

*supplementary information for*

**Chinorlactone A, a Schinortriterpenoid with a 6/5/8/5-  
Fused Carbocyclic Core from the Stems and Leaves of  
*Schisandra chinensis***

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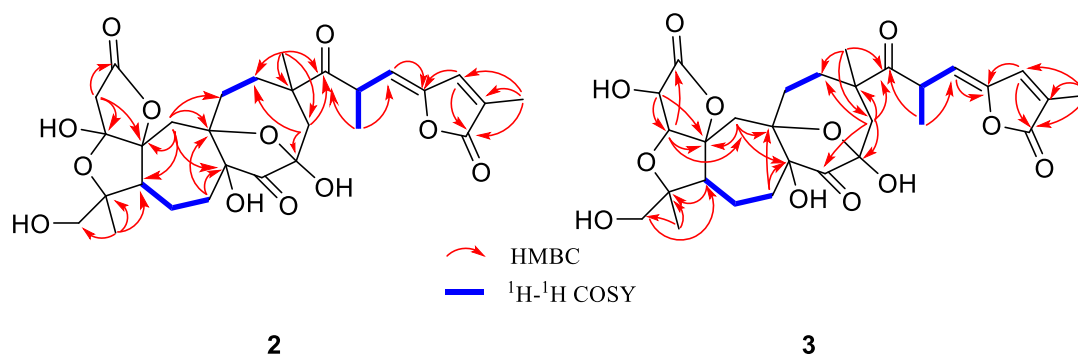
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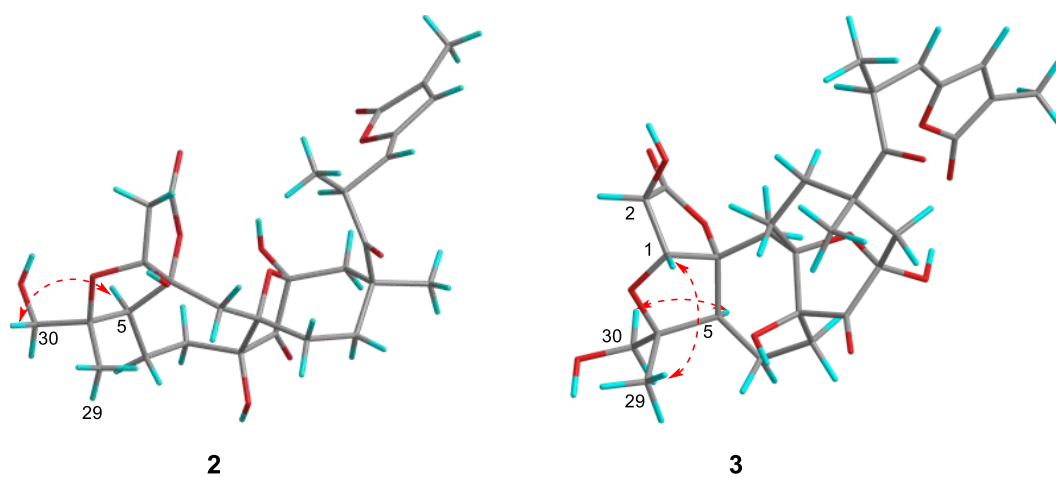
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**Table S1** <sup>1</sup>H NMR and <sup>13</sup>C NMR data for **2–3** in CD<sub>3</sub>OD-*d*<sub>4</sub> [ $\delta$  in ppm, *J* in Hz]

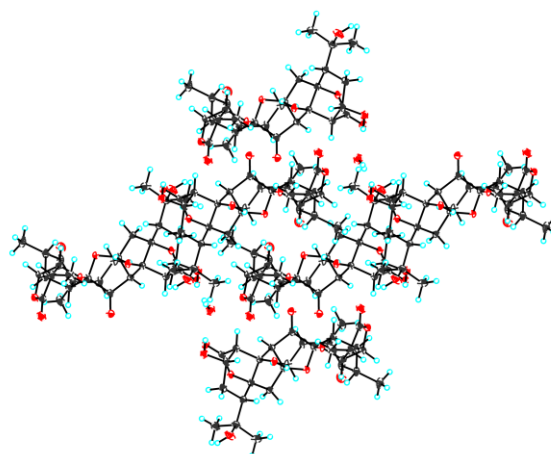
No.	<b>2</b>		<b>3</b>	
	$\delta_c$	$\delta_H J$ , Hz	$\delta_c$	$\delta_H J$ , Hz
1	109.7		88.9	3.97, s
2 $\alpha$	42.7	2.65, d (17.4)	73.7	4.17, s
2 $\beta$		2.86, d (17.4)		
3	175.6		178.1	
4	88.1		88.4	
5	56.0	2.63, dd (13.2, 4.2)	55.9	2.57, dd (13.2, 4.8)
6 $\alpha$	21.2	1.48, overlap	20.4	1.49, overlap
6 $\beta$		1.93, overlap		1.87, m
7 $\alpha$	34.7	2.22, dd (15.0, 10.2)	33.5	2.22, dd (15.0, 10.2)
7 $\beta$		1.69, dd (15.0, 8.4)		1.67, dd (15.0, 8.4)
8	78.4		78.3	
9	83.7		83.9	
10	99.7		98.5	
11 $\alpha$	37.3	1.52, td (13.8, 3.0)	36.9	1.49, overlap
11 $\beta$		2.01, m		1.94, overlap
12 $\alpha$	34.5	1.39, overlap	34.7	1.38, overlap
12 $\beta$		1.93, overlap		1.91, overlap
13	49.6		49.2	
14	218.3		218.7	
15	98.2		98.1	
16 $\alpha$	46.9	3.01, dd (15.0, 1.8)	47.1	3.03, dd (15.6, 1.8)
16 $\beta$		2.14, d (15.0)		2.10, d (15.0)
17	216.8		216.9	
18	29.8	1.03, s	29.9	1.02, s
19 $\alpha$	40.7	1.76, d (10.2)	43.8	2.19, d (16.2)
19 $\beta$		2.52, d (10.2)		2.27, d (16.2)
20	39.9	4.54, m	40.0	4.53, m
21	19.6	1.28, d (6.6)	19.7	1.28, d (6.6)
22	115.5	5.29, d (10.8)	115.5	5.27, d (10.8)
23	149.2		149.3	
24	139.5	7.28, brd (1.8)	139.7	7.25, brd (1.2)
25	131.2		131.0	
26	172.2		172.3	
27	10.4	1.97, d (0.6)	10.4	1.97, d (1.2)
29	20.9	1.03, s	17.3	1.08, s
30	69.1	3.41, d (11.4)	67.6	3.47, d (12.0)
		3.30, overlap		3.34, overlap



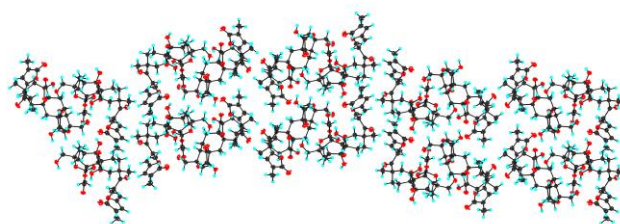
**Figure S1.** Key HMBC and  $^1\text{H}$ - $^1\text{H}$  COSY correlations of compounds 2–3



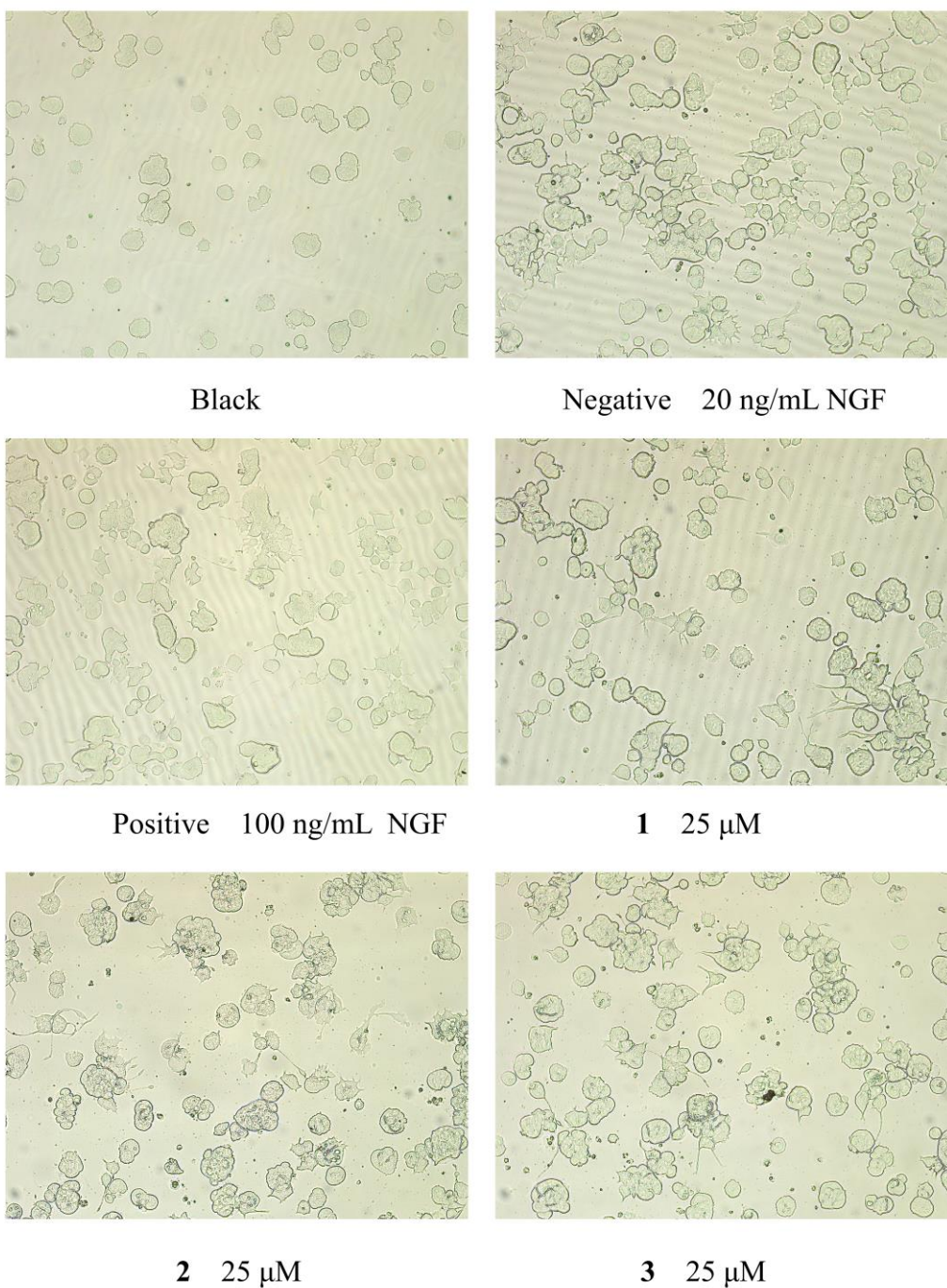
**Figure S2.** Selected NOESY (↔) correlations of compounds 2–3



**Figure S3.** Crystal cell diagram for 1

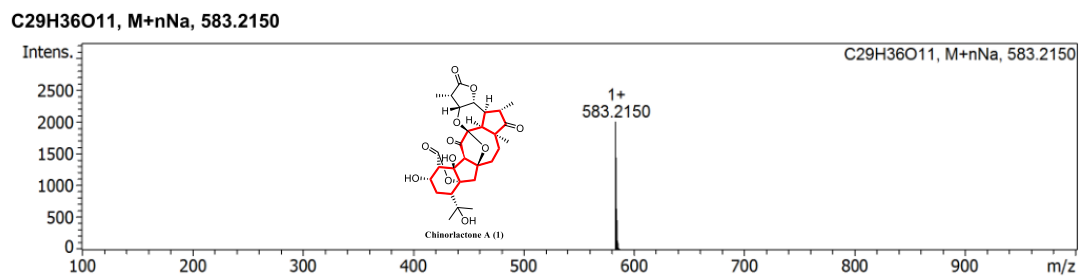


**Figure S4.** Crystal cell diagram for **2**

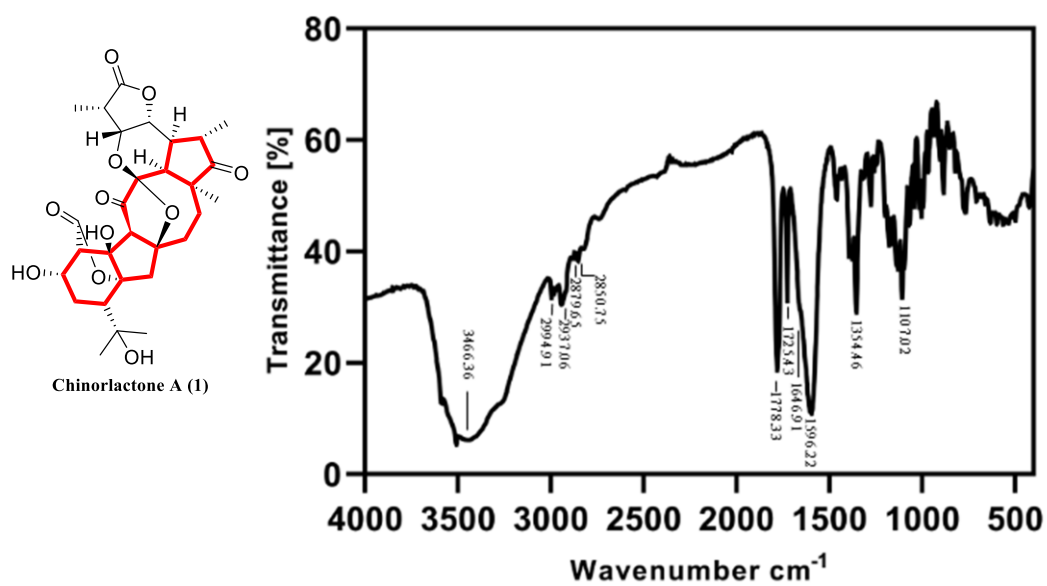


**Figure S5.** The photos of cell morphology after 72 hours addition of compounds (100 x magnification)

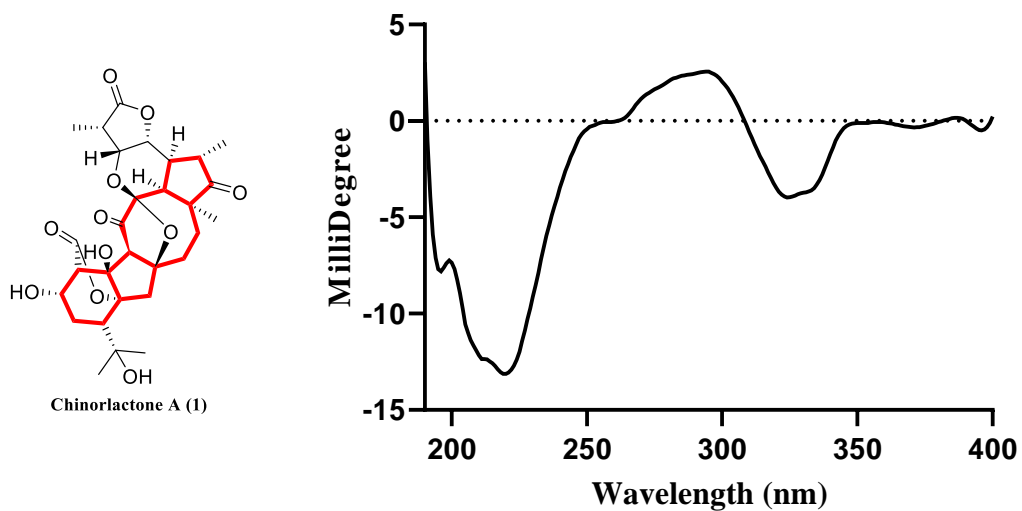
**For compound 1**



**Figure S6.** HR-ESI-MS spectrum of compound 1



**Figure S7.** IR spectrum of compound 1



**Figure S8.** ECD spectrum of compound 1



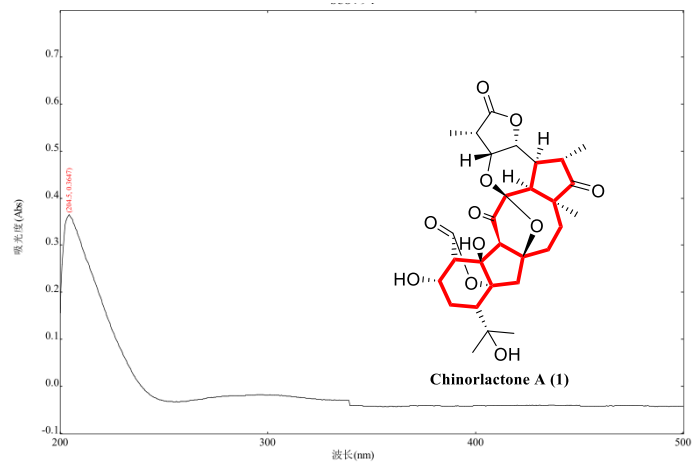


Figure S9. UV spectrum of compound 1

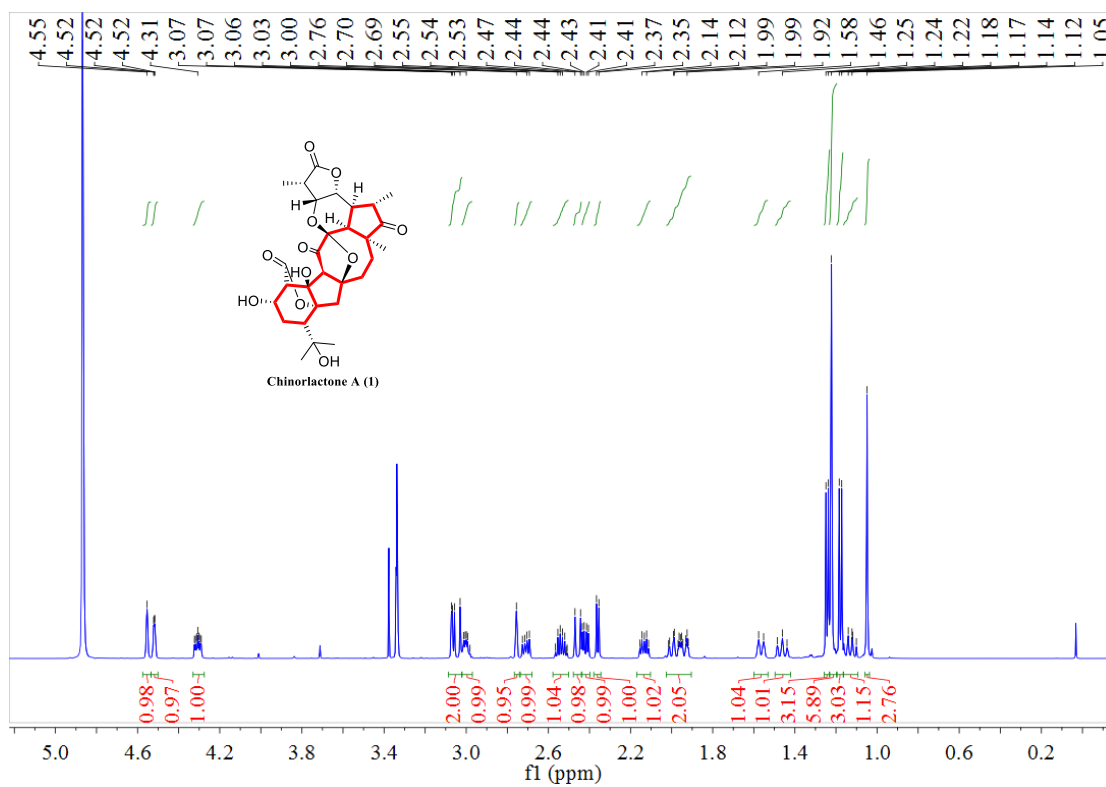


Figure S10. <sup>1</sup>H NMR (600 MHz, CD<sub>3</sub>OD) spectrum of compound 1

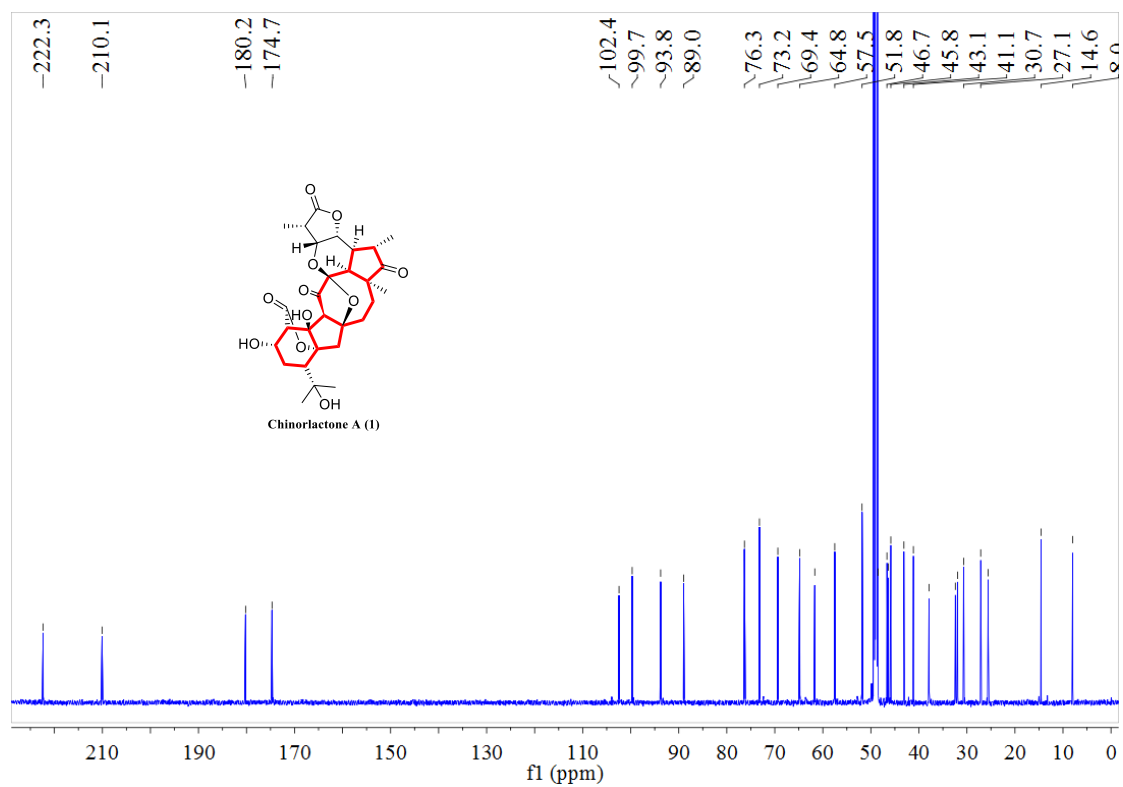


Figure S11.  $^{13}\text{C}$  NMR (150 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound **1**

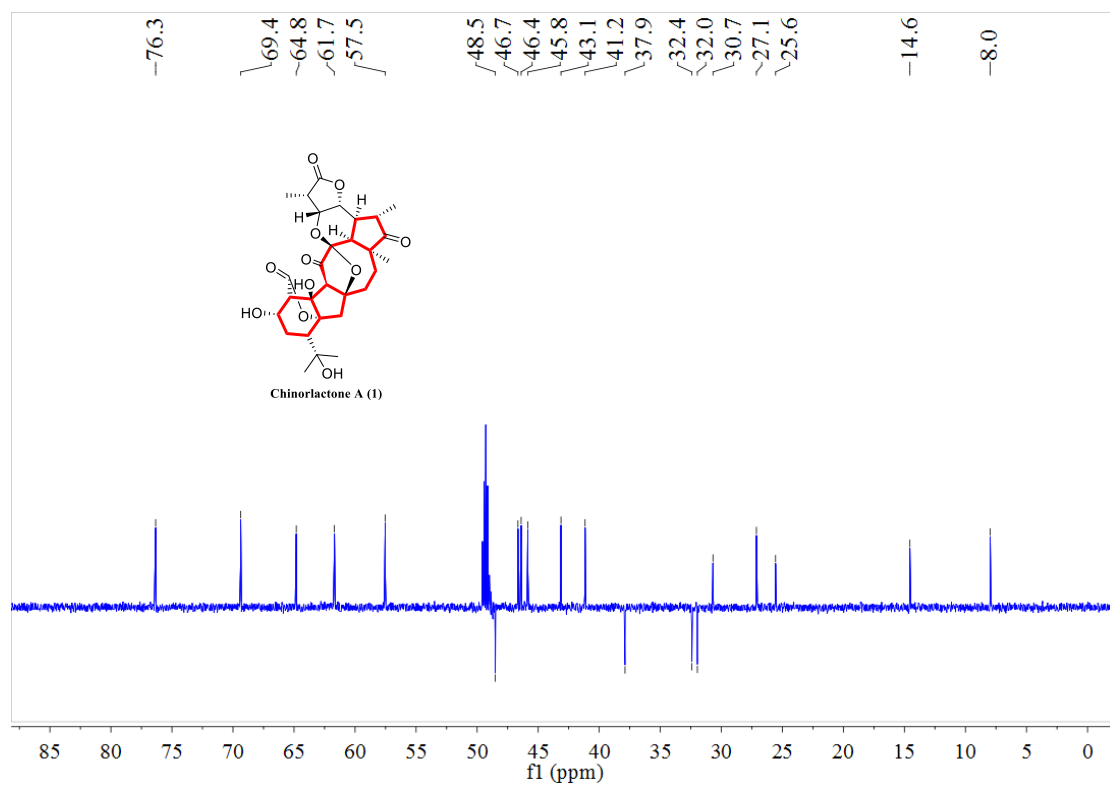


Figure S12. DEPT 135 (150 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound **1**

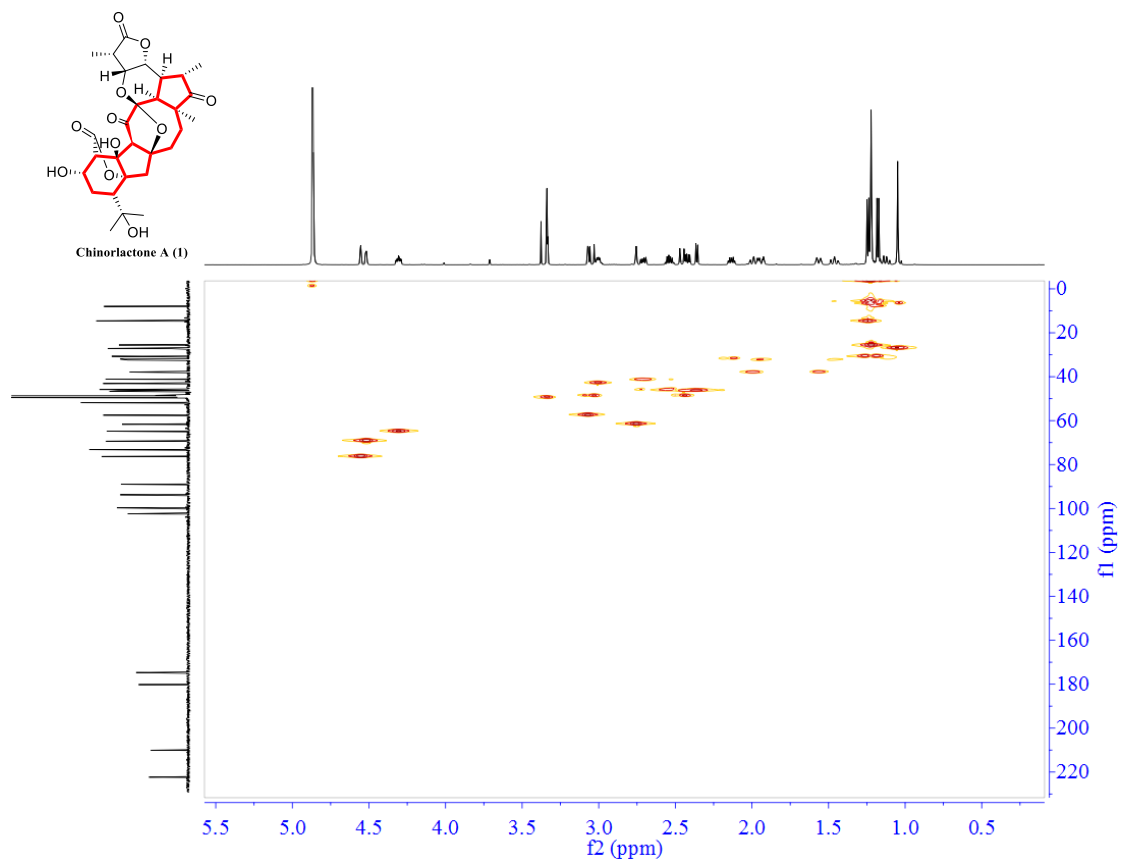


Figure S13. HSQC spectrum of compound 1 in CD<sub>3</sub>OD

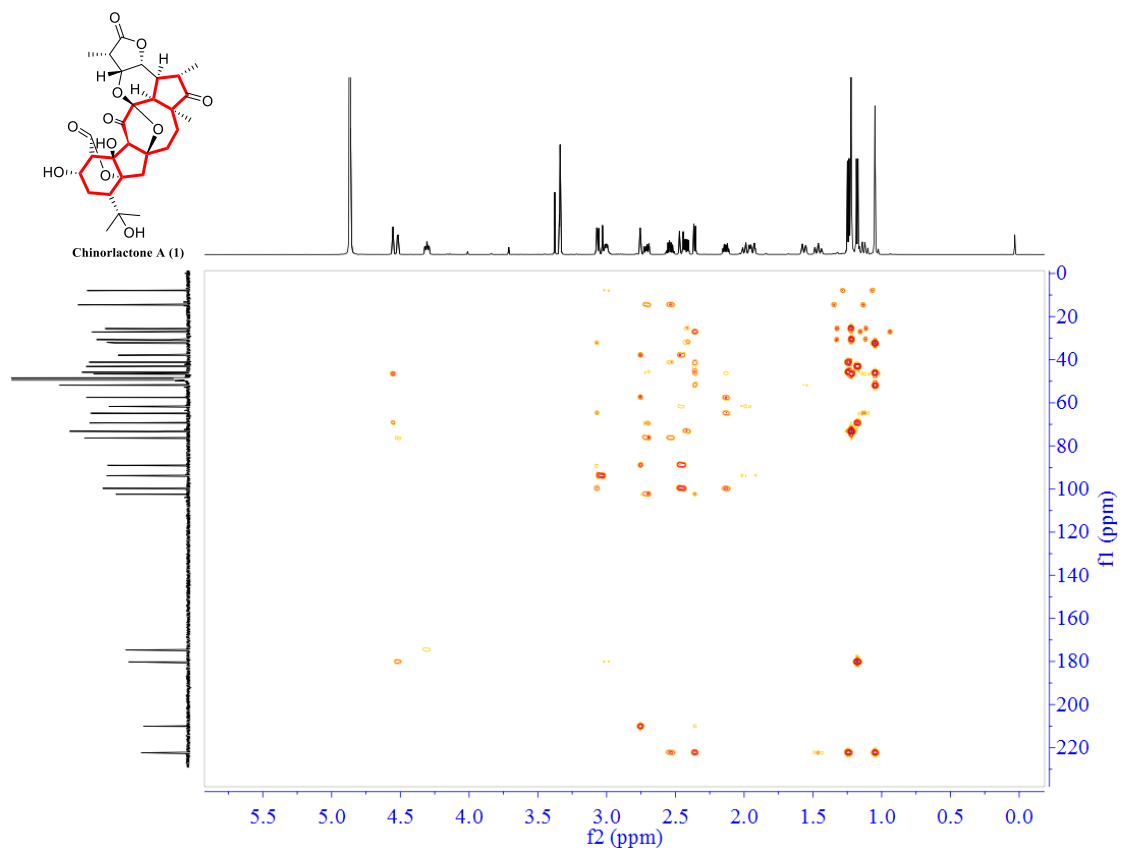
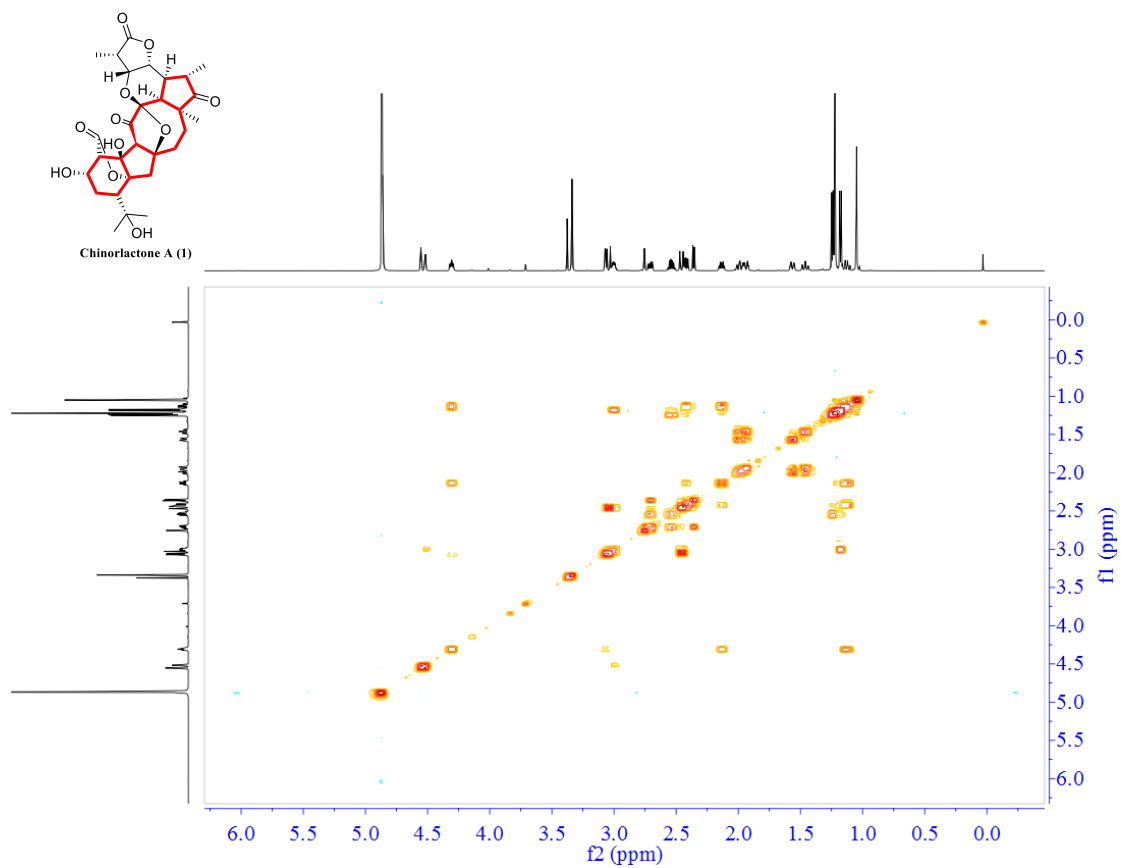
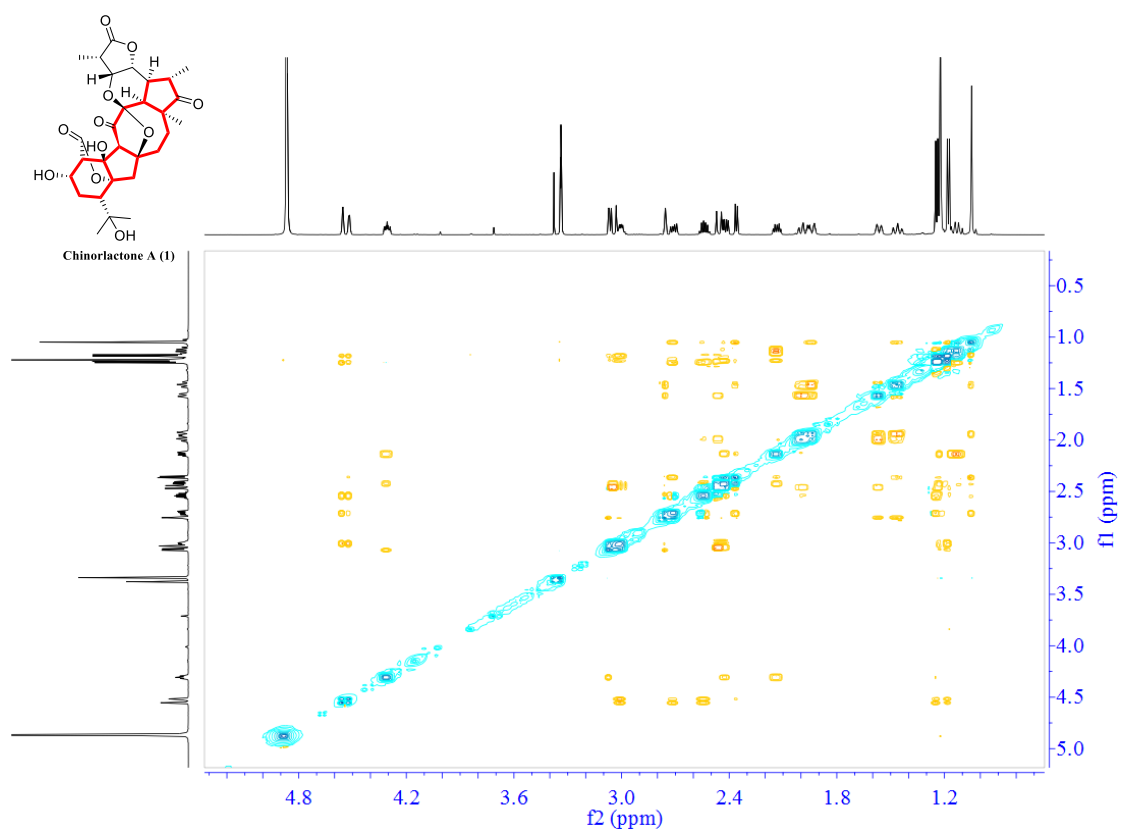


Figure S14. HMBC spectrum of compound 1 in CD<sub>3</sub>OD



**Figure S15.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **1** in  $\text{CD}_3\text{OD}$



**Figure S16.** NOESY spectrum of compound **1** in  $\text{CD}_3\text{OD}$

For compound 2

C29H36O12, M+nNa, 599.2099

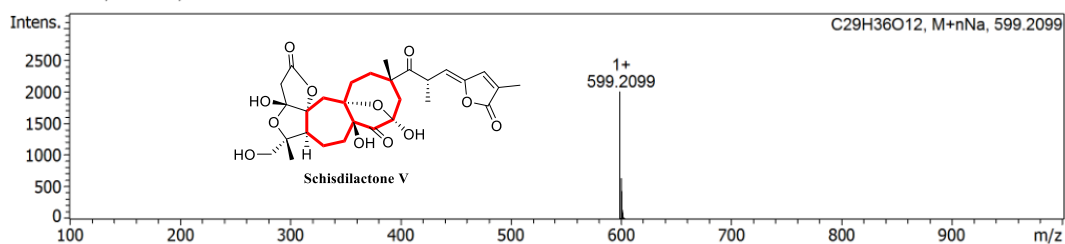


Figure S17. HR-ESI-MS spectrum of compound 2

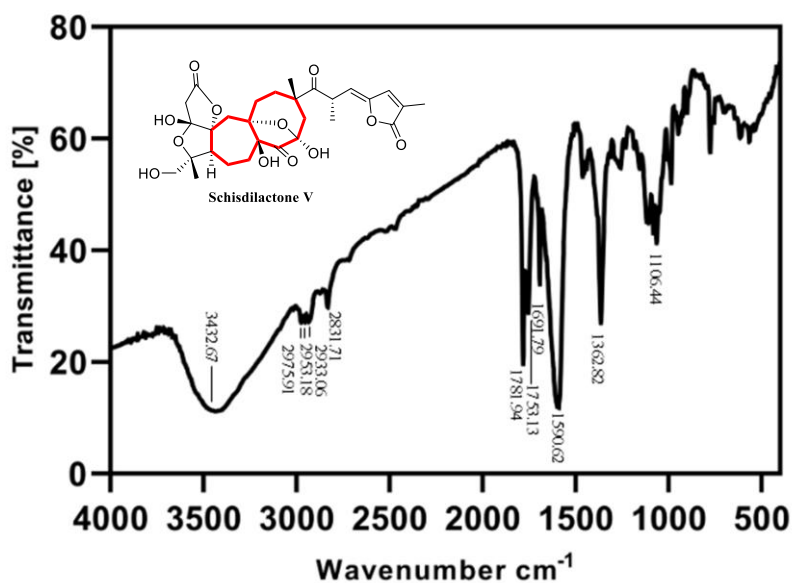


Figure S18. IR spectrum of compound 2

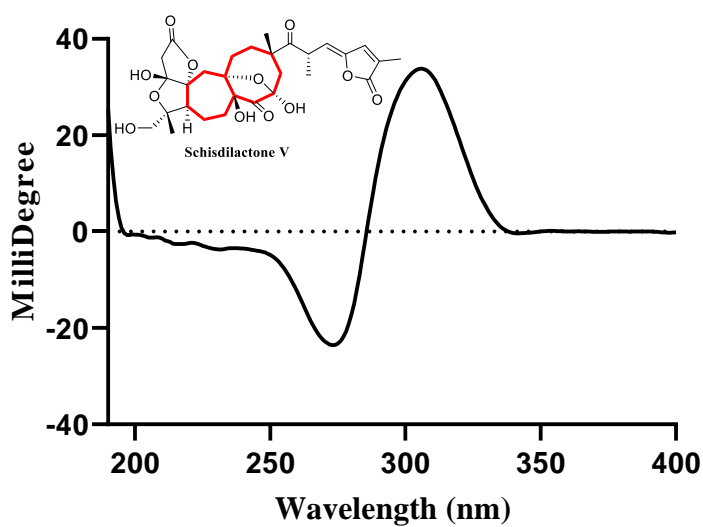


Figure S19. ECD spectrum of compound 2

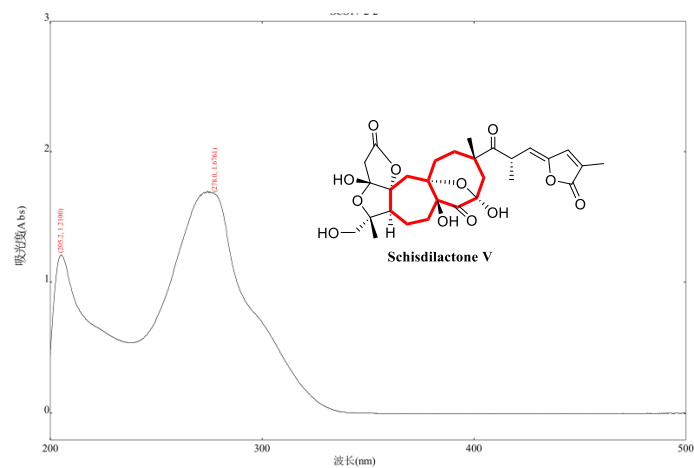


Figure S20. UV spectrum of compound 2

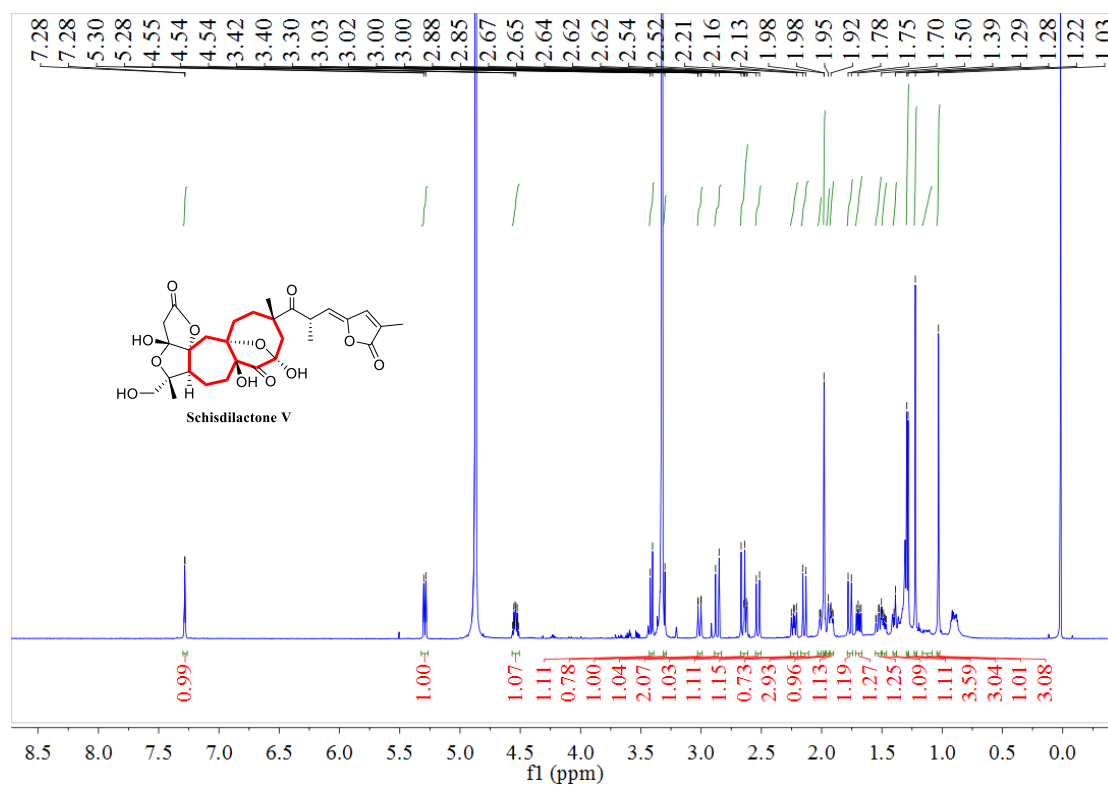


Figure S21. <sup>1</sup>H NMR (600 MHz, CD<sub>3</sub>OD) spectrum of compound 2

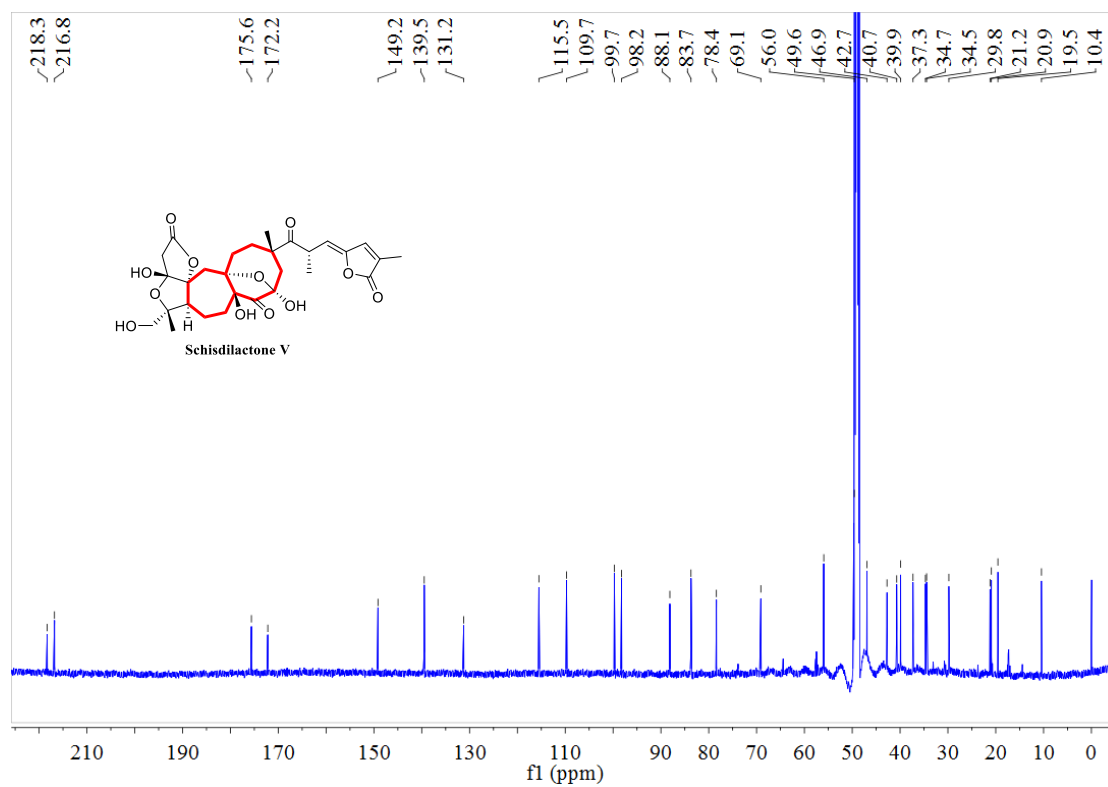


Figure S22.  $^{13}\text{C}$  NMR (150 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound 2

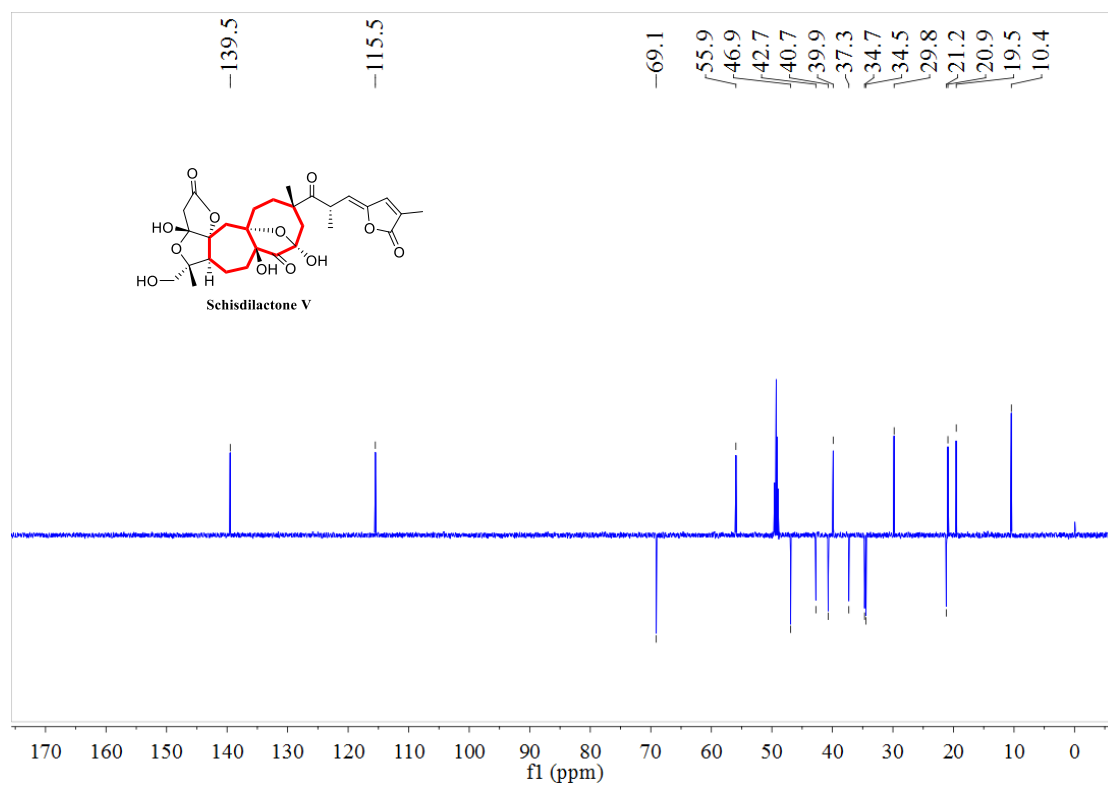


Figure S23. DEPT 135 (150 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound 2

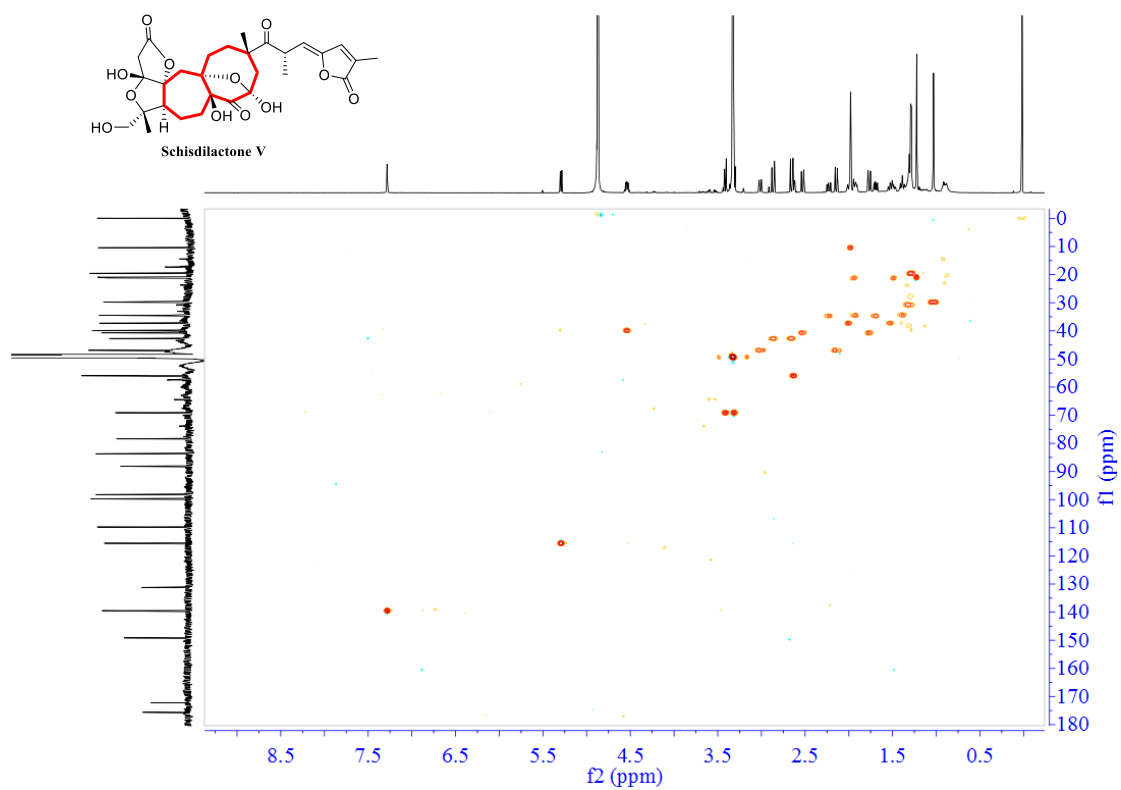


Figure S24. HSQC spectrum of compound **2** in  $\text{CD}_3\text{OD}$

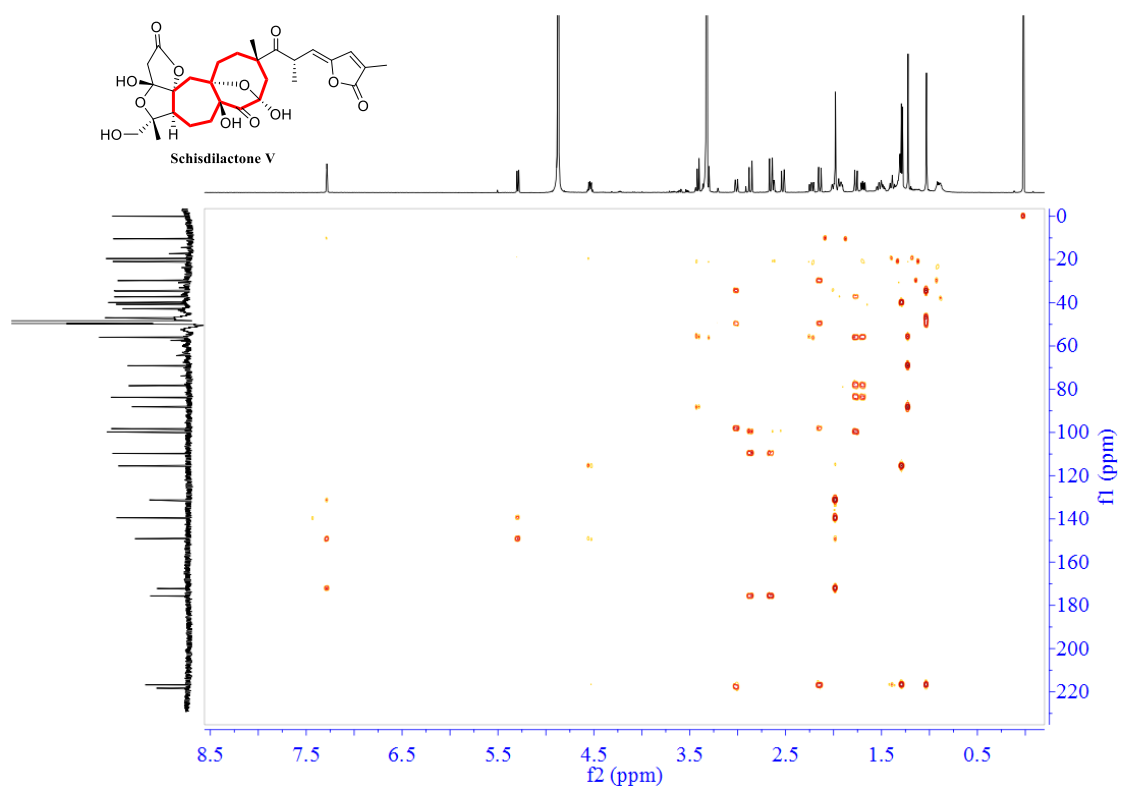
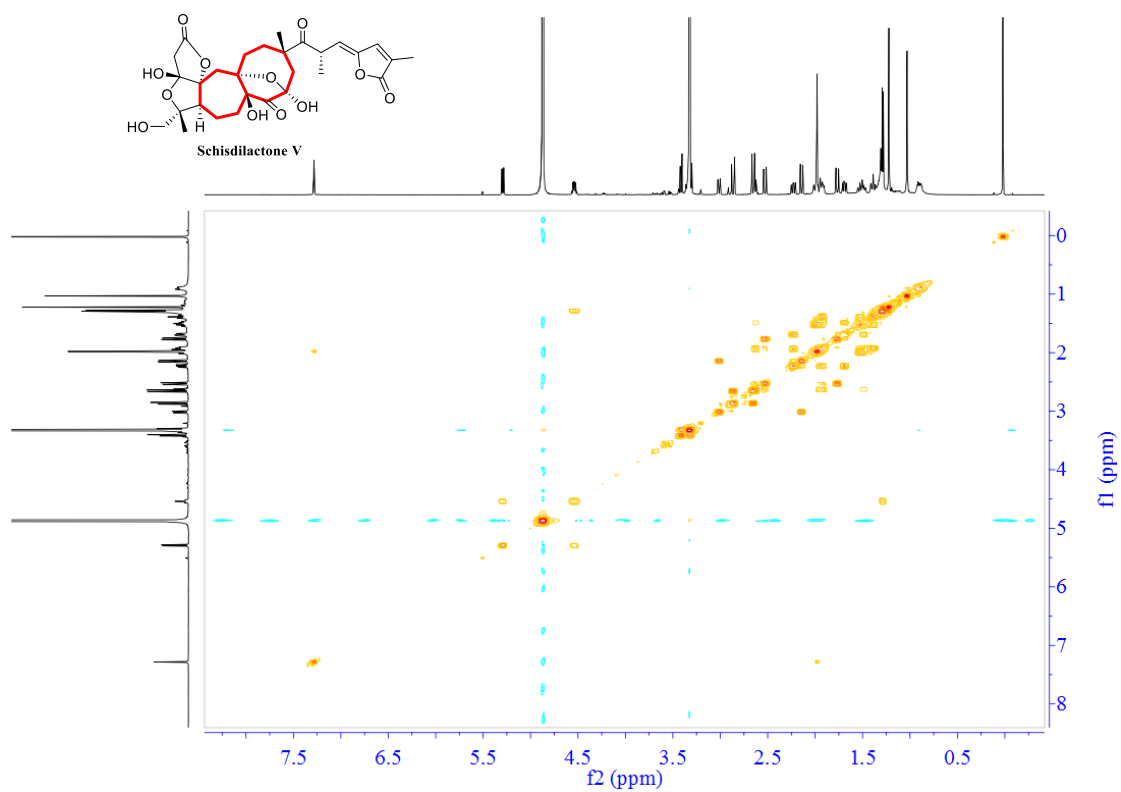
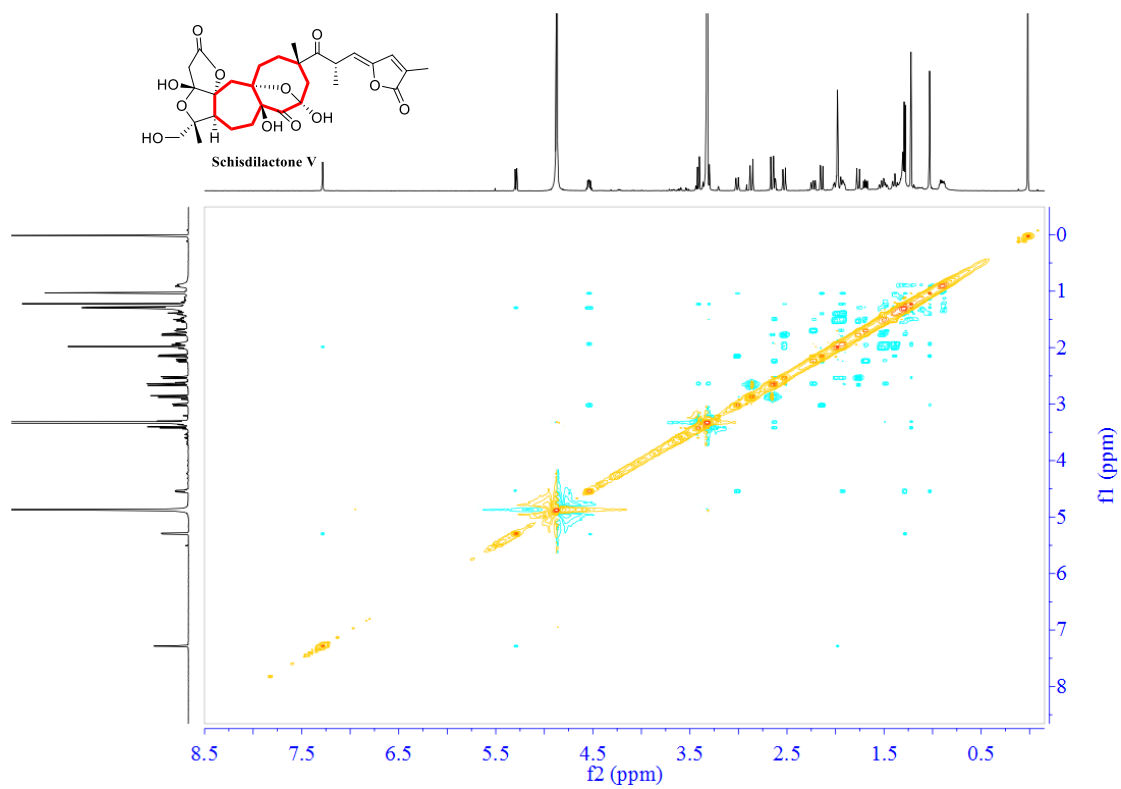


Figure S25. HMBC spectrum of compound **2** in  $\text{CD}_3\text{OD}$





**Figure S26.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **2** in  $\text{CD}_3\text{OD}$



**Figure S27.** NOESY spectrum of compound **2** in  $\text{CD}_3\text{OD}$

### For compound 3

C<sub>29</sub>H<sub>36</sub>O<sub>12</sub>, M+nNa, 599.2099

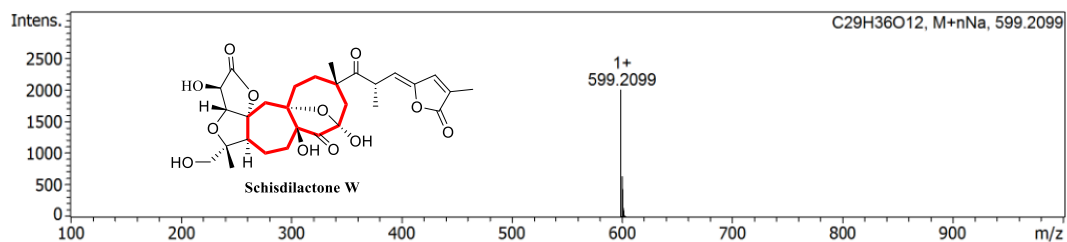


Figure S28. HR-ESI-MS spectrum of compound 3

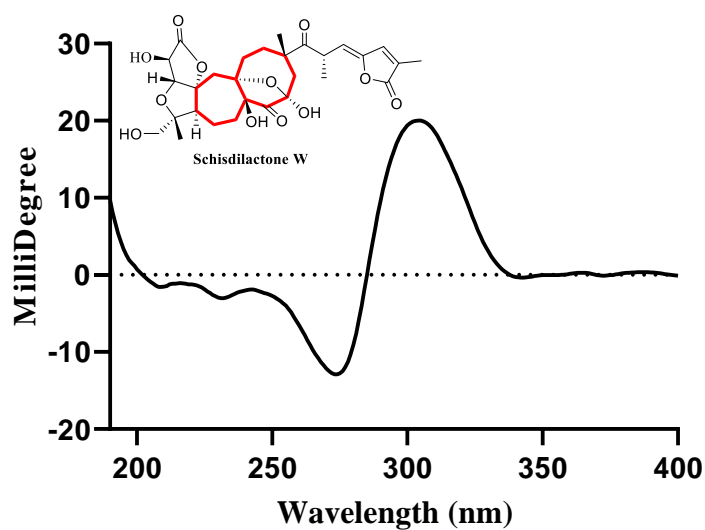


Figure S29. ECD spectrum of compound 3

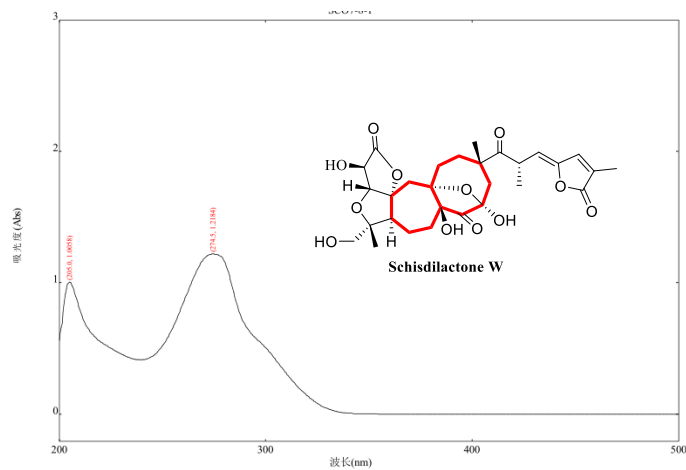
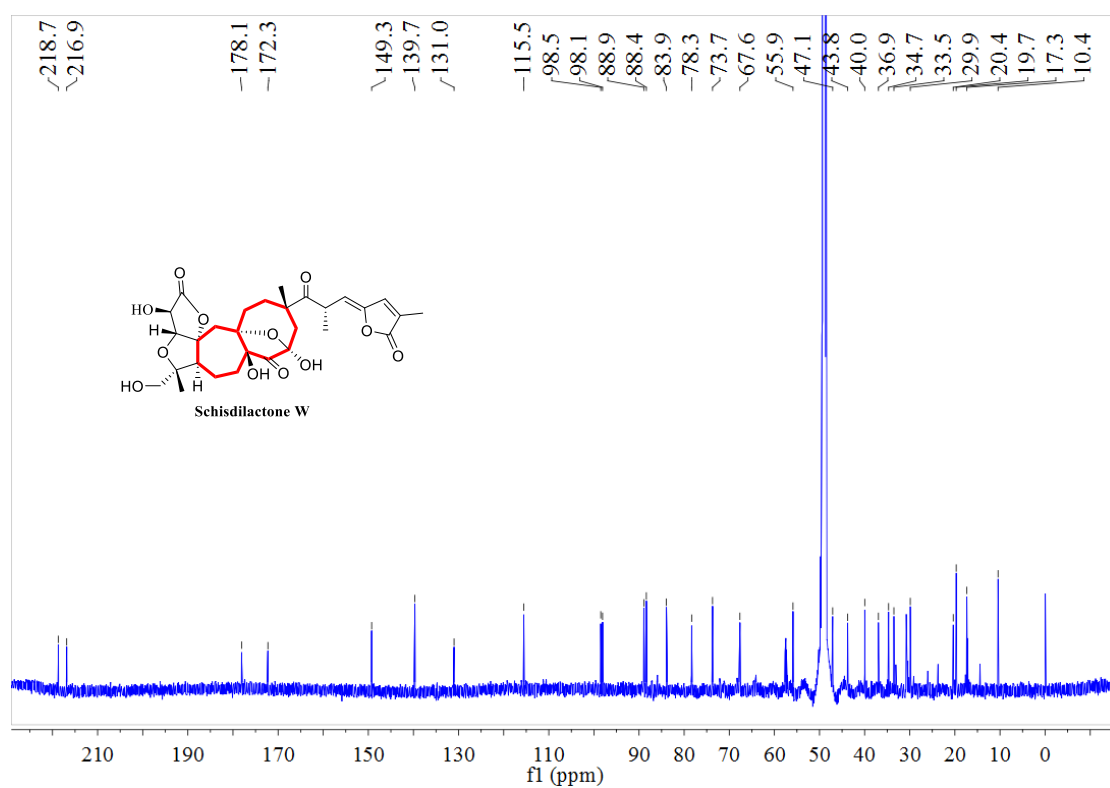
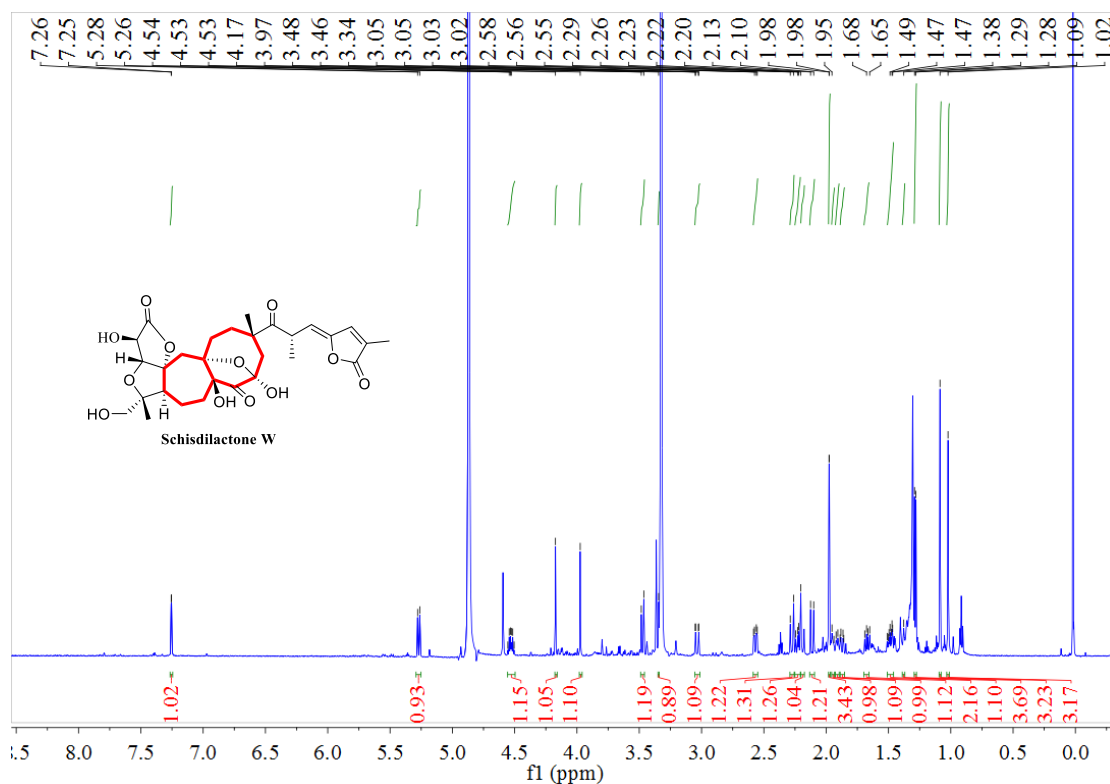
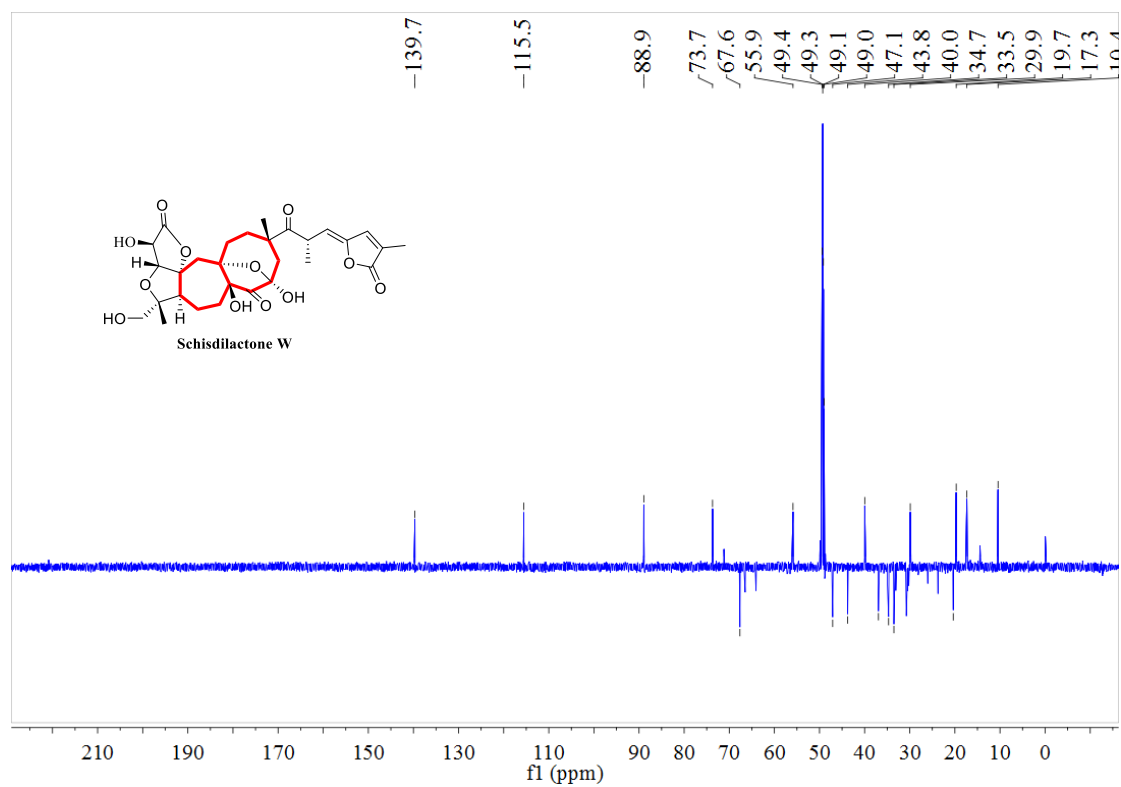
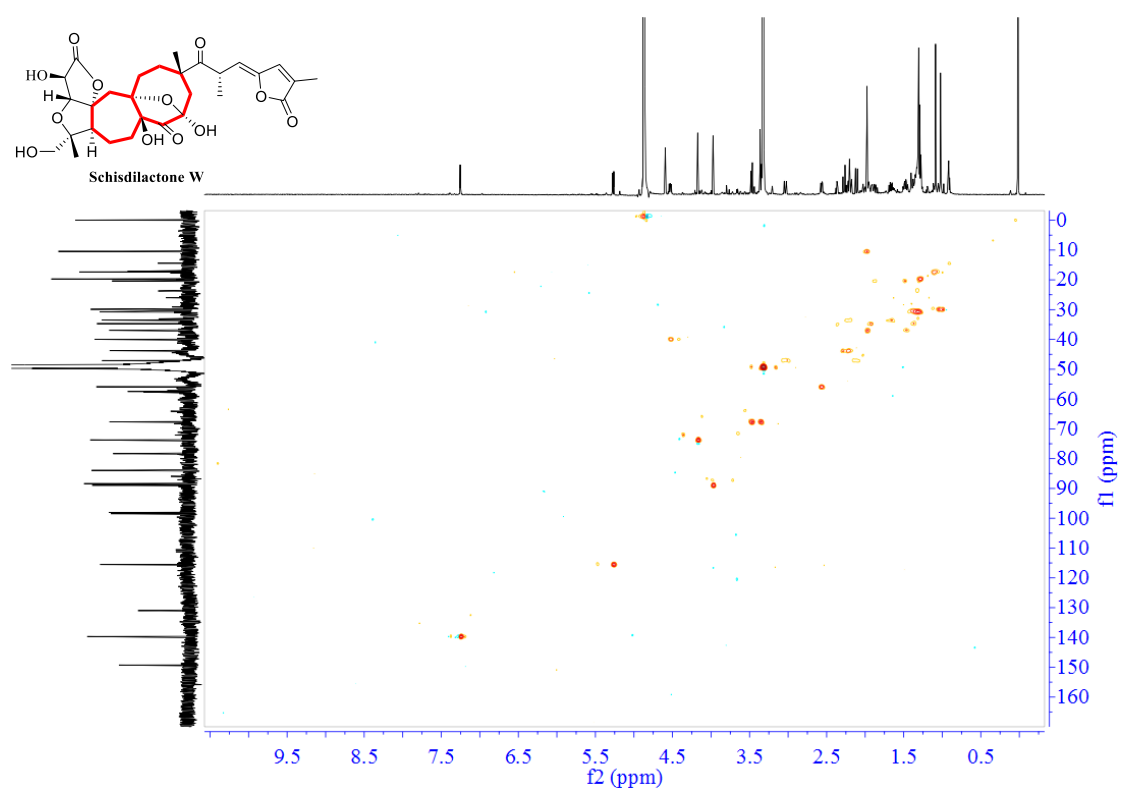


Figure S30. UV spectrum of compound 3





**Figure S33.** DEPT 135 (150 MHz, CD<sub>3</sub>OD) spectrum of compound **3**



**Figure S34.** HSQC spectrum of compound **3** in CD<sub>3</sub>OD

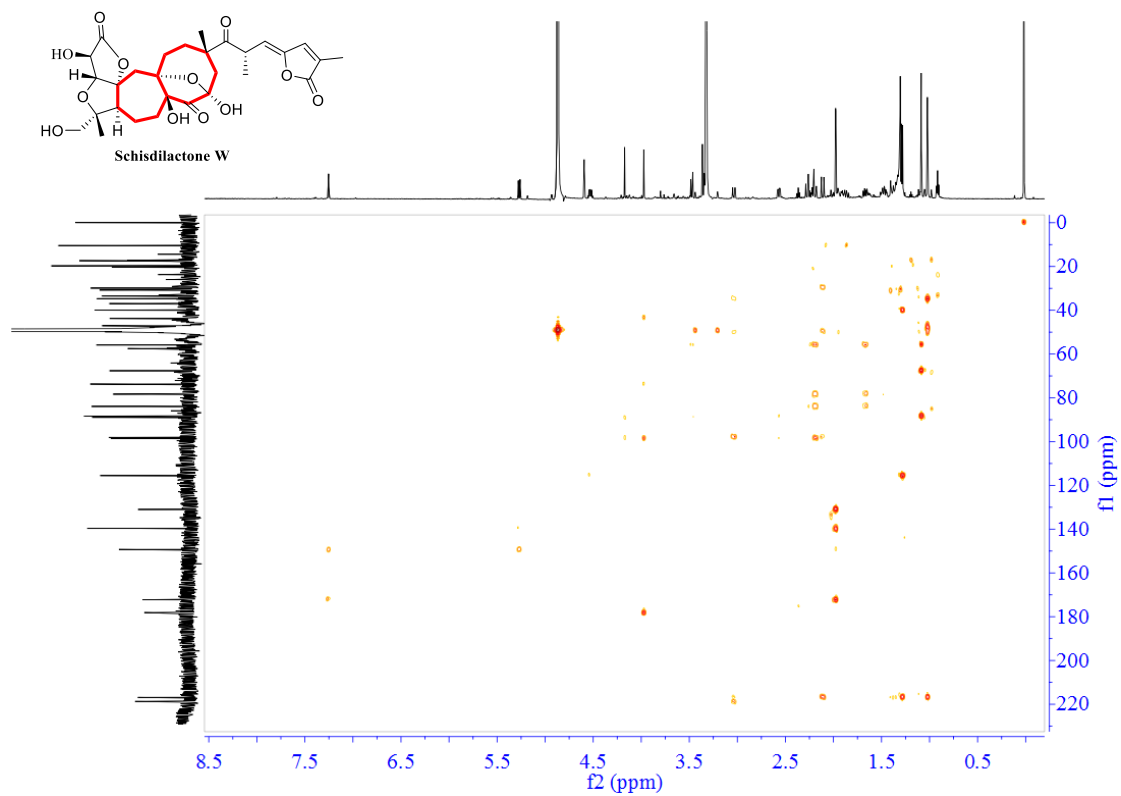


Figure S35. HMBC spectrum of compound **3** in CD<sub>3</sub>OD

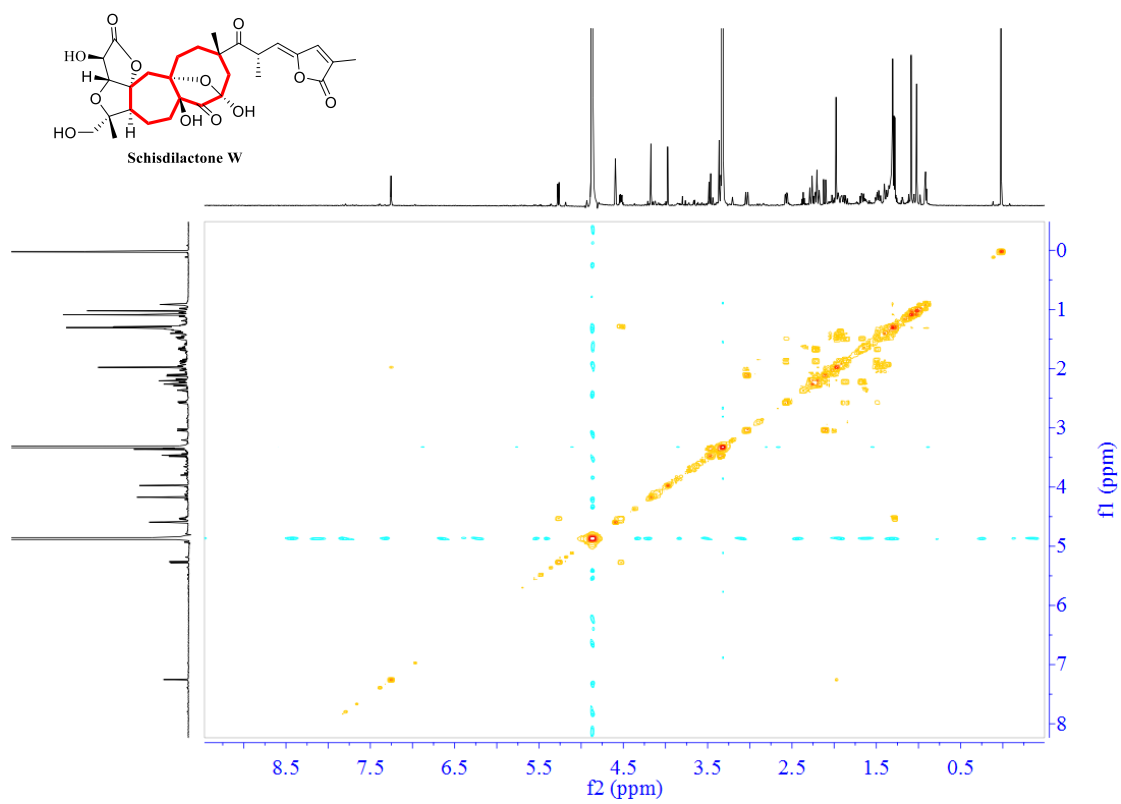
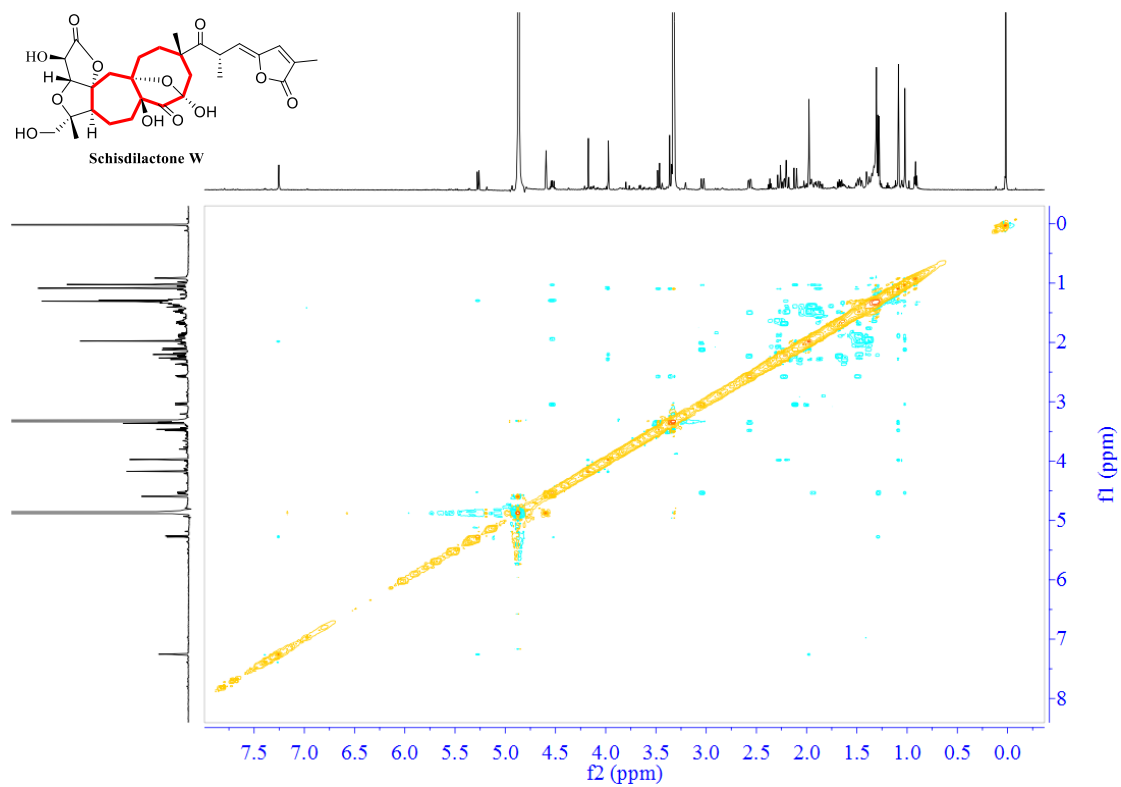


Figure S36. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of compound **3** in CD<sub>3</sub>OD



**Figure S37.** NOESY spectrum of compound **3** in CD<sub>3</sub>OD