

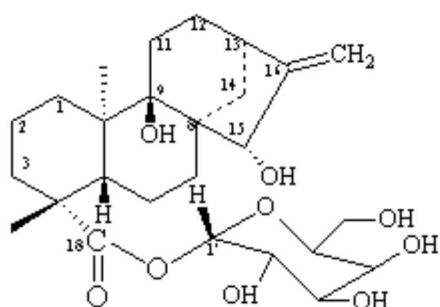
(-)-b-D-18–Glucopiranosyl-9,15-dihydroxy Kaurenoate, a New Diterpene Glycoside from *Ageratina vacciniaefolia*

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From leaves and flowers of *Ageratina vacciniaefolia* we have isolated several compounds: a flavonoid, a diterpene and a new compound identified as (-)-b-D-18–glucopiranosyl-9,15-dihydroxy kaurenoate (see the formula). The structure was established by using ^1H NMR, ^{13}C NMR, COSY, NOESY and HMBC spectroscopic techniques (See Table 1) [1,7].

The ethanolic extract of leaves and flowers of *A. vacciniaefolia* yielded white crystals after column chromatography eluted with CH_2Cl_2 , EtOAc and mixtures of these solvents.

M.p. 218–220°C.

$[\alpha]_D^{20} = -100$ (MeOH).

DCI-MS [isobutane] m/z : $(\text{M}^* + \text{H})^+$ 497; 479 (M-18); 377; 337; 335; 317; 299; 271; 230; 187; 163; 145 (100%); 127.

^1H NMR (400 MHz, $\text{C}_5\text{D}_5\text{N}$): d 1.15 (dt, 1H, CH_2 , $J=4.3$; 12.3); 1.33 (s, 3H, CH_3); 1.53 (s, 3H, CH_3); 1.55–1.70 (m, 2H, CH_2); 1.58–1.60 (m, 1H, CH_2); 1.66 (m, 1H, CH_2); 1.87 (ddd, 1H, CH_2 ; $J=12.0$; 3.8); 2.17–2.18 (m, 2H, CH_2); 2.25 (m, 1H, CH); 2.28 (m, 1H, CH_2); 2.30 (dq, 1H, CH_2 ; $J=3.2$; 12.4); 2.33 (m, 1H, CH_2); 2.44 (m, 1H, CH_2); 2.50 (dd, 1H, CH_2 ; $J=12.0$; 13.0); 2.75 (bs, 1H, CH); 4.06 (ddd, 1H, CH; $J=2.4$; 4.3; 9.5); 4.24 (bt, 1H, CH; $J=7.8$); 4.28 (t, 1H, CH; $J=8.0$); 4.35 (t, 1H, CH; $J=8.9$); 4.40 (dd, 1H, CH_2 ; $J=4.3$; 11.9); 4.46 (dd, 1H, CH_2 ; $J=2.4$; 11.9); 5.31 (bs, 1H, CH); 5.20/5.46 (bs, 2H, CH_2); 6.33 (d, 1H, CH; $J=7.8$, anomeric proton).

^{13}C NMR (100 MHz; $\text{C}_5\text{D}_5\text{N}$): d 18.6 ($-\text{CH}_3$, C20); 20.3 ($-\text{CH}_2$, C1); 22.5 ($-\text{CH}_2$, C6); 29.4 ($-\text{CH}_3$, C18); 30.0 ($-\text{CH}_2$, C11); 31.7 ($-\text{CH}_2$, C7); 33.3 (CH_2 , C1); 34.9 ($-\text{CH}_2$, C12); 37.7 ($-\text{CH}_2$, C14); 39.0 ($-\text{CH}_2$, C3); 42.4 ($-\text{CH}$, C13); 45.0 ($-\text{C}-$, C4); 45.7 ($-\text{C}-$, C10); 51.4 ($-\text{CH}$, C5); 54.3 ($-\text{C}-$, C8); 62.7 ($-\text{CH}_2\text{-O-}$, C6'); 71.6 ($-\text{CH}$, C4'); 74.6 ($-\text{CH}$, C2'); 77.4 ($-\text{C-OH}$, C9); 78.0 ($-\text{CH-OH}$, C15); 79.7 ($-\text{CH}$, C3'); 79.9 ($-\text{CH}$, C5'); 96.3 ($-\text{CH}$, C1'); 107.9 ($=\text{CH}_2$, C17); 162.3 ($=\text{C}$, C16); 178.0 ($-\text{COO}$, C19). For details, see table 1.

Table 1. Direct and long range NMR correlations and their assignments [2-6].

No. C	Type of C	d-ppm	C-H (JHz)	HMBC
19	COO-	178.0		6.33 2.25 1.33
16	C =	162.3		5.46 5.20 2.50 1.87
17	CH ₂ =	107.9	5.46, 5.20 s,b	
	CH - 1'	96.3	6.33 d (7.8)	4.24
	CH - 5'	79.9	4.06 ddd (2.4, 4.3, 9.5)	4.35
	CH - 3'	79.7	4.28 t (8.0)	4.35
15	CH	78.0	5.31 s,b	5.46 5.20 2.5
9	C - O	77.4		5.31 5.22 2.17 1.87, 1.6 1.53
	CH - 2'	74.6	4.24 bt (7.8)	4.28
	CH - 4'	71.6	4.35 t (8.9)	4.18 4.28
	CH ₂ -O-6'	62.7	4.46 dd (2.4 ;11.9)	4.35
			4.40 dd (4.3 ;11.9)	
8	C	54.3		5.22(OH), 2.75 2.5 2.33 2.17 1.87
5	CH	51.4	2.25 m.	2.66, 2.44, 2.17 1.66, 153, 1.33
10	C	45.7		2.25 4.66 1.53
4	C	45.0		2.44 2.25 1.33 1.15
13	CH	42.4	2.75 s.b	5.46 5.20 2.17 1.87
3	CH ₂	39.0	2.44 m	25. 2.25, 1.66, 1.33
			1.15 dt (4.3 ; 12.3)	
14	CH ₂	37.7	2.50 dd (12, 13)	531 2.17
			1.87 ddd (12, 3.8)	
12	CH ₂	34.9	1.55 - 1.7 m (2H)	2.5 2.17
1	CH ₂	33.3	2.33 m	2.44 1.53
			1.66 m	
7	CH ₂	31.7	2.18 d	2.66 2.25 1.87
11	CH ₂	30.0	2.17 m	5.22 (OH) 1.78
18	CH ₃	29.4	1.33 s	2.25 1.15
6	CH ₂	22.5	2.30 dq (3.2 ; 12.4)	2.25 2.17
			2.28 m	
1	CH ₂	20.3	2.33 m 1.60 m	1.15 2.3
			1.58 m	

20	CH ₃	18.6	1.53 s	2.17
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