Supporting Information

Electrochemical selective annulative amino-ketalization and amino-oxygenation of 1,6-enynes

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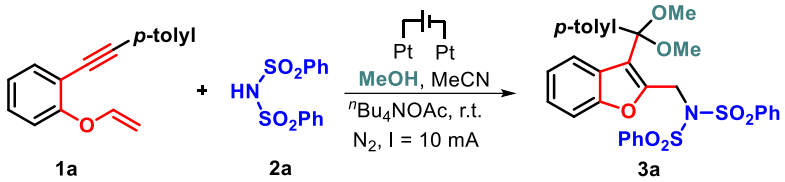
General Information

PE refers to petroleum ether (b.p. 60-90 °C) and EA refers to ethyl acetate, as well as DCE refers to dichloroethane. All other starting materials and solvents were commercially available and were used without further purification unless otherwise stated. ^{1}H NMR (^{13}C NMR) spectra were measured on a Bruker DPX 400 MHz spectrometer in $CDCl_3$ (or DMSO-d_6) with chemical shift (δ) given in ppm relative to TMS as internal standard [(s = singlet, d = doublet, m = multiplet), coupling constant (Hz)]. HRMS (APCI) was determined by using microTOF-QII HRMS/MS instrument (BRUKER). X-Ray crystallographic analysis was performed with a Siemens SMART CCD and a Siemens P4 diffractometer. The melting points were measured with digital melting point detector. CV curves were recorded using a three-electrode scheme. The working electrode was a platinum plate, A platinum wire served as counter electrode. Ag/AgCl electrode was used as the reference electrode. The working electrode was polished before recording each CV curve.

Table S1. Condition optimization for product **3a**[a]

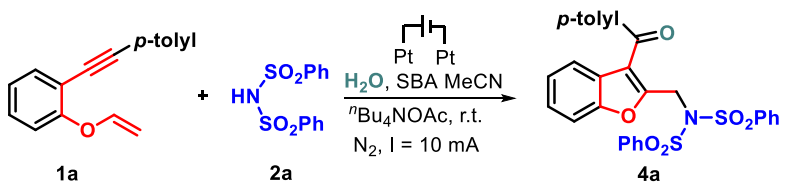


1a 2a 3a

entry	variation from the established conditions	yield (%)[b]
1	none	53
2	Air instead of N_2	18
3	5 mA instead of 10 mA	trace
4	20 mA instead of 10 mA	31
5[d,e]	MeOH/MeCN (2:3) as solvent	25
6[d,e]	MeOH/MeOH (1:4) as solvent	trace
7	DCE instead of MeCN	65
8	Toluene instead of MeCN	61
9	THF instead of MeCN	27
10	1,4-dioxane instead of MeCN	<5%
11	DMF instead of MeCN	<5%
12	30 °C instead of 25 °C	45
13	$^{n}Bu_4NBF_4$, $^{n}Bu_4NHSO_4$, $^{n}Bu_4NClO_4$ instead of $^{n}Bu_4NOAc$	N.D.
14[c]	GR(+)|Pt(-) instead of Pt(+)|Pt(-)	trace

[a]Reaction conditions: Pt anode, Pt cathode, undivided cell, constant current = 10 mA, **1a** (0.2 mmol), **2a** (0.6 mmol), and $^{n}Bu_4NOAc$ (0.6 mmol), MeOH (1.5 mL), and DCE (3.5 mL) under room temperature for 4 h. [b]Isolated yield based on substrate **1a**. [c]Graphite rod (GR) electrode. [d]Volume ratio. [e]Total solvent (5.0 mL).

Table S2. Optimization of the reaction conditions for forming **4a**[a]

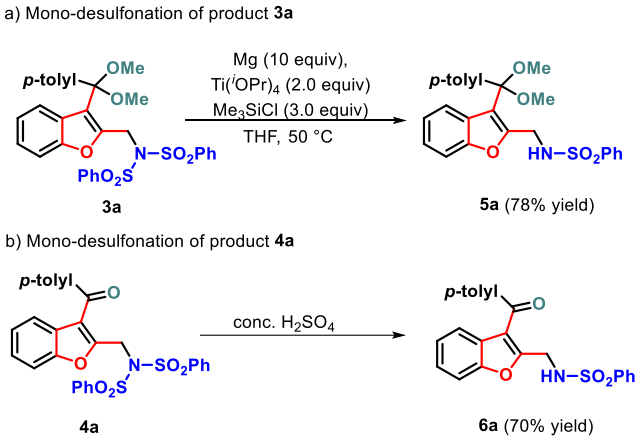


1a 2a 4a

entry	variation from the established conditions	yield (%)[b]

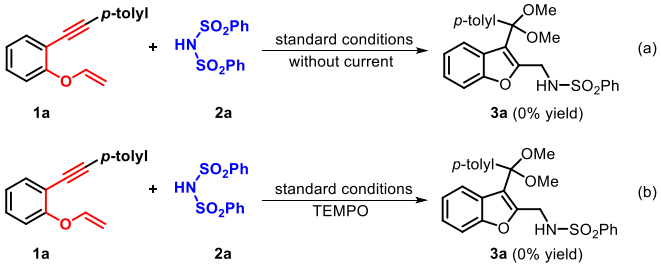
1	none	56
2	IPA (1.5 mL) instead of SBA	45
3	NBA (1.5 mL) instead of SBA	47
4	H_2O (1.5 mL) instead of SBA	23
5	1,4-dioxane instead of DCE	trace
6	Toluene instead of DCE	trace
7	DMSO instead of DCE	N.D.

[a]Reaction conditions: Pt anode, Pt cathode, undivided cell, constant current = 10 mA, **1a** (0.2 mmol), **2a** (0.6 mmol), and $^{n}Bu_4NOAc$ (0.6 mmol), SBA (1.5 mL), and DCE (3.5 mL) under room temperature for 4 h. [b]Isolated yield based on substrate **1a**. [c]Total solvent (5.0 mL). SBA = *sec*-butyl alcohol, IPA = *i*-propyl alcohol, NBA = *n*-butyl alcohol.



Scheme S1. Synthetic application of **3a** and **4a**

The presence of disulfonimides provides great possibilities for late-stage modifications (Scheme S1). For instance, mono-desulfonylation of compound **3a** in the presence of magnesium powder, $Ti(^{i}OPr)_4$ and Me_3SiCl gave sulfonamide-substituted benzofuran **5a** in 78% yield (Scheme S1a).[1] Next, mono-desulfonylation of compound **4a** in the presence of conc. H_2SO_4 afforded sulfonamide-substituted benzofuran **6a** in 70% yield (Scheme S1b).[2]



Scheme S2 Control experiments.

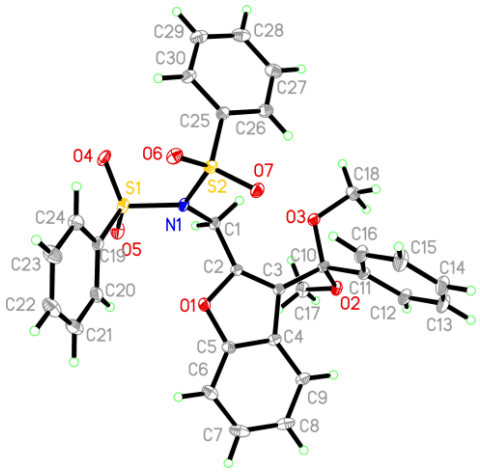


Figure S1 X-Ray structure of **3g** (CCDC 2189675)

A single crystal **3g** was obtained by slowly evaporating the mixed solvent of hexane and dichloromethane (V/V = 2:1) at room temperature under the air conditions.

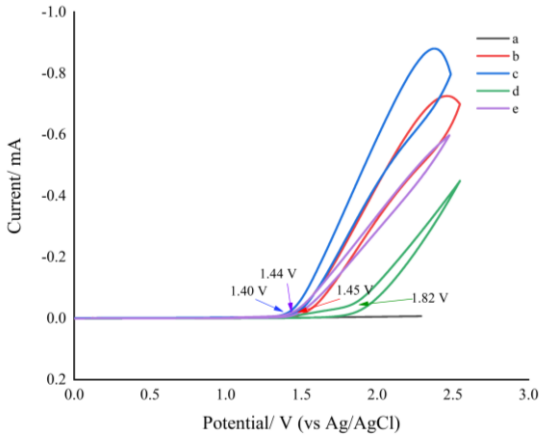
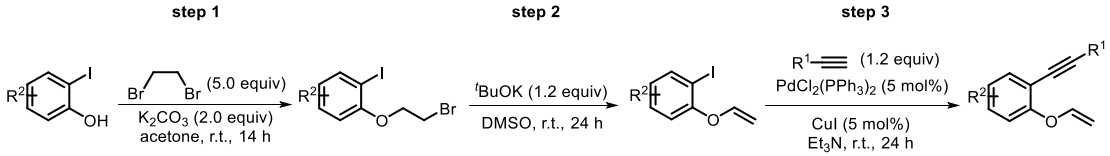


Figure S2. Cyclic voltammograms of the solution in DCE/MeOH (V/V 3.5/1.5) using a Pt wire working electrode, Pt disk, and Ag/AgCl (in saturated KCl solution) as counter and reference electrodes at a scan rate of 10 mV/s: (a) background; (b) $^{n}Bu_4NOAc$ (2 mmol/L); (c) **1a** (2 mmol/L), $^{n}Bu_4NOAc$ (2 mmol/L); (d) **2a** (2 mmol/L), $^{n}Bu_4NOAc$ (2 mmol/L); (e) **1a** (2 mmol/L), **2a** (2 mmol/L), and $^{n}Bu_4NOAc$ (2 mmol/L).

General procedure for the synthesis of 2-vinyloxy arylalkyne[1]



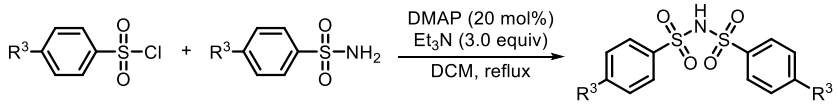
Step 1: To a solution of 2-iodophenol (5.0 mmol) and 1,2-dibromoethane (5.0 equiv) in acetone (50 mL) was added K_2CO_3 (2.0 equiv). The resulting mixture was stirred at room temperature for 14 h and then reflux for 6 h. The reaction was quenched with water and extracted with CH_2Cl_2. The organic layer was washed with brine, dried over Na_2SO_4, and concentrated. The crude product was purified by a silica gel column chromatography (petroleum ether (PE)/ ethyl acetate (EA) = 100:1 V/V) to give **A** (65~76% yields) as a colorless oil.

Step 2: To a solution of **A** (3.0 mmol) in DMSO (20 mL) was added $^{t}BuOK$ (1.5 equiv). The resulting mixture was stirred at room temperature for 2 h. The reaction mixture was filtered and washed with CH_2Cl_2. The combined filtrate was concentrated and the residue was purified by a silica gel column chromatography (PE/EtOAc = 100:1 V/V) to give **B** (81~95% yields) as a yellow oil.

Step 3: To a solution of **B** (1.0 mmol) and alkyne (1.1 equiv) in triethylamine (10 mL) was added $PdCl_2(PPh_3)_2$

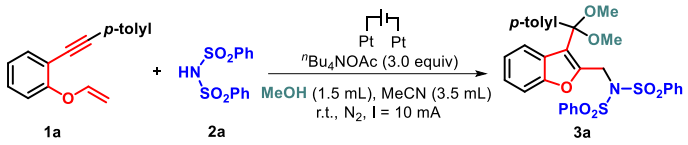
(5 mol%) and CuI (5 mol%). The resulting mixture was stirred at room temperature for 24~36 h. The reaction mixture was filtered and washed with Et_2O. The combined filtrate was concentrated and the residue was purified by a silica gel column chromatography (PE/EtOAc = 100:1 V/V) and recycling preparative GPC to give **1a-1t** (68~92% yields)

General procedure for the synthesis of disulfonimides 2[2]



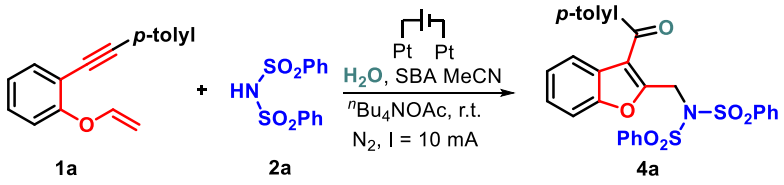
A mixture of $PhSO_2Cl$ (5.0 mmol), $PhSO_2NH_2$ (1.0 equiv), DMAP (20 mol%) and Et_3N (3.0 equiv) in DCM (5 mL) was refluxed for 2 h (monitored by TLC). After cooling to room temperature, the reaction was poured into 1 mol/L HCl (10 mL), extracted with DCM, and dried over anhydrous Na_2SO_4. The solvent was evaporated to afford the product as a colorless oil, which was used in the next step without purification (80%, yields).

General procedure for the synthesis of compounds 3



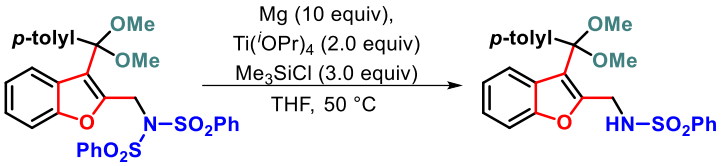
In an undivided flask (10 mL) equipped with a stir bar under nitrogen conditions, 1,6-enyne **1a** (0.2 mmol, 1.0 equiv, 47 mg), dibenzenesulfonimide (**2a**, 0.6 mmol, 3.0 equiv, 178 mg), ^{n}Bu$_4$NOAc (0.6 mmol, 3.0 equiv, 180 mg), and mixed solvent CH_3OH/DCE (V/V = 1.5/3.5, 5.0 mL) were added. The reaction flask was equipped with Pt disk as anode and cathode (1.0 × 1.5 cm^2). The solution was stirred and electrolyzed at a constant current (10 mA) without reference electrode for 4 h at room temperature until complete consumption of **1a** as monitored by TLC analysis. After the reaction was finished, the solution was concentrated under reduced pressure. The resulting residue was purified by silica gel column chromatography (PE/EA = 10:1 V/V) to afford the desired product **3a** (77 mg, 65% yield).

General procedure for the synthesis of compounds 4



In an undivided flask (10 mL) equipped with a stir bar under nitrogen conditions, 1,6-enyne **1a** (0.2 mmol, 1.0 equiv, 47 mg), dibenzenesulfonimide (**2a**, 0.6 mmol, 3.0 equiv, 178 mg), ^{n}Bu$_4$NOAc (0.6 mmol, 3.0 equiv, 180 mg), and mixed solvent SBA/DCE (V/V = 1.5/3.5, 5.0 mL) were added. The reaction flask was equipped with Pt disk as anode and cathode (1.0 × 1.5 cm^2). The solution was stirred and electrolyzed at a constant current (10 mA) without reference electrode for 4 h at room temperature until complete consumption of **1a** as monitored by TLC analysis. After the reaction was finished, the solution was concentrated under reduced pressure. The resulting residue was purified by silica gel column chromatography (PE/EA = 10:1 V/V) to afford the desired product **4a** (61 mg, 56% yield).

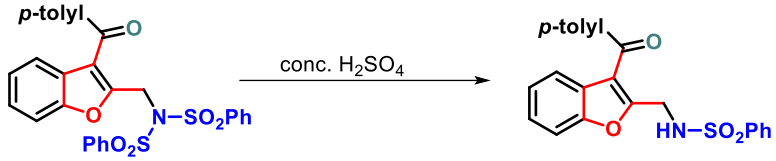
Synthetic Application of 3a[3]



3a (0.1 mmol) **5a** (78% yield)

To a Schlenk tube were added **3a** (0.1 mmol, 1.0 equiv, 59 mg), magnesium (1.0 mmol, 10.0 equiv, 24 mg), $Ti(^{i}OPr)_4$ (0.2 mmol, 2.0 equiv, 57 mg), Me_3SiCl (0.3 mmol, 3.0 equiv, 33 mg) and THF (2.0 mL) the protection with argon. The resulting mixture was heated at 50 °C. After the reaction was completed, the solution was concentrated in vacuo and purified by flash chromatography on silica gel (PE/EA= 10/1 V/V) to afford the desired product **5a** (35 mg, 78% yield) as the white solid.

Synthetic Application of 4a[4]

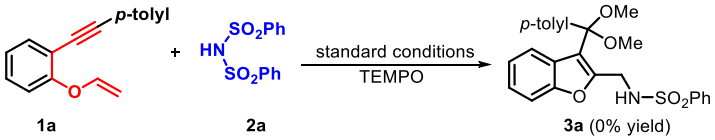


4a (0.05 mmol) **6a** (70% yield)

To a 5-mL pressure tube under air conditions, 1.5 mL conc. H_2SO_4 was added into **4a** (0.05 mmol, 1.0 equiv, 27 mg) and stirred at 25 °C for 1 hour. Upon completion, the mixture was poured into water and neutralized with NaOH solid. Then the mixture was extracted by EA. The organic layer was dried over anhydrous Na_2SO_4 and concentrated on rotavapor under reduced pressure. Finally, on silica gel (PE/EA = 10/1 V/V) to afford the desired product **6a** (16 mg, 78% yield) as the white solid.

Radical-Trapping Experiment:

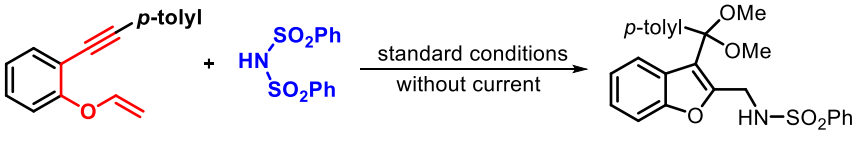
TEMPO as the radical trapping reagent — General procedure



1a **2a** **3a** (0% yield)

In an undivided flask (10 mL) under nitrogen, 1,6-enyne **1a** (0.2 mmol, 1.0 equiv, 47 mg), dibenzenesulfonimide (**2a**, 0.6 mmol, 3.0 equiv, 178 mg), $^{n}Bu_4NOAc$ (0.6 mmol, 3.0 equiv, 180 mg) and TEMPO (0.6 mmol, 3.0 equiv, 94 mg) in a mixed solvent of 1,2-dichloroethane (DCE) and methanol (V/V = 3.5/1.5, 5.0 mL) was stirred at 25 °C for 2 hours. The corresponding product **3a** was not detected according to TLC analysis.

Control Experiments



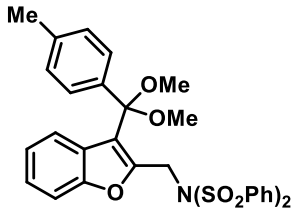
1a **2a** **3a** (0% yield)

In a tube (10 mL) equipped with a stir bar under nitrogen, **1a** (0.2 mmol, 1.0 equiv, 47 mg), **2a** (0.6 mmol, 3.0 equiv, 178 mg), $^{n}Bu_4NOAc$ (0.6 mmol, 3.0 equiv, 180 mg), and mixed solvent DCE/CH_3OH (V/V = 3.5/1.5, 5.0 mL) were added and stirred at 25 °C for 4 hours. The corresponding product (**3a**) was not detected according to

TLC analysis.

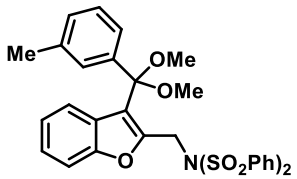
Characterization data

N-((3-(Dimethoxy(p-tolyl)methyl)benzofuran-2-yl)methyl)-N-(phenylsulfonyl)benzenesulfonamide (3a)



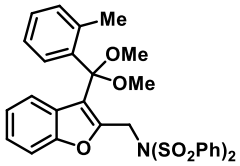
White solid, 77 mg, 65%; m.p. 129-130 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.07 (d, J = 8.0 Hz, 4H), 7.62 – 7.57 (m, 4H), 7.50 – 7.45 (m, 4H), 7.37 (d, J = 7.6 Hz, 1H), 7.14 (d, J = 8.0 Hz, 2H), 7.11 – 7.07 (m, 1H), 7.05 – 7.01 (m, 1H), 6.96 (d, J = 8.0 Hz, 1H), 5.55 (s, 2H), 3.16 (s, 6H), 2.31 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 153.7, 148.7, 139.7, 138.0, 137.6, 133.8, 128.9, 128.7, 127.0, 126.6, 124.1, 122.9, 121.4, 118.1, 110.9, 102.1, 49.3, 45.4, 21.3. IR (KBr, v, cm^{-1}) 1606, 1363, 1265, 1084, 907, 791, 774, 745. HR-MS (ESI) m/z calcd for $C_{31}H_{29}NNaO_7S_2$ $[M+Na]^+$ 614.1283, found 614.1265.

N-((3-(Dimethoxy(m-tolyl)methyl)benzofuran-2-yl)methyl)-N-(phenylsulfonyl)benzenesulfonamide (3b)



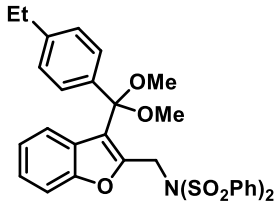
White solid, 56 mg 47%; m.p. 135-136 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.05 (d, J = 8.0 Hz, 4H), 7.61 – 7.57 (m, 2H), 7.52 (d, J = 9.2 Hz, 2H), 7.48 – 7.43 (m, 4H), 7.41 (d, J = 7.6 Hz, 1H), 7.22 (d, J = 7.6 Hz, 1H), 7.10 – 7.03 (m, 3H), 6.96 (d, J = 8.0 Hz, 1H), 5.55 (s, 2H), 3.17 (s, 6H), 2.33 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 153.7, 148.6, 140.5, 139.7, 137.8, 133.8, 129.0, 128.8, 128.7, 128.0, 127.6, 126.6, 124.2, 124.0, 122.9, 121.4, 118.2, 110.9, 102.1, 49.3, 45.5, 21.6. IR (KBr, v, cm^{-1}) 1605, 1361, 1259, 1169, 1084, 895, 865, 800, 720. HR-MS (ESI) m/z calcd for $C_{31}H_{29}NNaO_7S_2$ $[M+Na]^+$ 614.1283, found 614.1267.

N-((3-(Dimethoxy(o-tolyl)methyl)benzofuran-2-yl)methyl)-N-(phenylsulfonyl)benzenesulfonamide (3c)



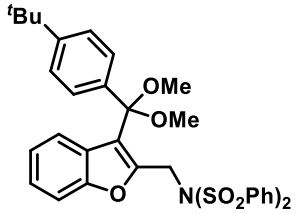
White solid, 56 mg, 47%; m.p. 166-167 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.13 – 8.07 (m, 5H), 7.68 – 7.64 (m, 2H), 7.57 – 7.52 (m, 4H), 7.29 (d, J = 7.2 Hz, 1H), 7.26 – 7.20 (m, 2H), 7.11 – 7.05 (m, 2H), 7.01 (d, J = 6.8 Hz, 1H), 6.96 (d, J = 4.4 Hz, 1H), 5.26 (s, 2H), 3.15 (s, 6H), 2.11 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm) 153.2, 139.1, 137.7, 136.5, 135.1, 132.3, 129.9, 129.2, 128.6, 128.4, 126.1, 124.7, 123.4, 111.3, 101.2, 49.0, 20.2. IR (KBr, v, cm^{-1}) 1601, 1362, 1084, 907, 807. HR-MS (ESI) m/z calcd for $C_{31}H_{29}NNaO_7S_2$ $[M+Na]^+$ 614.1283, found 614.1262.

N-((3-((4-Ethylphenyl)dimethoxymethyl)benzofuran-2-yl)methyl)-N-(phenylsulfonyl)benzenesulfonamide (3d)



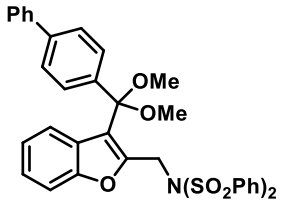
White solid, 42 mg, 39%; m.p. 123-124 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.07 (d, J = 8.0 Hz, 4H), 7.62 – 7.57 (m, 4H), 7.49 – 7.44 (m, 4H), 7.39 (d, J = 7.6 Hz, 1H), 7.16 (d, J = 8.0 Hz, 2H), 7.11 – 7.07 (m, 1H), 7.05 – 7.01 (m, 1H), 6.96 (d, J = 8.0 Hz, 1H), 5.55 (s, 2H), 3.17 (s, 6H), 2.64 – 2.58 (m, 2H), 1.21 – 1.17 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 153.7, 148.7, 144.2, 139.7, 137.8, 133.8, 128.8, 128.7, 127.6, 127.0, 126.6, 124.0, 122.8, 121.4, 118.2, 110.9, 102.2, 49.3, 45.4, 28.6, 15.4. IR (KBr, v, cm^{-1}) 1616, 1449, 1378, 1167, 1083, 929, 801. HR-MS (ESI) m/z calcd for $C_{32}H_{31}NNaO_7S_2$ $[M+Na]^+$ 628.1440, found 628.1419.

N-((3-((4-(tert-Butyl)phenyl)dimethoxymethyl)benzofuran-2-yl)methyl)-N-(phenylsulfonyl)benzenesulfonamide (3e)



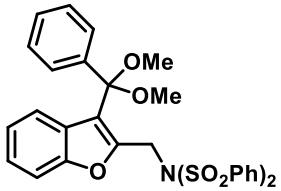
White solid, 65 mg, 51%; m.p. 149-150 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.05 (d, J = 8.0 Hz, 4H), 7.62 – 7.56 (m, 4H), 7.48 – 7.42 (m, 5H), 7.34 (d, J = 8.4 Hz, 2H), 7.11 – 7.07 (m, 1H), 7.06 – 7.02 (m, 1H), 6.96 (d, J = 8.0 Hz, 1H), 5.55 (s, 2H), 3.17 (s, 6H), 1.27 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 153.6, 151.1, 148.6, 139.6, 137.5, 133.8, 128.8, 128.7, 126.6, 125.0, 124.0, 122.8, 121.5, 118.2, 110.9, 102.2, 49.3, 45.4, 34.6, 31.4. IR (KBr, v, cm^{-1}) 1604, 1360, 1246, 1170, 1084, 910, 800. HR-MS (ESI) m/z calcd for $C_{34}H_{35}NNaO_7S_2$ $[M+Na]^+$ 656.1753, found 656.1729.

N-((3-([1,1'-Biphenyl]-4-yldimethoxymethyl)benzofuran-2-yl)methyl)-N-(phenylsulfonyl)benzenesulfonamide (3f)



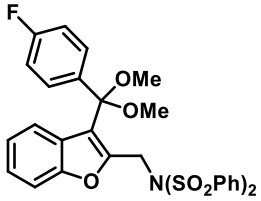
White solid, 95 mg, 73%; m.p. 110-111 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.04 (d, J = 7.2 Hz, 4H), 7.94 (d, J = 8.0 Hz, 2H), 7.73 (d, J = 8.4 Hz, 2H), 7.67 (d, J = 7.6 Hz, 2H), 7.63 – 7.59 (m, 2H), 7.53 – 7.46 (m, 7H), 7.44 – 7.40 (m, 1H), 7.29 (d, J = 7.6 Hz, 2H), 7.21 – 7.17 (m, 1H), 5.34 (s, 2H), 3.49 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 153.7, 148.9, 140.9, 140.6, 139.7, 139.6, 133.8, 128.8, 128.7, 127.6, 127.5, 127.1, 126.8, 126.6, 124.1, 122.9, 121.4, 117.9, 111.0, 102.1, 49.4, 45.4. IR (KBr, v, cm^{-1}) 1635, 1378, 1169, 1083, 1049, 801, 771, 750, 685. HR-MS (ESI) m/z calcd for $C_{36}H_{31}NNaO_7S_2$ $[M+Na]^+$ 676.1440, found 676.1413.

N-((3-(Dimethoxy(phenyl)methyl)benzofuran-2-yl)methyl)-N-(phenylsulfonyl)benzenesulfonamide (3g)



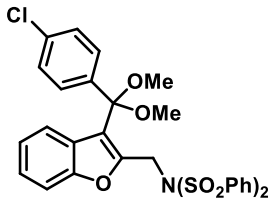
White solid, 70 mg, 61%; m.p. 172-173 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.07 (d, J = 8.0 Hz, 4H), 7.71 (d, J = 7.6 Hz, 2H), 7.62 – 7.57 (m, 2H), 7.49 – 7.45 (m, 4H), 7.38 – 7.32 (m, 3H), 7.28 (d, J = 7.2 Hz, 1H), 7.12 – 7.07 (m, 1H), 7.05 – 7.01 (m, 1H), 6.97 (d, J = 8.0 Hz, 1H), 5.56 (s, 2H), 3.18 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 153.6, 148.8, 140.5, 139.6, 134.0, 133.8, 128.8, 128.7, 128.2, 128.1, 127.0, 126.5, 124.0, 122.8, 121.3, 117.9, 110.9, 102.0, 49.2, 45.4. IR (KBr, v, cm^{-1}) 1601, 1363, 1169, 1084, 858, 774, 750. HR-MS (ESI) m/z calcd for $C_{30}H_{27}NNaO_7S_2$ $[M+Na]^+$ 600.1127, found 600.1102.

N-((3-((4-Fluorophenyl)dimethoxymethyl)benzofuran-2-yl)methyl)-N-(phenylsulfonyl)benzenesulfonamide (3h)



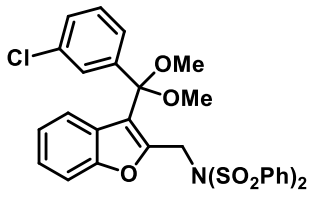
White solid, 67 mg 56%; m.p. 129-130 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.04 (d, J = 8.0 Hz, 4H), 7.91 – 7.86 (m, 2H), 7.64 – 7.60 (m, 2H), 7.53 – 7.49 (m, 4H), 7.32 – 7.27 (m, 2H), 7.19 – 7.15 (m, 4H), 5.31 (s, 2H), 3.49 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 153.7, 149.0, 139.6, 136.4, 133.9, 129.1, 129.0, 128.9, 128.7, 126.4, 124.2, 123.0, 121.1, 117.7, 115.1, 114.9, 111.0, 101.7, 49.3, 45.4. IR (KBr, v, cm^{-1}) 1601, 1363, 1123, 1068, 951, 775. HR-MS (ESI) m/z calcd for $C_{30}H_{26}FNNaO_7S_2$ $[M+Na]^+$ 618.1032, found 618.1035.

N-((3-((4-Chlorophenyl)dimethoxymethyl)benzofuran-2-yl)methyl)-N-(phenylsulfonyl)benzenesulfonamide (3i)



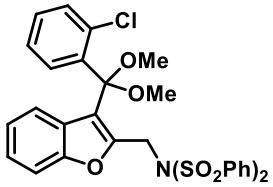
White solid, 72 mg, 59%; m.p. 174-175 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.07 (d, J = 8.0 Hz, 4H), 7.67 (d, J = 8.4 Hz, 2H), 7.61 (d, J = 7.6 Hz, 2H), 7.51 – 7.47 (m, 4H), 7.32 – 7.28 (m, 3H), 7.14 – 7.10 (m, 1H), 7.05 – 7.01 (m, 1H), 6.98 (d, J = 8.4 Hz, 1H), 5.53 (s, 2H), 3.15 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 153.7, 149.2, 139.6, 139.2, 134.2, 134.0, 131.1, 129.1, 128.9, 128.8, 128.4, 124.3, 123.0, 121.1, 111.1, 101.7, 49.4, 45.4. IR (KBr, v, cm^{-1}) 1604, 1363, 1169, 1084, 774. HR-MS (ESI) m/z calcd for $C_{30}H_{26}ClNNaO_7S_2$ $[M+Na]^+$ 634.0737, found 634.0713.

N-((3-((3-Chlorophenyl)dimethoxymethyl)benzofuran-2-yl)methyl)-N-(phenylsulfonyl)benzenesulfonamide (3j)



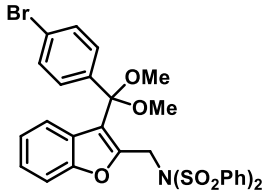
White solid, 61 mg, 50%; m.p. 150-151 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.07 (d, J = 8.0 Hz, 4H), 7.76 (s, 1H), 7.64 – 7.58 (m, 3H), 7.51 – 7.47 (m, 4H), 7.33 (d, J = 7.6 Hz, 1H), 7.29 (s, 1H), 7.25 (s, 1H), 7.14 – 7.10 (m, 1H), 7.07 – 7.03 (m, 1H), 6.98 (d, J = 8.4 Hz, 1H), 5.53 (s, 2H), 3.16 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 153.7, 149.1, 142.8, 139.7, 134.2, 133.9, 129.6, 128.9, 128.7, 128.5, 127.3, 126.3, 125.5, 124.3, 123.0, 121.1, 117.3, 111.0, 101.6, 49.4, 45.4. IR (KBr, v, cm^{-1}) 1605, 1363, 1169, 1084, 940, 857, 774, 685. HR-MS (ESI) m/z calcd for $C_{30}H_{26}ClNNaO_7S_2$ $[M+Na]^+$ 634.0737, found 634.0741.

N-((3-((2-Chlorophenyl)dimethoxymethyl)benzofuran-2-yl)methyl)-N-(phenylsulfonyl)benzenesulfonamide (3k)



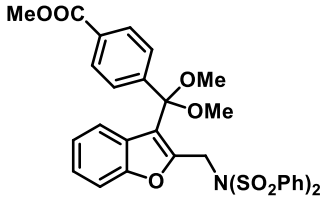
White solid, 60 mg, 49%; m.p. 129-130 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.07 (d, J = 8.0 Hz, 4H), 7.66 – 7.61 (m, 2H), 7.52 (d, J = 12.8 Hz, 5H), 7.48 (d, J = 8.8 Hz, 2H), 7.43 – 7.39 (m, 1H), 7.23 (d, J = 7.2 Hz, 1H), 7.15 – 7.11 (m, 2H), 6.86 (d, J = 7.6 Hz, 1H), 5.40 (s, 2H), 3.49 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 153.4, 139.7, 136.6, 133.9, 131.4, 130.3, 129.8, 128.9, 128.9, 126.4, 123.8, 122.7, 110.9, 100.7, 49.2, 46.3. IR (KBr, v, cm^{-1}) 1605, 1363, 1164, 1084, 929, 774. HR-MS (ESI) m/z calcd for $C_{30}H_{26}ClNNaO_7S_2$ $[M+Na]^+$ 634.0737, found 634.0735.

N-((3-((4-Bromophenyl)dimethoxymethyl)benzofuran-2-yl)methyl)-N-(phenylsulfonyl)benzenesulfonamide (3l)



White soild, 102 mg, 78%; m.p. 135-136 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.06 (d, J = 8.4 Hz, 4H), 7.64 – 7.59 (m, 4H), 7.51 – 7.45 (m, 6H), 7.28 (d, J = 7.6 Hz, 1H), 7.14 – 7.09 (m, 1H), 7.05 – 7.01 (m, 1H), 6.98 (d, J = 8.4 Hz, 1H), 5.53 (s, 2H), 3.15 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 153.6, 149.1, 139.6, 139.6, 133.8, 132.0, 131.3, 129.0, 128.8, 128.6, 126.2, 124.2, 122.9, 122.4, 121.0, 117.3, 111.0, 101.7, 49.3, 45.3. IR (KBr, v, cm^{-1}) 1602, 1355, 1169, 1084, 1050, 801. HR-MS (ESI) m/z calcd for $C_{30}H_{26}BrNNaO_7S_2$ $[M+Na]^+$ 678.0232, found 678.0202.

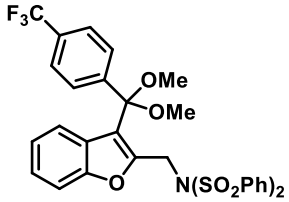
Methyl 4-(Dimethoxy(2-((N-(phenylsulfonyl)phenylsulfonamido)methyl)benzofuran-3-yl)methyl)benzoate (3m)



White solid, 41 mg, 32%; m.p. 136-137 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.06 (d, J = 8.0 Hz, 4H), 8.02 (d, J = 8.4 Hz, 2H), 7.81 (d, J = 8.0 Hz, 2H), 7.63 – 7.59 (m, 2H), 7.50 – 7.45 (m, 4H), 7.30 (d, J = 7.6 Hz, 1H), 7.12 – 7.08 (m, 1H), 7.04 – 7.00 (m, 1H), 6.97 (d, J = 8.0 Hz, 1H), 5.55 (s, 2H), 3.88 (s, 3H), 3.17 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 166.9, 153.7, 149.2, 145.5, 139.6, 133.9, 130.1, 129.6, 128.9, 128.7,

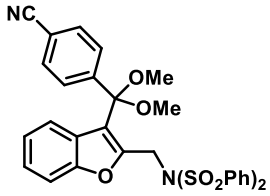
127.3, 126.2, 124.3, 123.0, 121.0, 117.3, 111.1, 101.8, 52.2, 49.5, 45.4. IR (KBr, *v*, cm^{-1}) 1718, 1610, 1449, 1379, 1279, 1169, 1084, 931, 859. HR-MS (ESI) m/z calcd for $C_{32}H_{29}NNaO_9S_2$ $[M+Na]^+$ 658.1181, found 658.1160.

N-((3-(Dimethoxy(4-(trifluoromethyl)phenyl)methyl)benzofuran-2-yl)methyl)-N-(phenylsulfonyl)benzenesulfonamide (3n)



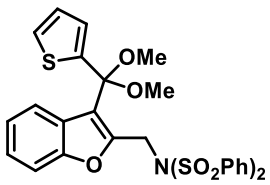
White solid, 57 mg, 44%; m.p. 135-136 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.07 (d, *J* = 8.0 Hz, 4H), 7.87 (d, *J* = 8.4 Hz, 2H), 7.64 – 7.59 (m, 4H), 7.52 – 7.47 (m, 4H), 7.28 (d, *J* = 8.0 Hz, 1H), 7.14 – 7.10 (m, 1H), 7.06 – 7.02 (m, 1H), 6.99 (d, *J* = 8.0 Hz, 1H), 5.55 (s, 2H), 3.17 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 153.7, 149.3, 144.5, 139.6, 133.9, 128.9, 128.7, 127.6, 126.1, 125.2, 124.4, 123.1, 120.9, 111.1, 101.6, 49.4, 45.3. IR (KBr, *v*, cm^{-1}) 1602, 1356, 1169, 1084, 930, 773. HR-MS (ESI) m/z calcd for $C_{31}H_{26}F_3NNaO_7S_2$ $[M+Na]^+$ 668.1000, found 668.1010.

N-((3-((4-Cyanophenyl)dimethoxymethyl)benzofuran-2-yl)methyl)-N-(phenylsulfonyl)benzenesulfonamide (3o)



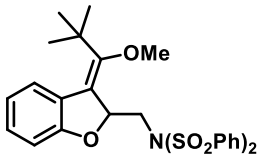
White solid, 99 mg, 82%; m.p. 155-156 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.07 (d, *J* = 8.0 Hz, 4H), 7.86 (d, *J* = 8.4 Hz, 2H), 7.63 – 7.58 (m, 4H), 7.51 – 7.47 (m, 4H), 7.28 (d, *J* = 8.0 Hz, 1H), 7.14 – 7.10 (m, 1H), 7.06 – 7.02 (m, 1H), 6.99 (d, *J* = 8.4 Hz, 1H), 5.55 (s, 2H), 3.17 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 153.7, 149.4, 144.5, 139.6, 133.9, 128.9, 128.7, 127.6, 126.2, 125.2, 124.4, 123.1, 121.0, 117.2, 111.1, 101.7, 49.4, 45.4. IR (KBr, *v*, cm^{-1}) 2230, 1604, 1362, 1257, 1169, 1027, 839. HR-MS (ESI) m/z calcd for $C_{31}H_{26}N_2NaO_7S_2$ $[M+Na]^+$ 625.1079, found 625.1092.

N-((3-(Dimethoxy(thiophen-2-yl)methyl)benzofuran-2-yl)methyl)-N-(phenylsulfonyl)benzenesulfonamide (3p)



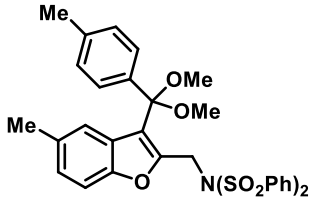
Yellow oil, 35 mg, 30%; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.07 (d, *J* = 8.0 Hz, 4H), 7.63 – 7.59 (m, 2H), 7.53 – 7.45 (m, 6H), 7.20 (d, *J* = 3.6 Hz, 1H), 7.15 – 7.11 (m, 1H), 7.09 – 7.05 (m, 1H), 6.99 (d, *J* = 8.0 Hz, 1H), 6.97 – 6.94 (m, 1H), 5.50 (s, 2H), 3.22 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 153.7, 149.0, 144.6, 139.7, 133.9, 128.9, 128.8, 127.1, 126.5, 126.4, 125.7, 124.3, 123.1, 121.4, 117.8, 111.0, 101.0, 49.6, 45.4. IR (KBr, *v*, cm^{-1}) 1608, 1361, 1169, 1084, 907, 750, 685. HR-MS (ESI) m/z calcd for $C_{28}H_{25}NNaO_7S_3$ $[M+Na]^+$ 606.0691, found 606.0670.

(Z)-N-((3-(1-Methoxy-2,2-dimethylpropylidene)-2,3-dihydrobenzofuran-2-yl)methyl)-N-(phenylsulfonyl)benzenesulfonamide (3r)



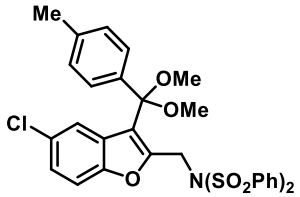
White solid, 36 mg, 34%; m.p. 129-130 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.12 (d, J = 8.0 Hz, 4H), 7.61 – 7.57 (m, 2H), 7.52 – 7.47 (m, 4H), 7.33 (d, J = 7.6 Hz, 1H), 7.17 – 7.13 (m, 1H), 6.96 – 6.91 (m, 2H), 5.49 – 5.44 (m, 1H), 4.15 – 4.08 (m, 1H), 4.05 – 3.99 (m, 1H), 3.27 (s, 3H), 1.33 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 157.3, 139.4, 133.9, 133.3, 128.9, 128.8, 122.5, 116.8, 115.8, 103.3, 75.0, 54.9, 50.6, 31.1, 28.3. IR (KBr, v, cm^{-1}) 1600, 1449, 1357, 1232, 1171, 1084, 887, 774, 721. HR-MS (ESI) m/z calcd for $C_{27}H_{29}NNaO_6S_2$ $[M+Na]^+$ 550.1334, found 550.1351.

N-((3-(Dimethoxy(p-tolyl)methyl)-5-methylbenzofuran-2-yl)methyl)-N-(phenylsulfonyl)benzenesulfonamide (3s)



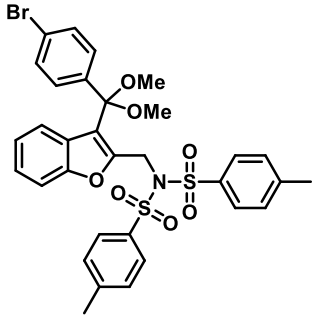
White solid, 67 mg, 55%; m.p. 130-131 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.00 (d, J = 7.6 Hz, 4H), 7.77 (d, J = 8.0 Hz, 2H), 7.62 – 7.57 (m, 2H), 7.50 – 7.46 (m, 4H), 7.30 (d, J = 7.6 Hz, 2H), 7.13 – 7.06 (m, 3H), 5.24 (s, 2H), 3.49 (s, 6H), 2.46 (s, 3H), 2.34 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 152.1, 148.8, 139.7, 137.9, 137.7, 133.8, 132.2, 128.8, 128.7, 127.0, 126.7, 125.4, 121.1, 117.8, 110.4, 102.1, 49.2, 45.5, 21.6, 21.3. IR (KBr, v, cm^{-1}) 1607, 1378, 1255 1169, 1084, 908, 774, 720. HR-MS (ESI) m/z calcd for $C_{32}H_{31}NNaO_7S_2$ $[M+Na]^+$ 628.1440, found 628.1419.

N-((5-Chloro-3-(dimethoxy(p-tolyl)methyl)benzofuran-2-yl)methyl)-N-(phenylsulfonyl)benzenesulfonamide (3t)



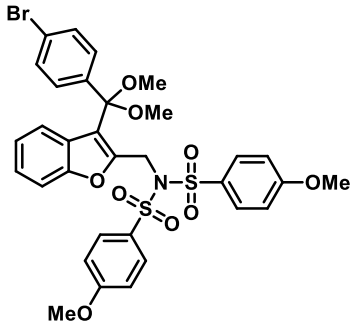
White solid, 58 mg, 46%; m.p. 129-130 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.00 (d, J = 7.6 Hz, 4H), 7.74 (d, J = 7.8 Hz, 2H), 7.63 – 7.59 (m, 2H), 7.51 – 7.46 (m, 5H), 7.32 (d, J = 8.0 Hz, 2H), 7.23 (d, J = 1.6 Hz, 1H), 7.15 (d, J = 8.8 Hz, 1H), 5.25 (s, 2H), 3.49 (s, 6H), 2.47 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 152.0, 150.2, 139.6, 138.2, 137.2, 133.9, 129.0, 128.9, 128.7, 128.5, 128.0, 126.9, 124.4, 121.0, 118.0, 111.9, 101.9, 49.3, 45.3, 21.2. IR (KBr, v, cm^{-1}) 1609, 1360, 1258, 1169, 1084, 932, 774, 720. HR-MS (ESI) m/z calcd for $C_{31}H_{28}ClNNaO_7S_2$ $[M+Na]^+$ 648.0893, found 648.0875.

N-((3-((4-Bromophenyl)dimethoxymethyl)benzofuran-2-yl)methyl)-4-methyl-N-tosylbenzenesulfonamide (3u)



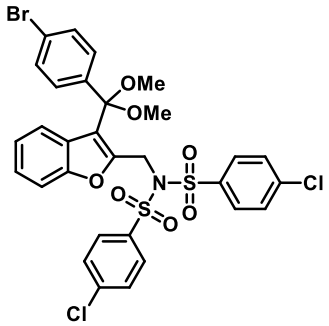
White solid, 88 mg, 64%; m.p. 126-127 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.93 (d, J = 8.0 Hz, 4H), 7.61 (d, J = 8.4 Hz, 2H), 7.46 (d, J = 8.4 Hz, 2H), 7.29 (d, J = 8.0 Hz, 3H), 7.24 (s, 2H), 7.14 – 7.10 (m, 1H), 7.05 – 7.00 (m, 2H), 5.50 (s, 2H), 3.15 (s, 6H), 2.41 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 153.7, 149.2, 144.9, 139.7, 136.8, 131.3, 129.6, 129.4, 129.1, 128.7, 126.3, 124.2, 122.9, 122.5, 121.1, 117.3, 111.0, 101.8, 49.3, 45.2, 27.0, 21.7. IR (KBr, v, cm^{-1}) 1609, 1359, 1166, 1084, 774. HR-MS (ESI) m/z calcd for $C_{32}H_{30}BrNNaO_7S_2$ $[M+Na]^+$ 706.0545, found 706.0523.

N-((3-((4-Bromophenyl)dimethoxymethyl)benzofuran-2-yl)methyl)-4-methoxy-N-((4-methoxyphenyl)sulfonyl)benzenesulfonamide (3v)



White solid, 47 mg, 33%; m.p. 146-147 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.97 (d, J = 8.8 Hz, 4H), 7.62 (d, J = 8.0 Hz, 2H), 7.47 (d, J = 8.4 Hz, 2H), 7.29 (d, J = 7.2 Hz, 1H), 7.15 – 7.10 (m, 1H), 7.06 – 7.02 (m, 2H), 6.90 (d, J = 8.8 Hz, 4H), 5.48 (s, 2H), 3.84 (s, 6H), 3.14 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 163.8, 153.8, 149.4, 139.8, 131.3, 131.2, 131.0, 129.1, 126.4, 124.2, 122.9, 122.5, 121.1, 117.3, 113.9, 111.0, 101.7, 55.8, 49.3, 45.1. IR (KBr, v, cm^{-1}) 1609, 1359, 1160, 1085, 774. HR-MS (ESI) m/z calcd for $C_{32}H_{30}BrNNaO_9S_2$ $[M+Na]^+$ 738.0443, found 738.0418.

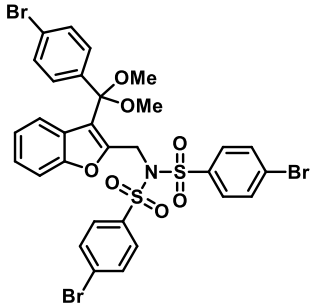
N-((3-((4-Bromophenyl)dimethoxymethyl)benzofuran-2-yl)methyl)-4-chloro-N-((4-chlorophenyl)sulfonyl)benzenesulfonamide (3w)



White solid, 46 mg, 32%; m.p. 154-155 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.96 (d, J = 8.4 Hz, 4H), 7.60 (d, J = 8.4 Hz, 2H), 7.47 (d, J = 8.4 Hz, 2H), 7.43 (d, J = 8.4 Hz, 4H), 7.32 (d, J = 7.6 Hz, 1H), 7.19 – 7.15 (m, 1H), 7.09 – 7.05 (m, 1H), 7.00 (d, J = 8.0 Hz, 1H), 5.50 (s, 2H), 3.15 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 153.7, 148.4, 140.8, 139.6, 137.9, 131.4, 130.1, 129.2, 129.0, 126.1, 124.7, 123.2, 122.6, 121.2, 117.9,

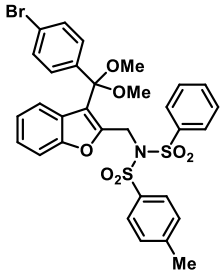
110.9, 101.7, 49.4, 45.5. IR (KBr, *v*, cm^{-1}) 1617, 1356, 1281, 1168, 1085, 1047, 773. HR-MS (ESI) m/z calcd for $C_{30}H_{24}Cl_2NNaO_7S_2$ $[M+Na]^+$ 745.9452, found 745.9468.

4-Bromo-N-((3-((4-bromophenyl)dimethoxymethyl)benzofuran-2-yl)methyl)-N-((4-bromophenyl)sulfonyl)benzenesulfonamide (3x)



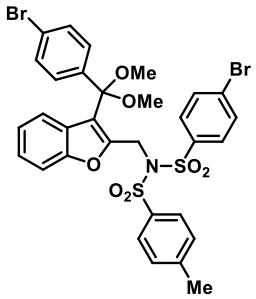
White solid, 64 mg, 39%; m.p. 117-118 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.87 (d, *J* = 8.0 Hz, 4H), 7.62 – 7.58 (m, 6H), 7.48 (d, *J* = 8.0 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 1H), 7.20 – 7.16 (m, 1H), 7.09 – 7.05 (m, 1H), 7.00 (d, *J* = 8.0 Hz, 1H), 5.50 (s, 2H), 3.15 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 153.6, 148.3, 139.6, 138.4, 132.2, 131.4, 130.1, 129.5, 128.9, 126.1, 124.8, 123.2, 122.6, 121.2, 117.9, 110.9, 101.7, 49.4, 45.6. IR (KBr, *v*, cm^{-1}) 1635, 1381, 1279, 1169, 1083, 773. HR-MS (ESI) m/z calcd for $C_{30}H_{24}Br_3NNaO_7S_2$ $[M+Na]^+$ 833.8442, found 833.8449.

N-((3-((4-Bromophenyl)dimethoxymethyl)benzofuran-2-yl)methyl)-4-methyl-N-(phenylsulfonyl)benzenesulfonamide (3y)



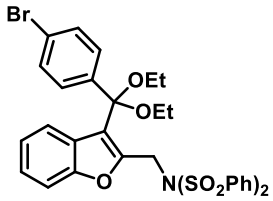
White solid, 62 mg, 41%; m.p. 105-106 ˚C; ^{1}H NMR (400 MHz, DMSO-d_6) (δ, ppm) 7.99 (d, *J* = 7.6 Hz, 2H), 7.84 (d, *J* = 8.0 Hz, 2H), 7.80 – 7.77 (m, 1H), 7.69 – 7.65 (m, 2H), 7.63 – 7.56 (m, 4H), 7.44 (d, *J* = 8.0 Hz, 2H), 7.28 (d, *J* = 7.6 Hz, 1H), 7.22 (d, *J* = 3.6 Hz, 2H), 7.14 – 7.09 (m, 1H), 5.55 (s, 2H), 3.12 (s, 6H), 2.41 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm) 153.5, 149.7, 145.9, 140.2, 139.4, 136.3, 135.0, 131.7, 130.3, 129.8, 129.5, 128.6, 128.5, 126.2, 125.1, 123.7, 122.2, 121.1, 117.3, 111.4, 101.7, 49.6, 45.2, 21.6. IR (KBr, *v*, cm^{-1}) 1655, 1378, 1280, 1167, 1051, 822, 753, 550. HR-MS (ESI) m/z calcd for $C_{31}H_{28}BrNNaO_7S_2$ $[M+Na]^+$ 692.0388, found 692.0402.

4-Bromo-N-((3-((4-bromophenyl)dimethoxymethyl)benzofuran-2-yl)methyl)-N-tosylbenzenesulfonamide (3z)



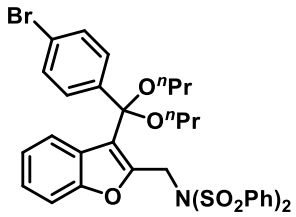
White solid, 60 mg, 40%; m.p. 110-111 ˚C; ^{1}H NMR (400 MHz, DMSO-d_6) (δ, ppm) 7.91 (s, 3H), 7.86 (d, J = 8.0 Hz, 2H), 7.62 – 7.54 (m, 5H), 7.44 (d, J = 7.6 Hz, 2H), 7.30 (d, J = 7.6 Hz, 1H), 7.23 (d, J = 4.0 Hz, 2H), 7.14 – 7.10 (m, 1H), 5.57 (s, 2H), 3.12 (s, 6H), 2.40 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm) 153.5, 149.4, 146.1, 140.2, 138.7, 136.1, 133.0, 131.7, 130.4, 130.3, 129.5, 129.2, 128.6, 126.1, 125.1, 123.7, 122.2, 121.2, 117.5, 111.4, 101.7, 54.9, 49.6, 45.3, 21.7. IR (KBr, v, cm^{-1}) 1588, 1450, 1377, 1167, 1051, 816, 750. HR-MS (ESI) m/z calcd for $C_{31}H_{27}Br_2NNaO_7S_2$ $[M+Na]^+$ 769.9493, found 769.9504.

N-((3-((4-Bromophenyl)diethoxymethyl)benzofuran-2-yl)methyl)-N-(phenylsulfonyl)benzenesulfonamide (3aa)



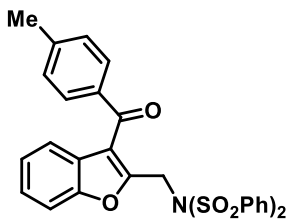
White solid, 115 mg, 84%; m.p. 99-100 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.07 (d, J = 8.0 Hz, 4H), 7.65 – 7.61 (m, 4H), 7.50 (d, J = 7.6 Hz, 3H), 7.48 – 7.43 (m, 3H), 7.29 (d, J = 8.0 Hz, 1H), 7.12 – 7.07 (m, 1H), 7.03 – 6.99 (m, 1H), 6.92 (d, J = 8.4 Hz, 1H), 5.58 (s, 2H), 3.39 – 3.33 (m, 4H), 1.20 – 1.15 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 153.6, 148.8, 140.6, 139.7, 133.9, 131.2, 129.0, 128.9, 128.7, 126.5, 124.1, 122.9, 122.3, 121.1, 117.8, 111.0, 101.0, 57.4, 45.6, 15.2. IR (KBr, v, cm^{-1}) 1609, 1359, 1169, 1084, 774. HR-MS (ESI) m/z calcd for $C_{32}H_{30}BrNNaO_7S_2$ $[M+Na]^+$ 706.0545, found 706.0518.

N-((3-((4-Bromophenyl)dipropoxymethyl)benzofuran-2-yl)methyl)-N-(phenylsulfonyl)benzenesulfonamide (3ab)



White solid, 77 mg, 54%; m.p. 92-93 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.04 (d, J = 8.0 Hz, 4H), 7.72 (d, J = 7.6 Hz, 2H), 7.66 – 7.61 (m, 4H), 7.55 – 7.49 (m, 4H), 7.32 – 7.26 (m, 2H), 7.20 – 7.14 (m, 2H), 5.31 (s, 2H), 3.65 – 3.57 (m, 4H), 1.63 – 1.56 (m, 4H), 0.99 – 0.90 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 153.5, 148.7, 140.6, 139.7, 133.9, 131.2, 128.9, 128.7, 126.5, 124.1, 122.9, 122.3, 121.1, 117.8, 111.0, 100.7, 63.3, 45.8, 23.0, 11.1. IR (KBr, v, cm^{-1}) 1609, 1357, 1248, 1169, 1083, 934, 774, 720. HR-MS (ESI) m/z calcd for $C_{34}H_{34}BrNNaO_7S_2$ $[M+Na]^+$ 734.0858, found 734.0830.

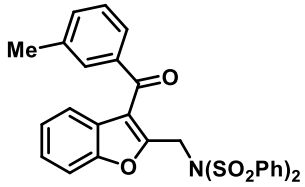
N-((3-(4-Methylbenzoyl)benzofuran-2-yl)methyl)-N-(phenylsulfonyl)benzenesulfonamide (4a)



White solid, 61 mg, 56%; m.p. 172-173 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.03 (d, J = 8.0 Hz, 4H), 7.76 (d, J = 8.0 Hz, 2H), 7.63 – 7.58 (m, 2H), 7.51 – 7.46 (m, 4H), 7.32 – 7.26 (m, 3H), 7.23 (d, J = 7.6 Hz, 2H), 7.19 – 7.15 (m, 1H), 5.30 (s, 2H), 2.46 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 191.0, 156.5, 153.8,

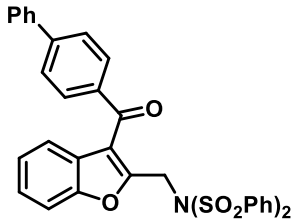
144.2, 139.3, 136.2, 134.0, 129.8, 129.4, 129.0, 128.6, 126.0, 125.4, 123.9, 122.0, 119.8, 111.4, 44.1, 21.9. IR (KBr, *v*, cm^{-1}) 1607, 1362, 1265, 1170, 1084, 907, 774, 686. HR-MS (ESI) m/z calcd for $C_{29}H_{23}NNaO_6S_2$ $[M+Na]^+$ 568.0864, found 568.0844.

N-((3-(3-Methylbenzoyl)benzofuran-2-yl)methyl)-N-(phenylsulfonyl)benzenesulfonamide (4b)



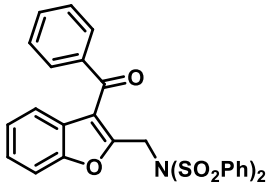
White solid, 55 mg, 50%; m.p. 97-98 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) (*δ*, ppm) 8.03 (d, *J* = 8.0 Hz, 4H), 7.69 (s, 1H), 7.63 – 7.58 (m, 3H), 7.53 – 7.47 (m, 4H), 7.45 (d, *J* = 7.6 Hz, 1H), 7.40 – 7.35 (m, 1H), 7.29 (d, *J* = 8.0 Hz, 1H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.19 – 7.14 (m, 1H), 5.31 (s, 2H), 2.42 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) (*δ*, ppm) 191.5, 156.8, 153.8, 139.4, 139.0, 138.6, 134.0, 129.8, 129.0, 128.6, 128.5, 126.8, 126.0, 125.4, 124.0, 122.0, 119.6, 111.4, 44.2, 21.5. IR (KBr, *v*, cm^{-1}) 1608, 1367, 1265, 1170, 1084, 896, 774. HR-MS (ESI) m/z calcd for $C_{29}H_{23}NNaO_6S_2$ $[M+Na]^+$ 568.0864, found 568.0881.

N-((3-([1,1'-Biphenyl]-4-carbonyl)benzofuran-2-yl)methyl)-N-(phenylsulfonyl)benzenesulfonamide (4c)



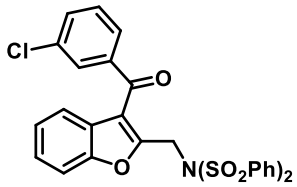
White solid, 89 mg, 73%; m.p. 199-200 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) (*δ*, ppm) 8.05 (d, *J* = 8.0 Hz, 4H), 7.95 (d, *J* = 8.0 Hz, 2H), 7.73 (d, *J* = 7.6 Hz, 2H), 7.67 (d, *J* = 8.0 Hz, 2H), 7.64 – 7.58 (m, 2H), 7.53 – 7.47 (m, 6H), 7.45 – 7.40 (m, 1H), 7.31 (d, *J* = 6.4 Hz, 2H), 7.26 (d, *J* = 3.6 Hz, 1H), 7.22 – 7.16 (m, 1H), 5.35 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) (*δ*, ppm) 190.8, 156.8, 153.8, 146.0, 139.9, 139.4, 137.5, 134.0, 130.2, 129.1, 129.0, 128.6, 128.4, 127.4, 127.3, 126.0, 125.5, 124.0, 122.0, 119.7, 111.5, 44.1. IR (KBr, *v*, cm^{-1}) 1605, 1380, 1244, 1170, 1084, 908, 800, 743. HR-MS (ESI) m/z calcd for $C_{34}H_{25}NNaO_6S_2$ $[M+Na]^+$ 630.1021, found 630.1037.

N-((3-Benzoylbenzofuran-2-yl)methyl)-N-(phenylsulfonyl)benzenesulfonamide (4d)



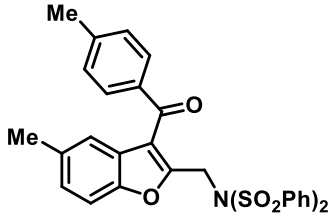
White solid, 44 mg, 41%; m.p. 190-191 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) (*δ*, ppm) 8.03 (d, *J* = 8.0 Hz, 4H), 7.85 (d, *J* = 8.0 Hz, 2H), 7.65 – 7.59 (m, 3H), 7.53 – 7.47 (m, 6H), 7.29 (d, *J* = 8.0 Hz, 1H), 7.23 (d, *J* = 8.0 Hz, 1H), 7.21 – 7.14 (m, 2H), 5.31 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) (*δ*, ppm) 191.3, 156.9, 153.7, 139.3, 138.8, 134.0, 133.2, 129.4, 128.9, 128.7, 128.6, 125.9, 125.4, 123.9, 121.9, 119.5, 111.4, 44.1. IR (KBr, *v*, cm^{-1}) 1608, 1379, 1242, 1170, 1084, 904, 750, 720. HR-MS (ESI) m/z calcd for $C_{28}H_{21}NNaO_6S_2$ $[M+Na]^+$ 554.0708, found 554.0723.

N-((3-(3-Chlorobenzoyl)benzofuran-2-yl)methyl)-N-(phenylsulfonyl)benzenesulfonamide (4e)



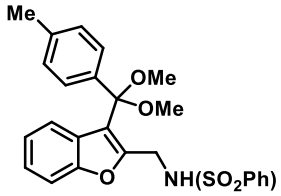
White solid, 51 mg, 45%; m.p. 128-129 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.05 (d, J = 8.0 Hz, 4H), 7.84 (s, 1H), 7.69 (d, J = 8.0 Hz, 1H), 7.65 – 7.59 (m, 3H), 7.54 – 7.49 (m, 4H), 7.45 – 7.41 (m, 1H), 7.32 – 7.26 (m, 2H), 7.21 – 7.17 (m, 1H), 7.15 (d, J = 7.6 Hz, 1H), 5.32 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 189.9, 157.5, 157.5, 153.7, 140.3, 139.3, 134.1, 133.1, 130.0, 129.2, 129.0, 128.6, 127.7, 125.6, 124.1, 121.6, 111.5, 43.9. IR (KBr, v, cm^{-1}) 1608, 1362, 1169, 1084, 774. HR-MS (ESI) m/z calcd for $C_{28}H_{20}ClNNaO_6S_2$ $[M+Na]^+$ 588.0318, found 588.0340.

N-((5-Methyl-3-(4-methylbenzoyl)benzofuran-2-yl)methyl)-N-(phenylsulfonyl)benzenesulfonamide (4f)



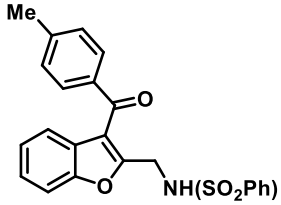
White solid, 66 mg, 59%; m.p. 169-170 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.00 (d, J = 8.4 Hz, 4H), 7.77 (d, J = 7.6 Hz, 2H), 7.62 – 7.57 (m, 2H), 7.50 – 7.45 (m, 4H), 7.30 (d, J = 8.0 Hz, 2H), 7.12 (d, J = 8.4 Hz, 1H), 7.08 (d, J = 8.4 Hz, 2H), 5.25 (s, 2H), 2.46 (s, 3H), 2.34 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 191.0, 156.3, 152.3, 144.1, 139.4, 136.2, 134.0, 133.6, 129.8, 129.4, 128.9, 128.6, 126.7, 126.1, 121.7, 119.6, 110.9, 44.2, 21.9, 21.5. IR (KBr, v, cm^{-1}) 1608, 1363, 1169, 1084, 774. HR-MS (ESI) m/z calcd for $C_{30}H_{25}NNaO_6S_2$ $[M+Na]^+$ 582.1021, found 582.1046.

N-((3-(Dimethoxy(p-tolyl)methyl)benzofuran-2-yl)methyl)benzenesulfonamide (5a)



White solid, 35 mg, 78%; m.p. 165-166 ˚C; ^{1}H NMR (400 MHz, DMSO-d_6) (δ, ppm) 8.30 – 8.24 (m, 1H), 7.83 (d, J = 9.6 Hz, 2H), 7.59 – 7.51 (m, 3H), 7.38 (d, J = 8.0 Hz, 2H), 7.33 (d, J = 8.0 Hz, 1H), 7.28 (d, J = 7.6 Hz, 1H), 7.19 – 7.14 (m, 1H), 7.08 (d, J = 8.4 Hz, 2H), 7.07 – 7.02 (m, 1H), 4.52 (d, J = 6.0 Hz, 2H), 2.94 (s, 6H), 2.22 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm) 153.7, 151.3, 141.1, 137.9, 137.8, 132.8, 129.5, 129.1, 127.1, 127.1, 126.5, 124.9, 123.3, 121.5, 118.3, 111.3, 101.9, 49.2, 21.2. IR (KBr, v, cm^{-1}) 1447, 1282, 1169, 1052, 750. HR-MS (ESI) m/z calcd for $C_{25}H_{25}NNaO_5S$ $[M+Na]^+$ 474.1351, found 474.1360.

N-((3-(4-Methylbenzoyl)benzofuran-2-yl)methyl)benzenesulfonamide (6a)



White solid, 14 mg, 70%; m.p. 171-172 ˚C; ^{1}H NMR (400 MHz, DMSO-d_6) (δ, ppm) 8.49 – 8.44 (m, 1H), 7.65 – 7.61 (m, 4H), 7.57 – 7.49 (m, 2H), 7.46 – 7.41 (m, 2H), 7.38 (d, J = 7.6 Hz, 1H), 7.35 (d, J = 7.6 Hz, 3H),

7.29 – 7.24 (m, 1H), 4.22 (d, J = 5.6 Hz, 2H), 2.42 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm) 190.4, 158.3, 153.7, 144.3, 140.5, 136.3, 132.8, 129.8, 129.7, 129.4, 126.8, 126.4, 126.0, 124.5, 121.8, 118.3, 111.9, 111.9, 39.2, 21.8. IR (KBr, v, cm^{-1}) 1644, 1449, 1332, 1170, 1093, 908, 752. HR-MS (ESI) m/z calcd for $C_{23}H_{19}NNaO_4S$ $[M+Na]^+$ 428.0932, found 428.0946.

Reference

[1] J. Sadhan, V. Ajay, K. Rahul and K. Sangit, *Chem. Sci.*, 2017, **8**, 6633.

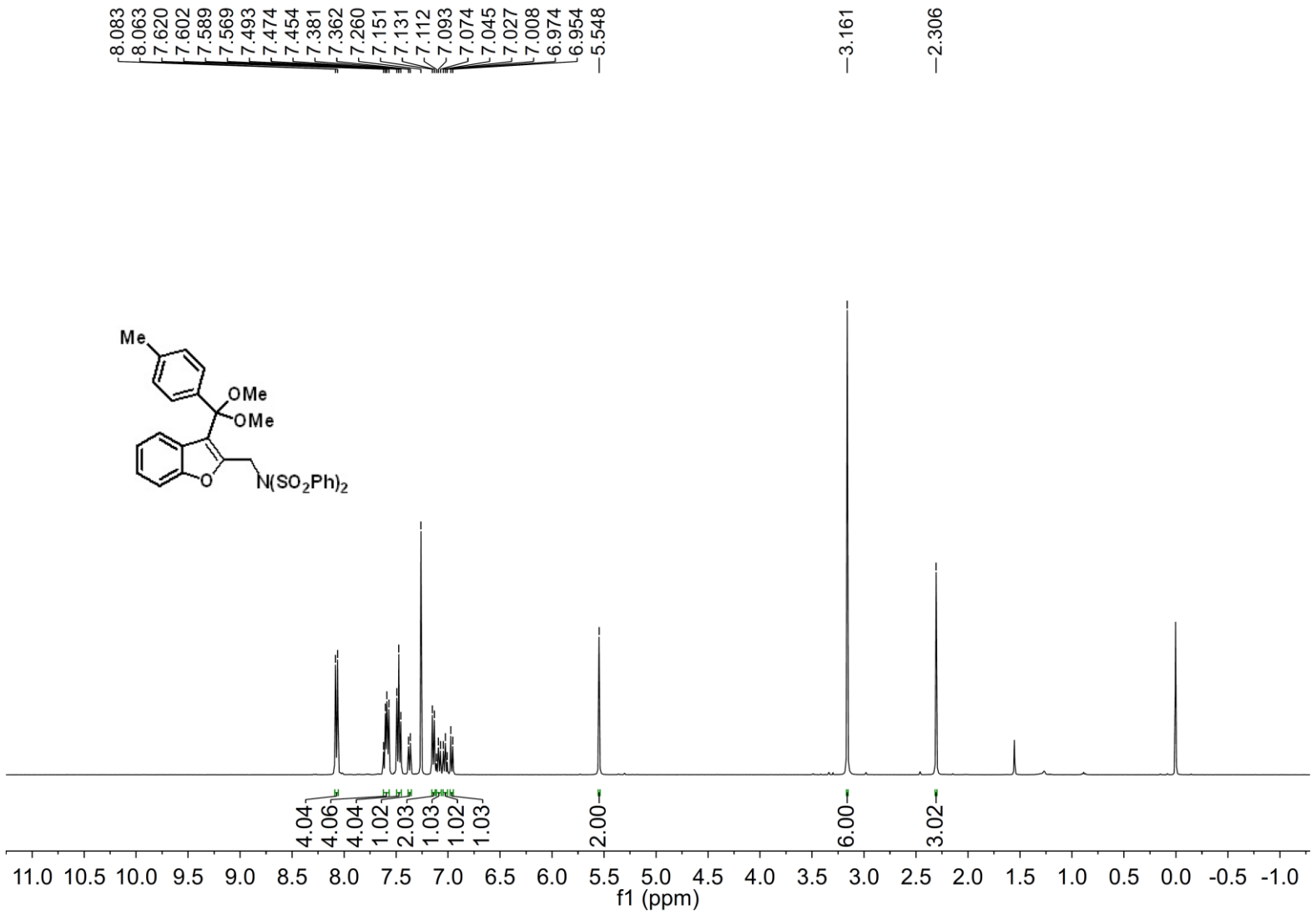
[2] X. Dong, R. Sang, Q. Wang, X.-Y. Tang and M. Shi, *Chem. Eur. J.*, 2013, **19**, 16910.

[3] X. Hu, G. Zhang, L. Nie, T. Kong and A. Lei, *Nat. Commun.*, 2019, **10**, 5467.

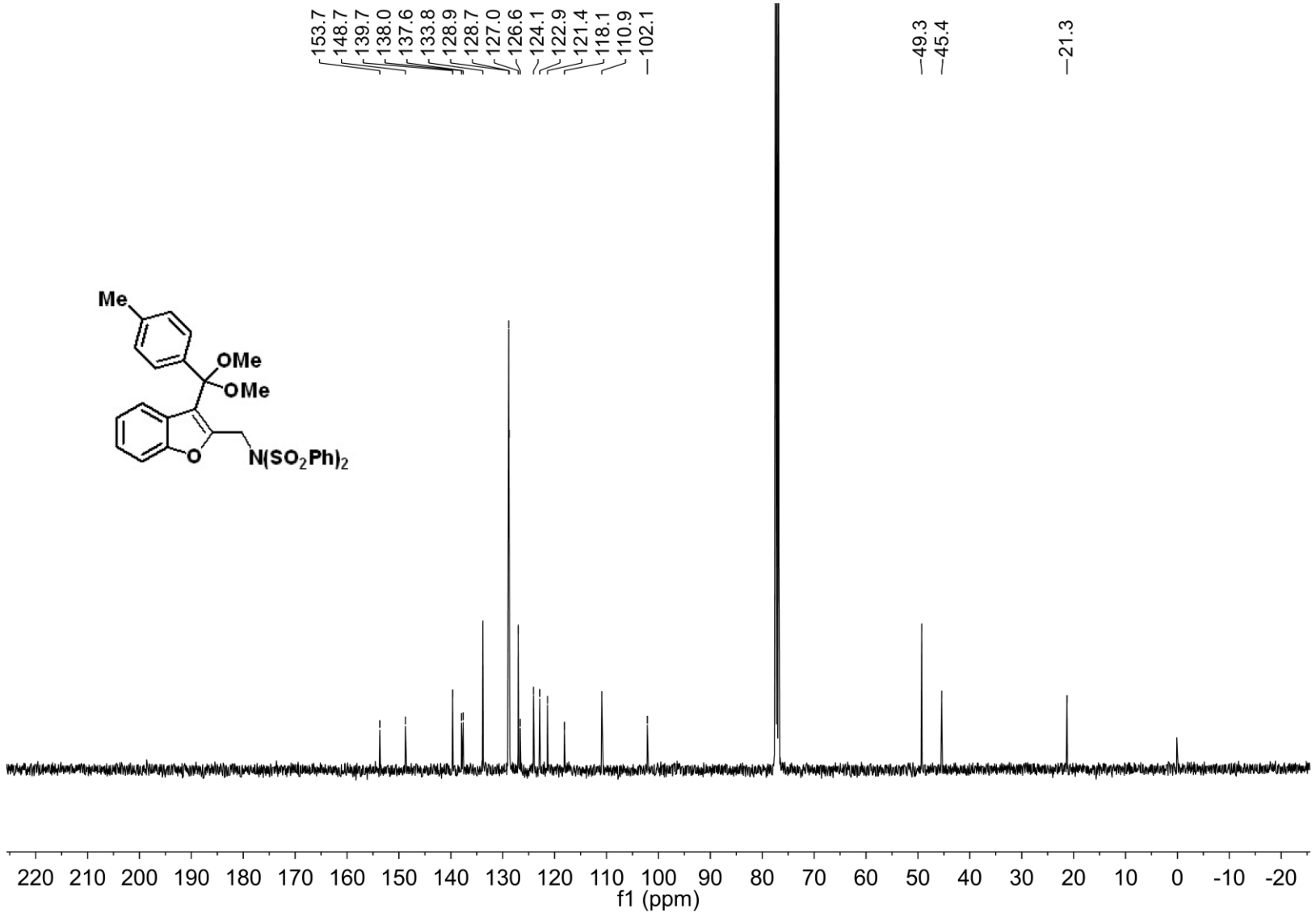
[4] D. Ji, X. He, Y. Xu, Z. Xu, Y. Bian, W. Liu, Q. Zhu and Y. Xu, *Org. Lett.*, 2016, **18**, 4478.

Copies of NMR Spectra

^{1}H spectra of compound 3a:



^{13}C spectra of compound 3a:



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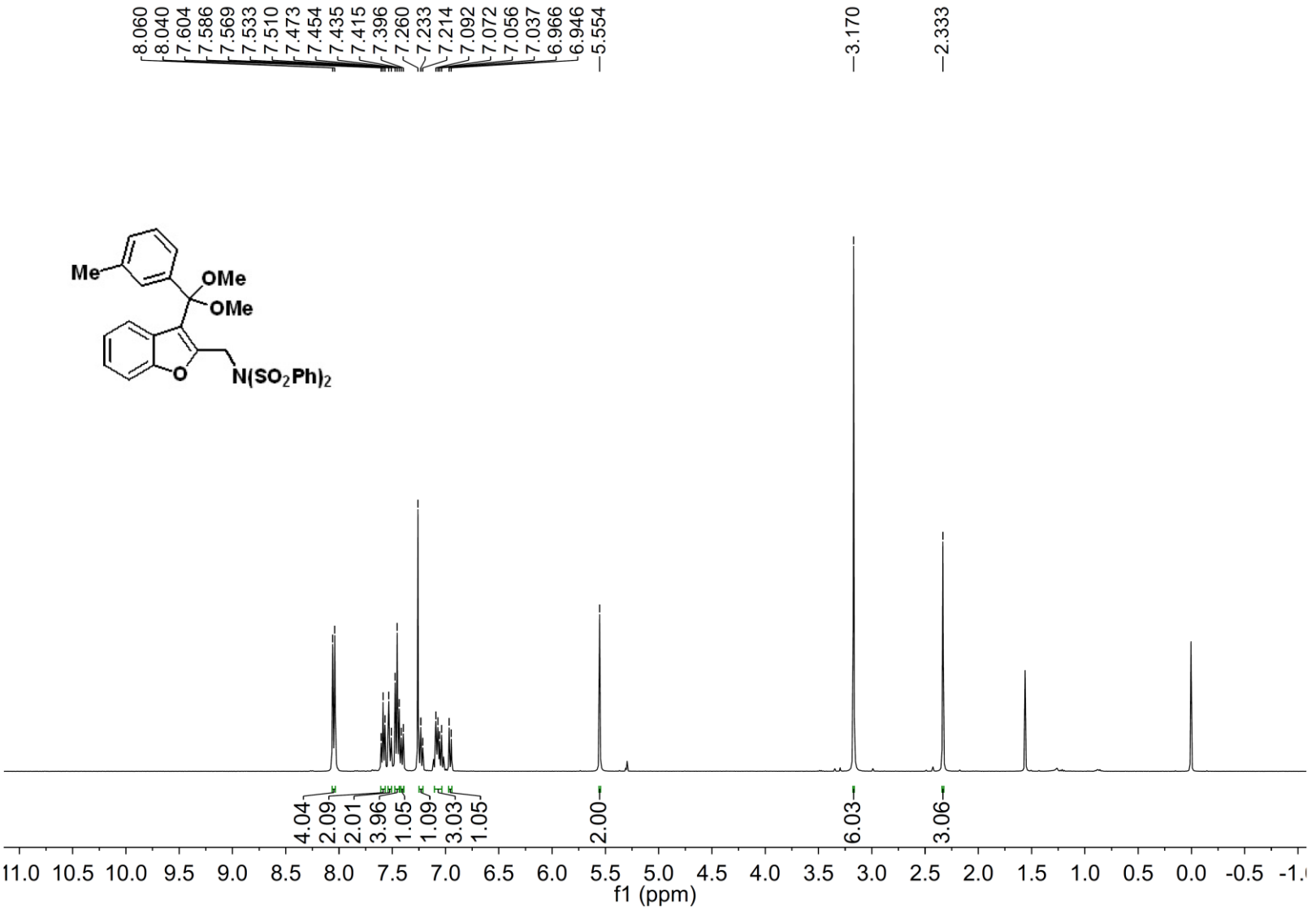
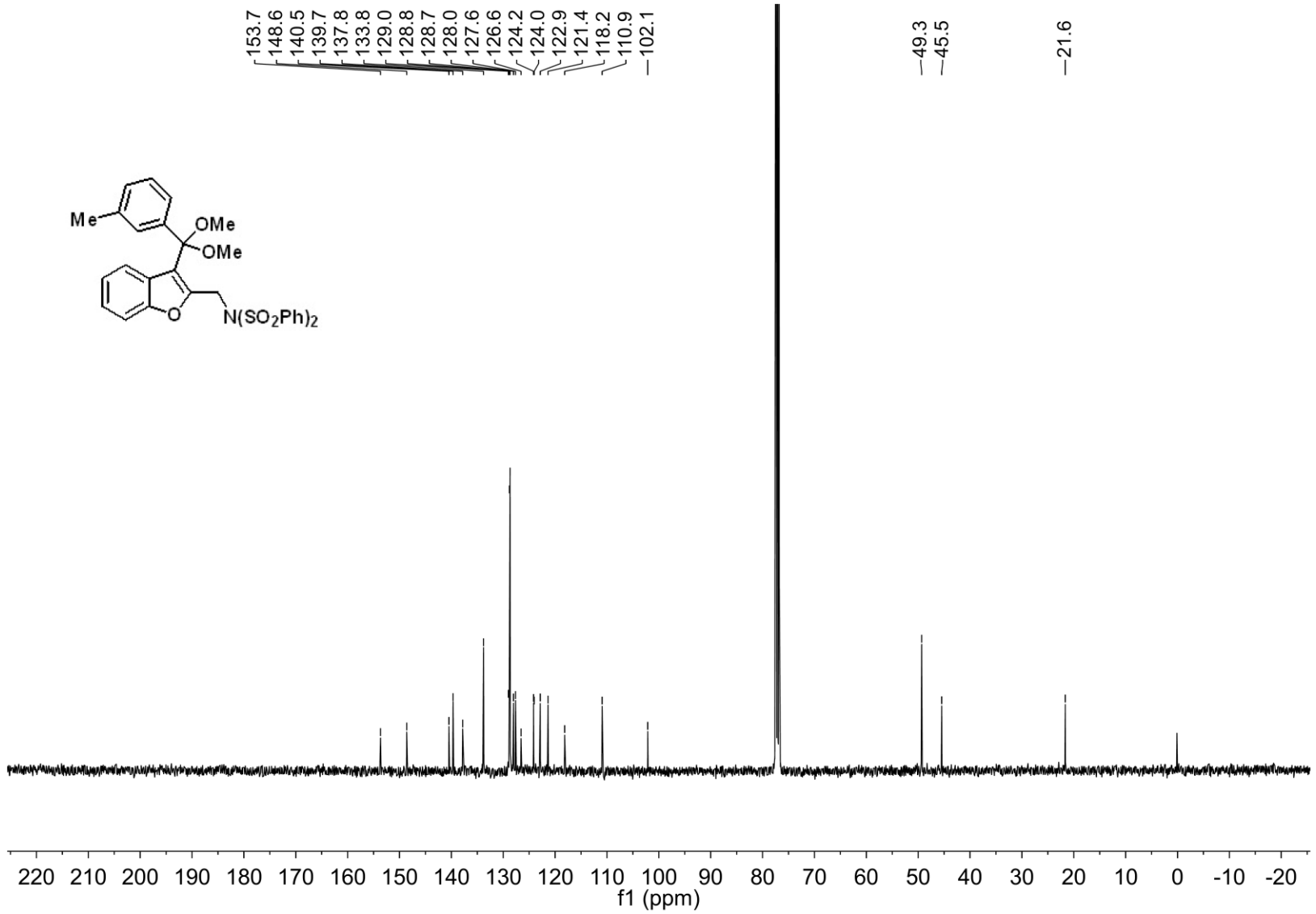


^{13}C spectra of compound 3b:



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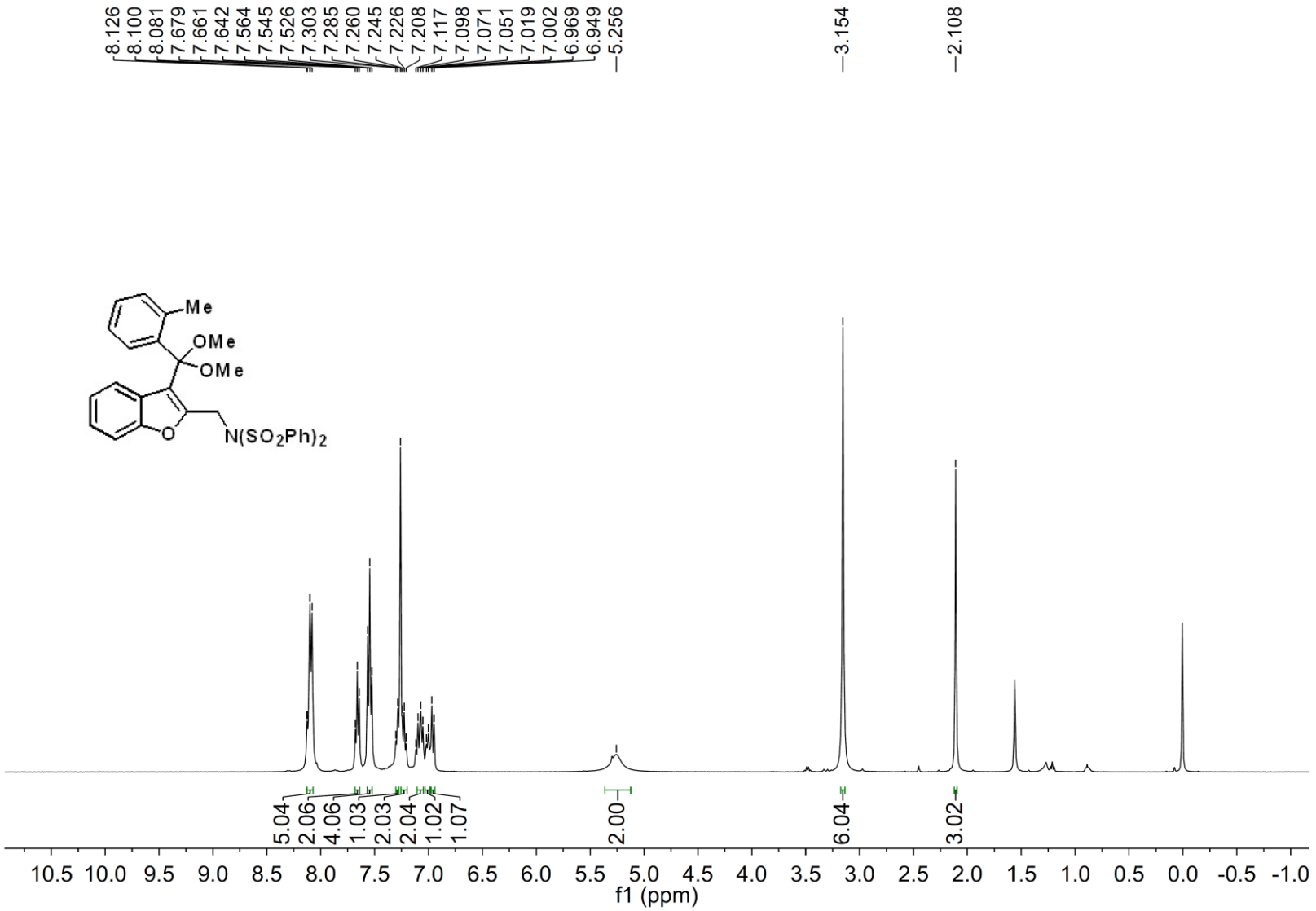
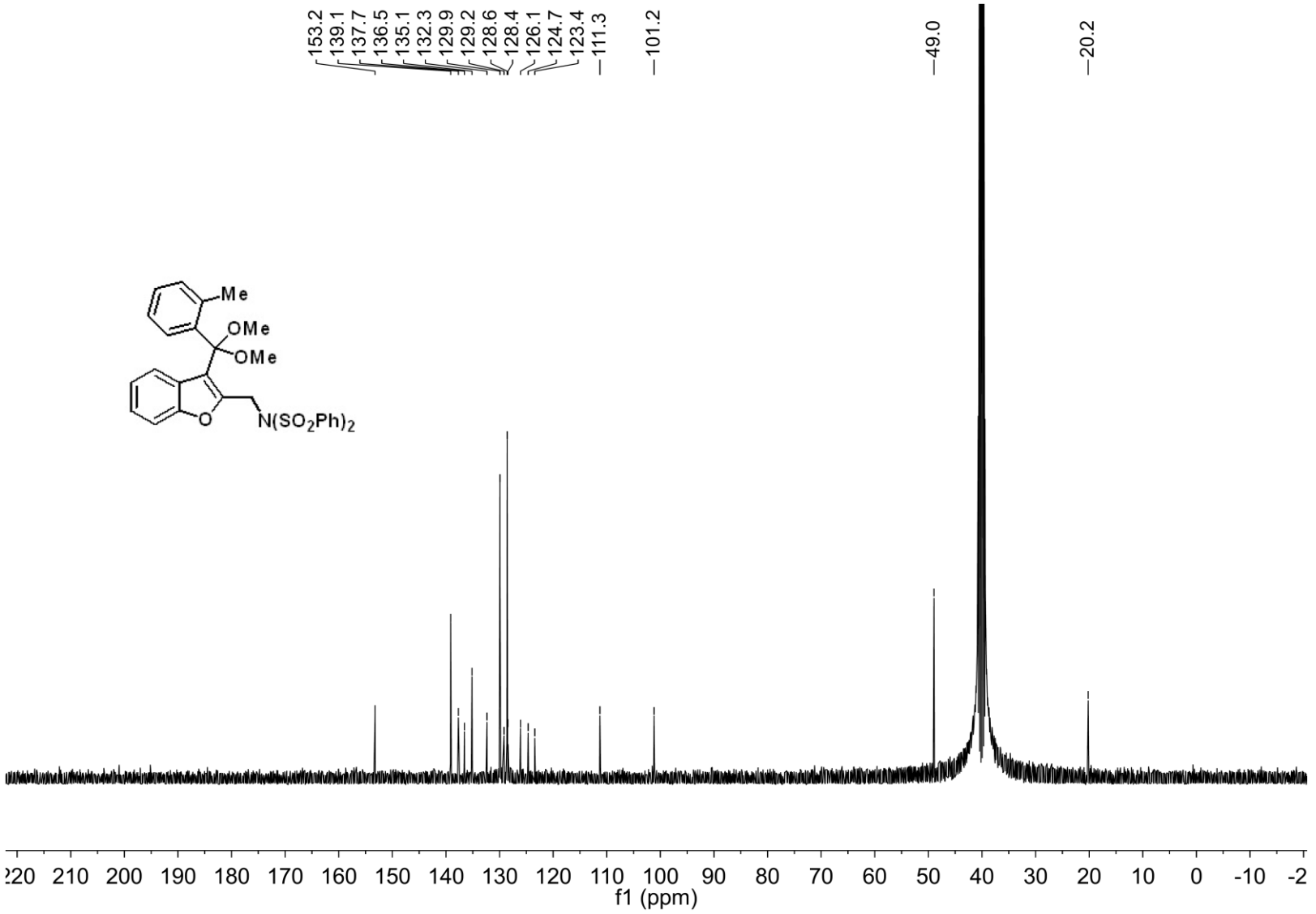


^{13}C spectra of compound 3c:



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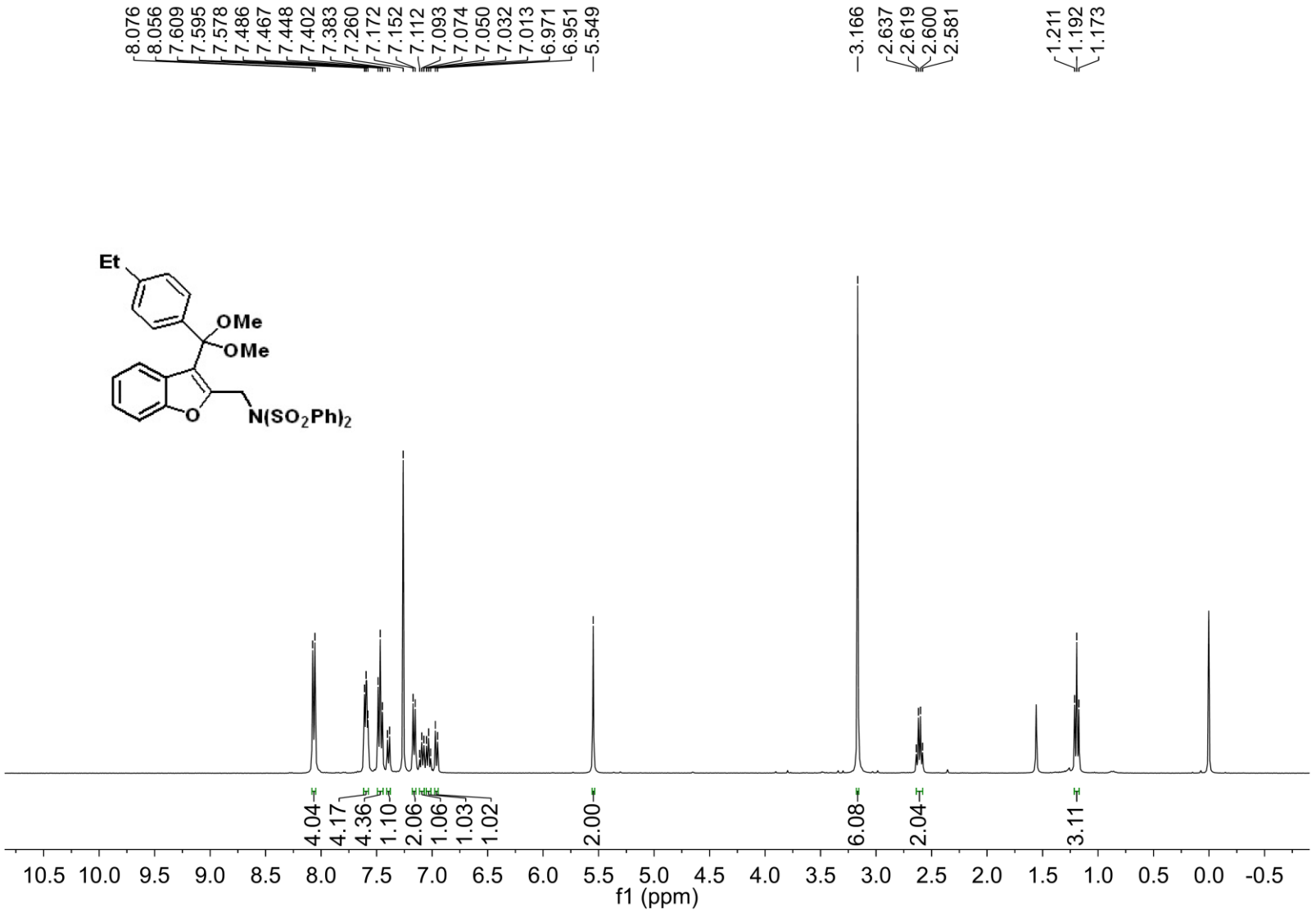
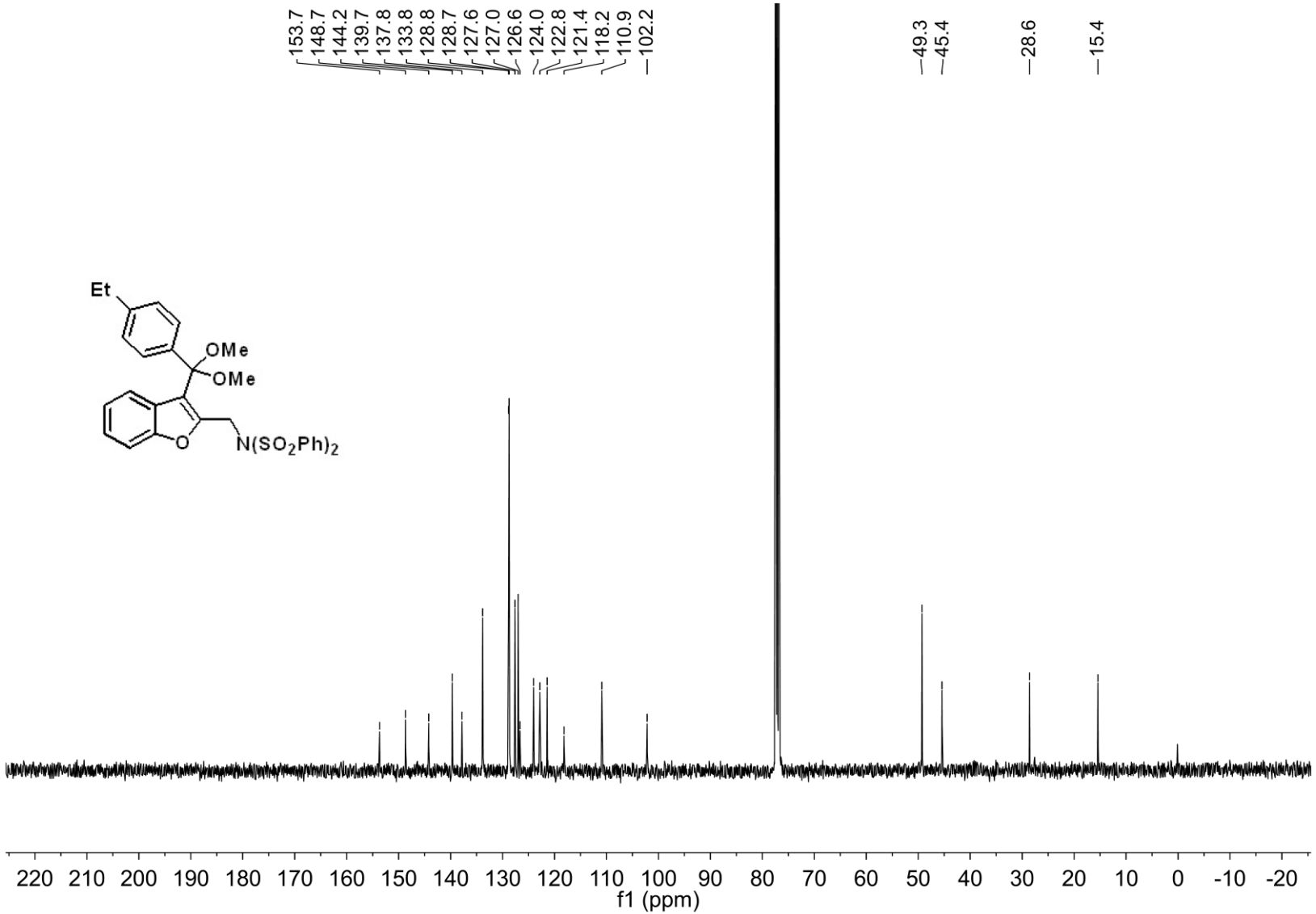


^{13}C spectra of compound 3d:



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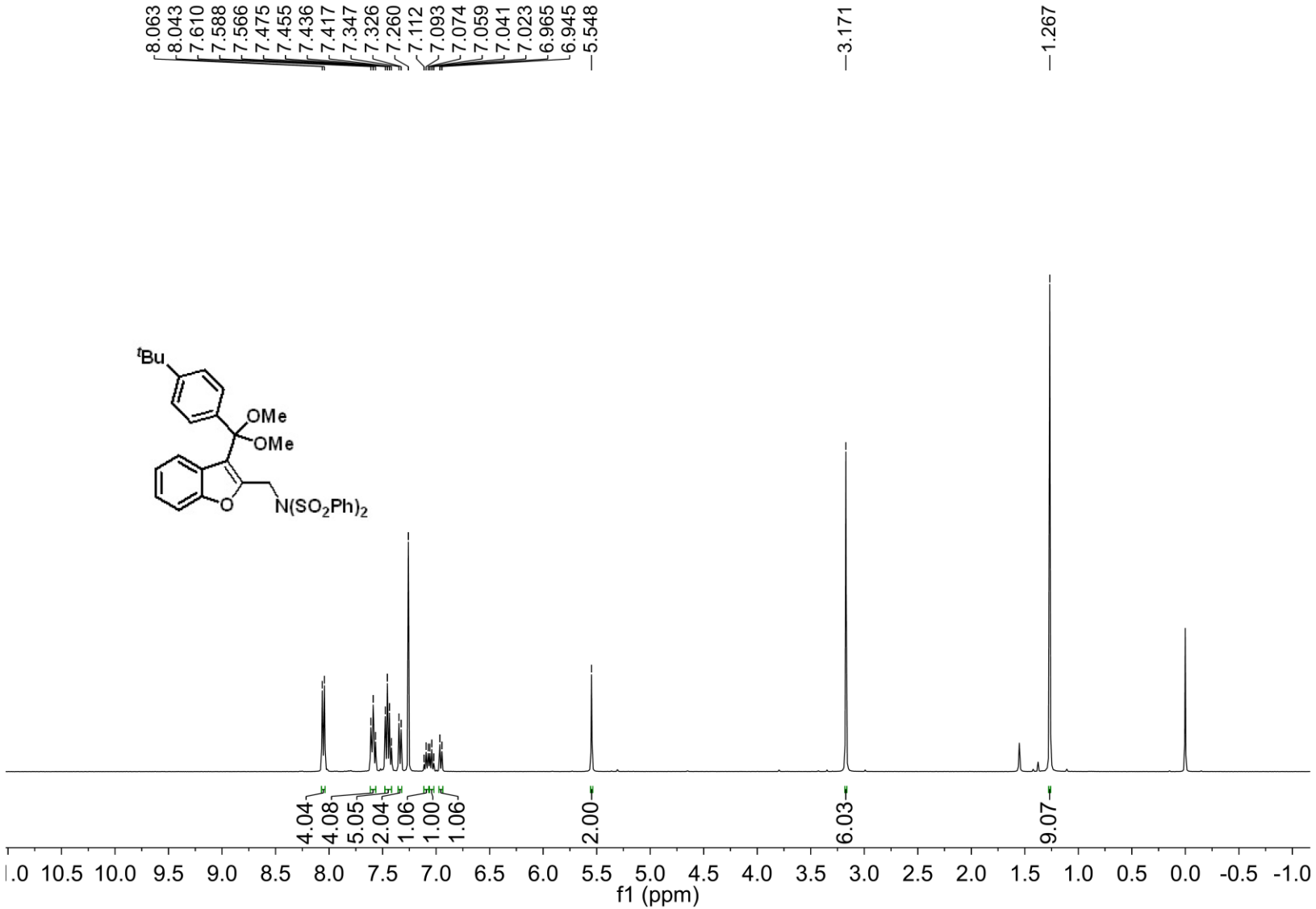

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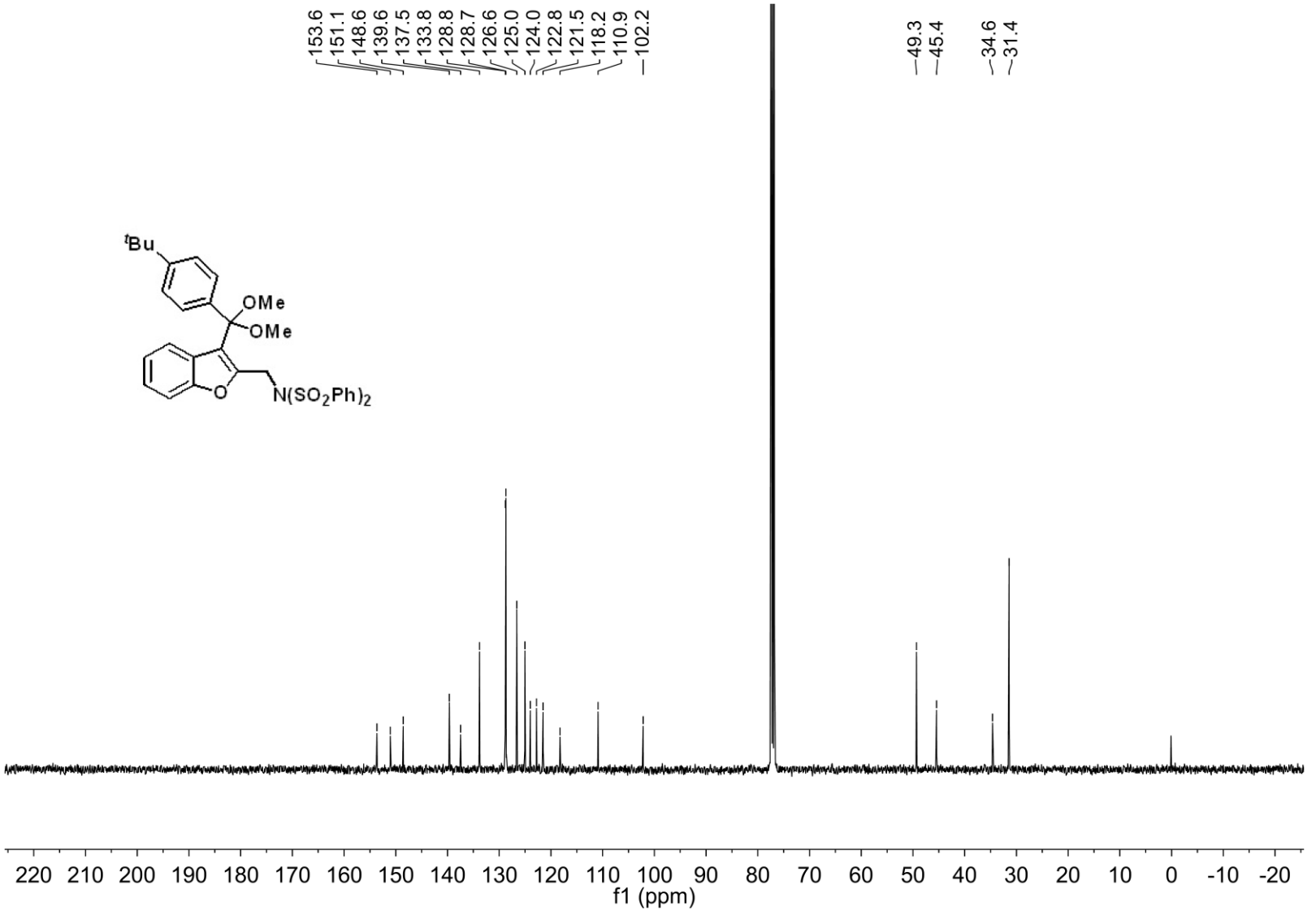

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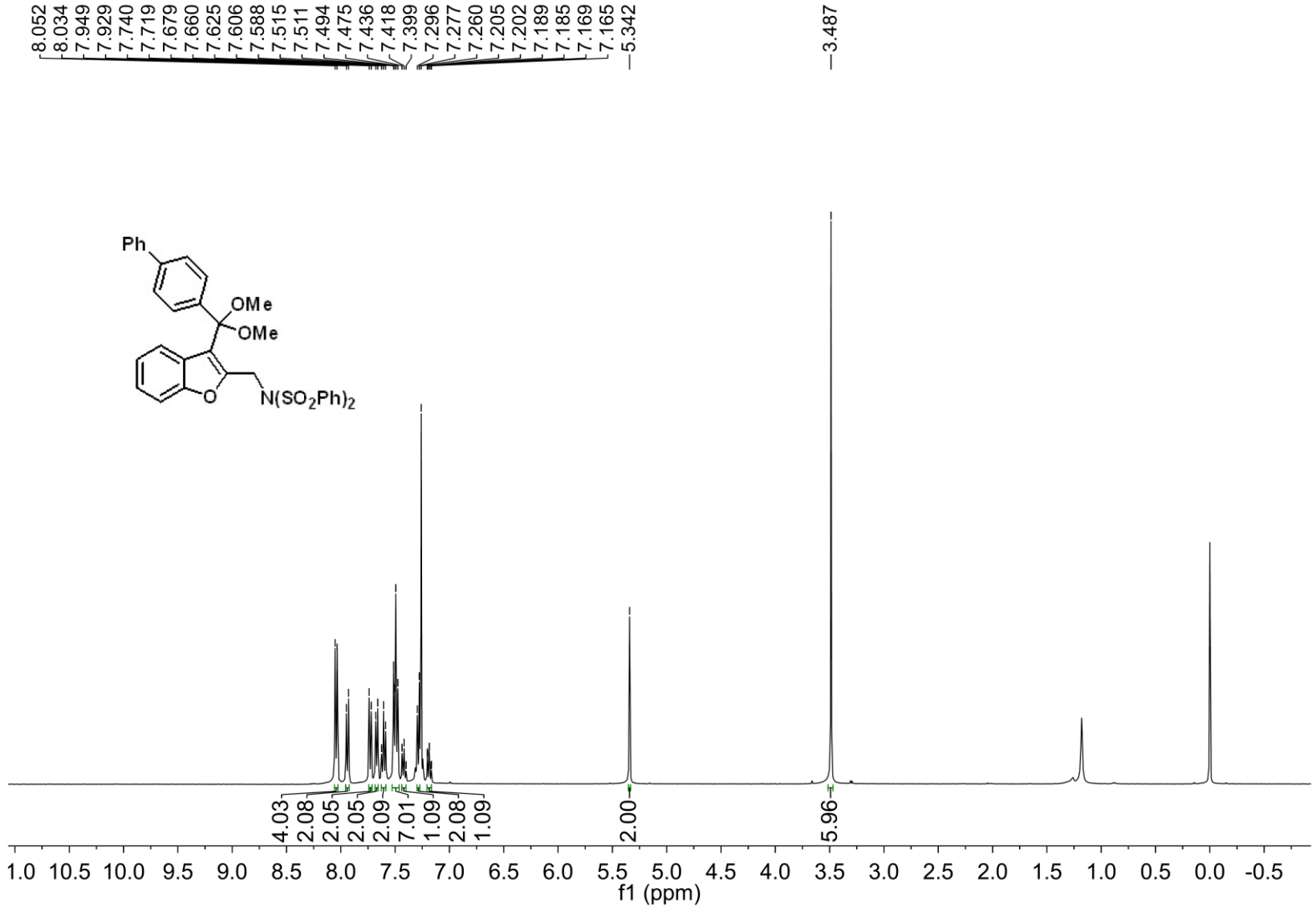
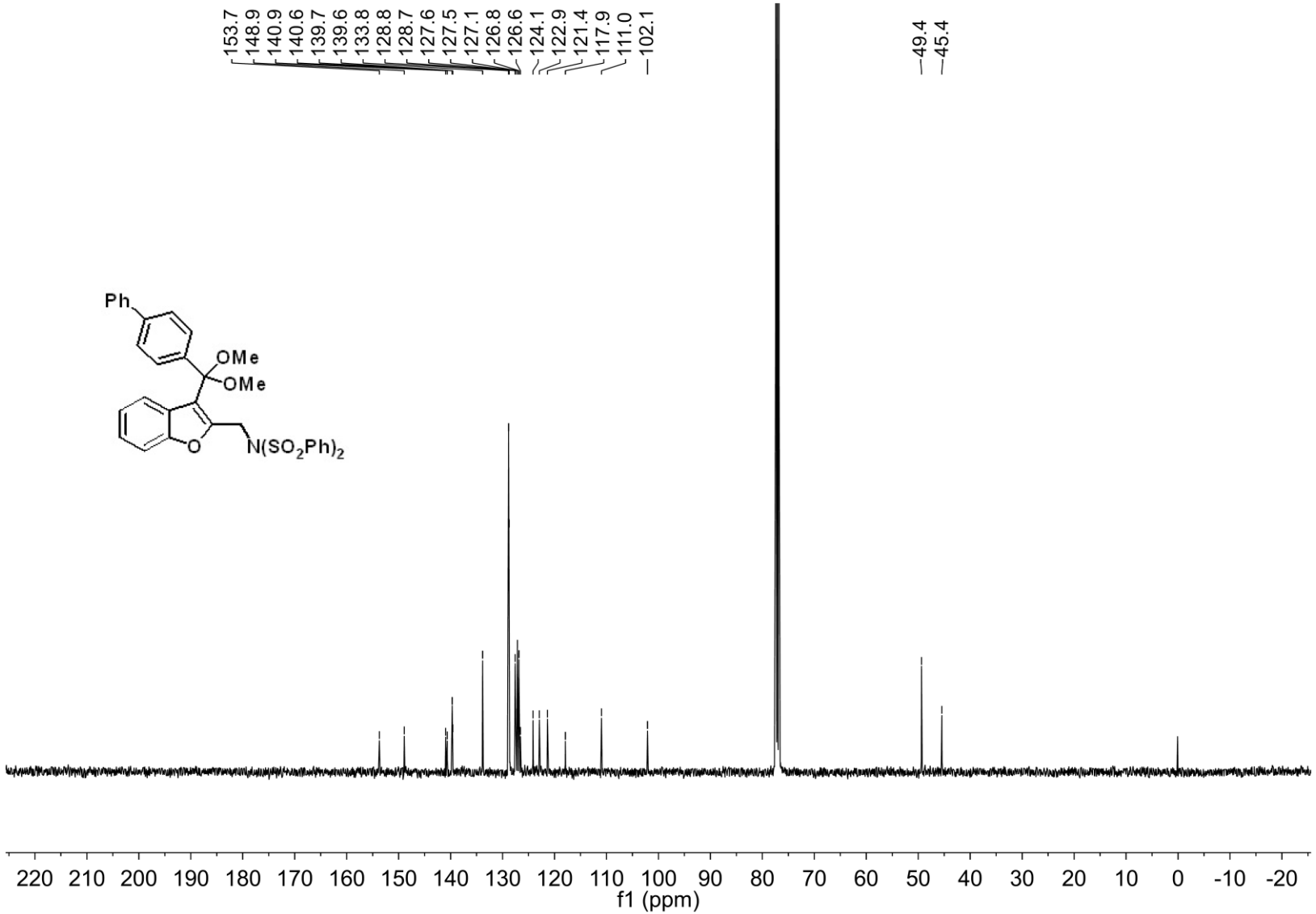


^{13}C spectra of compound 3f:



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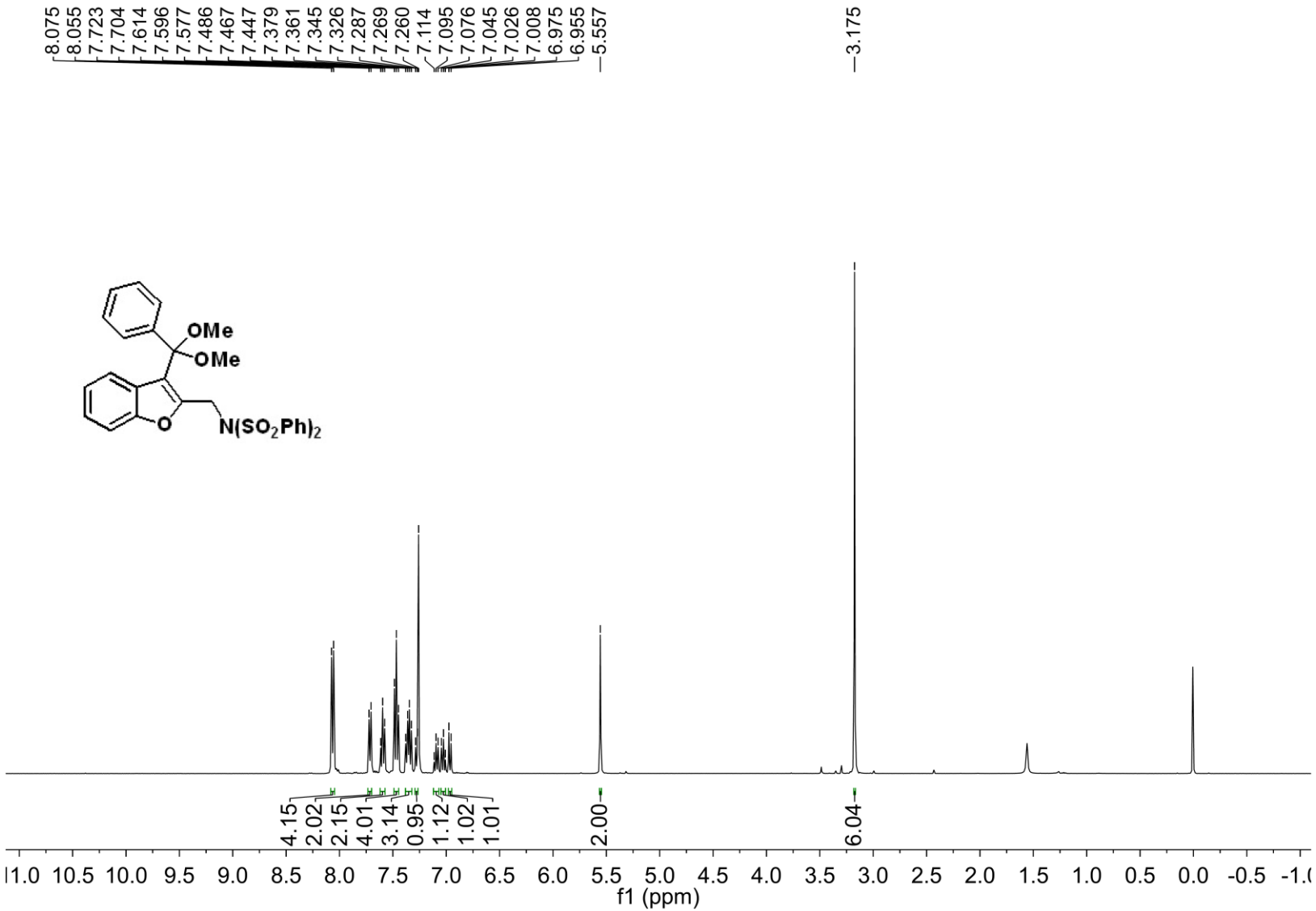

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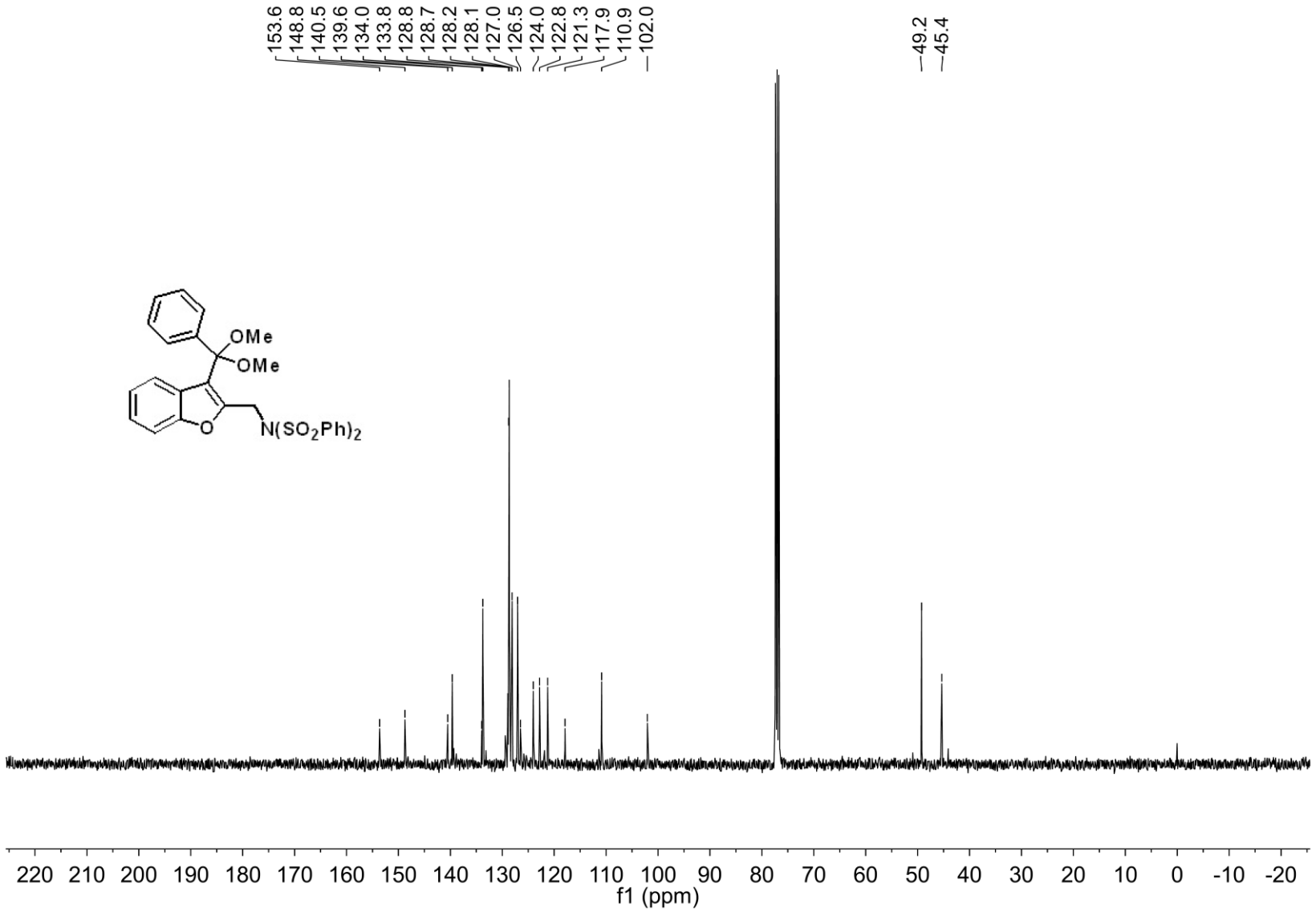

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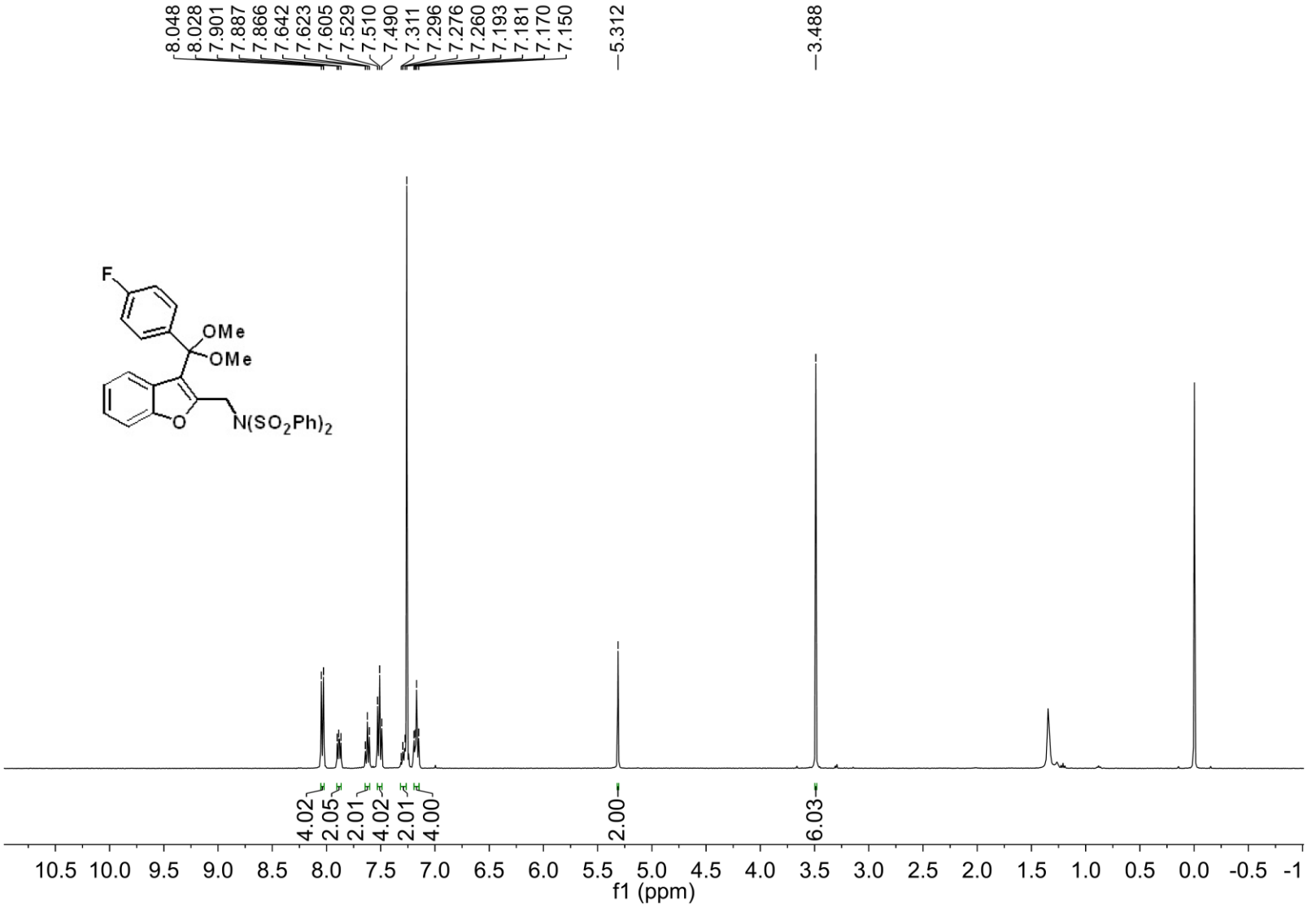

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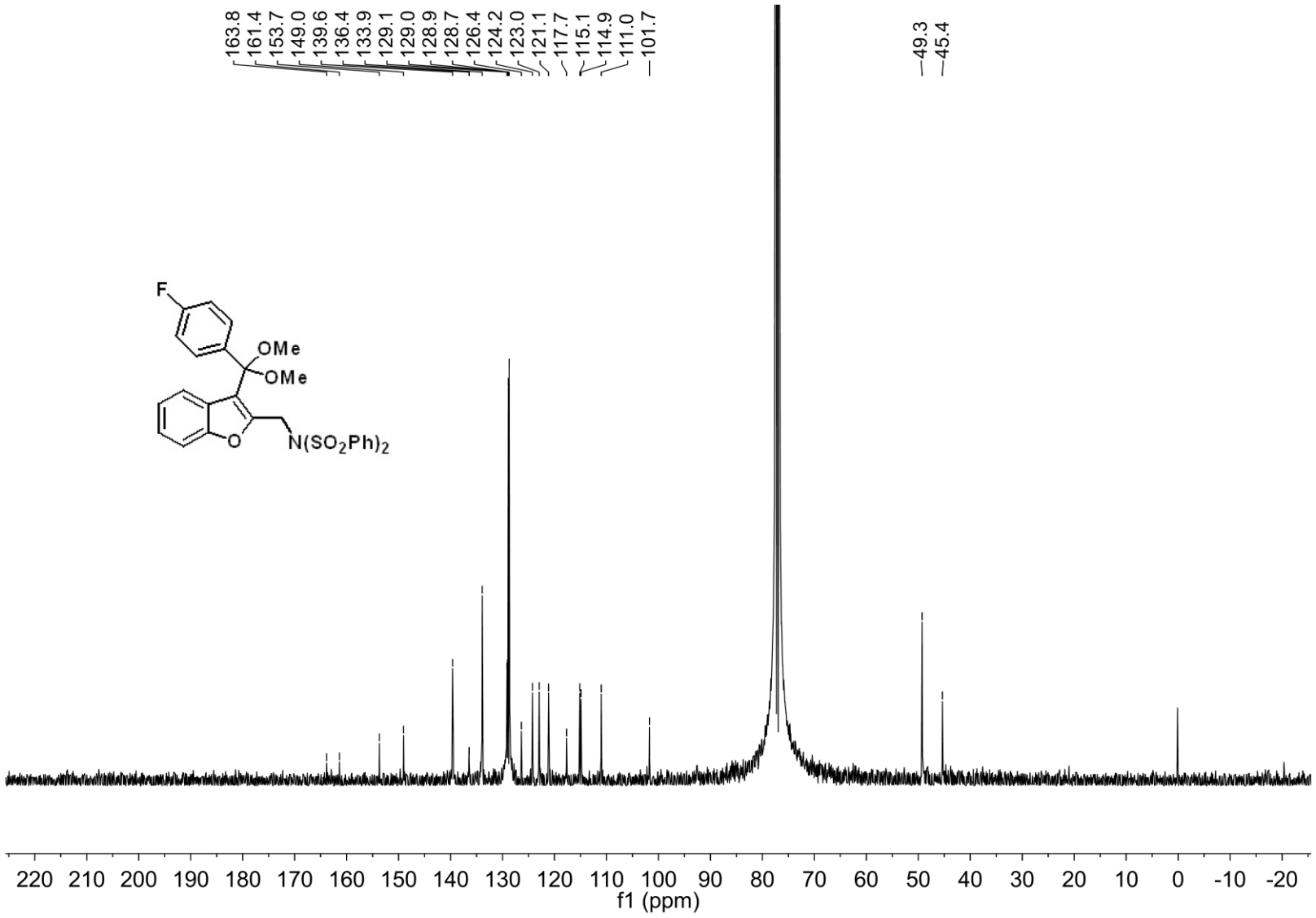

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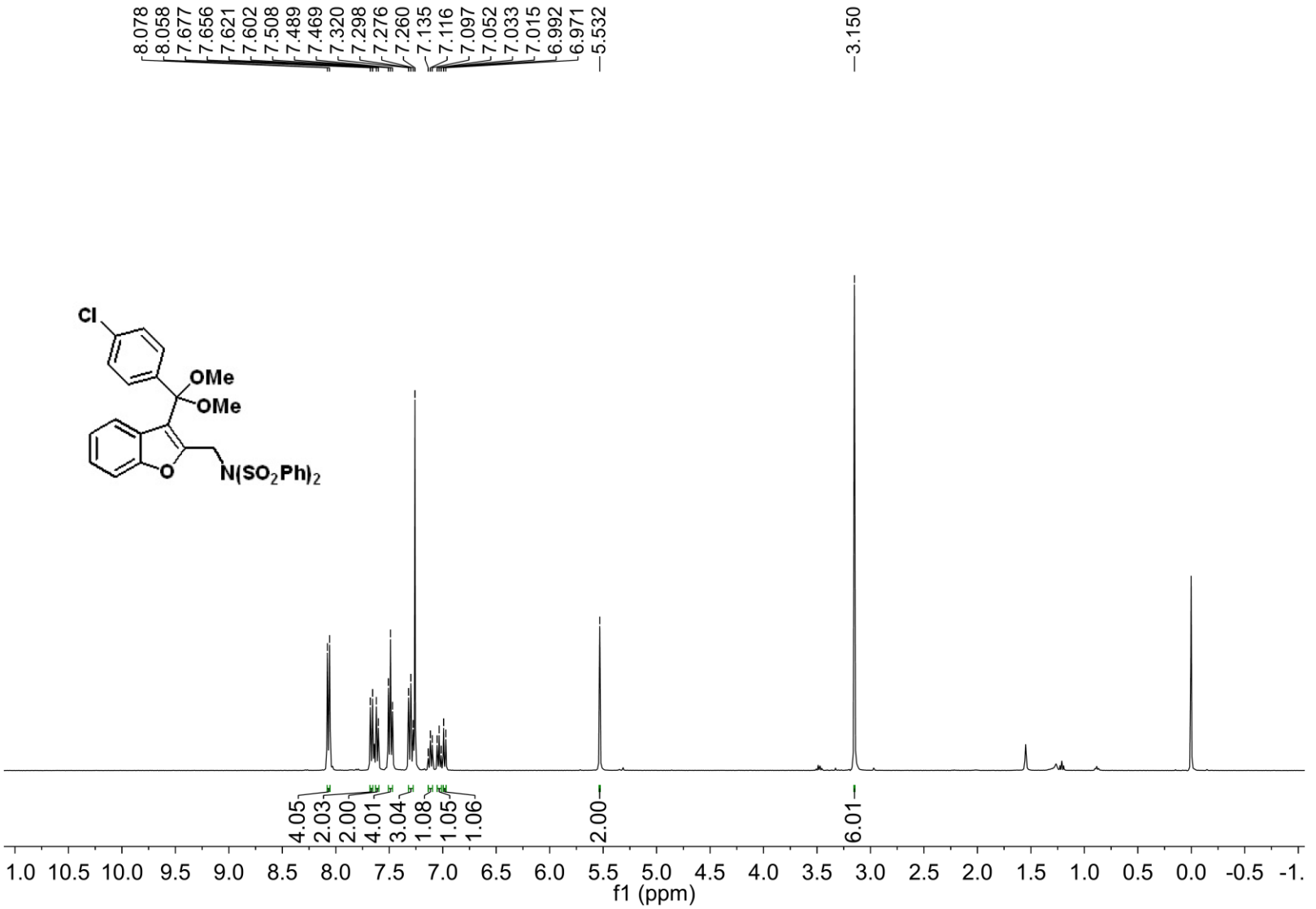

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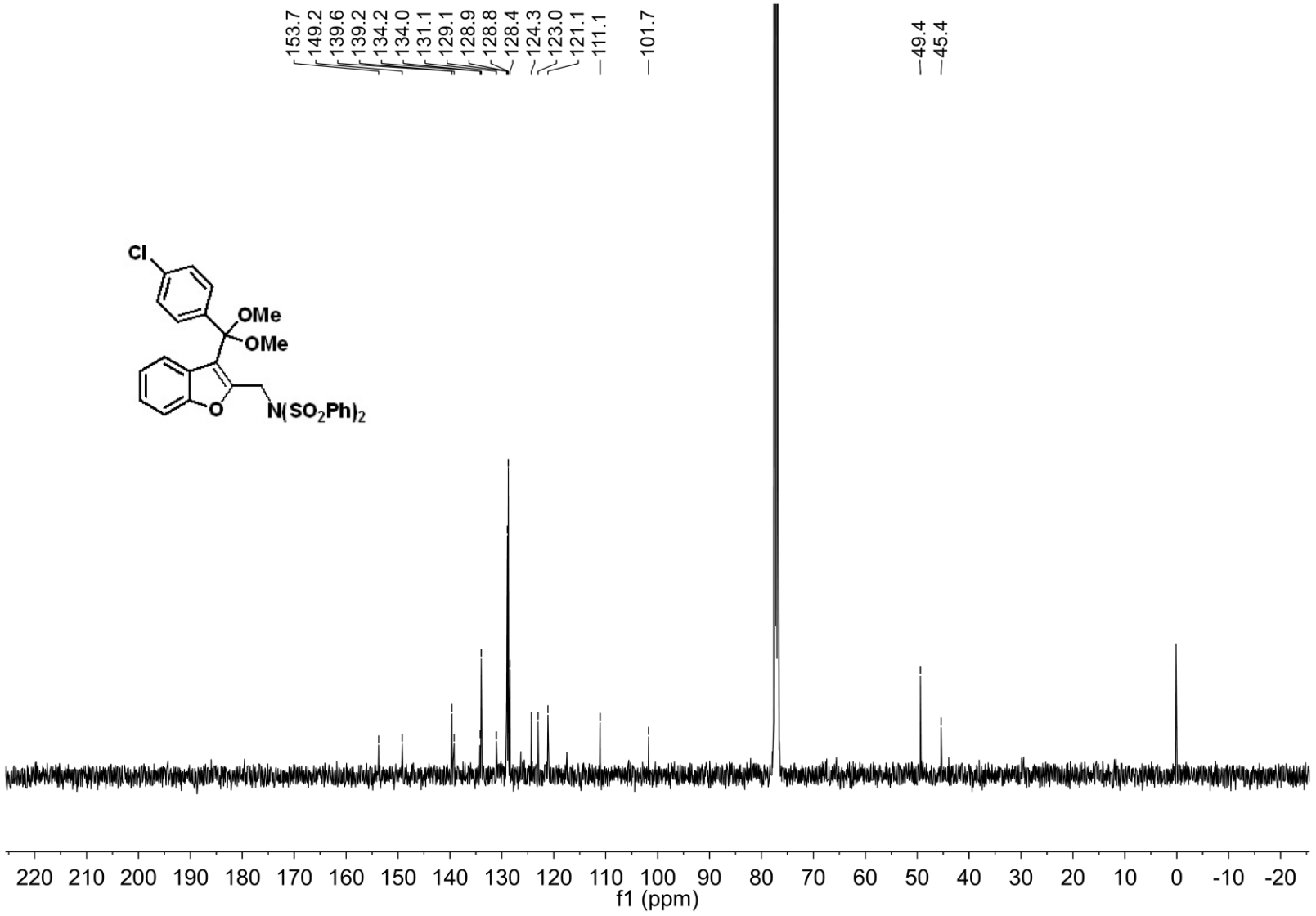

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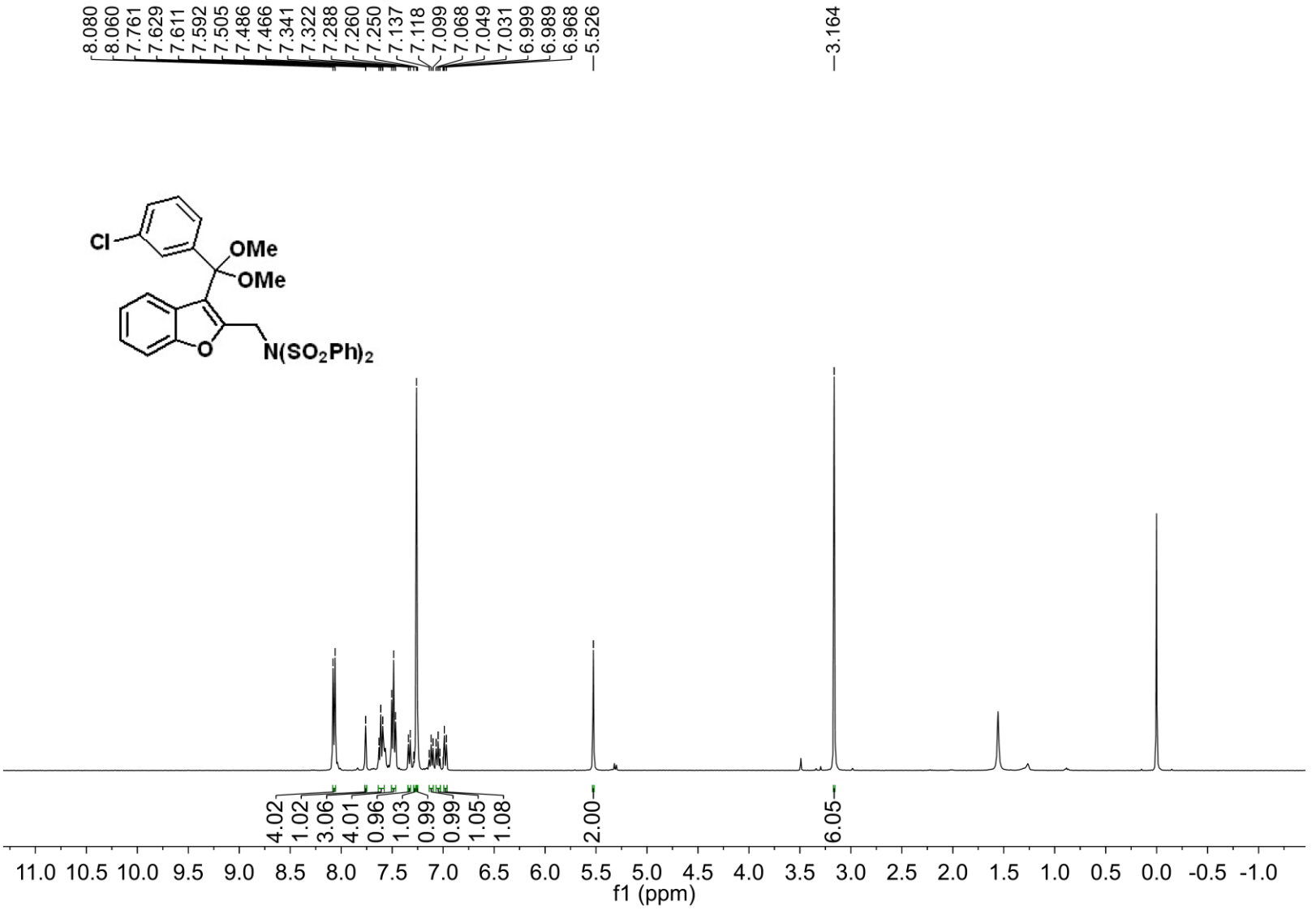

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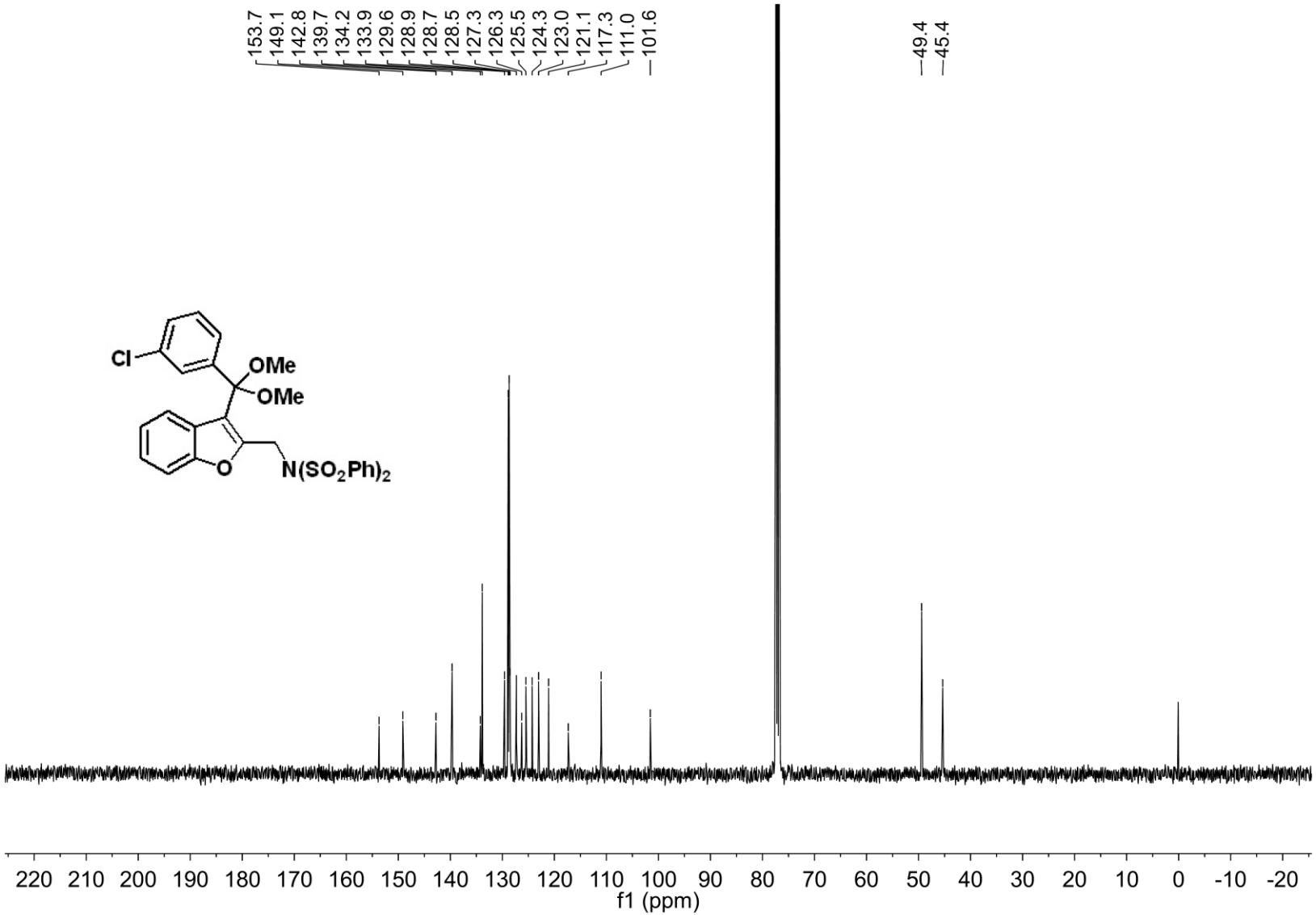

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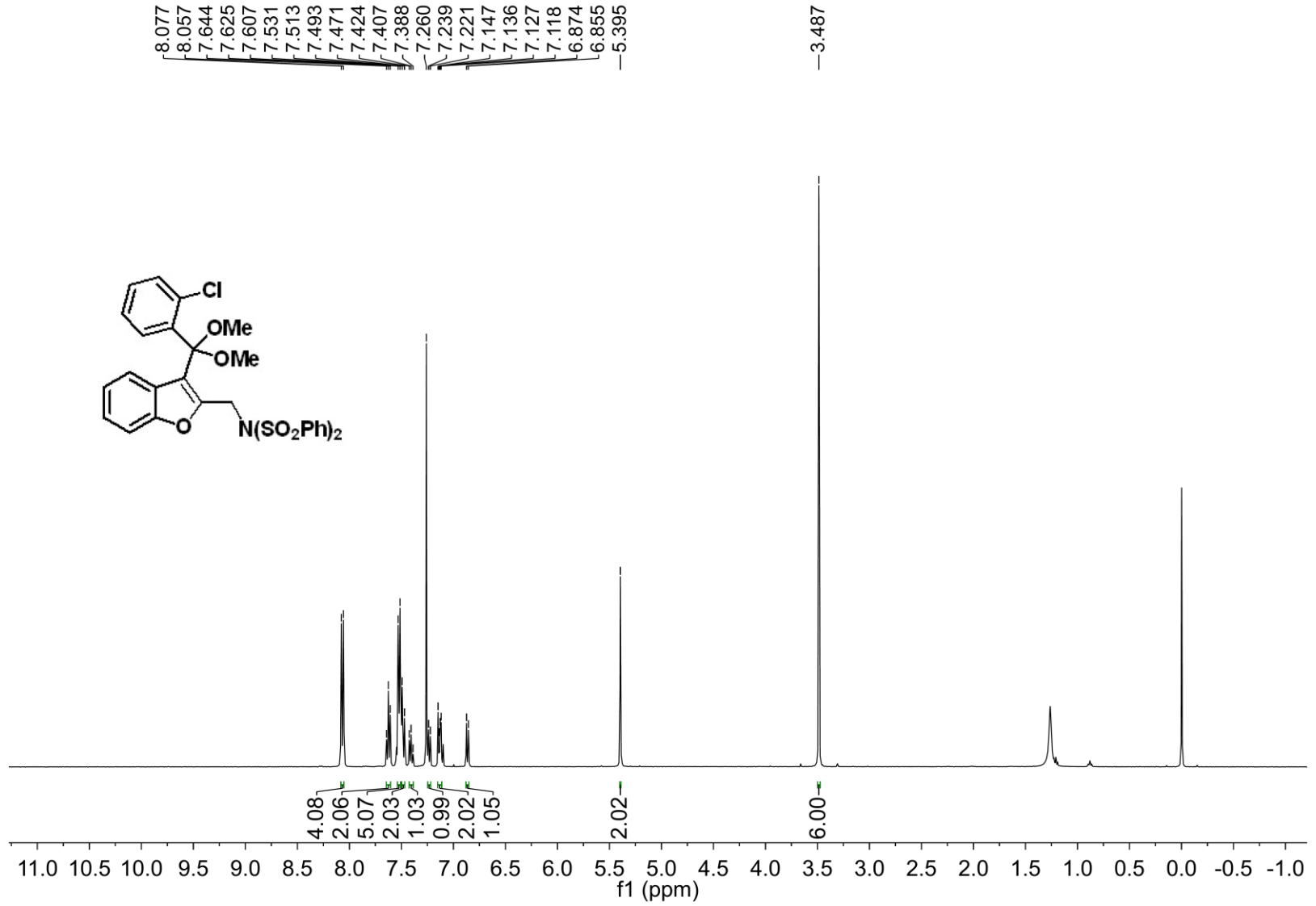

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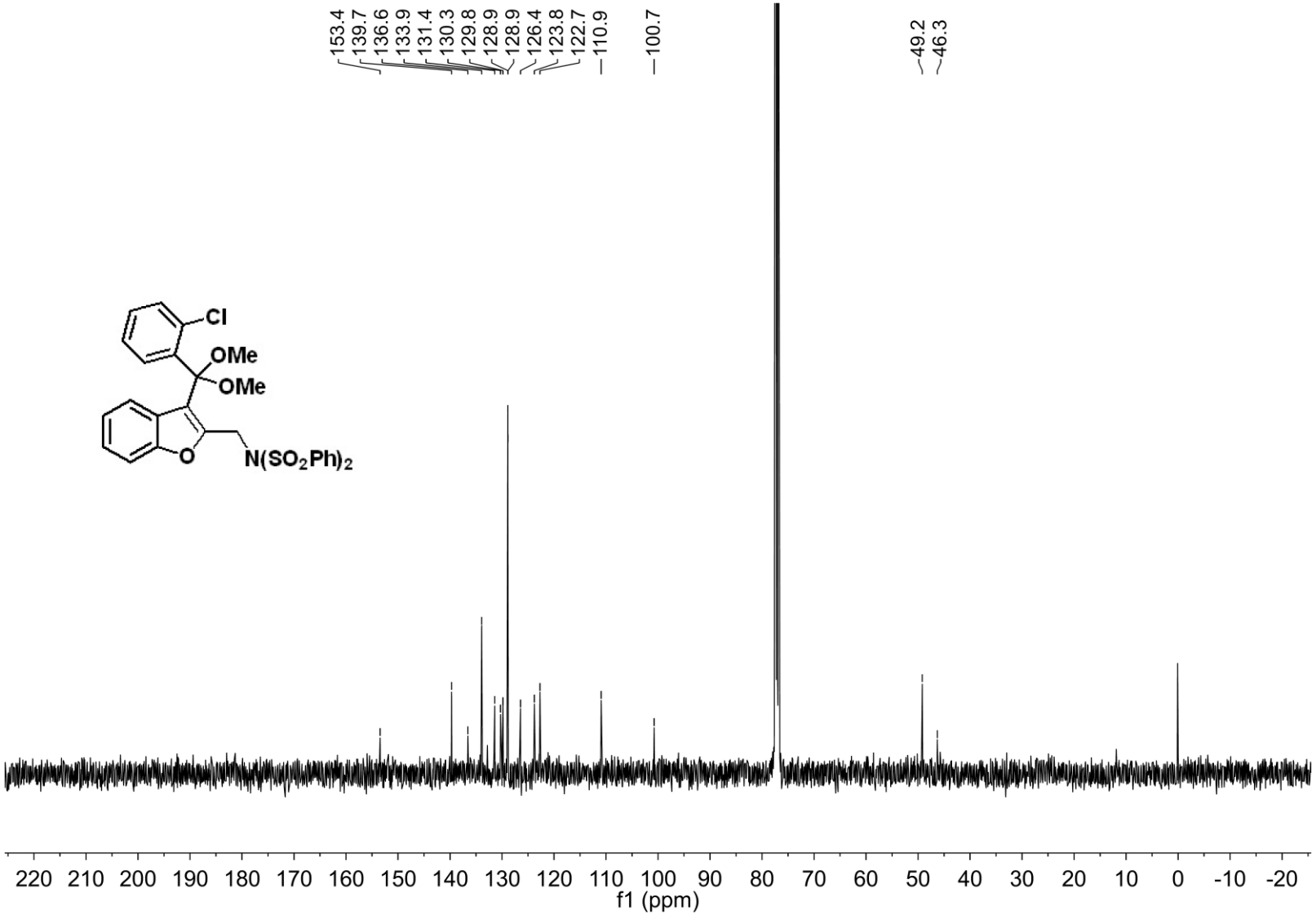

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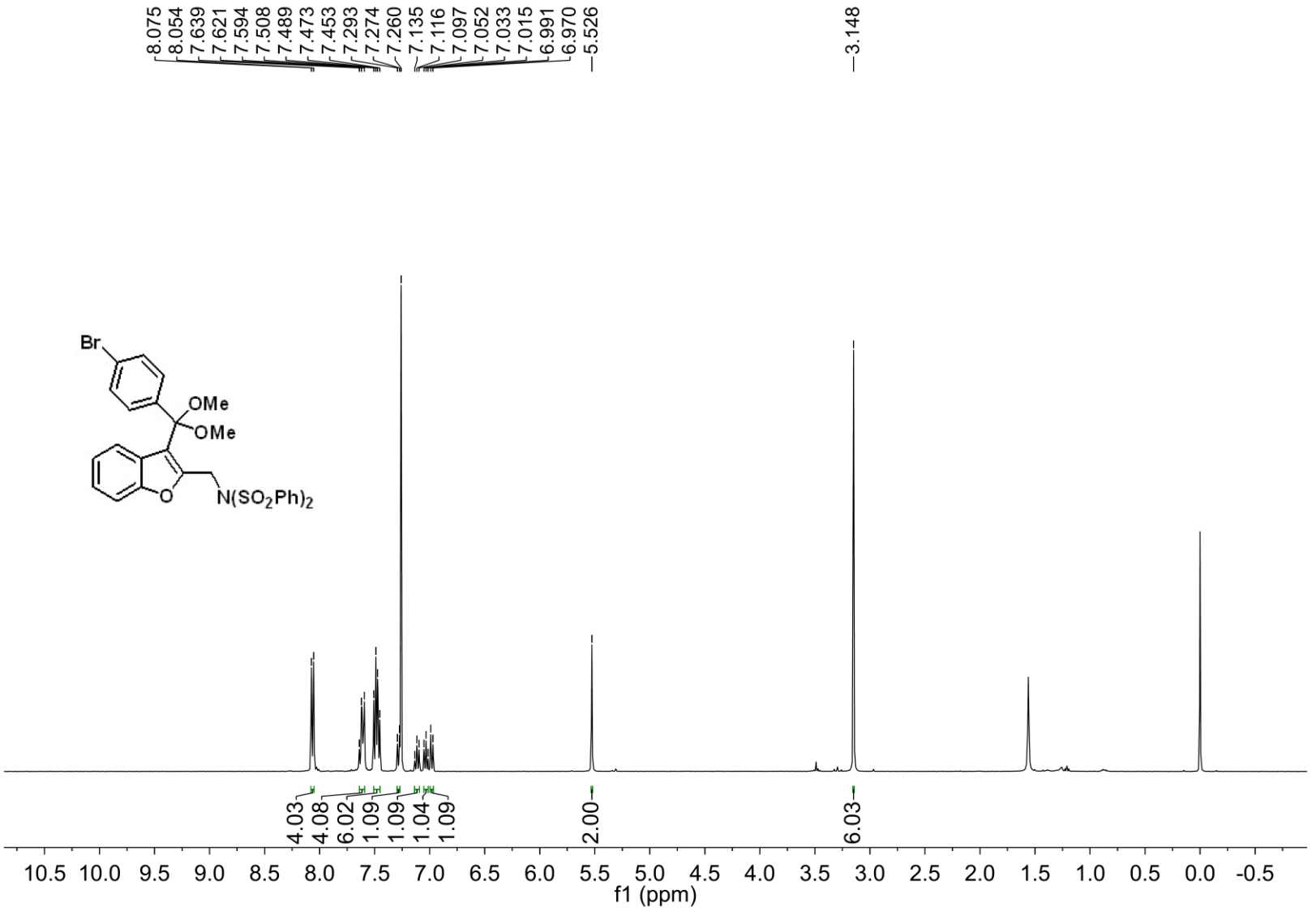
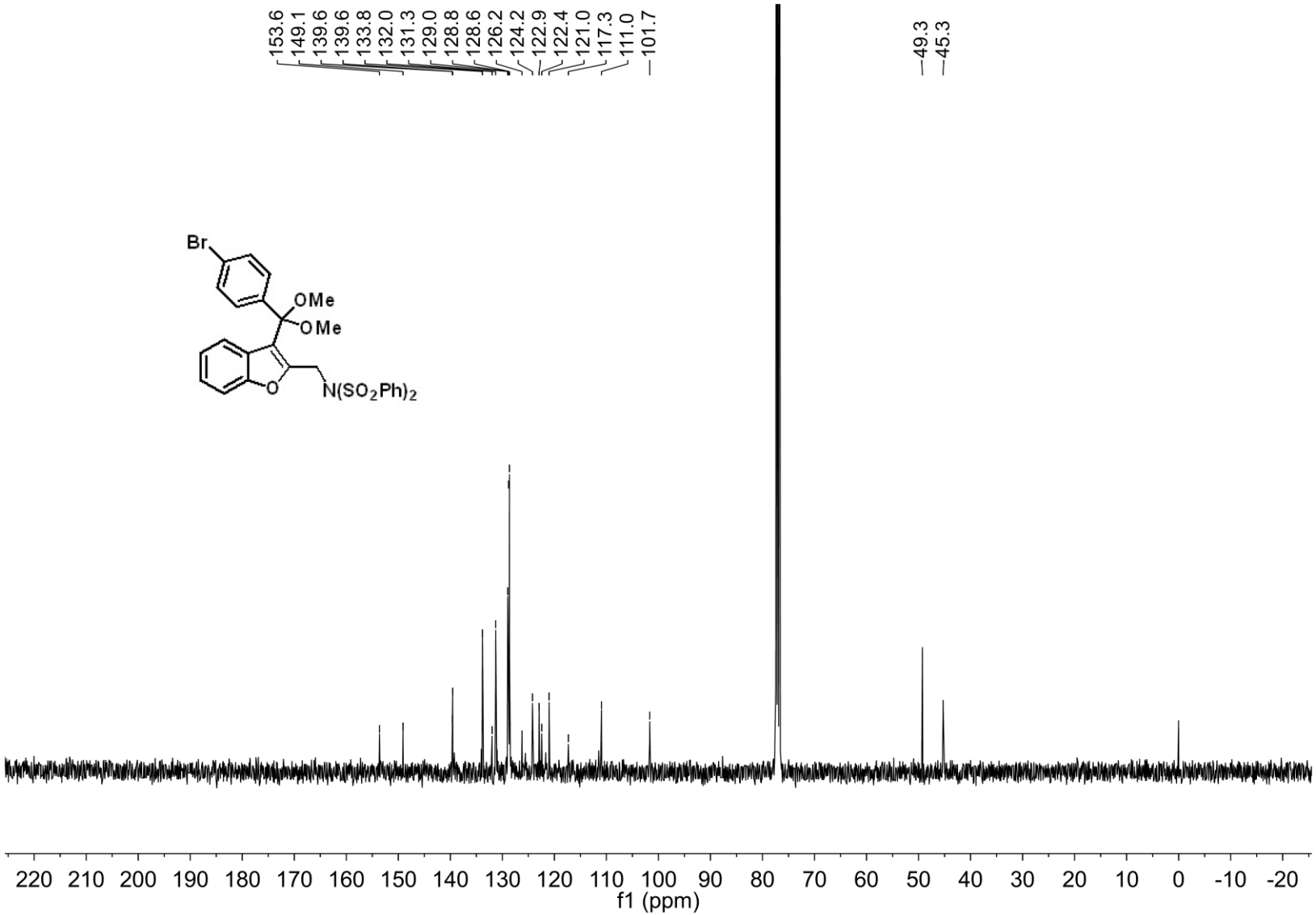


^{13}C spectra of compound 3l:



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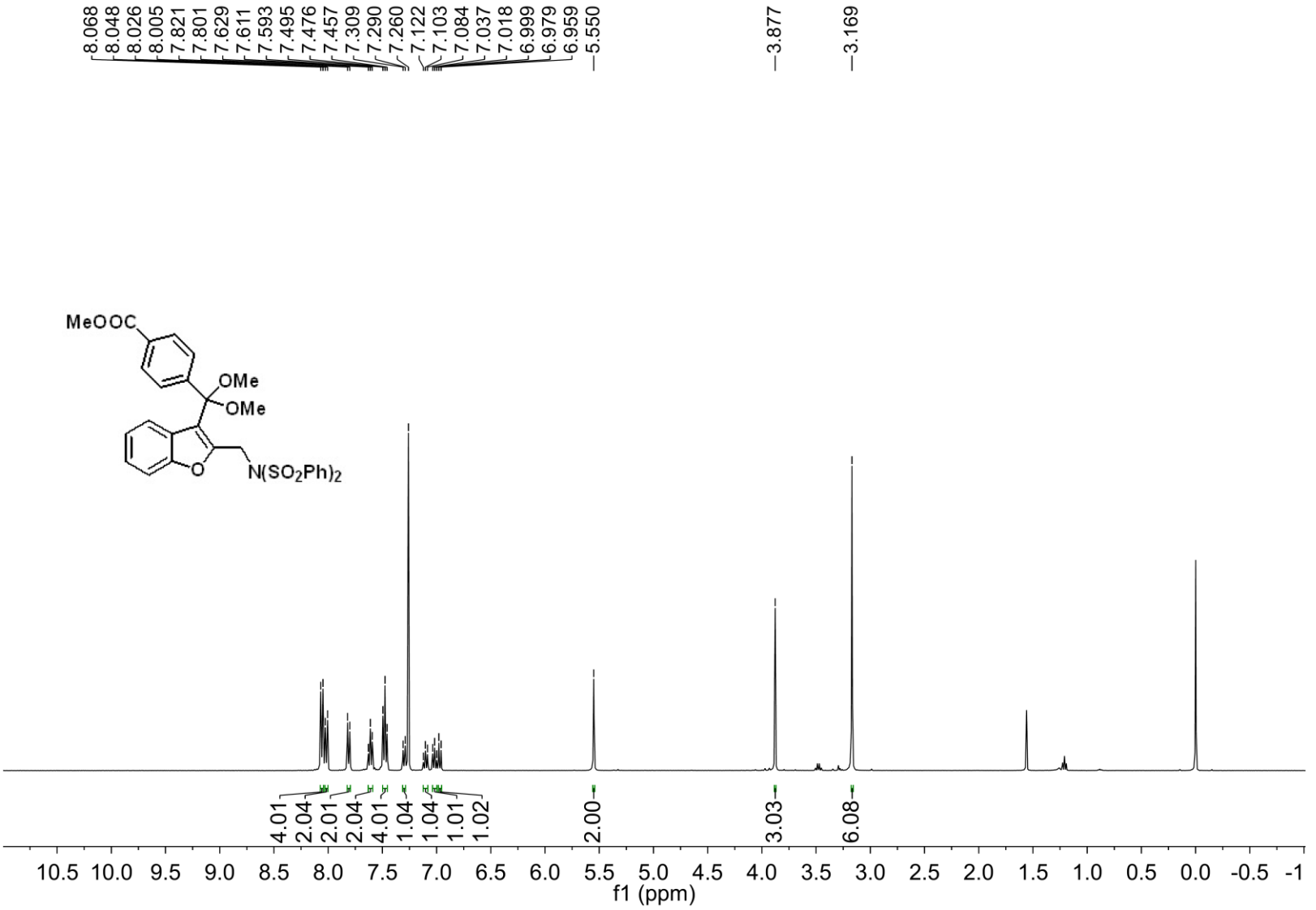

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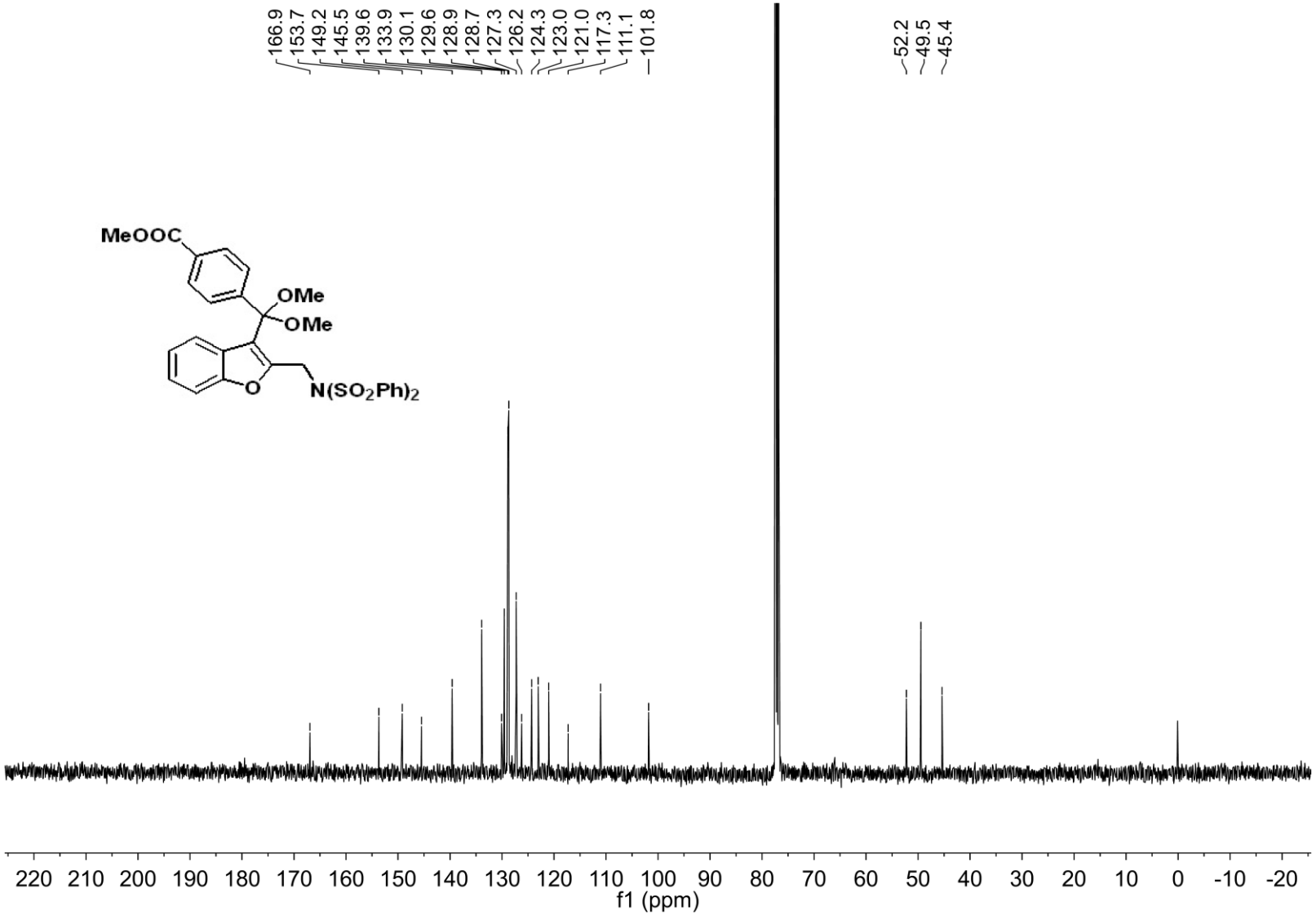

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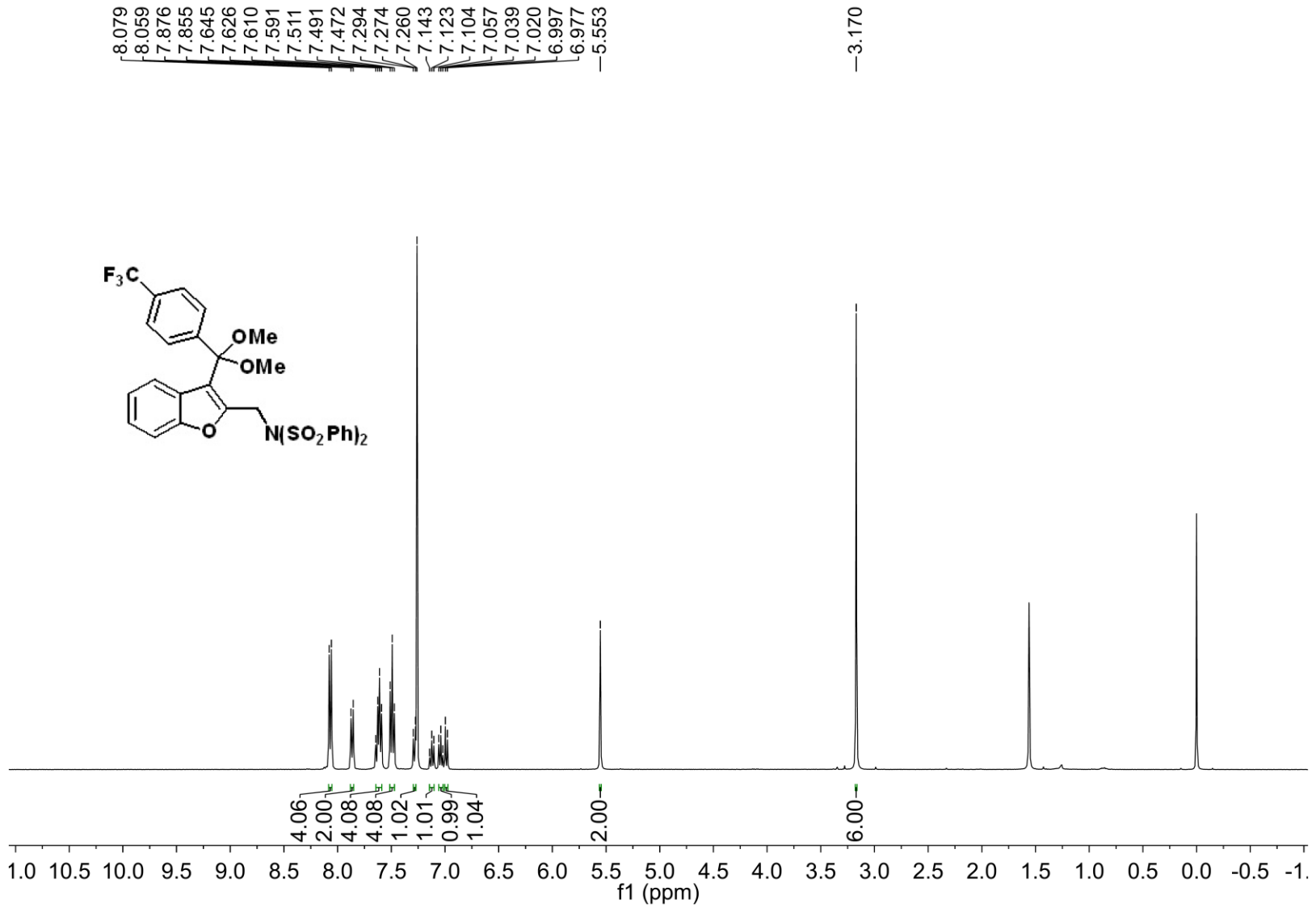

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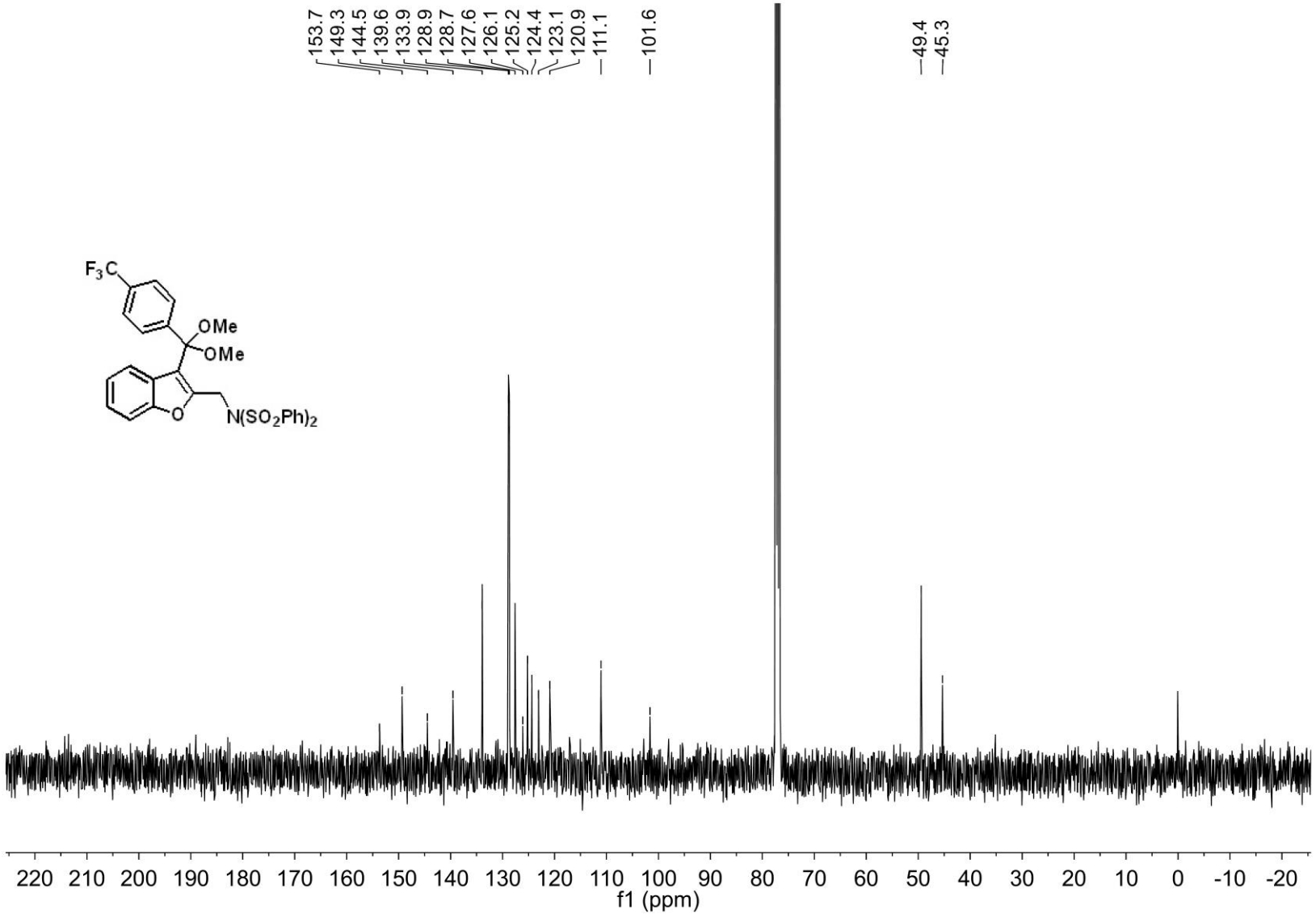

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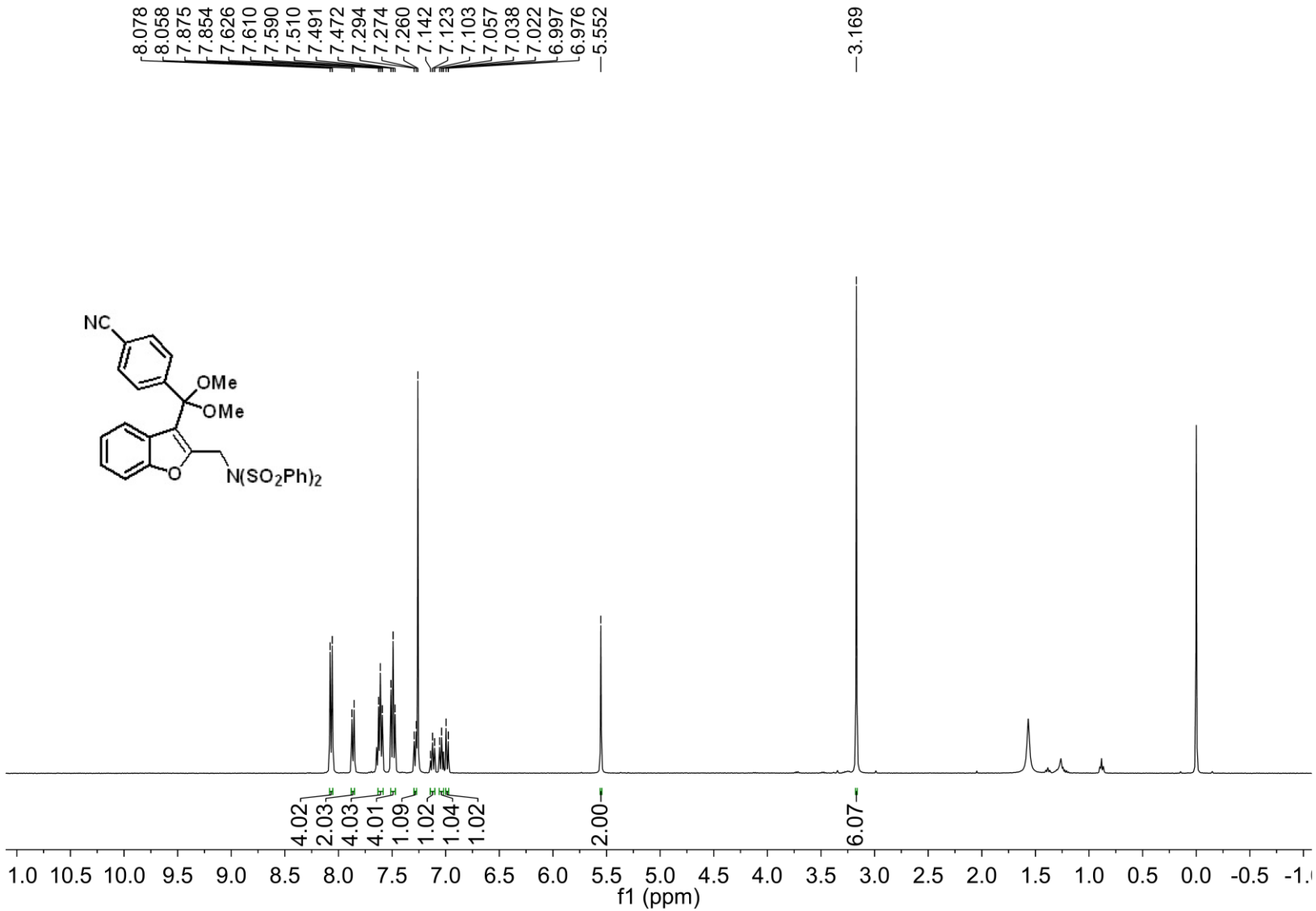

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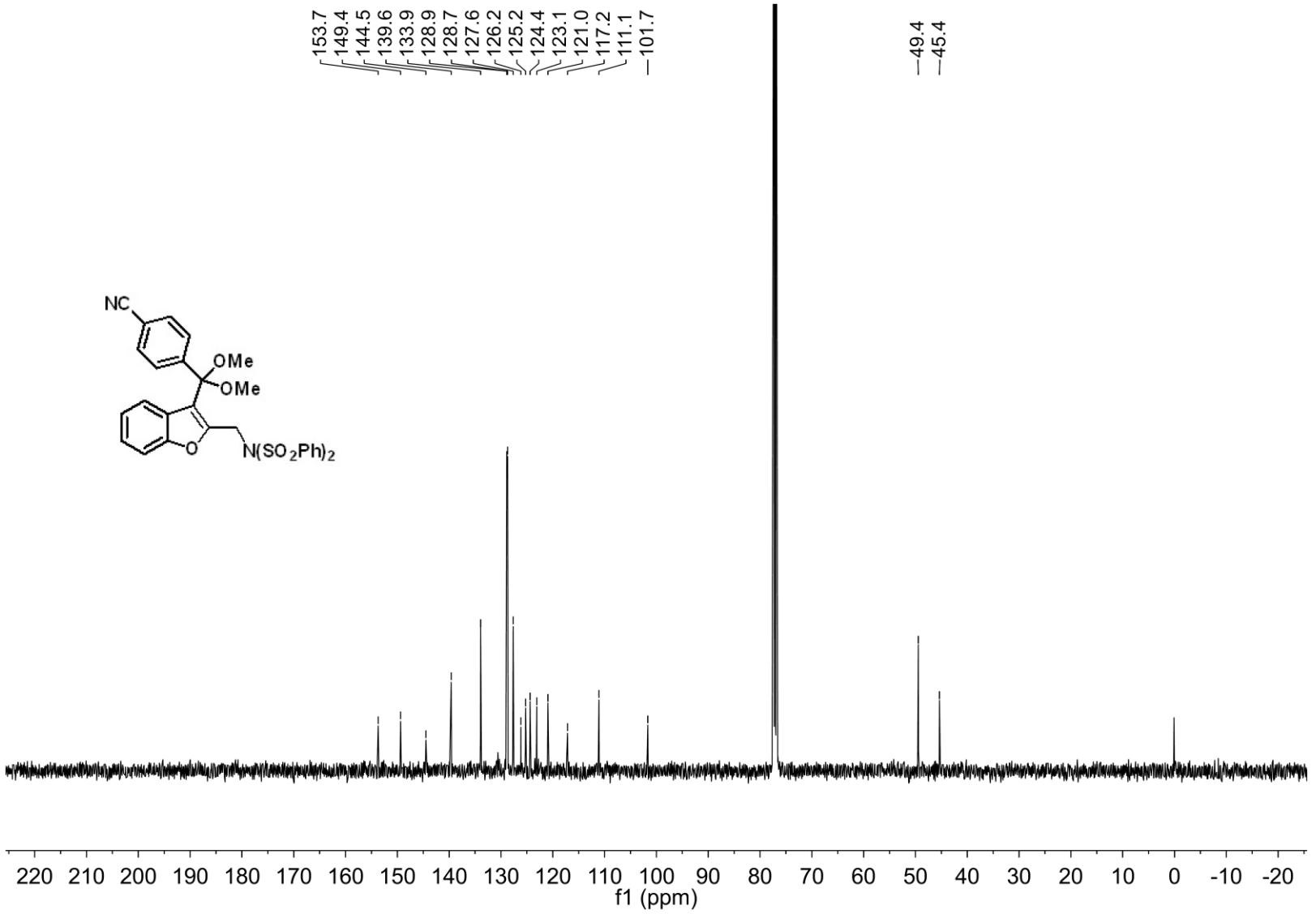

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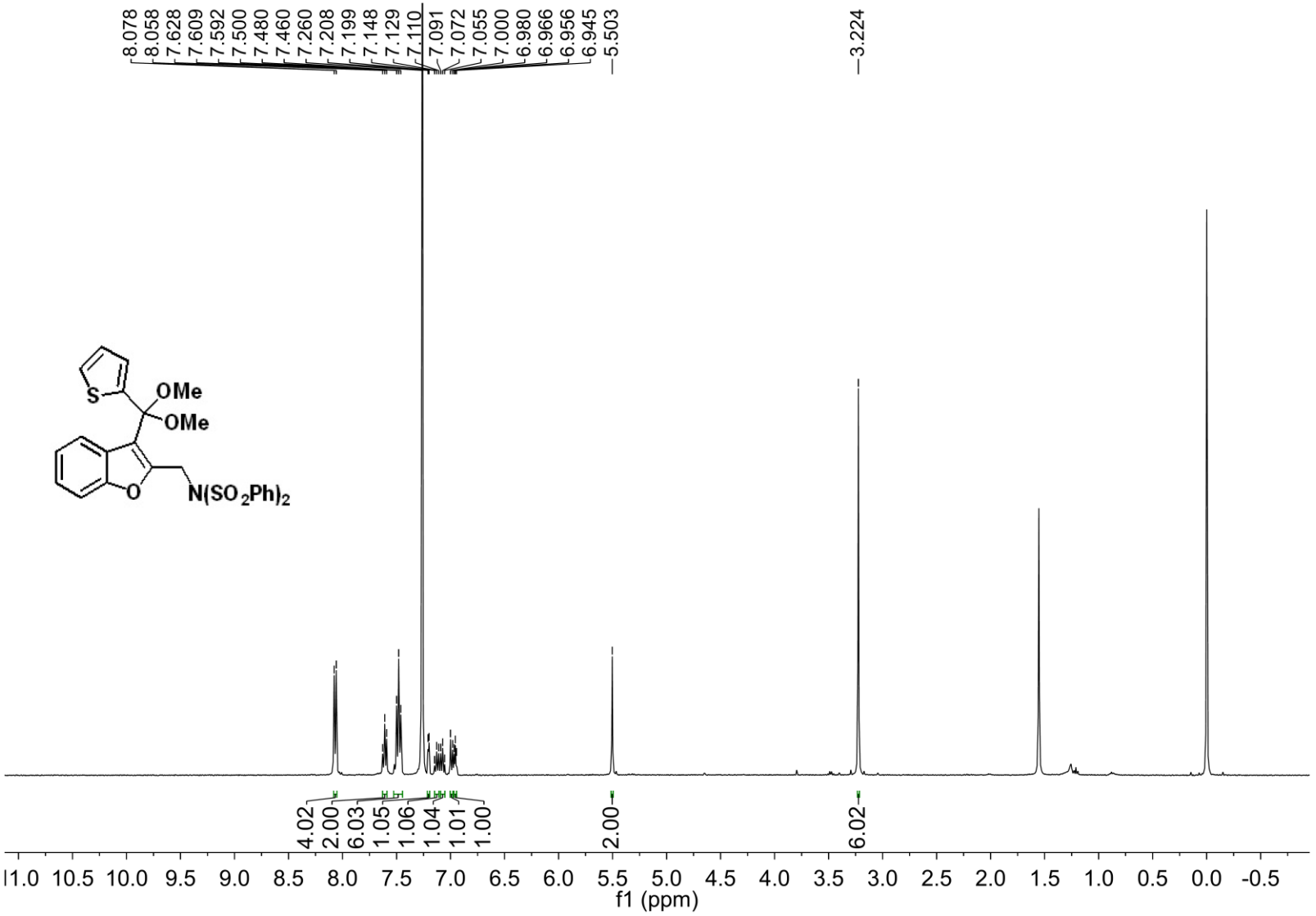

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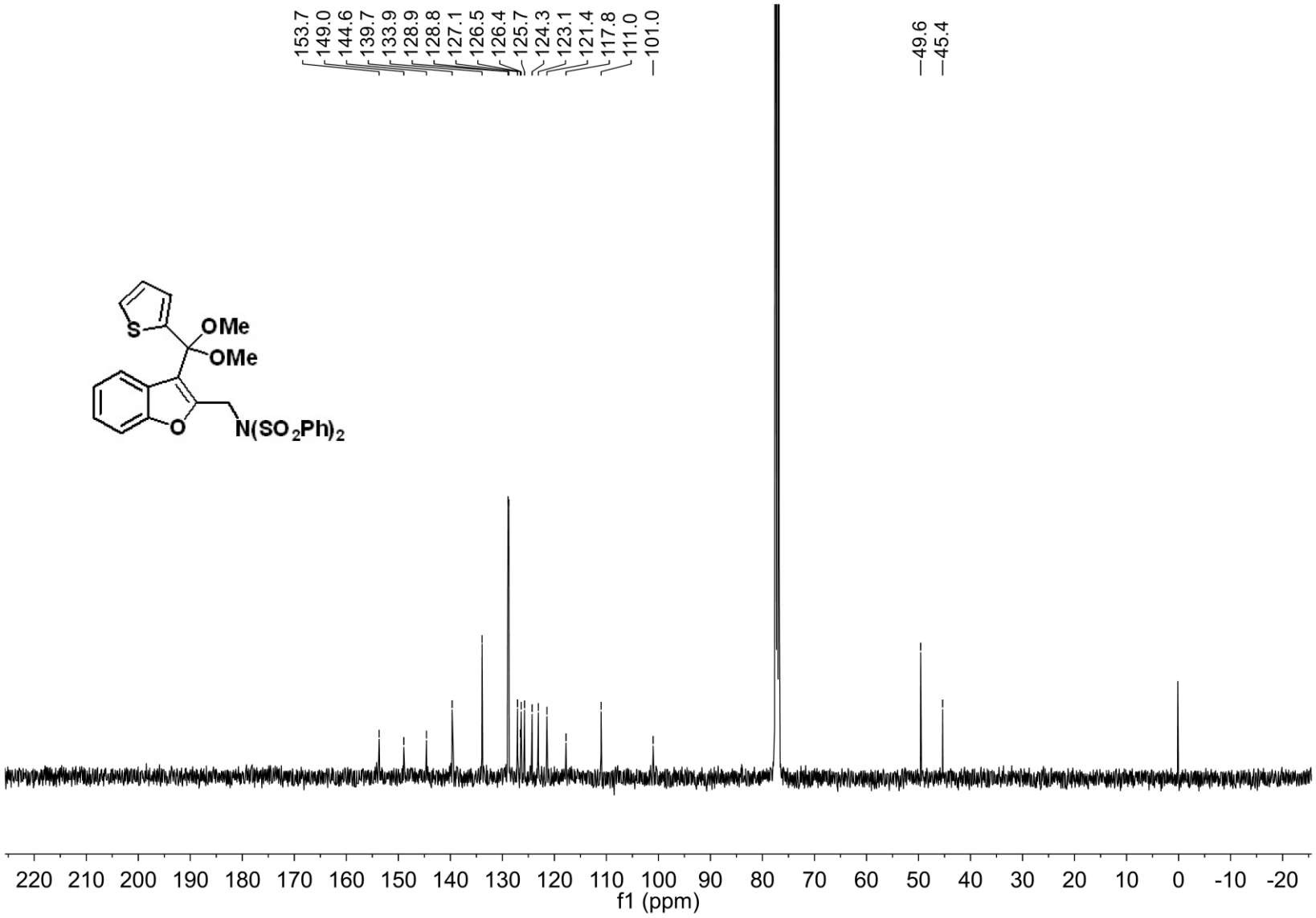

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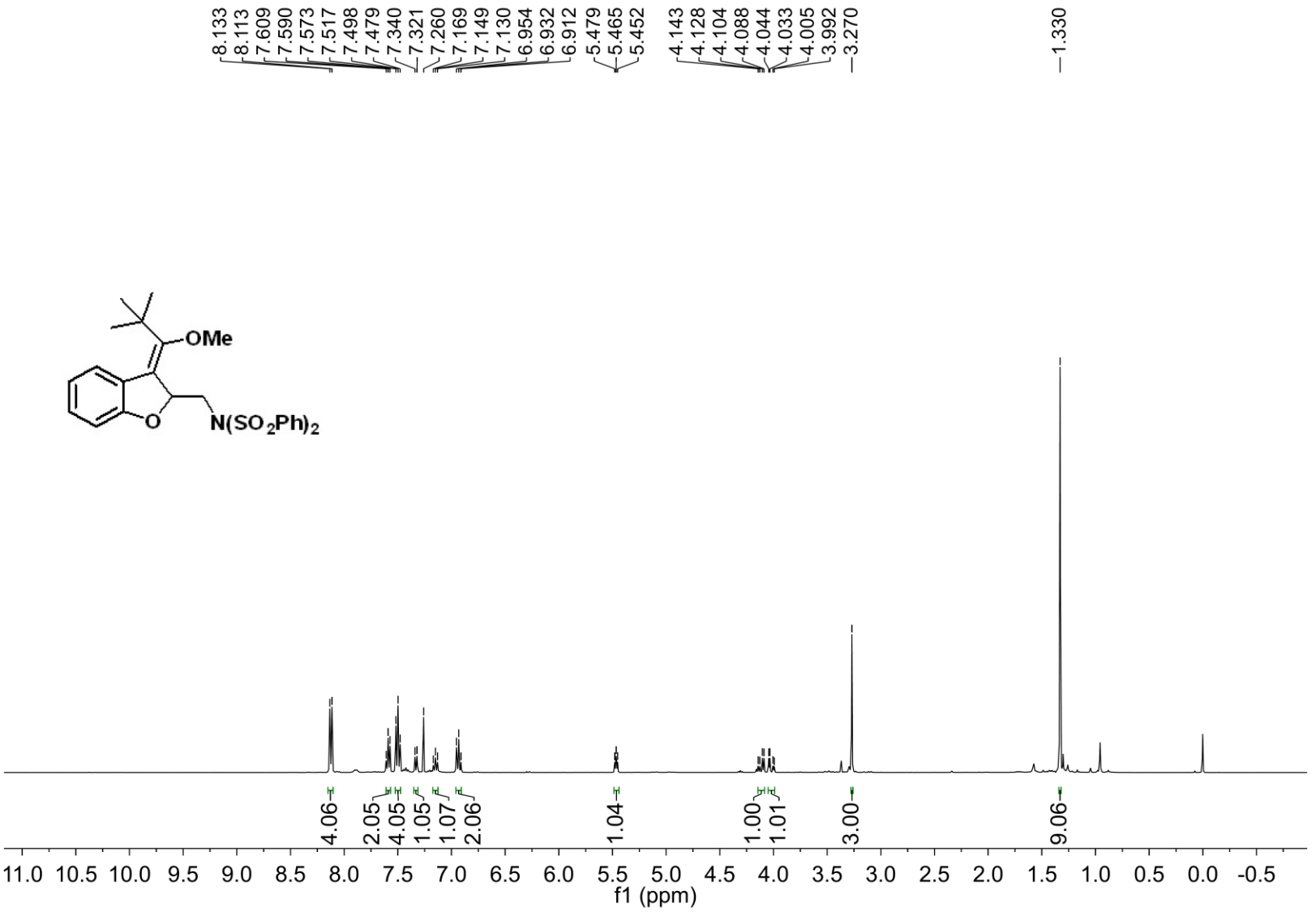

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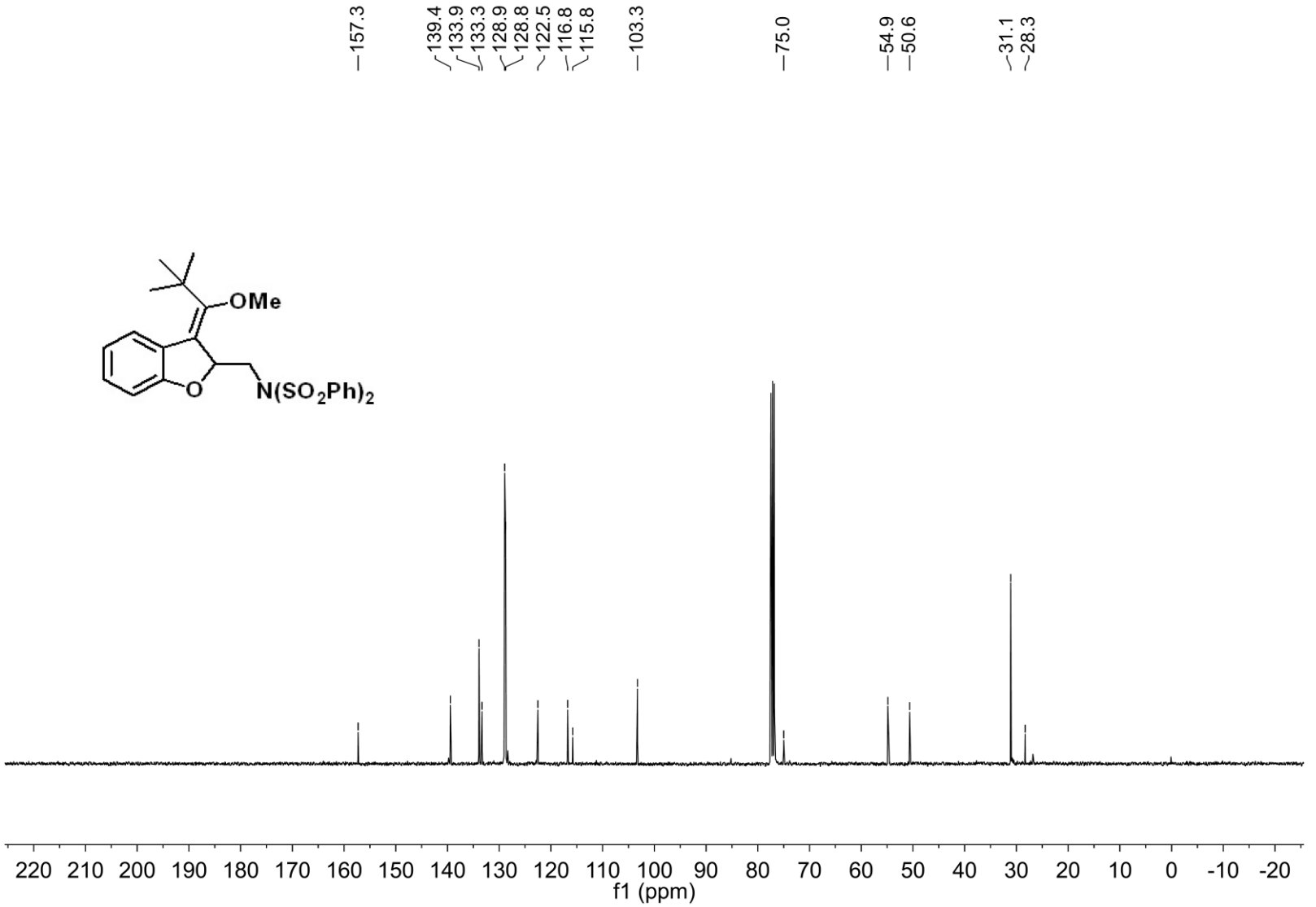

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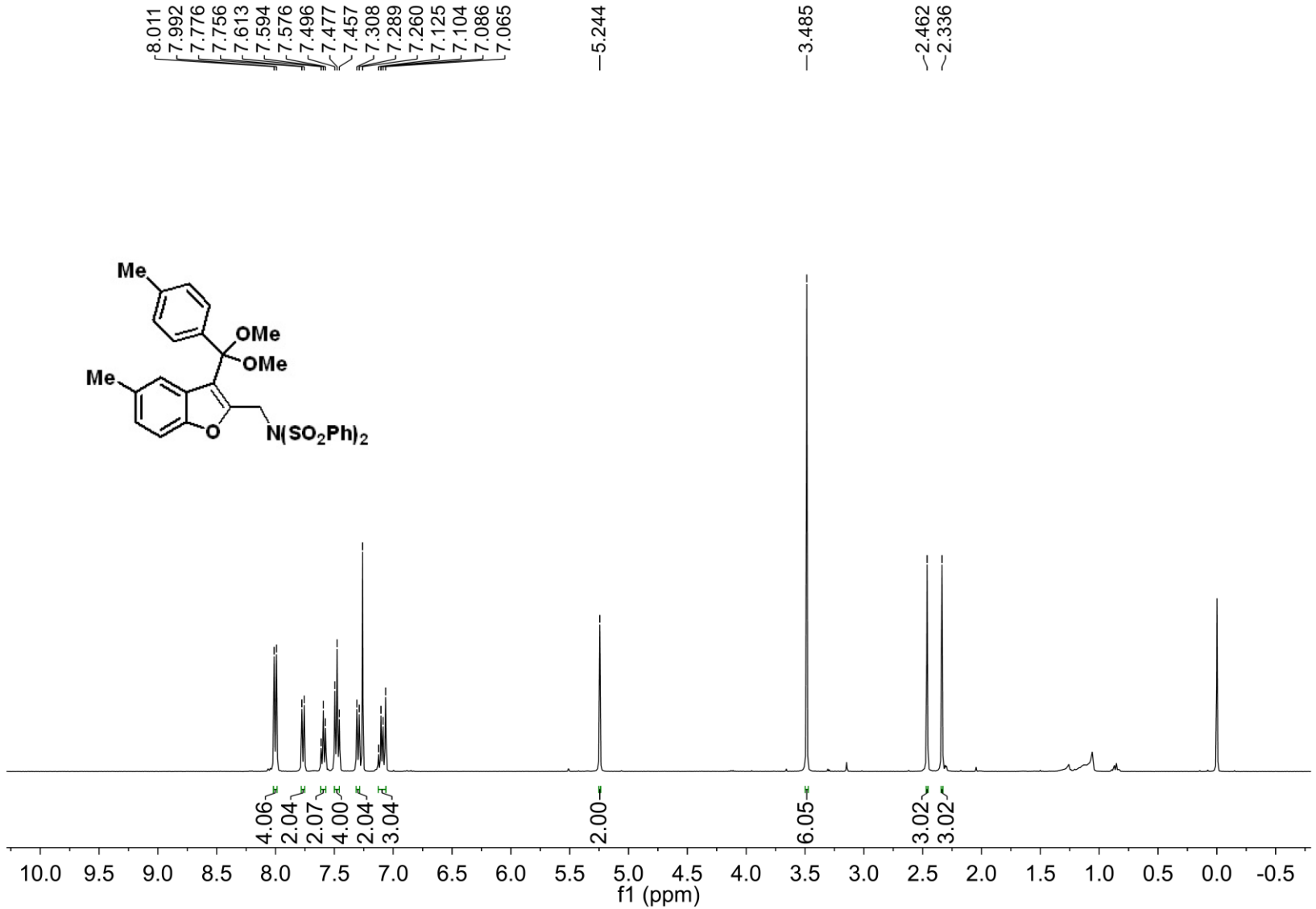

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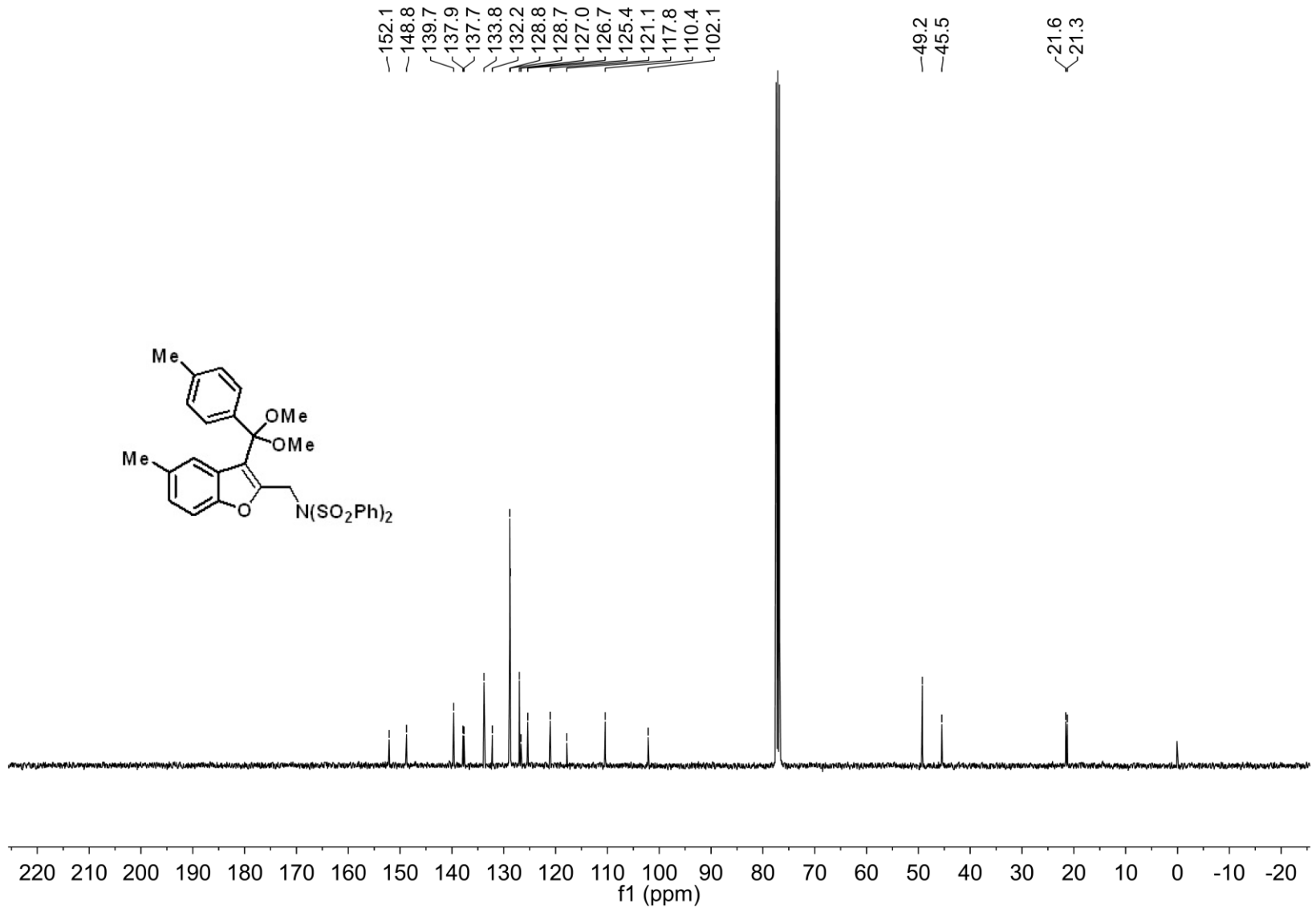

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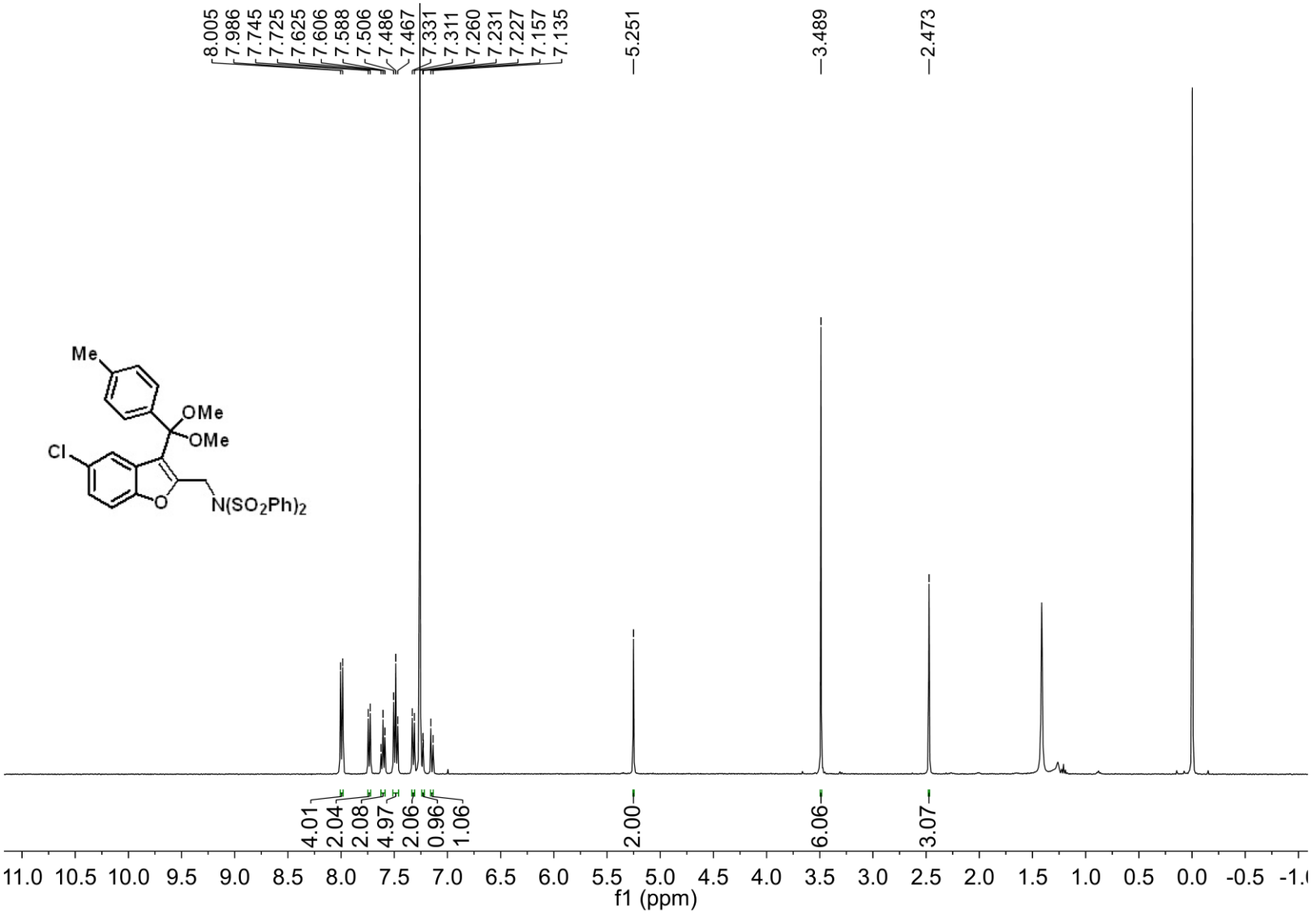

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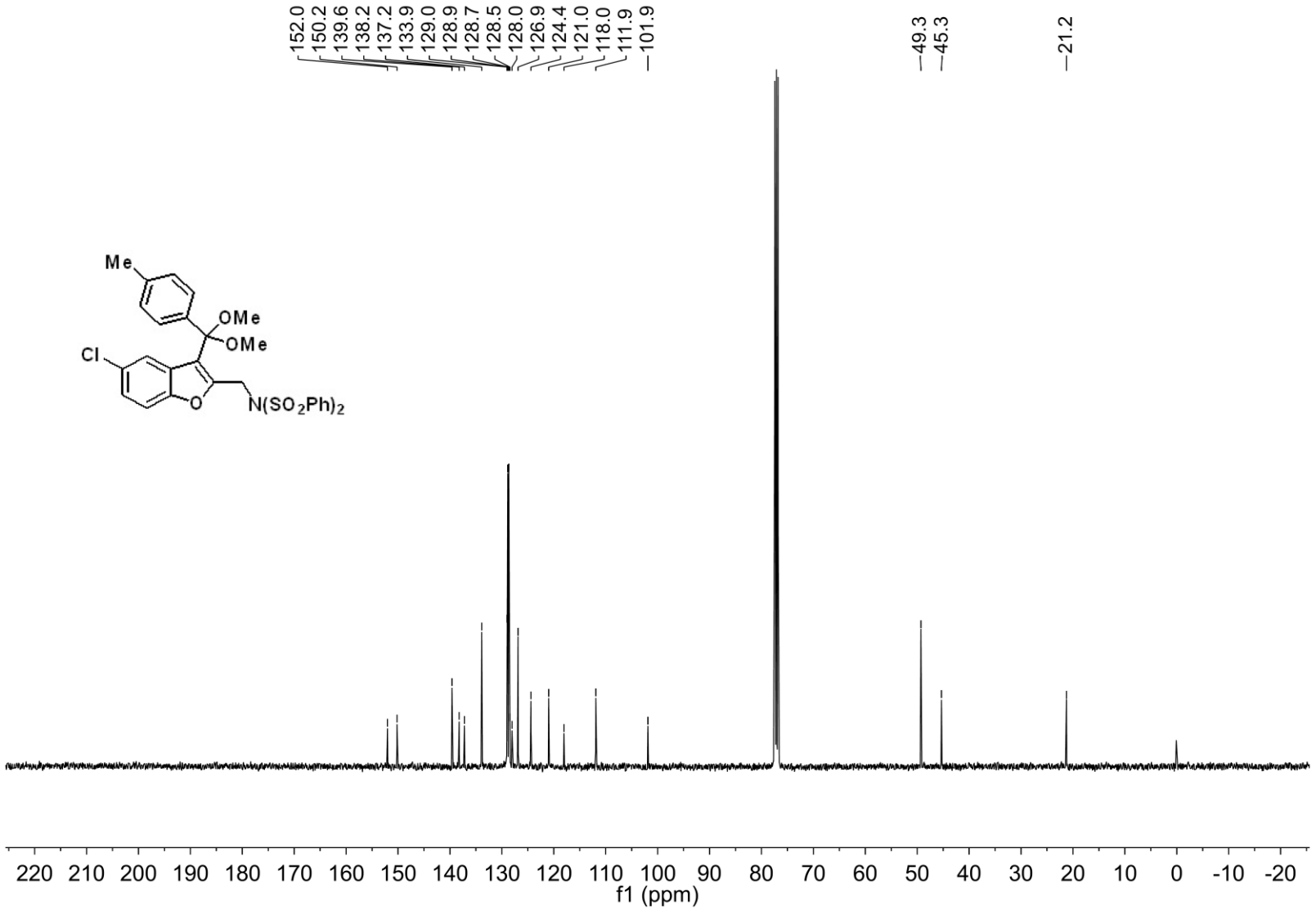

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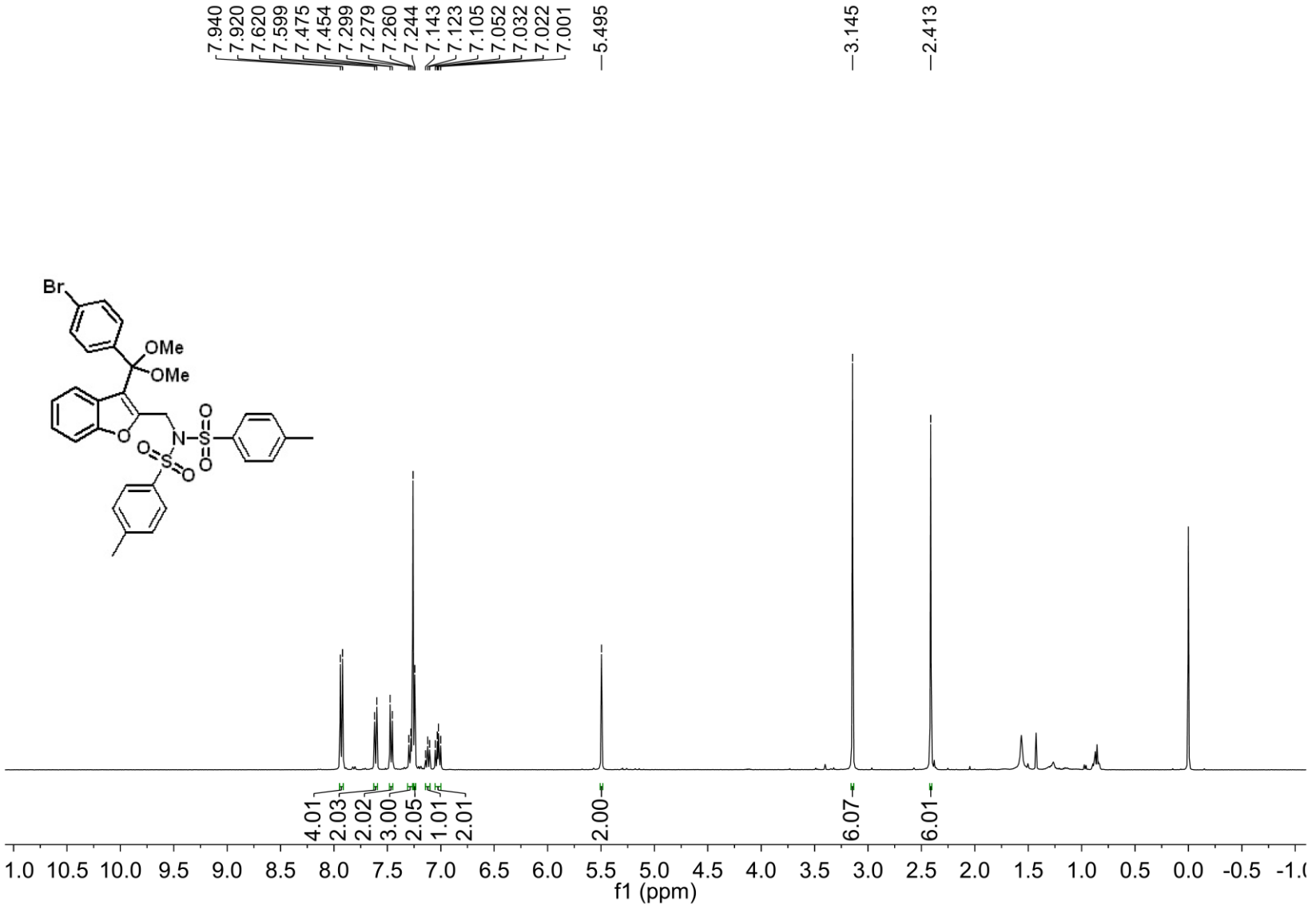

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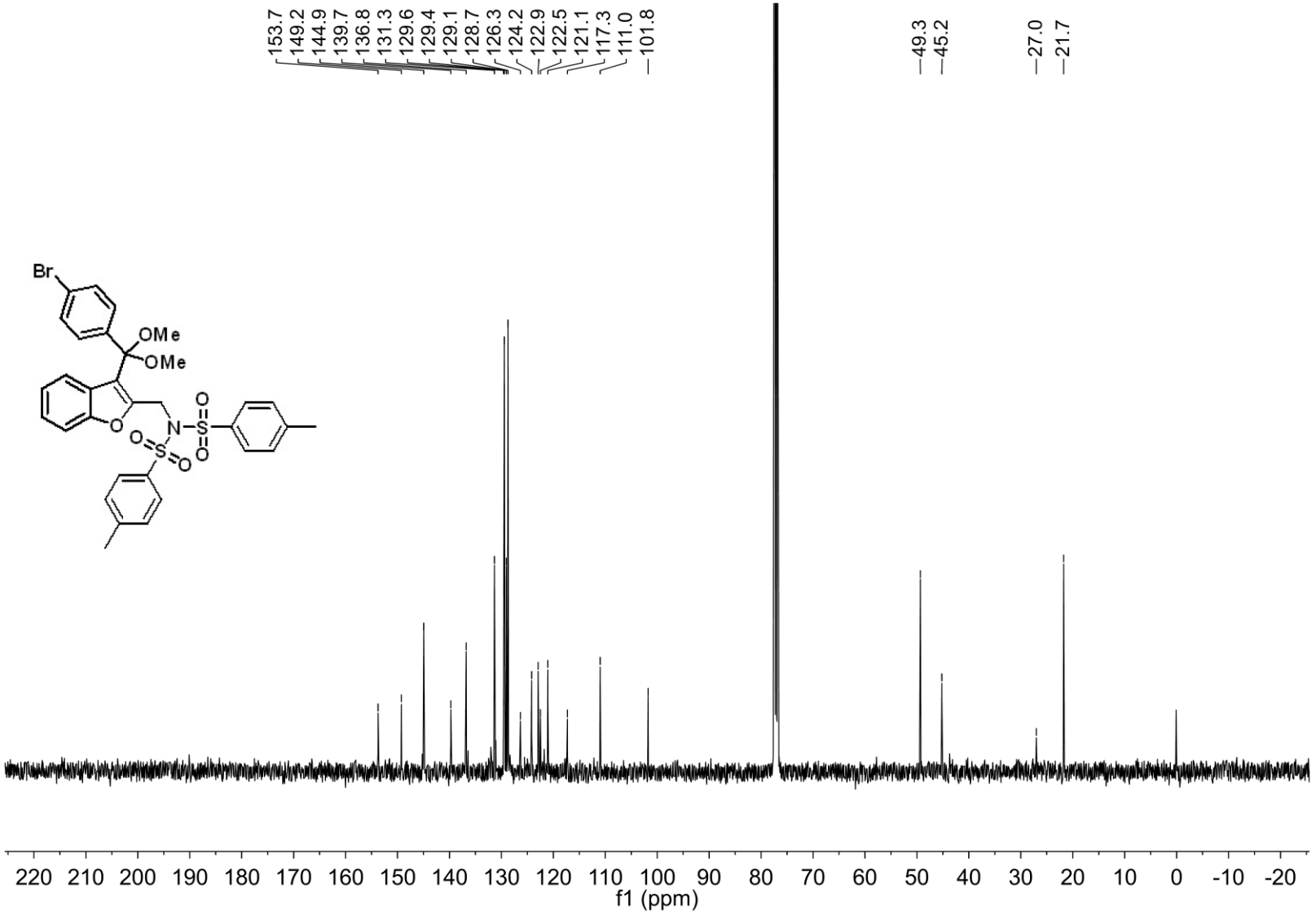

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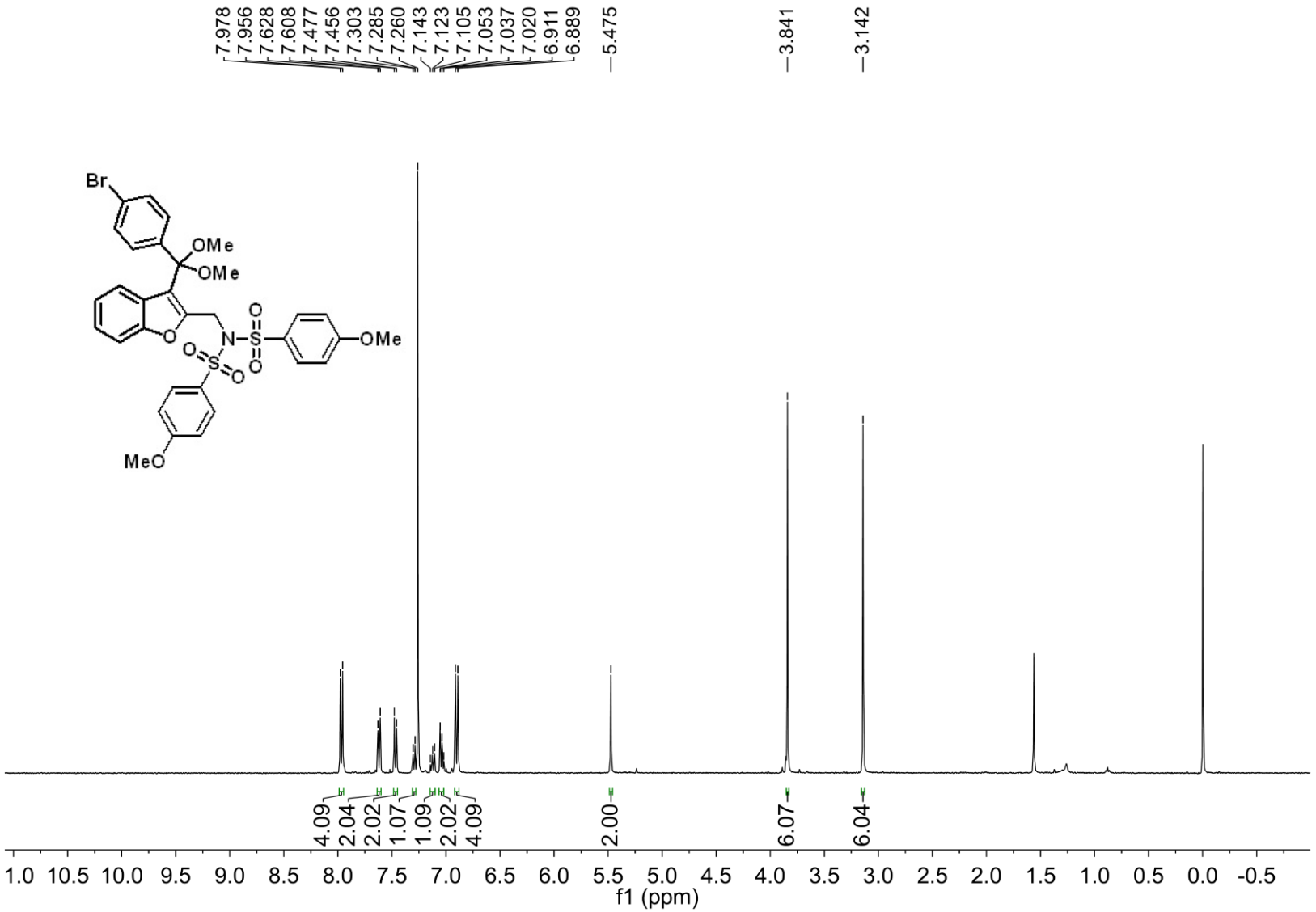

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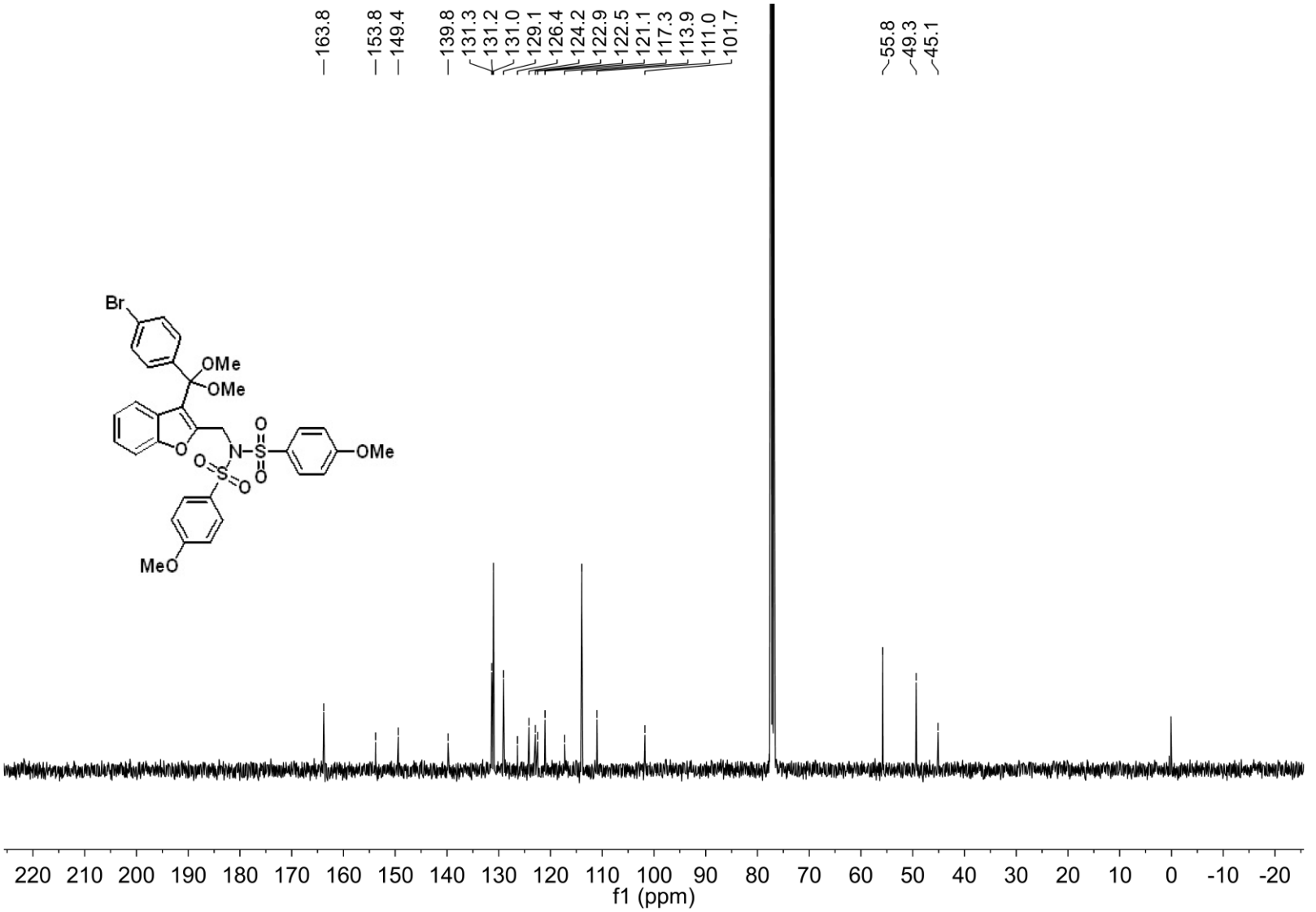

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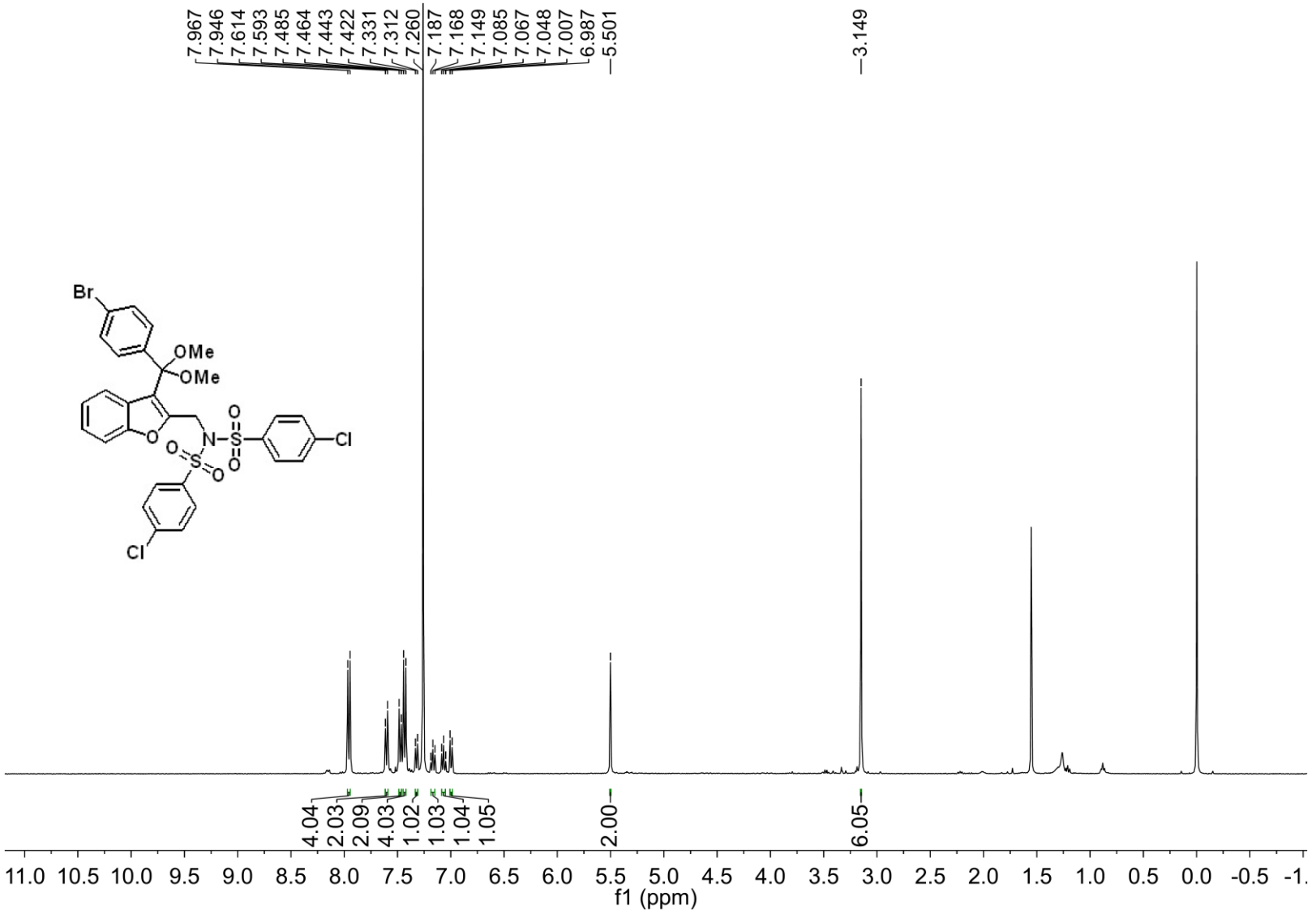

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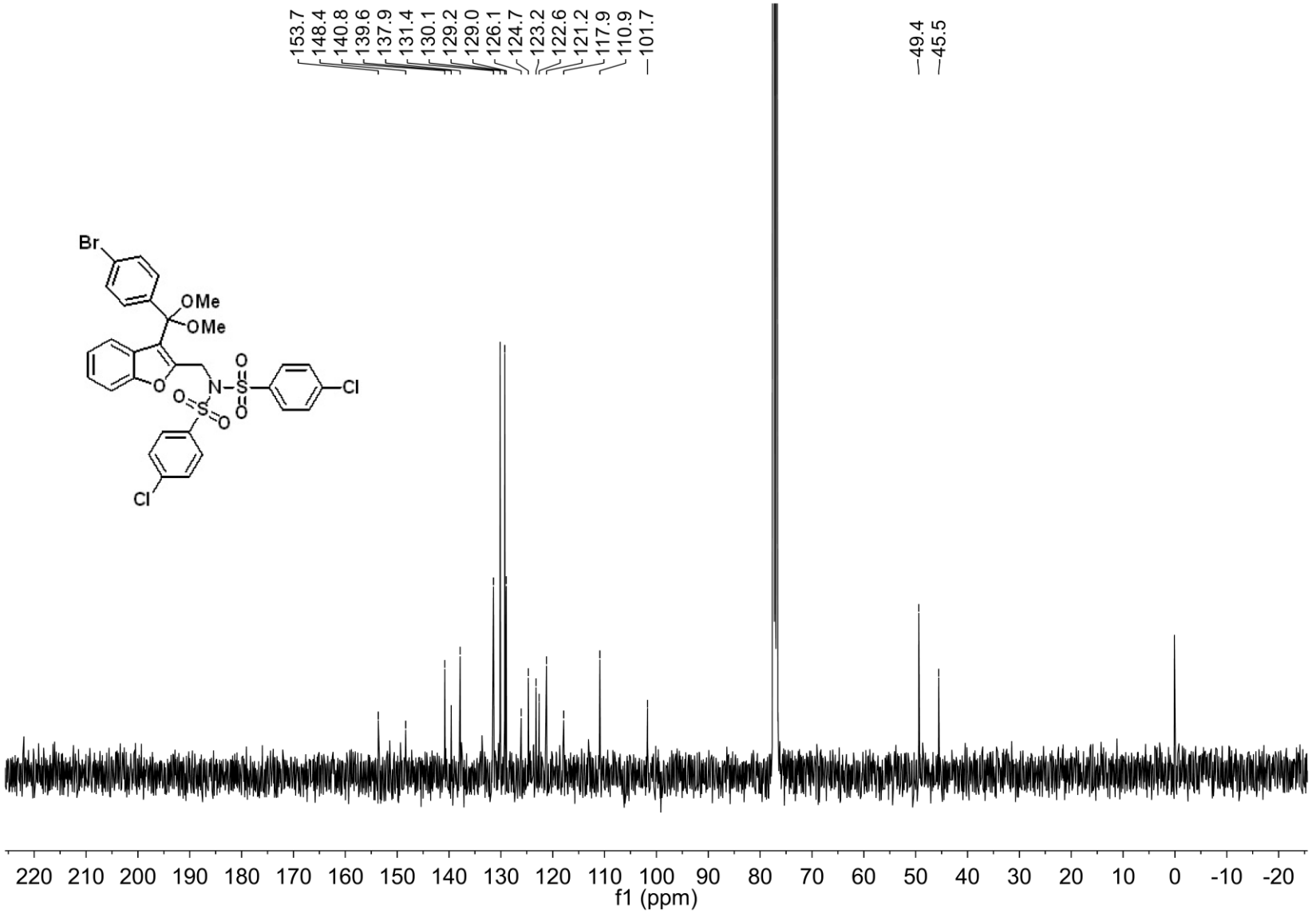

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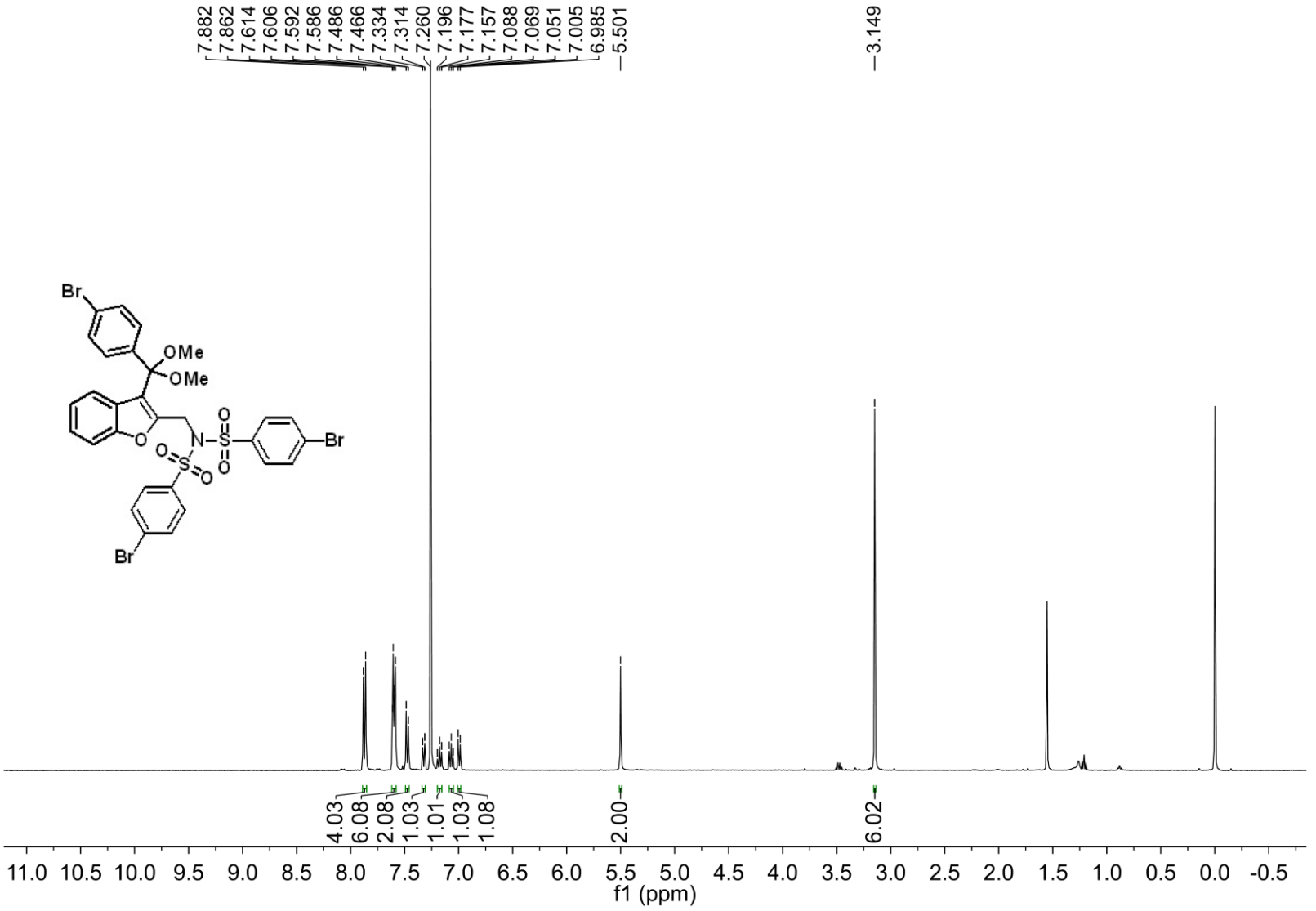

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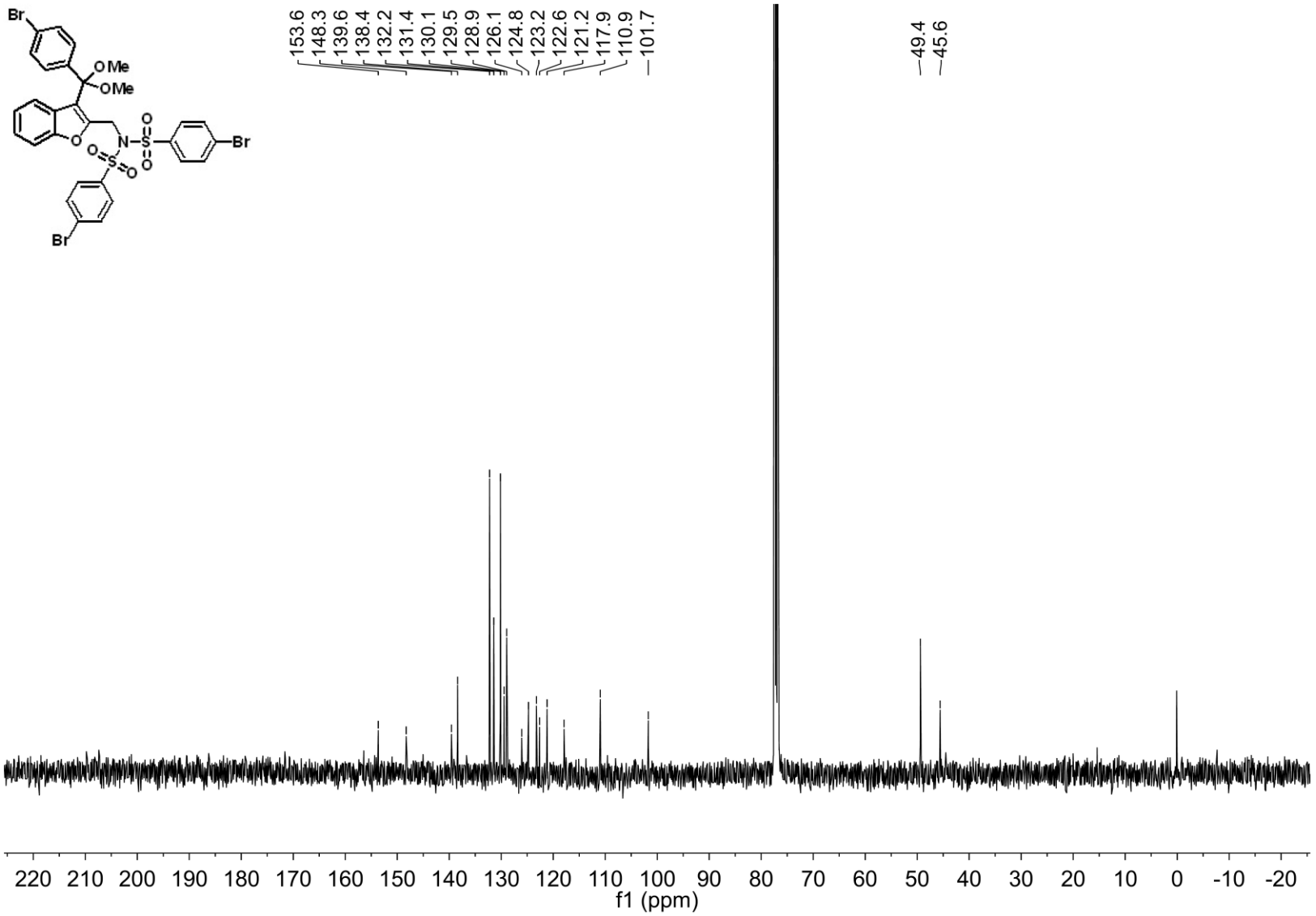

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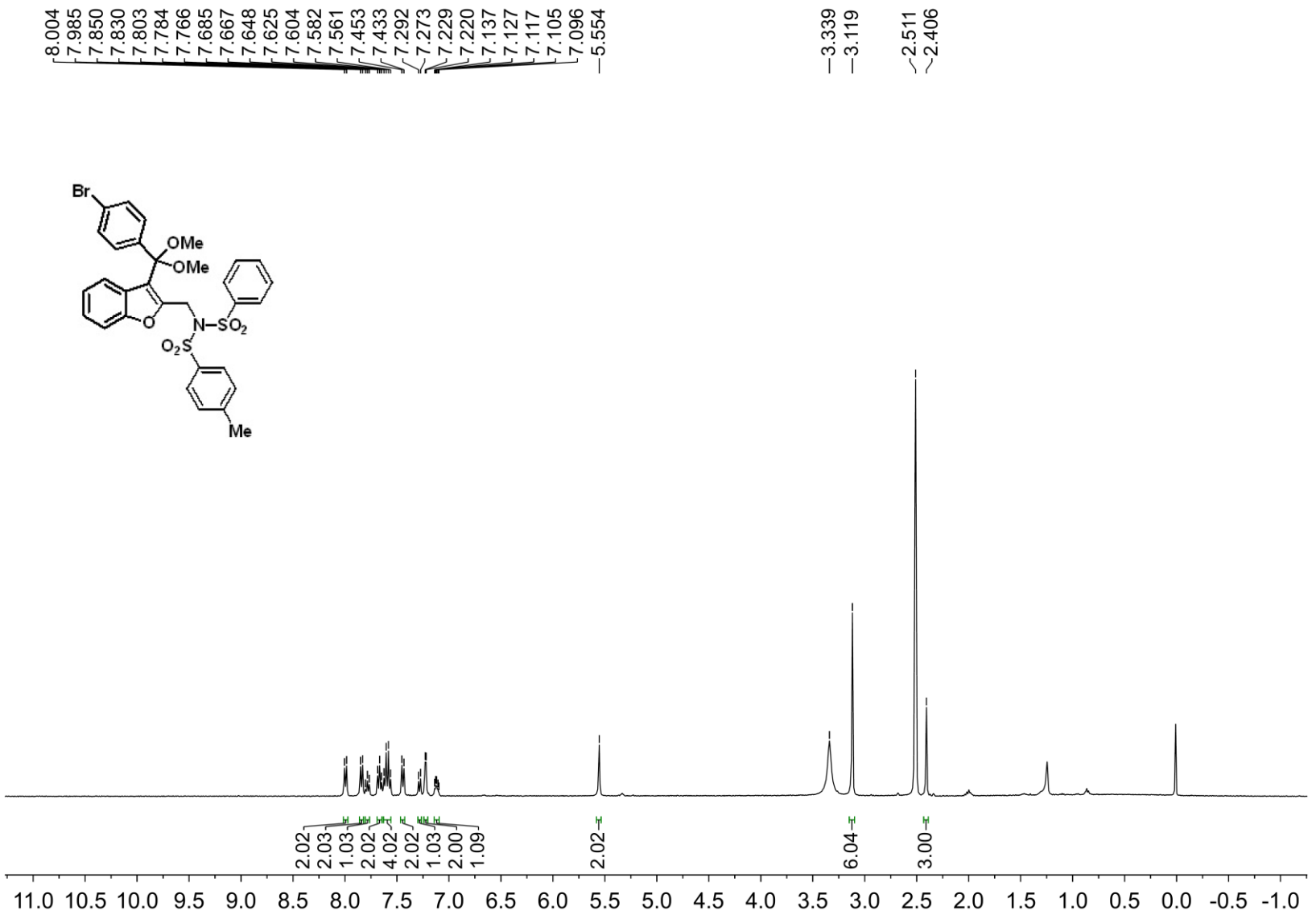

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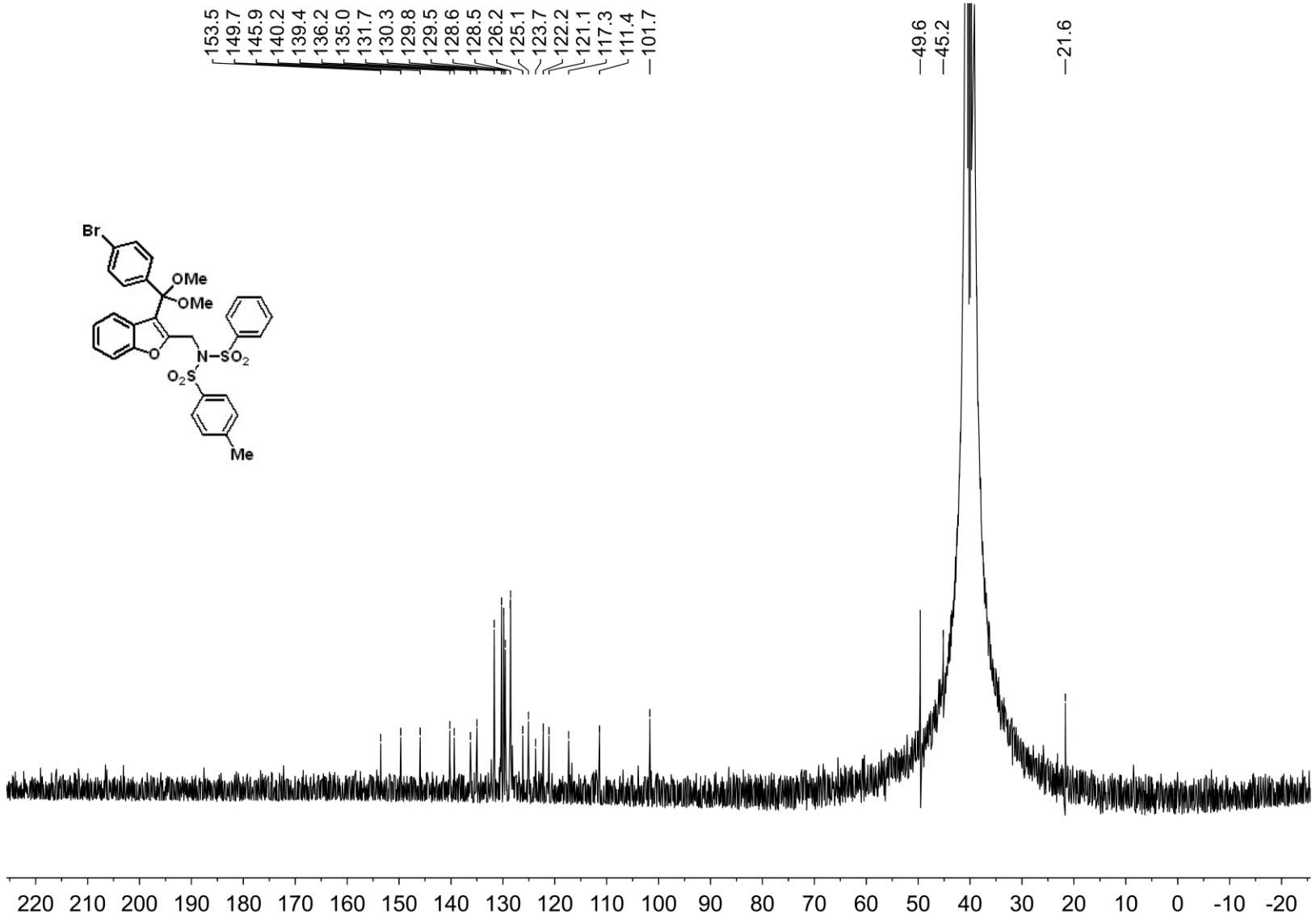

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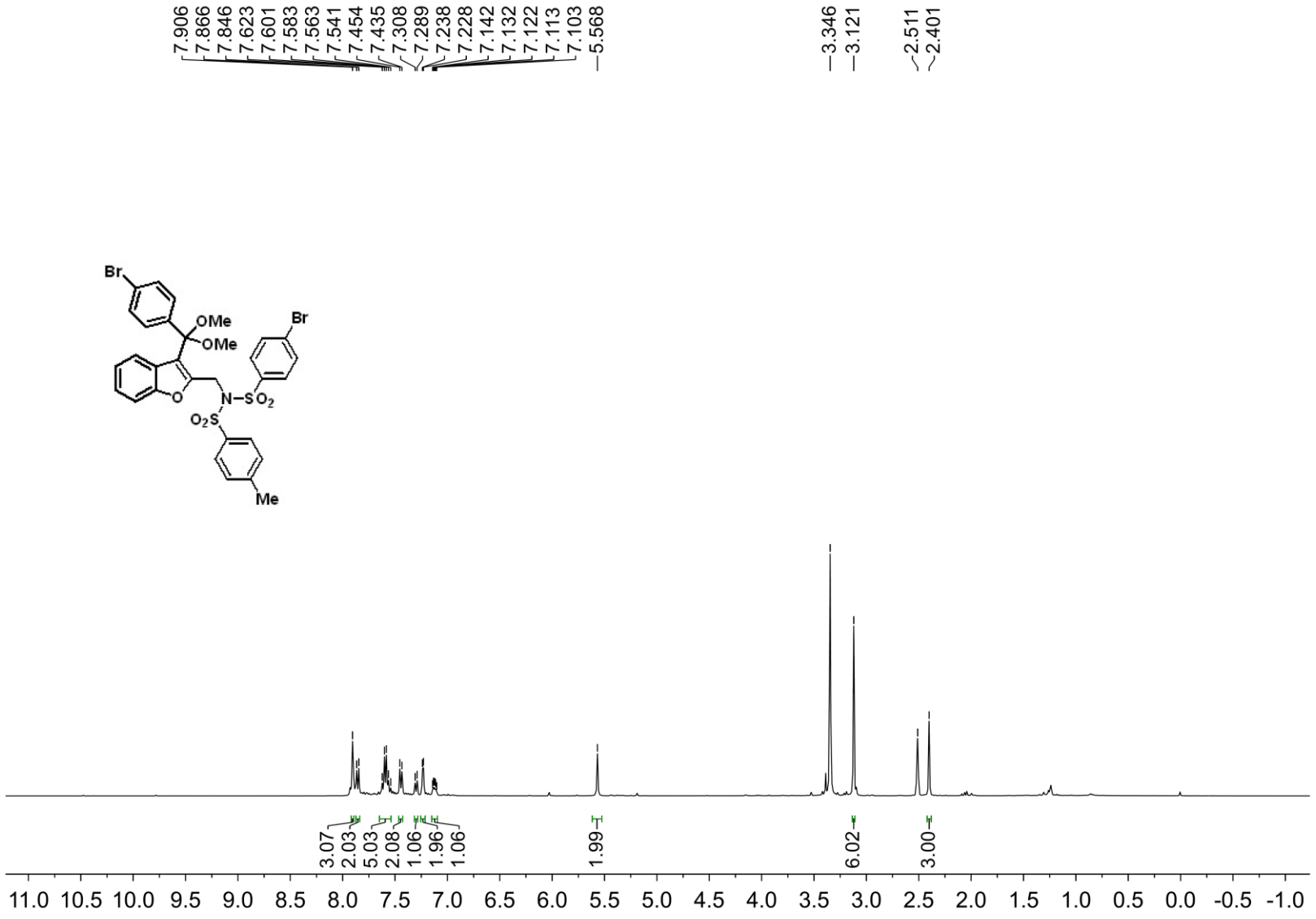

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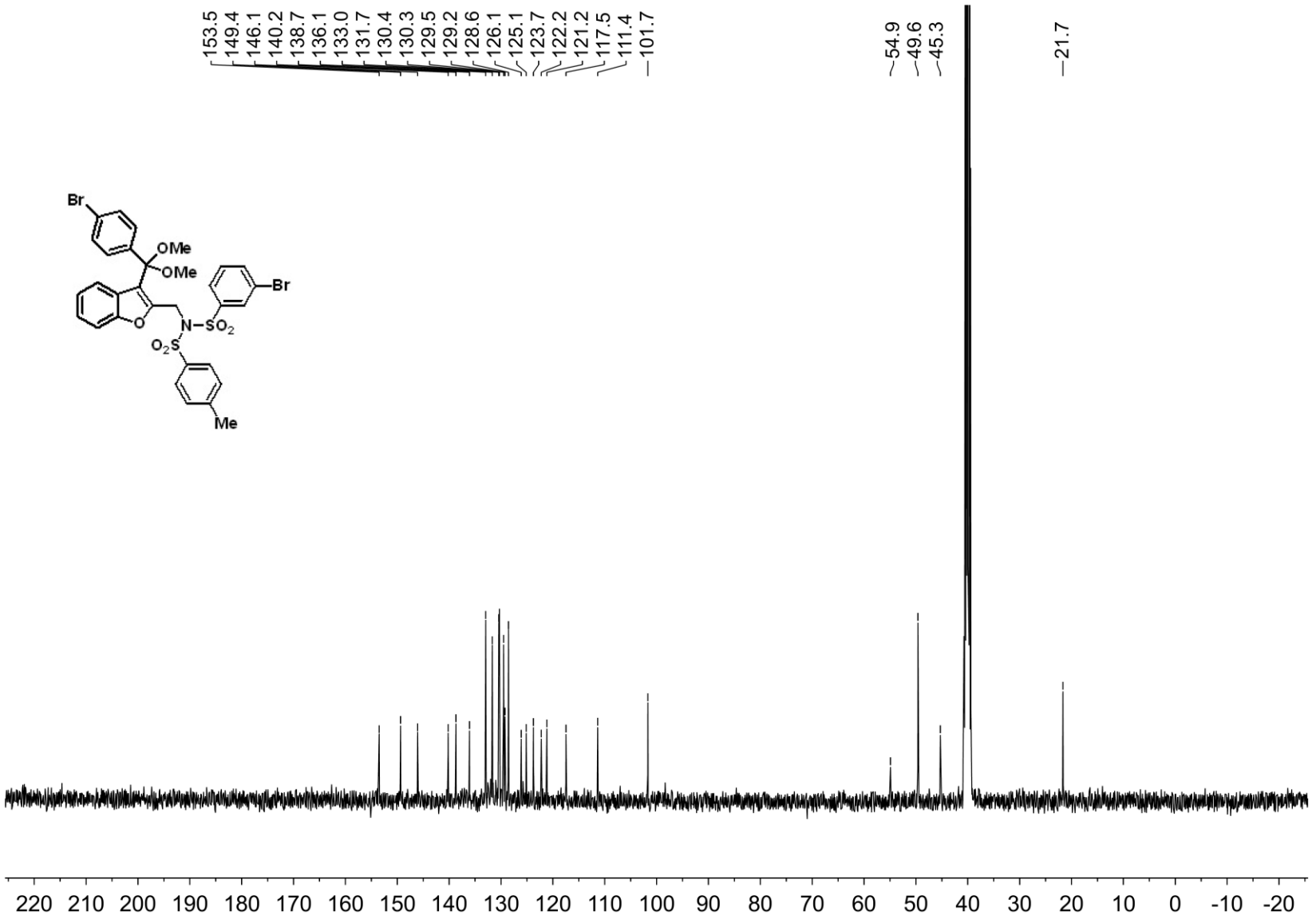

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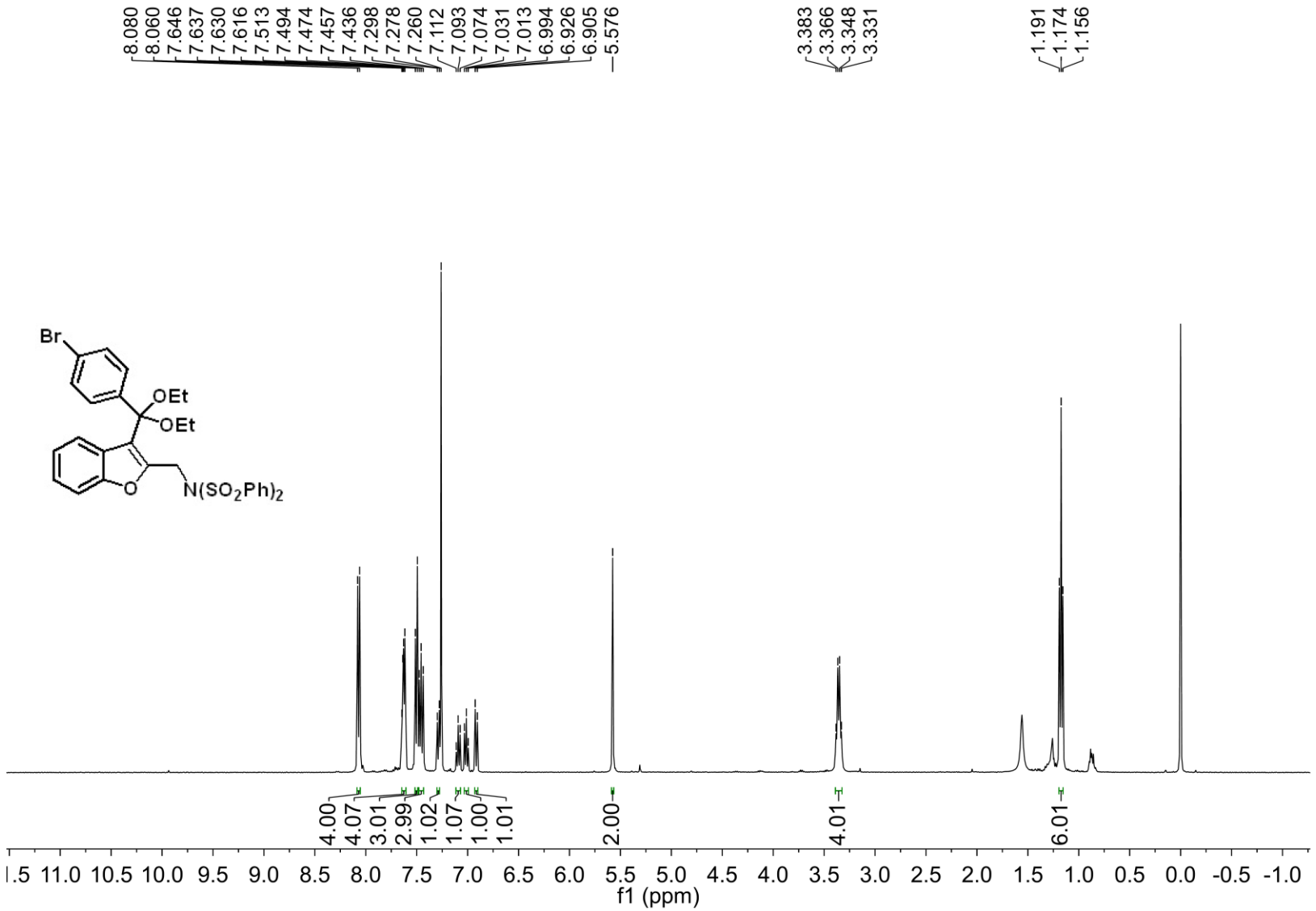

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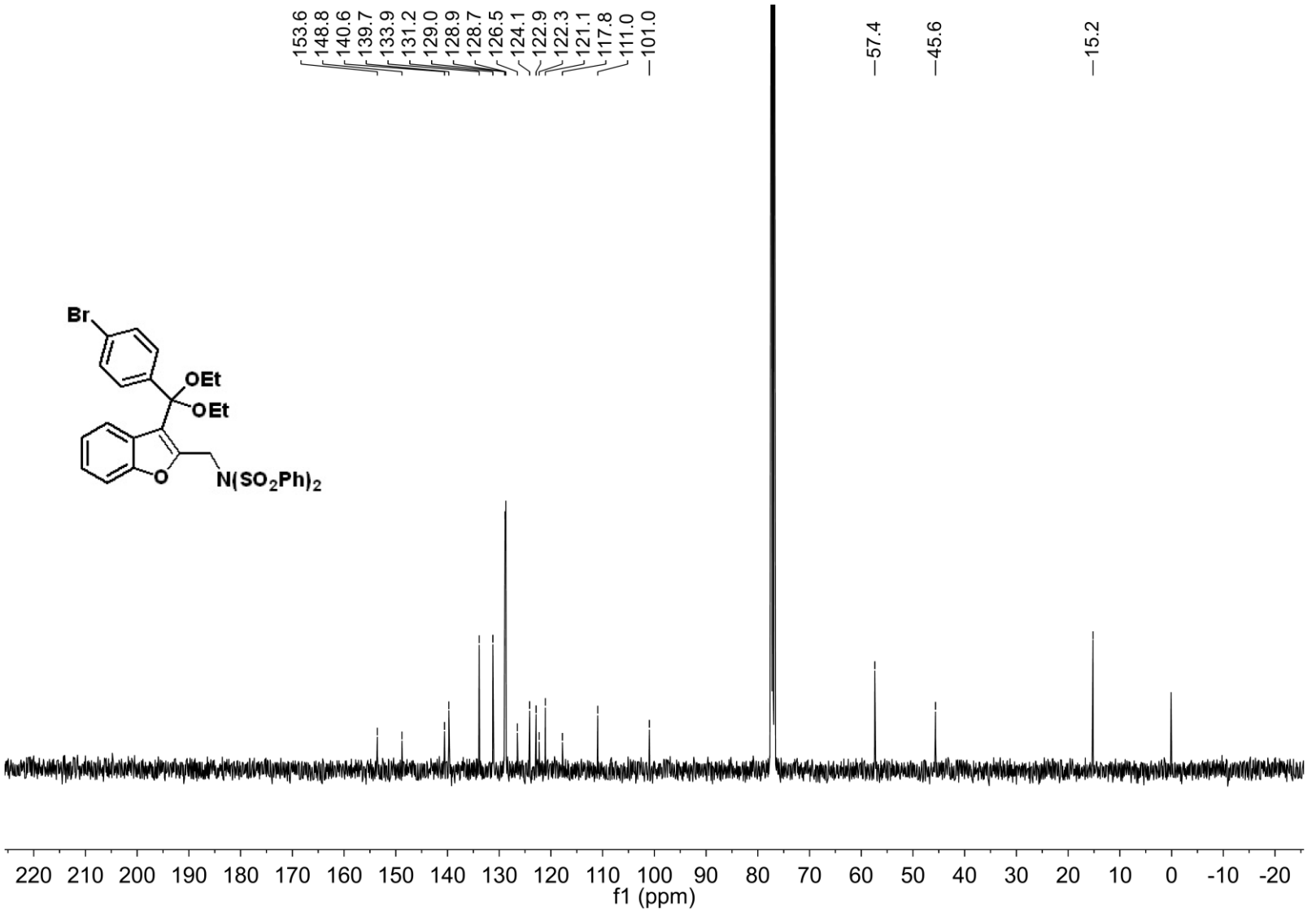
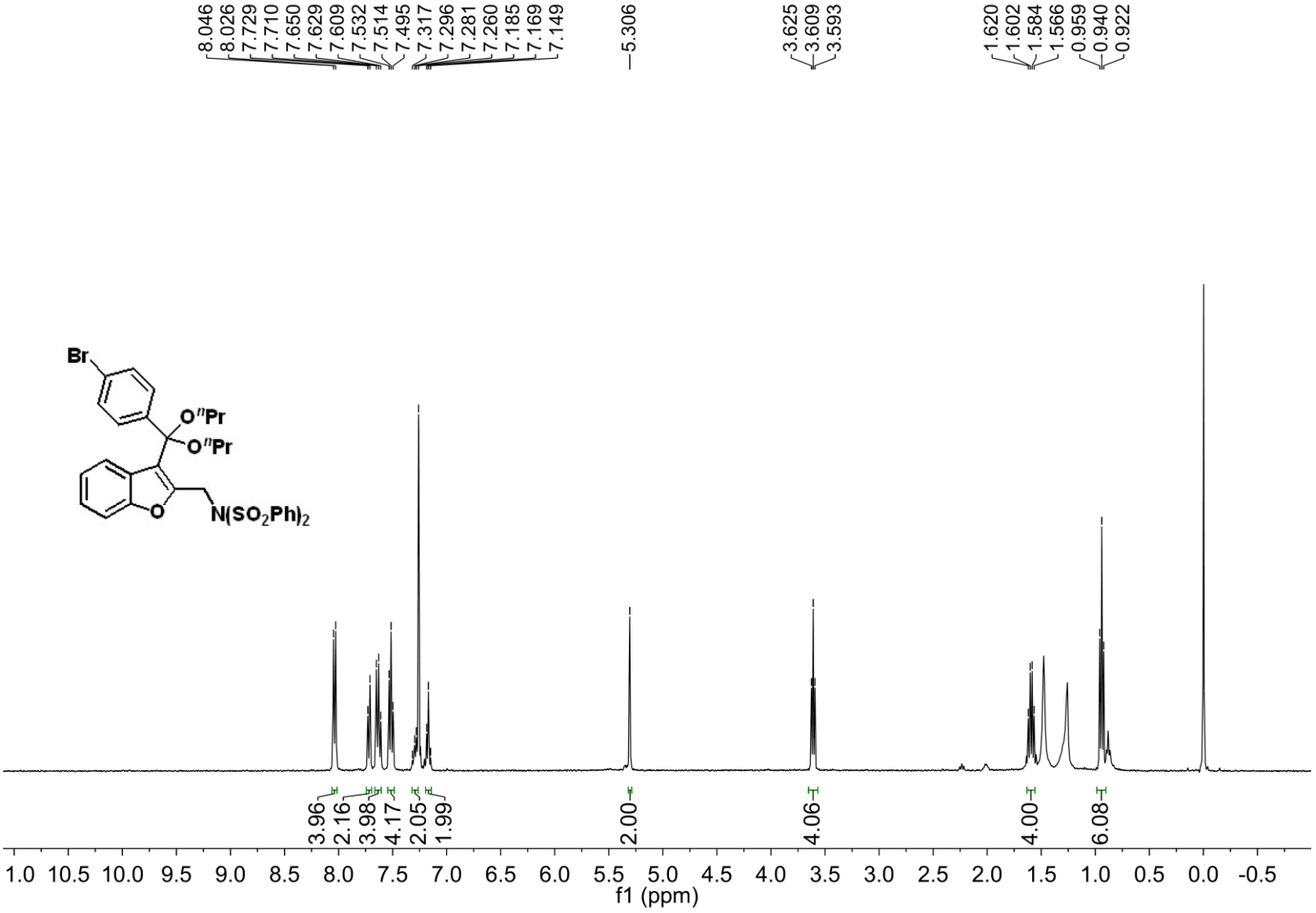
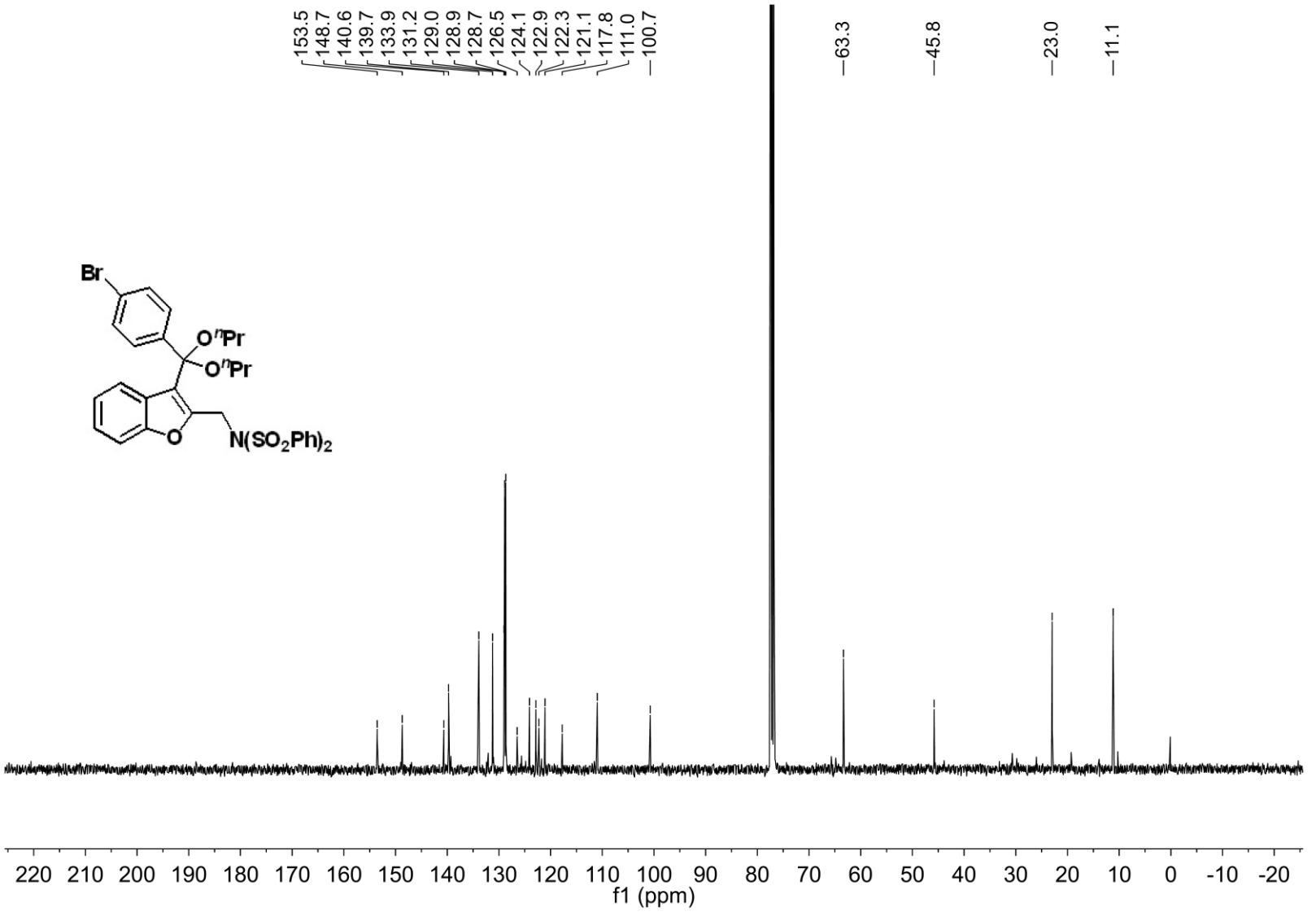


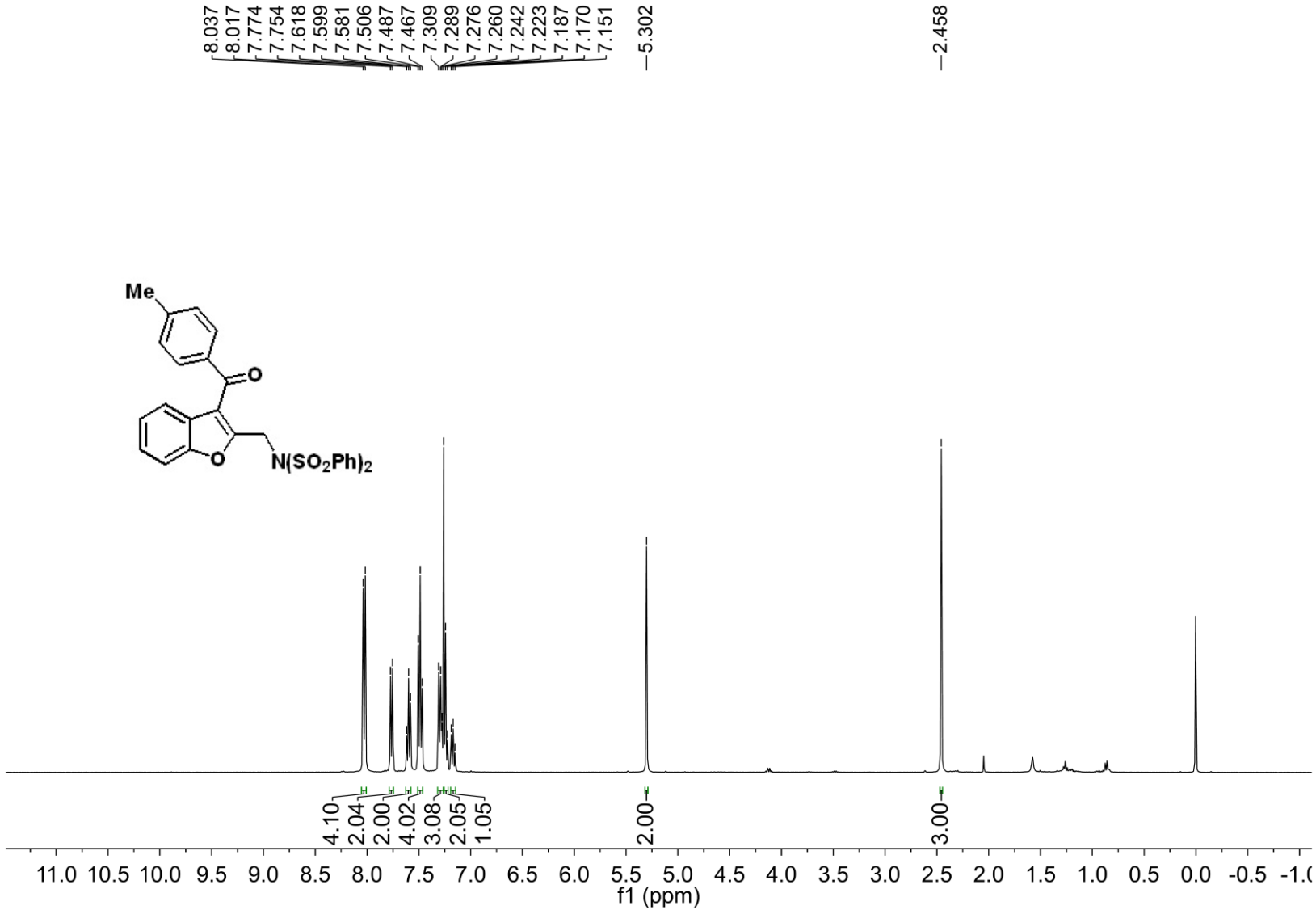
[1]H spectra of compound 3ab:



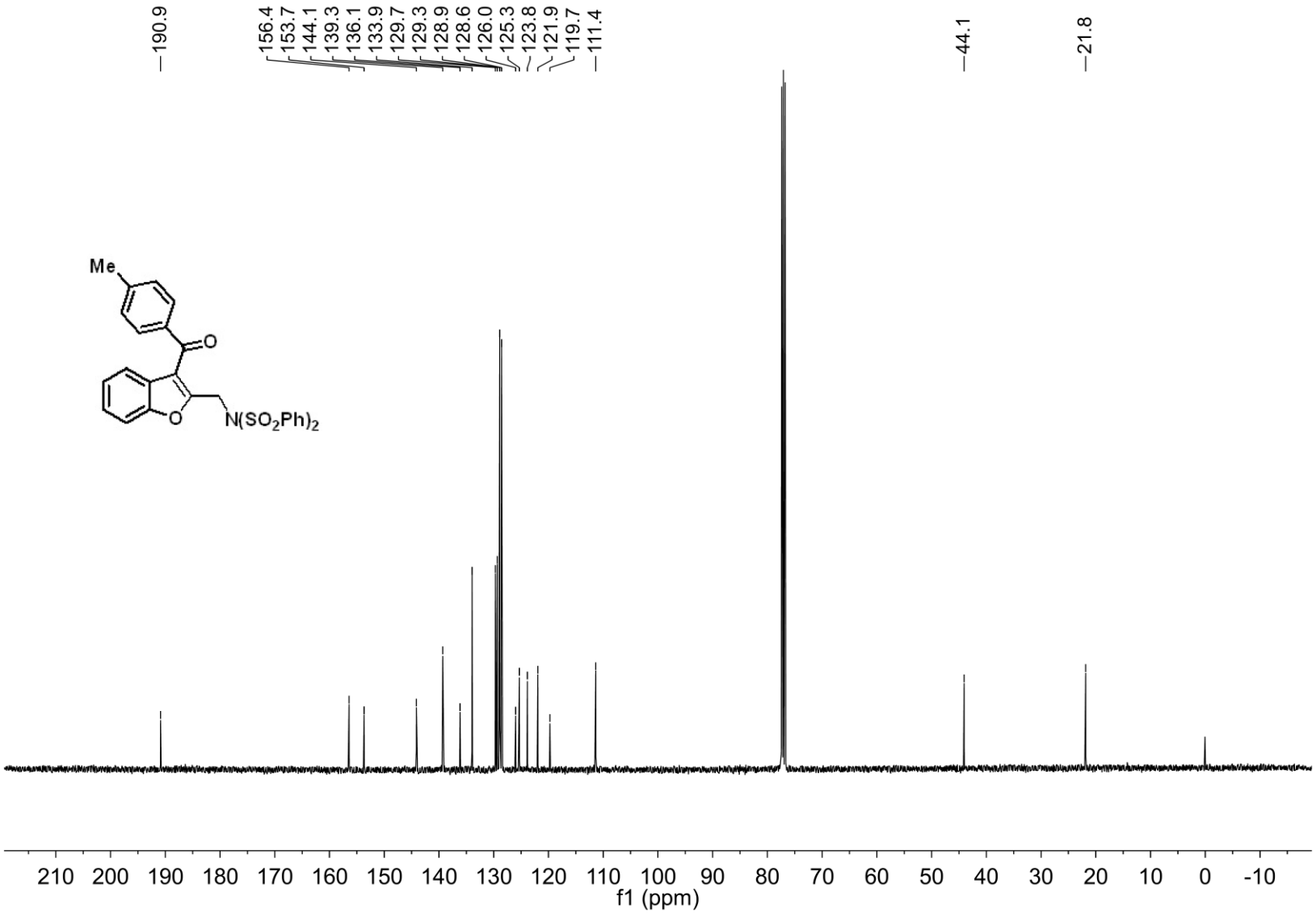
^{13}C spectra of compound 3ab:



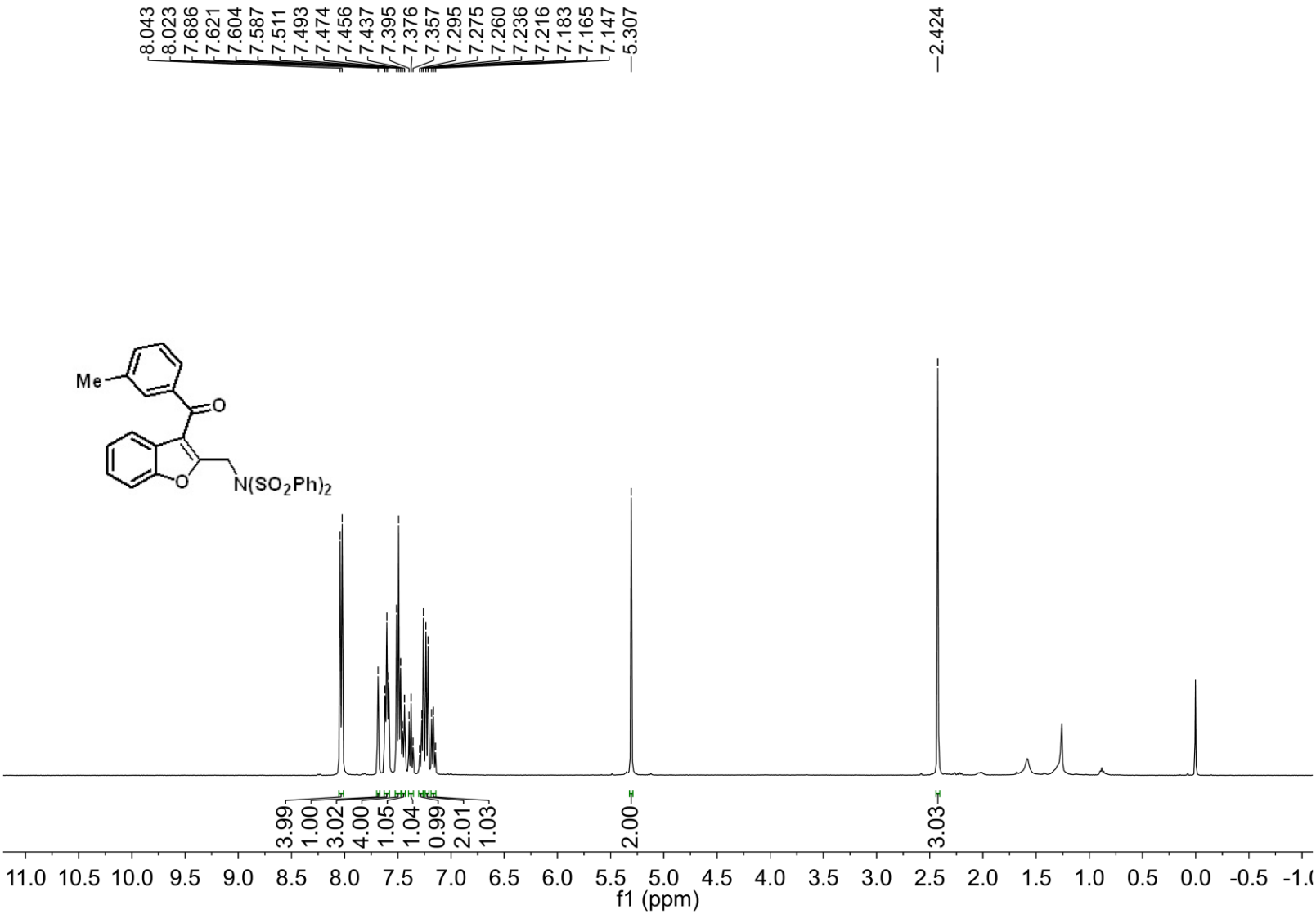
[1]H spectra of compound 4a:



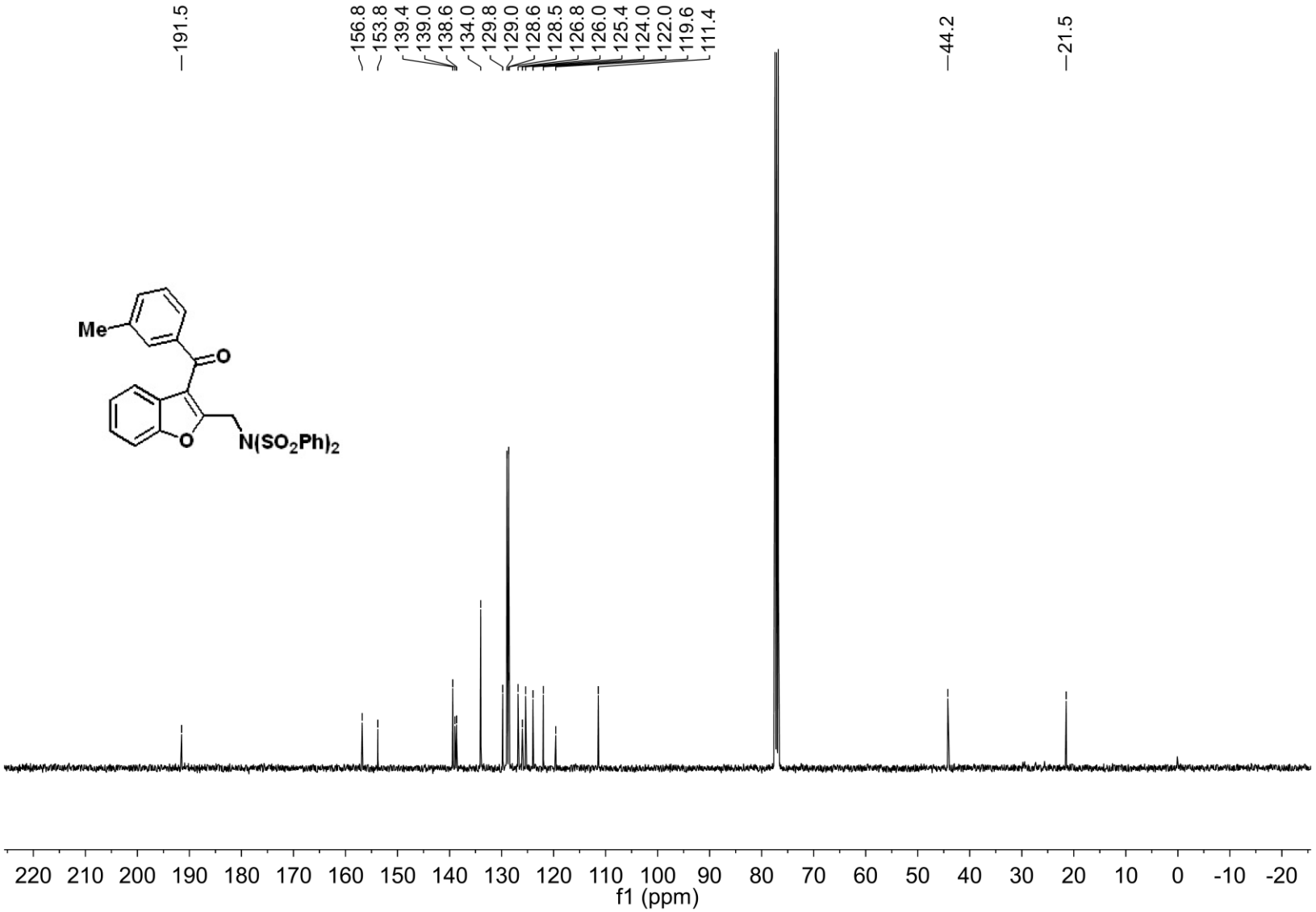
^{13}C spectra of compound 4a:



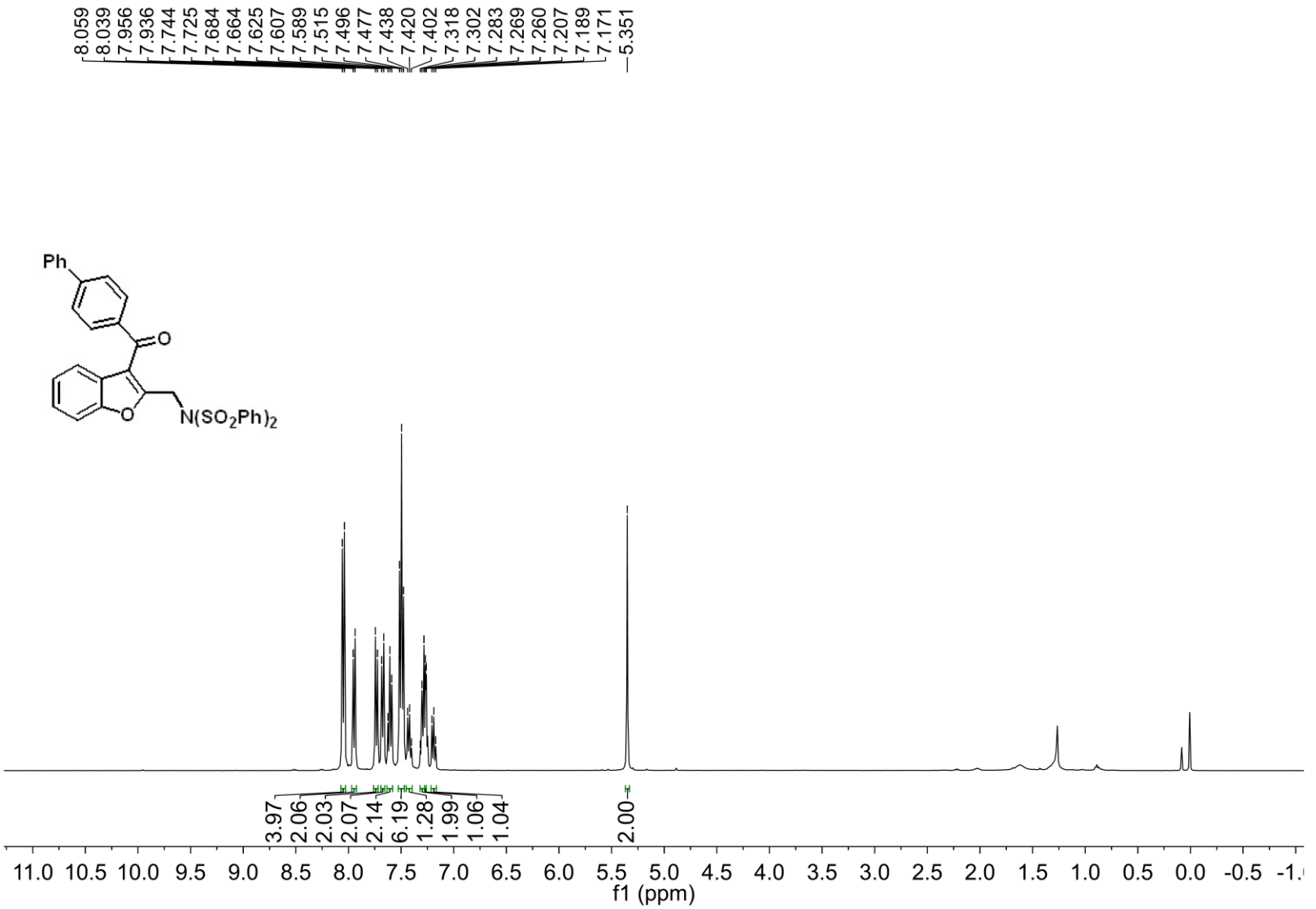
[1]H spectra of compound 4b:



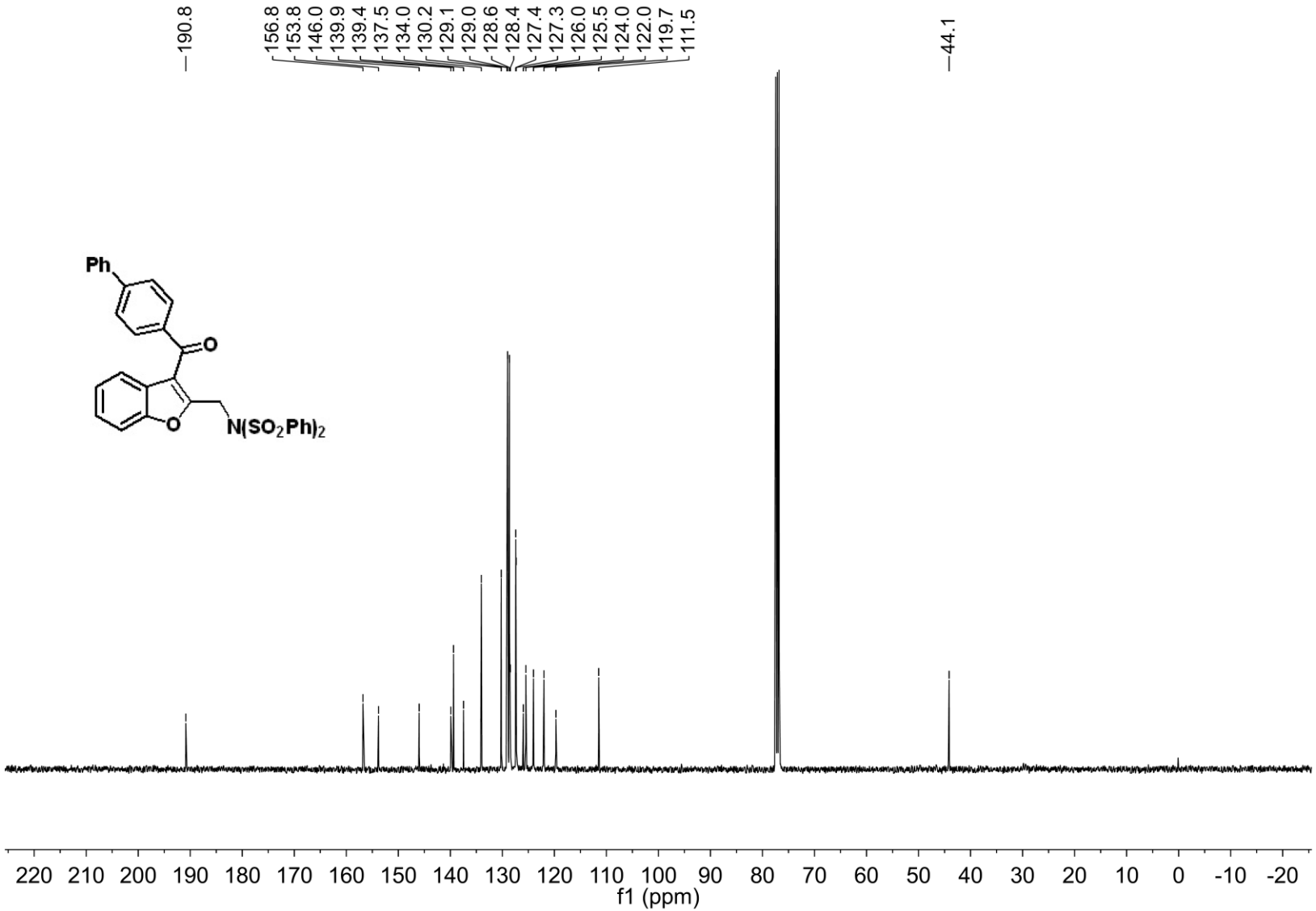
^{13}C spectra of compound 4b:



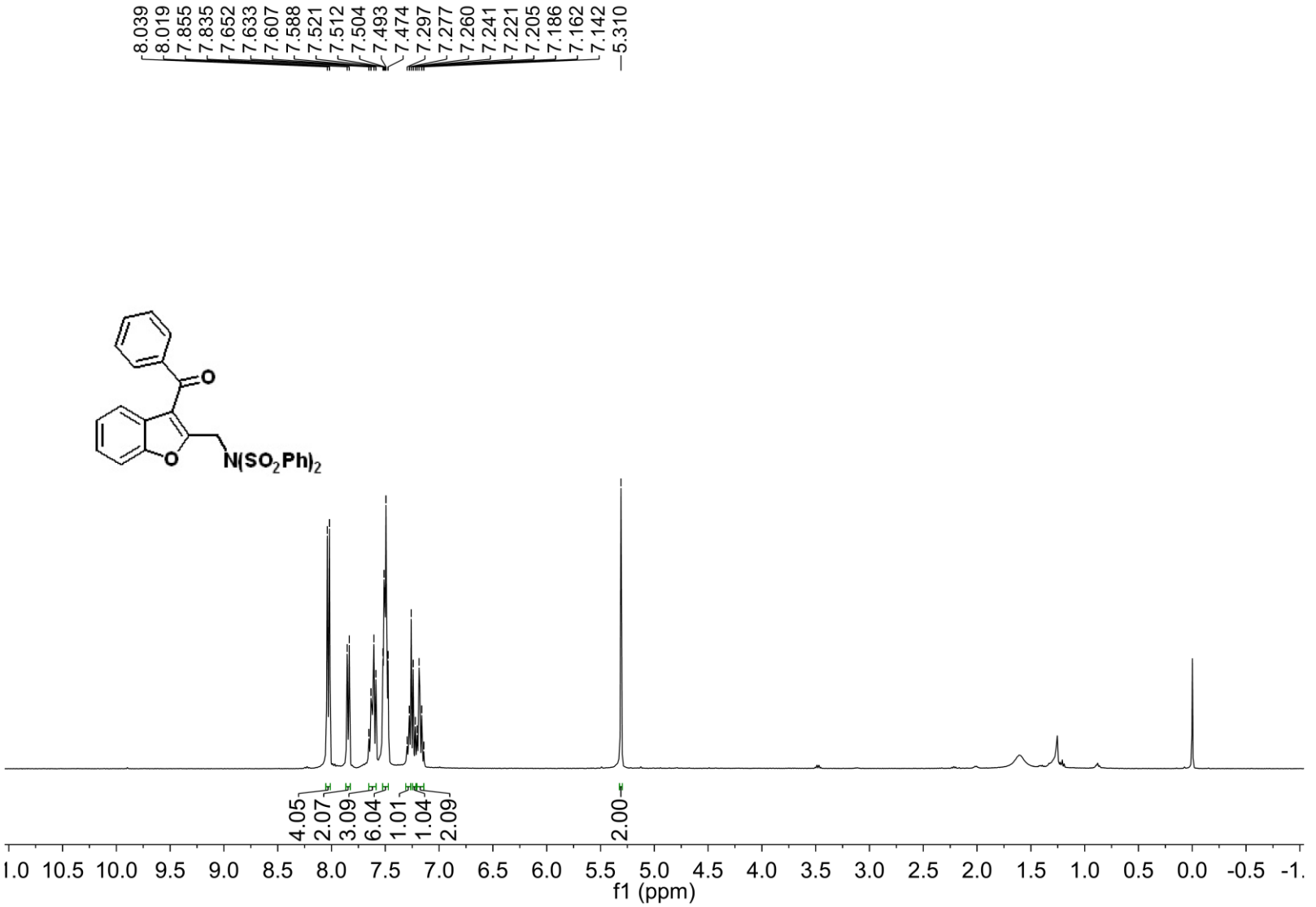
[1]H spectra of compound 4c:



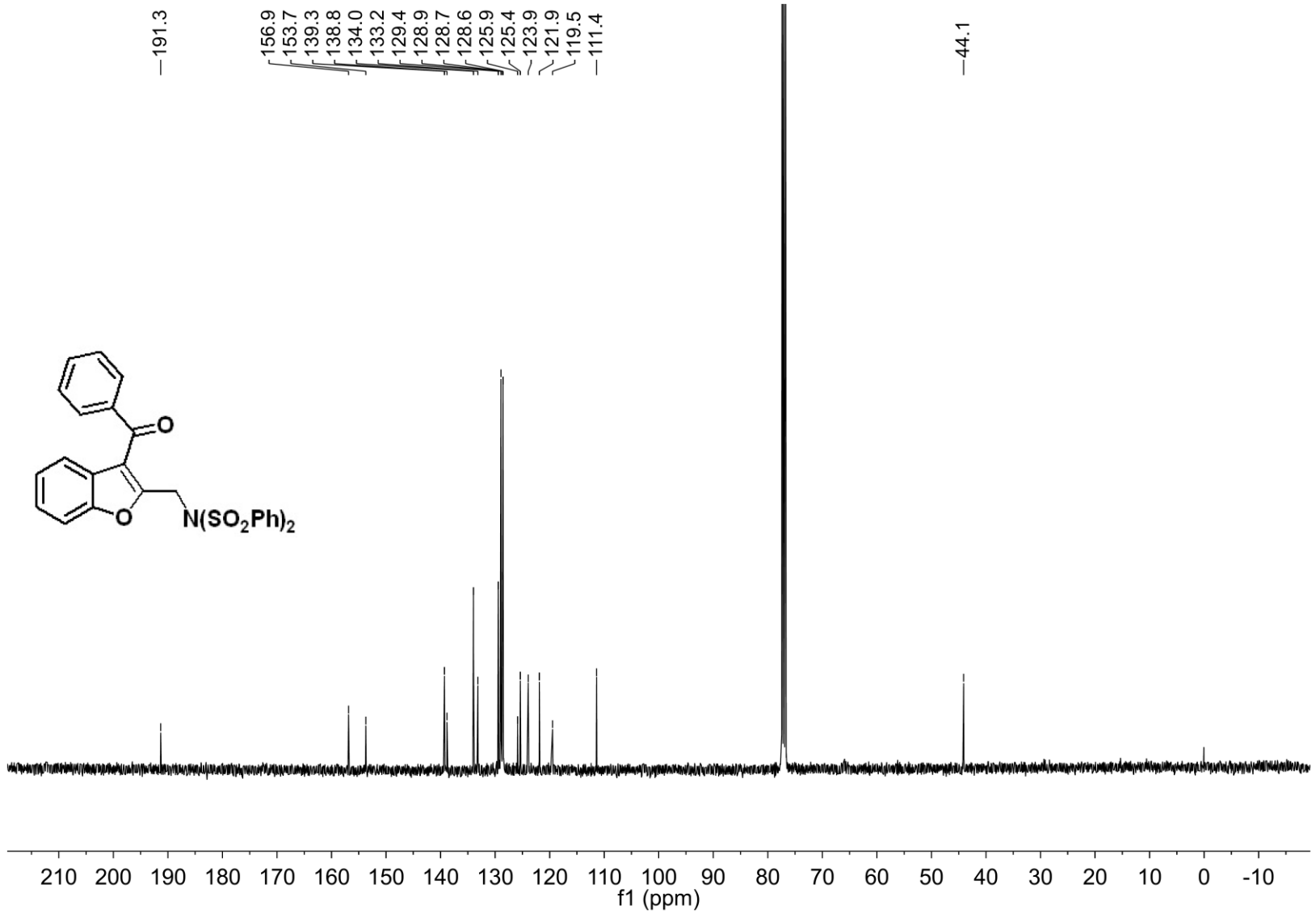
^{13}C spectra of compound 4c:



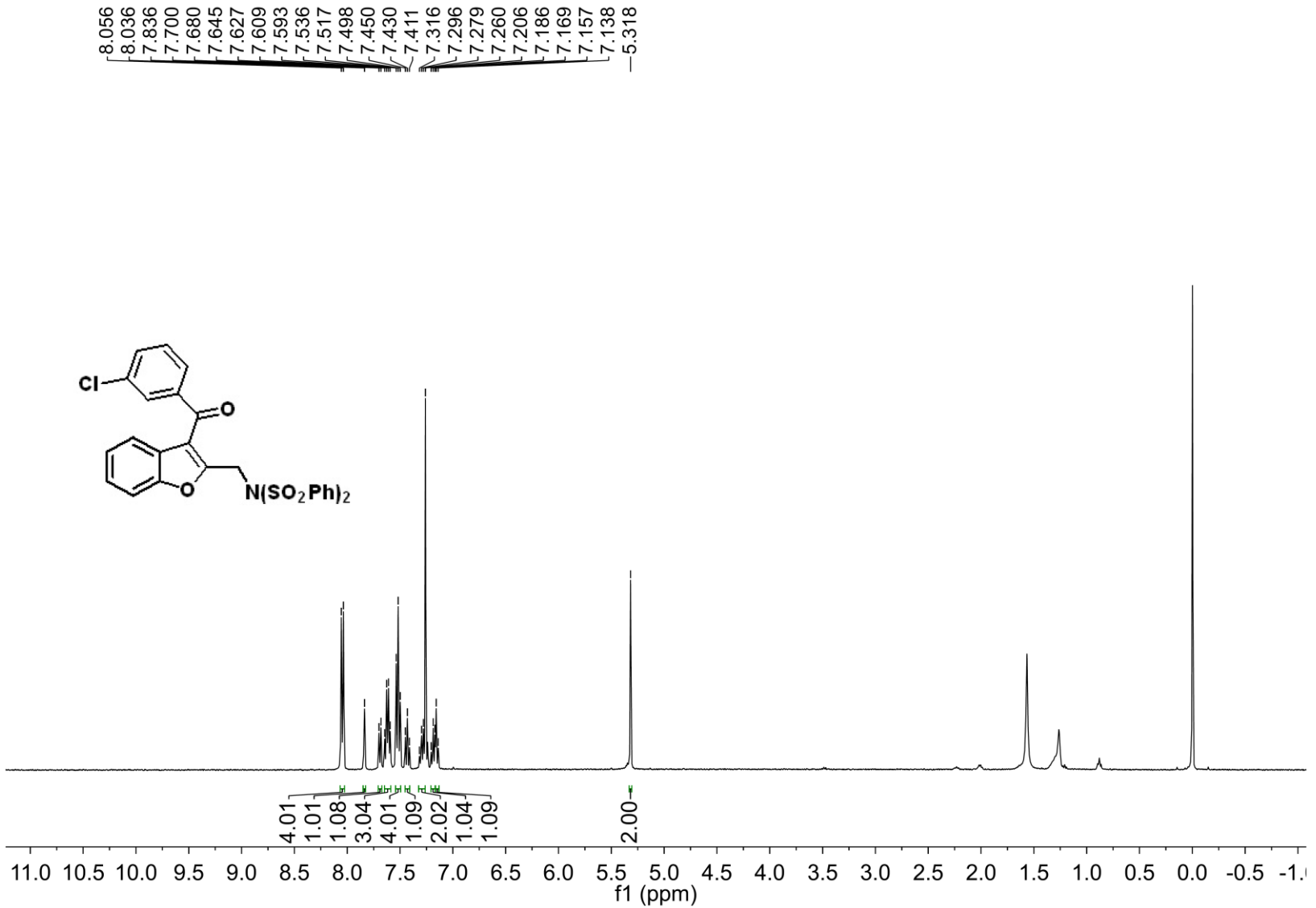
[1]H spectra of compound 4d:



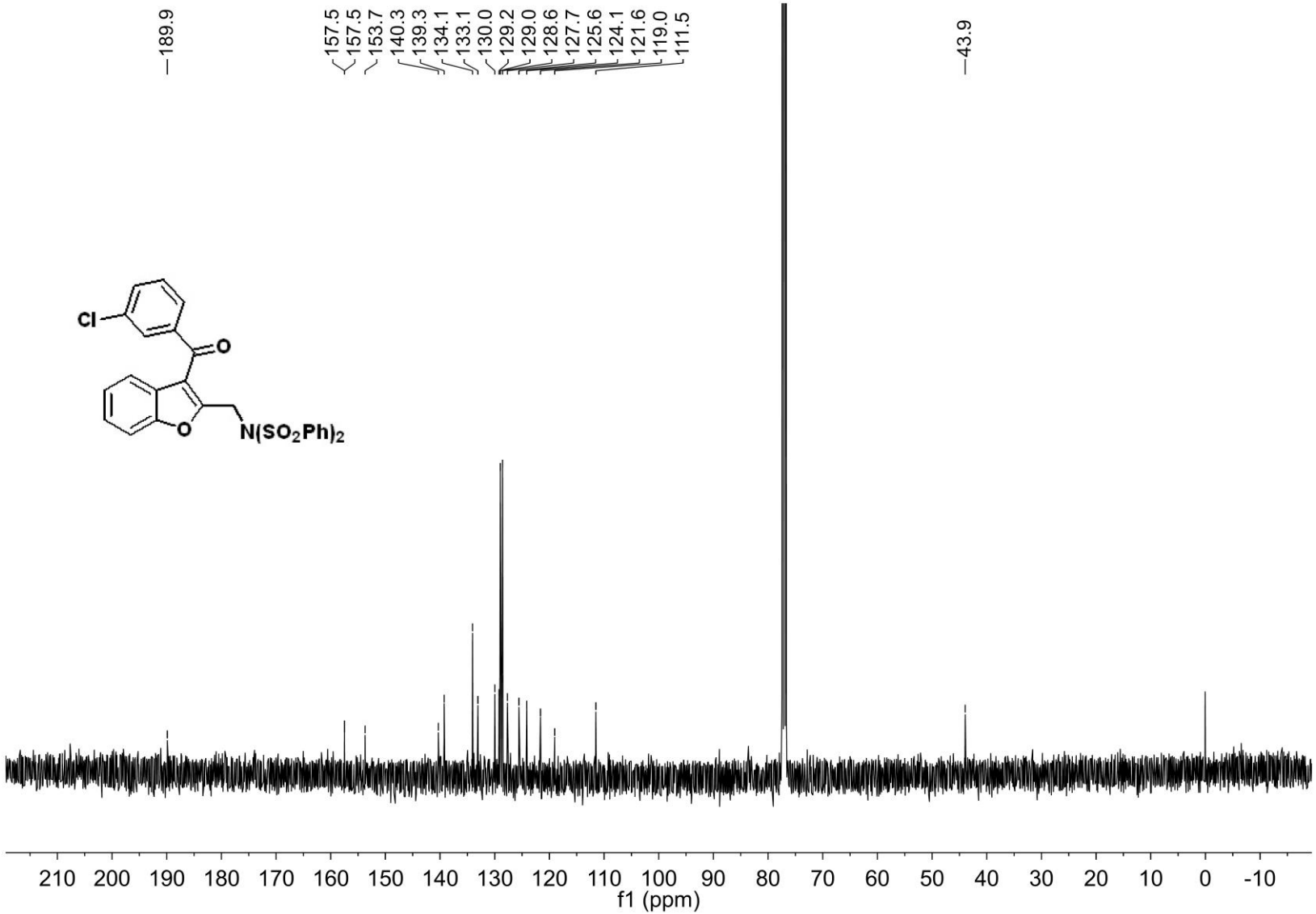
^{13}C spectra of compound 4d:



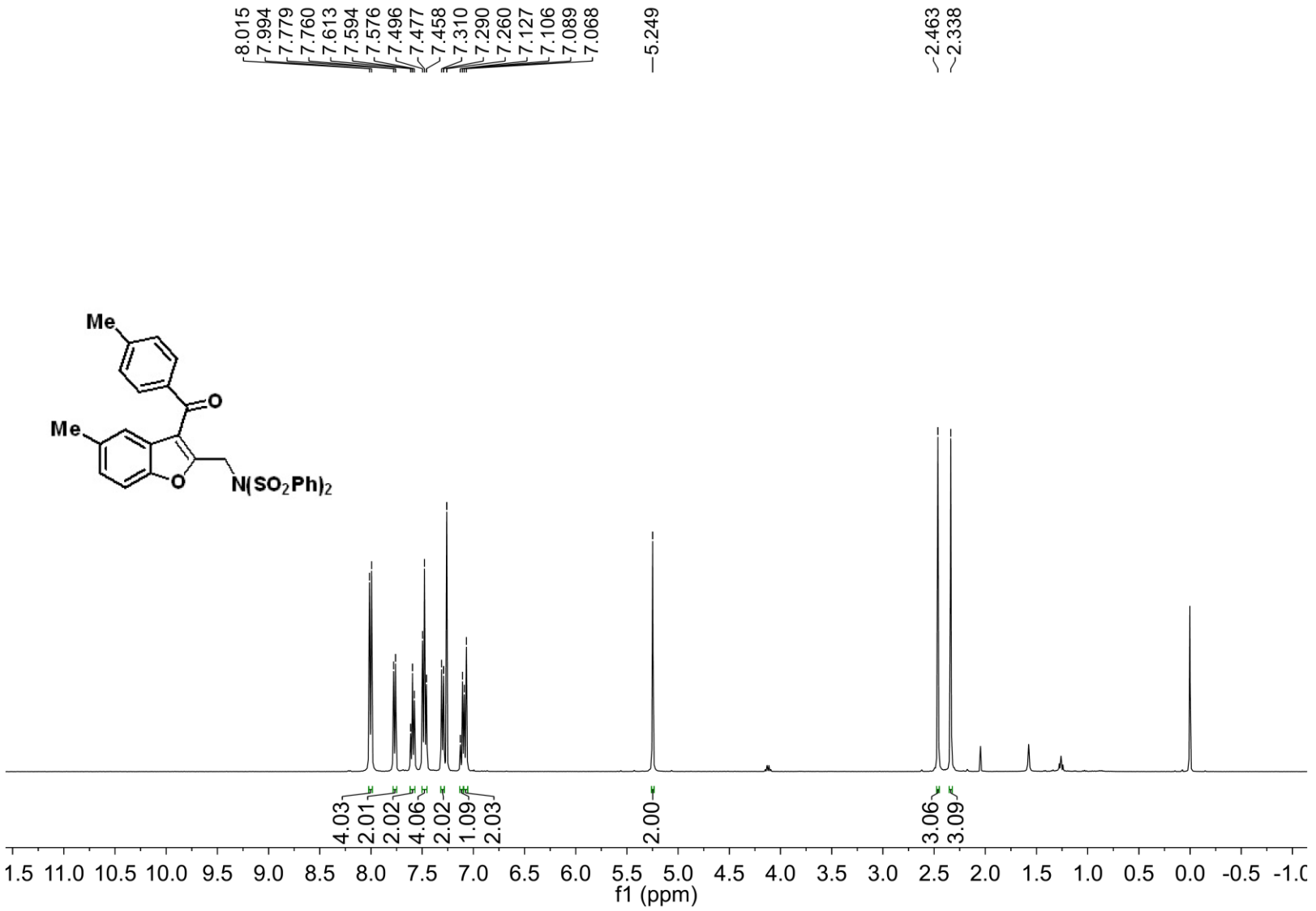
[1]H spectra of compound 4e:



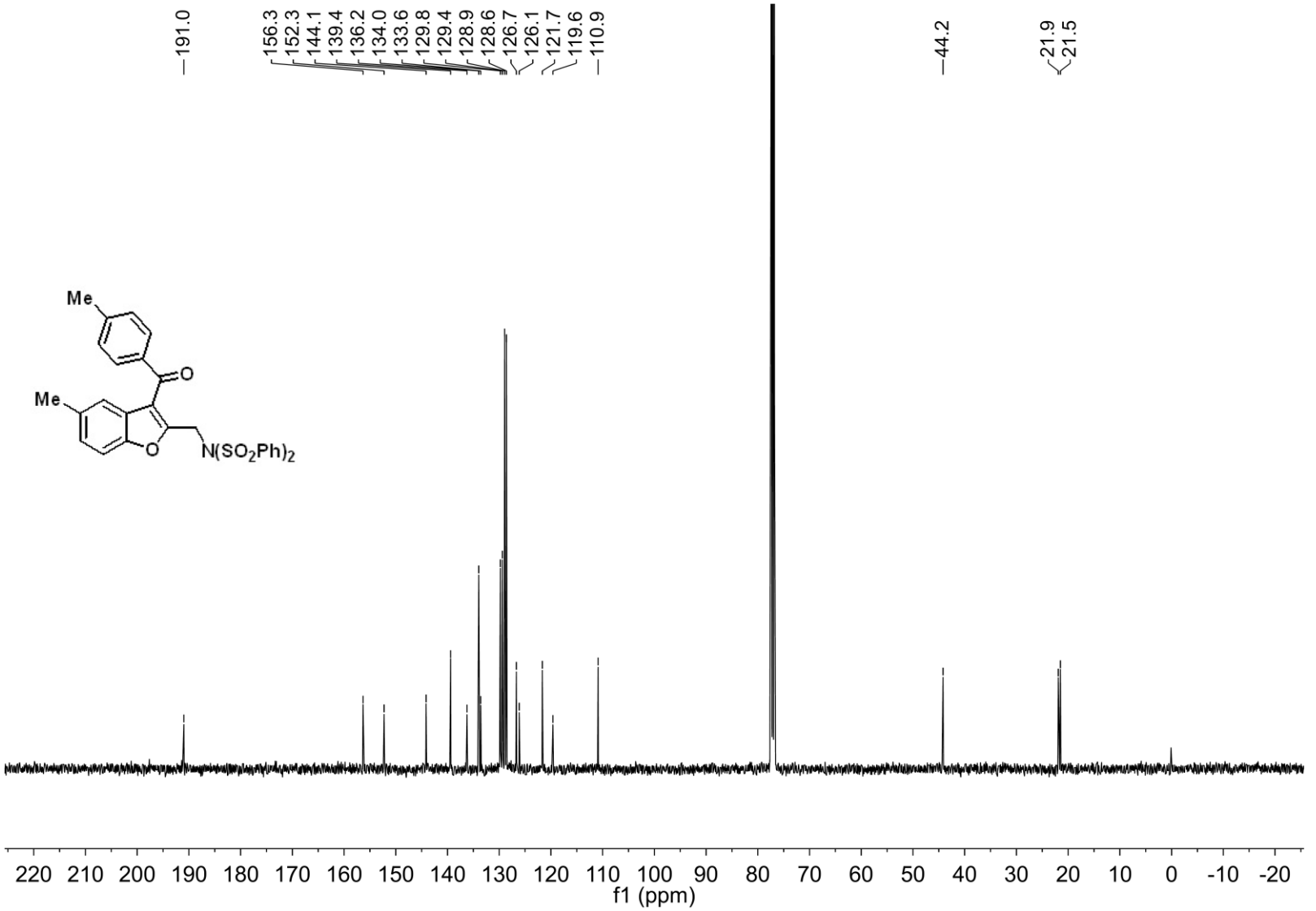
^{13}C spectra of compound 4e:



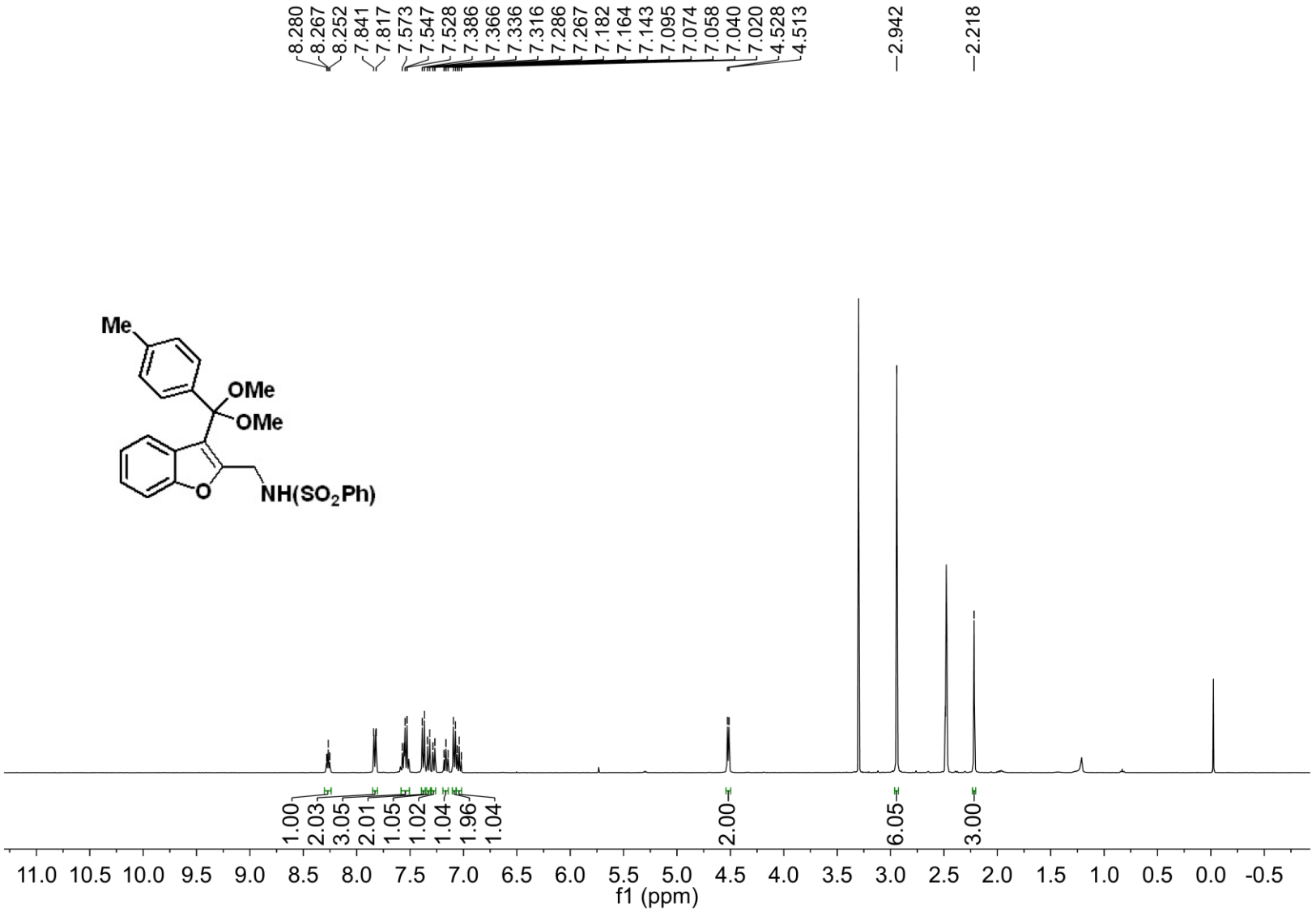
[1]H spectra of compound 4f:



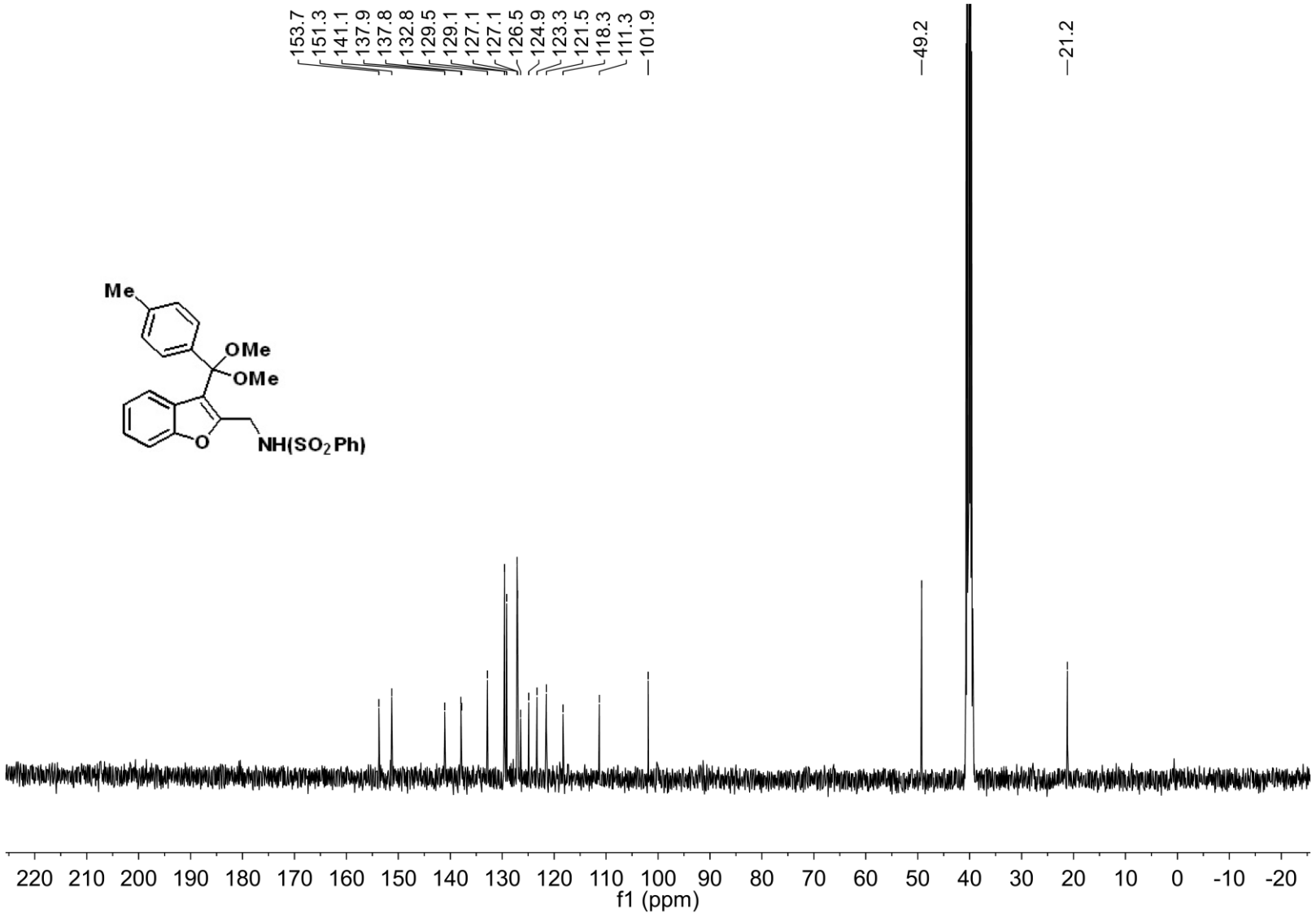
^{13}C spectra of compound 4f:



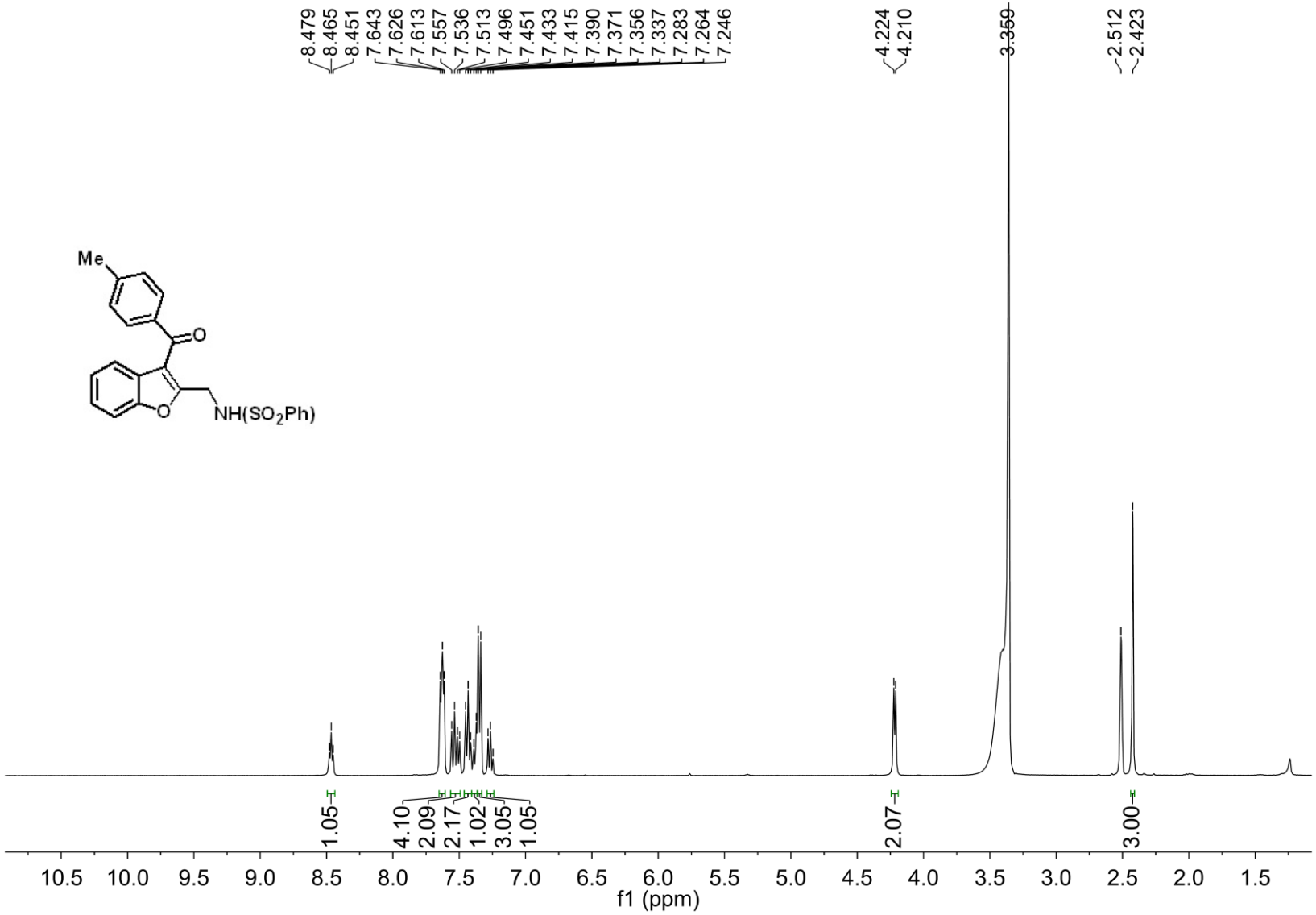
[1]H spectra of compound 5a:



^{13}C spectra of compound 5a:



[1]H spectra of compound 6a:



^{13}C spectra of compound 6a: