

SUPPLEMENTARY MATERIAL

A new sesquiterpenoid glycoside from *Saussurea involucrata*

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Abstract

Saussurea involucrata, known for the abundant bioactive components, is a precious traditional Chinese medicine. In this study, a novel guaiane sesquiterpenoid glycoside named (1*R*, 5*R*, 6*R*, 7*R*, 8*S*, 11*S*)-11, 13-dihydrodehydrocostuslactone-8-*O*-6'-2''(*E*)-butenoyl- β -D-glucopyranoside (**1**), together with seven known compounds (**2-8**) were isolated from the dried aerial part of *S. involucrata*. Their structures were elucidated by spectroscopic and physico-chemical analyses. The antioxidant and anti-inflammatory activities of compound **1** were investigated. And compound **1** showed weak radical scavenging activity and low inhibitory activity on nitric oxide (NO) production.

Keywords: *Saussurea involucrata*; sesquiterpenoid glycoside; antioxidant; anti-inflammatory

List of supplementary materials

Table S1. ^1H -NMR, ^{13}C -NMR, HMBC and NOESY spectral data of compound **1**

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Table S1

¹H-NMR, ¹³C-NMR, HMBC and NOESY spectral data of compound **1** (DMSO-*d*₆, δ in ppm, *J* in Hz)

Position	δ_{C}	δ_{H}	HMBC(H→C)	NOESY
1	46.5	2.88 (1H, dd, <i>J</i> = 13.8, 7.8 Hz)	C-7	H-7
2	31.9	2.38 (1H, m), 2.44 (1H, m)	C-4	
3	29.4	1.74 (1H, m), 1.82 (1H, m)	C-1	
4	152.2	-	-	
5	52.2	2.77 (1H, br t, <i>J</i> = 9.6 Hz)	C-1, 4, 6, 10, 15	
6	79.3	3.91 (1H, t, <i>J</i> = 9.6 Hz)	C-4, 7, 8	H-8
7	53.0	2.19 (1H, dd, <i>J</i> = 13.2, 9.6 Hz)	C-1, 5, 6, 8, 9, 11, 13	H-1, 5
8	83.3	3.65 (1H, td, <i>J</i> = 9.0, 5.4 Hz)	C-11	H-6, 11
9	44.1	2.18 (1H, m), 2.70 (1H, m)	C-1, 6, 8, 11, 14	
10	145.4	-	-	
11	40.2	2.67 (1H, dd, <i>J</i> = 10.8, 7.2 Hz)	C-7, 12, 13	H-6
12	178.8	-	-	
13	16.1	1.28 (3H, d, <i>J</i> = 7.2 Hz)	C-7, 11, 12	
14	113.6	4.78 (1H, br s), 4.86 (1H, br s)	C-9, 10, 11	
15	108.6	4.95 (1H, br s), 5.02 (1H, br s)	C-2, 7	
1'	103.7	4.35 (1H, d, <i>J</i> = 8.4 Hz)	C-8, 1''	
2'	76.8	3.17 (1H, t, <i>J</i> = 8.4 Hz)	C-3', 4', 5'	
3'	73.6	3.40 (1H, t, <i>J</i> = 8.4 Hz)	C-6'	
4'	70.3	3.06 (1H, t, <i>J</i> = 9.0 Hz)	C-2', 3', 5', 6'	
5'	73.7	2.99 (1H, m)	C-1'	
6'	63.5	4.10 (1H, dd, <i>J</i> = 11.4, 7.8 Hz), 4.38 (1H, dd, <i>J</i> = 12.0, 1.8 Hz)	C-3', 5', 1''	
1''	165.4	-	-	
2''	122.2	5.86 (1H, dd, <i>J</i> = 15.6, 1.8 Hz)	C-1'', 4''	
3''	145.3	6.88 (1H, m)		

4"	17.7	1.82 (3H, d, $J = 7.2$ Hz)	C-2", 3"
OH		5.21 (1H, d, $J = 5.4$ Hz), 5.09 (1H, s), 5.05 (1H, d, $J = 6.0$ Hz)	

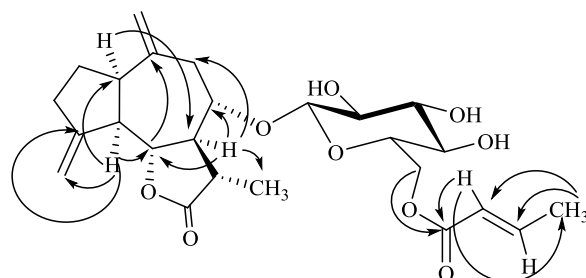


Figure S1. The key HMBC correlations of compound **1**.

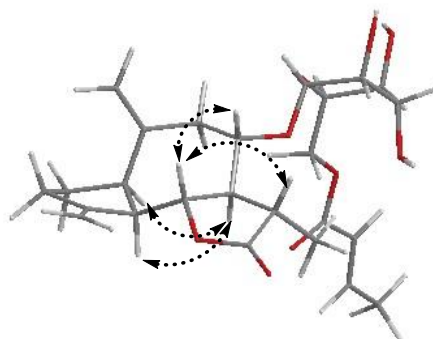


Figure S2. The key NOESY correlations of compound **1**.

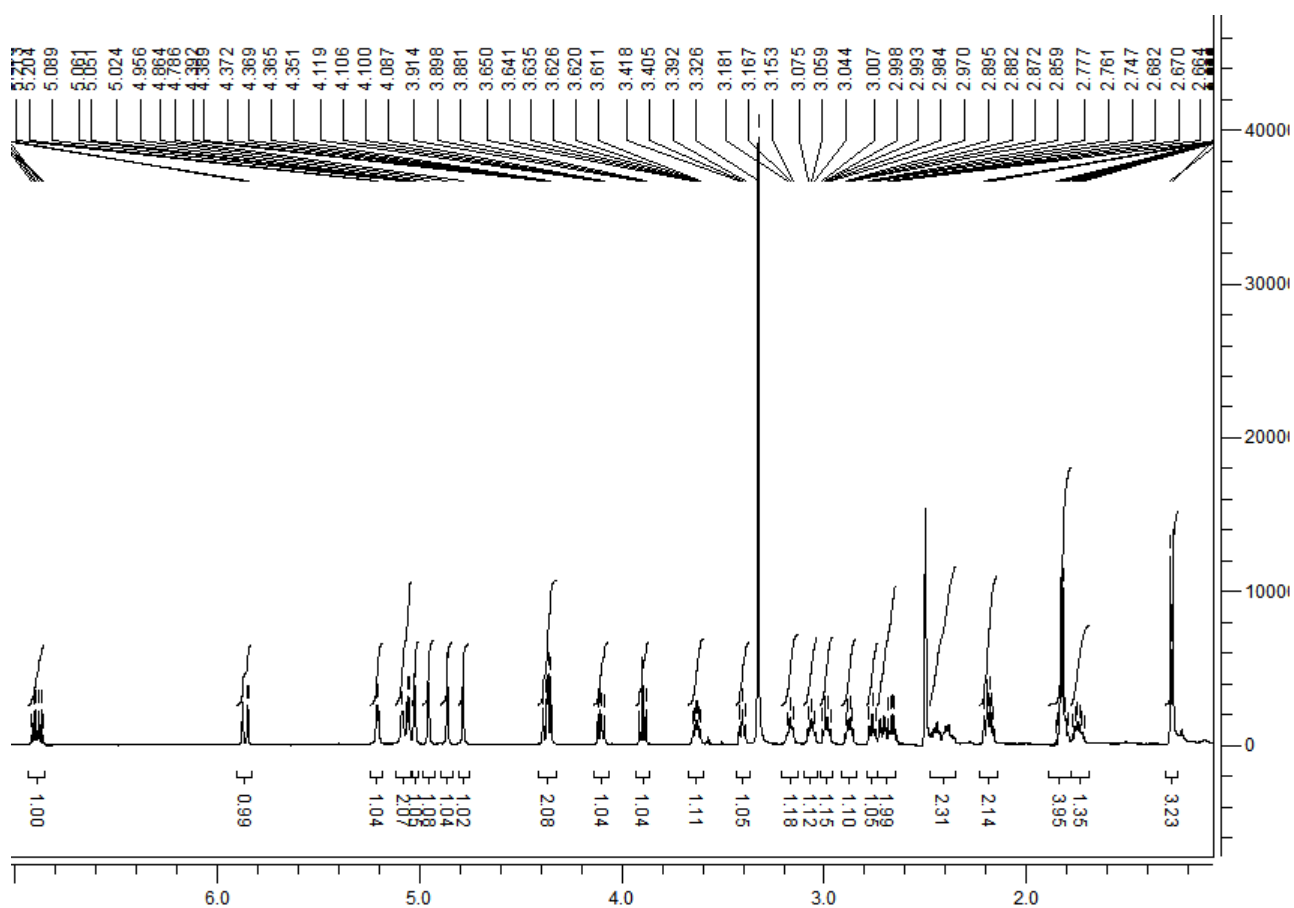


Figure S3. The ^1H -NMR spectrum of compound **1** ($\text{DMSO-}d_6$, 600 MHz)

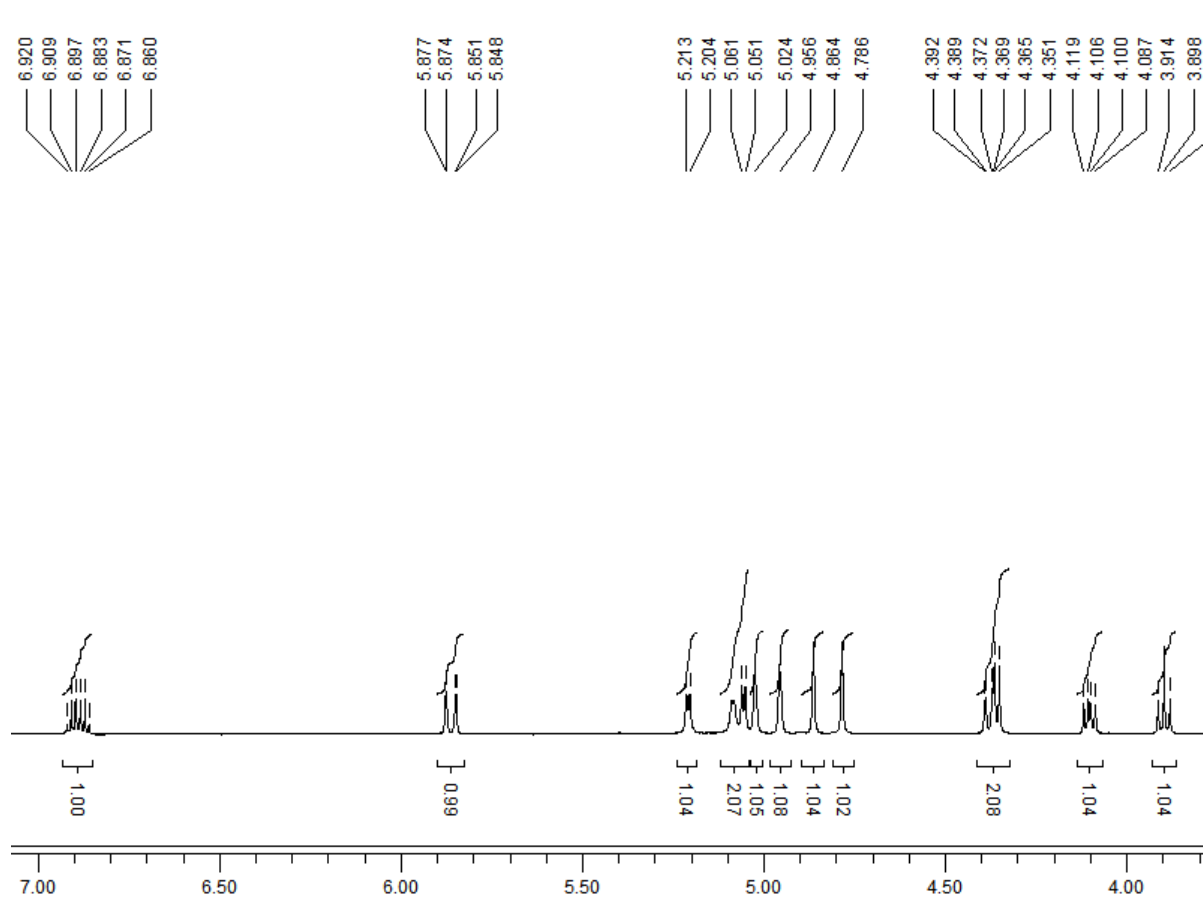


Figure S4. The ¹H-NMR spectrum of compound **1** (DMSO-*d*₆, 600 MHz)

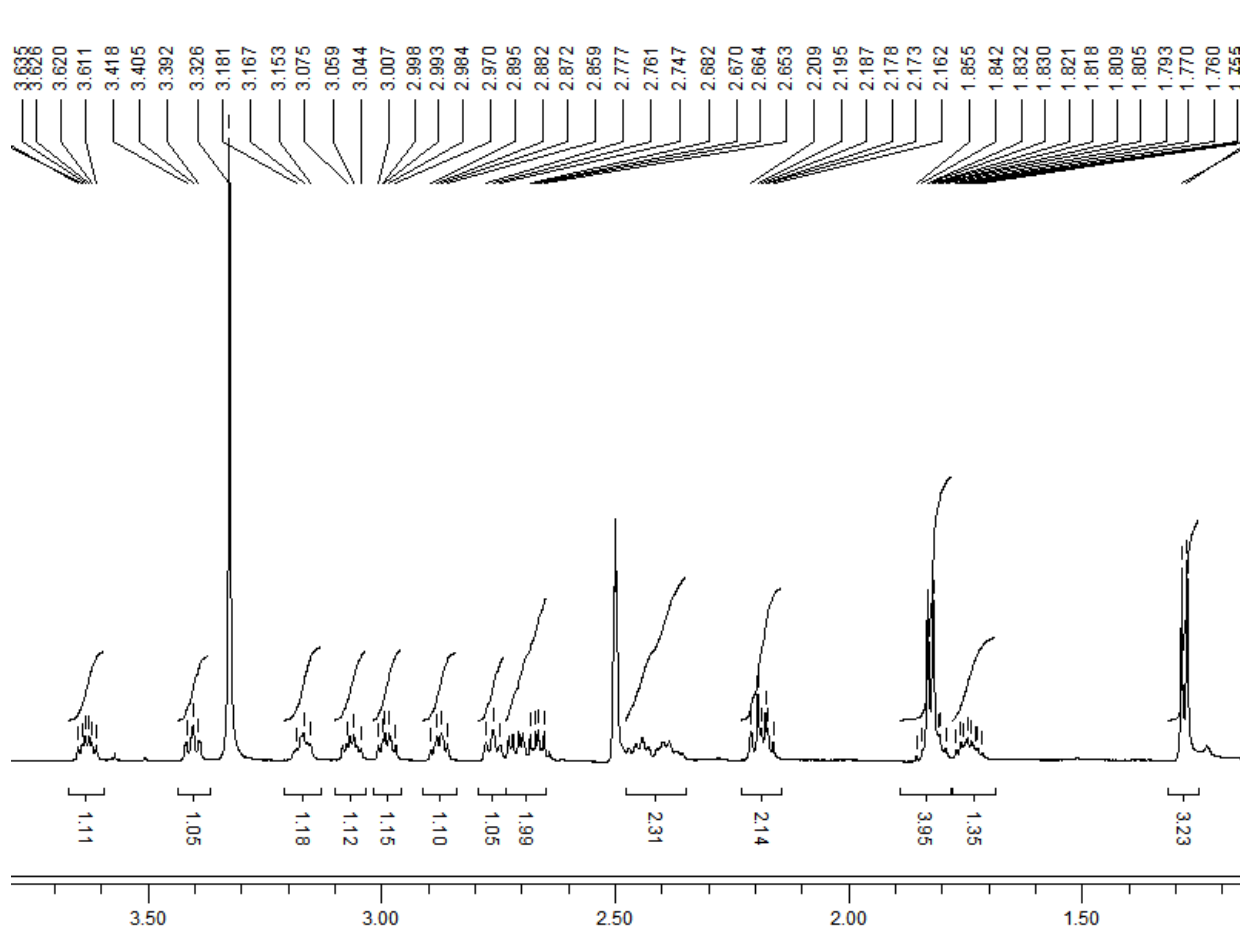


Figure S5. The ^1H -NMR spectrum of compound **1** ($\text{DMSO-}d_6$, 600 MHz)

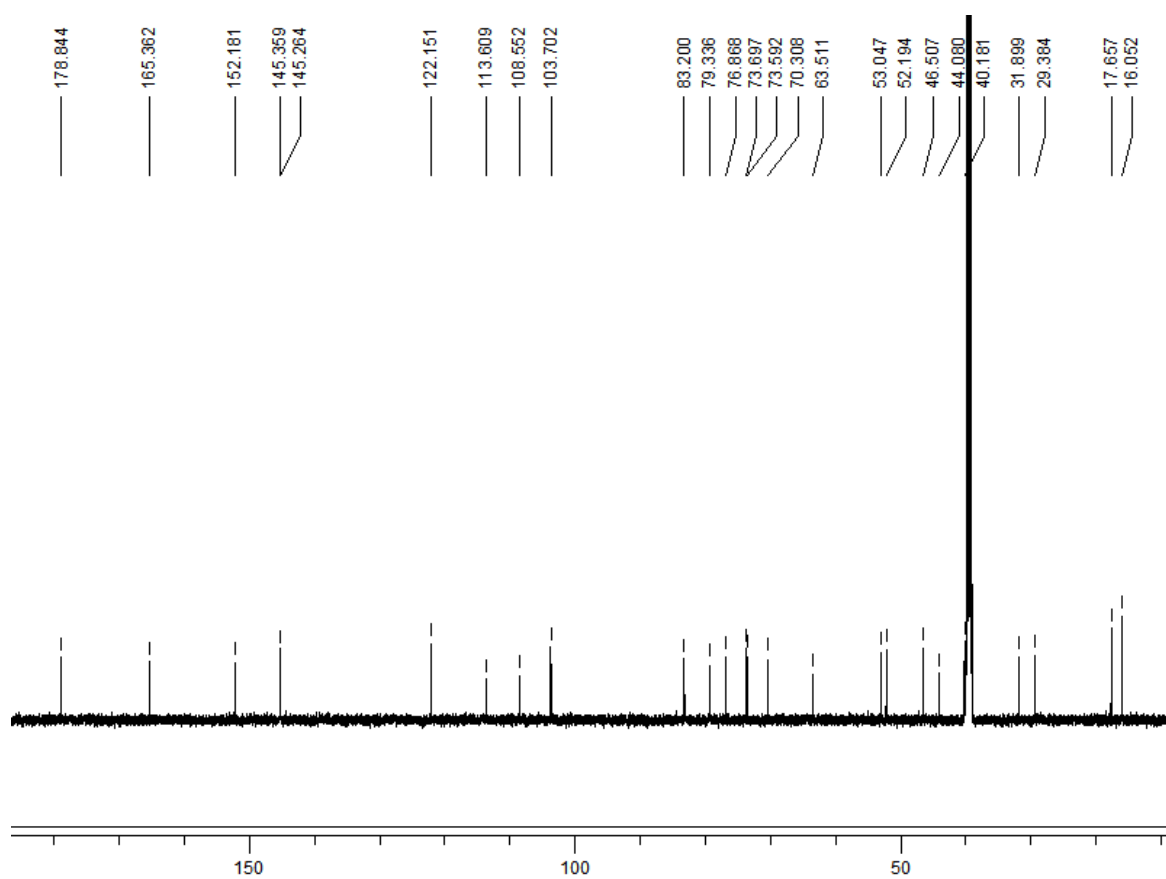


Figure S6. The ^{13}C -NMR spectrum of compound **1** ($\text{DMSO-}d_6$, 150 MHz)

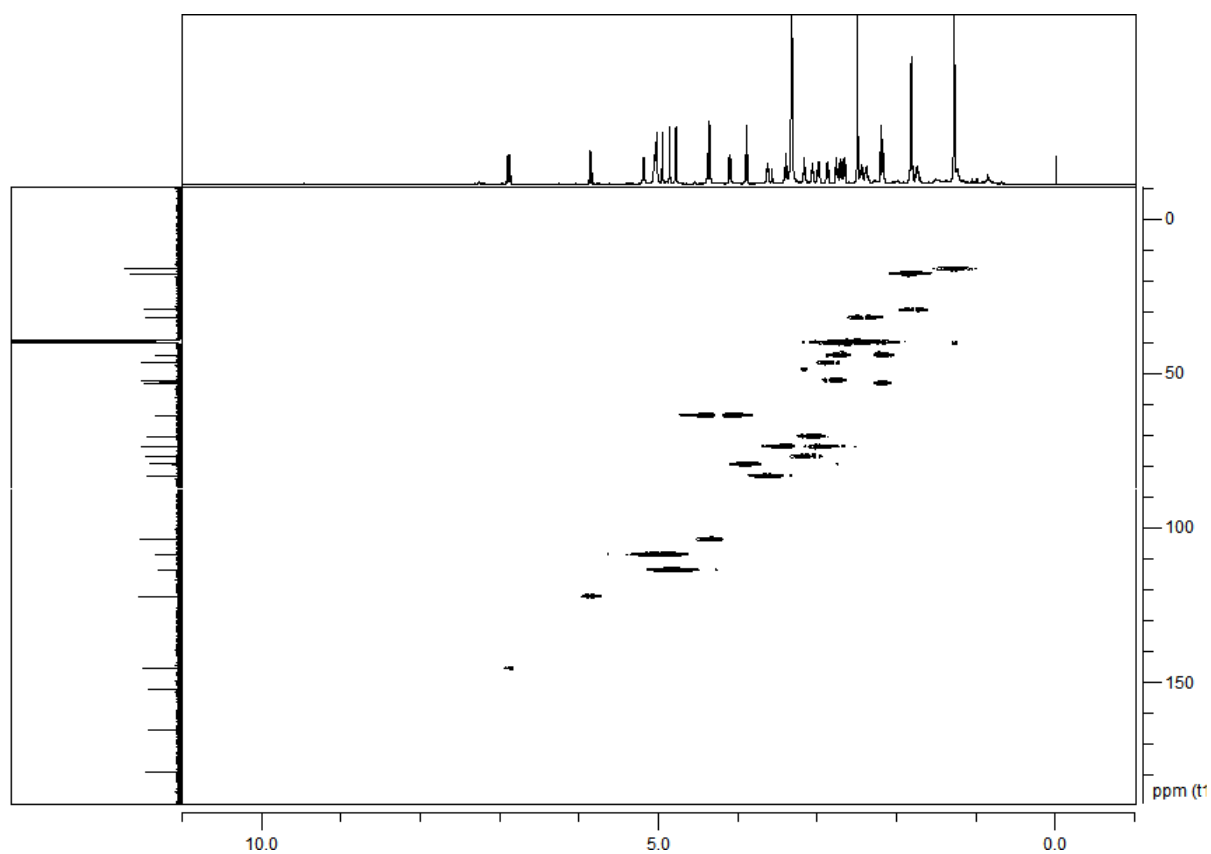


Figure S7. The HSQC spectrum of compound **1** (DMSO- d_6 , 600 MHz)

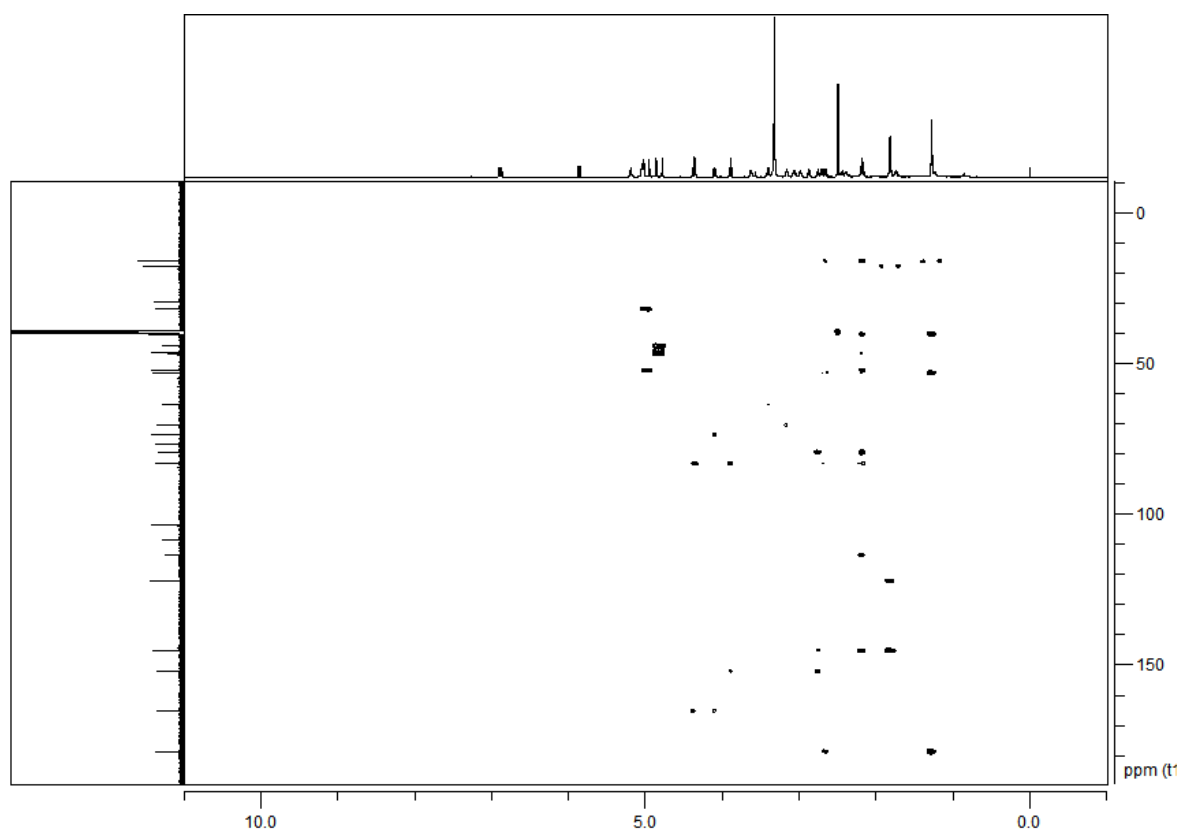


Figure S8. The HMBC spectrum of compound **1** (DMSO- d_6 , 600 MHz)

AV-600-NOESY
Sample:XXY-1

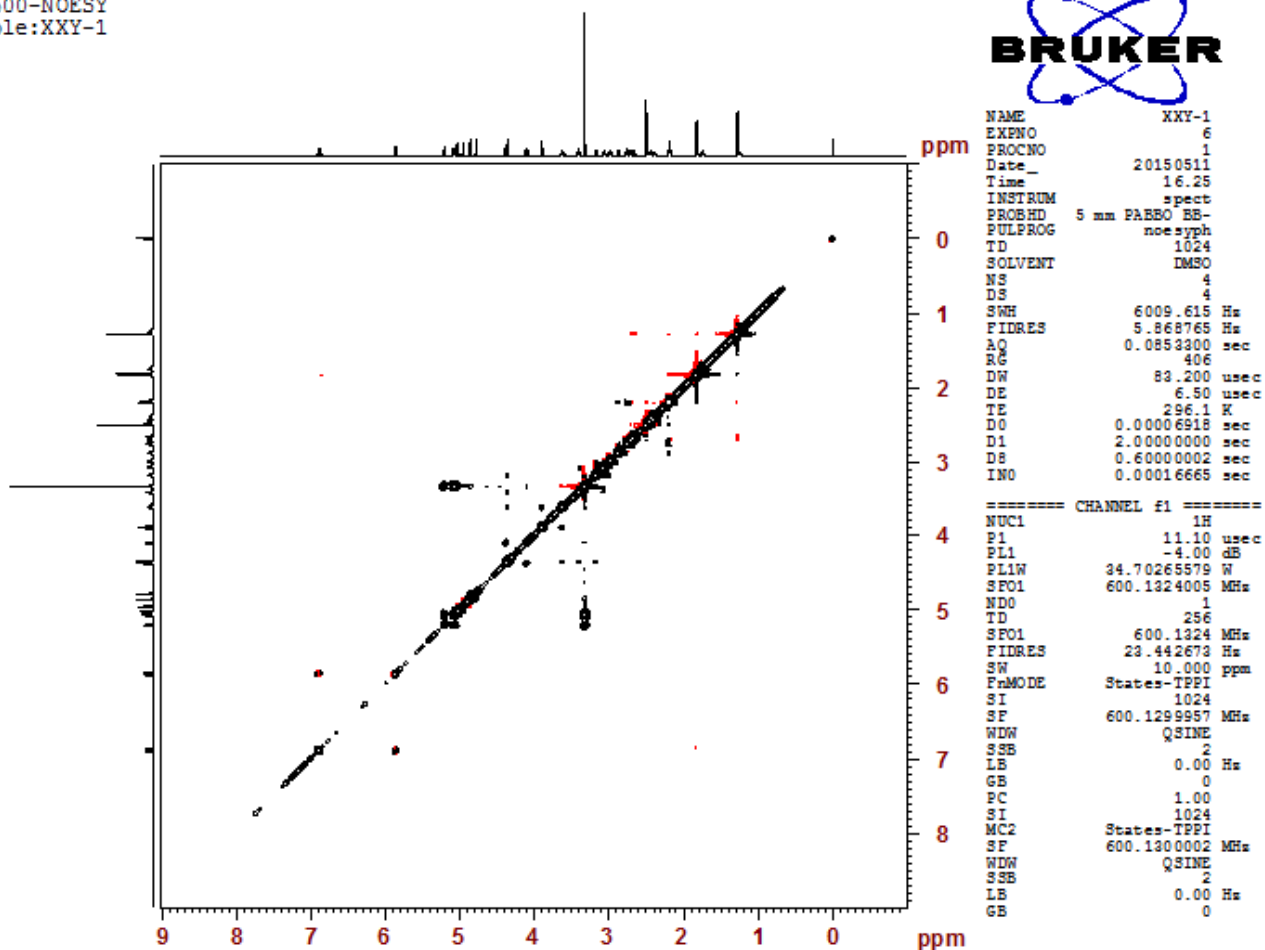


Figure S9. The NOESY spectrum of compound **1** (DMSO- d_6 , 600 MHz)

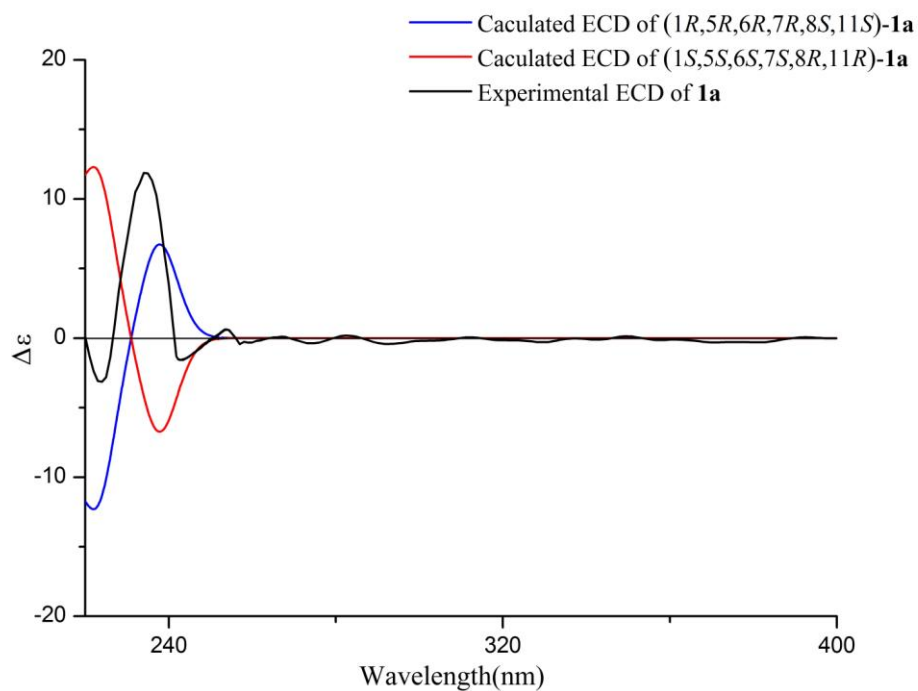


Figure S10. The ECD cotton effect of compound **1a**

Comment

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source

Generate Molecular Formula Parameter

Formula, min.		Tolerance	Charge
Formula, max.		Minimum	Maximum
Measured m/z		Electron Configuration	
Check Valence		Minimum	Maximum
Nitrogen Rule			
Filter H/C Ratio			
Estimate Carbon			

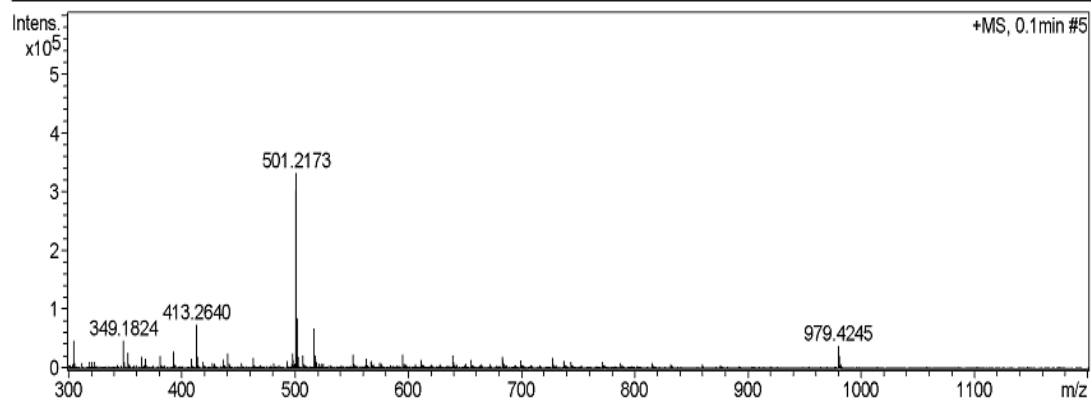


Figure S11. The HR-ESI-MS spectrum of compound **1**

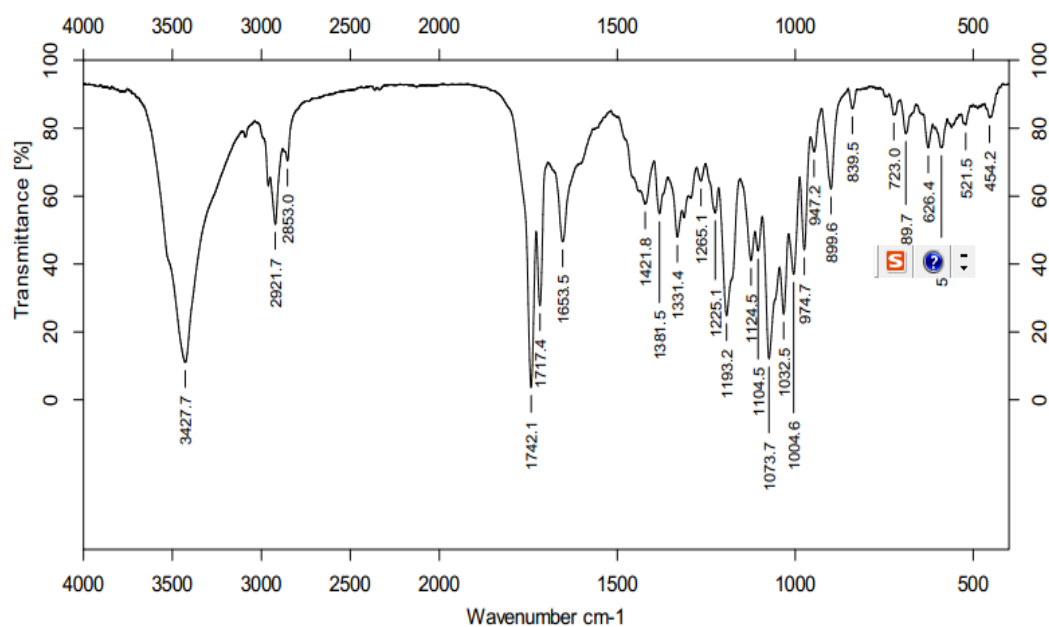


Figure S12. The IR spectrum of compound **1**

Reference

Wang XL, Gesang SL, Jiao W, Liao X, Ding LS. 2007. Two new sesquiterpenoid glucosides from the aerial parts of *Saussurea involucrate*. J Integr Plant Biol. 49: 609-614.

Xiao W, Li X, Li N, Bolati M, Wang XJ, Jia XG, Zhao, YQ. 2011. Sesquiterpene lactones from *Saussurea involucrata*. 82:983-987.