Supporting Information

Dimericursones A and B: two unprecedented hexacyclic dimeric diterpenoids from the root barks of *Jatropha curcas*

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TableS1. X-ray crystallographic data for **1**

TableS1. X-ray crystallographic data for 1	
Identification code	exp_4797
Empirical formula	$C_{79}H_{90}O_8$
Formula weight	1167.50
Temperature	293(2) K
Wavelength	1.54184 Å
Crystal system	Orthorhombic
Space group	P 21 21 2
Unit cell dimensions	a = 20.7367(6) Å α= 90°. b = 19.2582(5) Å β= 90°. c = 8.3754(3) Å γ= 90°.
Volume	3344.73(18) $Å^3$
Z	2
Density (calculated)	1.159 Mg/m^3
Absorption coefficient	0.574 mm^{-1}
F(000)	1256
Crystal size	0.31 x 0.22 x 0.18 mm^3
Theta range for data collection	4.264 to 71.810°
Index ranges	-25<=h<=24, -23<=k<=14, -10<=l<=7
Reflections collected	8862
Independent reflections	5467 [R(int) = 0.0235]
Completeness to theta = 67.684°	99.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.87523
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	5467/1/431
Goodness-of-fit on F^2	1.027
Final R indices [I>2sigma(I)]	R1 = 0.0467, wR2 = 0.1216
R indices (all data)	R1 = 0.0546, wR2 = 0.1285
Flack parameter	-1.8(2)
Extinction coefficient	n/a
Largest diff. peak and hole	0.731 and -0.205 $e.Å^{-3}$

TableS2. X-ray crystallographic data for **2**

TableS2. X-ray crystallographic data for 2	
Identification code	exp_4971
Empirical formula	$C_{82}H_{92}O_8$
Formula weight	1205.55
Temperature	293(2) K
Wavelength	1.54184 Å
Crystal system	Monoclinic
Space group	P 1 21 1
Unit cell dimensions	a = 9.8979(3) Å α= 90° b = 22.3751(8) Å β= 105.896(3)° c = 16.4276(5) Å γ= 90°
Volume	3499.0(2) $Å^3$
Z	2
Density (calculated)	1.144 Mg/m^3
Absorption coefficient	0.564 mm^{-1}
F(000)	1296
Crystal size	0.35 x 0.33 x 0.31 mm^3
Theta range for data collection	3.951 to 71.790°
Index ranges	-12<=h<=11,-27<=k<=26,-19<=l<=12
Reflections collected	15730
Independent reflections	10882 [R(int) = 0.0238]
Completeness to theta = 67.684°	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.80540
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10882/5/869
Goodness-of-fit on F^2	1.031
Final R indices [I>2sigma(I)]	R1 = 0.0496, wR2 = 0.1249
R indices (all data)	R1 = 0.0580, wR2 = 0.1345
Flack parameter	0.01(15)
Extinction coefficient	n/a
Largest diff. peak and hole	0.173 and -0.212 $e.Å^{-3}$

Figure S1. ^{1}H NMR spectrum of compound **1** in $CDCl_3$

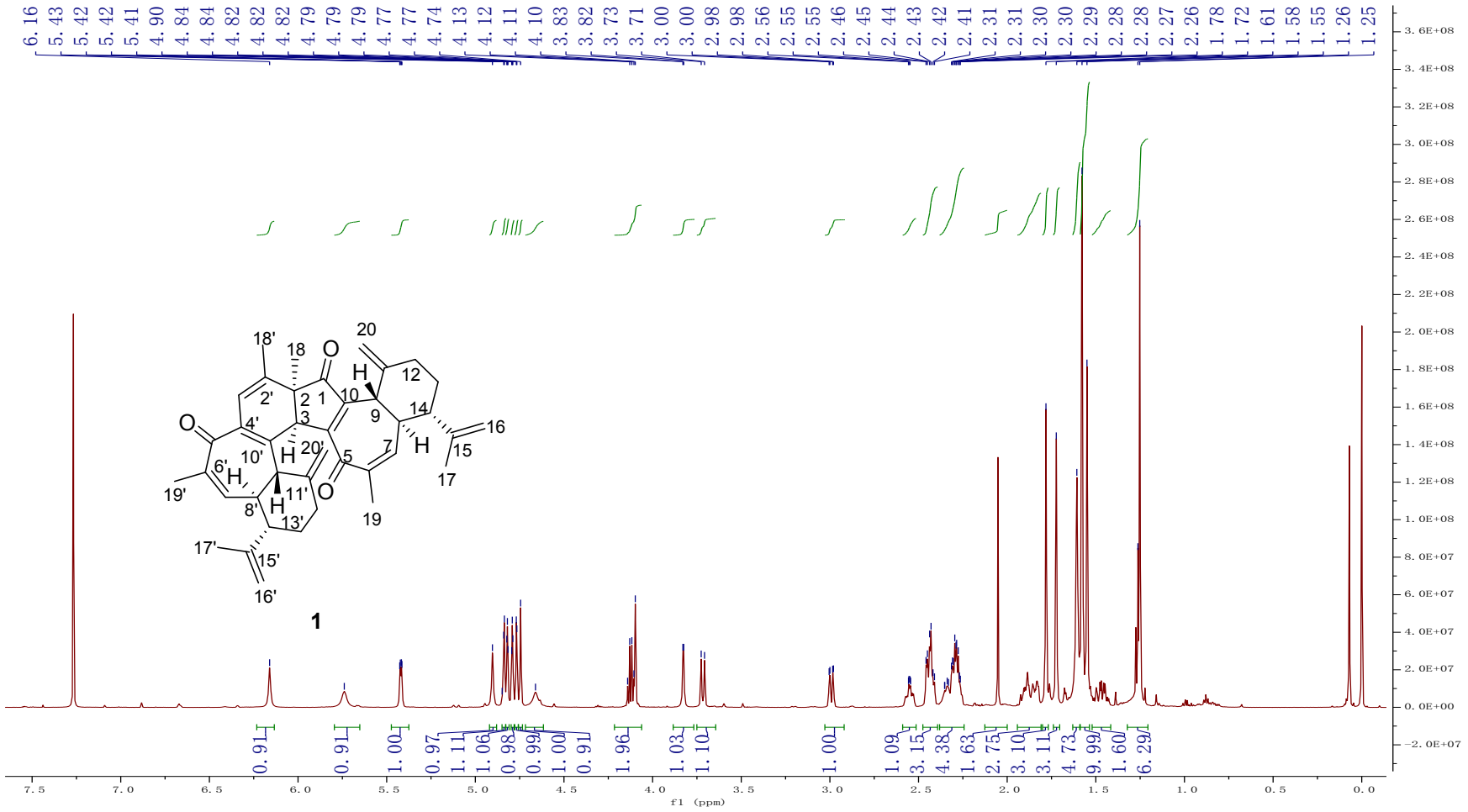


Figure S2. ^{13}C NMR spectrum of compound **1** in $CDCl_3$

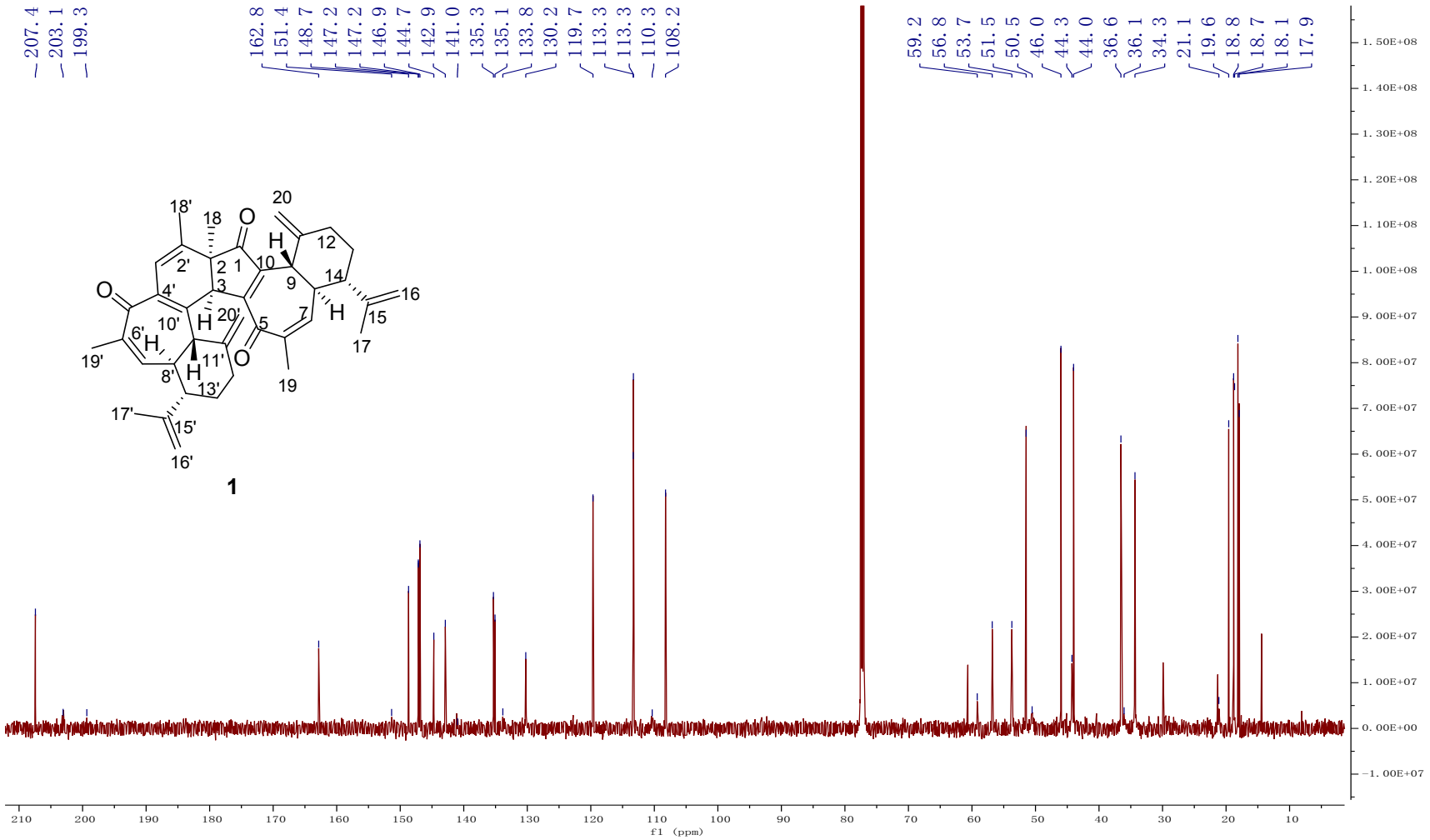


Figure S3. DEPT spectrum of compound **1** in $CDCl_3$

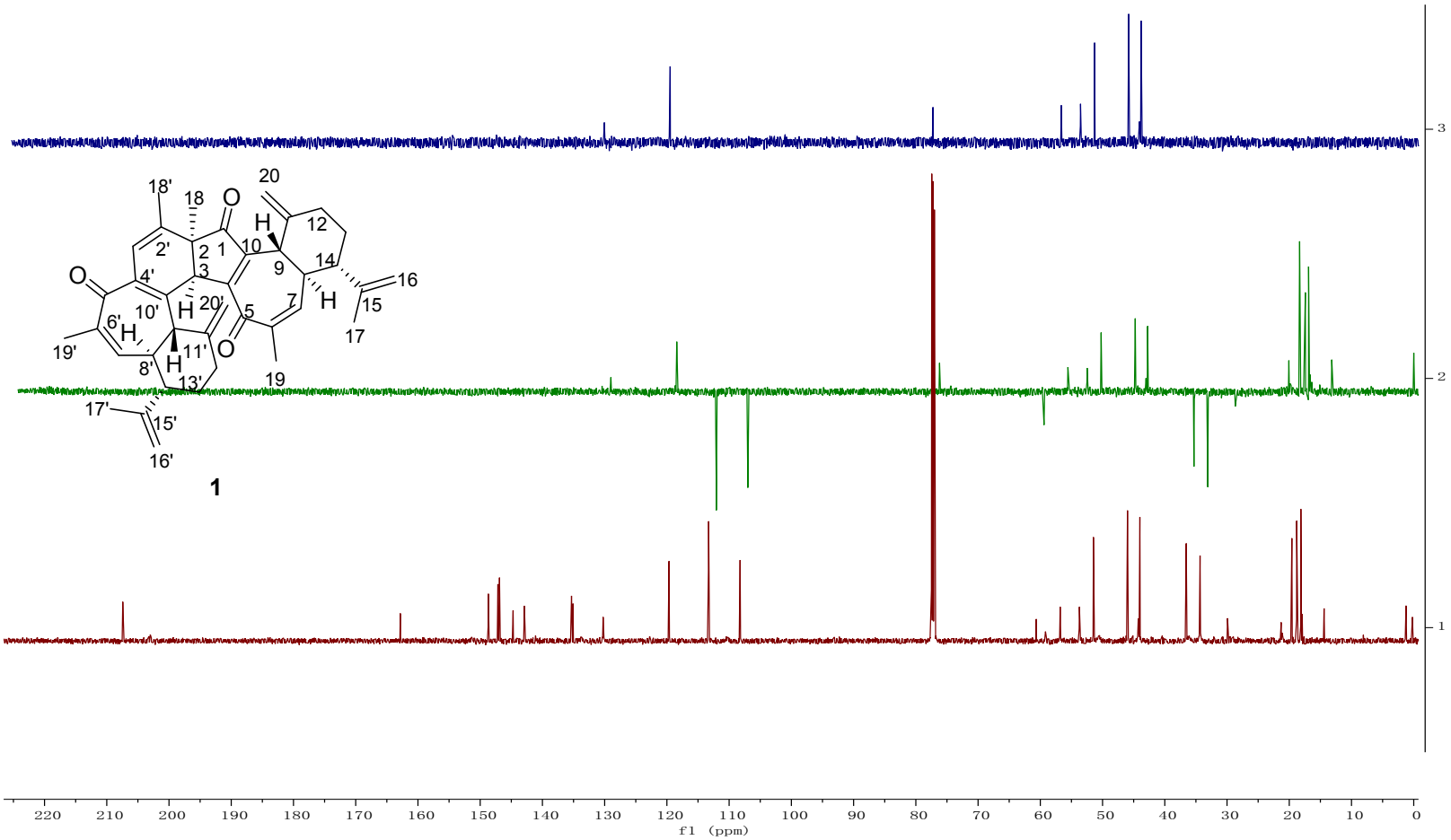


Figure S4. ^{1}H-^{1}H COSY spectrum of compound **1** in $CDCl_3$

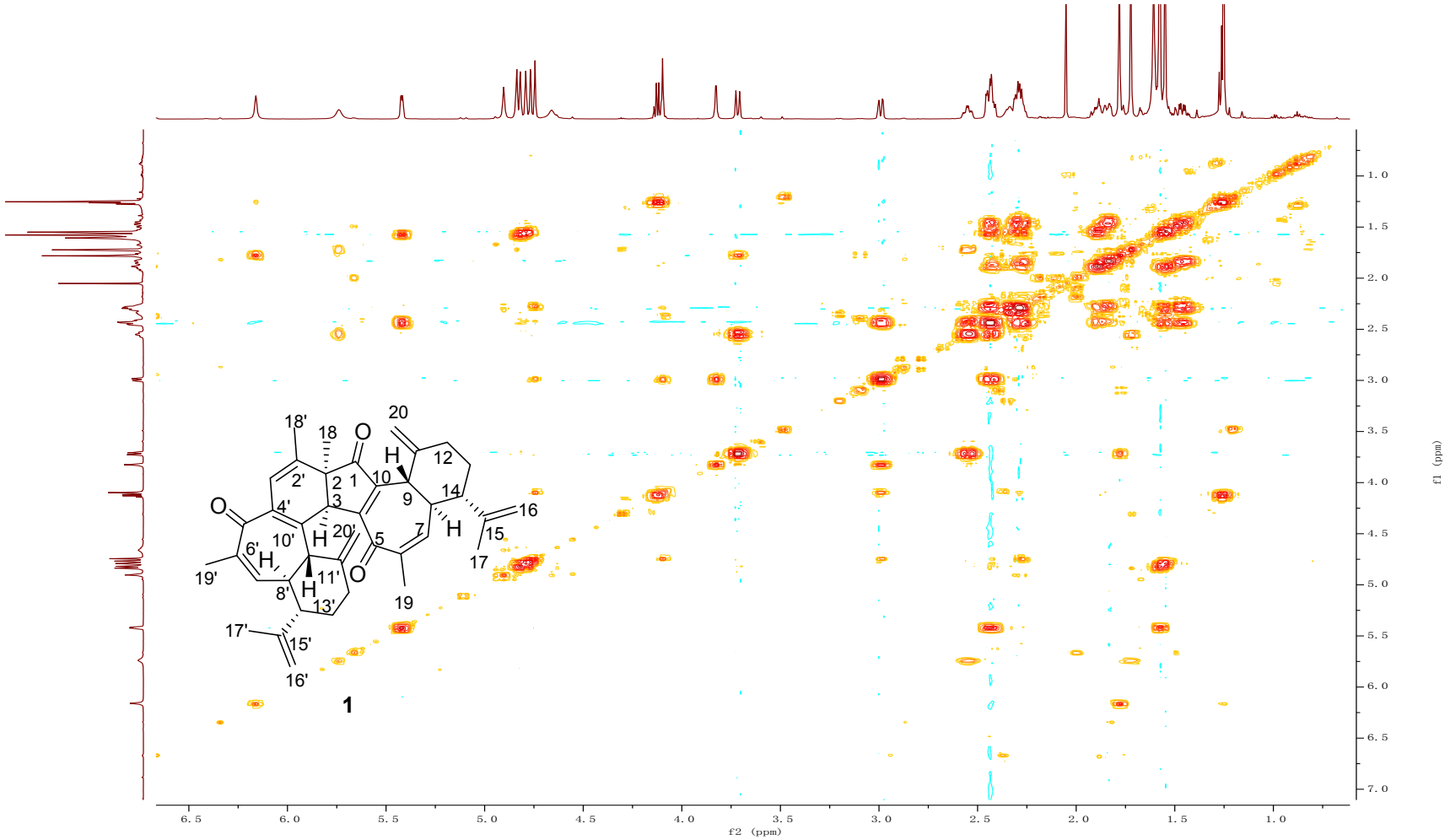


Figure S5. HSQC spectrum of compound **1** in $CDCl_3$

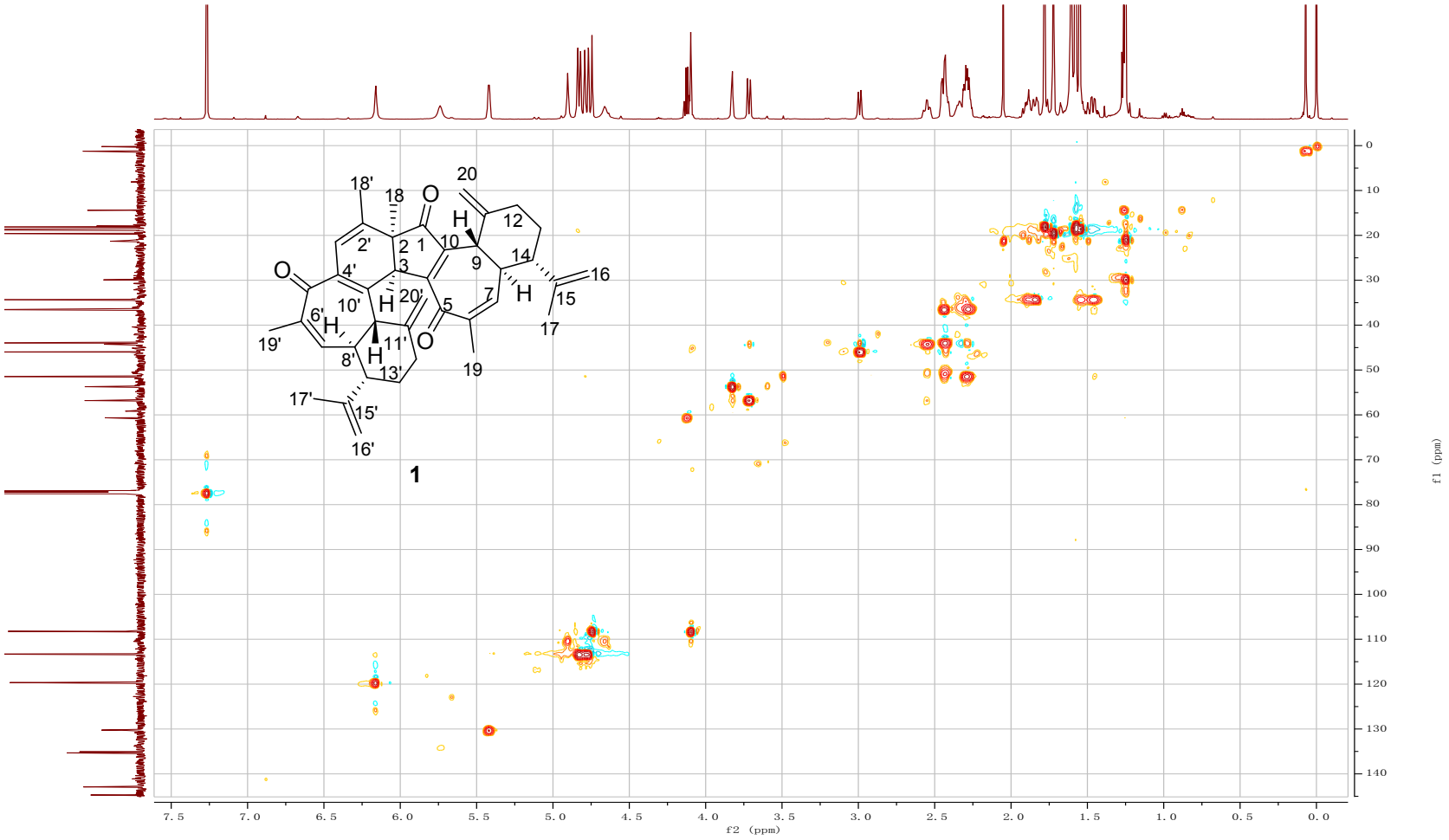


Figure S6. ROESY spectrum of compound **1** in $CDCl_3$

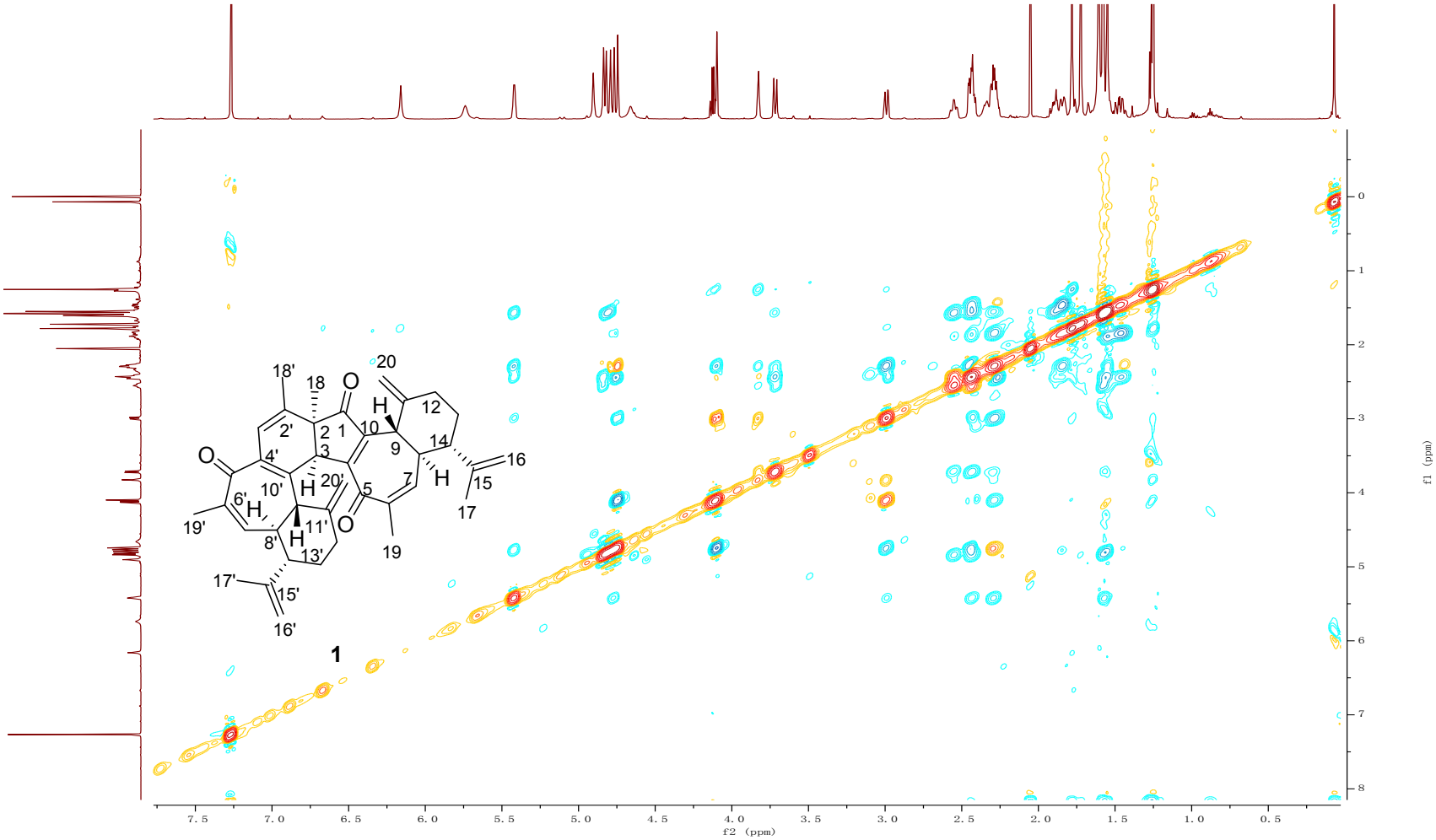


Figure S7. HMBC spectrum of compound **1** in $CDCl_3$

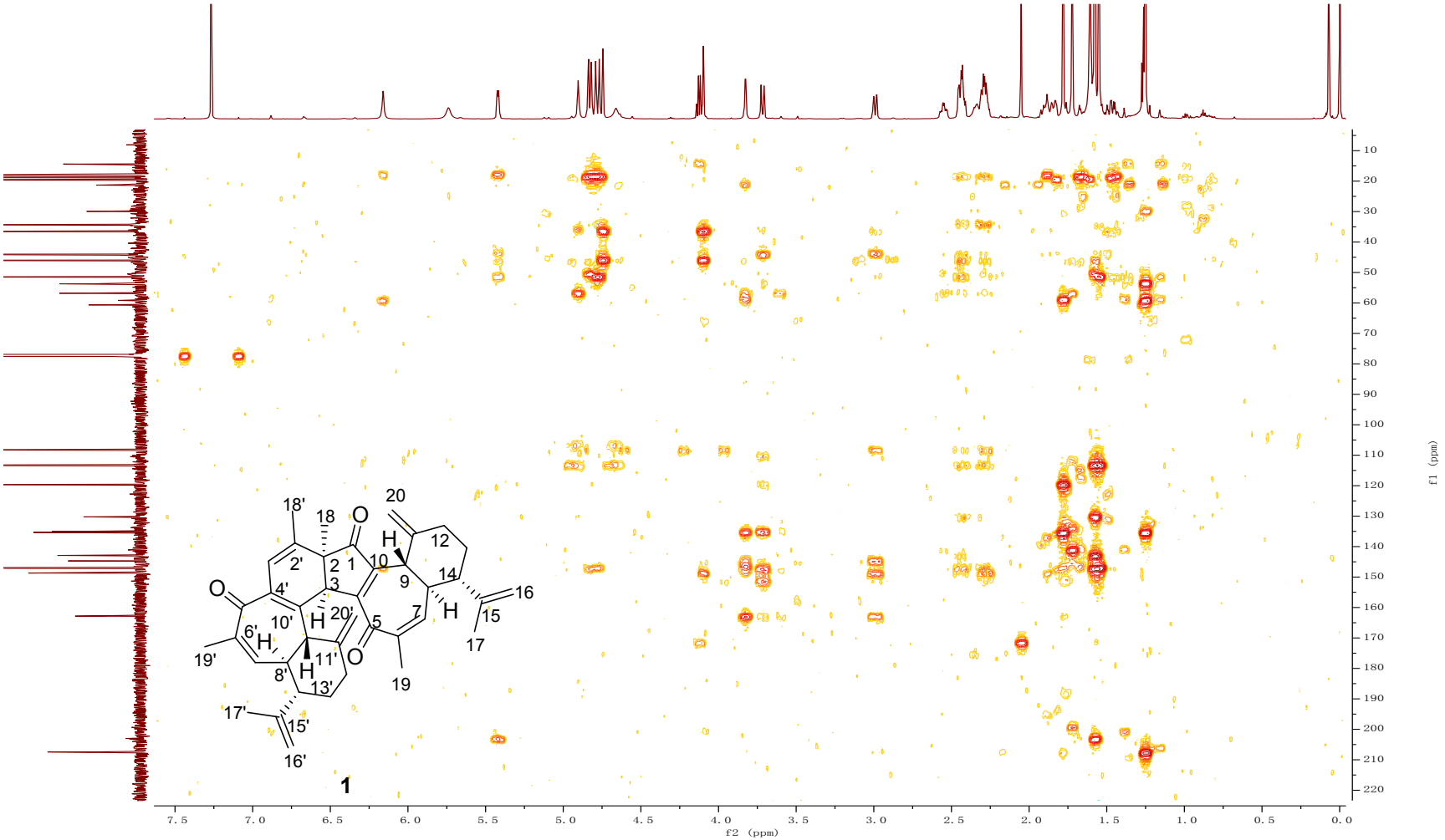


Figure S8. ^{1}H NMR spectrum of compound **2** in $CDCl_3$

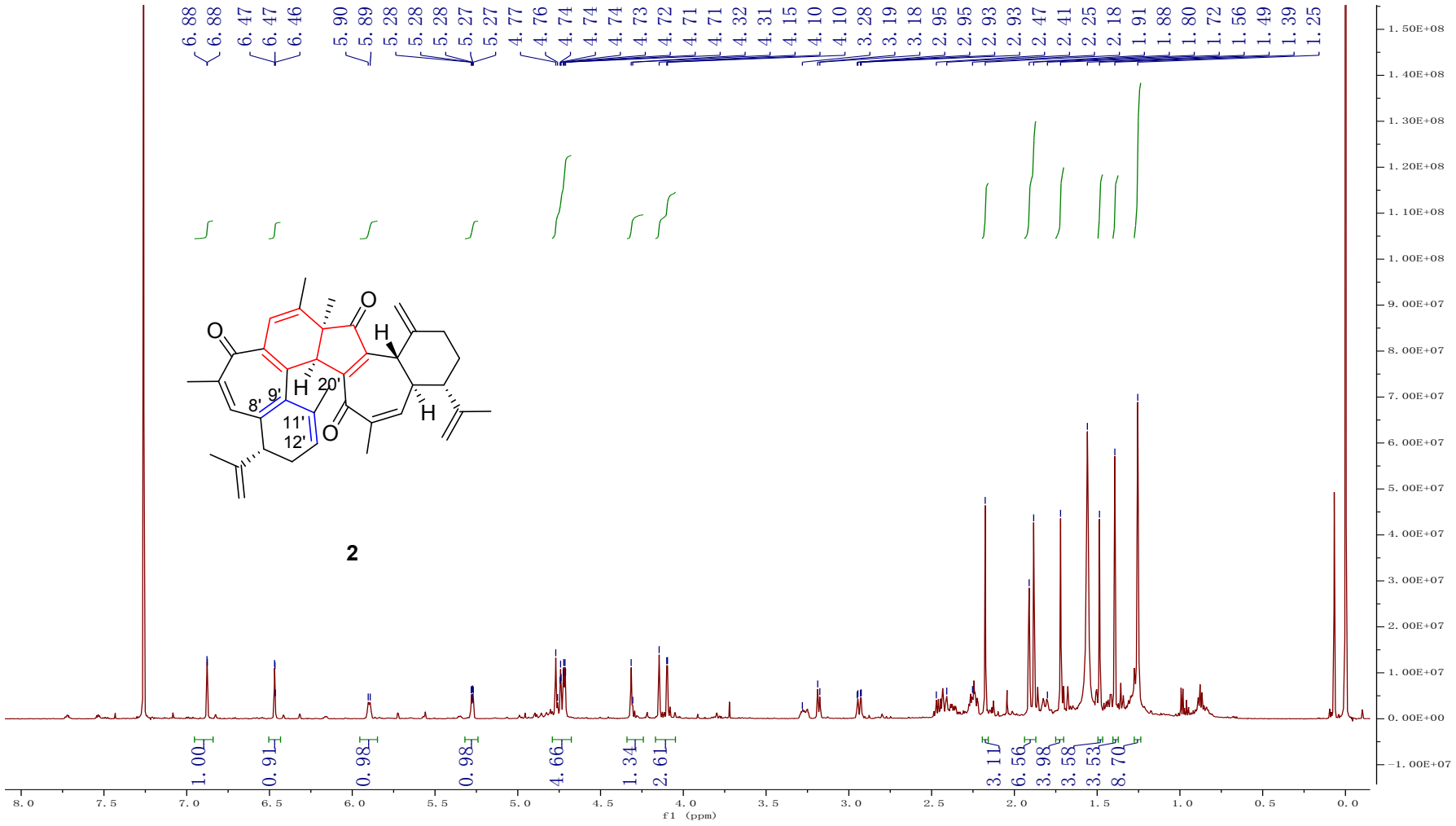

6.88
6.88
6.47
6.47
6.46
5.90
5.89
5.28
5.28
5.28
5.27
5.27
4.77
4.76
4.74
4.74
4.74
4.73
4.72
4.71
4.71
4.32
4.31
4.15
4.10
4.10
3.28
3.19
3.18
2.95
2.95
2.93
2.93
2.47
2.41
2.25
2.18
1.91
1.88
1.80
1.72
1.56
1.49
1.39
1.25
O
O
H
H
20'
8'
9'
11'
12'
O
H
2
1.00
0.91
0.98
0.98
4.66
1.34
2.61
3.11
6.56
3.98
3.58
3.53
8.70
f1 (ppm)

Figure S9. ^{13}C NMR spectrum of compound **2** in $CDCl_3$

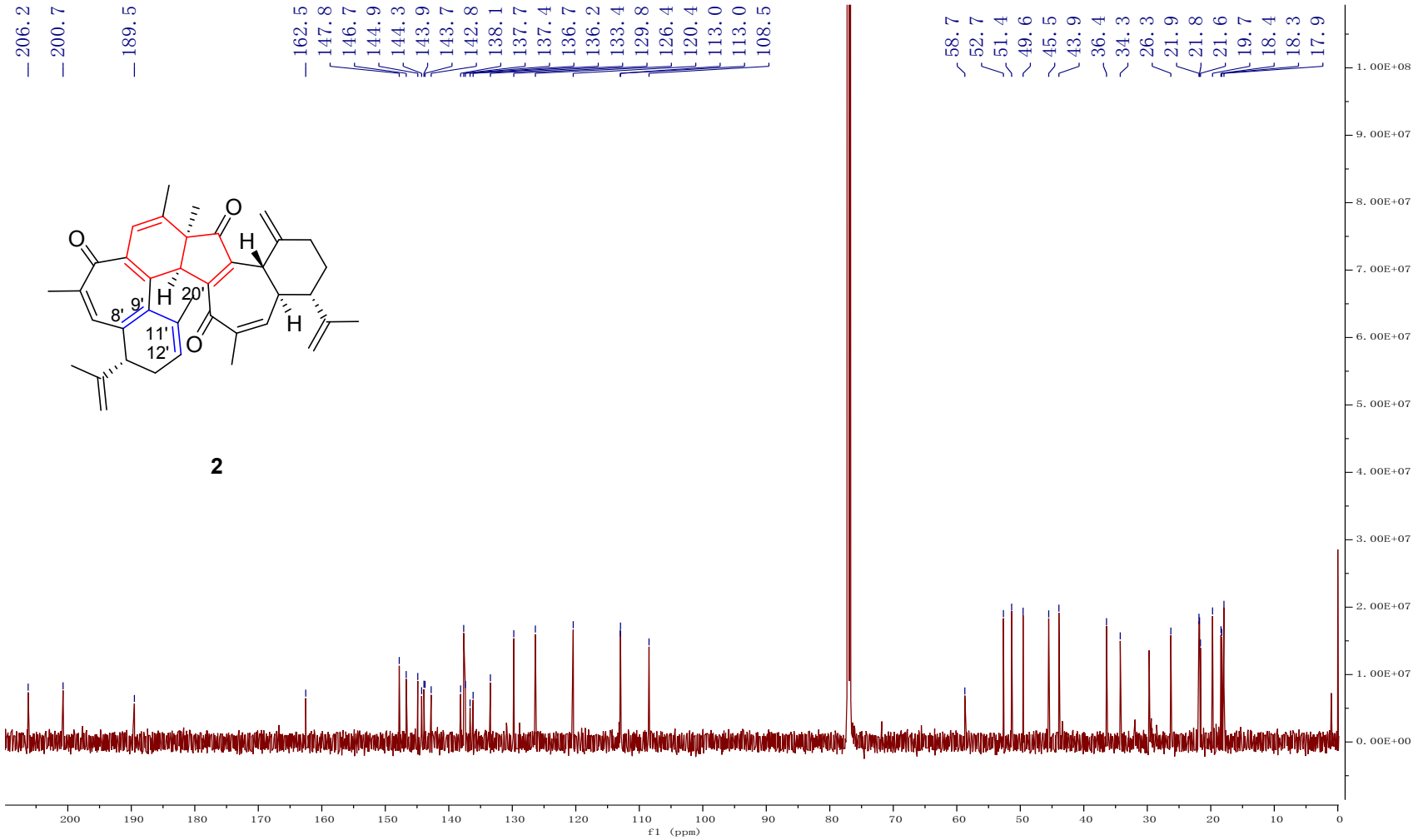


Figure S10. DEPT spectrum of compound **2** in $CDCl_3$

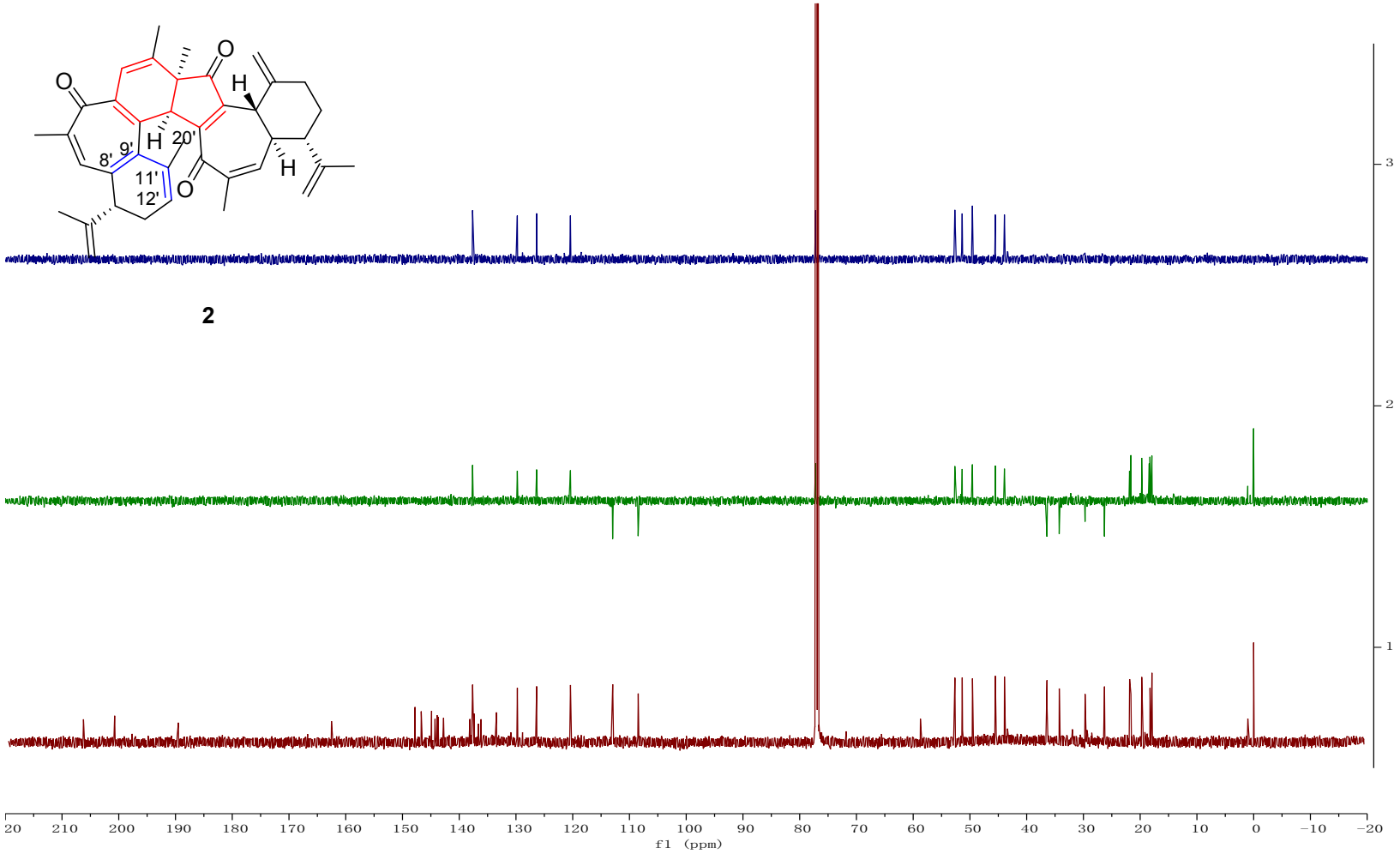


Figure S11. HSQC spectrum of compound **2** in $CDCl_3$

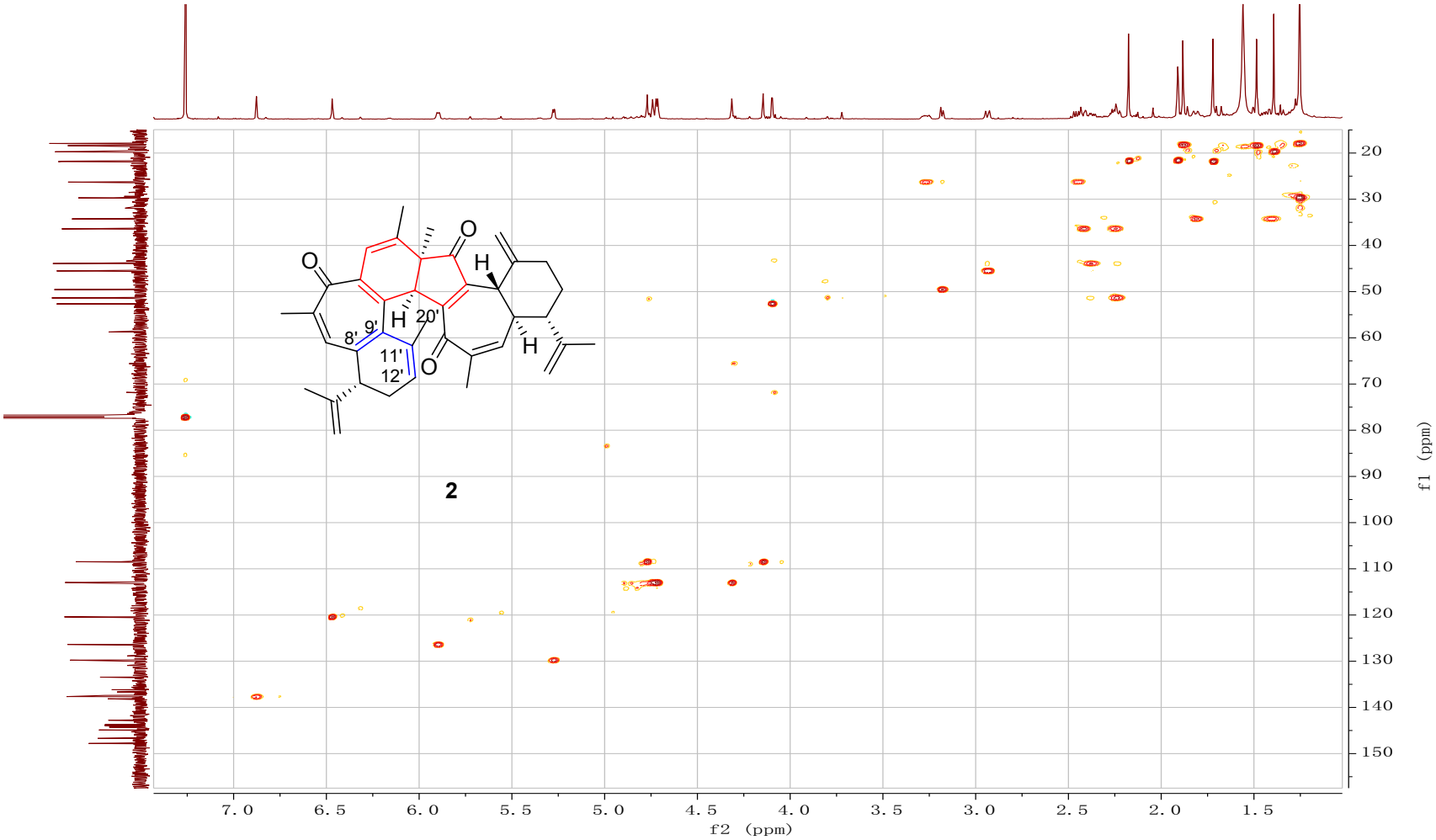


Figure S12. ^{1}H-^{1}H COSY spectrum of compound **2** in $CDCl_3$

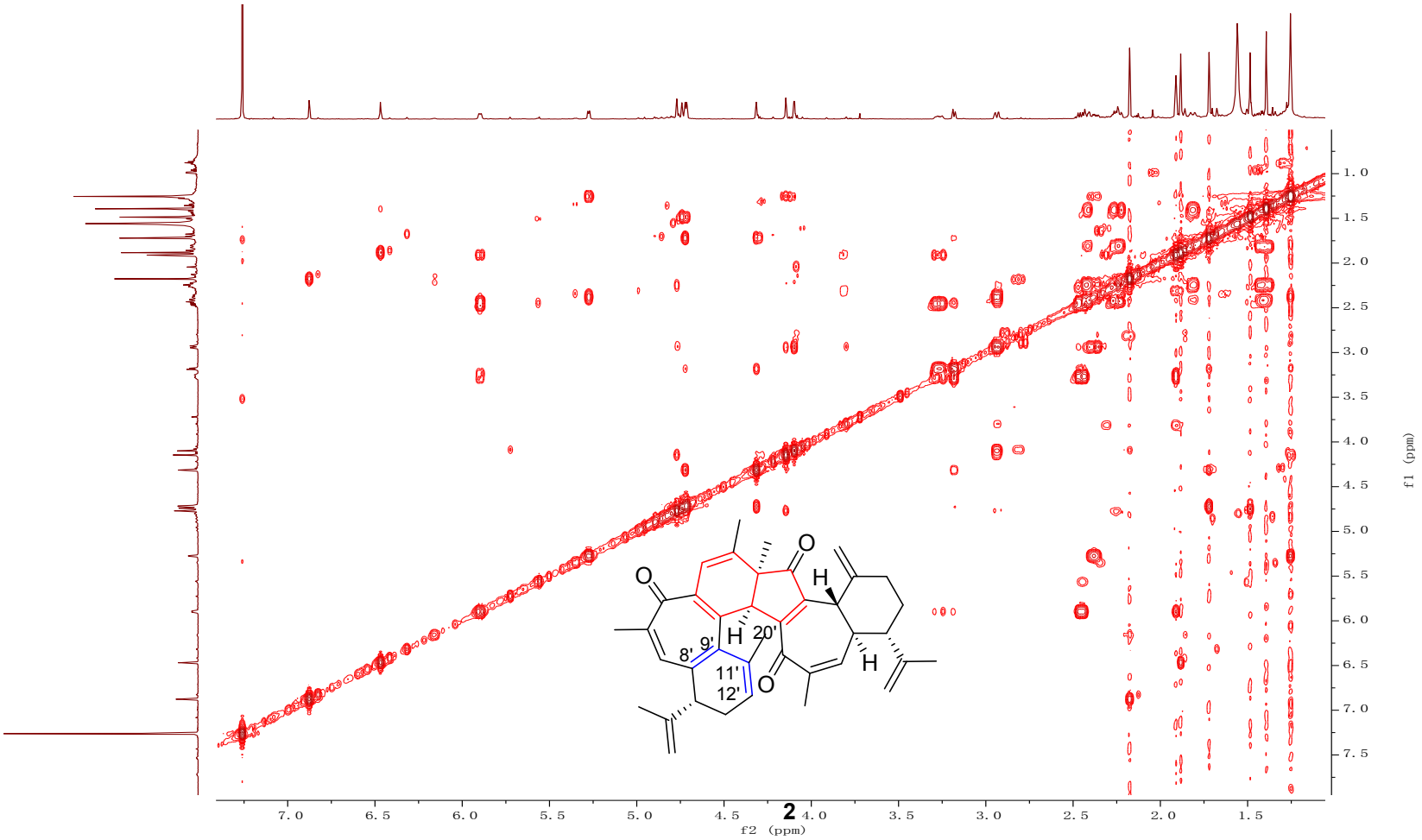


Figure S13. HMBC spectrum of compound **2** in $CDCl_3$

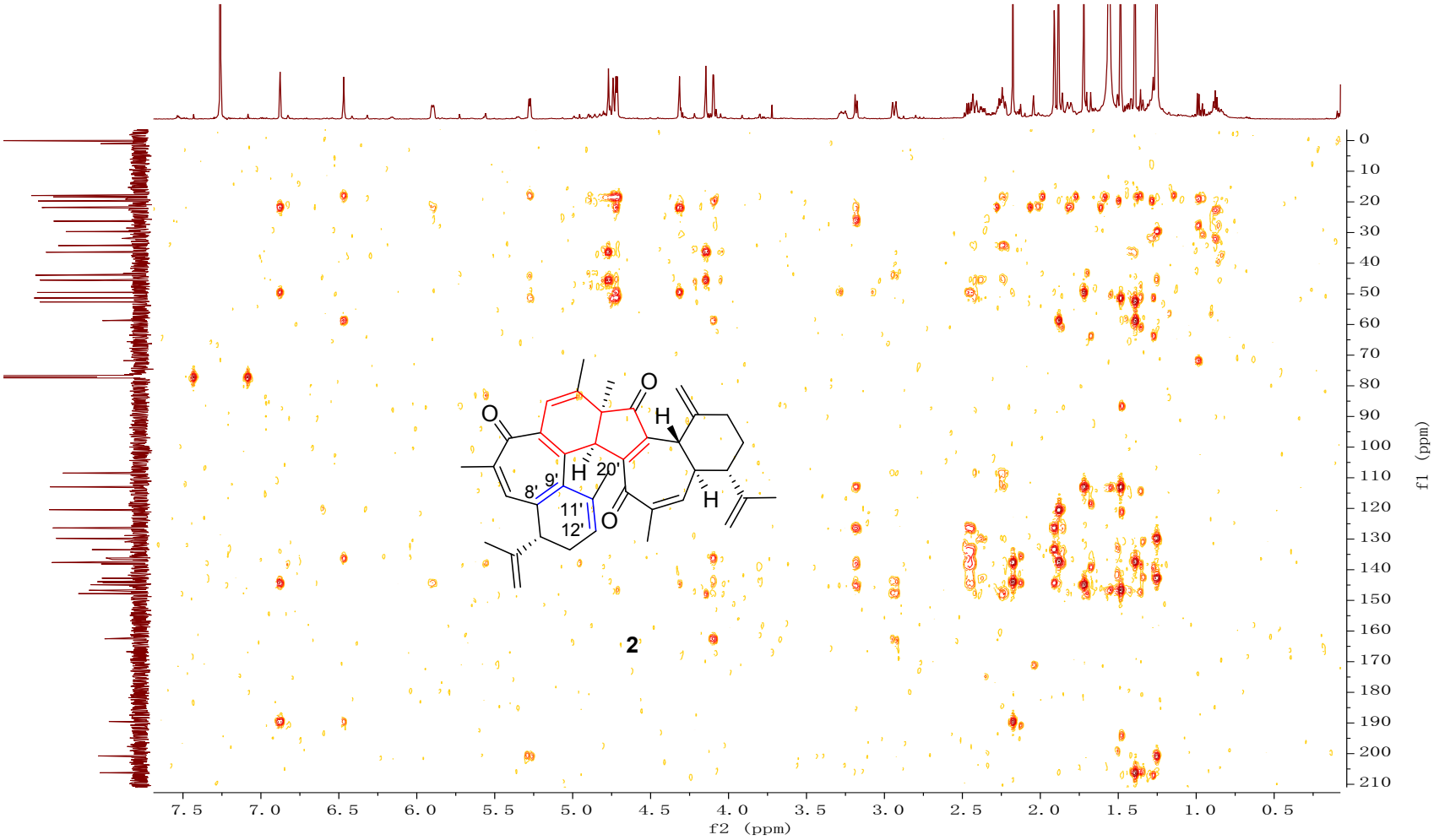
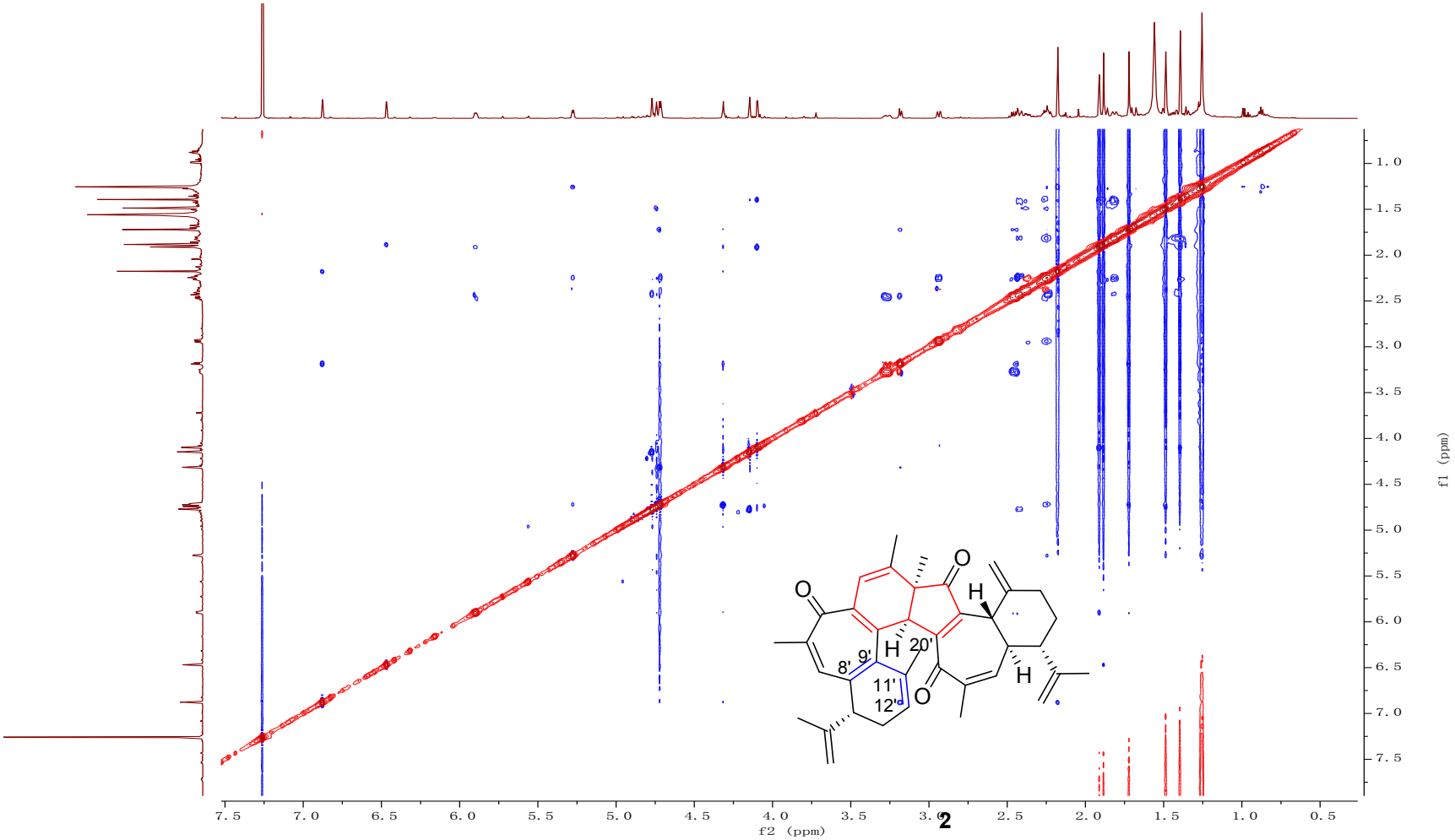


Figure S14. ROESY spectrum of compound **2** in $CDCl_3$



2

Figure S15. HRMS of compound **1**

Sample Name	Sample1	**Position**	P1-A1	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	LJQ1-1 2.d
ACQ Method	60-95%yijing5min.m	**Comment**		**Acquired Time**	11/10/2017 1:54:03 PM

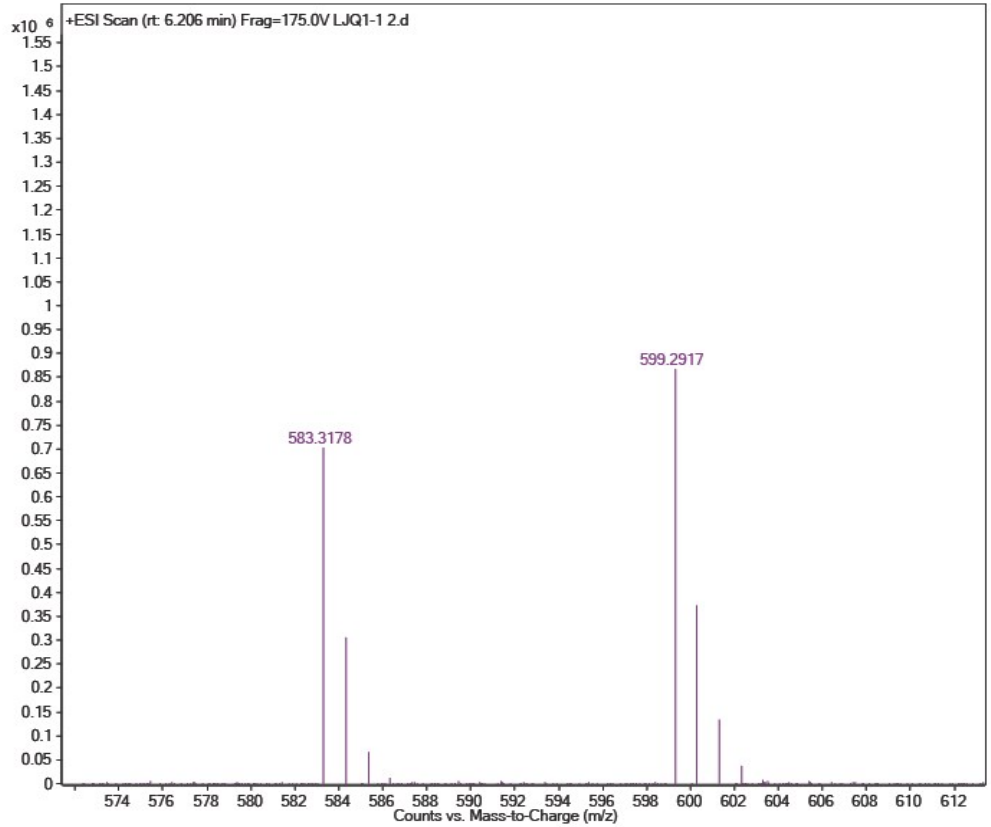


Figure S16. HRMS of compound **2**

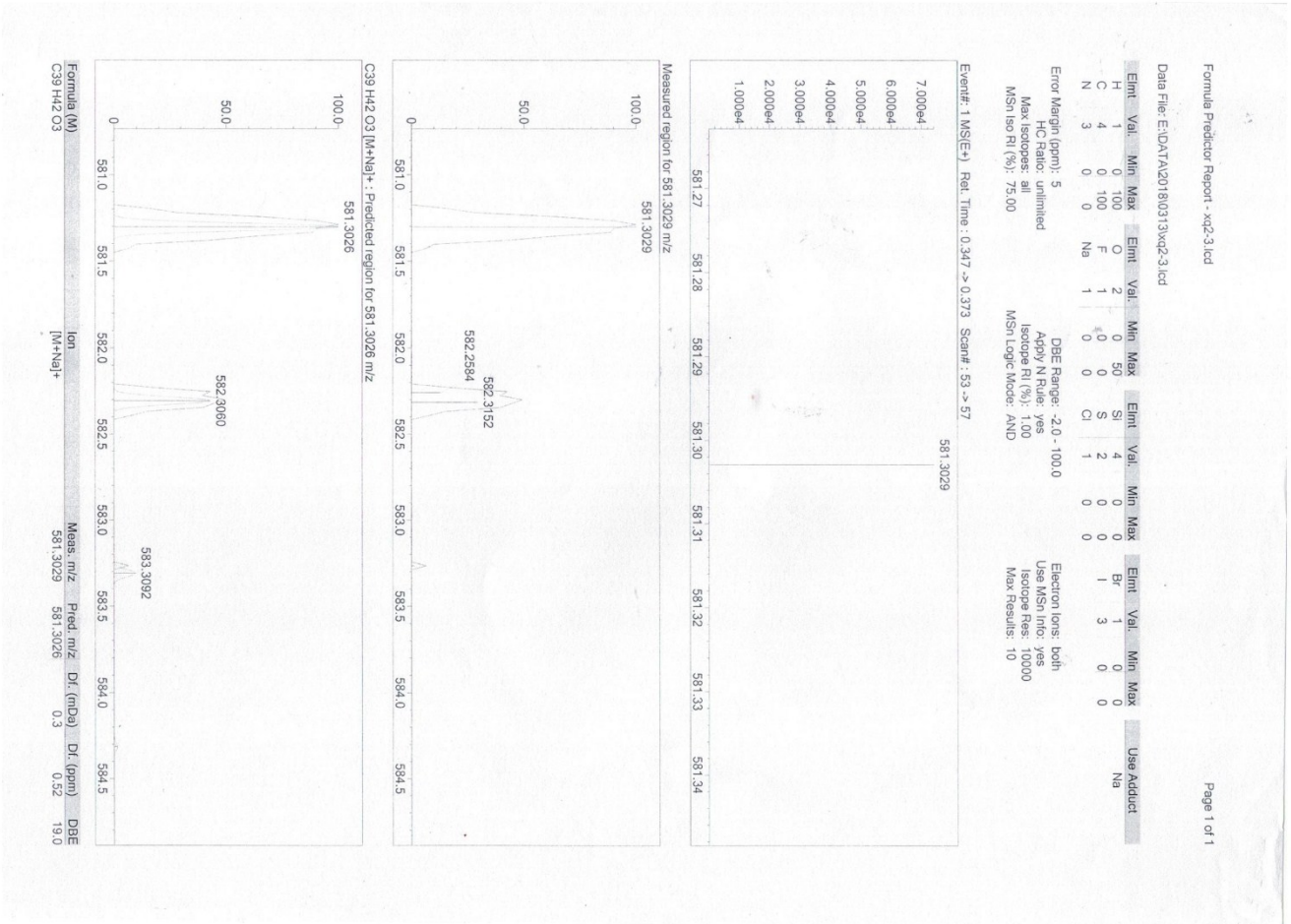


Table S3 The ^{1}H and ^{13}C NMR and the key HMBC, ^{1}H-^{1}H COSY and ROESY data for compound **1**.

	1						**1**				
no.	δ_C	δ_H (*J* in Hz)	HMBC	COSY	ROESY	*no.*	δ_C	δ_H (*J* in Hz)	HMBC	COSY	ROESY
1	207.4										
2	59.2					2′	135.3				
3	53.7	3.83 d (2.9)	18,2,2’,10’,4,10,4’	3/9	18	3′	119.7	6.16 s	2,4’,18’	3’/18’	
4	144.7					4′	135.1				
5	203.1					5′	199.3				
6	142.9					6′	141.0				
7	130.2	5.42 dd (5.5, 1.9)	5,8,9,19	7/19,7/8	17,14,8,16	7′	133.8	5.74 brs		7’/19’,7’/8’	
8	44.0	2.43 overlapped	7,9,11,13	8/9,8/14,8/7		8′	44.3	2.55 ddd (11.4, 4.5, 1.9)	9’	8’/9’,8’/14’,8’/7’	17’
9	46.0	2.99 dd (12.0, 2.9)	8,7,11,12	9/20,9/3,9/8	12,14	9′	56.8	3.72 d (11.4)	8’,11’,20’,10’,4’	9’/20’,9’/8’	12’,14’
10	162.8					10′	151.4				
11	148.7					11′	147.2				
12	36.6	2.43 overlapped	11,20,9,13,14	12/13		12′	36.1	2.44 overlapped	9’,11’,13’,14’20’	12’/13’	
		2,29 overlapped						2,29 overlapped			
13	34.3	1.86 overlapped	12,14	13/14,13/12		13′	34.3	1.86 overlapped	8’,12’	13’/14’,13’/12’	
		1.45 qd (12.8, 4.4)						1.45 qd (12.8, 4.4)			
14	51.5	2.29 overlapped	15,17,16,13	14/13,14/8		14′	50.5	2.43 overlapped	12’,13’,15’	14’/13’,14’/8’	
15	146.9					15′	147.2				
16	113.3	4.79 s	17,14,15	16/17	12	16′	113.3	4.83 s	14’,15’,17’	16’/17’	8’,12’,17’
		4.76 s						4.81 s			
17	18.7	1.55 s	14,15,16	17/16		17′	18.8	1.58 s	14’,15’,16’	17’/16’	
18	21.1	1.25 s	1,2,3,2’			18′	18.1	1.78 s	2,2’,3’		
19	17.9	1.58 s	5,6,7	19/7		19′	19.6	1.72 s	5’,6’,7’	19’/7’	
20	108.2	4.66 s	9,11,12	20/9	9,12	20′	110.3	4.90 s	9’,11’,12’	20’/9’	
		4.10 s						4.66 s			

[a] NMR data (δ) were measured at 600 MHz for ^{1}H and at 150 MHz for ^{13}C in $CDCl_3$. Proton coupling constants (*J*) In Hz are given in parentheses.

Table S4 The ^{1}H and ^{13}C NMR and the key HMBC, ^{1}H-^{1}H COSY and ROESY data for compound **2**.

	2						**2**				
no.	δ_C	δ_H (*J* in Hz)	HMBC	COSY	ROESY	*no.*	δ_C	δ_H (*J* in Hz)	HMBC	COSY	ROESY
1	206.2										
2	58.7					2′	137.4				
3	52.7	4.10 d (2.8)	18,2,10’ 4,10,4’	3/9	18	3′	120.4	6.47 d (1.5)	2,4’,18’,5’	3’/18’	
4	136.2					4′	136.7				
5	200.7					5′	189.5				
6	142.8					6′	143.9				
7	129.8	5.28 dd (5.7, 1.8)	5,8,9,19	7/19,7/8	17,14,8,16	7′	137.7	6.88 s	5’,9’,6’,14’,19’	7’/19’	
8	43.9	2.38 overlapped	7,9,11,13	8/9,8/14,8/7		8′	138.1				
9	45.5	2.93 dd (12.1, 2.7)	8,7,11,12	9/20,9/3,9/8	12,14	9′	144.3				
10	162.5					10′	143.7				
11	147.8					11′	133.4				
12	36.4	2.41 overlapped	11,20,9,13,14	12/13		12′	126.4	5.90 d (7.3)	9’, 20’	12’/13’,12’/20’	
		2.24 overlapped									
13	34.3	1.81 m	12,14	13/14,13/12		13′	26.3	3.27 m	8’,12’	13’/14’,13’/12’	
		1.41 m						2.44 overlapped			
14	51.4	2.24 overlapped	15,17,16,13	14/13,14/8		14′	49.6	3.18 d (7.8)	8’,9’,12’,13’,15’,16’	14’/13’	
15	146.7					15′	144.9				
16	113.0	4.31 s	17,14,15	16/17	12	16′	113.0	4.31 s	14’,15’,17’	16’/17’	8’,12’,17’
		4.72 s						4.72 s			
17	18.4	1.48 s				17′	21.9	1.72 s	14’,15’,16’	17’/16’	
18	19.7	1.39 s				18′	18.3	1.88 s	2,2’,3’		
19	17.9	1.25 s				19′	21.8	2.17 s	5’,6’,7’	19’/7’	
20	108.5	4.14 s				20′	21.6	1.91 s	9’,11’,12’	20’/9’	
		4.77 s									

[a] NMR data (δ) were measured at 600 MHz for ^{1}H and at 150 MHz for ^{13}C in $CDCl_3$. Proton coupling constants (*J*) In Hz are given in parentheses.