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In Silico Analytic of Antiacne Potential from Jamblang Flower's Essential Oil Formulation

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ABSTRACT

This study aims to determine the components of compounds contained in Jamblang flower essential oil (*Syzygium cumini* L.) as antiacne and mechanism of antiacne. Jamblang flower essential oil is obtained through a distillation process. The distilled oil was then analysed using a Gas Chromatography Mass Spectrophotometer (GC-MS). Analysis results GC-MS evaluated using the program MASSLAB. Data obtained from the tool GC-MS then analysed using software PubChem NCBI database (https://pubchem.ncbi.nlm.nih.gov/) and PASS Online. The results of the GC-MS analysis showed that there were 47 bioactive compounds in Jamblang flower essential oil. Analysis results PubChem showed 13 compounds have activity as an antibacterial. Analysis results PASS Online demonstrated an antibacterial mechanism, protein synthesis inhibitor, membrane permeability inhibitor dan cell wall synthesis inhibitor, with the highest Pa value of 0.804 in the compound Benzyl benzoate $$Benzoic acid, phenylmethyl ester (CAS) dan nilai Pa terendah 1H-Benzimidazole,2-(methylthio)-(CAS)$$2-thiomethylbenzimidazole.

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1. INTRODUCTION

Acne vulgaris (AV) is a chronic skin condition of multifactorial origin characterized by infections of the pilosebaceous units such as comedoes, papules, pustules, nodules, and cysts, predominantly affecting the face, neck, shoulders, chest, back, and upper arms. AV is a prevalent skin disorder affecting nearly 80% to 100% of the human population (Zaenglein *et al.,* 2012). The highest incidence occurs in adolescent males aged 16-19 years and females aged 14-17 years. According to the Global Burden of Disease (GBD) study, *Acne vulgaris* affects 85% of young individuals aged 12-25 years.

Acne vulgaris that remains untreated can lead to decreased self-confidence and contribute to mental stress and anxiety, particularly among adolescents (Samuels *et al.,* 2020). One contributing factor to acne development is the excessive colonization of Propionibacterium acnes bacteria (Platsidaki *et al.,* 2018). Propionibacterium acnes is a gram-positive bacterium commonly found on the skin in sebaceous glands (Desbois *et al.,* 2013).

Current treatments for acne infections typically involve the use of antibiotics, either orally or topically. However, antibiotic monotherapy can lead to bacterial resistance within a few weeks of use. This reduces treatment effectiveness and hinders the resolution of acne inflammation (Zaenglein, 2018). Therefore, there is a need for research and evaluation of natural substances with potential antibacterial properties from nature as alternative acne treatments.

Jamblang plant (*Syzygium cumini L.*) is a local fruit-bearing plant native to Indonesia but largely neglected by the population. Limited cultivation of the Jamblang plant has led to its increasing rarity. However, Jamblang is known for its numerous medicinal properties (Dalimartha, 2013). Various pharmacological activities have been attributed to specific parts of the Jamblang plant, which contain known compounds. β-sitosterol, sambetulinat, eugenin, quercetin, kaempferol, flavonoids, and tannins are found in the bark of Jamblang. The flower contain kaempferol, quercetin, myricetin, quercetin-3-glucoside, eugenol, and triterpenoids. Jamblang roots contain glycosides and isorhamnetin-3-O-rutinoside (Ayyanar & Pandurangan, 2012).

Analyzing bioactive compounds in plants typically involves an extraction process. One commonly used extraction method is distillation. Distillation is a process for extracting compounds that evaporate with water as the solvent to obtain essential oils from plants. This method is frequently used in essential oil production due to its simplicity and efficiency. To analyse the bioactive compound content in Jamblang flower essential oil, Gas Chromatography-Mass Spectrometry (GC-MS) analysis is conducted. GC-MS combines gas chromatography, which separates volatile compounds, with mass spectrometry. This method identifies compounds by their molecular weight and determines their molecular formula, offering detailed compound identification compared to other methods. This method is particularly suitable for volatile essential oils (Darmapatni *et al.,* 2016).

Essential oil is a secondary metabolite of plants that exists in an oily form and possesses volatile properties. Essential oils contain bioactive compounds that contribute beneficial properties to health. The use of essential oils is widespread across various industries including cosmetics, perfumery, food and beverage, pharmaceuticals, and antiviral applications (Julianto, 2016). Based on considerations, while bioactive compound content in the Jamblang plant is known, the specific bioactive compounds in Jamblang flower essential oil remain unidentified. Therefore, analysis of bioactive compounds in Jamblang flower essential oil and exploration of its anti-acne mechanisms are warranted.

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2. METHODS

This research employs an experimental study design utilizing an experimental method with computer software to investigate the bioactivity of phytochemical compounds in Jamblang essential oil. This involves gathering data on bioactive compounds, selecting and comparing potential anti-acne bioactive compounds present in Jamblang (*Syzygium cumini L.*) flower essential oil (Fitriani *et al.,* 2023).

3. RESULTS AND DISCUSSION

3.1. Jamblang Flower's Oil Extraction

The essential oil of Jamblang flower was obtained through distillation for approximately 8 hours after drying the plant material until it was completely devoid of moisture. This procedure aimed to maximize the yield of the essential oil. The resulting oil yield was 14.9 ml per 75 grams of plant material. The essential oils can be seen in **Figure 1**.

Figure 1. Essential oil extracted from Jamblang flower

3.2. GC-MS Analytic Result of Jamblang Flower Oil Components

The GC-MS analysis of the essential oil extract from Jamblang flower revealed the presence of a total of 47 compounds. Among these compounds, the highest retention peak was at 28.68 m/z and the lowest retention peak was at 5.40 m/z. The result of GC-MS analysis of Jamblang flower essential oil can be seen in **Table 1.**

Table 1. The result of GC-MS analysis of Jamblang flower essential oil.

No.	RT	Percentage Quality (%)	Library/ID
1.	5.40	93	6-Methyl-5-hepten-2-one $$ 5-Hepten-2-one, 6-methyl- (CAS) $$ Methylheptenone
2.	7.09	91	1,6-Octadien-3-ol, 3,7-dimethyl- $$ .beta.-Linalool $$ Linalol $$ Li nalool
3.	7.31	91	(E)-4,8-Dimethyl-1,3,7-nonatriene
4.	8.57	96	Methyl salicylate $$ Benzoic acid2-hydroxy-, methyl ester $$ Analgit

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No.	RT	Percentage Quality (%)	Library/ID
5.	9.48	97	$$ 4-allylphenol $$ para- ALLYL PHENOL $$ Phenol,4-(2-propenyl)-
6.	10.71	95	.alpha.-Cubebene $$ (-)-.alpha.-Cubebene
7.	11.32	98	Phenol, 2-methoxy-4-(2-propenyl)- (CAS) $$ Eugenol $$ Engenol $$ p-Eugenol
8.	11.61	95	Vanillin $$ Benzaldehyde, 4-hydroxy-3-methoxy- $$ Lioxin $$ Vanillaldehyde
9.	11.90	99	Caryophyllene $$ .beta.-Caryophyll en $$ .beta.-Caryophyllene
10.	12.25	98	.alpha.-Humulene (CAS) $$ Humulene $$ .alpha.-Caryophyllene $$ ALPHA –HUMULENE
11.	12.41	91	Naphthalene,1,2,3,5,6,8a-hexahydr o-4,7 dimethyl-1-(1-methylethyl)-, (1S-cis)-
12.	12.61	99	.beta.-Selinene (CAS) $$ Eudesma-4(14),11-diene (CAS) $$ .beta.-Eudesmene
13.	12.71	96	.alpha.-Gurjunene
14.	12.80	99	Guaia-1(10),11-diene $$ .alpha.-Bulnesene
15.	13.01	96	Naphthalene, 1,2,3,4-tetrahydro-1, 6-dimethyl-4-(1-methylethyl)-, (1S-cis)-
16.	13.26	72	Benzene,1-methyl-3-[(1-methylethylidene) cyclopropyl]-
17.	13.32	53	1-.alpha.,9-.alpha.-Dimethyl-cis bicyclo[4.3.0]non-7-en-2-one
18.	13.40	50	Triplal 1 (iff) $$ 2,4-dimethyl-3- cyclohexene-1-carbaldehyde
19.	13.64	72	Caryophyllenyl alcohol
20.	13.81	91	(-)-Caryophyllene oxide $$ (-)-.beta.-Caryophyllene epoxide
21.	13.96	78	Camphene (CAS) $$ Bicyclo[2.2.1]heptane, 2,2-dimethyl-3-methylene- (CAS)
22.	14.09	78	Naphthalene, decahydro- (CAS) $$ Dec $$ Decalin $$ Dekalin $$ Naphthan
23.	14.18	64	(1S-(1Alpha,2alpha,4beta))-1-isopropenyl-4-methyl-1,2-cyclohexanedio
24.	14.26	70	cadina-1,4-diene
25.	14.39	95	caryophylla-4(12),8(13)-dien-5.beta.-ol
26.	14.61	91	caryophylla-3,8(13)-dien-5.beta.-o
27.	14.76	86	Caryophyllenol-II $$ Caryophyllenol II
28.	15.54	95	2-Propenal, 3-(4-hydroxy-3-methoxyphenyl)-

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No.	RT	Percentage Quality (%)	Library/ID
29.	15.76	98	Benzyl benzoate $$ Benzoic acid, phenylmethyl ester (CAS) $$ Ascabin
30.	16.30	64	6-Hydroxycariophyllene
31.	16.38	45	trimethyl - perhydro – naphthalene $$ trimethyl –decalin
32.	16.43	90	Farnesol, acetate
33.	16.88	93	Benzoic acid, 2-hydroxy-, phenylmethyl ester $$ Salicylic acid, benzyl ester
34.	22.51	86	Dihydrophenanthropyrane
35.	22.75	76	4-Methylene-1-[4',6'- dimethylpyrimidin-2'-yl]-3,5,6-trimethyl-1H,3H, 6H-pyrim...
36.	22.86	83	Methyl 3-chloro-5-[(E)-3,7-dimethy l-2,6-octadienyl]-4,6-dimethoxy-2- methylbe...
37.	23.93	83	2-(5-Formyl-4-propyl-2-pyrrolyl)-5-(4-propyl-2-
38.	24.37	64	4,6-Dimethyl-2-mercaptopyridine-3- carbonitrile
39.	25.02	64	1H-Benzimidazole, 2-(methylthio)- (CAS) $$ 2-thiomethylbenzimidazole
39.	25.02	64	1H-Benzimidazole, 2-(methylthio)- (CAS) $$ 2-thiomethylbenzimidazole
40.	25.11	42	Benzotriazole, 1-(4-methyl-3-nitro benzoyl)-
41.	25.37	43	2-Methyl-6-methoxy-1-indenol
42.	25.61	72	cis-isoeugenol $$ cis-1-hydroxy-2- methoxy-4-propenyl-benzene $$ (e)- isoeugenol
43.	26.44	90	(Z)-5-tert-Butyl-8-(2-phenylethenyl) [2.2]metacyclophane
44.	26.61	64	3-Cyclopentylpropionamide, N-(3,4- dimethoxyphenethyl)-
45.	26.78	72	11-(1-Pyrenyl)undeca-10-ynal
46.	27.03	58	2'-Hydroxy-5'-methoxyacetophenone, acetate

Table 1 illustrates the presence of 47 phytochemical compounds in Jamblang flower essential oil, starting from 6-Methyl-5-hepten-2-one (CAS) to Vineomycinone B2 Methyl Ether, with retention times ranging from 5.40 to 28.68.

3.3. Results of Analysis of Anti-Acne Mechanisms Using PASS Online Software

Bioinformatics analysis is commonly used to design potential active substances for drug development using computerization. This process involves the selection and characterization of target molecules, visualization of target molecule structures, and designing drug-target or chemical compound interaction mechanisms based on the target molecules. The analysis tools utilized include the online software PubChem (http://pubchem.ncbi.nlm.nih.gov/) and

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PASS online. Subsequently, analysis is conducted using data obtained from NCBI, which serves as an internationally recognized library of chemical compounds. Identification of compounds from GC-MS results involves assessing molecular structure properties, and obtaining canonical smiles which function as codes for further analysis and other purposes using the online software PubChem.

3.4. Results of Anti-acne Bioactivity Analysis of Jamblang (Syzygium cumini L.) Flower Essential Oil

a) 1,6-Octadien-3-ol, 3,7-dimethyl-. beta.-Linalool $$ Linalol $$ Li nalool

This compound has PubChem CID 6549 with IUPAC name (3,7-dimethylocta-1,6-dien-3-ol) and other names Linalool, and 3,7-Dimethylocta-1,6-dien-3-ol. The canonical SMILES of this compound is CC(=CCCC(C)(C=C)O)C. It has a molecular formula of $C_{10}H_{18}O$. Molecular structure can be seen in **Figure 2.**

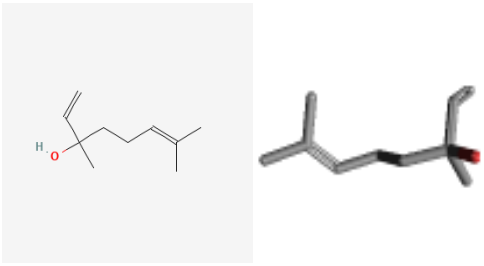

Figure 2. Molecular structure of 1,6-Octadien-3-ol, 3,7-dimethyl-. beta.-Linalool $$ Linalol $$ Linalool

b) .alpha.-Cubebene $$ (-)-.alpha.-Cubebene

This compound has PubChem CID 8669 with IUPAC name 4,10-dimethyl-7-propan-2-yltricyclo [4.4.0.0] dec-3-ene and other names alpha-Cubebene, alpha.-Cubebene, (-)-alpha.-Cubebene, and (-)alpha-Cubenene. The canonical SMILES of this compound is CC1CCC(C2C13C2C(=CC3)C)C(C)C. It has a molecular formula of $C_{15}H_{24}$. Molecular structure of .alpha.-Cubebene $$ (-)-.alpha.-Cubebene can be seen in **Figure 3.**

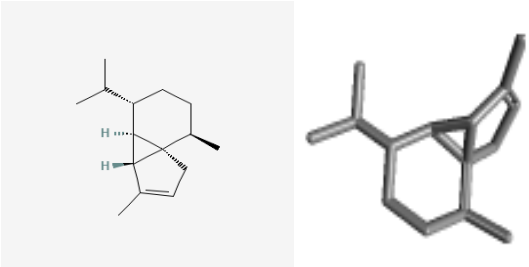

Figure 3. Molecular structure of .alpha.-Cubebene $$ (-)-.alpha.-Cubebene

c) Phenol, 2-methoxy-4-(2-propenyl)-(CAS) $$ Eugenol $$ Engenol $$ p-Eugenol

This compound has PubChem CID 442359 with IUPAC name (1R,5S,6R,7S,10R)-4,10 dimethyl-7-propan-2-yltricyclo[4.4.0.01,5]dec-3-ene and other names Eugenol, 4-Allyl-2-methoxyphenol, 4-Allylguaiacol, Eugenic acid. The canonical SMILES of this compound is COC1=C(C=CC(=C1)CC=C)O. It has a molecular formula of $C_{10}H_{12}O_2$. Molecullar structure of Phenol, 2-methoxy-4-(2-propenyl)-(CAS) EugenolEugenolEugenol Engenol $$ p-Eugenol can be seen in **Figure 4.**

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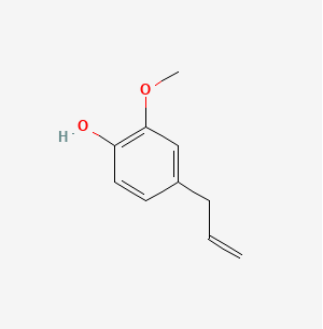

Figure 4. Phenol, 2-methoxy-4-(2-propenyl)-(CAS) $$ Eugenol $$ Engenol $$ p-Eugenol

d) .alpha.-Humulene (CAS) $$ Humulene $$ .alpha.-Caryophyllene $$ alpha –humulene
This compound has PubChem CID 5281520 with IUPAC name (1E,4E,8E)-2,6,6,9-tetramethylcycloundeca-1,4,8-triene and other names Humulene, alpha-Humulene, ALPHA-CARYOPHYLLENE, and 3,7,10-Humulatriene. The canonical SMILES of this compound is CC1=CCC(C=CCC(=CCC1)C)(C)C. It has a molecular formula of $C_{15}H_{24}$ and its chemical structure can be seen in **Figure 5.**

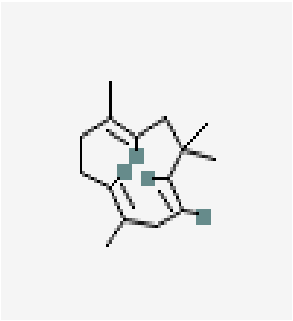

Figure 5. alpha.-Humulene (CAS) $$ Humulene $$ .alpha.-Caryophyllene $$ alpha –humulene

e) Naphthalene, 1,2,3,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1S-cis)-
This compound has PubChem CID 12306059 with IUPAC name (1S,8aS)-4,7-dimethyl-1-propan-2-yl-1,2,3,5,6,8a-hexahydronaphthalene and other names delta-Amorphene, .delta.-Cadinene, (+)-delta-amorphene. The canonical SMILES of this compound is CC1=CC2C(CCC(=C2CC1)C)C(C)C. It has a molecular formula of $C_{15}H_{24}$ and its chemical structure can be seen in **Figure 6**.

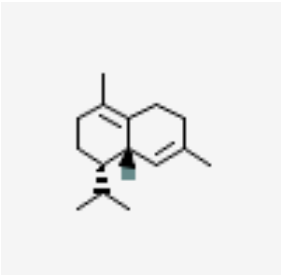

Figure 6. Naphthalene,1,2,3,5,6,8a-hexahydr o-4,7 dimethyl-1-(1-methylethyl)-, (1S-cis)-

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f) .beta.-Selinene (CAS) $$ Eudesma-4(14),11-diene (CAS) $$ .beta.-Eudesmene

This compound has PubChem CID 442393 with IUPAC name (3R,4aS,8aR)-8a-methyl-5-methylidene-3-prop-1-en-2-yl-1,2,3,4,4a,6,7,8-octahydronaphthalene and other names BETA-SELINENE, (+)-beta-Selinene, beta-Eudesmene, .beta,-Selinene. The canonical SMILES of this compound is CC(=C)C1CCC2(CCCC(=C)C2C1)C. It has a molecular formula of C15H24 and its chemical structure can be seen in **Figure 7**.

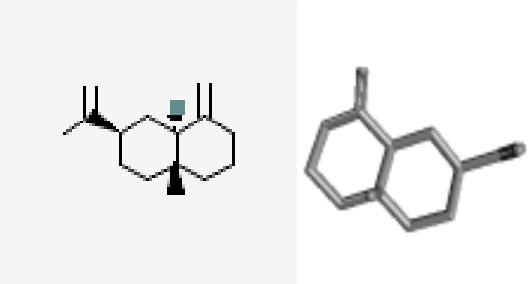

Figure 7. beta.-Selinene (CAS) $$ Eudesma-4(14), 11-diene (CAS) $$ .beta.-Eudesmene

g) .alpha.-Gurjunene

This compound has PubChem CID 521243 with IUPAC name 1,1,4,7-tetramethyl-1a,2,3,4,4a,5,6,7b-octahydrocyclopropa[e]azulene and other names (-)-alpha-Gurjunene, 1H-Cycloprop(e)azulene,1a,2,3,4,4a,5,6,7b-octahydro-1,1,4,7-tetramethyl,[1ar (1a.alpha.,4.alpha.,4a.beta.,7b.alpha.)]-, 1,1,4,7-Tetramethyl-1a,2,3,4,4a,5,6,7b-octahydro-1H-cyclopropa[e]azulene1H Cycloprop [e]azulene, 1a.beta.,2,3,4,4a.alpha.,5,6,7b.beta-octahydro-1,1,4.beta.,7-tetramethyl, Canonical SMILES CC1CCC2C(C2(C)C)C3=C(CCC13)C. It has a molecular formula of $C_{15}H_{24}$ and the molecular structure can be seen in **Figure 8.**

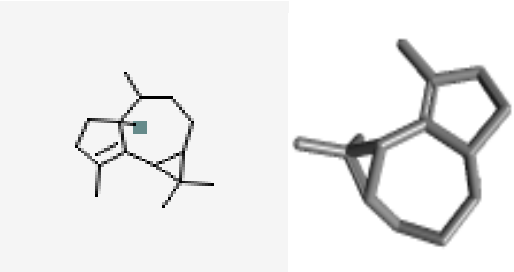

Figure 8. .alpha.-Gurjunene

h) (-)-Caryophyllene oxide $$ (-)-.beta.-Caryophyllene epoxide

This compound has PubChem CID 14350 with IUPAC name 4,12,12-trimethyl-9-methylidene-5-oxatricyclo[8.2.0.04,6]dodecane and other names Caryophyllene epoxide. The canonical SMILES of this compound is CC1(CC2C1CCC3(C(O3)CCC2=C)C)C. It has a molecular formula of $C_{15}H_{24}O$ and the molecular structure can be seen in **Figure 9**.

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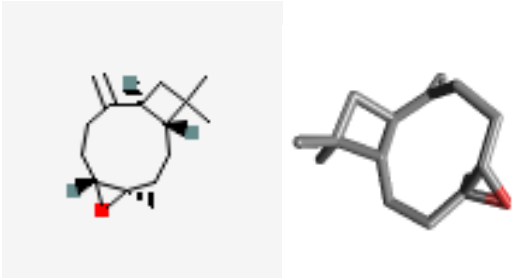

Figure 9. (-)-Caryophyllene oxide $$ (-)-.beta.-Caryophyllene epoxide

i) Cadina-1,4-diene

This compound has PubChem CID 642791 with IUPAC name (1S)-1,6-dimethyl-4-propan-2-yl-1,2,3,4,4a,7-hexahydronaphthalene and other names Cadina-1,4-diene, cis, Cadina-1(2)4-diene, and (1S,4S,4aR)-4-Isopropyl-1,6-dimethyl-1,2,3,4,4a,7-hexahydronaphthalene. The canonical SMILES of this compound is CC1CCC(C2C1=CCC(=C2)C)C(C)C. It has a molecular formula of $C_{15}H_{24}$ the molecular structure can be seen in **Figure 10.**

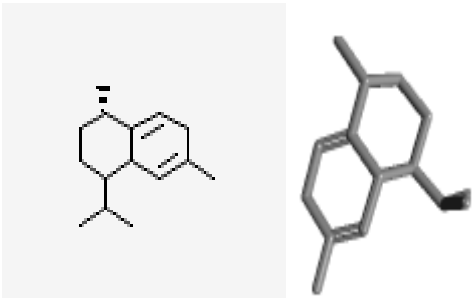

Figure 10. CADINA-1,4-DIENE

j) Caryophyllenol-II $$ Caryophyllenol II

This compound has PubChem CID 6438311 with IUPAC name (3Z)-4,11,11-trimethyl-8-methylidenebicyclo[7.2.0]undec-3-en-5-ol and other name Caryophyllenol 1. The canonical SMILES of this compound is CC1=CCC2C(CC2(C)C)C(=C)CCC1O. It has a molecular formula of $C_{15}H_{24}O$ and its molecular structure can be seen in **Figure 11.**

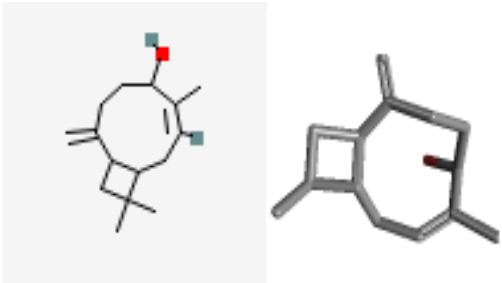

Figure 11. Caryophyllenol-II $$ Caryophyllenol II

k) Benzyl benzoate $$ Benzoic acid, phenylmethyl ester (CAS)

This compound has PubChem CID 2345 with IUPAC name benzyl benzoate and other names Ascobil, Novoscabin, Benylate. The canonical SMILES of this compound is

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C1=CC=C(C=C1)COC(=O)C2=CC=CC=C2. It has a molecular formula of $C_{14}H_{12}O_2$ and the molecular structure can be seen in **Figure 12.**

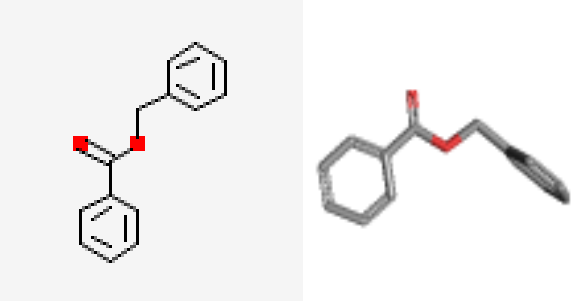

Figure 12. Benzyl benzoate $$ Benzoic acid, phenylmethyl ester (CAS)

l) 4,6-Dimethyl-2-mercaptopyridine-3-carbonitrile

This compound has PubChem CID 676510 with IUPAC name 4,6-dimethyl-2-sulfanylidene-1H-pyridine-3-carbonitrile and other names 2-Mercapto-4,6-dimethylnicotinonitrile, 4,6-dimethyl-2-thioxo-1,2-dihydropyridine-3-carbonitrile, 3-CYANO-4,6-DIMETHYL-2-MERCAPTOPYRIDINE. The canonical SMILES of this compound is CC1=CC(=C(C(=S)N1)C#N)C. It has a molecular formula of $C_8H_8N_2S$ and the molecular structure can be seen in **Figure 13.**

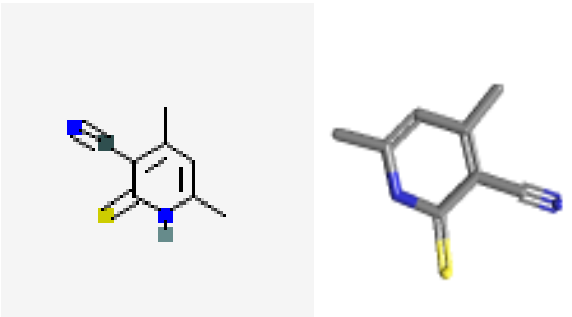

Figure 13. 4,6-Dimethyl-2-mercaptopyridine-3-carbonitrile

m) 1H-Benzimidazole, 2-(methylthio)- (CAS) $$ 2 thiomethylbenzimidazole

This compound has PubChem CID 23539 with IUPAC name 2-methylsulfanyl-1H-benzimidazole and other names 2-(Methylthio) benzimidazole, 2-Methylmercaptobenzimidazole, 2-(methylthio)-1H-benzo[d]imidazole. The canonical SMILES of this compound is CSC1=NC2=CC=CC=C2N1. It has a molecular formula of $C_8H_8N_2S$ and its molecular structure can be seen in **Figure 14.**

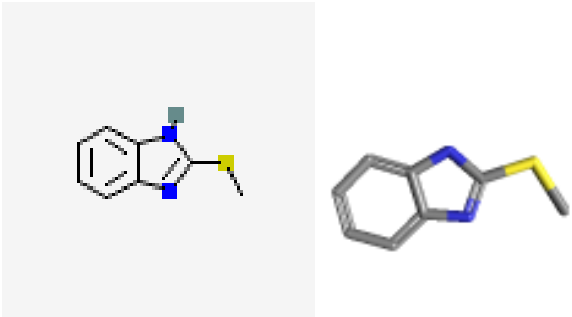

Figure 14. 1H-Benzimidazole, 2-(methylthio)-(CAS) $$ 2 thiomethylbenzimidazole

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3.4 Identification of Antiacne Compounds Using GC-MS

PASS online (Prediction of Activity Spectra for Substances) is a PC-based software used to predict the biological activities of a compound. Analysis with PASS has been extensively conducted, covering 205,000 compounds, resulting in more than 3,750 biological activities (Pramely & Raj, 2012). The result dan be seen in **Table 2.**

Based on the research procedure conducted, Jamblang flower contain 14.9 ml of essential oil per 75 grams. The essential oil obtained from Jamblang flower is characterized by its dark yellow color and distinctive aroma typical of Jamblang plants. Research by Prianto resulted in 17.2 ml of clove flower essential oil per 200 grams with steam-distillation lasting 8 hours (Prianto *et al.,* 2013). Meanwhile, research by Megawati obtained 15 ml of clove flower essential oil per 75 grams (Megawati *et al.,* 2010). According to Hendartomo, suboptimal oil yields can be attributed to factors such as poor raw materials, prolonged drying processes, and improper storage, which may affect the quality of the flower processed and the extraction of their oil, potentially leading to a reduction in Jamblang oil content (Hendartomo, 2005). Additionally, differences in isolation methods, origin of clove flower, and flower preparation before distillation can influence the yield of clove oil produced.

GC-MS analysis of Jamblang flower essential oil revealed the presence of various phytochemical compounds. According to GC-MS data on Jamblang flower essential oil in **Table 2**, phytochemical compounds range from 6-Methyl-5-hepten-2-one 5−Hepten−2−one,6−methyl−(CAS) Methylheptenone with the lowest retention time of 5.40 to vineomycinone B2 Methyl Ether with the highest retention time of 28.68. Thus, a total of 46 compounds were identified in Jamblang flower.

Table 2. Identification of antiacne compounds using GC-MS.

No	Compound Name	Pa Value	Pi Value	Antiacne Mechanism
1.	1,6-Octadien-3-ol, 3,7-dimethyl-. beta.-Linalool $$ Linalol $$ Li nalool	0,743	0,023	Membrane permeability inhibitor
2.	.alpha.-Cubebene $$ (-)-.alpha.-Cubebene	-	-	-
3.	Phenol, 2-methoxy-4-(2-propenyl)-(CAS) $$ Eugenol $$ Engenol $$ p-Eugenol	0,781	0,013	Membrane permeability inhibitor
4.	.alpha.-Humulene (CAS) $$ Humulene $$ .alpha.-Caryophyllene $$ ALPHA –HUMULENE	0,388	0,209	Membrane permeability inhibitor
5.	Naphthalene,1,2,3,5,6,8a-hexahydro-4,7 dimethyl-1-(1-methylethyl)-, (1S-cis)-	0,439	0,152	Membrane permeability inhibitor
6.	.beta.-Selinene (CAS) $$ Eudesma-4(14),11-diene (CAS) $$ .beta.-Eudesmene	0,304	0,052	DNA snthesis inhibitor
7.	.alpha.-Gurjunene	0,578	0,100	Membrane permeability inhibitor
8.	(-)-Caryophyllene oxide $$ (-)-.beta.-Caryophyllene epoxide	0,416	0,013	Protein synthesis inhibitor
9.	CADINA-1,4-DIENE	0,570	0,105	Membrane permeability inhibitor
10.	Caryophyllenol-II $$ Caryophyllenol II	0,381	0,018	Protein synthesis inhibitor

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Chemical components of essential oils vary depending on geographic location, plant species, local climate, seasons, and experimental conditions, as well as harvesting and post-harvest treatments, all of which can influence the composition of essential oils (Olonisakin *et al.,* 2006).

Based on the analysis from PubChem in **Table 2**, it is evident that there are 13 compounds exhibiting antibacterial bioactivity, include:

1. 1,6-Octadien-3-ol, 3,7-dimethyl-. beta.-Linalool (also known as Linalol or Li nalool)
2. alpha.-Cubebene (also known as (-)-alpha.-Cubebene)
3. Phenol, 2-methoxy-4-(2-propenyl)- (CAS) (also known as Eugenol, Engenol, or p-Eugenol)
4. alpha.-Humulene (CAS) (also known as Humulene or ALPHA-HUMULENE)
5. Naphthalene,1,2,3,5,6,8a-hexahydr o-4,7 dimethyl-1-(1-methylethyl)-, (1S-cis)-
6. beta.-Selinene (CAS) (also known as Eudesma-4(14),11-diene or .beta.-Eudesmene)
7. alpha.-Gurjunene
8. (-)-Caryophyllene oxide (also known as (-)-beta.-Caryophyllene epoxide)
9. CADINA-1,4-DIENE
10. Caryophyllenol-II (also known as Caryophyllenol II)
11. Benzyl benzoate (also known as Benzoic acid, phenylmethyl ester (CAS))
12. 4,6-Dimethyl-2-mercaptopyridine-3-carbonitrile
13. 1H-Benzimidazole, 2-(methylthio)- (CAS) (also known as 2-THIOMETHYLBENZIMIDAZOLE)

These compounds demonstrate bioactivity against bacteria, highlighting their potential applications in antimicrobial research and development.

Based on the analysis from PubChem in **Table 2**, a total of 13 phytochemical compounds exhibit antibacterial bioactivity. This indicates that PubChem serves as a database that collects and stores molecular data consisting of three interrelated databases: Substances, Components, and BioAssay (Kim *et al.,* 2016). According to the antibacterial mechanism analysis obtained from Table 4.3, there are 11 compounds that exhibit antibacterial mechanisms. The mechanisms identified from PASS Online analysis include Cell wall synthesis inhibitor, Protein synthesis inhibitor, and Membrane permeability inhibitor.

In the analysis results presented in **Table 1**, the highest Pa (Probable activity) value recorded is 0.804, and the Pi value is 0.115, indicating a membrane permeability inhibitor mechanism for the compound Benzyl benzoate $$ Benzoic acid, phenylmethyl ester (CAS) with Pa > 0.7. Therefore, there is a high likelihood of discovering the compound's activity experimentally. The comparison of Pa values for antibacterial compounds can also be visualized in Figure 4.3. Pa values indicate the potential of a compound for various biological activities based on Structure Activity Relationship between natural compounds and synthetic drugs (Pramely *et al.,* 2012).

Disruption of bacterial cell membrane permeability leads to leakage of proteins and nucleic acids. Leakage of proteins or nucleic acids signifies permanent damage and changes in the permeability of bacterial cell walls. Most antibacterials work by damaging the cytoplasmic membrane, which has the ability to release nucleic acids and proteins (Miksusanti *et al.*, 2008).

Yang's research studies have shown an increase in the amount of protein outside the bacterial cell of *Klebsiella pneumonia* after the application of lavender essential oil (*Lavandula angustifolia*) (Yang *et al.,* 2002). Nucleic acids in bacteria cause disturbances in the bacterial

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cell division process. The mechanism of action of an antibacterial can be observed from the leakage of nucleic acids and proteins in bacterial cells. Leakage of nucleic acids and proteins in bacteria leads to changes in the structure and function of bacterial proteins, ultimately damaging the bacterial cell wall.

4. CONCLUSION

From the total bioactive compounds found in Jamblang flower, it is known that there are 13 compounds exhibiting antibacterial bioactivity: yaitu 1,6-Octadien-3-ol, 3,7-dimethyl-. beta.-Linalool $$ Linalol $$ Li nalool ; .alpha.-Cubebene $$ (-)-.alpha.-Cubebene ; Phenol, 2-methoxy-4-(2-propenyl)- (CAS) $$ Eugenol $$ Engenol $$ p-Eugenol ; .alpha.-Humulene (CAS) $$ Humulene $$ .alpha.-Caryophyllene $$ ALPHA –HUMULENE ; Naphthalene,1,2,3,5,6,8a-hexahydr o-4,7 dimethyl-1-(1-methylethyl)-, (1S-cis)- ; beta.-Selinene (CAS) $$ Eudesma-4(14),11-diene (CAS) $$ .beta.-Eudesmene ; .alpha.-Gurjunene ; (-)-Caryophyllene oxide $$ (-)-.beta.-Caryophyllene epoxide ; CADINA-1,4-DIENE ; Caryophyllenol-II $$ Caryophyllenol II ; Benzyl benzoate $$ Benzoic acid, phenylmethyl ester (CAS ; 4,6-Dimethyl-2-mercaptopyridine-3- carbonitrile ; 1H-Benzimidazole, 2-(methylthio)- (CAS) $$ 2-THIOMETHYLBENZIMIDAZOLE. The mechanisms obtained from the antibacterial compounds in the study include membrane permeability inhibitor,protein synthesis inhibitor, and cell wall synthesis inhibitor with the highest Pa value of 0.804 found in Benzylbenzoate Benzoic acid, phenylmethyl ester (CAS) and the lowest Pa value of 0.115 in 1H-Benzimidazole, 2-(methylthio)- (CAS) $$ 2-THIOMETHYLBENZIMIDAZOLE.

5. AUTHORS' NOTE

The authors declare that there is no conflict of interest regarding the publication of this article. Authors confirmed that the paper was free of plagiarism.

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