Supporting Information for

One-Pot Synthesis of 6*H*-Benzo[*c*]chromene and 6,7-dihydrodibenzo[b,d]oxepine through Dearomatization and Dienone-Phenol Rearrangement

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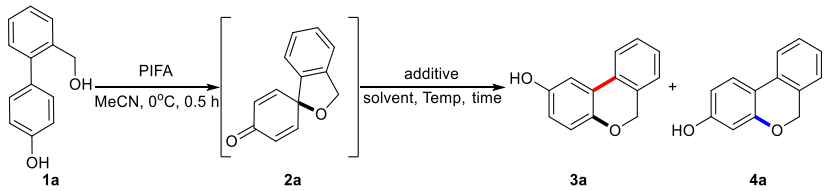
Part 1. General information

Nuclear magnetic resonance spectra were measured at 500 MHz (^{1}H NMR), and at 126 MHz (^{13}C NMR) on a Bruker 500 MHz instrument. ^{1}H NMR chemical shifts were reported in δ relative to the resonance of TMS (δ 0.00) and the residual solvent signals at δ 7.26 for $CDCl_3$. ^{13}C NMR chemical shifts were reported in δ relative to the residual solvent signals at δ 77.16 for $CDCl_3$. High resolution mass spectra (HRMS) were recorded by Bruker APEX II mass spectrometer (Varian, Palo Alto, CA). The melting points were determined by WRX-4 melting-point apparatus with a microscope (Shanghai Yice Apparatus & Equipment Co. Ltd., Shanghai, China).

Materials: All solvents and commercially available organic and inorganic reagents were purchased from professional chemical companies (Leyan, Shanghai, China; Bide, Shanghai, China; Energy chemical, Anhui, China) and used without further purification. Column chromatography was performed on 200-300 mesh silica gel (Cat No. C200011, Leyan, Shanghai, China). Known starting materials **1** were synthesized based on the reported procedures[1-2].

Sample preparation for X-ray diffraction analysis: White needle-shaped crystals of compound **3c** and **3w** were obtained by slowly evaporating mixed dichloromethane and methanol solution. A 0.27 × 0.24 × 0.23 mm^3 crystal of **3c** and a 0.36 × 0.21 × 0.20 mm^3 crystal of **3w** were selected for analysis.

Table S1. Screening of Conditions for the one-pot Synthesis of **3a**.[a,b]



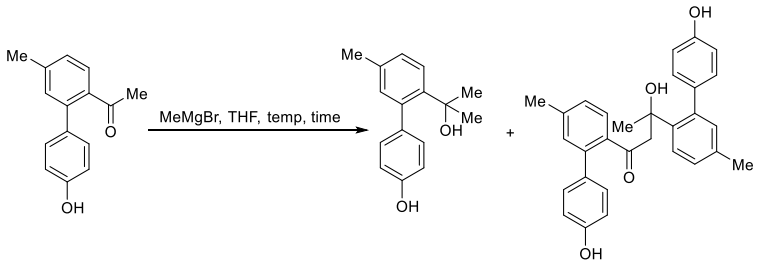
1a 2a 3a 4a

entry	additive	solvent	Temp. (°C)	t(h)	Yield of 3a (%)	Yield of 4a (%)
1	BCl_3	THF	rt	12	56	N.D.
2	$AlCl_3$	THF	rt	12	35	N.D.
3	$GaCl_3$	THF	rt	12	62	N.D.
4	$TiCl_4$	THF	rt	12	37	N.D.
5	$FeCl_3$	THF	rt	12	<5	N.D.
6	$ZnCl_2$	THF	rt	12	<5	N.D.
7	TsOH	THF	rt	12	44	N.D.
8	AcOH	THF	rt	12	31	N.D.
9[c]	$Ga_2(SO_4)_3$	THF	rt	12	70	N.D.
10	$Ga(OTf)_3$	THF	rt	12	75	N.D.
11	$Ga(Otf)_3$	Et_2O	rt	12	53	N.D.
12	$Ga(Otf)_3$	dioxane	rt	12	78	N.D.
13	$Ga(Otf)_3$	dioxane	60	12	83	N.D.
14	$Ga(Otf)_3$	dioxane	90	12	88	N.D.
15[d]	$Ga(Otf)_3$	dioxane	90	12	60	N.D.
16	$In(Otf)_3$	dioxane	90	12	75	N.D.
17	$In(Otf)_3$	dioxane	90	24	82	N.D.

18[e]	$In(Otf)_3$	dioxane	90	24	87	N.D.
19	$Ga(Otf)_3$	1.0 equiv.	90	24	85	N.D.
20	$Ga(Otf)_3$	0.5 equiv.	90	12	51	N.D.
21	$Ga(Otf)_3$	0.5 equiv.	90	24	65	N.D.
22	$Ga(Otf)_3$	0.5 equiv.	90	48	82	N.D.
23	$Ga(Otf)_3$	0.2 equiv.	90	24	43	N.D.
24	$Ga(Otf)_3$	0.2 equiv.	90	48	66	N.D.
25	$Ga(Otf)_3$	0.2 equiv.	90	96	83	N.D.
26	$Ga(Otf)_3$	0.1 equiv.	90	24	34	N.D.
27	$Ga(Otf)_3$	0.1 equiv.	90	48	52	N.D.
28	$Ga(Otf)_3$	0.1 equiv.	90	96	68	N.D.
29[f]	$Ga(Otf)_3$	0.2 equiv.	90	12	85	N.D.
30[f]	$Ga(Otf)_3$	0.2 equiv.	90	24	90	N.D.

[a] Reaction conditions: **1a** (0.2 mmol, 1.0 equiv.), PIFA (0.24 mmol, 1.2 equiv.), MeCN (5 mL), 3dditive (0.4 mmol, 2.0 equiv.), solvent (5 mL). [b] isolated yields. N.D.= not detected. [c] $Ga_2(SO_4)_3$ (0.2 mmol, 1.0 equiv.) was added. [d] $Ga(Otf)_3$ (0.2 mmol, 1.0 equiv.) was added. [e]The reaction was performed under N_2 atmosphere. [f]pure **2a** was used.

Table S2. Optimization for the Synthesis of product **6**

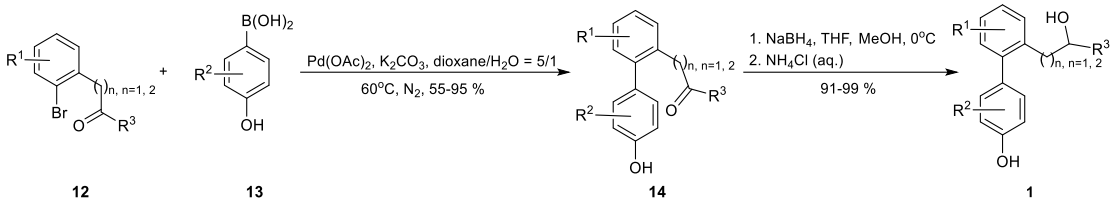


16 **6** **17**

entry	equivalency of MeMgBr (equiv.)	Temp. (°C)	t (h)	Yield of 6 (%)	Yield of 17 (%)	Recovery of 16 (%)
1	1.5	40	12	30	57	N.D.
2	1.5	rt	12	32	56	N.D.
3	1.5	0	12	39	49	N.D.
4	1.5	-10	12	46	43	N.D.
5	1.5	-20	12	56	39	5
6	1.5	-30	12	50	15	30
7	1.5	-40	12	30	5	50
8	1.5	-78	12	<5	<5	85
9	2.0	-20	12	54	42	N.D.
10	1.2	-20	12	52	35	8
11	1.0	-20	12	43	33	20
12	1.5	-20	24	56	40	5
13	1.5	-20	48	56	41	<5

[a]Reaction conditions: **16** (0.1 mmol, 22.6 mg, 1.0 equiv.), MeMgBr (3.0 mol/L in 2-methyl-THF), THF (1.5 mL). The yields of **6** and the recovery of **16** were determined by GCMS, and the yields of **17** were isolated yields. N.D.= not detected.

Scheme S1. Preparation of starting materials **1**.



Preparation of coupling substrates **14**:

As for the preparation of coupling substrates **14**, all manipulations of Suzuki-Miyaura coupling were performed under N_2 by standard Schlenk techniques unless otherwise noted.

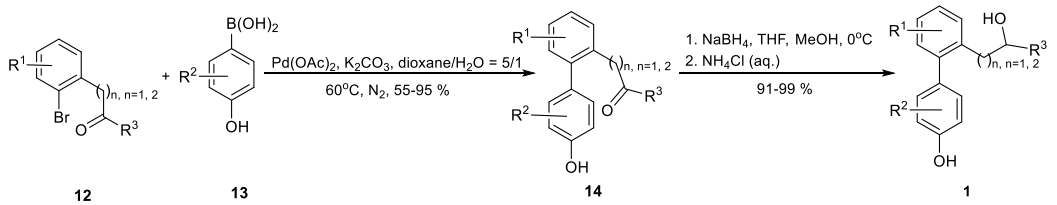
To an oven-dried Schlenk tube was added aryl bromide substrates **12** (0.5 mmol, 1.0 equiv.), various substituted (4-hydroxyphenyl)boronic acid **13** (0.6 mmol, 1.2 equiv.), K_2CO_3 (1.0 mmol, 2.0 equiv.), and $Pd(OAc)_2$ (5 mol %). Dioxane (5 mL) and H_2O (1 mL) were added via a syringe, and the reaction was protected under a N_2 atmosphere. The mixture was stirred at 60 °C in an oil bath for 12 h. The mixture was cooled and transferred into a separating funnel, extracted by EtOAc for 3 times. The organic phase was washed with brine and concentrated in *vacuo*. The crude product was purified by silica gel column chromatography (silica gel, 200–300 mesh, PE/EtOAc 15/1) to give intermediate coupling compounds **14**.

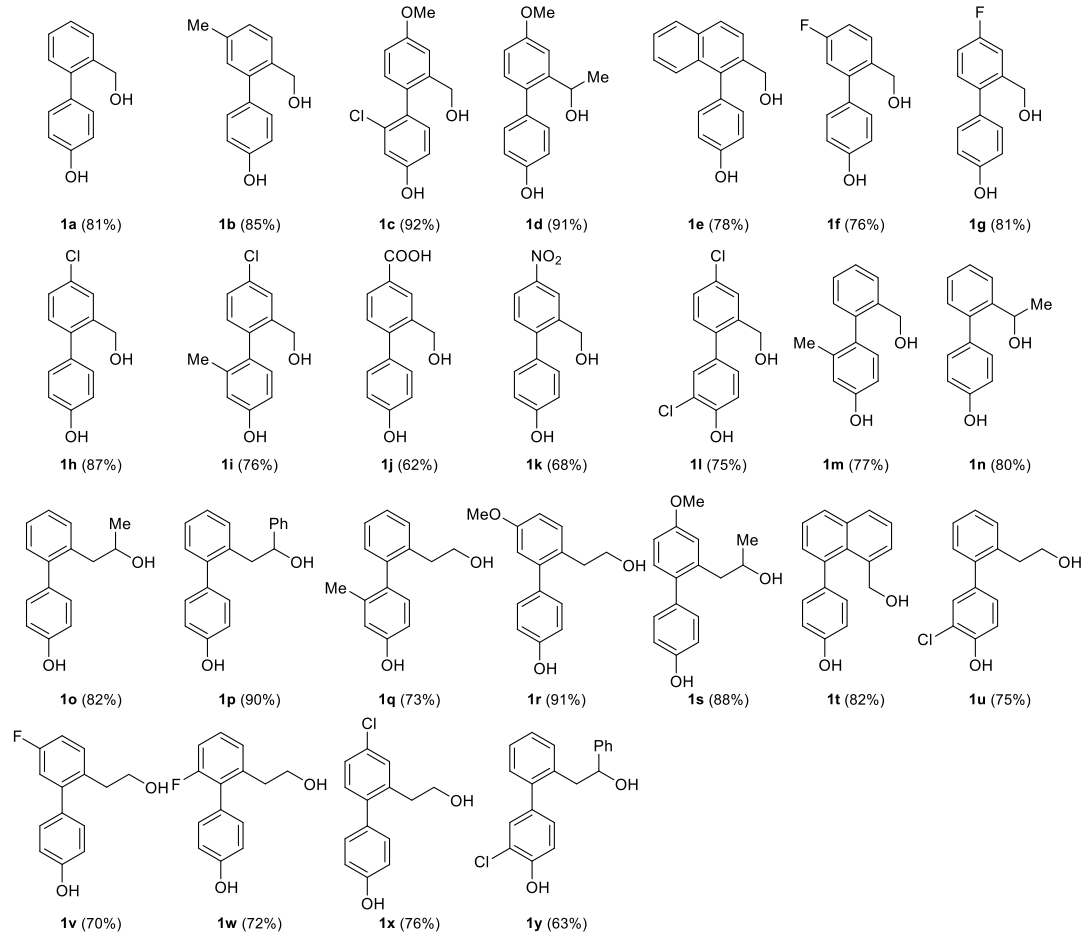
Preparation of alcohol **1**:

To an oven-dried round-bottom flask was added **14** (0.2 mmol, 1.0 equiv.), THF (3 mL), MeOH (3 mL), and $NaBH_4$ (0.6 mmol, 3.0 equiv.) at ice water bath, the mixture was stirred. After 4 h, the mixture was washed with saturated NH_4Cl aqueous solution for 3 times. The combined organic phase was washed with brine and concentrated under pressure. The crude product was purified by silica gel column chromatography (silica gel, 200–300 mesh, PE/EtOAc 3/1) to give starting materials **1**. The NMR and MS data of compounds **1** were identical with previous reports[1-2].

Scope of starting materials **1** was shown as **Scheme S2** as follows.

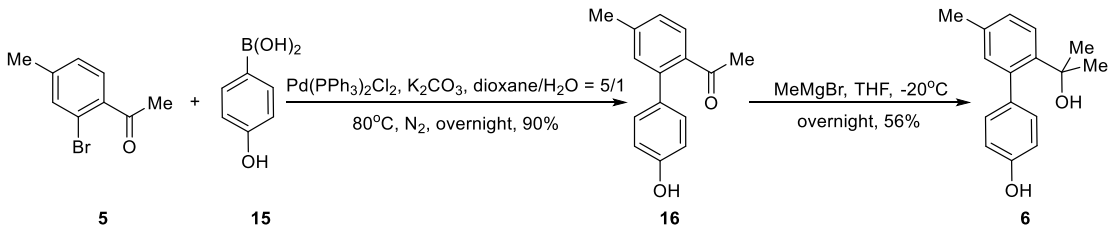
Scheme S2. Scope of starting materials **1**.





[a] Reaction conditions: Reactions were equipped under a N_2 atmosphere, **12** (0.5 mmol), **13** (0.6 mmol), K_2CO_3 (1.0 mmol) and $Pd(OAc)_2$ (5 mol %) in 5 mL of dioxane and 1 mL of H_2O at 60 °C and stirred for 12 h, and then purified coupling products (0.2 mmol, 1.0 equiv.), THF (3 mL), MeOH (3 mL), and $NaBH_4$ (0.6 mmol, 3.0 equiv.) were added at ice water bath for 4 h. [b] Isolated yields for two steps.

Scheme S3. Synthesis of compound **6**



To an oven-dried Schlenk tube was added 1-(2-bromo-4-methylphenyl)ethan-1-one **5** (0.5 mmol, 1.0 equiv.), (4-hydroxyphenyl)boronic acid **15** (0.6 mmol, 1.2 equiv.), K_2CO_3 (1.0 mmol, 2.0 equiv.), and $Pd(PPh_3)_2Cl_2$ (5 mol %). Dioxane (10 mL) and H_2O (2 mL) were added via a

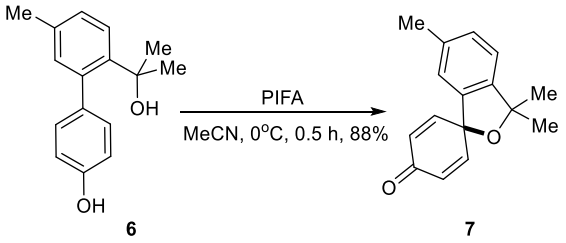
syringe under a N_2 atmosphere. The mixture was stirred at 80 °C in an oil bath overnight. The mixture was cooled and transferred into a separating funnel, extracted by EtOAc for 3 times. The combined organic phase was washed with brine and concentrated in *vacuo*. The crude product was purified by silica gel column chromatography (silica gel, 200–300 mesh, PE/EtOAc 10/1) to give intermediate coupling compounds **16** (102 mg, 90% yield).

Compound **16**, yellow oil, ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47 (d, J = 7.7 Hz, 1H), 7.21 – 7.15 (m, 4H), 6.88 (d, J = 8.6 Hz, 2H), 6.10 (s, 1H), 2.42 (s, 3H), 2.04 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 205.96, 155.96, 141.40, 140.66, 137.92, 133.10, 131.03, 130.12, 128.22, 127.75, 115.68, 30.41, 21.43. HRMS(ESI), m/z: calcd for $C_{15}H_{15}O_2$ $[M+H]^+$: 227.1072; found, 227.1074.

After coupling product **16** is obtained, to an oven-dried round-bottom flask was added **16** (0.2 mmol, 1.0 equiv.), THF (5 mL) and MeMgBr (0.3 mmol, 1.5 equiv., 1 M in THF) at -20 °C, the mixture was stirred for 4 h. After finished, the mixture was washed with saturated NH_4Cl aqueous solution for 3 times. The combined organic phase was washed with brine and concentrated under pressure. The crude product was purified by silica gel column chromatography (200–300 mesh, PE/EtOAc 2/1) to give tertiary alcohol **6** (27 mg, 56% yield).

Compound **6**, yellow oil, ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44 (d, J = 8.1 Hz, 1H), 7.21 – 7.11 (m, 3H), 6.89 (d, J = 2.1 Hz, 1H), 6.79 (d, J = 8.5 Hz, 2H), 5.80 (s, 1H), 2.32 (s, 3H), 2.13 (brs, 1H), 1.50 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.03, 143.25, 139.34, 135.73, 135.52, 133.32, 130.72, 128.04, 125.79, 114.92, 74.57, 32.63, 20.62. HRMS(ESI), m/z: calcd for $C_{16}H_{19}O_2$ $[M+H]^+$: 243.1385; found, 243.1388.

Scheme S4. Synthesis of compound **7**



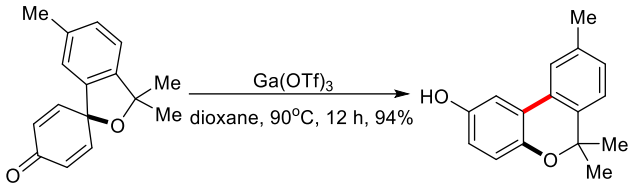
6 **7**

To an oven-dried Schlenk tube equipped with a magnetic stirrer was added **6** (0.4 mmol, 1.0 equiv.), MeCN (5 mL) was added via a syringe, and the reaction was protected under a N_2 atmosphere. The mixture was stirred at 0 °C in an ice-water bath, and then PIFA (0.48 mmol, 1.2 equiv.) was dissolved in 1 mL MeCN and slowly added to the tube. The reaction mixture was stirred for 30 min (the reaction was monitored by TLC using PE/EtOAc 5:1 as eluent by disappearance of the reactant). After completion of the reaction, the mixture was quenched by 0.5 M $NaHCO_3$ aqueous solution and transferred into a separating funnel, extracted by EtOAc for 3 times. The organic phase was concentrated in *vacuo* and the crude product was purified by silica gel column chromatography (200–300 mesh, PE/EtOAc 5/1) to give compound **7** (84 mg, 88% yield).

Compound **7**, white solid, ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.18 (dd, J = 7.8, 1.5 Hz, 1H), 7.09 (d, J = 7.7 Hz, 1H), 6.81-6.75 (m, 3H), 6.20 (d, J = 1.9 Hz, 1H), 6.18 (d, J = 1.9 Hz, 1H), 2.34 (s, 3H), 1.62 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 185.64, 150.65, 144.84, 138.46, 136.95, 130.19, 126.76, 122.63, 121.39, 87.59, 82.21, 30.94, 21.14. HRMS(ESI), m/z: calcd for

$C_{16}H_{17}O_2$ $[M+H]^+$: 241.1229; found, 241.1232.

Scheme S5. Synthesis of compound **8**



7 **8, Didehydroconicol**

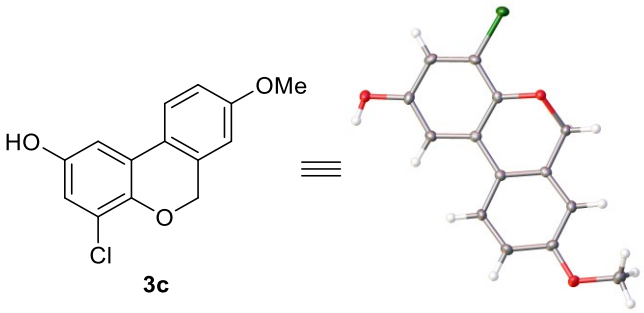
To an oven-dried round-bottom flask was added **7** (0.3 mmol, 1.0 equiv.), dioxane (5 mL) and $Ga(OTf)_3$ (0.6 mmol, 2.0 equiv.) and stirred for 12 h under 90°C. The reaction was monitored by TLC using PE/EtOAc 5:1 as eluent by disappearance of the reactant. After competition, the reaction mixture was quenched by saturated $NaHCO_3$ solution and was extracted by EtOAc for 3 times. The combined organic phase was dried over Na_2SO_4, and concentrated under reduced pressure. The crude was purified by 200-300 mesh silica-gel column chromatography using PE/EtOAc (10/1) to provide didehydroconicol, **8** (67 mg, 94% yield).

Compound **8**, yellow oil, ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 (d, J = 1.5 Hz, 1H), 7.20 (d, J = 2.9 Hz, 1H), 7.13-7.07 (m, 2H), 6.82 (d, J = 8.6 Hz, 1H), 6.70 (dd, J = 8.6, 3.0 Hz, 1H), 5.09 (s, 1H), 2.36 (s, 3H), 1.59 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 150.11, 146.72, 137.25, 137.12, 128.96, 128.25, 123.45, 123.17, 122.96, 118.77, 116.30, 109.42, 77.39, 27.45, 21.30. HRMS(ESI), m/z: calcd for $C_{16}H_{17}O_2$ $[M+H]^+$: 241.1229; found, 241.1231. The NMR and MS data of compounds **8** were identical with previous report[3].

References:

1. H. Ma, X. An, T. Zhang, X. He, Y. Li and M. Wang, *New J. Chem.*, 2024, **48**, 15846-15855.
2. X. An, T. Zhang, H. Ma, X. He and M. Wang, *Synthesis*, 2024, **56**, 3621-3629.
3. C. Shekhar and G. Satyanarayana, *Eur. J. Org. Chem.*, 2022, e202101444.

Part 2. The crystal structure parameters for compounds 3c and 3w



3c

Table S1. Crystal data and structure refinement for exp_10123 (compound **3c**, CCDC 2495484)

Identification code	exp_10123
Empirical formula	$C_{14}H_{11}ClO_3$
Formula weight	262.68
Temperature / K	117.60(14)
Crystal system	tetragonal
Space group	$I4_1/a$
a / Å, b / Å, c / Å	34.3840(8), 34.3840(8), 3.8114(4)
α/°, β/°, γ/°	90.00, 90.00, 90.00
Volume / Å^3	4506.0(5)
Z	16
ρ_{calc} / mg mm^{-3}	1.549
μ / mm^{-1}	2.989
F(000)	2176
Crystal size / mm^3	0.27 × 0.24 × 0.23
2Θ range for data collection	10.3 to 132.48°
Index ranges	$-37 \le h \le 40$, $-38 \le k \le 40$, $-4 \le l \le 1$
Reflections collected	5201
Independent reflections	1940[R(int) = 0.0382 (inf-0.9Å)]
Data/restraints/parameters	1940/0/165
Goodness-of-fit on F^2	1.039
Final R indexes [I>2σ (I) i.e. F_o>4σ (F_o)]	R_1 = 0.0345, wR_2 = 0.0835
Final R indexes [all data]	R_1 = 0.0398, wR_2 = 0.0886
Largest diff. peak/hole / e Å^{-3}	0.214/-0.266
Flack Parameters	N
Completeness	0.9923

Table S2. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for exp_10123. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Cl1	9300.95(13)	10757.79(12)	1569.6(13)	20.48(16)
O1	8033.6(4)	10098.9(4)	-1682(4)	20.3(3)
O2	9646.8(4)	8257.0(4)	6119(4)	20.8(3)
O3	9551.1(3)	9969.1(4)	3017(3)	15.3(3)
C4	9714.7(5)	8930.6(5)	4163(5)	14.3(4)
C5	9529.6(5)	9264.5(5)	2942(5)	12.8(4)
C6	9177.5(5)	9983.4(5)	1752(5)	13.3(4)
C7	8412.5(5)	10048.7(6)	-551(5)	15.9(4)
C8	8916.2(5)	8932.5(5)	3052(5)	15.3(4)
C9	9097.1(5)	8599.1(5)	4239(5)	17.0(4)
C10	8950.8(5)	9646.6(5)	1368(5)	13.4(4)
C11	9497.8(6)	8598.2(5)	4846(5)	15.8(4)
C12	10047.1(6)	8253.7(6)	7115(6)	22.5(5)
C13	8565.8(5)	9685.9(5)	220(5)	15.1(4)
C14	9126.7(5)	9273.0(5)	2426(5)	12.9(4)
C15	9017.0(5)	10342.5(5)	992(5)	14.4(4)
C16	8637.3(5)	10381.8(5)	-183(5)	16.0(4)
C17	9757.8(5)	9620.6(5)	2005(5)	14.1(4)

Table S3. Anisotropic Displacement Parameters ($Å^2×10^3$) for exp_10123. 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	18.3(2)	10.9(2)	32.2(3)	-1.18(19)	-2.1(2)	-1.89(17)
O1	14.0(7)	15.4(6)	31.5(8)	-4.4(6)	-5.5(6)	1.7(5)
O2	15.3(6)	14.3(6)	32.7(8)	6.9(6)	-4.1(6)	0.7(5)
O3	11.8(6)	11.9(6)	22.1(7)	-1.5(5)	-2.7(5)	-0.7(5)
C4	11.1(8)	15.9(9)	15.9(9)	-2.4(8)	-0.9(7)	0.2(7)
C5	14.4(9)	13.0(9)	11.1(9)	-2.6(7)	0.6(7)	-1.6(7)
C6	12.0(8)	16.1(9)	11.7(9)	-0.8(7)	0.9(7)	-0.3(7)
C7	13.0(9)	18.6(9)	16.1(9)	-3.1(8)	-0.9(8)	3.2(8)
C8	10.2(8)	14.6(9)	21.2(10)	-1.2(8)	0.1(8)	-1.0(7)
C9	15.6(9)	13.6(9)	21.9(10)	1.8(8)	1.3(8)	-3.3(7)
C10	15.2(9)	14.0(9)	11.2(9)	-1.9(7)	1.8(7)	0.4(7)
C11	18.1(9)	12.5(9)	16.8(9)	1.3(8)	1.8(8)	2.1(7)
C12	19.1(10)	19.1(10)	29.2(11)	2.6(9)	-4.0(9)	2.8(8)
C13	14.5(9)	13.8(9)	16.8(9)	-2.8(8)	0.5(8)	-1.7(7)
C14	13.8(9)	13.3(8)	11.7(9)	-1.5(7)	0.1(7)	-0.4(7)
C15	16.4(9)	11.3(8)	15.6(9)	-2.7(7)	1.9(8)	-2.1(7)

C16	18.7(9)	12.7(9)	16.5(9)	-1.5(8)	2.0(8)	3.7(7)
C17	11.9(8)	13.1(9)	17.2(9)	-0.9(7)	-0.5(7)	0.8(7)

Table S4. Bond Lengths for exp_10123.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl1	C15	1.7436(18)	C6	C10	1.404(3)
O1	C7	1.383(2)	C6	C15	1.383(3)
O2	C11	1.369(2)	C7	C13	1.386(3)
O2	C12	1.428(2)	C7	C16	1.389(3)
O3	C6	1.373(2)	C8	C9	1.380(3)
O3	C17	1.446(2)	C8	C14	1.397(3)
C4	C5	1.393(3)	C9	C11	1.397(3)
C4	C11	1.389(3)	C10	C13	1.401(3)
C5	C14	1.399(3)	C10	C14	1.476(3)
C5	C17	1.498(2)	C15	C16	1.387(3)

Table S5. Bond Angles for exp_10123.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C11	O2	C12	117.52(15)	C13	C10	C6	118.55(17)
C6	O3	C17	113.34(14)	C13	C10	C14	123.83(17)
C11	C4	C5	119.69(17)	O2	C11	C4	124.77(17)
C4	C5	C14	121.10(17)	O2	C11	C9	115.45(17)
C4	C5	C17	120.93(16)	C4	C11	C9	119.77(17)
C14	C5	C17	117.93(16)	C7	C13	C10	120.83(17)
O3	C6	C10	121.79(16)	C5	C14	C10	117.54(16)
O3	C6	C15	118.60(16)	C8	C14	C5	118.13(17)
C15	C6	C10	119.54(17)	C8	C14	C10	124.30(17)
O1	C7	C13	122.45(17)	C6	C15	Cl1	118.77(14)
O1	C7	C16	116.93(17)	C6	C15	C16	122.02(17)
C13	C7	C16	120.63(17)	C16	C15	Cl1	119.21(14)
C9	C8	C14	121.23(17)	C15	C16	C7	118.43(17)
C8	C9	C11	120.03(17)	O3	C17	C5	110.88(14)
C6	C10	C14	117.50(16)				

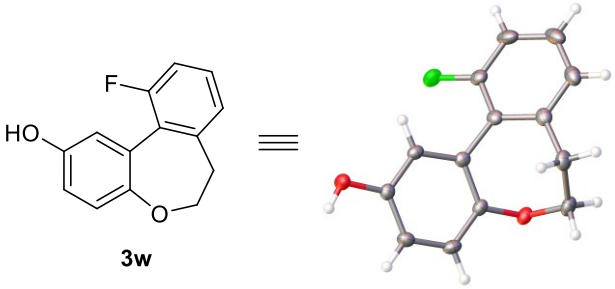
Table S6. Torsion Angles for exp_10123.

A	B	C	D	Angle/°
Cl1	C15	C16	C7	-178.55(14)
O1	C7	C13	C10	-179.83(17)
O1	C7	C16	C15	179.13(17)

O3	C6	C10	C13	176.99(16)
O3	C6	C10	C14	0.9(3)
O3	C6	C15	Cl1	1.6(2)
O3	C6	C15	C16	-177.83(17)
C4	C5	C14	C8	-2.2(3)
C4	C5	C14	C10	175.75(16)
C4	C5	C17	O3	-142.48(17)
C5	C4	C11	O2	-178.56(17)
C5	C4	C11	C9	1.2(3)
C6	O3	C17	C5	-52.8(2)
C6	C10	C13	C7	0.6(3)
C6	C10	C14	C5	-14.7(3)
C6	C10	C14	C8	163.12(18)
C6	C15	C16	C7	0.9(3)
C8	C9	C11	O2	178.11(17)
C8	C9	C11	C4	-1.7(3)
C9	C8	C14	C5	1.8(3)
C9	C8	C14	C10	-176.07(17)
C10	C6	C15	Cl1	178.76(14)
C10	C6	C15	C16	-0.7(3)
C11	C4	C5	C14	0.8(3)
C11	C4	C5	C17	-176.80(17)
C12	O2	C11	C4	6.0(3)
C12	O2	C11	C9	-173.81(17)
C13	C7	C16	C15	-0.4(3)
C13	C10	C14	C5	169.37(17)
C13	C10	C14	C8	-12.8(3)
C14	C5	C17	O3	39.9(2)
C14	C8	C9	C11	0.2(3)
C14	C10	C13	C7	176.42(17)
C15	C6	C10	C13	0.0(3)
C15	C6	C10	C14	-176.18(16)
C16	C7	C13	C10	-0.3(3)
C17	O3	C6	C10	34.0(2)
C17	O3	C6	C15	-148.96(16)
C17	C5	C14	C8	175.41(17)
C17	C5	C14	C10	-6.6(2)

Table S7. Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for exp_10123.

Atom	*x*	*y*	*z*	U(eq)
H1	7938	9882	-2203	30
H4	9988	8930	4527	17
H8	8643	8930	2654	18
H9	8949	8370	4644	20
H12A	10210	8279	5017	34
H12B	10107	8008	8308	34
H12C	10099	8472	8703	34
H13	8408	9461	-34	18
H16	8533	10631	-724	19
H17A	10013	9613	3208	17
H17B	9806	9625	-556	17



3w

Table S8. Crystal data and structure refinement for exp_10119 (compound **3w**, CCDC 2495483)

Identification code	exp_10119
Empirical formula	$C_{14}H_{11}FO_2$
Formula weight	230.23
Temperature / K	117.30(14)
Crystal system	orthorhombic
Space group	Pbca
a / Å, b / Å, c / Å	13.7379(4), 10.0334(3), 16.1142(4)
α/°, β/°, γ/°	90.00, 90.00, 90.00
Volume / Å^3	2221.14(12)
Z	8
ρ_{calc} / mg mm^{-3}	1.377
μ / mm^{-1}	0.854
F(000)	960
Crystal size / mm^3	0.36 × 0.21 × 0.20
2Θ range for data collection	10.98 to 132.92°
Index ranges	-16 ≤ h ≤ 15, -11 ≤ k ≤ 7, -19 ≤ l ≤ 18
Reflections collected	4512
Independent reflections	1907[R(int) = 0.0274 (inf-0.9Å)]

Data/restraints/parameters	1907/0/155
Goodness-of-fit on F^2	1.081
Final R indexes [I>2σ (I) i.e. F_o>4σ (F_o)]	R_1 = 0.0368, wR_2 = 0.1017
Final R indexes [all data]	R_1 = 0.0422, wR_2 = 0.1070
Largest diff. peak/hole / e Å^{-3}	0.236/-0.201
Flack Parameters	N
Completeness	0.9980

Table S9. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for exp_10119. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
F1	5120.6(7)	1688.1(9)	5453.7(6)	29.5(3)
O1	6755.9(7)	3040.7(10)	7795.2(6)	22.1(3)
O2	4043.2(8)	6128.6(11)	6148.8(7)	24.9(3)
C12	5200.8(10)	4403.0(15)	6147.7(9)	18.8(3)
C11	4716.3(10)	5398.7(14)	6575.9(9)	18.7(3)
C6	6511.0(11)	2658.6(15)	6068.1(9)	19.7(3)
C7	5920(1)	3642.6(14)	6533.5(9)	18.2(3)
C1	6108.7(11)	1745.0(15)	5523.4(9)	22.9(3)
C9	5629.7(11)	4864.3(16)	7802.7(9)	23.0(3)
C14	8003.8(10)	3608.9(17)	6753.1(11)	26.9(4)
C8	6117.8(10)	3878.2(14)	7374.6(9)	19.5(3)
C5	7534.9(11)	2665.9(16)	6147.8(9)	23.0(3)
C13	7784.2(11)	3272.4(18)	7656.7(10)	26.6(4)
C2	6646.7(13)	855.6(18)	5060.7(10)	31.2(4)
C10	4932.8(11)	5635.2(16)	7408.3(10)	23.1(3)
C3	7654.0(13)	905.6(18)	5125.3(10)	32.8(4)
C4	8088.3(12)	1804.2(17)	5663.6(10)	29.0(4)

Table S10. Anisotropic Displacement Parameters (Å^2×10^3) for exp_10119. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka\times b\times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F1	29.7(5)	29.5(5)	29.2(5)	-6.7(4)	-8.7(4)	-0.9(4)
O1	21.5(5)	24.3(6)	20.6(5)	4.8(5)	-4.3(4)	-0.8(4)
O2	26.8(6)	24.9(6)	22.8(6)	-3.0(5)	-5.0(4)	7.1(4)
C12	20.5(7)	20.6(7)	15.4(7)	1.1(6)	-0.8(6)	-4.6(6)
C11	17.3(6)	18.3(7)	20.6(7)	2.8(6)	-0.2(6)	-2.5(6)
C6	24.5(7)	19.0(7)	15.6(6)	4.6(6)	0.3(6)	1.7(6)

C7	19.1(7)	16.8(7)	18.7(7)	1.5(6)	0.6(6)	-4.1(6)
C1	28.7(8)	23.4(8)	16.6(7)	2.9(6)	-3.2(6)	3.0(6)
C9	28.1(7)	25.7(8)	15.4(7)	-1.2(6)	-0.8(6)	-3.3(6)
C14	18.9(7)	30.0(9)	31.9(9)	5.2(7)	0.2(7)	-1.7(6)
C8	19.4(7)	19.7(7)	19.4(7)	3.3(6)	-3.3(6)	-3.0(6)
C5	24.3(7)	23.0(8)	21.6(7)	7.6(6)	1.8(6)	1.9(6)
C13	20.3(7)	31.3(9)	28.2(8)	2.3(7)	-7.0(6)	-2.5(6)
C2	48.4(10)	28.1(9)	17.0(7)	-2.7(7)	-4.1(7)	8.6(8)
C10	26.0(7)	23.2(8)	20.1(7)	-2.6(7)	1.6(6)	0.5(6)
C3	45.3(10)	32.7(9)	20.3(8)	3.2(7)	6.0(7)	17.2(8)
C4	27.7(8)	32.9(9)	26.5(8)	8.9(8)	4.8(7)	8.9(7)

Table S11. Bond Lengths for exp_10119.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
F1	C1	1.3632(18)	C7	C8	1.402(2)
O1	C8	1.3907(17)	C1	C2	1.378(2)
O1	C13	1.4489(18)	C9	C8	1.380(2)
O2	C11	1.3656(18)	C9	C10	1.385(2)
C12	C11	1.385(2)	C14	C5	1.504(2)
C12	C7	1.394(2)	C14	C13	1.525(2)
C11	C10	1.394(2)	C5	C4	1.391(2)
C6	C7	1.482(2)	C2	C3	1.389(3)
C6	C1	1.384(2)	C3	C4	1.386(3)
C6	C5	1.413(2)			

Table S12. Bond Angles for exp_10119.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C8	O1	C13	116.27(11)	C8	C9	C10	120.45(14)
C11	C12	C7	120.88(13)	C5	C14	C13	113.29(13)
O2	C11	C12	117.48(13)	O1	C8	C7	119.43(13)
O2	C11	C10	122.54(13)	C9	C8	O1	119.72(13)
C12	C11	C10	119.98(14)	C9	C8	C7	120.65(13)
C1	C6	C7	122.91(13)	C6	C5	C14	119.26(14)
C1	C6	C5	117.31(14)	C4	C5	C6	119.35(15)
C5	C6	C7	119.74(14)	C4	C5	C14	121.39(14)
C12	C7	C6	121.80(13)	O1	C13	C14	112.05(12)
C12	C7	C8	118.42(13)	C1	C2	C3	118.07(16)
C8	C7	C6	119.68(13)	C9	C10	C11	119.59(14)

F1	C1	C6	118.53(13)	C4	C3	C2	119.96(15)
F1	C1	C2	117.54(14)	C3	C4	C5	121.34(15)
C2	C1	C6	123.90(15)				

Table S13. Torsion Angles for exp_10119.

A	B	C	D	Angle/°
F1	C1	C2	C3	179.89(15)
O2	C11	C10	C9	-179.47(13)
C12	C11	C10	C9	-0.3(2)
C12	C7	C8	O1	173.20(12)
C12	C7	C8	C9	-1.7(2)
C11	C12	C7	C6	-174.24(13)
C11	C12	C7	C8	2.2(2)
C6	C7	C8	O1	-10.3(2)
C6	C7	C8	C9	174.79(13)
C6	C1	C2	C3	-2.0(2)
C6	C5	C4	C3	-2.3(2)
C7	C12	C11	O2	177.97(13)
C7	C12	C11	C10	-1.2(2)
C7	C6	C1	F1	-4.5(2)
C7	C6	C1	C2	177.43(14)
C7	C6	C5	C14	4.5(2)
C7	C6	C5	C4	-175.36(13)
C1	C6	C7	C12	-46.7(2)
C1	C6	C7	C8	136.92(15)
C1	C6	C5	C14	-177.96(13)
C1	C6	C5	C4	2.2(2)
C1	C2	C3	C4	2.0(2)
C14	C5	C4	C3	177.90(15)
C8	O1	C13	C14	-39.57(18)
C8	C9	C10	C11	0.8(2)
C5	C6	C7	C12	130.76(15)
C5	C6	C7	C8	-45.6(2)
C5	C6	C1	F1	177.99(13)
C5	C6	C1	C2	-0.1(2)
C5	C14	C13	O1	-48.24(18)
C13	O1	C8	C7	78.90(16)
C13	O1	C8	C9	-106.12(16)
C13	C14	C5	C6	67.66(18)

C13	C14	C5	C4	-112.52(16)
C2	C3	C4	C5	0.1(2)
C10	C9	C8	O1	-174.68(13)
C10	C9	C8	C7	0.2(2)

Table S14. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for exp_10119.

Atom	***x***	***y***	***z***	**U(eq)**
H2	3800	6705	6465	37
H12	5041	4236	5584	23
H9	5773	5016	8372	28
H14A	7774	4525	6636	32
H14B	8717	3593	6668	32
H13A	8154	2466	7817	32
H13B	8004	4016	8014	32
H2A	6337	226	4708	37
H10	4604	6321	7703	28
H3	8045	324	4801	39
H4	8778	1832	5703	35

Part 3. Copies of ^{1}H and ^{13}C NMR spectra of products

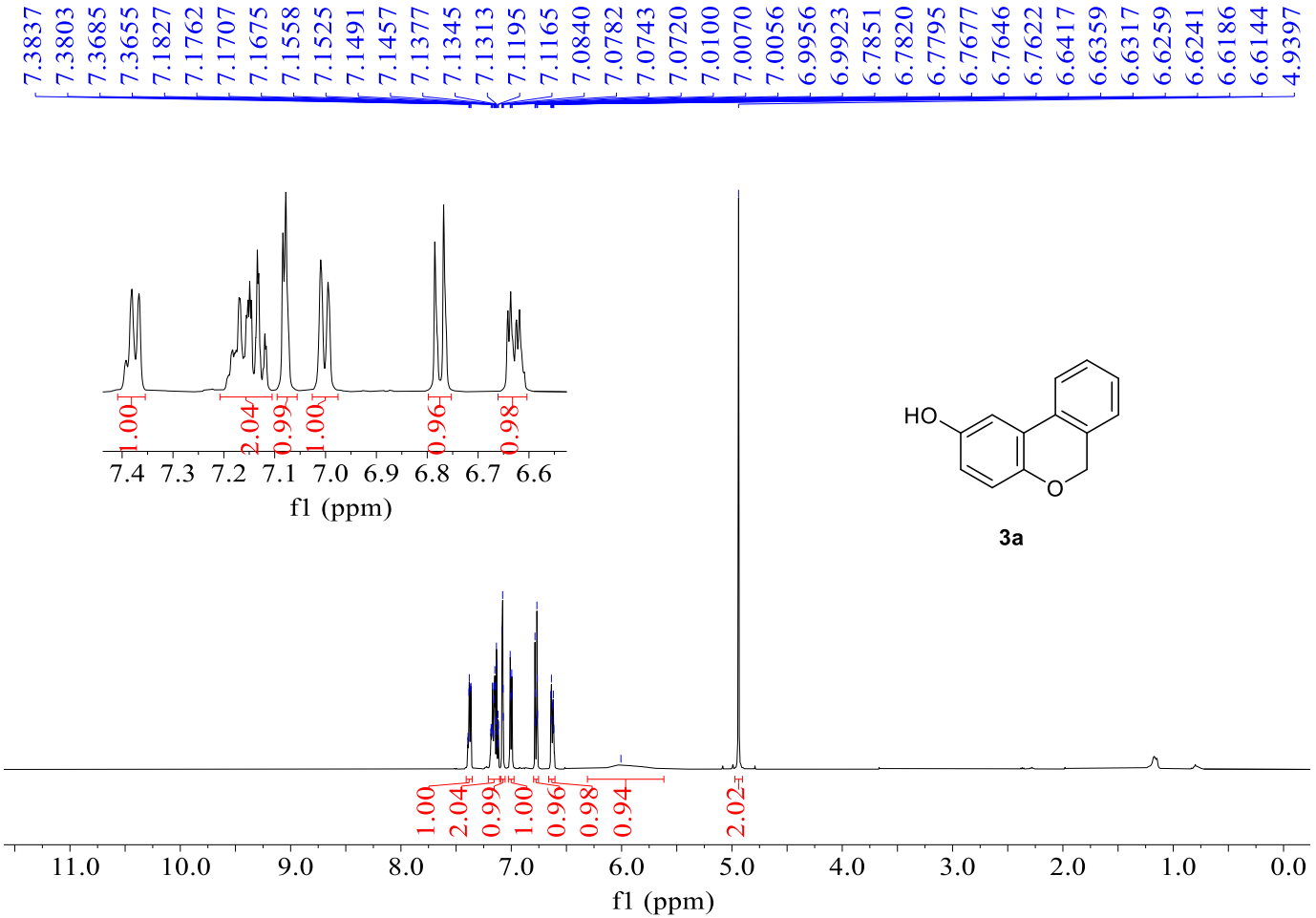


Figure S1 ^{1}H NMR of compound **3a** (500 MHz, $CDCl_3$)

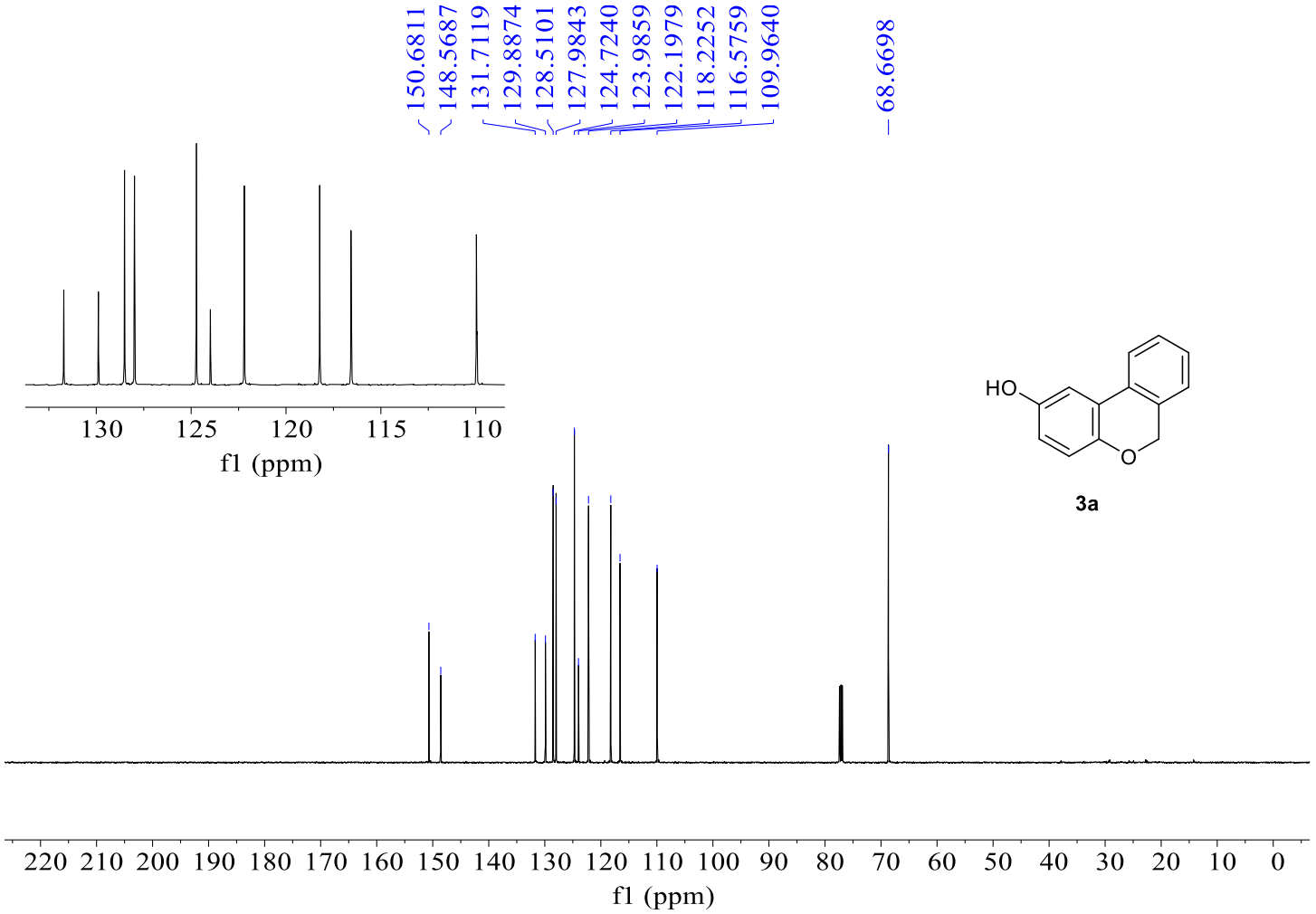


Figure S2 ^{13}C NMR of compound **3a** (126 MHz, $CDCl_3$)

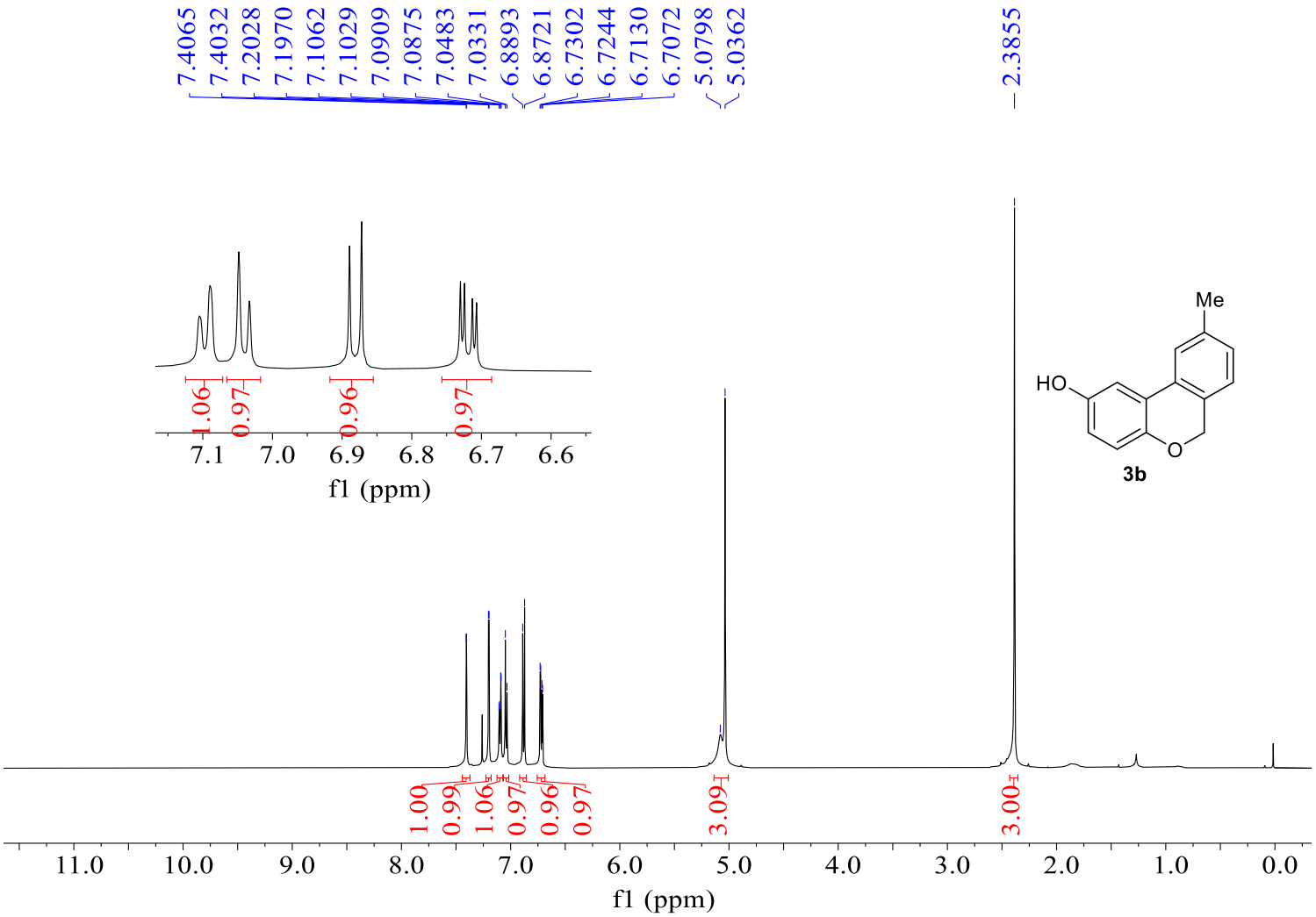


Figure S3 ^{1}H NMR of compound **3b** (500 MHz, $CDCl_3$)

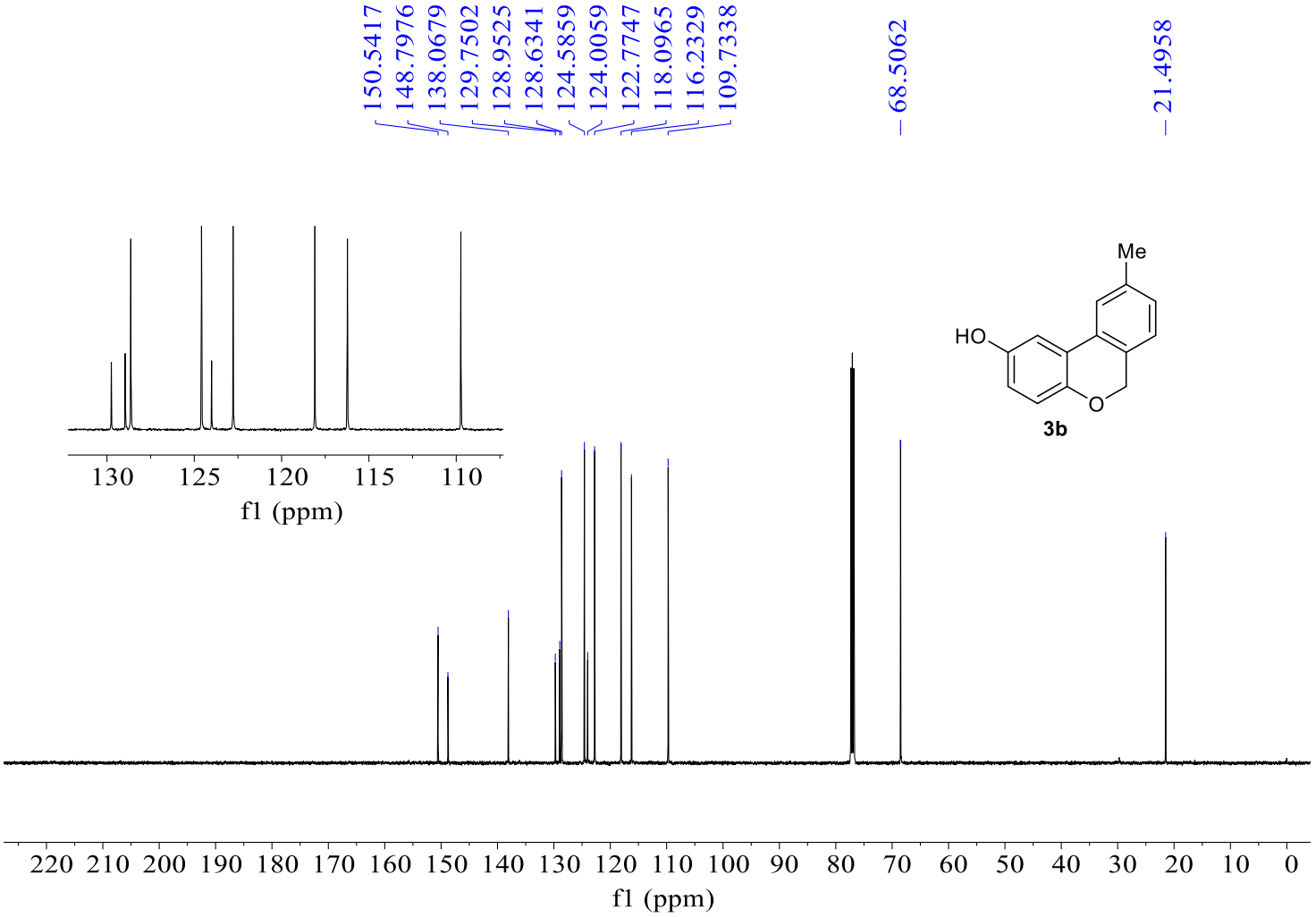


Figure S4 ^{13}C NMR of compound **3b** (126 MHz, $CDCl_3$)

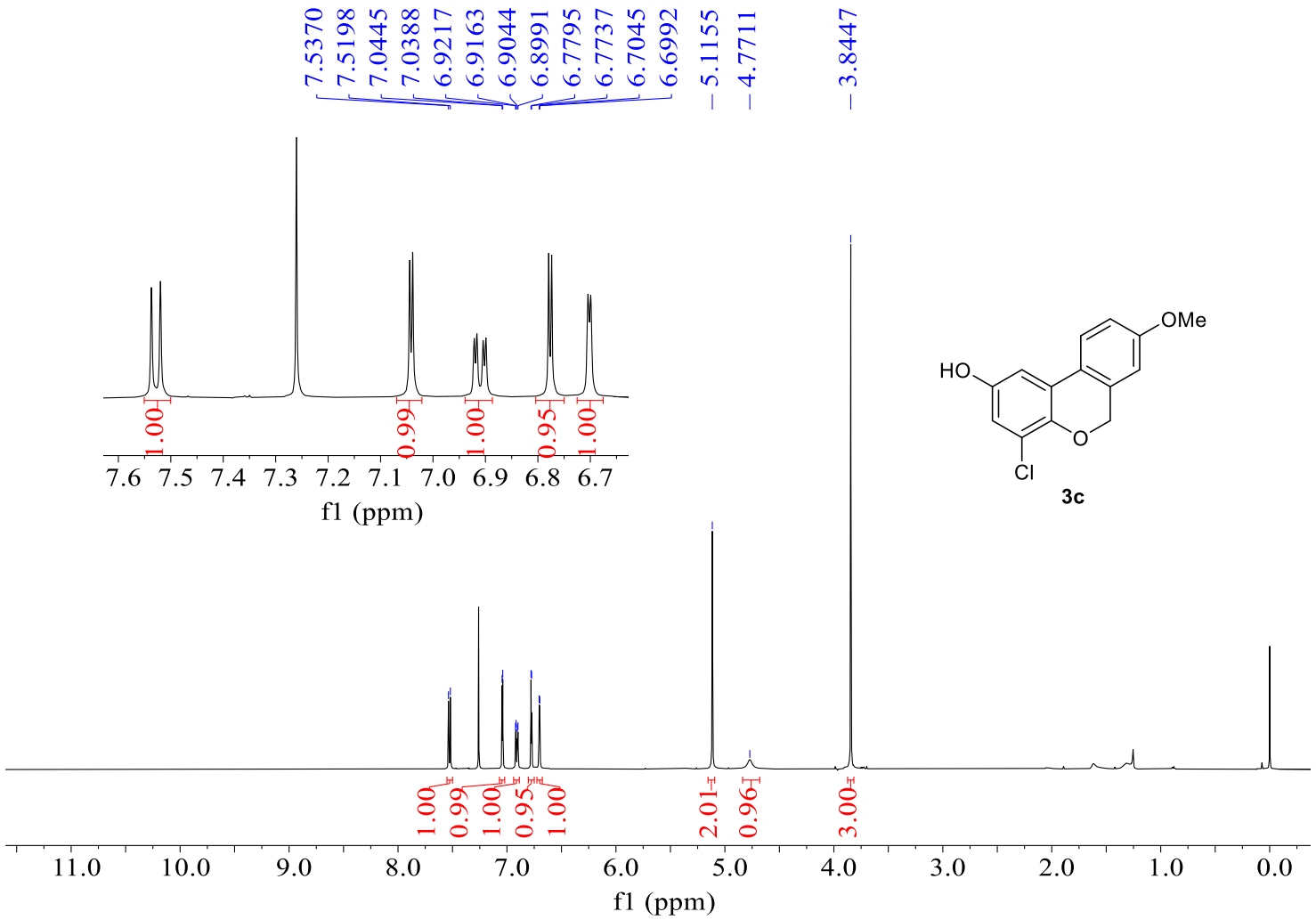


Figure S5 ^{1}H NMR of compound **3c** (500 MHz, $CDCl_3$)

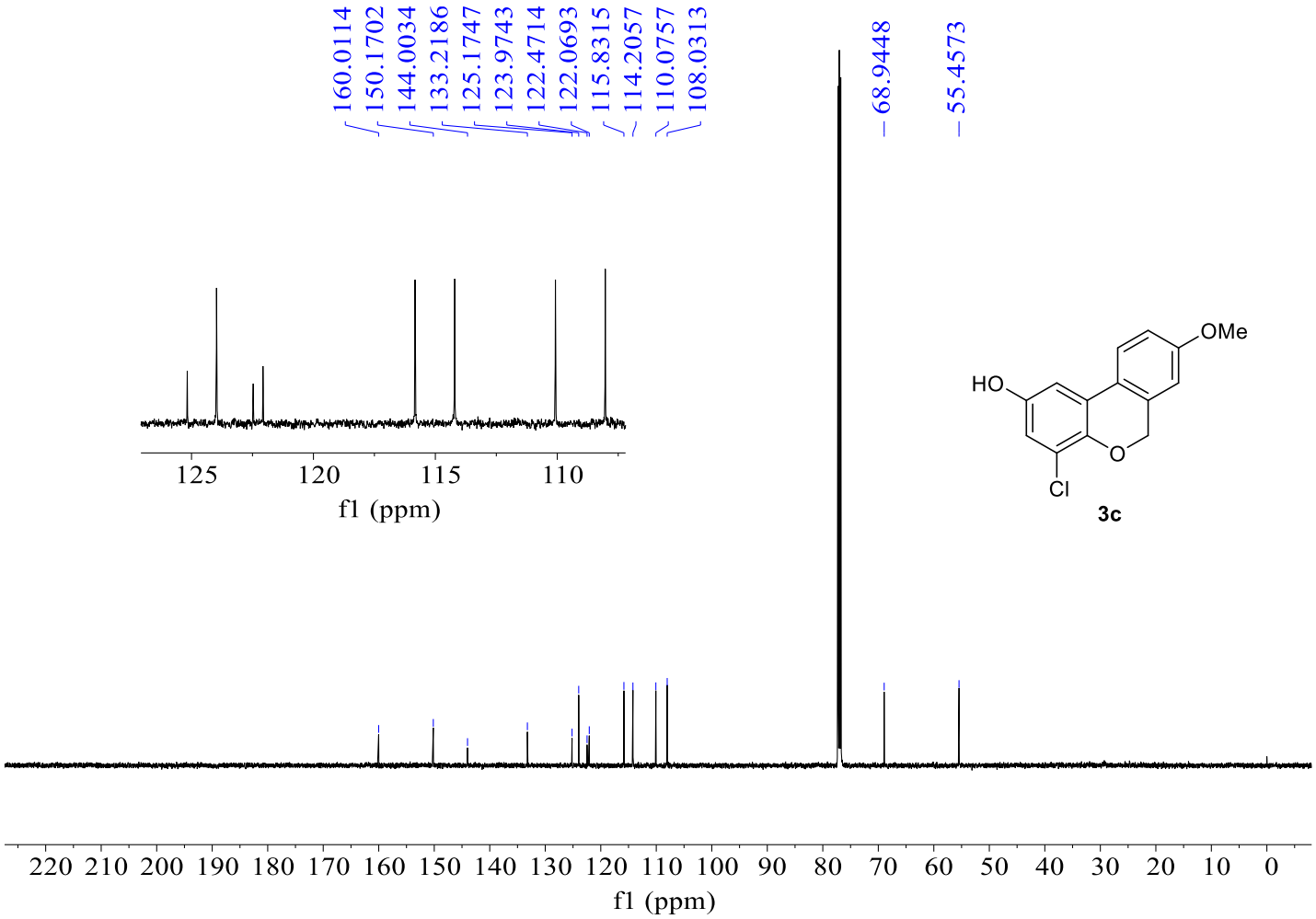


Figure S6 ^{13}C NMR of compound **3c** (126 MHz, $CDCl_3$)

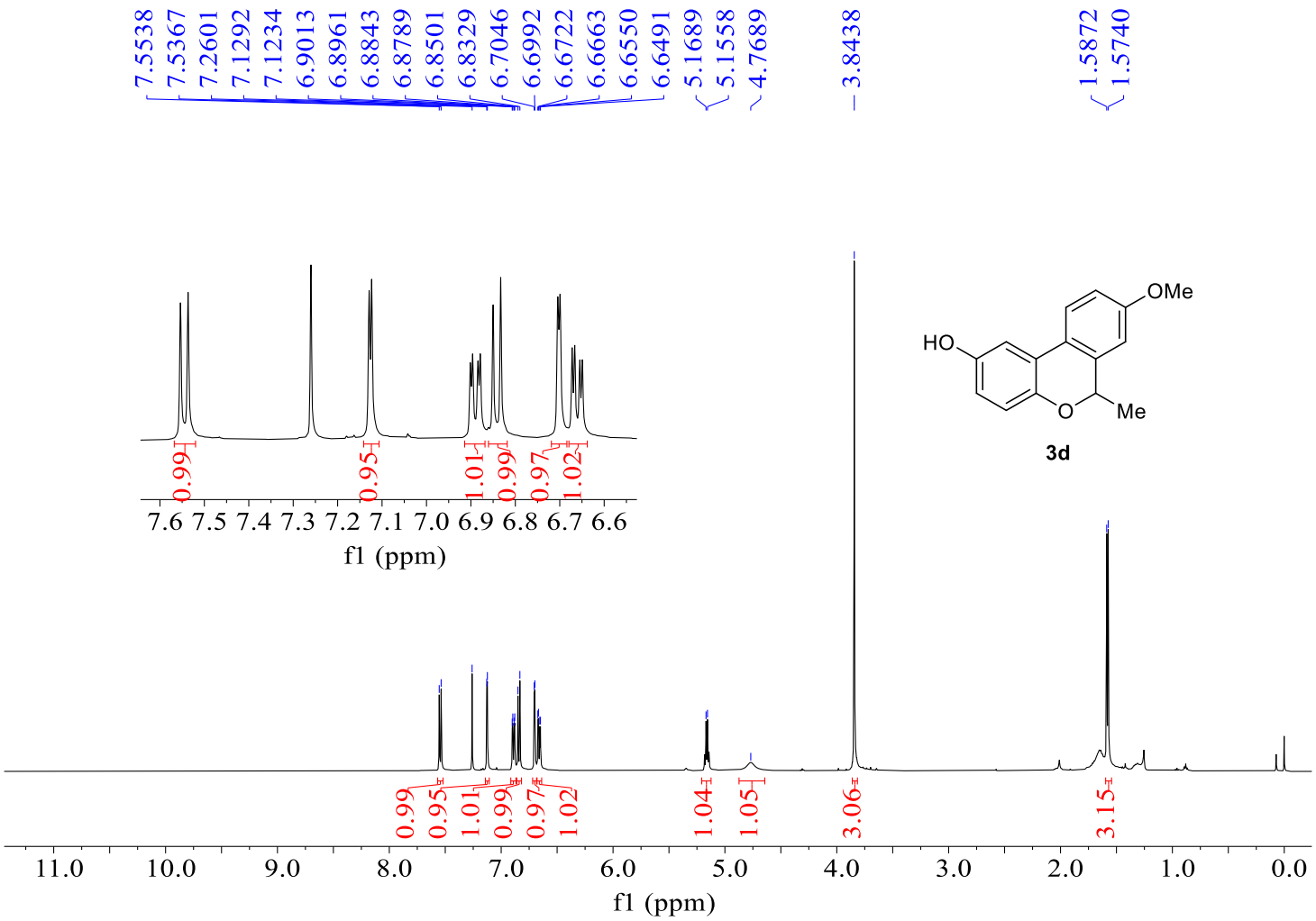


Figure S7 ^{1}H NMR of compound **3d** (500 MHz, $CDCl_3$)

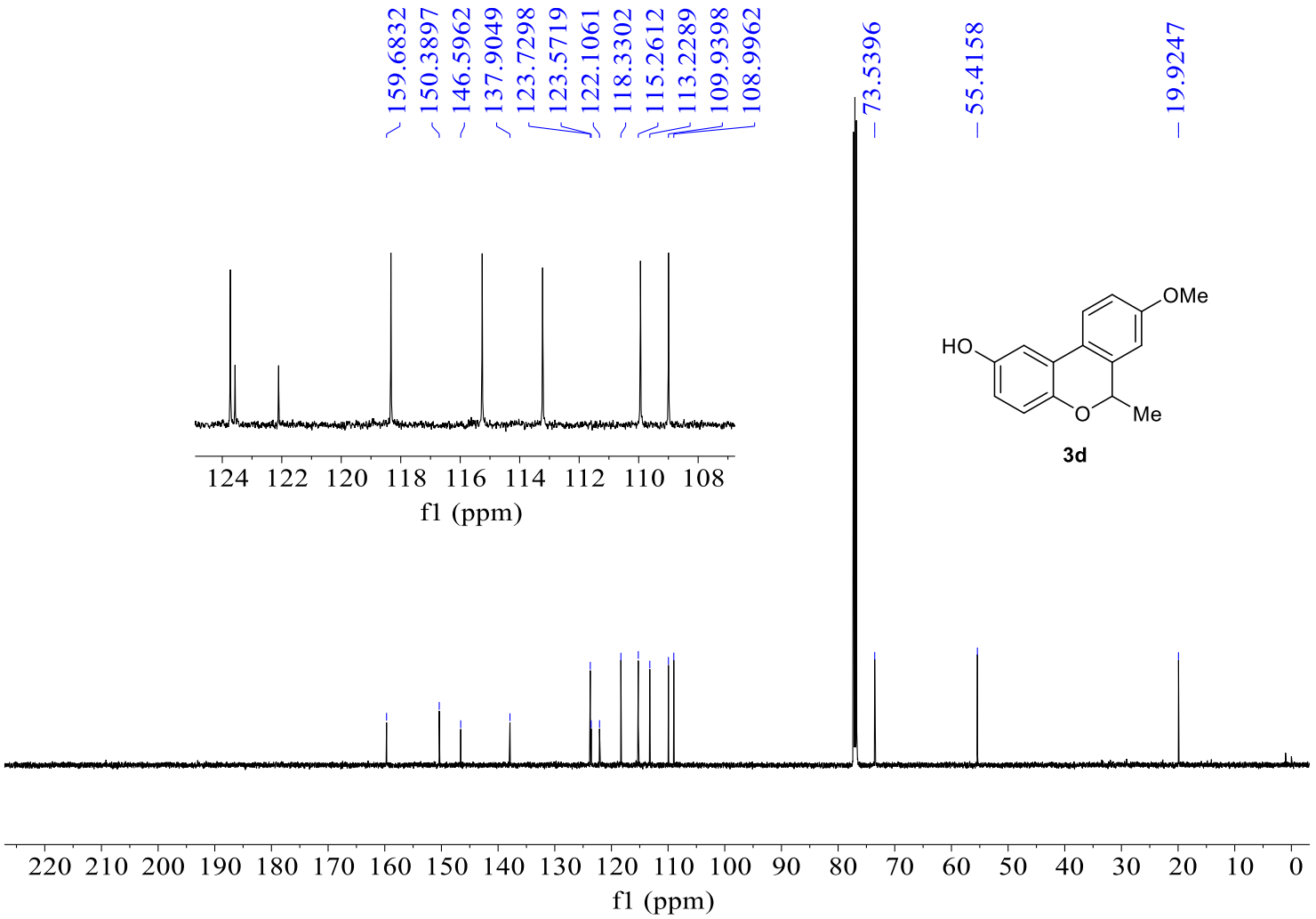


Figure S8 ^{13}C NMR of compound **3d** (126 MHz, $CDCl_3$)

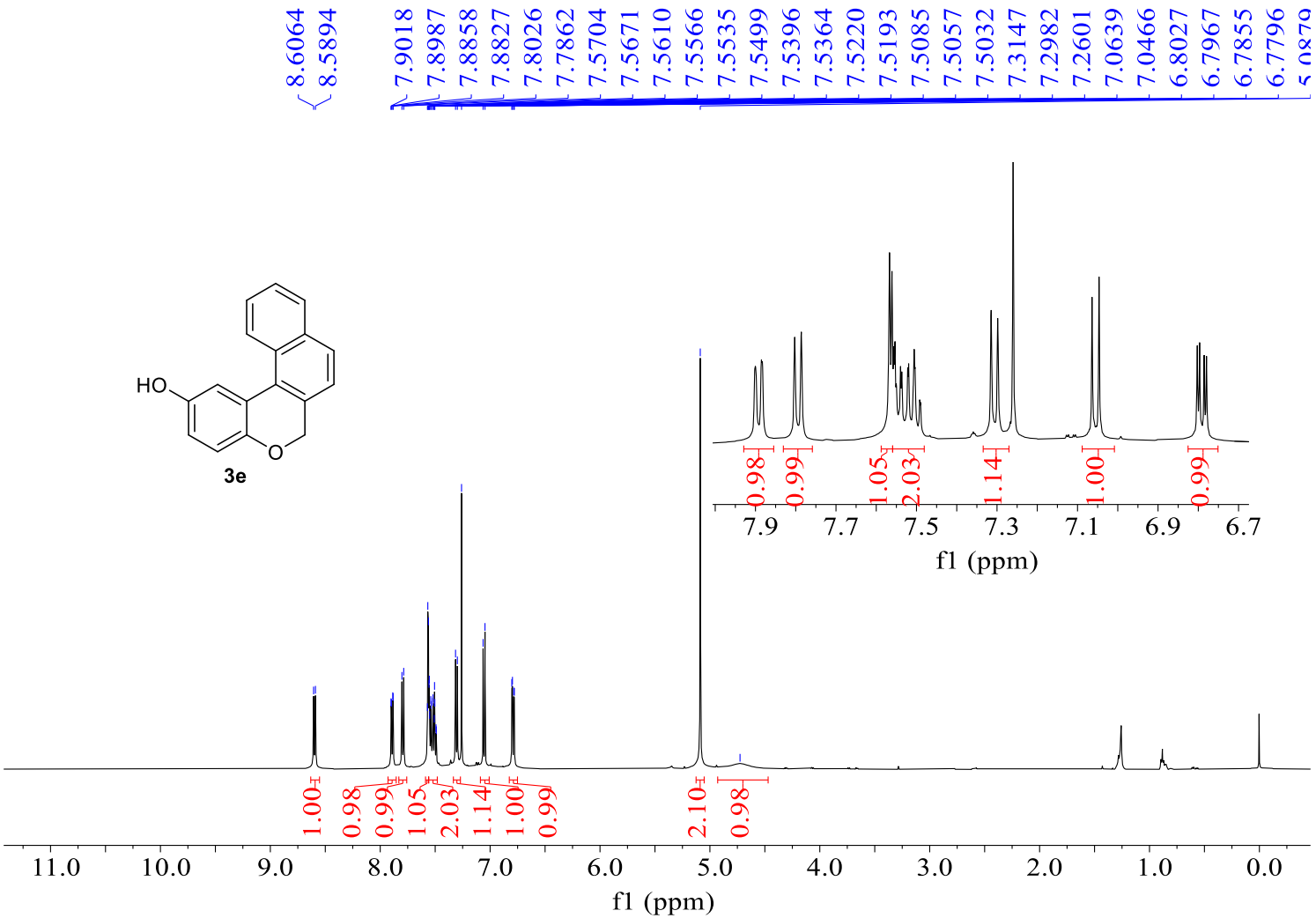


Figure S9 ^{1}H NMR of compound **3e** (500 MHz, $CDCl_3$)

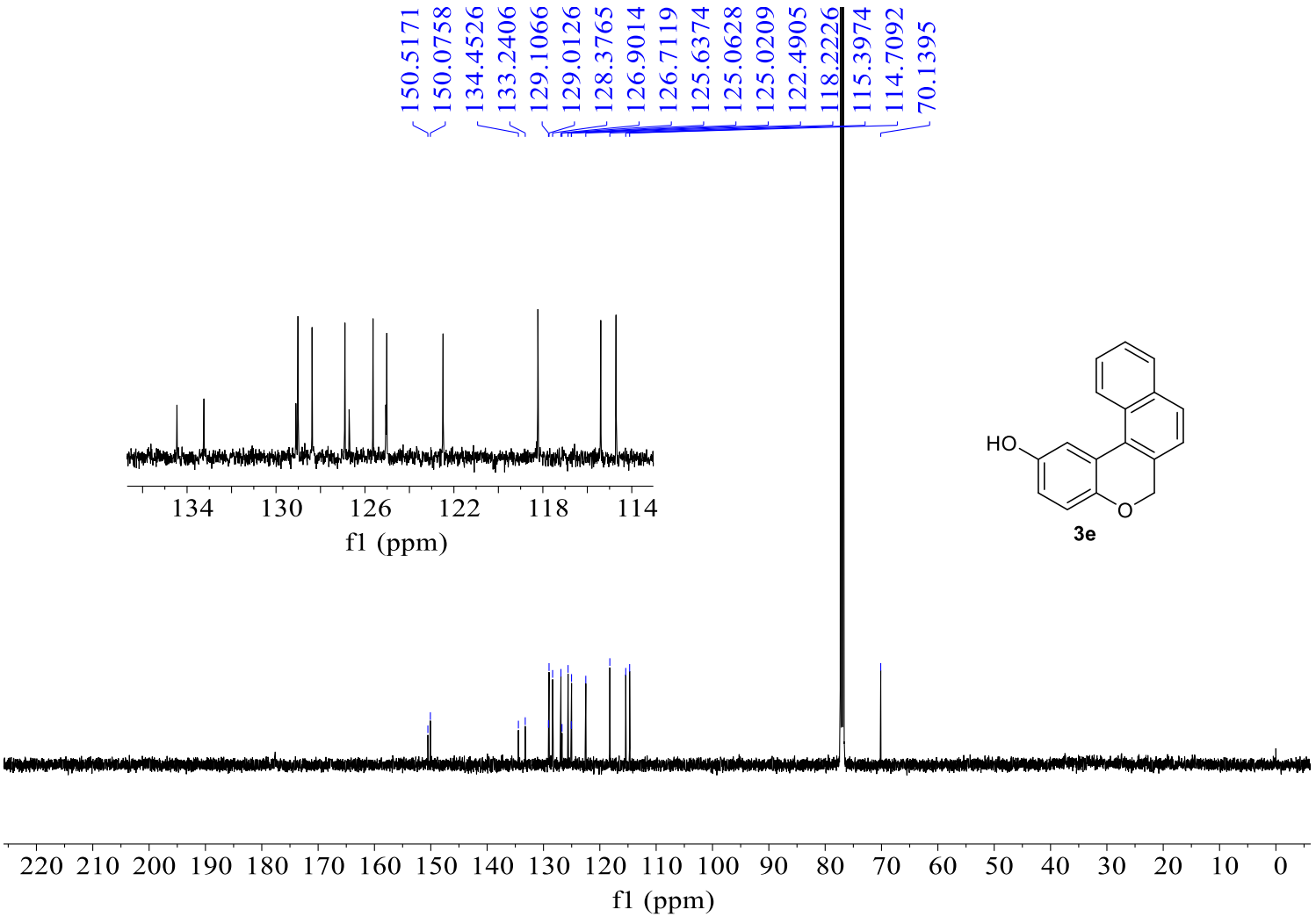


Figure S10 ^{13}C NMR of compound **3e** (126 MHz, $CDCl_3$)

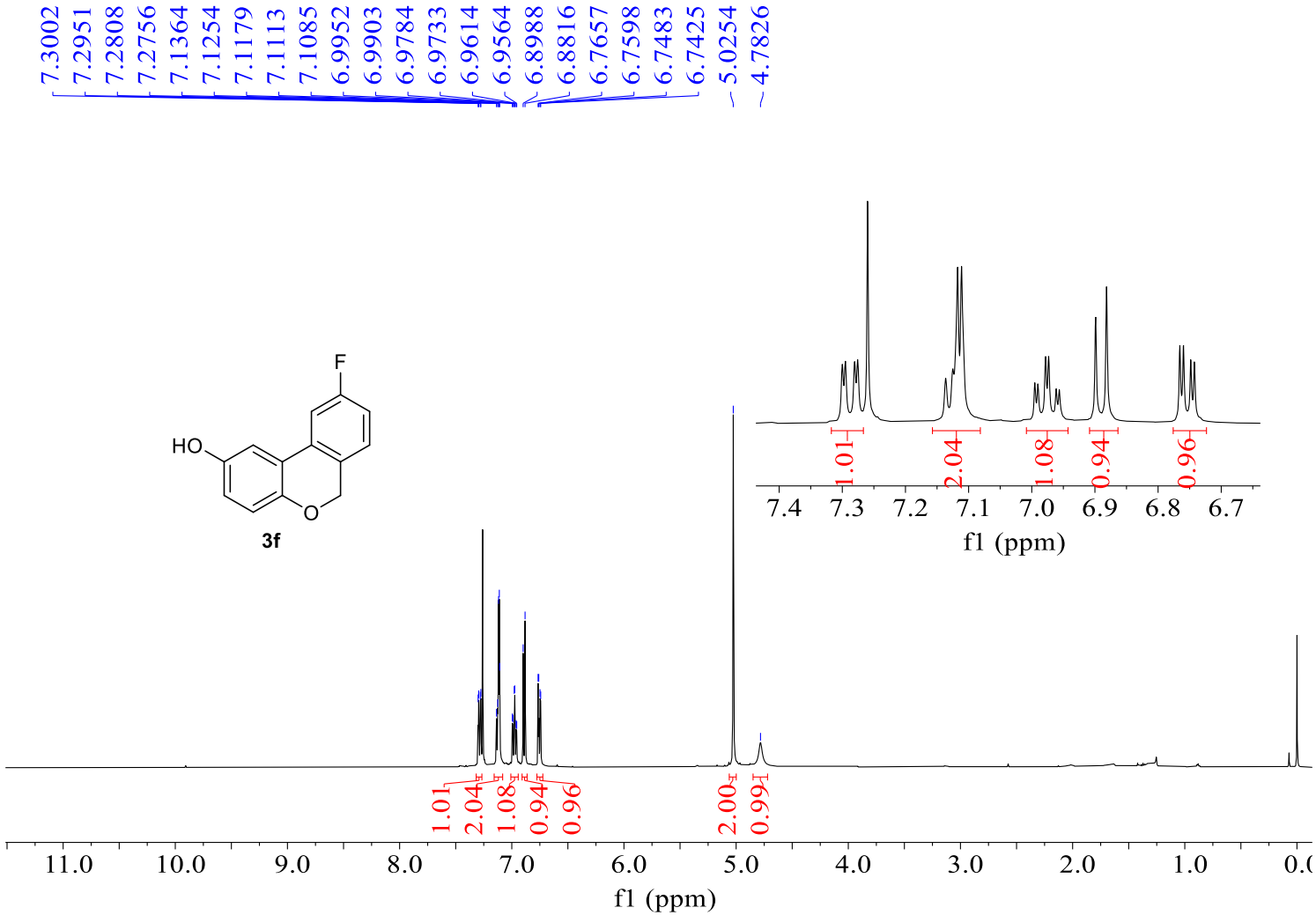


Figure S11 ^{1}H NMR of compound **3f** (500 MHz, $CDCl_3$)

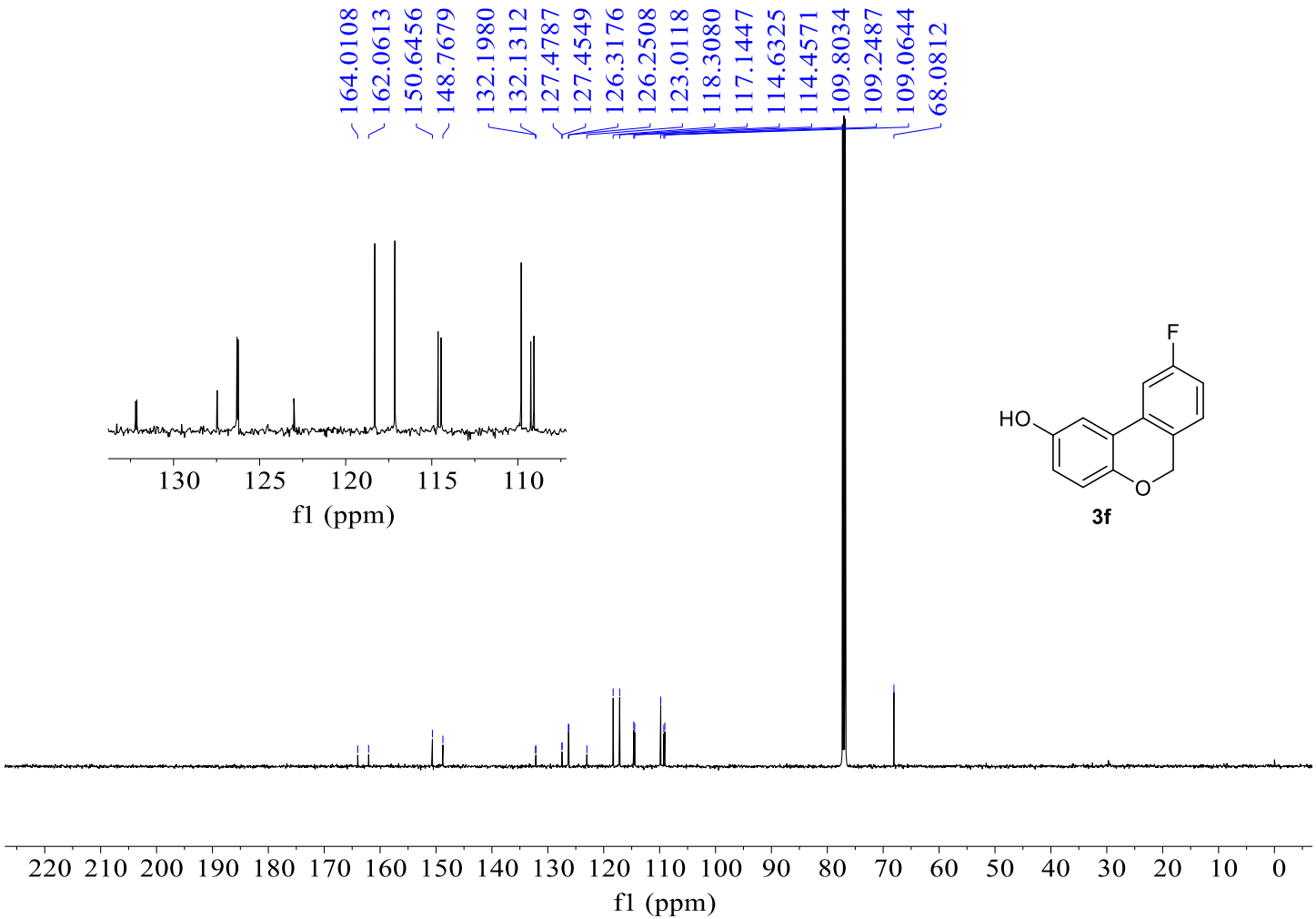


Figure S12 ^{13}C NMR of compound **3f** (126 MHz, $CDCl_3$)

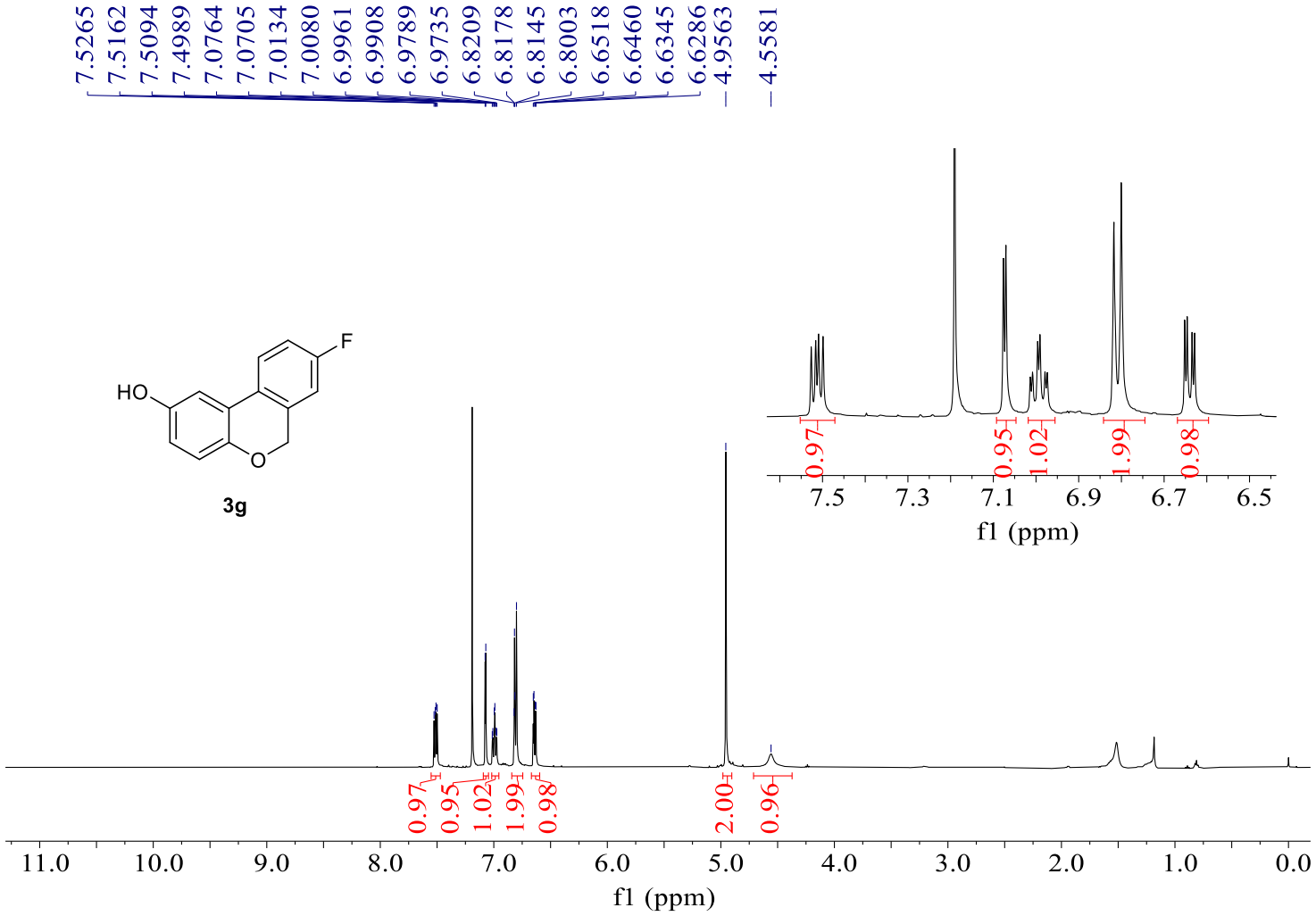


Figure S13 ^{1}H NMR of compound **3g** (500 MHz, $CDCl_3$)

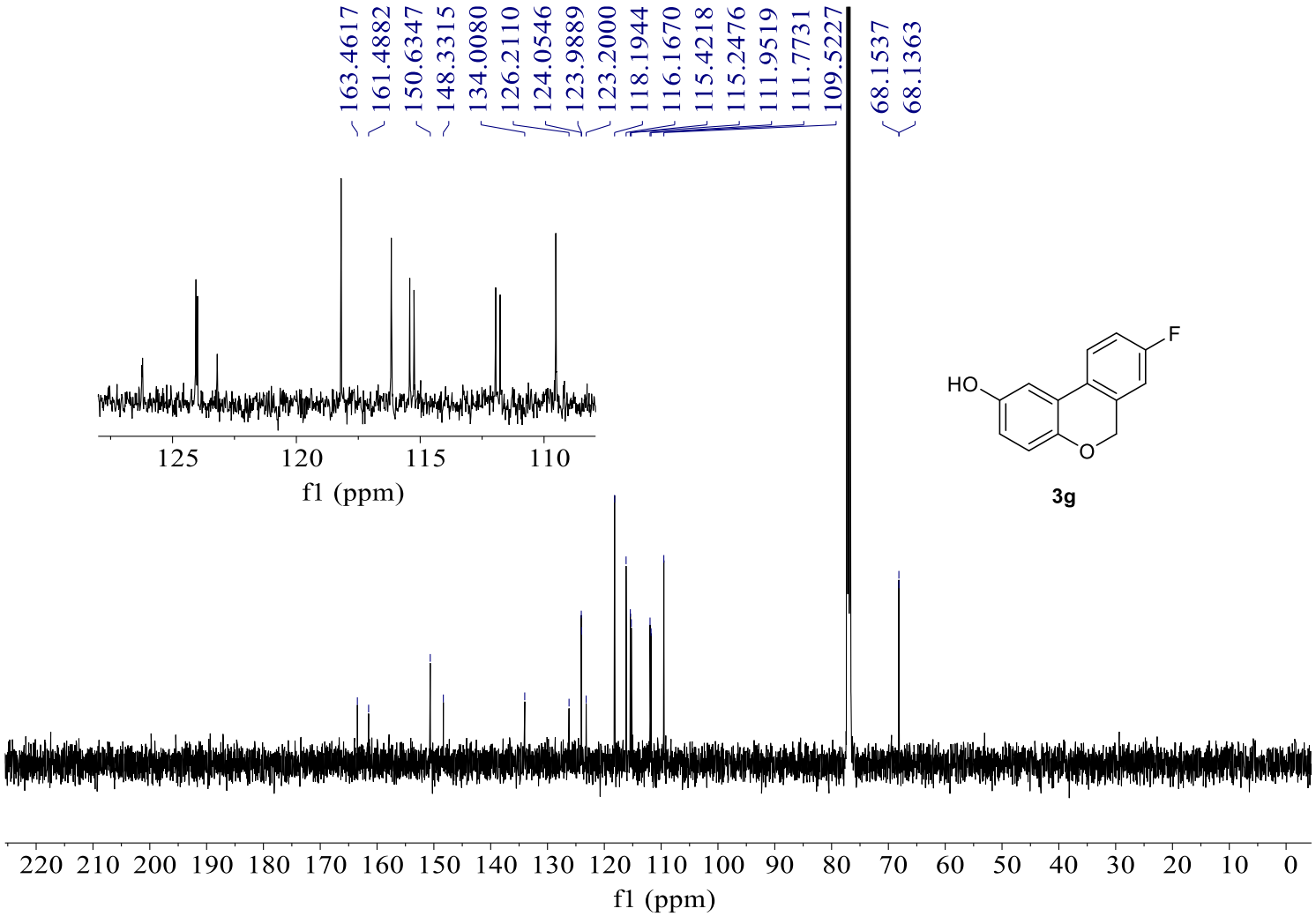


Figure S14 ^{13}C NMR of compound **3g** (126 MHz, $CDCl_3$)

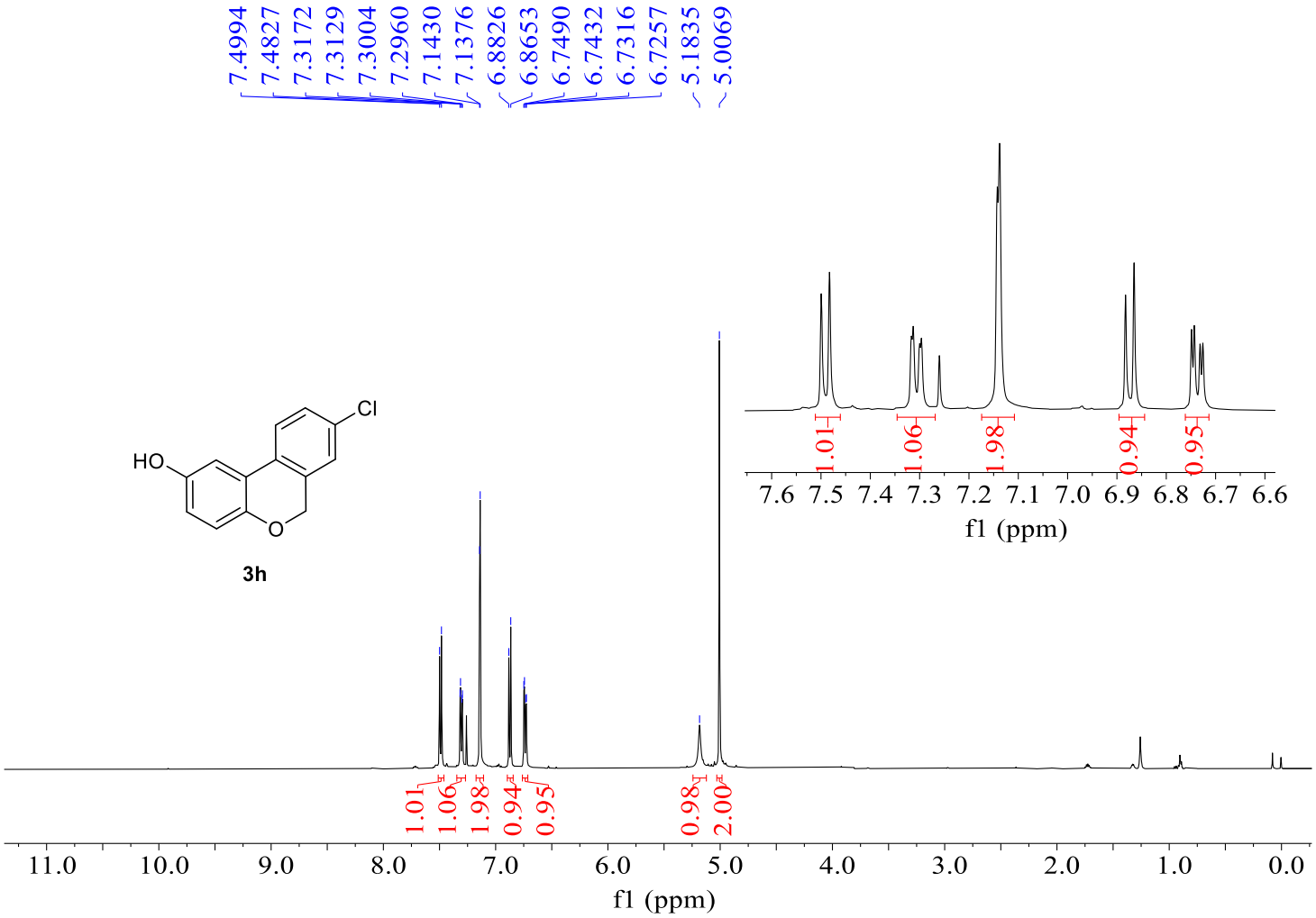


Figure S15 ^{1}H NMR of compound **3h** (500 MHz, $CDCl_3$)

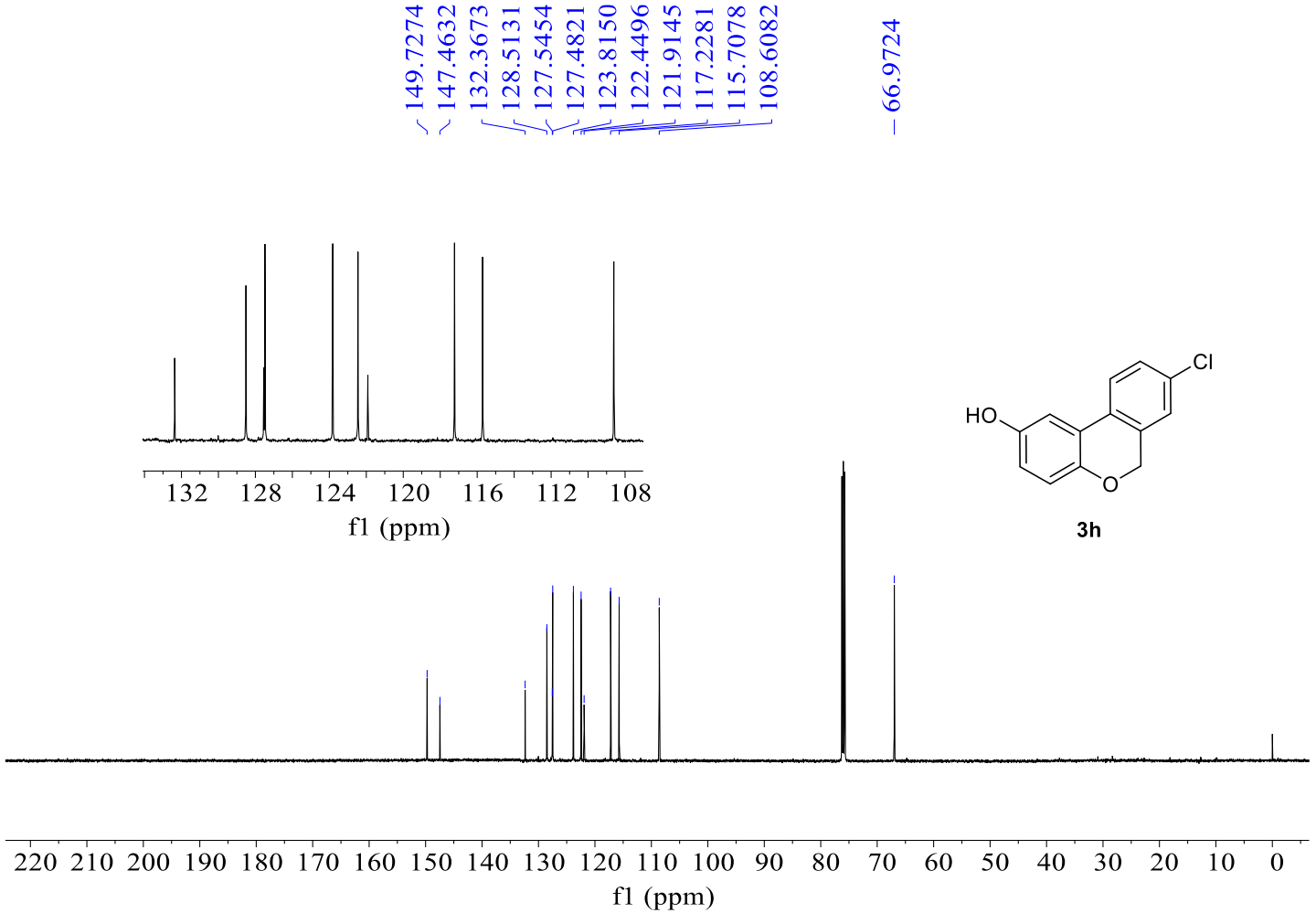


Figure S16 ^{13}C NMR of compound **3h** (126 MHz, $CDCl_3$)

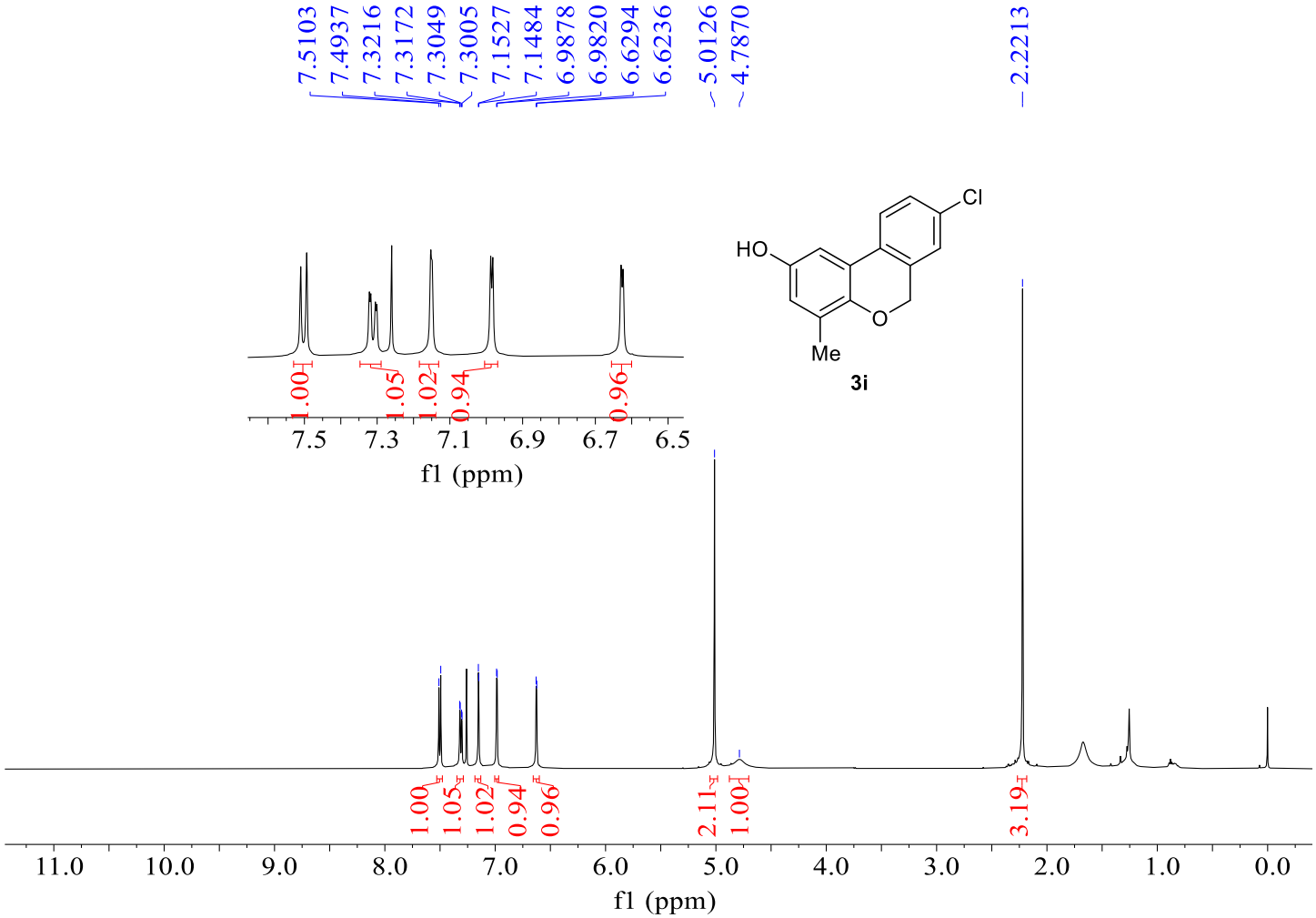


Figure S17 ^{1}H NMR of compound **3i** (500 MHz, $CDCl_3$)

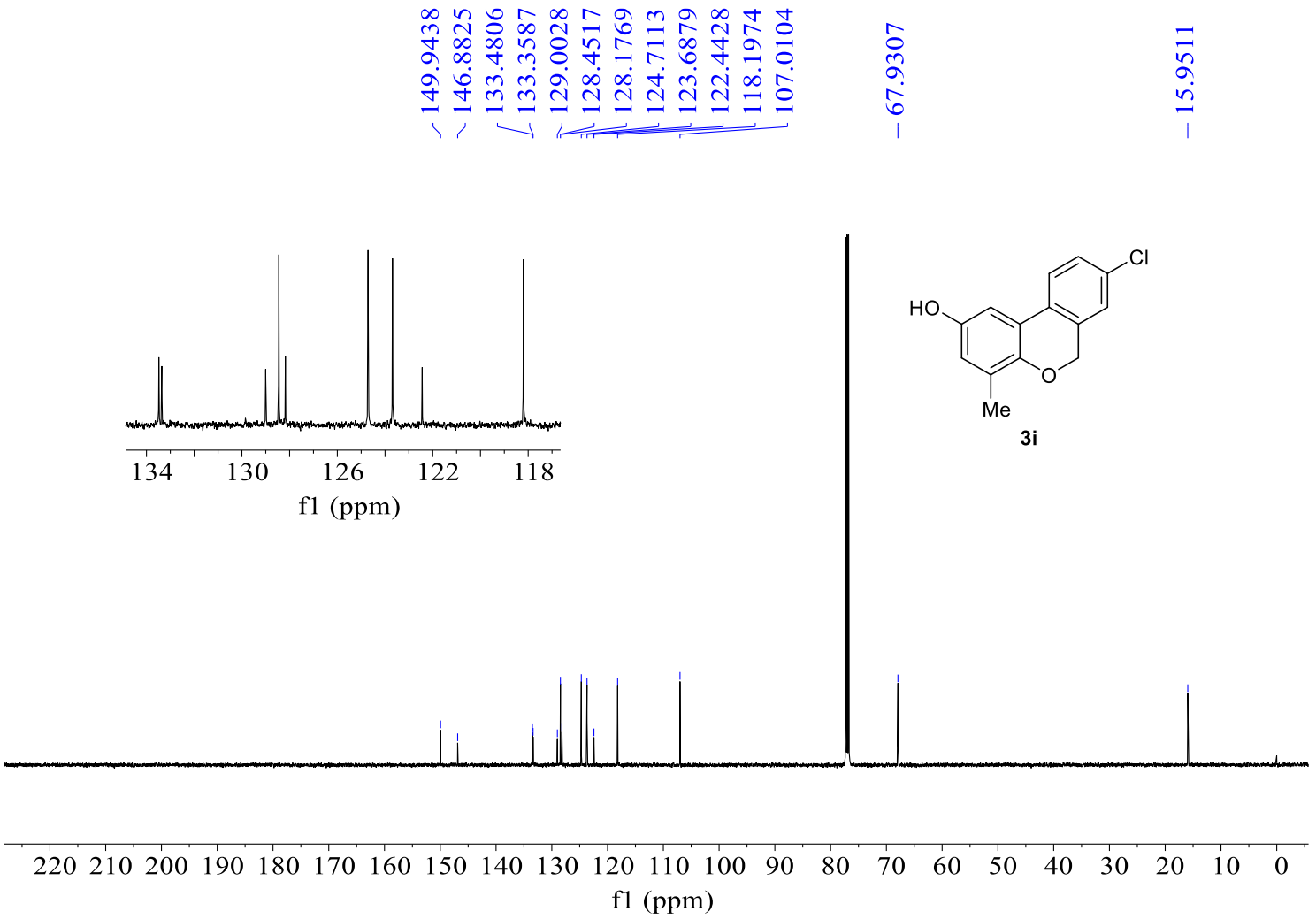


Figure S18 ^{13}C NMR of compound **3i** (126 MHz, $CDCl_3$)

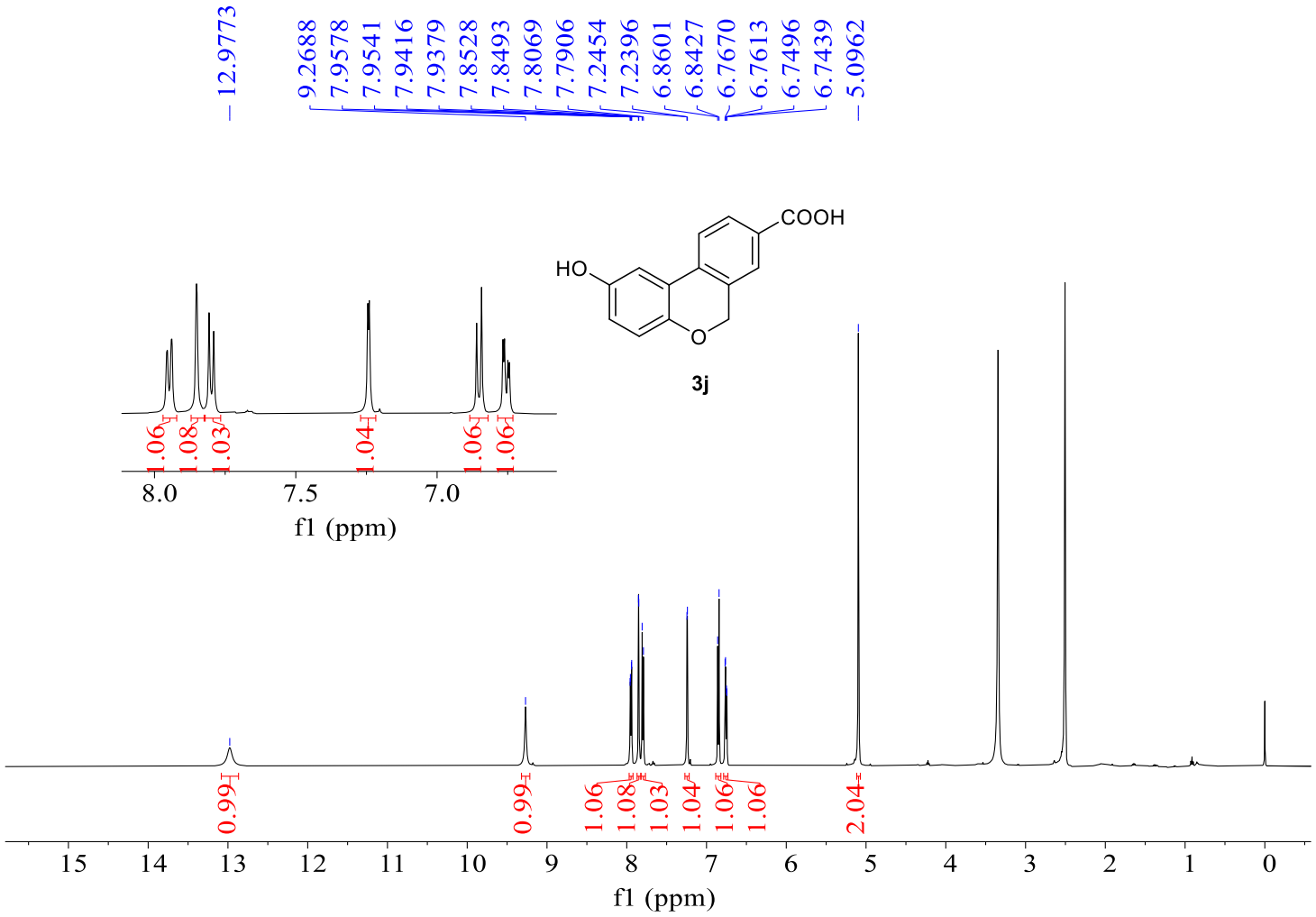


Figure S19 ^{1}H NMR of compound **3j** (500 MHz, DMSO-d_6)

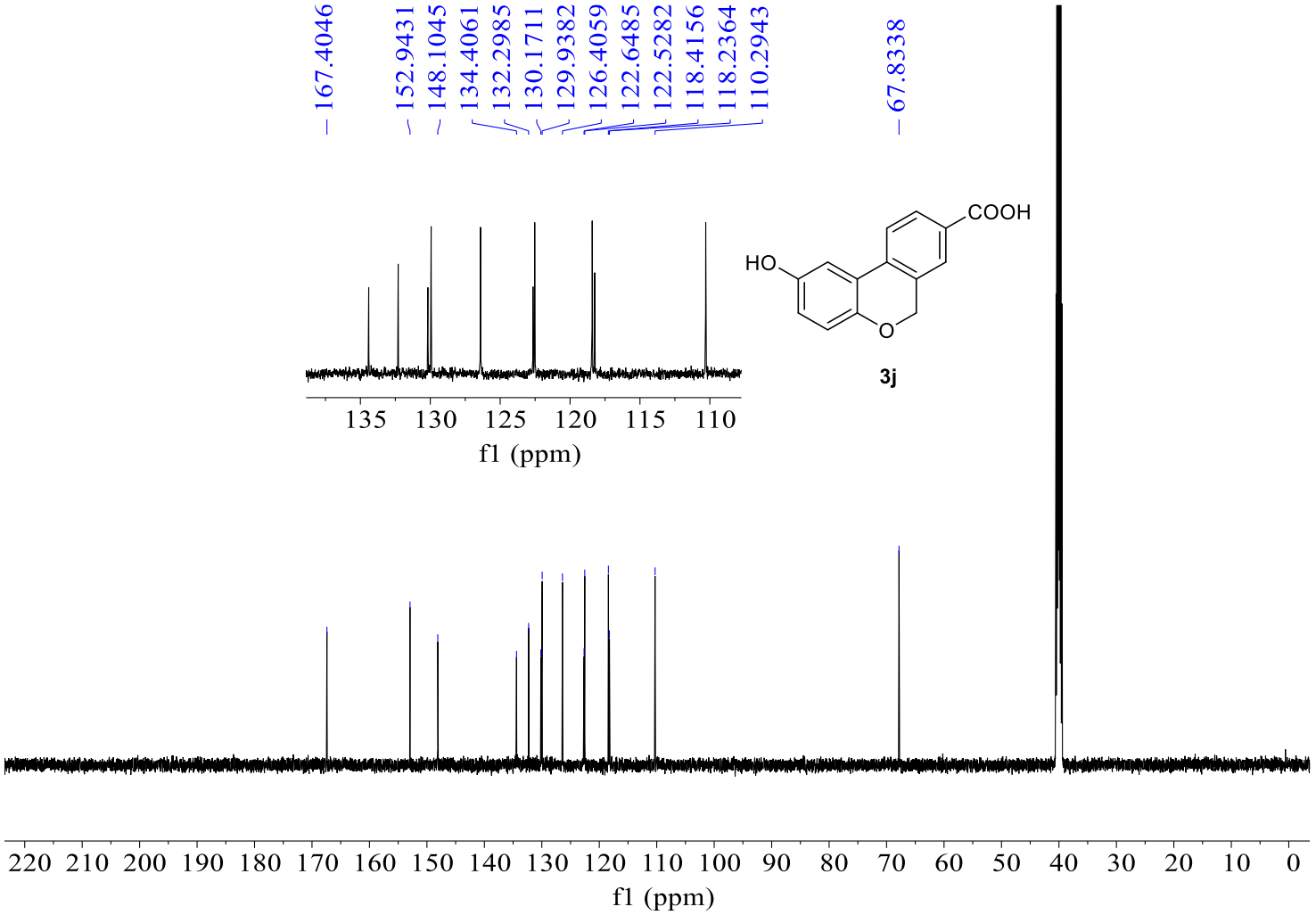


Figure S20 ^{13}C NMR of compound **3i** (126 MHz, DMSO-d_6)

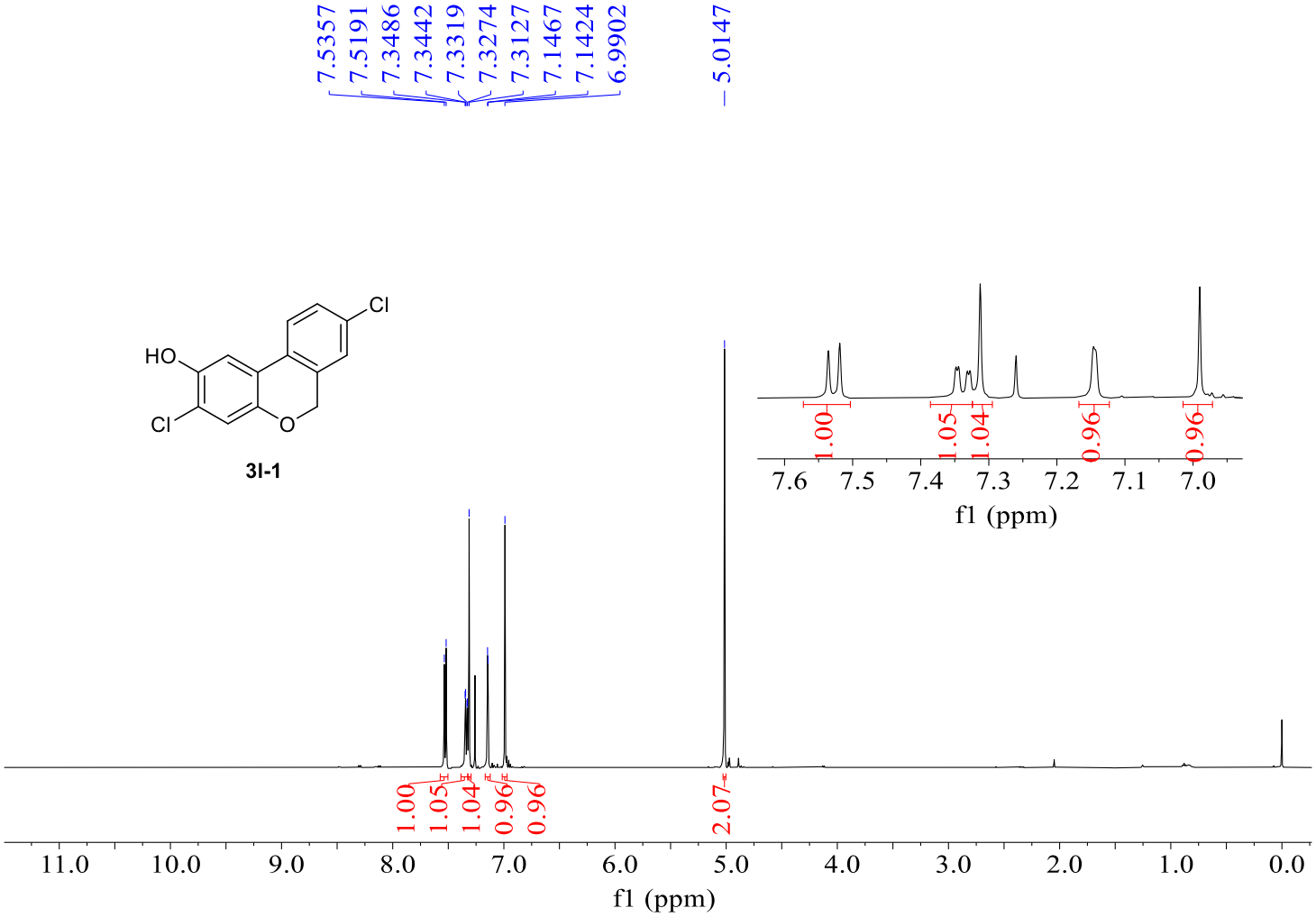


Figure S21 ^{1}H NMR of compound **3l-1** (500 MHz, $CDCl_3$)

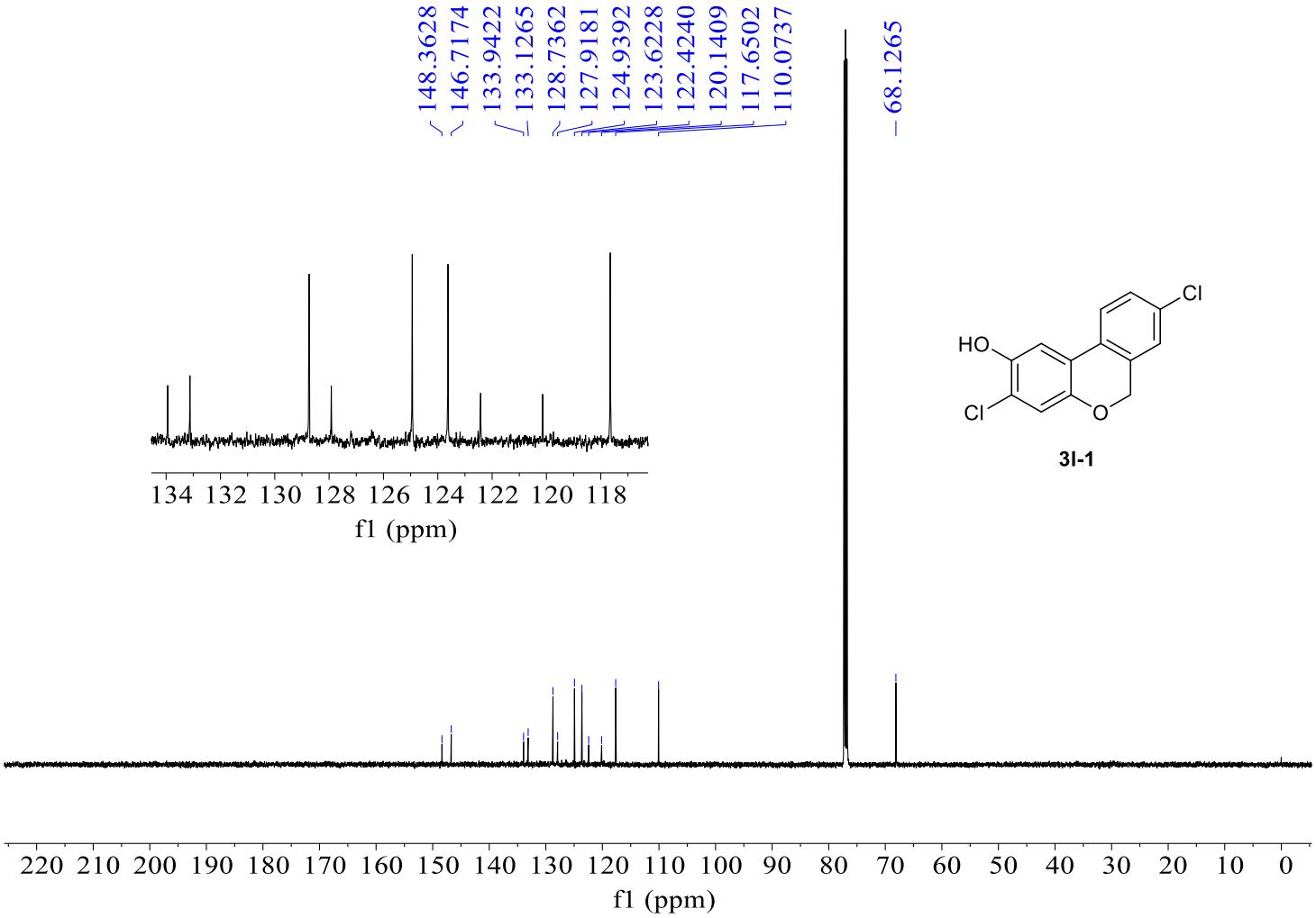


Figure S22 ^{13}C NMR of compound **3l-1** (126 MHz, $CDCl_3$)

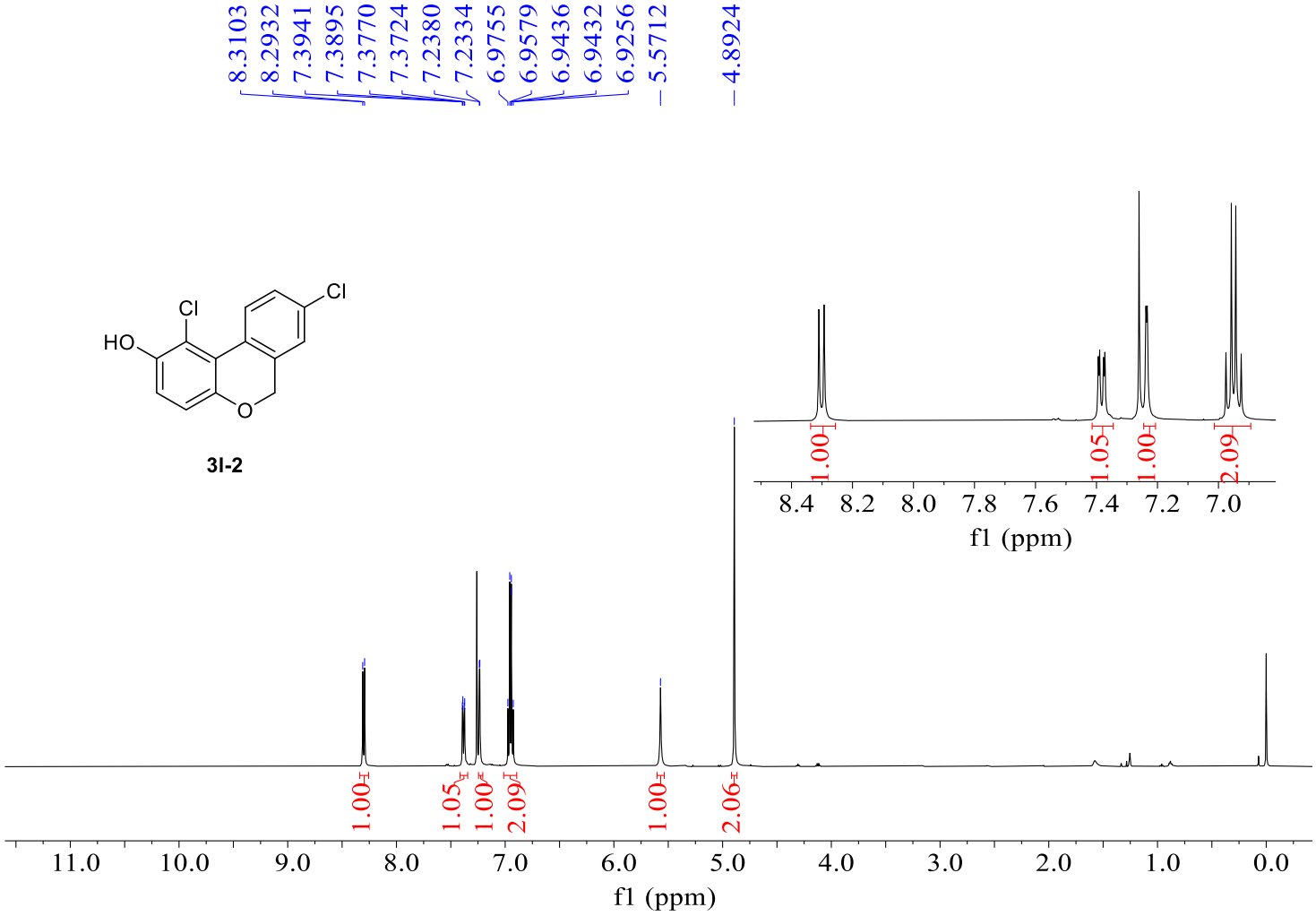


Figure S23 ^{1}H NMR of compound **3l-2** (500 MHz, $CDCl_3$)

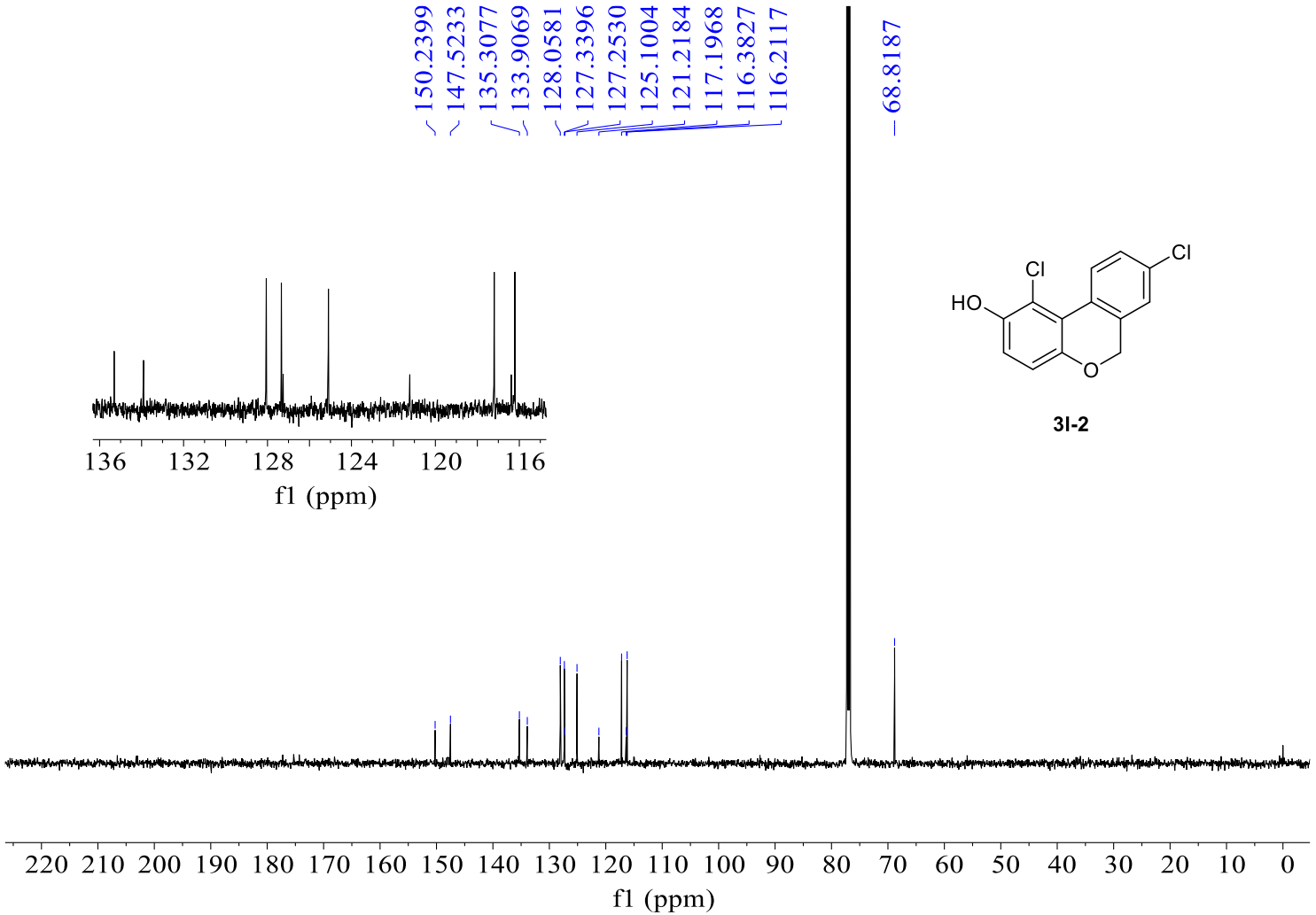


Figure S24 ^{13}C NMR of compound **3l-2** (126 MHz, $CDCl_3$)

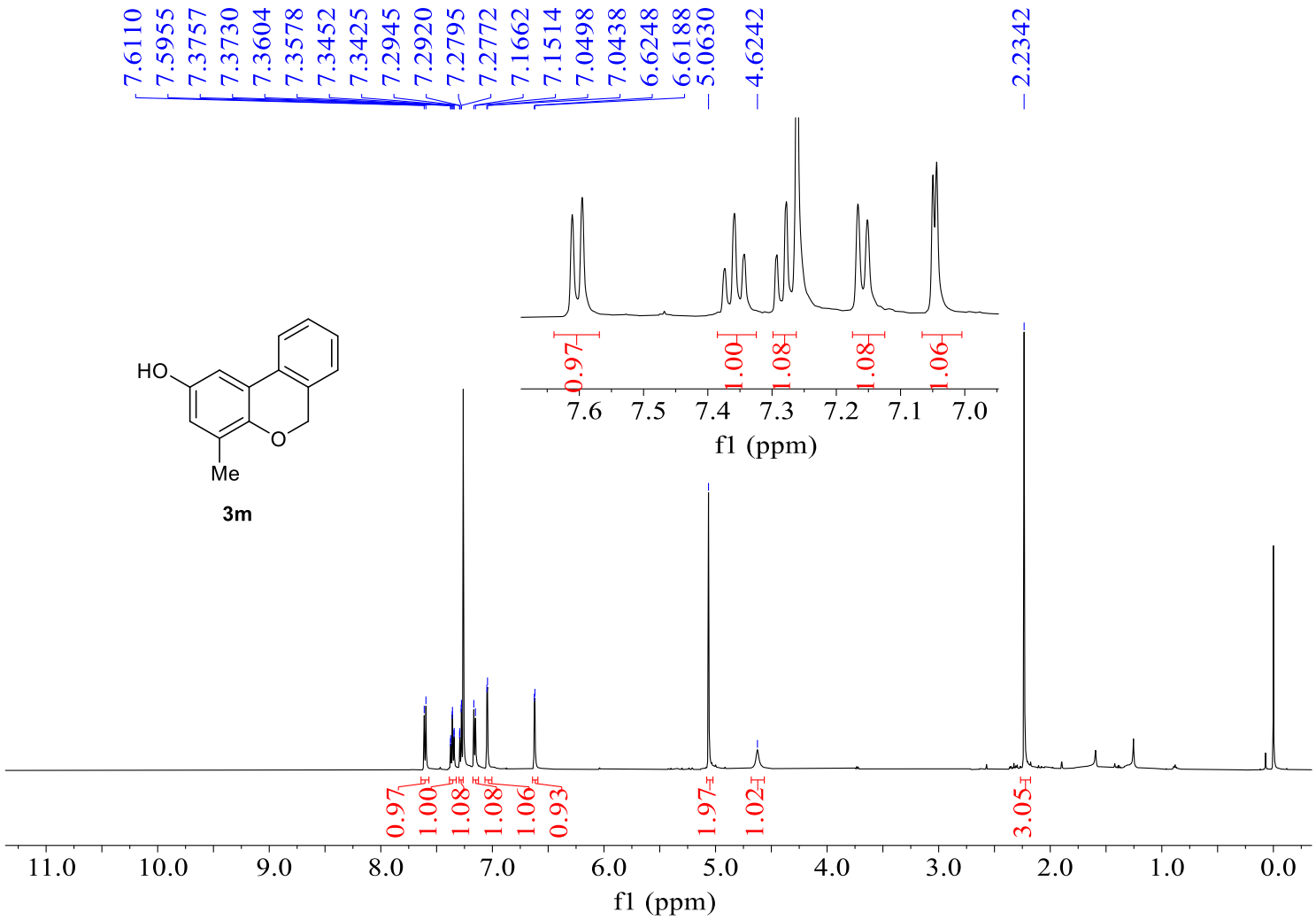


Figure S25 ^{1}H NMR of compound **3m** (500 MHz, $CDCl_3$)

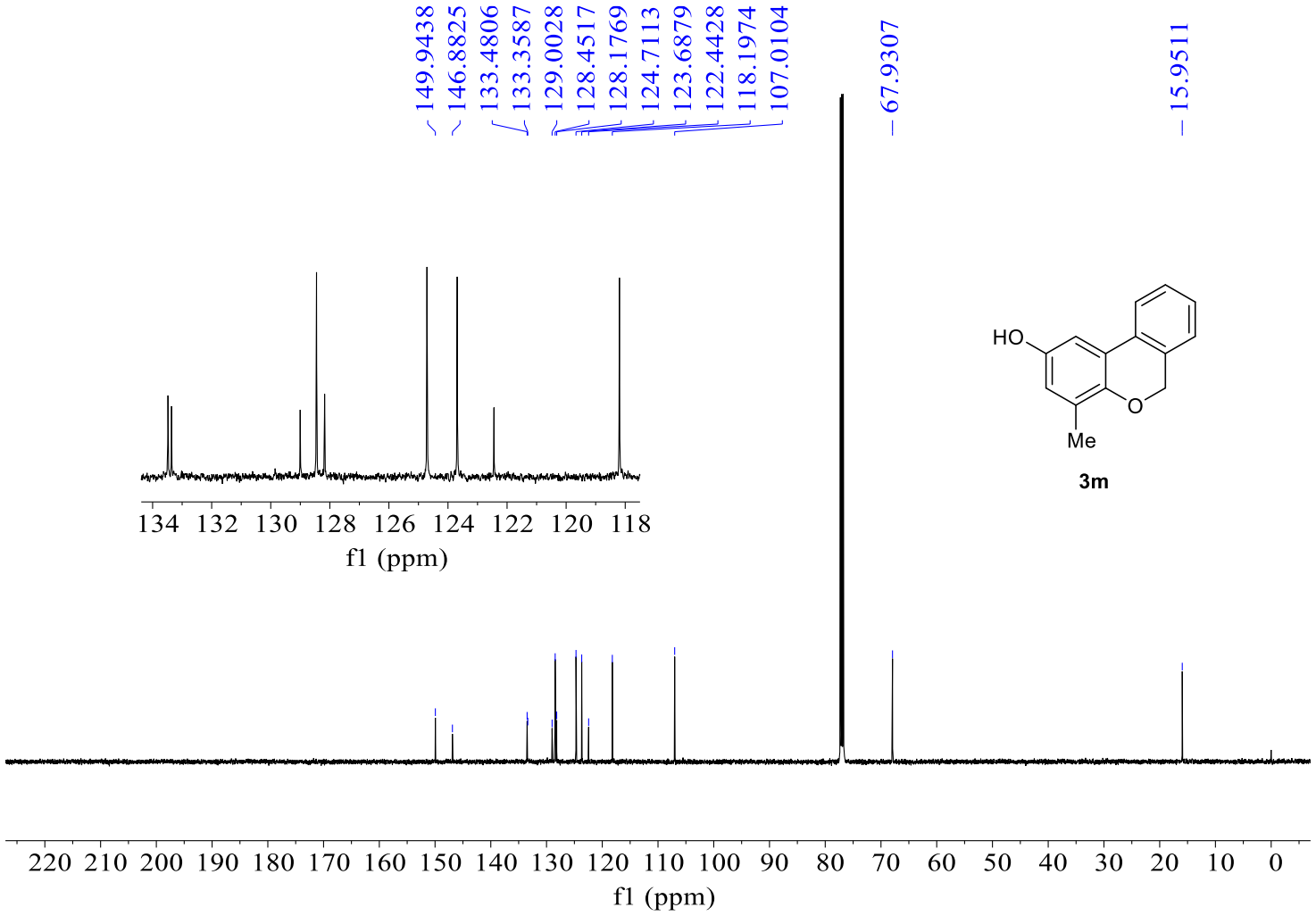


Figure S26 ^{13}C NMR of compound **3m** (126 MHz, $CDCl_3$)

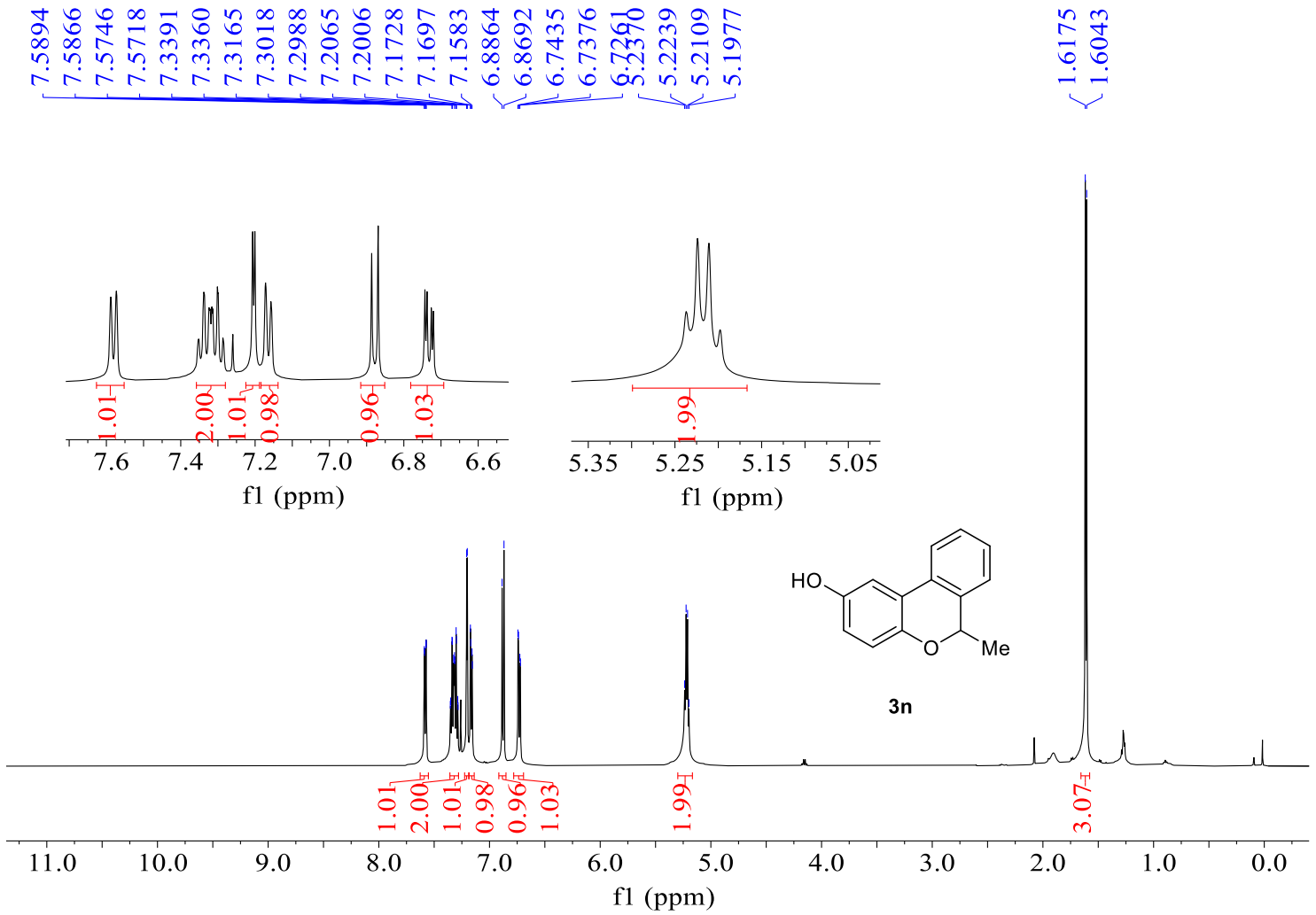


Figure S27 ^{1}H NMR of compound **3n** (500 MHz, $CDCl_3$)

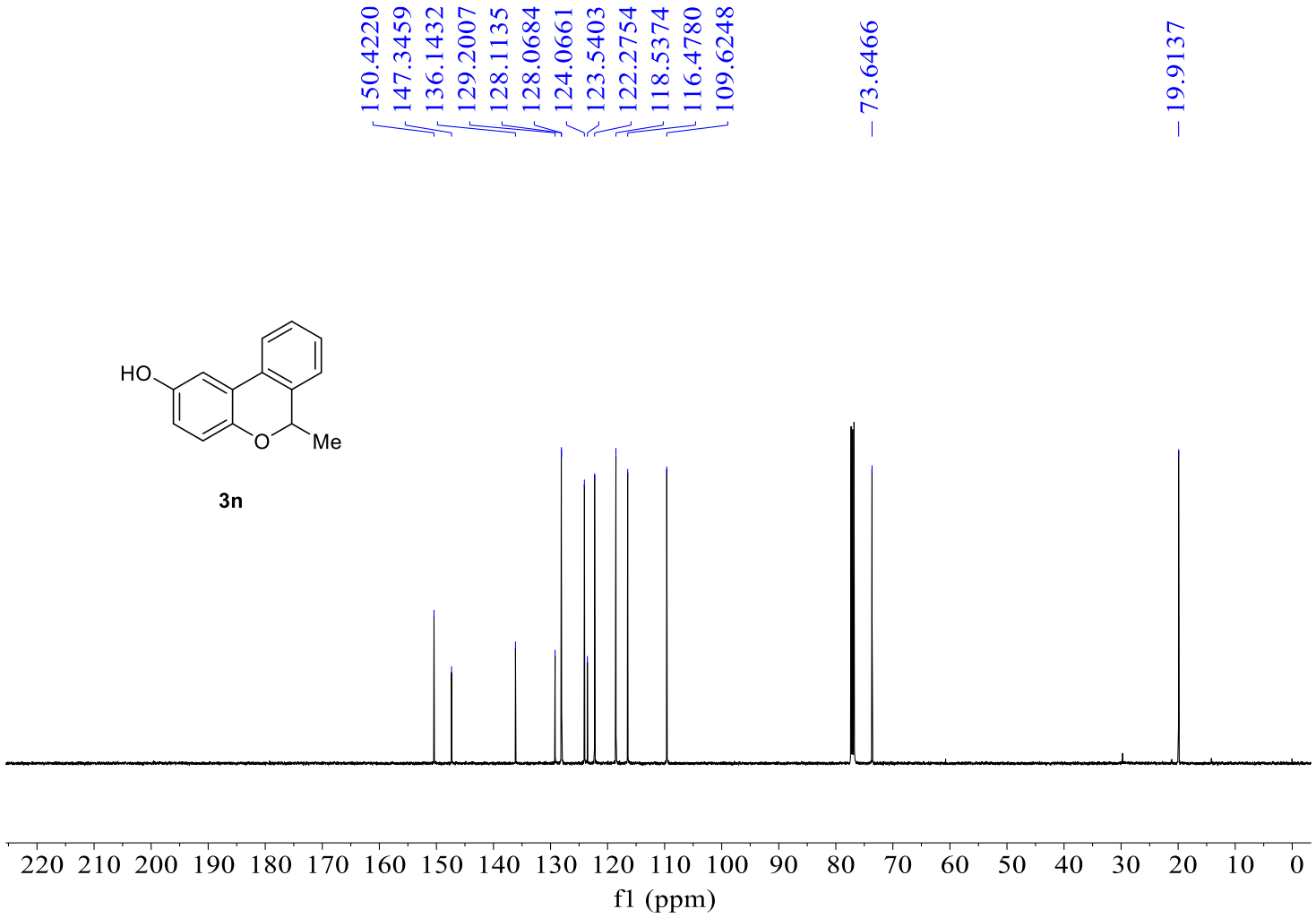


Figure S28 ^{13}C NMR of compound **3n** (126 MHz, $CDCl_3$)

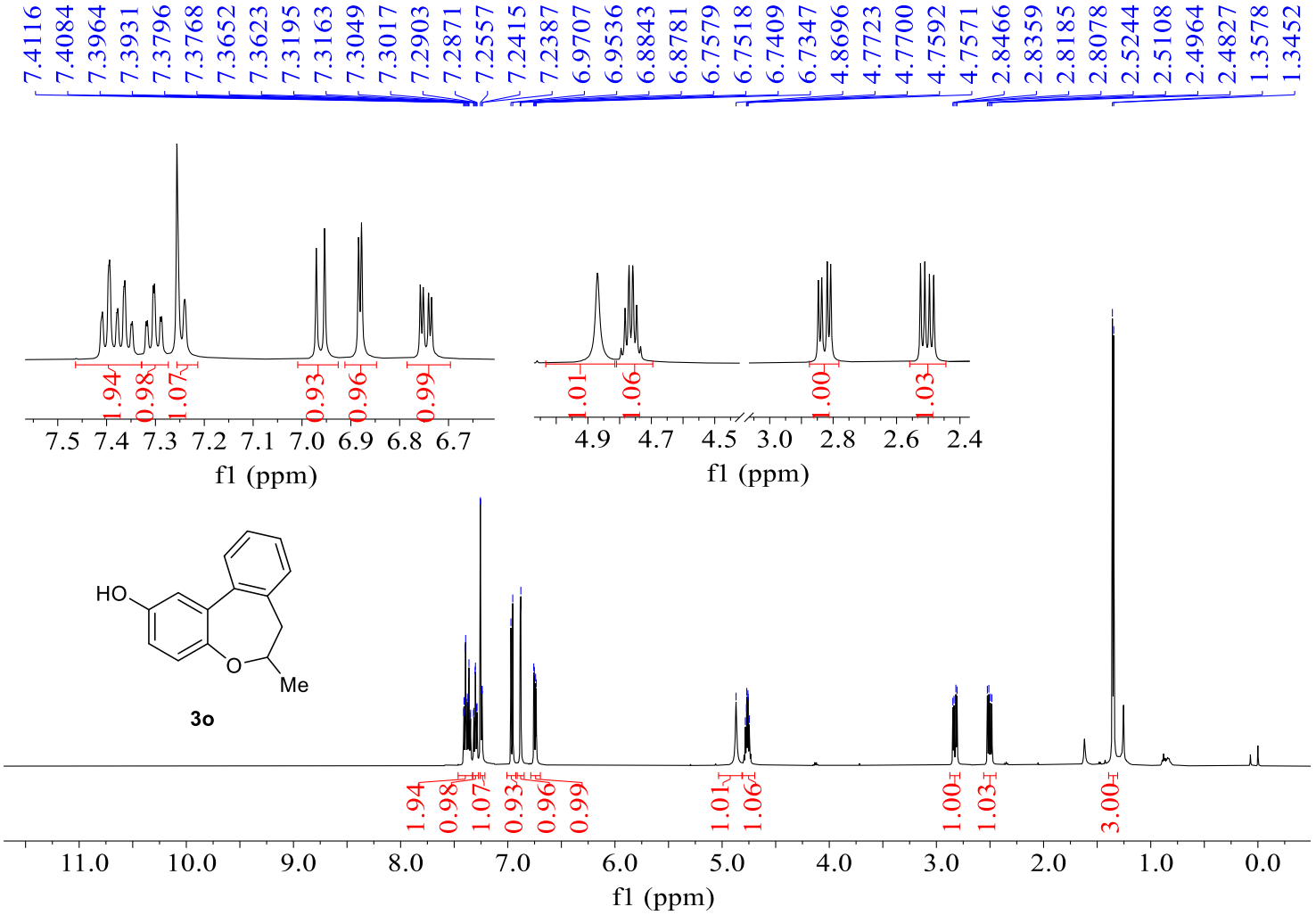


Figure S29 ^{1}H NMR of compound **3o** (500 MHz, $CDCl_3$)

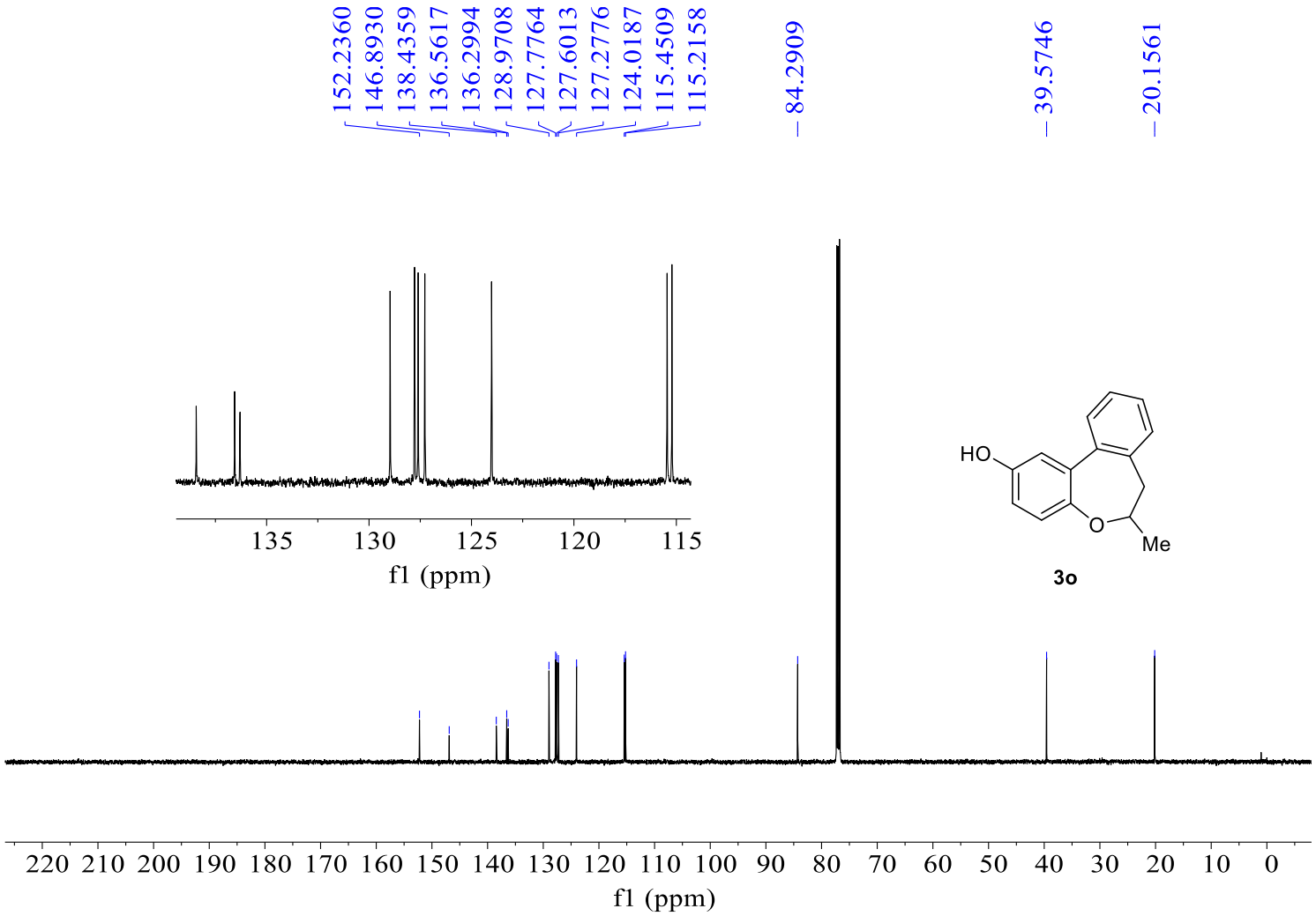


Figure S30 ^{13}C NMR of compound **3o** (126 MHz, $CDCl_3$)

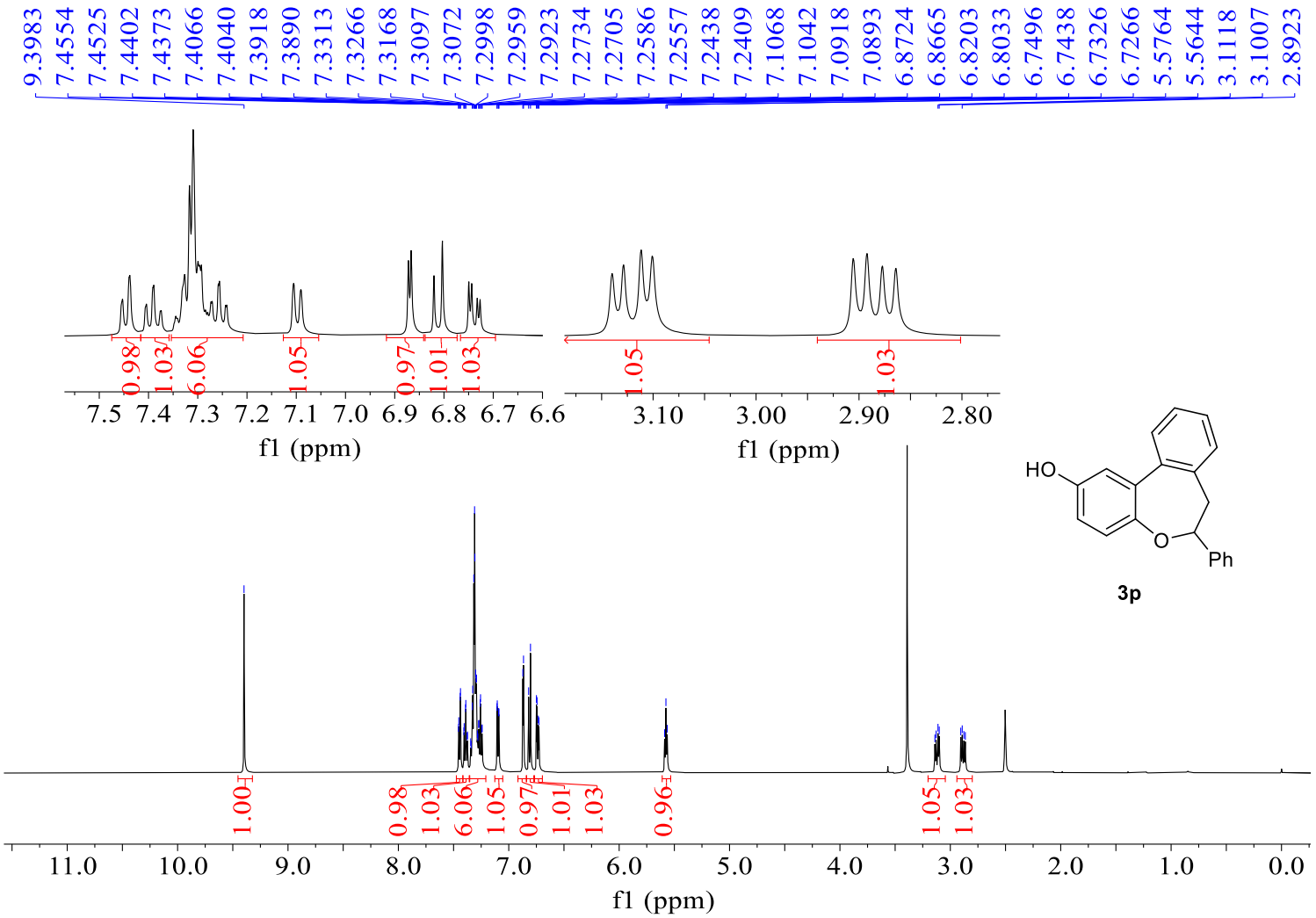


Figure S31 ^{1}H NMR of compound **3p** (500 MHz, DMSO-d_6)

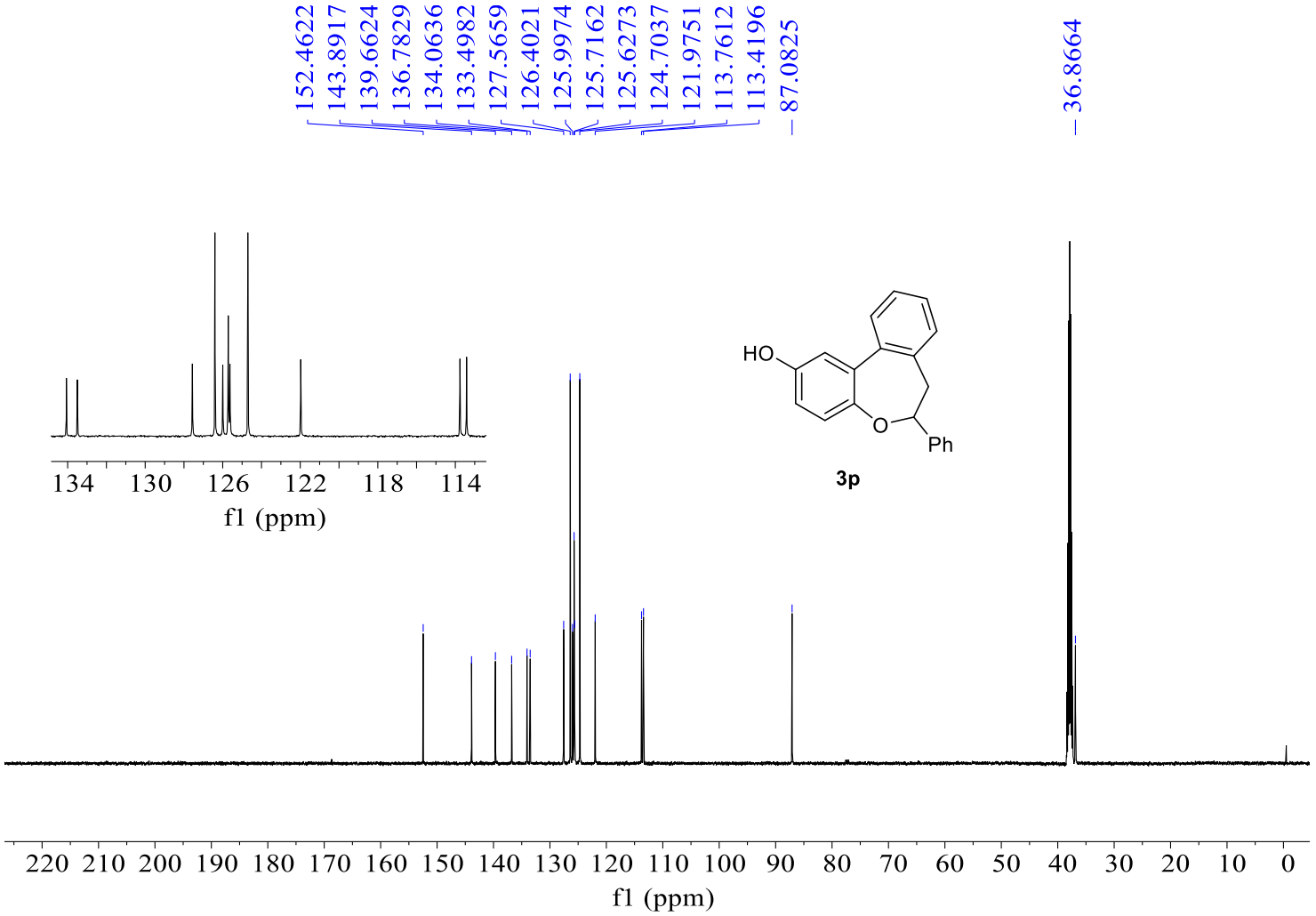


Figure S32 ^{13}C NMR of compound **3p** (126 MHz, DMSO-d_6)

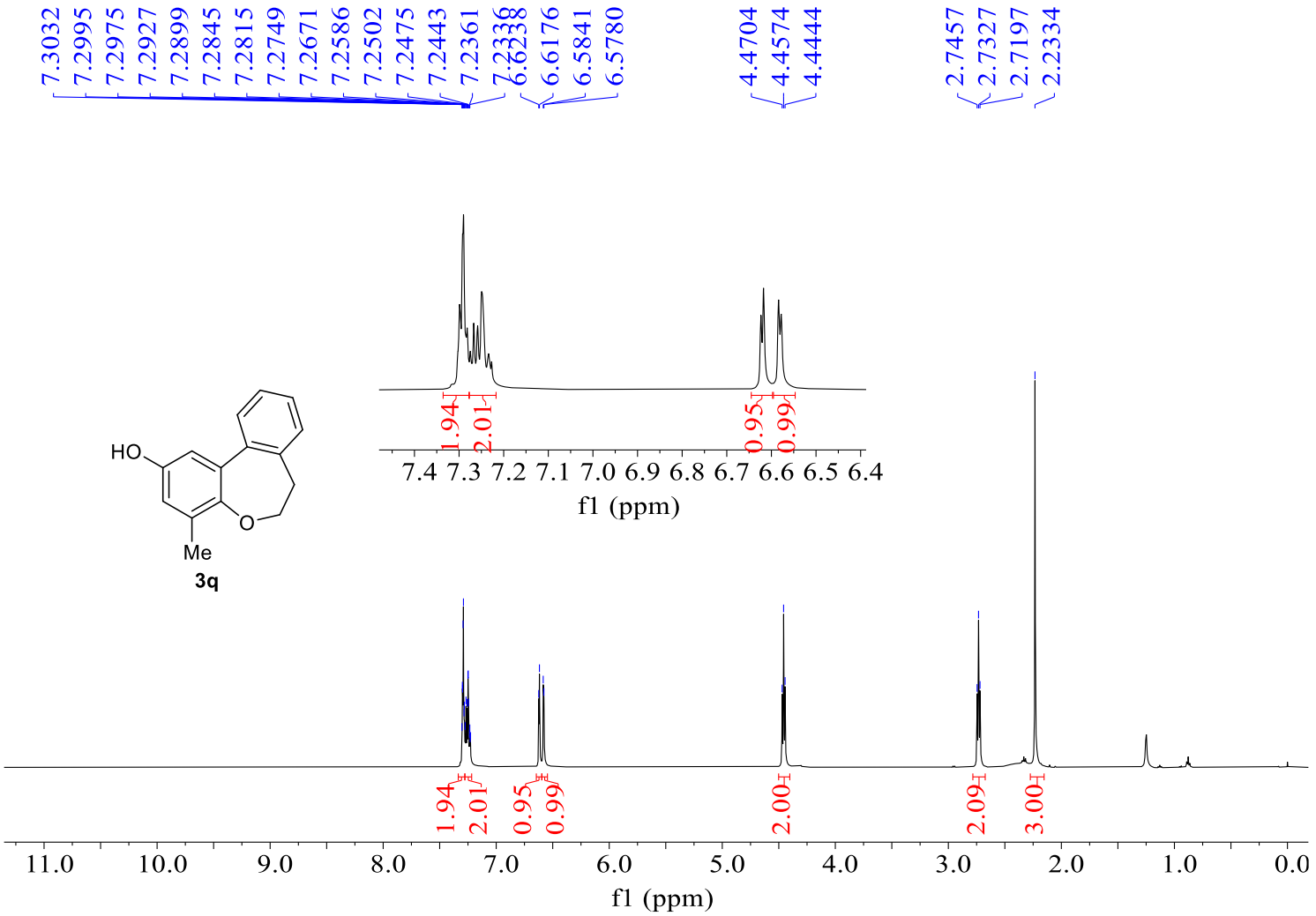


Figure S33 ^{1}H NMR of compound **3q** (500 MHz, $CDCl_3$)

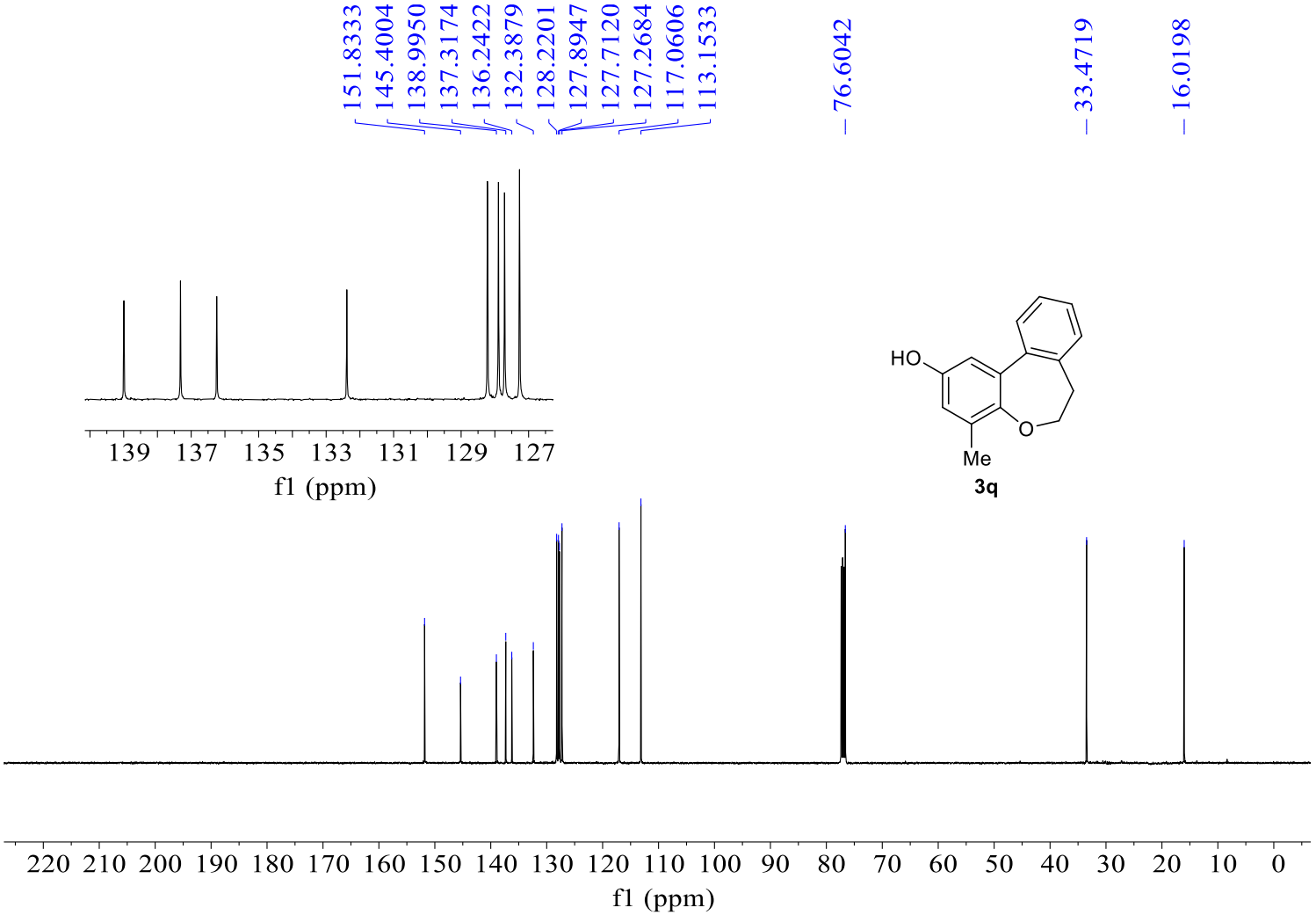


Figure S34 ^{13}C NMR of compound **3q** (126 MHz, $CDCl_3$)

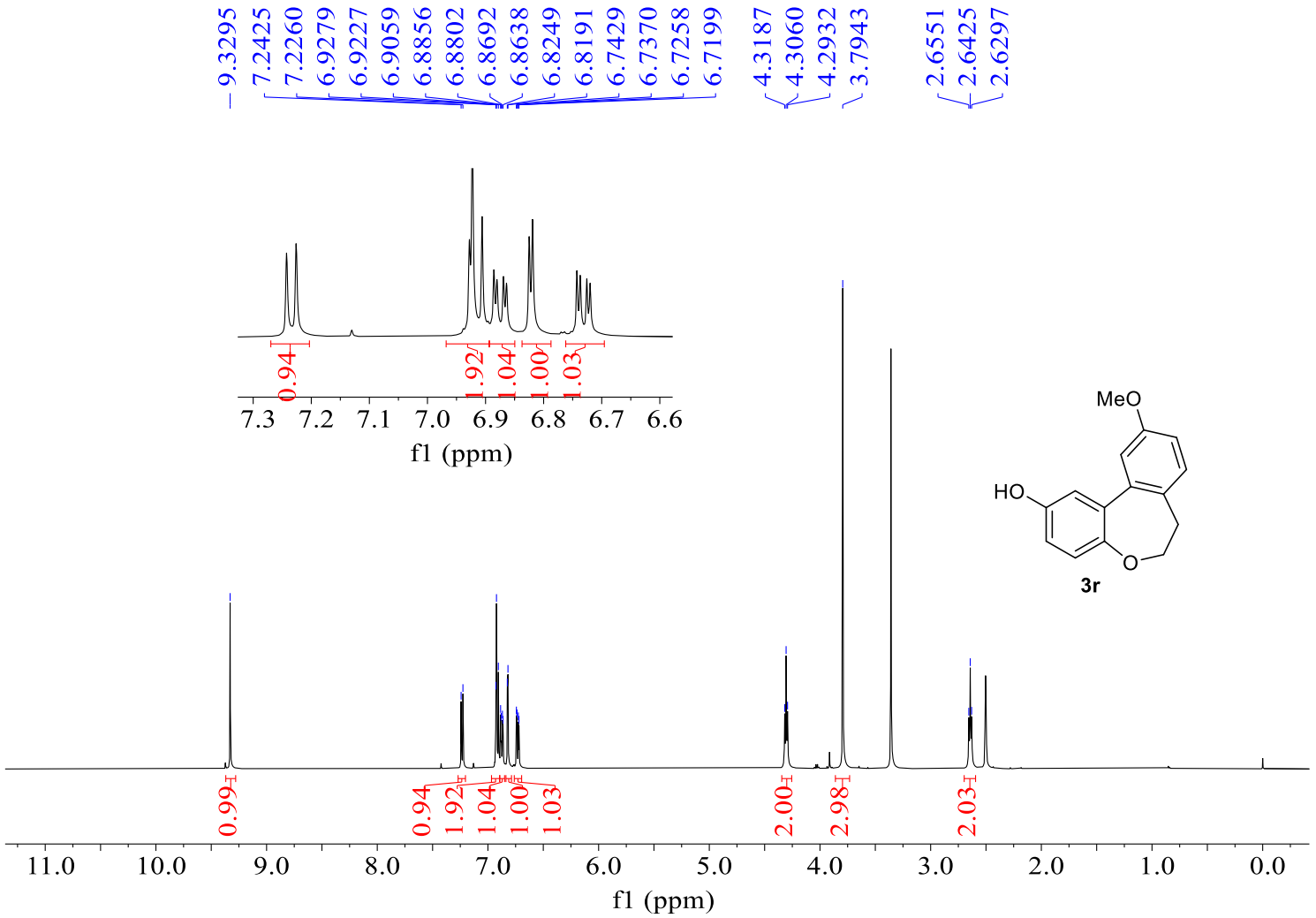


Figure S35 ^{1}H NMR of compound **3r** (500 MHz, DMSO-d_6)

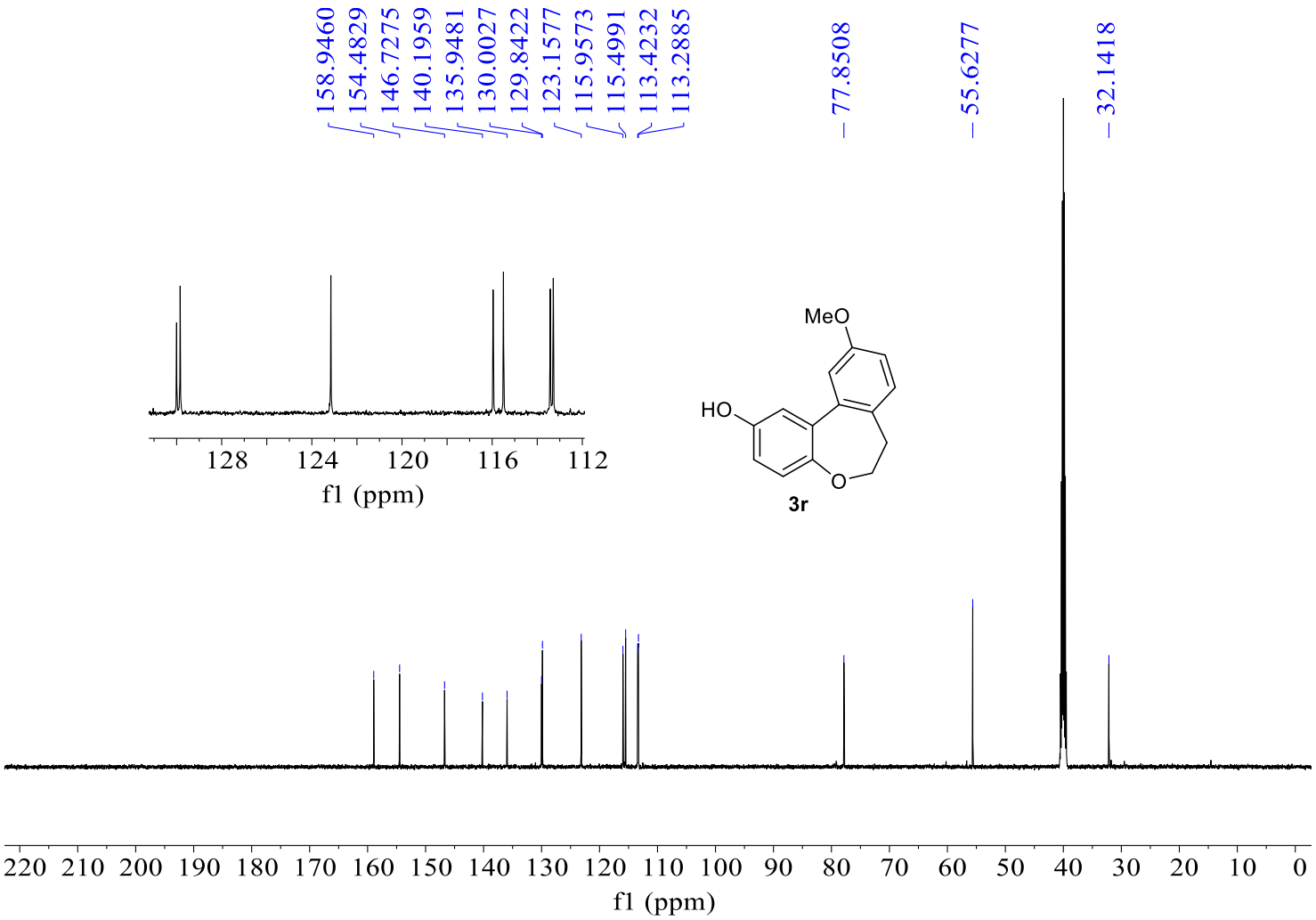


Figure S36 ^{13}C NMR of compound **3r** (126 MHz, DMSO-d_6)

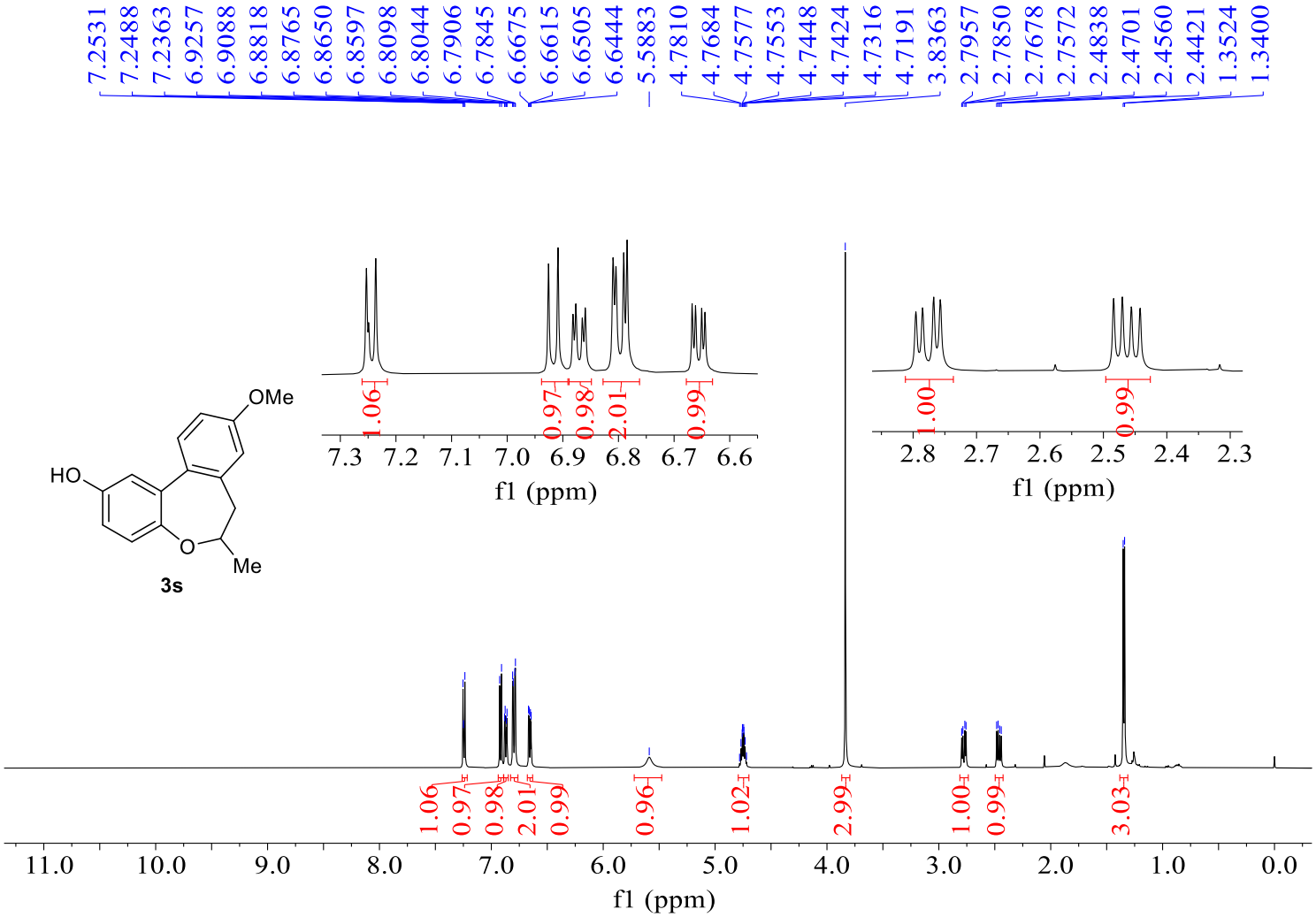


Figure S37 ^{1}H NMR of compound **3s** (500 MHz, $CDCl_3$)

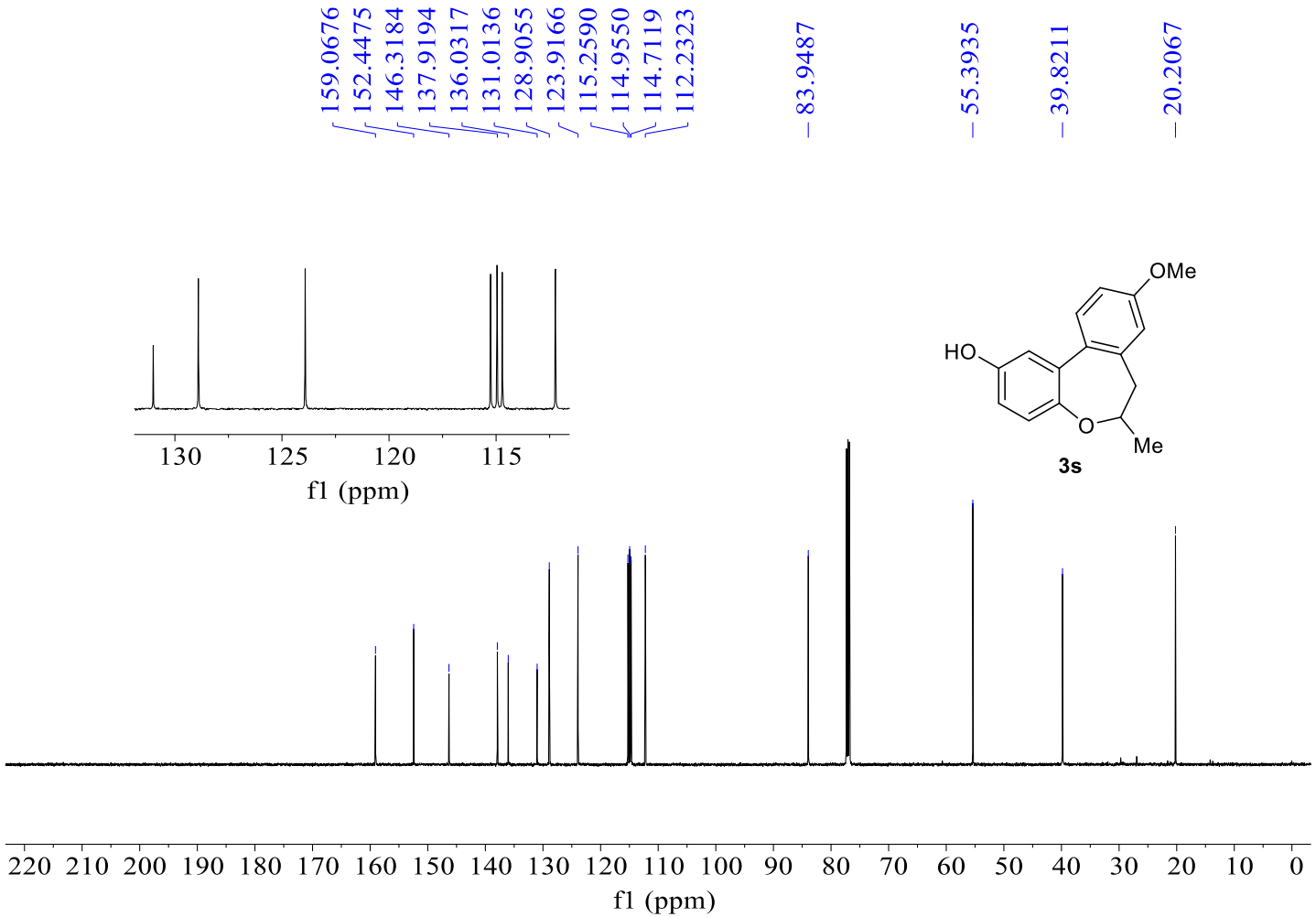


Figure S38 ^{13}C NMR of compound **3s** (126 MHz, $CDCl_3$)

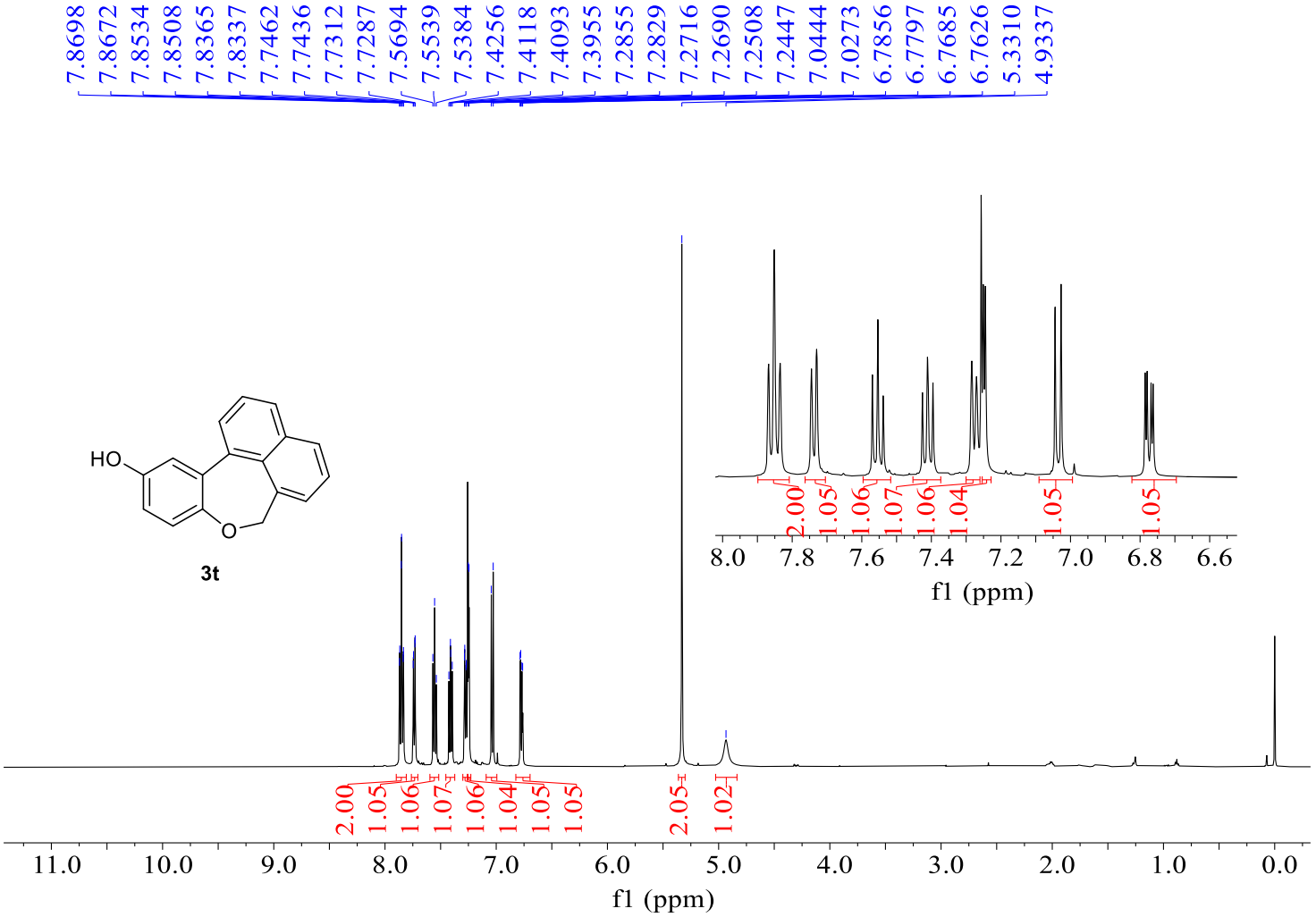


Figure S39 ^{1}H NMR of compound **3t** (500 MHz, $CDCl_3$)

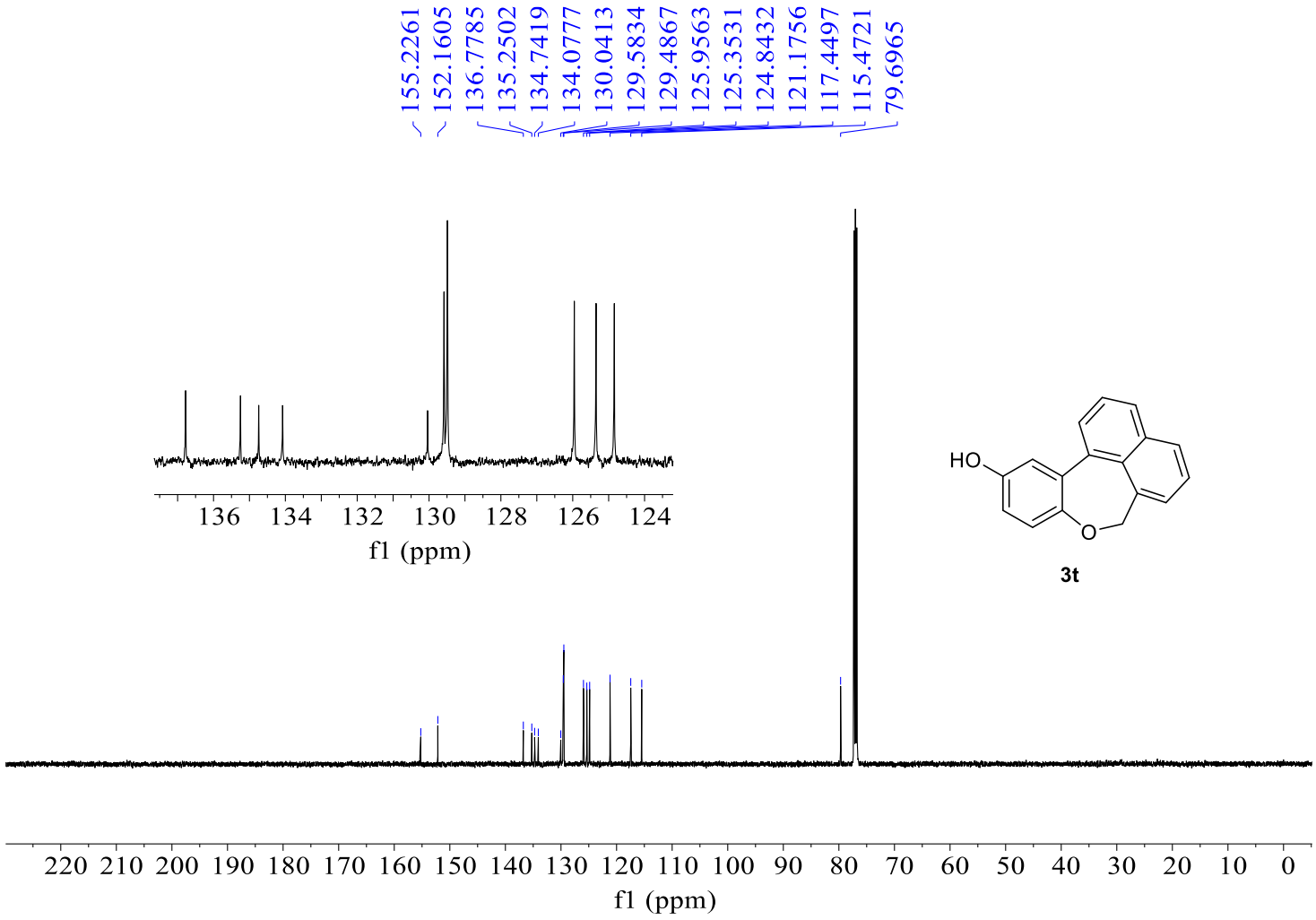


Figure S40 ^{13}C NMR of compound **3t** (126 MHz, $CDCl_3$)

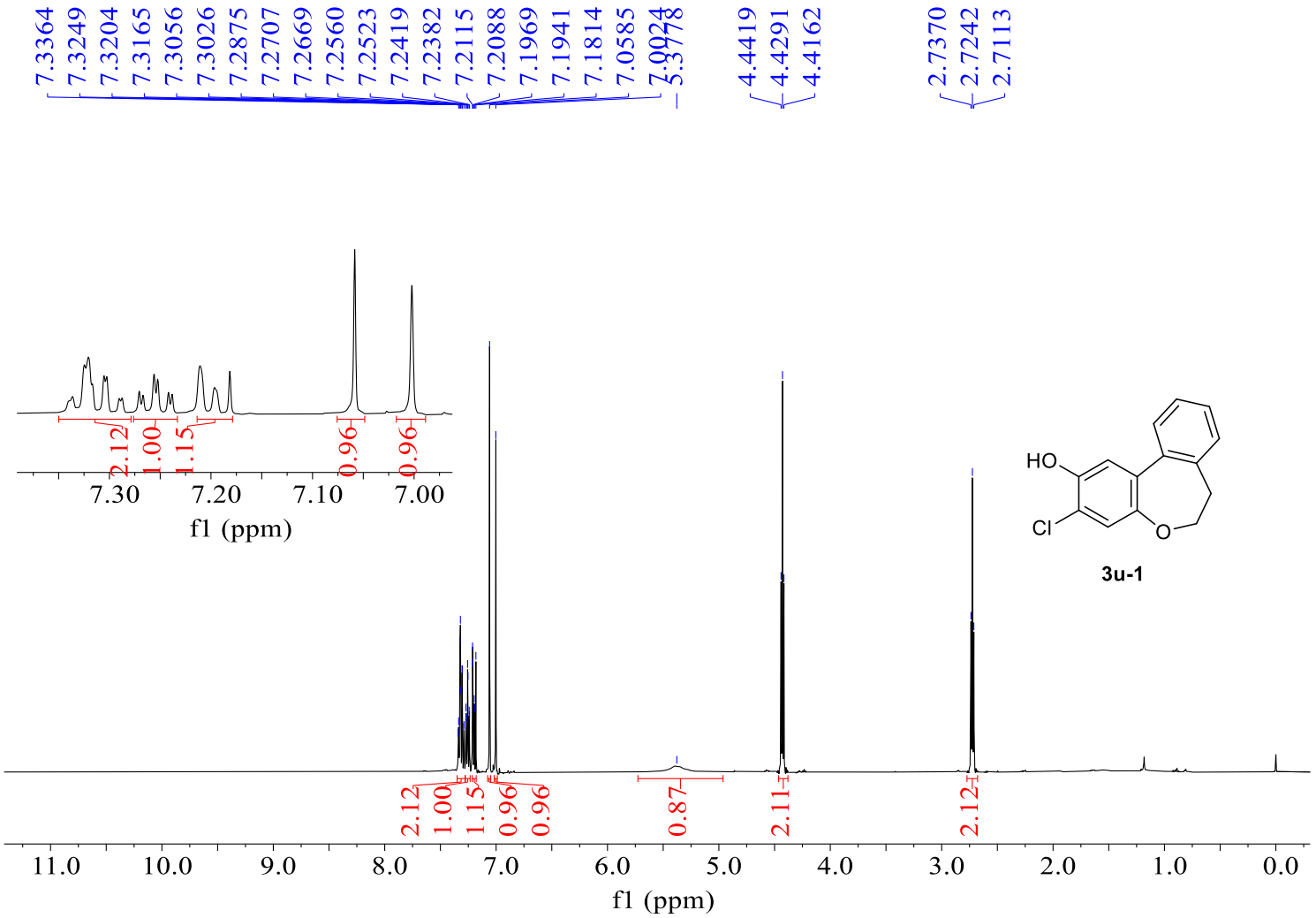


Figure S41 ^{1}H NMR of compound **3u-1** (500 MHz, $CDCl_3$)

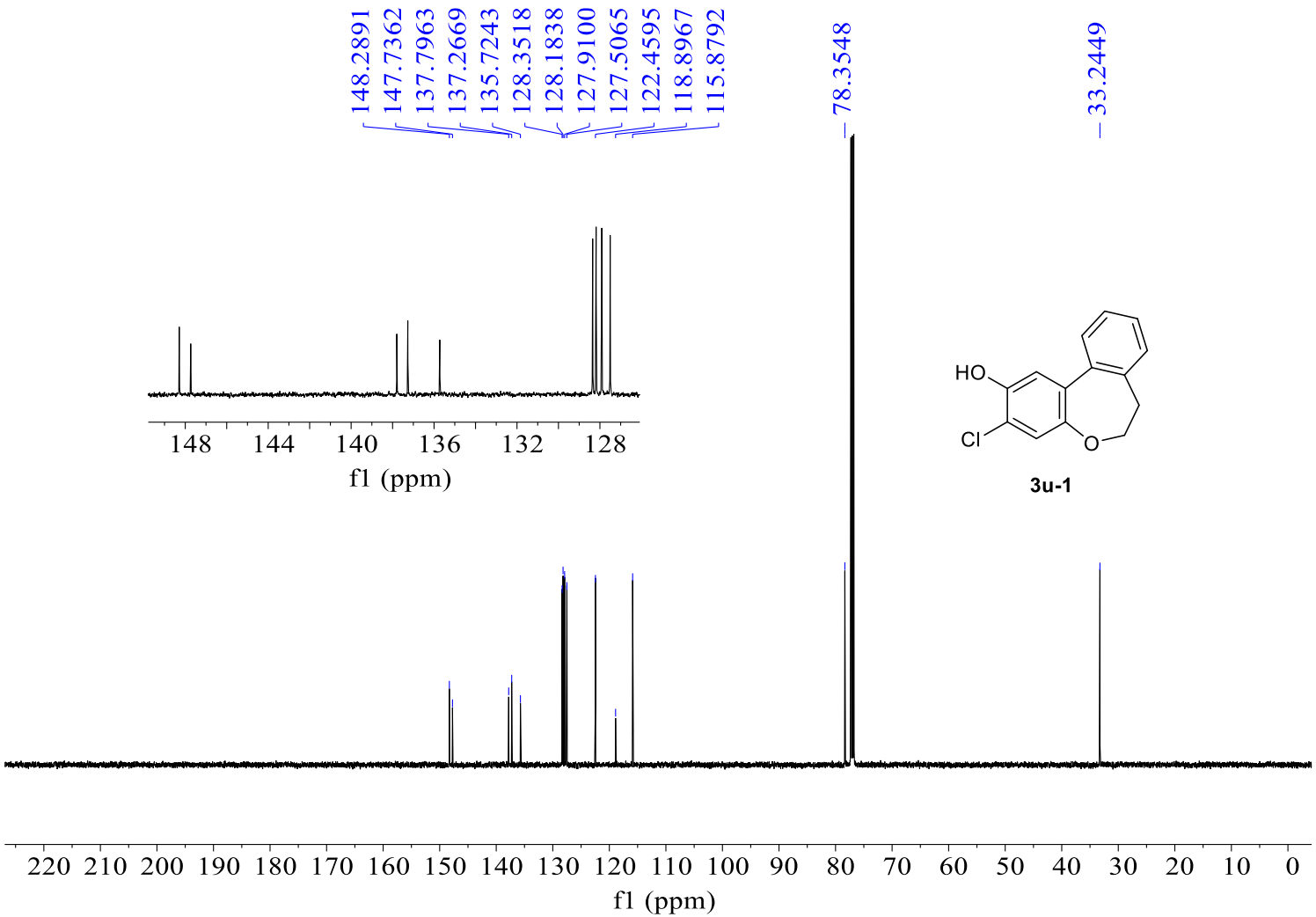


Figure S42 ^{13}C NMR of compound **3u-1** (126 MHz, $CDCl_3$)

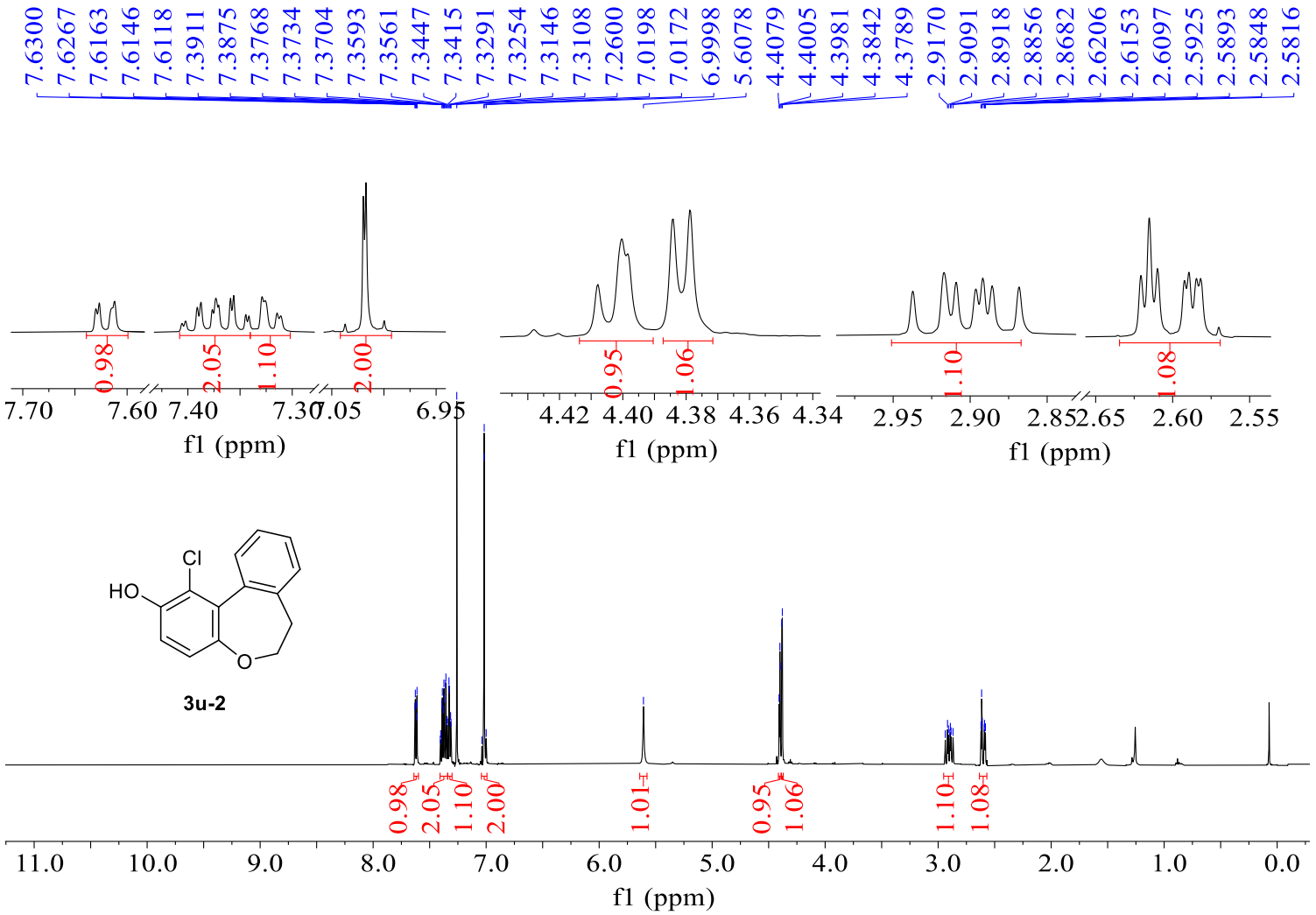


Figure S43 ^{1}H NMR of compound **3u-2** (500 MHz, $CDCl_3$)

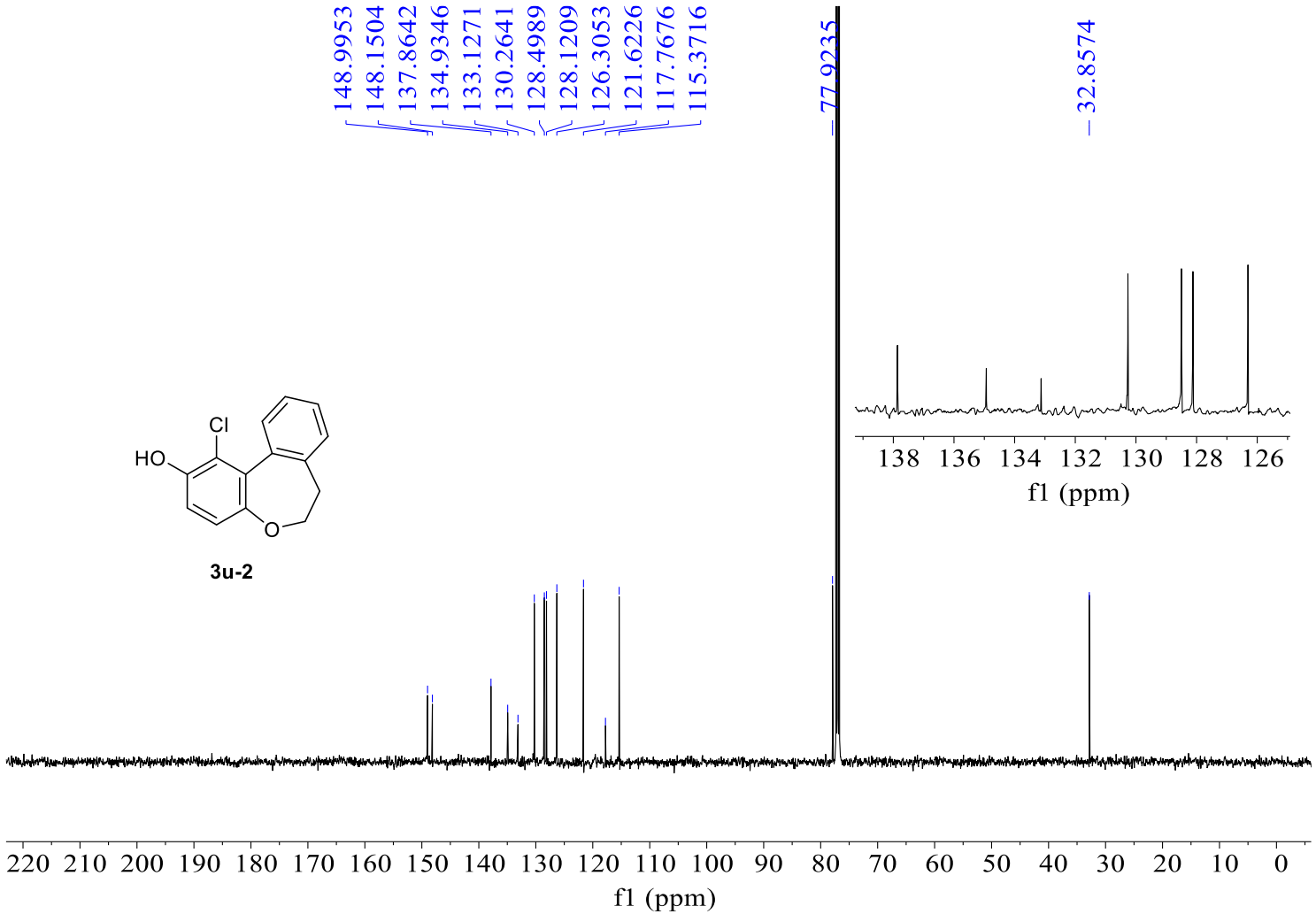


Figure S44 ^{13}C NMR of compound **3u-2** (126 MHz, $CDCl_3$)

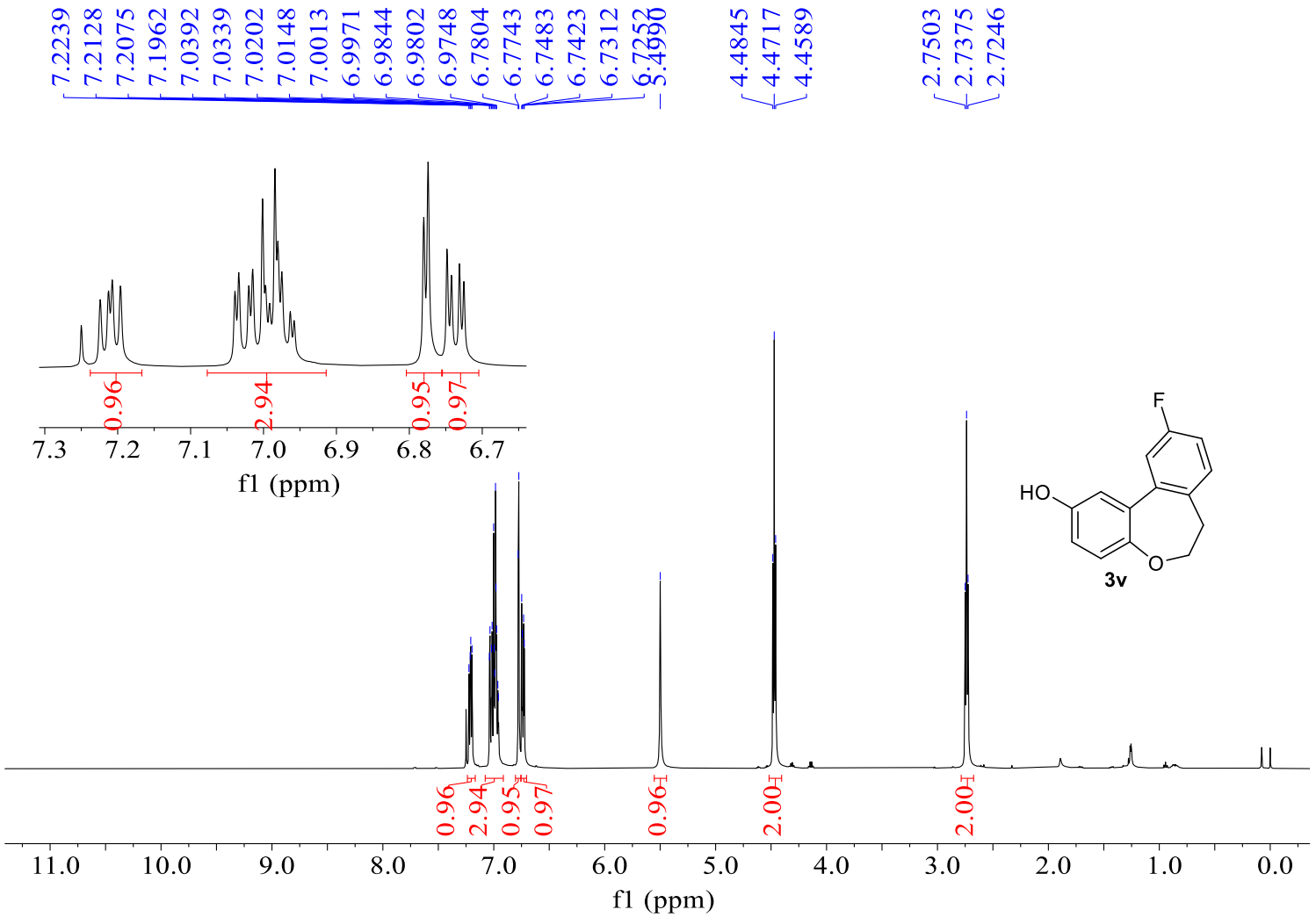


Figure S45 ^{1}H NMR of compound **3v** (500 MHz, $CDCl_3$)

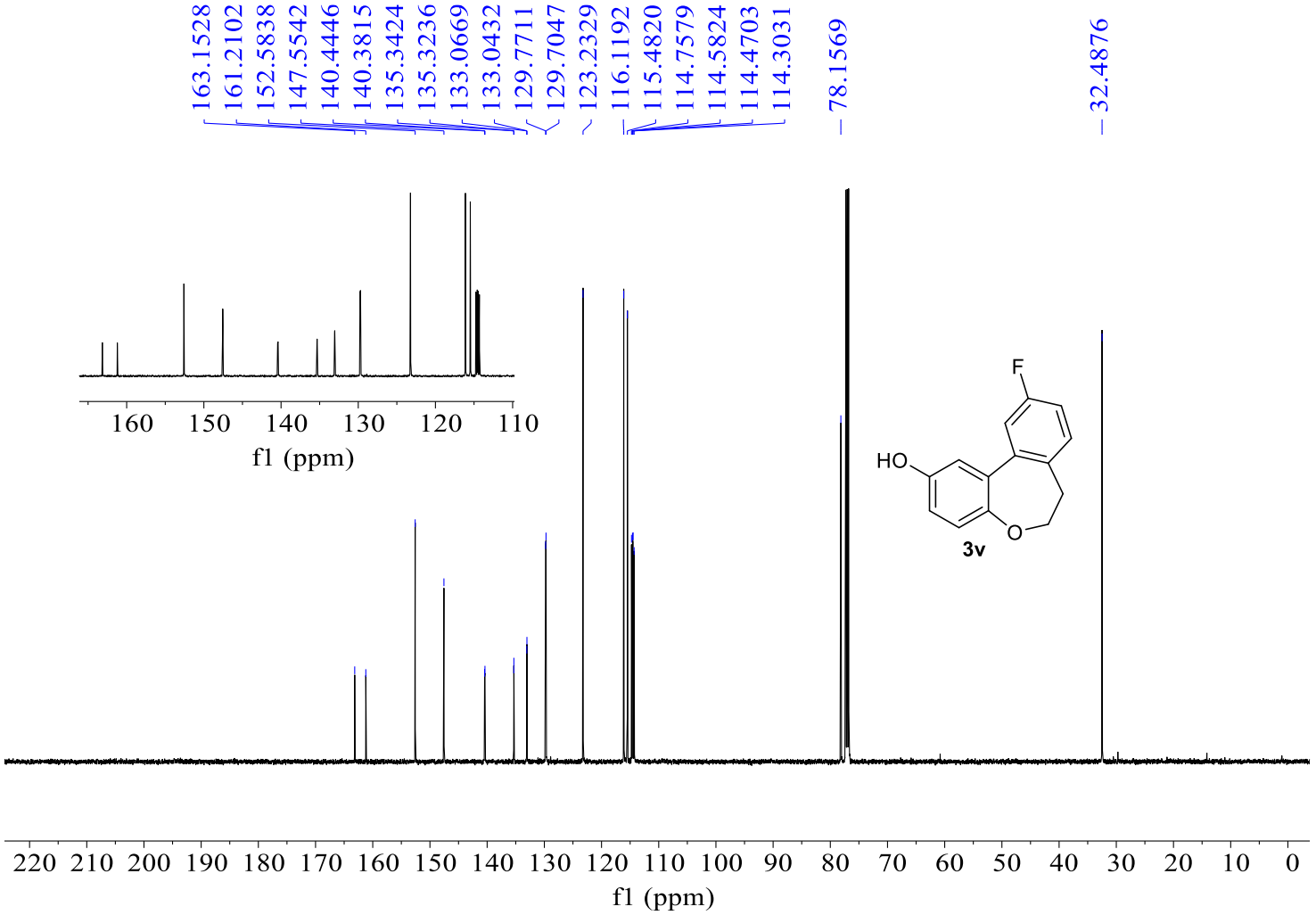


Figure S46 ^{13}C NMR of compound **3v** (126 MHz, $CDCl_3$)

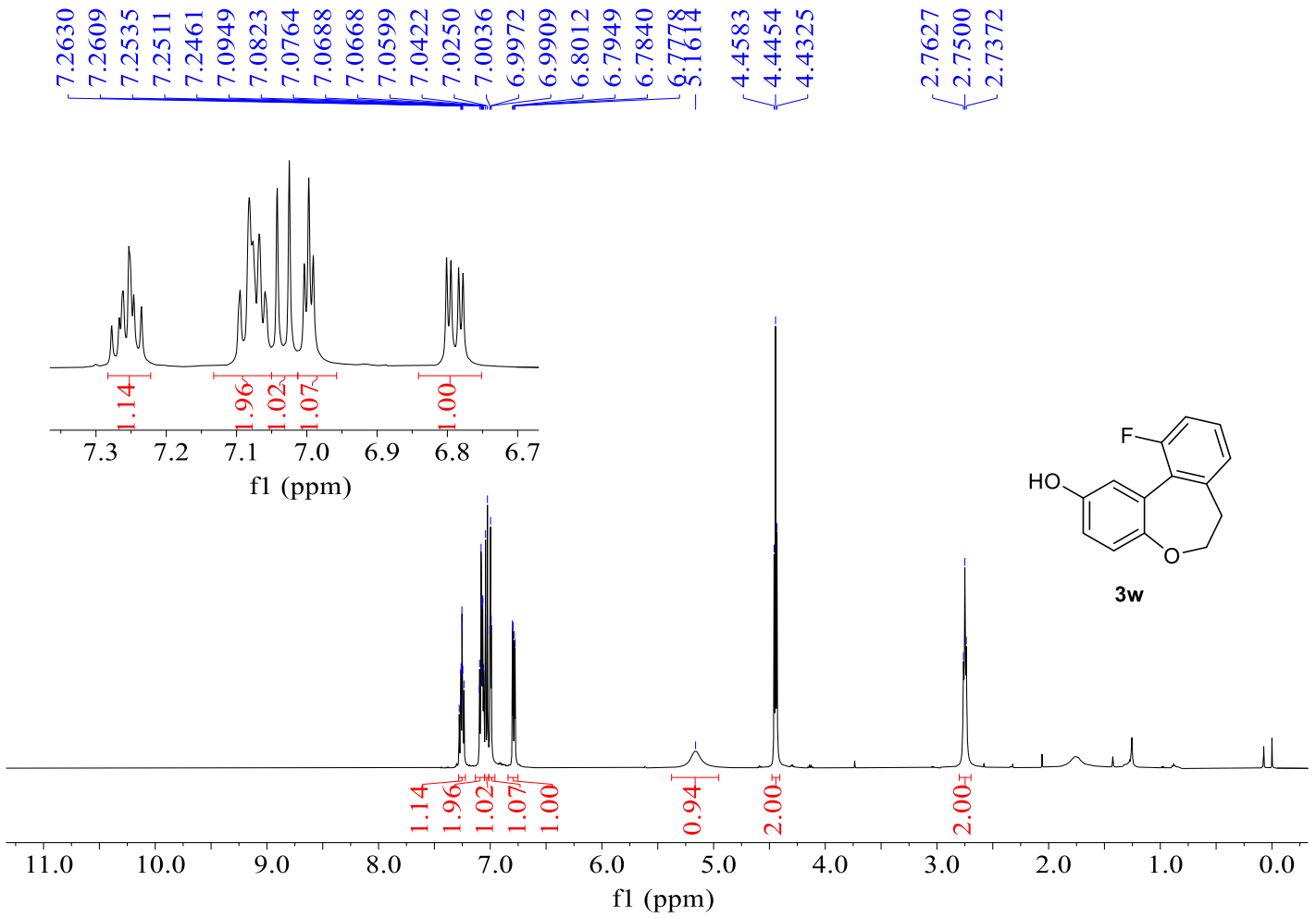


Figure S47 ^{1}H NMR of compound **3w** (500 MHz, $CDCl_3$)

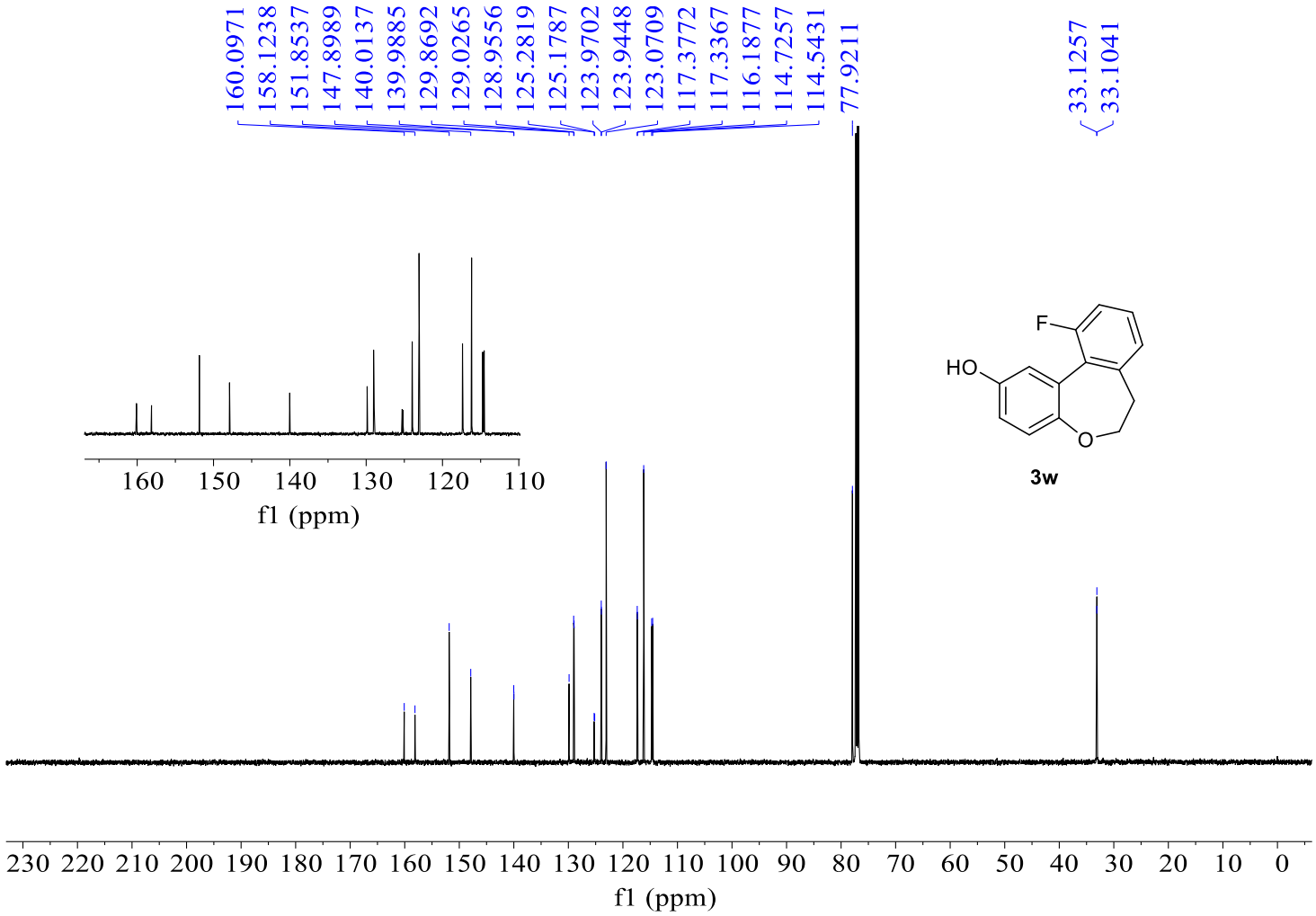


Figure S48 ^{13}C NMR of compound **3w** (126 MHz, $CDCl_3$)

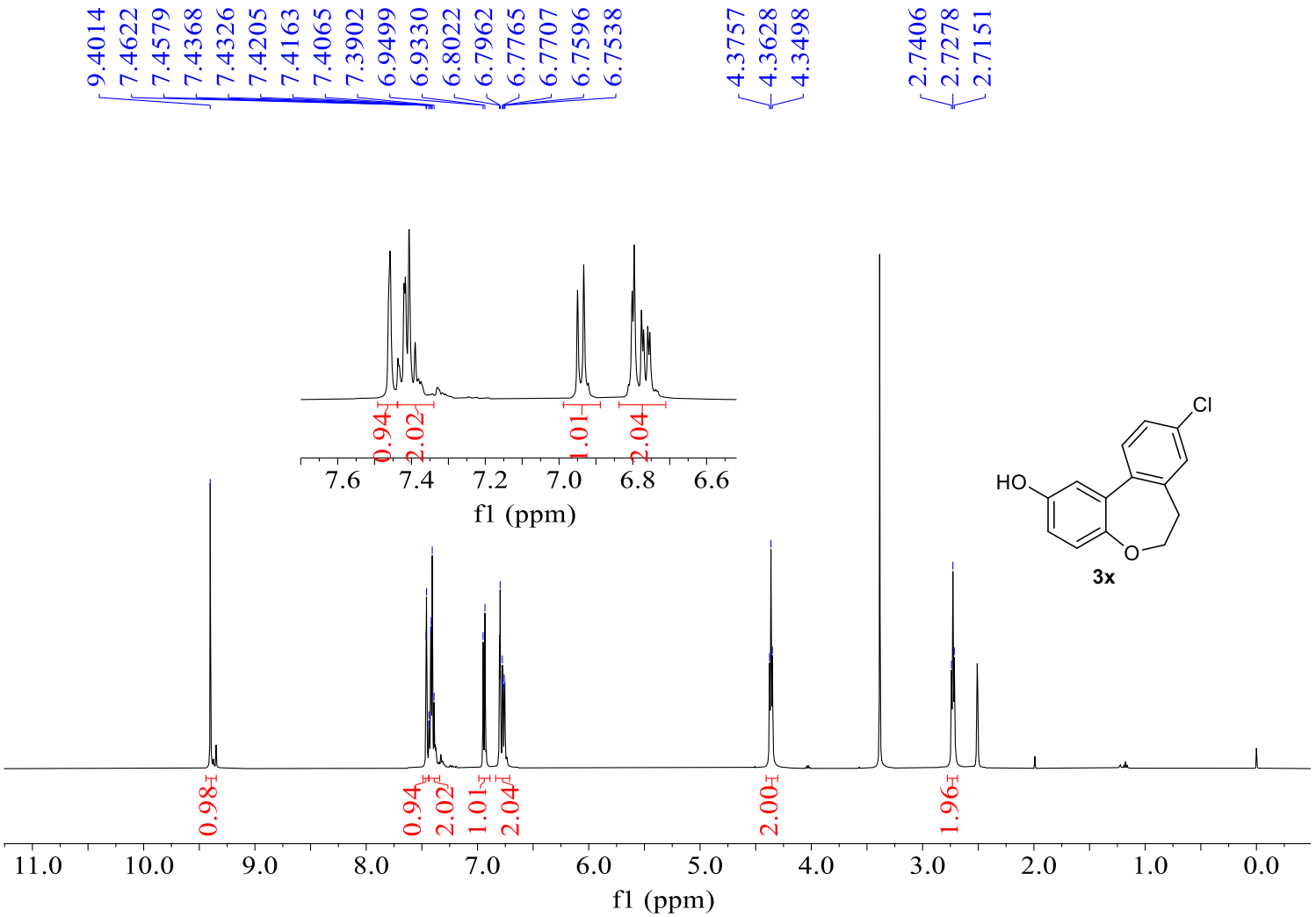


Figure S49 ^{1}H NMR of compound **3x** (500 MHz, DMSO-d_6)

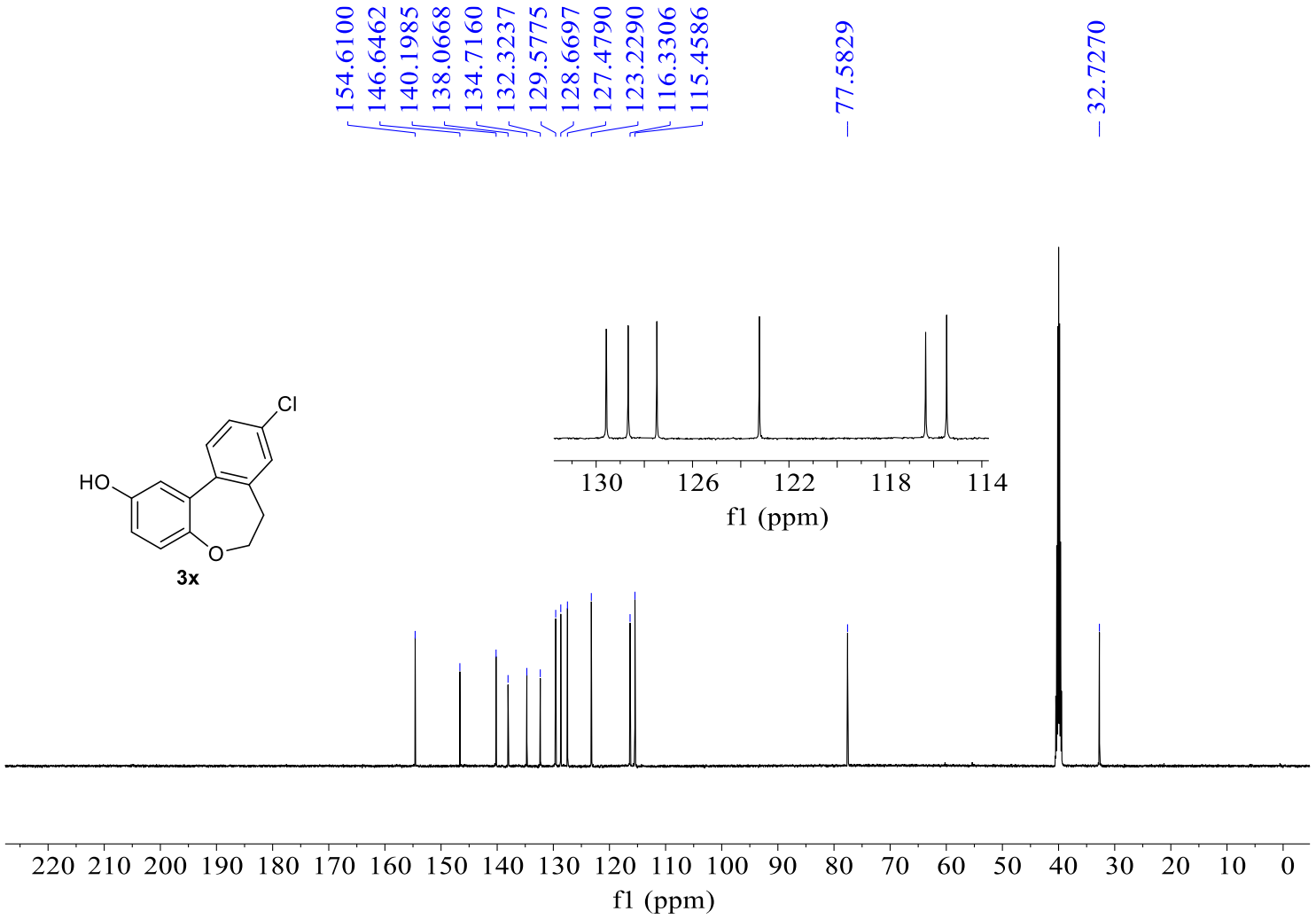


Figure S50 ^{13}C NMR of compound **3x** (126 MHz, DMSO-d_6)

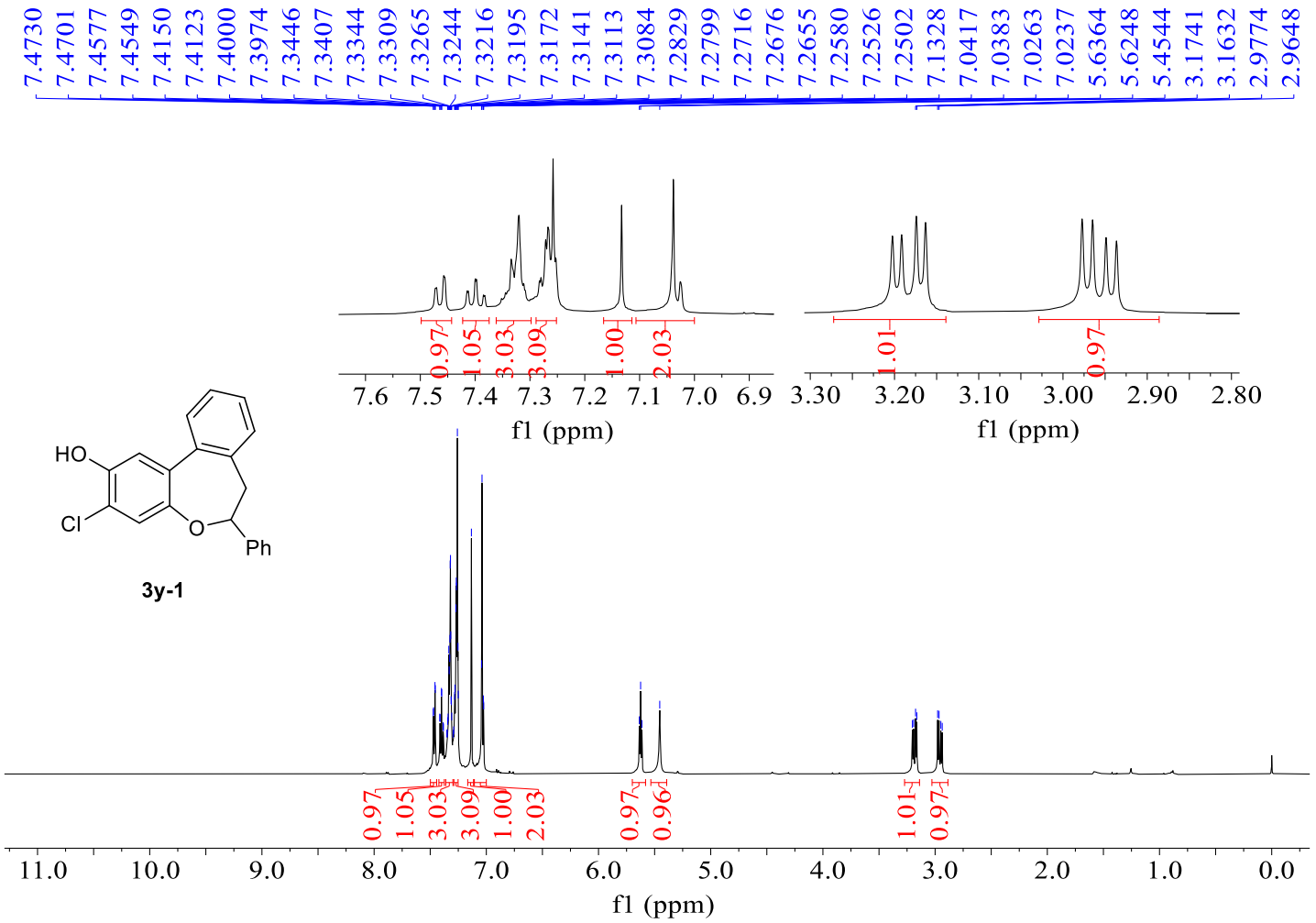


Figure S51 ^{1}H NMR of compound **3y-1** (500 MHz, $CDCl_3$)

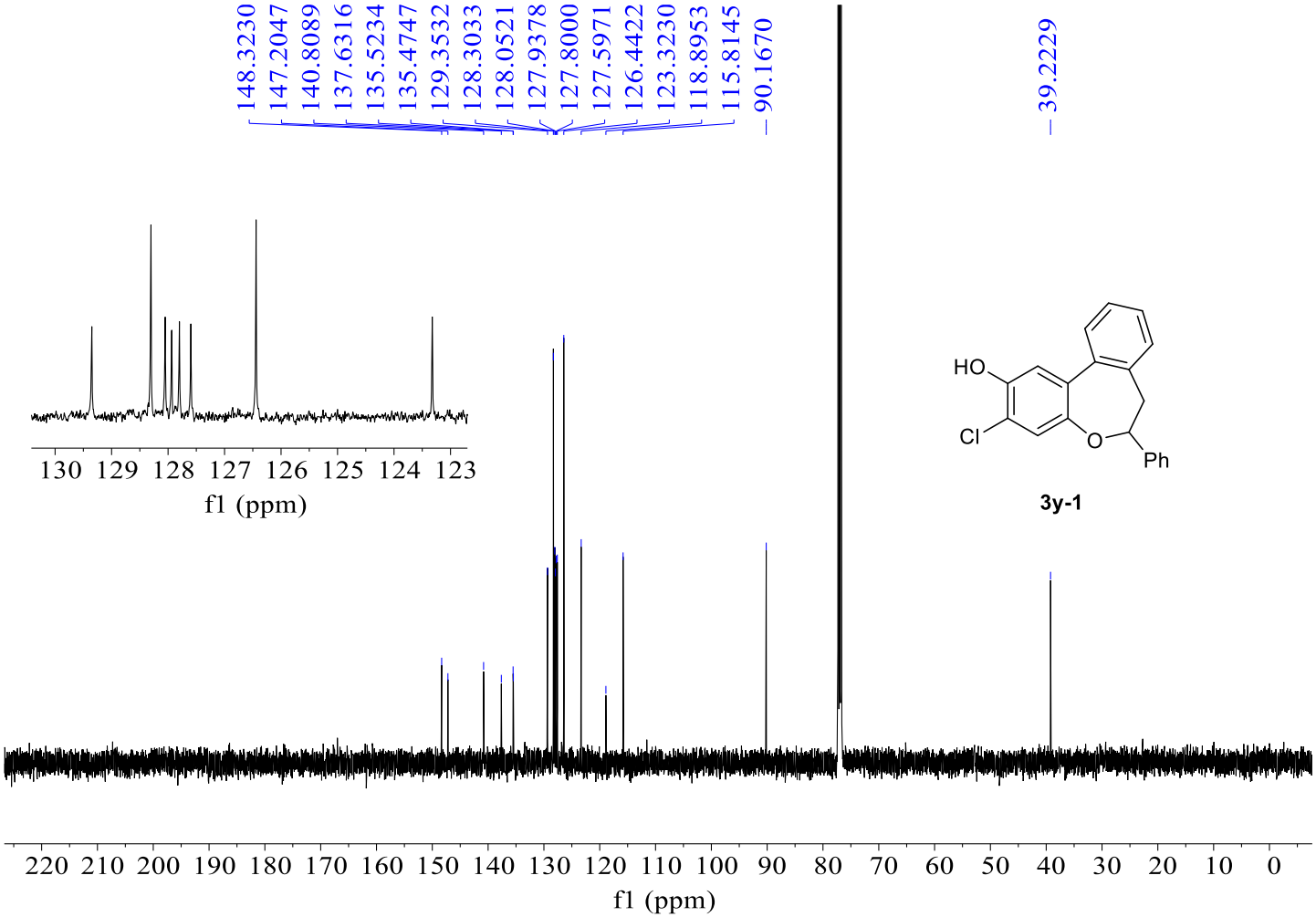


Figure S52 ^{13}C NMR of compound **3y-1** (126 MHz, $CDCl_3$)

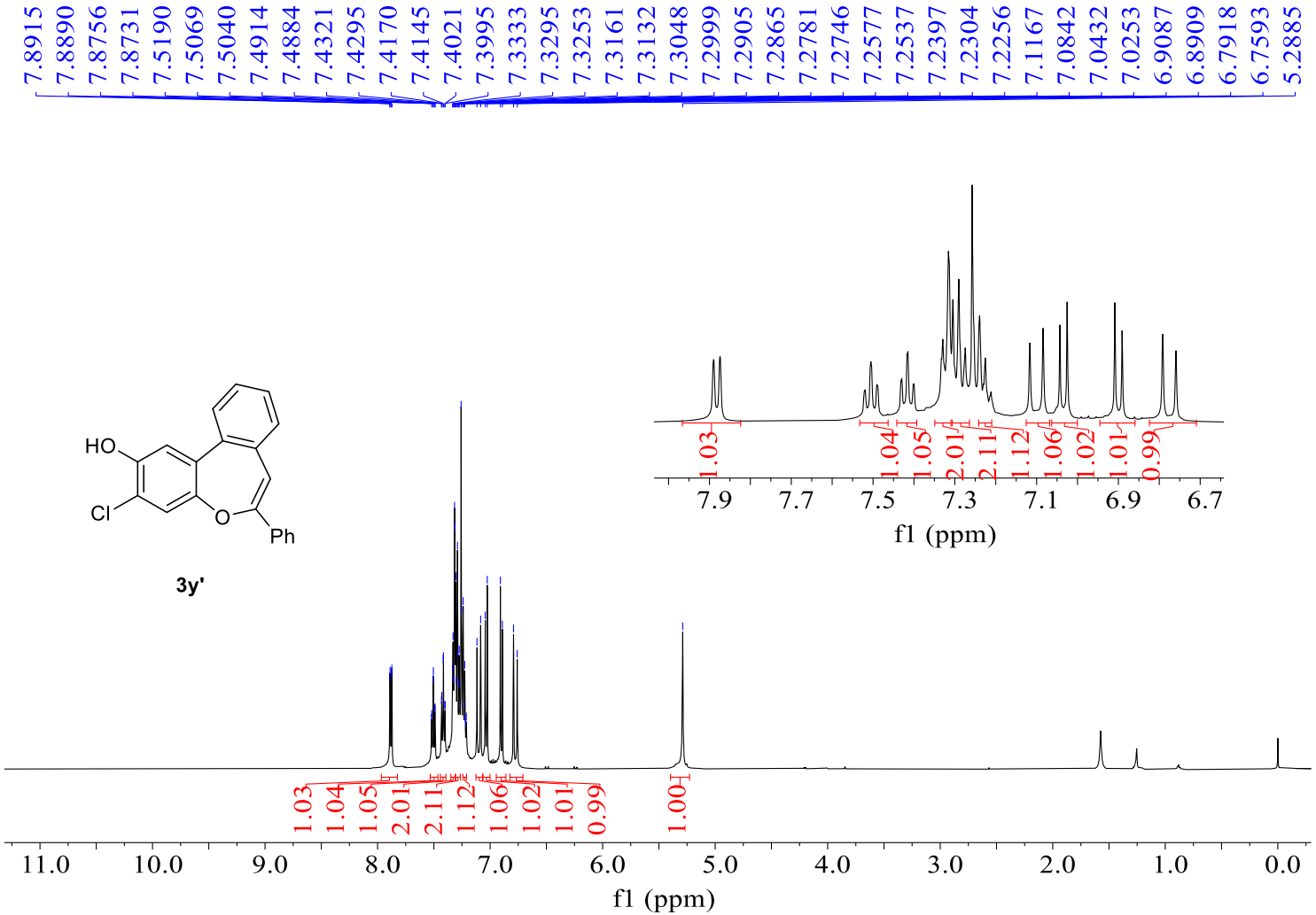


Figure S53 ^{1}H NMR of compound **3y'** (500 MHz, $CDCl_3$)

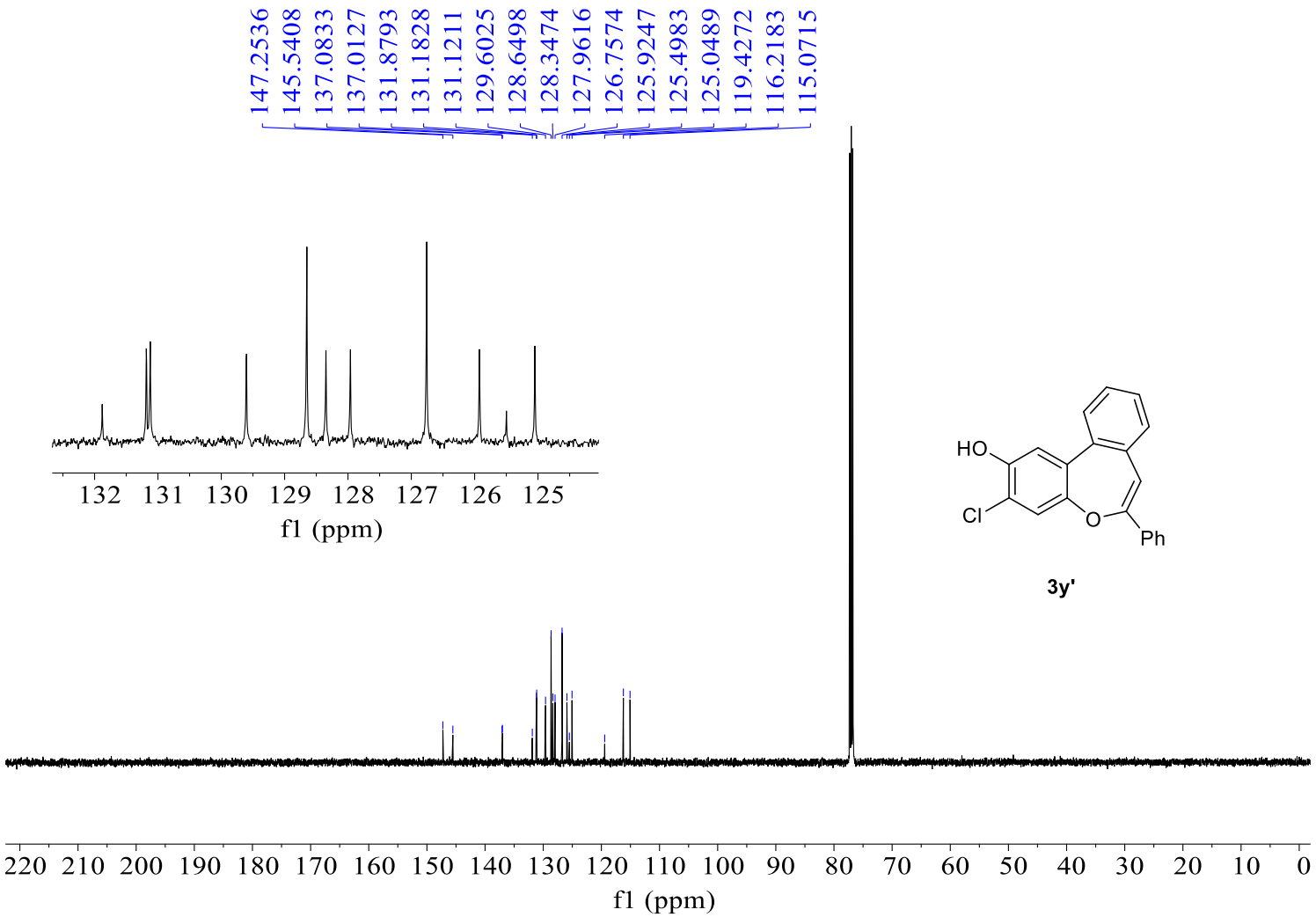


Figure S54 ^{13}C NMR of compound **3y'** (126 MHz, $CDCl_3$)

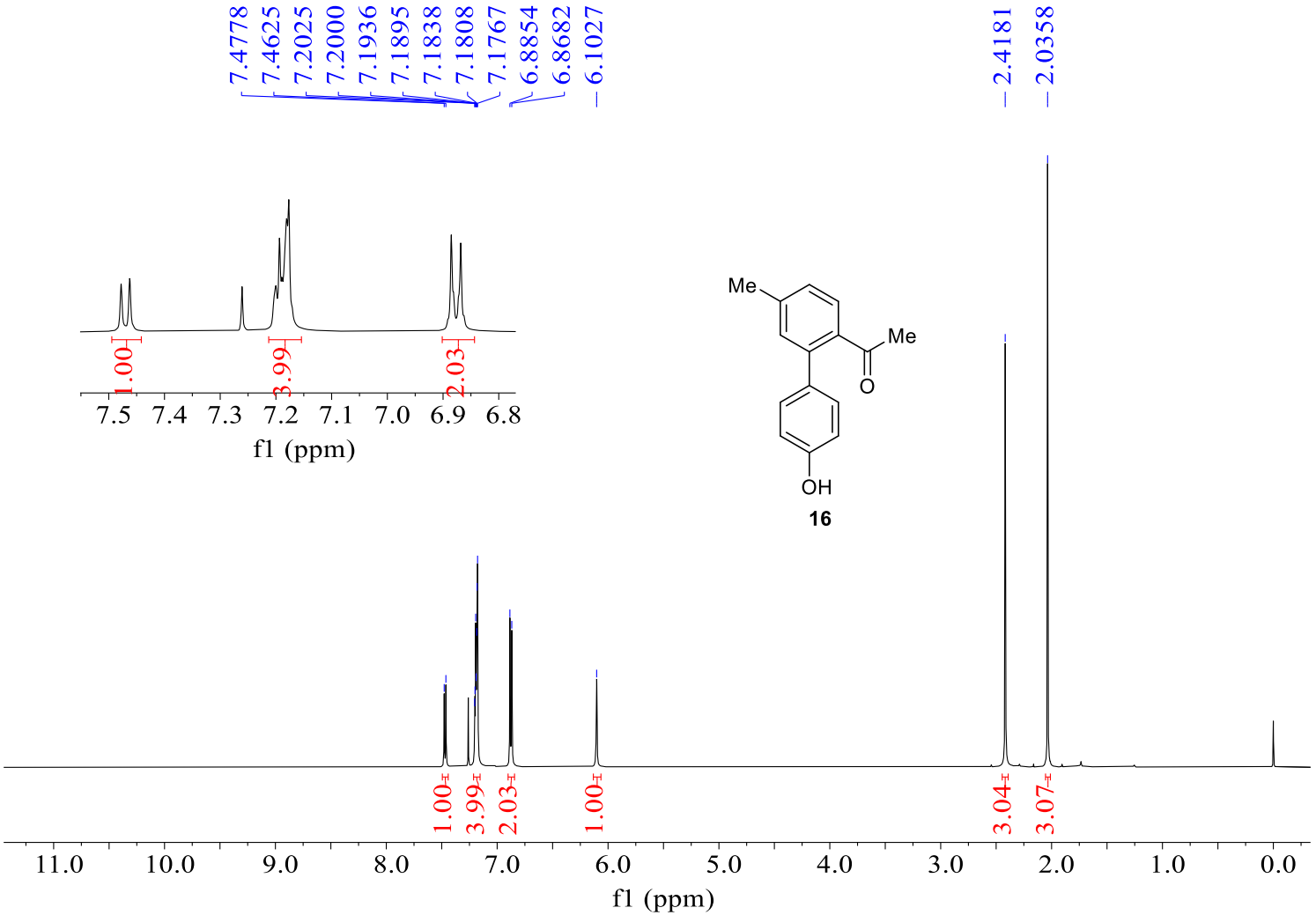


Figure S55 ^{1}H NMR of compound **16** (500 MHz, $CDCl_3$)

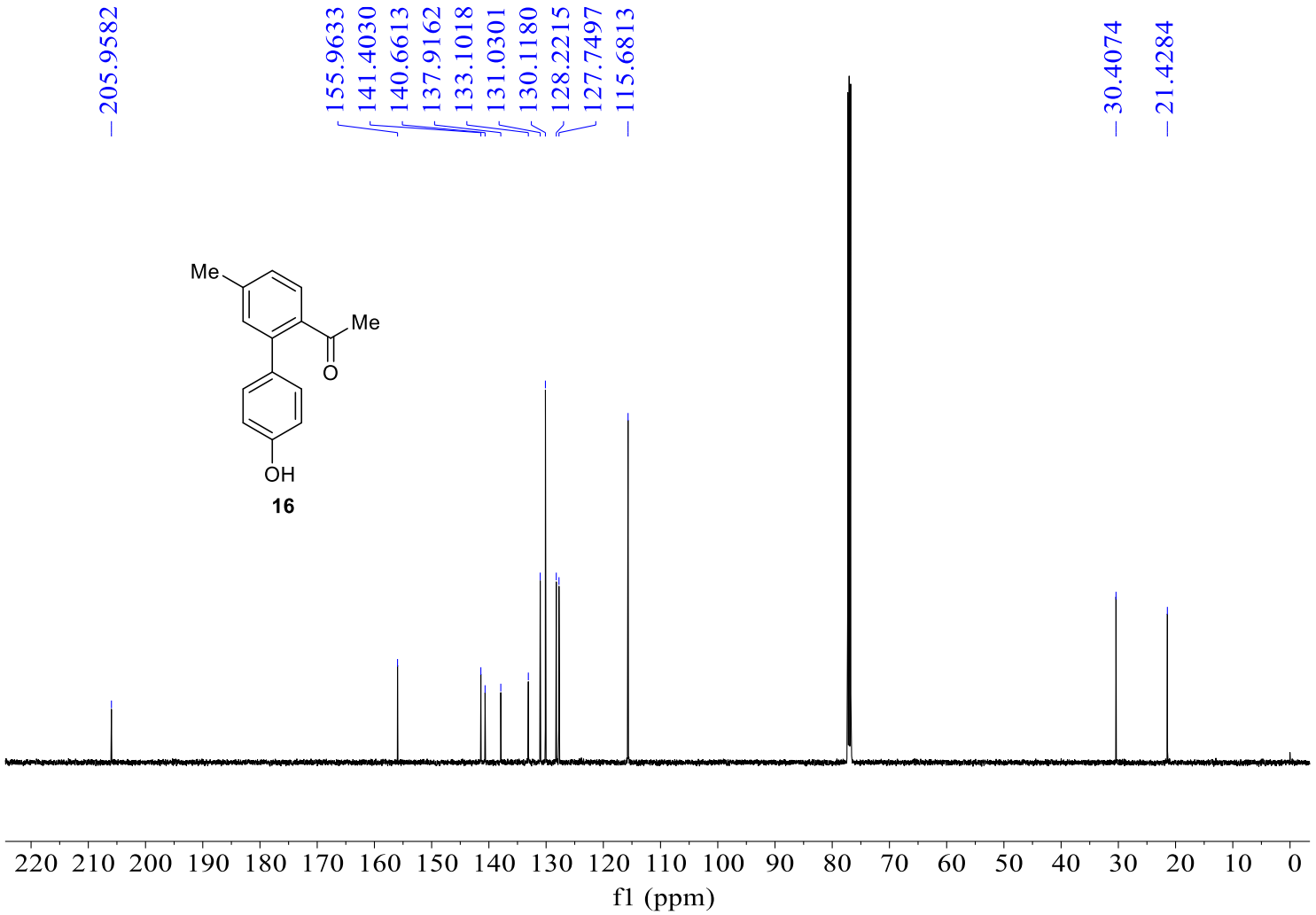


Figure S56 ^{13}C NMR of compound **16** (126 MHz, $CDCl_3$)

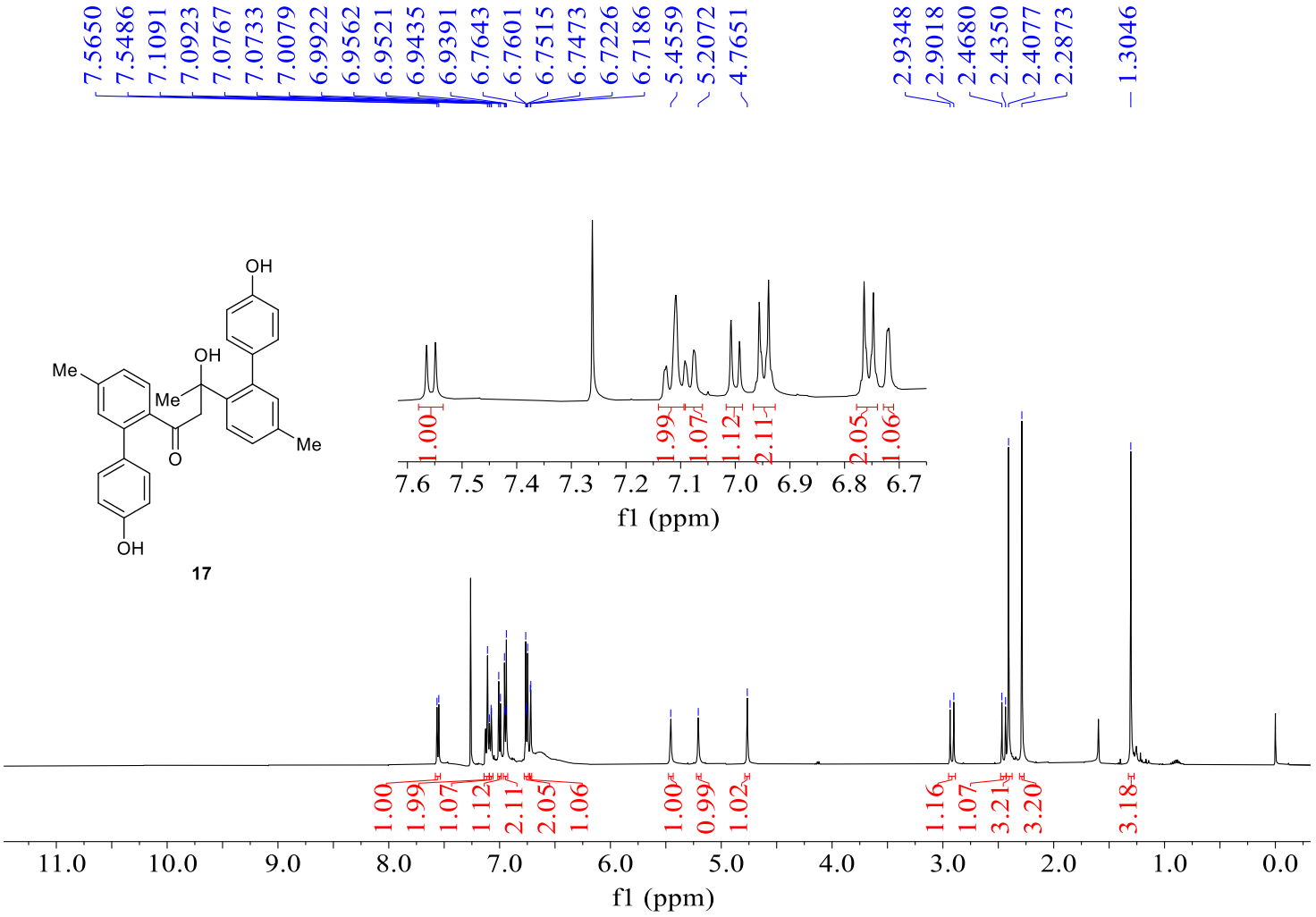


Figure S57 ^{1}H NMR of compound **17** (500 MHz, $CDCl_3$)

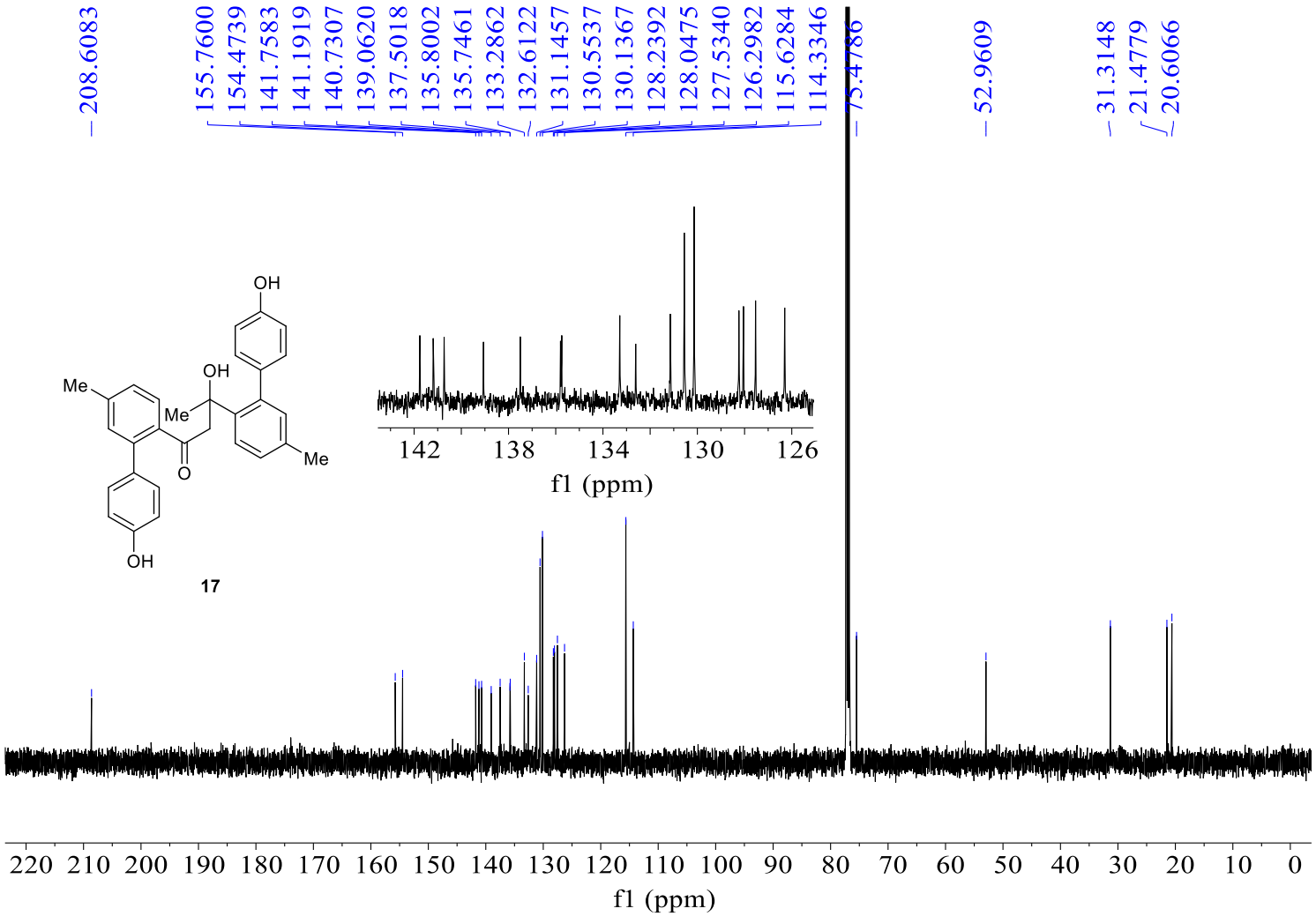


Figure S58 ^{13}C NMR of compound **17** (126 MHz, $CDCl_3$)

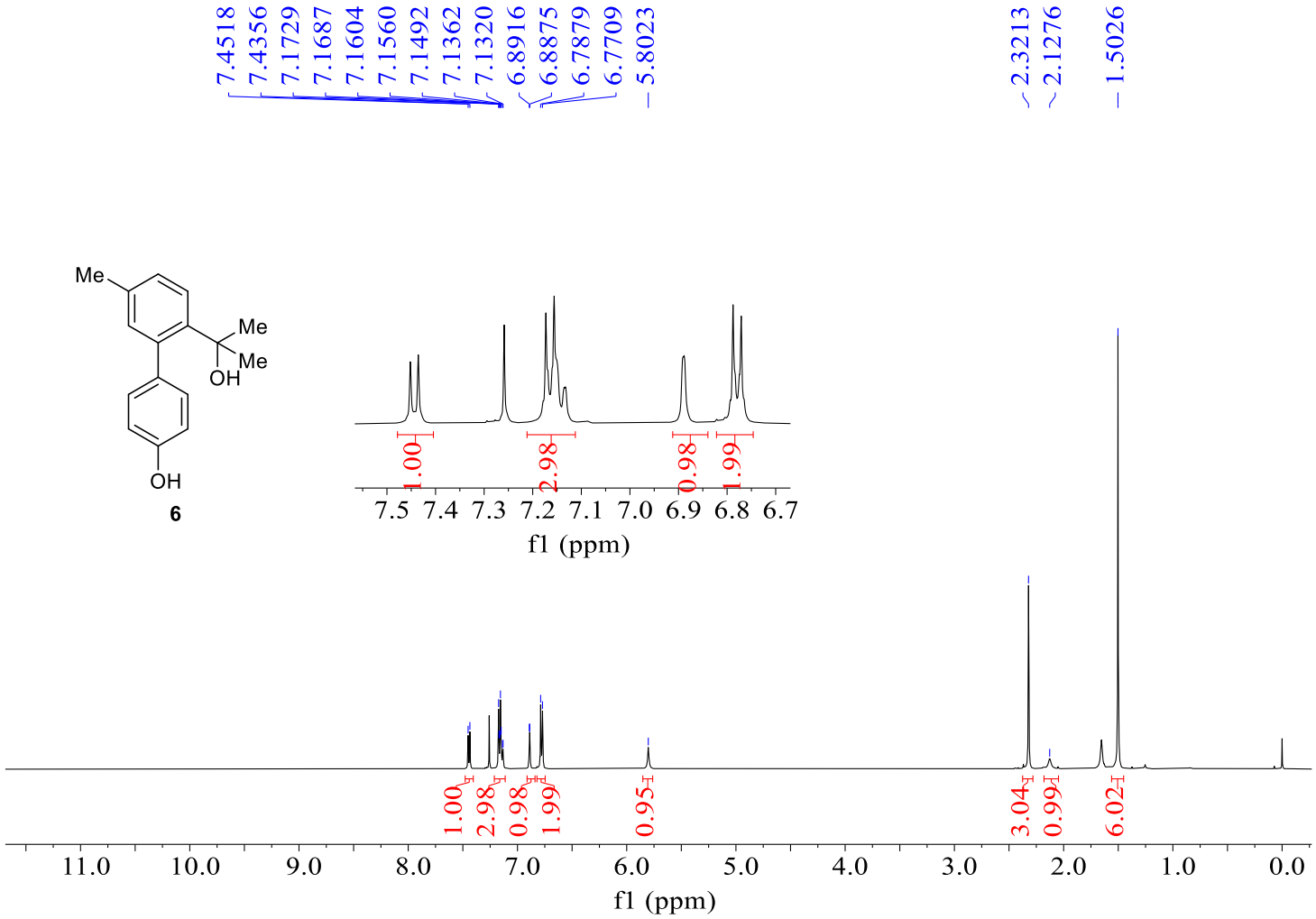


Figure S59 ^{1}H NMR of compound **6** (500 MHz, $CDCl_3$)

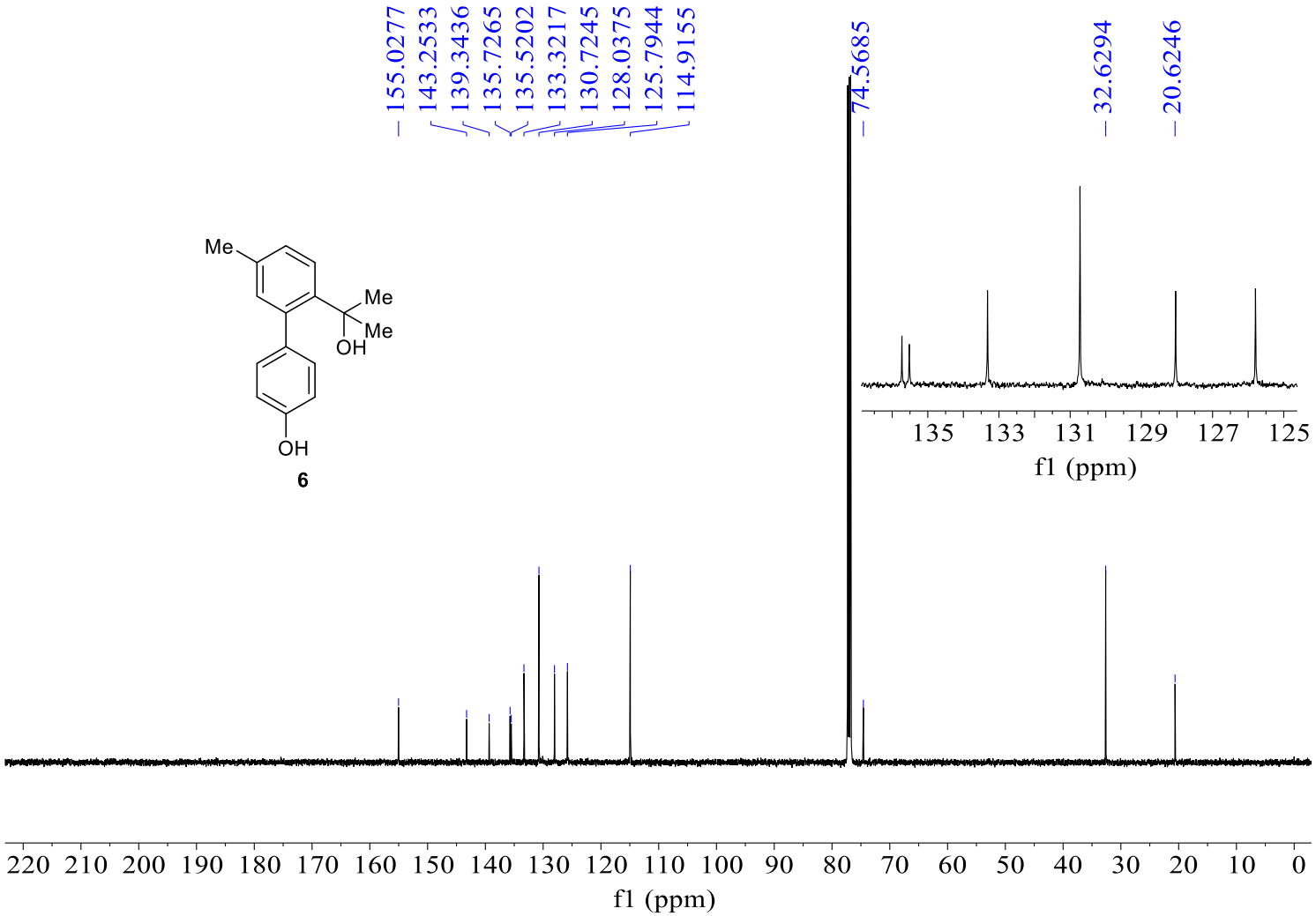


Figure S60 ^{13}C NMR of compound **6** (126 MHz, $CDCl_3$)

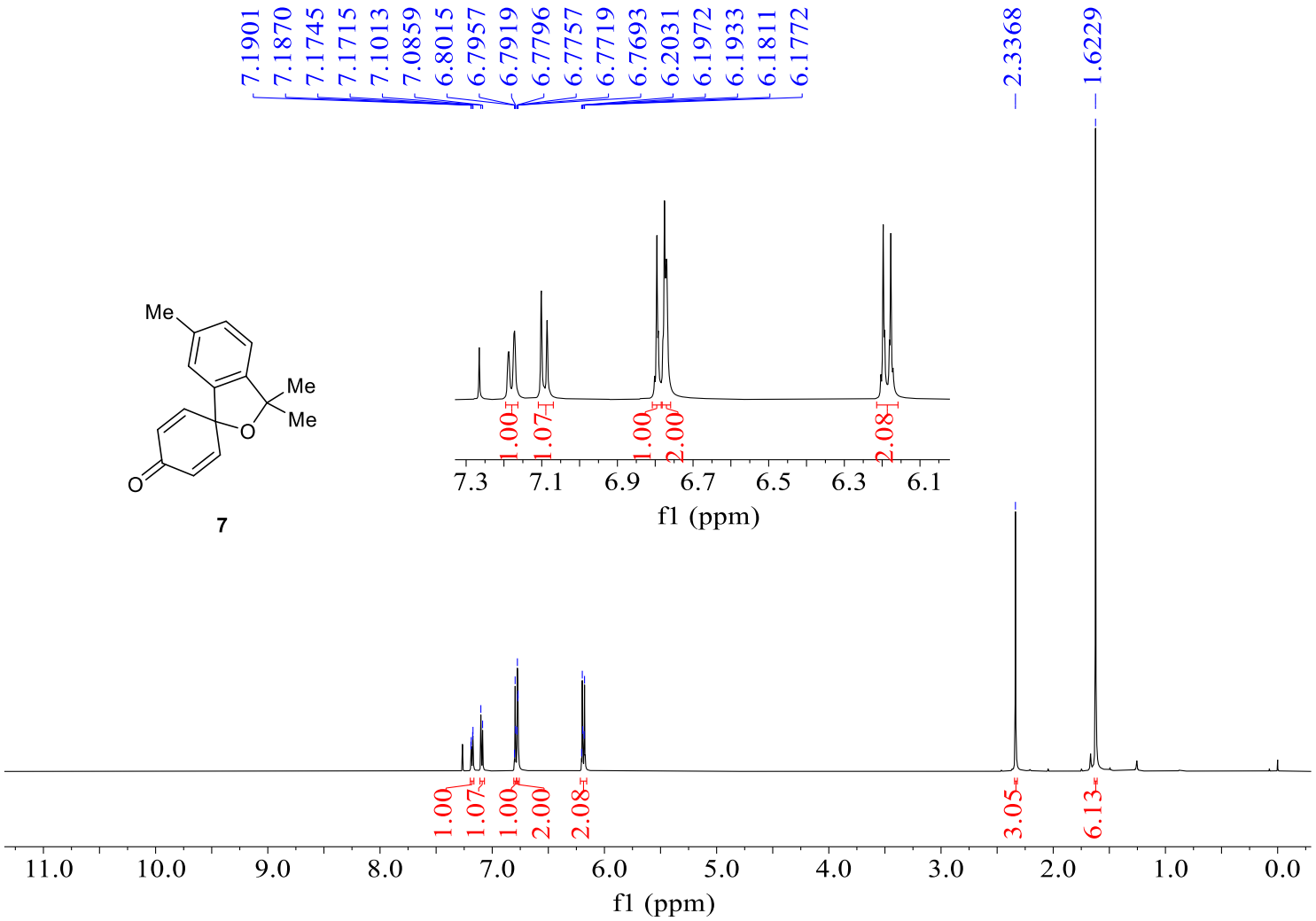


Figure S61 ^{1}H NMR of compound **7** (500 MHz, $CDCl_3$)

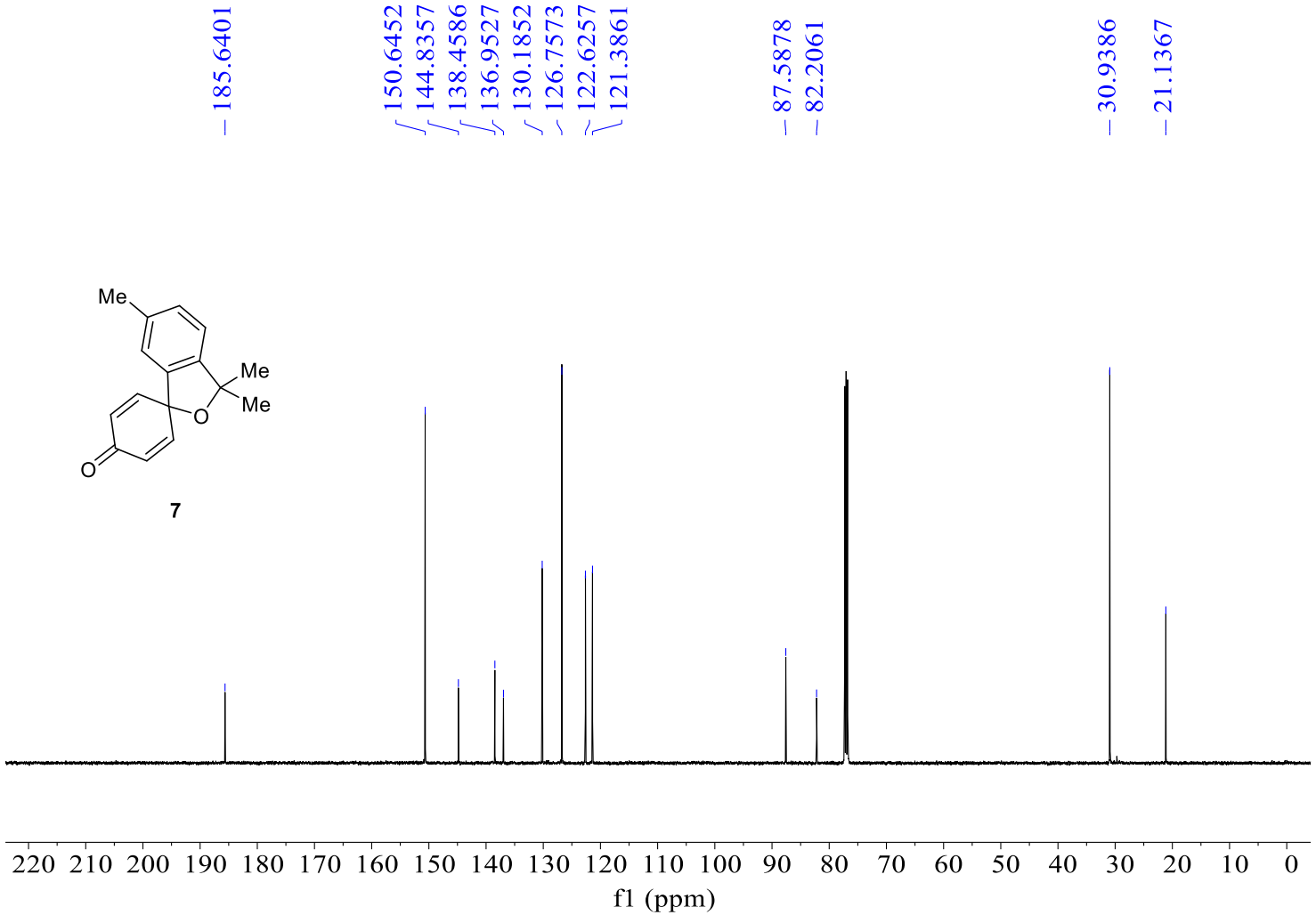


Figure S62 ^{13}C NMR of compound **7** (126 MHz, $CDCl_3$)

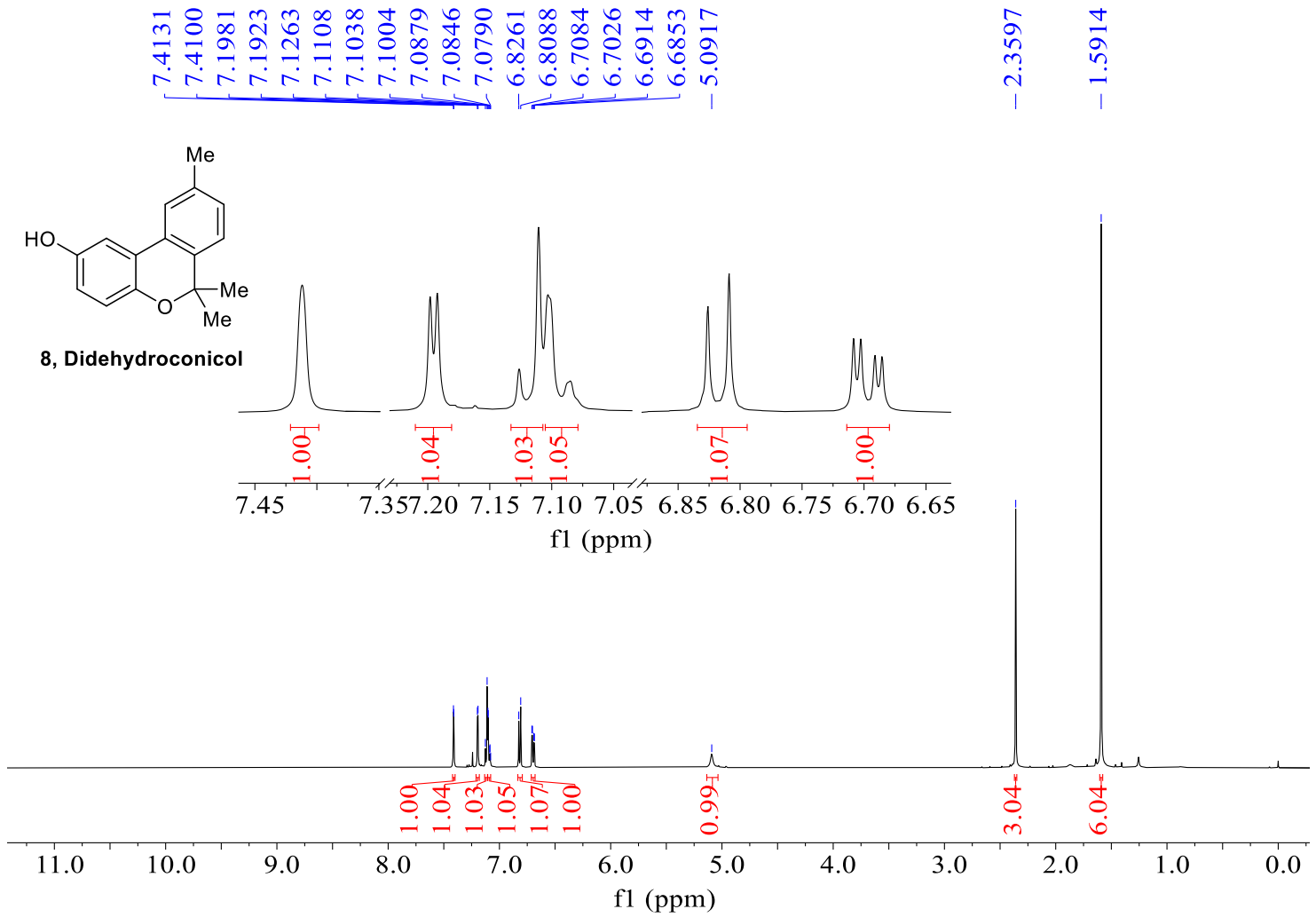


Figure S63 ^{1}H NMR of compound **8** (500 MHz, $CDCl_3$)

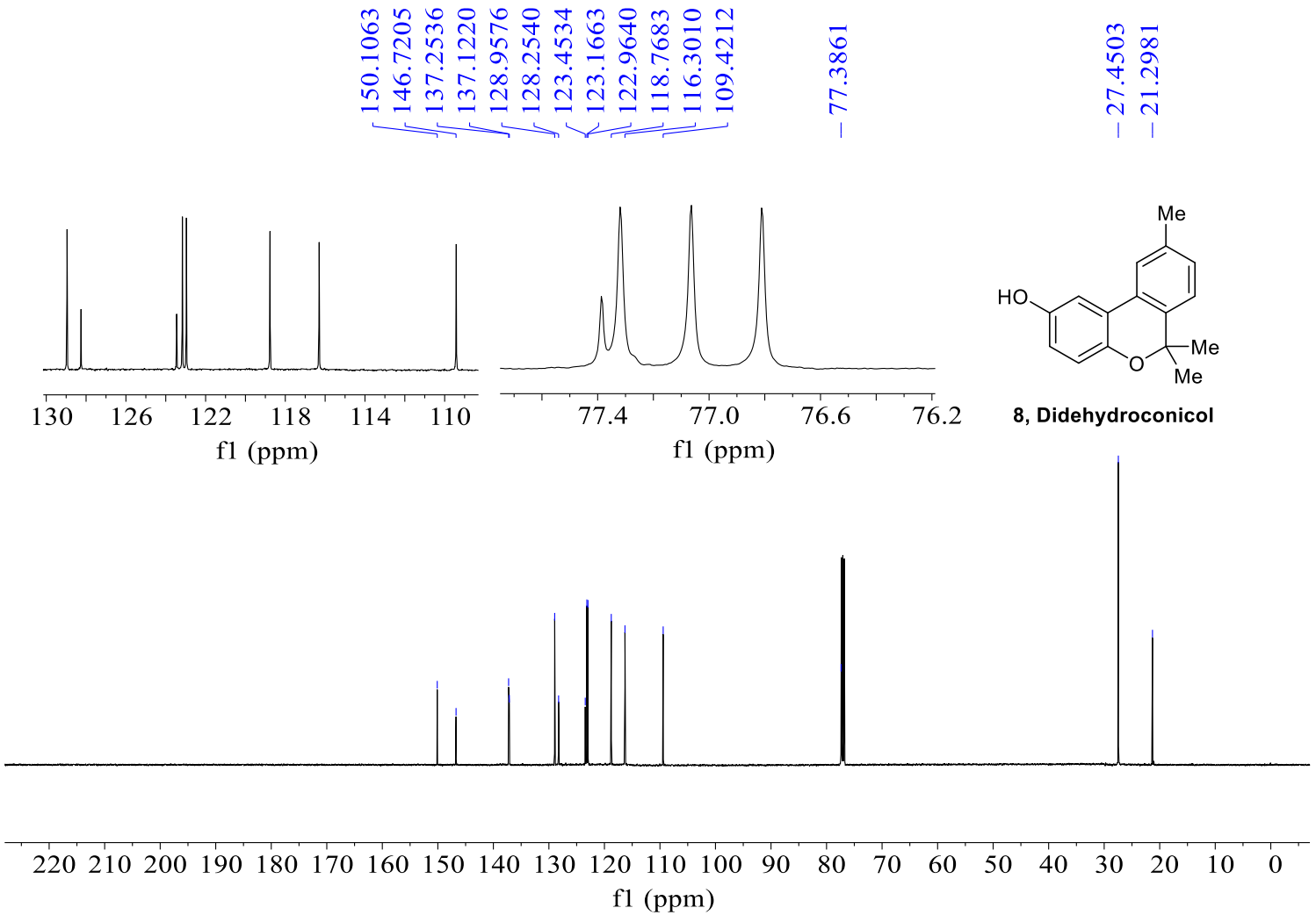
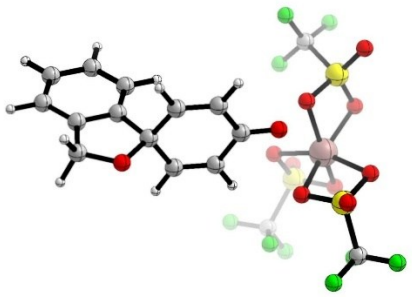


Figure S64 ^{13}C NMR of compound **8** (126 MHz, $CDCl_3$)

Part 4. Mechanistic studies and DFT calculation

Cartesian coordinates of all the optimized structures and transient state vibrational frequencies for all species.

2a+Ga(OTf)$_3$



Zero-point correction=	0.284339 (Hartree/Particle)
Thermal correction to Energy=	0.323754
Thermal correction to Enthalpy=	0.324698
Thermal correction to Gibbs Free Energy=	0.200736
Sum of electronic and zero-point Energies=	-5458.838826
Sum of electronic and thermal Energies=	-5458.799411
Sum of electronic and thermal Enthalpies=	-5458.798467
Sum of electronic and thermal Free Energies=	-5458.922429

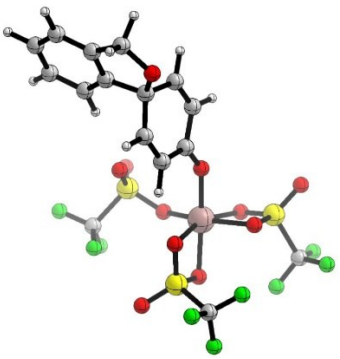
Cartesian coordinates

0 1

O	-2.83274400	-0.68136200	-1.79710800
S	-1.92504200	-1.90598500	-1.60723400
O	-1.08893200	-1.43076800	-0.40488500
C	-3.03954200	-3.24380700	-0.90587100
F	-3.64274600	-2.80311600	0.19354800
F	-2.28779400	-4.30129800	-0.61504400
F	-3.94352200	-3.56363400	-1.82429100
O	-1.26360200	-2.47540100	-2.75752300
O	-2.84515100	2.12101700	-0.83815800
C	-1.00008400	4.08815100	-0.51797700
F	-0.84684600	3.70353800	0.74384400
F	-1.90989200	5.05321700	-0.59332000
F	0.15942000	4.51319300	-1.00876900
O	-1.71015100	3.10993500	-2.91579600
O	-1.26628500	0.77975900	1.53838800
S	-2.59377600	0.47167700	2.24522200
O	-3.44257900	0.00858400	1.05786500
C	-2.26832000	-1.07384200	3.25634000
F	-1.82804700	-2.04511800	2.46320500

F	-3.40476500	-1.44228200	3.83708900
F	-1.35449500	-0.78914800	4.17769800
O	-3.13905500	1.46541700	3.14570700
Ga	-1.98318800	0.37168900	-0.30678100
O	-0.61027400	1.49629200	-1.25121300
S	-1.58924300	2.63984400	-1.55287200
O	1.30103500	-0.52990100	-2.49489300
C	2.36756800	-0.75417900	-1.93057000
C	2.43295100	-1.40826600	-0.60168900
C	3.66340100	-0.40755400	-2.56038800
C	3.60082700	-1.61487000	0.02149000
H	1.48480200	-1.72137600	-0.17471100
C	4.82870000	-0.61183700	-1.93238400
H	3.61019700	0.00561600	-3.56377000
H	3.64966500	-2.11304800	0.98718600
H	5.77824100	-0.37071200	-2.40516800
C	4.92920300	-1.15160900	-0.52515500
C	7.03025000	-1.97166300	0.26941700
H	7.91639700	-1.99992400	-0.38193100
H	7.15543100	-2.75244700	1.03272700
C	5.57106100	-0.12133400	0.40306600
C	6.79274800	-0.60864200	0.85934800
O	5.85756700	-2.26251200	-0.50485300
C	7.57884400	0.15211900	1.72281100
H	8.53429100	-0.22020800	2.08410600
C	5.10079900	1.12990400	0.79227600
H	4.14545200	1.50176000	0.43194300
C	5.88541500	1.89437100	1.65904100
H	5.53820800	2.87318500	1.97786600
C	7.11466500	1.40887900	2.12020400
H	7.71377000	2.01465700	2.79447400

2a-Ga(OTf)$_3$



Zero-point correction= 0.285971 (Hartree/Particle)
Thermal correction to Energy= 0.324775
Thermal correction to Enthalpy= 0.325719
Thermal correction to Gibbs Free Energy= 0.206905
Sum of electronic and zero-point Energies= -5458.873975
Sum of electronic and thermal Energies= -5458.835171
Sum of electronic and thermal Enthalpies= -5458.834227
Sum of electronic and thermal Free Energies= -5458.953041

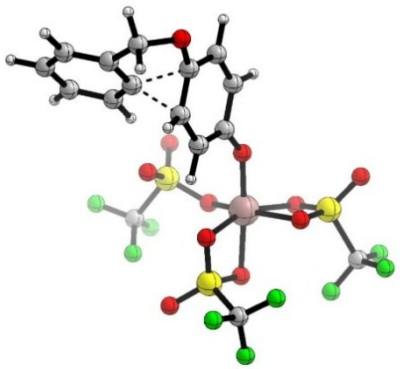
Cartesian coordinates

0 1

O	-2.33907500	-0.62857600	-2.03452300
S	-2.83227900	-1.93114800	-1.39948300
O	-2.27753800	-1.79903900	0.01437200
C	-4.68838900	-1.74126000	-1.24107000
F	-4.98185000	-0.61775300	-0.59741700
F	-5.15980600	-2.78590000	-0.56296400
F	-5.21749900	-1.71732100	-2.46057400
O	-2.60778700	-3.17100100	-2.11837100
O	-0.62250500	1.48281300	-1.36827000
C	0.48666400	3.75643700	-0.70185200
F	0.18227200	3.55643400	0.58357300
F	-0.51073100	4.40595200	-1.29816500
F	1.60160800	4.48833400	-0.77938000
O	1.07540500	2.39697500	-2.93355500
O	-0.87853900	0.34491600	1.53926100
S	-2.13998300	1.19699200	1.75870400
O	-2.81143700	1.06287400	0.40031600
C	-3.19083900	0.22132300	2.96696900
F	-3.38661700	-1.01415500	2.52533700
F	-4.35768600	0.84543300	3.10086200
F	-2.55654500	0.18776500	4.13701700
O	-1.97956100	2.51381400	2.34083500
Ga	-1.26966700	-0.02947900	-0.42781000
O	1.79588400	1.44233000	-0.70480700
S	0.78627000	2.11710500	-1.53464600
O	0.27729000	-1.13703700	-0.77756900
C	1.41037200	-1.42088200	-0.29896500
C	1.83243000	-1.04501100	1.04098000
C	2.30252300	-2.21017800	-1.13654600
C	3.07412700	-1.35355500	1.45680200
H	1.12776600	-0.52658200	1.67897600
C	3.54913300	-2.49450000	-0.72358000
H	1.90621500	-2.54133400	-2.09081200

H	3.40898100	-1.10280800	2.45947100
H	4.22812700	-3.08168100	-1.33572200
C	4.11599300	-1.96894700	0.56688200
C	6.22954200	-2.77927800	1.31164500
H	6.74439400	-3.57906200	0.76074200
H	6.55652600	-2.82962500	2.35835300
C	5.20385400	-0.92635300	0.25526700
C	6.42842000	-1.42448200	0.69351500
O	4.80774400	-3.01221800	1.26739500
C	7.58939800	-0.67318000	0.52155100
H	8.55248200	-1.04810400	0.85819400
C	5.08826000	0.32003200	-0.35460500
H	4.12498000	0.70601600	-0.67757700
C	6.25451400	1.07093300	-0.52367000
H	6.19593500	2.04828500	-0.99340800
C	7.49163800	0.57855700	-0.09206900
H	8.38693800	1.17771600	-0.23209600

TS1



Zero-point correction= 0.284731 (Hartree/Particle)
Thermal correction to Energy= 0.322947
Thermal correction to Enthalpy= 0.323891
Thermal correction to Gibbs Free Energy= 0.207356
Sum of electronic and zero-point Energies= -5458.834515
Sum of electronic and thermal Energies= -5458.796299
Sum of electronic and thermal Enthalpies= -5458.795355
Sum of electronic and thermal Free Energies= -5458.911890

Cartesian coordinates

0 1

O	-2.45500900	-0.41497700	-1.95230900
S	-2.84853200	-1.79324700	-1.41875200
O	-2.11165700	-1.83645900	-0.09168200
C	-4.66430000	-1.65464800	-0.99079600

F	-4.87155600	-0.63306100	-0.16760100
F	-5.04658700	-2.78849500	-0.40223700
F	-5.35700100	-1.47677400	-2.11354100
O	-2.73416000	-2.92883600	-2.31654300
O	-0.72785200	1.68451100	-1.28979700
C	0.19812100	4.05351400	-0.74944200
F	-0.31652300	3.96346600	0.47769300
F	-0.69210500	4.61774300	-1.56475000
F	1.29951500	4.81303800	-0.70921800
O	1.12703800	2.52044900	-2.74123300
O	-0.50888300	0.14072900	1.47209000
S	-1.73058300	0.93287500	1.95256300
O	-2.58438800	0.94177100	0.69850400
C	-2.59943800	-0.19298500	3.17136700
F	-2.85463000	-1.37484500	2.62440900
F	-3.73853900	0.38762700	3.54236200
F	-1.80853200	-0.35209800	4.23344300
O	-1.49815500	2.17636600	2.66180100
Ga	-1.13785100	0.00659600	-0.47659400
O	1.58745100	1.81558200	-0.35971200
S	0.66300200	2.35961600	-1.36836100
O	0.32247400	-0.94286500	-1.19722100
C	1.46383700	-1.41861200	-0.80394900
C	1.96362100	-1.39322000	0.49829600
C	2.26525800	-2.04979400	-1.84087200
C	3.23598700	-1.95514400	0.78473700
H	1.40639700	-0.91699700	1.29420200
C	3.48537700	-2.59661800	-1.59555200
H	1.83753000	-2.05677100	-2.83867300
H	3.47588100	-2.19130100	1.81730300
H	4.07874900	-3.07260100	-2.36882400
C	4.01726200	-2.56266000	-0.26395200
C	5.96340200	-2.85109300	0.99796100
H	6.94857400	-3.27903500	0.80244400
H	5.63672500	-3.17494400	1.99778200
C	4.68038100	-0.90928300	0.33043400
C	5.90302200	-1.35544200	0.83516400
O	5.07797600	-3.38088200	-0.00711500
C	6.92931500	-0.43519700	1.02785700
H	7.89487000	-0.75825100	1.40763800
C	4.43803800	0.41421700	-0.02264000
H	3.46414700	0.75069400	-0.36696600
C	5.48552300	1.31986100	0.15853000

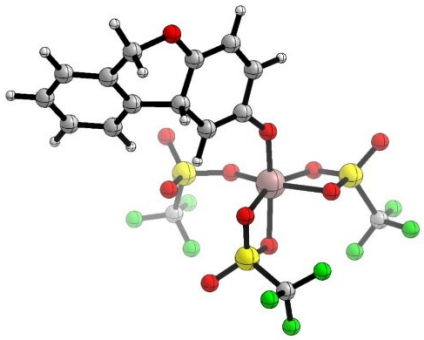
H	5.32719300	2.36237500	-0.09971700
C	6.71215600	0.90454700	0.68865900
H	7.51068500	1.62724900	0.82791200

Vibrational frequencies

1	-463.32	153.1776	40	316.50	0.8080	79	770.26	0.4775
2	10.80	0.4018	41	317.92	16.1738	80	779.35	52.9180
3	16.20	0.8692	42	324.67	0.7256	81	836.57	9.1570
4	19.81	0.1594	43	327.96	2.1320	82	845.81	31.7429
5	22.83	0.0282	44	376.45	8.0007	83	870.16	52.0493
6	25.96	0.5616	45	382.99	27.1789	84	890.14	25.9490
7	27.45	0.2164	46	389.83	11.7552	85	896.40	10.0068
8	30.96	0.3765	47	395.37	15.4416	86	940.55	658.3144
9	35.53	0.2028	48	403.65	41.3725	87	950.41	11.1314
10	37.40	0.5715	49	407.36	21.7483	88	951.81	127.0734
11	47.59	1.0674	50	450.53	15.6663	89	970.93	342.2289
12	55.74	0.3498	51	472.76	13.8251	90	978.15	5.8798
13	60.80	1.5564	52	481.21	17.3470	91	985.96	0.7820
14	70.85	0.3486	53	491.53	1.5042	92	1007.35	1.8240
15	74.32	1.7495	54	494.12	23.2336	93	1019.01	6.7019
16	92.92	0.3908	55	495.44	8.9154	94	1020.80	33.5304
17	94.96	0.4456	56	506.88	0.4433	95	1030.54	6.2882
18	112.40	0.9885	57	528.53	11.5065	96	1037.05	37.4550
19	117.14	1.0153	58	539.96	25.4791	97	1039.33	11.4083
20	121.81	10.3920	59	541.60	9.1343	98	1059.08	227.6682
21	141.59	0.4749	60	543.78	34.5158	99	1061.64	0.8547
22	151.73	9.4519	61	558.75	5.4294	100	1132.26	284.6779
23	160.81	0.6221	62	561.45	0.1110	101	1136.29	3.0991
24	171.05	0.1607	63	562.49	2.9830	102	1152.31	1.3182
25	181.20	2.1329	64	572.46	12.1682	103	1190.59	94.6452
26	197.10	2.4243	65	581.64	49.0987	104	1194.25	28.1084
27	199.49	2.0225	66	586.22	69.3089	105	1194.47	173.3867
28	211.38	6.0650	67	605.96	44.6454	106	1200.74	1.8492
29	218.59	29.4763	68	616.94	145.1972	107	1213.37	46.6756
30	226.55	25.6642	69	634.60	8.2383	108	1222.01	92.4272
31	232.96	1.1868	70	637.29	3.9996	109	1235.86	4.3456
32	248.38	8.8241	71	653.18	133.5567	110	1248.44	224.1135
33	253.86	2.9499	72	656.32	14.3631	111	1257.48	18.4455
34	269.80	6.4315	73	665.42	334.7994	112	1258.89	367.8127
35	275.23	15.3590	74	704.37	18.4464	113	1260.31	158.4368
36	278.30	4.9122	75	716.88	3.3760	114	1263.35	141.6405
37	298.79	24.2904	76	763.91	31.2279	115	1275.11	168.6116
38	310.43	9.7372	77	764.69	13.2041	116	1278.04	107.0335
39	314.32	18.6851	78	769.33	0.6854	117	1311.20	66.7013

118	1318.64	85.6141	127	1498.44	37.1297	136	3142.20	12.2575
119	1319.49	453.0343	128	1504.35	51.8981	137	3195.04	2.1211
120	1323.72	504.5103	129	1517.21	300.1928	138	3201.69	1.0452
121	1333.56	85.4204	130	1534.86	9.4697	139	3206.84	78.8866
122	1354.58	16.4348	131	1581.75	730.9782	140	3212.17	19.5160
123	1372.47	11.7876	132	1626.95	19.6541	141	3220.94	0.2761
124	1395.90	39.4252	133	1638.73	36.4716	142	3223.50	17.3494
125	1413.12	60.4351	134	1666.92	192.9384	143	3234.94	0.1715
126	1477.18	21.1053	135	3021.19	31.4414	144	3261.79	15.6178

INT1



Zero-point correction= 0.286182 (Hartree/Particle)
Thermal correction to Energy= 0.324688
Thermal correction to Enthalpy= 0.325632
Thermal correction to Gibbs Free Energy= 0.207713
Sum of electronic and zero-point Energies= -5458.867291
Sum of electronic and thermal Energies= -5458.828785
Sum of electronic and thermal Enthalpies= -5458.827841
Sum of electronic and thermal Free Energies= -5458.945760

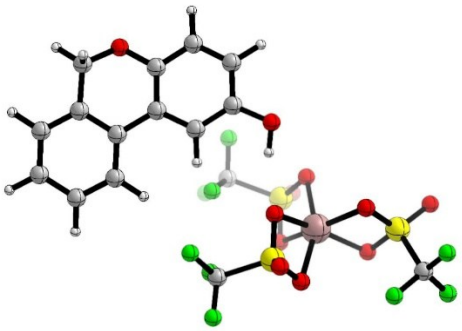
Cartesian coordinates

0 1

O	-2.46119400	-0.59035700	-1.89259100
S	-3.10812100	-1.80368600	-1.22276400
O	-2.39169400	-1.84487100	0.11121200
C	-4.85916300	-1.26906900	-0.84552000
F	-4.85599900	-0.13796300	-0.14743900
F	-5.45394000	-2.22990100	-0.13730200
F	-5.51286000	-1.08857100	-1.99147400
O	-3.21966500	-3.02752900	-1.99709500
O	-0.42581400	1.17858400	-1.54085300
C	-0.13509300	3.76923900	-1.23932100
F	-1.03486400	3.76484700	-0.25592800
F	-0.74839200	3.99878500	-2.40099400

F	0.75778900	4.73938100	-1.01542000
O	1.65706600	2.19353100	-2.44851600
O	-0.39461700	-0.14213600	1.51547800
S	-1.41338800	0.91686300	1.93371100
O	-2.25256100	1.03125700	0.66650000
C	-2.51026000	0.08671400	3.20625700
F	-3.01738300	-1.04545100	2.73684100
F	-3.49601000	0.92528400	3.52106800
F	-1.77361300	-0.16695500	4.28912900
O	-0.93734100	2.13088600	2.56770500
Ga	-1.08794100	-0.25579500	-0.44624000
O	1.33283200	1.94848800	0.04392000
S	0.75907800	2.13566500	-1.30012600
O	0.17418300	-1.53618500	-0.97166400
C	1.42298700	-1.80521900	-0.67650500
C	2.23143600	-1.14698500	0.22434200
C	2.00163800	-2.91589300	-1.39513600
C	3.62411100	-1.58542100	0.49873200
H	1.85160600	-0.31241500	0.80014800
C	3.29371600	-3.37913600	-1.23004000
H	1.34547900	-3.40591200	-2.11025300
H	3.59715000	-1.98933500	1.53767800
H	3.67714200	-4.21402500	-1.80666400
C	4.12044400	-2.73951100	-0.30954000
C	6.19478900	-2.44758200	0.80555100
H	7.20799200	-2.79290000	0.60083000
H	5.89158800	-2.80510100	1.80020100
C	4.71405700	-0.49764900	0.50028500
C	6.02435900	-0.96641700	0.65463700
O	5.35561400	-3.16614500	-0.15557200
C	7.09668400	-0.07433100	0.64972700
H	8.11372800	-0.44368900	0.75490500
C	4.46512200	0.86348000	0.33193500
H	3.45651800	1.23639200	0.18515900
C	5.54346100	1.75337300	0.34813100
H	5.35192600	2.81453900	0.22074000
C	6.85080800	1.29242200	0.50871800
H	7.68035400	1.99329400	0.50950900

3a+Ga(OTf)$_3$



Zero-point correction=	0.286747 (Hartree/Particle)
Thermal correction to Energy=	0.325379
Thermal correction to Enthalpy=	0.326323
Thermal correction to Gibbs Free Energy=	0.207438
Sum of electronic and zero-point Energies=	-5458.886078
Sum of electronic and thermal Energies=	-5458.847446
Sum of electronic and thermal Enthalpies=	-5458.846502
Sum of electronic and thermal Free Energies=	-5458.965387

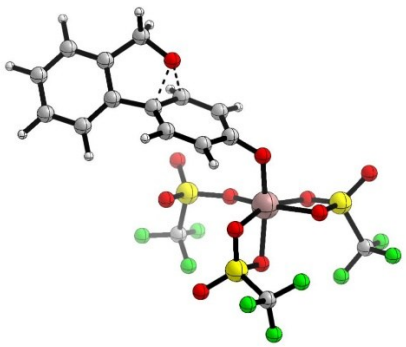
Cartesian coordinates

0 1

O	-2.40664400	-1.84217100	0.25701100
S	-1.23441700	-2.08943900	-0.69468400
O	-0.67079900	-0.65884500	-0.80178700
C	0.05535700	-3.02388300	0.29919000
F	0.27090200	-2.40131300	1.45062300
F	1.17806800	-3.05316200	-0.41760100
F	-0.38379600	-4.25532900	0.51414300
O	-1.46766400	-2.82884800	-1.91555200
O	-4.00637400	0.57712300	0.95886900
C	-5.71470100	-0.20726500	-1.01527900
F	-6.79483200	-0.11631500	-0.24925900
F	-5.18741300	-1.42219600	-0.92323000
F	-6.02048400	0.06528200	-2.27768000
O	-3.19226300	0.78307200	-1.24477800
O	-1.16355900	1.88083600	0.67093600
S	-0.78948500	1.53406500	2.12211300
O	-1.37378900	0.11301700	2.21561500
C	1.07602000	1.29691900	2.10341000
F	1.36540400	0.22874200	1.36267900
F	1.48451700	1.10622500	3.35121800
F	1.63381400	2.38058800	1.59021300
O	-1.10725400	2.48378600	3.16522600

Ga	-2.13153800	0.15870600	0.34874300
O	-5.08270700	2.36500900	-0.53182500
S	-4.46424400	1.06199800	-0.42605000
C	2.05761100	1.47365800	-2.05951600
C	2.77135000	0.43717200	-1.45727300
C	2.70071700	2.68390900	-2.35293600
C	4.13106300	0.58631800	-1.13532600
H	2.26372200	-0.49773600	-1.23776700
C	4.05149100	2.83787200	-2.06449100
H	2.13170100	3.48065400	-2.82100300
H	4.57203800	3.76174300	-2.29620200
C	4.76781400	1.79604700	-1.47304500
C	6.89640300	0.82516300	-1.26185000
H	7.89136100	1.11674600	-0.91625100
H	6.97534000	0.51867000	-2.31885000
C	4.91990900	-0.42715000	-0.40930300
C	6.32295500	-0.29344000	-0.42867900
O	6.09544100	2.00792500	-1.18562100
C	7.12838800	-1.19339000	0.26627100
H	8.20937900	-1.07238500	0.24611600
C	4.35596600	-1.47647400	0.33211600
H	3.27747000	-1.57901000	0.39492200
C	5.16755000	-2.38426600	1.01098200
H	4.71342200	-3.19357700	1.57680300
C	6.55648100	-2.24782400	0.98046700
H	7.18887700	-2.95007000	1.51636500
O	0.73711900	1.36740800	-2.39962800
H	0.39078000	0.50970700	-2.10332500

TS2



Zero-point correction= 0.284196 (Hartree/Particle)
Thermal correction to Energy= 0.322548
Thermal correction to Enthalpy= 0.323492
Thermal correction to Gibbs Free Energy= 0.206662

Sum of electronic and zero-point Energies= -5458.816646
Sum of electronic and thermal Energies= -5458.778294
Sum of electronic and thermal Enthalpies= -5458.777350
Sum of electronic and thermal Free Energies= -5458.894180

Cartesian coordinates

0 1

O	-2.28697100	-1.53849600	-1.40178700
S	-3.27941300	-2.15660500	-0.41409500
O	-2.87870300	-1.48666500	0.88722000
C	-4.94007400	-1.42966100	-0.87399100
F	-4.87326200	-0.10281600	-0.90302200
F	-5.83700300	-1.81322300	0.03447200
F	-5.29263700	-1.88874000	-2.07321200
O	-3.45311200	-3.59736500	-0.43759000
O	-0.05471400	0.04668300	-1.42958600
C	0.62040700	2.31440500	-2.55663200
F	-0.35605400	2.94848200	-1.90871900
F	0.16447500	1.87906800	-3.73147000
F	1.63409000	3.16150000	-2.76555400
O	2.24169500	0.20542000	-2.36639000
O	-0.90544000	0.69934500	1.63704200
S	-1.79676100	1.82908000	1.12497300
O	-2.35014600	1.20750700	-0.15194100
C	-3.23628500	1.90980200	2.32056900
F	-3.78245600	0.71144600	2.48249700
F	-4.14195200	2.75642600	1.83385000
F	-2.78422500	2.35947200	3.49143800
O	-1.25466100	3.17302400	1.06887200
Ga	-1.22910200	-0.52160400	-0.00514000
O	1.66135800	1.43633000	-0.24617500
S	1.23862400	0.88154300	-1.53864300
O	-0.11744300	-1.86241800	0.72551600
C	1.18423700	-1.71690300	0.77754100
C	1.72885800	-0.95878800	1.92023500
C	2.02945200	-2.14959600	-0.21171100
C	3.02491900	-0.57928500	1.99791200
H	1.01355600	-0.68287500	2.68802900
C	3.40875300	-1.75815500	-0.18477400
H	1.62992000	-2.65024400	-1.08457200
H	3.40165600	0.01848300	2.82085500
H	3.92974900	-1.70883300	-1.13636000
C	3.91611000	-0.90758600	0.91371000
C	5.77602900	-2.61303300	0.43650800

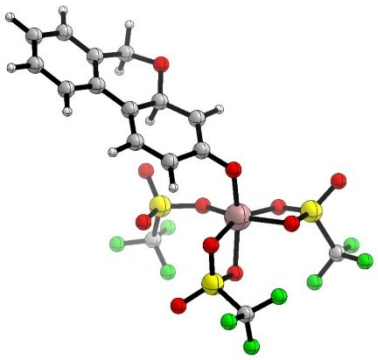
H	5.85202900	-3.08240700	-0.55276400
H	6.27927400	-3.24922800	1.17210000
C	5.23919000	-0.27881700	0.74890900
C	6.26372600	-1.18547000	0.45152800
O	4.37866200	-2.60434700	0.83112400
C	7.56041100	-0.73064800	0.23662300
H	8.36475800	-1.42766400	0.01719600
C	5.49199700	1.09107100	0.83733800
H	4.68008600	1.78564400	1.02958700
C	6.79448500	1.54402700	0.61872300
H	7.00830200	2.60695800	0.67375800
C	7.81955300	0.64091200	0.32391300
H	8.83005600	1.00529200	0.16435800

Vibrational frequencies

1	-378.70	54.6249	30	230.96	17.4234	59	540.55	31.9539
2	10.67	1.8100	31	235.89	1.0659	60	542.58	11.8845
3	18.33	1.3501	32	236.44	3.9412	61	551.41	1.8286
4	19.24	0.4907	33	245.89	11.9559	62	557.75	3.8440
5	22.39	0.0472	34	270.24	17.9623	63	560.98	1.0017
6	25.66	0.1016	35	283.65	11.7652	64	562.76	2.8289
7	29.27	0.1500	36	300.22	18.4040	65	581.60	55.2628
8	29.78	0.0877	37	308.47	11.9262	66	585.99	60.0112
9	34.00	0.1376	38	312.61	10.6325	67	592.97	32.5018
10	42.01	0.4289	39	315.25	8.8432	68	607.44	80.6309
11	45.00	0.7107	40	316.21	7.5215	69	616.45	107.9548
12	55.69	0.4809	41	317.47	16.1569	70	623.68	5.5127
13	60.46	1.7465	42	322.03	0.9119	71	652.42	123.1147
14	66.37	0.1079	43	328.13	4.0683	72	664.88	358.9733
15	77.92	0.6065	44	364.71	28.0507	73	676.39	4.5096
16	85.89	1.9689	45	372.93	1.1510	74	688.77	38.2499
17	90.06	0.1340	46	383.03	40.3202	75	718.94	1.5046
18	97.27	0.4677	47	394.33	59.2002	76	733.76	20.2081
19	114.80	1.7284	48	394.86	15.0418	77	765.28	1.6648
20	131.23	0.9167	49	427.55	43.1680	78	769.14	0.1120
21	133.43	10.2201	50	440.43	103.0250	79	769.90	0.0271
22	147.22	3.1976	51	452.71	2.3841	80	777.18	38.6494
23	157.04	4.6162	52	482.39	10.3837	81	824.27	13.5969
24	169.15	3.2029	53	491.86	27.9852	82	837.18	7.0778
25	185.80	1.4865	54	494.37	2.4403	83	850.05	101.7327
26	196.86	4.0288	55	500.89	31.0248	84	860.87	18.5997
27	200.38	3.5214	56	517.39	74.9367	85	890.91	0.3198
28	213.11	17.8336	57	522.62	13.9856	86	945.70	508.4646
29	217.28	6.1620	58	531.06	89.0241	87	952.69	161.4772

88	958.10	13.5249	107	1219.52	92.5485	126	1458.60	255.2142
89	967.73	373.5188	108	1225.69	4.0425	127	1476.11	146.5913
90	976.51	144.3738	109	1230.14	0.5012	128	1503.16	17.3672
91	979.17	6.6280	110	1251.04	249.8154	129	1517.29	1.9859
92	1001.78	0.1132	111	1256.58	88.8145	130	1532.46	6.3709
93	1006.36	1.4858	112	1258.80	321.3995	131	1601.65	428.9899
94	1028.28	14.6398	113	1260.71	171.4460	132	1638.32	6.9853
95	1032.74	10.8269	114	1273.80	120.1727	133	1659.67	15.2202
96	1035.91	72.0637	115	1278.00	135.5684	134	1673.93	96.8489
97	1055.92	153.4536	116	1287.65	1.3249	135	3051.06	25.3218
98	1060.62	7.9304	117	1303.50	160.7147	136	3107.96	6.8813
99	1067.06	28.6223	118	1314.47	23.9020	137	3194.10	2.5576
100	1129.06	77.2343	119	1322.66	787.4766	138	3205.92	6.0568
101	1134.54	157.2374	120	1327.09	194.6871	139	3209.53	1.3546
102	1163.90	4.7802	121	1333.83	42.4540	140	3215.44	9.1120
103	1190.20	131.5940	122	1344.30	1.5834	141	3219.51	0.4228
104	1195.09	161.8733	123	1358.35	41.4533	142	3225.16	7.9649
105	1198.33	0.5117	124	1374.89	139.9458	143	3239.64	0.2094
106	1202.64	20.6194	125	1389.86	7.2147	144	3249.76	1.5856

INT2



Zero-point correction= 0.285225 (Hartree/Particle)
Thermal correction to Energy= 0.323585
Thermal correction to Enthalpy= 0.324530
Thermal correction to Gibbs Free Energy= 0.208252
Sum of electronic and zero-point Energies= -5458.856245
Sum of electronic and thermal Energies= -5458.817885
Sum of electronic and thermal Enthalpies= -5458.816941
Sum of electronic and thermal Free Energies= -5458.933218

Cartesian coordinates

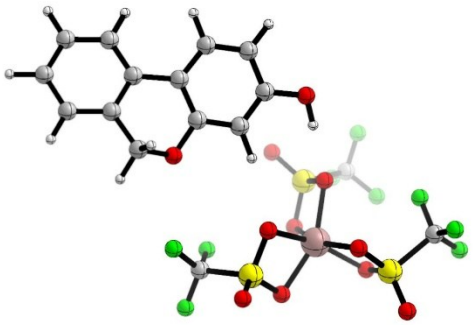
0 1

O	2.07779100	-1.76148100	1.17041500
S	2.97798400	-2.41621600	0.12138900

O	2.71109500	-1.55312900	-1.09851400
C	4.72401400	-2.01330600	0.65621500
F	4.86806800	-0.70143800	0.81453100
F	5.56606900	-2.44619300	-0.28174900
F	4.97592000	-2.63543200	1.80633400
O	2.92350400	-3.86016000	-0.01532800
O	0.08232000	0.09546500	1.36491000
C	-0.32764600	2.22454800	2.85087700
F	0.87112400	2.69130300	2.50868000
F	-0.22368600	1.49835200	3.96378600
F	-1.15975000	3.24643100	3.06679100
O	-2.26697700	0.60751500	1.97865200
O	1.17166100	0.98649300	-1.62699400
S	2.18829700	1.90156400	-0.94899400
O	2.55812700	1.06565800	0.27438000
C	3.69990900	1.88055400	-2.05571800
F	4.09226000	0.63639300	-2.29758000
F	4.67644700	2.55068100	-1.44632900
F	3.38739900	2.48465400	-3.20198500
O	1.86126700	3.30108100	-0.75895700
Ga	1.22155400	-0.44284400	-0.11721200
O	-1.06180100	2.02672100	0.27554000
S	-1.00778800	1.17634400	1.46847300
O	-0.07698700	-1.49378400	-0.97712500
C	-1.36401500	-1.20761800	-0.92964700
C	-1.89529600	-0.10671700	-1.67924900
C	-2.25874200	-1.93977900	-0.17125300
C	-3.24761200	0.22854100	-1.71347700
H	-1.18608000	0.47213300	-2.26346100
C	-3.63560200	-1.46542300	0.00859300
H	-1.92026400	-2.76431900	0.44726200
H	-3.55539000	1.05410500	-2.34570600
H	-3.41862300	-0.75086300	0.87579600
C	-4.18050800	-0.47777600	-0.96132300
C	-5.72212300	-1.90142900	0.94940400
H	-5.47997300	-1.33098200	1.86395500
H	-6.35849400	-2.74283300	1.23343100
C	-5.61746400	-0.27708200	-0.97663100
C	-6.40897800	-1.00853200	-0.05537600
O	-4.52686700	-2.46699400	0.41534000
C	-7.79373700	-0.85571900	-0.06208900
H	-8.39847100	-1.41877500	0.64429500
C	-6.25376800	0.58851100	-1.89188600

H	-5.66573200	1.14107300	-2.61682400
C	-7.63373300	0.73123500	-1.88557300
H	-8.11180900	1.39892100	-2.59565600
C	-8.40663000	0.01033800	-0.96778700
H	-9.48735300	0.11875000	-0.96474400

4a+Ga(OTf)$_3$



Zero-point correction= 0.286680 (Hartree/Particle)
Thermal correction to Energy= 0.325422
Thermal correction to Enthalpy= 0.326366
Thermal correction to Gibbs Free Energy= 0.206419
Sum of electronic and zero-point Energies= -5458.887443
Sum of electronic and thermal Energies= -5458.848700
Sum of electronic and thermal Enthalpies= -5458.847756
Sum of electronic and thermal Free Energies= -5458.967703

Cartesian coordinates

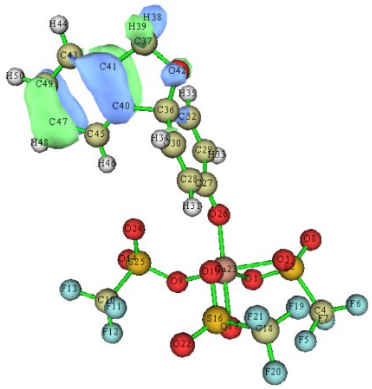
0 1

O	1.59056600	-0.05900600	-1.98923100
S	1.12192700	1.32942500	-1.53878200
O	1.31040500	1.18665400	-0.01209300
C	2.46684700	2.52600600	-2.07536600
F	3.63381900	2.12493600	-1.58321000
F	2.16163200	3.72792600	-1.60641000
F	2.50746600	2.54078300	-3.40089700
O	-0.14115200	1.82774900	-2.03262000
O	1.71904900	-2.68859400	-0.59613000
C	-0.89220400	-3.06833900	-1.33285200
F	-0.66537400	-4.25425200	-1.88607800
F	-0.72601100	-2.10468700	-2.23010200
F	-2.11328500	-3.02072000	-0.82303500
O	0.12348100	-1.37642200	0.53083400
O	2.74949900	-0.80761900	1.71582300
S	4.18790700	-0.80104100	1.17973400

O	3.91508700	-0.66580700	-0.32815300
C	4.90091800	0.85734400	1.69019500
F	4.08468800	1.82798900	1.28930000
F	6.08940200	0.99599600	1.11541200
F	5.02159700	0.87752900	3.01071000
O	5.10140500	-1.82893700	1.62715700
Ga	1.91465800	-0.74580600	-0.12483100
O	0.13803800	-3.89702700	1.02145500
S	0.33701900	-2.82784100	0.06827100
C	-2.03695100	2.42834000	1.13971000
C	-3.11889900	3.31555100	1.23384300
C	-2.26720100	1.06579600	0.93544600
C	-4.41291500	2.83435600	1.08580100
H	-2.92439400	4.36733400	1.41516400
C	-3.57415300	0.60387300	0.79611200
H	-1.45764400	0.34577200	0.89719800
H	-5.24114200	3.53332100	1.16032200
C	-4.68108400	1.47584400	0.84595200
C	-4.96654200	-1.27877900	1.06450300
H	-4.90567600	-1.31054300	2.16515800
H	-5.00652200	-2.30726100	0.69676000
C	-6.01600900	0.92191900	0.56624500
C	-6.16400600	-0.47866800	0.62097900
O	-3.73665900	-0.73758000	0.56115700
C	-7.38773000	-1.07456600	0.32239500
H	-7.48154300	-2.15797100	0.36277700
C	-7.12667800	1.69788600	0.20036900
H	-7.02848500	2.77600000	0.11424800
C	-8.35410200	1.09854100	-0.07719800
H	-9.20299200	1.71785000	-0.35492900
C	-8.49104800	-0.28983400	-0.01835200
H	-9.44487800	-0.75804500	-0.24485900
O	-0.78270500	2.94644300	1.28223600
H	-0.12173500	2.25490300	1.10898900

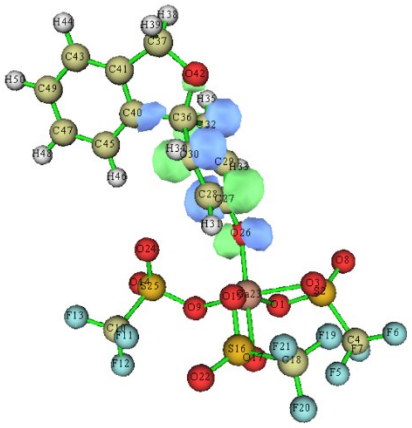
HOMO and LUMO respective orbital coefficients of each atom in **2a-Ga(OTf)$_3$**

2a-Ga(OTf)$_3$-HOMO



Atom	1(O)	0.00%	Atom	26(O)	0.00%
Atom	2(S)	0.00%	Atom	27(C)	-0.06%
Atom	3(O)	0.00%	Atom	28(C)	0.91%
Atom	4(C)	0.00%	Atom	29(C)	0.73%
Atom	5(F)	0.00%	Atom	30(C)	0.82%
Atom	6(F)	0.00%	Atom	31(H)	0.18%
Atom	7(F)	0.00%	Atom	32(C)	1.22%
Atom	8(O)	0.00%	Atom	33(H)	0.21%
Atom	9(O)	0.00%	Atom	34(H)	0.26%
Atom	10(C)	0.00%	Atom	35(H)	0.19%
Atom	11(F)	0.00%	Atom	36(C)	0.44%
Atom	12(F)	0.00%	Atom	37(C)	3.19%
Atom	13(F)	0.00%	Atom	38(H)	3.96%
Atom	14(O)	0.00%	Atom	39(H)	3.56%
Atom	15(O)	-0.01%	**Atom**	**40(C)**	**13.96%**
Atom	16(S)	0.01%	**Atom**	**41(C)**	**21.96%**
Atom	17(O)	0.00%	**Atom**	**42(O)**	**5.37%**
Atom	18(C)	0.00%	Atom	43(C)	3.48%
Atom	19(F)	0.00%	Atom	44(H)	0.02%
Atom	20(F)	0.00%	Atom	45(C)	3.08%
Atom	21(F)	0.00%	Atom	46(H)	0.02%
Atom	22(O)	0.00%	**Atom**	**47(C)**	**24.11%**
Atom	23(Ga)	0.02%	Atom	48(H)	0.18%
Atom	24(O)	0.02%	**Atom**	**49(C)**	**12.08%**
Atom	25(S)	0.01%	Atom	50(H)	0.08%

2a-Ga(OTf)$_3$-LUMO



Atom	1(O)	0.04%	**Atom**	**26(O)**	**13.38%**
Atom	2(S)	0.07%	**Atom**	**27(C)**	**30.13%**
Atom	3(O)	0.11%	Atom	28(C)	1.48%
Atom	4(C)	-0.02%	Atom	29(C)	3.01%
Atom	5(F)	0.00%	**Atom**	**30(C)**	**21.47%**
Atom	6(F)	0.00%	Atom	31(H)	0.00%
Atom	7(F)	0.00%	**Atom**	**32(C)**	**21.63%**
Atom	8(O)	0.00%	Atom	33(H)	0.00%
Atom	9(O)	-0.14%	Atom	34(H)	0.21%
Atom	10(C)	0.07%	Atom	35(H)	0.19%
Atom	11(F)	0.00%	Atom	36(C)	1.29%
Atom	12(F)	0.00%	Atom	37(C)	0.77%
Atom	13(F)	0.00%	Atom	38(H)	0.00%
Atom	14(O)	0.05%	Atom	39(H)	0.03%
Atom	15(O)	0.03%	Atom	40(C)	8.63%
Atom	16(S)	-0.04%	Atom	41(C)	1.62%
Atom	17(O)	-0.01%	Atom	42(O)	0.44%
Atom	18(C)	0.01%	Atom	43(C)	-0.35%
Atom	19(F)	0.00%	Atom	44(H)	0.15%
Atom	20(F)	0.00%	Atom	45(C)	-2.14%
Atom	21(F)	0.00%	Atom	46(H)	-0.33%
Atom	22(O)	0.00%	Atom	47(C)	-2.87%
Atom	23(Ga)	0.98%	Atom	48(H)	0.08%
Atom	24(O)	-0.08%	Atom	49(C)	-0.11%
Atom	25(S)	0.22%	Atom	50(H)	0.01%

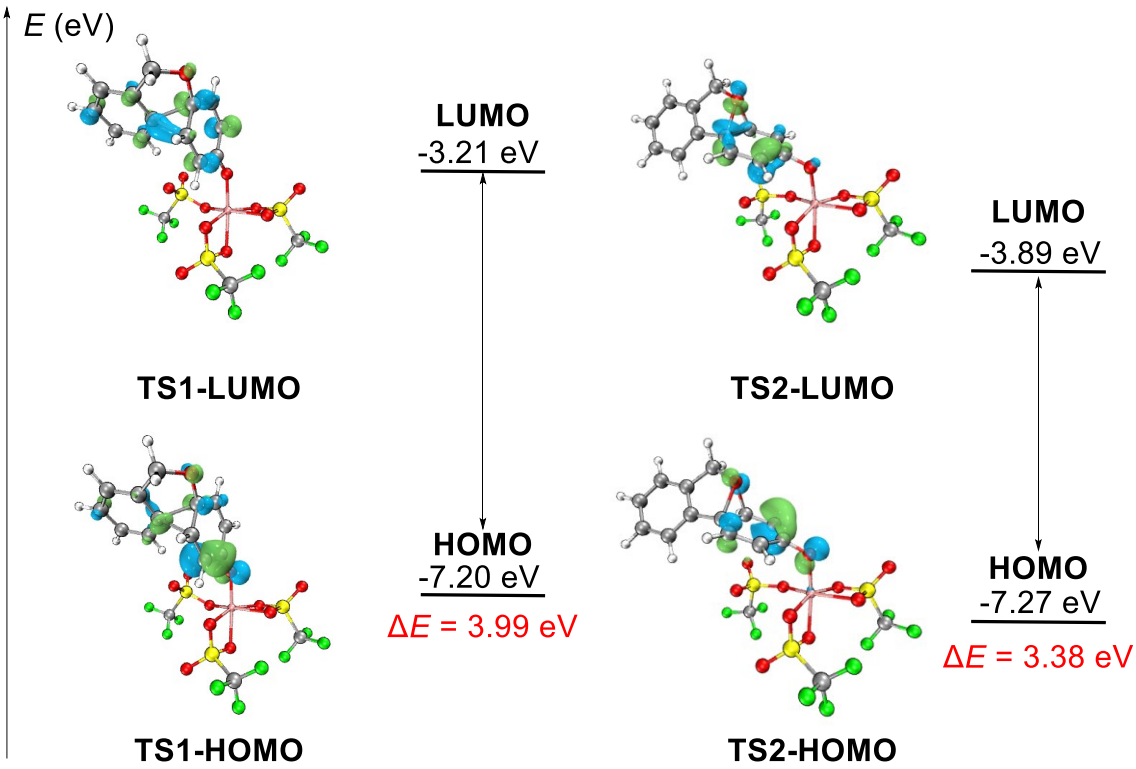


Figure S65 Optimized geometries, HOMO and LUMO of **TS1** and **TS2**