Supporting Information for

UPLC-MS-ELSD-PDA as A Powerful Dereplication Tool to Facilitate Compound Identification from Small Molecule Natural Product Libraries

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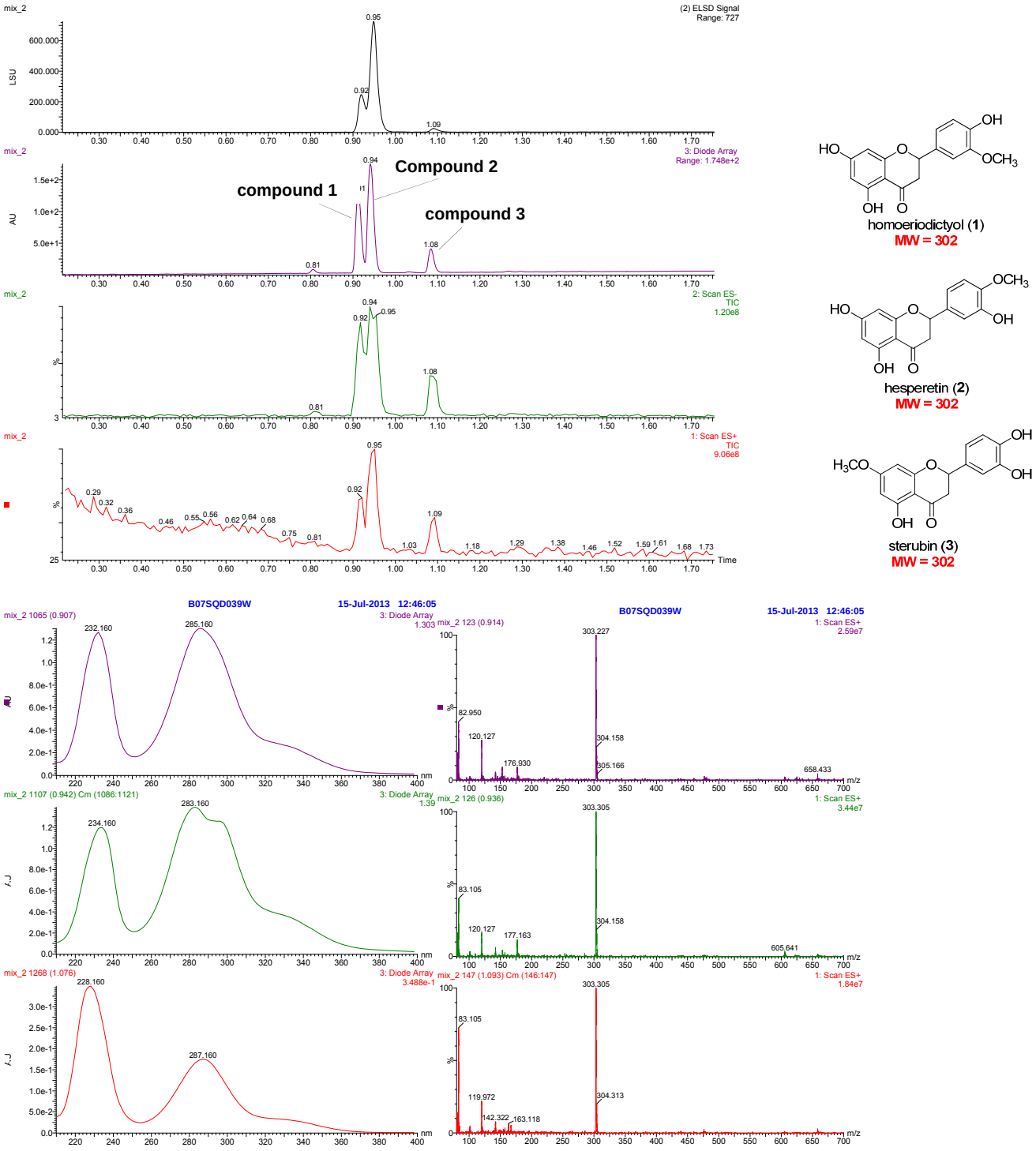


Figure S1. UPLC-MS-ELSD-PDA analysis of a mixture of authentic samples homoeriodictyol (**1**), hesperetin (**2**) and sterubin (**3**). Compounds **1** and **2** were from the commercial source Indofine and compound **3** was from our NCNPR repository.

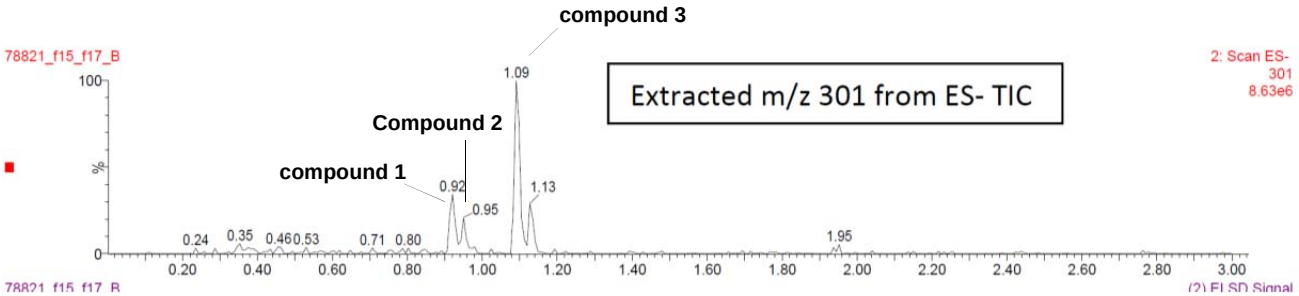


Figure S2. UPLC-MS-ELSD-PDA analysis of hit 78821-c4 cont aining homoeriodictyol (**1**), hesperetin (**2**) and sterubin (**3**).

MS Conditions:

Waters SQD MS with ESI source
Operated in Positive/Negative mode with switching every 0.02 sec.
Capillary Voltage: 4.0 KV
Extractor Voltage: 44.0 V
RF lens Voltage: 0.10 V
Source Temperature: 150^{o} C
Desolvation Temperature: 250^{o} C
Desolvation Gas Flow (nitrogen): 500 L/Hr
Cone Gas Flow (nitrogen): 30 L/Hr

UPLC Conditions:

Waters Acquity UPLC Classic
Column: Waters BEH C18 - 1.7 um, 5 x 2.1 mm
Column Temp: 50^{o} C
Mobile Phase A: Water/0.1% formic acid
Mobile Phase B: Acetonitrile/0.1% formic acid
Gradient:

Time-min.	Flow-ml/min	%A	%B
I	1.0	85	15
0.20	1.0	80	20
2.85	1.0	5	95
2.95	1.0	5	95
3.0	1.0	85	20

Data Acquisition: MassLynx Software

Figure S3. 400 MHz ^{1}H NMR spectrum of acetylated mixture of compounds **5a** and **5b** in $CDCl_3$.

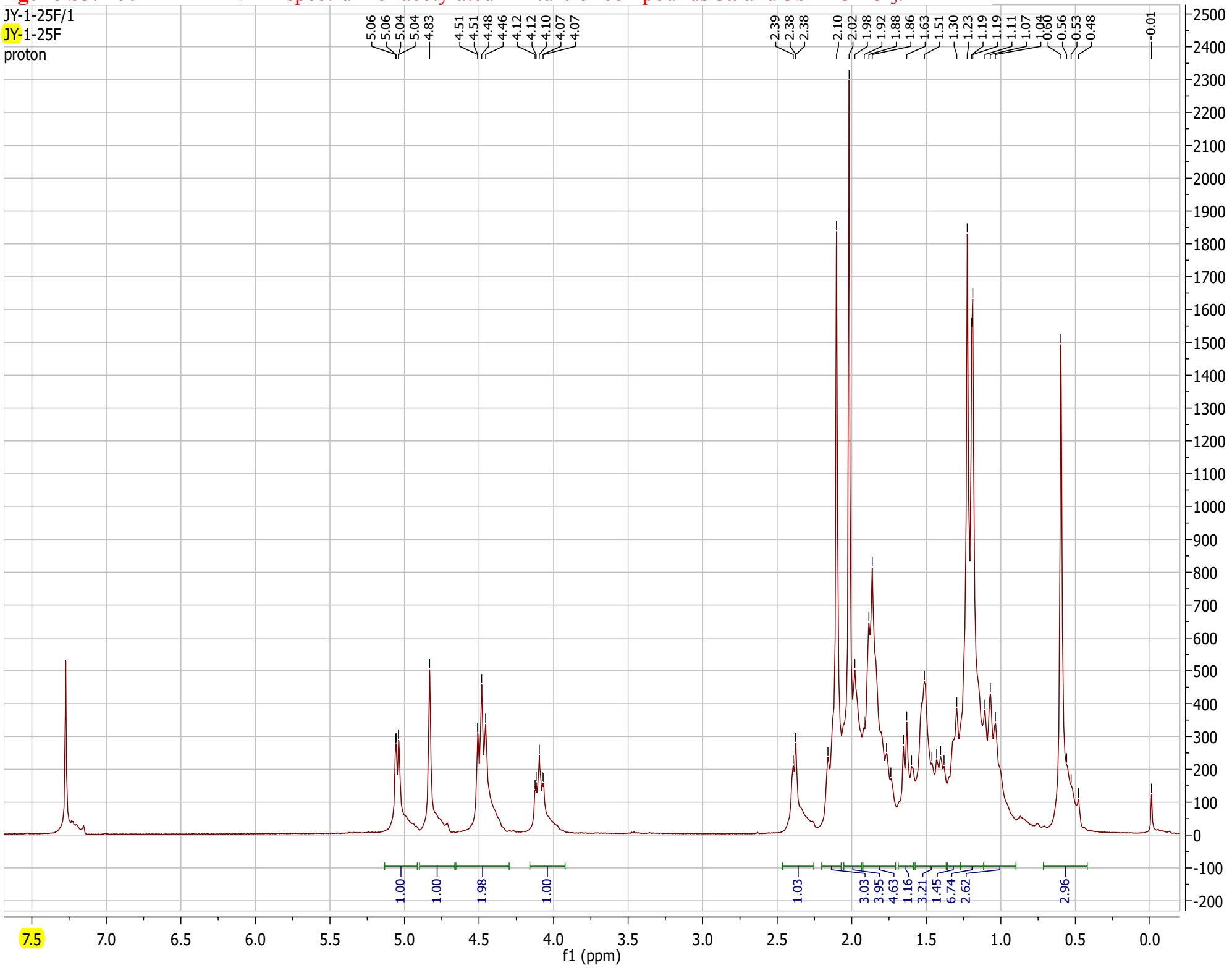


Figure S4. 100 MHz ^{13}C NMR spectrum of acetylated mixture of compounds **5a** and **5b** in $CDCl_3$.

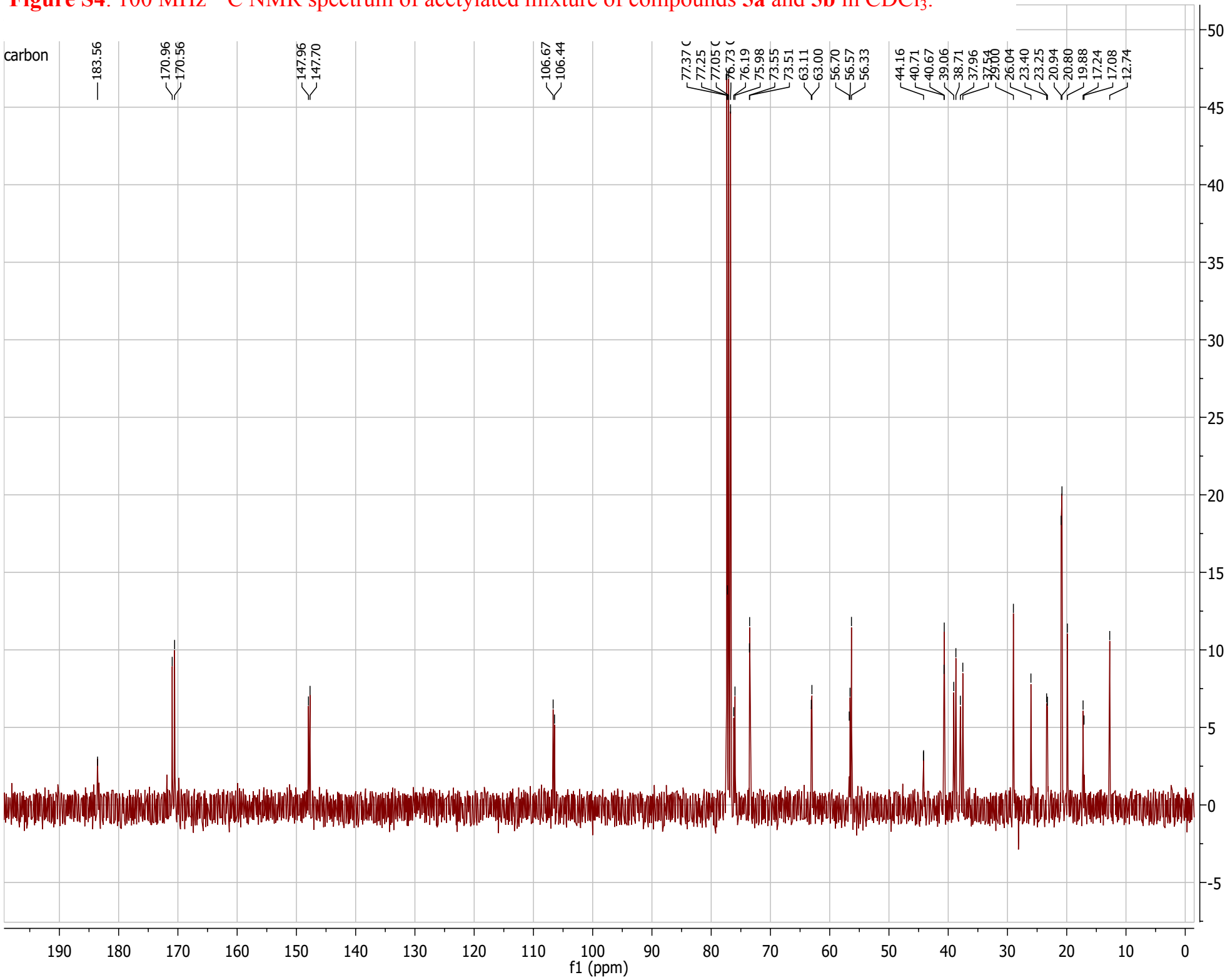


Figure S5. 400 MHz ^{1}H NMR spectrum of of compound **9** in $CDCl_3$.

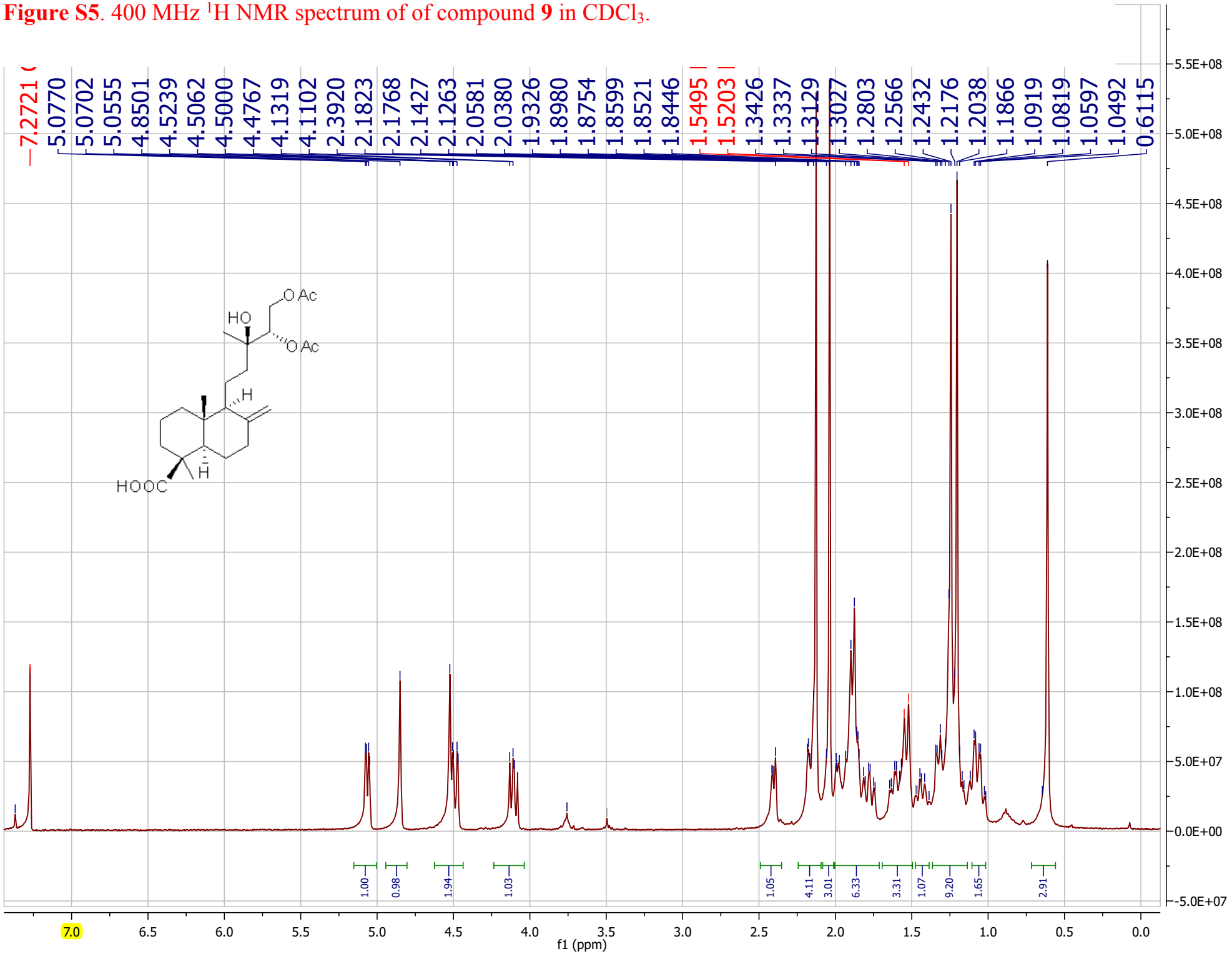


Figure S6. 100 MHz ^{13}C NMR spectrum of of compound **9** in $CDCl_3$.

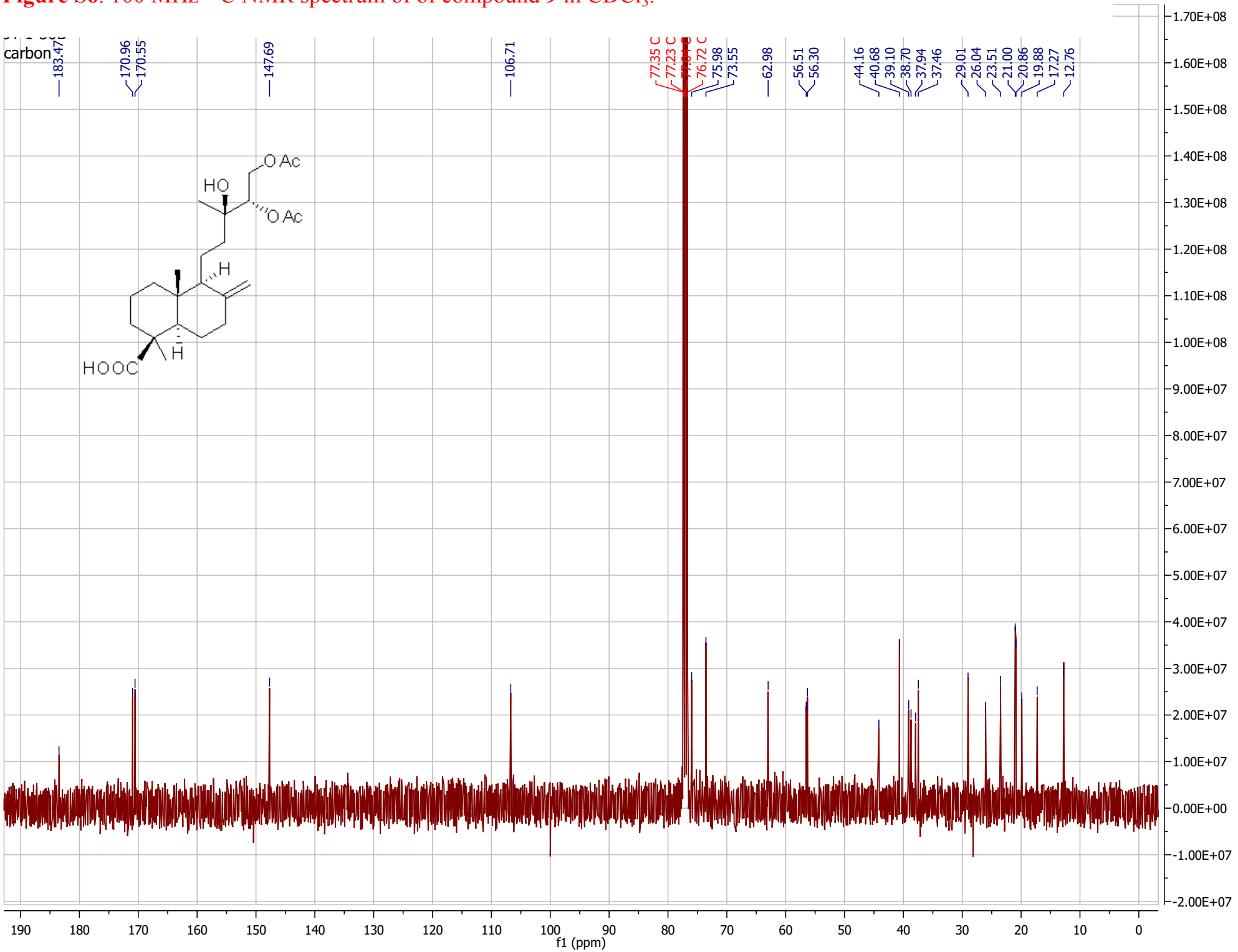


Figure S7. 400 MHz HMQC spectrum of of compound **9** in $CDCl_3$.

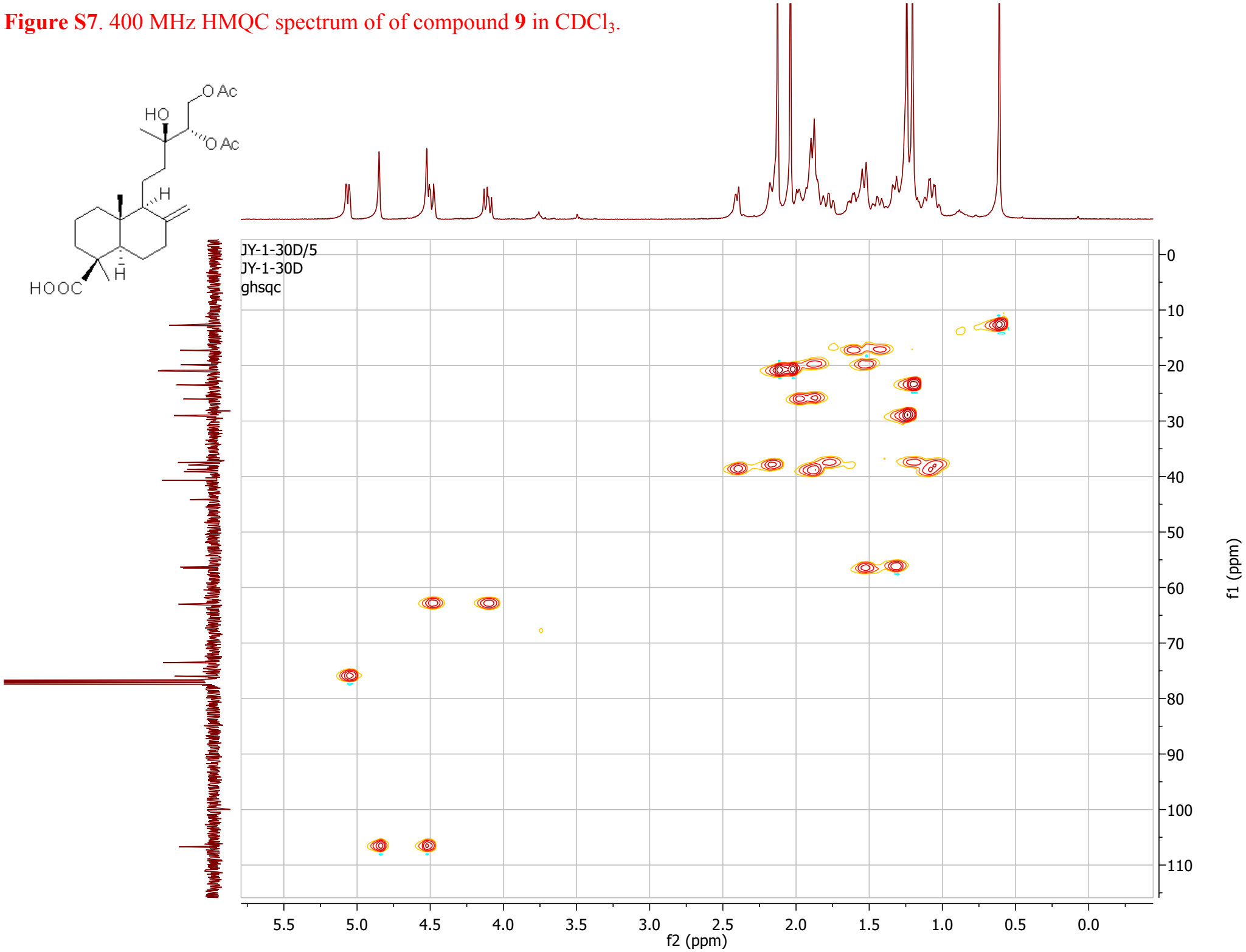


Figure S8. 400 MHz HMBC spectrum of of compound **9** in $CDCl_3$.

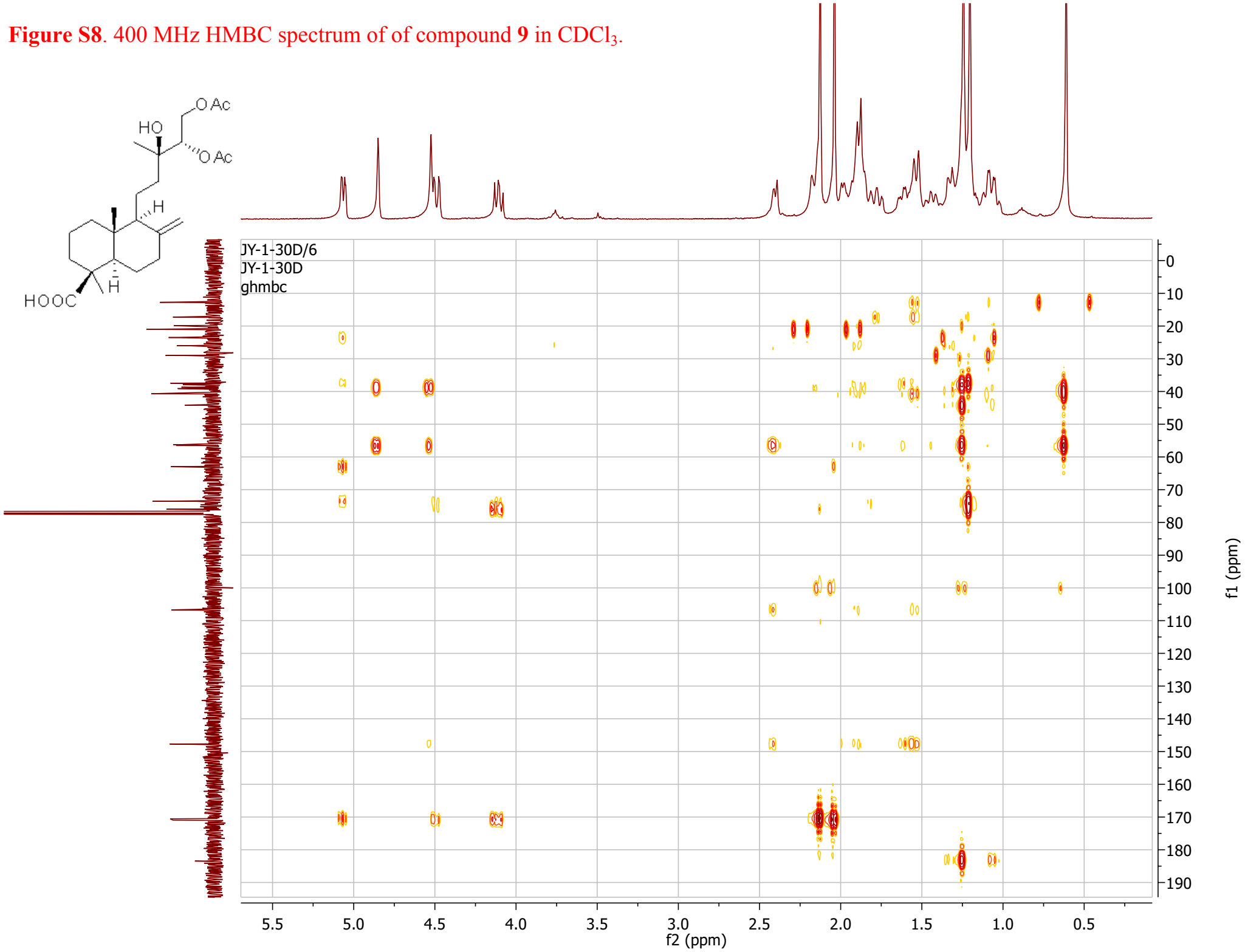


Figure S9. 400 MHz NOESY spectrum of of compound **9** in $CDCl_3$.

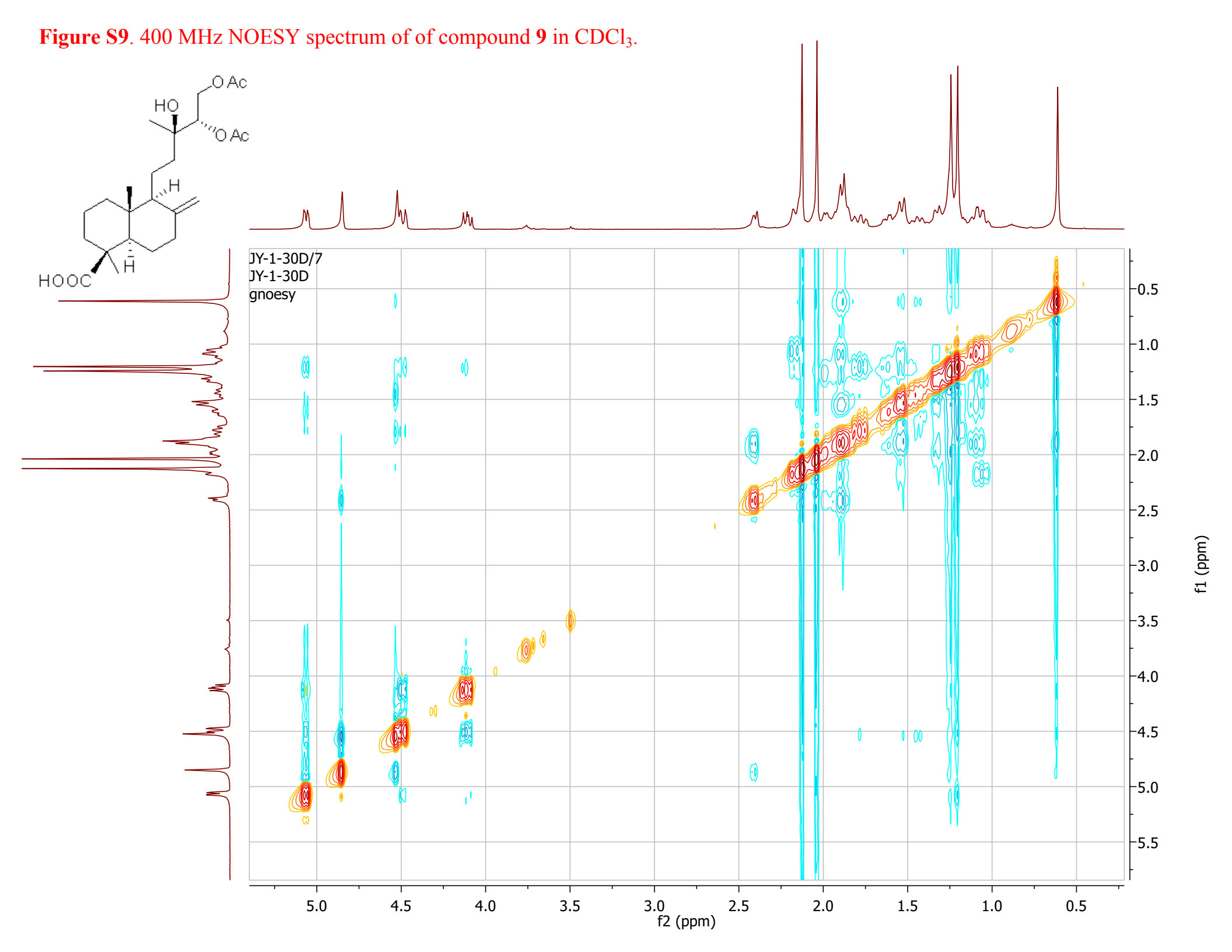


Figure S10. 400 MHz ^{1}H NMR spectrum of of compound **10** in $CDCl_3$.

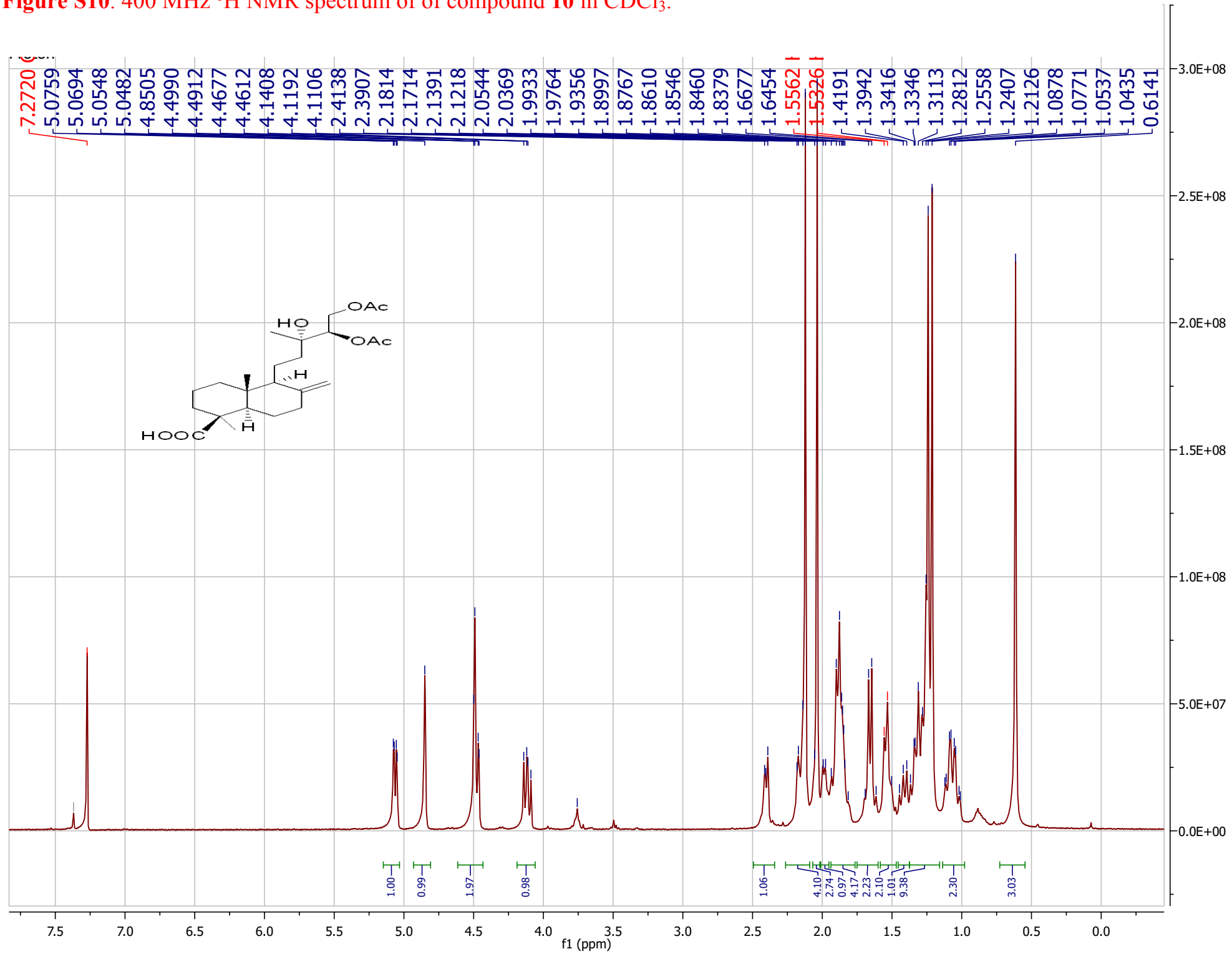


Figure S11. 100 MHz ^{13}C NMR spectrum of of compound **10** in $CDCl_3$.

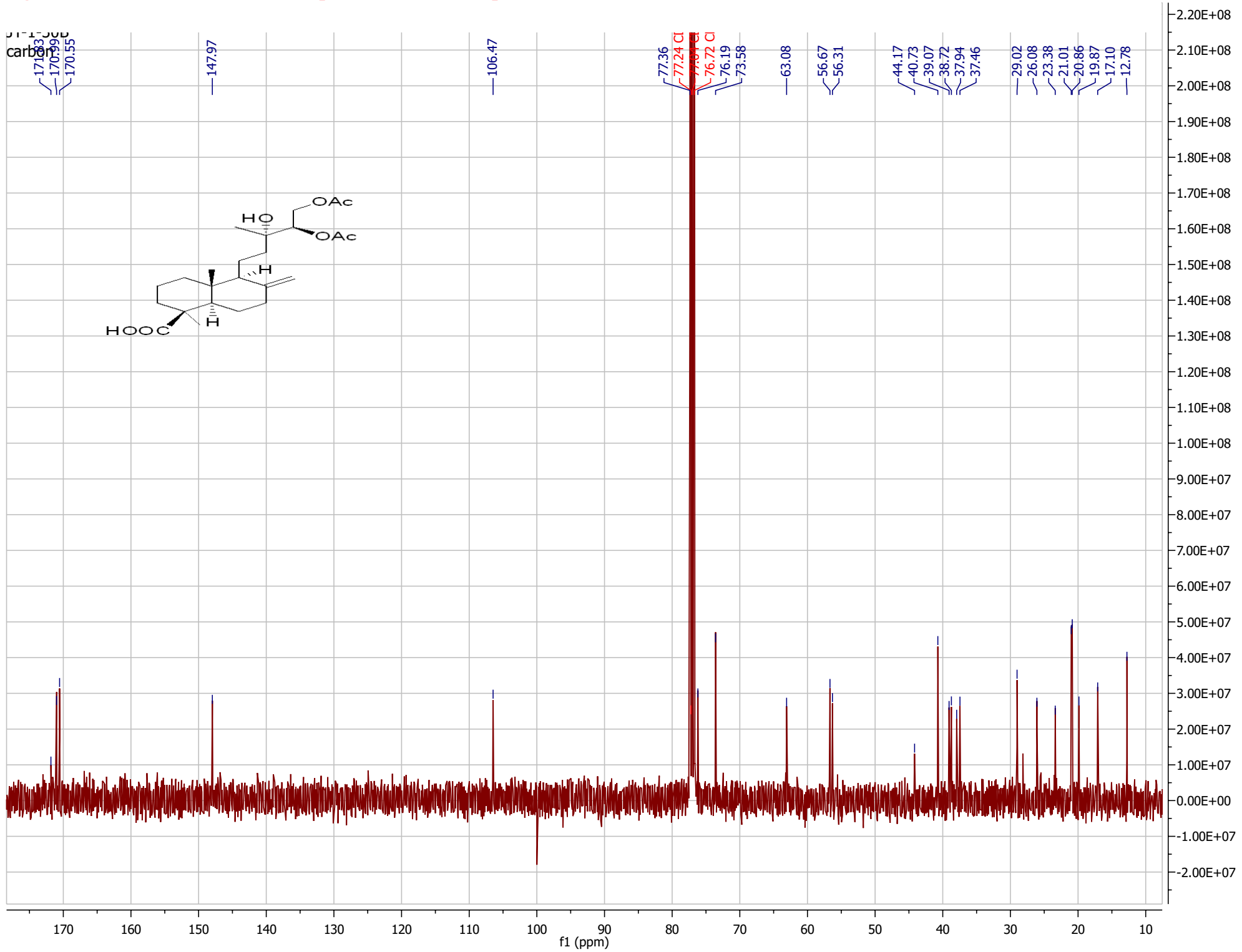
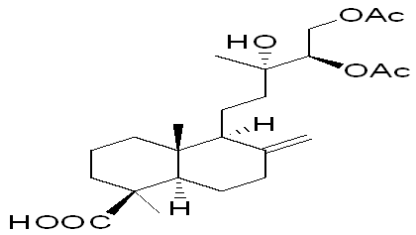


Figure S12. 400 MHz HMQC spectrum of of compound **10** in $CDCl_3$.



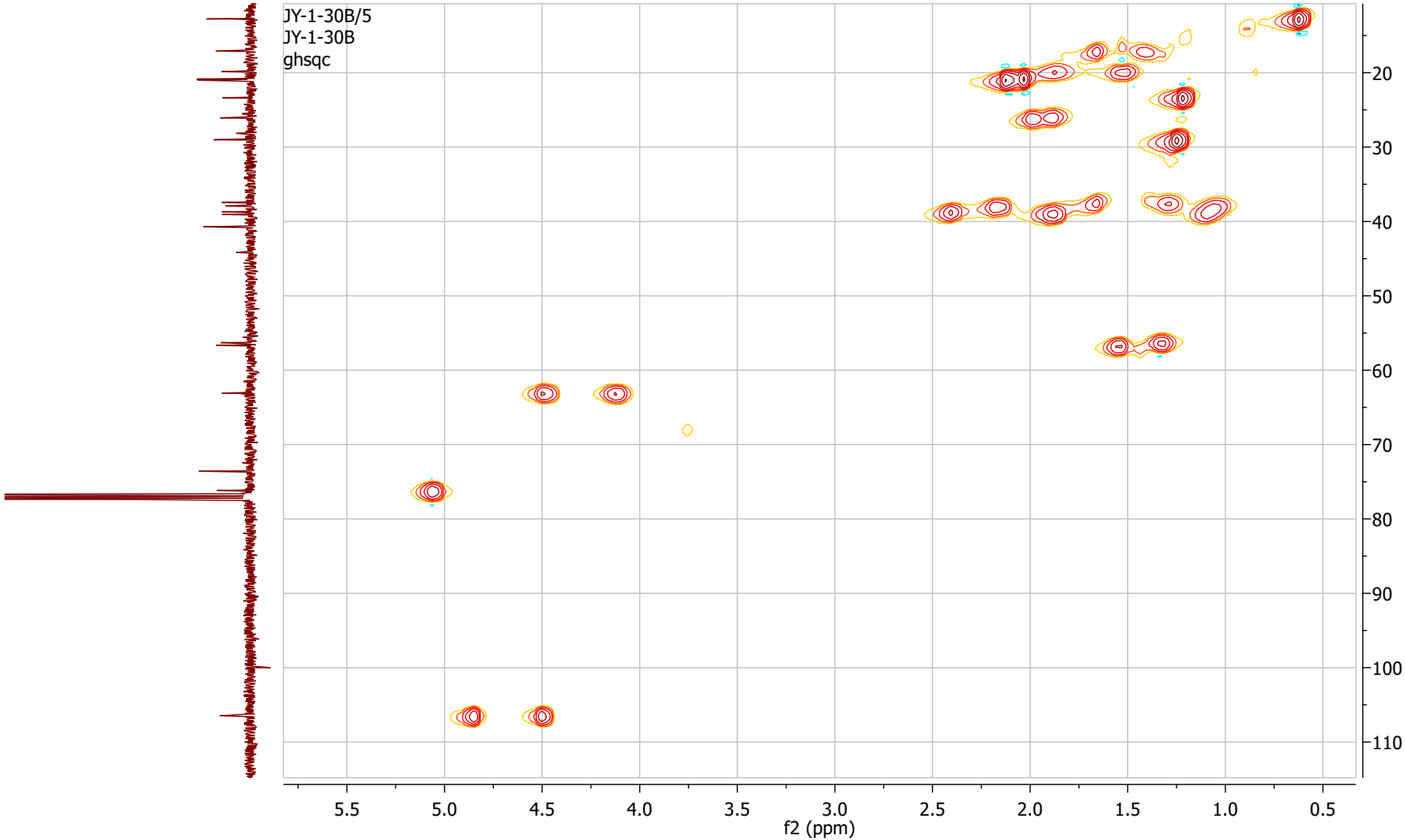


Figure S13. 400 MHz HMBC spectrum of of compound **10** in $CDCl_3$.

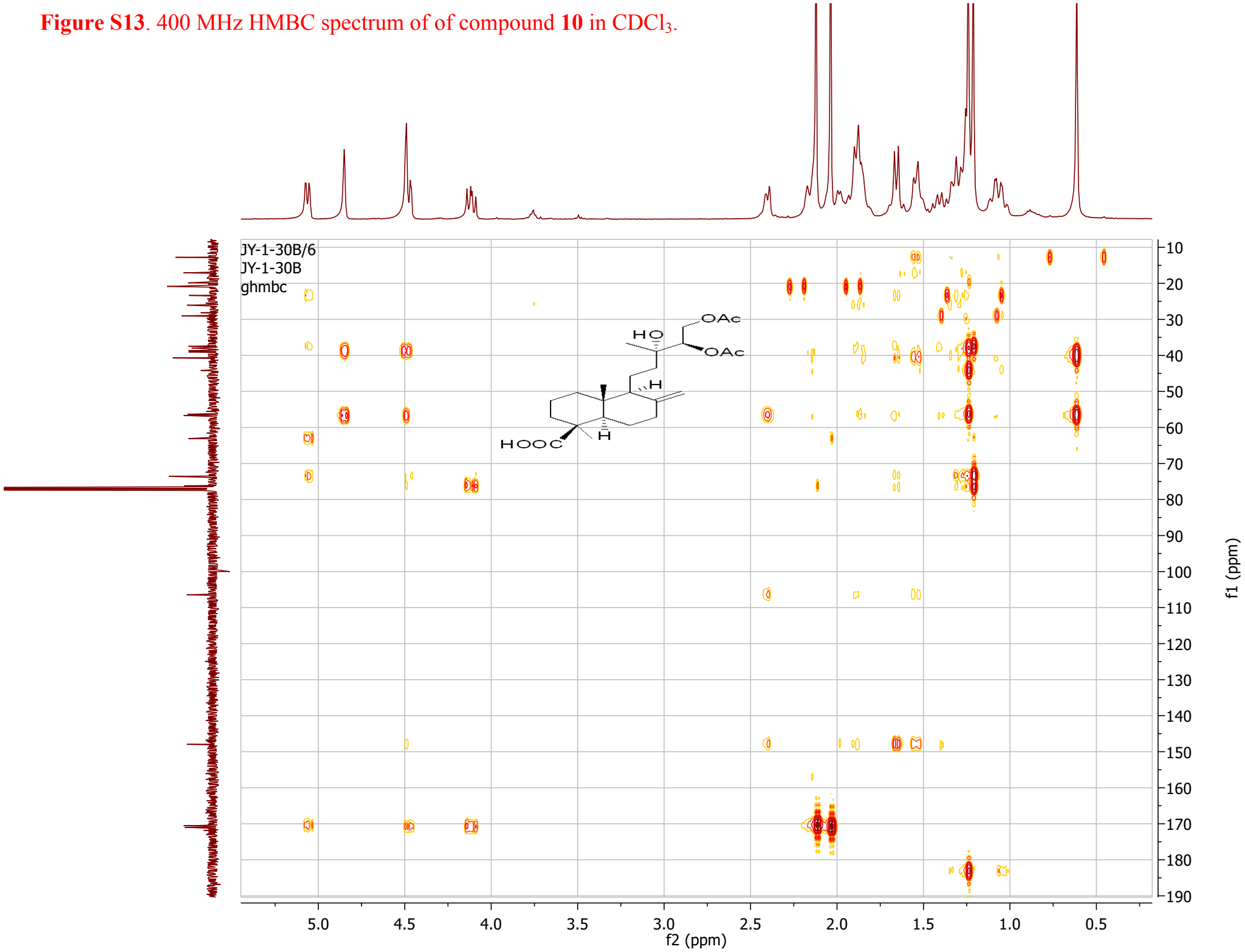


Figure S14. UPLC-MS data showing deoxypodorhizone in 79864-c9 from the stem of *Thuja occidentalis.*

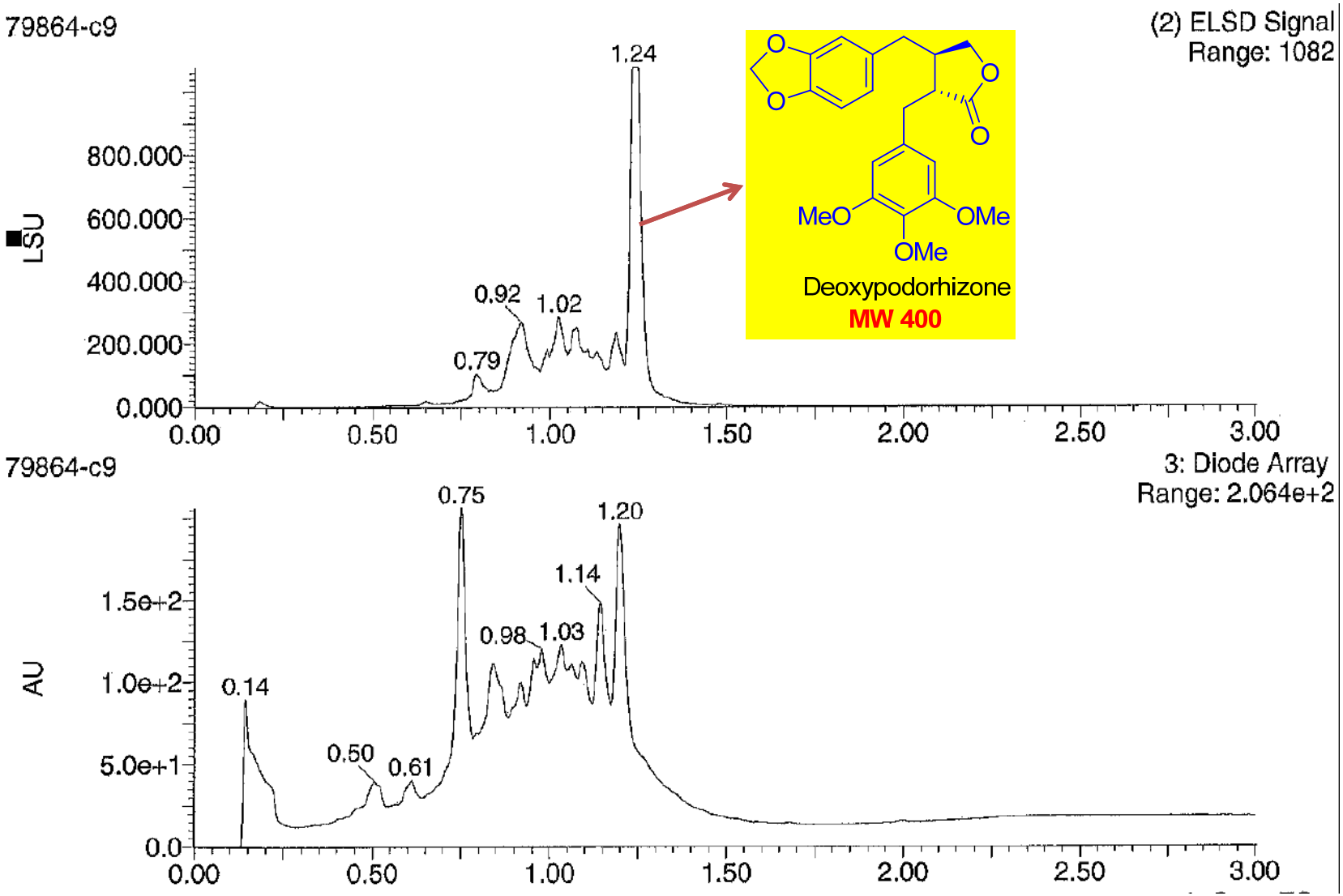


Figure S15. 400 MHz ^{1}H NMR spectrum of 79864-c9 (0.4 mg) indicating the presence of doxypodorhizone.

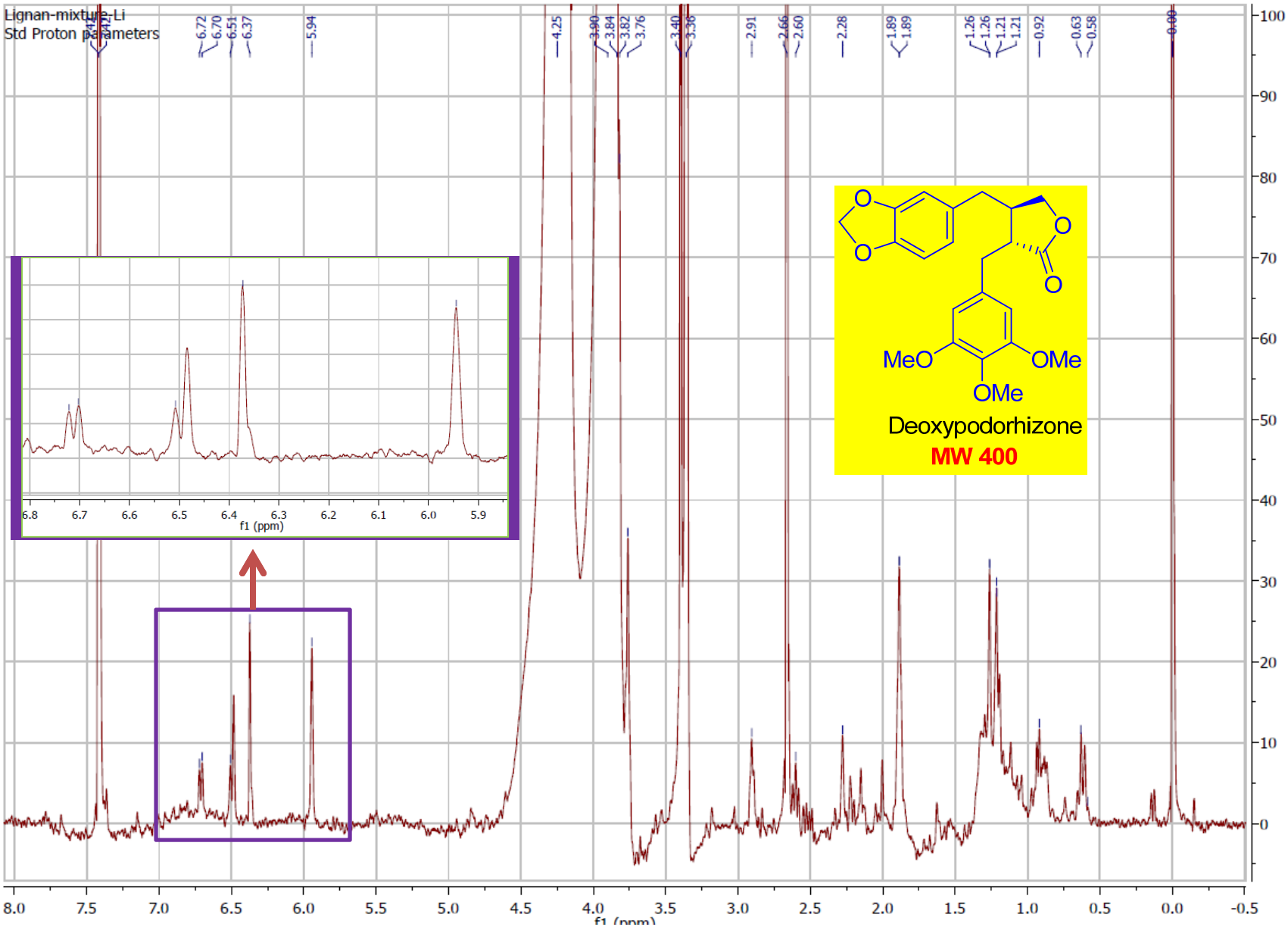


Figure S16. HRESIMS Spectrum of Compound **9**.

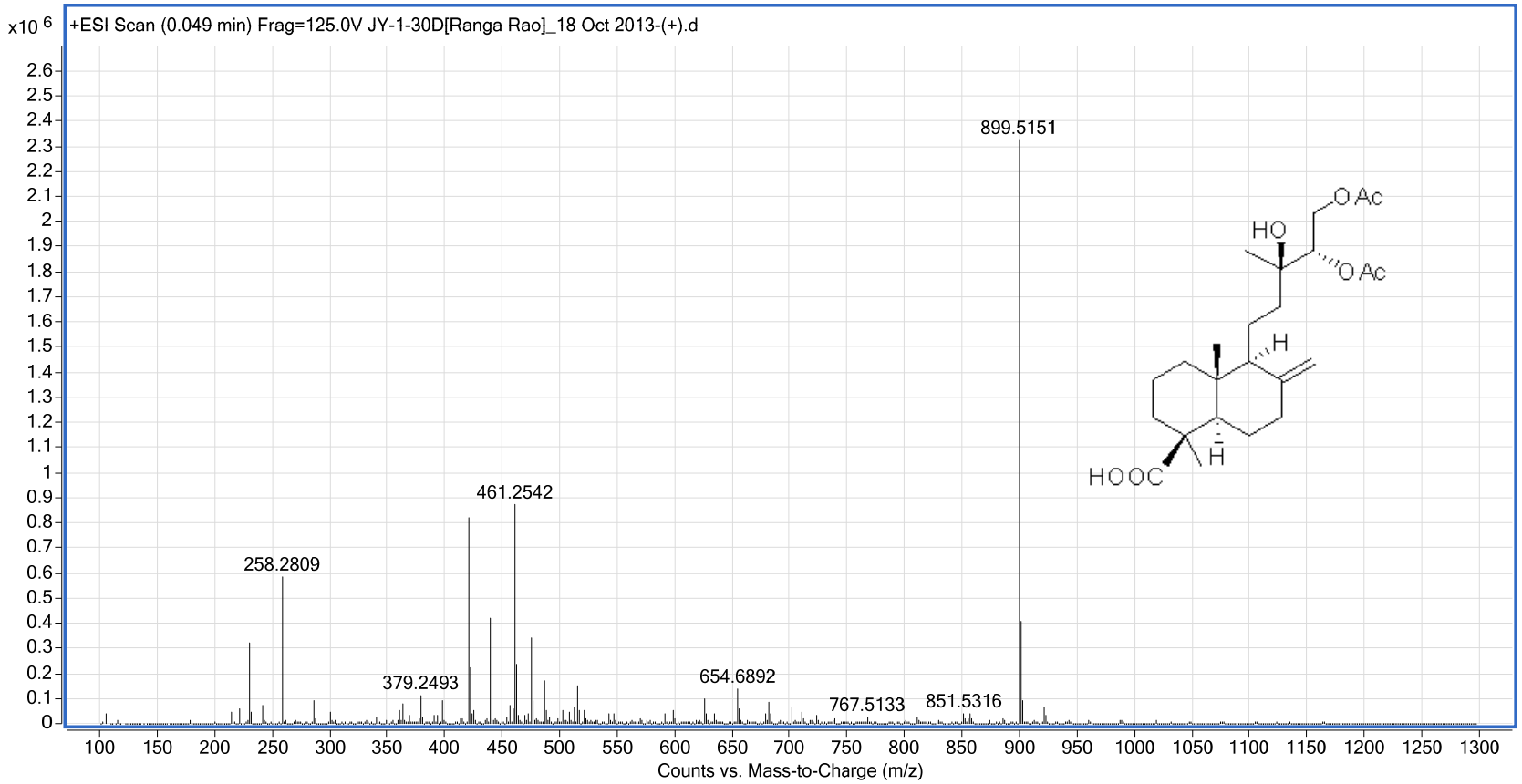


Figure S17. HRESIMS Spectrum of Compound **10**.

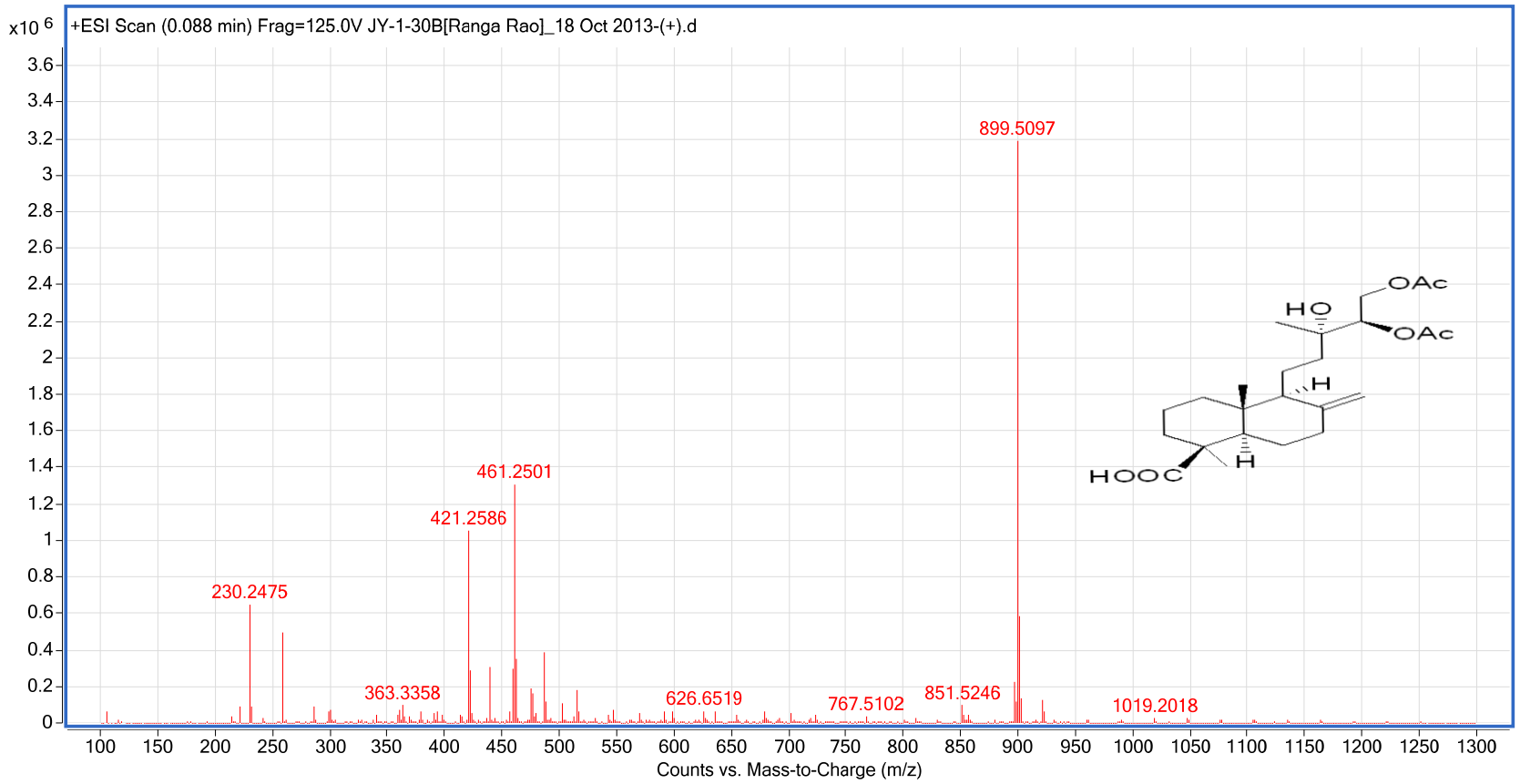


Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound_**9**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	3355(2)	5322(1)	9437(2)	32(1)
O(2)	1354(2)	5539(1)	11619(2)	27(1)
O(3)	817(2)	9658(1)	9641(2)	21(1)
O(4)	4810(2)	9338(1)	5597(2)	22(1)
O(5)	4577(2)	8406(1)	4839(2)	32(1)
O(6)	1223(2)	9760(1)	6171(2)	19(1)
O(7)	1010(2)	9416(1)	3318(2)	30(1)
C(1)	4245(3)	7069(1)	8856(3)	22(1)
C(2)	5266(3)	6504(1)	8498(3)	26(1)
C(3)	5845(3)	6205(1)	10268(3)	26(1)
C(4)	4189(3)	6095(1)	11527(3)	22(1)
C(5)	3169(3)	6680(1)	11861(2)	19(1)
C(6)	1639(3)	6661(1)	13301(2)	22(1)
C(7)	956(3)	7265(1)	13773(3)	24(1)
C(8)	295(3)	7561(1)	12047(2)	21(1)
C(9)	1851(3)	7616(1)	10676(2)	18(1)
C(10)	2529(2)	7004(1)	10077(2)	18(1)
C(11)	1364(3)	8033(1)	9105(2)	19(1)
C(12)	1326(3)	8644(1)	9879(2)	19(1)
C(13)	601(2)	9129(1)	8640(2)	18(1)
C(14)	1758(2)	9202(1)	6918(2)	17(1)
C(15)	3876(3)	9217(1)	7279(2)	20(1)
C(16)	-1476(3)	9051(1)	8092(3)	23(1)
C(17)	-1490(3)	7718(1)	11776(3)	26(1)
C(18)	2931(3)	5619(1)	10717(3)	23(1)
C(19)	5004(3)	5859(1)	13358(3)	29(1)
C(20)	926(3)	6699(1)	9005(2)	20(1)
C(21)	5055(2)	8884(1)	4480(3)	23(1)
C(22)	6032(3)	9062(1)	2787(3)	32(1)
C(23)	927(2)	9811(1)	4377(2)	20(1)
C(24)	468(3)	10413(1)	3829(3)	29(1)

Table S1. Crystal data and structure refinement for compound_**9**.

Identification code	shelx	
Empirical formula	C24 H38 O7	
Formula weight	438.54	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 7.0889(2) Å	α= 90°.
	b = 23.3669(5) Å	β= 91.7930(10)°.
	c = 7.3183(2) Å	γ = 90°.
Volume	1211.65(5) $Å^3$	
Z	2	
Density (calculated)	1.202 Mg/m^3	
Absorption coefficient	0.712 mm^{-1}	
F(000)	476	
Crystal size	0.400 x 0.200 x 0.190 mm^3	
Theta range for data collection	3.783 to 69.591°.	
Index ranges	-8<=h<=8, -27<=k<=27, -8<=l<=8	
Reflections collected	9933	
Independent reflections	3954 [R(int) = 0.0209]	
Completeness to theta = 67.679°	98.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8767 and 0.7639	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3954 / 1 / 288	
Goodness-of-fit on F^2	1.039	
Final R indices [I>2sigma(I)]	R1 = 0.0259, wR2 = 0.0693	
R indices (all data)	R1 = 0.0260, wR2 = 0.0694	
Absolute structure parameter	0.09(3)	
Extinction coefficient	0.0031(6)	
Largest diff. peak and hole	0.198 and -0.152 $e.Å^{-3}$	

Table S3. Bond lengths [Å] and angles [°] for compound_**9**.

O(1)-C(18)	1.212(2)
O(2)-C(18)	1.330(2)
O(2)-H(2)	0.8400
O(3)-C(13)	1.444(2)
O(3)-H(3)	0.8400
O(4)-C(21)	1.355(2)
O(4)-C(15)	1.444(2)
O(5)-C(21)	1.197(3)
O(6)-C(23)	1.329(2)
O(6)-C(14)	1.458(2)
O(7)-C(23)	1.208(2)
C(1)-C(2)	1.532(3)
C(1)-C(10)	1.539(3)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-C(3)	1.517(3)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.536(3)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(18)	1.533(3)
C(4)-C(19)	1.545(3)
C(4)-C(5)	1.570(2)
C(5)-C(6)	1.536(2)
C(5)-C(10)	1.564(2)
C(5)-H(5)	1.0000
C(6)-C(7)	1.534(3)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(8)	1.501(3)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(17)	1.327(3)
C(8)-C(9)	1.520(3)

C(9)-C(11)	1.538(2)
C(9)-C(10)	1.574(2)
C(9)-H(9)	1.0000
C(10)-C(20)	1.536(2)
C(11)-C(12)	1.537(2)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.530(2)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(16)	1.525(2)
C(13)-C(14)	1.535(2)
C(14)-C(15)	1.517(2)
C(14)-H(14)	1.0000
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9500
C(17)-H(17B)	0.9500
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-C(22)	1.497(3)
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-C(24)	1.495(3)
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800

C(18)-O(2)-H(2)	109.5

C(13)-O(3)-H(3)	109.5
C(21)-O(4)-C(15)	115.52(14)
C(23)-O(6)-C(14)	118.78(13)
C(2)-C(1)-C(10)	113.56(15)
C(2)-C(1)-H(1A)	108.9
C(10)-C(1)-H(1A)	108.9
C(2)-C(1)-H(1B)	108.9
C(10)-C(1)-H(1B)	108.9
H(1A)-C(1)-H(1B)	107.7
C(3)-C(2)-C(1)	111.60(16)
C(3)-C(2)-H(2A)	109.3
C(1)-C(2)-H(2A)	109.3
C(3)-C(2)-H(2B)	109.3
C(1)-C(2)-H(2B)	109.3
H(2A)-C(2)-H(2B)	108.0
C(2)-C(3)-C(4)	113.42(15)
C(2)-C(3)-H(3A)	108.9
C(4)-C(3)-H(3A)	108.9
C(2)-C(3)-H(3B)	108.9
C(4)-C(3)-H(3B)	108.9
H(3A)-C(3)-H(3B)	107.7
C(18)-C(4)-C(3)	109.61(15)
C(18)-C(4)-C(19)	105.84(15)
C(3)-C(4)-C(19)	107.95(15)
C(18)-C(4)-C(5)	115.25(15)
C(3)-C(4)-C(5)	108.21(15)
C(19)-C(4)-C(5)	109.76(15)
C(6)-C(5)-C(10)	113.25(14)
C(6)-C(5)-C(4)	114.82(14)
C(10)-C(5)-C(4)	114.47(14)
C(6)-C(5)-H(5)	104.2
C(10)-C(5)-H(5)	104.2
C(4)-C(5)-H(5)	104.2
C(7)-C(6)-C(5)	111.19(15)
C(7)-C(6)-H(6A)	109.4
C(5)-C(6)-H(6A)	109.4
C(7)-C(6)-H(6B)	109.4

C(5)-C(6)-H(6B)	109.4
H(6A)-C(6)-H(6B)	108.0
C(8)-C(7)-C(6)	109.03(15)
C(8)-C(7)-H(7A)	109.9
C(6)-C(7)-H(7A)	109.9
C(8)-C(7)-H(7B)	109.9
C(6)-C(7)-H(7B)	109.9
H(7A)-C(7)-H(7B)	108.3
C(17)-C(8)-C(7)	121.67(17)
C(17)-C(8)-C(9)	125.88(17)
C(7)-C(8)-C(9)	112.35(16)
C(8)-C(9)-C(11)	113.37(15)
C(8)-C(9)-C(10)	109.96(14)
C(11)-C(9)-C(10)	115.48(14)
C(8)-C(9)-H(9)	105.7
C(11)-C(9)-H(9)	105.7
C(10)-C(9)-H(9)	105.7
C(20)-C(10)-C(1)	109.59(14)
C(20)-C(10)-C(5)	113.12(14)
C(1)-C(10)-C(5)	108.62(14)
C(20)-C(10)-C(9)	109.60(15)
C(1)-C(10)-C(9)	108.99(14)
C(5)-C(10)-C(9)	106.81(14)
C(12)-C(11)-C(9)	108.62(14)
C(12)-C(11)-H(11A)	110.0
C(9)-C(11)-H(11A)	110.0
C(12)-C(11)-H(11B)	110.0
C(9)-C(11)-H(11B)	110.0
H(11A)-C(11)-H(11B)	108.3
C(13)-C(12)-C(11)	118.61(14)
C(13)-C(12)-H(12A)	107.7
C(11)-C(12)-H(12A)	107.7
C(13)-C(12)-H(12B)	107.7
C(11)-C(12)-H(12B)	107.7
H(12A)-C(12)-H(12B)	107.1
O(3)-C(13)-C(16)	108.74(14)
O(3)-C(13)-C(12)	107.81(13)

C(16)-C(13)-C(12)	111.84(15)
O(3)-C(13)-C(14)	105.63(13)
C(16)-C(13)-C(14)	109.48(14)
C(12)-C(13)-C(14)	113.05(14)
O(6)-C(14)-C(15)	106.86(13)
O(6)-C(14)-C(13)	105.57(13)
C(15)-C(14)-C(13)	114.25(14)
O(6)-C(14)-H(14)	110.0
C(15)-C(14)-H(14)	110.0
C(13)-C(14)-H(14)	110.0
O(4)-C(15)-C(14)	109.48(14)
O(4)-C(15)-H(15A)	109.8
C(14)-C(15)-H(15A)	109.8
O(4)-C(15)-H(15B)	109.8
C(14)-C(15)-H(15B)	109.8
H(15A)-C(15)-H(15B)	108.2
C(13)-C(16)-H(16A)	109.5
C(13)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(13)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(8)-C(17)-H(17A)	120.0
C(8)-C(17)-H(17B)	120.0
H(17A)-C(17)-H(17B)	120.0
O(1)-C(18)-O(2)	122.38(18)
O(1)-C(18)-C(4)	123.99(18)
O(2)-C(18)-C(4)	113.53(16)
C(4)-C(19)-H(19A)	109.5
C(4)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(4)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(10)-C(20)-H(20A)	109.5
C(10)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5

C(10)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
O(5)-C(21)-O(4)	123.72(17)
O(5)-C(21)-C(22)	125.65(18)
O(4)-C(21)-C(22)	110.62(17)
C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
O(7)-C(23)-O(6)	123.76(17)
O(7)-C(23)-C(24)	124.19(17)
O(6)-C(23)-C(24)	112.05(16)
C(23)-C(24)-H(24A)	109.5
C(23)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(23)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for compound_**9**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	37(1)	24(1)	35(1)	-10(1)	5(1)	-2(1)
O(2)	36(1)	18(1)	26(1)	-4(1)	2(1)	-9(1)
O(3)	32(1)	17(1)	14(1)	0(1)	0(1)	4(1)
O(4)	22(1)	22(1)	21(1)	2(1)	3(1)	-2(1)
O(5)	37(1)	24(1)	35(1)	-2(1)	11(1)	-1(1)
O(6)	25(1)	16(1)	15(1)	0(1)	0(1)	2(1)
O(7)	51(1)	22(1)	16(1)	0(1)	-3(1)	4(1)
C(1)	24(1)	20(1)	23(1)	1(1)	2(1)	-1(1)
C(2)	24(1)	24(1)	30(1)	-2(1)	7(1)	1(1)
C(3)	23(1)	21(1)	35(1)	-4(1)	0(1)	2(1)
C(4)	26(1)	16(1)	24(1)	1(1)	-4(1)	1(1)
C(5)	24(1)	14(1)	20(1)	-1(1)	-3(1)	-2(1)
C(6)	32(1)	17(1)	18(1)	2(1)	1(1)	-1(1)
C(7)	36(1)	19(1)	18(1)	0(1)	5(1)	0(1)
C(8)	28(1)	14(1)	20(1)	-2(1)	3(1)	-2(1)
C(9)	21(1)	16(1)	17(1)	0(1)	1(1)	-1(1)
C(10)	21(1)	16(1)	18(1)	0(1)	0(1)	-1(1)
C(11)	24(1)	17(1)	16(1)	1(1)	0(1)	1(1)
C(12)	22(1)	18(1)	16(1)	0(1)	0(1)	0(1)
C(13)	21(1)	16(1)	17(1)	-1(1)	1(1)	2(1)
C(14)	22(1)	14(1)	15(1)	1(1)	-1(1)	2(1)
C(15)	22(1)	20(1)	18(1)	2(1)	2(1)	-1(1)
C(16)	23(1)	24(1)	21(1)	3(1)	2(1)	2(1)
C(17)	28(1)	23(1)	29(1)	2(1)	6(1)	-1(1)
C(18)	30(1)	14(1)	23(1)	3(1)	-3(1)	2(1)
C(19)	36(1)	20(1)	31(1)	0(1)	-9(1)	5(1)
C(20)	23(1)	18(1)	19(1)	-1(1)	0(1)	-1(1)
C(21)	18(1)	28(1)	24(1)	-1(1)	2(1)	2(1)
C(22)	30(1)	41(1)	26(1)	0(1)	6(1)	-1(1)
C(23)	23(1)	21(1)	17(1)	0(1)	1(1)	-1(1)
C(24)	46(1)	22(1)	21(1)	3(1)	-3(1)	5(1)