Biomimetic Synthesis of C_{23} Terpenoids: Structural Revision of Salyunnanin A and Confirmation of Hassanane

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Supporting information

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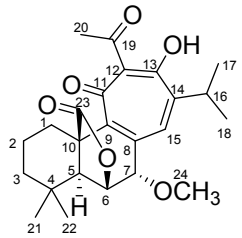
1. **General information:** All moisture or oxygen-sensitive reactions were carried out under an argon atmosphere in oven flasks. Solvents were purified and dried by standard methods prior to use. All commercially available reagents were used without further purification unless otherwise noted. Column chromatography was performed on silica gel (200–300 mesh). NMR spectra were recorded on Bruker 400 MHz and Oxford 600 MHz spectrometers in $CDCl_3$, acetone d_6 or methanol d_4. Chemical shifts are reported as δ values relative to internal chloroform (δ 7.26 for ^{1}H NMR and 77.16 for ^{13}C NMR), acetone-d_6 (δ 2.05 for ^{1}H NMR and 29.84 for ^{13}C NMR) and methanol d_4 (δ 3.31 for ^{1}H NMR and 49.00 for ^{13}C NMR). High resolution mass spectra (HRMS) were obtained on a 4G mass spectrometer by using electrospray ionization (ESI) analyzed by quadrupole time-of-flight (Q-TOF). Optical rotations were measured on a Rudolph Autopol IV polarimeter. The IR spectra were recorded on

Nicolet Nexus 670 FT-IR spectrometer. The X-ray single-crystal determination was performed on an Agilent SuperNova single crystal X-ray diffractometer.

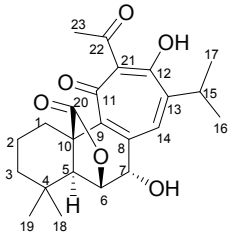
2. Comparison of the Spectra and Data of Natural and Synthetic (+)-Salyunnain A and (+)-Hassanane



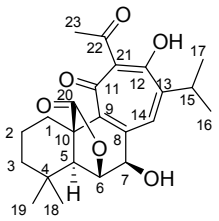
(+)-Hassanane (**6**)

Position	nature sample δ (J in Hz)	synthetic sample δ (J in Hz)	Δ_{n-s}	nature sample δ	synthetic sample δ	Δ_{n-s}
1α	2.75 (d, 13.3, 1H)	2.84 (d, 12.8, 1H)	-0.09	26.40 (t)	26.54	-0.14
1β		1.14-1.11 (m, 1H)				
2α		1.61-1.54 (m, 1H)		18.60 (t)	18.75	-0.15
2β		1.61-1.54 (m, 1H)				
3α		1.48-1.45 (m, 1H)		38.14 (t)	38.28	-0.14
3β		1.18-1.16 (m, 1H)				
4				31.34 (q)	31.37	-0.03
5	2.03 (s, 1H)	2.02 (s, 1H)	0.01	50.18 (d)	50.32	-0.14
6	4.63 (d, 1.8, 1H)	4.62 (d, 2.8, 1H)	0.01	73.02 (d)	73.15	-0.13
7	4.01 (d, 1.8, 1H)	4.00 (d, 2.8, 1H)	0.01	79.45 (d)	79.59	-0.14
8				132.07 (s)	132.23	-0.16
9				146.62 (s)	146.76	-0.14
10				45.83 (s)	45.97	-0.14
11				189.11 (s)	189.29	-0.18
12				119.82 (s)	119.96	-0.14
13				175.71 (s)	175.87	-0.16
14				149.08 (s)	149.23	-0.15
15	6.56 (s, 1H)	6.55 (s, 1H)	0.01	132.00 (s)	132.15	-0.15
16	3.29 (hept, 6.8, 1H)	3.32-3.25 (m, 1H)		30.20 (d)	30.34	-0.14
17	1.24 (d, 6.8, 3H)	1.23 (d, 6.8, 3H)	0.01	22.76 (q)	22.92	-0.16
18	1.09 (d, 6.8, 3H)	1.08 (d, 6.8, 3H)	0.01	22.34 (s)	22.50	-0.16
19				203.12 (s)	203.30	-0.18
20	2.46 (s, 3H)	2.46 (s, 3H)	0.00	28.08 (q)	28.26	-0.18
21	1.01 (s, 3H)	1.00 (s, 3H)	0.01	31.34 (q)	31.49	-0.15

22	0.93 (s, 3H)	0.92 (s, 3H)	0.01	21.88 (q)	22.04	-0.16
23				175.41 (s)	175.59	-0.18
24	3.65 (s, 3H)	3.64 (s, 3H)	0.01	59.19 (q)	59.35	-0.16



(+)-Salyunnanin A (**2**)



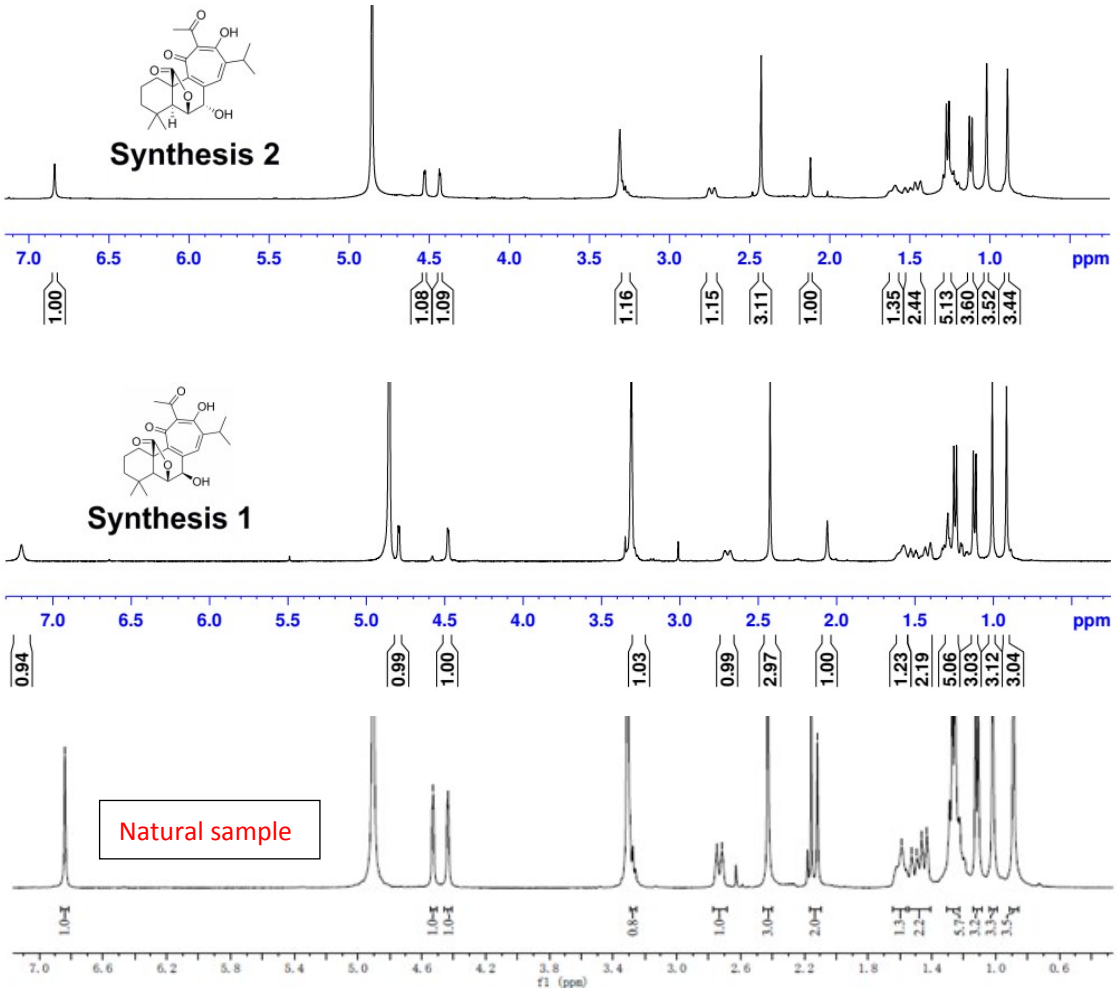
7-epi-Salyunnanin A (**1**)

Position	nature sample δ (J in Hz)	Synthetic sample **2** δ (J in Hz)	Δ_{n-s2}	Synthetic sample **1** δ (J in Hz)	Δ_{n-s1}
1α	2.72 (d, 13.2, 1H)	2.74 (d, 13.2, 1H)	-0.02	2.70 (d, 13.2, 1H)	0.02
1β	1.27-1.25 (m,1H)[1]	1.27-1.25 (m, 1H)		1.33-1.29 (m, 1H)	
2α	1.59 (m,1H)	1.62-1.59 (m,1H)		1.61-1.57 (m,1H)	
2β	1.51 (m,1H)	1.53-1.43 (m,1H)		1.53-1.40 (m,1H)	
3α	1.44 (m,1H)	1.53-1.43 (m,1H)		1.53-1.40 (m,1H)	
3β	1.27-1.25 (m, 1H) [1]	1.27-1.25 (m, 1H)		1.33-1.29 (m, 1H)	
4					
5	2.11 (s, 1H)	2.12 (s, 1H)	-0.01	2.06 (s, 1H)	0.05
6	4.52 (d, 3.0, 1H)	4.53 (d, 2.8, 1H)	-0.01	4.79 (d, 2.8, 1H)	-0.27
7	4.43 (d, 3.0, 1H)	4.43 (d, 2.8, 1H)	0.00	4.48 (d, 2.4, 1H)	-0.05
8					
9					
10					
11					
12					
13					
14	6.83 (s, 1H)	6.84 (s, 1H)	-0.01	7.20 (s, 1H)	-0.37
15	3.25 (sept, 6.6, 1H)	3.29-3.26 (m, 1H)		3.29-3.27 (m, 1H)	
16	1.11 (d, 6.6, 3H)	1.12 (d, 6.8, 3H)	-0.01	1.12 (d, 6.8, 3H)	-0.01
17	1.25 (d, 6.6, 3H)	1.26 (d, 6.8, 3H)	-0.01	1.24 (d, 6.8, 3H)	0.01
18	1.01 (s, 3H)	1.02 (s, 3H)	-0.01	1.01 (s, 3H)	0.00
19	0.88 (s, 3H)	0.89 (s, 3H)	-0.01	0.92 (s, 3H)	-0.04
20					
21					
22					
23	2.42 (s, 3H)	2.43 (s, 3H)	-0.01	2.42 (s, 3H)	0.00

[1] Recording error by isolated author.

Position	nature sample δ	synthetic sample **2** δ	Δ_{n-s2}	synthetic sample **1** δ	Δ_{n-s1}
1α	27.4	27.5	-0.1	26.5	0.9
1β					
2α	19.6	19.7	-0.1	18.6	1.0
2β					
3α	39.1	39.1	0.0	38.0	1.1
3β					
4	32.1	32.2	-0.1	31.8	0.3
5	50.8	50.8	0.0	55.2	-4.4
6	78.6	78.7	-0.1	77.4	1.2
7	71.1	71.1	0.0	70.1	1.0
8	135.5	135.6	-0.1	133.9	1.6
9	149.8	149.8	0.0	149.1	0.7
10	47.1	47.2	-0.1	47.3	-0.2
11	190.8[1]	190.9	-0.1	189.1	1.7
12	175.7	175.7	0.0	175.4	0.3
13	147.5	147.6	-0.1	145.7	1.8
14	134.2	134.3	-0.1	130.2	4.0
15	31.6	31.6	0.0	30.7	0.9
16	22.1	22.2	-0.1	22.8	-0.7
17	22.5	22.6	-0.1	22.8	-0.3
18	31.5	31.6	-0.1	31.6	-0.1
19	23.0	23.1	-0.1	21.9	1.1
20	178.0	178.0	0.0	175.6	2.4
21	120.8	120.8	0.0	119.8	1.0
22	204.6	204.7	-0.1	203.2	1.4
23	28.3	28.5	-0.2	28.3	0.0

[1] **2**-C-MeOD, **1**-C-$CDCl_3$.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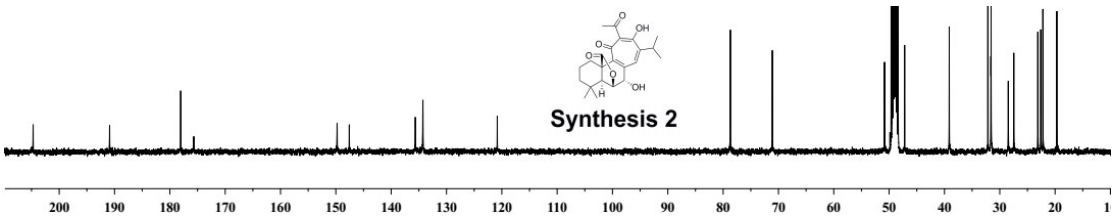
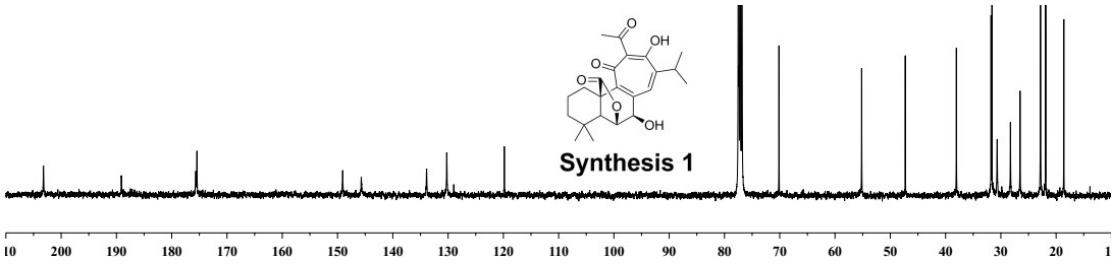
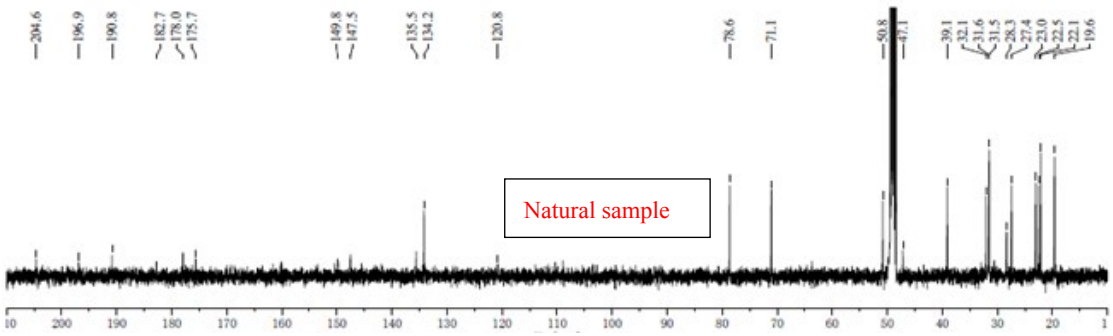
1.00 1.08 1.09 1.16 1.15 3.11 1.00 1.35 2.44 5.13 3.60 3.52 3.44
Synthesis 1
7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
0.94 0.99 1.00 1.03 0.99 2.97 1.00 1.23 2.19 5.06 3.03 3.12 3.04
Natural sample
f1 (ppm)


Synthesis 2


Synthesis 1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149.8
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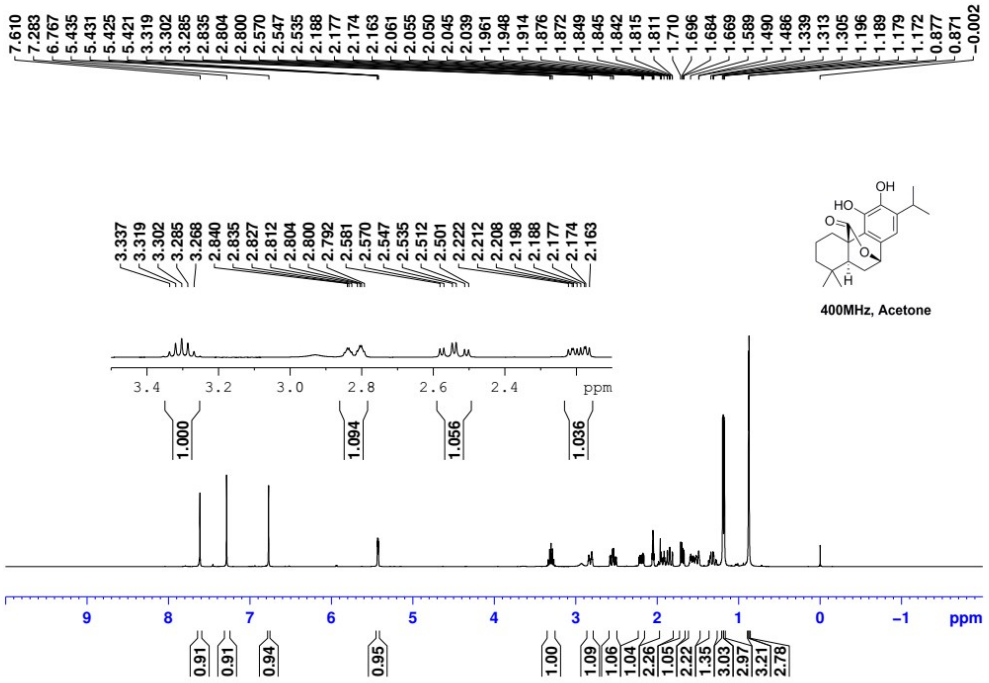
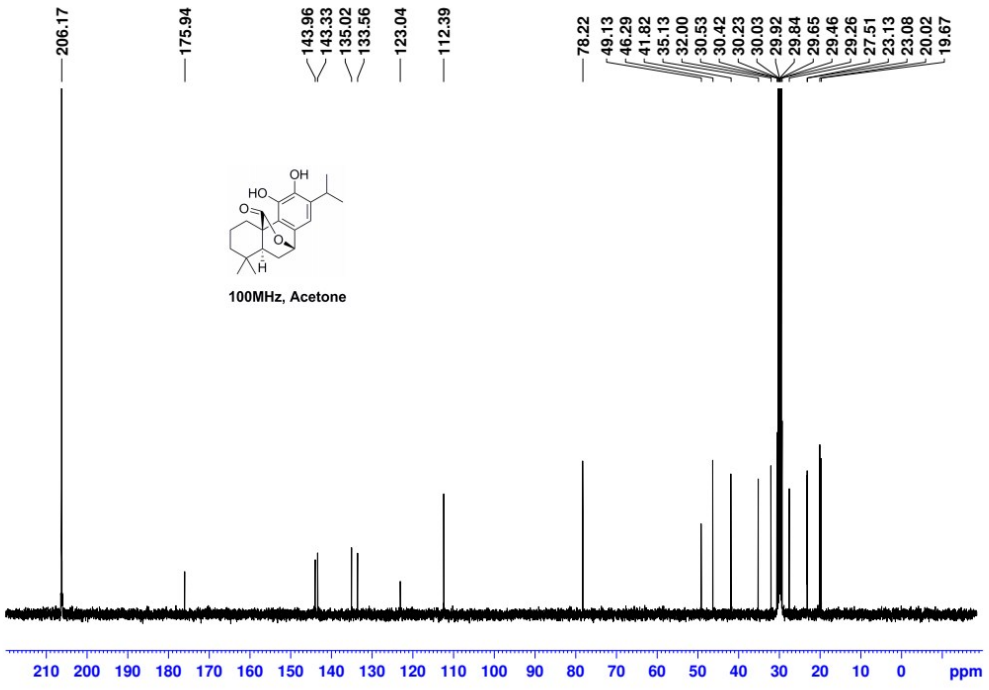
78.6
71.1
50.8
47.1
39.1
32.1
31.6
31.5
28.3
27.4
23.0
22.5
22.1
19.6
Natural sample

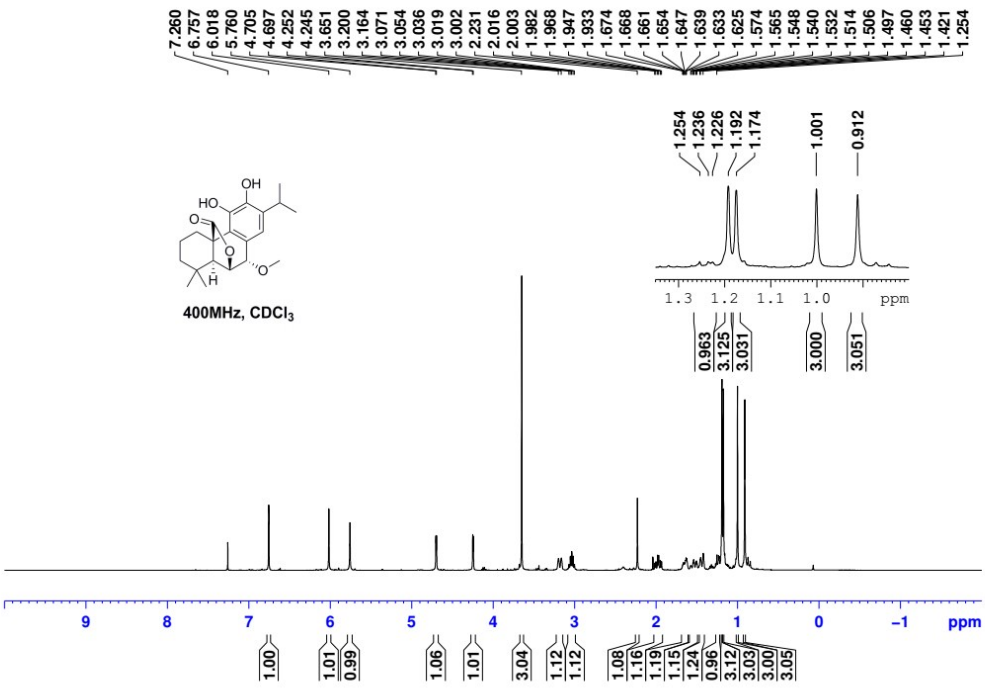
3 ^{1}H and ^{13}C NMR spectra of new compounds

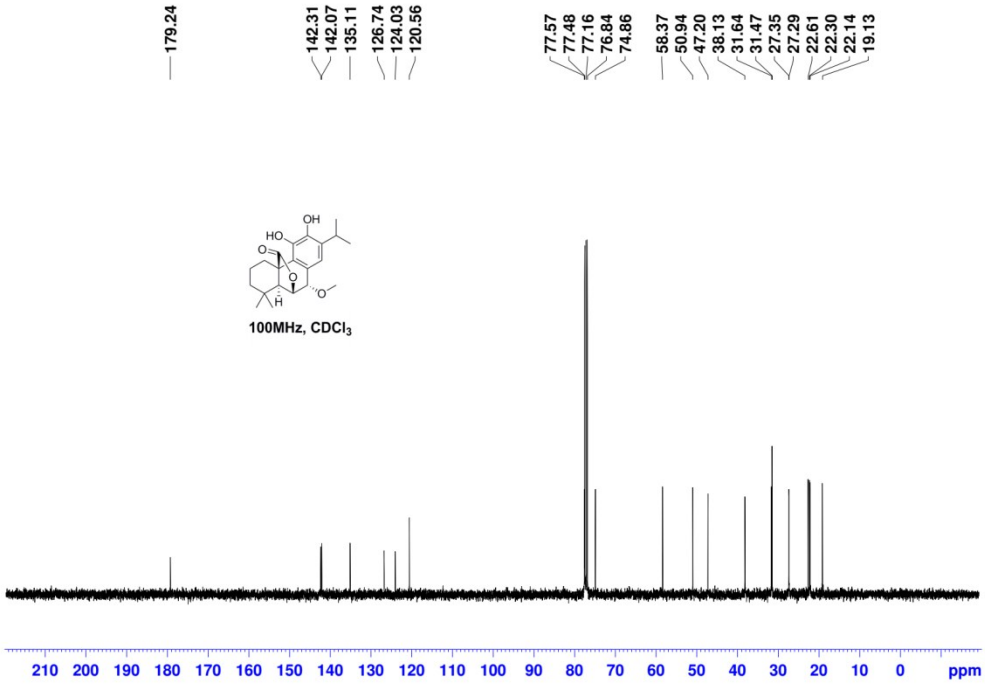
^{1}H and ^{13}C NMR spectra of compound **15**:



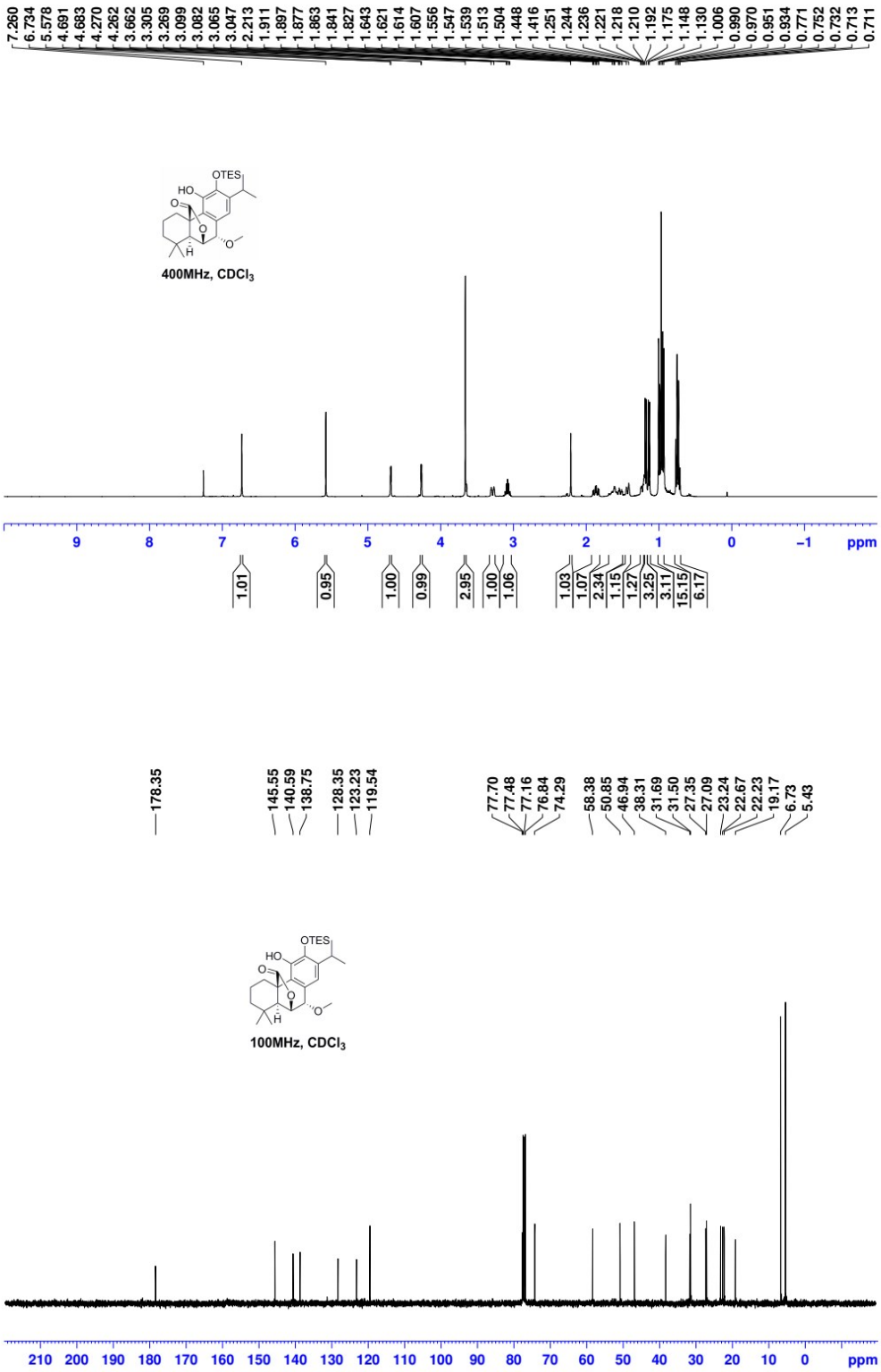


^{1}H and ^{13}C NMR spectra of compound **14**:

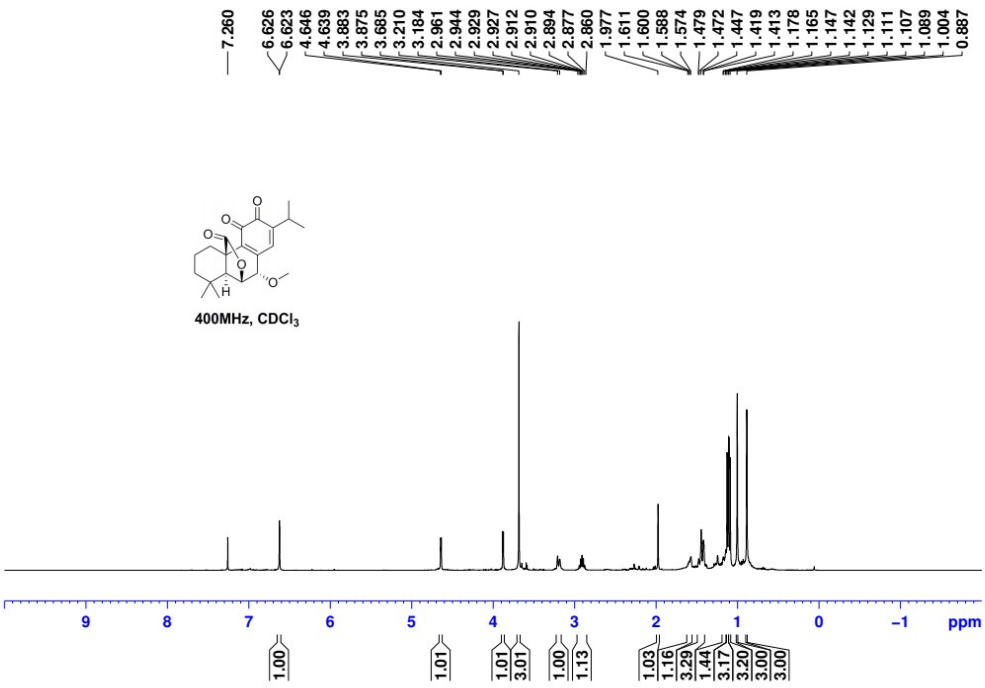


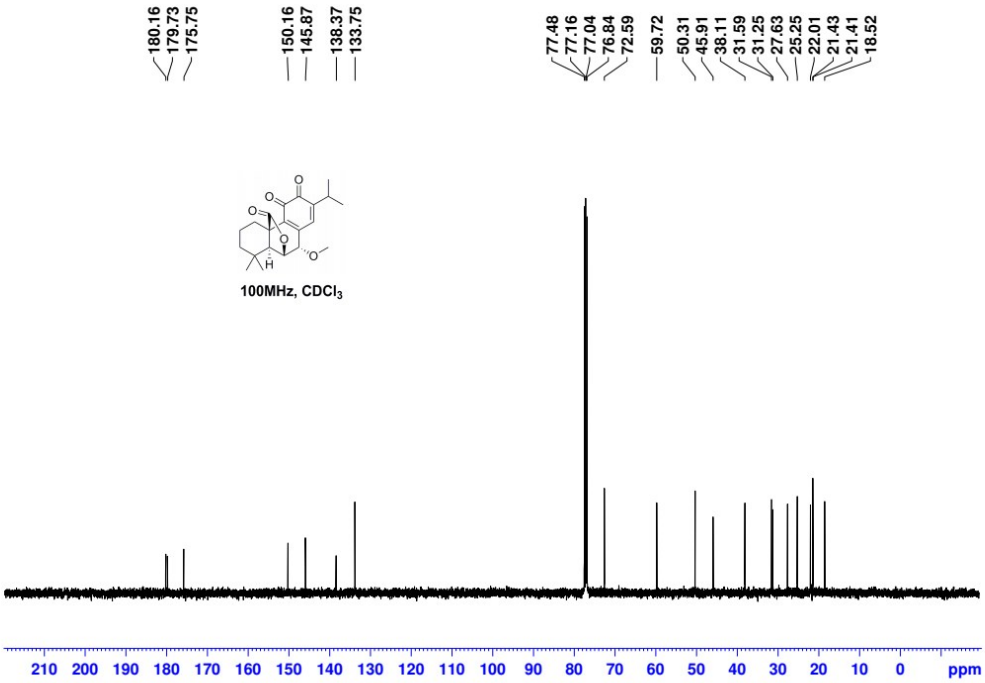


^{1}H and ^{13}C NMR spectra of compound **16**:

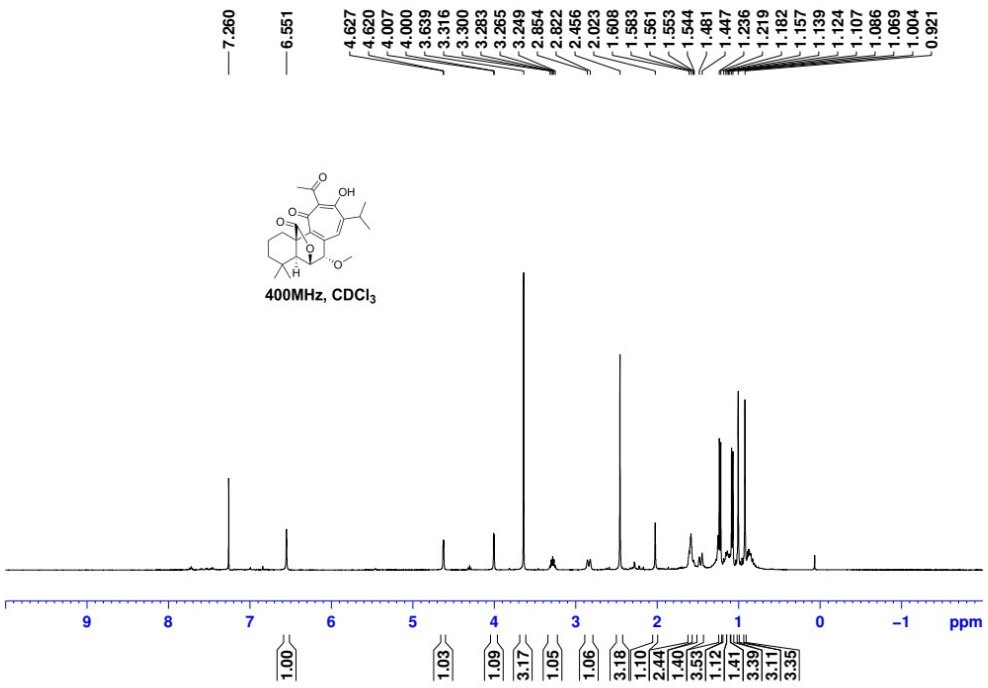


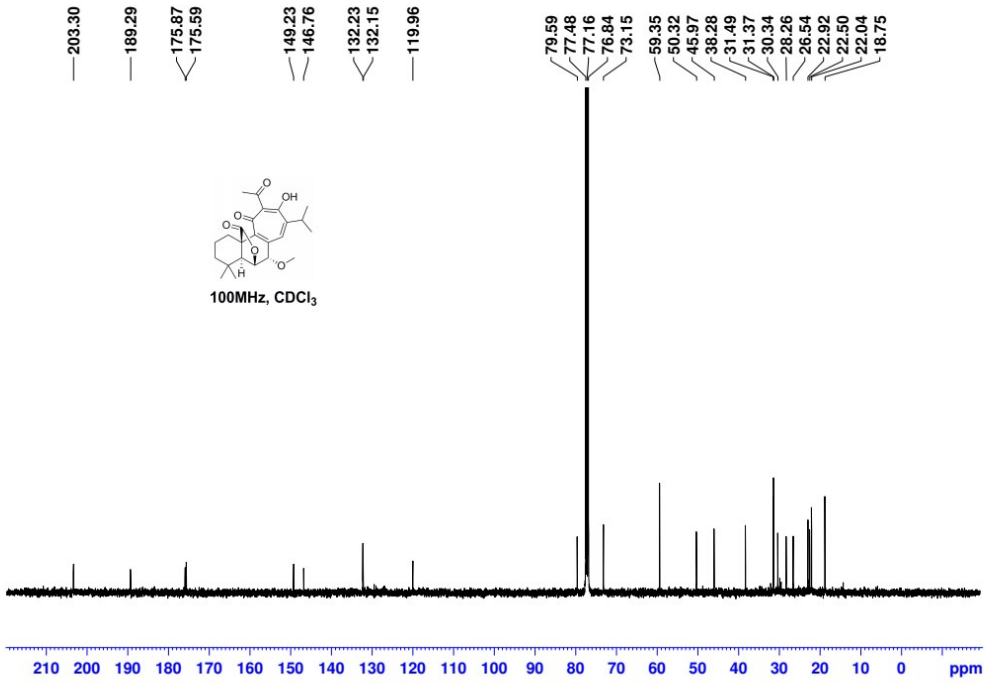
^{1}H and ^{13}C NMR spectra of compound **17**:

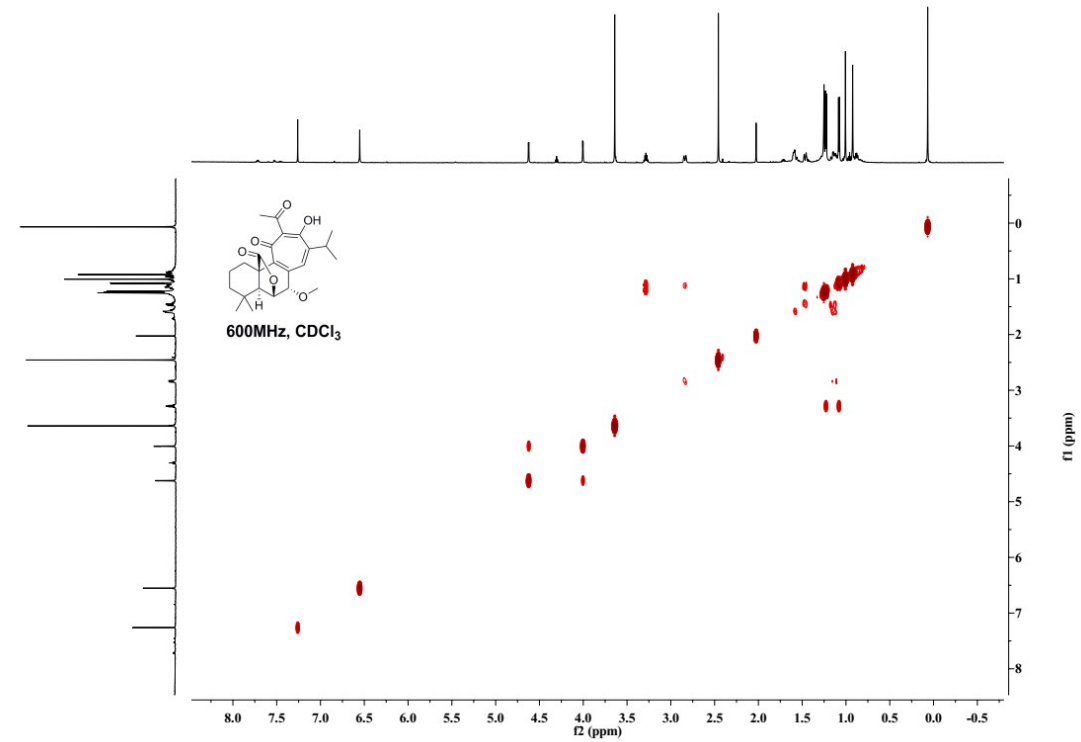




^{1}H and ^{13}C NMR spectra and H – H COSY and HMQC and HMBC of compound **6**:



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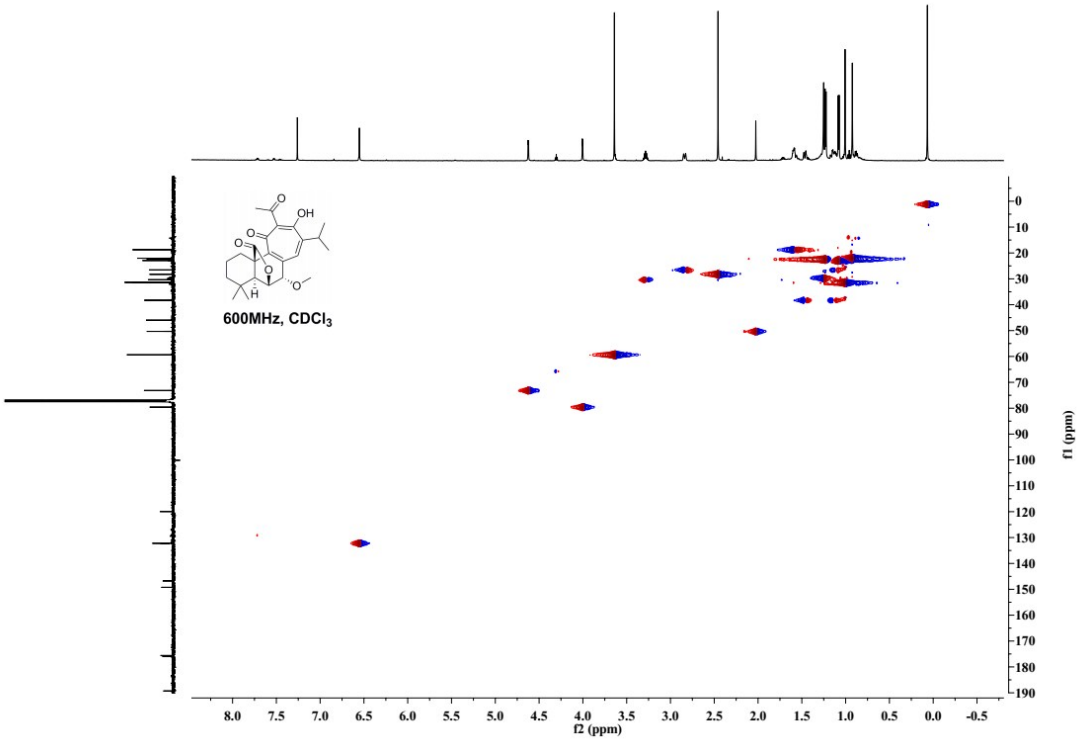
f1 (ppm)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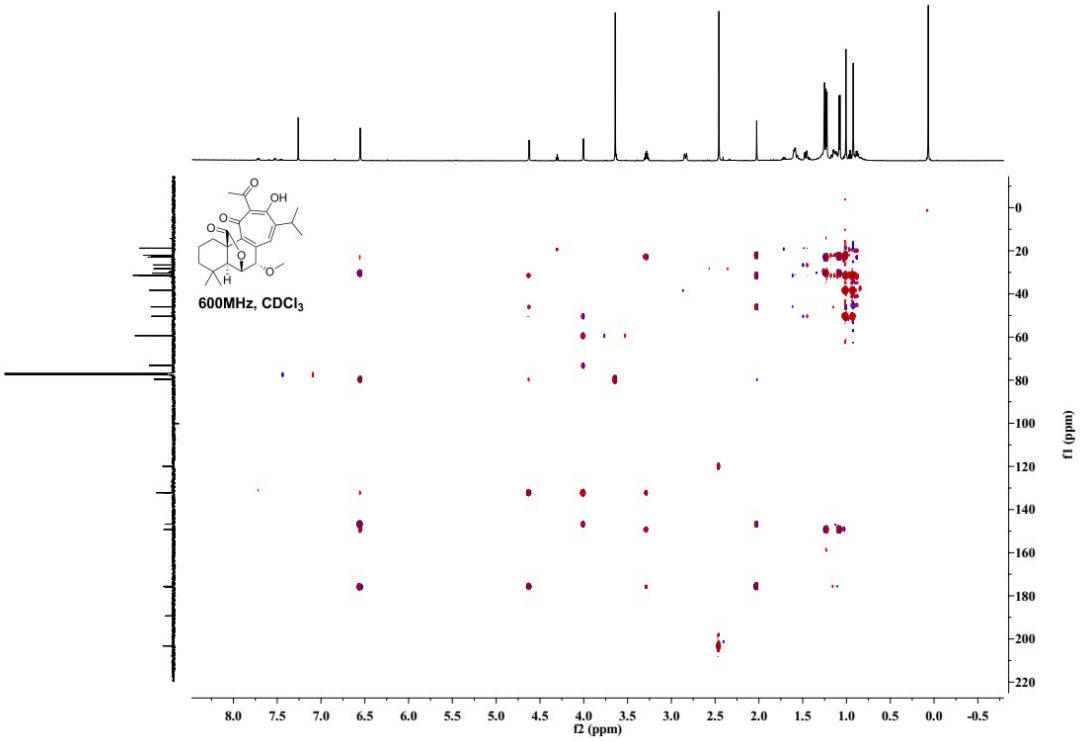
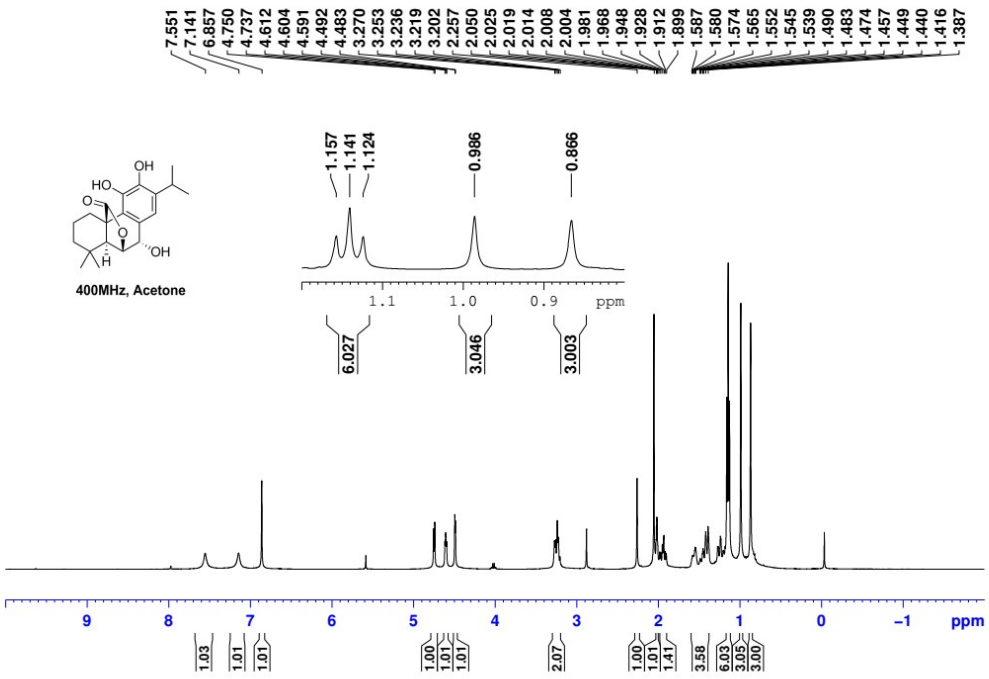
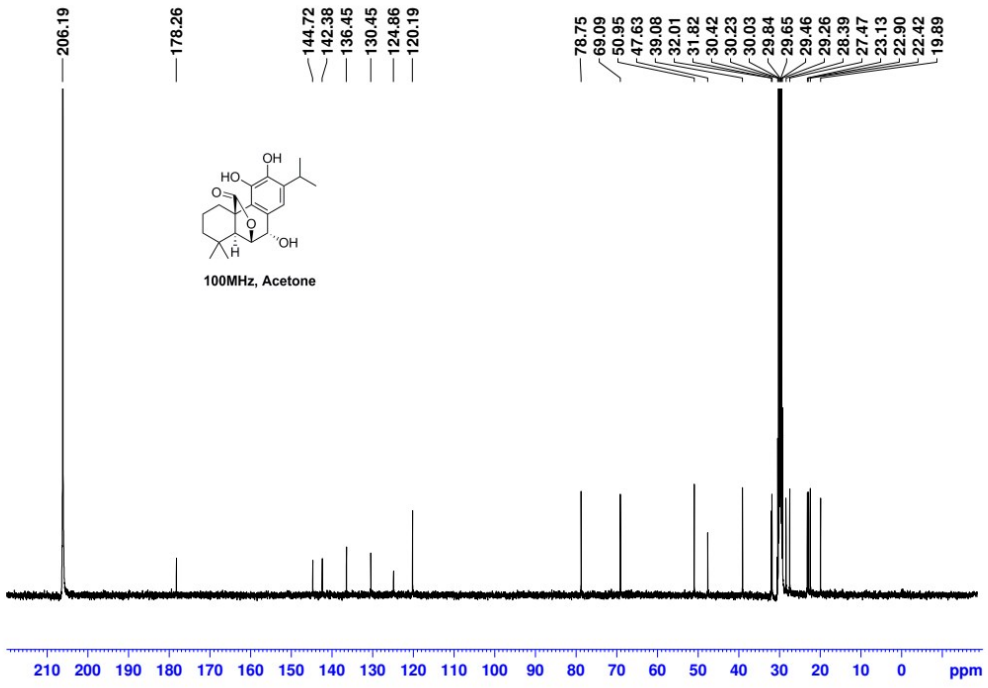
f1 (ppm)

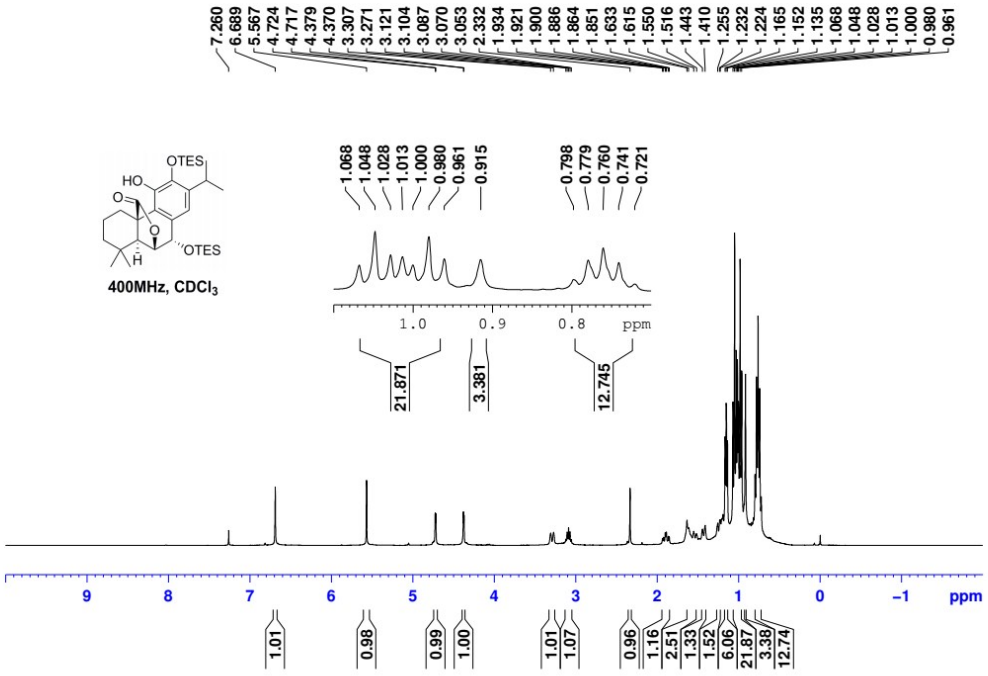


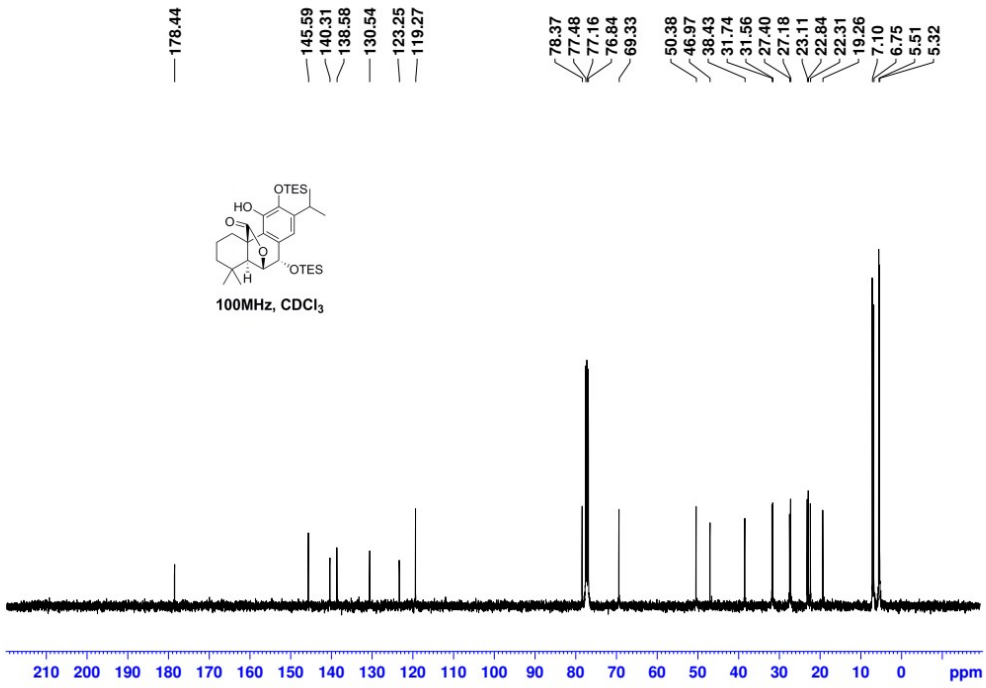
^{1}H and ^{13}C NMR spectra of compound **10**:



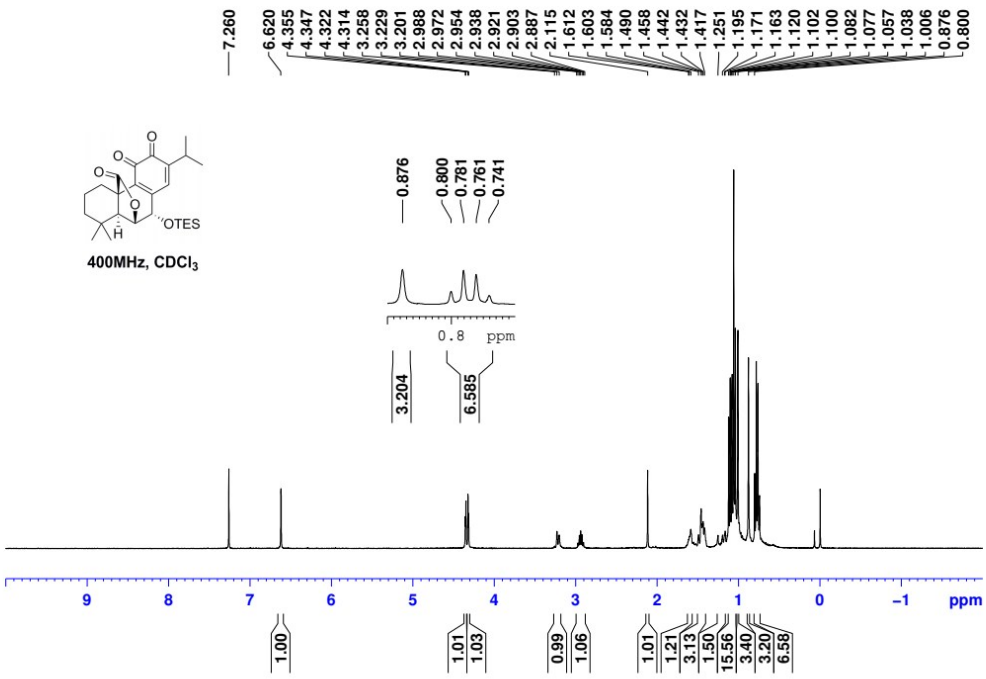


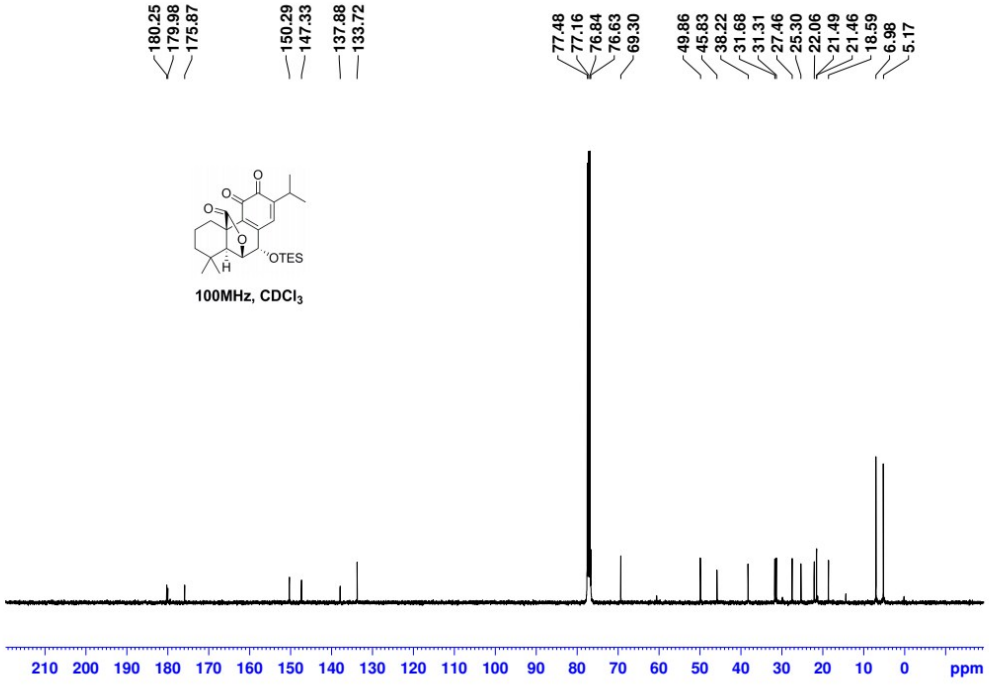
^{1}H and ^{13}C NMR spectra of compound **19**:



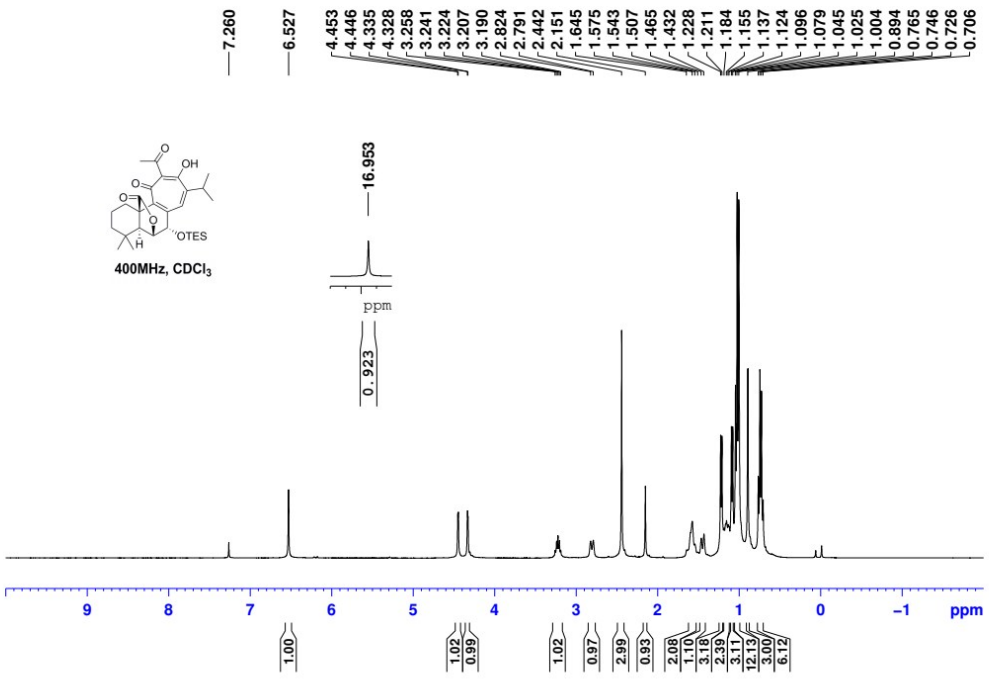


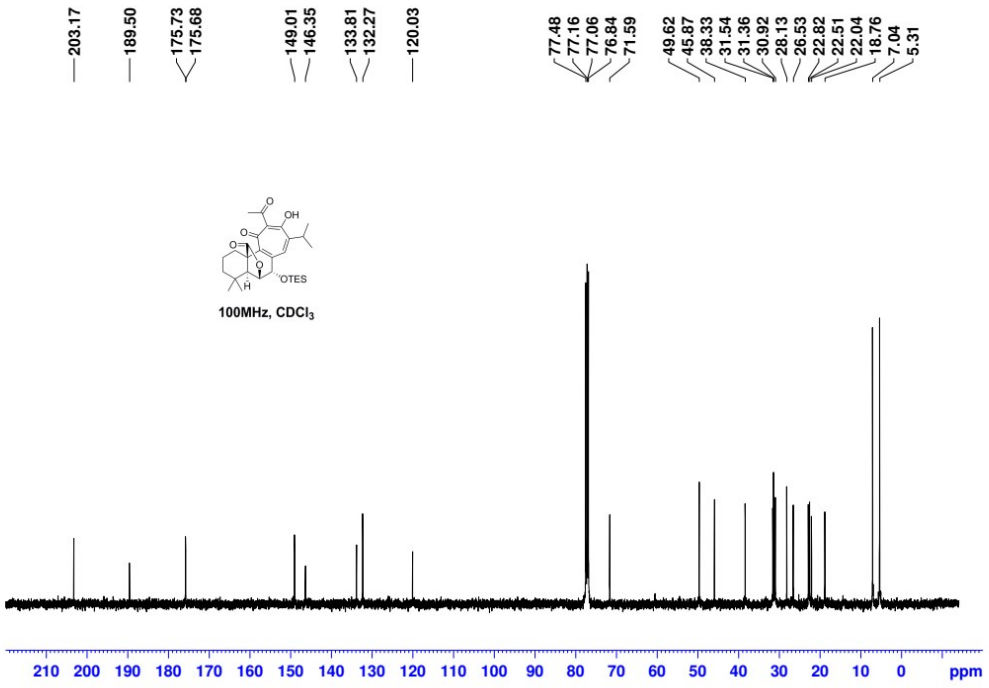
^{1}H and ^{13}C NMR spectra of compound **20**:



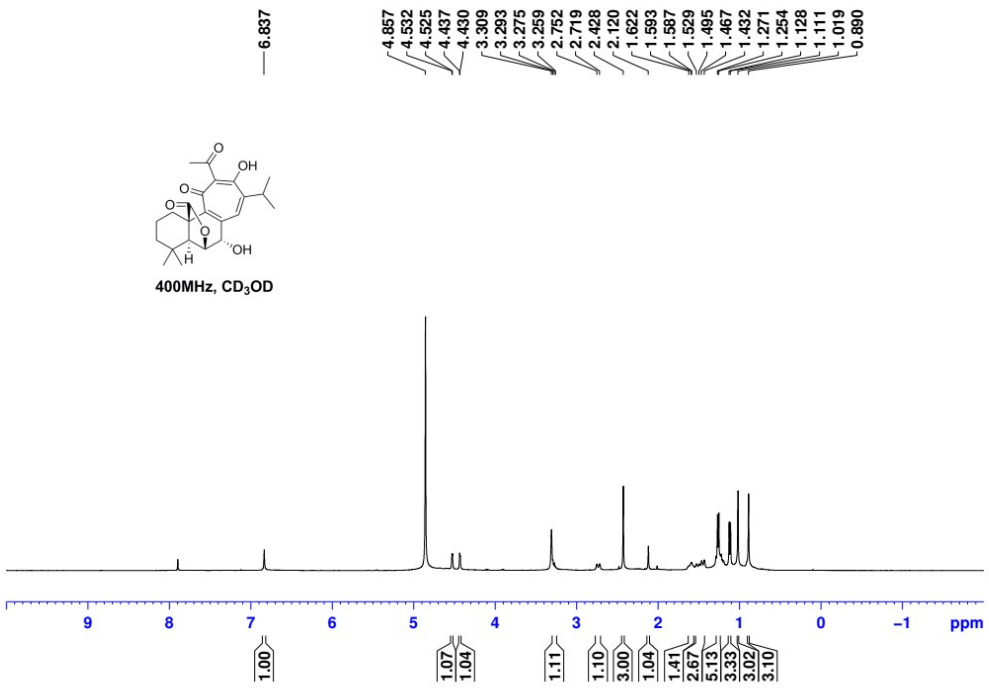


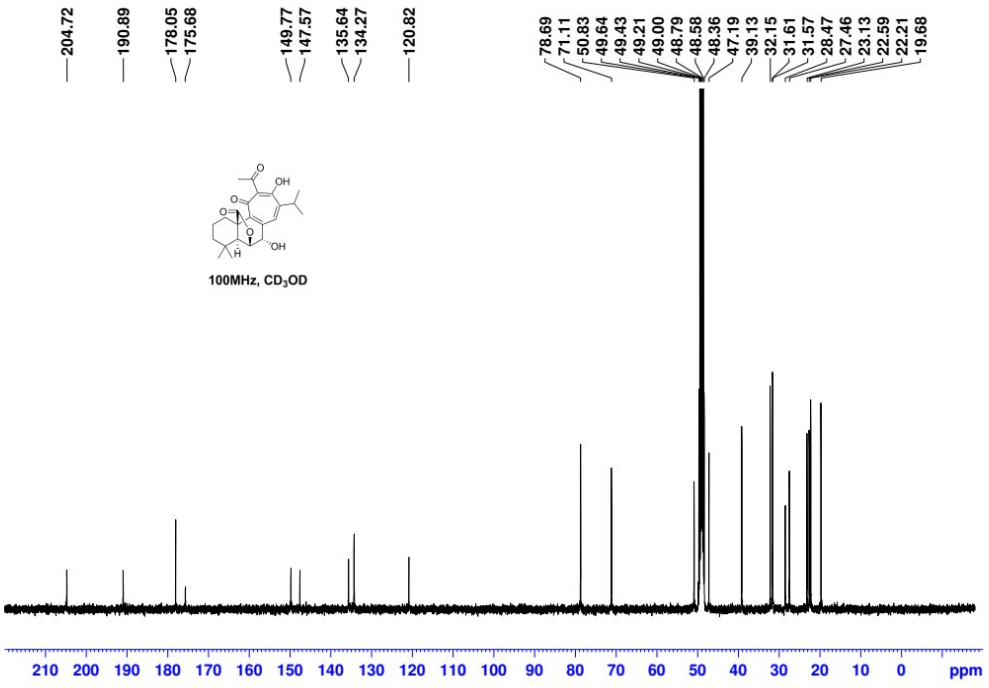
^{1}H and ^{13}C NMR spectra of compound **21**:





^{1}H and ^{13}C NMR spectra and H – H COSY and HSQC and HMBC of compound **2**:

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78.69
71.11
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49.64
49.43
49.21
49.00
48.79
48.58
48.36
47.19
39.13
32.15
31.61
31.57
28.47
27.46
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22.59
22.21
19.68
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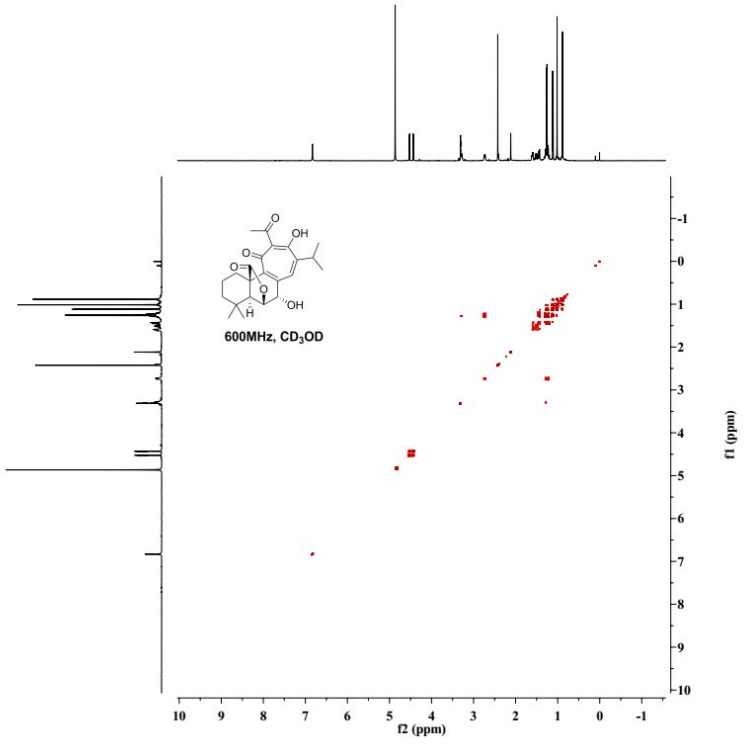
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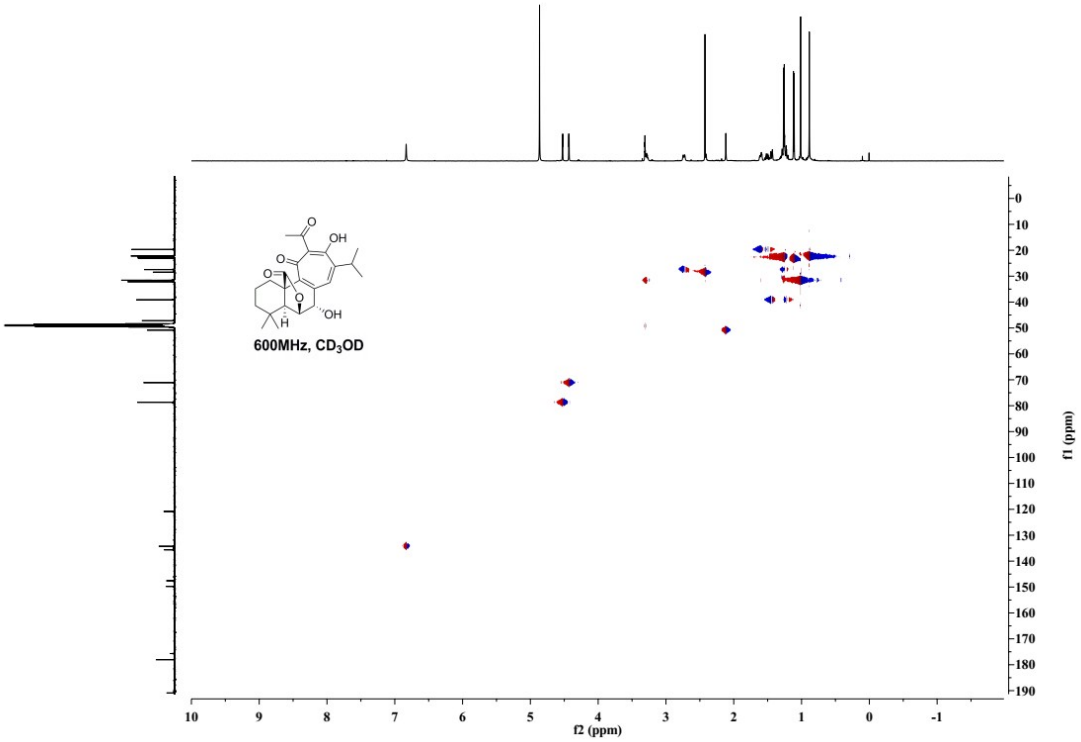
f1 (ppm)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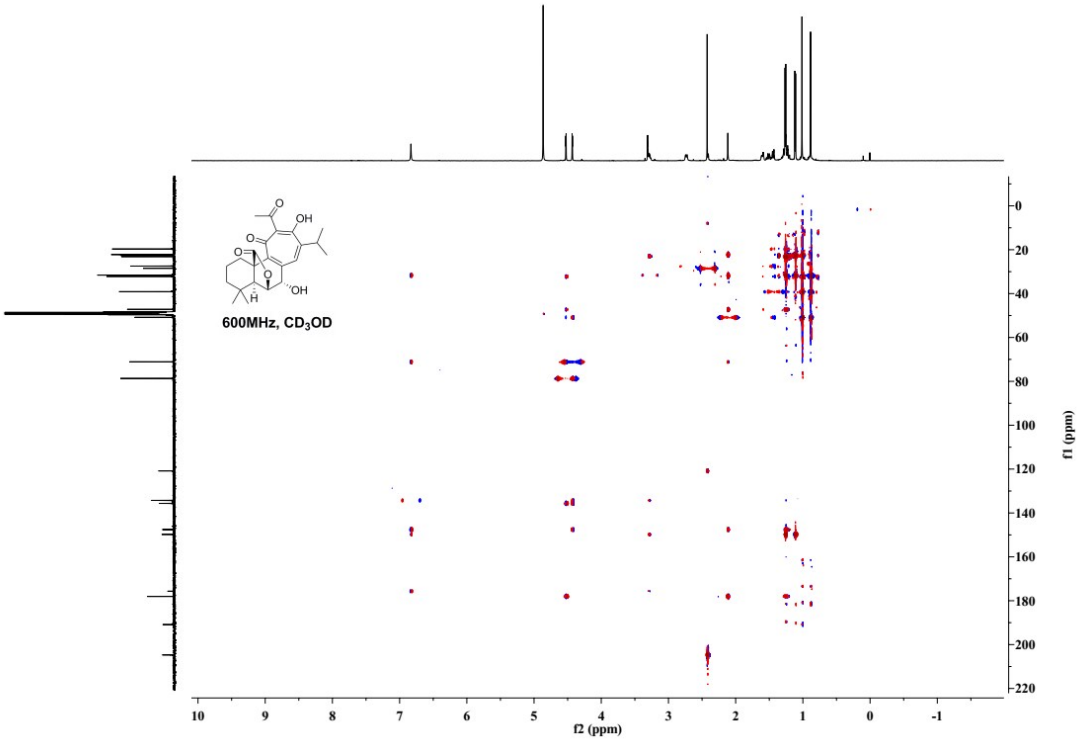
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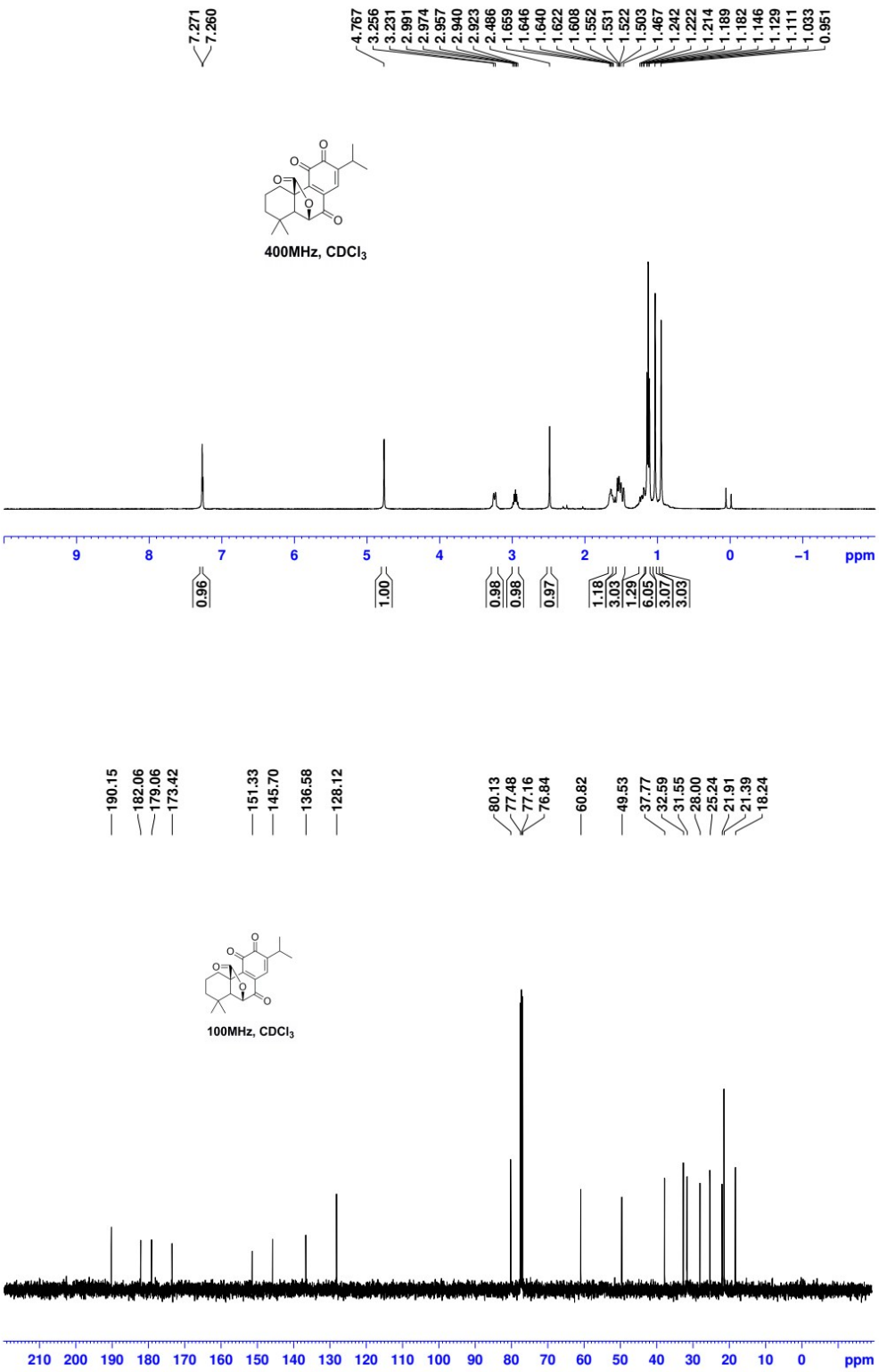
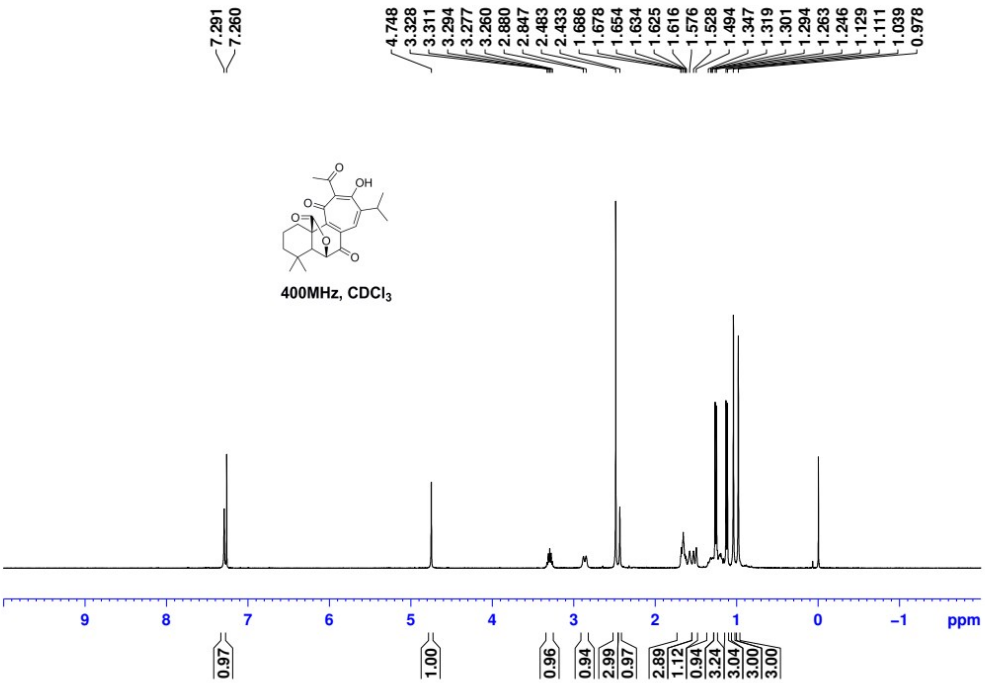
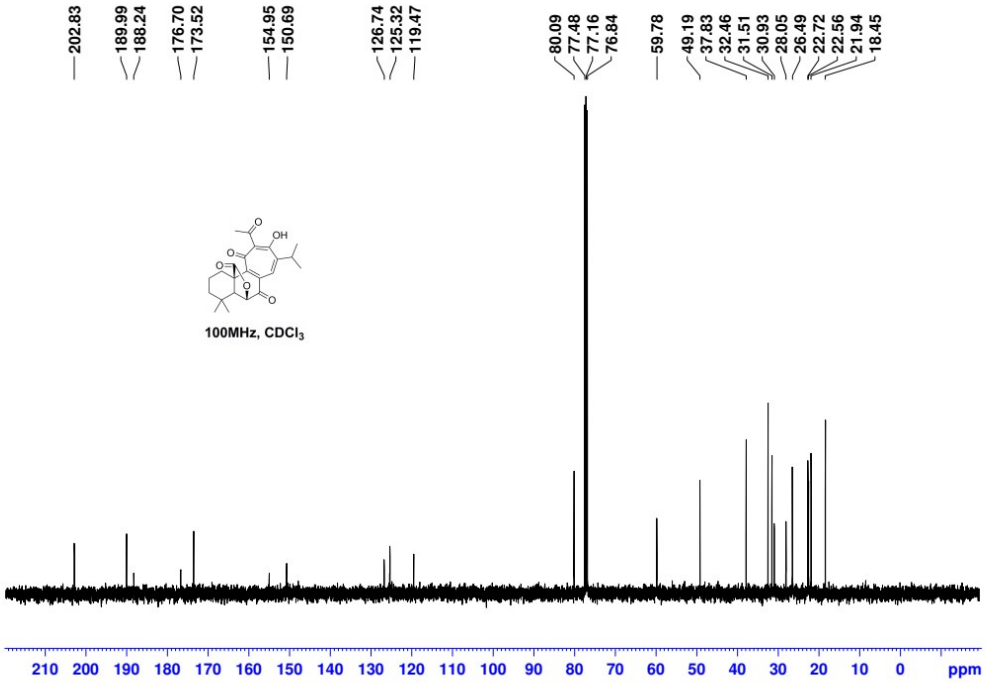
f2 (ppm)
f1 (ppm)

^{1}H and ^{13}C NMR spectra of compound **23**:

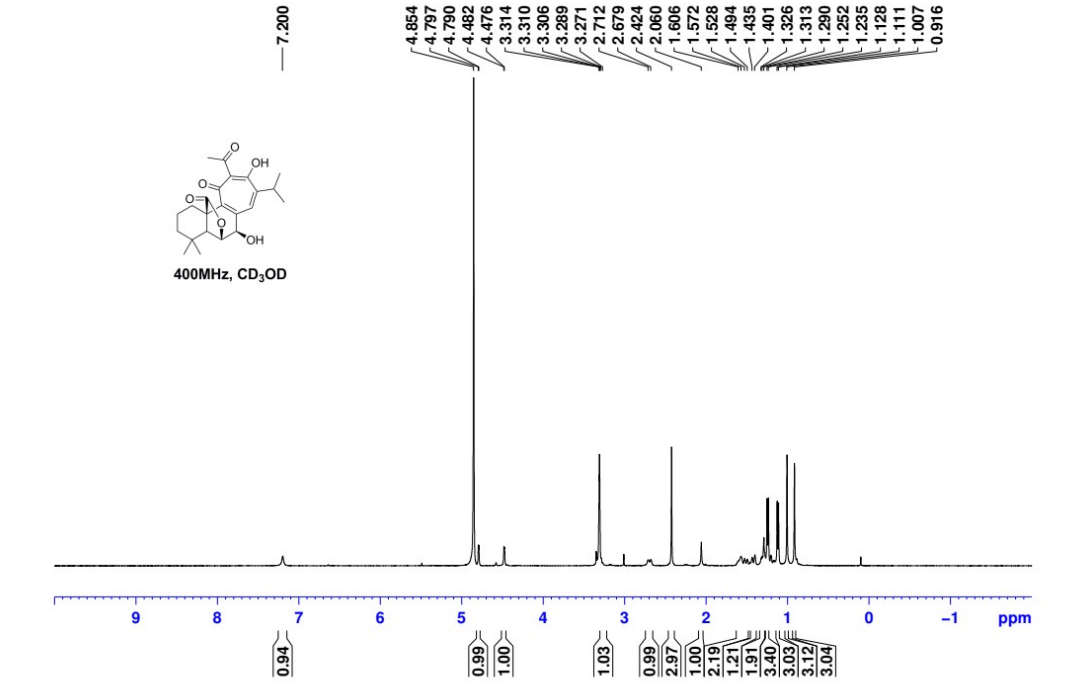


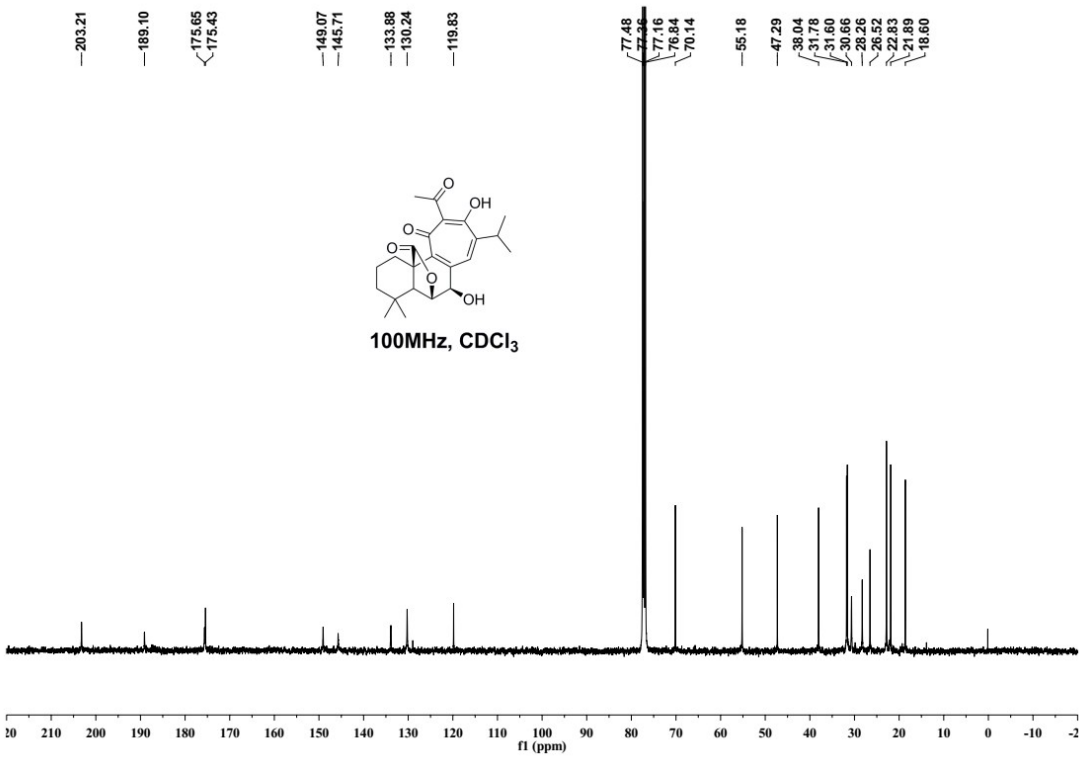
^{1}H and ^{13}C NMR spectra of compound **22**:

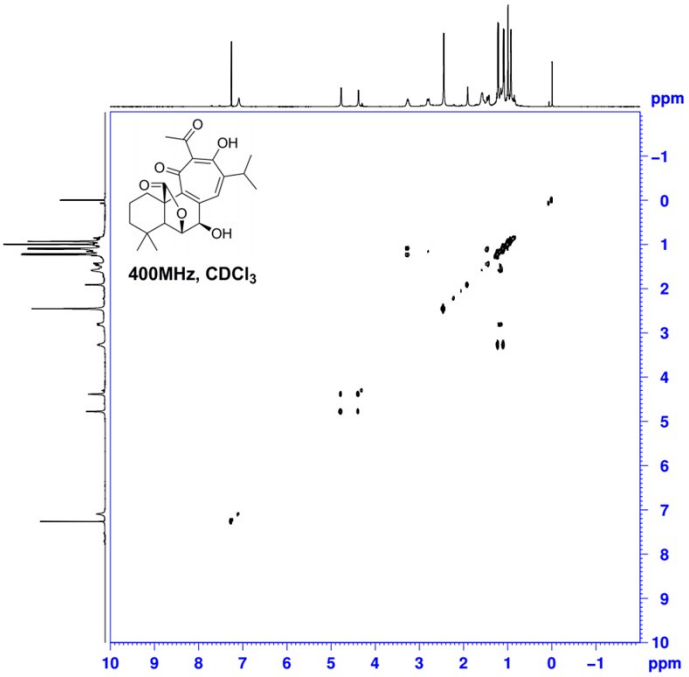




^{1}H and ^{13}C NMR spectra and H – H COSY and HMQC and HMBC of compound **1**:



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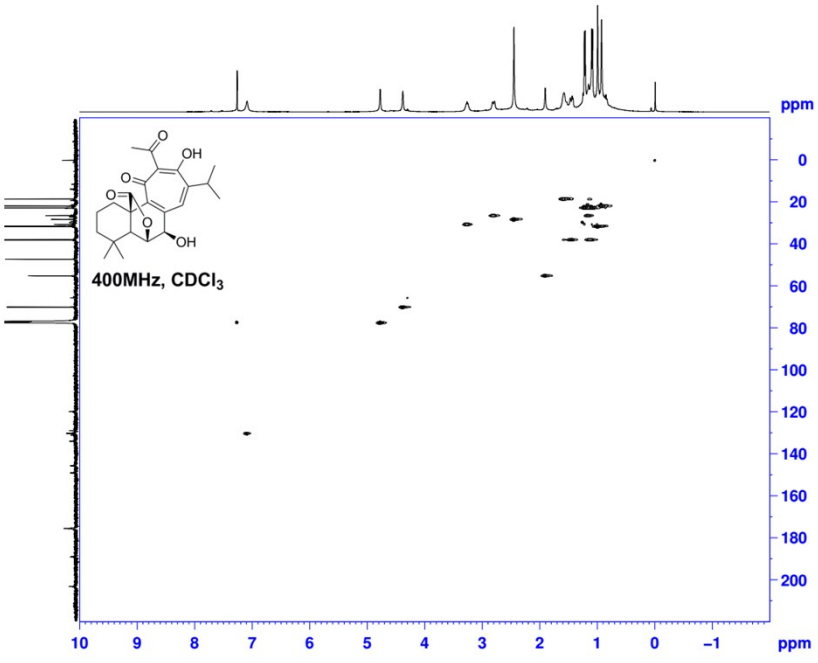
O
O
OH
400MHz, CDCl3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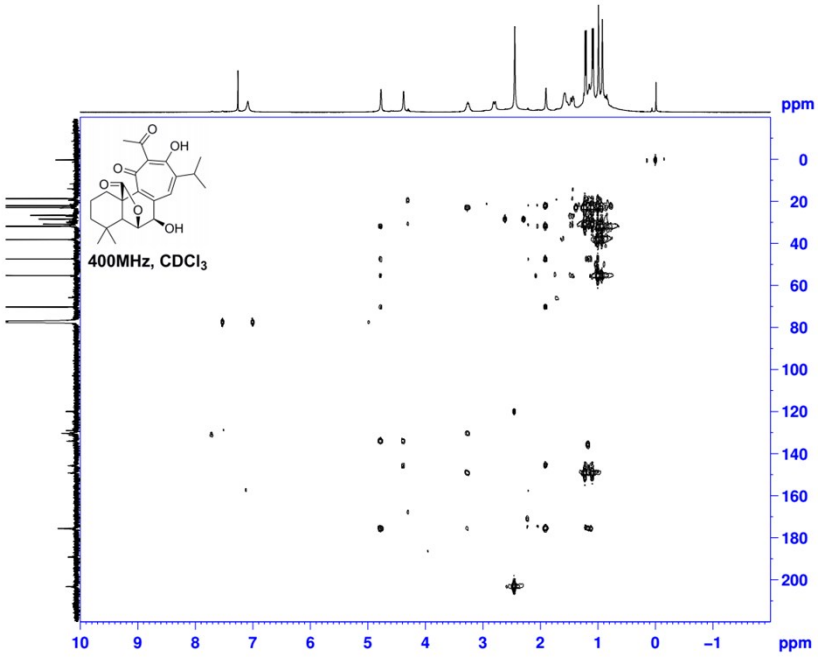
400MHz, CDCl3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OH
400MHz, CDCl3
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7
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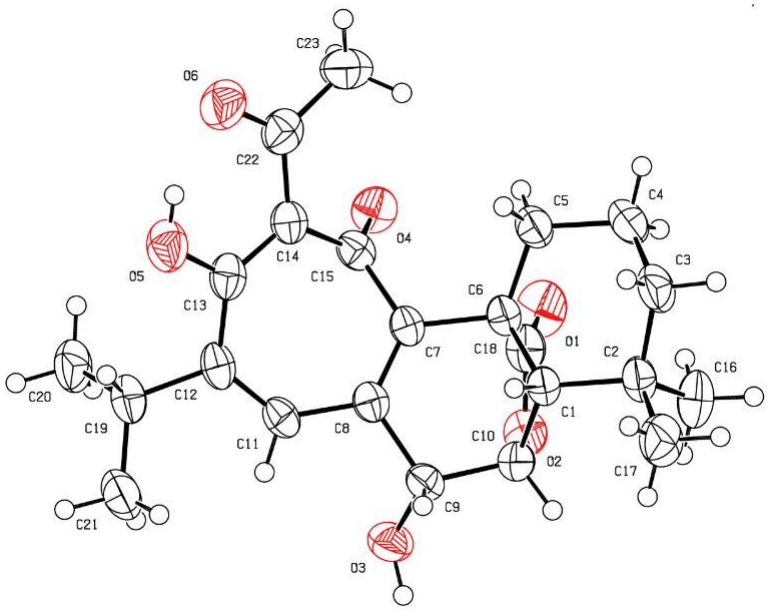
3
2
1
0
−1
ppm

4. X-ray crystallography of compound 1

(CCDC 1856524)



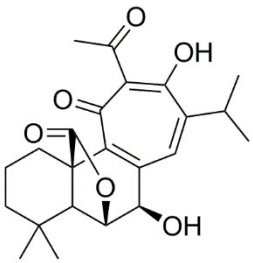


Table 1 Crystal data and structure refinement for zhangxun_0718.

Identification code	zhangxun_0718
Empirical formula	$C_{23}H_{28}O_6$
Formula weight	400.45
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	7.3005(4)
b/Å	12.1224(5)
c/Å	11.9121(6)
α/°	90.00
β/°	105.259(6)
γ/°	90.00
Volume/Å^3	1017.06(9)
Z	2
ρ_{calc}g/cm^3	1.308
μ/mm^{-1}	0.769
F(000)	428.0
Crystal size/mm^3	0.21 × 0.15 × 0.14
Radiation	CuKα (λ = 1.54184)

2Θ range for data collection/°	12.9 to 133.16
Index ranges	-8 ≤ h ≤ 8, -14 ≤ k ≤ 14, -11 ≤ l ≤ 14
Reflections collected	6953
Independent reflections	3388 [R_{int} = 0.0484, R_{sigma} = 0.0420]
Data/restraints/parameters	3388/1/272
Goodness-of-fit on F^2	1.040
Final R indexes [I>=2σ (I)]	R_1 = 0.0506, wR_2 = 0.1379
Final R indexes [all data]	R_1 = 0.0514, wR_2 = 0.1395
Largest diff. peak/hole / e $Å^{-3}$	0.21/-0.21
Flack parameter	0.0(2)

Table 2 Fractional Atomic Coordinates (×104) and Equivalent Isotropic Displacement Parameters (Å2×103) for zhangxun_0718. Ueq is defined as 1/3 of of the trace of the orthogonalised UIJ tensor.

Atom	***x***	***y***	***z***	**U(eq)**
O1	-2940(4)	-1134.3(16)	-5410(2)	64.1(6)
O2	-4278(2)	411.6(15)	-4991.0(16)	48.5(4)
O3	-6328(3)	2260.3(17)	-6206.0(18)	51.9(5)
O4	-1388(3)	-247.0(15)	-7605.8(17)	50.3(4)
O5	-696(3)	3015(2)	-9436.3(19)	59.7(5)
O6	1813(3)	1660(2)	-9222(2)	67.2(6)
C1	-1487(3)	1494.7(18)	-4384.8(19)	35.0(5)
C2	-515(4)	1191(2)	-3107(2)	44.8(6)
C3	1541(4)	851(3)	-3060(2)	54.7(7)
C4	1641(4)	-111(3)	-3860(3)	56.7(7)
C5	688(4)	161(2)	-5129(2)	46.1(6)
C6	-1285(3)	652.5(18)	-5319.3(19)	35.9(5)
C7	-2022(3)	1223.8(18)	-6514.1(19)	33.7(5)
C8	-3366(3)	2017.6(19)	-6694(2)	36.0(5)
C9	-4340(3)	2301.7(19)	-5739(2)	38.5(5)
C10	-3650(3)	1550(2)	-4698(2)	40.4(5)
C11	-4076(3)	2636(2)	-7764(2)	39.0(5)
C12	-3287(3)	2855(2)	-8651(2)	40.4(5)
C13	-1459(4)	2435(2)	-8732(2)	42.5(5)

C14	-559(3)	1477(2)	-8227(2)	40.0(5)
C15	-1354(3)	755.2(19)	-7485(2)	37.9(5)
C16	-1503(5)	266(3)	-2601(3)	66.2(8)
C17	-462(5)	2226(3)	-2376(3)	65.7(9)
C18	-2866(4)	-151(2)	-5256(2)	45.7(6)
C19	-4291(4)	3592(2)	-9662(2)	47.9(6)
C20	-5060(4)	2877(3)	-10746(2)	58.9(7)
C21	-5857(5)	4315(3)	-9430(3)	61.8(8)
C22	1171(4)	1111(2)	-8531(2)	48.7(6)
C23	2262(5)	108(3)	-8008(3)	62.0(7)

Table 3 Anisotropic Displacement Parameters (Å2×103) for zhangxun_0718. The Anisotropic displacement factor exponent takes the form: -2π2[h2a*2U11+2hka*b*U12+…].

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
O1	88.4(16)	35.1(10)	70.4(14)	-1.0(9)	23.4(12)	-17.8(9)
O2	41.6(9)	49.5(10)	54.2(10)	7.1(8)	12.1(8)	-10.2(7)
O3	39.2(10)	61.2(12)	52.7(11)	-3.7(9)	7.3(8)	8.3(8)
O4	61.5(11)	38.3(9)	50.7(10)	-9.3(8)	14.1(8)	-6.0(8)
O5	54.3(11)	69.3(13)	55.3(12)	19.9(10)	14.0(9)	-6.0(9)
O6	51.4(11)	95.6(18)	57.8(12)	11.8(12)	20.1(9)	-2.2(11)
C1	39.3(11)	33.1(10)	30.5(11)	2.5(9)	5.5(8)	0.4(9)
C2	51.6(14)	45.1(13)	32.8(12)	5.0(10)	2.5(10)	2.6(10)
C3	51.4(15)	63.9(17)	39.0(13)	4.6(12)	-5.6(10)	8.8(13)
C4	56.3(15)	58.5(17)	48.9(15)	9.0(13)	2.2(12)	20.2(13)
C5	50.9(14)	43.2(12)	40.7(13)	3.8(10)	5.7(10)	9.2(10)
C6	40.0(11)	31.7(10)	32.6(11)	2.2(9)	3.8(8)	-0.4(9)
C7	32.2(11)	32.1(10)	32.6(10)	0.3(8)	1.1(8)	-4.8(8)
C8	32.2(10)	36.9(10)	35.1(11)	-0.4(9)	2.3(8)	-5.2(9)
C9	34.3(11)	38.8(11)	39.9(12)	0.7(9)	5.5(9)	4.3(8)
C10	40.5(12)	43.6(12)	36.0(11)	0.3(9)	8.5(9)	1.5(9)
C11	32.8(10)	39.2(11)	38.6(12)	0.3(9)	-2.0(8)	0.2(9)
C12	40.8(11)	38.7(11)	33.1(11)	1.3(9)	-5.4(8)	-7.8(9)
C13	41.3(12)	48.6(13)	32.6(11)	-1.0(10)	0.9(9)	-10.8(10)
C14	38.0(11)	44.1(12)	32.9(11)	-4.1(9)	0.3(8)	-5.2(10)
C15	33.3(10)	36.7(12)	38.1(12)	-4.9(9)	-0.3(8)	-2.0(8)
C16	84(2)	69.4(19)	43.8(15)	19.2(14)	15.3(14)	-2.9(17)
C17	80(2)	67(2)	40.8(14)	-11.4(13)	-0.3(13)	7.7(15)
C18	54.4(14)	37.1(13)	43.4(13)	3.0(10)	8.8(11)	-8.4(10)
C19	47.7(14)	52.2(14)	37.2(13)	8.1(11)	-0.3(10)	-2.5(11)

C20	56.7(15)	74.6(19)	36.0(13)	2.9(12)	-4.2(11)	-1.1(13)
C21	64.7(17)	60.8(17)	52.3(15)	14.2(13)	2.2(13)	14.2(13)
C22	43.5(13)	60.5(15)	38.8(13)	-7.5(11)	5.1(10)	-8.3(11)
C23	54.8(15)	65.5(18)	68.7(19)	-8.4(15)	21.6(14)	9.2(13)

Table 4 Bond Lengths for zhangxun_0718.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C18	1.206(3)	C6	C7	1.547(3)
O2	C10	1.467(3)	C6	C18	1.527(3)
O2	C18	1.341(4)	C7	C8	1.351(3)
O3	C9	1.412(3)	C7	C15	1.482(3)
O4	C15	1.223(3)	C8	C9	1.531(3)
O5	C13	1.324(3)	C8	C11	1.452(3)
O6	C22	1.242(4)	C9	C10	1.514(3)
C1	C2	1.545(3)	C11	C12	1.356(4)
C1	C6	1.546(3)	C12	C13	1.455(4)
C1	C10	1.526(3)	C12	C19	1.524(3)
C2	C3	1.544(4)	C13	C14	1.392(4)
C2	C16	1.540(4)	C14	C15	1.467(3)
C2	C17	1.521(4)	C14	C22	1.471(4)
C3	C4	1.519(4)	C19	C20	1.533(4)
C4	C5	1.525(3)	C19	C21	1.522(4)
C5	C6	1.520(3)	C22	C23	1.497(5)

Table 5 Bond Angles for zhangxun_0718.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C18	O2	C10	108.81(19)	C10	C9	C8	110.72(19)
C2	C1	C6	116.49(19)	O2	C10	C1	104.80(19)
C10	C1	C2	115.4(2)	O2	C10	C9	110.83(19)
C10	C1	C6	98.15(18)	C9	C10	C1	109.0(2)
C3	C2	C1	106.8(2)	C12	C11	C8	131.2(2)
C16	C2	C1	114.7(2)	C11	C12	C13	124.7(2)
C16	C2	C3	110.0(3)	C11	C12	C19	121.0(2)
C17	C2	C1	107.7(2)	C13	C12	C19	114.3(2)
C17	C2	C3	108.8(2)	O5	C13	C12	113.8(2)
C17	C2	C16	108.7(3)	O5	C13	C14	119.2(2)
C4	C3	C2	112.9(2)	C14	C13	C12	126.9(2)
C3	C4	C5	111.8(2)	C13	C14	C15	122.8(2)
C6	C5	C4	113.6(2)	C13	C14	C22	118.9(2)
C1	C6	C7	106.92(18)	C15	C14	C22	118.0(2)

C5	C6	C1	114.71(19)	O4	C15	C7	118.2(2)
C5	C6	C7	113.53(19)	O4	C15	C14	121.4(2)
C5	C6	C18	116.2(2)	C14	C15	C7	120.3(2)
C18	C6	C1	99.71(19)	O1	C18	O2	122.1(3)
C18	C6	C7	104.30(17)	O1	C18	C6	128.9(3)
C8	C7	C6	121.8(2)	O2	C18	C6	109.0(2)
C8	C7	C15	121.6(2)	C12	C19	C20	109.1(2)
C15	C7	C6	116.13(19)	C21	C19	C12	115.0(2)
C7	C8	C9	120.2(2)	C21	C19	C20	110.6(2)
C7	C8	C11	125.7(2)	O6	C22	C14	120.0(3)
C11	C8	C9	114.1(2)	O6	C22	C23	117.3(3)
O3	C9	C8	109.23(19)	C14	C22	C23	122.7(3)
O3	C9	C10	112.8(2)				

Table 6 Torsion Angles for zhangxun_0718.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
A	B	C	D	Angle/°	A	B	C	D	Angle/°
O3	C9	C10	O2	55.4(3)	C8	C9	C10	C1	47.5(3)
O3	C9	C10	C1	170.27(19)	C8	C11	C12	C13	3.2(4)
O5	C13	C14	C15	-176.8(2)	C8	C11	C12	C19	-176.4(2)
O5	C13	C14	C22	-2.6(3)	C9	C8	C11	C12	159.1(2)
C1	C2	C3	C4	-58.4(3)	C10	O2	C18	O1	172.0(3)
C1	C6	C7	C8	-28.7(3)	C10	O2	C18	C6	-8.2(3)
C1	C6	C7	C15	158.77(18)	C10	C1	C2	C3	163.9(2)
C1	C6	C18	O1	-147.6(3)	C10	C1	C2	C16	41.7(3)
C1	C6	C18	O2	32.6(2)	C10	C1	C2	C17	-79.5(3)
C2	C1	C6	C5	-42.6(3)	C10	C1	C6	C5	-166.4(2)
C2	C1	C6	C7	-169.45(19)	C10	C1	C6	C7	66.8(2)
C2	C1	C6	C18	82.3(2)	C10	C1	C6	C18	-41.5(2)
C2	C1	C10	O2	-85.7(2)	C11	C8	C9	O3	50.0(3)
C2	C1	C10	C9	155.6(2)	C11	C8	C9	C10	174.73(19)
C2	C3	C4	C5	60.3(3)	C11	C12	C13	O5	-159.2(2)
C3	C4	C5	C6	-49.2(4)	C11	C12	C13	C14	25.7(4)
C4	C5	C6	C1	40.5(3)	C11	C12	C19	C20	-107.3(3)
C4	C5	C6	C7	163.8(2)	C11	C12	C19	C21	17.7(3)
C4	C5	C6	C18	-75.2(3)	C12	C13	C14	C15	-2.0(4)
C5	C6	C7	C8	-156.3(2)	C12	C13	C14	C22	172.2(2)
C5	C6	C7	C15	31.2(3)	C13	C12	C19	C20	73.2(3)
C5	C6	C18	O1	-23.7(4)	C13	C12	C19	C21	-161.9(2)
C5	C6	C18	O2	156.5(2)	C13	C14	C15	O4	134.6(3)

C6	C1	C2	C3	49.5(3)	C13	C14	C15	C7	-49.5(3)
C6	C1	C2	C16	-72.6(3)	C13	C14	C22	O6	0.5(4)
C6	C1	C2	C17	166.2(2)	C13	C14	C22	C23	178.4(2)
C6	C1	C10	O2	38.8(2)	C15	C7	C8	C9	166.4(2)
C6	C1	C10	C9	-79.9(2)	C15	C7	C8	C11	-11.1(3)
C6	C7	C8	C9	-5.7(3)	C15	C14	C22	O6	175.0(3)
C6	C7	C8	C11	176.81(19)	C15	C14	C22	C23	-7.1(3)
C6	C7	C15	O4	45.7(3)	C16	C2	C3	C4	66.7(3)
C6	C7	C15	C14	-130.4(2)	C17	C2	C3	C4	-174.3(2)
C7	C6	C18	O1	102.0(3)	C18	O2	C10	C1	-20.4(2)
C7	C6	C18	O2	-77.8(2)	C18	O2	C10	C9	97.1(2)
C7	C8	C9	O3	-127.8(2)	C18	C6	C7	C8	76.3(3)
C7	C8	C9	C10	-3.0(3)	C18	C6	C7	C15	-96.2(2)
C7	C8	C11	C12	-23.3(4)	C19	C12	C13	O5	20.3(3)
C8	C7	C15	O4	-126.8(2)	C19	C12	C13	C14	-154.7(2)
C8	C7	C15	C14	57.1(3)	C22	C14	C15	O4	-39.6(3)
C8	C9	C10	O2	-67.3(2)	C22	C14	C15	C7	136.3(2)

Table 7 Hydrogen Atom Coordinates (Å×104) and Isotropic Displacement Parameters (Å2×103) for zhangxun_0718.

Atom	***x***	***y***	***z***	**U(eq)**
H3	-6990(60)	2670(40)	-5830(40)	77(12)
H5	291	2718	-9483	90
H1	-997	2209	-4560	42
H3A	2199	1478	-3277	66
H3B	2193	650	-2268	66
H4A	1025	-748	-3628	68
H4B	2960	-299	-3781	68
H5A	1480	678	-5410	55
H5B	598	-508	-5588	55
H9	-3995	3060	-5485	46
H10	-4088	1816	-4036	48
H11	-5281	2934	-7858	47
H16A	-1474	-405	-3025	99
H16B	-2797	469	-2666	99
H16C	-854	155	-1796	99
H17A	158	2064	-1577	99
H17B	-1735	2471	-2438	99
H17C	225	2794	-2652	99
H19	-3332	4085	-9829	57

H20A	-4042	2454	-10900	88
H20B	-5602	3343	-11401	88
H20C	-6017	2388	-10615	88
H21A	-6895	3859	-9358	93
H21B	-6292	4821	-10065	93
H21C	-5372	4721	-8722	93
H23A	2282	58	-7201	93
H23B	3539	159	-8080	93
H23C	1664	-538	-8409	93