw oedema caused by carrageenin and vascular permeability induced by acteic acid in rats.[19][25]

This study aims to analyze and determine the potential of chemical compound contained in this medicinal plant. A bioinformatic analysis via this database is expected can provide information and knowledge about the potential of a chemical compound contained in this plant a drug molecule, molecular shape, 3D structure, analysis influence the movement of molecules, the nergy produced by these molecules and see the parts that cannot be directly observed by the eye without the aid of a tool.[20]

Figure 1. Morphology of *Clitoria ternatea*

3. EXPERIMENTAL

This analysis uses a laptop device. The laptop used is the HP Notebook brand Model 14-an004AU. This laptop is equipped with *Chemoffice* 14.0 software which consists of ChemDraw Pro 12.0 which is used to determine the structure of the compound and Chem3D 16.0 for describing compounds in three-dimensional form Research. This is done in several stages, namely as follows :

Compound and target preparation

The medicinal plant samples to be analyzed were *Clitoria ternatea*, then searched chemical compounds contained in it at Dr. Duke's Phytochemical and Ethnobotanical databases / *phytochem.nal.usda.gov/phytochem/search*. Next the chemical compounds obtained were analyzed for the 3D structure of Pubchem *https://pubchem.ncbi.nlm.nih.gov/*.

Druglikeness analysis

The target compound that has been obtained from the database, thn the potential is predicted as a drug molecules on the server http://swisstargetprediction.ch/ by pasting the SMILES obtained from PubChem.From this server, the compound belonging to the group are obtained drug molecules.

2D dan 3D molecule structure analyzers

After obtaining a structural analysis from PubChem, it is then proven by using *Chemoffice* 14.0 *Software*. This research was conducted in several stages (1) Molecular analysis of Genistein (5,7-dihydroxy-3-(4-hydroxyphenyl)chromen-4-one) two-dimensional using ChemDraw Pro 12.0 ; (2) Analysis of the Genistein molecule (5,7-dihydroxy-3-(4-hydroxyphenyl)chromen-4-one) in three dimensions using Chem3D 16.0 ; (3) Analysis of the effect of molecular movement 5,7-dihydroxy-3-(4-hydroxyphenyl) chromen-4-one with respect to the energy prodcedand the bonds to the molecule.

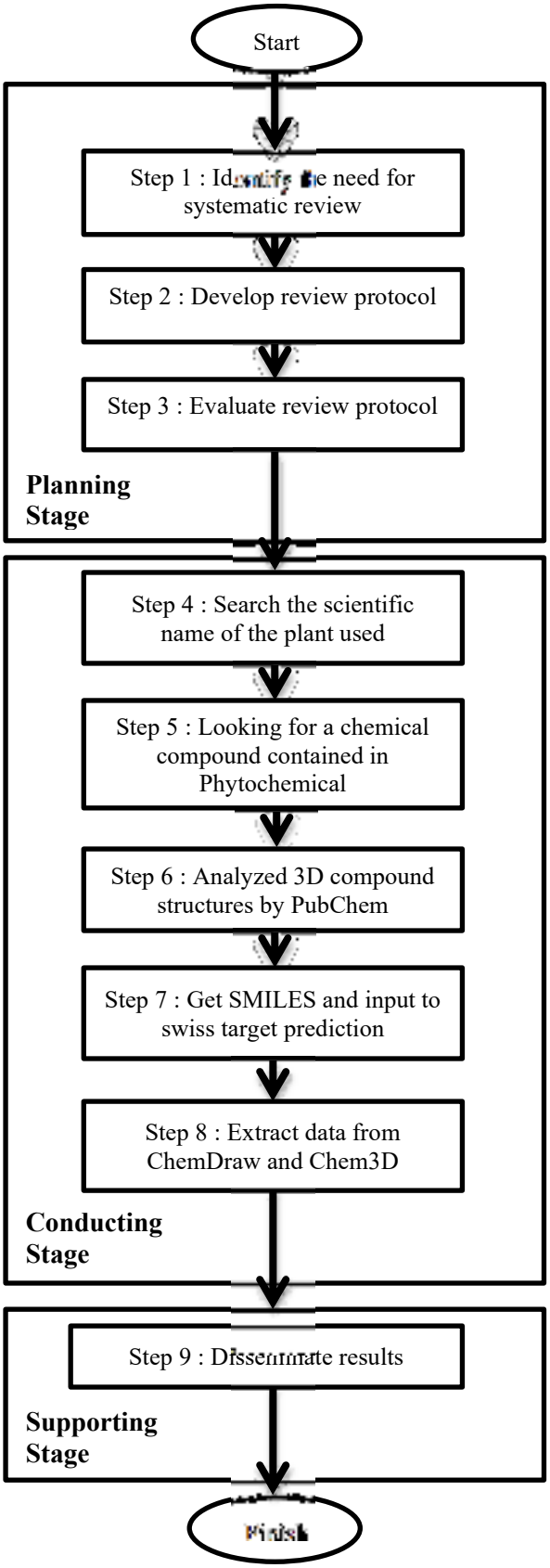

Figure 2. Systematic Review Diagram

Table 1. PICOC Criteria

Population	Inflammantory
Intervention	-
Comparison	-
Outcomes	Treat disease problems inflammantoty in community
Context	Observational descriptive research retrospectively

4. RESULTS AND DISCUSSION

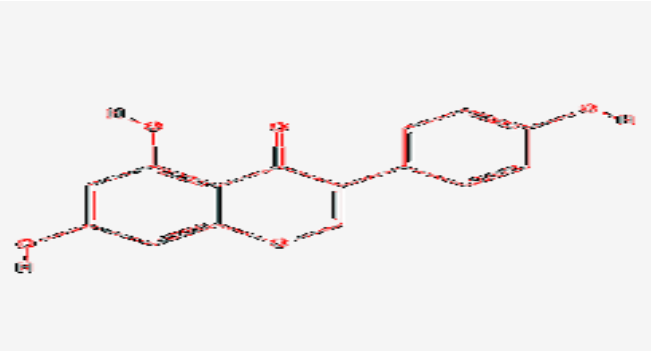

Figure 3. Chemical Structure Depiction by PubChem

IUPAC Name
5,7-dihydroxy-3-(4-hydroxyphenyl)chromen-4-one

Canonical SMILES
C1=CC(=CC=C1C2=COC3=CC(=CC(=C3C2=O)O)O)O

Table 2. Active Compound in Clitoria ternatea by PubChem

Chemical	*Part*	*Low Ppm*	*High Ppm*	*Stddev*
Genistein	*Leaf Diffusate*	*--*	*25.0*	*1.63*

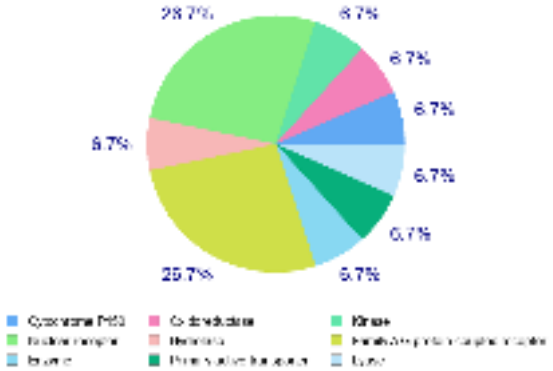

Figure 4. Diagram Target Classes by swiss target prediction

Figure 5. Tabel Target Classes by swiss target prediction

a. Potential Chemical Compounds of *Clitoria ternatea* as drug molecules

One type of active chemical compound in *Clitoria ternatea* has been obtained from Dr. Duke's Phytochemical and Ethnobotanical databases. Identified compound active in this plant, namely Genistein atau 5,7-dihydroxy-3-(4-hydroxyphenyl)chromen-4-one. Furthermore, the compound were analyzed using PubChem databases https://pubchem.ncbi.nlm.nih.gov/ to get the structure 3D compound target in structured data format (.sdf). To predict target class used server Swiss Target Prediction http://www.swisstargetprediction.ch/.

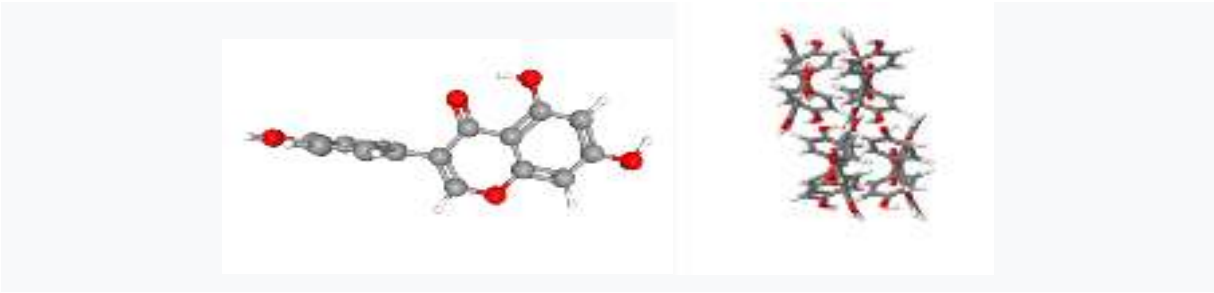

Figure 6. 3D structure and crystal structure of Clitoria ternatea by Pubchem

The target chemical compound is then analyzed using the Human Metabolome Database http://www.hmdb.ca/citing. From these databases, it is obtained that data Genistein compounds are soy-derived isoflavones and phytoestrogens with antinoplastick activity. Genistein has a weak estrogenic effect viz can bind and inhibit protein-tyrosine kinase, thus interfering signal transduction and induces cell differential. Genistein shows activity antioxidant, antiangiogenic, and immunosuppressive.

Genistein is a relatively bad antioxidant. However, genistein can protects against factor-induced vascular endothelial barrier dysfunction proinflammatory and inhibits leukocyte-endothelial

interactions, which are capable of modulates vascular inflammation, a major event in the pathogenesis of atherosclerosis.

Genistein uses non-genomic actions by targeting molecules important signaling in vaskular endothelial celss (EC). Genistein on the fly activates endothelial nitric oxide synthase and nitric oxide production in ECs. Effect genistein is new because it does not depend on a known, but mediated, effect by the cyclic adenosine monophosphate or protein kinase A (cAMP / PKA) cascade.

Genistein directly stimulates adenylate cyclase associated with plasma membranes, leading to activation of the cAMP signaling pathway. In addition, genistein activates receptors that activate peroxisome proliferators, core receptors that are activated ligands that are essential for normal vascular function. Furthermore, genistein reduces reactive oxygen species(ROS) by attenuating expression ROS-producing enzymes. These findings reveal a role for genistein in regulation vascular function and provides a basis for further investigating its potential therapeutic for inflammatory-related vascular disease. Currently Genistein is studied in clinical trials as a treatment for prostate cancer.

b. 2D Molecular Analysis 5,7-dihydroxy-3-(4-hydroxyphenyl)chromen-4-one

In the analysis stage of the 5,7-dihydroxy-3-(4-hydroxyphenyl) chromen-4-one molecule 2D used ChemDraw Pro 12.0.

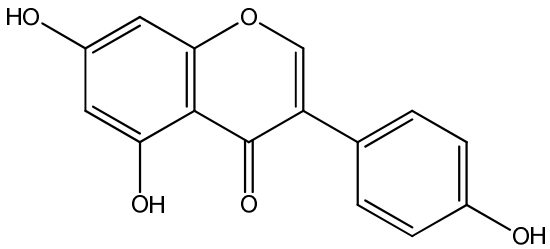

Figure 7. 2D Molecular Analysis 5,7-dihydroxy-3-(4-hydroxyphenyl)chromen-4-one

Molecular Weight: 270,24
Elemental Analysis: C, 66.67; H, 3.73; O, 29.60
Boiling Point: 957,59 [K]
Melting Point: 785,56 [K]
Critical Temp: 957 [K]
Critical Pres: 56,62 [Bar]
Critical Vol: 671,5 [cm3/mol]
Gibbs Energy: -305,27 [kJ/mol]
Log P: 1,74
MR: 71,74 [cm3/mol]
Henry's Law: 17,78
Heat of Form: -559,68 [kJ/mol]
tPSA: 86.99

c. 3D Molecular Analysis 5,7-dihydroxy-3-(4-hydroxyphenyl)chromen-4-one

Analysis molecule 5,7-dihydroxy-3-(4-hydroxyphenyl)chromen-4-one using computational methods created with *ChemDraw* Pro 12.0 Software . Then projected on Chem3D for analysis of its three-dimensional structure. This process shows how the optimal molecular movement pattern is.

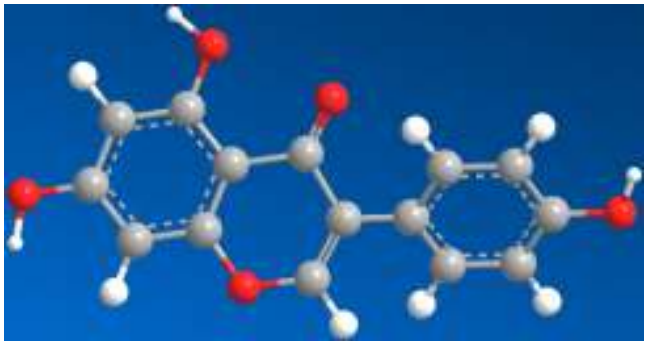

Figure 8. 5,7-dihydroxy-3-(4-hydroxyphenyl)chromen-4-one molecule before optimized

Table 3. Active Compound in 5,7-dihydroxy-3-(4-hydroxyphenyl)chromen-4-one

	Atom	Bond Atom	Bond Length	Angle Atom	Angle (°)	2nd Angle Atom	2nd Angle	2nd Angle Type
1.	C(3)							
2.	C(5)	C(3)	1.401					
3.	C(1)	C(3)	1.504	C(5)	120.353			
4.	C(6)	C(3)	1.401	C(1)	120.532	C(5)	119.115	Pro-S
5.	O(9)	C(5)	1.378	C(3)	122.704	C(1)	0.001	Dihedral
6.	C(10)	C(5)	1.395	C(3)	120.582	O(9)	116.714	Pro-S
7.	C(12)	C(6)	1.396	C(3)	120.277	C(1)	-179.999	Dihedral
8.	C(15)	C(10)	1.395	C(5)	119.909	C(3)	0.002	Dihedral
9.	C(4)	C(1)	1.495	C(3)	112.597	C(5)	0.005	Dihedral
10.	C(7)	O(9)	1.375	C(5)	117.952	C(3)	-0.008	Dihedral
11.	C(8)	C(4)	1.337	C(1)	119.335	C(7)	119.335	Pro-R
12.	C(13)	C(8)	1.395	C(4)	119.999	C(1)	-144.000	Dihedral
13.	C(14)	C(8)	1.395	C(4)	119.999	C(13)	120.003	Pro-R
14.	C(16)	C(13)	1.395	C(8)	119.997	C(4)	-179.994	Dihedral
15.	C(17)	C(14)	1.395	C(8)	120.000	C(4)	179.999	Dihedral
16.	C(19)	C(16)	1.395	C(13)	120.000	C(8)	-0.006	Dihedral
17.	O(11)	C(6)	1.355	C(3)	119.862	C(12)	119.862	Pro-S
18.	O(18)	C(15)	1.355	C(10)	120.014	C(12)	120.014	Pro-S
19.	O(20)	C(19)	1.355	C(16)	119.998	C(17)	119.998	Pro-R
20.	O(2)	C(1)	1.208	C(3)	123.702	C(4)	123.702	Pro-R
21.	H(21)	C(7)	1.100	C(4)	117.468	O(9)	117.468	Pro-R
22.	H(22)	C(10)	1.100	C(5)	120.045	C(15)	120.045	Pro-R
23.	H(24)	C(12)	1.100	C(6)	119.927	C(15)	119.927	Pro-S
24.	H(25)	C(13)	1.100	C(8)	120.002	C(16)	120.002	Pro-R
25.	H(26)	C(14)	1.100	C(8)	120.000	C(17)	120.000	Pro-R
26.	H(27)	C(16)	1.100	C(13)	120.000	C(19)	120.000	Pro-S
27.	H(28)	C(17)	1.100	C(14)	120.001	C(19)	120.001	Pro-R
28.	H(23)	O(11)	0.972	C(6)	108.000	C(3)	-180.000	Dihedral
29.	H(29)	O(18)	0.972	C(15)	108.000	C(10)	0.000	Dihedral
30.	H(30)	O(20)	0.972	C(19)	108.000	C(16)	-180.000	Dihedral

5. CONCLUSION

Based on the analysis of compounds in *Clitoria ternatea.* there are active chemical compound namely Genistein or 5,7-dihydroxy-3-(4-hydroxyphenyl)chromen-4-one. Which one Genistein compounds are isoflavones and phytoestrogens derived from soybeans with antinoplastick activity. Genistein is a relatively bad antioxidant. Genistein reduces reactive oxygen species (ROS) by attenuating anzyme expressing ROS generator. These findings reveal the role of Genistein in the regulation of function vascular and provides a basis for further investigating its therapeutic potential for inflammatory-related vascular disease. Genistein is currently being studied in trials clinical as a treatment for prostate cancer. The energy obtained after the compound Genistein optimized using Chem3D was obtained at 29.698 kcal/mol.

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