

Identification of Chemical Compounds of Ylang Ylang Flower Essential Oil (*Cananga Odorata*) and Kaffir Lime Essential Oil (*Citrus Hystrix*) Using Gas Chromatography- Mass Spectrophotometry (Gc-Ms)

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Article Info

Article history:

Received May 7, 2024

Revised June 22, 2024

Accepted June 22, 2024

Keywords: (A-Z)

Chemical component

D-limonen

Linalool

ABSTRACT

Essential oils are substances that have an aroma contained in plants, these oils are usually also referred to as volatile oils and are usually in liquid form and can be isolated from plant parts such as roots, stems, leaves, flowers, fruit and seeds. This research aims to determine the chemical components of kaffir lime essential oil (*Citrus hystix*), ylang ylang (*Cananga odorata*) using the GC-MS method. The conclusion from the research results is that there is a main compound produced by kaffir lime (*Citrus hystix*) essential oil, namely the chemical compound D-limonane (15.15%) while the chemical compound linalool contained in kaffir lime (*citrus hystrix*) essential oil is only 1.04 % so that the essential oil of kaffir lime (*citrus hystrix*) does not meet the quality standard requirements for the chemical compound linalool of 3.5-5.5%. The main compound produced by ylang-ylang oil (*Cananga odorata*) is the chemical compound Linalool (17.85%). In this case, efforts need to be made to improve the quality of essential oils in order to increase added value and meet the requirements for essential oil quality standards.

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1. INTRODUCTION

Indonesia is a country with a very high level of plant diversity in producing essential oils (Qodri, 2020). Until now, the essential oil trade is quite developed because the uses of essential oils are quite specific and have economic value. The essential oils that have been studied include clove oil, patchouli, nutmeg, vetiver, cinnamon, and lemongrass (Lunggela et al., 2022).

Essential oils are substances that have an aroma contained in plants, these oils are usually also referred to as volatile oils and are usually in liquid form and can be isolated from plant parts such as roots, stems, leaves, flowers, fruit and seeds (Lunggela et al., 2022). Essential oils are also widely used in the health, food, cosmetics and pharmaceutical industries, where they are useful for meeting needs (Qodri, 2020).

Kaffir limes are quite famous in Indonesian society. Kaffir lime is a plant from the Citrus genus and is a plant that produces essential oils. Kaffir lime contains bioactive compounds including vitamin C, flavonoids, carotenoids, limonoids and minerals important for health and can inhibit the growth of *Staphylococcus Aureus* bacteria. Kaffir lime essential oil is an essential oil that comes from Indonesia (Warsito et al., 2017). According to scientific research sources, kaffir lime contains essential oils which can inhibit bacterial growth (Megumi, 2017).

Ylang-ylang is a plant that is used as an essential oil. One of the flower plants that is popular with many people because it has many uses. Ylang-ylang is a plant native to Indonesia, especially Bali, especially Ylang-ylang from the species *Cananga odorata* forma *macrophylla* which can produce ylang-ylang oil. Until now, ylang-ylang is a plant that produces essential oils (Ayuni et al., 2021).

According to the results of research by Anwar et al. in 2023, using the GC-MS method, the content of the main chemical compound, namely linalyl acetate, was 20.59%. Linalyl acetate has various pharmacological effects, including anti-hypertensive, anti-diabetic, neuroprotective, anti-inflammatory, and antioxidant properties (Shin & Seol, 2023). Meanwhile, according to the results of research by Sry Iryani and Deka in 2018, the results of the essential oil content of kaffir lime (*Citrus Hystrix*) using the GC-MS method showed that the content of the main chemical compound, namely limonene, was 16.45%. D-limonene is one of the most common terpenes in nature. D-limonene is the main constituent in several citrus oils (Fitrianti et al., 2016).

The main content of ylang ylang essential oil (*Cananga Odorata*) according to the results of research by Anwar et al. in 2023 using the GC-MS method, it was found that the content of the main chemical compound, namely caryophyllene, was 14.36%. Caryophyllene has antibacterial functions, antioxidant effects, anti-fungal activity and strong cytotoxic properties against cancer cells from essential oils (Jelita et al., 2018). Meanwhile, according to Maulidya et al.'s research in 2016, the results of the essential oil content of ylang-ylang flowers (*Cananga Odorata*) using the GC-MS method showed that the main content was caryophyllene but with a higher percentage compared to Anwar et al.'s research in 2023, namely 29.60%.

The chemical compound content of kaffir lime essential oil (*Citrus Hystrix*) and ylang ylang flower essential oil (*Cananga Odorata*) from several research results shows that the results of the essential oil content are different for each identification, therefore it is necessary to re-identify to find out the essential oil content that will be used. used as raw material for a product. The method commonly used to determine essential oil content is by using the gas chromatography-mass spectrometry (GC-MS) method (Lunggela et al., 2022).

Gas chromatography-mass spectrometry (GC-MS) is a method that combines gas chromatography and mass spectrometry for the purpose of identifying various compounds in sample analysis. This means that the sample to be tested is identified first using a GC (Gas Chromatography) tool, then the sample is identified using an MS (Mass Spectrometry) tool. Gas Chromatography – Mass Spectrometry (GC-MS) is able to detect drug concentrations 1µ g/L and requires a relatively short processing time (Pratiwi et al., 2022)

The GC-MS identification method was used to determine the chemical compound content in kaffir lime essential oil (*Citrus Hystrix*) and ylang-ylang essential oil (*Cananga Odorata*). The advantages of the GC-MS method are fast identification time, high sensitivity, good separation capability and long-term use of the instrument. Based on the background above, analysis of essential oils was carried out with the aim of finding out in more detail the chemical components contained therein.

2. RESEARCH METHOD

The type of research used is experimental. Experimental research is research conducted to determine the chemical compounds of ylang ylang flower essential oil (*Cananga odorata*) and kaffir lime essential oil (*Citrus Hystrix*) using the GC-MS method.

The materials used in this research were two types of essential oils obtained from farmers and refineries in PT. Syailendra Bumi Investama Wonorejo Gondangrejo Karanganyar Village Central Java, namely kaffir lime oil (*Citrus Hystrix*) and ylang-ylang oil (*Cananga Odorata*). The essential oil produced was obtained using the steam distillation method which was carried out for 8-10 hours. The steam distillation method is the method most often used by the essential oil industry because the process is easy and uses simple equipment. The essential oils obtained were identified at the BRIN (National Research and Innovation Agency) chemical laboratory in Tangerang, Banten using GC-MS instrument, Merek: Agilent, Tipe: Agilent 7890B (GC) and 5977A (MSD) with a data base system: NIST 20. The mobile phase and stationary phase used in GC-MS were Agilent 19091S-433 type: 93.92873 DB-5MS UI 5% Phenyl Methyl Siloxane and injection volume of 1 mL.

3. RESULT AND DISCUSSION

From the results of the research carried out, the composition of the chemical compounds of kaffir lime essential oil (*Citrus Hystrix*) was obtained which were analyzed using Gas Chromatography-Mass Spectra (GC-MS). The following is the chemical content of kaffir lime essential oil (*citrus hystrix*) was show in figure 1.

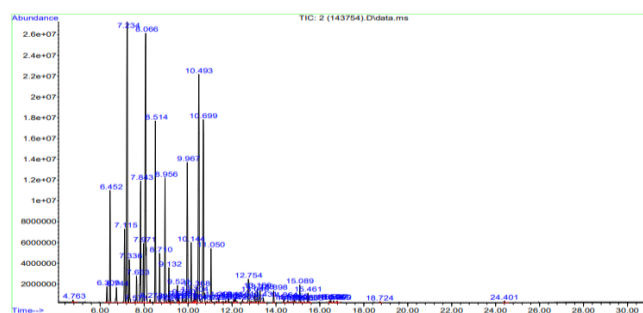


Figure- 1. GC-MS chromatogram of kaffir lime (*Citrus hystrix*)

Based on the results of identifying kaffir lime essential oil originating from Central Java using GC-MS, the results showed that kaffir lime essential oil has 65 identified components and 10 components with the highest peaks as seen in Figure 1, where five peaks are the dominant components, that is D-limonane (15.15%), Bicyclo [3.1.1] heptane, 6,6-dimethy 1-2-methylene-, (1S)-. beta. -pinene (14.68%), Terpinen-4-ol (10.92%), Alpha tepineol (9.21%), Isopugeol (6.21%).

Table 1. Chemical components of kaffir lime

Peak	Retention Time (Rt)	Compound	Area (%)	Qual
1	6.305	Bicyclo [3.1.0] hex-2-ene, 4-methyl-1- (1-methylethyl)-	0.52	94
2	7.238	Bicyclo [3.1.1] heptane, 6,6-dimethy 1-2-methylene-, (1S)-. beta. -pinene	14.68	97
3	7.578	Ethylane oxide	0.04	5
4	7.666	Alpha. -phellandrene	1.05	91
5	7.843	1,3-cyclohexadine, 1-methyl-4-(1-methylethyl)-	5.00	98
6	8.070	D-Limonene	15.15	99
7	8.511	Gamma. -Terpinene	5.98	96
8	8.952	Cyclohexene, 1-methyl-4-(1-methylethylidene)-	4.04	97
9	9.027	Acetaldehyde	0.06	3
10	9.128	Linalool	1.04	96
11	9.204	1,3-Butanediamine	0.08	40
12	9.519	4-isoprophyl-1-methylcyclohex-2-eno	0.21	87
13	9.973	Isopulegol	6.21	99
14	10.250	2-Propenamamide	2.06	97
15	10.300	Cyclohexanol, 5-methyl-2-(1-methylethenyl)-	0.35	99
16	10.489	Terpinen-4-ol	10.92	96
17	10.704	Alpha. -terpineol	9.21	91
18	11.044	Citronellol	1.70	96
19	13.048	Geranyl acetate	0,48	91
20	13.892	Caryophylene	0.39	99
21	14.359	Humulene	0.13	96
22	15.090	1-isopropyl-4, 7-dimethyl-1,2,3,4,5,6, 8a-hexahydronaphthalene	0.65	96

Based on the results of identifying kaffir lime essential oil using the GC-MS method, the chemical compounds of kaffir lime produced can be seen in table 1. There are 5 dominant components contained in kaffir lime essential oil (*Citrus Hystrix*) which is marked in red, namely D-limonane (15.15%), Bicyclo [3.1 .1] heptane, 6,6-dimethy 1-2-methylene-, (1S)-. beta. -pinene (14.68%), Terpinen-4-ol (10.92%), Alpha tepineol (9.21%), Isopugeol (6.21%). The analysis results obtained show that the main compound in kaffir lime essential oil (*Citrus Hystrix*) is D-limonene with the molecular formula $C_{10}H_{16}$, a retention time of 8.07 minutes and with an area percentage of 15.15% which is found in the 6th peak. There are several other compounds in kaffir lime essential oil (*Citrus Hystrix*). The compounds that appear are compounds that are also found in kaffir lime essential oil but are present in very small amounts.

The results of this research are supported by other research conducted by Yustinah in 2016. The sample used for analysis was taken with a variable amount of 500 ml of 1 ml of solvent, then the results of the analysis obtained the main compound in the form of limonene with the molecular formula $C_{10}H_{16}$ in essential oil from orange peel with a retention time of 7.01 minutes and an area percentage of 96. 79% (Yustinah & Fanandara, 2016). The percentage of area produced from the chemical compound D-limonene from Yustinah's 2016 research was greater than this research, namely 15.15%.

The results of this identification are different from research conducted by Anwar in 2023 regarding the identification of chemical compounds from kaffir lime essential oil (*Citrus Hystrix*) obtained from Central Java. The identification results showed that there were 44 chemical compounds with 5 main components, namely Linalyl acetate (20.59%), D-limonene (17.77%), Linalool (15.19%), Geranyl acetate (7.64%), 1, 3-cyclohexadiene, and 1-methyl-4 alpha-terpinyl acetate (6.42%). The chemical compound Linalyl acetate shows

the most dominant compound with a percentage area (20.59%) showing a higher percentage produced with this identification result. Meanwhile, the most dominant compound in this study was D-limonene with a percentage area of 15.15%.

In general, differences in the composition of essential oils identified by various researchers are caused by differences in the type of plant produced, climatic conditions, soil where it is grown, age of harvest, extraction methods used, and how the oil is stored. According to research conducted by Dacosta et al in 2017 who conducted research on the comparison of essential oil content from different locations, the results showed that the content of essential oils produced from highland locations was higher than those in lowland areas, but the quality of the essential oils produced from plain locations low is better than the quality of essential oils from the highlands.

Table 2. orange oil quality requirement

Parameter	Test result	Condition (ISO 3140-2011)
Color	Light yellow	Colorless - yellow
Aroma	Typical kaffir lime	Standard
Linalool	1.04%	3.5-5.5%

The organoleptic test results of kaffir lime essential oil (*Citrus Hystrix*) showed a light yellow color, a typical orange aroma with a concentration of the chemical compound linalool 1.04%; these results does not meet the quality requirements of ISO 3140-2011. The quality of kaffir lime essential oil (*Citrus Hystrix*) can be influenced by several factors, including the selection of quality kaffir lime seeds, appropriate cultural techniques and proper separation and purification (Yuliana et al., 2020).

From the results of the research carried out, the composition of the chemical compounds of ylang-ylang essential oil (*Cananga Odorata*) was obtained which were analyzed using Gas Chromatography-Mass Spectra (GC-MS). The following is the chemical content of ylang-ylang essential oil (*Cananga Odorata*) was show in figure 2.

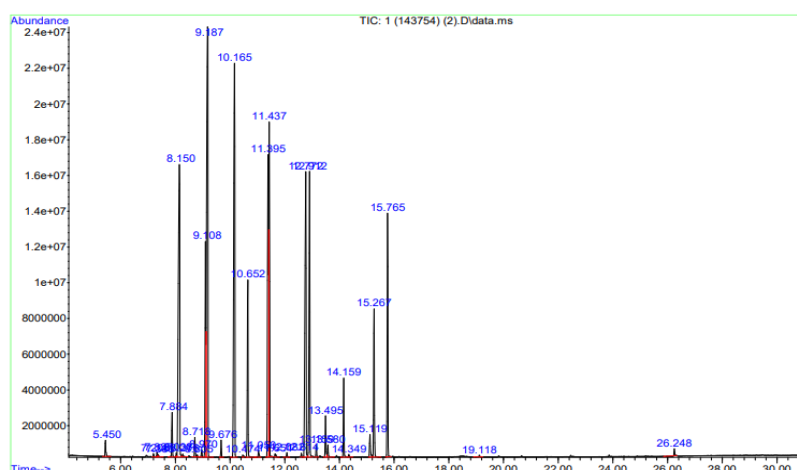


Figure- 2. GC-MS chromatogram of Ylang oil (*Cananga odorata*)

Based on the results of identifying ylang ylang essential oil originating from Central Java using GC-MS, the results showed that ylang-ylang essential oil (*Cananga odorata*) has 35 identified components and 10 components with the highest peaks as seen in Figure 1, where five peaks are the dominant components, that is Linalool (17.85%), Benzyl alcohol (12.49%), Acetic acid (13.46%), Piperonal (10.08%), Eugenol (7.17%).

Table 3. Chemical components of Cananga essential oil

Peak	Retention Time (Rt)	Compound	Area (%)	Qual
1	5.448	1- Butanol, 3-methyl-, acetate	0.37	80
2	7.389	2-Chloro-1, 1, 2-trifluoroethyl ethyl 1 ether	0.05	9
3	8.145	Benzyl alcohol	12.49	98
4	8.271	Acetic acid, chloro-, ethyl ester	0.09	7
5	9.103	Benzoic acid, methyl ester	4.35	97
6	9.191	Linalool	17.85	97

Peak	Retention Time (Rt)	Compound	Area (%)	Qual
7	10.162	Acetic acid, phenylmethyl ester	13.46	98
8	10.653	Methyl salicylate	4.00	97
9	11.044	2,6-Octadien-1-0l, 3,7-dimethyl-, (z)-	0.17	93
10	11.397	Linalyl acetate	8.35	91
11	11.435	Geraniol	7.15	96
12	11.649	3, 4-Pyridinediamine	0.11	43
13	12.771	Piperonal	10.08	97
14	12.909	Eugenol	7.17	98
15	13.161	Geranyl acetate	0.24	91
16	13.577	Phenol, 2-methoxy-4- (1-propenyl)-, (z)	0.29	98
17	14.157	Phenol, 2-methoxy-4- (1-propenyl)-	1.48	98
18	15.115	2-Propanone, 1- (4-hydroxy-3-methoxyphenyl)-	0.57	91
19	15.266	Benzoic acid, 2-hydroxy-, 2-methyl butyl ester	3.37	98
20	15.770	Benzoic acid, 2-hydroxy-, penthyl ester	5.14	96
21	19.122	Benzoic acid, 2-hydroxy-, phenylmethyl ester	0.04	86
22	15.090	Licarin A	0.06	98

Based on the results of identifying ylang-ylang essential oil (*Cananga odorata*) using the GC-MS method, the chemical compounds of ylang-ylang produced can be seen in table 3. There are 5 dominant components contained in ylang-ylang essential oil (*Cananga odorata*) which is marked in red, namely Linalool (17.85%), Benzyl alcohol (12.49%), Acetic acid (13.46%), Piperonal (10.08%), Eugenol (7.17%). The analysis results obtained show that the main compound in ylang-ylang essential oil (*Cananga odorata*) is linalool with the molecular formula $C_{10}H_{18}O$, a retention time of 9.19 minutes and with an area percentage of 17.85% which is found in the 6th peak. There are several other compounds in ylang-ylang essential oil (*Cananga odorata*). The compounds that appear are compounds that are also found in ylang-ylang essential oil (*Cananga odorata*) but are present in very small amounts.

The results of this research are supported by other research conducted by Anggia in 2014, namely from the results of the analysis it was found that the main compound was linalool with a molecular formula $C_{10}H_{18}O$ and area percentage of 12.79% (Anggia *et al*, 2014). The percentage area of the chemical compound linalool resulting from Anggia's research is smaller than this research, namely 17.85%.

The results of this identification are different from research conducted by Anwar in 2023 regarding the identification of chemical compounds from ylang-ylang essential oil (*Cananga odorata*) obtained from West Java. The identification results showed that there were 73 compounds with the main component being caryophyllene with an area percentage of 14.36%, indicating a chemical compound composition that was different from this research. While the chemical compound caryophyllene in this study was not detected (Anwar *et al*, 2023).

In general, differences in the composition of essential oils identified by various researchers are caused by differences in the type of plant produced, climatic conditions, soil where it is grown, age of harvest, extraction methods used, and how the oil is stored (Rudini, 2017).

Table 4. Ylang oil quality requirements

Parameter	Test result	Condition (SNI 06-3949-1005)
Color	Light yellow	Light yellow-dark yellow
Aroma	Typical ylang-ylang oil	Fresh, typical ylang ylang oil
Solubility in 95% ethanol	Soluble	1:0,5 clear

Characterization of the physical properties of ylang ylang essential oil (*Cananga odorata*) include light yellow-dark yellow color, fresh smell typical of ylang ylang, refractive index measurement of 0.904-0.920 gr/ml (27° C), specific gravity of 1.493-1.503 (27° C) and soluble in alcohol based on in SNI 06-3949-1005. This aims to determine the quality of the essential oil produced (Pujiarti *et al.*, 2015).

4. CONCLUSION

Based on the results of identifying essential oils obtained from Central Java using the GC-MS method, it was found that in kaffir lime essential oil (*Citrus Hystrix*) there was a main component, namely D-limonene with a percentage area of 15.15%, while in ylang-ylang essential oil (*Cananga Odorata*) there was a main component, namely linalool with a percentage area 17.85%. Meanwhile, based on the parameters of the quality requirements for kaffir lime essential oil (*Citrus Hystrix*), it does not meet the quality standards because the percentage area of the chemical compound linalool produced is 1.04% and does not meet the quality standards, namely 3.5-5.5%. In this case, efforts need to be made to improve the quality of essential oils so that they can improve added value, while ylang ylang essential oil (*Cananga Odorata*) meets quality standards.

5. ACKNOWLEDGEMENT

I would like to thank those who have helped in preparing this journal. thank BRIN for facilitating GC-MS testing, PT. Syailendra Bumi Investama, farmers and processors of kaffir lime essential oil (*Citrus Hystrix*) and ylang ylang essential oil (*Cananga Odorata*) as well as supervisors and colleagues who have helped in the preparation and publication of this journal.

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