SHORT REPORT

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A New Cytotoxic Alkenylresorcinol from *Embelia schimperi*

Blanche L. Ndontsa[1], Faustine L. M. Dongmo[1], Michel F. Tala[1,2], Hippolyte K. Wabo[1], Guang-Zhi Zeng[2], Ning-Hua Tan[2] and Pierre Tane[1*]

[1] *Department of Chemistry, University of Dschang, P.O. Box 67, Dschang, Cameroon*
[2] *State Key Laboratory of Phytochemistry and Plant Resources in West China, Kunming Institute of Botany, Chinese Academy of Sciences, Kunming 650201, Yunnan, P.R. China*

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Abstract: An investigation of MeOH extract of *Embelia schimperi* stem led to the isolation of a new resorcinol derivative, 5-(7'*Z*-pentadecenyl)resorcinol (**1**), along with the known compounds lupeol (**2**) and *β*-sitosterol glucoside (**3**). The structures of isolated compounds were elucidated using spectroscopic methods. Compound **1** exhibited moderate *in vitro* cytotoxic activity against human Hela cell line.

Keywords: *Embelia schimperi*; Myrsinaceae; alkenylresorcinol; 5-(7'*Z*-pentadecenyl)resorcinol; cytotoxic activity.

1. Plant Source

Embelia is a genus of Myrsinaceae consisting of approximately 30 species [1]. *Embelia schimperi* Vatke is a shrub that grows in Mount Oku and Mount Mwanengouba in Cameroon [2, 3]. Its stem is used in folk medicine as antibiotic. The stem of *Embelia schimperi* was collected at Mount Oku (altitude, about 3000 m), in the North-West Region of Cameroon, in January 2011. The plant material was identified by Dr. Caroline S. Momo, a botanist at the Department of Plant Biology of the University of Dschang, Cameroon. A voucher specimen (No 37430 HNC/Cam) is deposited at the Cameroon National Herbarium, Yaoundé.

2. Previous Studies

Previous phytochemical studies on *E. schimperi* reported the isolation of long alkyl chain substituted benzoquinones [3], pentacyclic triterpenoids [4, 5], anthraquinones [6], and flavonoids [7].

3. Present Study

Chromatography of the MeOH extract of stem of *E. schimperi* over silica gel and Sephadex LH-20 afforded a new alkenylresorcinol derivative, 5-(7'*Z*-pentadecenyl)resorcinol (**1**), along with the known lupeol (**2**) and *β*-sitosterol glucoside (**3**). Their structures (Fig. 1) were established by MS and NMR spectral analysis and comparison with literature data.

* Corresponding author: E-mail: ptane@yahoo.com; Phone: +237 77619546; Fax: +237 33451202

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5-(7'*Z*-pentadecenyl)Resorcinol (**1**): orange oil, ^{1}H and ^{13}C NMR: see Table 1; HREIMS: *m/z* 318.2550 $[M]^+$ (Calcd. for $C_{21}H_{34}O_2$ 318.2559); ESIMS: *m/z* (rel. int. %) = 319 $[M + H]^+$ (11), 313 (22), 301 (100), 299 (18), 275 (20), 230 (42), 219 (44), 206 (48), 193 (7); EIMS: *m/z* (int. rel. %) = 318 $[M]^+$ (8), 222 (4), 191(4), 166 (6), 137 (19), 124 (100), 55 (28), 69 (20), 123 (35).

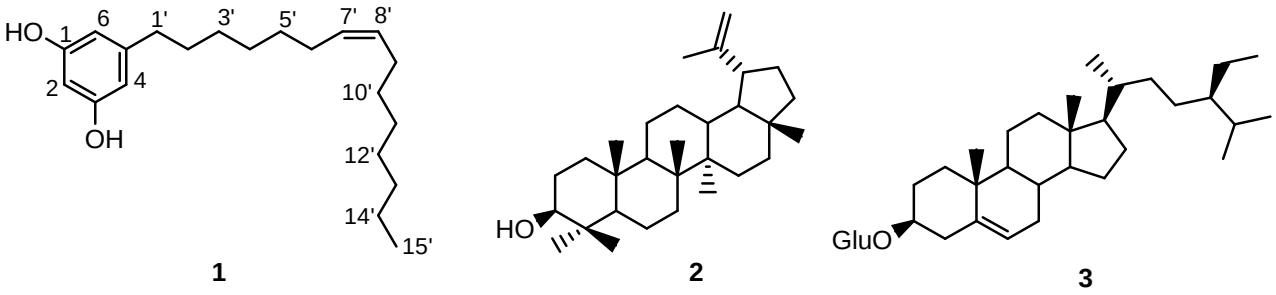

Figure 1. Structures of **1**-**3**.

Compound **1** was obtained as orange oil. It reacted positively to $FeCl_3$ reagent, suggesting the presence of phenolic hydroxyl group in the molecule. The molecular formula $C_{21}H_{34}O_2$ accounting for 5 degrees of unsaturation was determined from the HREIMS which showed a molecular ion peak at *m/z* 318.2550, in conjunction with NMR data. The ^{1}H NMR spectrum (Table 1) showed three aromatic protons at δ_H 6.17 (2H, brs, H-4 and H-6) and 6.11 (1H, brs, H-2) and a long alkenyl side chain with signals at δ_H 5.28 (2H, m, H-7'and H-8'), 2.41 (2H, t, *J* = 7.6 Hz, H-1'), 1.97 (4H, m, H-6' and H-9'), 1.60 (2H, m, H-2'), 1.18-1.35 (16H, m) and 0.86 (3H, t, *J* = 7.3 Hz, H-15'). The ^{13}C NMR spectrum (Table 1) exhibited signals of three aromatic quaternary carbons at δ_C 156.8 (C-1 and C-3), 146.0 (C-5) and three aromatic methine carbons at δ_C 108.2 (C-4 and C-6) and 100.3 (C-2), characteristic of a three substituted aromatic ring of a resorcinol moiety [8, 9]. This spectrum also showed the signals of two olefinic carbons of an alkenyl chain at δ_C 130.0 (C-7') and 130.2 (C-8'). The length of the alkenyl chain was deduced to be C_{15} by substraction of the benzene moiety ($C_6H_5O_2$) from the molecular formula. The configuration of the double bond was assigned as *Z* on the basis of the diagnostic chemical shift value of the allylic carbons (C-6' and C-9') signals observed around δ_C 27 [9]. The position of the double bond was determined by the presence of fragment ions peaks resulting from the vinylic cleavage of the side chain at *m/z* 191 [M-C_9H_{17}-2H] and *m/z* 222 [M-C_7H_{15}+3H] in the EIMS spectrum (Fig. 2) and at *m/z* 193 [M-C_9H_{17}] and *m/z* 219 [M-C_7H_{15}] in the ESI spectrum. These data also confirmed the length of the alkenyl chain. Compound **1** was thus characterized as 5-(7'*Z*-pentadecenyl)resorcinol. Bilobol or 5-(8'*Z*-pentadecenyl)resorcinol, an isomer of this compound was isolated from *Ginkgo biloba* [8].

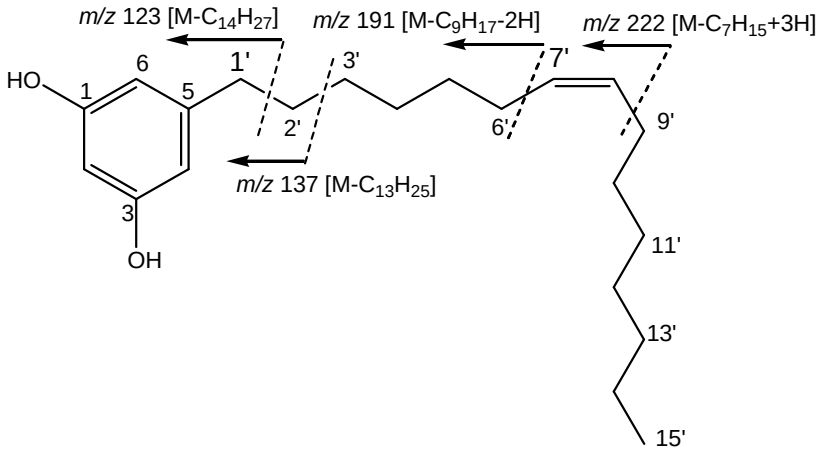

Figure 2. Fragment ions observed in EIMS spectrum of **1**.

Table 1. ^{1}H and ^{13}C NMR data for compound **1** (600 and 150 MHz, in $CDCl_3$), δ in ppm, *J* in Hz

Position	δ_C	δ_H (mult., *J* in Hz)	HMBC (H ⟶ C)
1	156.8	-	-
2	100.3	6.11 (brs)	C-4, C-6
3	156.8	-	-
4	108.2	6.17 (brs)	C-1', C-2, C-3, C-6
5	146.0	-	-
6	108.2	6.17 (brs)	C-1, C-2, C-1', C-4
1'	36.0	2.41 (t, *J* = 7.6 Hz)	C-4, C-6, C-5, C-2'
2'	32.0	1.60 (m)	C-1'
3'-5'	29.2-29.9	1.18-1.35 (m)	C-7'
6'	27.4	1.97 (m)	C-8'
7'	130.0	5.28 (m)	C-9'/ C-6'
8'	130.2	5.28 (m)	C-6'/ C-9'
9'	27.4	1.97 (m)	C-7'
10'-12'	29.2-29.9	1.18-1.35 (m)	C-9', C-15'
13'	31.3	1.18 (m)	C-8', C-15'
14'	22.9	1.18 (m)	C-15'
15'	14.4	0.86 (t, *J* = 7.3 Hz)	C-13', C-14'

The cytotoxic activity of 5-(7'*Z*-pentadecenyl)resorcinol was evaluated against Hela cell line by the SRB method as previously described by Xu et al.[10]. 5-(7'*Z*-pentadecenyl)resorcinol showed moderate cytotoxic activity against Hela cell line, with IC_{50} value of 12.13 μg/mL. The IC_{50} value of taxol, used as reference drug in this study was 0.37 μg/mL.

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Supporting Information

Supporting Information accompanies this paper on http://www.acgpubs.org/RNP

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