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Supporting Information

Total Synthesis and Preliminary SAR Study of (±)-Merochlorins A and B

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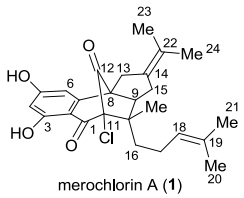
I: Comparison of NMR Data of Natural and Synthetic Merochlorins

Note: Some of the NMR data of natural product **1** and **2** were misreported in the original isolation paper, which have been corrected in the following synthetic work by George[1] and Trauner,[2] respectively. The NMR data of our samples are in good agreement with those reported in reference 1 and 2.

1) Merochlorin A



merochlorin A (**1**)

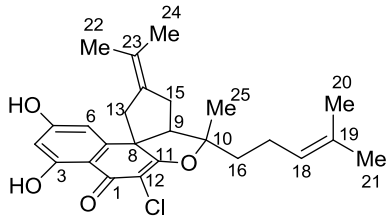
No.	**Natural** (600 MHz)	**Synthetic (Ref.1)** (400 MHz)	**Synthetic (This work)** (400 MHz)
	^{1}**H NMR δ_H** [ppm, mult, *J* (Hz)] d_6-DMSO		
1			
2			
4	6.16, d (2.0)	6.28, d (2.0)	6.28, d (2.0)
5			
6	6.38, d (2.0)	6.46, d (2.0)	6.46, d (2.0)
7			
8			
9	2.24, dd (9.4, 4.0)	2.33, dd (9.1, 4.2)	2.33, dd (8.1, 4.5)
12			
13	2.87, d (13.0); 2.65, d(13.0)	2.95, d (15.2); 2.73, d (15.2)	2.95, d (15.2); 2.73, d (15.2)
14			
15	2.36, dd (14.0, 4.0); 2.33, dd (14.0, 9.4)	2.45-2.38, m	2.46-2.38, m
16	1.14, q (6.0); 1.40, dt (14.8, 4.8)	1.20, dt (13.2, 4.9); 1.47, dt (13.2, 4.9)	1.20, dt (12.9, 4.1); 1.46, dt (13.4, 4.9)
17	2.03, m; 1.75m	2.10, m;1.83, m	2.10, m;1.83, m
18	4.92, t (6.5)	5.01, t (7.1)	5.01, t (7.1)
19			
20	1.45, s	1.54, s	1.54, s
21	1.53, s	1.61, s	1.61, s
22	1.56, s	1.63, s	1.63, s
23			
24	1.65, s	1.73, s	1.73, s
25	0.81, s	0.88, s	0.88, s
3-OH	11.9, br, s	12.00, br, s	11.99, br, s
5-OH		11.35, br, s	11.36, br, s

Ref 1: J. P. Pepper and J. H. George, *Angew. Chem. Int. Ed.*, 2013, **52**, 1-5.

Ref 2: R. Meier, S. Strych, D. Trauner, *Org. Lett.*, 2014, **16**, 2634-2637.

No.	^{13}C NMR δ_c [ppm] d_6-DMSO		
	Natural (150 MHz)	**Synthetic (Ref.1)** (100 MHz)	**Synthetic (This work)** (100 MHz)
1	193.2	193.0	193.0
2	109.8	109.6	109.6
3	165.4	165.8	165.8
4	102.1	101.8	101.8
5	166.5	166.6	166.6
6	103.7	103.3	103.3
7	150.5	150.3	150.3
8	61.5	61.3	61.3
9	58.8	58.1	58.1
10	45.3	45.1	45.1
11	91.3	91.0	91.0
12	200.1	199.8	199.8
13	29.3	29.0	29.0
14	132.1	132.4	132.4
15	31.9	31.9	31.7
16	39.2	39.4	39.4
17	22.8	22.6	22.5
18	124.2	124.3	124.3
19	131.6	131.6	131.6
20	18.1	17.9	17.9
21	26.1	25.8	25.8
22	20.9	21.0	21.0
23	123.1	123.0	123.0
24	21.1	21.3	21.3
25	16.5	16.5	16.5
3-OH			
5-OH			

1) Merochlorin B



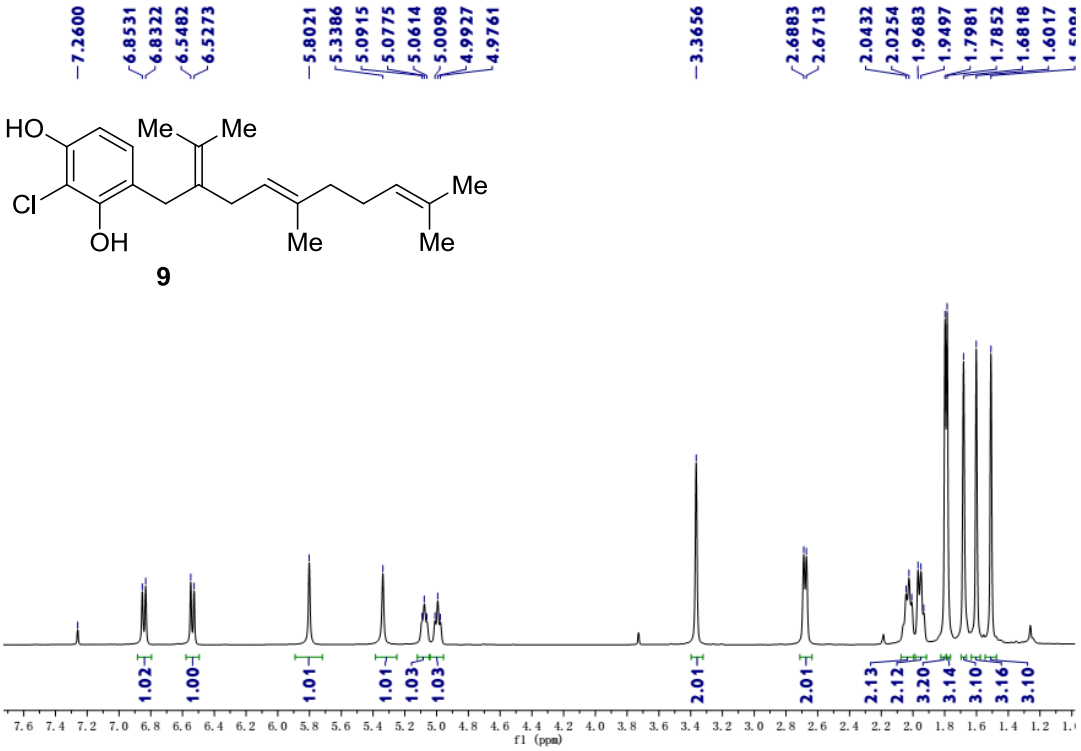
merochlorin B (**2**)

	^{1}H NMR δ_H [ppm, mult, *J* (Hz)] d_6-DMSO		
	Natural	**Synthetic (Ref.2)**	**Synthetic (This work)**
	(600 MHz)	(400 MHz)	(400 MHz)
1			
2			
3			
4	6.17, d (2.0)	6.18, d (2.1)	6.18, d (2.0)
5			
6	6.15, d (2.0)	6.16, d (2.2)	6.16, d (2.0)
7			
8			
9	2.99, d (7.8)	3.00, d (7.9)	2.99, d (7.6)
10			
11			
12			
13	2.81, d (17.0); 2.47, d(17.0)	2.82, d (18.6); 2.48, d (18.2)	2.81, d (18.4); 2.47, d (18.3)
14			
15	2.82, d (17.8); 2.70, d (17.8)	2.89, d (18.6); 2.73, d (18.6)	2.85, d (18.6); 2.72, d (17.9)
16	1.73-1.74, m	1.77-1.71, m	1.76-1.71, m
17	1.99, m; 1.74, m	2.04-1.93, m	2.04-1.93, m
18	5.05, t (7.5)	5.05, t (7.0)	5.05, t (6.6)
19			
20	1.48, s	1.48, s	1.48, s
21	1.57, s	1.57, s	1.56, s
22	1.70, s	1.48, s	1.48, s
23			
24	1.62, s	1.70, s	1.70, s
25	1.41, s	1.41, s	1.41, s
3-OH	12.9, br, s	12.91, br, s	12.91, br, s
5-OH		10.55, br, s	10.55, br, s

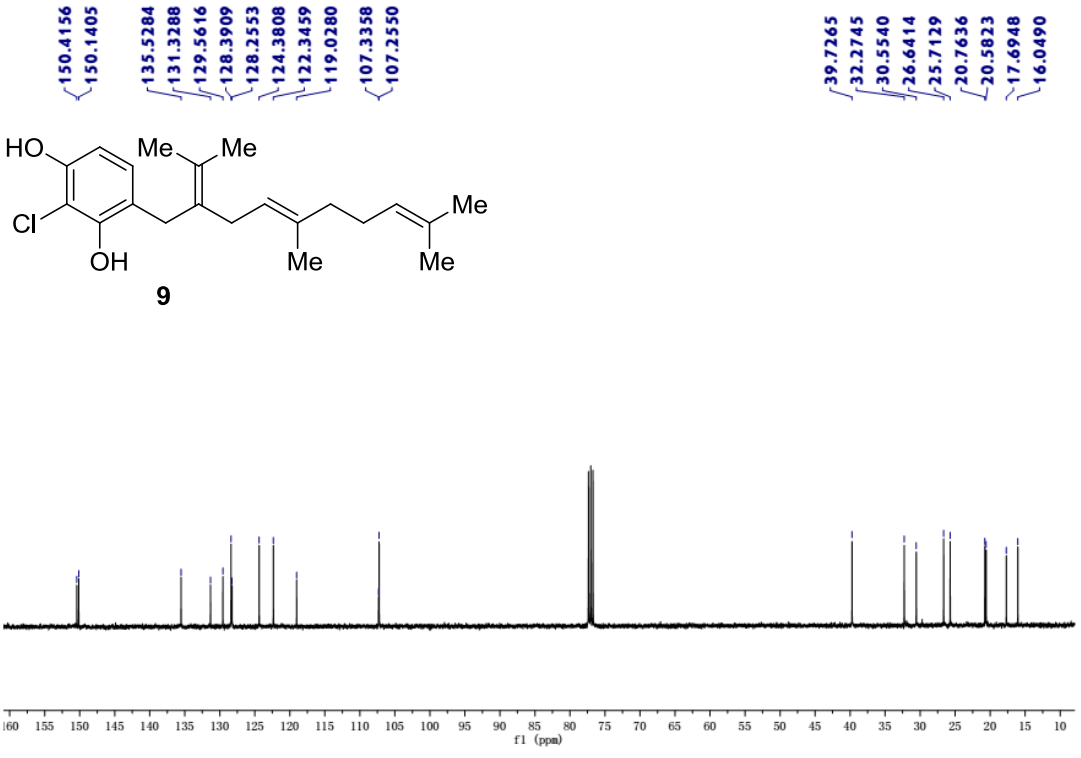
No.	^{13}C NMR δ_c [ppm] d_6-DMSO		
	Natural (150 MHz)	**Synthetic (Ref.1)** (100 MHz)	**Synthetic (This work)** (100 MHz)
1	184.0	184.1	184.1
2	106.4	105.9	105.9
3	163.7	163.4	163.4
4	101.9	101.0	101.0
5	163.0	163.3	163.3
6	104.4	103.6	103.6
7	148.4	147.7	147.7
8	60.7	60.1	60.1
9	52.5	52.0	52.0
10	98.6	97.9	97.9
11	174.0	176.0	176.0
12	99.8	99.7	99.7
13	49.8	49.1	49.1
14	131.0	130.6	130.6
15	35.3	34.4	34.4
16	42.9	43.2	43.2
17	22.6	21.9	21.9
18	124.5	123.3	123.3
19	131.4	131.3	131.3
20	18.1	17.4	17.4
21	25.6	25.4	25.4
22	21.9	21.3	21.3
23	126.2	125.5	125.5
24	17.0	21.3	21.3
25	22.6	22.1	22.1
3-OH			
5-OH			

II: NMR Spectrum

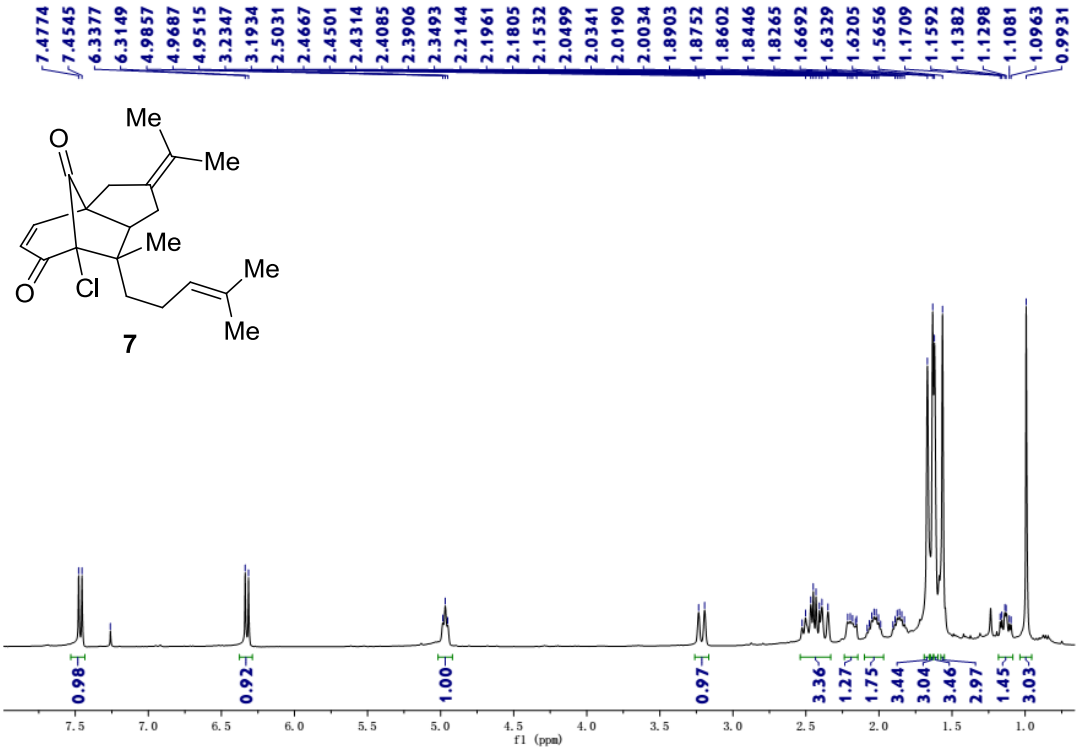
^{1}H-NMR spectrum for **9** ($CDCl_3$, 400 MHz)



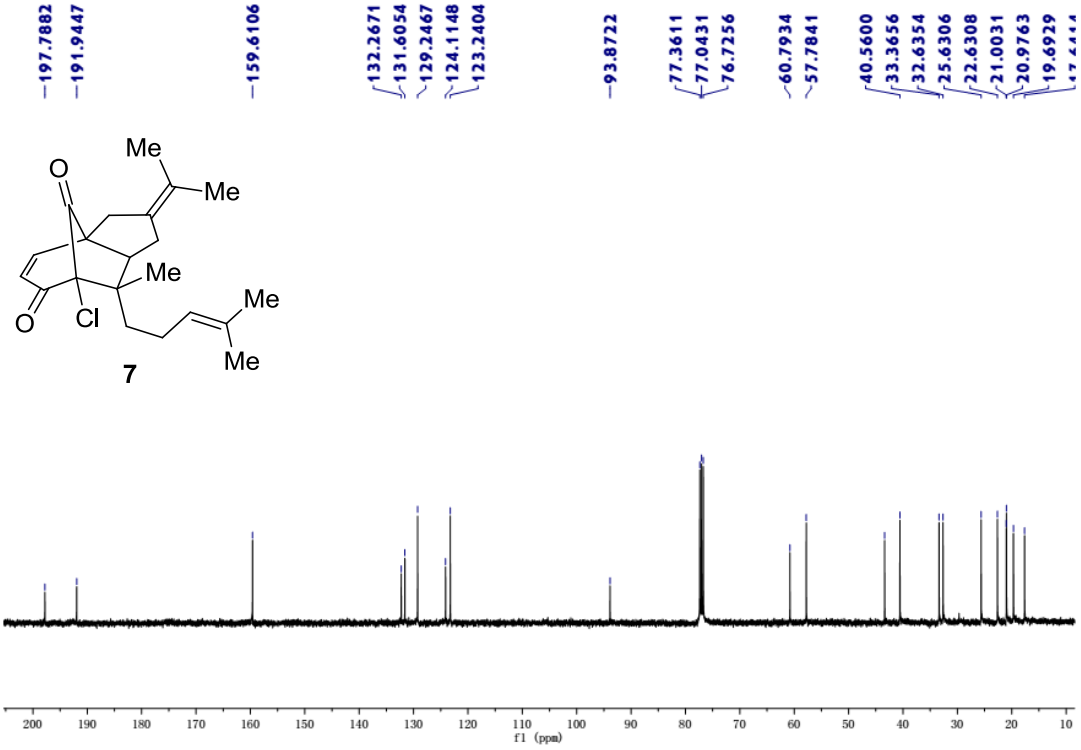
^{13}C-NMR spectrum for **9** ($CDCl_3$, 100 MHz)



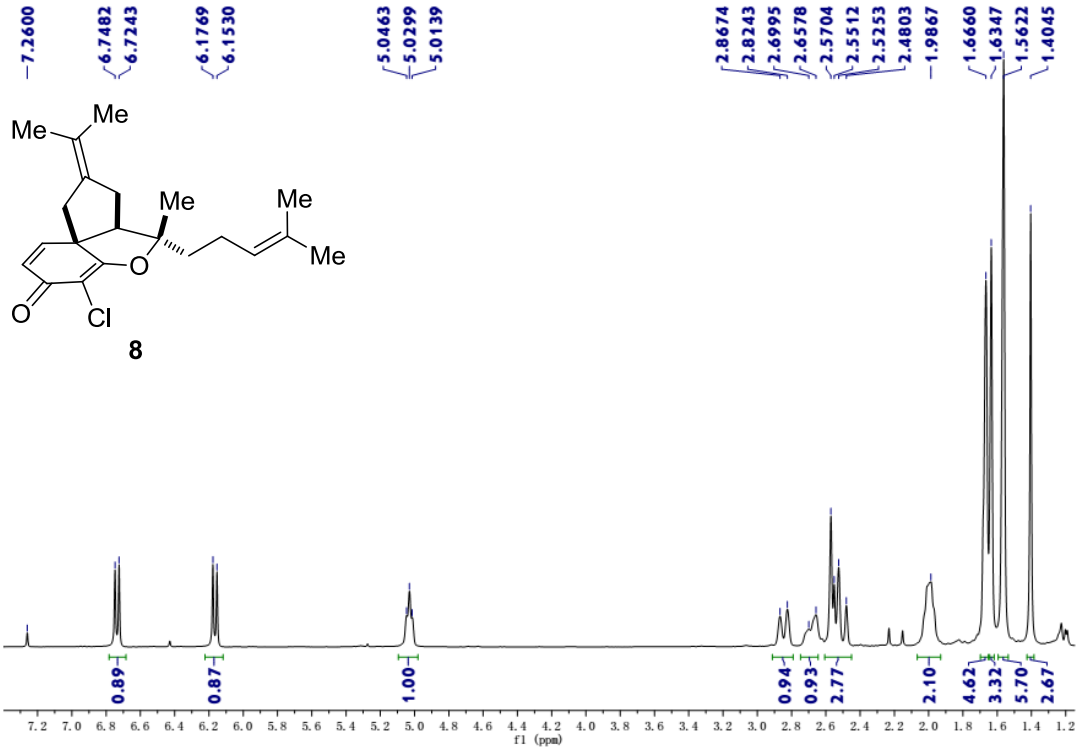
^{1}H-NMR spectrum for **7** ($CDCl_3$, 400 MHz)



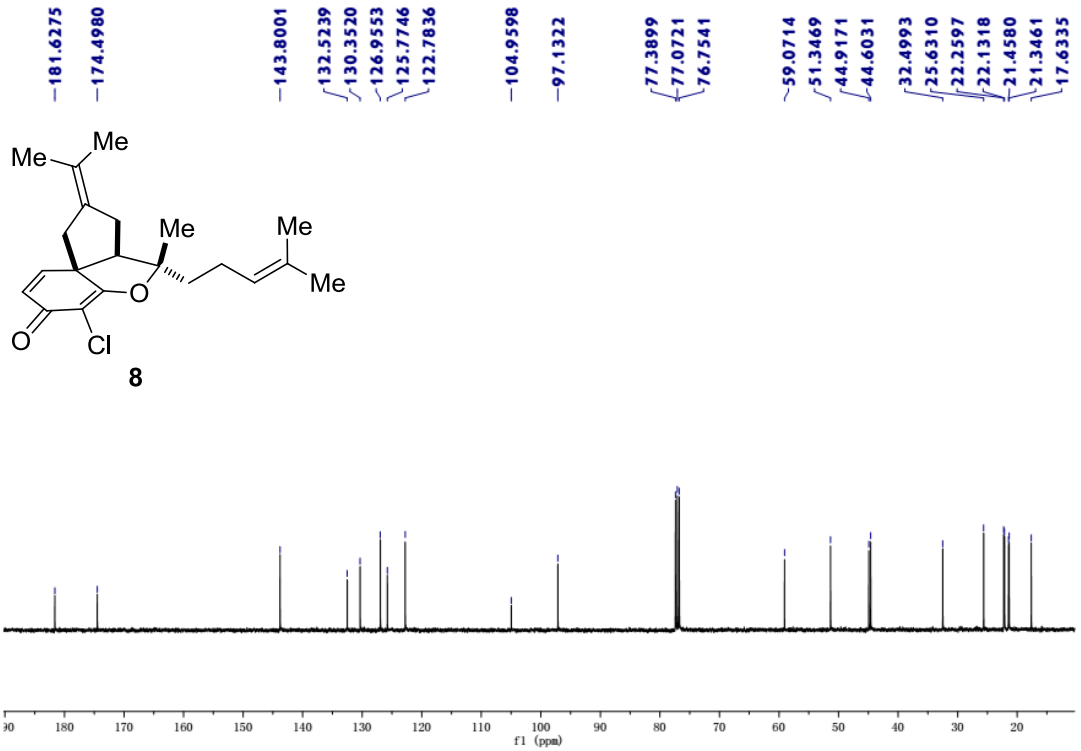
^{13}C-NMR spectrum for **7** ($CDCl_3$, 100 MHz)



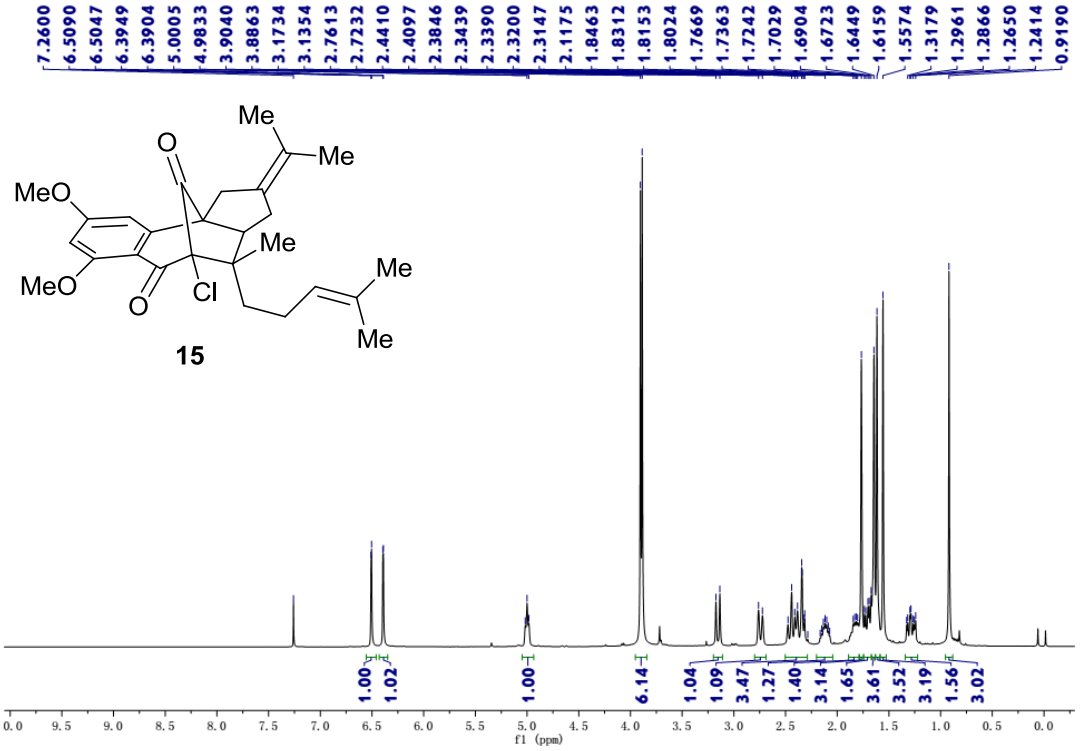
^{1}H-NMR spectrum for **8** ($CDCl_3$, 400 MHz)



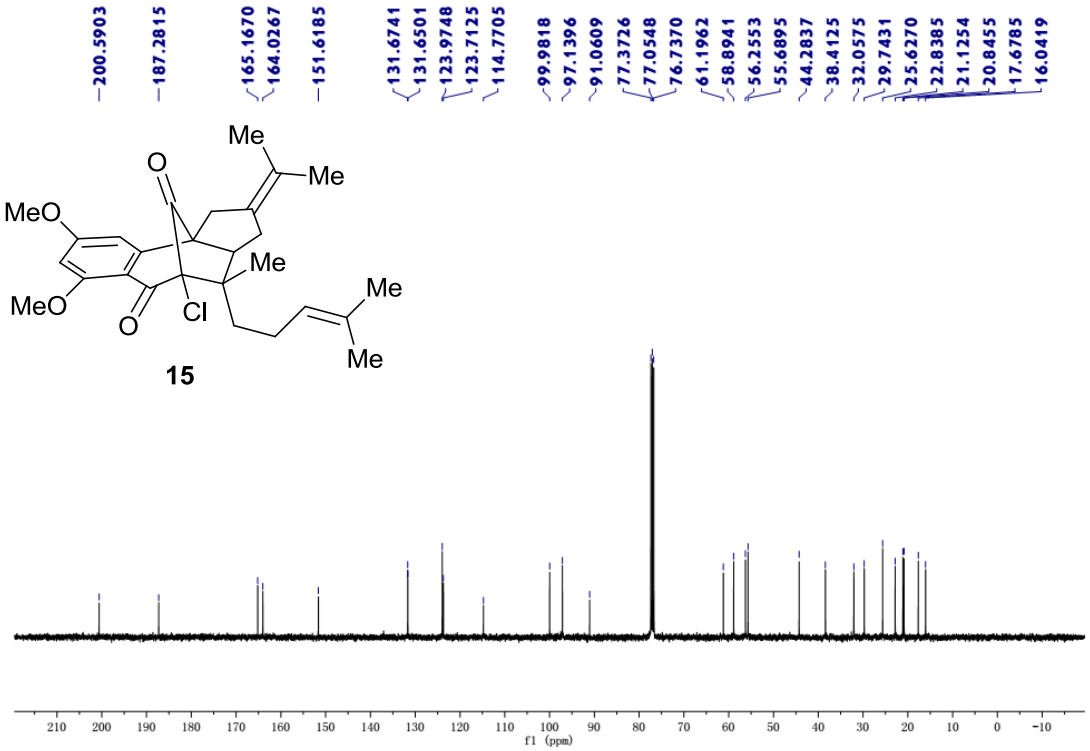
^{13}C-NMR spectrum for **8** ($CDCl_3$, 100 MHz)



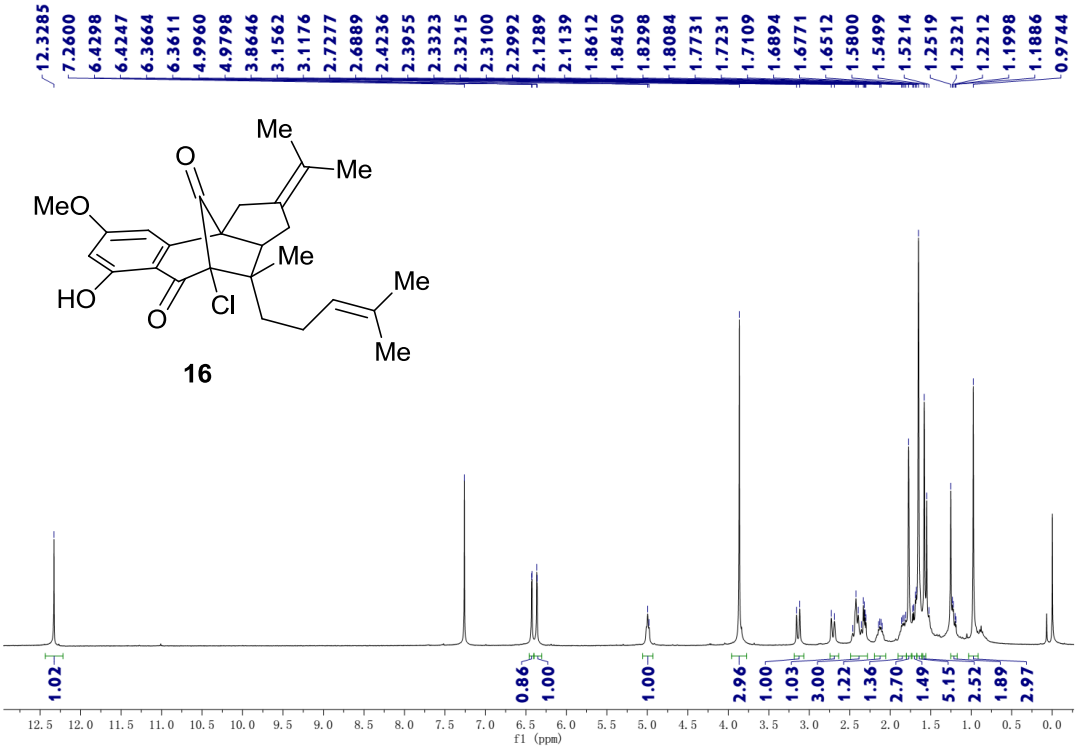
^{1}H-NMR spectrum for **15** ($CDCl_3$, 400 MHz)



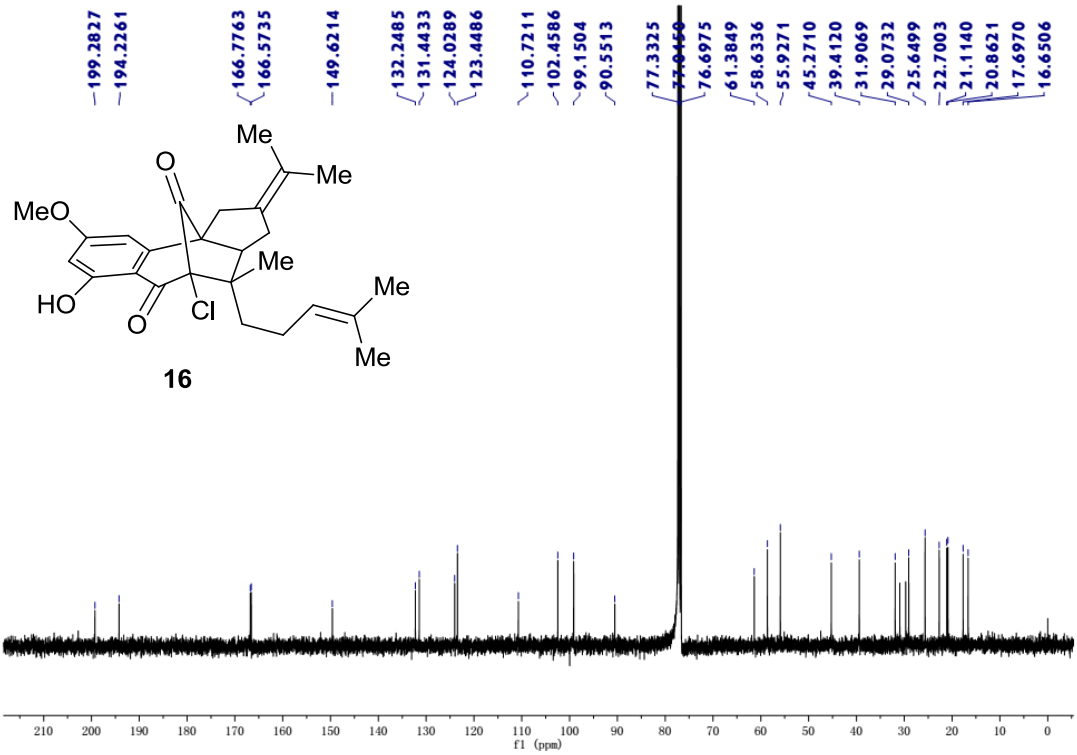
^{13}C-NMR spectrum for **15** ($CDCl_3$, 100 MHz)



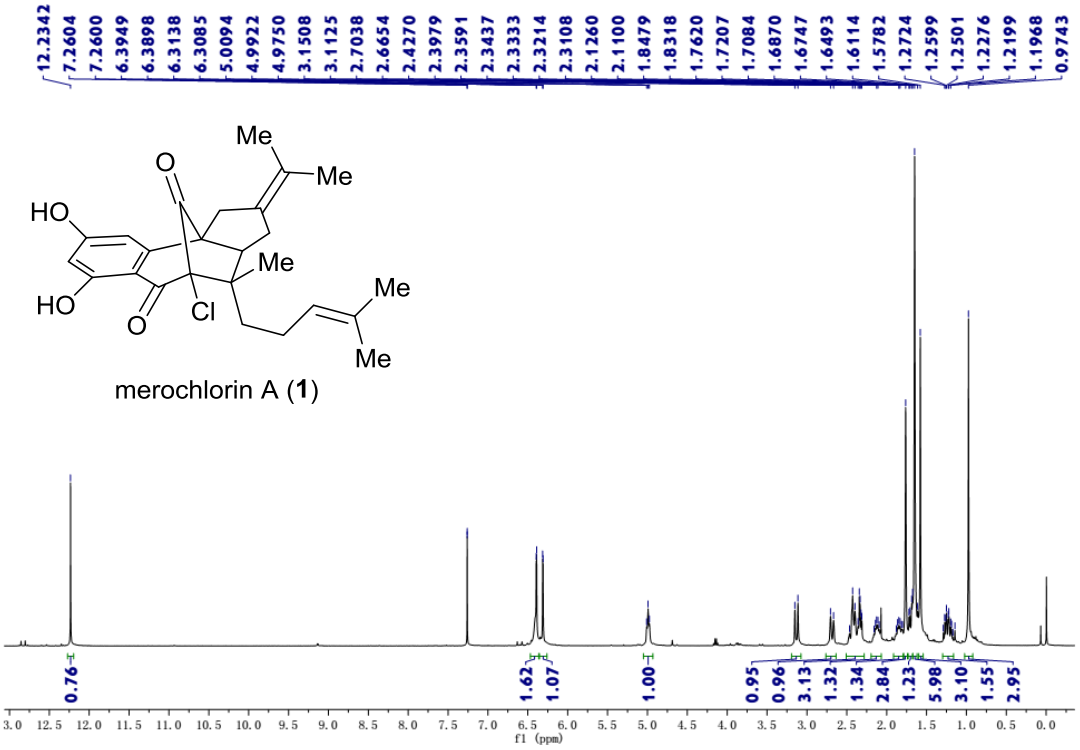
^{1}H-NMR spectrum for **16** ($CDCl_3$, 400 MHz)



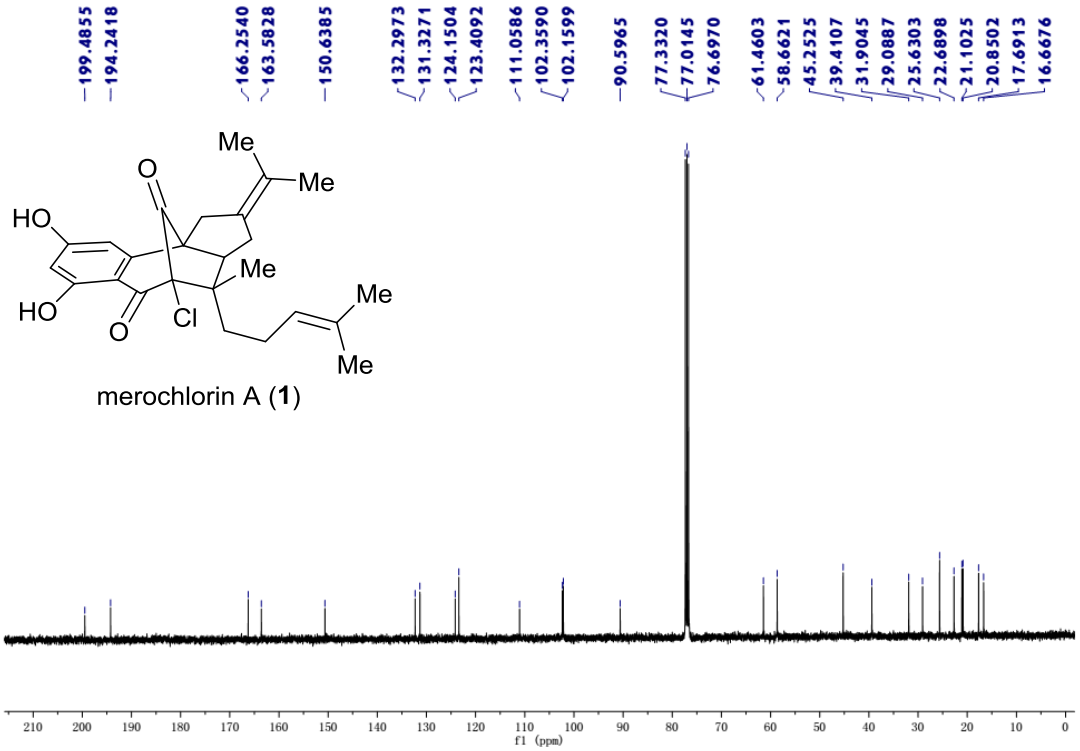
^{13}C-NMR spectrum for **16** ($CDCl_3$, 100 MHz)



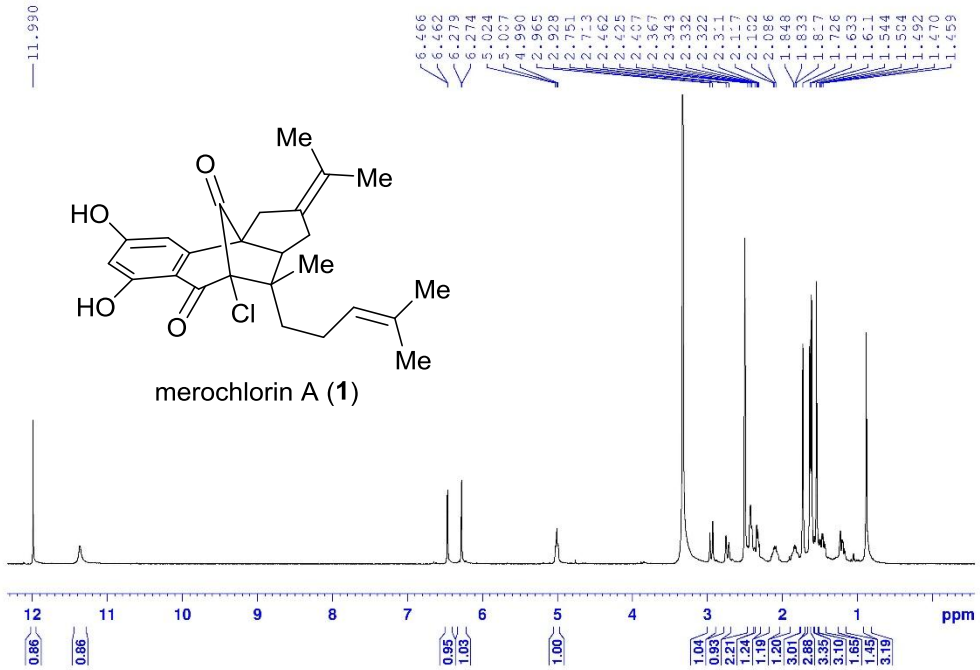
^{1}H-NMR spectrum for **1** ($CDCl_3$, 400 MHz)



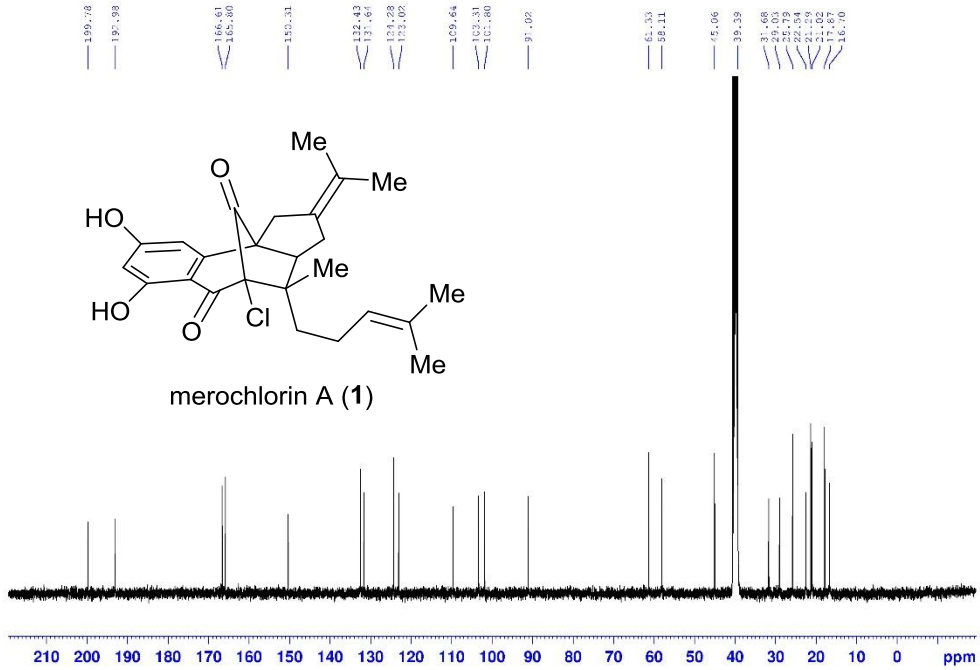
^{13}C-NMR spectrum for **1** ($CDCl_3$, 100 MHz)



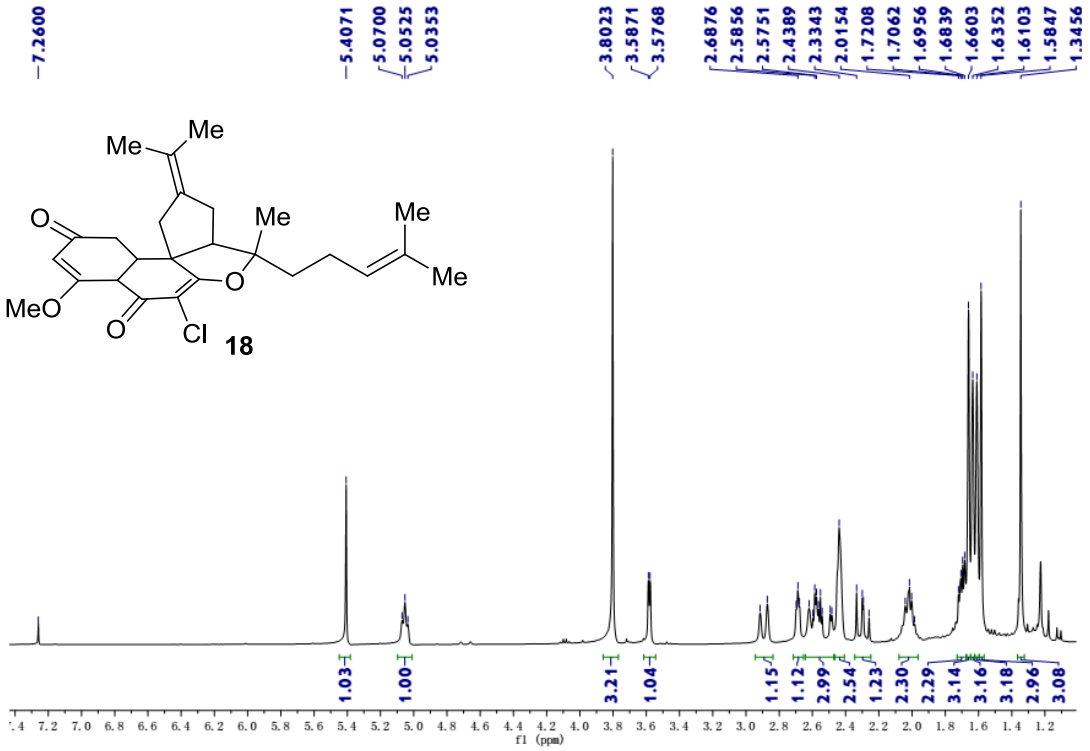
^{1}H-NMR spectrum for **1** (d_6-DMSO, 400 MHz)



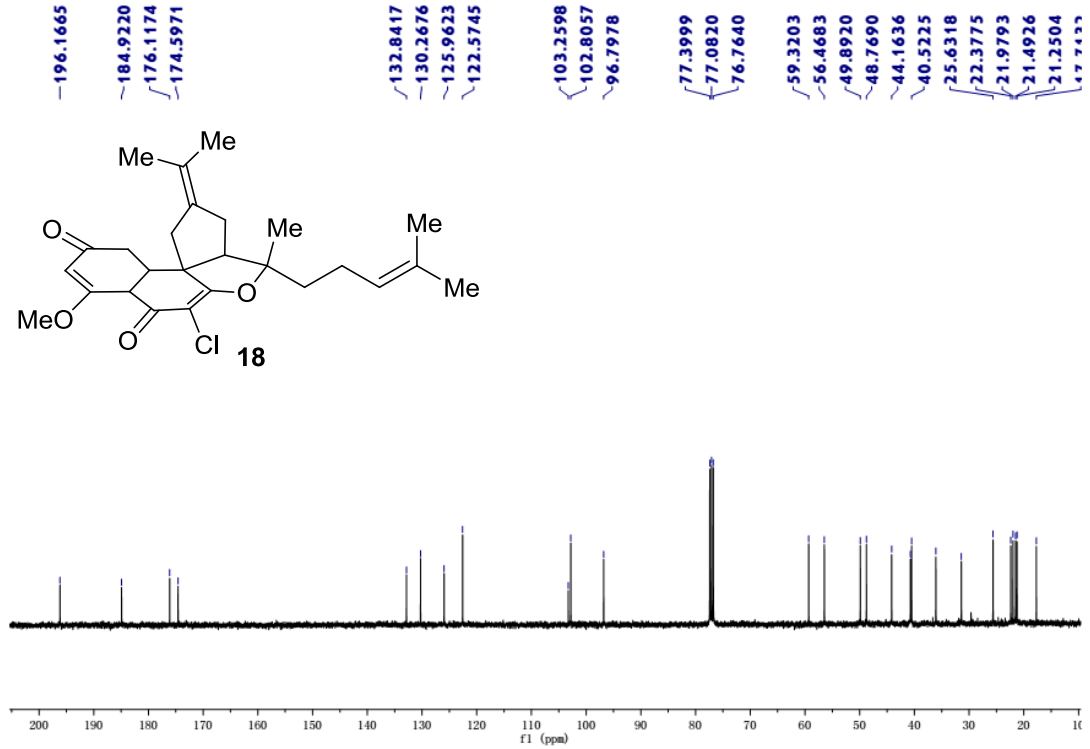
^{13}C-NMR spectrum for **1** (d_6-DMSO, 100 MHz)



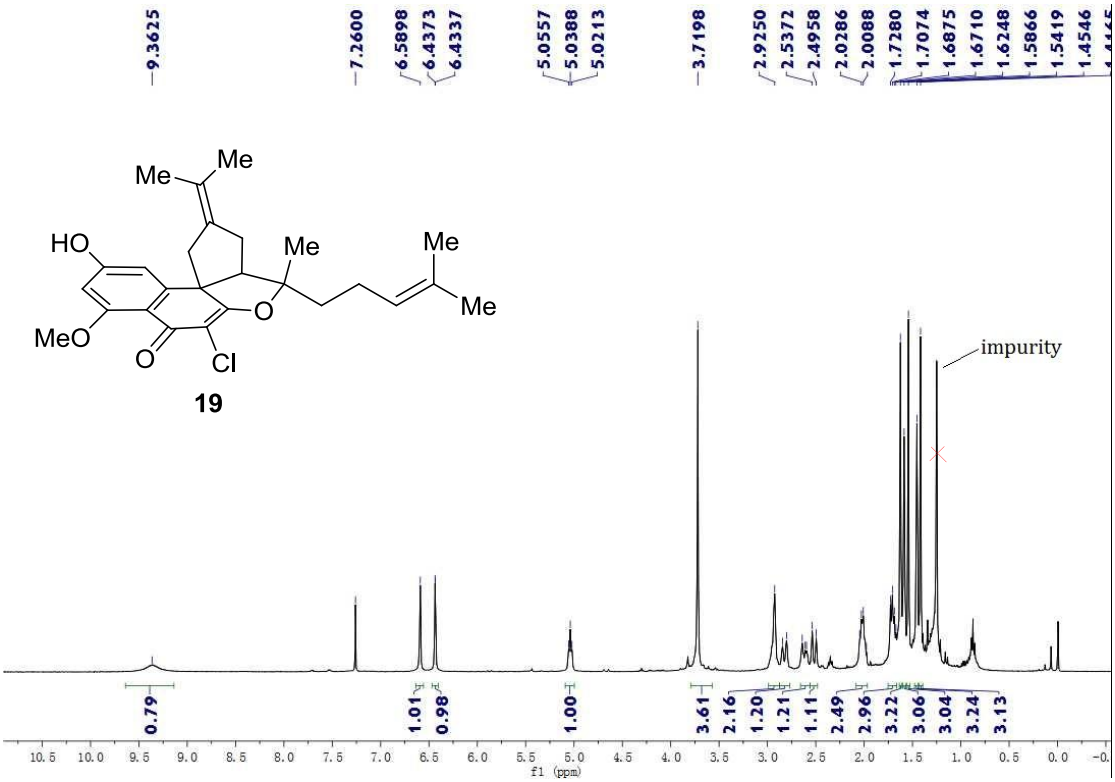
^{1}H-NMR spectrum for **18** ($CDCl_3$, 400 MHz)



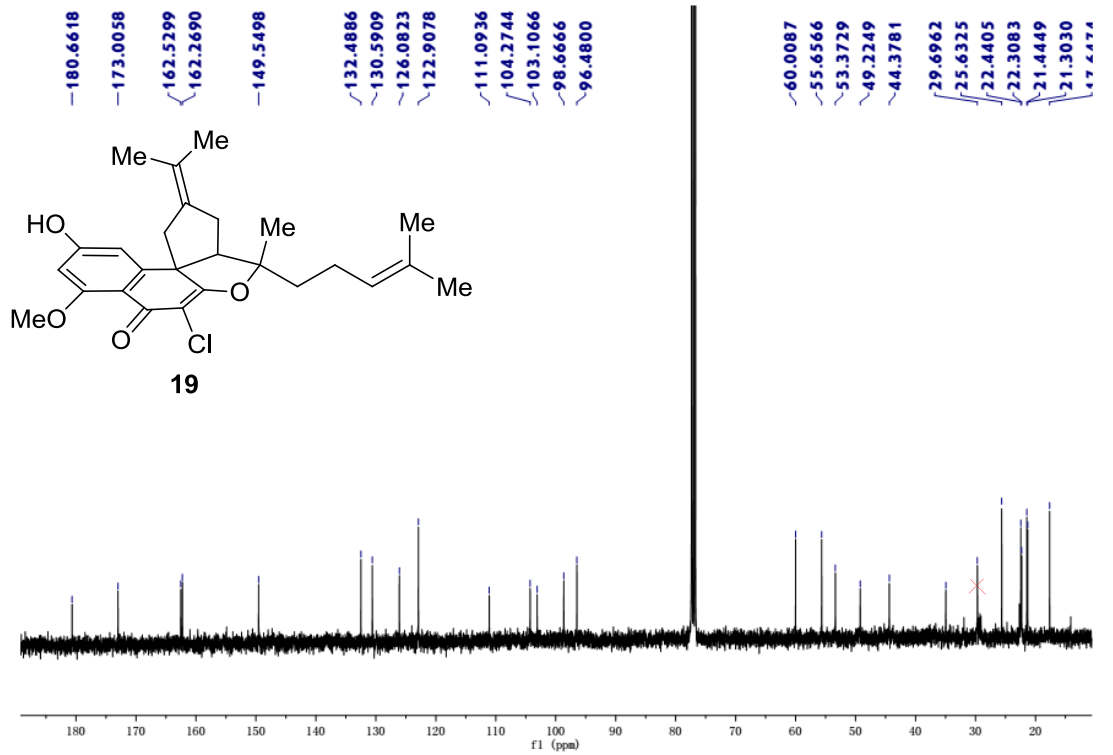
^{13}C-NMR spectrum for **18** ($CDCl_3$, 100 MHz)



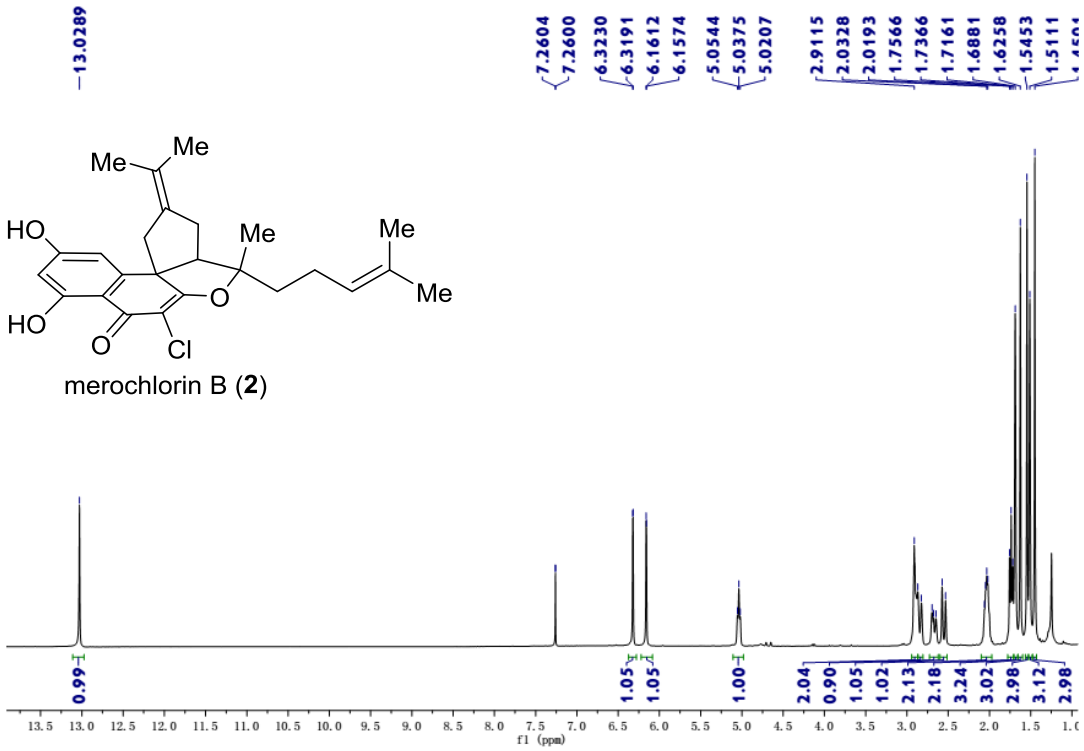
^{1}H-NMR spectrum for **19** ($CDCl_3$, 400 MHz)



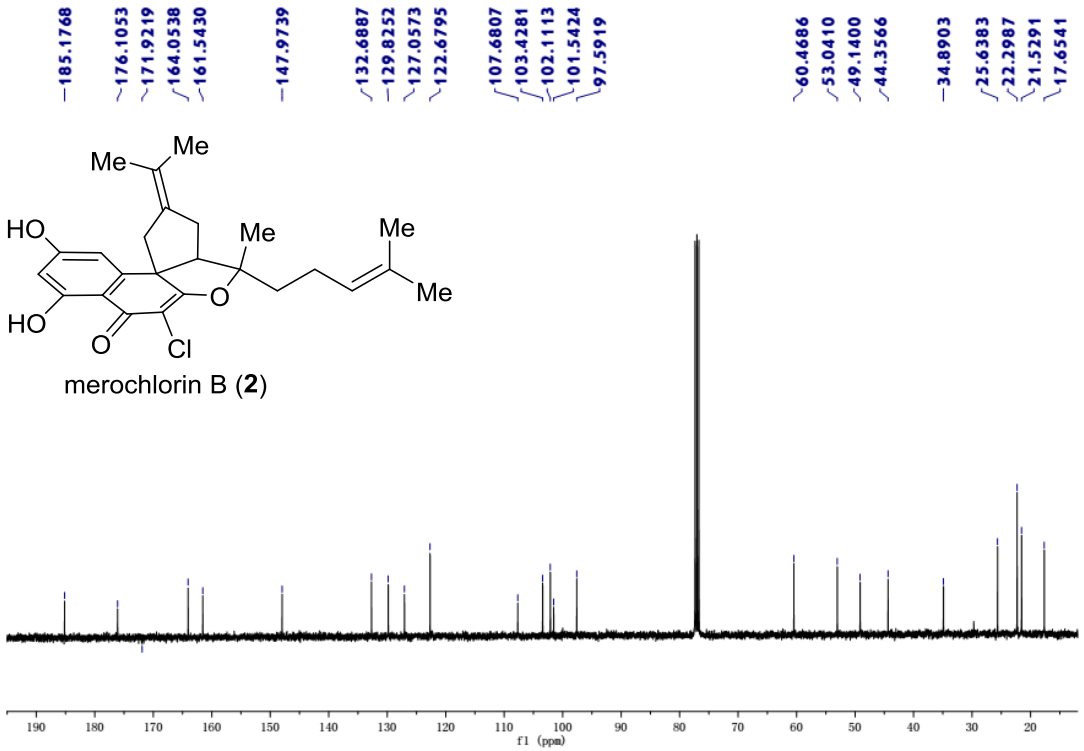
^{13}C-NMR spectrum for **19** ($CDCl_3$, 100 MHz)



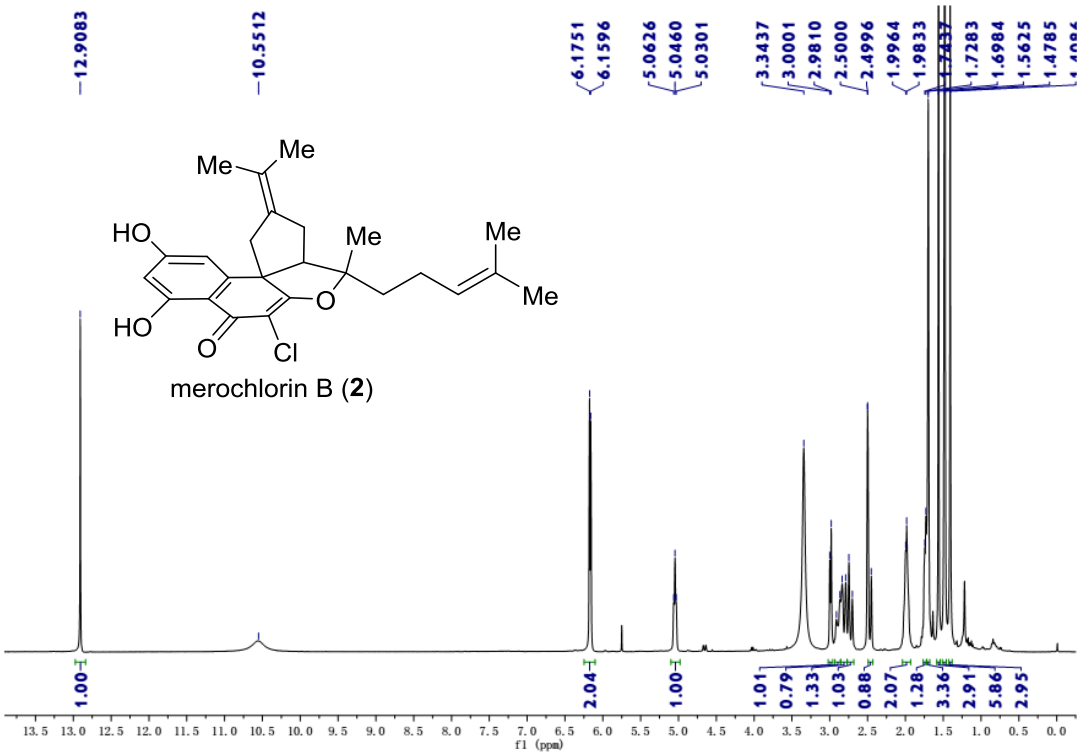
^{1}H-NMR spectrum for **2** ($CDCl_3$, 400 MHz)



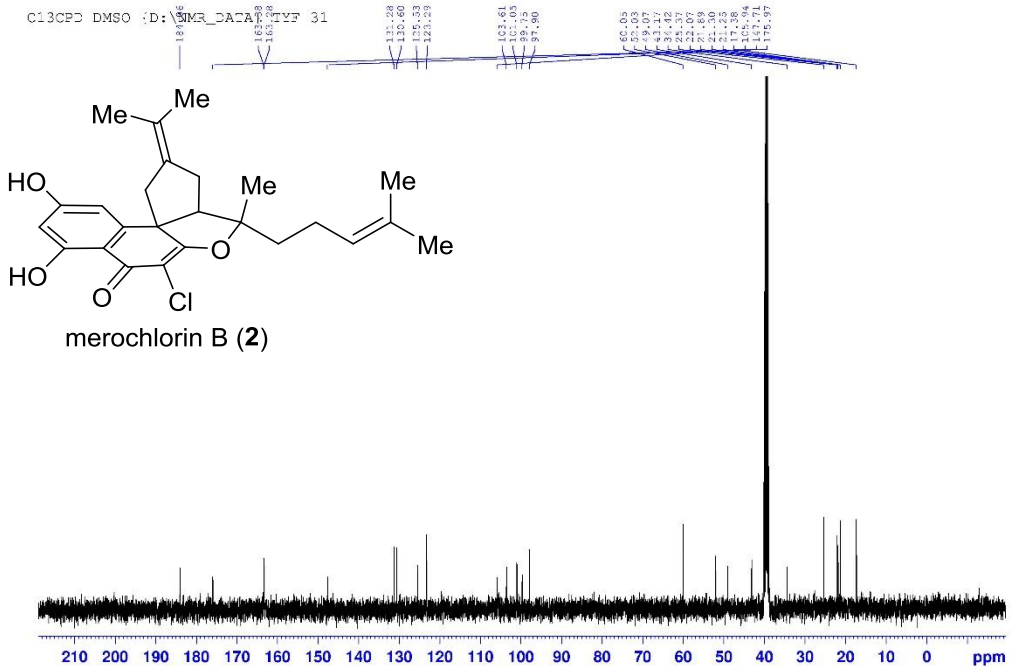
^{13}C-NMR spectrum for **2** ($CDCl_3$, 100 MHz)



^{1}H-NMR spectrum for **2** (d_6-DMSO, 400 MHz)



^{13}C-NMR spectrum for **2** (d_6-DMSO, 100 MHz)



III: X-ray Crystallographic Study

1) X-ray Crystallographic Study for 8

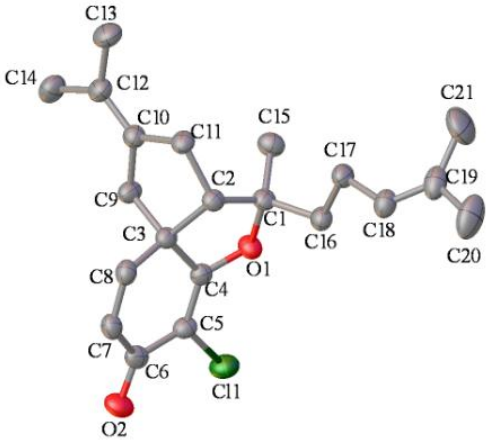


Figure S-1. X-ray structure of **8**

Table S-1. Details crystallographic data for **8**

Compound	**8**
formula	$C_{21}H_{27}ClO_2$
FW	346.88
crystal system	triclinic
space group	*P-1*
a/Å	9.418(2)
b/Å	10.301(3)
c/Å	10.919(3)
α/deg	75.398(15)
β/deg	77.071(16)
γ/deg	72.538(15)
V/Å^3	965.1(5)
Z	2
D_c/g cm^{-3}	1.194
μ/mm^{-1}	0.208
R_1[a]($I > 2\sigma$)	0.0654
wR_2[b] (all data)	0.1530
GOF	1.143

2) X-ray Crystallographic Study for 18

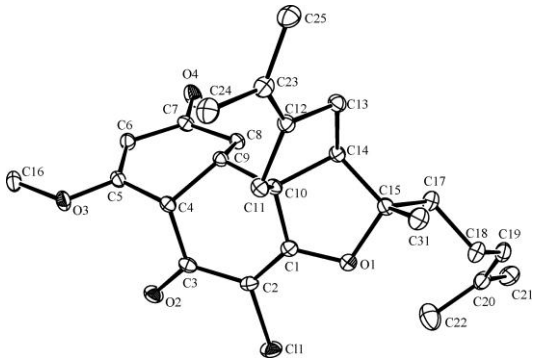


Figure S-2. X-ray structure of **18**

Table S-2. Details crystallographic data for **18**

Compound	**18**
formula	$C_{26}H_{33}ClO_4$
FW	444.97
crystal system	monoclinic
space group	P 1 21/c 1
a/Å	12.8200(5)
b/Å	14.6670(7)
c/Å	12.6709(7)
α/deg	90
β/deg	101.774(5)
γ/deg	90
V/Å^3	2332.4(2)
Z	4
D_c/g cm^{-3}	1.267
μ/mm^{-1}	0.193
R_1[a]($I > 2\sigma$)	0.0488
wR_2[b] (all data)	0.1114
GOF	1.030