Electronic Supplementary Material (ESI) for *RSC Adv.*
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Supporting information

Total Synthesis of Palmarumycin BGs, C_1 and Guignardin E

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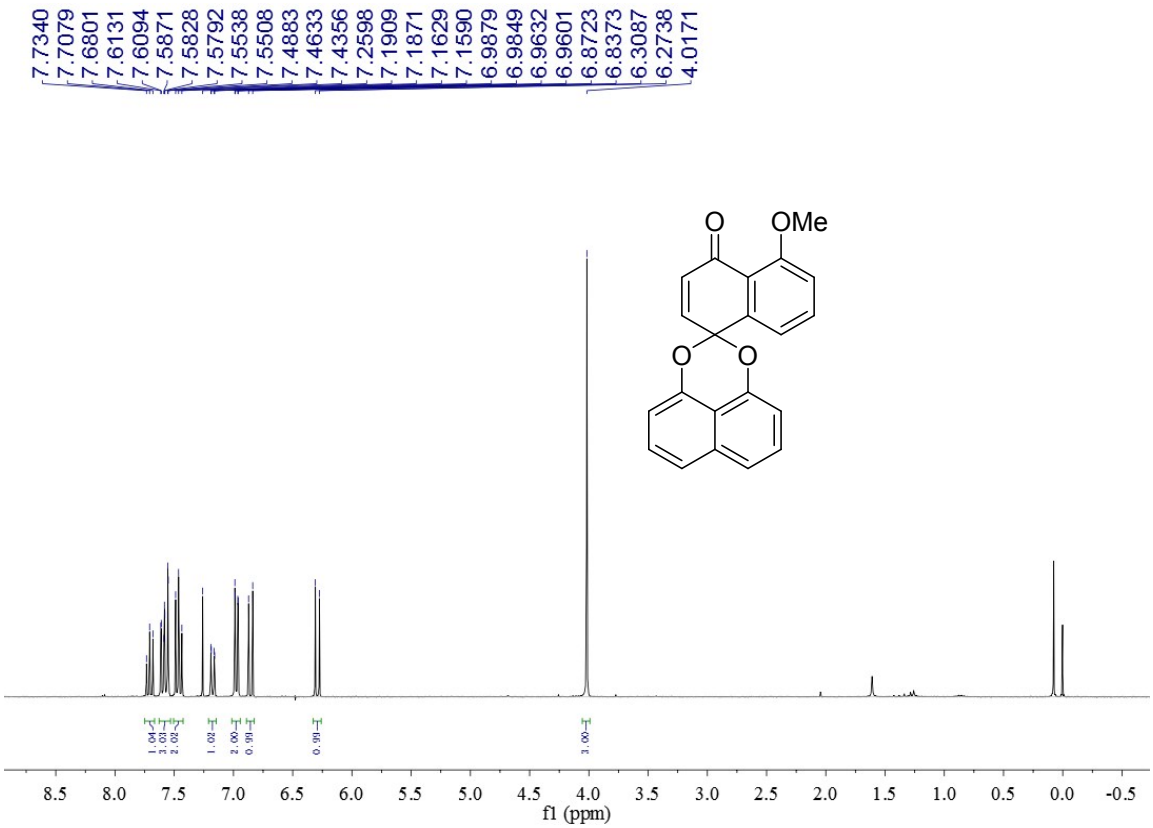


Figure S1 ^{1}H NMR of compound **10**

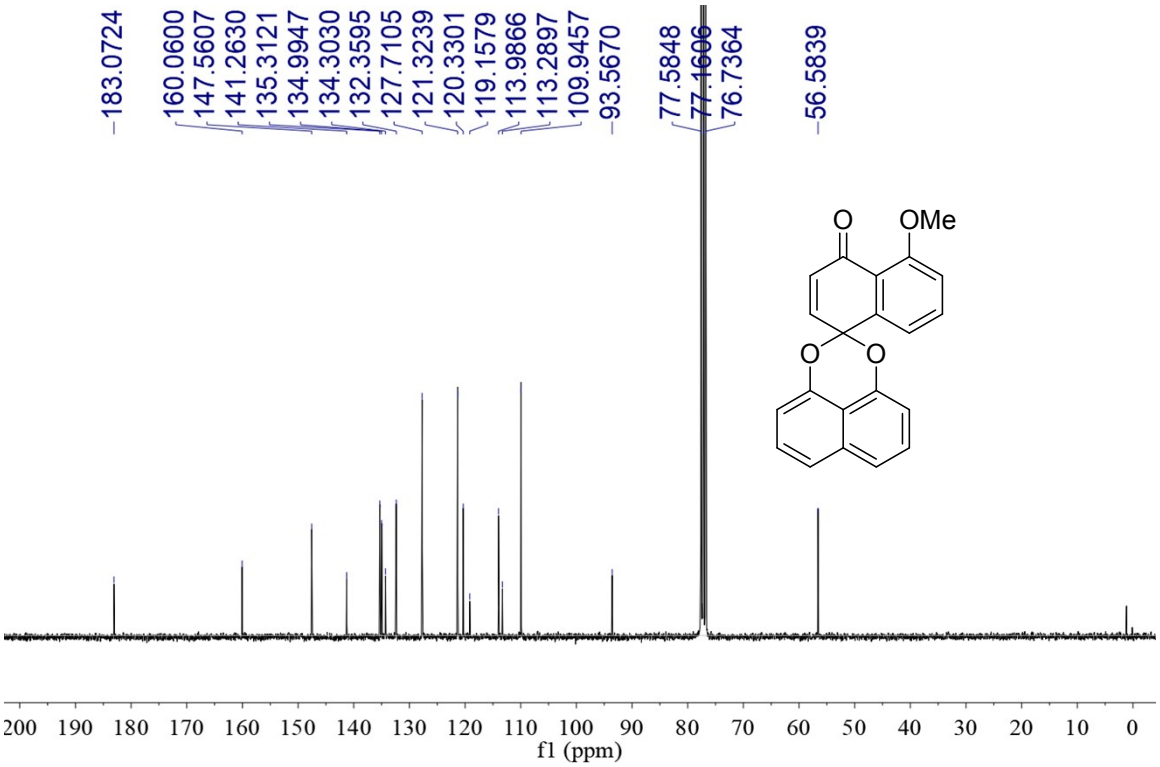


Figure S2 ^{13}C NMR of compound **10**

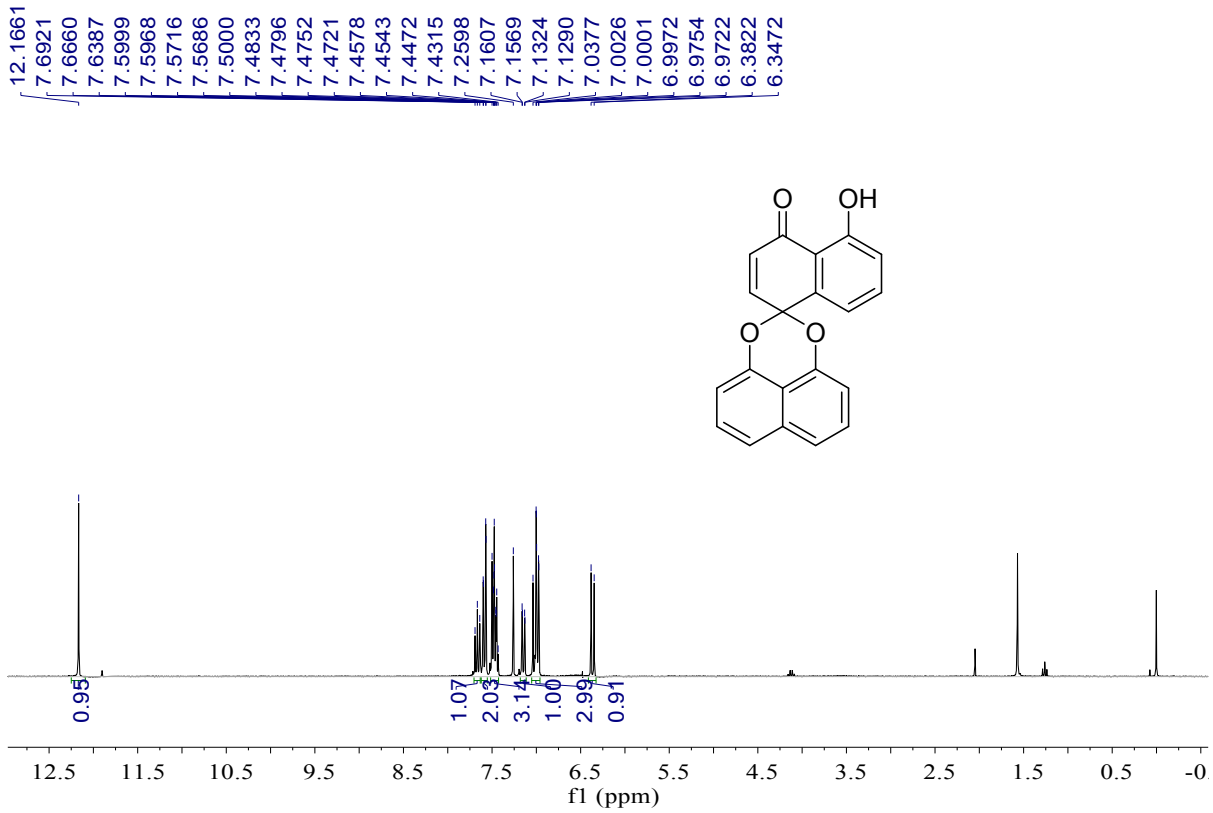


Figure S3 ^{1}H NMR of compound **11**

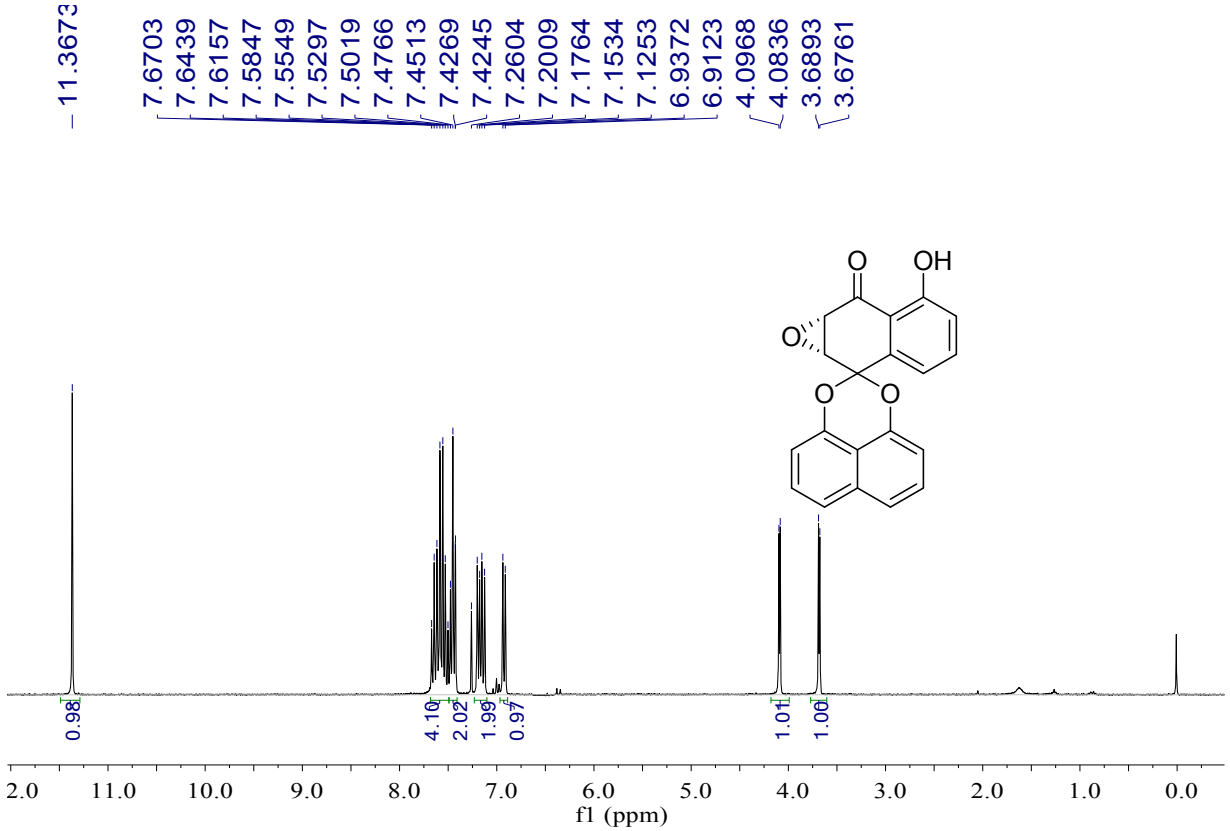


Figure S4 ^{1}H NMR of compound **12**

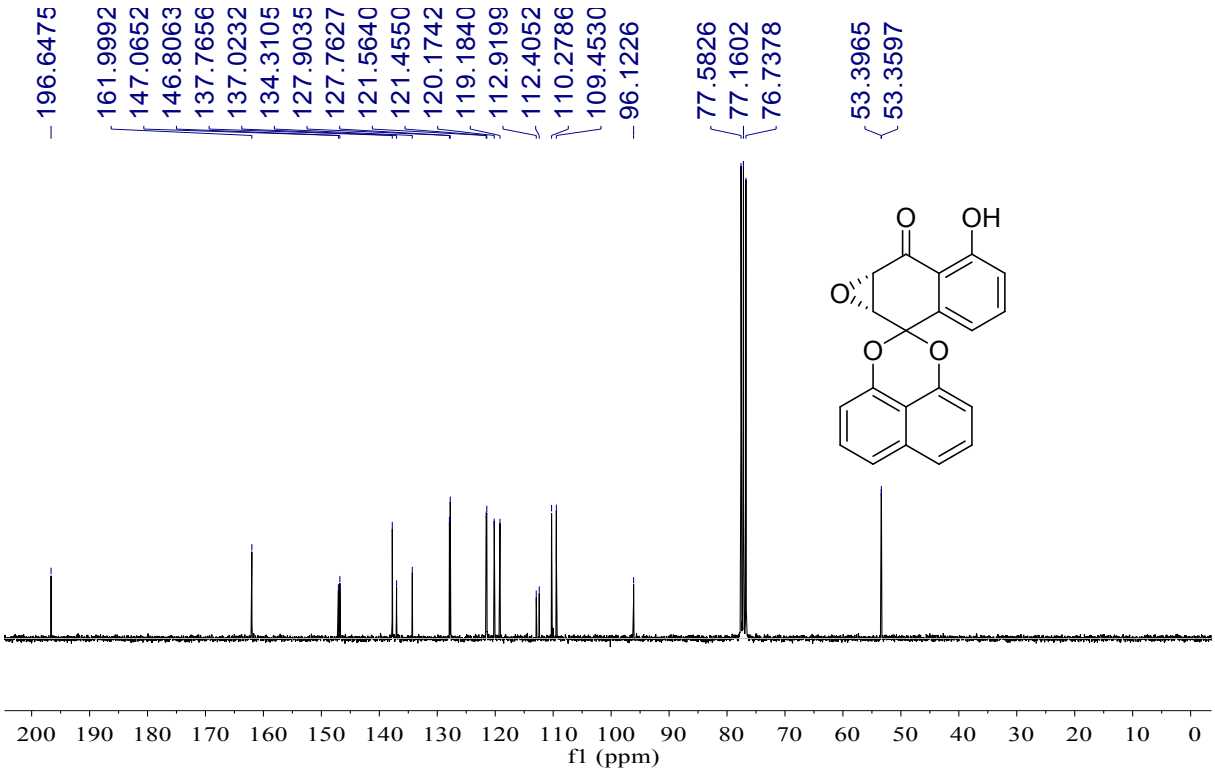
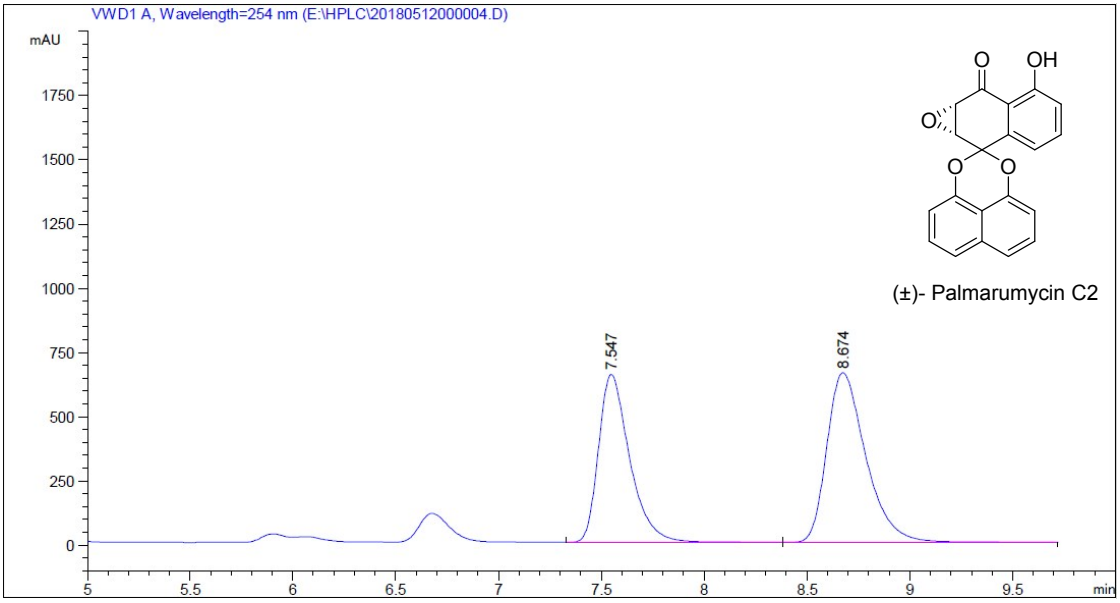
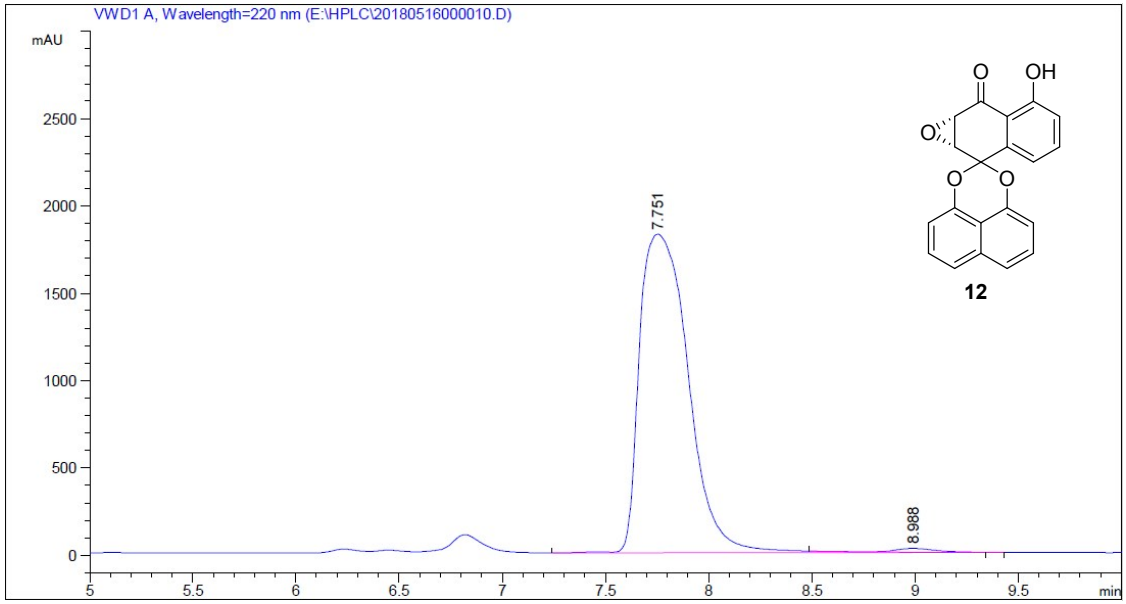


Figure S5 ^{13}C NMR of compound **12**



Peak#	Ret. Time [min]	Area [mAU*s]	Height [mAU]	Conc. [%]
1	7.547	6875.209	652.997	44.172
2	8.674	8689.386	659.877	55.823
Total		15564.595		



Peak#	Ret. Time [min]	Area [mAU*s]	Height [mAU]	Conc. [%]
1	7.751	3.0038e4	1824.567	98.989
2	8.988	306.8433	22.421	1.011
Total		3.0344e4		

Figure S6 HPLC profiles of compound **(±)-** and (-) Palmarumycin $\mathbf{C_2}$ (**12**)

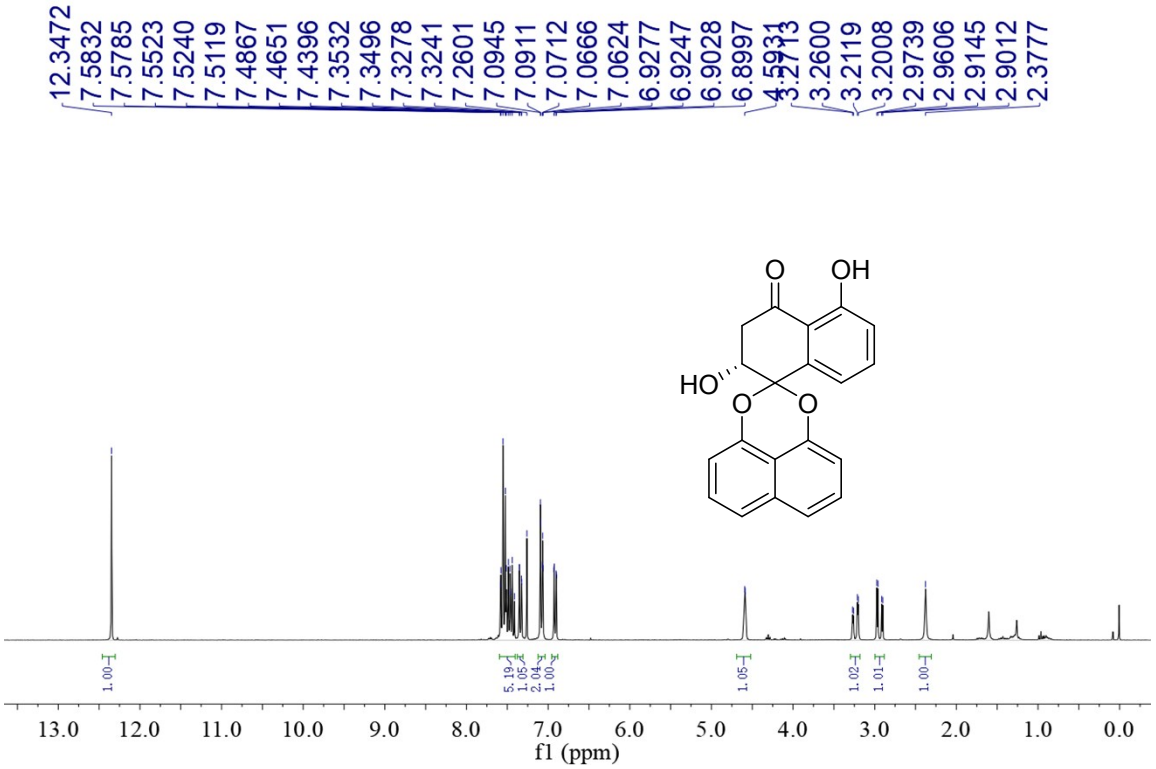


Figure S7 ^{1}H NMR of compound **1**

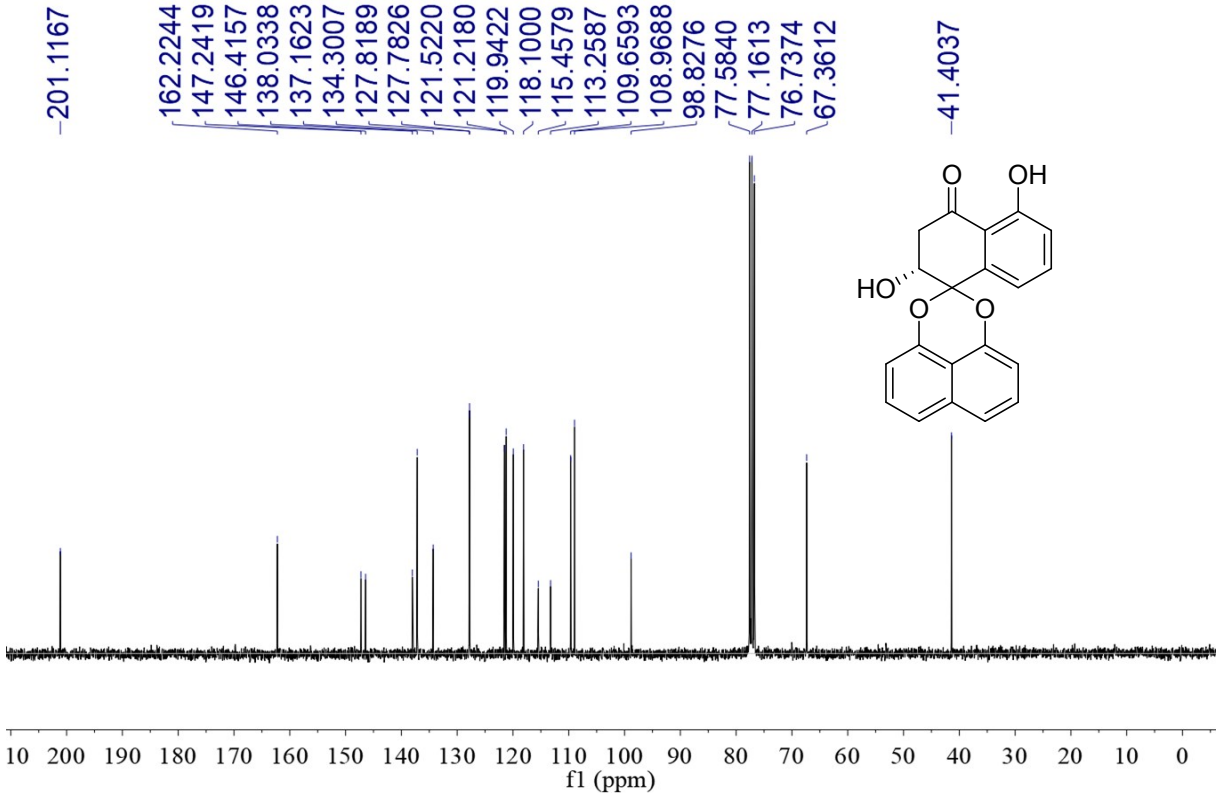


Figure S8 ^{13}C NMR of compound **1**

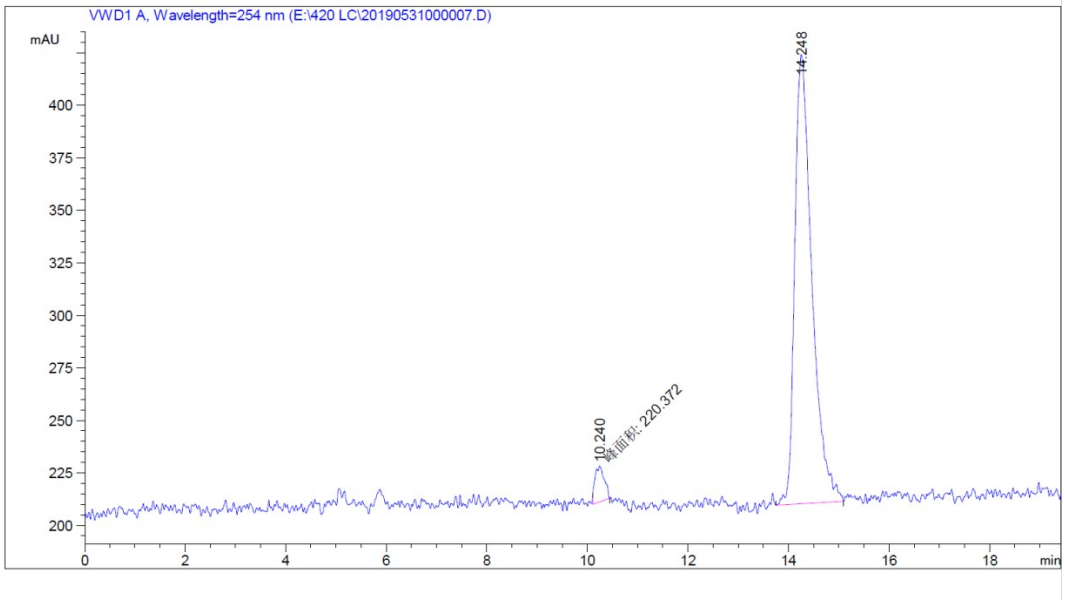


Figure S9 HPLC profile of compound **1**

Peak#	Ret. Time [min]	Area [mAU*s]	Height [mAU]	Conc. [%]
1	10.240	220.3720	17.0249	4.165
2	14.248	5069.9824	213.7812	95.835
Total		5290.3544		

Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z
1	$C_{20}H_{14}O_5$	[M-H]-	333.0791	333.0768

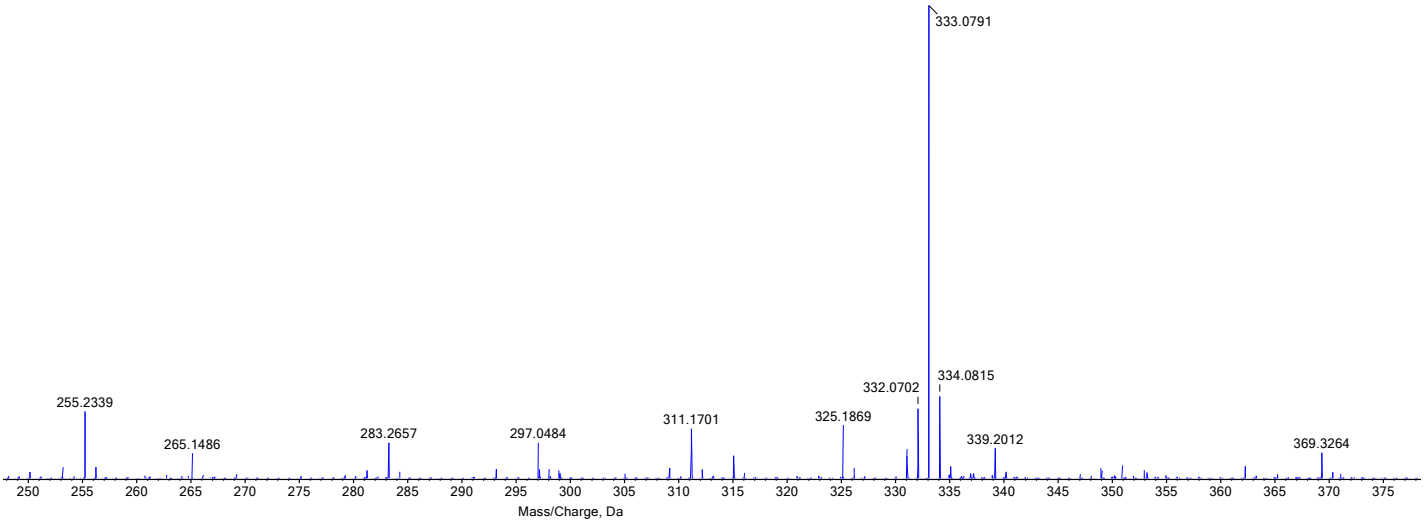


Figure S10 HR-ESI-MS of compound **1**

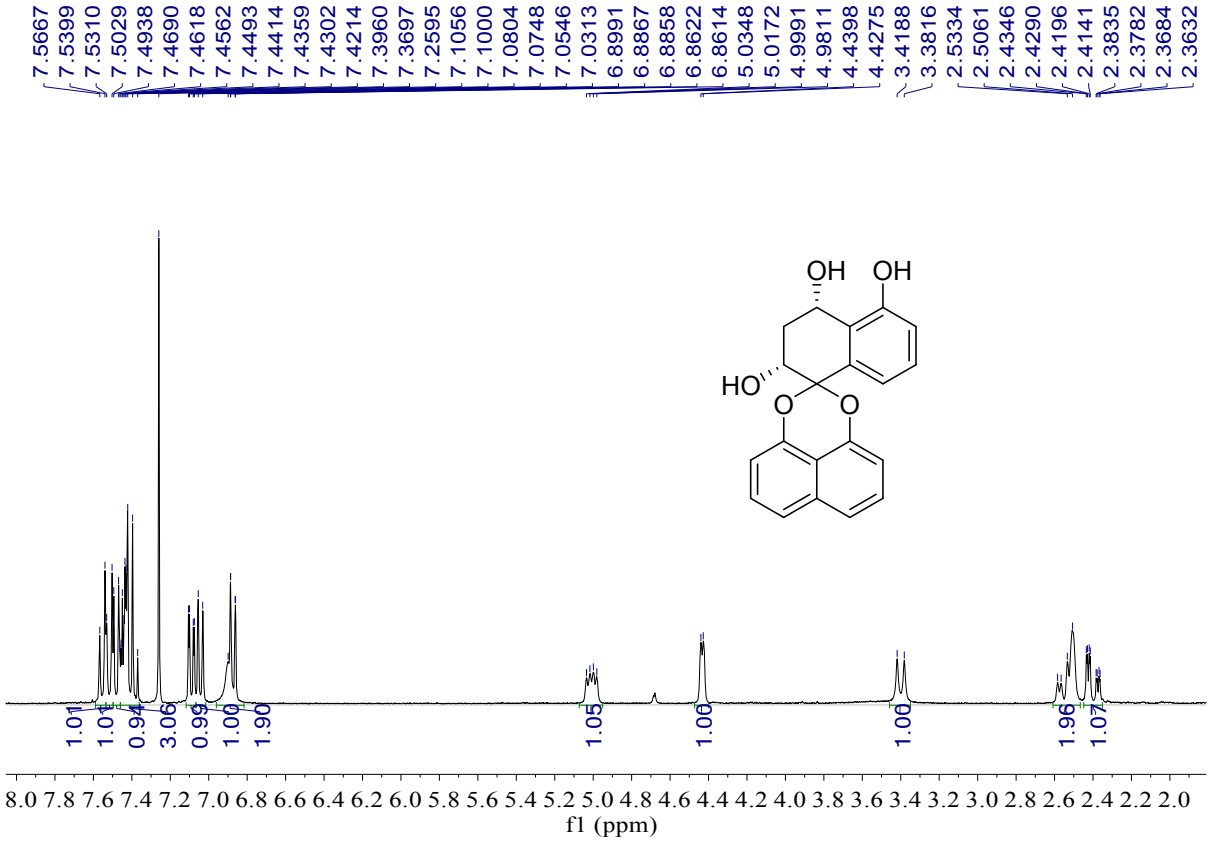


Figure S11 ^{1}H NMR of compound **2**

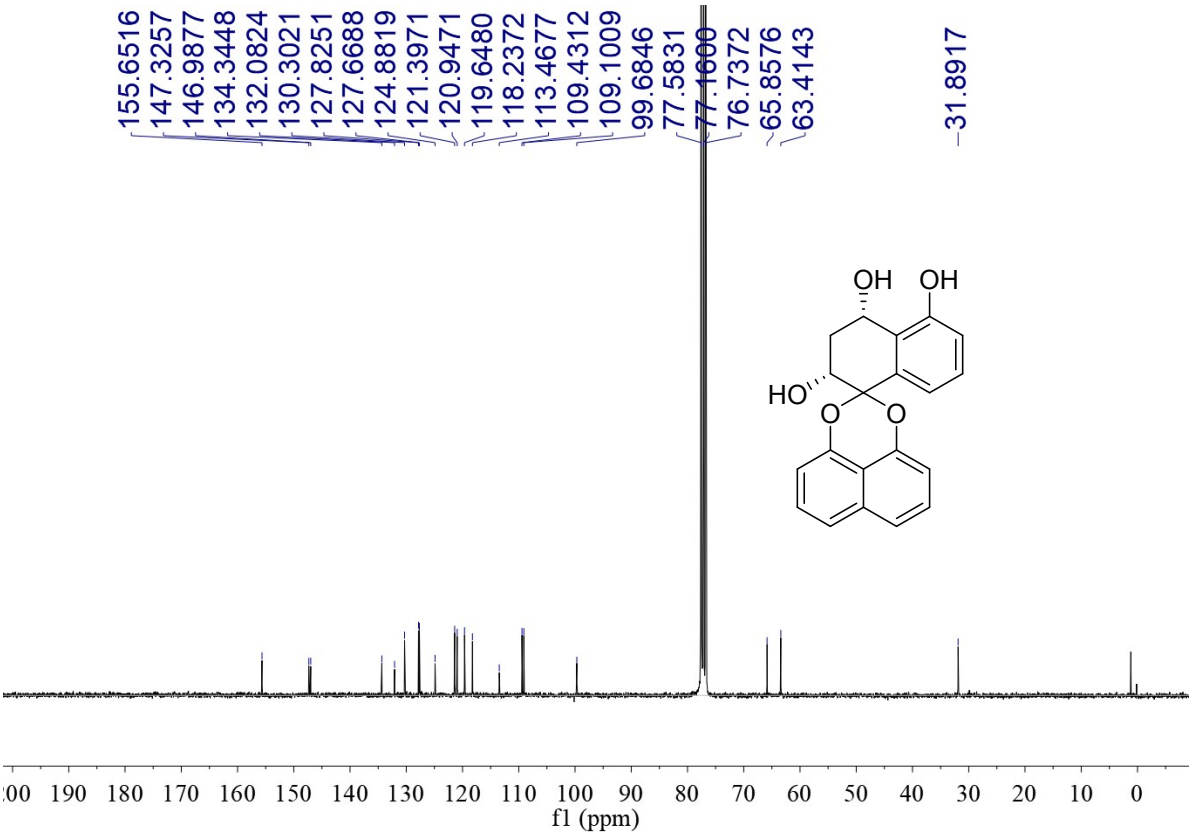


Figure S12 ^{13}C NMR of compound **2**

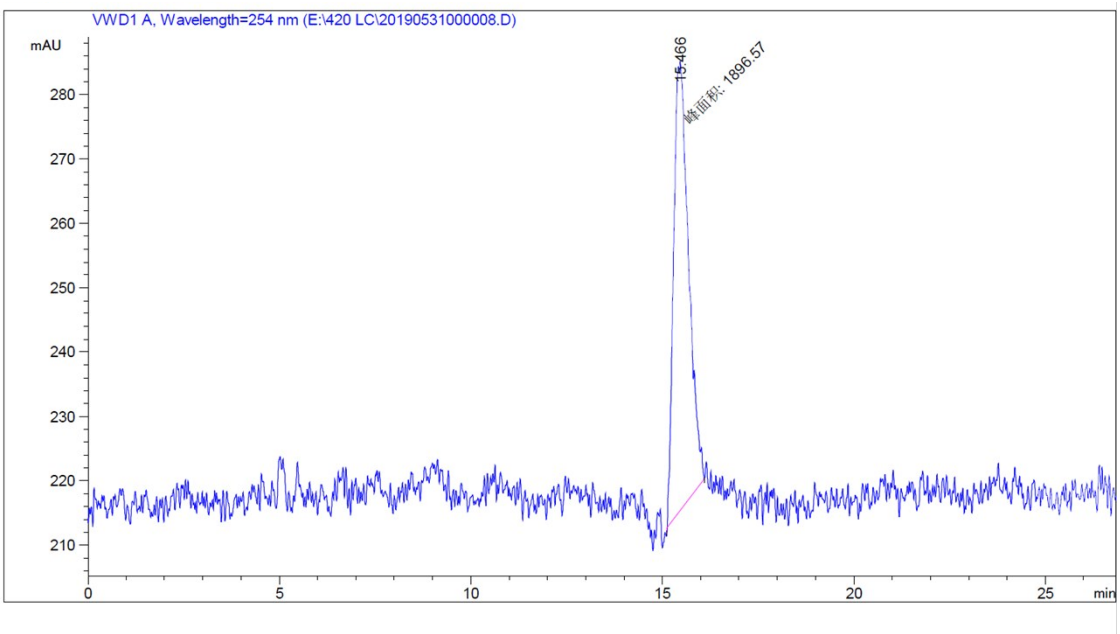


Figure S13 HPLC profile of compound **2**

Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z
2	$C_{20}H_{16}O_5$	[M-H]-	335.0954	335.0925

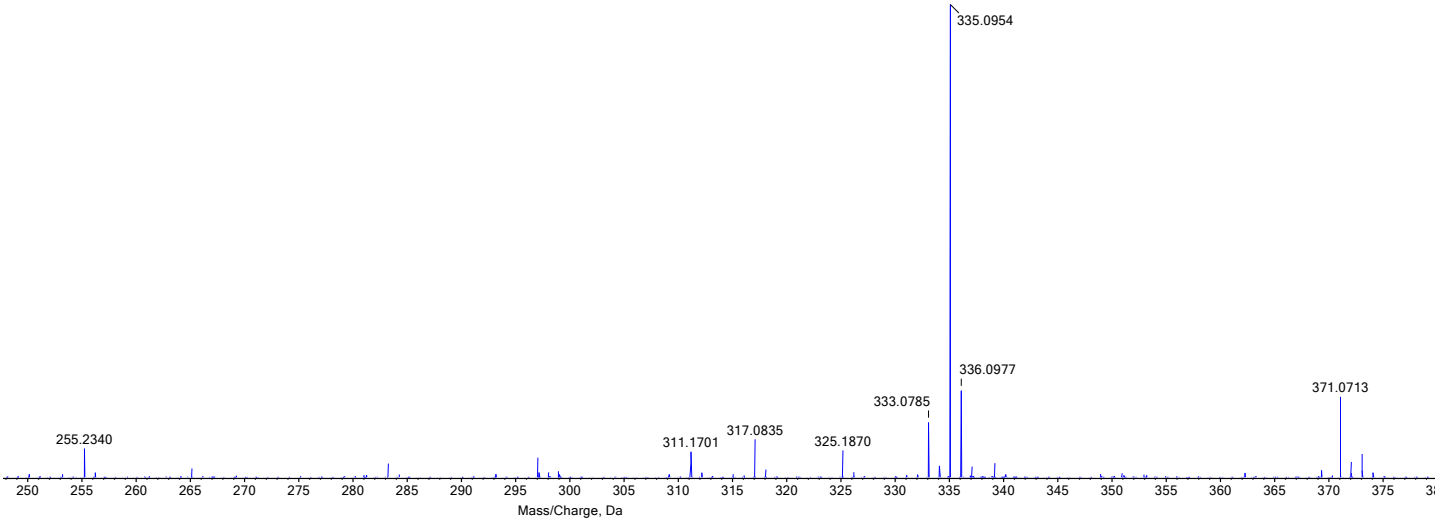


Figure S14 HR-ESI-MS of compound **2**

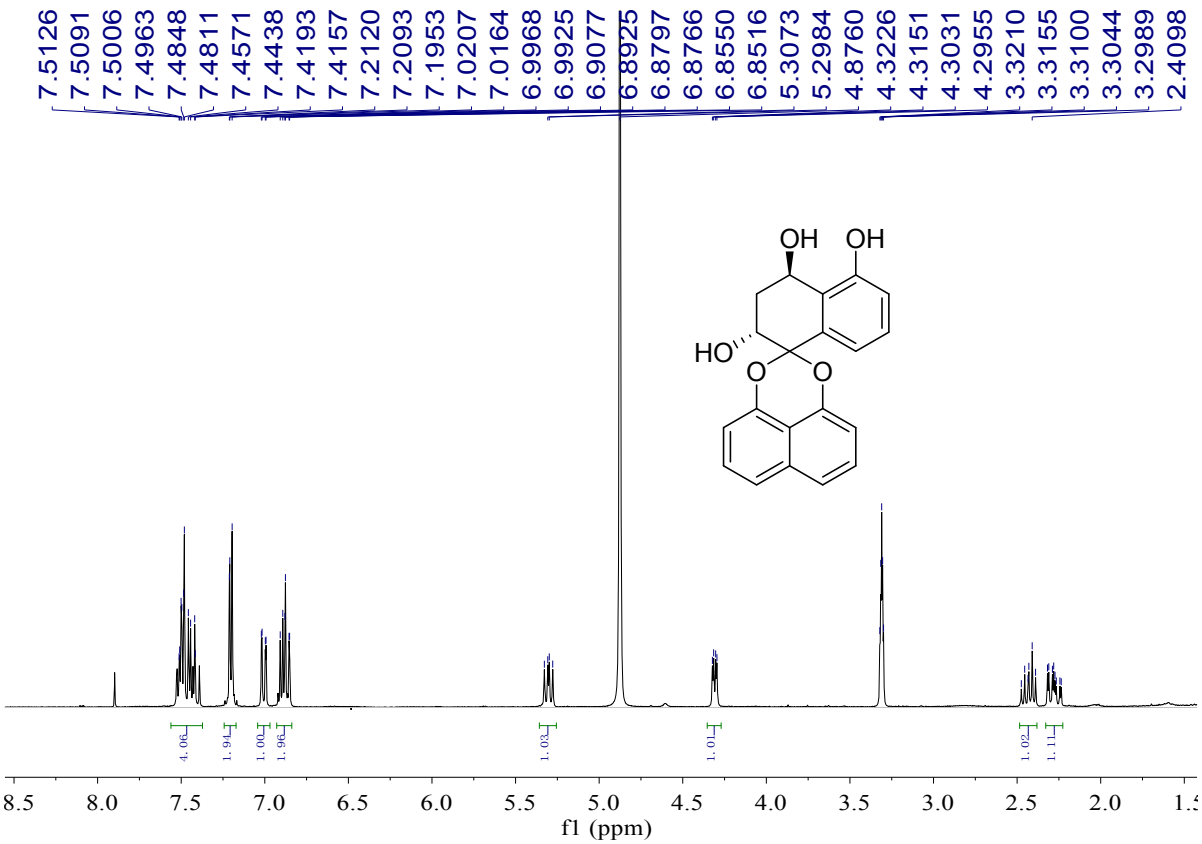


Figure S15 ^{1}H NMR of compound **3**

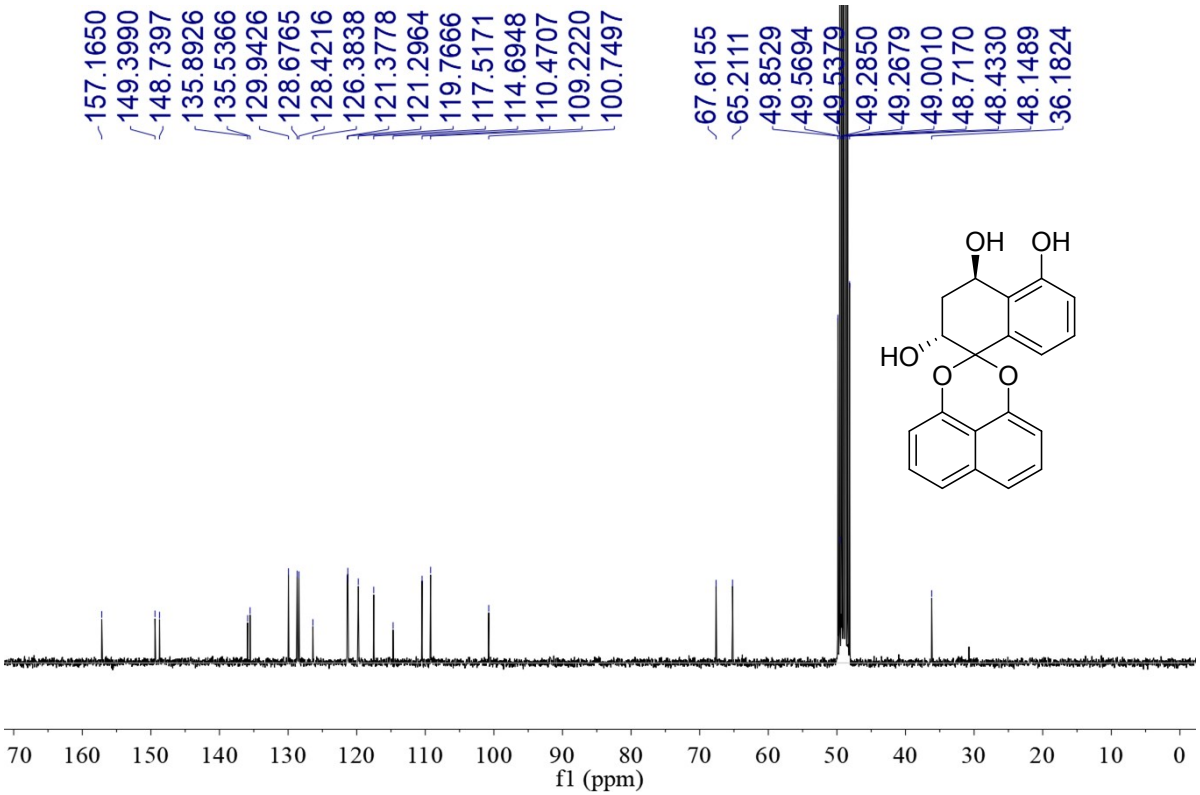


Figure S16 ^{13}C NMR of compound **3**

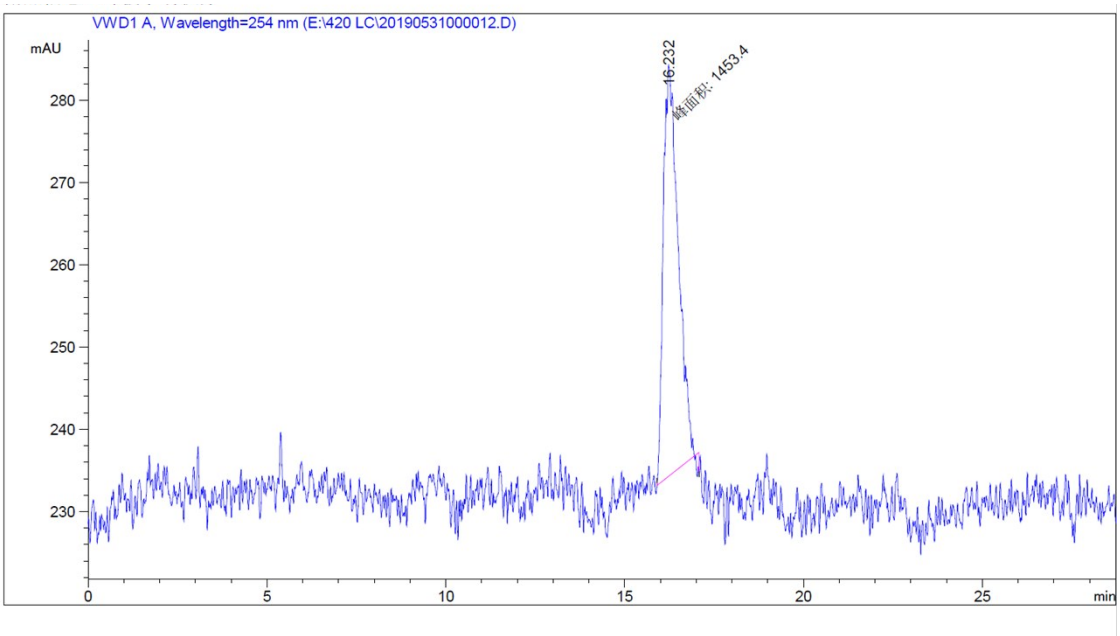


Figure S17 HPLC profile of compound **3**

Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z
3	$C_{20}H_{16}O_5$	[M-H]-	335.0939	335.0925

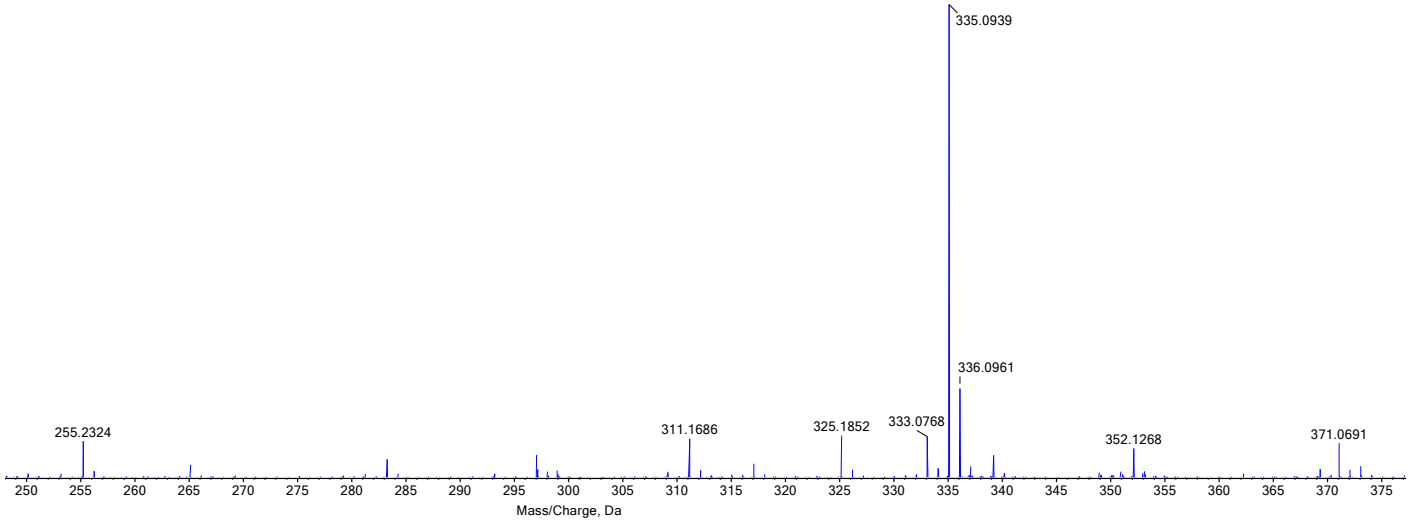


Figure S18 HR-ESI-MS of compound **3**

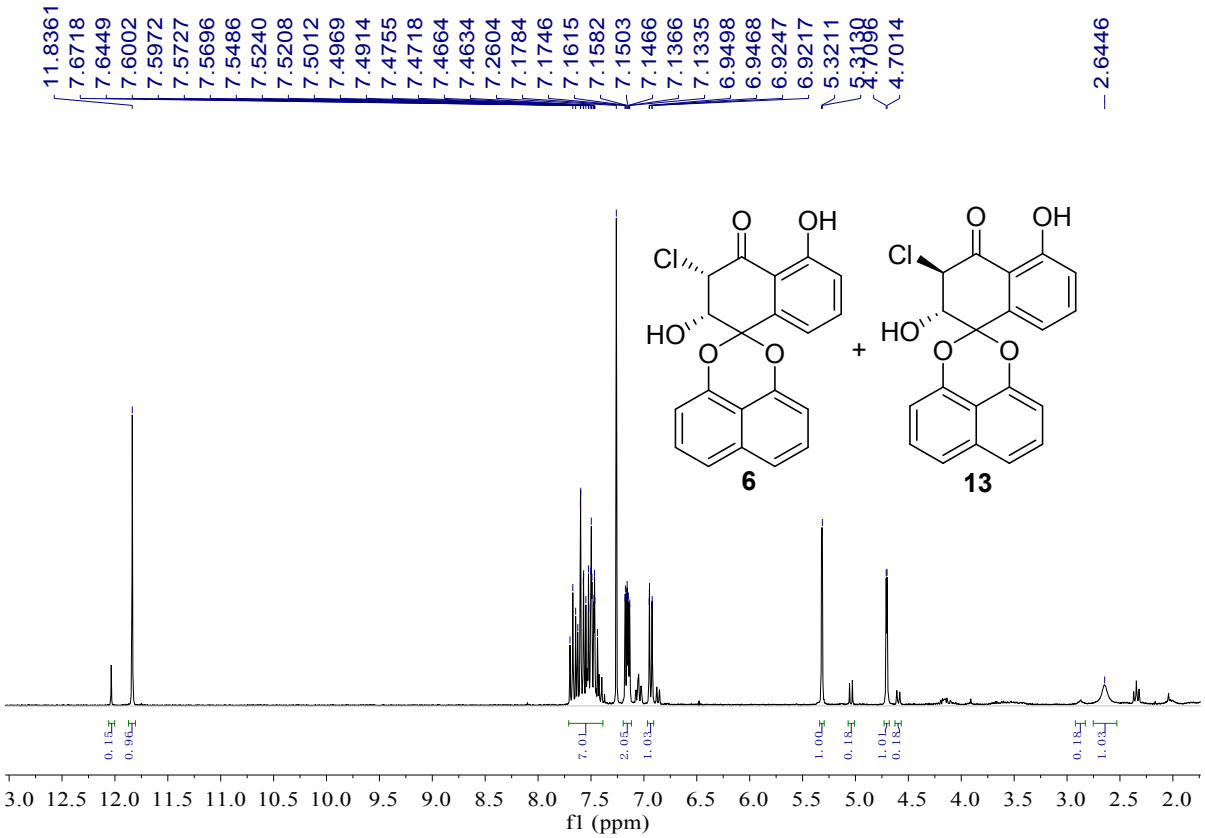


Figure S19 ^{1}H NMR of the mixture of compound **6** and its C-3 epimer **13** (*dr* = 5.7: 1)

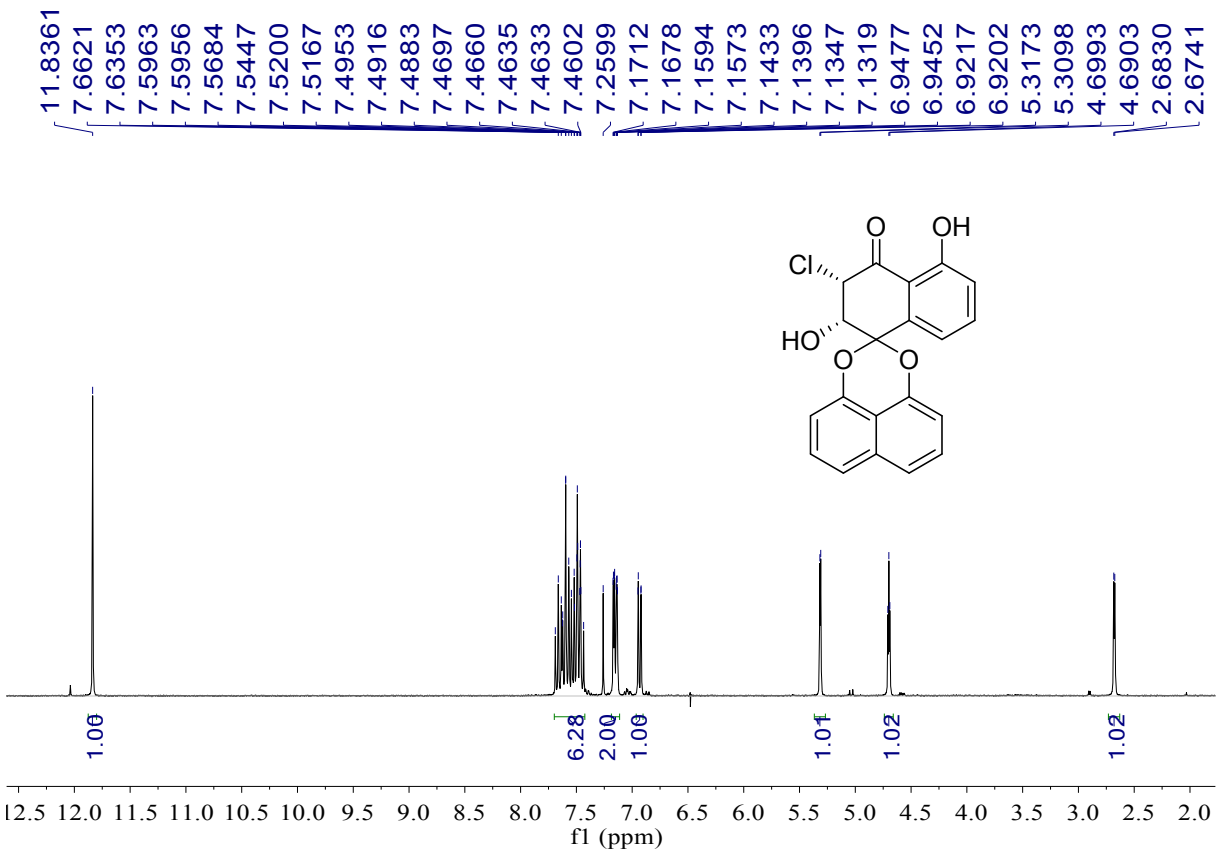


Figure S20 ^{1}H NMR of compound **6**

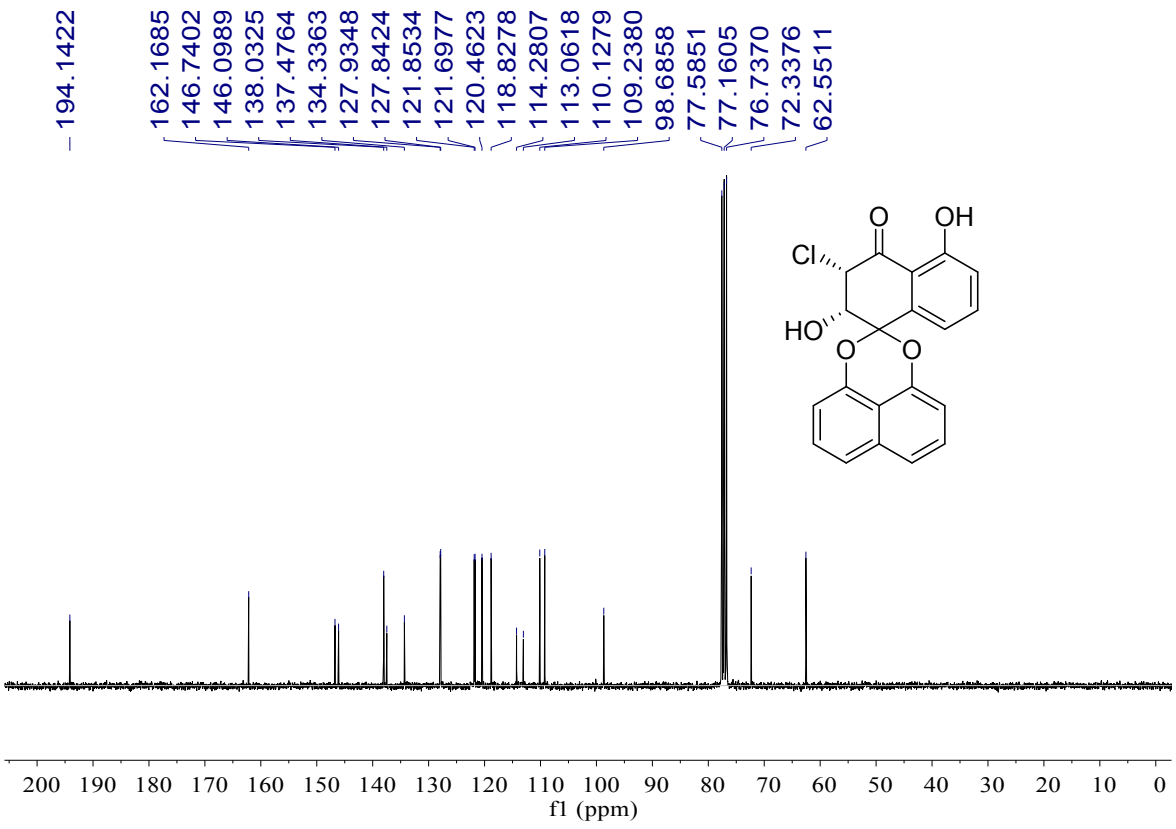


Figure S21 ^{13}C NMR of compound **6**

Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z
6	$C_{20}H_{13}ClO_5$	[M-H]-	367.0397	367.0379

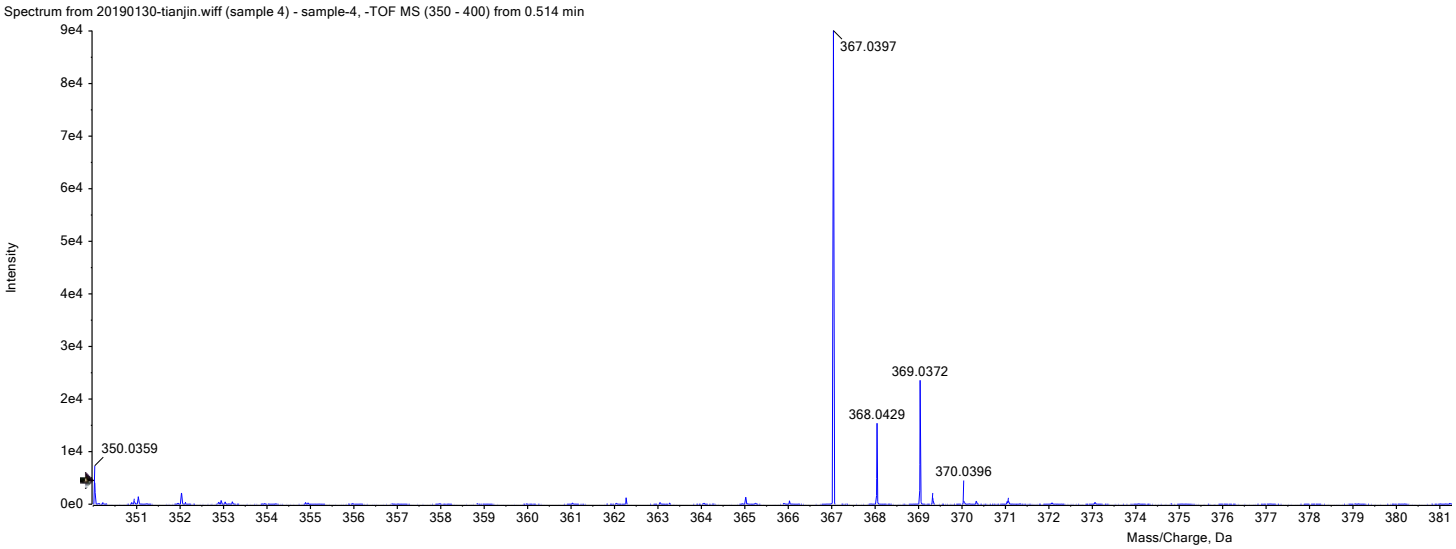


Figure S22 HR-ESI-MS of compound **6**

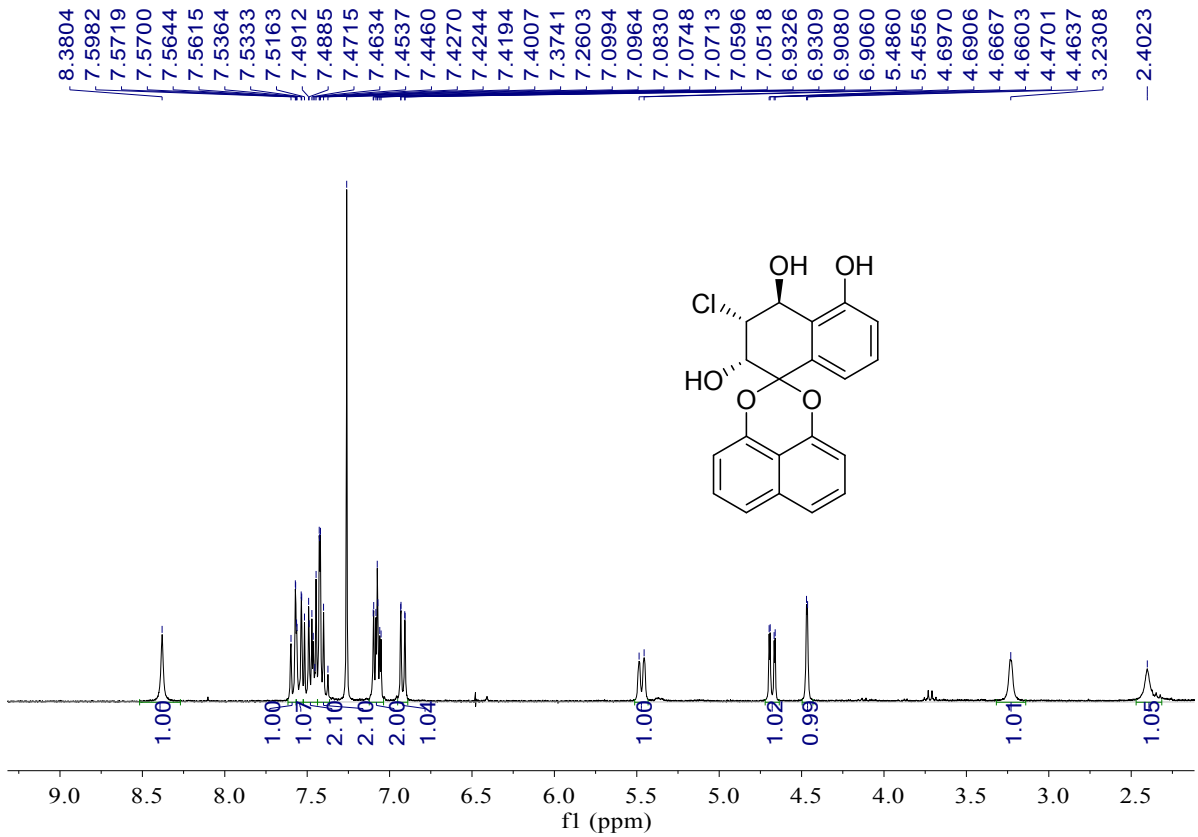


Figure S23 ^{1}H NMR of compound **4**

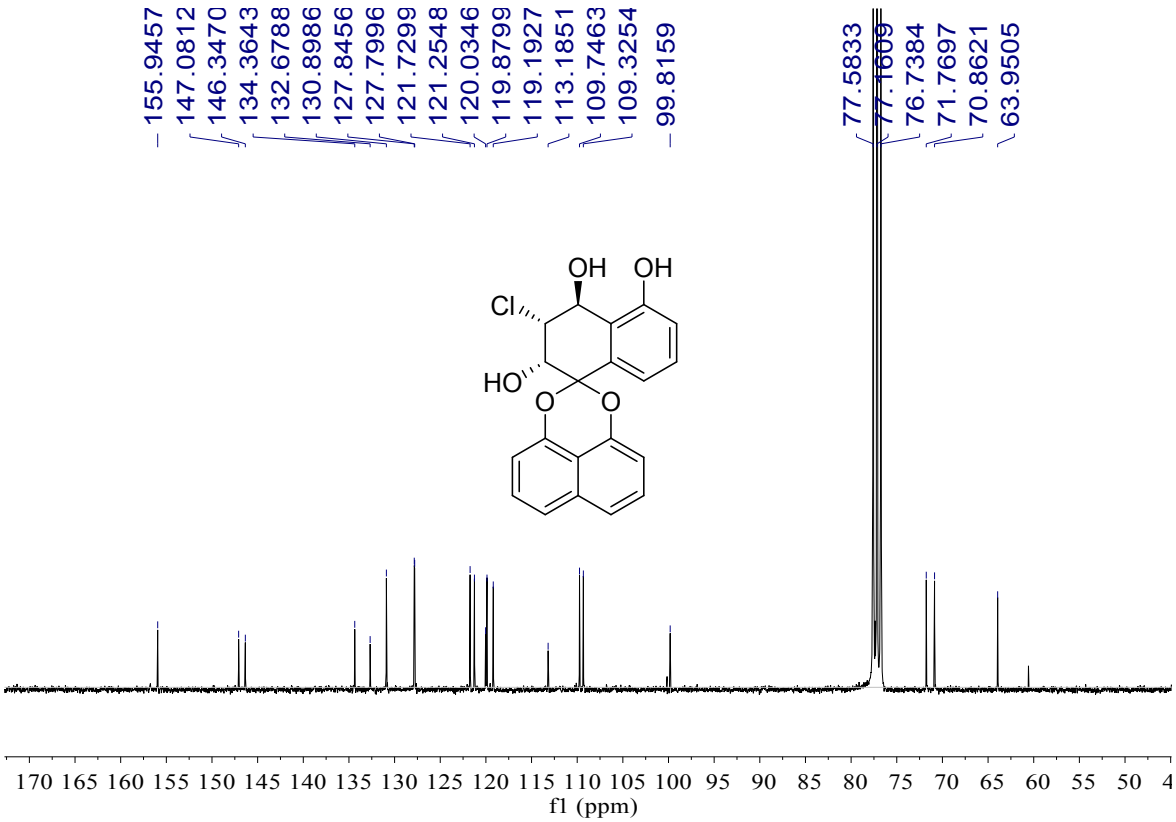


Figure S24 ^{13}C NMR of compound **4**

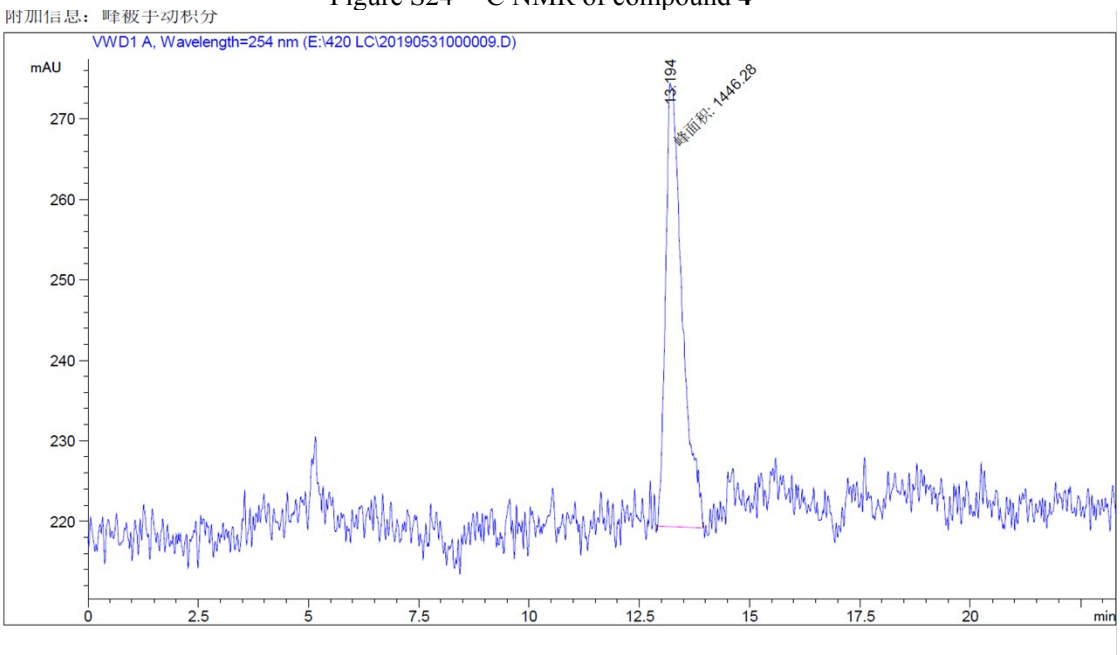


Figure S25 HPLC profile of compound **4**

Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z
4	$C_{20}H_{15}ClO_5$	[M-H]-	369.0548	369.0535

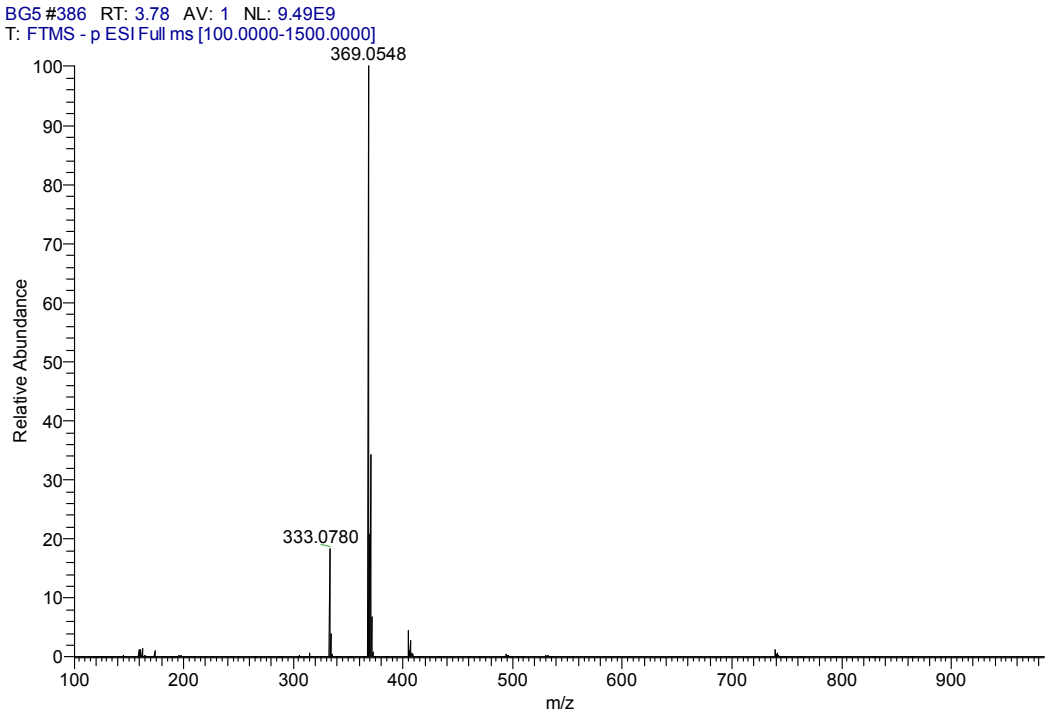


Figure S26 HR-ESI-MS of compound **4**

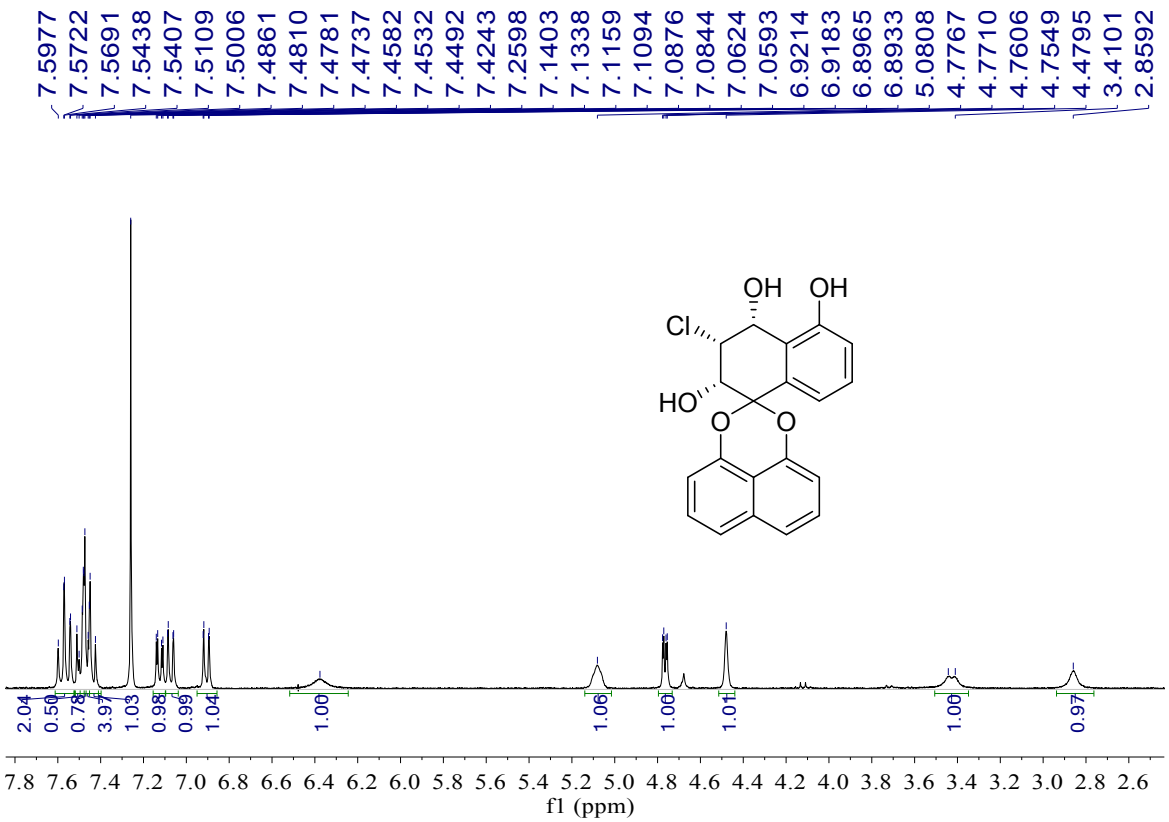


Figure S27 ^{1}H NMR of compound **14**

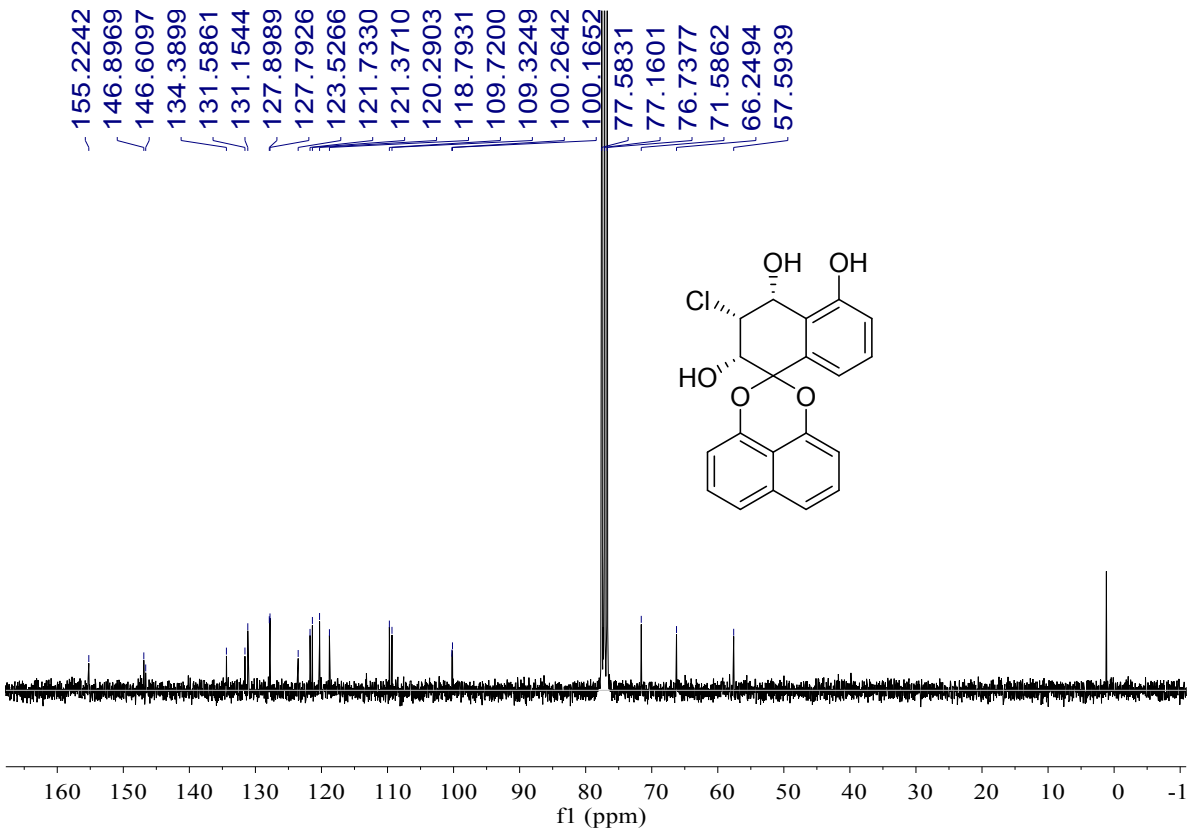


Figure S28 ^{13}C NMR of compound **14**

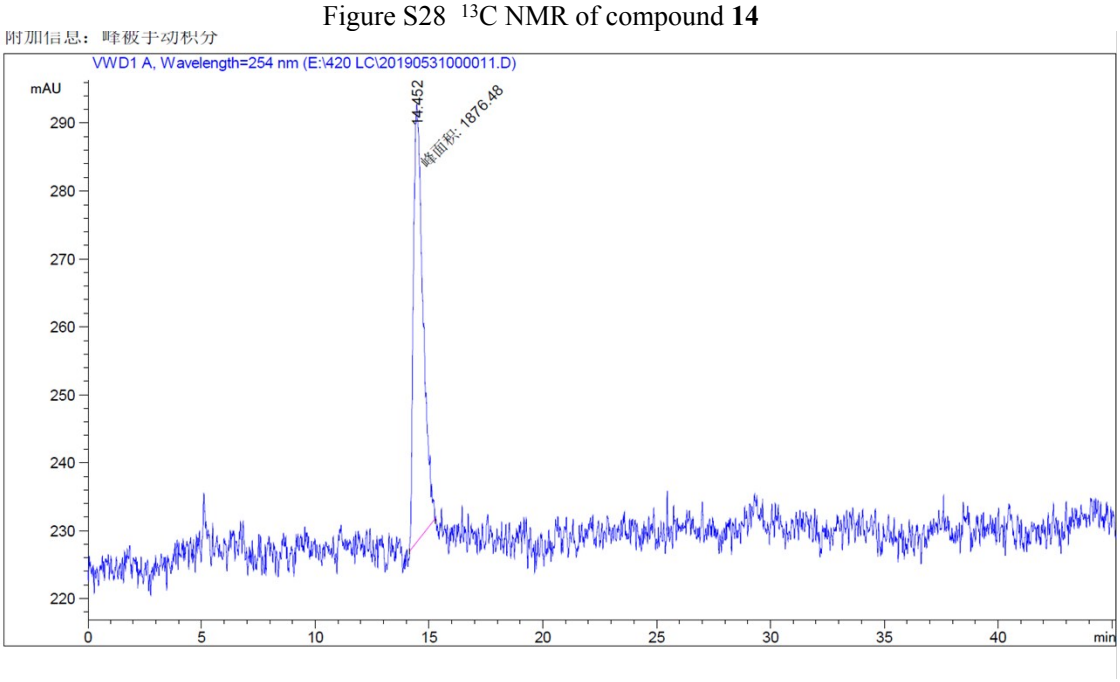


Figure S29 HPLC profile of compound **14**

Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z
14	$C_{20}H_{15}ClO_5$	[M-H]-	369.0547	369.0535

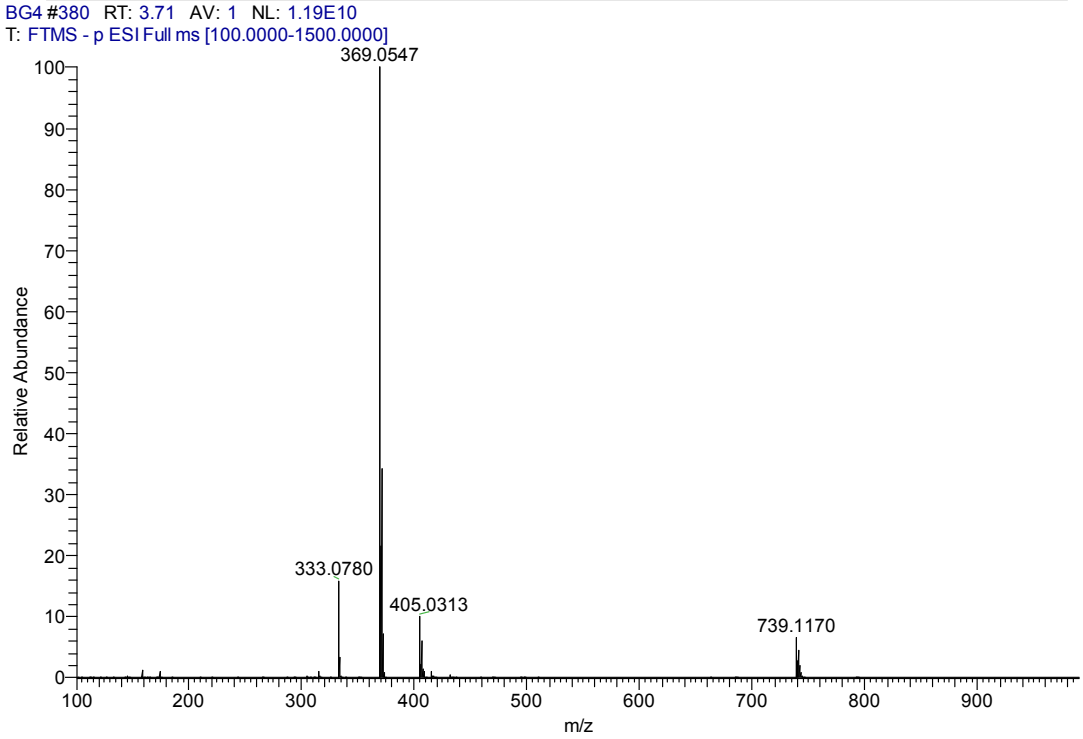


Figure S30 HR-ESI-MS of compound **14**

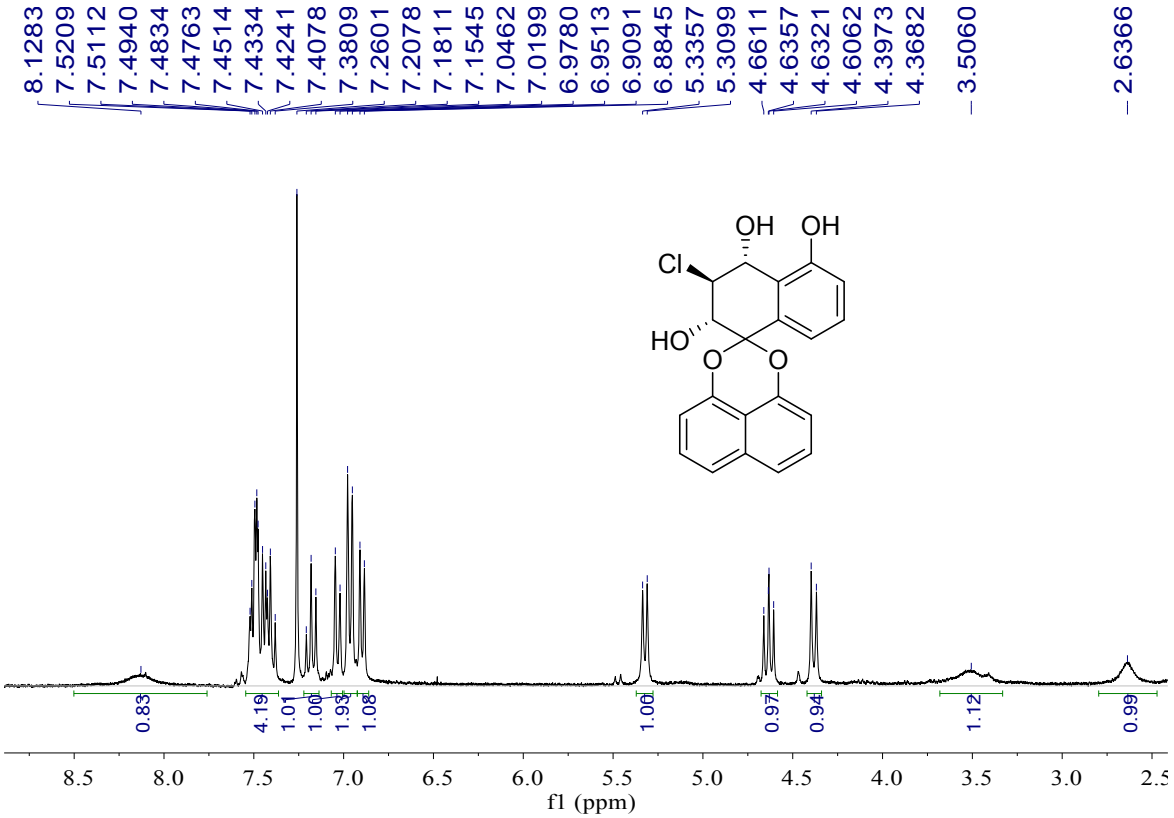


Figure S31 ^{1}H NMR of compound **5**

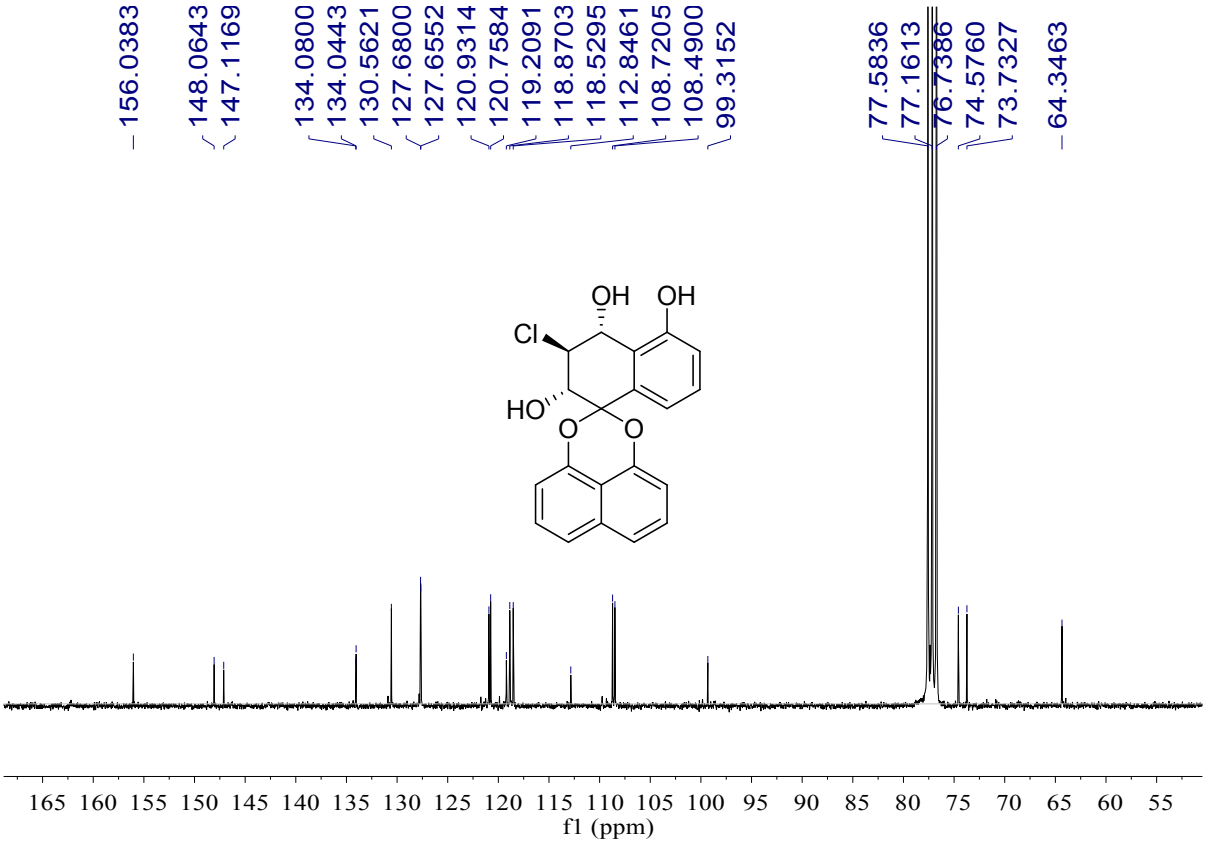


Figure S32 ^{13}C NMR of compound **5**

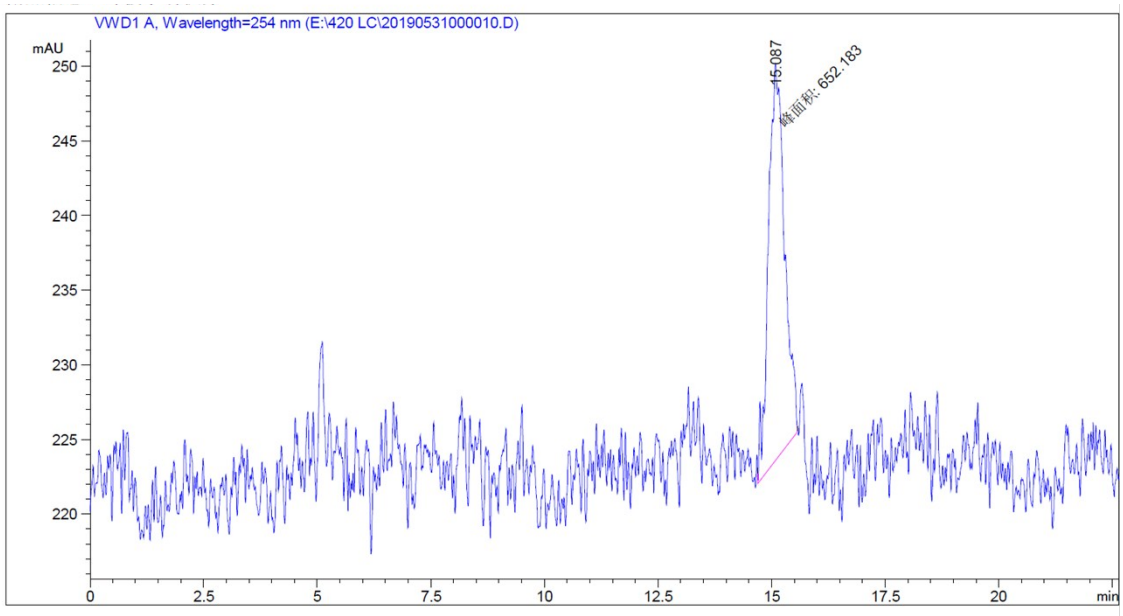


Figure S33 HPLC profile of compound **5**

Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z
5	$C_{20}H_{15}ClO_5$	[M-H]-	369.0547	369.0535

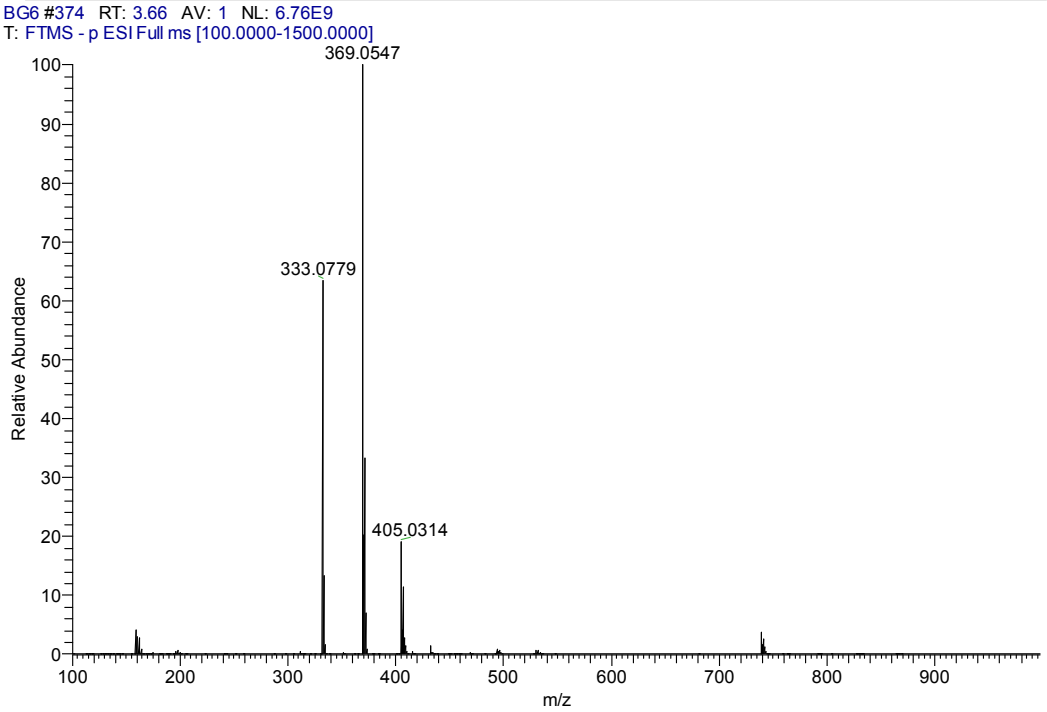


Figure S34 HR-ESI-MS of compound **5**

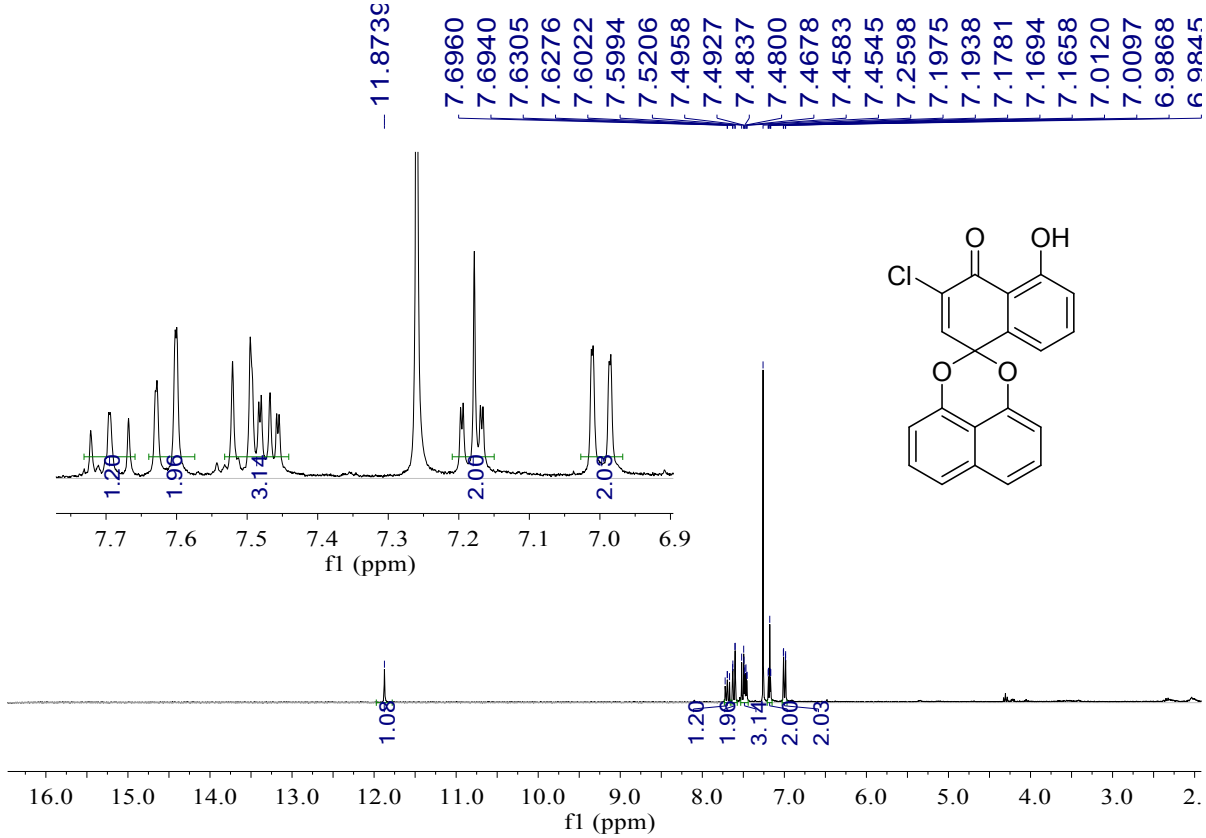


Figure S35 ^{1}H NMR of compound **7**

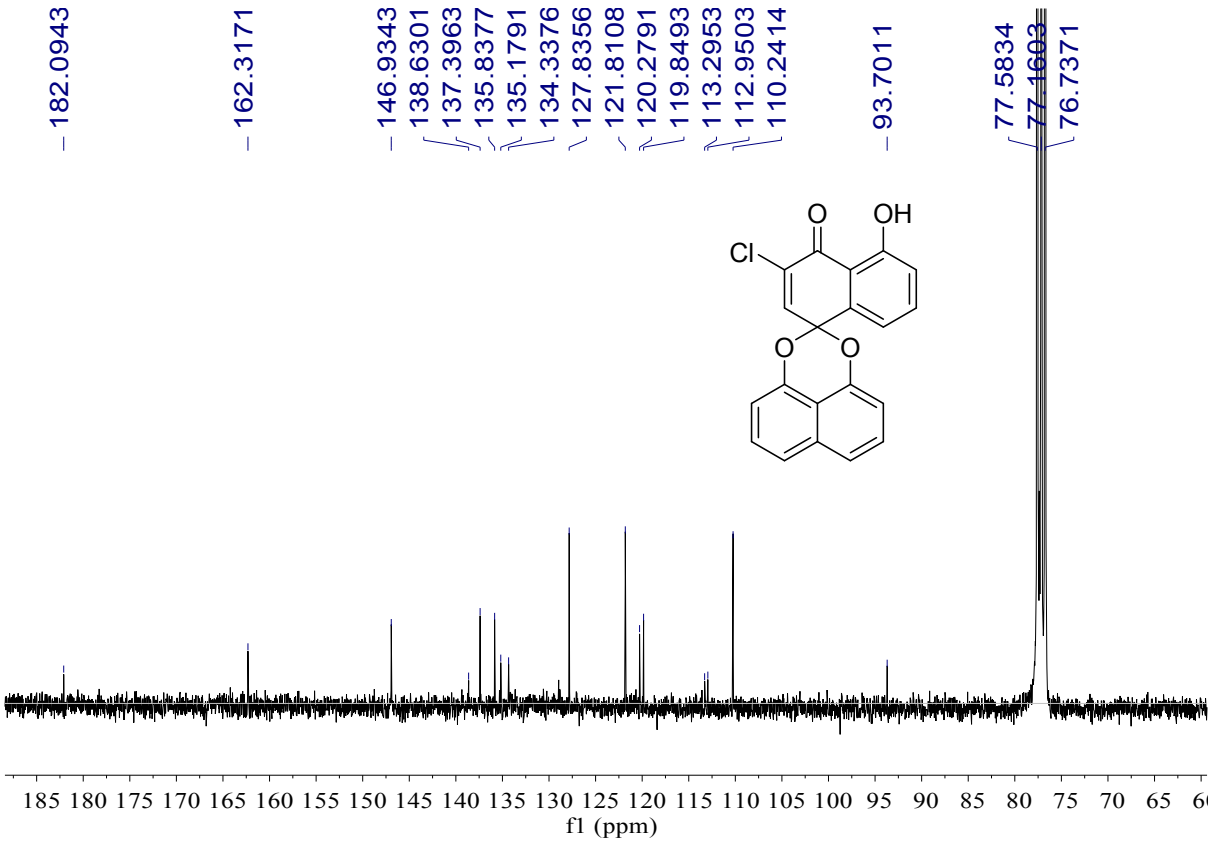


Figure S36 ^{13}C NMR of compound **7**

2. The crystal structure parameters for compound 14

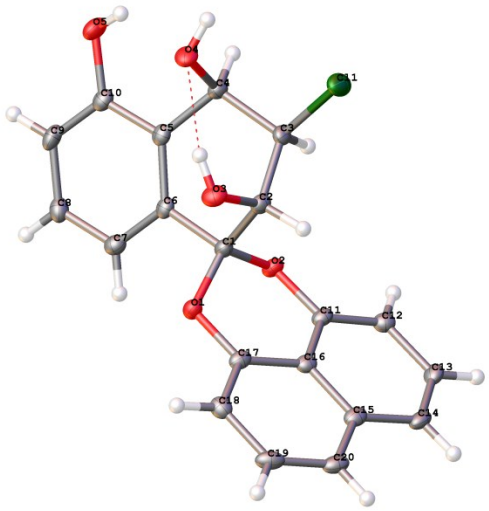


Table 1: Crystal data and structure refinement for exp_6109

Identification code	exp_6109
Empirical formula	$C_{20}H_{15}ClO_5$
Formula weight	370.77
Temperature / K	114.0(4)
Crystal system	monoclinic
Space group	$P2_1$
a / Å, b / Å, c / Å	8.7889(3), 10.1048(5), 8.8667(3)
α/°, β/°, γ/°	90.00, 93.111(3), 90.00
Volume / Å^3	786.30(6)
Z	2
ρcalc / mg mm^{-3}	1.566
μ / mm^{-1}	2.434
F(000)	384
Crystal size / mm^3	0.35 × 0.24 × 0.03
2Θ range for data collection	10.08 to 142.34°
Index ranges	$-10 \le h \le 10$, $-11 \le k \le 12$, $-9 \le l \le 10$
Reflections collected	6127
Independent reflections	2729 [R(int) = 0.0362 (inf-0.9 Å)]
Data/restraints/parameters	2729/1/238
Goodness-of-fit on F^2	1.042
Final R indexes [I>2σ (I) i.e. F_o>4σ (F_o)]	R_1 = 0.0379, wR_2 = 0.0975
Final R indexes [all data]	R_1 = 0.0394, wR_2 = 0.0990
Largest diff. peak/hole / e Å^{-3}	0.358/-0.316
Flack Parameters	0.006(16)
Completeness	0.9993

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for exp_6109. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
Cl1	1905.7(7)	1342.1(7)	1431.9(7)	28.48(18)
O1	397.2(18)	6008.5(18)	3231.1(17)	16.1(4)
O2	53.0(19)	4145.1(18)	4783.0(18)	15.7(4)
O5	-3985.4(19)	2522(2)	-55.5(19)	22.7(4)
O3	1290(2)	4482(2)	919.3(18)	20.5(4)
C3	536(3)	2442(3)	2204(3)	16.5(5)
C18	2499(3)	7489(3)	3709(2)	17.7(5)
C11	1363(3)	4437(3)	5655(2)	15.1(5)
C17	1745(2)	6352(3)	4038(2)	15.2(5)
C7	-2694(3)	5405(3)	3076(3)	17.7(5)

C20	4362(3)	7058(3)	5788(3)	19.9(5)
C16	2235(3)	5550(3)	5271(3)	15.2(5)
C15	3567(3)	5898(3)	6175(2)	17.4(5)
C4	-966(3)	2368(3)	1229(3)	16.1(5)
C19	3828(3)	7837(3)	4603(3)	20.5(5)
O4	-724(2)	2487(2)	-358.4(17)	20.3(4)
C14	3970(3)	5083(3)	7444(3)	18.6(5)
C13	3093(3)	4015(3)	7785(3)	17.8(5)
C10	-3519(3)	3461(3)	978(3)	17.2(5)
C6	-1612(3)	4496(3)	2633(2)	14.9(5)
C5	-2024(3)	3482(3)	1632(2)	15.2(5)
C8	-4175(3)	5346(3)	2458(3)	19.9(5)
C9	-4582(3)	4389(3)	1386(3)	19.6(5)
C12	1748(3)	3687(3)	6906(3)	17.1(5)
C1	21(3)	4632(3)	3269(2)	14.5(5)
C2	1146(3)	3839(3)	2336(3)	16.2(5)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for exp_6109. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka×b×U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl1	20.8(3)	27.9(4)	36.1(3)	-12.6(3)	-3.7(2)	9.7(3)
O1	16.1(8)	15.6(10)	16.3(7)	1.0(6)	-1.3(6)	-1.1(6)
O2	15.3(7)	18.7(11)	12.9(8)	-0.7(6)	-0.4(6)	-4.1(7)
O5	17.6(8)	28.9(12)	21.1(8)	-5.2(8)	-3.9(6)	-0.5(8)
O3	23.3(8)	24.2(11)	14.2(7)	-2.3(7)	3.1(6)	-2.6(7)
C3	15.1(11)	16.6(14)	17.6(11)	-2.8(9)	-0.6(8)	4.5(9)
C18	20.8(12)	18.1(14)	14.8(10)	0.7(9)	5.3(8)	1.4(10)
C11	14(1)	19.5(14)	11.9(10)	-3.7(9)	1.0(8)	-0.6(9)
C17	12.3(10)	20.3(13)	13.3(10)	-3.6(10)	2.9(7)	-1.5(10)
C7	19.3(12)	18.5(14)	15.0(11)	-0.3(9)	0.3(9)	-1.9(10)
C20	17.8(12)	23.8(15)	18.2(11)	-8.8(10)	3.4(9)	-3.6(10)
C16	15.0(11)	17.1(14)	13.6(10)	-3.9(9)	2.7(8)	0.8(9)
C15	15.1(11)	22.6(15)	14.8(11)	-5.9(9)	2.9(8)	0.6(9)
C4	15.1(11)	16.6(13)	16.1(10)	-2.2(9)	-1.8(8)	-0.8(9)
C19	20.1(12)	20.8(14)	21.3(12)	-7.3(10)	8.2(9)	-7.7(10)
O4	24.2(9)	23.4(11)	13.1(8)	-5.2(7)	0.7(6)	3.8(8)
C14	15.8(11)	24.3(15)	15.3(10)	-7.9(10)	-1.9(8)	1.2(10)
C13	20.8(12)	21.7(14)	10.8(10)	-1.9(9)	-1.2(9)	3.4(10)
C10	17.2(11)	21.3(14)	13(1)	1.8(9)	-0.3(8)	-1.7(10)
C6	14.6(10)	18.4(13)	11.6(10)	3.2(9)	0.1(8)	-0.1(9)
C5	16.0(11)	18.0(14)	11.7(10)	3.5(9)	0.7(8)	-0.2(9)
C8	18.8(12)	23.5(15)	17.4(11)	2.8(10)	1.3(9)	5.6(10)
C9	13.7(11)	29.4(16)	15.4(10)	3.1(10)	-2.2(8)	0.6(10)
C12	18.1(12)	18.0(15)	15.5(11)	-2.5(9)	2.7(8)	-0.7(10)
C1	15.4(11)	13.6(13)	14.3(10)	0.2(9)	-1.6(8)	-1.3(9)
C2	12.9(10)	19.4(14)	16.3(10)	-2.2(9)	-0.1(8)	0.0(9)

Table 4 Bond Lengths for exp_6109.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl1	C3	1.800(2)	C7	C8	1.386(3)
O1	C17	1.394(3)	C20	C15	1.417(4)
O1	C1	1.431(3)	C20	C19	1.375(4)
O2	C11	1.383(3)	C16	C15	1.426(3)
O2	C1	1.428(3)	C15	C14	1.423(4)
O5	C10	1.366(3)	C4	O4	1.440(3)
O3	C2	1.426(3)	C4	C5	1.516(3)
C3	C4	1.540(3)	C14	C13	1.369(4)
C3	C2	1.512(4)	C13	C12	1.419(3)
C18	C17	1.365(4)	C10	C5	1.407(3)
C18	C19	1.420(3)	C10	C9	1.386(4)
C11	C16	1.413(4)	C6	C5	1.390(4)
C11	C12	1.371(3)	C6	C1	1.520(3)
C17	C16	1.410(3)	C8	C9	1.389(4)
C7	C6	1.394(4)	C1	C2	1.546(3)

Table 5 Bond Angles for exp_6109.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C17	O1	C1	114.88(19)	C13	C14	C15	120.7(2)
C11	O2	C1	115.14(17)	C14	C13	C12	121.7(2)
C4	C3	Cl1	109.09(16)	O5	C10	C5	121.8(2)
C2	C3	Cl1	111.37(17)	O5	C10	C9	117.6(2)
C2	C3	C4	112.2(2)	C9	C10	C5	120.6(2)
C17	C18	C19	118.9(2)	C7	C6	C1	118.7(2)
O2	C11	C16	118.8(2)	C5	C6	C7	120.5(2)
C12	C11	O2	119.7(2)	C5	C6	C1	120.8(2)
C12	C11	C16	121.4(2)	C10	C5	C4	117.5(2)
O1	C17	C16	118.1(2)	C6	C5	C4	123.8(2)
C18	C17	O1	120.6(2)	C6	C5	C10	118.7(2)
C18	C17	C16	121.2(2)	C7	C8	C9	120.2(2)
C8	C7	C6	120.0(2)	C10	C9	C8	119.8(2)
C19	C20	C15	120.5(2)	C11	C12	C13	118.5(2)
C11	C16	C15	120.0(2)	O1	C1	C6	107.1(2)
C17	C16	C11	119.8(2)	O1	C1	C2	109.65(18)
C17	C16	C15	120.1(2)	O2	C1	O1	111.35(18)
C20	C15	C16	117.9(2)	O2	C1	C6	106.69(18)
C20	C15	C14	124.5(2)	O2	C1	C2	110.1(2)
C14	C15	C16	117.6(2)	C6	C1	C2	111.90(19)
O4	C4	C3	112.13(18)	O3	C2	C3	113.89(19)
O4	C4	C5	107.08(19)	O3	C2	C1	109.0(2)
C5	C4	C3	110.47(19)	C3	C2	C1	106.94(19)
C20	C19	C18	121.4(2)				

Table 6 Torsion Angles for exp_6109.

A	B	C	D	Angle/°
Cl1	C3	C4	O4	-48.4(3)
Cl1	C3	C4	C5	-167.80(16)
Cl1	C3	C2	O3	69.8(2)
Cl1	C3	C2	C1	-169.81(15)
O1	C17	C16	C11	0.0(3)
O1	C17	C16	C15	-177.0(2)
O1	C1	C2	O3	-47.2(2)
O1	C1	C2	C3	-170.77(17)
O2	C11	C16	C17	1.3(3)
O2	C11	C16	C15	178.2(2)
O2	C11	C12	C13	-179.6(2)
O2	C1	C2	O3	-170.08(18)
O2	C1	C2	C3	66.4(2)
O5	C10	C5	C4	-4.0(3)
O5	C10	C5	C6	177.6(2)
O5	C10	C9	C8	178.5(2)
C3	C4	C5	C10	-172.3(2)
C3	C4	C5	C6	6.1(3)
C18	C17	C16	C11	174.9(2)
C18	C17	C16	C15	-2.0(4)
C11	O2	C1	O1	-50.6(3)
C11	O2	C1	C6	-167.1(2)
C11	O2	C1	C2	71.3(3)
C11	C16	C15	C20	-177.0(2)
C11	C16	C15	C14	0.4(3)
C17	O1	C1	O2	51.8(2)
C17	O1	C1	C6	168.11(16)
C17	O1	C1	C2	-70.3(2)
C17	C18	C19	C20	-0.2(4)
C17	C16	C15	C20	-0.1(3)
C17	C16	C15	C14	177.4(2)
C7	C6	C5	C4	-172.9(2)
C7	C6	C5	C10	5.4(3)
C7	C6	C1	O1	-42.9(3)
C7	C6	C1	O2	76.4(3)

C7	C6	C1	C2	-163.1(2)
C7	C8	C9	C10	2.5(4)
C20	C15	C14	C13	176.5(2)
C16	C11	C12	C13	-2.8(4)
C16	C15	C14	C13	-0.7(4)
C15	C20	C19	C18	-1.8(4)
C15	C14	C13	C12	-0.8(4)
C4	C3	C2	O3	-52.9(3)
C4	C3	C2	C1	67.6(2)
C19	C18	C17	O1	177.0(2)
C19	C18	C17	C16	2.1(4)
C19	C20	C15	C16	1.9(3)
C19	C20	C15	C14	-175.3(2)
O4	C4	C5	C10	65.4(3)
O4	C4	C5	C6	-116.3(2)
C14	C13	C12	C11	2.5(4)
C6	C7	C8	C9	-0.6(4)
C6	C1	C2	O3	71.4(2)
C6	C1	C2	C3	-52.1(2)
C5	C10	C9	C8	-0.4(4)
C5	C6	C1	O1	137.3(2)
C5	C6	C1	O2	-103.4(2)
C5	C6	C1	C2	17.1(3)
C8	C7	C6	C5	-3.4(4)
C8	C7	C6	C1	176.8(2)
C9	C10	C5	C4	174.9(2)
C9	C10	C5	C6	-3.5(3)
C12	C11	C16	C17	-175.6(2)
C12	C11	C16	C15	1.4(4)
C1	O1	C17	C18	158.1(2)
C1	O1	C17	C16	-26.9(3)
C1	O2	C11	C16	24.6(3)
C1	O2	C11	C12	-158.5(2)
C1	C6	C5	C4	6.9(3)
C1	C6	C5	C10	-174.8(2)
C2	C3	C4	O4	75.5(3)
C2	C3	C4	C5	-43.9(3)