SUPPLEMENTARY MATERIAL

A new sesquiterpene lactone from yacon leaves

Ying Yuan^a, Khin Khin Win Aung^{†ac}, Xiao-Ku Ran^a, Xiao-Tong Wang^a,
De-Qiang Dou^{a*} and Feng Dong^b

^a *College of Pharmacy, Liaoning University of Traditional Chinese Medicine, Dalian 116600, P.R. China.*

^b *Zhen-Ao Co.Ltd, Dalian 11660, P.R. China*

^c *Pharmaceutical Research Department, Ministry of Science and Technology, Yangon 999091, Myanmar*

The chemical constituents of 60% EtOH extract of yacon leaves were separated to yield a new compound, together with four known compounds, which were isolated for the first time from this plant. The structure of the new compound was characterized and named as chlorodalin (**1**) on the basis of NMR (1D and 2D), HR-MS and other spectral methods. The effects of **1–5** were evaluated on cytotoxic activities against two human cancer cell lines. The new compound showed significant cytotoxic activity.

Keywords: *Smallanthus sonchifolius*; yacon; sesquiterpene lactone; chemical constituent; cytotoxic activity.

Table S1. ¹³C-NMR, ¹H-NMR, HMBC and NOESY of compound **1** (CDCl₃)

No.	¹³ C-NMR	¹ H-NMR	HMBC	NOESY
1	148.4	7.01 (1H, dd, <i>J</i> =7.7 and 10.2 Hz)	2, 3, 9	2, 3, 9, 15
2a	26.1	2.46 (1H, m)	1, 3	1, 3, 9
2b		2.69 (1H, m)		
3a	36.9	2.05 (1H, d, <i>J</i> =11.9 Hz)	1, 2, 5, 18	1, 2, 5, 18
3b		2.40 (1H, m)		
4	130.7		2, 3, 5, 6	
5	126.6	4.96 (1H, d, <i>J</i> =10.4 Hz)	3, 6, 7, 18	3, 6, 7, 9, 18
6	75.0	5.12 (1H, td, <i>J</i> =10.0 and 6.5 Hz)	5, 7, 8	5, 7, 9, 18, 3', 5'
7	50.9	2.79 (1H, m)	5, 6, 8, 13	5, 6, 8, 9, 13
8	72.3	6.65 (1H, dd, <i>J</i> =0.9 and 8.3 Hz)	6, 7, 9	7, 9, 13, 17
9	71.0	5.41 (1H, dd, <i>J</i> =8.4 and 0.9 Hz)	1, 8	5, 6, 7, 8, 17, 5'
10	138.2		2	
11	133.7		7, 8, 13	
12	169.0		13	
13a	122.3	5.76 (1H, d, <i>J</i> =3.1 Hz)	7	7, 8
13b		6.28 (1H, d, <i>J</i> =3.4 Hz)		
14	165.8		9, 15	
15	52.3	3.81 (3H, s)		1
16	170.2		9, 17	
17	21.0	1.99 (3H, s)		8, 9
18	16.9	2.00 (3H, s)	3, 5	2, 3, 5, 6
1'	173.3		8, 3', OH, 4', 5'	
2'	76.8		OH, 4', 5'	
3'	61.7	4.15 (1H, q, <i>J</i> =6.7 Hz)	4', 5'	6, 4', 5'
4'	18.0	1.49 (3H, d, <i>J</i> =6.8 Hz)	3'	3', 5', OH
5'	23.0	1.31 (3H, s)	3'	9, 3', 4', OH
OH		3.19 (1H, s)		4', 5'

Table S2. ^{13}C -NMR, ^1H -NMR, HMBC and NOESY of compound **2** (CD_3OD)

No.	^{13}C -NMR	^1H -NMR	HMBC	NOESY
1	37.0		2, 8, 11, 12	
2a	47.2	2.22 (1H, br. d, $J=11.9\text{ Hz}$);	3, 4, 8, 11, 12	3, 4, 11, 12
2b		1.49 (1H, t, $J=$ 11.9 Hz)		
3	73.5	4.96 (1H, br. t, $J=11.9\text{ Hz}$)	2, 4	2, 4, 11, 13
4a	47.3	2.48 (1H, br. d, $J=11.9\text{ Hz}$)	2, 3, 8, 13	2, 3, 11, 12, 13
4b		1.55 (1H, t, $J=$ 11.9 Hz)		
5	72.4		4, 8, 13	
6	119.7		2, 4, 8, 11, 12, 13	
7	211.4		8, 10	
8	101.2	5.84 (1H, s)	10	10, 12, 13
9	200.8		8, 10	
10	26.6	2.20 (3H, s)	8	8
11	29.3	1.42 (3H, s)	2, 8, 12	2, 3, 4
12	32.1	1.17 (3H, s)	2, 11	2, 4, 8
13	30.6	1.39 (3H, s)	4	3, 4, 8,

Figure S1. (a-b) HR-MS of compound **1**, (c-e) UPLC/TOF-MS of compound **1** in yacon leaves

Figure S2. The key HMBC and NOESY correlations of compound 1

Figure S3. HR-MS of compound 1

Note: m/z 485.1571 $[M+H]^+$

Figure S4. HR-MS of compound 2

Note: m/z 225.1500 $[M+H]^+$

Figure S5. CD of compound 2 (experimental in CH_2Cl_2)

Note: -91.3 (226)

Figure S6. CD of compound 2 (experimental in Dioxane)

Note: +4.8 (215), +2.3 (240), +4.8(290)

Figure S7 (a). ¹³C-NMR of compound 1

Figure S7 (b). ¹³C-NMR of compound 1

Figure S8 (a). ¹H-NMR of compound 1

Figure S8 (b). ¹H-NMR of compound 1

Figure S8 (c). ¹³C-NMR of compound 1

Figure S9 (a). HSQC of compound 1

Figure S9 (b). HSQC of compound 1

Figure S9 (c). HSQC of compound 1

Figure S10 (a). HMBC of compound 1

Figure S10 (b). HMBC of compound 1

Figure S10 (c). HMBC of compound 1

Figure S11 (a). NOESY of compound 1

Figure S11 (b). NOESY of compound 1

Figure S11 (c). NOESY of compound 1

Figure S12. ¹³C-NMR of compound 2

Figure S13 (a). ¹H-NMR of compound 2

Figure S13(b). ^1H -NMR of compound 2

Figure S14. HSQC of compound 2

Figure S15 (a). HMBC of compound 2

Figure S15 (b). HMBC of compound 2

Figure S16. NOESY of compound 2

Figure S17. ¹³C-NMR of compound 3

Figure S18. ¹H-NMR of compound 3

Figure S19. ¹³C-NMR of compound 4

Figure S20. ¹H-NMR of compound 4

Figure S21. ¹³C-NMR of compound 5

Figure S22. ¹H-NMR of compound 5