

A New Diterpene from *Spiraea japonica* var. *ovalifolia*

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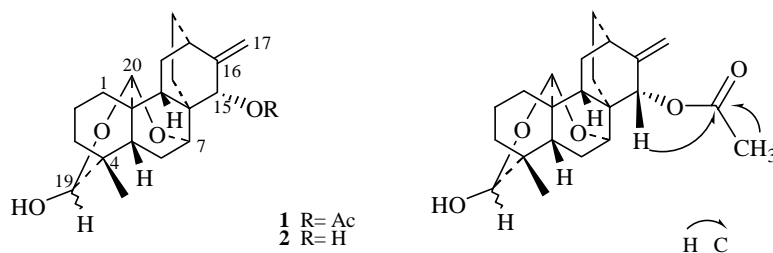
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Abstract: A new diterpenoid, 15-*O*-acetylspiraminol (**1**), was isolated from the aerial parts of *Spiraea japonica* L. f. var. *ovalifolia*. The structure was characterized mainly based on spectral analysis.

Keywords: Rosaceae, *Spiraea japonica* L. f. var. *ovalifolia*, diterpenoids.

In the previous paper, we have reported five new diterpenoid alkaloids from *Spiraea japonica* L. f. var. *ovalifolia* (Rosaceae), a shrub originated in Songming, Yunnan¹. Further investigation of the plant material led to the isolation of a new non-alkaloid component, 15-acetylspiraminol (**1**), together with its known 15-deacetyl analogue, spiraminol (**2**). Their structures were elucidated mainly by 1D and 2D NMR methods.



Compound **1**, colorless needles with mp 171~172°C (Me₂CO) and $[\alpha]_D^{22} -70.31$ (*c* 7.20, CHCl₃), was determined to have the molecular formula of C₂₂H₃₀O₅ by HREIMS (374.2103, calcd. 374.2093). The ¹H and ¹³C NMR spectra of **1** was similar to those of spiraminol (**2**)². Three oxygen-substituted methines were demonstrated by the NMR signals at δ_C 95.0 (d, C-19) and δ_H 5.19 (s, 1H, H-19), δ_C 74.1 (d, C-15) and δ_H 5.26 (s, 1H, H-15 β), as well as δ_C 70.7 (d, C-7) and δ_H 3.71 (dd, 1H, J 4.4, 6.8 Hz, H-7 β). The

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difference between the NMR spectra of **1** and **2** was the additional acetyl signals in **1** [δ_{H} 2.06 (s, 3H, $\underline{\text{CH}_3}$), δ_{C} 21.2 (q, $\underline{\text{CH}_3}$) and 171.2 (s, $\underline{\text{CO}}$)]. The IR signals at 3465 and 1714 cm^{-1} indicated the presence of O-H and C=O functionalities, respectively, which was further supported by the EIMS m/z (%) 374 (M^+ , 10), 358 ($\text{M} - 1 - \text{OH}$, 40), and 331 ($\text{M} - \text{CH}_3\text{CO}$, 10). The cross peak between H-15 β and $\underline{\text{COCH}_3}$ in HMBC confirmed the acetyl group was designated at C-15-*O*-position. Hence, **1** was determined to be 15-*O*-acetylspiraminol. All the NMR assignments were thoroughly carried out on the basis of 2D NMR experiments and compared with those of **2**² (Table 1).

Table 1 NMR data of compound **1** (δ ppm, CDCl_3).

	^1H	^{13}C	HMBC (H to C)
1	2.03 (dd, 2H, 4.4, 5.5)	33.7t	C-2, 3, 4, 20
2	1.42 (m, 2H)	25.2t	C-1, 3, 4, 20
3	1.73 (dd, 1H, 4.0, 8.5)	29.5t	C-2, 1, 4
4	/	37.5s	/
5	1.36 (m, 1H)	45.6d	C-4, 6, 10, 18, 19
6	1.58 (m, 1H)	25.8t	C-4, 5, 7, 8
	1.70 (m, 1H)		
7	3.61 (m, 1H)	70.7d	C-6, 8, 9, 15
8	/	41.0s	/
9	1.06 (t, 1H, 6.6)	43.4d	C-7, 10, 11, 14
10	/	34.0s	/
11	1.02 (m, 2H)	22.7t	C-8, 9, 10, 12, 20
12	2.45 (t, 1H, 4.3)	36.6d	C-9, 11, 13, 16
13	1.71, 1.86 (m, 2H)	20.6t	C-11, 12, 14, 16
14	1.71, 1.86 (m, 2H)	20.4t	C-7, 8, 9, 14, 15
15	5.26 (s, 1H)	74.1d	$\underline{\text{CO}}$, C-8, 9, 14, 16
16	/	149.9s	/
17	5.07 (br s, 2H)	114.4t	C-12, 15
18	0.86 (s, 3H)	22.2q	C-4, 5, 19
19	5.19 (s, 1H)	95.0d	C-3, 4, 5, 20
20	5.27 (s, 1H)	98.0d	C-1, 9, 10, 15
CH_3	2.06 (s, 3H)	21.2q	$\underline{\text{CO}}$
CO	/	171.2s	/

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References and Notes

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3. ^{13}C NMR (400 MHz, CDCl_3 , ppm) of **2**: δ 33.6 (t, C-1), 25.2 (t, C-2), 29.5 (t, C-3), 37.6 (s, C-4), 45.7 (d, C-5), 25.8 (t, C-6), 70.6 (d, C-7), 40.8 (s, C-8), 43.7 (d, C-9), 34.0 (s, C-10), 22.7 (t, C-11), 36.9 (d, C-12), 20.6 (t, C-13), 20.4 (t, C-14), 74.2 (d, C-15), 155.2 (s, C-16), 112.3 (t, C-17), 22.3 (q, C-18), 95.0 (d, C-19), 98.2 (d, C-20), 21.2 (q, $\underline{\text{CH}_3}$), 171.2 (s, $\underline{\text{CO}}$).

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