Bioinformatics Study of *Cymbopogon nardus* Compound as a Mosquito Repellent

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Abstract. Cymbopogon nardus is a plant of the Poaceae family which is an herbal plant that is used by the community as room and clothing fragrances, relieves wound pain, improves digestion, beautifies the skin and bites the body of mosquitoes. Several previous studies have applied Citronella plants (Cymbopogon nardus) as mosquito repellents. Mosquitoes are very annoying insects because they cause pain and pain, they can also cause skin lesions due to mosquito bites and infections. Sensible mosquito repellent in the form of spray, burn or liquid where chemical compounds are harmful to human health, namely propoxur, tranflutrin, bioaleterin, dikiorvos, dalletherine, octachiorophil ether. The purpose of this study was to see the bioactivity of plants in Serai Wangi (Cymbopogon nardus). The method used is a computational study using various bioinformatics applications. From the research it was found that the plants in Serai Wangi (Cymbopogon nardus) were very effective as mosquito repellents

1. Introduction

Geographically, Indonesia is an area that is in accordance with the place where the mosquito species live as vectors of disease. High rainfall causes a lot of standing water everywhere and there are swamps, so that mosquitoes will breed easily [6]. As a result of mosquitoes that easily breed, various diseases are caused by mosquitoes. So efforts are needed to overcome it, one of which is the use of mosquito repellents, which of course contain insecticides of several chemical compounds [1]. Insecticides that contain several chemical compounds, one of which is a class of pesticides where pesticides are part of a toxic zone [5].

Anti-mosquito drugs circulating in the market are in the form of sprays, burns and liquids which contain chemical compounds that are harmful to human health, namely propoxur, tranflutrin, bioaleterin, dikiorvos, dalletherine, octachiorophil ether [4]. The active substances contained in electric mosquito repellent and mosquito coils when used routinely can gradually affect and cause abnormalities in human organs, one of which is the lungs [2]. To prevent the occurrence of abnormalities in the organs of the body due to mosquito repellents derived from chemicals, it is necessary to look for mosquito repellents derived from natural ingredients.

Indonesia is a country that is very rich in biodiversity. Among the thousands of plants that grow in Indonesia, there are various plants that are unique and have multiple functions. Not only can it be used as decoration, cooking spices, or plant filler, the richness of Indonesian flora in the form of mosquito repellent plants has turned out to be a mosquito repellent [7]. For a long time, people have known various

types of mosquito repellent plants that can thrive in Indonesia. Several types of plants in Indonesia that have the potential to act as anti / mosquito repellents are lemongrass [9].

Cymbopogon nardus . L is a type of essential oil plant that is classified as well-developed. From the results of the distillation of the leaves, citronella oil is obtained which in the trading world is known as Citronella Oil. Citronella oil is obtained from citronella plants which contain about 32-45% citronellal compounds, 10-12% geraniol, 11-15% citronellol, 3-8% geranil acetate, 2-4% citronellal acetate and contain little sesquiterpenes and compounds other. Of the various medicinal plants available, fragrant lemongrass *(Cymbopogon nardus L)* is a plant that has many benefits. The results showed that the antibacterial activity of lemongrass essential oil was greater against S. aureus bacteria [10]. Based on the description, a computative study was conducted on the Bioactivity Test of Citronella Plant Extract (Cybopogon nardus) as a Mosquito Drug

2. Methodology

This study uses the literature review method or the SLR (systematic literature review) approach to examine research, assess and interpret and gather information about the compounds contained in white turmeric and their role in helping cure cancer. To determine the content, phytochemicals were used, then chemdraw ultra 12.0 and chem 3 D pro 12.0 to make the structure of the compound that was in the previous https://pub parameter (internal and cartesian coordinate table). In addition, http://swisstargetprediction.ch/ is also used to predict that these compounds are more active in healing any disease. cbi.nlm.nih.gov/ and specify.

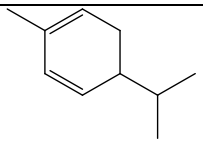
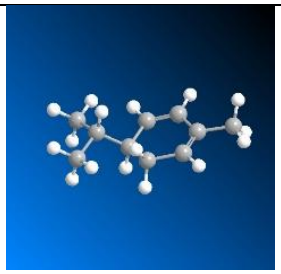
3. Result and Discussion

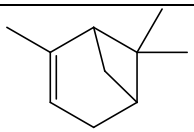
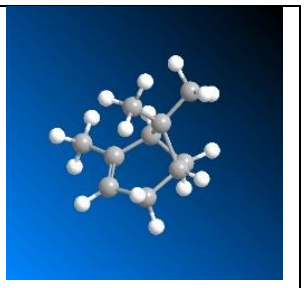
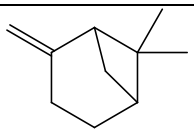
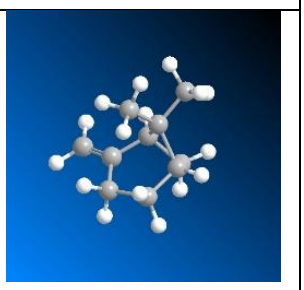
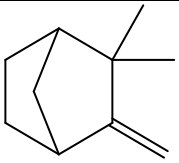
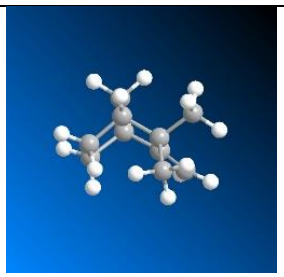
The citronella plant *(Cymbopogon nardus L*) has 20 chemical compounds and there are 14 active chemical compounds, which are as follows:

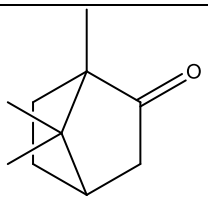
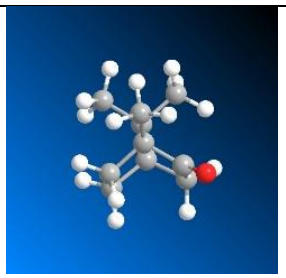
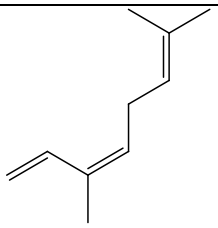
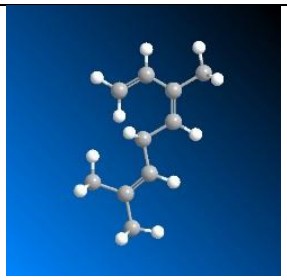
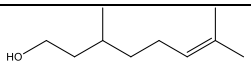
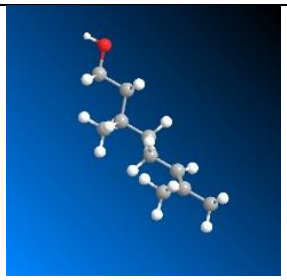
Activity	Chemical	Part	Low PPM	High PPM	StdDev
0	1-CARVOTANACETONE	Plant	327.0	1284.0	
11	ALPHA-PHELLANDRENE	Plant	24.0	96.0	-0.5
28	ALPHA-PINENE	Plant	78.0	312.0	-0.26
23	ALPHA-TERPINEOL	Plant	-	-	
13	BETA-PINENE	Plant	-	-	
0	BOURBONENE	Plant	30.0	120.0	
9	CAMPHENE	Plant	150.0	960.0	1.04

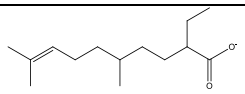
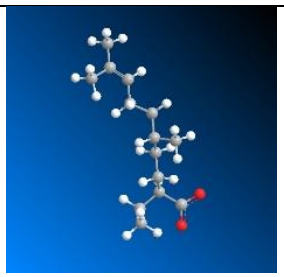
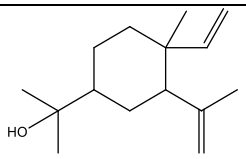
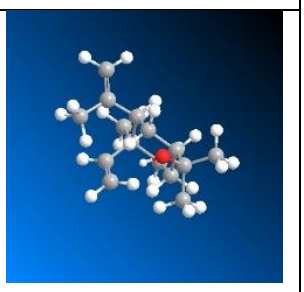
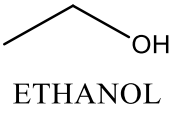
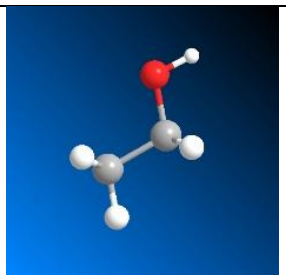
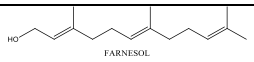
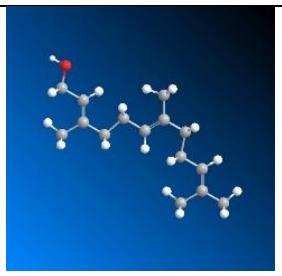
41	CAMPHOR	Plant	15.0	60.0	-0.62
31	CARYOPHYLLENE	Plant	96.0	348.0	-0.07
3	CIS-OCIMENE	Plant	42.0	168.0	0.05
15	CITRONELLOL	Plant	252.0	1008.0	1.71
1	CITRONELLYL-BUTYRATE	Plant	-	-	
0	D-CITRONELLAL	Plant	126.0	1800.0	
0	D-CITRONELLOL-ACETATE	Plant	57.0	228.0	
0	D-CITRONELLOL-N- BUTYRATE	Plant	-	-	
8	DELTA-3-CARENE	Plant	-	-	
2	ELEMOL	Plant	51.0	204.0	0.85
0	EO	Plant	3000.0	12000.0	0.17
24	ETHANOL	Plant	75.0	300.0	
17	FARNESOL	Plant	6.0	36.0	-0.47

Several active compounds in Cymbopogon nardus. L can be identified using Chemdraw and Chem3D, so the results can be seen in the following table:

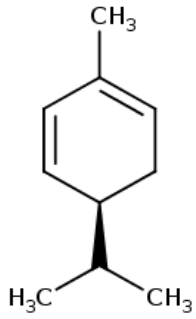
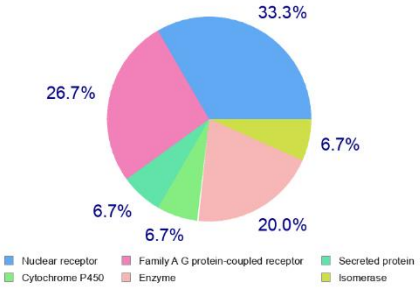
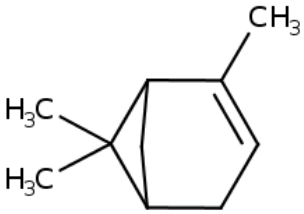
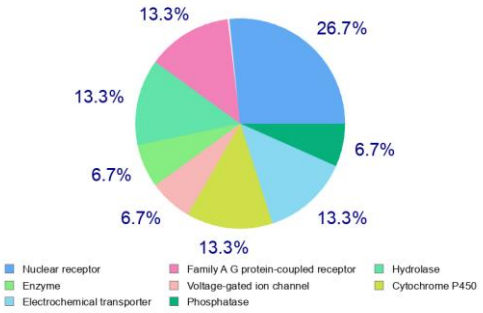
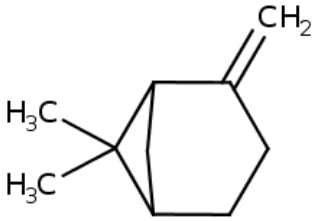
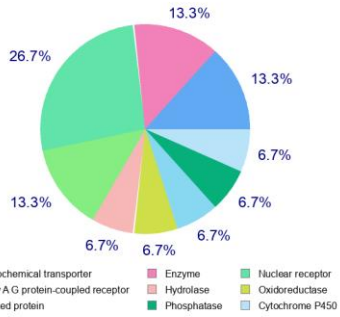
Elements/ Compound	**Chemical Properties**	**Structure 2D**	**Structure 3D**
ALPHA- PHELL ANDRENE	Boiling Point: 450.81 [K] Melting Point: 208.38 [K] Critical Temp: 639.45 [K] Critical Pres: 27.47 [Bar] Critical Vol: 494.5 [cm3/mol] Gibbs Energy: 105.62 [kJ/mol] Log P: 3.12 MR: 48.71 [cm3/mol] Henry's Law: -1.1 Heat of Form: -96.6 [kJ/mol] tPSA: 0 CLogP: 4.412 CMR: 4.5872	 ALPHA- PHELLANDRENE	

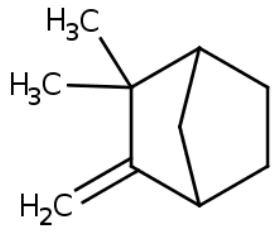
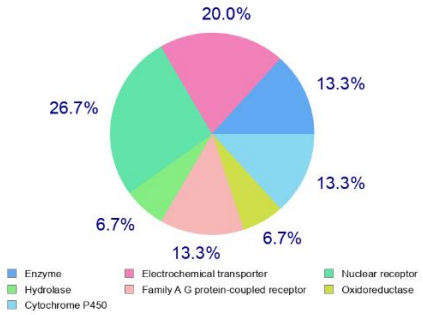
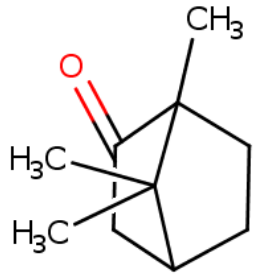
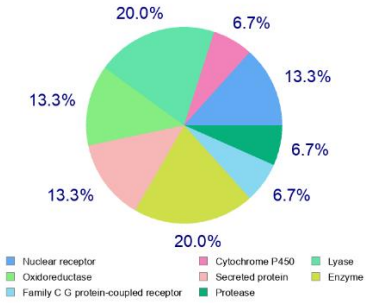
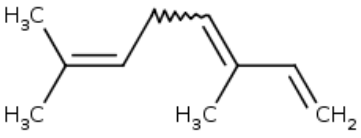
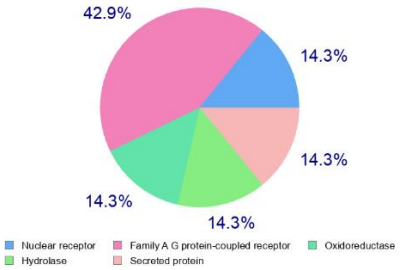
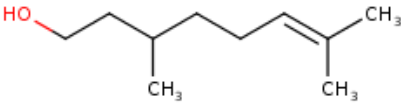
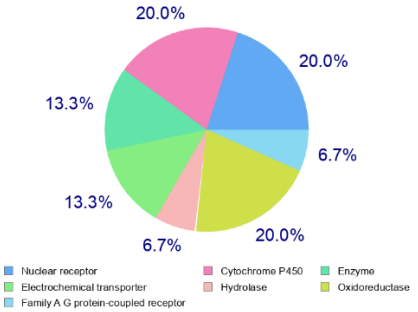
ALPHA-PINENE	Boiling Point: 445.86 [K] Melting Point: 267.26 [K] Critical Temp: 632.45 [K] Critical Pres: 28.91 [Bar] Critical Vol: 484.5 [cm3/mol] Gibbs Energy: 149.85 [kJ/mol] Log P: 2.9 MR: 45.05 [cm3/mol] Henry's Law: -0.64 Heat of Form: -69.08 [kJ/mol] tPSA: 0 CLogP: 4.702 CMR: 4.4352	 ALPHA-PINENE	
BETA-PINENE	Boiling Point: 440.88 [K] Melting Point: 267.66 [K] Critical Temp: 623.65 [K] Critical Pres: 28.84 [Bar] Critical Vol: 482.5 [cm3/mol] Gibbs Energy: 182.6 [kJ/mol] Log P: 2.95 MR: 43.74 [cm3/mol] Henry's Law: -0.57 Heat of Form: -31.15 [kJ/mol] tPSA: 0 CLogP: 4.702 CMR: 4.4352	 BETA-PINENE	
CAMPHENE	Boiling Point: 440.88 [K] Melting Point: 267.66 [K] Critical Temp: 623.65 [K] Critical Pres: 28.84 [Bar] Critical Vol: 482.5 [cm3/mol] Gibbs Energy: 182.6 [kJ/mol] Log P: 2.95 MR: 43.74 [cm3/mol] Henry's Law: -0.57 Heat of Form: -31.15 [kJ/mol] tPSA: 0 CLogP: 4.702 CMR: 4.4352	 CAMPHENE	

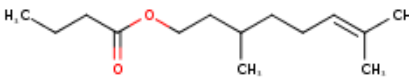
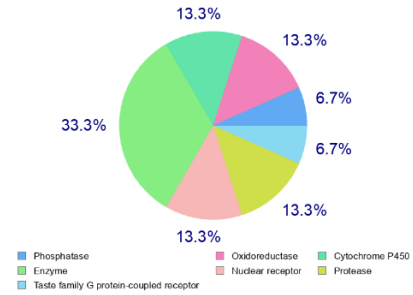
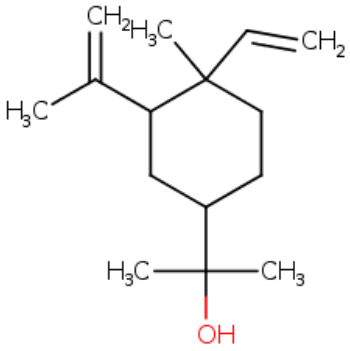
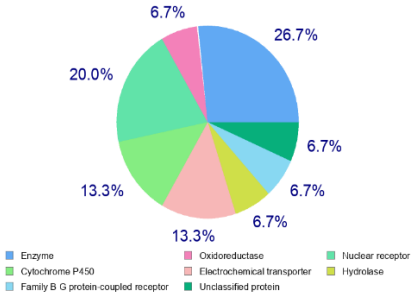
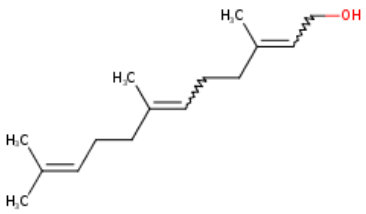
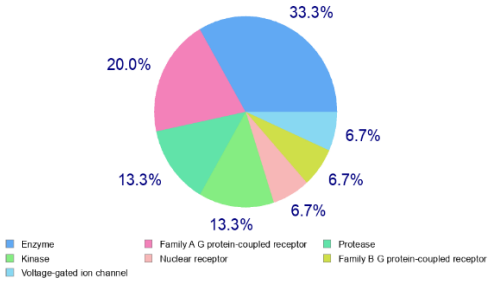
CAMPHOR	Boiling Point: 509.78 [K] Melting Point: 346.1 [K] Critical Temp: 695.08 [K] Critical Pres: 30.83 [Bar] Critical Vol: 503.5 [cm3/mol] Gibbs Energy: 1.44 [kJ/mol] Log P: 2.92 MR: 44.37 [cm3/mol] Henry's Law: 2.54 Heat of Form: -237.85 [kJ/mol] tPSA: 17.07 CLogP: 2.177 CMR: 4.4963	 CAMPHOR	
CIS-OCIMENE	Boiling Point: 433.16 [K] Melting Point: 162.12 [K] Critical Temp: 629.06 [K] Critical Pres: 24.46 [Bar] Critical Vol: 538.5 [cm3/mol] Gibbs Energy: 264.5 [kJ/mol] Log P: 3.28 MR: 50.32 [cm3/mol] Henry's Law: -1.4 Heat of Form: 90.56 [kJ/mol] tPSA: 0 CLogP: 4.332 CMR: 4.8912	 CIS-OCIMENE	
CITRONELLOL	Boiling Point: 524.18 [K] Melting Point: 228.74 [K] Critical Temp: 664.48 [K] Critical Pres: 24.48 [Bar] Critical Vol: 589.5 [cm3/mol] Gibbs Energy: -34.27 [kJ/mol] Log P: 2.82 MR: 50.82 [cm3/mol] Henry's Law: 2.83 Heat of Form: -299.81 [kJ/mol] tPSA: 20.23 CLogP: 3.253 CMR: 4.9431	 CITRONELLOL	

CITRONELLYL- BUTYRATE	Boiling Point: 598.67 [K] Melting Point: 286.53 [K] Critical Temp: 714.05 [K] Critical Pres: 17.38 [Bar] Critical Vol: 803.5 [cm3/mol] Gibbs Energy: -47.75 [kJ/mol] Log P: 3.72 MR: Henry's Law: 1.71 Heat of Form: -424.41 [kJ/mol] tPSA: 40.13 CLogP: 1.19 CMR: 6.7453	 CITRONELLYL-BUTYRATE	
ELEMOL	Boiling Point: 635.44 [K] Melting Point: 326.87 [K] Critical Temp: 721.81 [K] Critical Pres: 19.34 [Bar] Critical Vol: 775.5 [cm3/mol] Gibbs Energy: 112.11 [kJ/mol] Log P: 3.84 MR: 70.46 [cm3/mol] Henry's Law: 2.77 Heat of Form: -243.96 [kJ/mol] tPSA: 20.23 CLogP: 4.64 CMR: 7.0593	 ELEMOL This name appears to be ambiguous	
ETHANOL	Boiling Point: 337.54 [K] Melting Point: 172.62 [K] Critical Temp: 500.51 [K] Critical Pres: 57.57 [Bar] Critical Vol: 166.5 [cm3/mol] Gibbs Energy: -170.86 [kJ/mol] Log P: 0.07 MR: 12.84 [cm3/mol] Henry's Law: 3.64 Heat of Form: -236.84 [kJ/mol] tPSA: 20.23 CLogP: -0.235 CMR: 1.2581	 ETHANOL	
FARNESOL	Boiling Point: 647.1 [K] Melting Point: 262.01 [K] Critical Temp: 756.36 [K] Critical Pres: 17.43 [Bar] Critical Vol: 837.5 [cm3/mol] Gibbs Energy: 153.61 [kJ/mol] Log P: 4.01 MR: 75.63 [cm3/mol] Henry's Law: 2.19 Heat of Form: -182.87 [kJ/mol] tPSA: 20.23 CLogP: 5 CMR: 7.2113	 FARNESOL	

The active compound from Cymbopogon nardus is obtained after the 2D and 3D structures are then identified using the Swiss target prediction.

Elements/ Compound	Query Molecule	Target classes
ALPHA-PHELLANDRENE		
ALPHA-PINENE		
BETA-PINENE		

CAMPHENE		
CAMPHOR		
CIS-OCIMENE		
CITRONELLOL		

CITRONELLY L-BUTYRATE		
ELEMOL		
FARNESOL		

Lemongrass (Cymbopogon nardus) is a type of plant that can be used as a mosquito repellent in accordance with the repellent requirements, namely that it does not interfere with its use, is made from natural ingredients that are not sticky or sticky, smells good, is non-toxic and does not irritate the skin and takes advantage of the yard environment and easy to cultivate. Lemongrass is an upright, chronic grassy plant that has very deep and strong roots. The stems form clumps, are short, massive and round. The cross section of the bar is red. Lemongrass leaves are single, complete and cylindrical leaf midribs,

bald, often the inner surface is red, the tip of the tongue (ligula), strands, more than half hanging, the squeeze smells aromatic. The flower arrangement is panicle or compound grains, stemmed or seated, real protective leaves, usually the same color, generally white.

The content of lemongrass, especially essential oils with 32-45% citronellal components, 12-18% geraniol, 11-15% citronellol, 3-8% geranil acetate, 2-4% citronellyl acetate, citral, kavikol, eugenol , elemol, cadinol, cadinene, vanillin, limonene, camphen. Lemongrass oil contains 3 main components, namely citronellal, citronellol and geraniol [6]. The distillation of Andropogon nardus L can be obtained by an essential oil called Oleumcitronellae, mainly consisting of geraniol and citronellal which can be used to repel mosquitoes [10]. Ash from the leaves and stalks of lemongrass contains 45% silica which is the cause of desiccation (continuous discharge) on the skin of insects so that the insects will die from drying out. Citronellol and geraniol are active ingredients that are not liked and are highly avoided by insects, including mosquitoes, so the use of these materials is very useful as mosquito repellents [7].

Citronellal compounds have dehydrating toxicity (desiscant) which can lead to death of mosquitoes due to continuous fluid loss, graniol compounds are substances that can protect against insects and volatile compounds are substances that have a smell that mosquitoes do not like, properties possessed by geraniol and volatile compounds This is what gives effect to the effectiveness of mosquito repellents.

4. Conclusion

Based on research that has been done by several people and several literature reviews, it can be concluded that lemongrass (Cymbopogon nardus) has benefits as a mosquito repellent that can repel mosquitoes because this plant contains namely citronellal, citronellol and geraniol which are active ingredients which are not liked by mosquitoes

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