Anti-meningitis agent potentially of Syzygium Cumini
Essential oil by GC-MS

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Abstract. The essential oil from fruit of Syzygium cumini (Myrtaceae), endemic to Indonesia, was investigated by using GC and GC-MS. Forty-six components represented of the total oil were identified. The major components of the essential oil were 1,2,3-Propanetriol (20.32%), octadecanoic acid (16.13%), glycerine-1-oleate-3-palmitate (12.00%), 9,12-Octadecadienoic acid (6.49%) and Heptadecyl acetate (5.52%). The bio-activity of the major components of essential oil of S. cumini was investigated by the PASS-online bio-activity prediction software. The major components of essential oil of S. cumini exhibited antibacterial activities. The antibacterial activity present in the essential oil of S. cumini has the potential to be used as an anti-meningitis bacterial. Further research is needed to test the definitive antibacterial ability of the compounds contained in S. cumini essential oil.

1. Introduction
The genus Syzygium, comprising more than 100 species, is one of the largest genera of the Myrtaceae family [1]. Syzygium cumini growing in Indonesia are endemic [2]. In Sumatra, S. cumini species is known as jamblang and are used as fruit for diet and antioxidants [3]. In traditional medicine, this species has been used to treat diabetes, antioxidant, antibacterial, inflammatory tumors, and cancer [4,5]. Since they possess S. cumini has activity as anti-diabetic, antioxidant, anti-inflammatory, either the whole plant or the leaves have been consumed as a tea in phytotherapy [6]. Also, the extracts or components of S. cumini species possess significant antibacterial anti-inflammatory [7].

S. cumini is an endemic medicinal plant that is distributed in north-south Sumatra. Chemical studies have been reported for S. cumini species [8], as well as various biological properties, such as radical scavenging [9], antioxidants due to polyphenol content [9], anti-inflammatory [7], and antibacterial [8] activities. A literature survey showed that 1,2,3-Propanetriol, octadecanoic acid, glycerine-1-oleate-3-palmitate, 9,12-Octadecadienoic acid, and Heptadecyl acetate were the most encountered essential oil components of S. cumini species [7]. The essential oils and/or the activity of forty-six S. cumini species growing in Sumatra were investigated previously [4,5].

This study aimed to determine the chemical composition of the essential oil of S. cumini, and the antimeningitis bacterial activity of its oil, its major components. Forty-six components were identified by a library search. This is the first report of the essential oil of this species and its anti-meningitis bacterial activity.
2. Method

**Plant material:** The fruit parts of *Syzygium cumini* were collected at the harvest period in February 2020 from the Banda Aceh region of Aceh has been deposited in the Department of Biology, Faculty of Sciences and Technology of Ar-Raniry State Islamic University, Banda Aceh, Indonesia.

**Isolation of the essential oil:** The essential oil of the air-dried aerial parts of *S. cumini* (2000g) was obtained by hydrodistillation for 4h by using a Clevenger type apparatus, according to the recommendation of the European Pharmacopoeia [9]. The essential oil was dried by treatment with anhydrous sodium sulfate and was then stored under nitrogen in a sealed vial until required.

**Isolation of the main component:** The essential oil of *S. cumini* was subjected to column chromatography, using silica gel 60 F254 (70-230 mesh) and eluting with n-hexane containing 1% increasing amounts of diethyl ether. The main component of the essential oil, trans-β-caryophyllene, was obtained from the n-hexane: diethyl ether fractions (80:20, v/v) [10].

**Gas chromatography:** GC analyses of the essential oil were performed using a Shimadzu GC-17 AAF, V3, 230V LV Series (Kyoto, Japan) gas chromatography, equipped with an FID and an Optima5 fused silica column [30m x 0.25 mm (i.d.), film thickness 0.25 μm]; the oven temperature was held at 40°C for 15 min., then programmed to 220°C at 3°C/min and held isothermal for 15 min; injector and detector temperatures were 250°C and 270°C respectively; carrier gas was He at a flow rate of 1.3 mL/min; Sample size, 1.0 μL; split ratio, 50:1. The percentage composition of the essential oil was determined with a Class-GC 10 computer program [10,11].

**Gas chromatography-mass spectrometry:** The analysis of the essential oil was performed using a Varian Saturn 2100 (Old York Rd., Ringoes, NJ, USA), E. I Quadrupole machine, equipped with a ZEBRON–5 MS fused silica capillary column [60 m x 0.25 mm (i.d.), film thickness 0.25 μm]. For GC–MS detection, an electron ionization system with ionization energy of 70eV was used. The carrier gas was helium (20 psi) at a flow rate of 1.7 mL/min. Injector and MS transfer line temperatures were set at 220°C and 290°C, respectively. The oven temperature was held at 40°C for 5 min, then increased up to 220°C with 2°C/min increments and held at this temperature for 10 min. Diluted samples (1/100, v/v, in methylene chloride) of 1.0 μL were injected manually in the splitless mode. The relative percentages of the oil constituents were expressed as percentages [10].

**Identification of components:** Identification of components of the essential oil was based on GC retention indices and computer matching with the Wiley and NIST, 2005 Library, as well as by comparison of the fragmentation patterns of the mass spectra with those reported in the literature, and when possible, by co-injection with authentic samples. The identity of the main component of the essential oil was also assigned by 1 H-NMR spectroscopy at 300 MHz, on a Varian-300 Spectrometer, using CDCl3 as solvent and TMS as the internal standard. The NMR spectroscopic data of trans-β-caryophyllene were in agreement with data given in the literature [12].

3. Results and Discussions

The essential oil, which was a clear yellow color, was obtained by steam distillation (0.15%, v/w) of the dried fruit of the plant. The chemical constitution of the essential oil is in Table 1. The essential oil was analyzed by GC-MS and resulted in the identification of 46 components representing the total oil. The major components of the oil were 1,2,3-Propanetriol (20.32%), octadecanoic acid (16.13%), glycerine-1-oleate-3-palmitate (12.00%), 9,12-Octadecadienoic acid (6.49%) and Heptadecyl acetate (5.52%) (Table1).

The principal components of the essential oil of *S. cumini* species previously studied showed chemical variations that could be chemotaxonomically important for *S. cumini* species [8,9]. The analysis results of Chebi software and PASS online showed the bioactivity of the phytochemical compounds contained in S. cumini essential oil (Tabel 2).
| Pk# | RT  | Area % | Library/ID | CAS#             | Qual |
|-----|-----|--------|------------|-----------------|------|
| 1   | 2.403 | 4.04   | 3-D-4-methyl-2-pentanol | 13412 028080-81-1 | 64   |
| 2   | 2.873 | 5.54   | 2-Pentanol | 6608 006032-29-7 | 64   |
| 3   | 3.309 | 20.32  | Glycerin   | 7590 000056-81-5 | 83   |
| 4   | 5.481 | 2.14   | 1,2,3-Propanetriol | 7585 000056-81-5 | 83   |
| 5   | 5.840 | 0.85   | Z,-4,5-dimethylhex-2-en-4-ol | 71780 007786-61-0 | 89   |
| 6   | 6.635 | 2.43   | 1-Dodecanol | 163697 000112-53-8 | 62   |
| 7   | 7.122 | 0.97   | Heneicosanoic acid | 612579 002363-71-587 | 25   |
| 8   | 7.378 | 3.56   | Nonanoic acid, | 130798 003788-56-5 | 47   |
| 9   | 7.549 | 1.34   | 1,1-Dichloro-2-methoxyfluoroethene | 480974 000057-11-4 | 35   |
| 10  | 7.678 | 3.53   | Nonanedioic acid, monomethyl ester | 208359 002104-19-0 | 38   |
| 11  | 8.191 | 5.52   | Heptadecyl acetate | 526444 000822-20-8 | 38   |
| 12  | 10.046 | 0.40 | Cyclohexanecarboxylic acid, 3-pentadecyl ester | 116071 000116-07-1 | 35   |
| 13  | 10.191 | 1.97  | n-Hexadecanoic acid | 387914 000057-10-3 | 99   |
|     |       |        | Hexadecanoic acid | 387924 000057-10-3 | 98   |
| 14 | 11.302 | 6.49 | 9,12-Octadecadienoic acid (Z,Z)-Linoelaidic acid | 467189 000060-33-3 | 99 |
| 15 | 13.345 | 2.40 | Hexadecanoic acid, 2,3-dihydroxypropyl ester Glycerol 1-palmitate | 624473 000542-44-9 | 58 |
| 16 | 14.072 | 1.13 | Cyclohexanecarboxylic acid, tetradecyl ester 2-Pentenoic acid, 5-bromo-4-methoxy-, methyl ester, (E)-(,+)- | 606454 200606-45-4 | 49 |
| 17 | 14.209 | 0.55 | Z-5-Methyl-6-tetradecen-1-ol acetate Oxacyclohexadecan-2-one, 13-methyl | 427925 200427-92-5 | 81 |
| 18 | 14.277 | 1.29 | 9,12-Octadecadien-1-one 7-Pentadecyne octadecanoic acid, 2-[(1-oxo-hexadecyl)oxy]-1-[[1-oxo-hexadecyloxy]methyl]ethyl ester 5,5',7,7'-Tetrabromoindigo | 421179 001577-52-2 | 96 |
| 19 | 16.705 | 16.13 | 2-(4-oxo-hexadecyl)-1-[[1-oxo-hexadecyloxy]methyl]ethyl ester 5,5',7,7'-Tetrabromoindigo | 947088 002177-97-1 | 10 |
| 20 | 17.226 | 2.89 | Cyclopentanecarboxylic acid, methoxyphenyl)-2-oxo-, ethyl ester 6-Methyl-3-(trifluoromethyl)benzo[c][1,6]naphthyridine | 1-(4-oxo-5)-1H-pyrrolo[2,1-c][1,4]benzothiazine GLYCERINE-1-OLEATE-3-PALMITATE .beta.-Tocopherol (R)-6-Methoxy-2,8-dimethyl-2-((4R,8R)-4,8,12-trimethyltridecyl)chroman | 922227 2000922-22-7 | 11 |
| 21 | 17.509 | 2.45 | Ascorbic acid, 4TBDMS derivative | 933906 200933-90-6 | 10 |
| 22 | 21.407 | 12.00 | 4,4-Diphenyl-4H-pyrrolo[2,1-c][1,4]benzothiazine GLYCERINE-1-OLEATE-3-PALMITATE | 647284 200647-28-4 | 37 |
| 23 | 27.485 | 2.03 | | 927193 003343-30-4 | 17 |

GLYCERINE-1-OLEATE-3-PALMITATE 810763 000148-03-8 | 64 |
### Tabel 2. Bioactivity of the phytochemical compounds contained in *S. cumini* essential oil

| Phytochemical compounds | Structure | Bio-activity                                                                 |
|-------------------------|-----------|-------------------------------------------------------------------------------|
| 1,2,3-Propanetriol     | ![structure](image) | Antibacterial, Antiviral, inflammation, Antifungal, Antidiabetic, Antiprotozoal (Leishmania), Antipsoriatic, Antipruritic non-allergic, Antiparkinsonian rigidity relieving, antioxidant, Antineurogenic pain |
| octadecanoic acid       | ![structure](image) | Antieczematic, Antiseborrheic, Antihypoxic, Antimutagenic, Antiinflammatory, intestinal, Antisecretoric, Antiviral (Picornavirus), Antihyperamonemic, Antibacterial, Antiviral (Influenza A) |
| glycerine-1-oleate-3-palmitate | ![structure](image) | Antibacterial, Antiviral (Influenza A), Anticoagulant, Antineoplastic (bone cancer), Antiallergic, Antianorexic, Anticholelithogenic |
| 9,12-Octadecadienoic acid | ![structure](image) | Antimutagenic, Antihypercholesterolemic, Antiseborrheic, Antisecretoric, Antithrombotic, Antiinflammatory, Antiulcerative, Antipruritic, Antiinfective, Antiviral (Influenza), Antiviral (Picornavirus) |
| Heptadecyl acetate      | ![structure](image) | Antieczematic, Antiseborrheic, Antihypoxic, Antiviral (Picornavirus), Antiinflammatory, Antihelmintic (Nematodes), Antipruritic, Antiprotozoal (Leishmania), Antihypercholesterolemic |

Five phytochemical compounds were analyzed by Chebi and PASS online tended to be anti-inflammatory. Bacterial meningitis is caused by bacteria. In this study, of the five compounds analyzed, only 1,2,3-Propanetriol showed great potential as antibacterial. This 1,2,3-Propanetriol compound will later be tested for its antibacterial ability to inhibit the growth of bacteria that cause meningitis. It also needs to be done with other compounds from *S. cumini* essential oil so that the results of this research can be more comprehensive.
4. Conclusions
One of five major components of essential oil of *S. cumini* exhibited antibacterial activities namely 1,2,3-Propanetriol. The antibacterial activity present in the essential oil of *S. cumini* has the potential to be used as an anti-meningitis bacterial. Further research is needed to test the definitive antibacterial ability of the compounds contained in *S. cumini* essential oil.

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