Supporting Information for

Photoinduced hydroxylation of arylboronic acids with molecular oxygen under photocatalyst-free conditions

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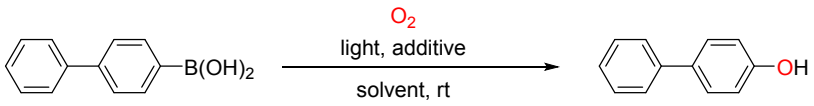
1. General Information

Unless otherwise noted, all materials were obtained from commercial suppliers (TCI, Sigma-Aldrich, Alfa Aesar, Acros and Meryer) and used without further purification. All reactions were conducted using standard Schlenk techniques. A 15W UV lamp was used for photoirradiation. Column chromatography was performed using EM silica gel 60 (300−400 mesh). ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra were measured on a 500 MHz Bruker AVANCE spectrometer (500 MHz for ^{1}H, 125 MHz for ^{13}C and 470 MHz for ^{19}F), or 400 MHz Zhongke-Niujin spectrometer (400 MHz for ^{1}H and 100 MHz for ^{13}C), using DMSO-d_6 or $CDCl_3$ as the solvent with tetramethylsilane (TMS) as the internal standard at room temperature. Chemical shifts δ were given in ppm, the coupling constants J were given in Hz. Peak multiplicities were designated by the following abbreviations: s, singlet; d, doublet; t, triplet; m, multiplet. ^{1}H NMR spectra were referenced to DMSO-d_6 (2.50 ppm) or $CDCl_3$ (7.28 ppm), and ^{13}C NMR spectra were referenced to DMSO-d_6 (39.5 ppm) or $CDCl_3$ (77.0 ppm). Analysis of crude reaction mixture was done on the Varian 4000 GC/MS and Agilent 7890A/5975C.

2. Experimental Section

2.1 Optimization of Reaction Conditions[a]

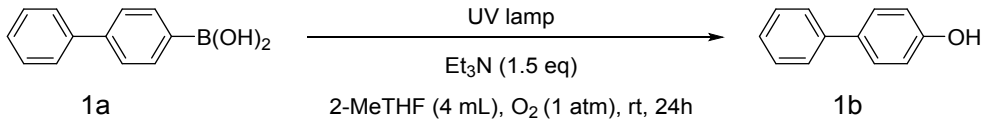


1a 1b

entry	light source	additive	solvent	Yield(%)
1	UV lamp	--	DMF	23
2	UV lamp	Et_3N	DMF	87
3	UV lamp	Et_3N	dioxane	40
4	UV lamp	Et_3N	THF	53
5	UV lamp	Et_3N	CH_3CN	77
6	UV lamp	Et_3N	toluene	41
7	UV lamp	Et_3N	DCM	23
8	UV lamp	Et_3N	DMSO	33
9	UV lamp	Et_3N	2-MeTHF	92
10	UV lamp	DIPEA	2-MeTHF	82
11	UV lamp	$(Me)_2EtN$	2-MeTHF	83
12	UV lamp	$(Me)_2{}^nBuN$	2-MeTHF	65
13[b]	UV lamp	Et_3N	2-MeTHF	58
14[c]	UV lamp	Et_3N	2-MeTHF	0
15	filament lamp	Et_3N	2-MeTHF	10
16	green LED	Et_3N	2-MeTHF	83
17	blue LED	Et_3N	2-MeTHF	80
18	dark	Et_3N	2-MeTHF	trace

[a]Reaction conditions: **1a** (0.3 mmol), O_2 (1 atm), light source (15 W), addition (0.45 mmol), solvent (4 mL), rt, 24 h, isolated yields. [b]Under the air atmosphere. [c]Under the N_2 atmosphere.

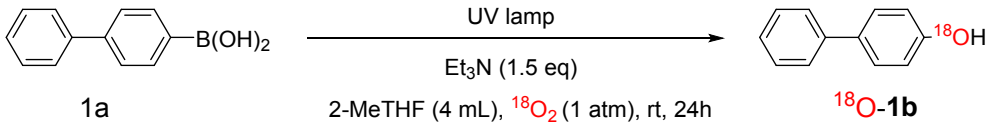
2.2 General Procedure for Synthesis of Phenols



1a 1b

An oven-dried 20 mL quarz test tube equipped with a magnetic stir bar was charged with [1,1'-biphenyl]-4-ylboronic acid (59.4 mg, 0.3 mmol, 1.0 equiv),and the quartz test tube was evacuated and backfilled with O_2 three times. Under O_2, Et_3N (62.5 μL, 0.45 mmol, 1.5 equiv) and 2-MeTHF (4 mL) were added in turn via syringe. The resulting mixture was stirred for 5 minutes, and then the quartz test tube transferred to photoreactor. The tube was placed approximately 2 cm from a 15 W UV lamp. The reaction mixture was stirred and irradiated for 24 h. After the indicated time period, the crude product was diluted with ethyl ether, filtered through a pad of silica gel and concentrated under reduced pressure. The residue was then purified by flash chromatography on silica gel (EtOAc/PE = 1/10) directly to give the desired product 1b (92% yield, white solid).

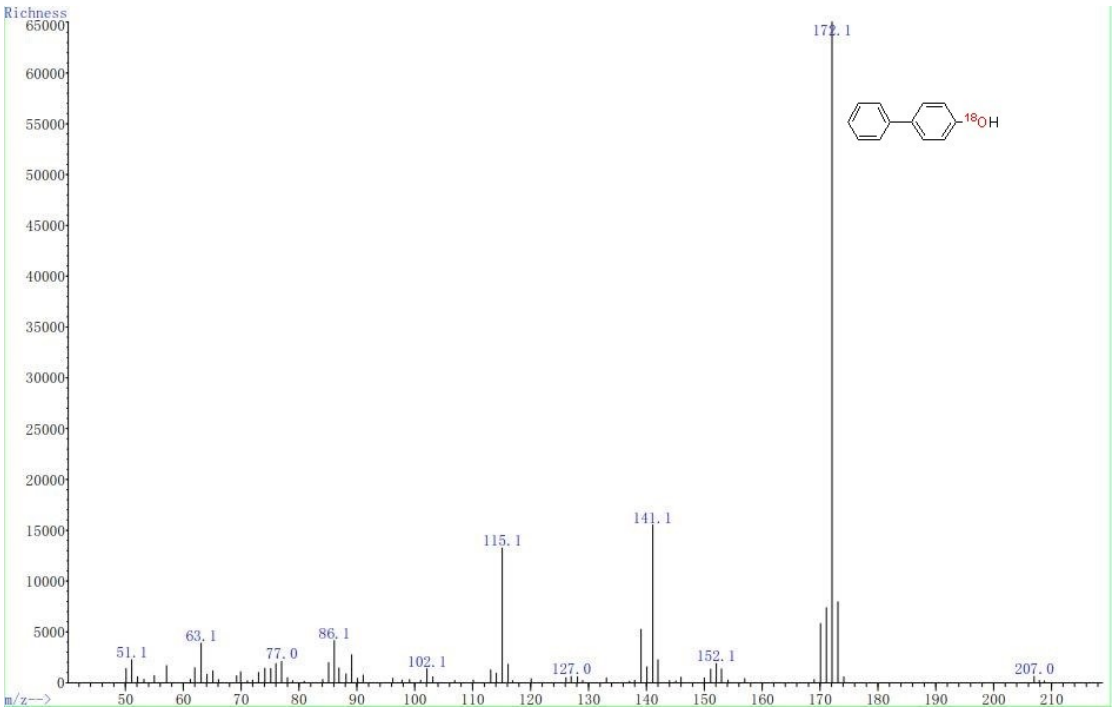
3. ^{18}O-Labeling Experiments



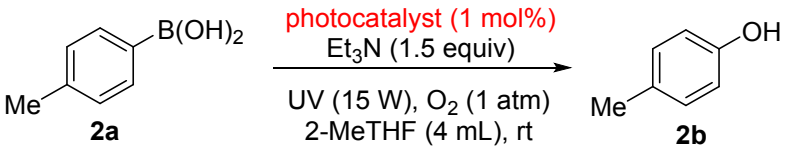
1a ^{18}O-**1b**

An oven-dried 20 mL quarz test tube equipped with a magnetic stir bar was charged with [1,1'-biphenyl]-4-ylboronic acid (59.4 mg, 0.3 mmol, 1.0 equiv),and the quartz test tube was evacuated and backfilled with $^{18}O_2$ three times. Under $^{18}O_2$, Et_3N (62.5 μL, 0.45 mmol, 1.5 equiv) and 2-MeTHF (4 mL) were added in turn via syringe. The resulting mixture was stirred for 5 minutes, and then the quartz test tube was transferred to photoreactor. The tube was placed approximately 2 cm from a 15 W UV lamp. The reaction mixture was stirred and irradiated for 24 h. After the indicated time period, the crude product was diluted with ethyl ether, filtered through a pad of silica gel and concentrated under reduced pressure. The residue was then purified by flash chromatography on silica geldirectly to give the desired product ^{18}O-**1b**.

The GC-MS shows a m/z peak of 172, which is in good agreement with that of ^{18}O-**1b**



4. Controlled Experiment



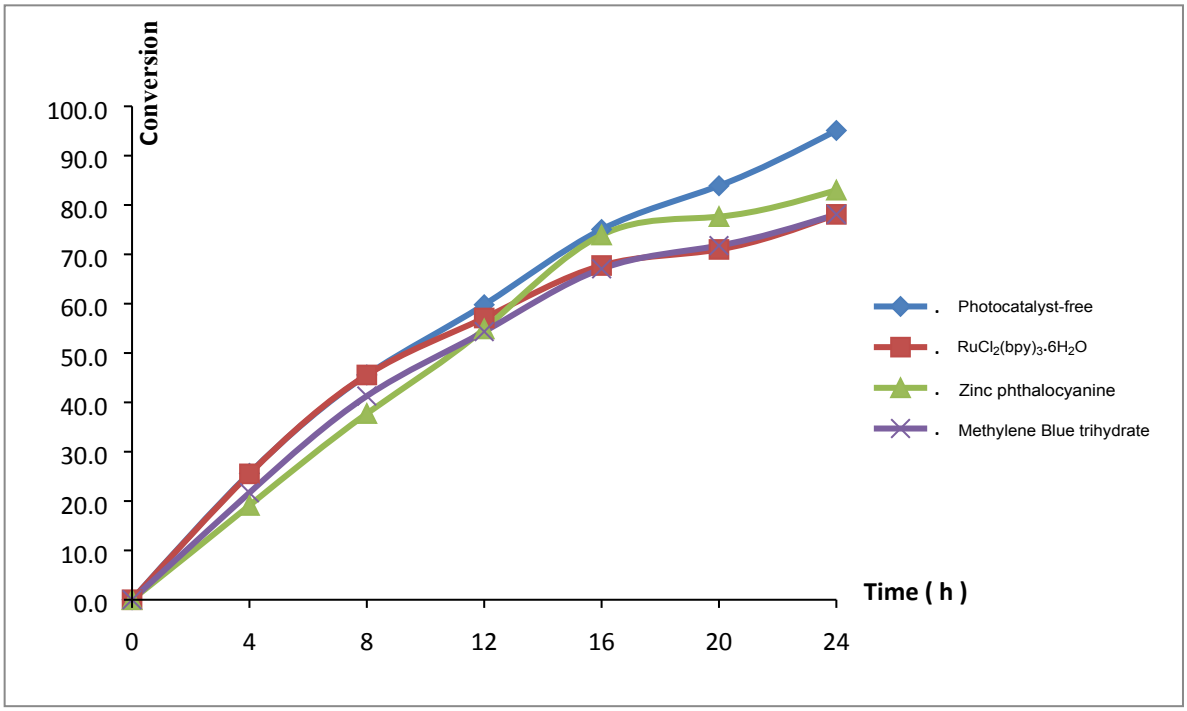
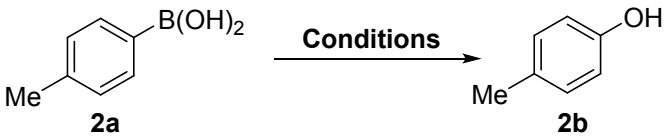


Figure S1. Conversion vs time plot for the reactions of **2a** with different photocatalysts or without photocatalyst. The conversion was determined by GC.



Condition A (standard reaction condition): Et_3N (1.5 equiv), UV (15 W), O_2 (1 atm), 2-MeTHF (4 mL), rt;

Condition B: Et_3N (1.5 equiv), 2,6-dimethyl phenol **36b** (1.5 equiv), UV (15 W), O_2 (1 atm), 2-MeTHF (4 mL), rt;

Condition C: 2,6-dimethyl phenol **36b** (1.5 equiv), UV (15 W), O_2 (1 atm), 2-MeTHF (4 mL), rt;

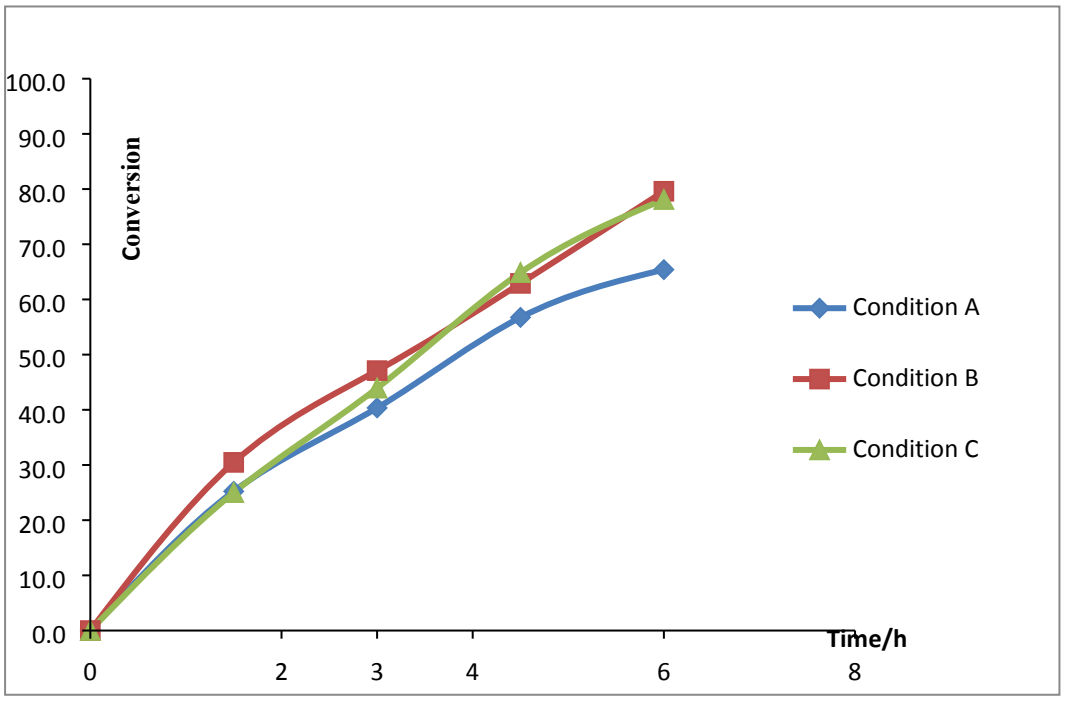
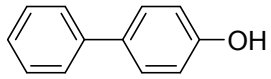


Figure S2. Conversion vs time plot for the reaction of **2a** under different conditions. The conversion was determined by GC.

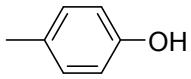
5. Characterization of Products in Details

4-Phenylphenol (1b)[1]



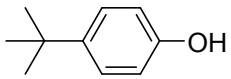
White solid (46.9 mg, 92% yield); EtOAc/PE = 1/10. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.61 (s, 1H), 7.60 (d, J = 8.0 Hz, 2H), 7.52 (d, J = 8.8 Hz, 2H), 7.45-7.41 (m, 2H), 7.32-7.28 (m, 1H), 6.89 (d, J = 8.8 Hz, 2H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 157.1, 140.2, 130.9, 128.7, 127.7, 126.3, 125.9, 115.7.

p-Cresol (2b)[1]



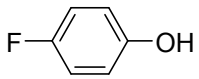
Faint yellow liquid (32.1 mg, 99% yield); EtOAc/PE = 1/10. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.11 (s, 1H), 6.98 (d, J = 8.0 Hz, 2H), 6.67 (d, J = 8.4 Hz, 2H), 2.20 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 155.0, 129.6, 127.1, 115.0, 20.0.

4-Tert-Butylphenol (3b)[2]



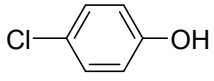
White solid (38.7 mg, 86% yield); EtOAc/PE = 1/10. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.16 (s, 1H), 7.19 (d, J = 8.8 Hz, 2H), 6.71 (d, J = 8.8 Hz, 2H), 1.25 (s, 9H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 154.9, 140.8, 125.8, 114.6, 33.6, 31.4.

4-Fluorophenol (4b)[3]



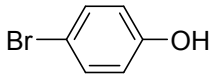
Yellow solid (31.9 mg, 95% yield); EtOAc/PE = 1/10. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.37 (s, 1H), 7.03-6.98 (m, 2H), 6.79-6.75 (m, 2H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 155.5 (d, $J_{C\text{-}F}$ = 231.3 Hz), 153.6 (d, $J_{C\text{-}F}$ = 2.5 Hz), 116.0 (d, $J_{C\text{-}F}$ = 7.5 Hz), 115.5 (d, $J_{C\text{-}F}$ = 22.5 Hz); ^{19}F NMR (470 MHz, DMSO-d_6) δ -126.4 (s, 1F).

4-Chlorophenol (5b)[1]



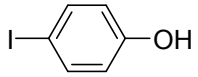
White solid (32.9 mg, 85% yield); EtOAc/PE = 1/10. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.70 (s, 1H), 7.23-7.19 (m, 2H), 6.82-6.78 (m, 2H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 156.3, 129.1, 122.3, 116.9.

4-Bromophenol (6b)[3]



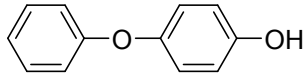
Yellow solid (26.8 mg, 52% yield); EtOAc/PE = 1/10. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.71 (s, 1H), 7.35-7.31 (m, 2H), 6.77-6.73 (m, 2H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 156.7, 132.0, 117.5, 109.9.

4-Iodophenol (7b)[3]



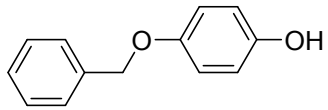
Off white solid (16.0 mg, 24% yield); EtOAc/PE = 1/10. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.70 (s, 1H), 7.50-7.46 (m, 2H), 6.66-6.62 (m, 2H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 157.3, 137.8, 118.2, 80.6.

4-Phenoxyphenol (8b)[4]



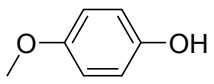
Faint yellow solid (40.6 mg, 73% yield); EtOAc/PE = 1/5. ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.35 (s, 1H), 7.33-7.31 (m, 2H), 7.05-7.02 (m, 1H), 6.88 (d, J = 7.5 Hz, 4H), 6.78 (d, J = 7.6 Hz, 2H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 158.4, 153.8, 147.8, 129.7, 122.2, 120.9, 116.9, 116.2.

4-(Phenylmethoxy)-phenol (9b)[5]



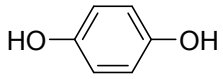
White solid (39.9 mg, 67% yield); EtOAc/PE = 1/5. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.97 (s, 1H), 7.46-7.38 (m, 4H), 7.36-7.32 (m, 1H), 6.86-6.83 (m, 2H), 6.72-6.68 (m, 2H), 5.01 (s, 2H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 151.3, 151.2, 137.5, 128.3, 127.6, 127.5, 115.8, 115.7, 69.7.

4-Methoxyphenol (10b)[1]



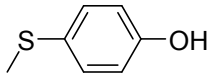
Clear colorless soild (26.5 mg, 71% yield); EtOAc/PE = 1/5. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.93 (s, 1H), 6.79-6.75 (m, 2H), 6.72-6.68 (m, 2H), 3.68 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 152.1, 151.1, 115.7, 114.6, 55.3.

Hydroquinone (11b)[1]



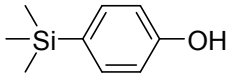
Off white soild (30.1 mg, 91% yield); EtOAc/PE = 1/5. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.64 (s, 2H), 6.56 (s, 4H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 149.7, 115.6.

4-(Methylthio)phenol (12b)[3]



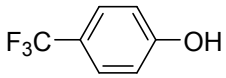
White solid (29.4 mg, 70% yield); EtOAc/PE = 1/5. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.48 (s, 1H), 7.19-7.15 (m, 2H), 6.78-6.74 (m, 2H), 2.41 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 155.9, 129.8, 125.9, 116.1, 17.2.

4-(Trimethylsilyl)phenol (13b)[6]



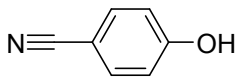
Off white solid (47.4 mg, 95% yield); EtOAc/PE = 1/5. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.50 (s, 1H), 7.33 (d, J = 8.4 Hz, 2H), 6.79 (d, J = 8.4 Hz, 2H), 0.21 (s, 9H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 159.0, 135.3, 129.0, 115.8, 0.0.

4-(Trifluoromethyl)phenol (14b)[3]



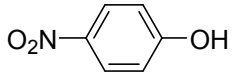
Yellow solid (40.8 mg, 84% yield); EtOAc/PE = 1/10. ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.30 (s, 1H), 7.55 (d, J = 8.4 Hz, 2H), 6.95 (d, J = 8.8 Hz, 2H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 160.7, 126.85 (q, $J_{C\text{-}F}$ = 3.8 Hz), 124.77 (q, $J_{C\text{-}F}$ = 268.8 Hz), 119.44 (q, $J_{C\text{-}F}$ = 31.3 Hz), 115.6; ^{19}F NMR (470 MHz, DMSO-d_6) δ -59.6 (s, 3F).

4-Cyanophenol (15b)[1]



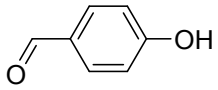
Off white solid (32.4 mg, 91% yield); EtOAc/PE = 1/5. ^{1}H NMR (400 MHz, DMSO-d_6) δ10.64 (s, 1H), 7.66 (d, J = 8.8 Hz, 2H), 6.93 (d, J = 8.8 Hz, 2H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 161.6, 134.2, 119.5, 116.4, 101.0.

4-Nitrophenol (16b)[3]



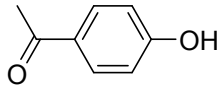
Faint yellow solid (37.9 mg, 91% yield); EtOAc/PE = 1/3. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.08 (s, 1H), 8.16-8.12 (m, 2H), 6.98-6.93 (m, 2H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 163.9, 139.6, 126.1, 115.7.

4-Hydroxybenzaldehyde (17b)[3]



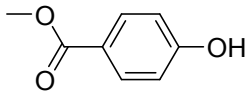
Faint yellow solid (34.4 mg, 94% yield); EtOAc/PE = 1/2. ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.61 (s, 1H), δ 9.79 (s, 1H), 7.76 (d, J = 8.0 Hz, 2H), 6.94 (d, J = 8.0 Hz, 2H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 190.8, 163.3, 132.0, 128.4, 115.8.

4'-Hydroxyacetophenone (18b)[2]



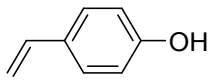
White solid (29.8 mg, 73% yield); EtOAc/PE = 1/3. ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.34 (s, 1H), 7.83 (d, J = 7.5 Hz, 2H), 6.84 (d, J = 7.5 Hz, 2H), 2.47 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 195.9, 162.0, 130.6, 128.6, 115.1, 26.2.

Methylparaben (19b)[3]



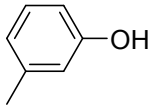
White solid (42.5 mg, 93% yield); EtOAc/PE = 1/5. ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.35 (s, 1H), 7.82 (d, J = 8.0 Hz, 2H), 6.85 (d, J = 6.8 Hz, 2H), 3.78 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 166.0, 161.9, 131.3, 120.3, 115.3, 52.5.

4-Hydroxystyrene (20b)[3]

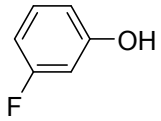


Clear colorless liquid (20.9 mg, 58% yield); EtOAc/PE = 1/5. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.56 (s, 1H), 7.32-7.29 (m, 2H), 6.79-6.75 (m, 2H), 6.63 (dd, J_1 = 10.8 Hz, J_2 = 17.6 Hz, 1H), 5.61 (dd, J_1 = 1.2 Hz, J_2 = 17.6 Hz, 1H), 5.06 (dd, J_1 = 0.8 Hz, J_2 = 10.8 Hz, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 157.3, 136.4, 128.3, 127.4, 115.3, 110.5.

m-Cresol (21b)[1]

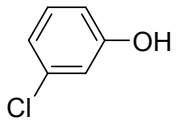


Brown liquid (30.0 mg, 93% yield); EtOAc/PE = 1/7. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.26 (s, 1H), 7.07-7.04 (m, 1H), 6.61-6.57 (m, 2H), 6.60 (s, 1H), 2.24 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 157.2, 138.6, 129.1, 119.5, 115.8, 112.3, 21.0. **3-Fluorophenol (22b)[7]**



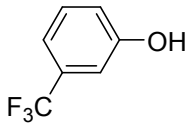
Brown liquid (23.6 mg, 70% yield); EtOAc/PE = 1/10. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.88 (s, 1H), 7.23-7.18 (m, 1H), 6.64-6.55 (m, 3H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 163.0 (d, J_{C-F} = 241.3 Hz), 159.0 (d, J_{C-F} = 11.3 Hz), 130.5 (d, J_{C-F} = 11.3 Hz), 111.52 (d, J_{C-F} = 2.5 Hz), 105.4 (d, J_{C-F} = 21.3 Hz), 102.4 (d, J_{C-F} = 23.8 Hz); ^{19}F NMR (470 MHz, DMSO-d_6) δ -112.5 (s, 1F).

3-Chlorophenol (23b)[7]



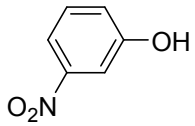
Faint yellow liquid (25.7 mg, 67% yield); EtOAc/PE = 1/5. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.93 (s, 1H), 7.22-7.18 (m, 1H), 6.85-6.83 (m, 2H), 6.78-6.75 (m, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 158.5, 133.4, 130.7, 118.7, 115.2, 114.2.

3-(Trifluoromethyl)phenol (24b)[7]



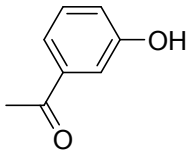
Yellow liquid (46.8 mg, 96% yield); EtOAc/PE = 1/10. ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.12 (s, 1H), 7.45-7.41 (m, 1H), 7.15 (s, 1H), 7.13-7.07 (m, 2H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 157.8, 130.6, 130.2 (q, J_{C-F} = 31.3 Hz), 124.1 (q, J_{C-F} = 270.0 Hz), 119.4, 115.3 (q, J_{C-F} = 3.8 Hz), 111.5 (q, J_{C-F} = 3.8 Hz); ^{19}F NMR (470 MHz, DMSO-d_6) δ -61.3 (s, 3F).

3-Nitrophenol (25b)[1]



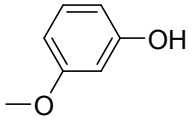
Faint yellow solid (38.9 mg, 93% yield); EtOAc/PE = 1/10. ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.46 (s, 1H), 7.67 (d, J = 8.0 Hz, 1H), 7.57 (s, 1H), 7.49-7.46 (m, 1H), 7.23 (d, J = 8.5 Hz, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 158.2, 148.7, 130.5, 122.3, 113.7, 109.5.

3'-Hydroxyacetophenone (26b)[2]



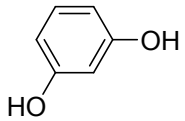
White solid (27.9 mg, 68% yield); EtOAc/PE = 1/3. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.26 (s, 1H), 7.42 (d, J = 7.6 Hz, 1H), 7.36-7.33 (m, 2H), 7.05 (d, J = 8.0 Hz, 1H), 2.55 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 197.7, 157.5, 138.2, 129.7, 120.2, 119.2, 114.2, 26.7.

3-Methoxyphenol (27b)[8]



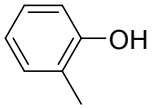
Light yellow liquid (36.8 mg, 99% yield); EtOAc/PE = 1/10. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.39 (s, 1H), 7.07-7.03 (m, 1H), 6.36-6.32 (m, 2H), 6.32 (s, 1H), 3.69 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 160.5, 158.5, 129.8, 107.8, 104.6, 101.2, 54.8.

Resorcinol (28b)[8]



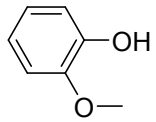
Faint yellow solid (32.3 mg, 98% yield); EtOAc/PE = 1/5. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.17 (s, 2H), 6.96-6.92 (m, 1H), 6.24-6.20 (m, 2H), 6.21 (s, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 158.4, 129.7, 106.2, 102.5.

o-Cresol (29b)[1]



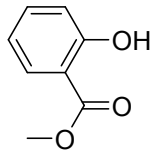
White solid (20.3 mg, 63% yield); EtOAc/PE = 1/10. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.26 (s, 1H), 7.06 (d, J = 7.4 Hz, 1H), 7.02-6.98 (m, 1H), 6.79 (d, J = 8.0 Hz, 1H), 6.72-6.68 (m, 1H), 2.14 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 155.6, 130.7, 126.8, 123.9, 118.9, 114.8, 16.1.

Guaiacol (30b)[1]



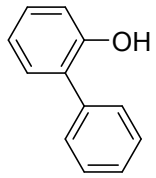
Light yellow liquid (25.5 mg, 69% yield); EtOAc/PE = 1/10. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.93 (s, 1H), 6.95-6.91 (m, 1H), 6.81-6.73 (m, 3H), 3.77 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 147.9, 146.9, 121.2, 119.4, 115.9, 112.7, 55.8.

Methyl salicylate (31b)[9]



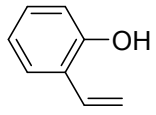
Clear colorless liquid (29.6 mg, 65% yield); EtOAc/PE = 1/15. ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.55 (s, 1H), 7.82-7.80 (m, 1H), 7.57-7.53 (m, 1H), 7.03-7.00 (m, 1H), 6.99-6.95 (m, 1H), 3.92 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 169.2, 160.0, 135.6, 129.9, 119.4, 117.4, 113.0, 42.4.

2-Phenylphenol (32b)[3]



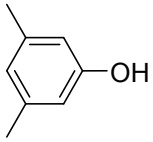
White solid (44.0 mg, 86% yield); EtOAc/PE = 1/15. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.56 (s, 1H), 7.56 (d, J = 8.0 Hz, 2H), 7.43-7.40 (m, 2H), 7.33-7.36 (m, 2H), 7.21-7.16 (m, 1H), 6.97 (d, J = 8.0 Hz, 1H), 6.92-6.88 (m, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 154.2, 138.6, 130.3, 129.0, 128.4, 127.9, 127.7, 126.4, 119.4, 116.0.

2-Hydroxystyrene (33b)[10]



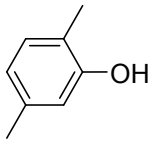
Clear colorless liquid (8.1 mg, 23% yield); EtOAc/PE = 1/15. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.65 (s, 1H), 7.46-7.44 (m, 1H), 7.13-7.09 (m, 1H), 6.96 (dd, J_1 = 11.2 Hz, J_2 = 17.6 Hz, 1H), 6.87-6.84 (m, 1H), 6.82-6.78 (m, 1H), 5.78 (dd, J_1 = 1.6 Hz, J_2 = 18.0 Hz, 1H), 5.21 (dd, J_1 = 1.6 Hz, J_2 = 11.2 Hz, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 154.7, 131.8, 128.7, 126.2, 123.9, 119.1, 115.7, 113.5.

3,5-Dimethylphenol (34b)[3]



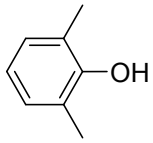
White solid (19.5 mg, 53% yield); EtOAc/PE = 1/10. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.14 (s, 1H), 6.42 (s, 1H), 6.39 (s, 2H), 2.19 (s, 6H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 157.5, 138.6, 120.8, 113.3, 21.3.

2,5-Dimethylphenol (35b)[9]



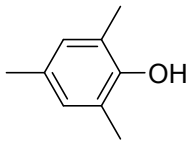
White solid (26.7 mg, 73% yield); EtOAc/PE = 1/10. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.13 (s, 1H), 6.93 (d, J = 7.6 Hz, 1H), 6.61 (s, 1H), 6.51 (d, J = 7.6 Hz, 1H), 2.20 (s, 3H), 2.09 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 155.1, 135.6, 130.2, 120.5, 119.4, 115.3, 20.7, 15.5.

2,6-Dimethylphenol (36b)[1]



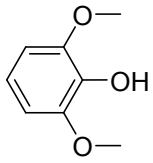
Faint yellow solid (20.3 mg, 55% yield); EtOAc/PE = 1/15. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.19 (s, 1H), 6.91 (d, J = 7.2 Hz, 2H), 6.67-6.63 (m, 1H), 2.17 (s, 6H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 153.1, 128.1, 124.1, 119.1, 16.5.

2,4,6-Trimethylphenol (37b)[8]



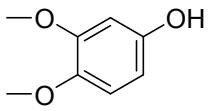
White solid (31.8 mg, 78% yield); EtOAc/PE = 1/10. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.93 (s, 1H), 6.72 (s, 2H), 2.15 (s, 3H), 2.14 (s, 6H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 150.7, 128.6, 127.3, 124.0, 20.0, 16.4.

2,6-Dimethoxyphenol (38b)[3]



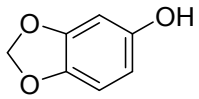
Off white solid (35.2 mg, 76% yield); EtOAc/PE = 1/5. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.28 (s, 1H), 6.74-6.70 (m, 1H), 6.63-6.61 (m, 2H), 3.77 (s, 6H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 148.2, 135.7, 118.1, 105.8, 56.0.

3,4-Dimethoxyphenol (39b)[7]



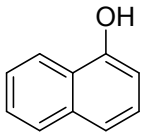
Faint yellow solid (36.9 mg, 80% yield); EtOAc/PE = 1/5. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.97 (s, 1H), 6.76 (d, J = 8.4 Hz, 1H), 6.43 (d, J = 2.8 Hz, 1H), 6.29-6.26 (m, 1H), 3.72 (s, 3H), 3.67 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 151.9, 149.8, 141.8, 113.8, 105.6, 100.9, 56.4, 55.3.

Benzo[d][1,3]dioxol-5-ol (40b)[6]



White solid (36.5 mg, 88% yield); EtOAc/PE = 1/5. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.15 (s, 1H), 6.72 (d, J = 8.4 Hz, 1H), 6.40 (d, J = 2.4 Hz, 1H), 6.23-6.20 (m, 1H), 5.92 (s, 2H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 152.5, 147.6, 139.6, 108.1, 106.2, 100.5, 97.8.

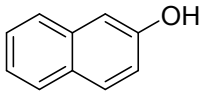
Naphthalen-1-ol (43b)[1]



Off white solid (35.5 mg, 82% yield); EtOAc/PE = 1/10. ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.32 (s, 1H), 8.34 (d, J = 7.0 Hz, 1H), 8.01 (d, J = 6.5 Hz, 1H), 7.67-7.46 (m,

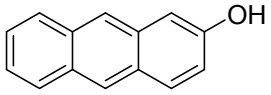
4H), 7.08 (d, J = 5.0 Hz, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 153.1, 134.4, 127.3, 126.4, 126.0, 124.6, 124.5, 121.9, 118.3, 108.0.

Naphthalen-2-ol (44b)[1]

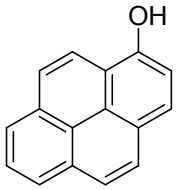


White solid (34.2 mg, 79% yield); EtOAc/PE = 1/10. ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.74 (s, 1H), 7.77-7.74 (m, 2H), 7.67 (d, J = 8.0 Hz, 1H), 7.39-7.37 (m, 1H), 7.27-7.24 (m, 1H), 7.12 (s, 1H), 7.10-7.08 (m, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 155.3, 134.6, 129.2, 127.7, 127.5, 126.1, 125.9, 122.6, 118.6, 108.6.

Anthracen-2-ol (45b)[6]

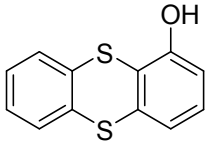


Yellow solid (29.2 mg, 50% yield); EtOAc/PE = 1/5. ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.94 (s, 1H), 8.42 (s, 1H), 8.27 (s, 1H), 7.97-7.96 (m, 3H), 7.43-7.38 (m, 2H), 7.24 (s, 1H), 7.17 (d, J = 8.0 Hz, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 154.8, 132.9, 131.7, 129.8, 129.3, 128.1, 127.3, 126.0, 125.4, 124.0, 122.8, 120.6, 106.5. **1-Hydroxypyrene (46b)[1]**



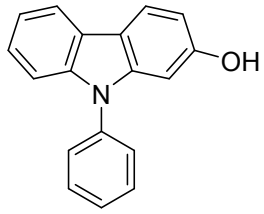
Yellow solid (46.2 mg, 71 % yield); EtOAc/PE = 1/5. ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.72 (s, 1H), 8.38 (d, J = 8.8 Hz, 1H), 8.15-8.13 (m, 3H), 8.08-7.97 (m, 3H), 7.92 (d, J = 8.8 Hz, 1H), 7.64 (d, J = 8.4 Hz, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 152.2, 131.4, 131.3, 127.4, 126.1, 126.1, 125.5, 125.4, 124.5, 123.9, 123.8, 123.6, 123.6, 121.4, 118.1, 113.2.

1-Thianthrenol (47b)[11]



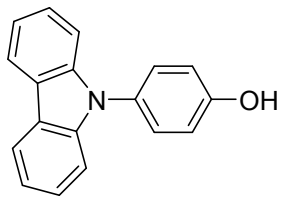
Yellow solid (51.1 mg, 73 % yield); EtOAc/PE = 1/5. ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.48 (s, 1H), 7.60-7.53 (m, 2H), 7.36-7.31 (m, 2H), 7.18-7.14 (m, 1H), 7.01 (d, J = 7.6 Hz, 1H), 6.89 (d, J = 8.0 Hz, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 155.0, 134.7, 134.6, 128.7, 128.4, 128.0, 127.9, 120.9, 119.4, 114.2.

9-Phenyl-9H-carbazol-2-ol (48b) [12]



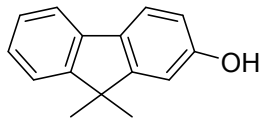
Faint yellow solid (66.1 mg, 85% yield); EtOAc/PE = 1/5. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.57 (s, 1H), 8.09 (d, J = 7.6 Hz, 1H), 8.02 (d, J = 8.4 Hz, 1H), 7.73-7.69 (m, 2H), 7.63-7.61 (m, 2H), 7.57-7.53 (m, 1H), 7.34-7.28 (m, 2H), 7.25-7.21 (m, 1H), 6.80-6.76 (m, 2H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 157.0, 141.9, 140.1, 137.0, 130.1, 127.5, 126.6, 124.3, 123.3, 121.3, 119.9, 119.2, 115.2, 109.6, 109.1, 95.3.

N-(4-hydroxyphenyl)carbazole (49b)[13]



Faint yellow liquid (54.8 mg, 71% yield); EtOAc/PE = 1/5. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.89 (s, 1H), 8.24 (d, J = 7.6 Hz, 2H), 6.45-7.38 (m, 4H), 7.31-7.26 (m, 4H), 7.07 (d, J = 8.4 Hz, 2H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 156.9, 140.7, 128.2, 127.8, 126.0, 122.3, 120.3, 119.5, 116.6, 109.5.

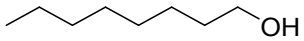
9,9-Dimethyl-9H-fluoren-2-ol (50b)[14]



Yellow solid (53.4 mg, 85% yield); EtOAc/PE = 1/5. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.52 (s, 1H), 7.66 (d, J = 7.2 Hz, 1H), 7.62 (d, J = 8.0 Hz, 1H), 7.48 (d, J = 7.2 Hz, 1H), 7.31-7.27 (m, 1H), 7.23-7.19 (m, 1H), 6.93 (d, J = 2.0 Hz, 1H), 6.77 (dd, J_1 =

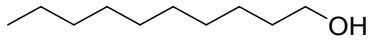
2.4 Hz, J_2 = 8.4 Hz, 1H), 1.41 (s, 6H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 157.5, 155.2, 152.6, 139.0, 129.7, 126.8, 125.6, 122.4, 120.9, 118.7, 114.1, 109.8, 46.1, 27.0.

1-Octanol (51b)[15]



Clear colorless liquid (27.7 mg, 71% yield); EtOAc/PE = 1/10. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.65-3.61 (m, 2H), 1.83 (s, 1H), 1.60-1.53 (m, 2H), 1.40-1.27 (m, 10H), 0.88 (t, J = 6.8 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 63.1, 32.8, 31.9, 29.4, 29.3, 25.8, 22.7, 14.1.

Decan-1-ol (52b) [12]



Clear colorless liquid (47.7 mg, 99% yield); EtOAc/PE = 1/10. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.63 (t, J = 6.8 Hz, 2H), 2.04 (s, 1H), 1.60-1.53 (m, 2H), 1.36-1.28 (m, 14H), 0.88 (t, J = 6.8 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 63.1, 32.9, 32.0, 19.7, 29.6, 29.5, 29.4, 25.8, 22.7, 14.1.

Reference:

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6. NMR spectra

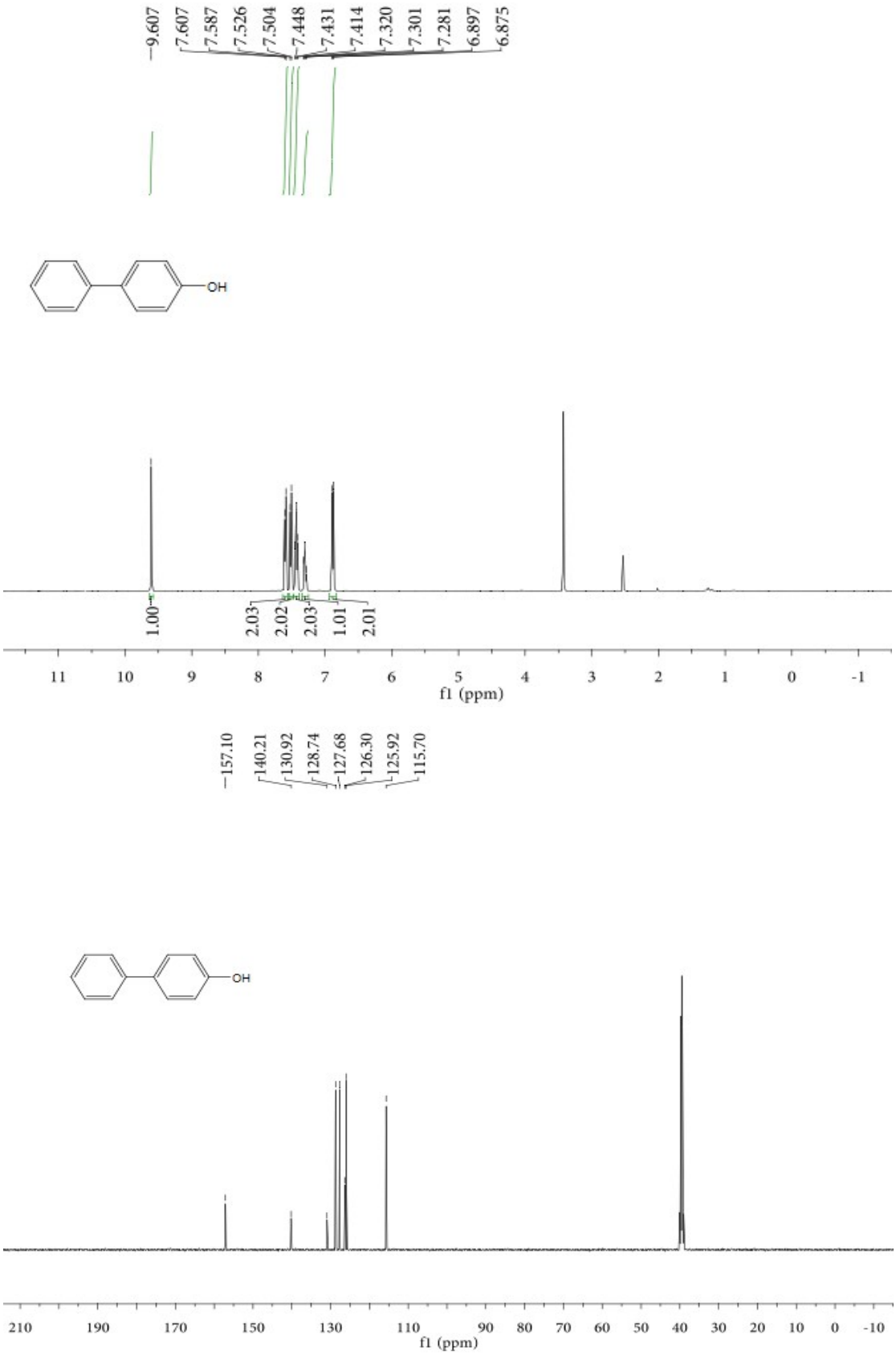


Figure S3. ^{1}H NMR of **1b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **1b** (125 MHz, DMSO-d_6)

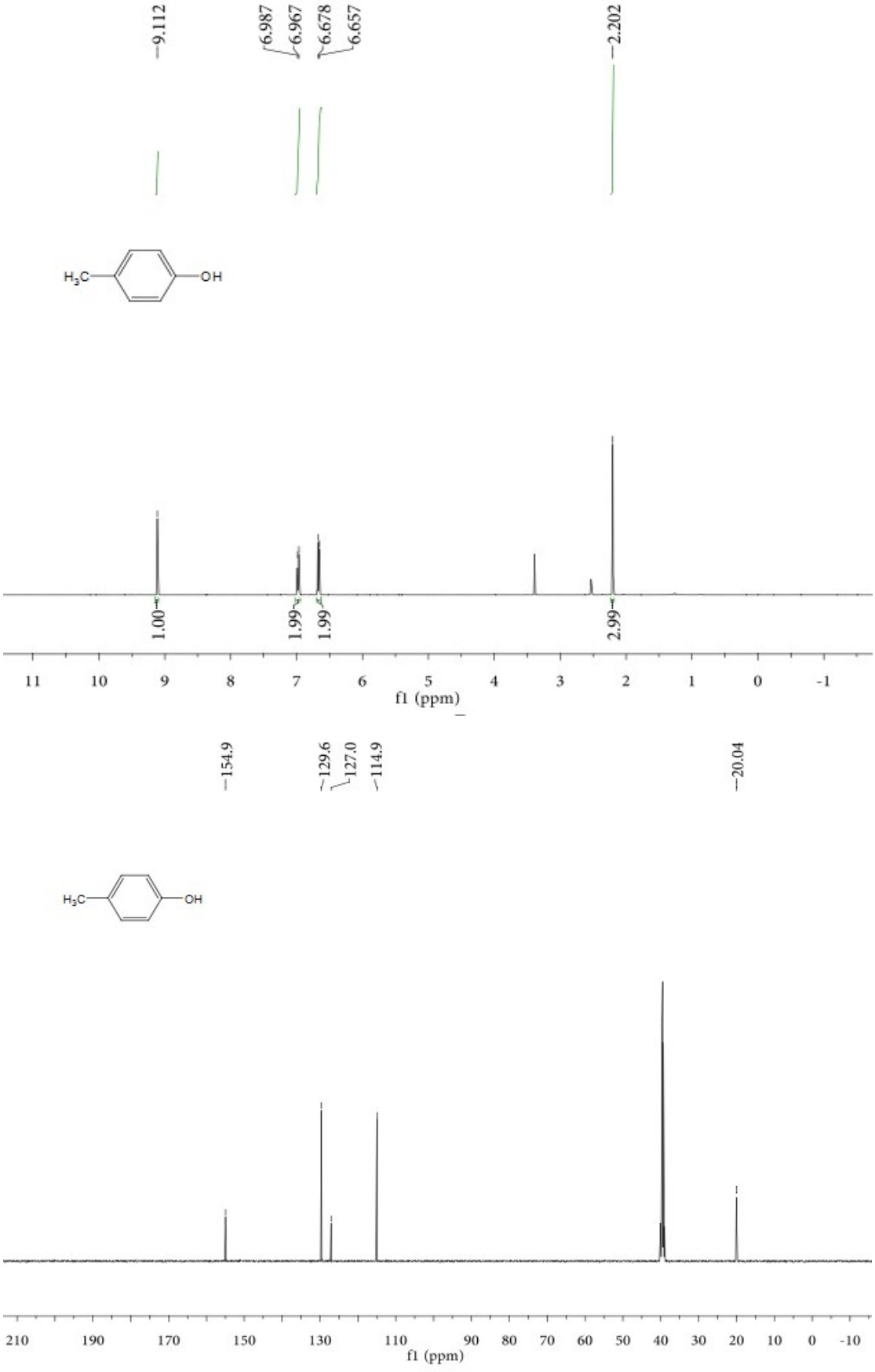


Figure S4. ^{1}H NMR of **2b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **2b** (125 MHz, DMSO-d_6)

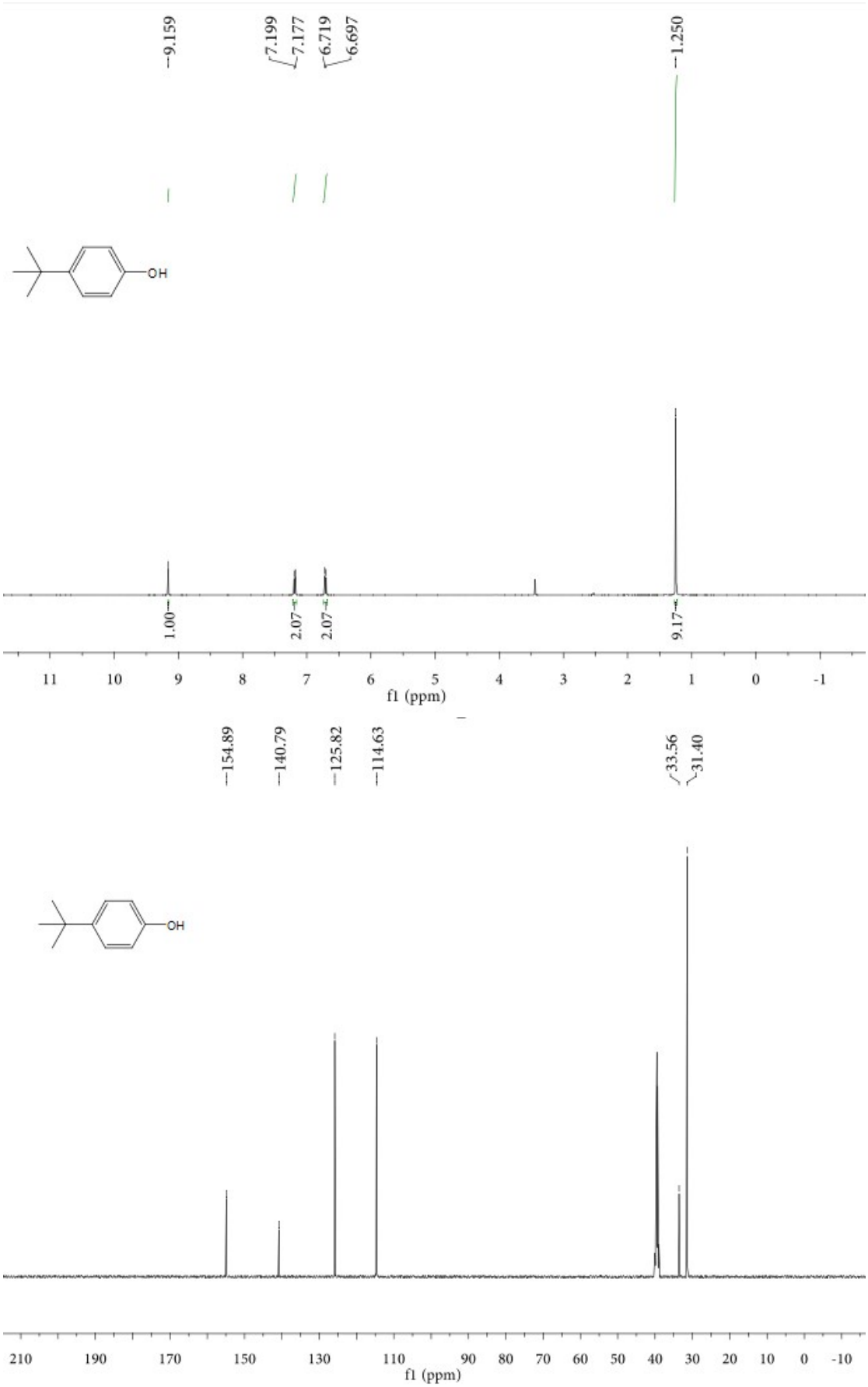
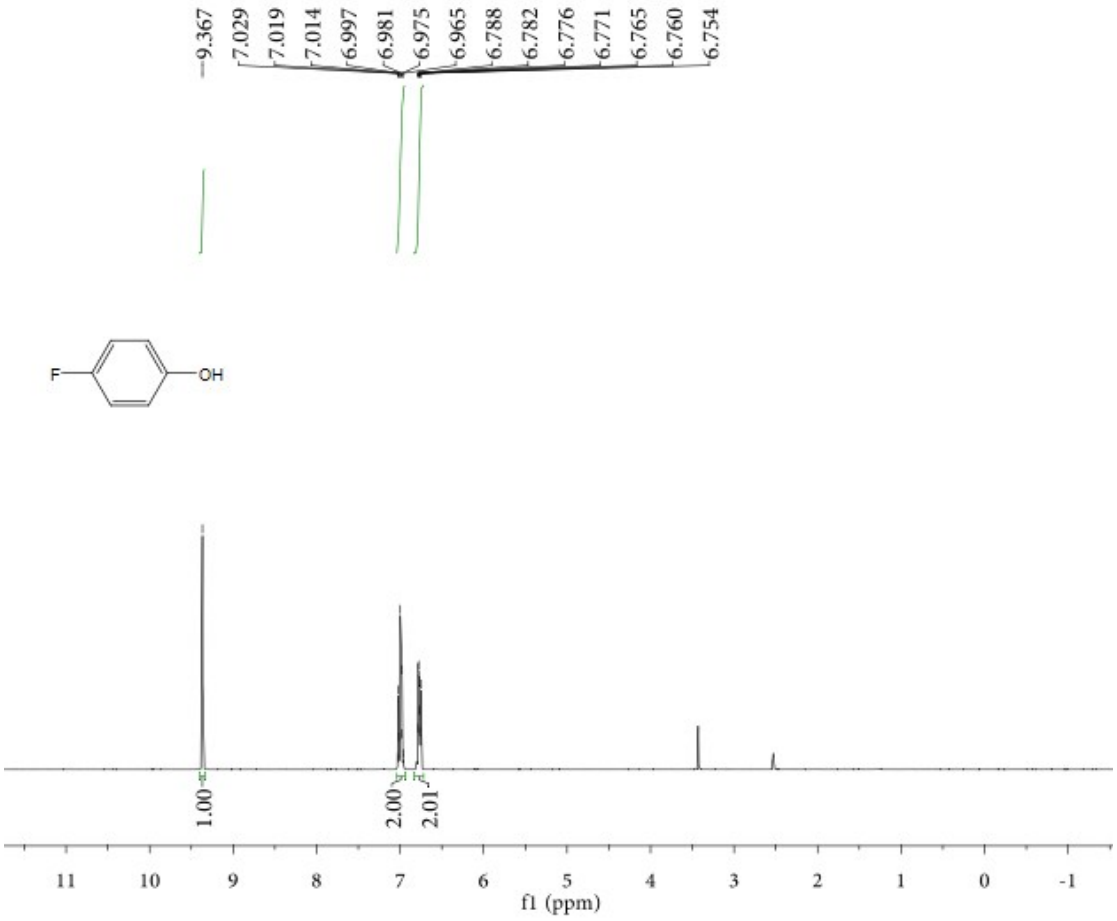
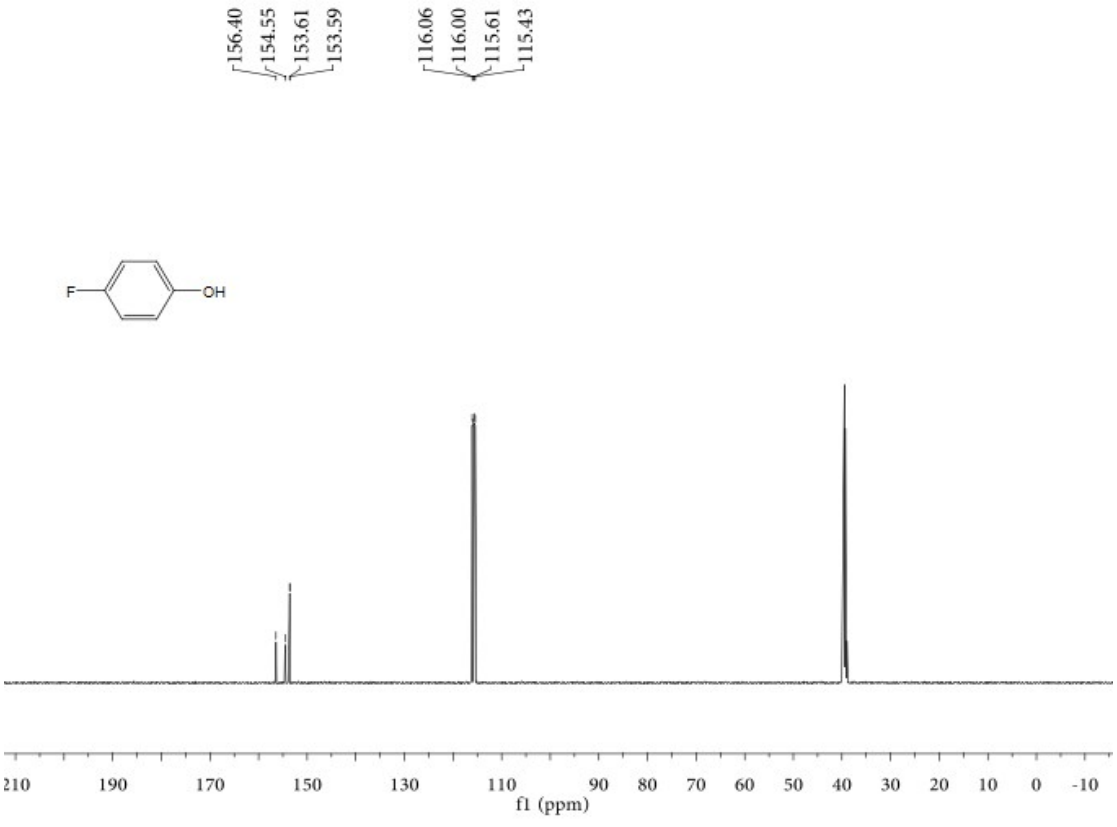


Figure S5. ^{1}H NMR of **3b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **3b** (125 MHz, DMSO-d_6)


9.367
7.029
7.019
7.014
6.997
6.981
6.975
6.965
6.788
6.782
6.776
6.771
6.765
6.760
6.754
F
OH
1.00
2.00
2.01
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)


156.40
154.55
153.61
153.59
116.06
116.00
115.61
115.43
F
OH
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

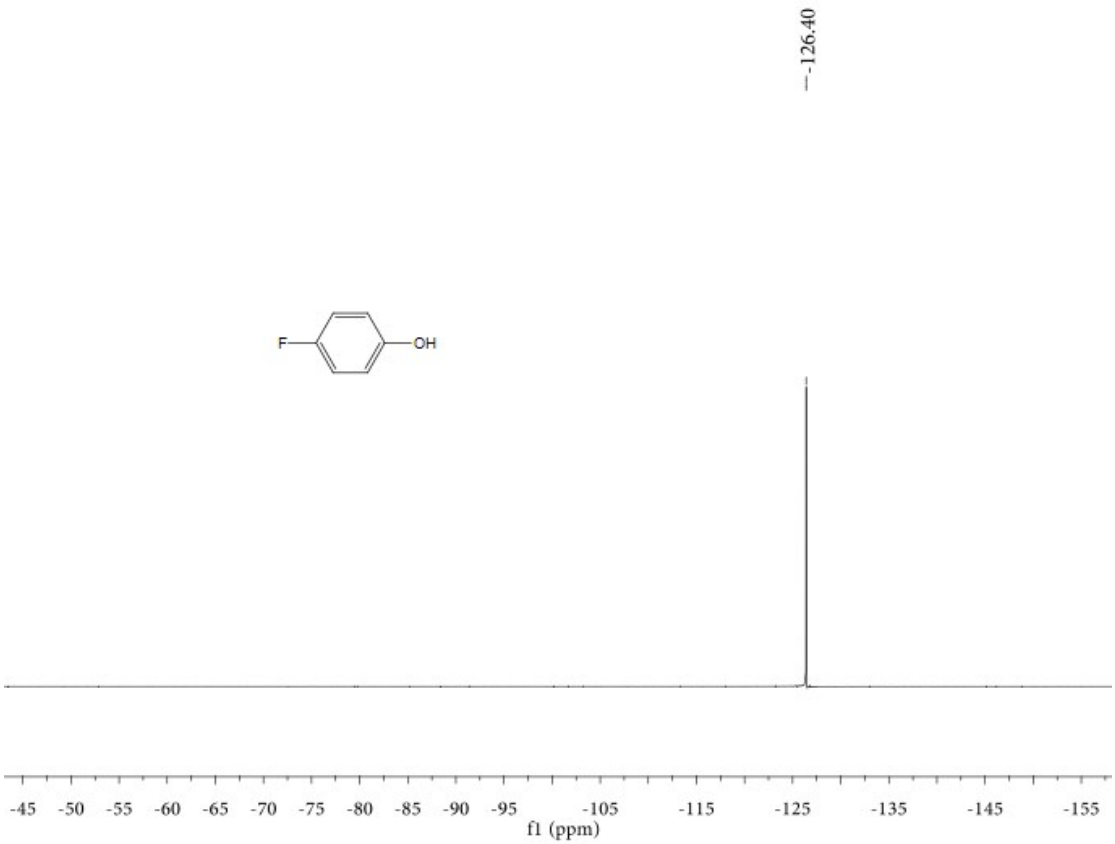


Figure S6. ^{1}H NMR of **4b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **4b** (125 MHz, DMSO-d_6) and^{19}F NMR of **4b** (470 MHz, DMSO-d_6)

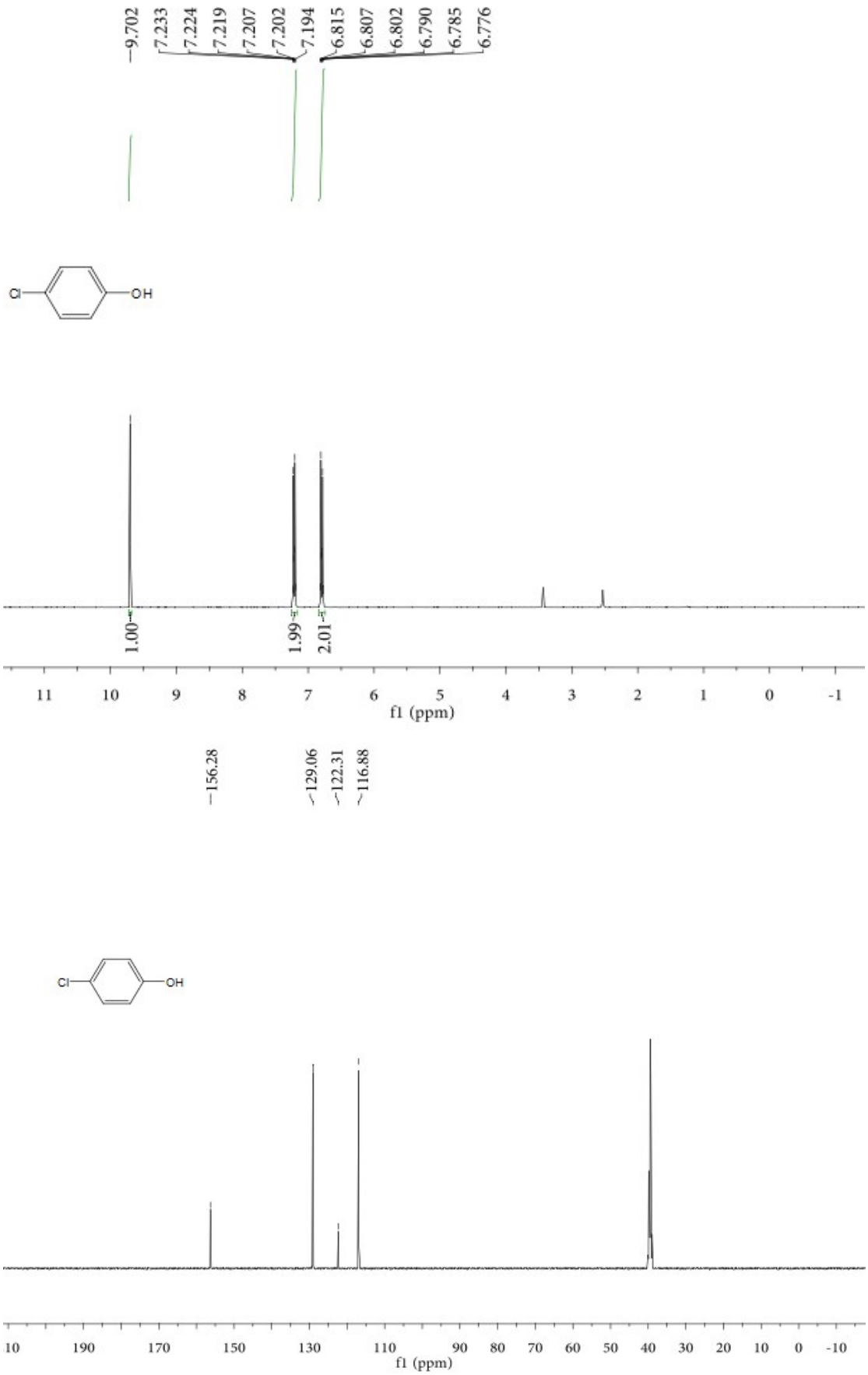


Figure S7. ^{1}H NMR of **5b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **5b** (125 MHz, DMSO-d_6)

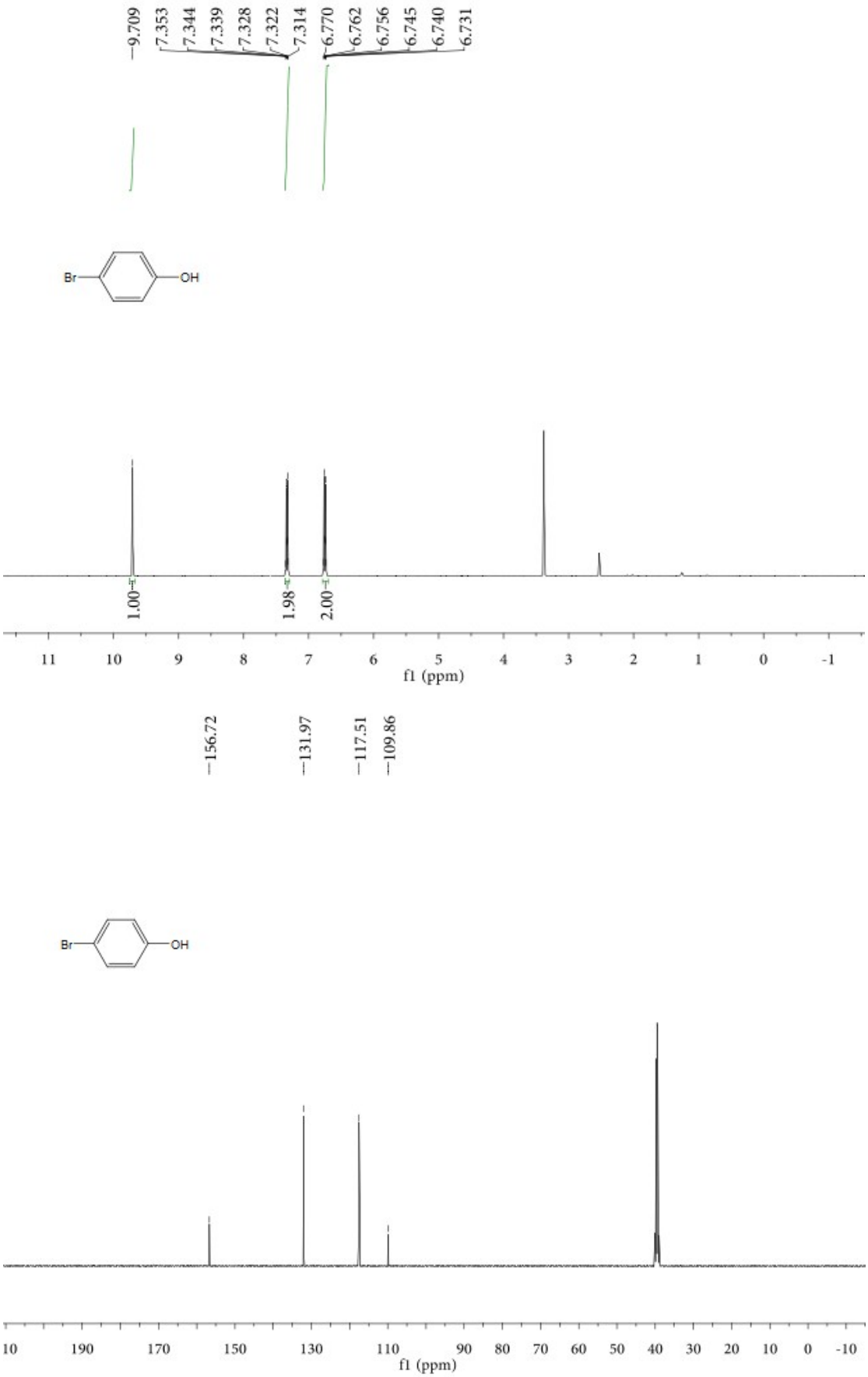


Figure S8. ^{1}H NMR of **6b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **6b** (125 MHz, DMSO-d_6)

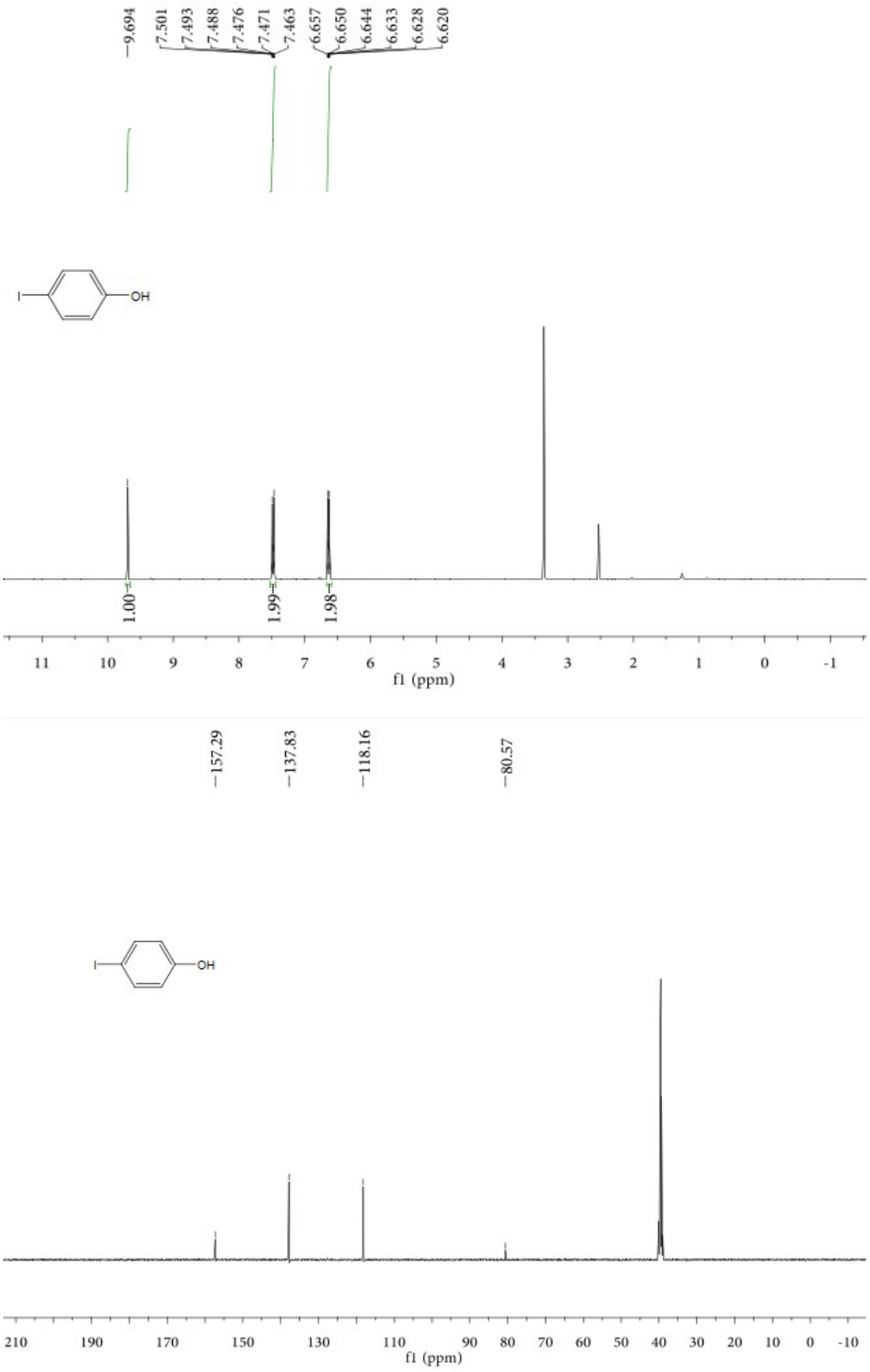


Figure S9. ^{1}H NMR of **7b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **7b** (125 MHz, DMSO-d_6)

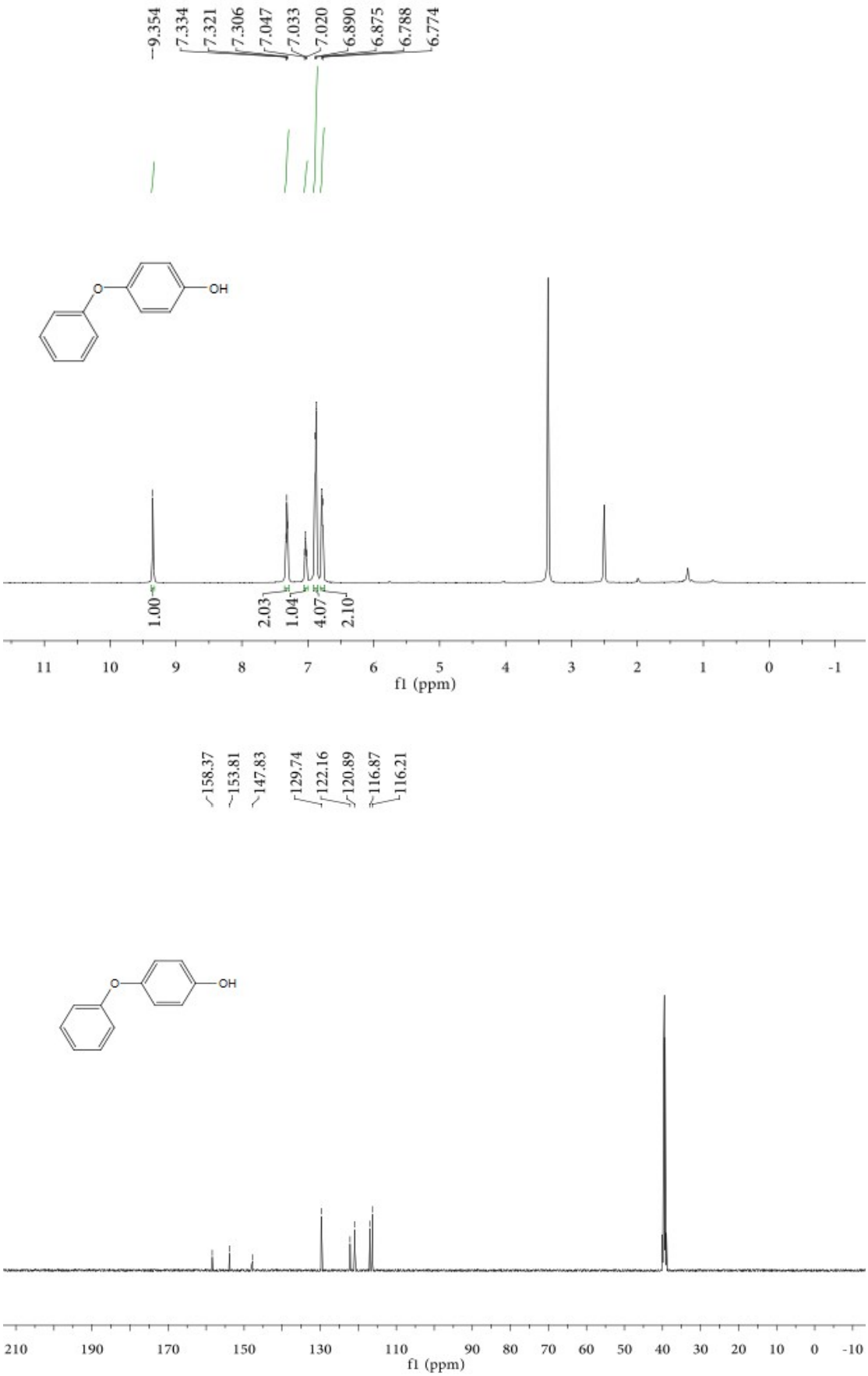


Figure S10. ^{1}H NMR of **8b** (500 MHz, DMSO-d_6) and ^{13}C NMR of **8b** (125 MHz, DMSO-d_6)

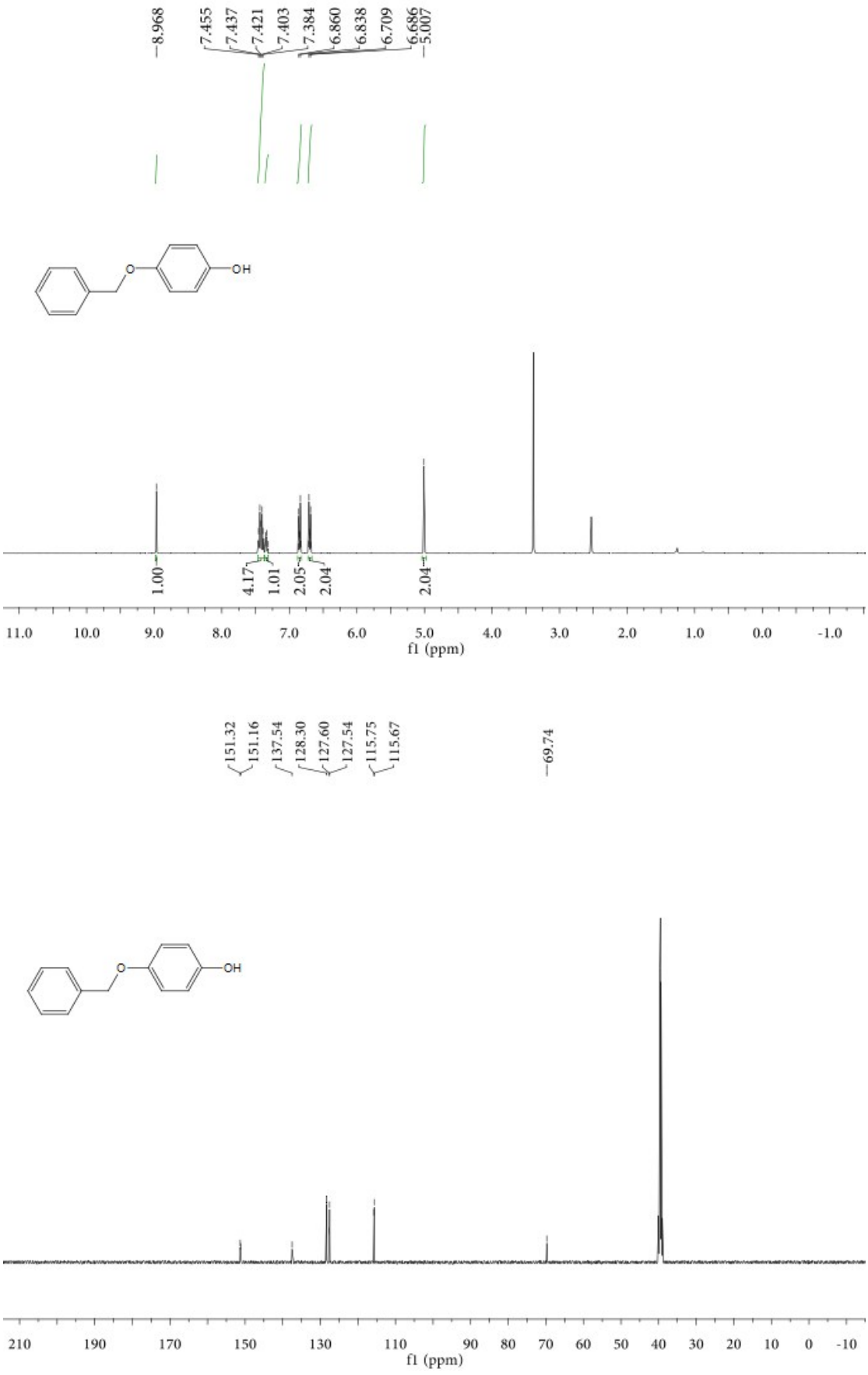


Figure S11. ^{1}H NMR of **9b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **9b** (125 MHz, DMSO-d_6)

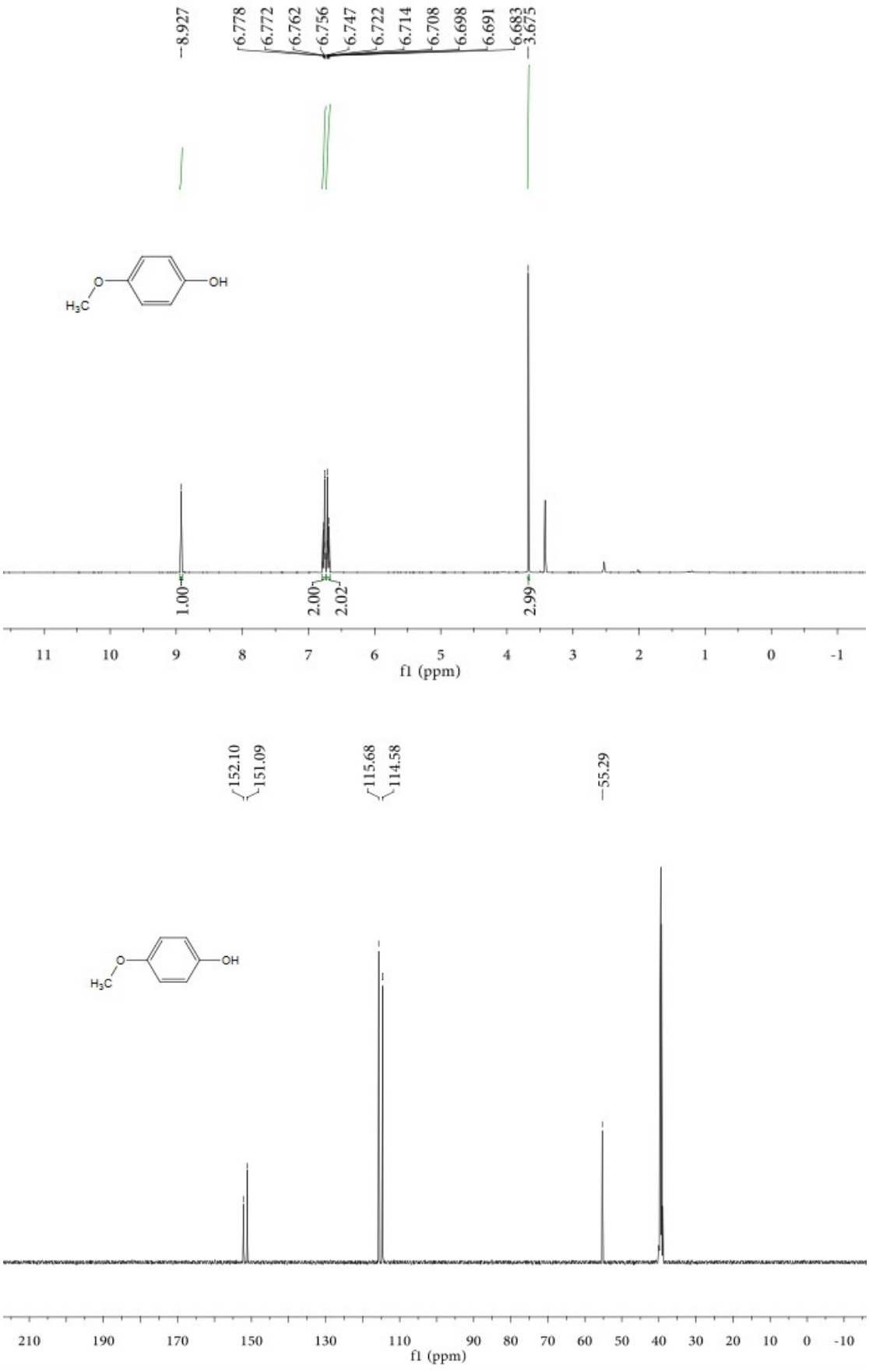


Figure S12. ^{1}H NMR of **10b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **10b** (125 MHz, DMSO-d_6)

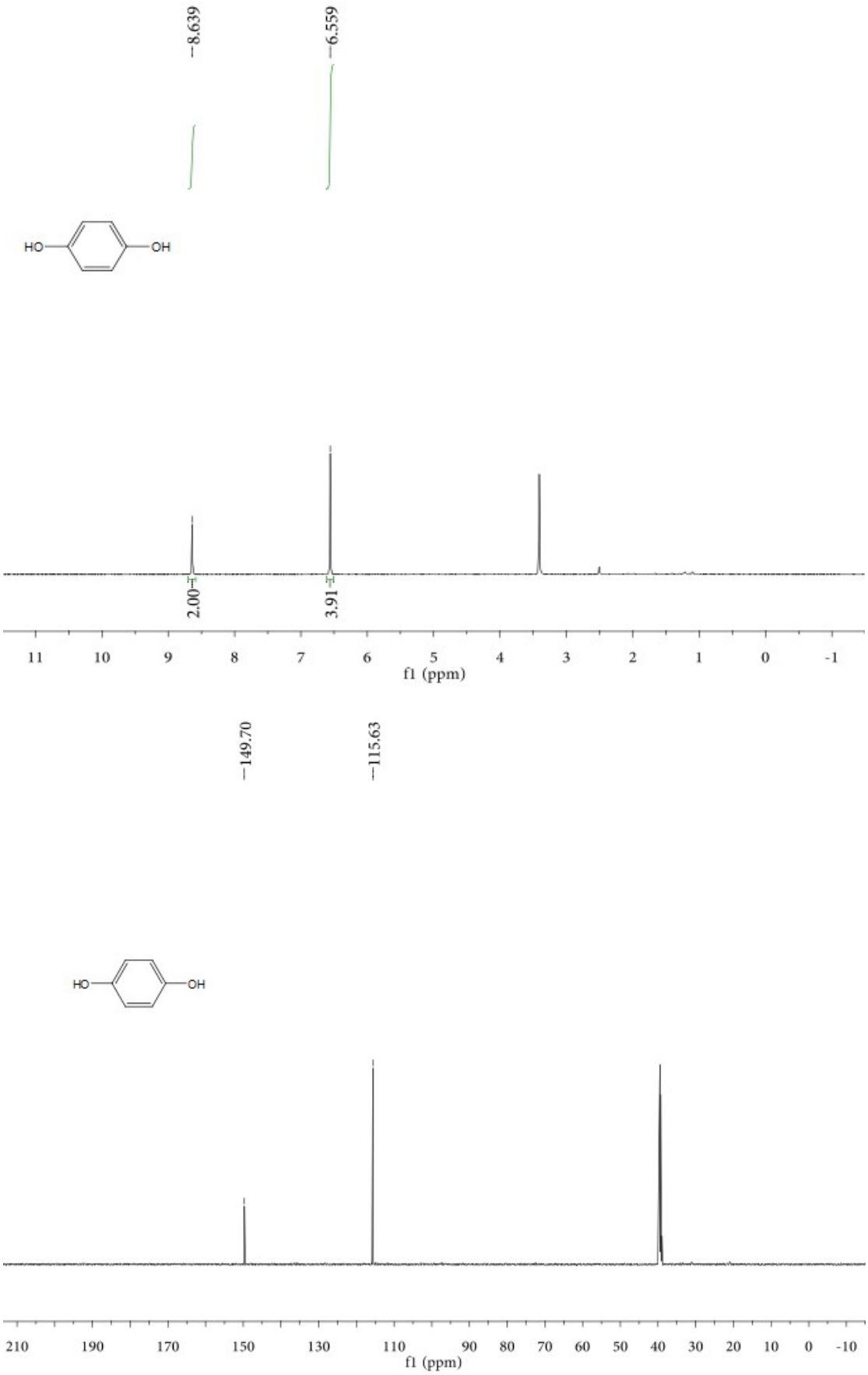


Figure S13. ^{1}H NMR of **11b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **11b** (125 MHz, DMSO-d_6)

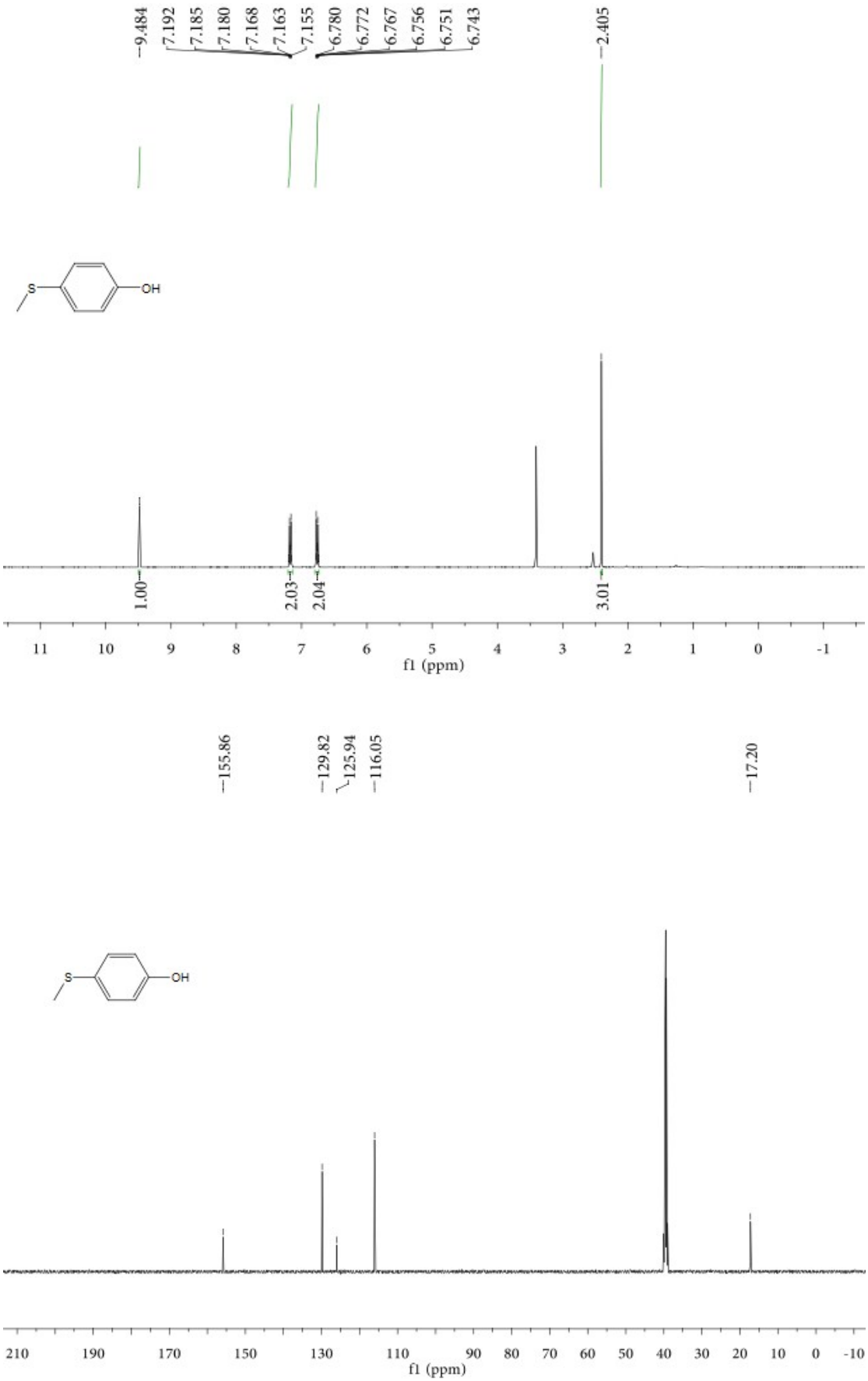


Figure S14. ^{1}H NMR of **12b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **12b** (125 MHz, DMSO-d_6)

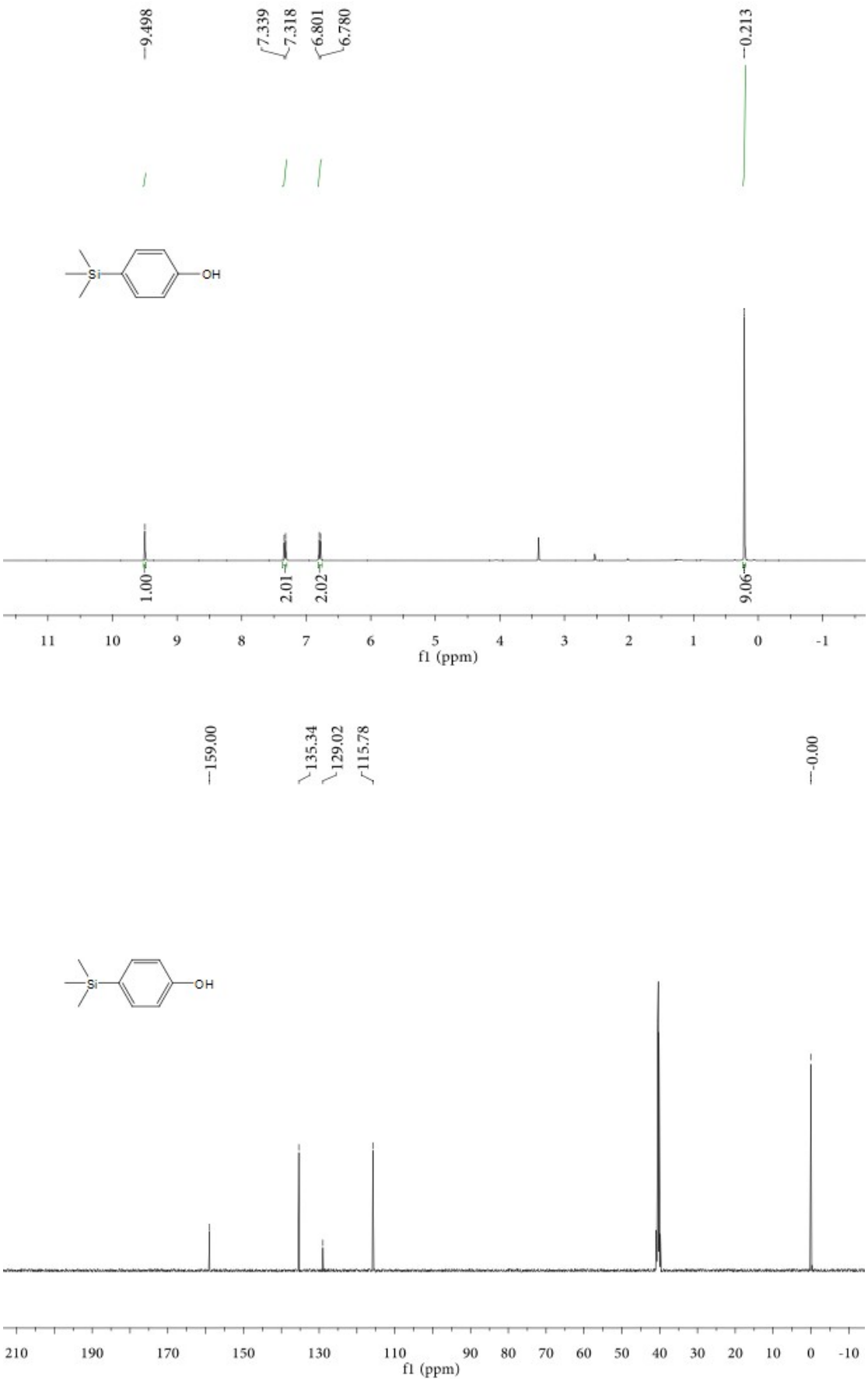
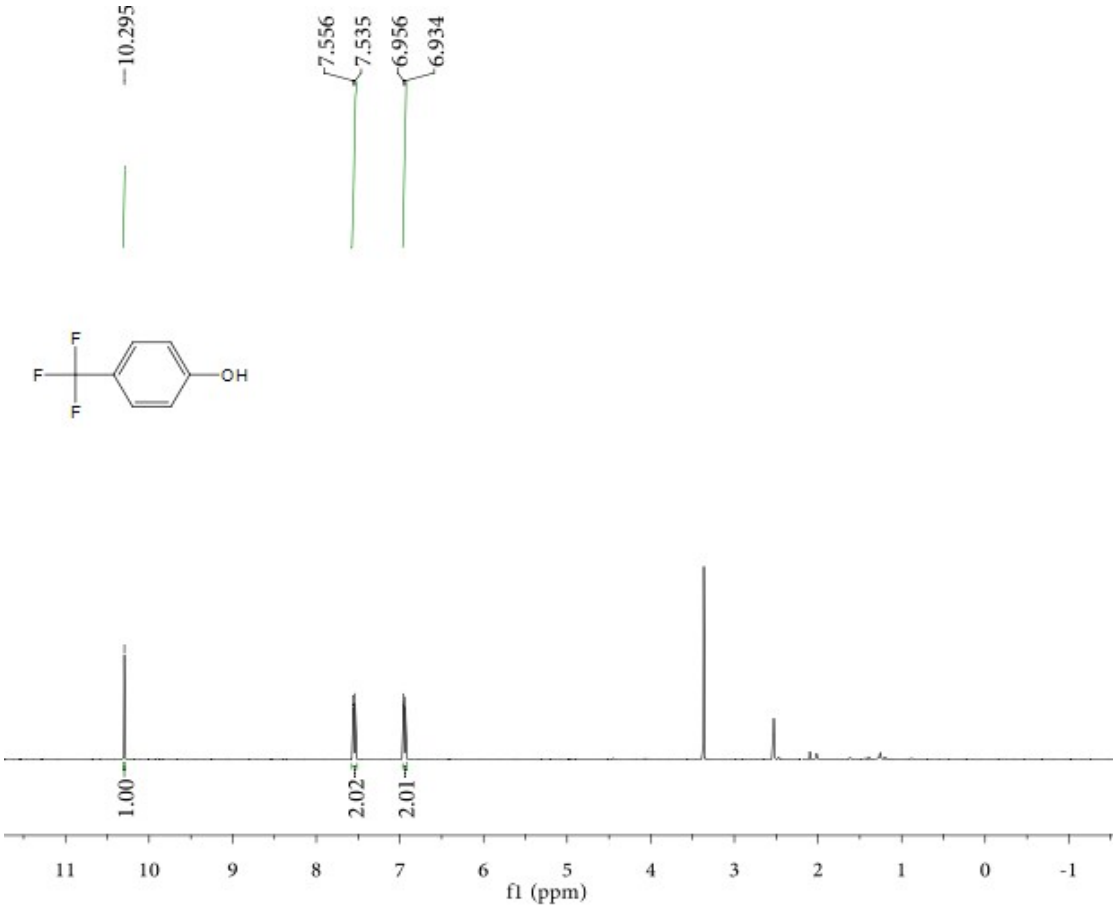
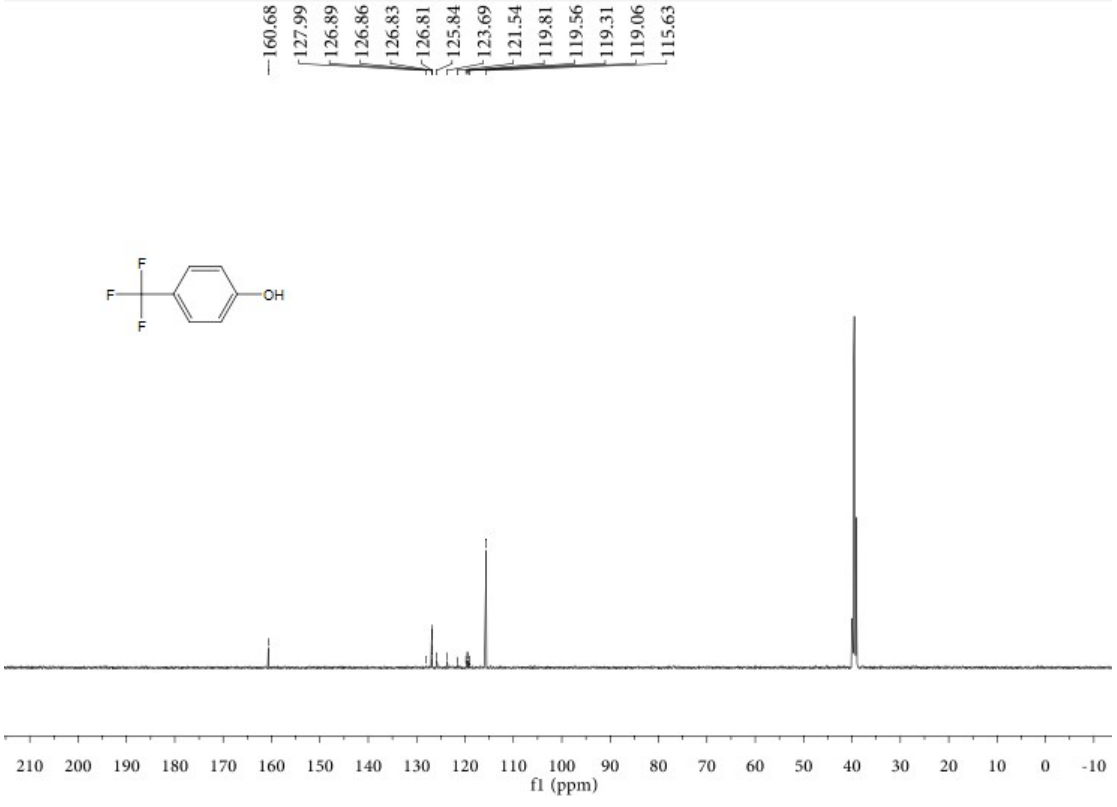


Figure S15. ^{1}H NMR of **13b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **13b** (125 MHz, DMSO-d_6)


10.295
7.556
7.535
6.956
6.934
F
F
F
OH
1.00
2.02
2.01
11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


160.68
127.99
126.89
126.86
126.83
126.81
125.84
123.69
121.54
119.81
119.56
119.31
119.06
115.63
F
F
F
OH
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

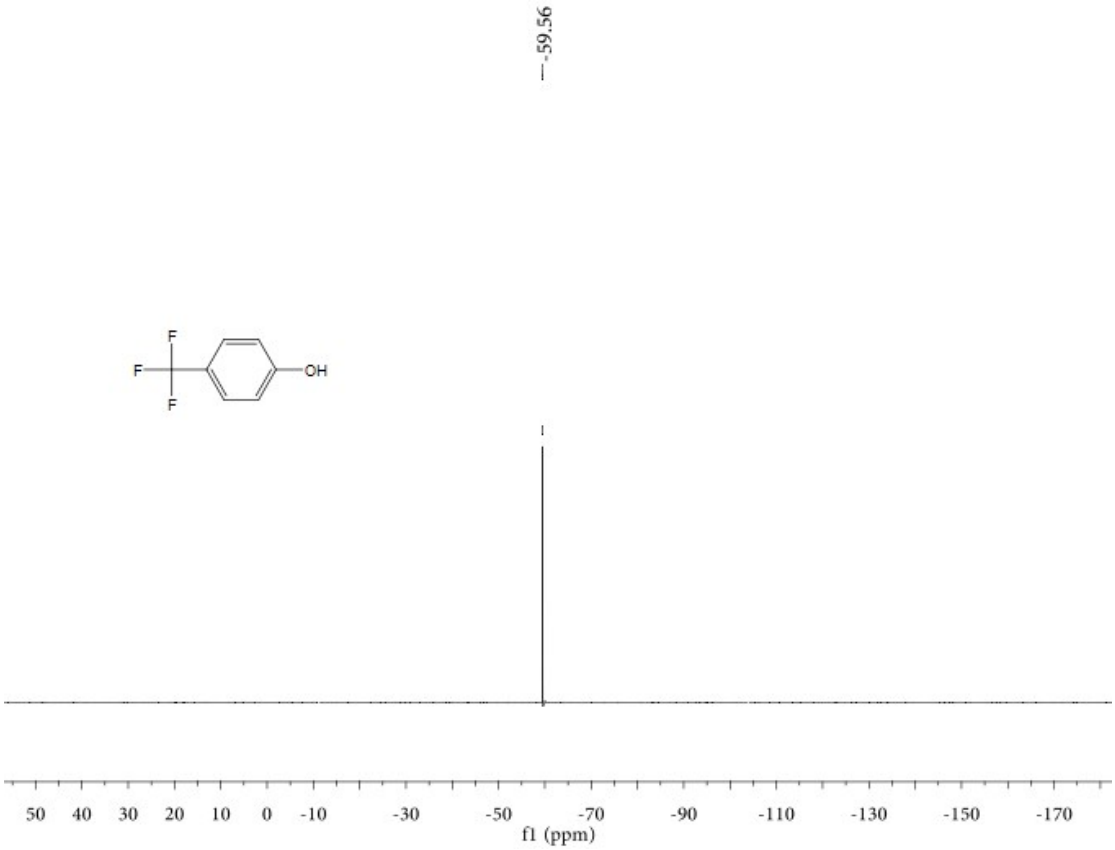


Figure S16. ^{1}H NMR of **14b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **14b** (125 MHz, DMSO-d_6) and ^{19}F NMR of **14b** (470 MHz, DMSO-d_6)

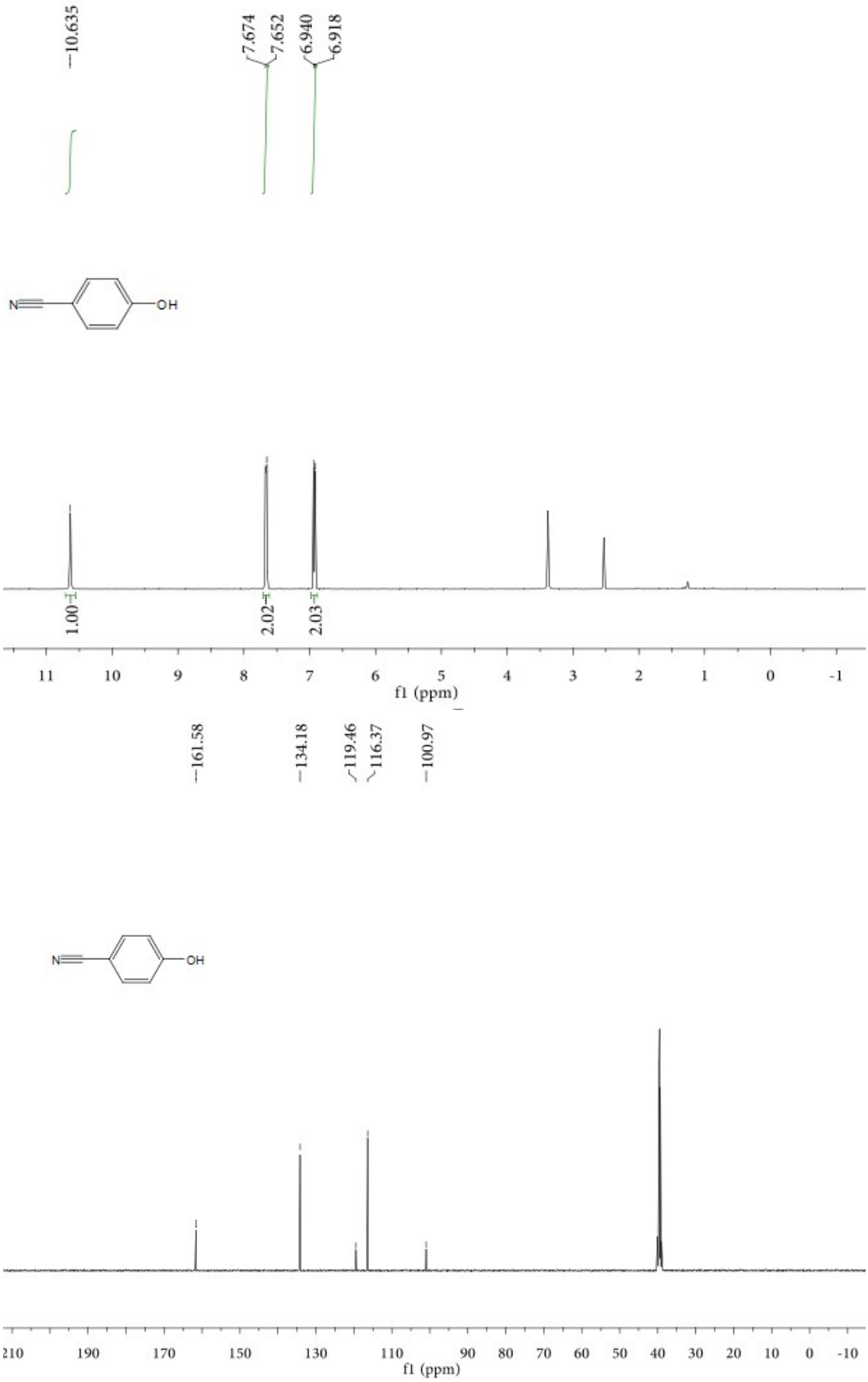


Figure S17. ^{1}H NMR of **15b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **15b** (125 MHz, DMSO-d_6)

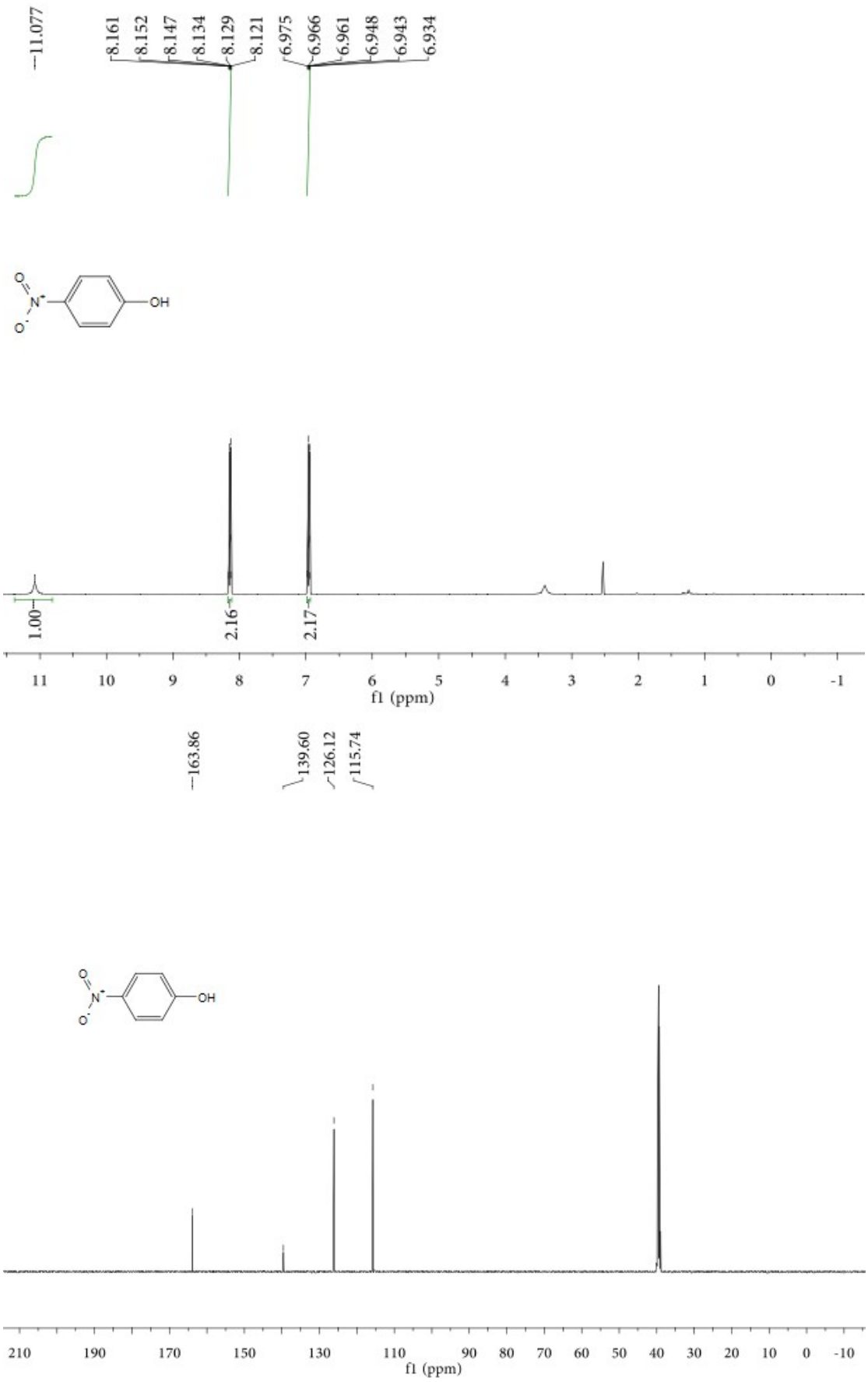


Figure S18. ^{1}H NMR of **16b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **16b** (125 MHz, DMSO-d_6)

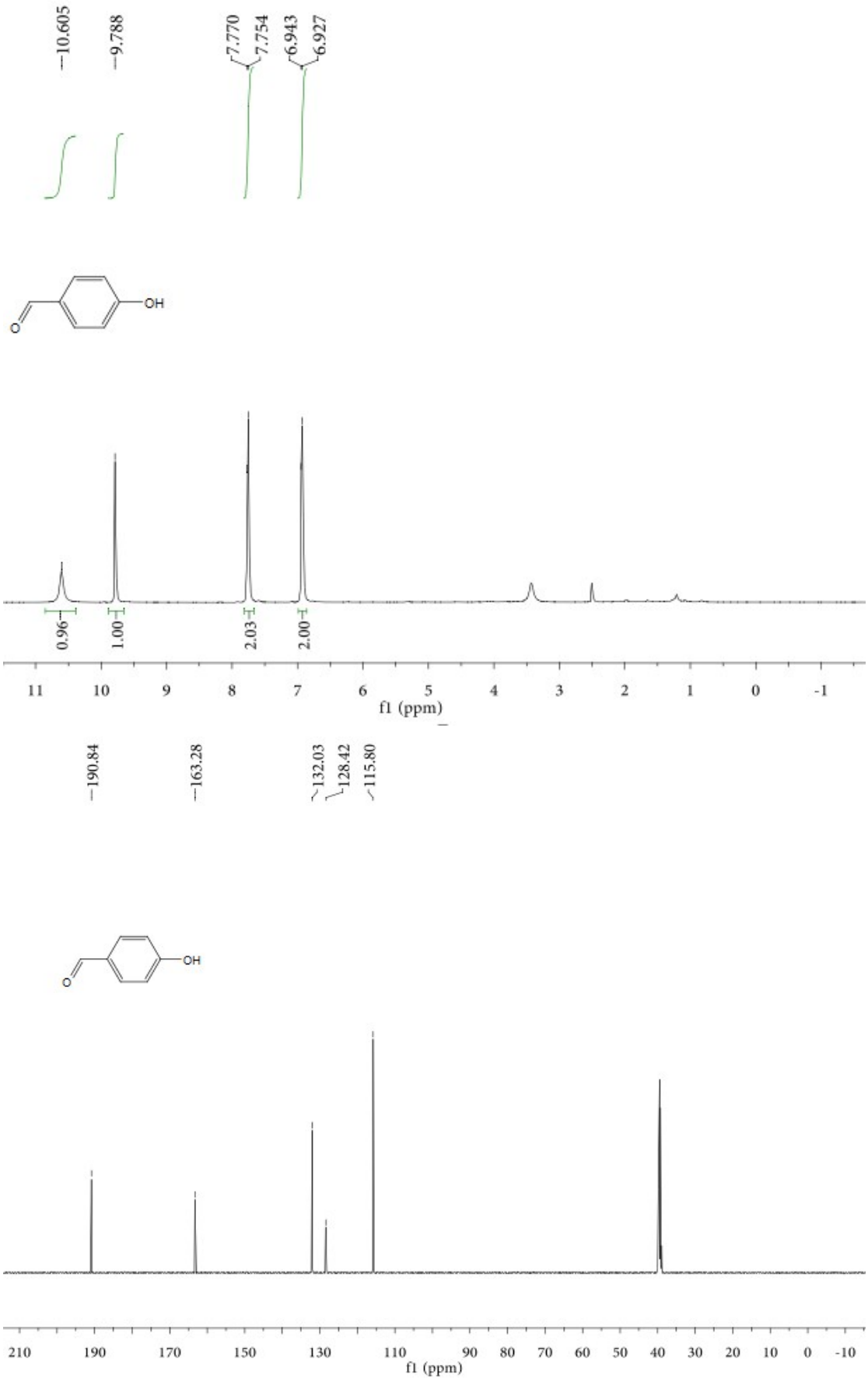


Figure S19. ^{1}H NMR of **17b** (500 MHz, DMSO-d_6) and ^{13}C NMR of **17b** (125 MHz, DMSO-d_6)

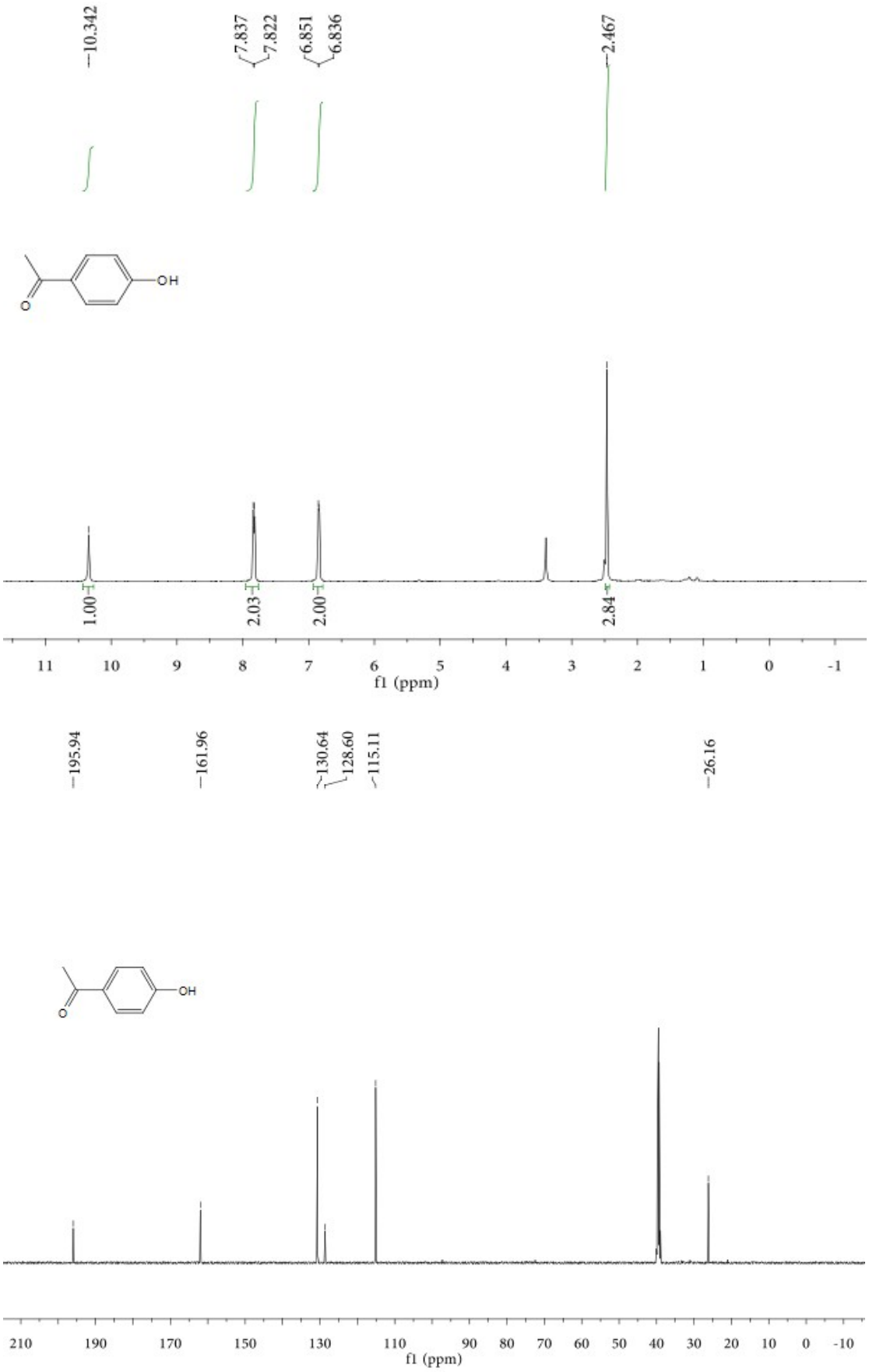


Figure S20. ^{1}H NMR of **18b** (500 MHz, DMSO-d_6) and ^{13}C NMR of **18b** (125 MHz, DMSO-d_6)

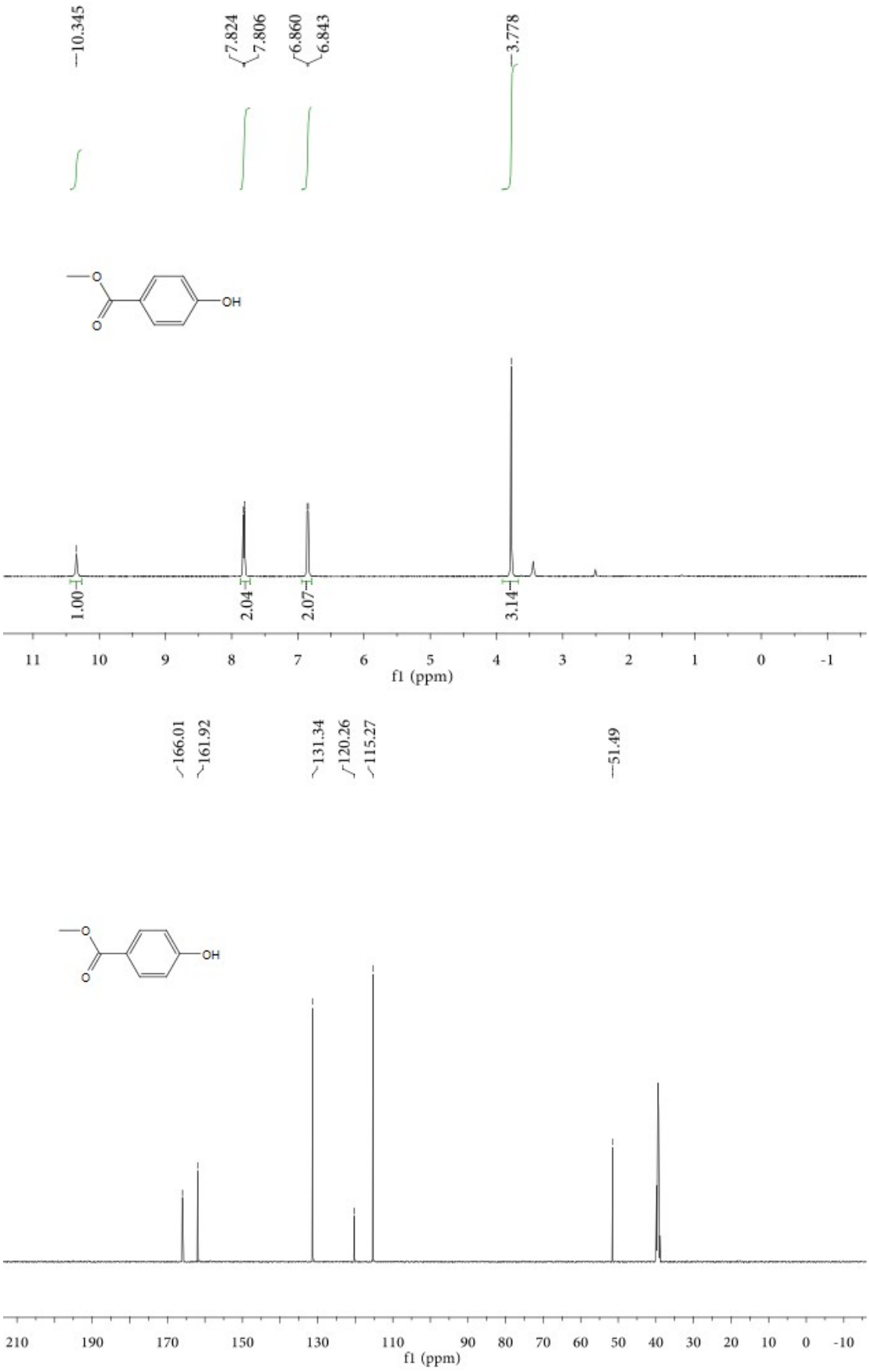


Figure S21. ^{1}H NMR of **19b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **19b** (125 MHz, DMSO-d_6)

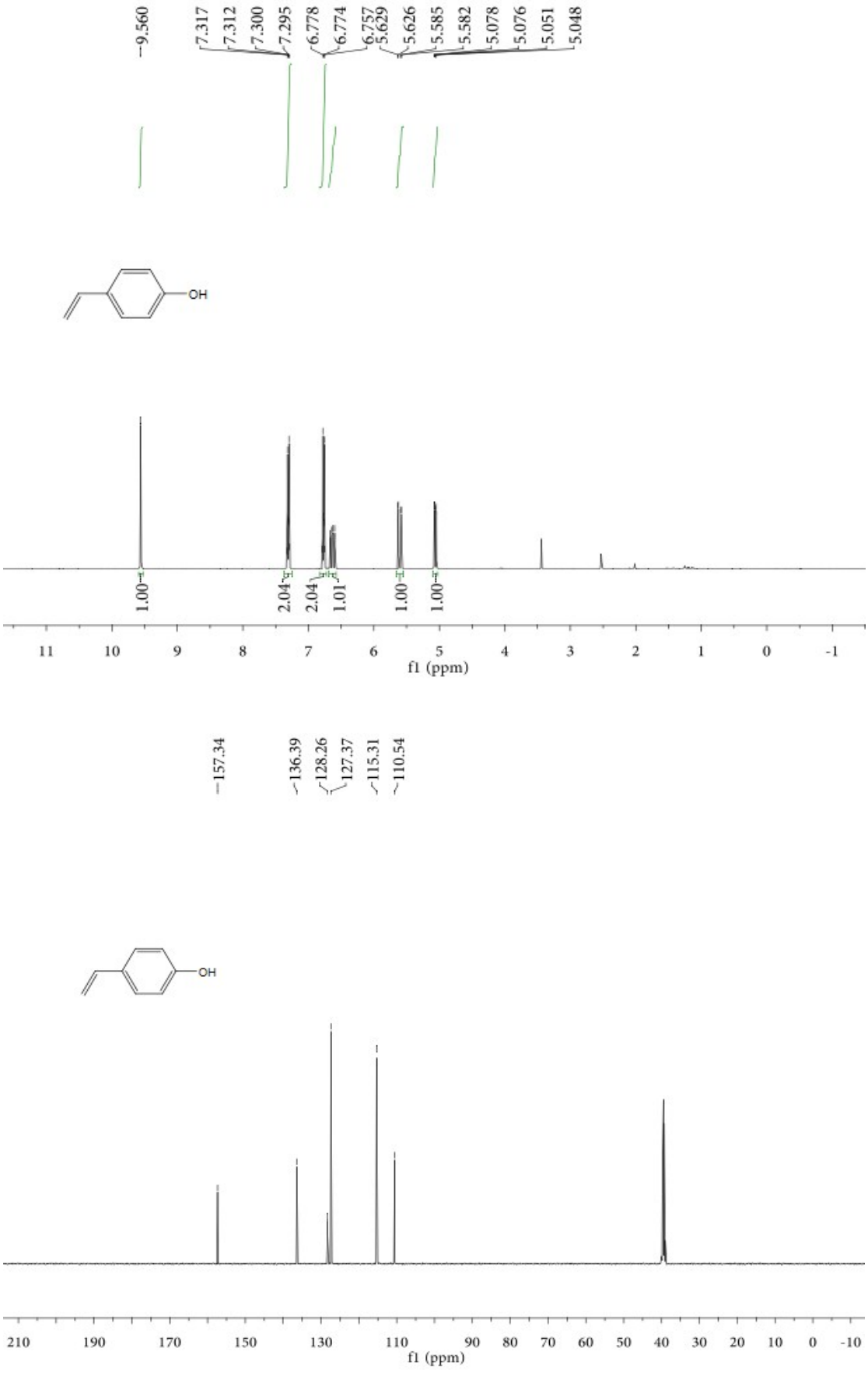


Figure S22. ^{1}H NMR of **20b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **20b** (125 MHz, DMSO-d_6)

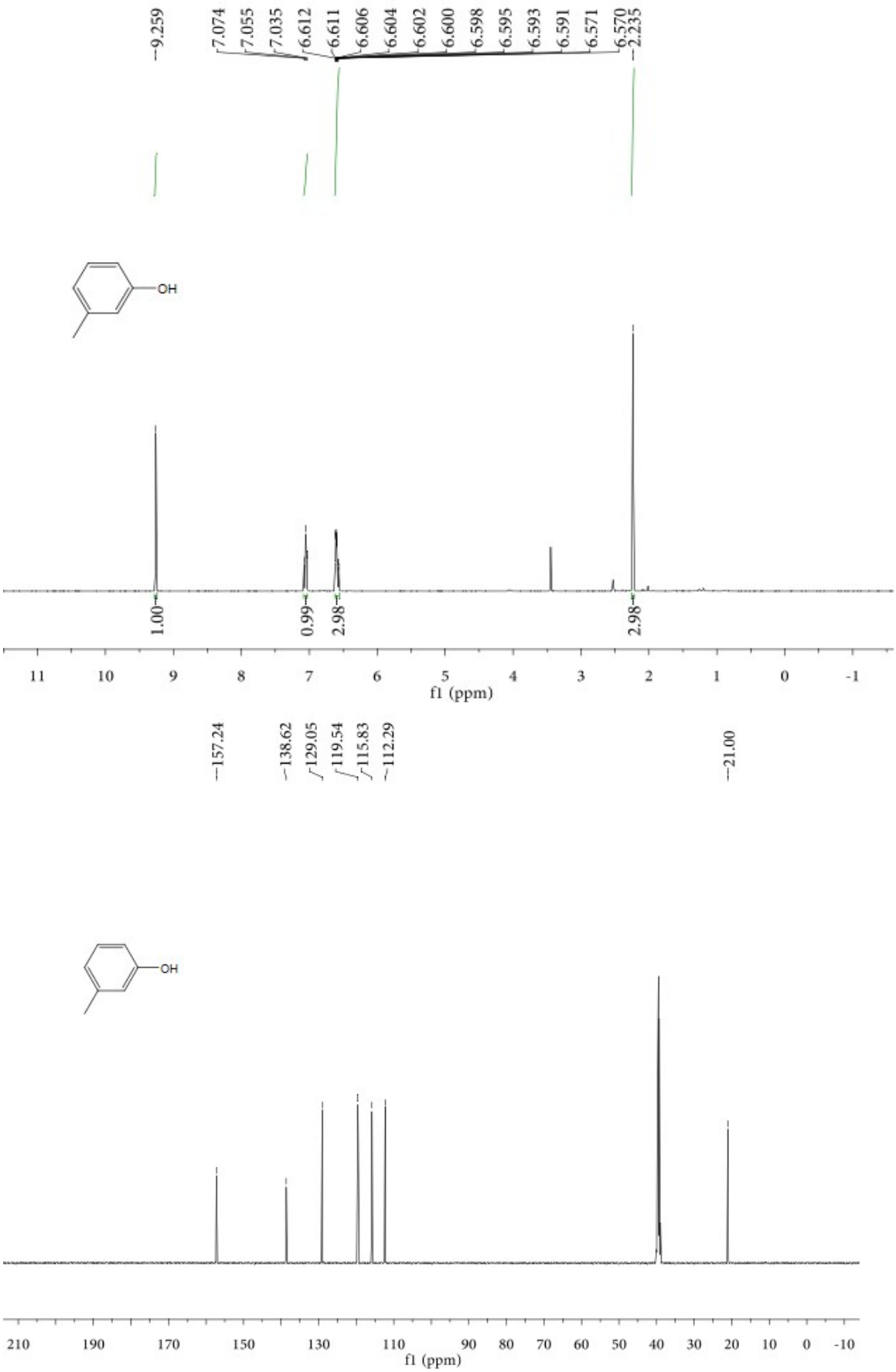
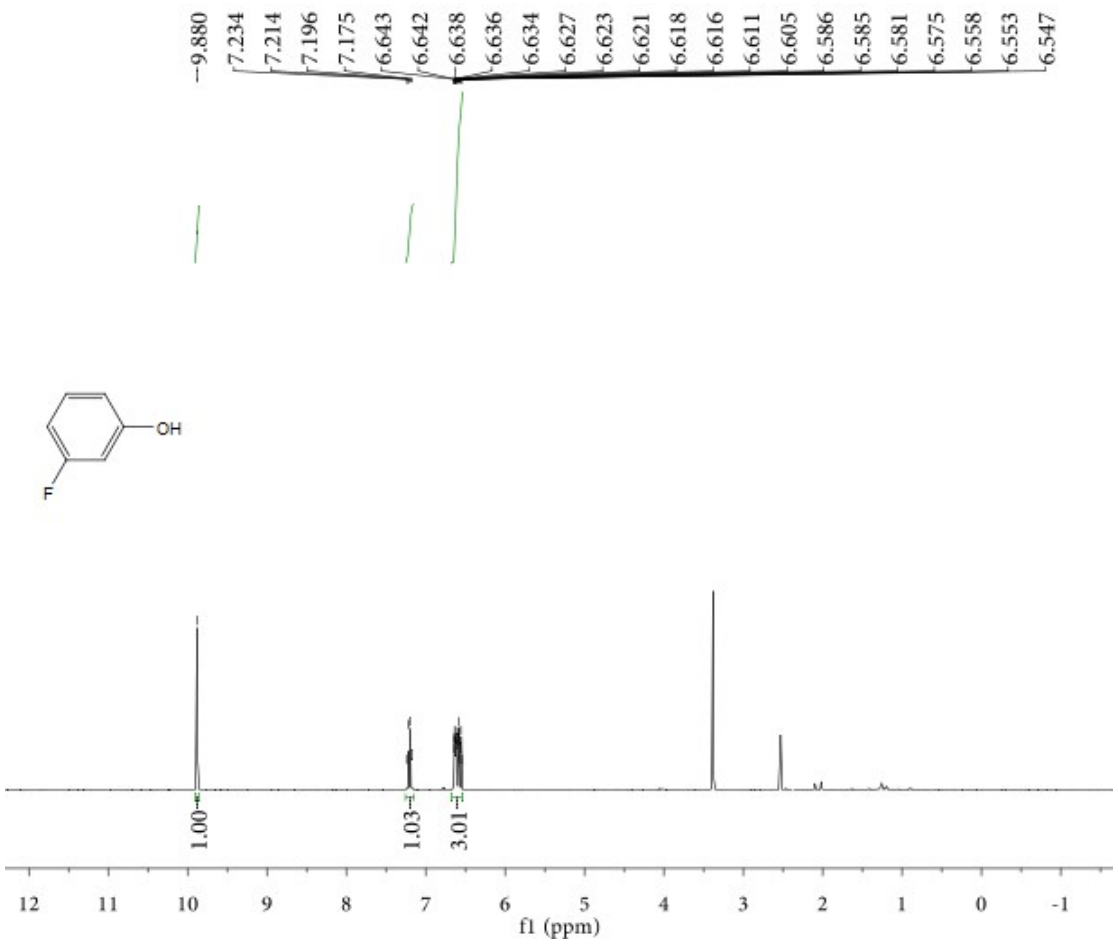
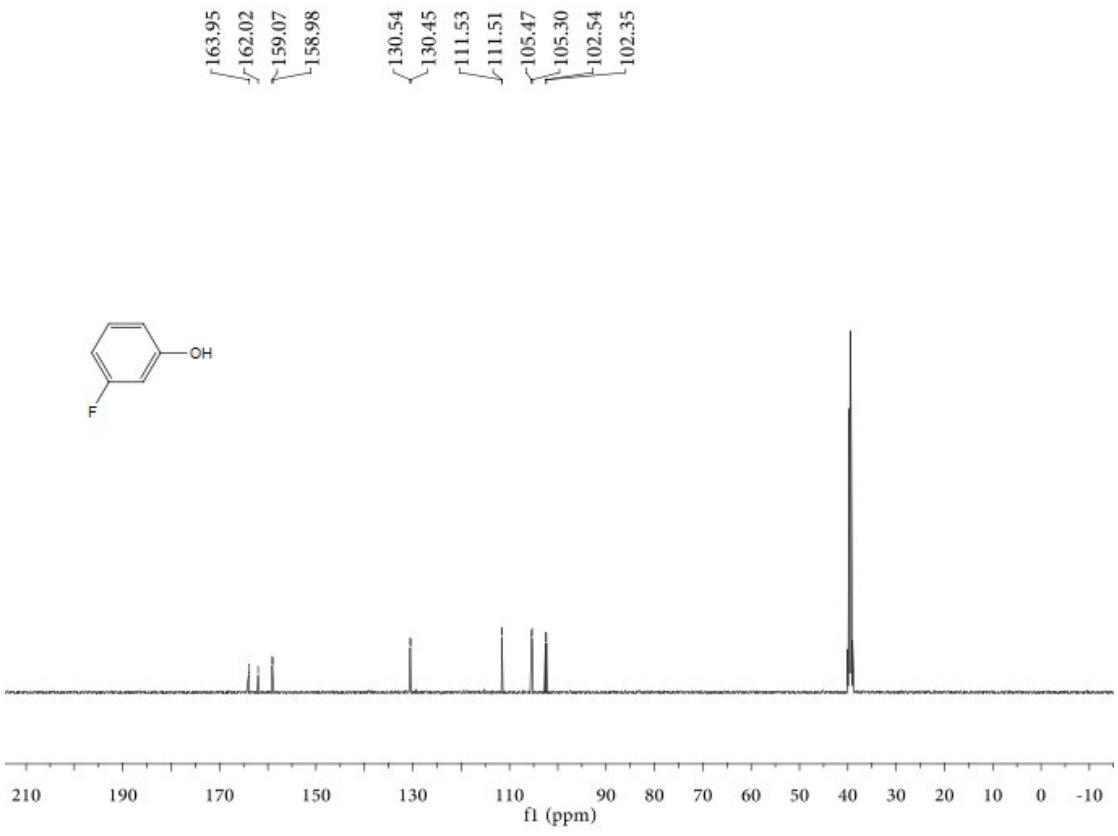


Figure S23. ^{1}H NMR of **21b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **21b** (125 MHz, DMSO-d_6)


9.880
7.234
7.214
7.196
7.175
6.643
6.642
6.638
6.636
6.634
6.627
6.623
6.621
6.618
6.616
6.611
6.605
6.586
6.585
6.581
6.575
6.558
6.553
6.547
OH
F
1.00
1.03
3.01
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)


163.95
162.02
159.07
158.98
130.54
130.45
111.53
111.51
105.47
105.30
102.54
102.35
OH
F
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

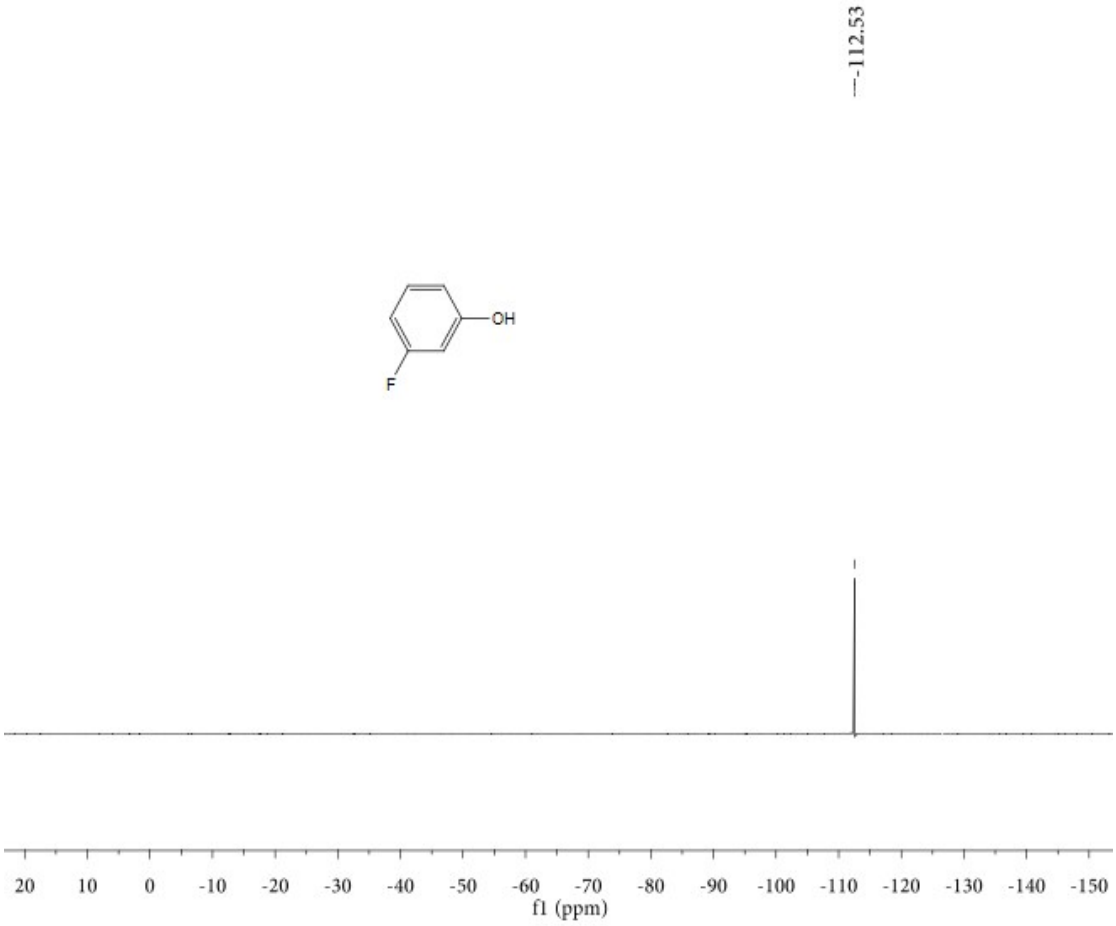


Figure S24. ^{1}H NMR of **22b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **22b** (125 MHz, DMSO-d_6) and ^{19}F NMR of **22b** (470 MHz, DMSO-d_6)

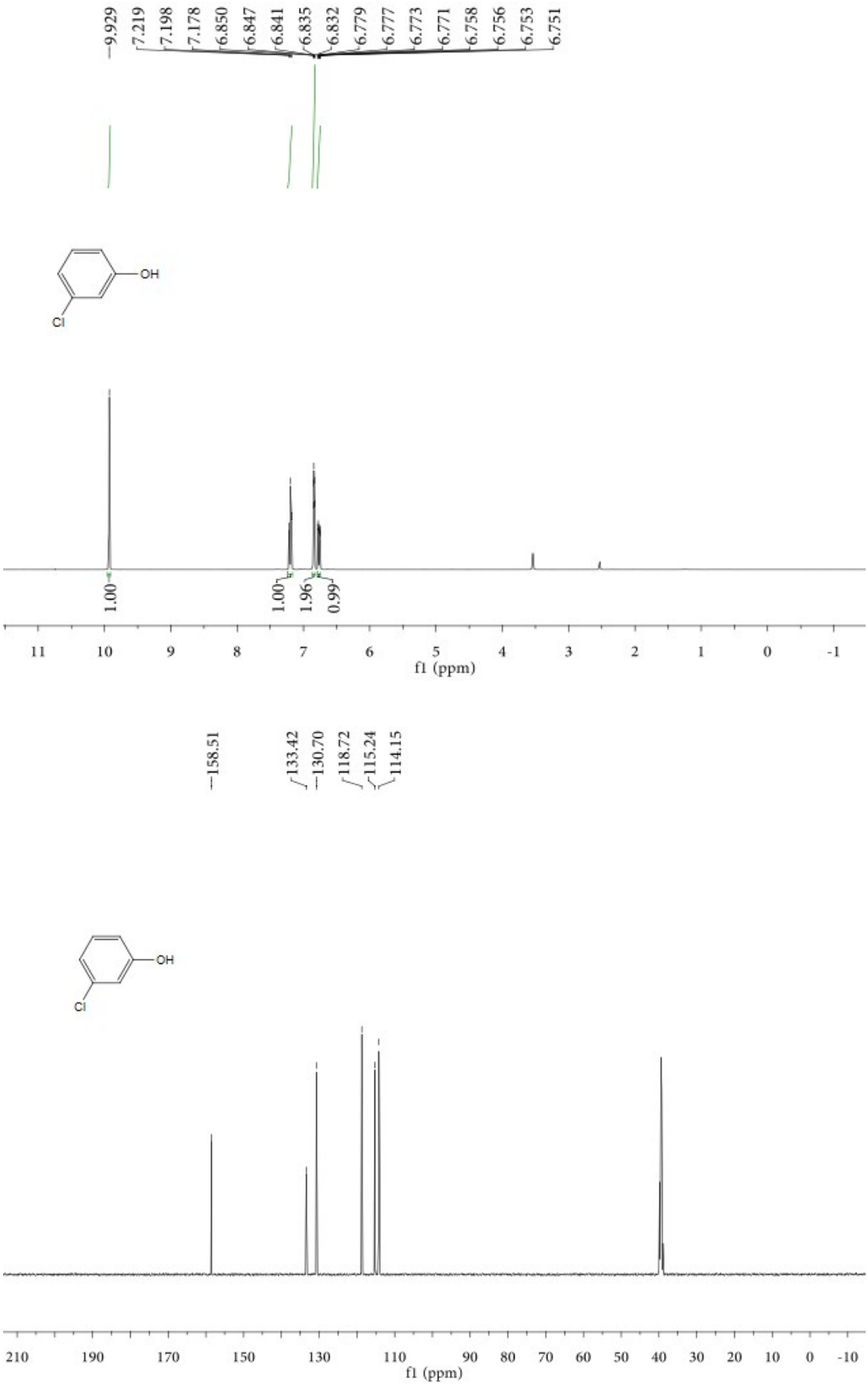
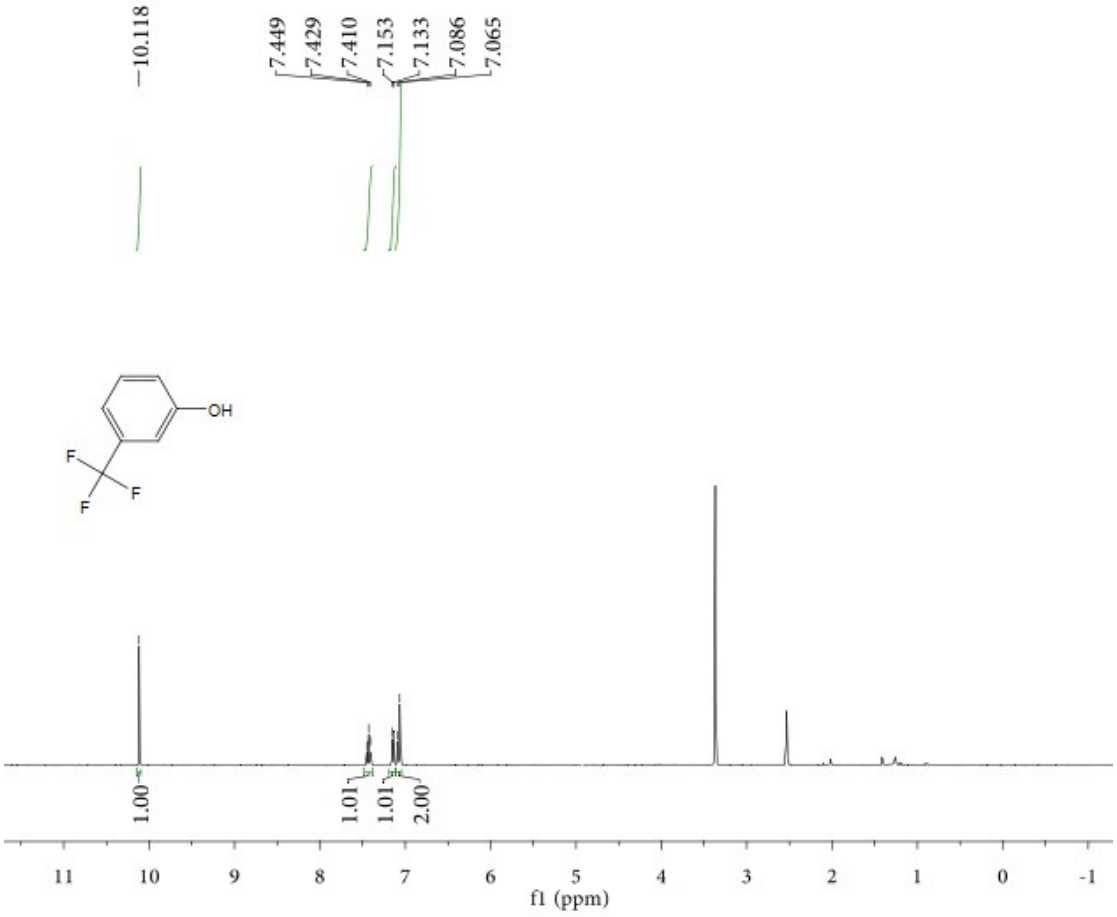
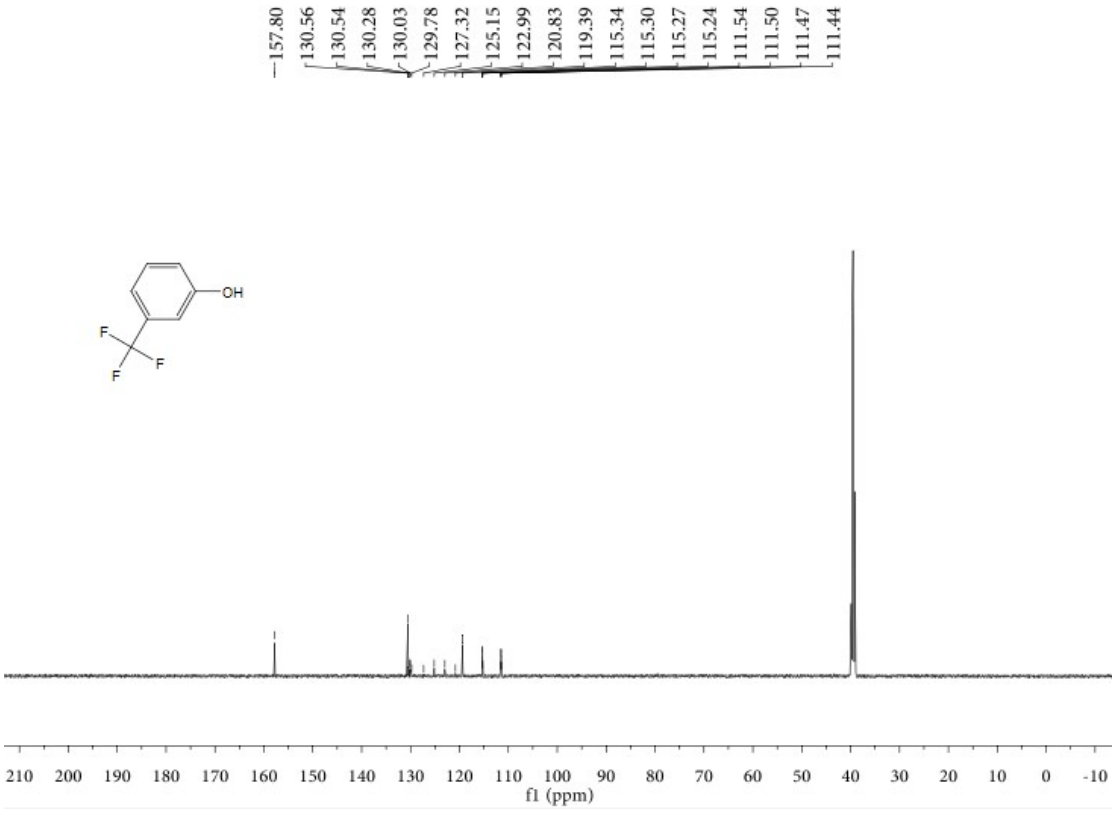


Figure S25. ^{1}H NMR of **23b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **23b** (125 MHz, DMSO-d_6)


10.118
7.449
7.429
7.410
7.153
7.133
7.086
7.065
OH
F
F
F
1.00
1.01
1.01
2.00
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)


157.80
130.56
130.54
130.28
130.03
129.78
127.32
125.15
122.99
120.83
119.39
115.34
115.30
115.27
115.24
111.54
111.50
111.47
111.44
OH
F
F
F
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

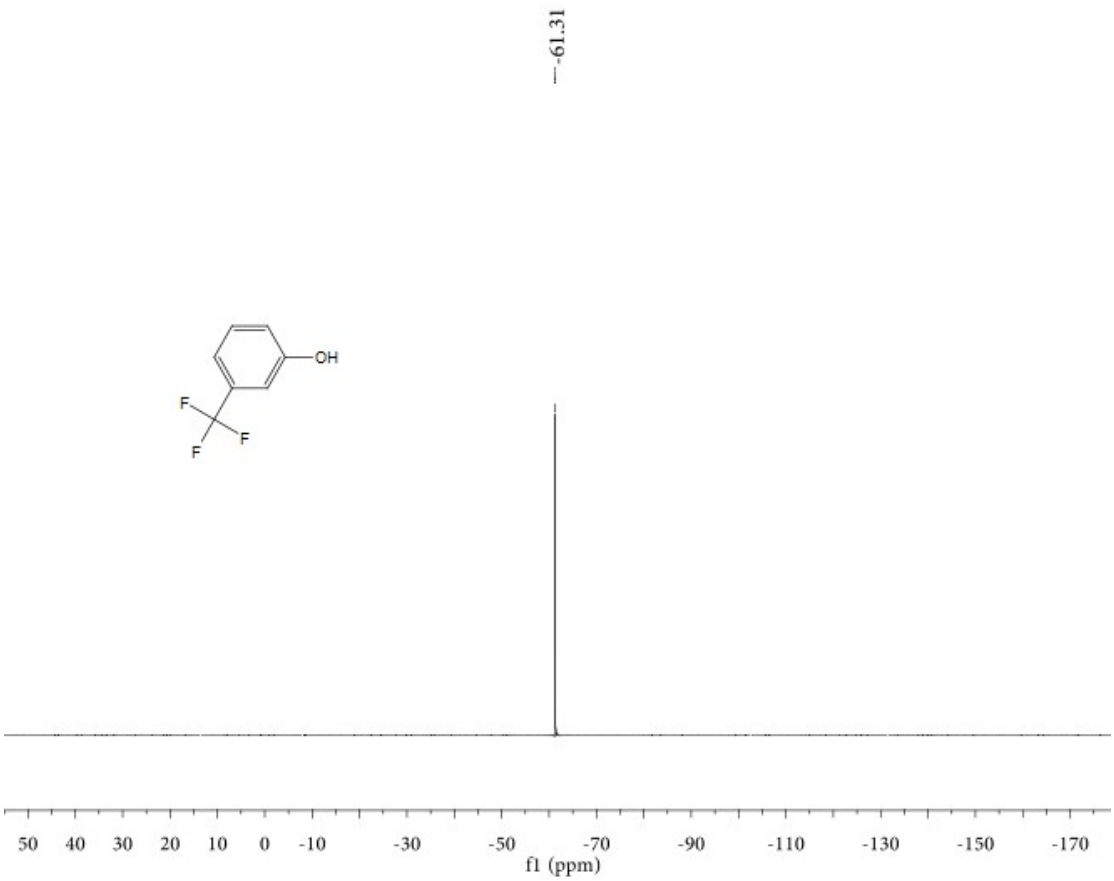


Figure S26. ^{1}H NMR of **24b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **24b** (125 MHz, DMSO-d_6) and ^{19}F NMR of **24b** (470 MHz, DMSO-d_6)

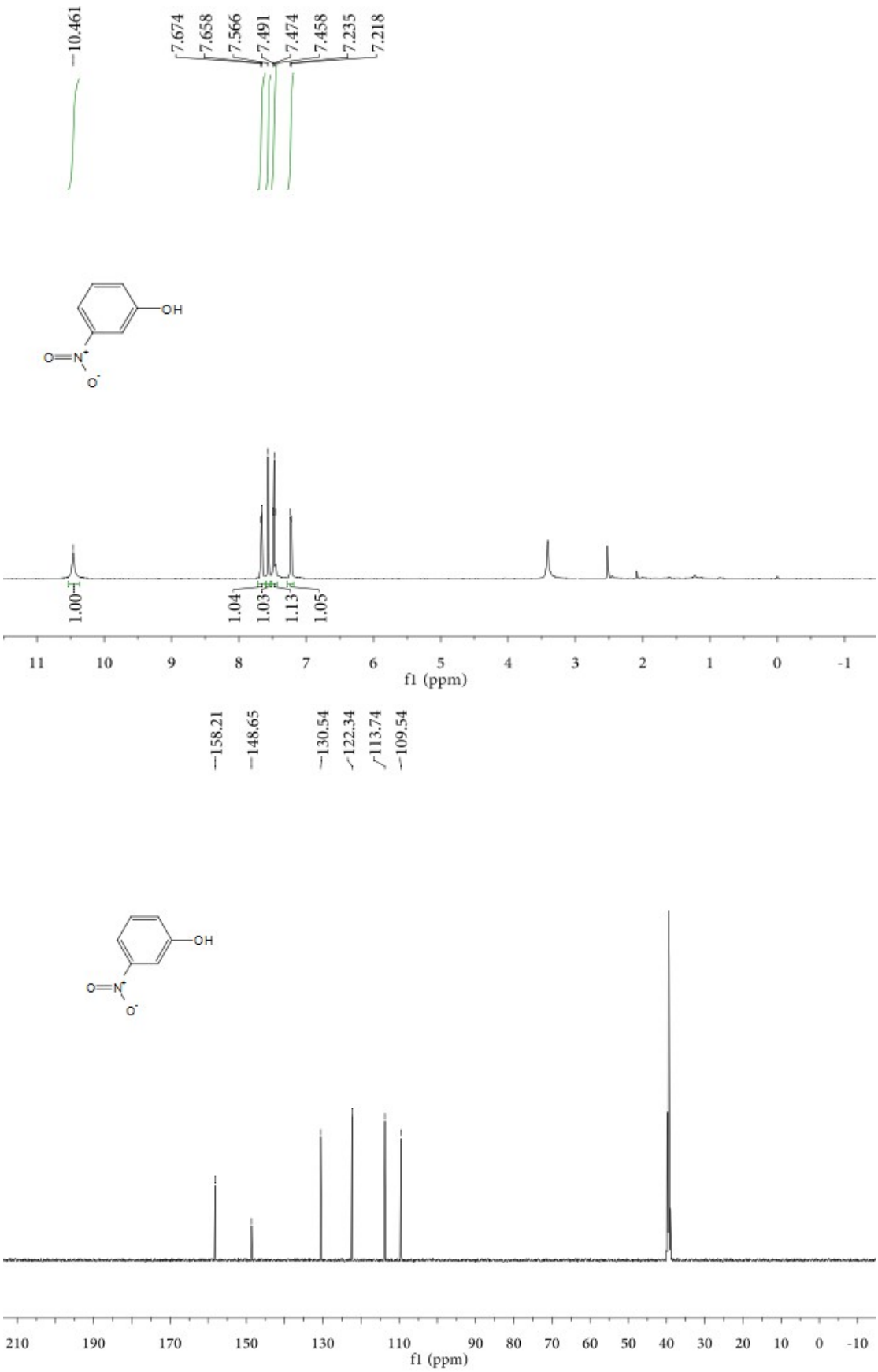


Figure S27. ^{1}H NMR of **25b** (500 MHz, DMSO-d_6) and ^{13}C NMR of **25b** (125 MHz, DMSO-d_6)

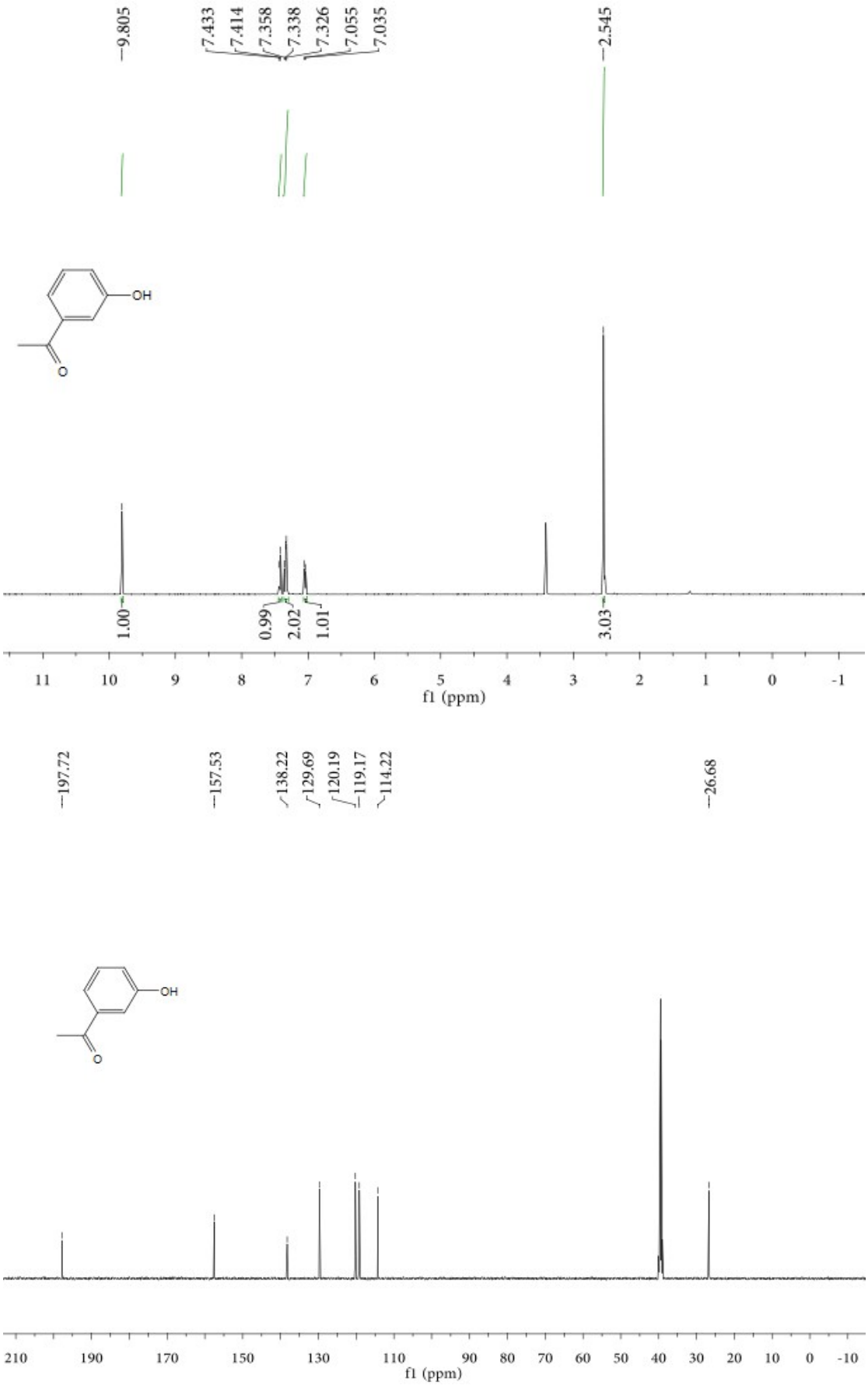


Figure S28. ^{1}H NMR of **26b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **26b** (125 MHz, DMSO-d_6)

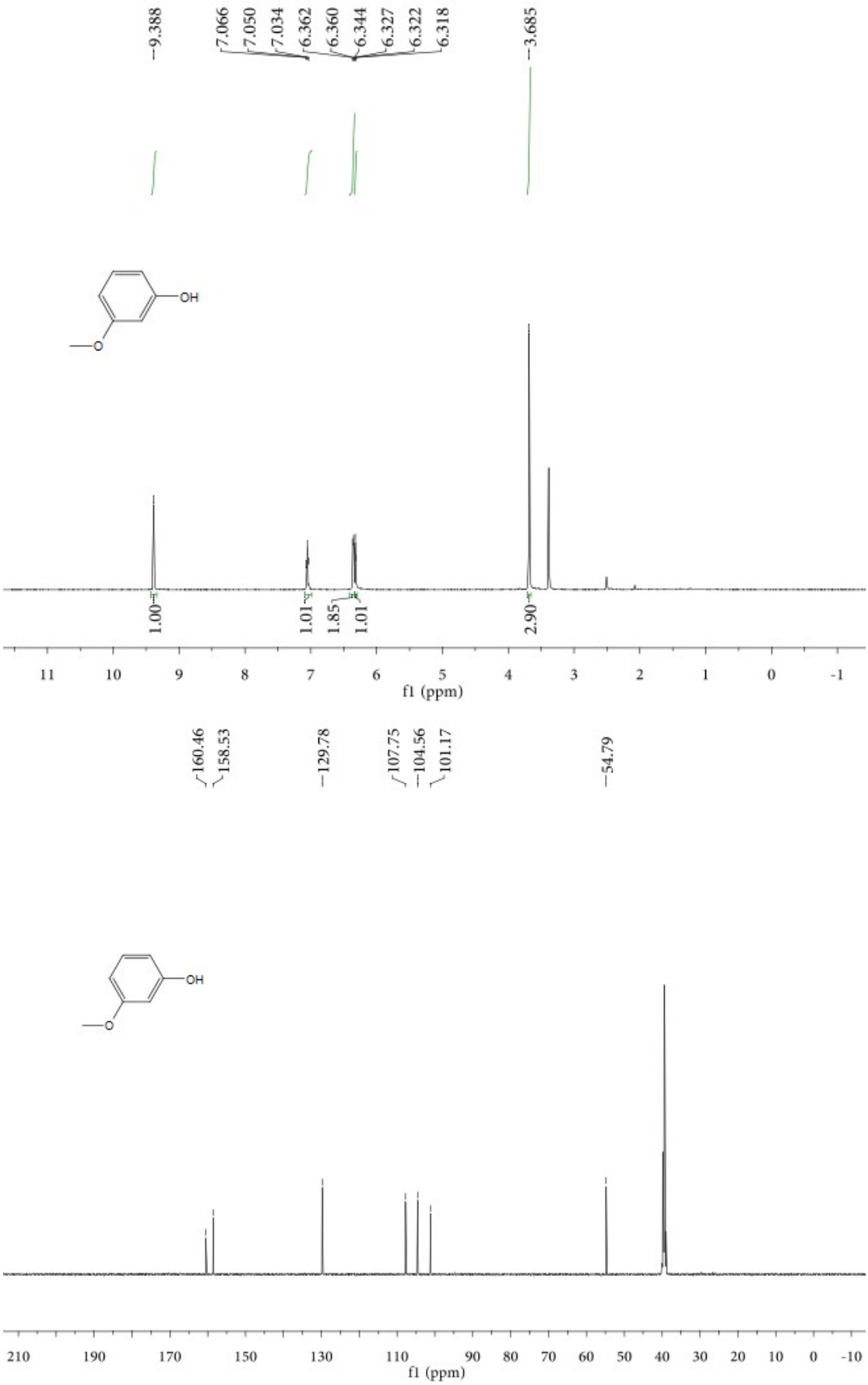


Figure S29. ^{1}H NMR of **27b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **27b** (125 MHz, DMSO-d_6)

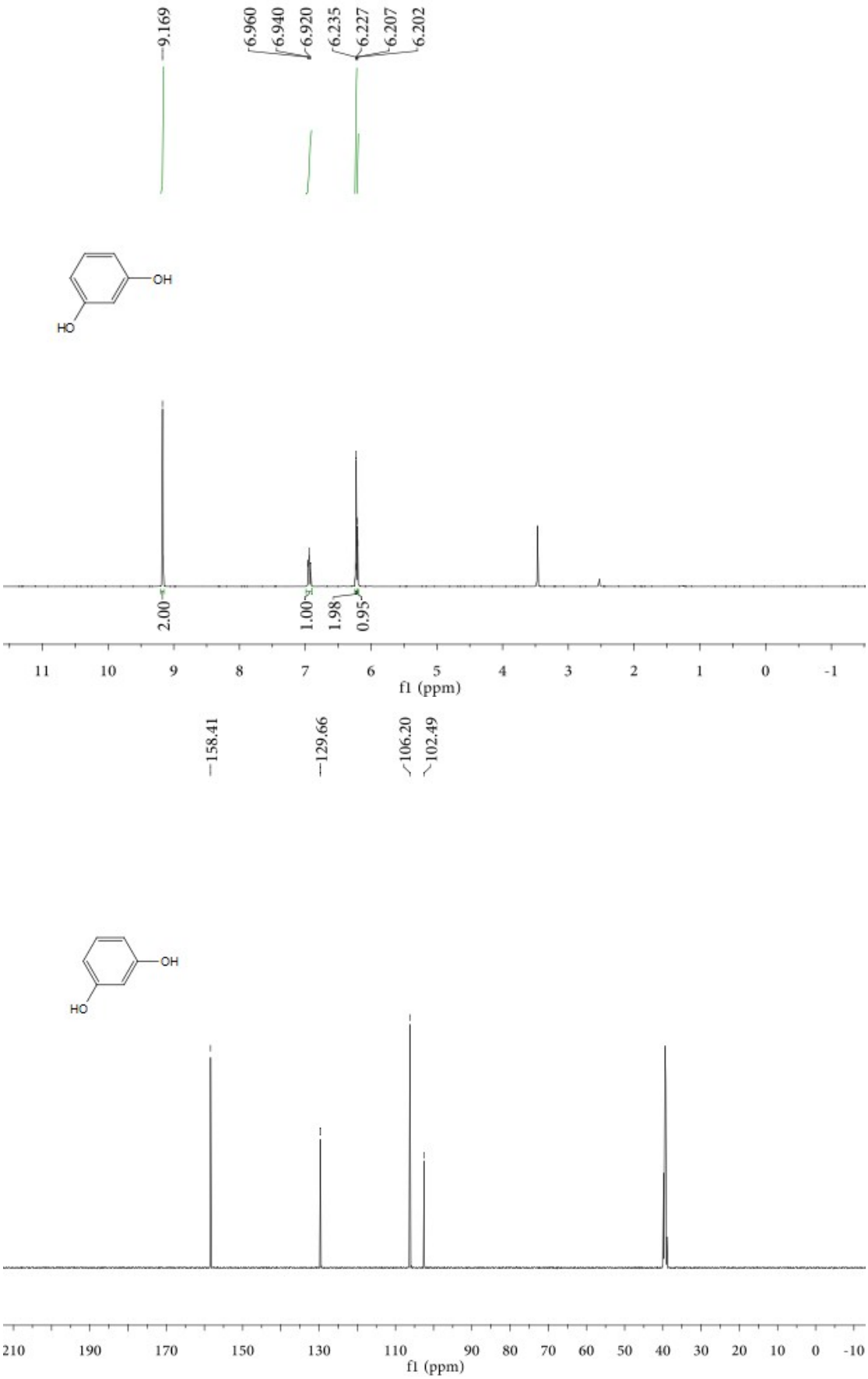


Figure S30. ^{1}H NMR of **28b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **28b** (125 MHz, DMSO-d_6)

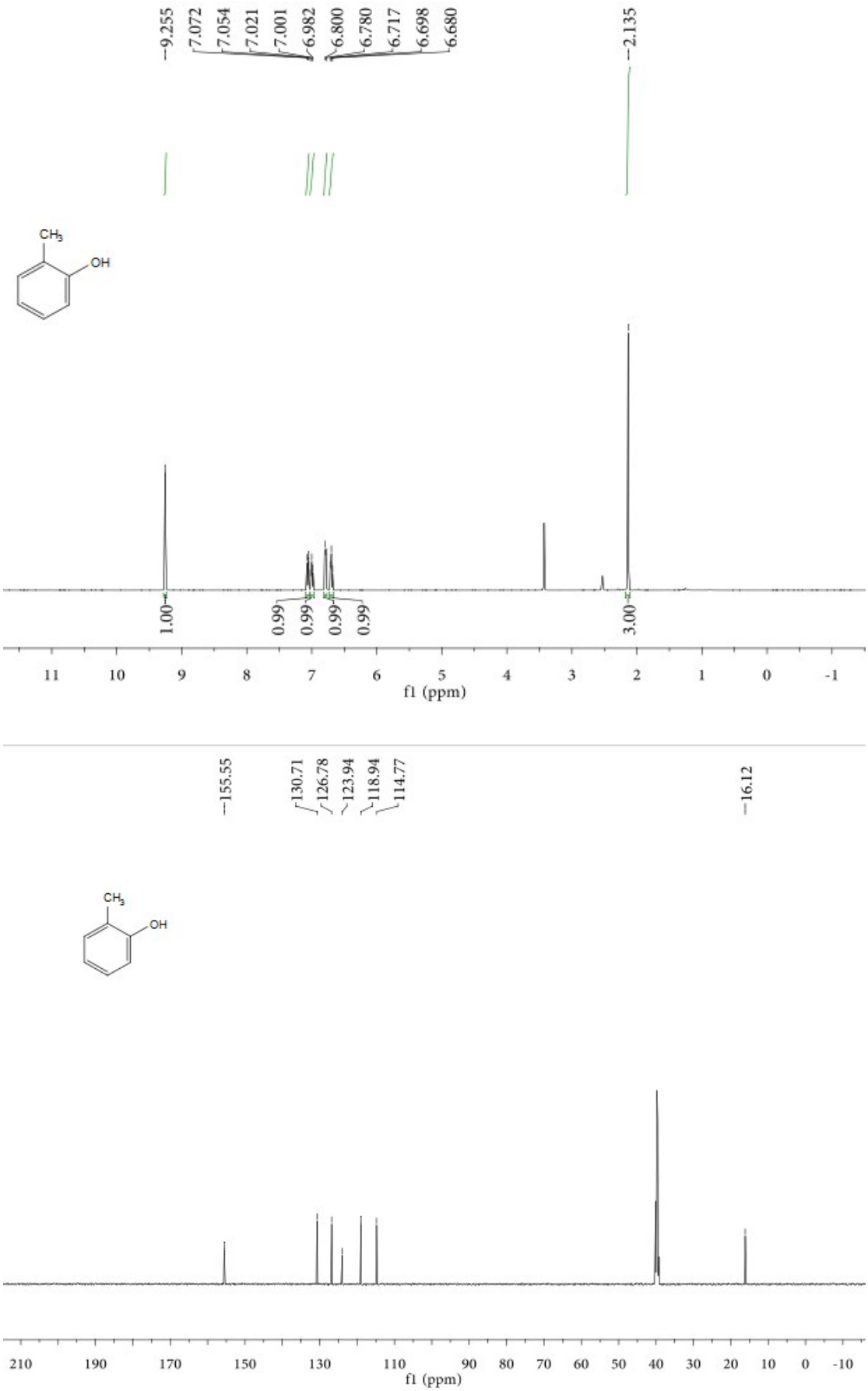


Figure S31. ^{1}H NMR of **29b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **29b** (125 MHz, DMSO-d_6)

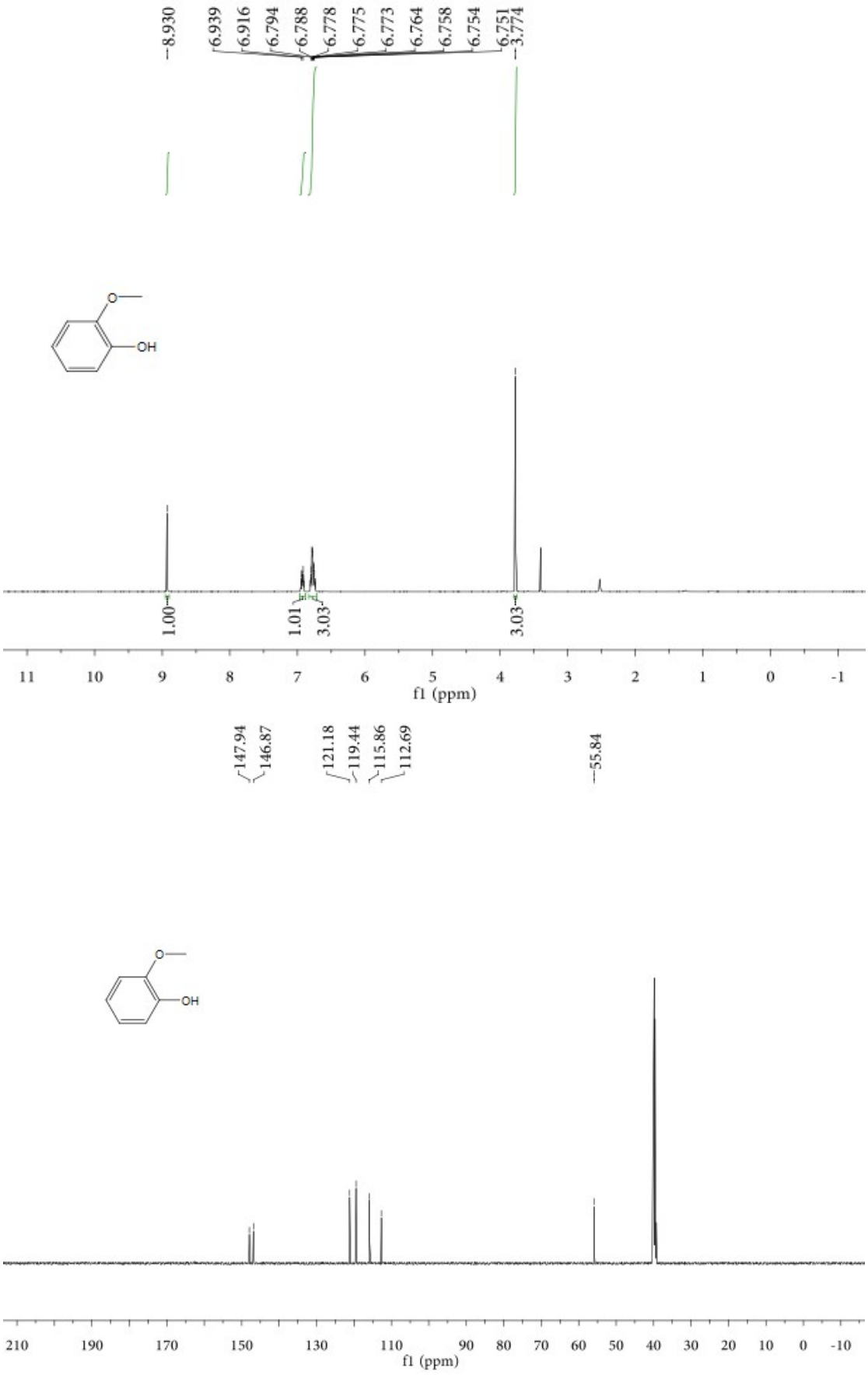


Figure S32. ^{1}H NMR of **30b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **30b** (125 MHz, DMSO-d_6)

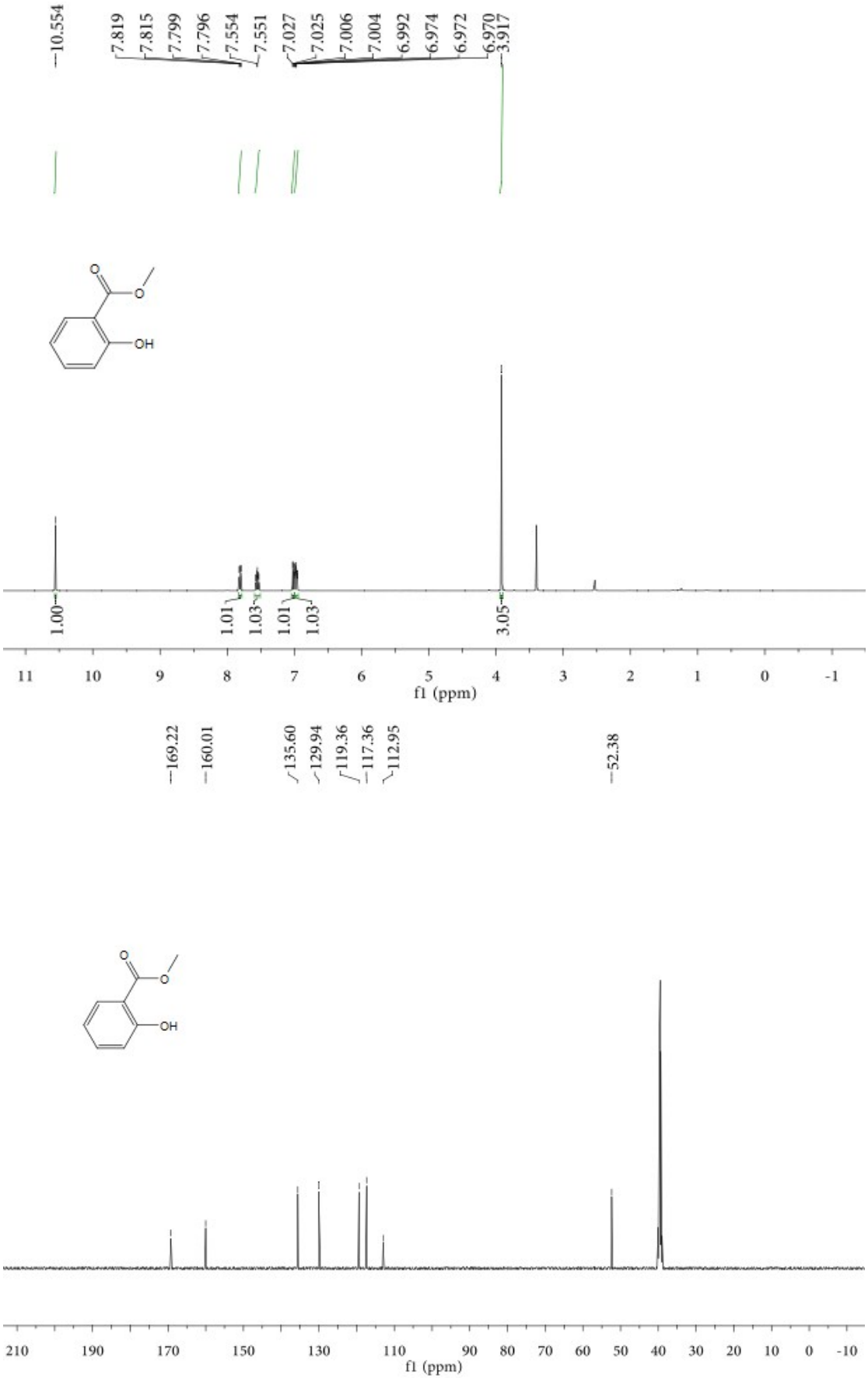


Figure S33. ^{1}H NMR of **31b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **31b** (125 MHz, DMSO-d_6)

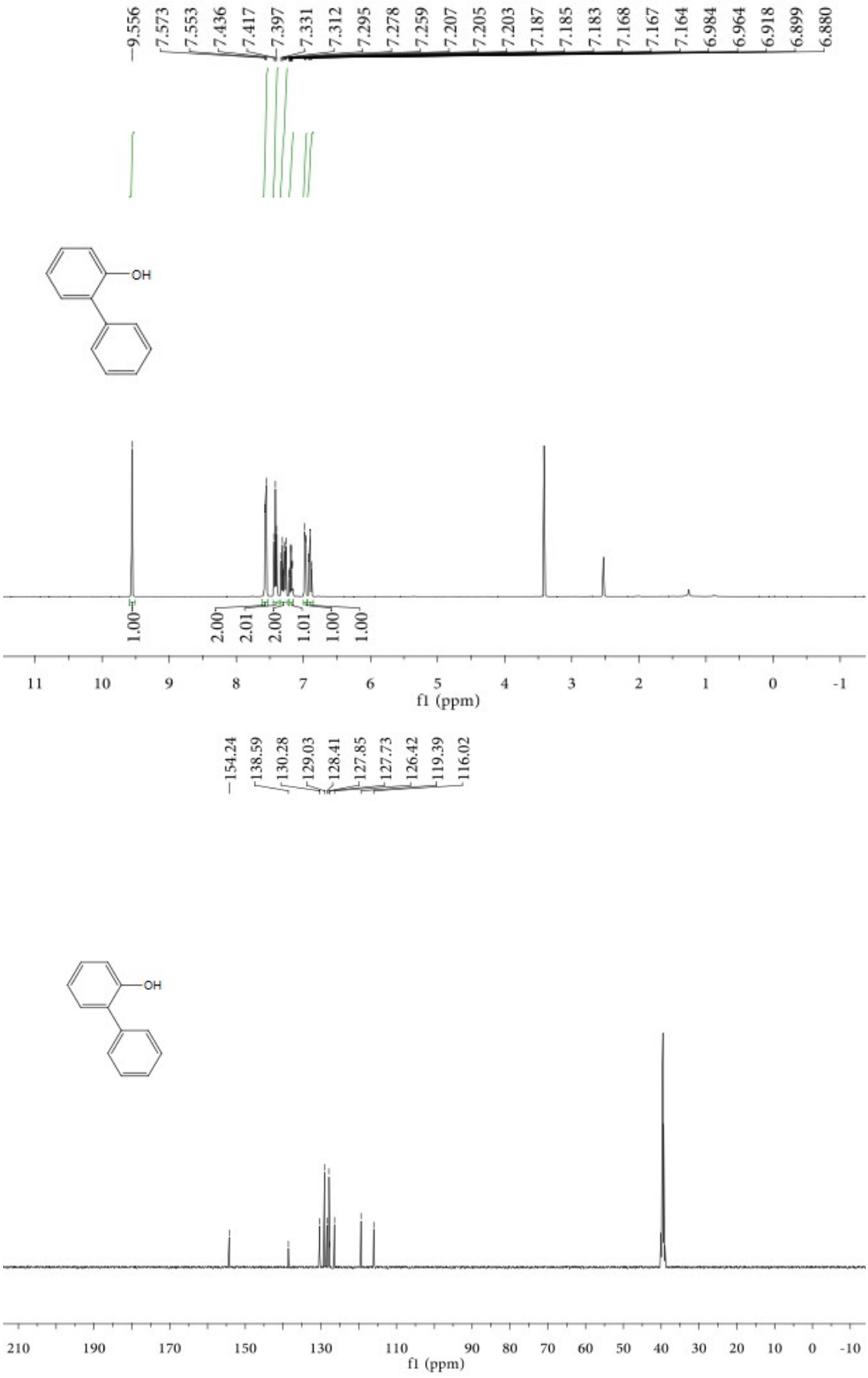


Figure S34. ^{1}H NMR of **32b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **32b** (125 MHz, DMSO-d_6)

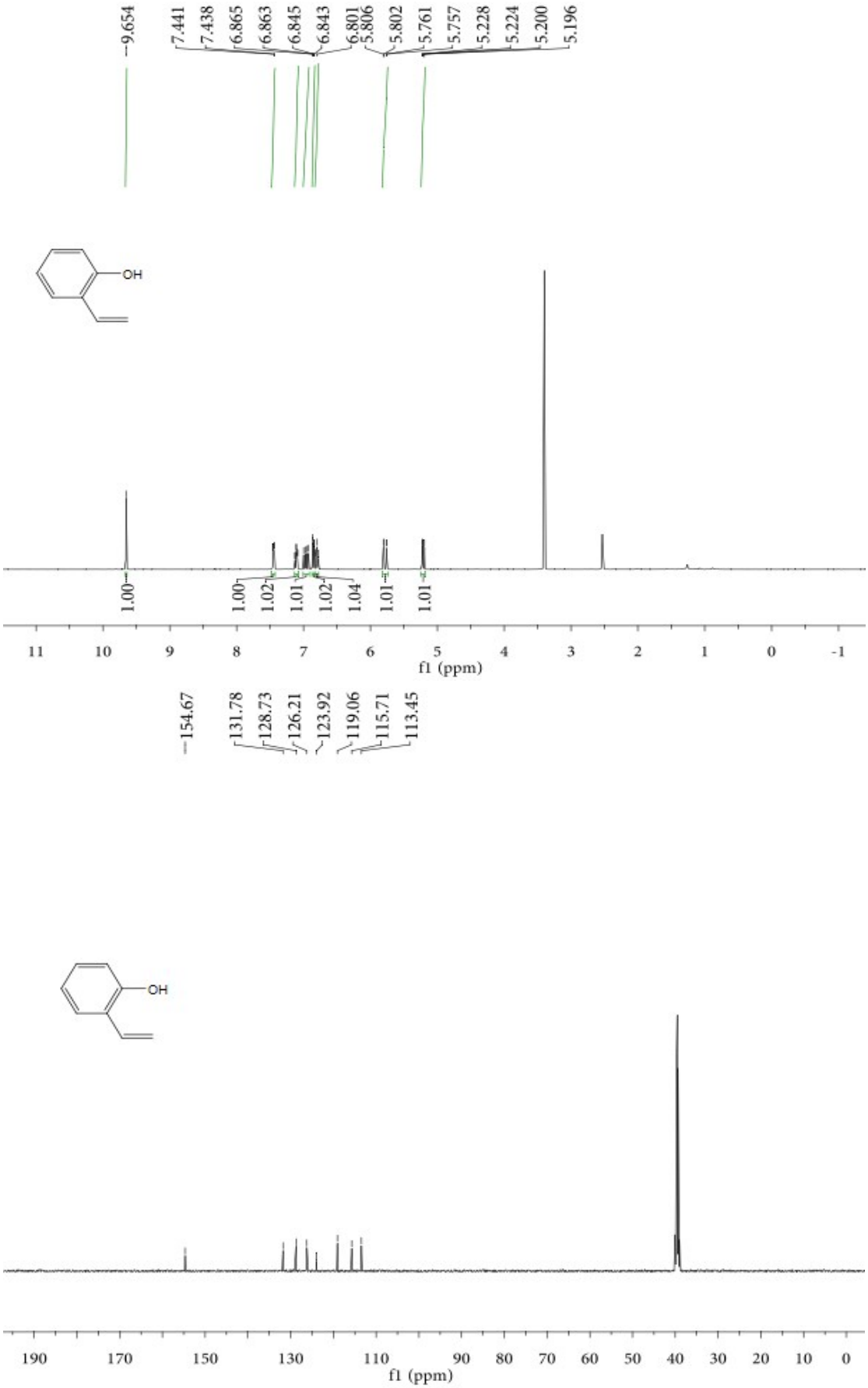


Figure S35. ^{1}H NMR of **33b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **33b** (125 MHz, DMSO-d_6)

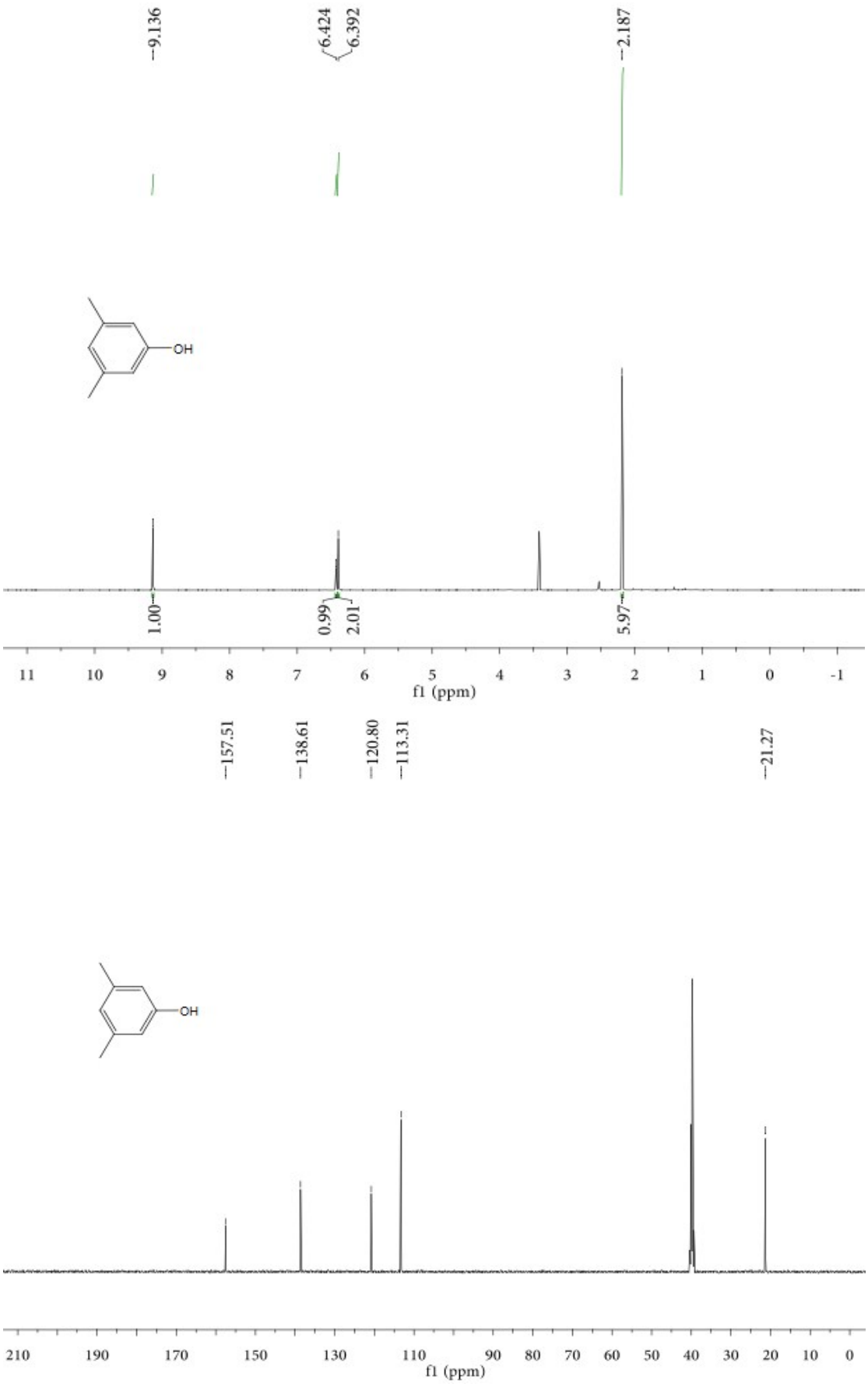


Figure S36. ^{1}H NMR of **34b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **34b** (125 MHz, DMSO-d_6)

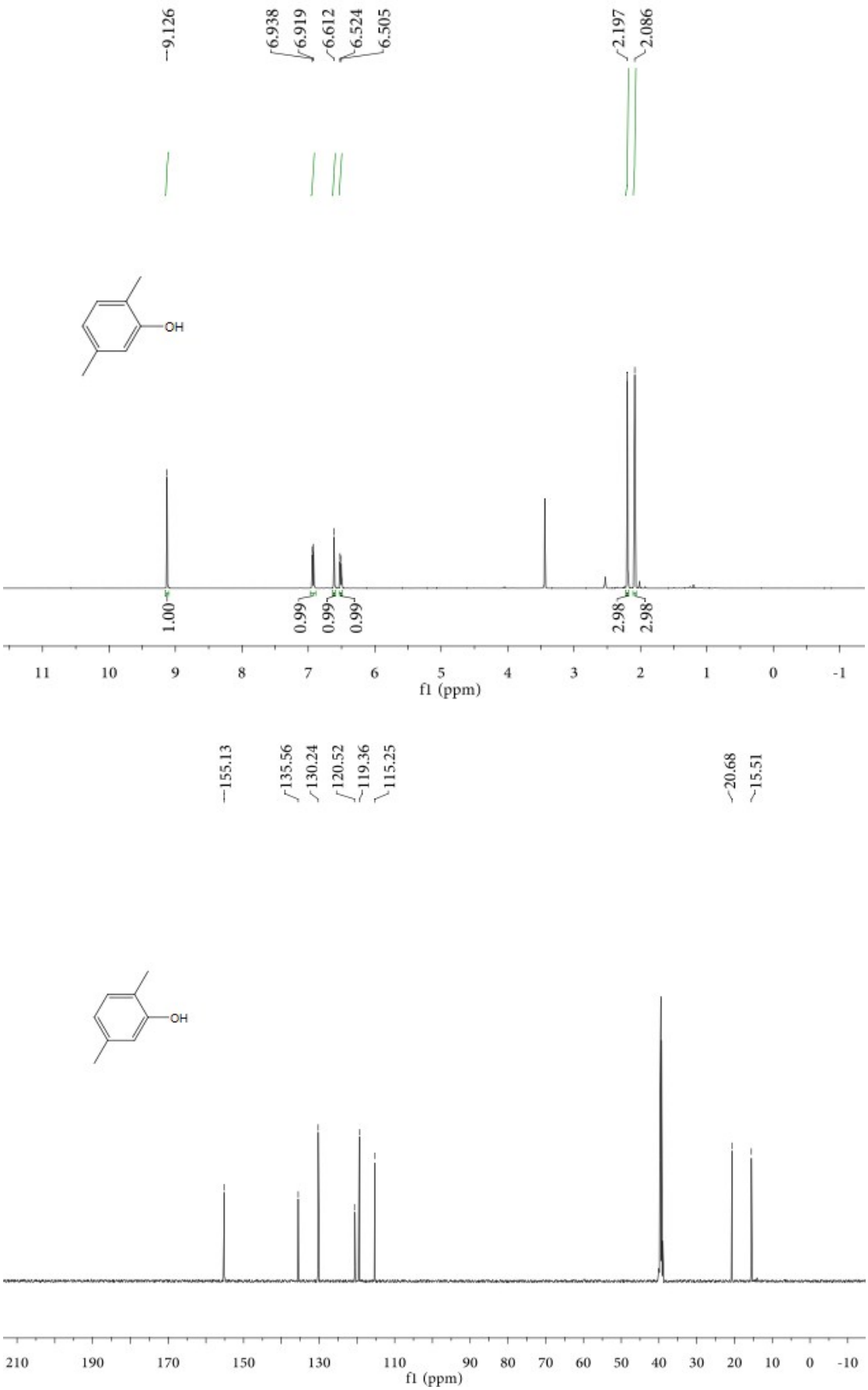


Figure S37. ^{1}H NMR of **35b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **35b** (125 MHz, DMSO-d_6)

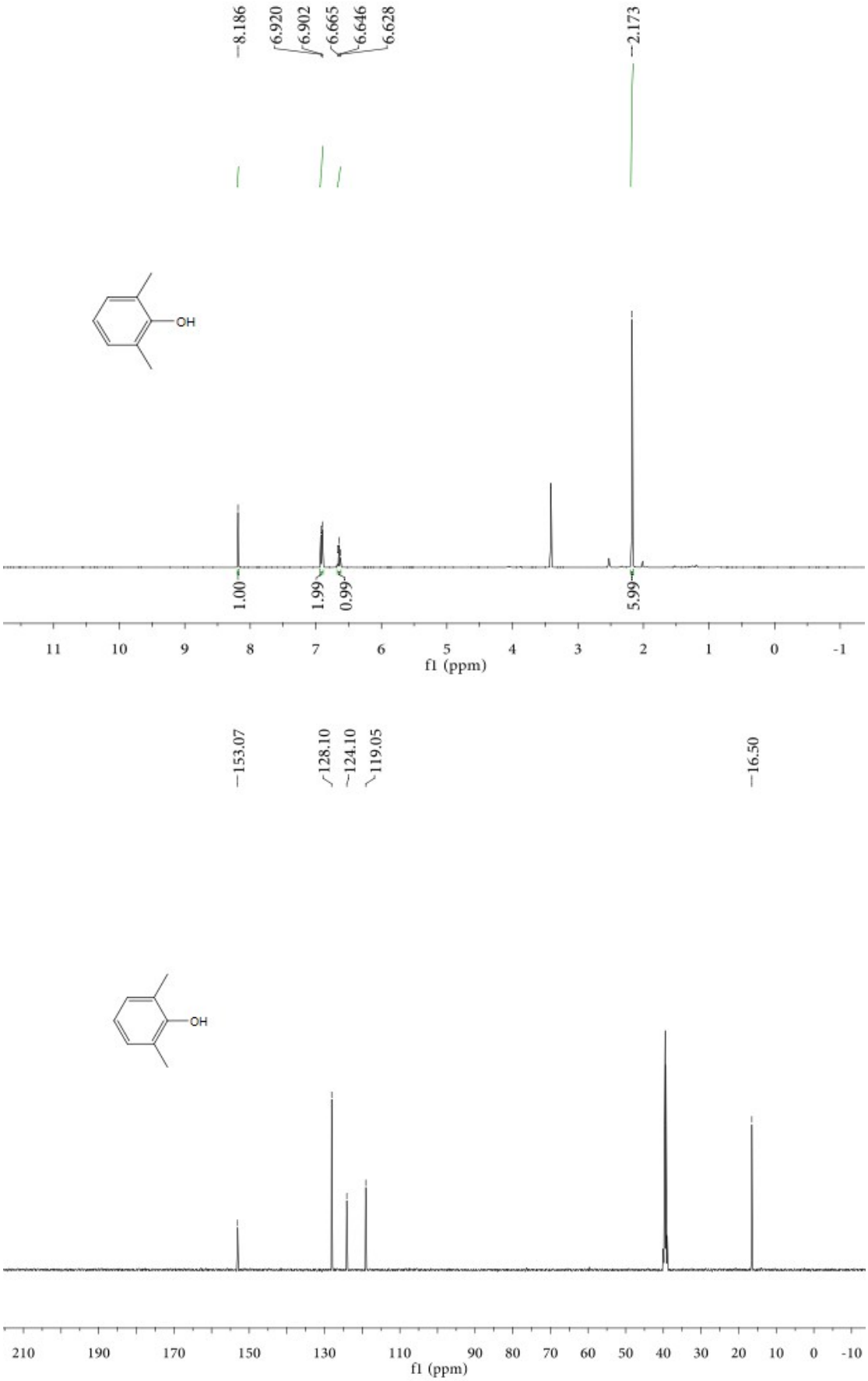


Figure S38. ^{1}H NMR of **36b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **36b** (125 MHz, DMSO-d_6)

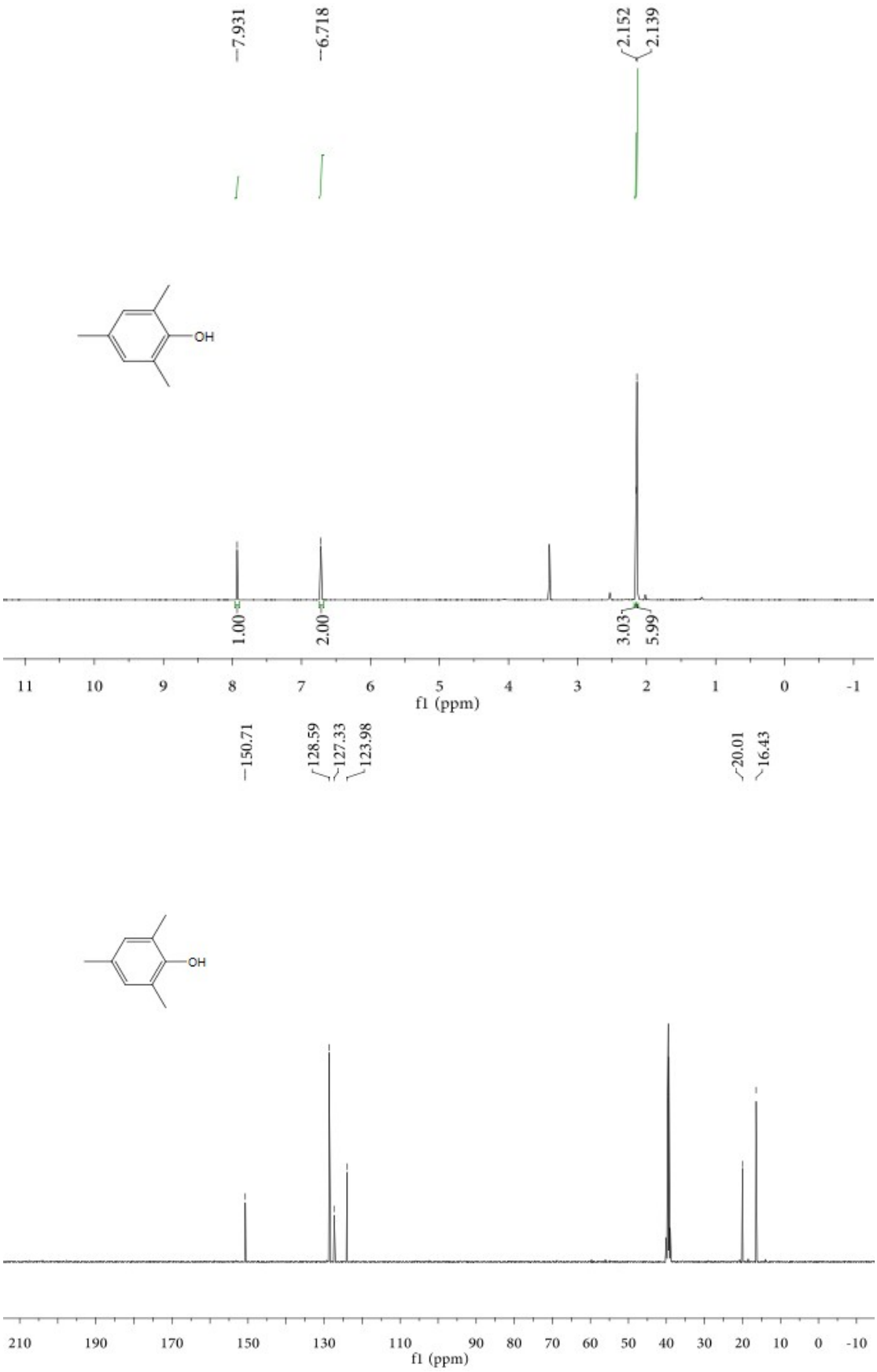


Figure S39. ^{1}H NMR of **37b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **37b** (125 MHz, DMSO-d_6)

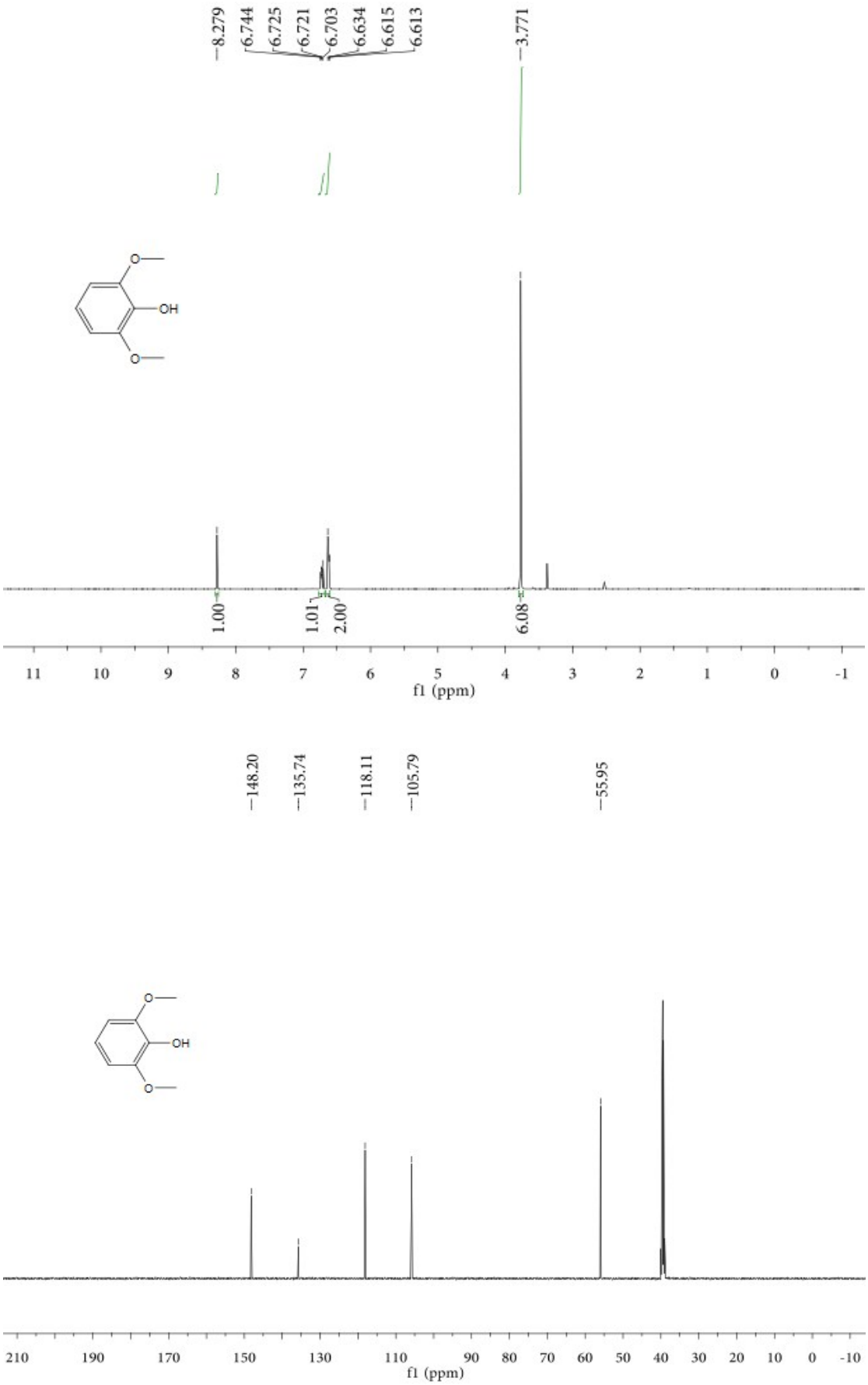


Figure S40. ^{1}H NMR of **38b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **38b** (125 MHz, DMSO-d_6)

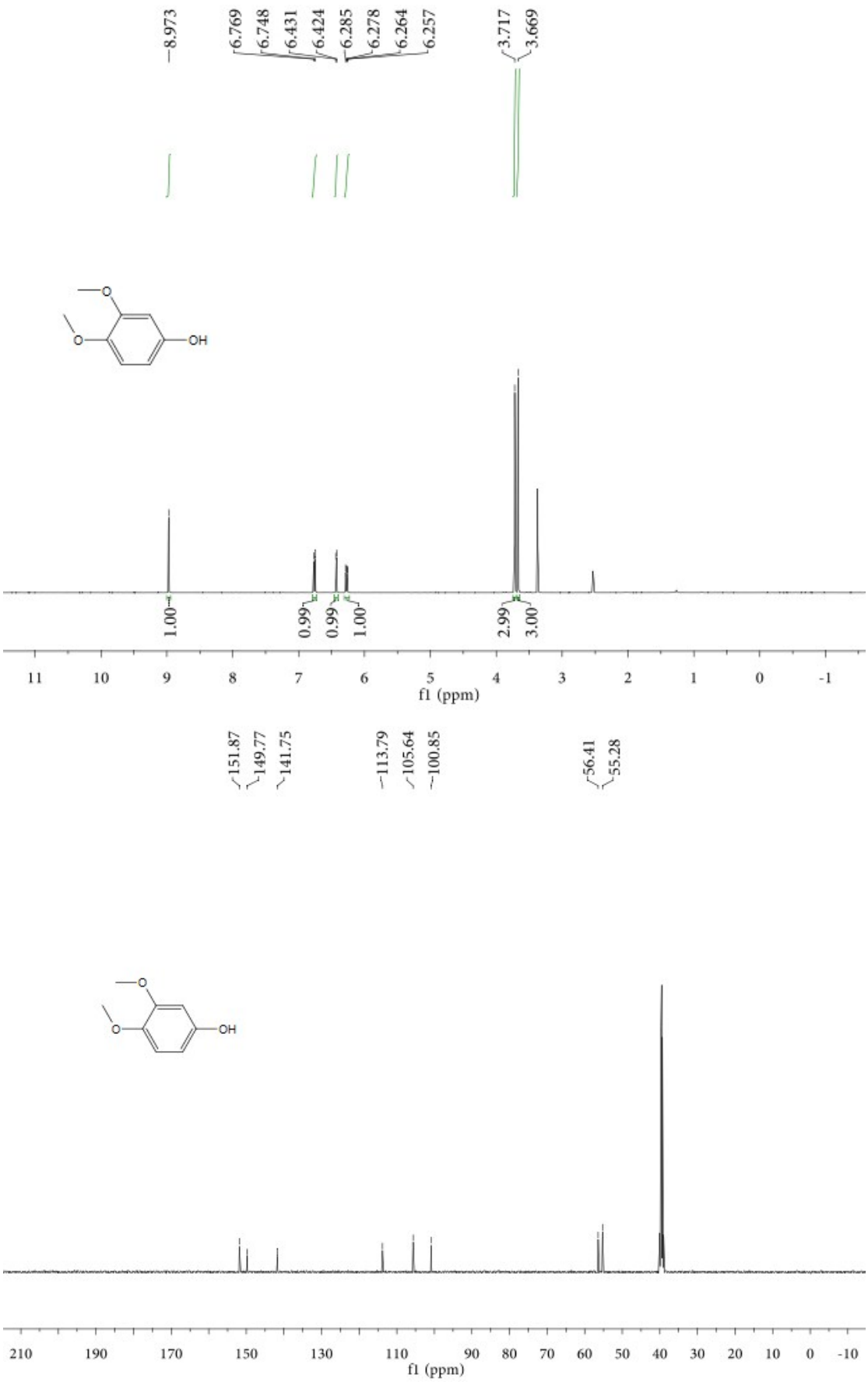


Figure S41. ^{1}H NMR of **39b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **39b** (125 MHz, DMSO-d_6)

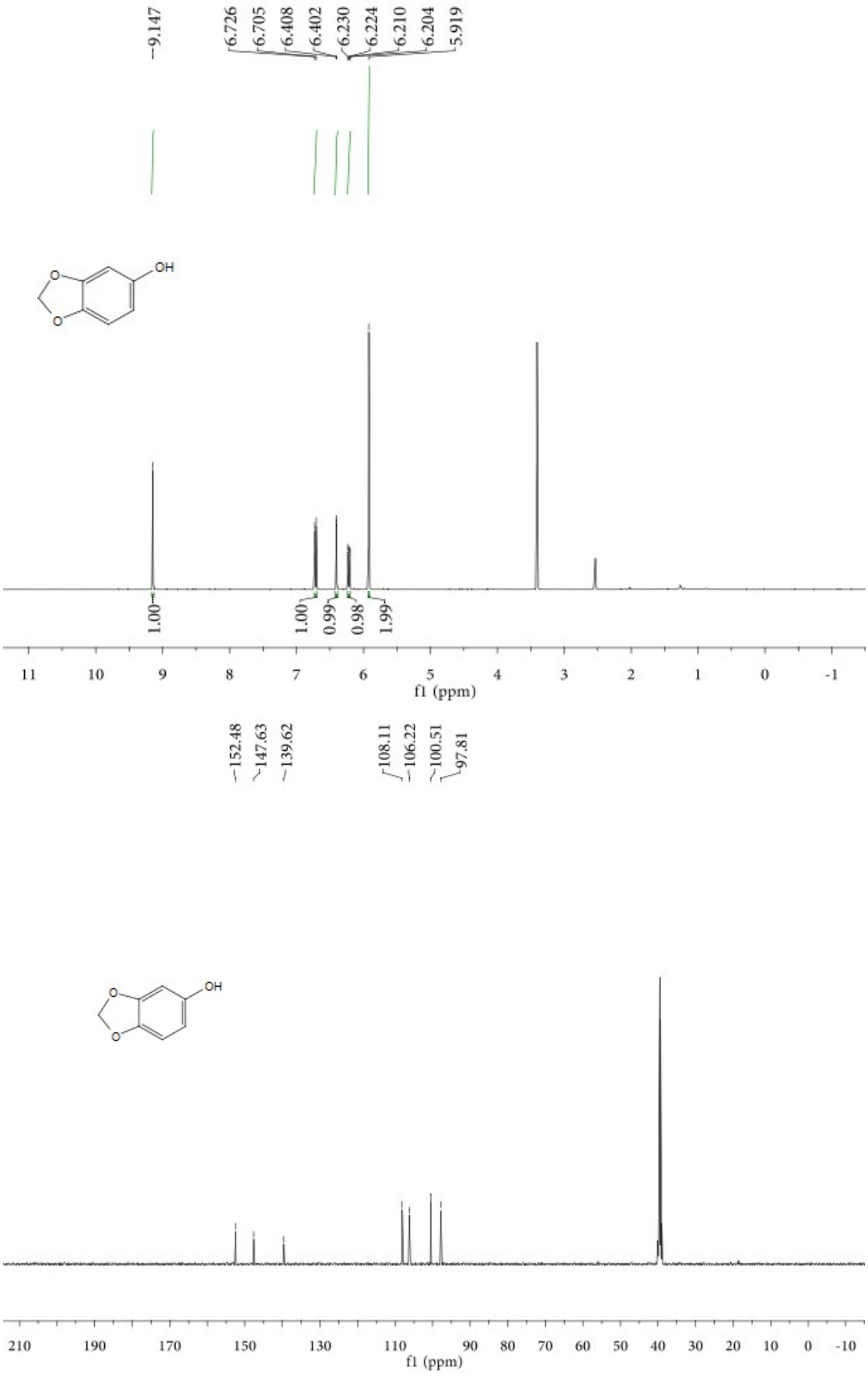


Figure S42. ^{1}H NMR of **40b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **40b** (125 MHz, DMSO-d_6)

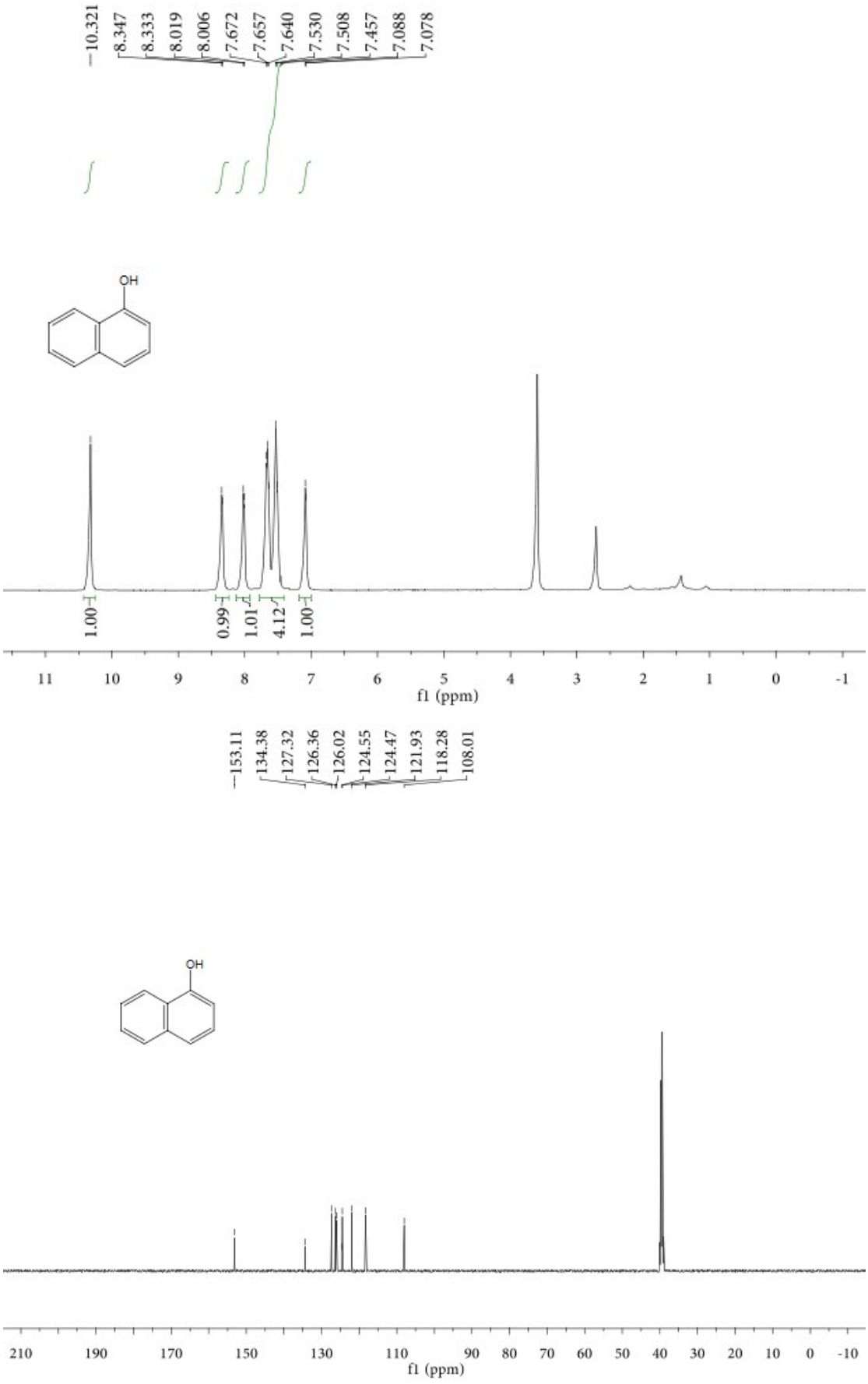


Figure S43. ^{1}H NMR of **43b** (500 MHz, DMSO-d_6) and ^{13}C NMR of **43b** (125 MHz, DMSO-d_6)

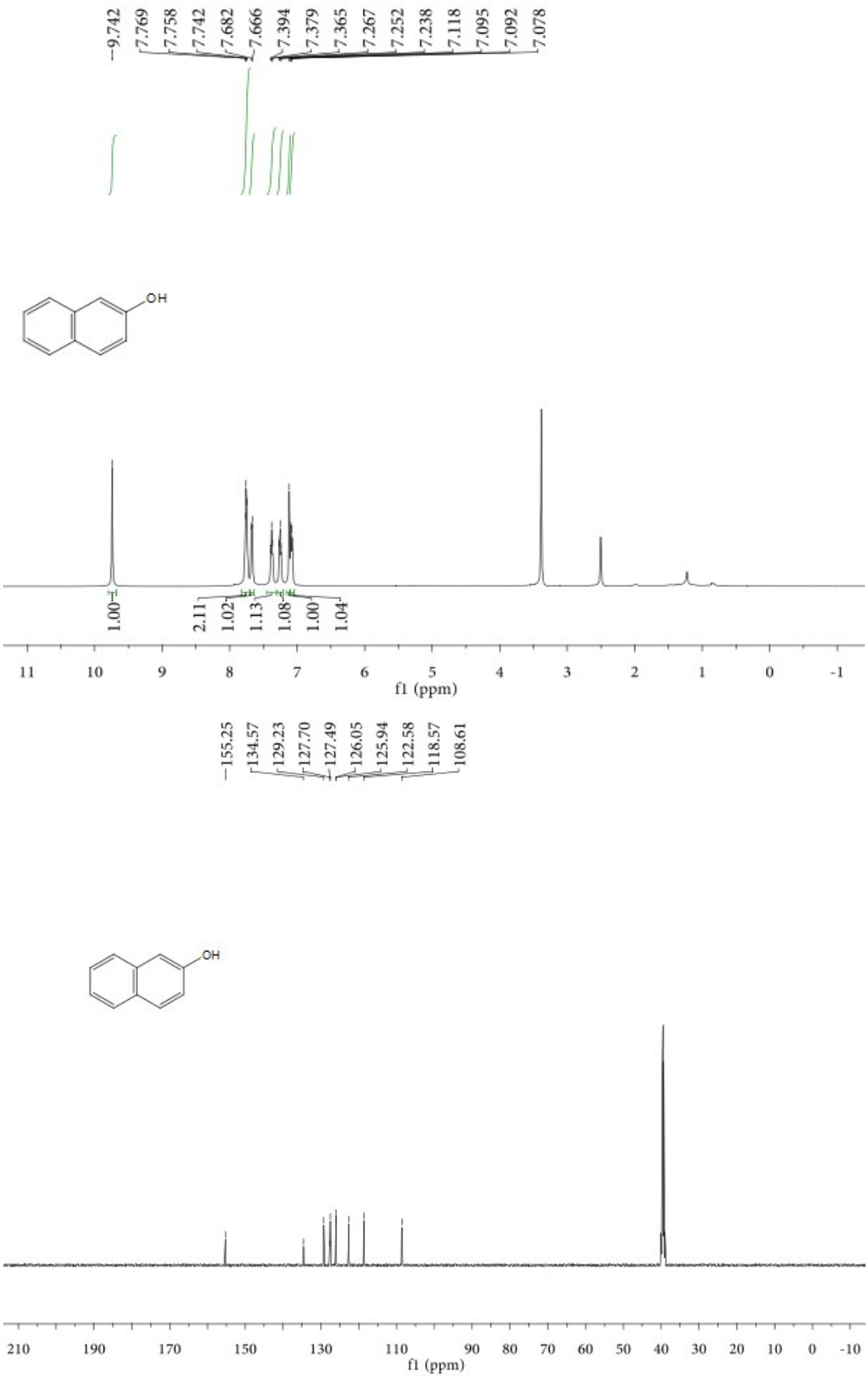


Figure S44. ^{1}H NMR of **44b** (500 MHz, DMSO-d_6) and ^{13}C NMR of **44b** (125 MHz, DMSO-d_6)

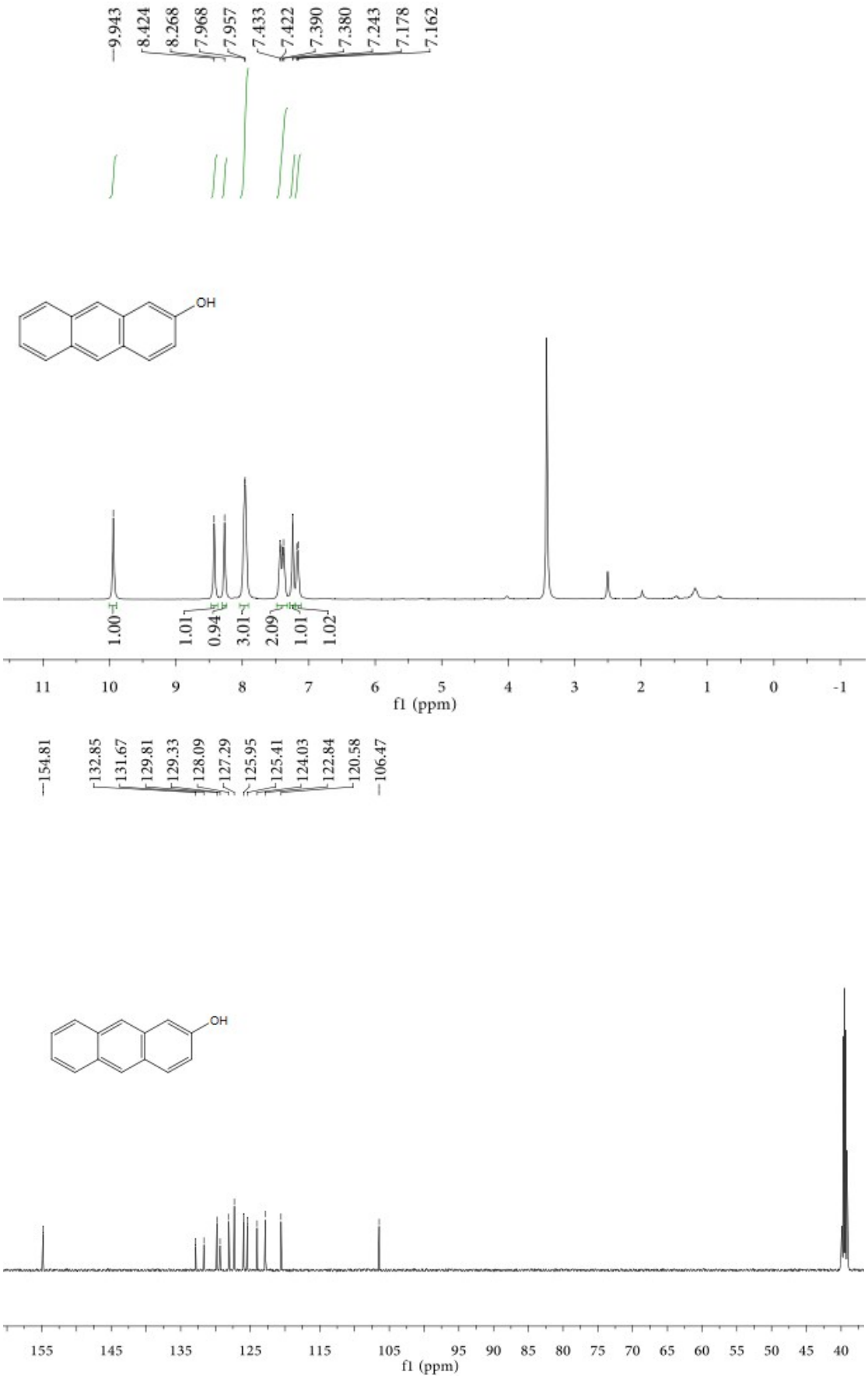


Figure S45. ^{1}H NMR of **45b** (500 MHz, DMSO-d_6) and ^{13}C NMR of **45b** (125 MHz, DMSO-d_6)

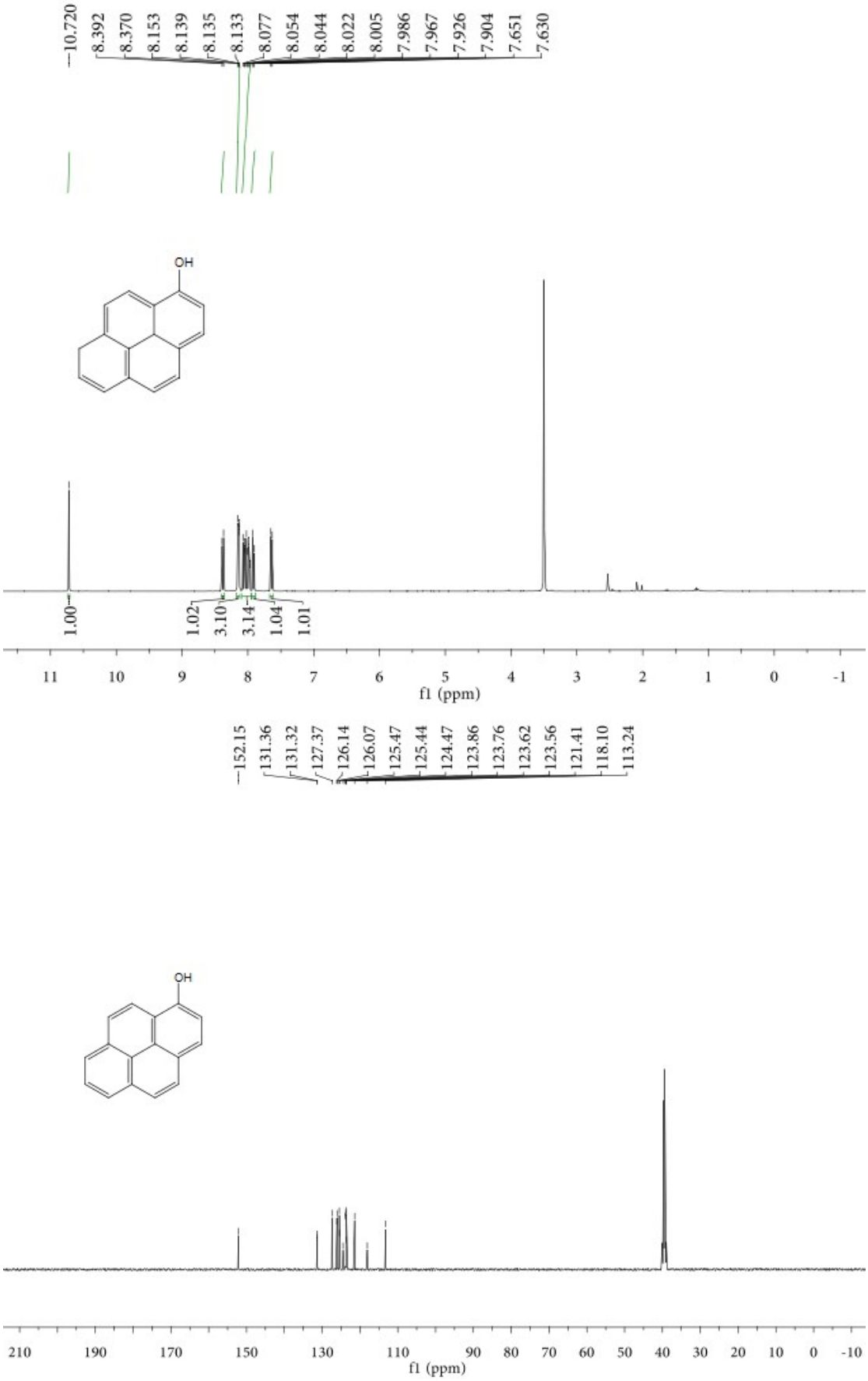


Figure S46. ^{1}H NMR of **46b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **46b** (125 MHz, DMSO-d_6)

Figure S47. ^{1}H NMR of **47b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **47b** (125 MHz, DMSO-d_6)

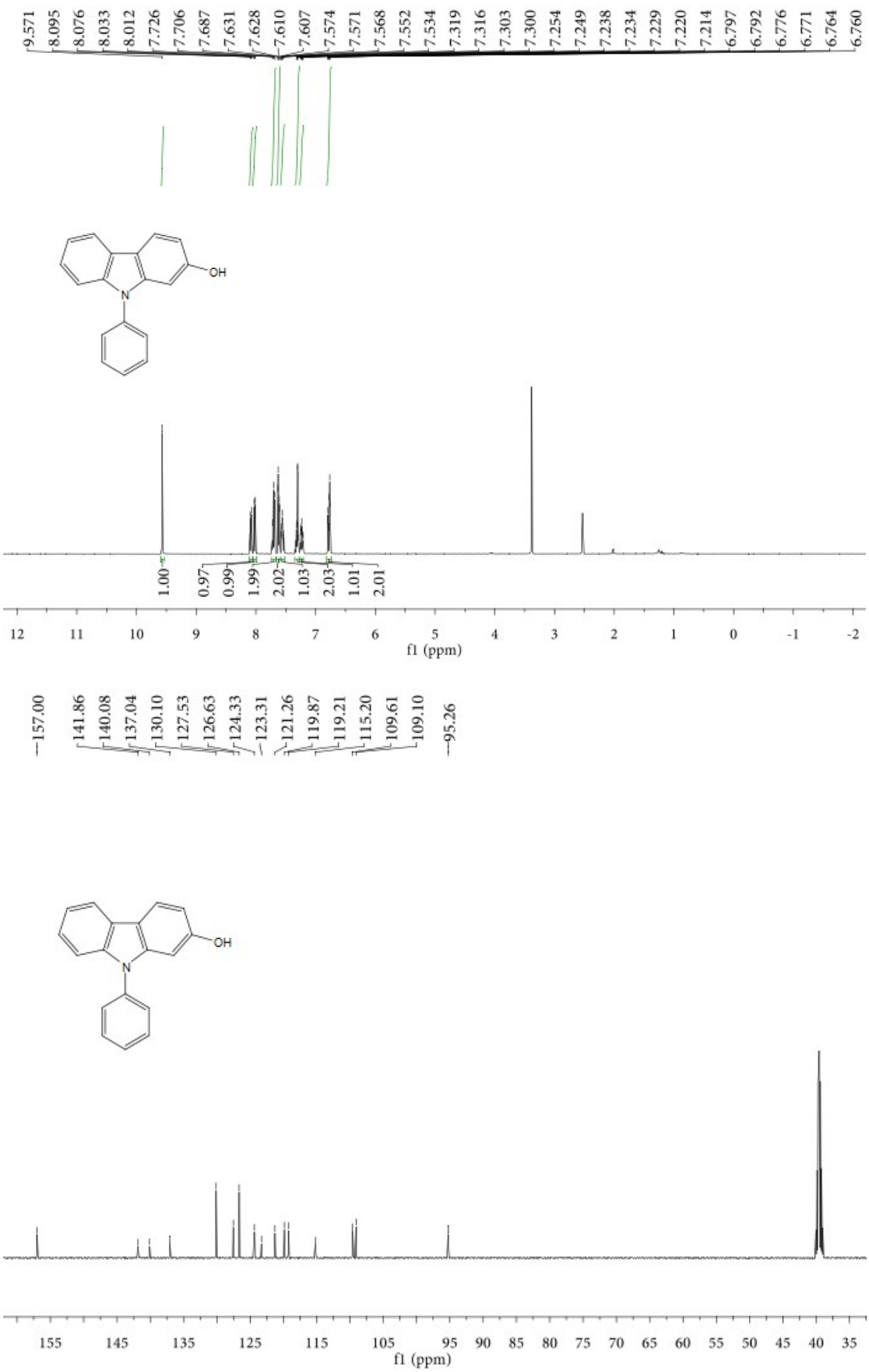


Figure S48. ^{1}H NMR of **48b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **48b** (125 MHz, DMSO-d_6)

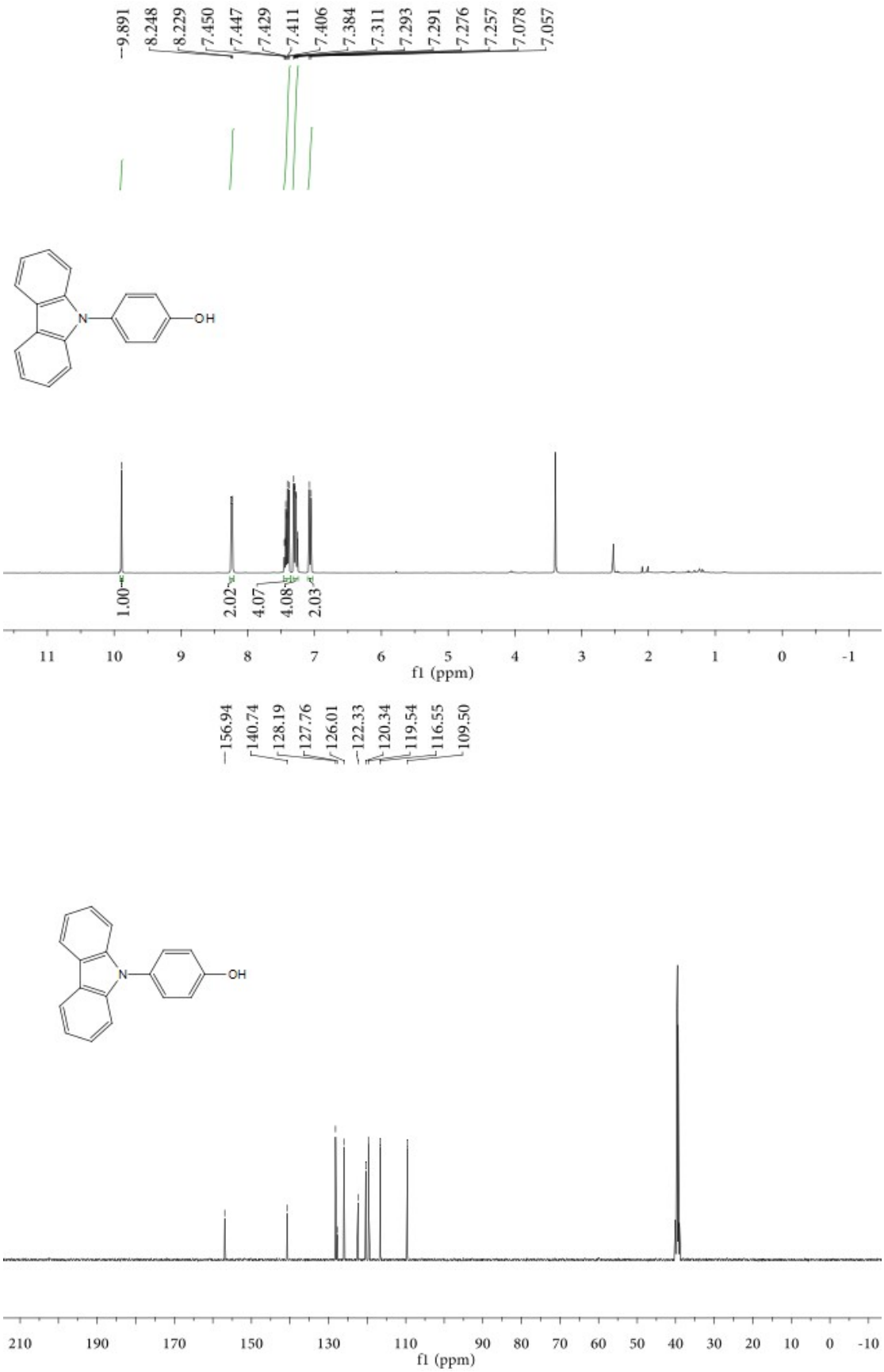


Figure S49. ^{1}H NMR of **49b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **49b** (125 MHz, DMSO-d_6)

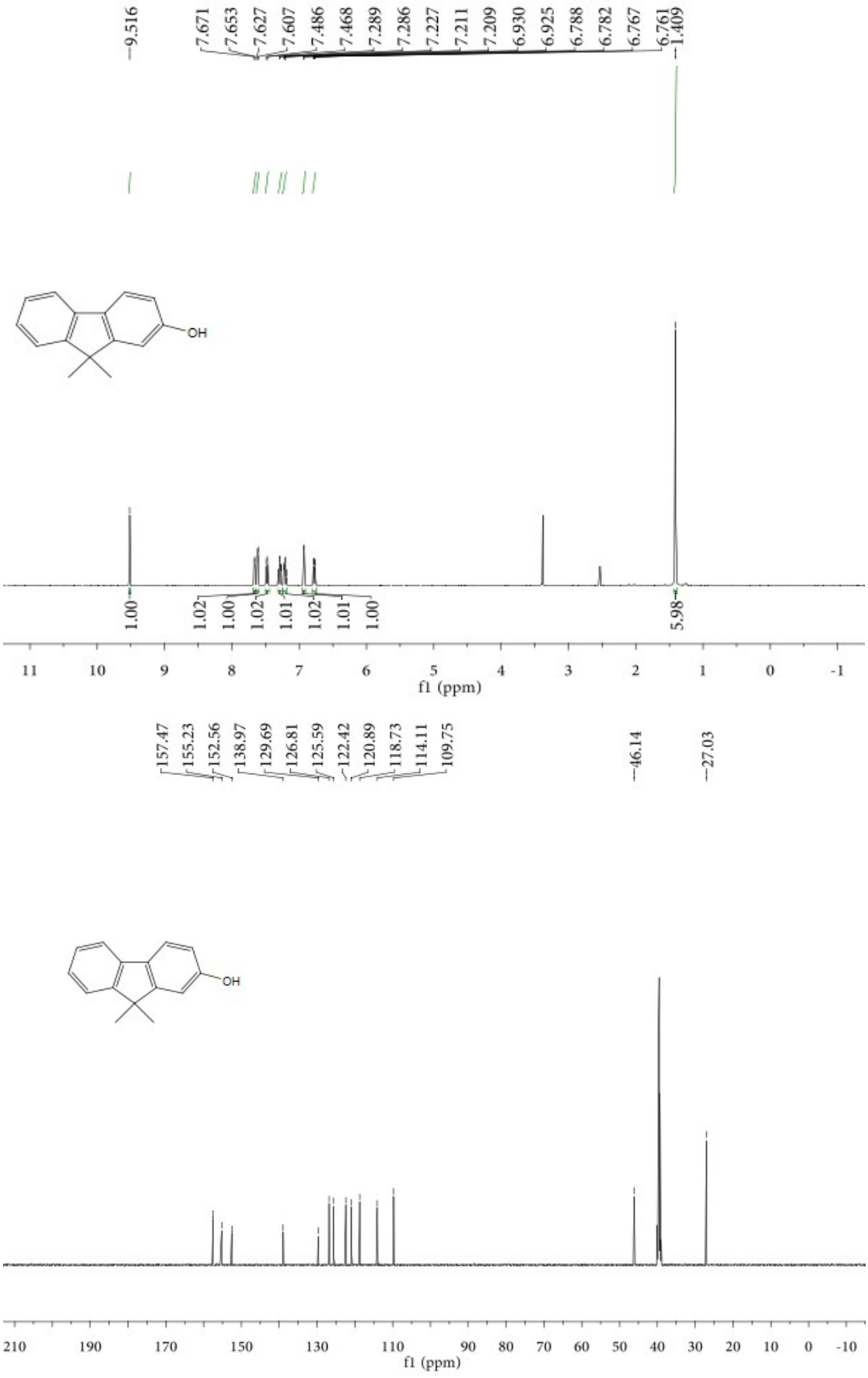


Figure S50. ^{1}H NMR of **50b** (400 MHz, DMSO-d_6) and ^{13}C NMR of **50b** (125 MHz, DMSO-d_6)

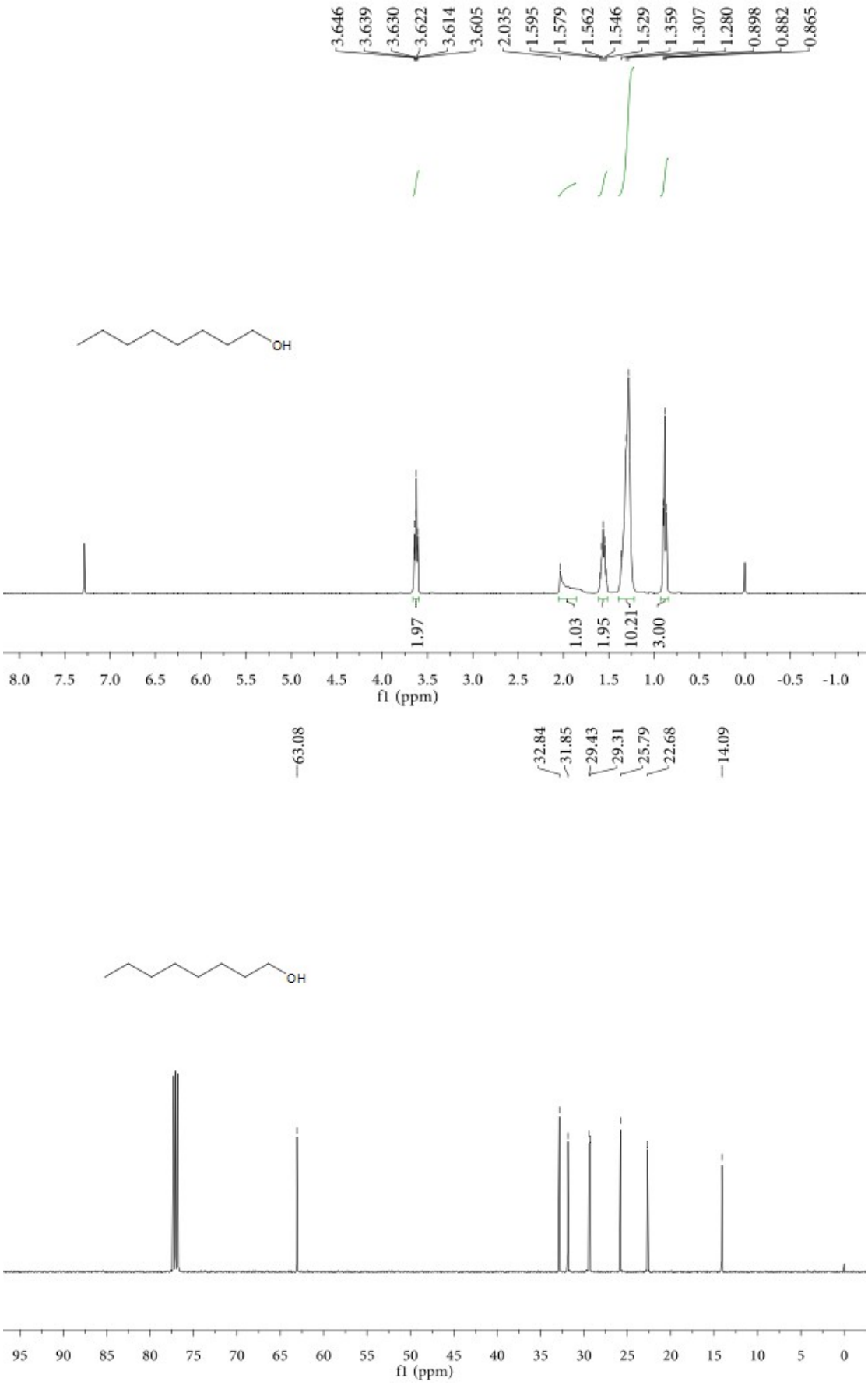


Figure S51. ^{1}H NMR of **51b** (400 MHz, $CDCl_3$) and ^{13}C NMR of **51b** (125 MHz, $CDCl_3$)

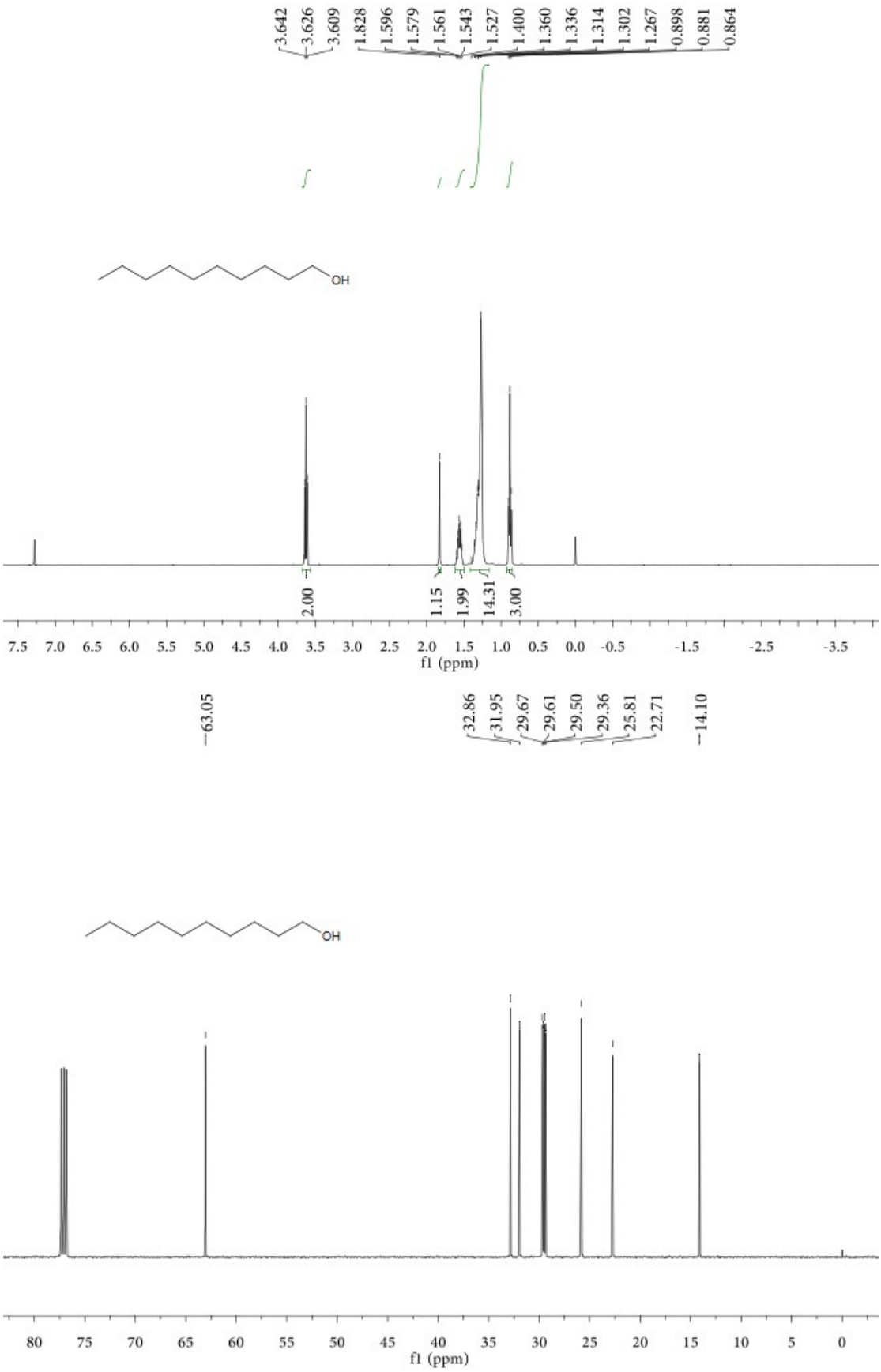


Figure S52. ^{1}H NMR of **52b** (400 MHz, $CDCl_3$) and ^{13}C NMR of **52b** (125 MHz, $CDCl_3$)