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PHYTOCHEMICAL INVESTIGATION OF ENGKABANG (*SHOREA MACROPHYLLA*): CHARACTERIZATION AND POTENTIAL SIGNIFICANCE OF 1-OCTADECANOL

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SUMMARY

This pioneering study focused on the isolation and structural elucidation of phytochemicals from the stem bark of Engkabang (*Shorea macrophylla*), a species belonging to the family Dipterocarpaceae, known for its diverse bioactive compounds and traditional uses. The hexane extract of its stem bark underwent multiple chromatographic techniques, including thin-layer chromatography (TLC), vacuum liquid chromatography (VLC), and gravity column chromatography (GCC), successfully isolating the fatty alcohol and 1-octadecanol. The structure of the isolated compound reached validation through various spectroscopic techniques, including ^{1}H and ^{13}C NMR, as well as 2D NMR methods (COSY, HMBC, HSQC), and Fourier Transform Infrared (FT-IR) spectroscopy. The discovery of 1-octadecanol highlights the potential of *S. macrophylla* as a source of bioactive compounds with possible applications in pharmaceuticals, cosmetics, and biofuels. This research work marks the first report of a fatty alcohol from *S. macrophylla*, contributing significantly to the phytochemical understanding of this species.

Keywords: Engkabang (*S. macrophylla*), spectroscopy, bioactive compounds, fatty alcohol, 1-octadecanol, phytochemicals

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Key findings: The presented study reports the first isolation of 1-octadecanol from *S. macrophylla* stem bark, as confirmed through spectroscopy. The finding highlights the ecological role of fatty alcohols in plant adaptation and suggests potential applications in cosmetics, pharmaceuticals, and biofuels, considerably contributing to the phytochemical properties of the species.

INTRODUCTION

Engkabang (*Shorea macrophylla*), a member of the family Dipterocarpaceae, has a common name of Tengkawang in Indonesia (Manshoor *et al*., 2013) (Figure 1). This tropical tree prevails throughout the rainforest areas of Southeast Asia. It has traditionally served as timber used in various other applications, such as in furniture, construction, and boat building (Suganya *et al*., 2014). Beyond its industrial functions, species within the genus *Shorea* have gained extensive studies for their diverse phytochemical constituents, which include triterpenoids, ellagic acid, flavonoids, coumarins, alkaloids, and resveratrol oligomers (Yee *et al*., 2022; Musa *et al*., 2024a, b). These bioactive compounds contribute to the pharmaceutical potential of *Shorea* species, underscoring their significance in natural product research.

Despite the well-documented phytochemical diversity in *Shorea* species, comprehensive investigations into the biochemical constituents of *S. macrophylla*, particularly in its stem barks, remain limited. This knowledge gap presents an opportunity to explore its chemical composition and potential bioactivities. This study reports the isolation and structural elucidation of 1-octadecanol from the n-hexane extract of *S. macrophylla* stem bark, marking the first identification of this fatty alcohol in this species (Pollard *et al*., 2008). The discovery contributes to the expanding phytochemical profile of *S. macrophylla* and highlights its potential as a natural source of fatty alcohols (Gupta *et al*., 2013).

Fatty alcohols, including 1-octadecanol, are well-known for their industrial applications in the cosmetics, pharmaceuticals, and biofuel industries. Additionally, their considerable role in plant physiology, particularly in stress response and environmental adaptation, underscores the ecological significance of these findings (Molina *et al*., 2006; Mudge *et al*., 2010). The promising research results enriched the phytochemical knowledge of the genus *Shorea* and provided a base for further exploration of Engkabang (*S. macrophylla*) as a source of bioactive compounds with potential industrial and ecological relevance.

MATERIALS AND METHODS

Experimental procedure

Thin layer chromatography, vacuum liquid chromatography, and gravity column chromatography succeeded in using silica gel TLC 60 GF254 (0.25 mm), silica gel G60 Merck (0.200-0.500 mm), and Kiesel gel 60 (F254, Merck), respectively. The initial visualization of spots utilized a UV lamp (lambda-40) before spraying with anisaldehyde and being heated on a hot plate. The FTIR spectrum, as recorded, used a Shimadzu IR Tracer-100 FTIR spectrophotometer. The ^{1}H and ^{13}C-NMR spectra, along with the 2D spectra, proceeded to record on a 600 MHz Bruker AVANCE spectrometer.

Plant material

The stem bark collection of *S. macrophylla* began in September 2023 in Borneo, Central Kalimantan, Indonesia. The plant, when identified, received a designated voucher specimen (002/03.314JI.Genbinesia) at Yayasan Generation Biology, Indonesia.

Extraction and isolation

Stem barks of *S. macrophylla* sustained cleaning and air-drying at room temperature for three days before grinding. Dried stem bark

Figure 1. Tree of *Shorea macrophylla.*

powder samples (3.5 kg) underwent extraction by maceration using methanol, which incurred repetitions three times at room temperature. The resulting mixture's filtration had the subsequent filtrate evaporated with a rotary evaporator, yielding a concentrated methanol crude extract. The methanol crude extract's partitioning with *n*-hexane separated hexane and methanol residue fractions. The *n*-hexane extract was concentrated to a constant weight of 31 g. The initial step of the isolation process involved using vacuum liquid chromatography (VLC) to separate the main fractions into sub-fractions. The *n*-hexane extract underwent analysis by thin-layer chromatography (TLC) to determine the eluent during column chromatography. Then, separating the extract by VLC used step gradient solvent mixtures of *n*-hexane:ethyl acetate (from 100% to 95:5) to yield 21 main fractions. Fraction-18 further sustained gravity column chromatography, being eluted with *n*-hexane:dichloromethane gradient elution (from 100:0 to 0:100). This resulted in compound-1. The pure compound obtained gained more testing for purity using three different eluent systems. Further analysis continued to determine the structure of the compound using an FT-IR spectrophotometer and NMR spectroscopy.

RESULTS AND DISCUSSION

Structure elucidation

The identified compound-1 (14 mg) appeared as white-waxy flakes, with a melting point of 58 °C-59 °C, consistent with prior reports of 1-octadecanol from natural sources (Gupta *et al*., 2013). Its structure's further elucidation employed various spectroscopic analyses, i.e., FT-IR (Figure 2), ^{1}H-NMR (Figure 3), ^{13}C-NMR (Figure 4), and 2D techniques, such as COSY, HSQC, and HMBC. The FT-IR spectra revealed characteristic bands at 3304 cm^{-1} (associated with the OH group), 2918 cm^{-1} (indicating C-H asymmetric stretching), 2848 cm^{-1} (indicating C-H symmetric stretching), 1064 cm^{-1} (C-O stretching), and 1467 cm^{-1} and 725 cm^{-1} (out-of-plane and in-plane deformation of the OH group).

These spectral features were comparable to the FT-IR data of fatty alcohols reported in previous studies on plant-derived cuticular wax components (Pollard *et al*., 2008). The ^{1}H NMR spectral analysis ($CDCl_3$, 600 MHz) (δ ppm): 3.64 (2H, t, *J* = 6.6 Hz, H-1), 1.57 (2H, dq, *J* = 8.1 Hz, 6.6 Hz, H-2), 1.36 (2H, m, H-3), and 0.88 (3H, t, *J* = 7 Hz, H-18). The ^{13}C NMR spectral analysis ($CDCl_3$,

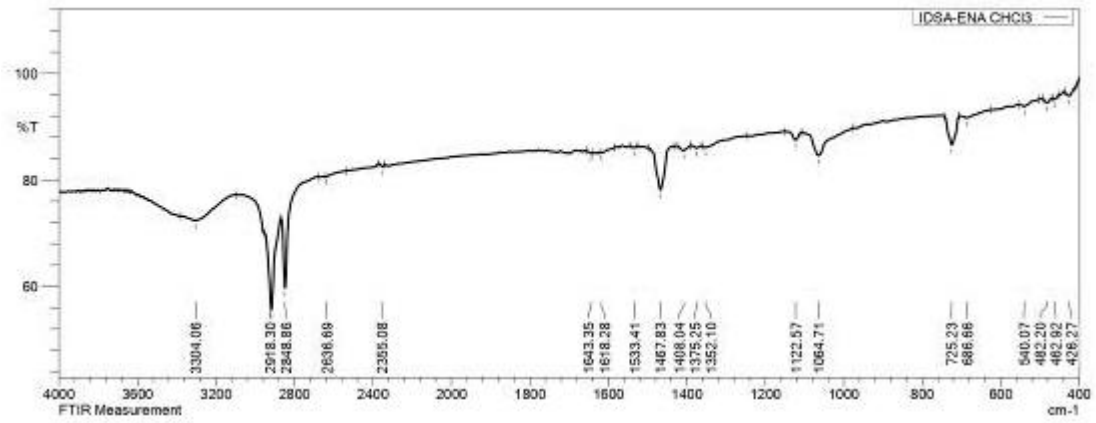

Figure 2. FT-IR spectrum of 1-octadecanol.

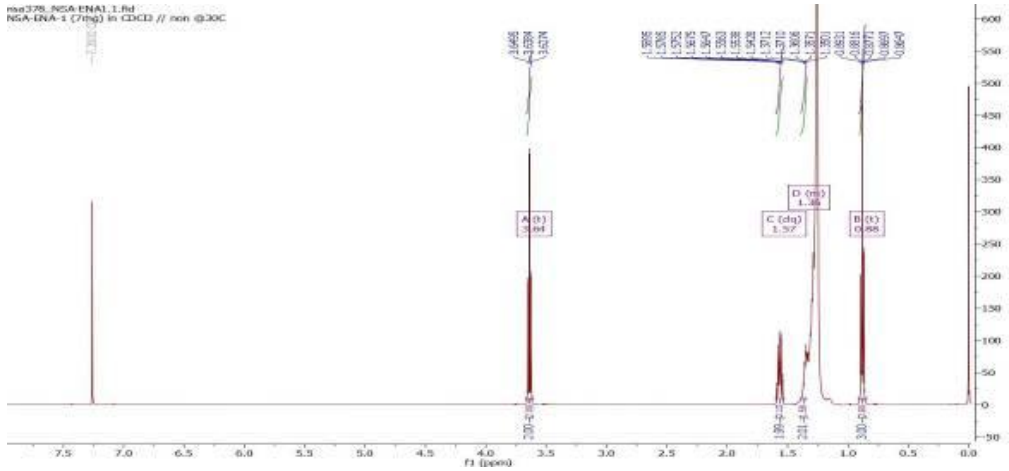

Figure 3. [1]H NMR spectrum of 1-octadecanol.

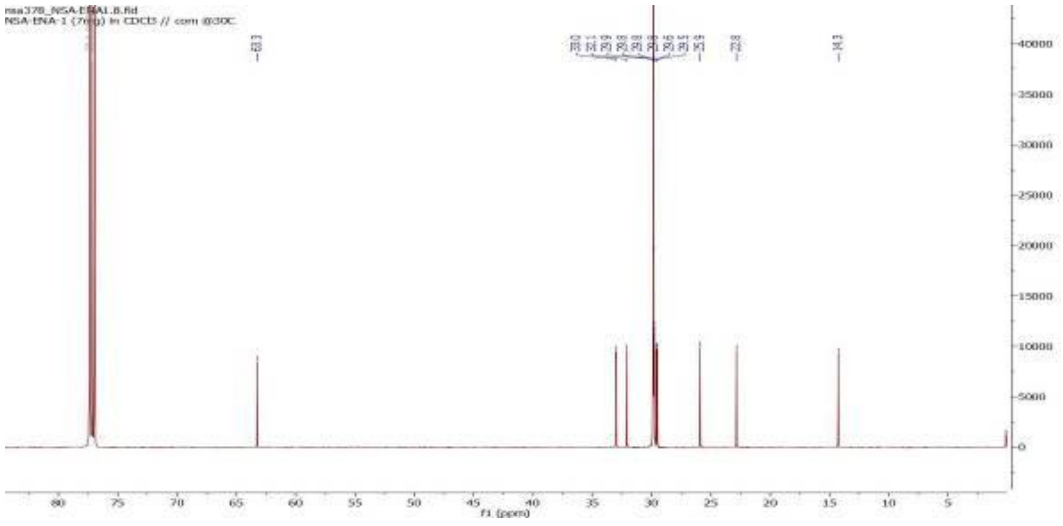

Figure 4. [13]C NMR spectrum of 1-octadecanol.

600 MHz) (δ ppm): 63.2 (C-1), 32.9 (C-2), 32.0, 29.8, 29.8, 29.7, 29.7, 29.6, 29.5, 25.9 (C-3), 22.8 (C-17), and 14.2 (C-18). In the ^{1}H NMR spectrum, the detected chemical shift at δ_H 0.88 ppm was the methyl proton, while δ_H 3.64, 1.57, and 1.36 ppm comprised the methylene group. The OH group presence makes the methylene group at 3.64 very deshielded. Moreover, the ^{13}C NMR spectrum revealed the presence of one methyl carbon at δ_C 14.2 ppm. Carbon (C-1) was also distinct as a methylene carbon (R-CH_2-OH).

The COSY spectrum revealed a series of diagonal peaks along the proton chemical shift axis, which correspond to the individual protons in the sample. By analyzing the COSY spectrum data, a proton-proton interaction occurred at δ 3.64/1.57 ppm, indicating a coupling between protons H-1 and H-2, which were adjacent in the molecular structure. The HMBC can detect the long-range couplings (2–4 bonds) between protons and carbon, which provides crucial information about the molecular structure. Between the proton at 3.64 ppm and the carbon at 25.9 and 32.9 ppm, the correlation also confirmed the position of the -CH_2OH (C-1) group relative to two other groups, -CH_2 (C-2) and -CH_2 (C-3), in the molecule. Based on these findings, the identification of compound-1 (Figure 5a, b, and c) proved to be 1-octadecanol, with the molecular formula $C_{18}H_{38}O$ (Table 1).

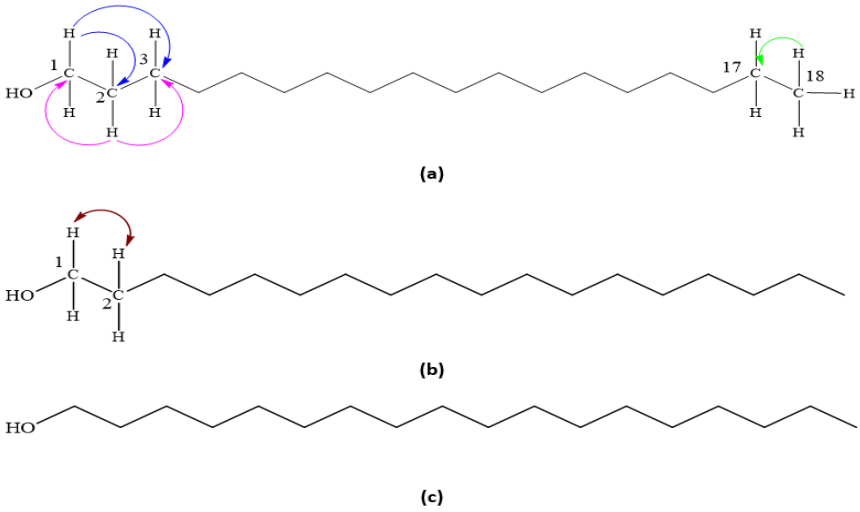

Figure 5. Chemical structure of HMBC (a), COSY (b), and 1-octadecanol (c).

Table 1. ^{1}H and ^{13}C NMR (600 MHz) spectral data ($CDCl_3$ solution) of Compound-1.

Position	δ ^{13}C (ppm)	δ ^{1}H (ppm)	m; *J* (Hz)	HMBC ^{1}H to ^{13}C	COSY ^{1}H to ^{1}H
1	63.2	3.64	t, J = 6.6 Hz	C-2, C-3	C-2
2	32.9	1.57	dq, J = 8.1, 6.6 Hz	C-1, C-3	C-1
	32.0	1.26	-	-	-
	29.8	1.26	-	-	-
	29.8	1.26	-	-	-
	29.7	1.26	-	-	-
	29.7	1.26	-	-	-
	29.6	1.26	-	-	-
	29.5	1.26	-	-	-
3	25.9	1.36	-	-	-
17	22.8	1.26	-	-	-
18	14.2	0.88	t, J = 7 Hz	C-17	-

Fatty alcohols' role in the adaptation of *S. macrophylla*

In the stem bark of *S. macrophylla*, the isolated fatty alcohol could play a crucial role in the plant's adaptation to its existing environment. Fatty alcohols are the widely recognized essential components of plant cuticular waxes, contributing to reduced water loss, protection against microbial diseases, and UV radiation resistance (Pollard *et al*., 2008; Chen *et al*., 2011). These protective mechanisms are particularly essential for tropical forest species like *S. macrophylla*, which endure high humidity and intermittent drought conditions.

Previous studies have demonstrated the antimicrobial properties of fatty alcohols, such as their ability to inhibit fungal spore germination and bacterial growth at various stages in crop plants (Steen *et al*., 2010). These findings align with the potential ecological role of 1-octadecanol in protecting *S. macrophylla* against pathogens prevalent in its humid native habitat. Furthermore, studies on related species suggested that fatty alcohols play a vital role in the chemical defense mechanisms, such as herbivore deterrence, and the adding of another layer of protection for the plant (Gupta *et al*., 2013). Similarly, fatty alcohols have garnered attention as potential biofuels due to their high energy density, biodegradability, and low toxicity. They can be effective as fuel additives or converted into fatty alcohol-based biodiesel, which enhances combustion efficiency and reduces emissions (Schirmer *et al*., 2010). Additionally, recent advancements in biotechnological production methods, such as microbial fermentation and enzymatic conversion, have improved the sustainability and viability of fatty alcohols as renewable energy sources (Liu *et al*., 2010).

The ecological significance of 1-octadecanol gained more recognition for its potential contribution to water retention and structural integrity in the stem bark (Molina *et al*., 2006; Mudge *et al*., 2010). Its ability to enhance the plant's resilience under environmental stress conditions, such as drought and pathogen load, warrants further investigation (Steen *et al*., 2010). Future research must evaluate its bioactivity against local pathogens, its distribution across plant tissues, and its accumulation under diverse environmental conditions. The significant findings emphasize the remarkable role of fatty alcohols as multifunctional biomolecules crucial for the survival and ecological fitness of *S. macrophylla*.

CONCLUSIONS

The *n*-hexane extract of *S. macrophylla* stem bark, as separated and purified, employed various chromatographic techniques. From a specific fraction of the extract, the isolation of a fatty alcohol compound was effective, with its structure confirmed through NMR and FT-IR spectroscopic methods. This study reports the first successful isolation of 1-octadecanol from the *S. macrophylla* plant. This marked a significant contribution to the phytochemical profile of the species, as previous documentation of 1-octadecanol did not exist in this plant. Therefore, the isolation of 1-octadecanol from *S. macrophylla* suggests the plant may serve as a valuable source of fatty alcohols, which are known for their numerous uses in cosmetics, pharmaceuticals, and biofuels.

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