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RESEARCH NOTE

Secondary Metabolites from *Schefflera odorata* Blanco

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The leaves of *Schefflera odorata* afforded oleanolic acid (1), lutein (2), fatty alcohols, and hydrocarbons. The structure of 1 was elucidated by extensive 1D and 2D NMR analyses, while the structure of 2 was deduced by comparison of its ^{1}H NMR spectral data with those of lutein.

Key Words: Araliaceae, oleanolic acid, lutein, hydrocarbons, fatty alcohols

INTRODUCTION

Schefflera odorata Blanco, commonly known as "five fingers" is a famous indoor plant. The biological activities of the plant include treatment of asthma, liver diseases, rheumatism, arthritis, sprains, fracture, stomach pain, antipyretic, anti-inflammatory, analgesic, migraine, and general tonic (Quisumbing 1978). A saponin was reported to be potential modulator of the cell-signalling pathway (De Castro-Bernas & Ramos 2001). Although there is only one reported study on *S. odorata*, a number of studies have been reported on the congener of the plant. A betulinic acid glycoside was isolated from *S. venulosa* (Purohit et al. 1991). Oleanolic acid, a bidesmosidic triterpene saponin, and a trisaccharide were isolated from *S. octophylla* (Sung et al. 1991). *S. lucantha* afforded triterpenoid glycosides (Pancharoen et al. 1994). The aerial parts of *S. divaricata* produced triterpenoid saponins (De Tommasi et al. 1997). Triterpenoid saponins, along with oleanolic acid (Srivastava & Jain 1989) and a new triterpene (Shrivastava 1992) were obtained from *S. impressa*. The leaves of *S. bodinieri* afforded triterpenoids and a triterpene glycoside (Zho et al. 1996), while the roots of the plant afforded triterpene glycosides (Zho et al. 1996).

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We now report the isolation, and full structure elucidation by 1D and 2D NMR spectroscopy of oleanolic acid (**1**) from *S. odorata*. Lutein (**2**), fatty alcohols, and hydrocarbons were also obtained from the dichloromethane extract of the air-dried leaves of the plant.

MATERIALS AND METHODS

General

NMR spectra were recorded on a Bruker Avance 400 in $CDCl_3$ at 400 MHz for ^{1}H NMR and 100 MHz for ^{13}C NMR. Column chromatography was performed with silica gel 60 (70-230 mesh); TLC was performed with plastic backed plates coated with silica gel F_{254}; plates were visualized by spraying with vanillin-H_2SO_4 and warming.

Sample Collection and Extraction

Fresh leaves of the plant material were collected from Tandang Sora Ave., Quezon City in May 2001. The plant was identified as *Schefflera odorata* at the Philippine National Museum by Wilfredo F. Vendivil and a voucher specimen # 040 is kept at the Chemistry Department, De La Salle University.

Isolation

The air-dried leaves (937.90 g) of *S. odorata*, was extracted with CH_2Cl_2 to afford a crude extract (338.00 g) which was chromatographed with increasing proportions of $(CH_3)_2CO$ in CH_2Cl_2 at 10% increments as eluents. The 50-60% $(CH_3)_2CO$ in CH_2Cl_2 fraction from the first column was rechromatographed using 8:1:1 by volume, CH_2Cl_2:Et_2O:CH_3CN as eluent. Fraction 3 eluted from this column was triturated with petroleum ether to produce **1** (colorless crystals, 10 mg) after recrystallization from diethyl ether. Fraction 4 was chromatographed in the same solvent system to produce **2** (15 mg, orange crystals) after washing with diethyl ether. The 10-40% $(CH_3)_2CO$ in CH_2Cl_2 fraction from the first column was rechromatographed in 8:1:1 by volume, CH_2Cl_2:Et_2O:CH_3CN as eluent. Fraction 2 produced fatty alcohols (12 mg, colorless solid) after washing with petroleum ether. The CH_2Cl_2 fraction from the first column was rechromatographed using 10% ethyl acetate in petroleum ether. Fractions 1-8 produced hydrocarbons (15 mg, colorless solid) after washing with petroleum ether.

RESULTS AND DISCUSSION

The dichloromethane extract of the leaves of *S. odorata* produced **1**, **2**, (Figure 1) fatty alcohols, and hydrocarbons. The structure of **1** was elucidated by extensive 1D and 2D NMR spectroscopy as follows.

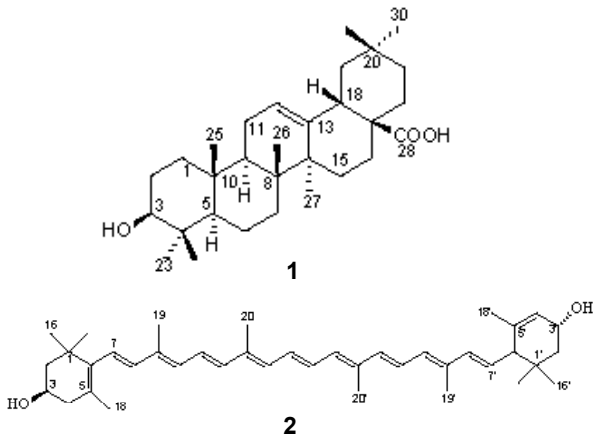

Figure 1. Structure of oleanolic acid (**1**) and lutein (**2**) from *Schefflera odorata* Blanco. by 1D and 2D NMR spectroscopy

The ^{1}H-NMR spectrum of **1** (Table 1) indicated resonances for an olefinic proton at δ 5.28 (1H, t), a carbinyl proton at δ 3.20 (1H, dd, J= 5.0, 11.0 Hz), and seven methyl singlets at δ 1.13 (3H), 0.98 (3H), 0.92 (3H), 0.91 (3H), 0.90 (3H), 0.77(3H), and 0.75 (3H). The large coupling constant (11 Hz) of the carbinyl proton indicates that it is in the axial position. The ^{13}C-NMR spectral data of 1 (Table 1) indicated resonances for thirty carbon atoms with the following functionalities: a carbonyl carbon of a carboxylic acid at δ 182.66; two olefinic carbons at δ 143.26 and 122.6; a carbinyl carbon at δ 79.01; and twenty-six methyl, methylene, methine, and quaternary carbons that resonate

Table 1. The 400 MHz 1H and 13C spectral data of oleanolic acid (**1**) from *Schefflera odorata* Blanco

Position	dC	dH mult. (J Hz)	HMBC Correlations	NOESY Correlations
1	38.37	0.98a,	H-25	-
		1.62		H-11
2	27.15	1.56,		H-23
		1.6		-
3	79.01	3.20 dd (5.0, 11.0)	H-1', H-2, H-23, H-24	H-5, H-23
4	38.74	-----	H-6', H-24	
5	55.18	0.75 t	H-1', H-23, H-24, H-25	H-9, H-23, H-27
6	18.27	1.38,	H-5	H-24, H-26
		1.54		H-23, H-27, H-6
7	32.59	1.29,		H-26
		1.44		H-27
8	39.23	-----	H-26, H-27	
9	47.6	1.54	H-12, H-25, H-26	H-5, H-23, H-27, H-6
10	37.05	-----	H-25	
11	23.37	0.91,	H-9	
		1.88		H-12, H-26, H-25

Table 1 continuation . . .

Position	dC	dH mult. (J Hz)	HMBC Correlations	NOESY Correlations
12	122.61	5.28 t (3.6)	H-9, H-11, H-18	
13	143.26	-----	H-27, H-18	
14	41.59	-----	H-12, H-27, H-26	
15	27.66	1.10, 1.72		H-15’
16	22.91	1.61, 1.97		H-16’, H-22’ H-16, H-29
17	46.47	-----	H-19	
18	40.98	2.81 dd (3.6, 13.6)	H-19’	H-12, H-19, H-26
19	45.84	1.16, 1.63	H-29, H-30	H-12, H-18, H-19’, H-29 H-27
20	30.66	-----	H-19’, H-29, H-30	
21	33.77	1.22, 1.33		H-21’ H-21
22	32.4	1.58, 1.77		H-29, H-22’ H-22
23	28.08	0.98 s (Me)	H-24	H-3, H-5, H-24
24	15.52	0.75 s (Me)		H-25, H-2’
25	15.3	0.91 s (Me)	H-5, H-9	H-24, H-6’
26	17.08	0.77 s (Me)		H-24, H-25, H-11’, H-6’
27	25.91	1.13 s (Me)		H-22’, H-9, H-7’
28	182.66	-----	H-22’	
29	33.05	0.92 s (Me)		
30	23.66	0.90 s (Me)	H-19, H-21, H-29	

[a]multiplets unless otherwise indicated

at δ 55.18, 47.60, 46.47, 45.84, 41.59, 40.98, 39.27, 38.74, 38.37, 37.05, 33.77, 33.05, 32.59, 32.40, 30.66, 28.08, 27.66, 27.15, 25.91, 23.66, 23.37, 22.91, 18.27, 17.08, 15.52, and 15.30. These resonances are characteristics of a triterpene with an olefin and an alcohol functionalities (Huang & Hsu 2001).

The COSY 2D NMR spectrum of **1** showed correlations of six spin systems as follows: H2-1/H2-2/H-3, H-5/H2-6/H2-7, H-9/H2-11/H-12, H2-15/H-2-16, H-18/H2-19, H2-21/H2-22 (Figure 2).

The ^{1}H and ^{13}C assignments of **1** (Table 1) were verified by 2D Heteronuclear Single-Quantum Correlation (HSQC) experiments, while connectivities were verified by Heteronuclear Multibond Shift Correlation (HMBC) (Table 1 and Figure 2). The hydroxyl was attached to C-3 due to long-range correlations between this carbon and H-1, H-2, H-23, and H-24. The double bond was placed on C-12 due to its long-range correlations with H-9, H-11, and H-18. The carboxylic acid was placed at C-28 since a long-range correlation was observed between this carbon and H-22. All long-range correlations observed are consistent with the structure of **1**.

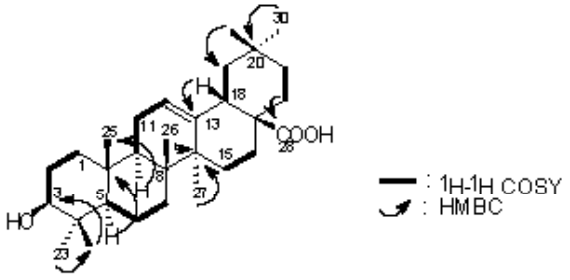

Figure 2. ^{1}H-^{1}H COSY and key ^{1}H-^{13}C long-range correlations of oleanolic acid (**1**) from *Schefflera odorata* Blanco.

The NOESY spectral data of **1** (Table 1 and Figure 3) indicated that the carbinyl proton (H-3) is close in space to the H-5 and the methyl singlet (H-23). NOE correlations were observed between the methyl singlets (H-24 and H-25). This indicated that the bridgehead protons (H-5 and H-25) are trans to each other. NOE correlations were also observed between H-9, H-5, and H-27, indicating the relative stereochemistry in structure **1**. No correlation was observed between H-9 and H-26, which correlates to H-25, suggesting a trans configuration for the bridgehead protons (H-9 and H-26). This confirms the structure of **1**, which was identified as oleanolic acid. Comparison of the ^{1}H-NMR and ^{13}C-NMR spectral data of **1** and oleanolic acid (Huang & Hsu 2001) indicated similar resonances. However, in the literature some of the ^{1}H and ^{13}C assignments were different from our assignments. Furthermore, only the resonances for H-3, H-12, H-18, and all the methyl singlets were reported in the literature.

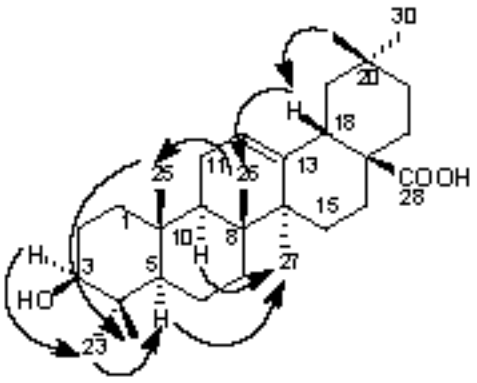

Figure 3. Key NOESY correlations for oleanolic acid (**1**) from *Schefflera odorata* Blanco

The ^{1}H NMR spectrum of **2** (Table 2) indicated resonances for carbinyl protons at δ 4.00 and 4.25; olefinic protons at δ 5.45, 5.55, 6.64, 6.12, 6.16, 6.27, and 6.36; methyl protons at δ 0.85, 1.00, and 1.07; and allylic methyl protons at δ 1.97, 1.91, 1.74, and 1.63. Compound 2 was identified by comparison of its ^{1}H NMR spectral data (Table 2) with those reported in the literature for lutein (Largo et al. 1997). The spectra matched in all essential respects.

The fatty alcohols and hydrocarbons were deduced from their ^{1}H NMR spectral data as follows. The ^{1}H NMR spectrum for the fatty alcohols indicated resonances for a long chain of methylene groups at δ 1.26, carbinyl protons at δ 3.65, and terminal methyl triplets at δ 0.88. The 1H NMR spectrum of the hydrocarbons indicated long chain methylene groups of the hydrocarbons at δ 1.27 and almost overlapping methyl triplets at 0.87 and 0.89.

Table 2. Comparision of the 300 MHz 1H NMR spectral data of Lutein (**2**) from *Schefflera odorata* Blanco with other literature

Position	Lutein (2)	Lutein (Largo et al. 1997)
	δH	δH
H-2	1.44, 1.81	1.45, 1.80
H-3	4.00	4.0
H-4	2.0, 2.40	2.0, 2.40
H-2'	1.40, 1.87	1.40, 1.90
H-3'	4.25	4.2
H-4'	5.55	5.5
H-6'	2.4	2.4
H-7'	5.45	5.4
Allylic Me	1.97 (9H, s), 1.91 (3H),	1.95 (9H, s), 1.90 (3H, s)
	1.74 (3H, s), 1.63 (3H, s)	1.72 (3H, s), 1.61 (3H, s)
Ring B Me	0.85 (3H, s), 1.00 (3H, s)	0.84 (3H, s), 0.97 (3H, s)
Ring A Me	1.07 (6H, s)	1.06 (6H, s)
Olefinic H	6.64 (4H), 6.12 (5H), 6.16 (2H),	6.6 (4H), 6.1 (5H), 6.2 (2H),
	6.27 (1H), 6.36 (1H)	6.3 (1H), 6.4 (1H)

Literature search revealed that oleanolic acid has anti-inflammatory, hepatoprotective, gastroprotective, anti-ulcer, and immunoregulatory effect (Vachalkova et al. 2004), gastroprotective effect on experimentally induced gastric lesions in rats and mice (Astudillo et al. 2002), inhibits mouse skin tumor (Oguro 1998), protects against hepatotoxicants and is used in China to treat hepatitis (Lui et al. 1993), and significant antitumor activity on human colon carcinoma cell line HCT 15 (Li et al. 2002). Thus, some of the known biological activities of *S. odorata*, such as treatment of liver diseases, stomach pain, and anti-inflammatory may be attributed to this compound.

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