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Identification of Chemical Compounds of *Cymbopogon Nardus* (L.) Rendle and *Ocimum Basilicum* (L.) using Gas Chromatography-Mass Spectrometry (GC-MS)

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ABSTRACT
Citronella essential oil (*Cymbopogon nardus* (L.) and basil leaf essential oil (*Ocimum basilicum* (L.) offer various benefits, including antibacterial properties. This study aims to identify the chemical compounds present in these oils obtained through local distillation at PT Syailendra Bumi Investama in Wonorejo Village, Gondangrejo, Karanganyar, Central Java. Gas Chromatography-Mass Spectrometry (GC-MS) analysis was conducted at the BRIN (National Innovation Research Agency) in Serpong, South Tangerang, Banten, to characterize citronella essensial oil and basil essential oil. The findings indicate that citronella essential oil meets the criteria of SNI 06-3953-1995, with three compounds showing significant concentrations: Geraniol (26.49%), citronellol (14.53%), and citronellal (10.95%). Similarly, research on basil leaf essential oil conforms to ISO 11043 - 1998 standards, revealing high concentrations of two compounds: Estragole (55.80%) and linalool (22.35%).

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1. INTRODUCTION

As a tropical nation, Indonesia boasts abundant biodiversity, including a wide variety of essential oils. Renowned as one of the leading producers globally, Indonesia benefits from its natural and geographical features that facilitate the growth of numerous plants yielding essential oils. Following refining processes, these essential oils become sought-after commodities, extensively exported to various nations (Maputo, 2021).

Essential oils, often termed volatile oil, are plant-derived substances distinguished by their volatility, bitter taste, and aromatic fragrance reflective of their botanical origins. With numerous benefits, essential oils find applications across various domains, including medicinal uses due to their diverse biological activities. These activities encompass antiseptic, analgesic, diuretic, antispasmodic, antirheumatic, antidepressant, insecticidal, antifungal, antibacterial properties, among others. Presently, citronella essential oil and basil essential oil are extensively investigated for their potential as primary components in antibacterial hand sanitizer formulations (Putri et all., 2020).

Citronella with the Latin name (*Cymbopogon nardus* (L.) is a plant known as the "Citronella Oil of Java" is an annual plant of the Poaceae family (Munda et al., 2020). Citronella contains three main components, namely geraniol, citronellol, and citronellal (Anwar et al., 2020). Citronella plants (*Cymbopogon nardus* (L.) have fibrous roots and herbaceous habitus (grass group). The stem is between 50-100 cm high, flat round, white- brown in colour. The leaves are lanceolate, parallel leaf bones, green in colour and rough leaf surface. The main content in citronella plants generally contains flavonoids, saponins, polyphenols and essential oils (Depkes RI, 2001).

Basil plants known as (*Ocimum basilicum* L.) have more than 30 species that are included in the Lamiaceae family and the genus Ocimum. This plant can grow in subtropical and tropical areas at high and low altitudes with altitudes reaching 1,100 metres above sea level. Basil plants have petioles with a length of 0.25-3 cm with round to elliptical leaf shapes, pointed ends, and elongated. The leaves and flower shoots of the basil plant are a source of essential oil. Basil leaf essential oil contains alkaloids, aldehydes, beta carotene, ascorbic acid, cineole, eugenol, eugenolmeter-ether, glycosides, linalool, methyl chavicol, ursolic acid, n-triacontanol, and phenol (Verrillo et all., 2021).

Gas Chromatography-Mass Spectrometry (GC-MS) is employed in analytical techniques to discern the primary constituents within essential oils. This method combines the separations capabilities of gas-liquid chromatography, which isolates compounds, with *mass spectrometry's* capacity to identify substances in the sample. GC-MS divides analytes based on mass for identification, while *Gas chromatography* isolates volatile and thermally stable compounds. The fusion of these techniques enables the separation, identification, and quantification of individual components within complex mixtures like essential oils, offering crucial insights into their chemical makeup (Chauhan, 2014).

Certainly, examining the chemical makeup of essential of essential oils holds significant importance, particulary when they serve as primary ingredients in formulations. Given citronella essential oil's frequent utilization across various products owing to its antibacterial attributes, pispointing its chemical compounds assumes paramount significance. Consequently, *Gas Chromatography-Mass Spectrometry* (GC-MS) was employed to identify the chemical constituents present in citronella oil (Sari et all., 2023).

Therefore, this research was conducted to discuss the identification of citronella and basil with the aim of knowing the components of chemical compounds contained in citronella oil and basil leaf oil using *Gas Chromatography-Mass Spectrometry* (GC-MS).

2. RESEARCH METHOD

The materials used in this study were citronella essential oil and basil leaf essential oil obtained from local distillation using the water vapour distillation method at 80°C for 8 hours at PT Syailendra Bumi Investama, Wonorejo Village, Gondangrejo Karanganyar, Central Java. The essential oil obtained was identified through the BRIN (National Research and Innovation Agency) chemical laboratory in Serpong, South Tangerang, Banten, Indonesian using GC-MS instrument. The essential oil composition was identified using Aligent 7890B (GC) and 5977A (MSD) Mass Spectrophotometry Gas Chromatography (GC), 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 1 mL injection volume.

3. RESULT AND DISCUSSION

Chemical Content of Essensial Oil of *Cymbopogon nardus* (L.) Rendle was show in figure 1

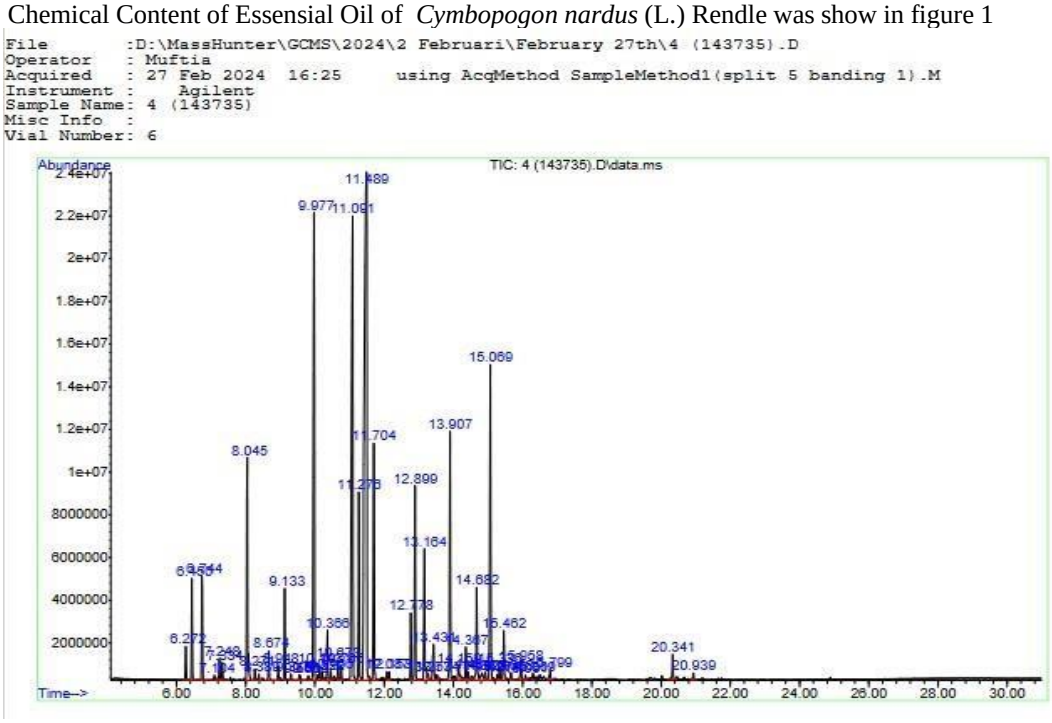

Figure 1. Chromatogram of *Cymbopogon nardus* (L.) Rendle

Based on the results of identification using *Gas Chromatography-Mass Spectrometry* (GC-MS), the essential oil obtained from a local refinery in PT. Syailendra Bumi Investama Wonorejo Gondangrejo Karanganyar Village, Central Java 39 compounds, of which there were 3 compounds with high content, namely Geraniol (26,49%), Citronellol (14,53%) dan Citronellal (10,95%)

Table 1. Chemical compounds of *Cymbopogon nardus* (L.) Rendle

Peak	Retention time (RT)	Area %	Compound	Qual
1	6.746	1.91	Camphene	97
2	7.339	0.32	beta.-Myrcene	96
3	8.044	4.36	D-Limonene	98
4	8.271	0.23	1,3,6-Octatriene, 3,7-dimethyl-, (Z)	98
5	8.385	0.10	5-Heptenal,2,6-dimethyl	93
6	8.675	0.58	4-Nonanone	94
7	8.952	0.24	Cyclohexene, 1-methyl-4-(1- methyle thylidene)	98
8	9.128	1.38	Linalool	96
9	9.128	1.38	Linalool	96
10	**9.973**	**10.95**	**Citronellal**	**87**
11	10.225	0.16	2-((3,3Dimethyloxiran-2-yl)methyl -3-methylfuran	96
12	10.363	0.90	endo-Borneol	94
13	10.363	0.90	Bicyclo	90
14	10.464	0.17	Terpinen-4-ol	94
15	10.678	0.35	Terpineol	90
16	10.767	0.29	Decanal	90
17	**11.094**	**14.53**	**Citronellol**	**98**
18	11.271	3.32	Neral	95
19	11.271	3.32	Citral	74
20	**11.485**	**26.49**	**Geraniol**	**96**
21	11.699	4.53	Citral	96
22	12.153	0.17	Citronellic acid	98
23	12.783	1.05	2,6-Octadiene, 2,6-dimethyl	98
24	12.783	1.05	2,6-Octadiene, 2,6-dimethyl	98
25	12.783	3.51	Eugenol	98
26	13.426	2.48	Geranyl isobutyrate	91
27	13.426	1.06	Cyclohexane, 1-ethenyl-1-1-methyl-2,4-bis (1-methylethenyl)	99
28	13.905	4.34	Caryophyllene	99
29	14.157	0.45	Pheno,2-methoxy-4-(1-propenyl)	98
30	14.371	0.62	Humulene	97
31	14.434	0.17	Muurola-4(15),5-diene	98
32	14.686	1.85	Germacrene D	99

Peak	Retention time (RT)	Area %	Compound	Qual
33	14.825	0.32	Zonarene	94
34	15.064	6.05	Naphthalene,1,2,3,4,4a,5,6,8a-oct ahydro-7-methyl-4-methylene-1-(1-methylethyl)	99
35	15.064	6.05	Naphthalene,1,2,4a,5,6,8a- hexahydro-4,7-dimethyl-1-(1- methylethyl)	99
36	15.342	0.24	Naphthalene,1,2,4a,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)	99
37	15.468	1.00	Cyclohexanemethanol 4-ethenyl-alpha.,alpha.,4-trimethyl-3-(1-methylethenyl)	95
38	15.669	0.50	Caryophyllene oxide	93
39	16.804	0.27	2Naphthalenemethanol, 1,2,3,4,4a, 5,6,8a	96

Specific quality standards for citronella oil are outlined in SNI 06-3953-1995. Citronella oil should have a refractive index between 1.466 and 1.475 and a light yellow to yellow-brown colour according too this standard. This oil should contain a minimum 0f 85% total Geraniol and 35% Citronellal. It should also be readily soluble in 80% ethanol at a ratio of 1:2 and appear clear to slightly cloudy without additives such as oils, fats, or alcohol. Citronella oil should have a distinctive and fresh aroma, an optical rotation of –(-6), and a flash point of 76-84 °C (Wijayati et al., 2023).

Table 2. Comparison of inspection results of citronella essential oil and SNI 06-3953-1995 standard

No	Parameters	Results	SNI 06-3953-1995
1	Colour	Brown - Yellowish	Bright yellow – Yellow with a hint of brown
2	Aroma	Specific aroma of citronella	Specific aroma of citronella
3	Solubility in alcohol	Solute	80% solute in alcohol
4	Citronellal	10,95%	Minimum 35%
5	Geraniol	26,49%	Minimum 85%

The chemical compounds Geraniol, Sitronellal and Sitronellol are the 3 most compounds that make up essential oils (Sukandar, D., et al., 2022). The identification results in this study can also be supported by other studies which also found that of the many chemical compounds contained in Cymbopogon nardus (L.) Rendle essential oil are citronellal (35.72%), citronellol (15.09%), and geraniol (12.89%) (Kumala et al., 2019). Both identification results show citronellol, citronellal, and geraniol compounds as constituents of almost all citronella essential oils. Therefore, there are differences in the percentage of identification results using citronella essential oil samples from Wonorejo Gondangrejo village, Karanganyar, Central Java. This difference can be explained by comparing various factors that affect plant growth and development, such as age, genetics, season, and plant location. The identification results of this study are very different from previous findings, where the compounds with the highest percentage of Geraniol, Citronellol, and Citronellal have a percentage of 26.49%, 14.53%, and 10.95% respectively. One of the three chemical compounds which is the main constituent of citronella essential oil is Geraniol with a percentage of 26.49%, this is different from the SNI 06-3953-1995 quality standard, geraniol with a percentage of 85%.

These compounds are of great interest in the pharmaceutical, food, and perfume industries. Citronella essential oil, which has a distinctive odor, and is used as an antimicrobial (Munda, et all. 2020). Chemical Content of Essensial Oil of *Basilicum Ocimum* (L.) was show in figure 2.

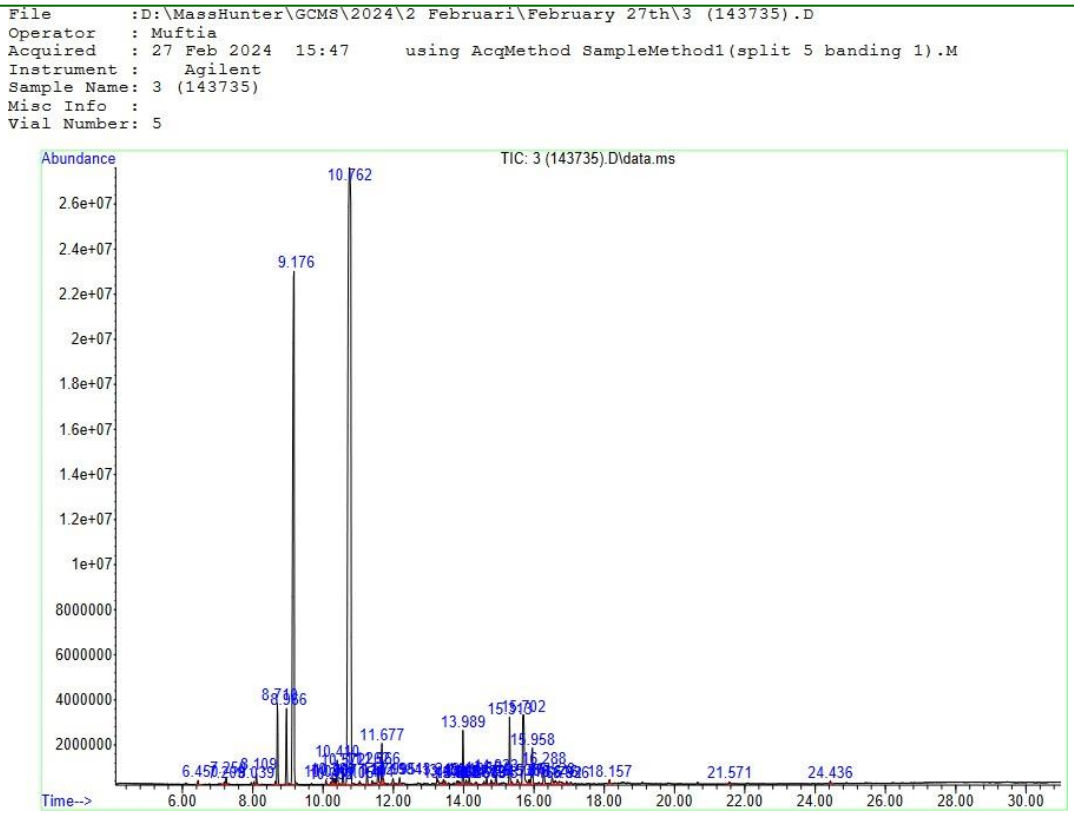

Figure 2. Chromatogram of Basil Leaf (*Ocimum basilicum* L.)

Based on the results of identification using *Gas Chromatography-Mass Spectrometry* (GC-MS), the essential oil obtained from a local refinery in PT. Syailendra Bumi Investama Wonorejo Gondangrejo Karanganyar Village Central Java 28 compounds, of which there were 2 compounds with high content, namely Estragole (55,80%) and Linalool (22,35%)

Table 3. Chemical compounds of Basil Leaves (*Ocimum basilicum* L.)

Peak	Retention time (RT)	Area %	Compound	Qual
1	6.444	0.09	Trimethylbicyclo	93
2	8.108	0.30	Eucalyptol	99
3	8.713	2.21	2-Furanmethanol, 5-ethenyltetrahyd	91
4	8.965	1.91	Ethyl 2-(5-methyl-5- vinyltetrahydrofuran	91
5	**9.179**	**22.35**	**Linalool**	**97**
6	10.414	0.70	Levomenthol	91
7	10.578	0.70	dl-Menthol	91
8	10.578	0.48	3,7-Octadiene-2,6-diol, 2,6-dimethyl-	72
9	**10.767**	**55.80**	**Estragole**	**99**
10	11.258	0.40	Citral	58
11	11.258	0.40	Neral	95
12	11.397	0.17	Geraniol	76
13	11.561	0.59	Benzaldehyde, 4-methoxy-	97
14	11.561	0.59	Benzaldehyde, 4-methoxy	97
15	11.674	1.03	2,6-Octadienal, 3,7- dimethyl	97
16	11.989	0.26	Anethole	98

Peak	Retention time (RT)	Area %	Compound	Qual
17	11.989	0.26	Benzene, 1-methoxy-4-(1-propenyl)	98
18	12.178	0.23	Benzene, 1-methoxy-4- propyl	87
19	13.250	0.33	cis-3-Hexenyl cis-3- hexenoate 71411 5-Heptenal, 2,6-dimethyl	74
20	13.993	1.26	Bergamotene	99
21.	13.993	1.26	Bicyclo	98
22	14.661	0.18	(4-methylpent-3-en-1- yl)bicyclo heptane	96
23	14.661	0.18	Farnesene	97
24	14.926	0.27	Bisabolene	96
25	15.317	1.62	Cyclohexene	99
26	15.707	3.76	Methoxycinnamaldehyde	99
27	15.959	1.36	Caryophyllene oxide	90
28	16.287	0.61	(1R,3E,7E,11R)-1,5,5,8-Tetramethyl	99

ISO 11043-1998 specifies specific quality standards for basil leaf essential oil. According to ISO 11043- 1998, basil leaf essential oil has a slightly yellow or amber colour and a refractive index that ranges between
1.510 and 1.520. It should have 55% Linalool and 87% Estragole, with an optical rotation between -1 and +2, and a flash point of 75°C. Basil leaf essential oil should have a fresh aroma, with an optical rotation between -1 and
+2, and an alcohol soluble ratio of 1:1 (ISO, 1998).

Table 4. Comparison of inspection results of Basil Leaf (*Ocimum basilicum* L.) essential oil and ISO 11043- 1998 standards

No	Parameters	Results	ISO 11043 – 1998
1.	Colour	Light yellow	Amber yellow or pale yellow
2.	Aroma	Specific aroma of basil essential oil	Specific aroma of basil essential oil
3.	Solubility in alcohol	Solute	1:1 Solute in alcohol
4.	Linallol	22.35%	Minimum 55.8%
5.	Estragole	55.80 %	Minimum 87 %

Basil leaf essential oil contains chemical compound components such as Camphor, Sitral, Geraniol, Limonene, and Linalool. This study found differences with other studies that found many chemical compounds contained in Ocimum basilicum (L.) essential oil. Among the many compounds in Ocimum basilicum (L.) essential oil, Neral (55.97%), Sitral (46.19%), and Geraniol (2.99%) are the most commonly found compounds (Tanrisanah, et al, 2023), The identification results showed Neral, Sitral, and Geraniol as the main constituents in almost all essential oils of basil leaves. (Tanrisanah, et al, 2023) obtained from Sungguminasa, Gowa Regency, South Sulawesi, 2023) obtained from Sunggumin, 2023) obtained from Sungguminasa, Gowa Regency, and tested in the laboratory, while the essential oil of basil leaves in this study was obtained from Central Java. The identification results in this study using samples from PT Syailendra Bumi Investama in Wonorejo Gondangrejo, Karanganyar, Central Java, of the many components of chemical compounds there are Linalool compounds (22.35%) and Estragole (55.80%) as the main components contained in the essential oil of basil leaves. This difference can be explained by various factors related to plant growth and development, such as genetics, plant

age, season, or location (Kumala S, et al., 2019), such as basil leaves in mountainous areas have good growth from a greener and wider leaf colour and sufficient water needs while basil leaves in plain areas tend to have small, thin and pale green leaves because the weather in plain areas is hotter which is a factor in the difference in the components of chemical compounds contained in the essential oil of basil leaves (Hakim, L., et al., 2015), et al., 2015), In this study, the chemical compound component with the highest percentage found was Estragole (55.80%), this is different from the quality requirements of ISO 11043 - 1998, Estragole with a percentage of 87%

Chemical molecular structure of Estragole as a phenolic compound was show in figure 3.

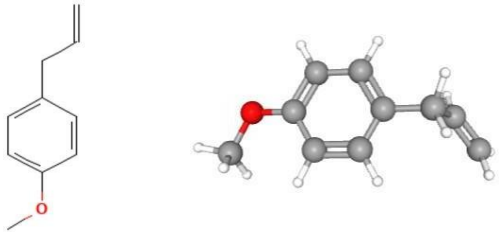

Figure 3. Molecular structure of Estragole

This type of compound is indispensable in the pharmaceutical industry, perfumes, and food raw materials. Industry. The Estragole compound which is a derivative of phenolic compounds. Phenolic compounds occur when a methyl or ethyl group is attached to a benzene ring through an oxygen molecule (Tisserand, 2014) which has an antiseptic effect and works by damaging the bacterial cell membrane, until now Estragole compounds have been widely isolated and used for antibacterial purposes. Estragole, which is a monoterpene, is used as an antibacterial in vitro proven to inhibit the growth of *Staphylococcus aureus* and *Eschericia coli* (Batista, et all, 2023). So that with the content of basil leaves, basil leaves can be used as an alternative to traditional medicine (Pejic et all., 2020)

4. CONCLUSION

Based on the results obtained, essential oil *Cymbopogon nardus* (L.) Rendle and essential oil *Ocimum basilicum* (L.) obtained from local distillation in Wonorejo Village Gondangrejo Karanganyar-Central Java, from GC-MS results obtained essential oil contained in citronella essential oil is Geraniol and the compound contained in basil leaf essential oil is Estragole. The dominant essential oil of basil leaves is Estragole with the largest percentage area of 55.80%, while the percentage area in accordance with the requirements of ISO 11043 - 1998 standard is 87%. The dominant essential oil of citronella is Geraniol with the largest percentage area of 26.49%, while the percentage area in accordance with the SNI 06-3953-1995 standard is 85%. Further research pays more attention to the raw materials of citronella and basil leaves that will be distilled using GC-MS tools to meet quality standards.

5. ACKNOWLEDGEMENT

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