Supporting information

Antimicrobial phenalenone derivatives from the marine-derived fungus *Coniothyrium cereale*

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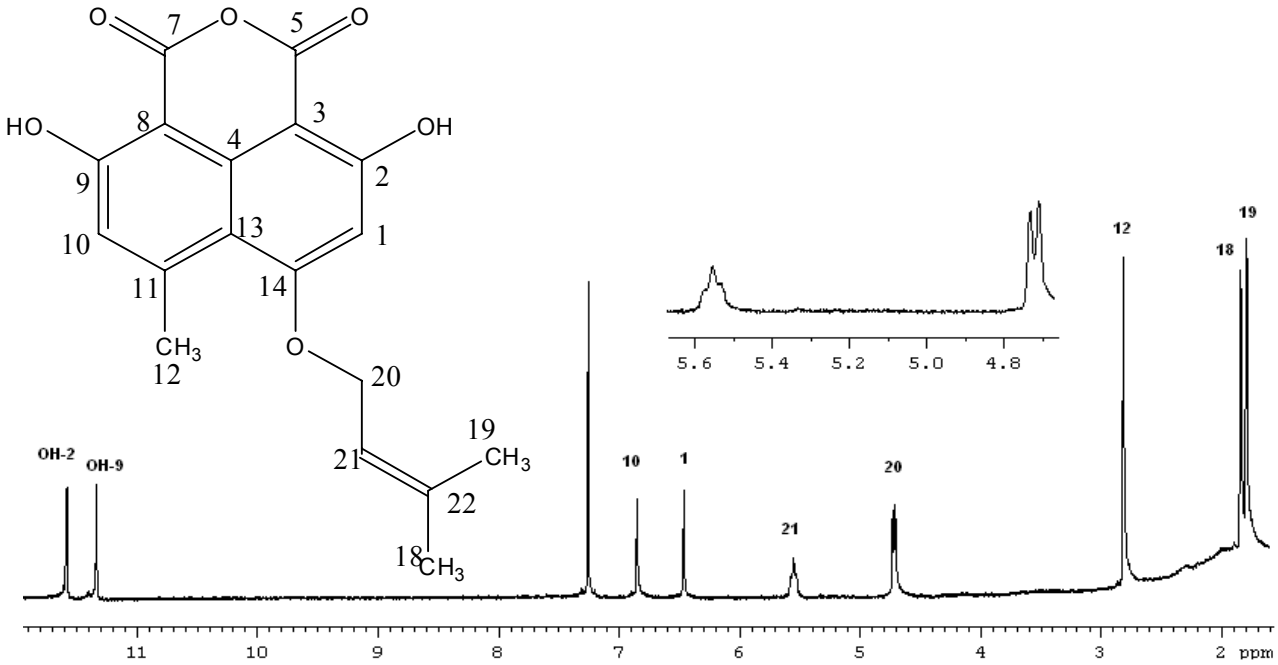
S1. NMR spectroscopic data of compound **1** in $CDCl_3$.

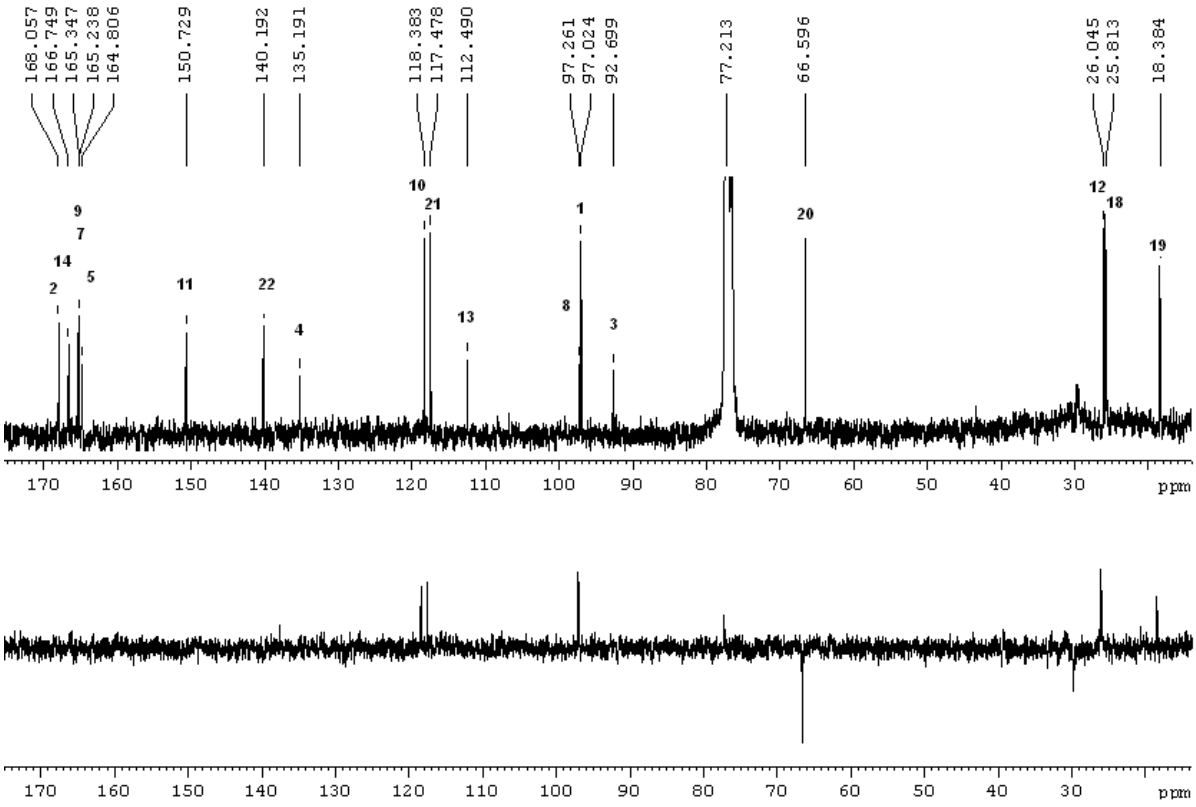
No.	$\delta^{13}C$ (ppm)	multiplicity	δ ^1H (ppm), *J* in Hz	^1H-^1H COSY	^1H- ^{13}C HMBC (H to C)
1	97.0	CH	6.46, s		2, 3, 13, 14
2	168.0	C			
3	92.6	C			
4	135.1	C			
5	164.7*	C			
6	-				
7	165.2*	C			
8	97.2	C			
9	165.3	C			
10	118.3	CH	6.84, s	12	8, 9, 12, 13
11	150.7	C			
12	26.0	CH_3	2.81, s	10	10, 11, 13
13	112.4	C			
14	166.7	C			
15	-				
16	-				
17	-				
18	25.8	CH_3	1.85, s	21	19, 21, 22
19	18.4	CH_3	1.80, s	21	18, 21, 22
20	66.6	CH_2	4.72, d, 6.6	18, 19, 21	14, 18, 19, 21
21	117.5	CH	5.55, br t, 6.6	18, 19, 20	18, 19
22	140.2	C			
OH-2			11.57, s		1, 2, 3
OH-9			11.33, s		8, 9, 10

*interchangeable

S2. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **1**.



S3. ^{13}C NMR (75 MHz, $CDCl_3$, upper line) and DEPT 135 (lower line) spectra of compound **1**.

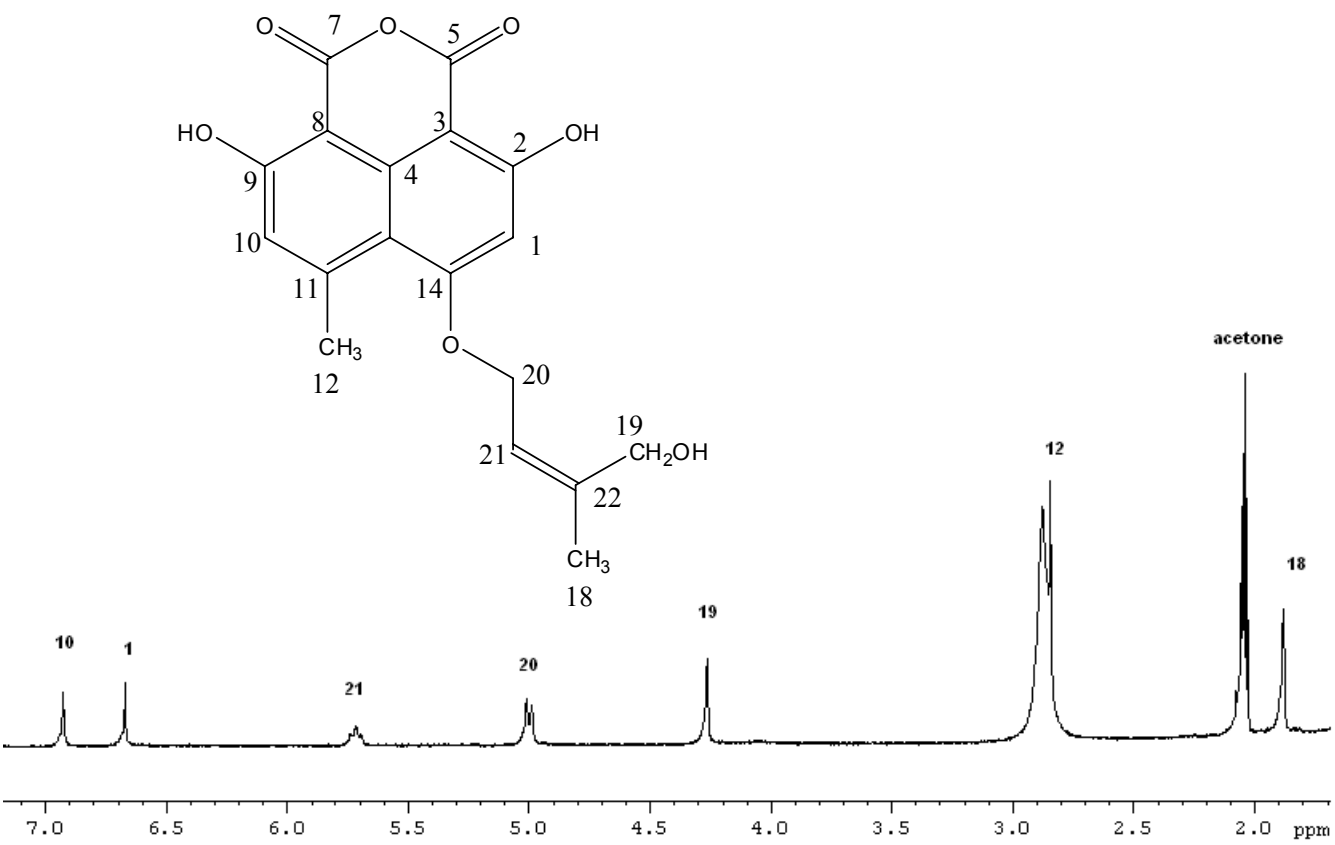


S4. NMR spectroscopic data of compound **2** in acetone-d_6.

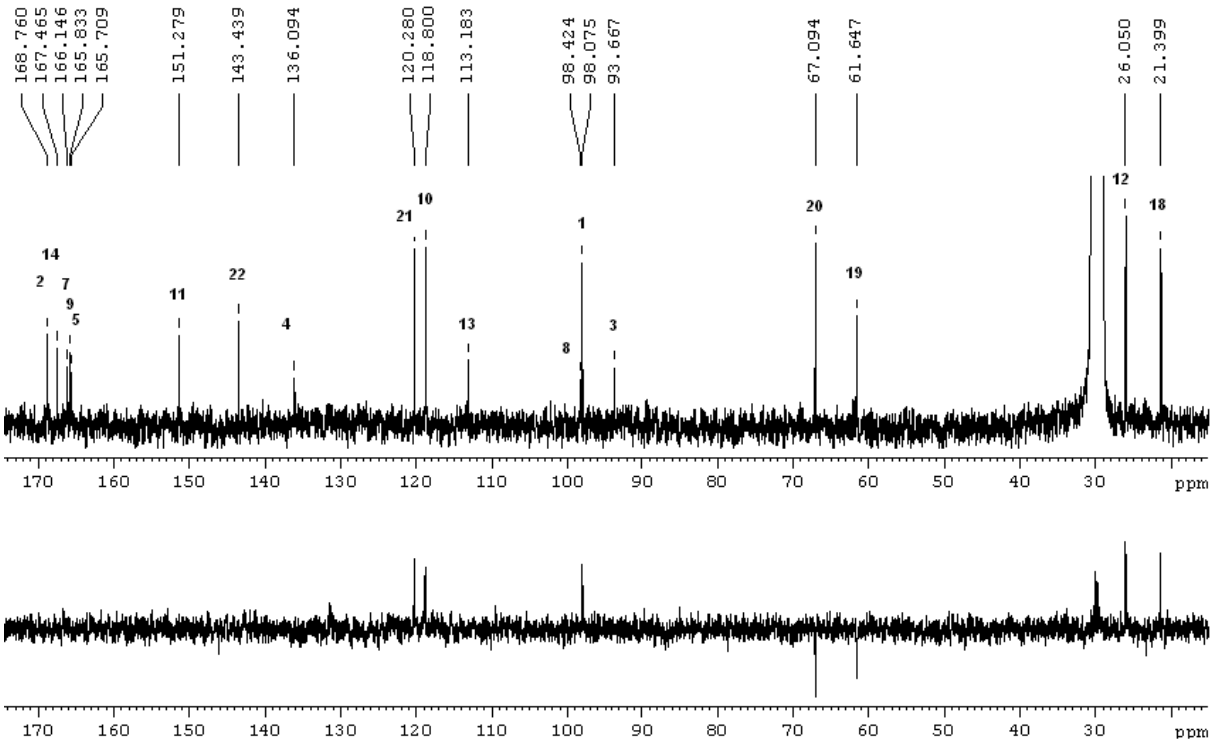
No.	$\delta^{13}C$ (ppm)[a]	multiplicity	δ ^1H (ppm), J in Hz	^1H-^1H COSY	^1H- ^{13}C HMBC (H to C)
1	98.1	CH	6.67, s		2 (w)
2	168.7	C			
3	93.7	C			
4	136.1	C			
5	165.7*	C			
6	-				
7	166.1*	C			
8	98.4	C			
9	165.8	C			
10	118.8	CH	6.93, s		8, 9, 12, 13
11	151.3	C			
12	26.0	CH_3	2.84, s		10, 11, 13
13	113.2	C			
14	167.5	C			
15	-				
16	-				
17	-				
18	21.4	CH_3	1.87, s	21	19, 21, 22
19	61.6	CH_2	4.26, s		18, 21, 22
20	67.1	CH_2	5.00, d, 6.6	18, 21	14 (w), 21
21	120.3	CH	5.71, br t, 6.6	18, 20	
22	143.4	C			

w: weak signal; *interchangeable

S5.[1]H NMR spectrum (300 MHz, acetone-d_6) of compound **2**. **(*Z*)-coniosclerodinol**



S6.[13]C NMR (75 MHz, acetone-d_6, upper line) and DEPT 135 (lower line) spectra of compound **2**.

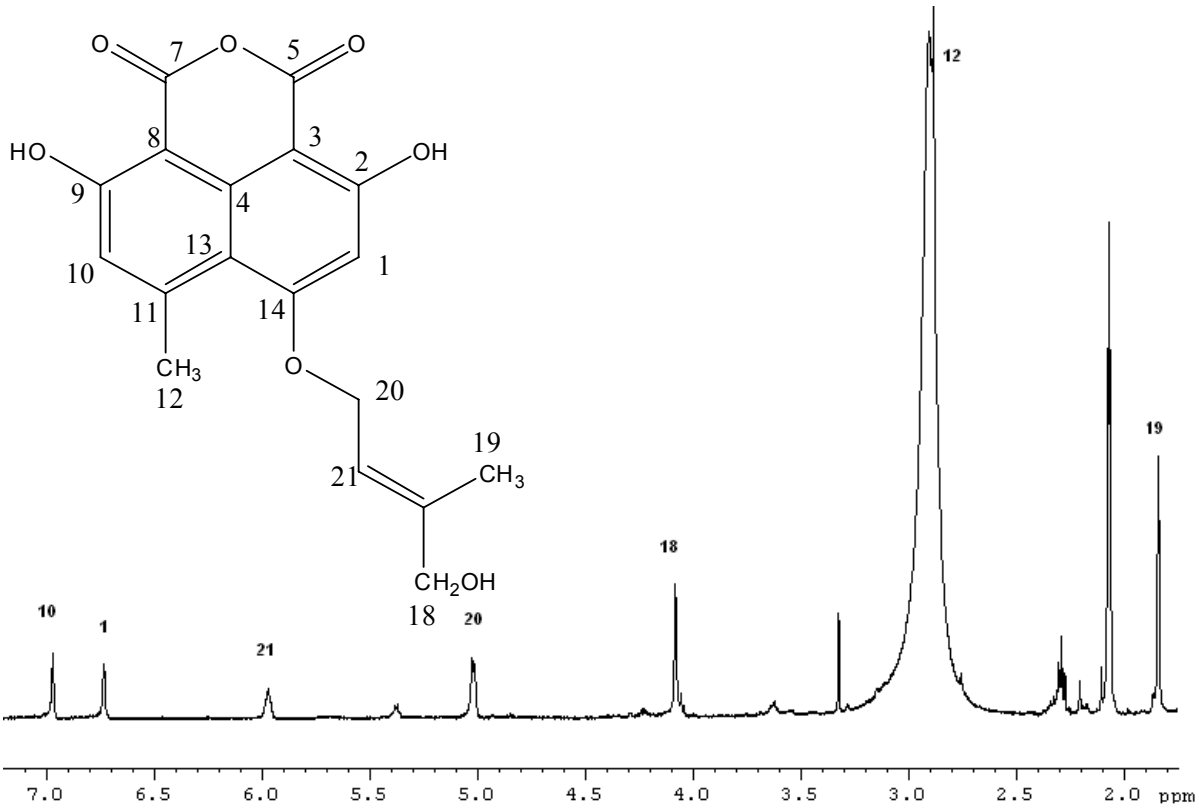


S7. NMR spectroscopic data of compound **3** in acetone-d_6.

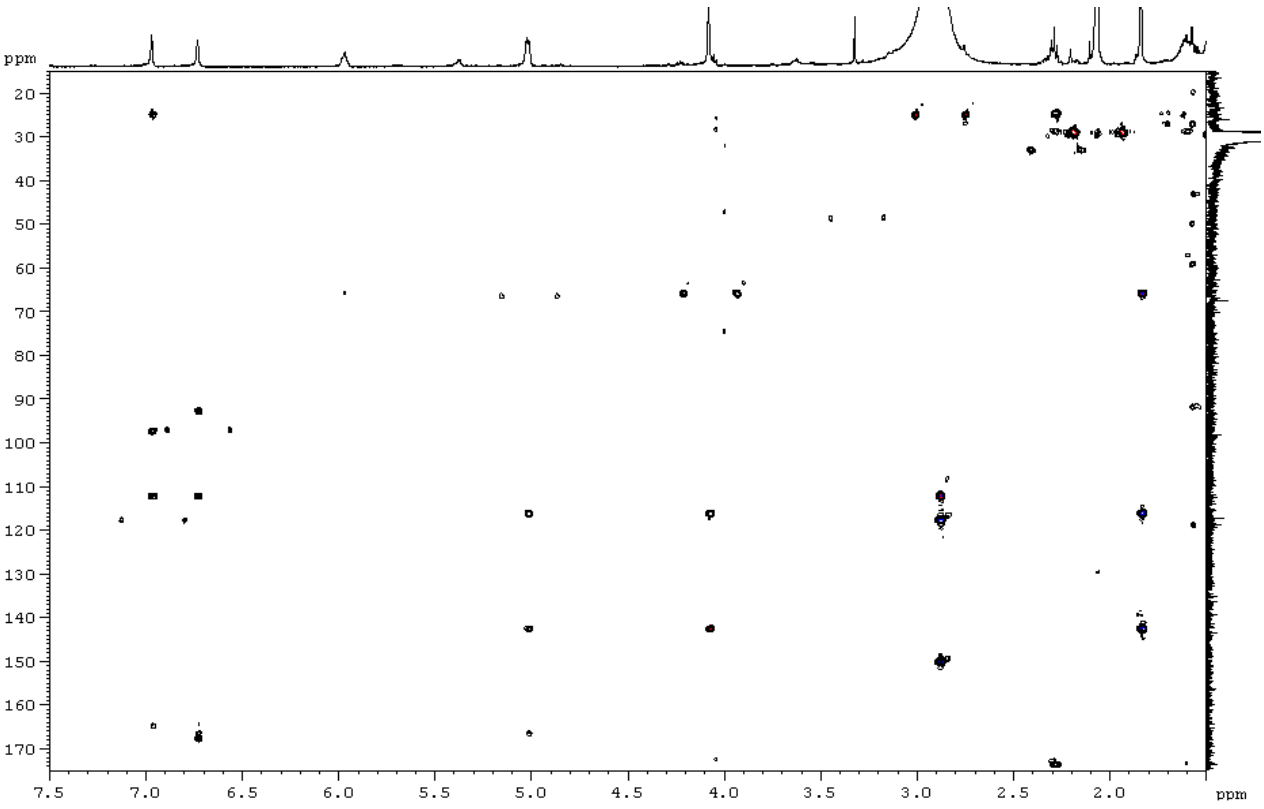
No.	$\delta^{13}C$ (ppm)[a]	multiplicity	δ ^1H (ppm), J in Hz	^1H-^1H COSY	^1H- ^{13}C HMBC (H to C)
1	98.1	CH	6.70, s		2, 3, 5, 13, 14
2	168.8	C			
3	93.9	C			
4	136.1	C			
5	165.6	C			
6	-				
7	n.d.[b]	C			
8	98.6	C			
9	165.9	C			
10	118.8	CH	6.94, s	12	8, 9, 12, 13
11	151.3	C			
12	26.1	CH_3	2.86, s	10	10, 11, 13
13	113.4	C			
14	167.7	C			
15	-				
16	-				
17	-				
18	66.8	CH_2	4.05, s	18, 20, 21	18, 21, 22
19	14.3	CH_3	1.81, s	19, 20, 21	21, 22
20	67.5	CH_2	4.99, d, 6.3	18, 19, 21	14, 21, 22
21	117.2	CH	5.94, br t, 6.3	18, 19, 20	18, 20
22	143.5	C			

[a]partly determined from ^1H-^{13}C HMBC cross peak correlations (500 MHz). [b]not detected

S8. ^{1}H NMR spectrum (300 MHz, acetone-d_6) of compound **3**.



S9.^{1}H ^{13}C HMBC spectrum (500 MHz, acetone-d_6) of compound **3**.

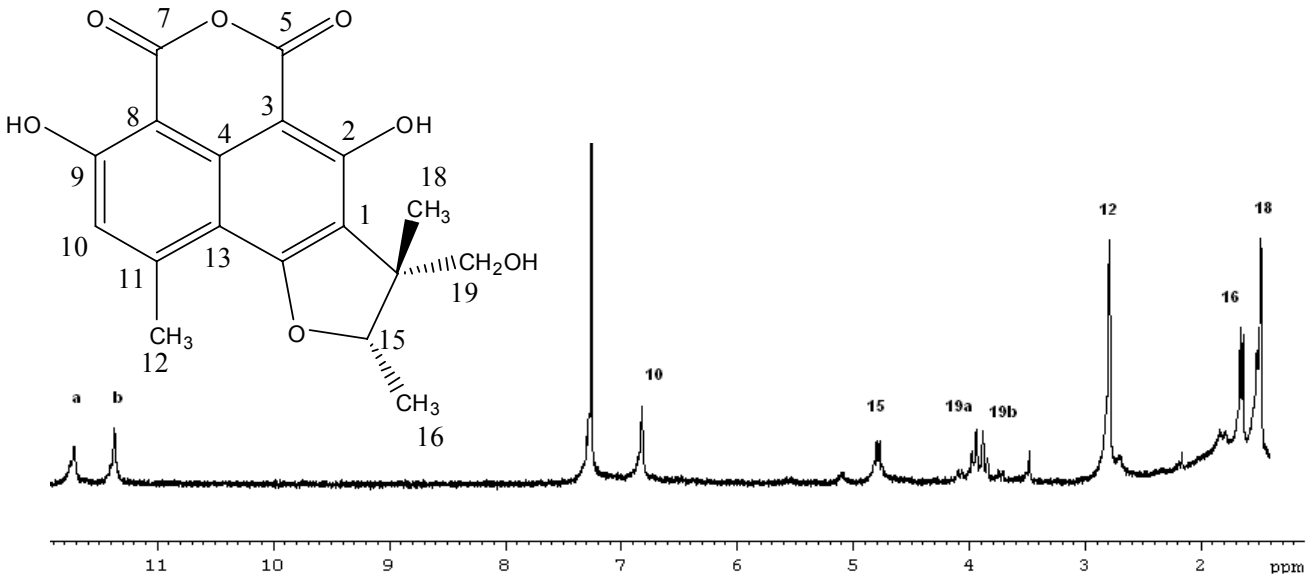


S10. NMR spectroscopic data of compound **4** in acetone-d_6.

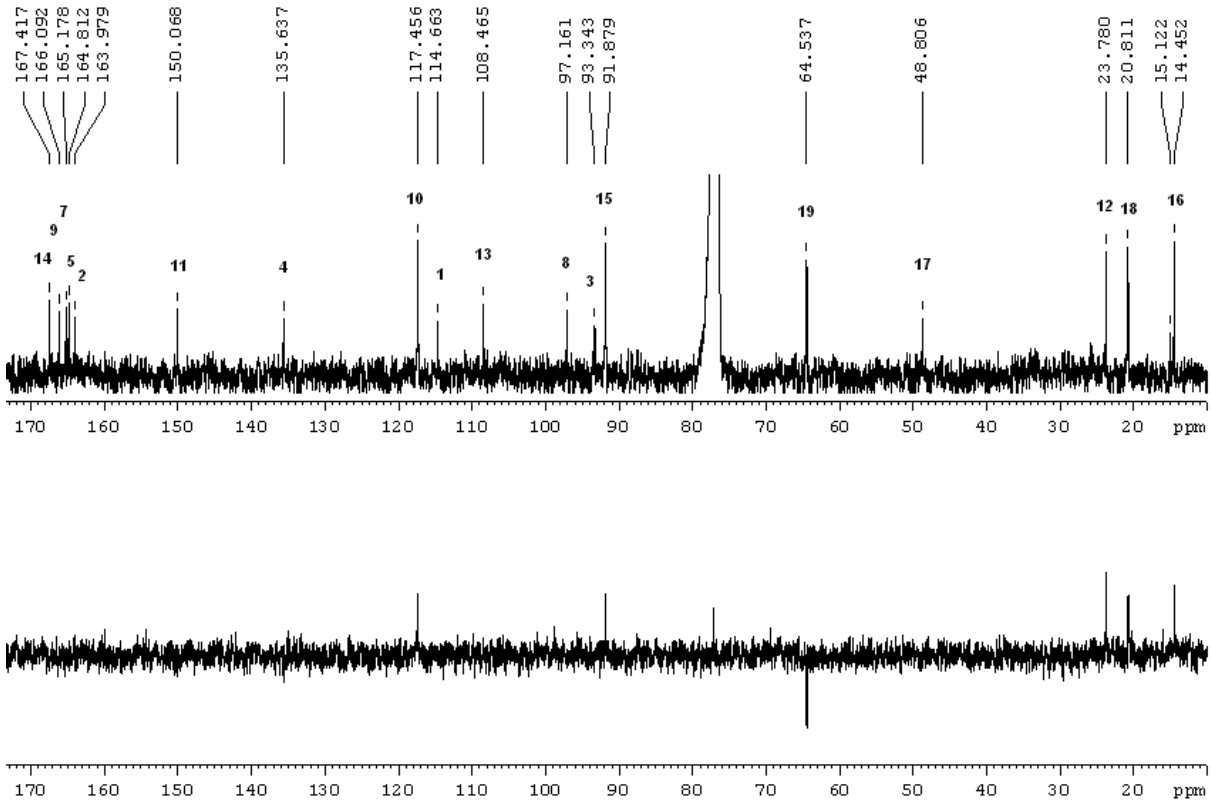
No.	$\delta^{13}C$ (ppm)	mulitiplicity	δ ^1H (ppm), J in Hz	^1H-^1H COSY	^1H- ^{13}C HMBC (H to C)	2D-NOESY
1	114.7	C				
2	164.0	C				
3	93.3	C				
4	135.6	C				
5	164.8*	C				
6	-					
7	165.2*	C				
8	97.2	C				
9	166.1	C				
10	117.5	CH	6.82, s	12	8, 9, 12, 13	12
11	150.1	C				
12	23.8	CH_3	2.80, s	10	10, 11, 13	10
13	108.5	C				
14	167.4	C				
15	91.9	CH	4.77, q, 6.6	16	17, 18, 19	16, 18
16	14.5	CH_3	1.65, d, 6.6	15	15, 17	15
17	48.8	C				
18	20.8	CH_3	1.49, s		1, 15, 17, 19	15
19	64.5	CH_2	a: 3.96, d, 11.7	19b	1, 15, 17, 18	19b
			b: 3.86, d, 11.7	19a	1, 15, 17, 18	19a
OH-2			11.72, s			
OH-9			11.37, s			

*interchangeable

S11.[1]H NMR spectrum (300 MHz, $CDCl_3$) of compound **4**.



S12.[13]C NMR (75 MHz, $CDCl_3$, upper line) and DEPT 135 (lower line) spectra of compound **4**.

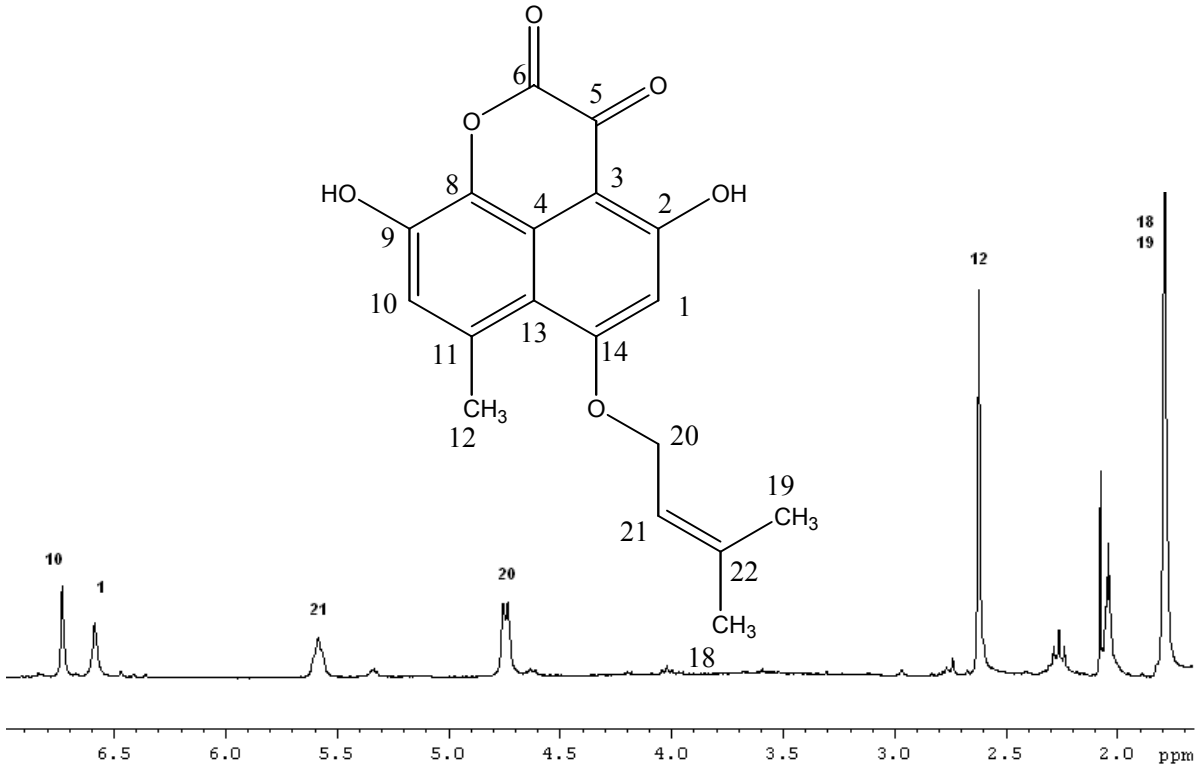


S13. NMR spectroscopic data of compound **5** in acetone-d_6.

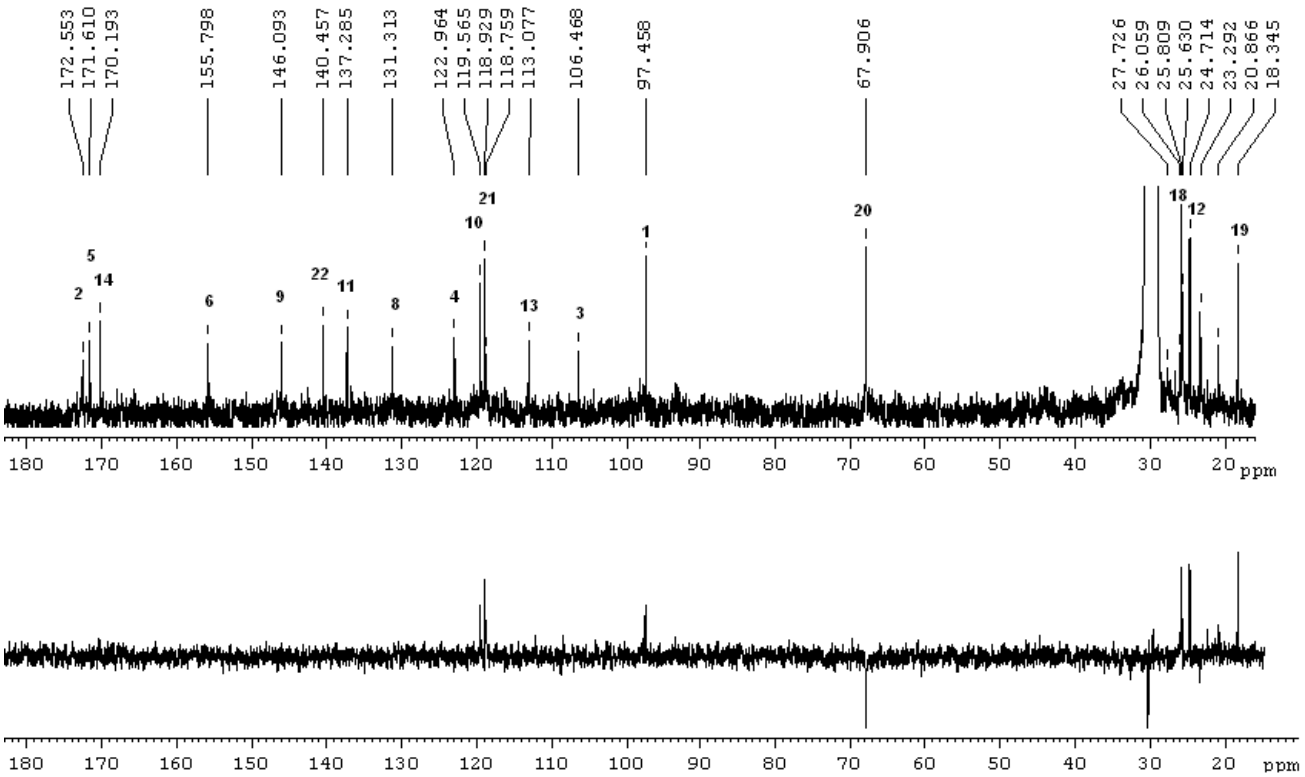
No.	δ^{13}C (ppm)	multiplicity[a]	δ ^{1}H (ppm), *J* in Hz	^{1}H-^{1}H COSY	^{1}H- ^{13}C HMBC (H to C)
1	97.5	CH	6.56, s		13
2	171.6*	C			
3	106.5	C			
4	122.9	C			
5	172.6*	C			
6	155.8	C			
7	-				
8	131.3	C			
9	146.1	C			
10	119.6	CH	6.93, s		
11	137.3	C			
12	24.7	CH_3	2.70, s		10, 11, 13
13	113.1	C			
14	170.2*	C			
15	-				
16	-				
17	-				
18	25.8	CH_3	1.83, s	20, 21	19, 21, 22
19	18.3	CH_3	1.83, s	20, 21	18, 21, 22
20	67.9	CH_2	4.91, d, 6.6	18, 19, 21	18, 22
21	118.9	CH	5.66, br t, 6.6	18, 19, 20	
22	140.5	C			

*interchangeable

S14.[1]H NMR spectrum (300 MHz, acetone-d_6) of compound **5**.



S15. [13]C NMR (75 MHz, acetone-*d6,* upper line) and DEPT 135 (lower line) spectra of compound **5**.

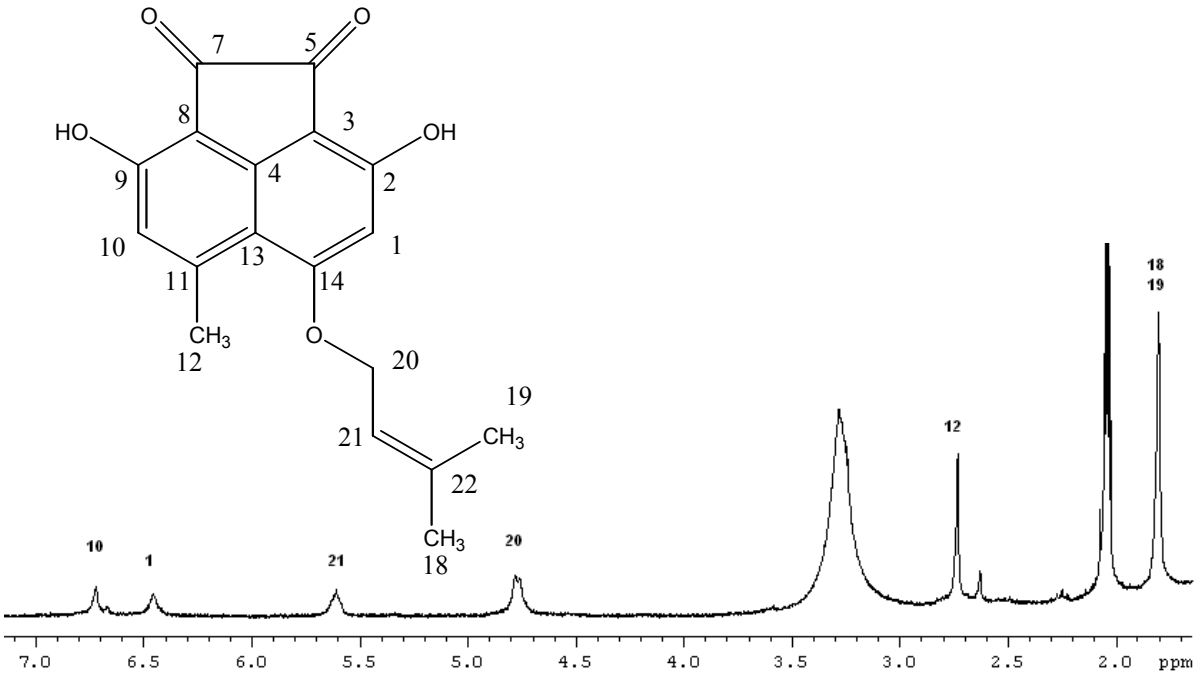


S16. NMR spectroscopic data of compound **6** in acetone-d_6.

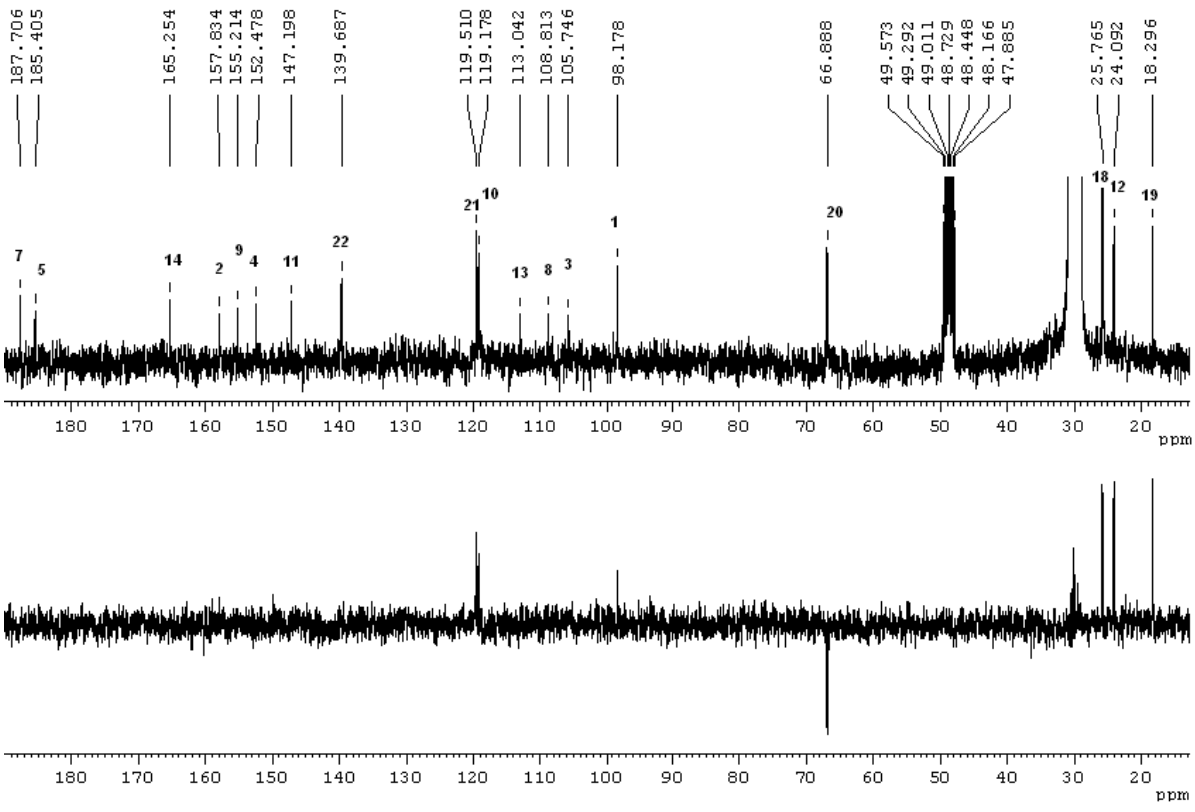
No.	$\delta^{13}C$ (ppm)	multiplicity[a]	δ ^1H (ppm), *J* in Hz	^1H-^1H COSY	^1H- ^{13}C HMBC (H to C)
1	98.2	CH	6.46, s		2, 3, 13
2	157.8	C			
3	105.7	C			
4	152.5	C			
5	185.4*	C			
6	-				
7	187.7*	C			
8	108.8	C			
9	155.2	C			
10	119.2	CH	6.72, s		8, 12, 13
11	147.2	C			
12	24.1	CH_3	2.73, s		10, 11, 13
13	113.0	C			
14	165.3	C			
15					
16					
17					
18	25.8	CH_3	1.80, s	19, 20, 21	19, 21, 22
19	18.3	CH_3	1.80, s	18, 20, 21	18, 21, 22
20	66.9	CH_2	4.77, d, 6.3	18, 19, 21	14, 21, 22
21	119.5	CH	5.61, br t, 6.3	18, 19, 20	18, 19
22	139.7	C			

*interchangeable

S17.[1]H NMR spectrum (300 MHz, acetone-d_6) of compound **6**.



S18. [13]C NMR (75 MHz, acetone-*d6,* upper line) and DEPT 135 (lower line) spectra of compound **6**.

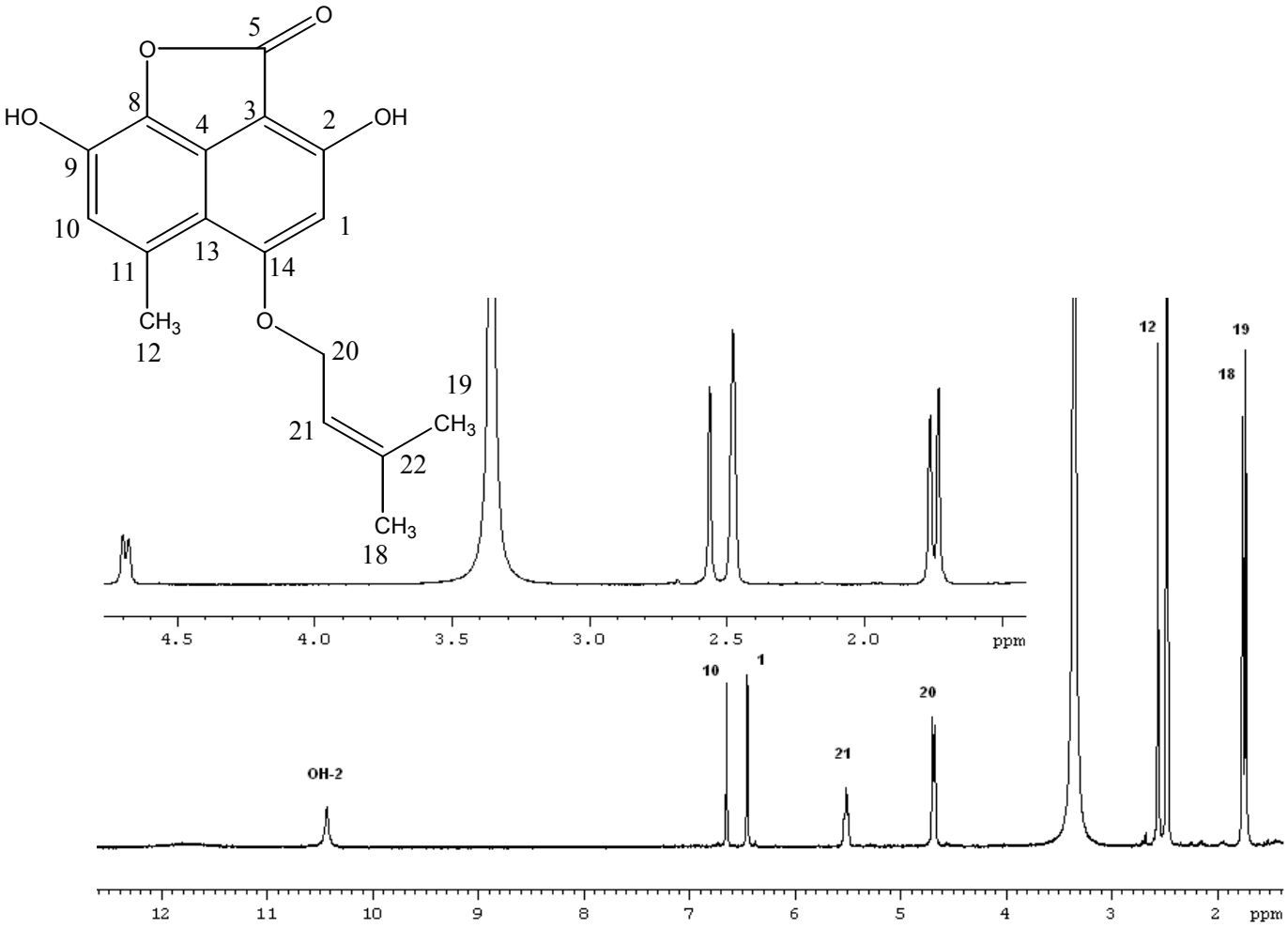


S19. NMR spectroscopic data of compound **7** in dmso-d_6.

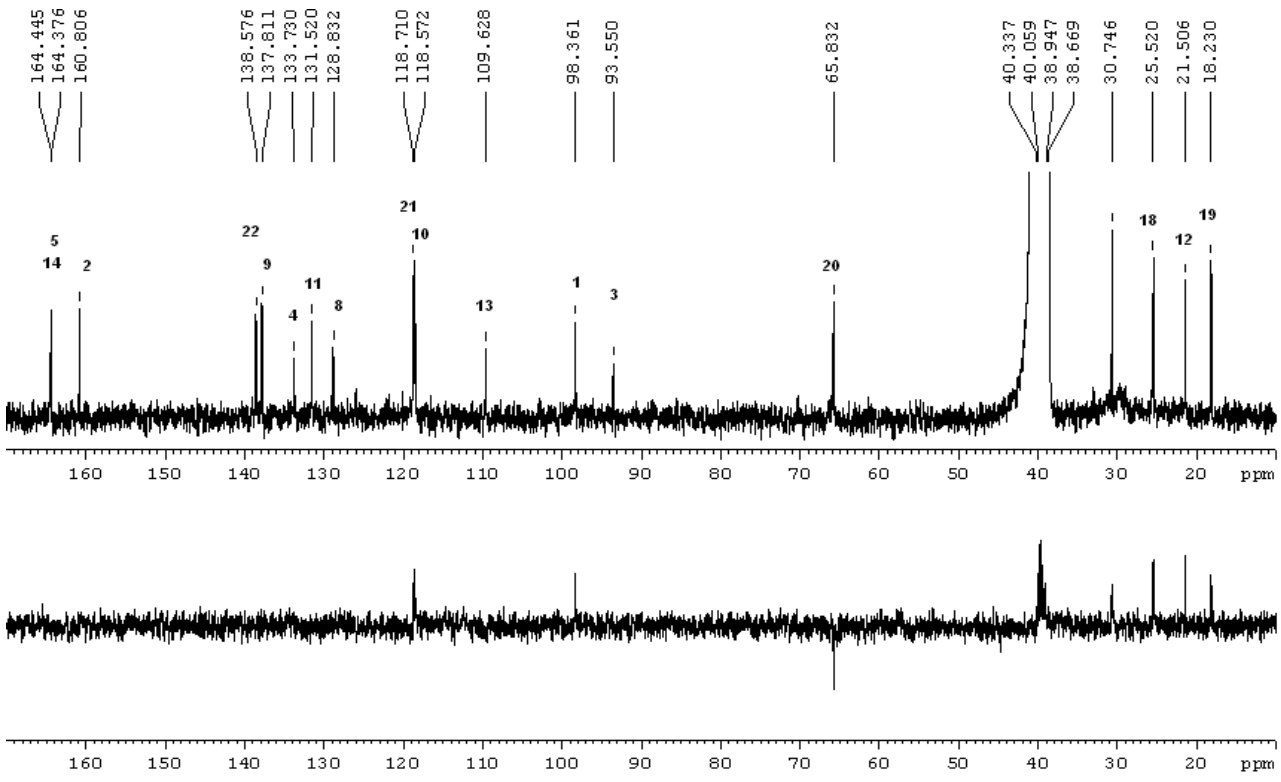
No.	$\delta^{13}C$ (ppm)	multiplicity	δ ^1H (ppm), *J* in Hz	^1H-^1H COSY	^1H-^{13}C HMBC (H to C)
1	98.4	CH	6.47, s		2, 3, 13, 14
2	160.8	C			
3	93.5	C			
4	133.7	C			
5	164.44*	C			
6	-				
7	-	C			
8	128.8	C			
9	137.8	C			
10	118.6	CH	6.67, s	12	8, 9, 12, 13
11	131.5	C			
12	21.5	CH_3	2.58, s	10	10, 11, 13, 14
13	109.6	C			
14	164.37*	C			
15	-				
16	-				
17	-				
18	25.5	CH_3	1.78, s		19, 21, 22
19	18.2	CH_3	1.75, s		18, 21, 22
20	65.8	CH_2	4.71, d, 6.6	21	14, 21, 22
21	118.7	CH	5.54, br t, 6.6	18, 19, 20	18, 19
22	138.6	C			
OH-2			10.47, s		

*interchangeable

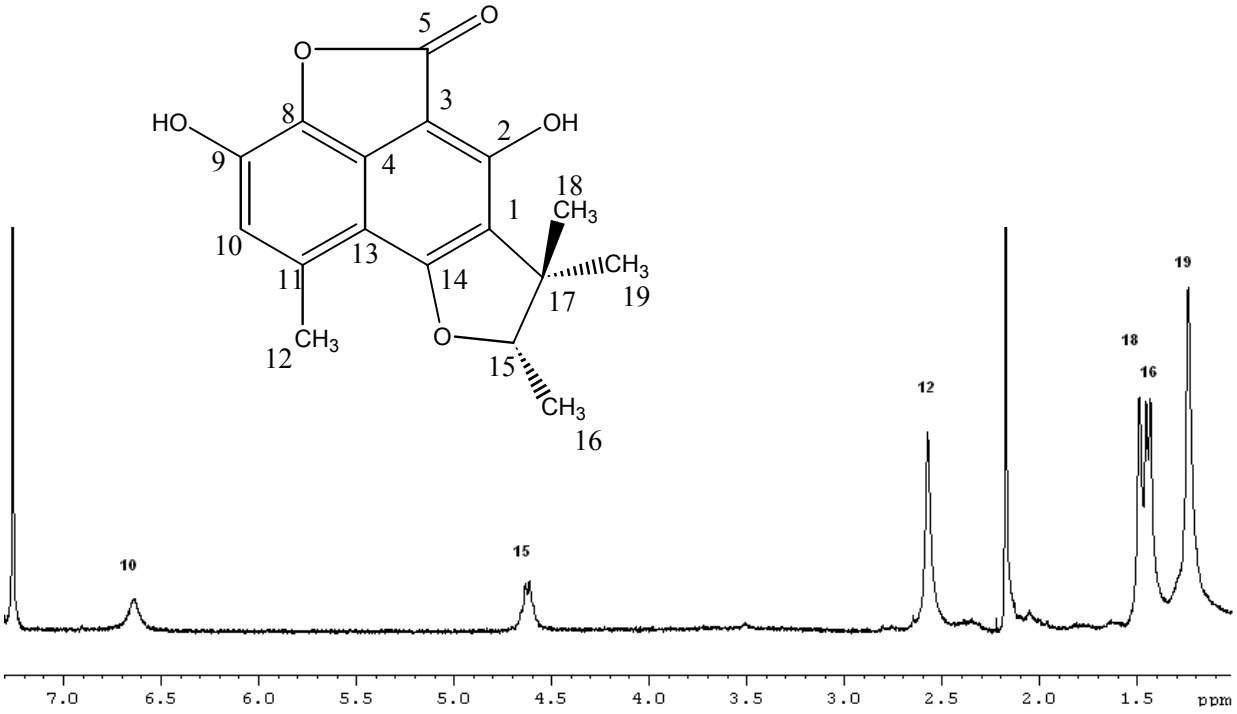
S20. ^{1}H NMR spectrum (300 MHz, dmso-d_6) of compound **7**.



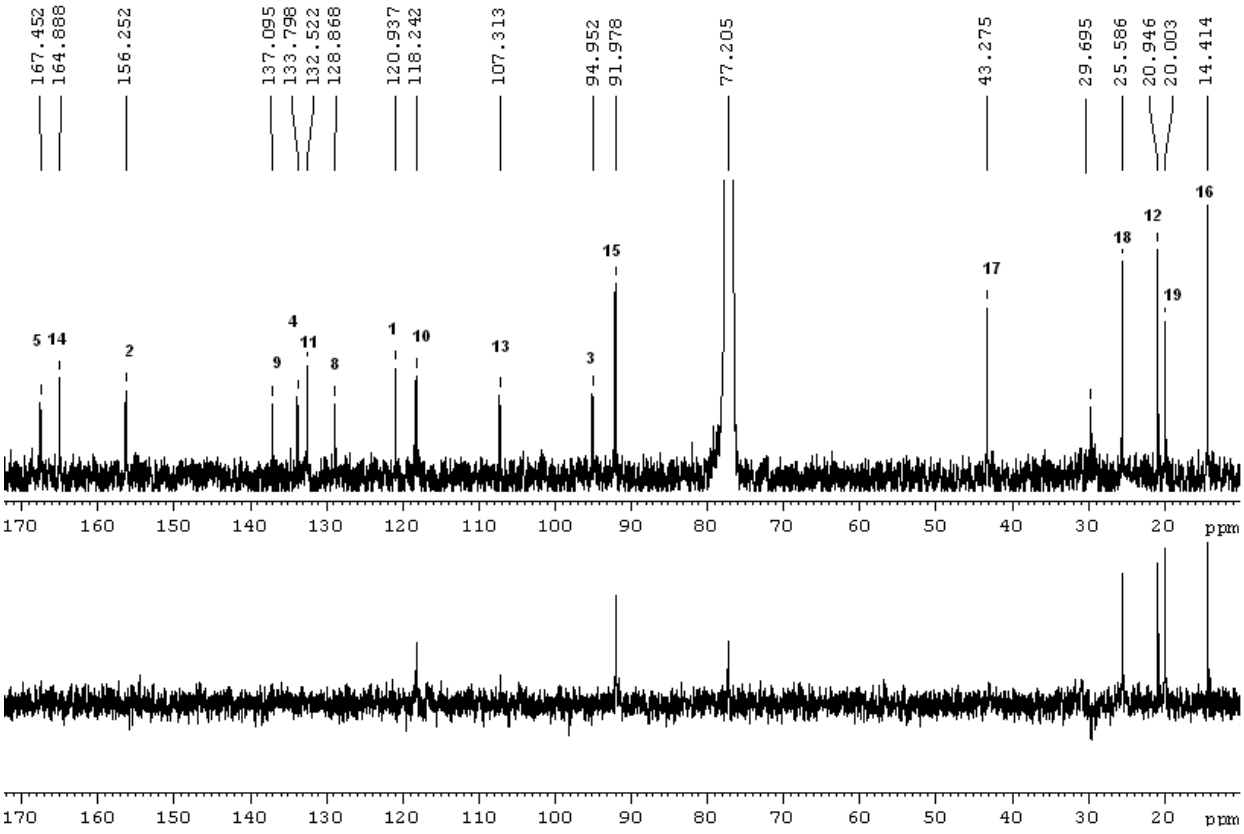
S21. ^{13}C NMR (75 MHz, dmso-*d6,* upper line) and DEPT 135 (lower line) spectra of compound **7**.



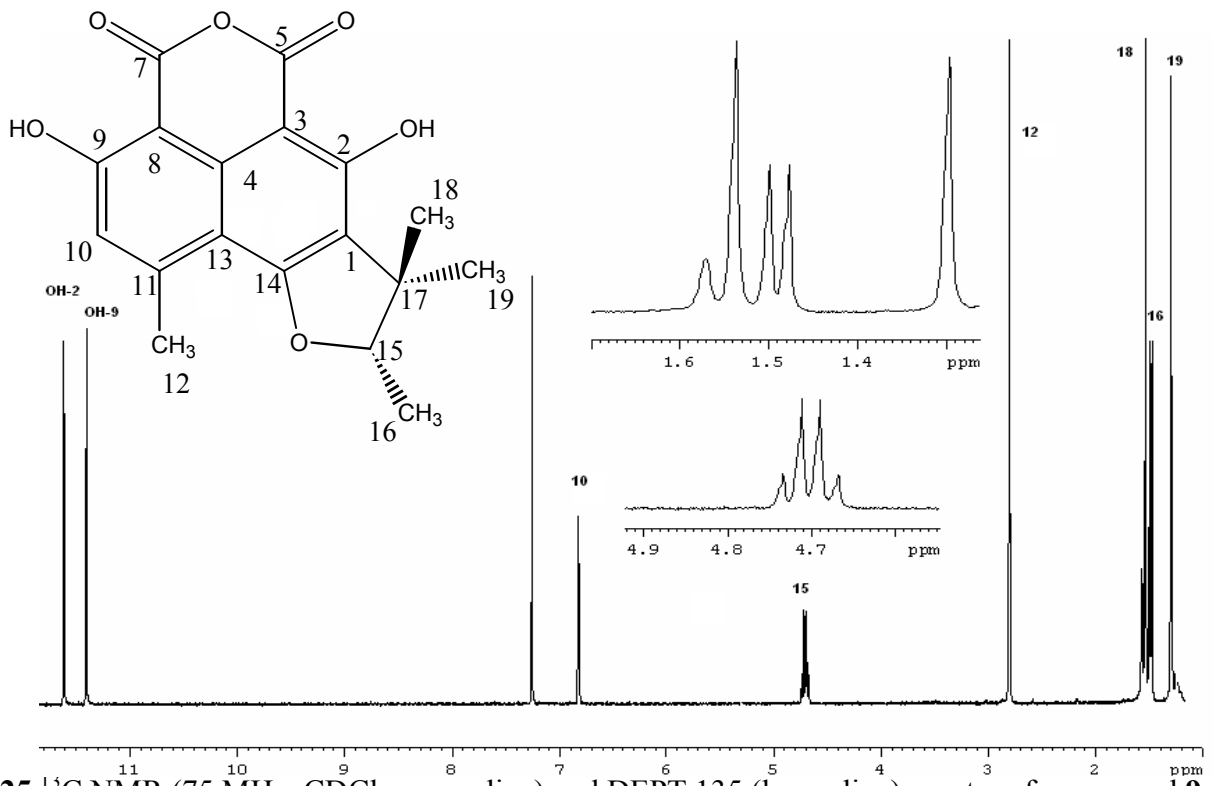
S22.[1]H NMR spectrum (300 MHz, $CDCl_3$) of compound **8**.



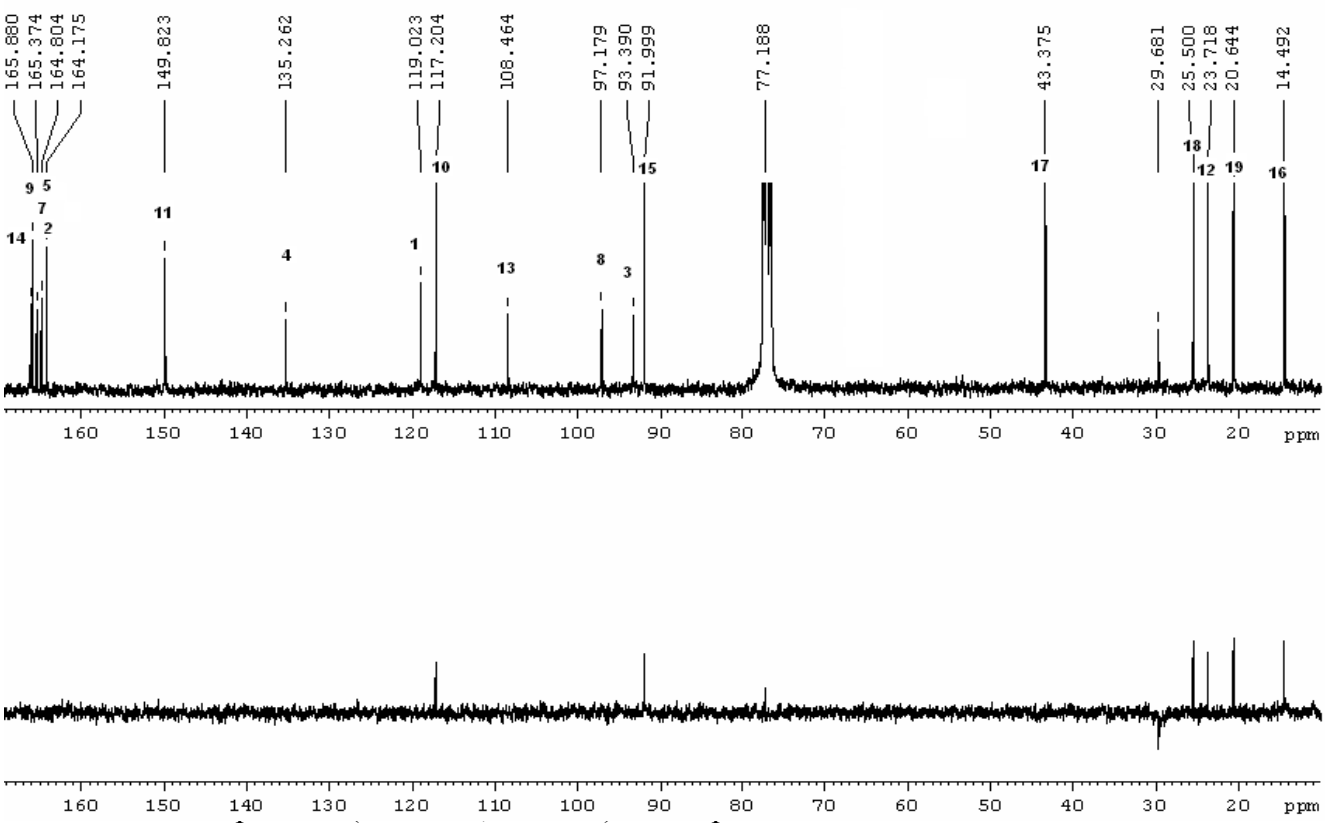
S23.[13]C NMR (75 MHz, $CDCl_3$, upper line) and DEPT 135 (lower line) spectra of compound **8**.

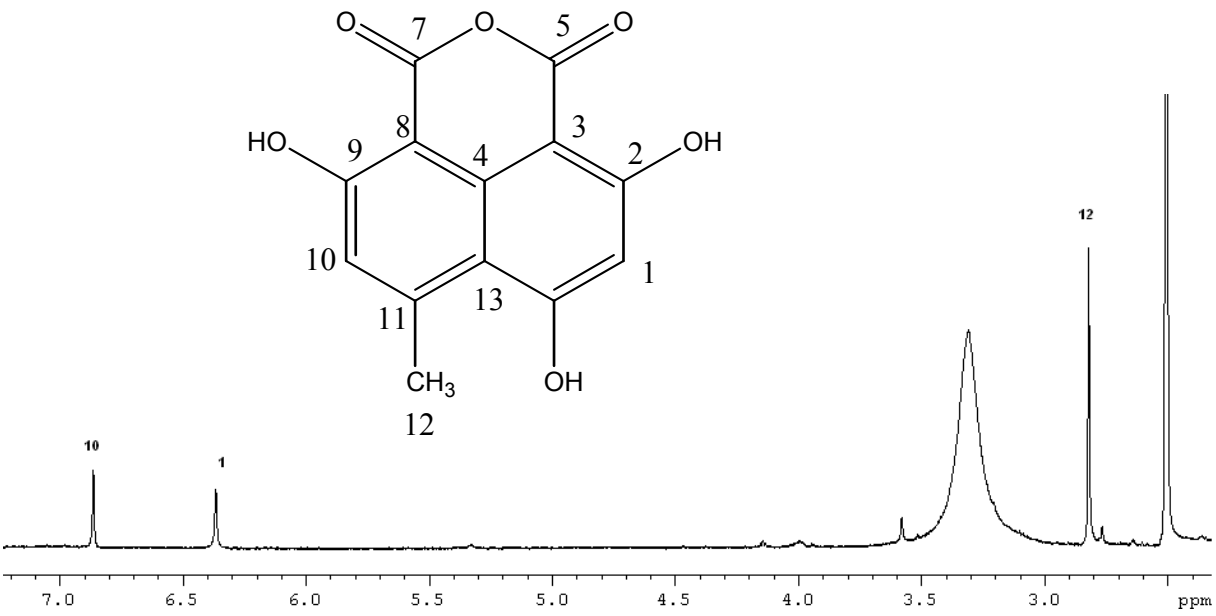


S24.[1]H NMR spectrum (300 MHz, $CDCl_3$) of compound **9**.

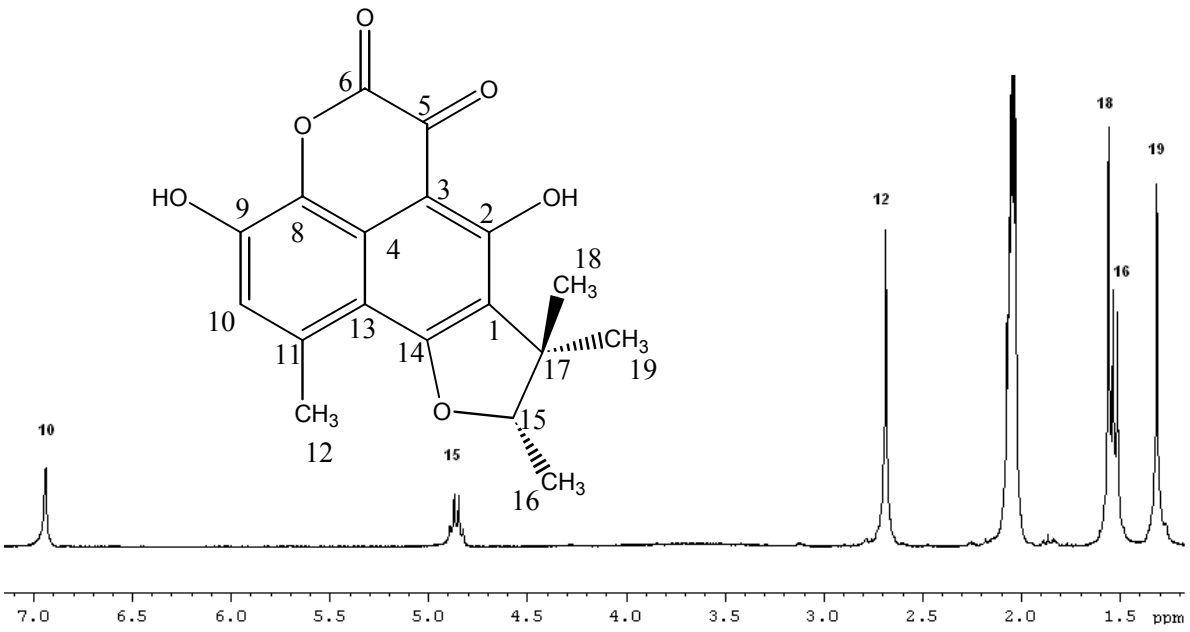


S25.[13]C NMR (75 MHz, $CDCl_3$, upper line) and DEPT 135 (lower line) spectra of compound **9**.

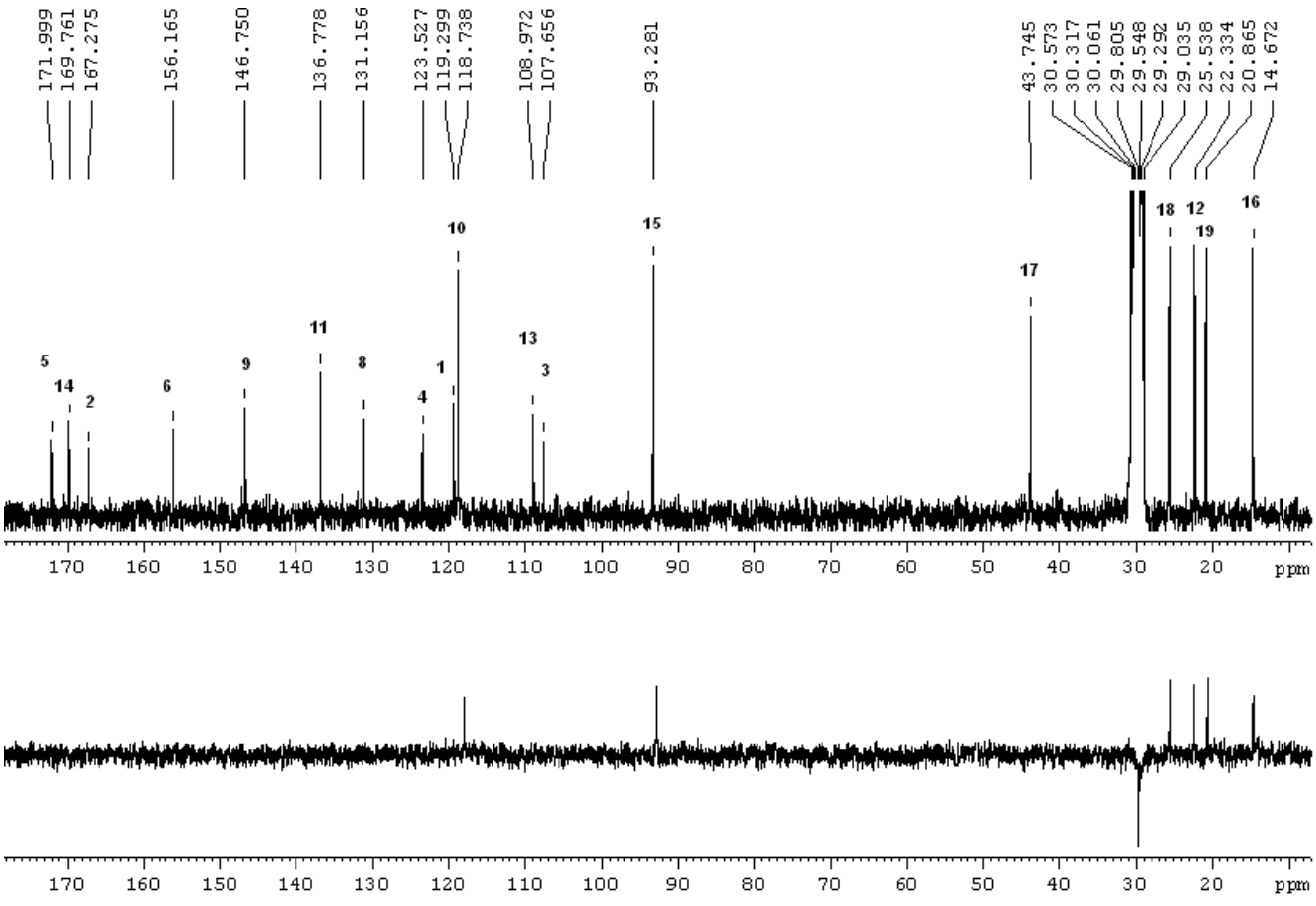




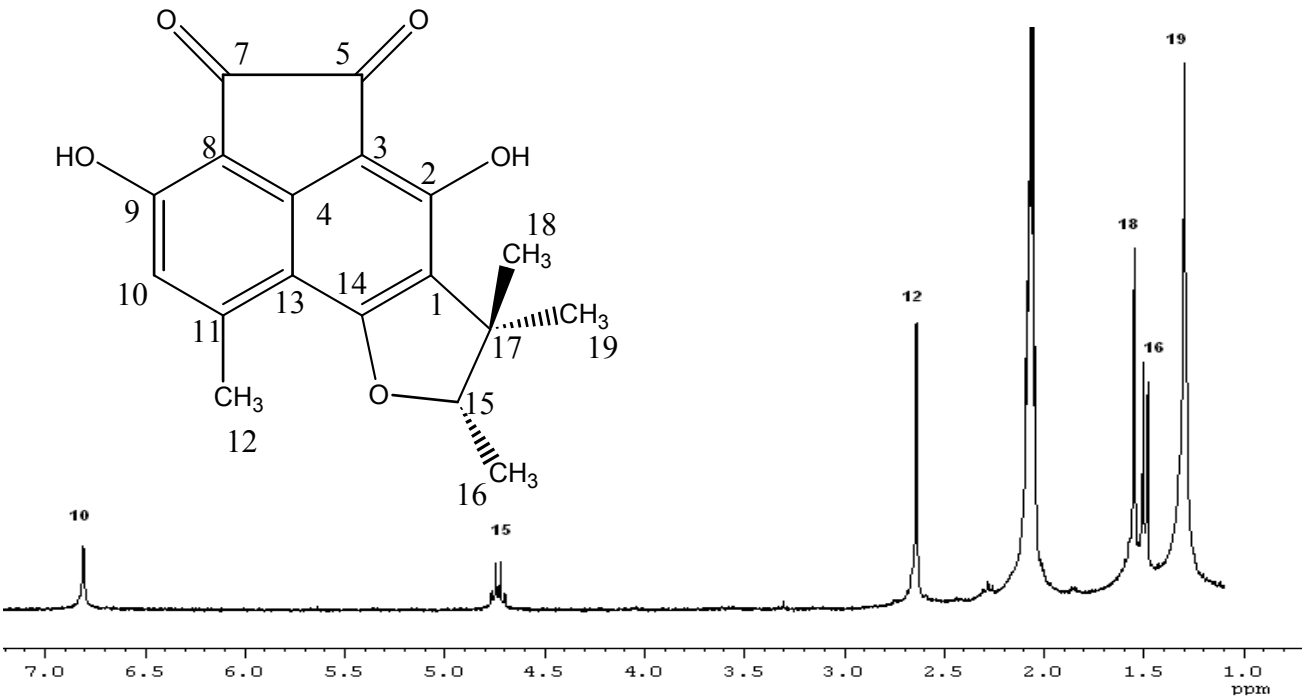
S27.[1]H NMR spectrum (300 MHz, acetone-d_6) of compound **11**.



S28.[13]C NMR (75 MHz, acetone-d_6, upper line) and DEPT 135 (lower line) spectra of compound **11**.



S29.[1]H NMR spectrum (300 MHz, acetone-d_6) of compound **12**.



S30.[13]C NMR (75 MHz, acetone-d_6, upper line) and DEPT 135 (lower line) spectra of compound **12**.