Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Dirhodium-Catalyzed One-Step Cascade Intermolecular 1,4-Diamination via Cyclopropanation

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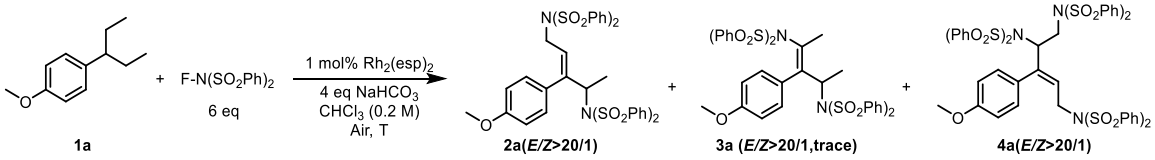
1.General Information

If not explicitly stated, all reactions requiring anhydrous conditions were conducted by standard procedures under air atmosphere. $Rh_2(esp)_2$ and its derivatives was prepared as described.[1] Unless otherwise noted, all reagents were obtained from commercial suppliers and used without further purification. Yields reported are for isolated yields unless otherwise noted. ^{1}H and ^{13}C NMR spectra were obtained on a Bruker 400 spectrometer at 400 MHz and 101 MHz. ^{19}F NMR spectra were obtained on a Bruker 400 spectrometer at 376 MHz. The ^{1}H NMR (400 MHz) chemical shifts were recorded relative to $CDCl_3$ as the internal reference ($CDCl_3$: δ H = 7.26 ppm). The ^{13}C NMR (101 MHz) chemical shifts were given using $CDCl_3$ as the internal standard ($CDCl_3$: δ C = 77.16 ppm). ^{1}H NMR data are reported as: chemical shift (ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublet, etc), and coupling constant (Hz). High resolution mass spectrometric measurements were carried out using a Bruker autoflex MALDITOF mass spectrometer and Waters-Q-TOF Premier (ESI). Melting points were recorded on a Buchi Melting Point B-545.

2. Reaction Optimization

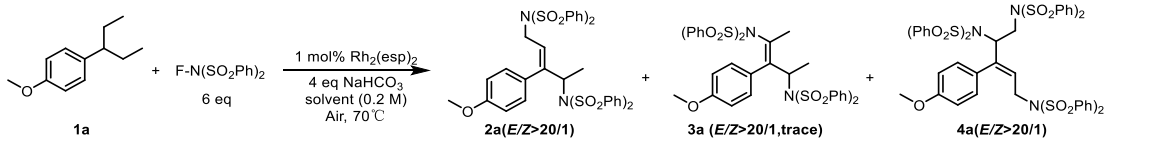
Table S1. Selection of reaction temperature for the formation of 1,4-diamine from alkane.[a]



Entry	T(℃)	Yield of 2a[b]	Ratio(2a/3a)[b]	Ratio(2a/4a)[b]
1	rt		No Reaction	
2	50	38%	>10/1	>10/1
3	60	56%	>15/1	>10/1
4	70	63%	>20/1	>10/1
5	80	49%	>15/1	>10/1
6[c]	70	62%	>20/1	>10/1

[a]All reactions were performed with **1a** (0.4 mmol)，$Rh_2(esp)_2$ (0.004 mmol), NFSI (6 equiv, 2.4 mmol), $NaHCO_3$ (4 equiv, 1.6 mmol), $CHCl_3$ (2 mL), **Temperature**，1 h under air. NFSI = N-Fluorobenzenesulfonmide. [b]As determined by ^1H NMR spectroscopy using $C_2H_2Cl_4$ as the internal standard. [c]Ar instead of air.

Table S2. Selection of reaction solvent for the formation of 1,4-diamine from alkane.[a]

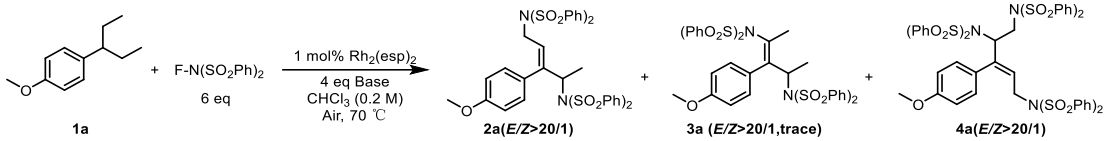


Entry	Solvent	Yield of 2a[b]	Ratio(2a/3a)[b]	Ratio(2a/4a)[b]
1	DCE	40%	>20/1	>6/1
2	$CHCl_3$	63%	>20/1	>10/1
3	DME		No Reaction	
4	EA	25%	>8/1	>10/1
5	CH_3CN	32%	>15/1	>10/1

6	1,4-dioxane		No Reaction	
7	THF		No Reaction	
8	MeOH		No Reaction	
9	acetone	19%	>8/1	>10/1
10	hexane		No Reaction	
11	DCM	37%	>10/1	>10/1
12	Ph		No Reaction	

[a]All reactions were performed with **1a** (0.4 mmol)，$Rh_2(esp)_2$ (0.004 mmol), NFSI (6 equiv, 2.4 mmol), $NaHCO_3$ (4 equiv, 1.6 mmol), **Solvent** (2 mL), 70℃， 1 h under air. NFSI = N-Fluorobenzenesulfonmide. [b]As determined by ^1H NMR spectroscopy using $C_2H_2Cl_4$ as the internal standard.

Table S3. Selection of reaction base for the formation of 1,4-diamine from alkane.[a]

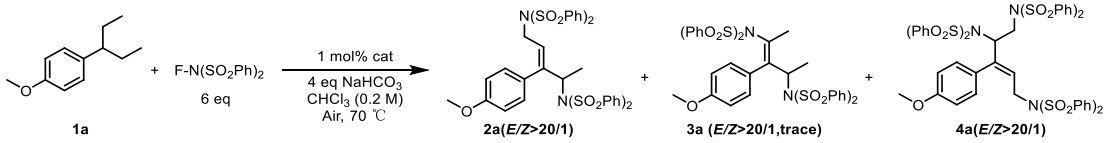


Entry	Base	Yield of 2a[b]	Ratio(2a/3a)[b]	Ratio(2a/4a)[b]
1	No Base		No Reaction	
2	$NaHCO_3$	63%	>20/1	>10/1
3	K_2HPO_4	52%	>10/1	>5/1
4	KH_2PO_4	49%	>15/1	>5/1
5	K_3PO_4	27%	>20/1	>5/1
6	NaOAc		trace	
7	Na_2CO_3	47%	>10/1	>6/1
8	NaOH	47%	>15/1	>5/1
9	K_2CO_3	41%	>10/1	>6/1
10	KOAc		trace	
11	MgO	25%	>10/1	>10/1

[a]All reactions were performed with **1a** (0.4 mmol), $Rh_2(esp)_2$ (0.004 mmol), NFSI (6

equiv, 2.4 mmol), **Base** (4 equiv, 1.6 mmol), $CHCl_3$ (2 mL), 70℃, 1 h under air. NFSI = N-Fluorobenzenesulfonmide. [b]As determined by ^1H NMR spectroscopy using $C_2H_2Cl_4$ as the internal standard.

Table S4. Selection of reaction catalyst for the formation of 1,4-diamine from alkane.[a]

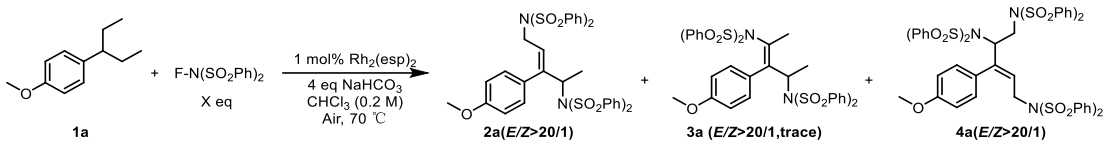


Entry	Catalyst	Yield of 2a[b]	Ratio(2a/3a)[b]	Ratio(2a/4a)[b]
1	$Rh_2(h\text{-}esp)_4$	41%	>20/1	>5/1
2	$Rh_2(3\text{-}Me\text{-}esp)_2$	50%	>15/1	>3/1
3	$Rh_2(3\text{-}tBu\text{-}esp)_2$	52%	>20/1	>3/1
4	$Rh_2(oct)_4$	31%	>20/1	>10/1
5	$Rh_2(OPiv)_4$	36%	>20/1	>10/1
6	$Rh_2(5\text{-}Br\text{-}esp)_2$	31%	>10/1	>4/1
7	$Rh_2(TFA)_4$		No Reaction	
8	$Rh_2(6\text{-}F\text{-}esp)_2$	44%	>20/1	>5/1
9	$Rh_2(esp)_2$	63%	>20/1	>10/1
10[c]	$Rh_2(esp)_2$	52%	>20/1	>10/1
11	$Rh_2(OAc)_4$	42%	>20/1	>10/1
12	No Catalyst		No Reaction	
13	$Rh_2(cap)_4$		No Reaction	
14	$FeCl_3$		No Reaction	
15	$Cu(OAc)_2$		No Reaction	
16	$Co(OAc)_2$		No Reaction	
17	$Mn(OAc)_2$		No Reaction	
18	$CuCl_2$		No Reaction	
19	$Cu(acac)_2$		No Reaction	
20	$Mn(acac)_2$		No Reaction	

21	$Ni(acac)_2$	No Reaction
22	$Co(acac)_2$	No Reaction
23	$Fe(acac)_3$	No Reaction
24	CuI	No Reaction
25	CuCl	No Reaction

[a]All reactions were performed with **1a** (0.4 mmol), **Catalyst** (0.004 mmol), NFSI (6 equiv, 2.4 mmol), $NaHCO_3$ (4 equiv, 1.6 mmol), $CHCl_3$ (2 mL), 70℃， 1 h under air. NFSI = N-Fluorobenzenesulfonmide. [b]As determined by ^1H NMR spectroscopy using $C_2H_2Cl_4$ as the internal standard. [c]0.5 mol% $Rh_2(esp)_2$ was used.

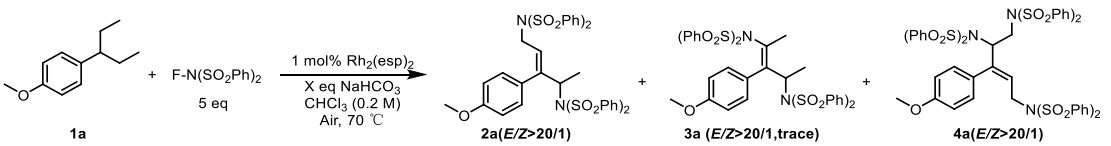
Table S5. Selection of NFSI equivalent for the formation of 1,4-diamine from alkane.[a]



Entry	X equiv	Yield of 2a[b]	Ratio(2a/3a)[b]	Ratio(2a/4a)[b]
1	3	56%	>20/1	>10/1
2	4	66%	>20/1	>10/1
3	5	68%	>20/1	>10/1
4	6	63%	>20/1	>10/1

[a]All reactions were performed with **1a** (0.4 mmol), **catalyst** (0.004 mmol), NFSI (**x** equiv), $NaHCO_3$ (4 equiv, 1.6 mmol), $CHCl_3$ (2 mL), 70℃， 1 h under air. NFSI = N-Fluorobenzenesulfonmide. [b]As determined by ^1H NMR spectroscopy using $C_2H_2Cl_4$ as the internal standard.

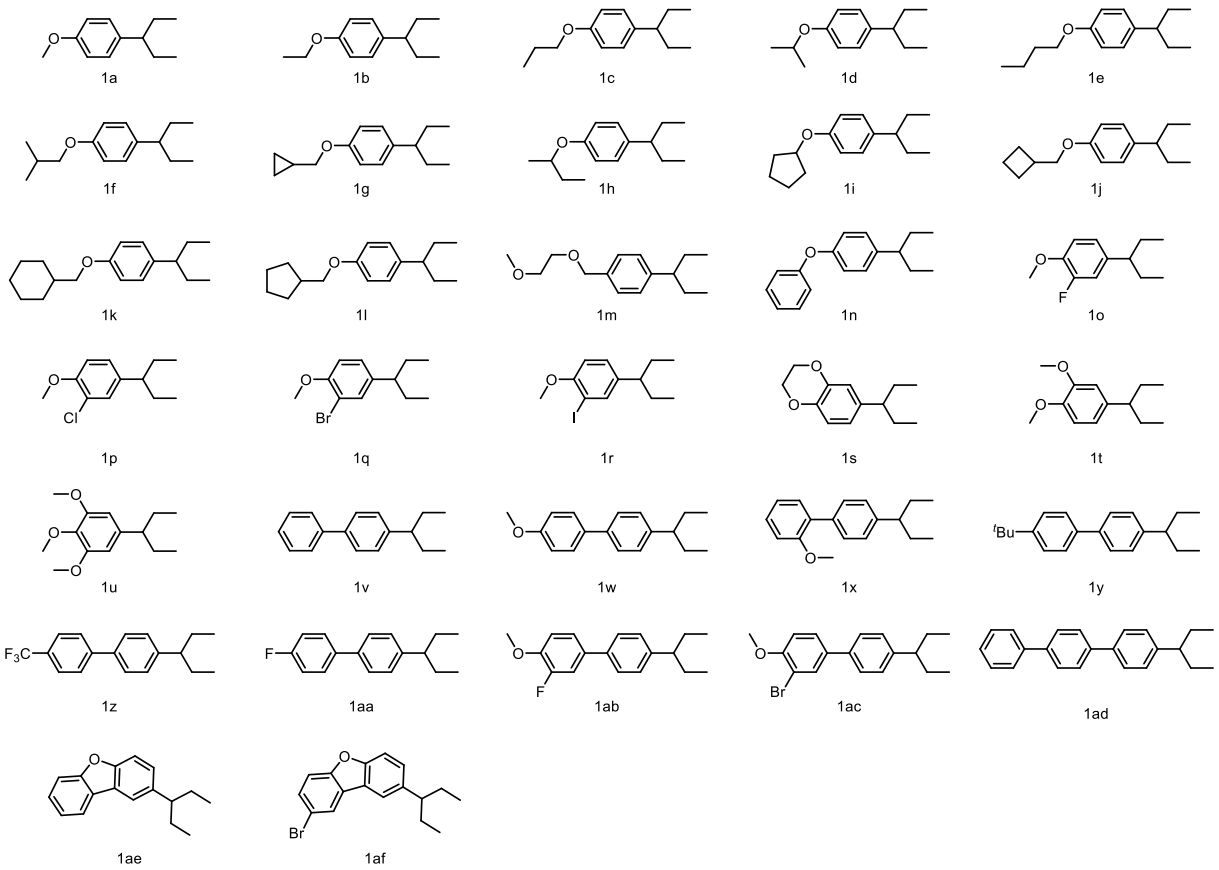
Table S6. Selection of $NaHCO_3$ equivalent for the formation of 1,4-diamine from alkane.[a]



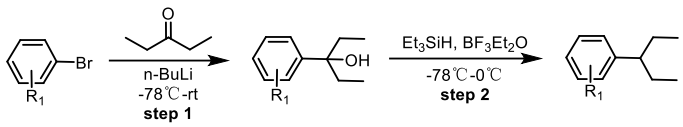
Entry	X equiv	Yield of 2a[b]	Ratio(2a/3a)[b]	Ratio(2a/4a)[b]
1	3	48%	>20/1	>10/1
2	4	68%	>20/1	>10/1
3	5	60%	>20/1	>10/1
4	6	58%	>20/1	>10/1

[a]All reactions were performed with **1a** (0.4 mmol), $Rh_2(esp)_2$ (0.004 mmol), NFSI (6 equiv, 2.4 mmol), **NaHCO$_3$** (**x** equiv), $CHCl_3$ (2 mL), 70℃， 1 h under air. NFSI = N-Fluorobenzenesulfonmide. [b]As determined by ^{1}H NMR spectroscopy using $C_2H_2Cl_4$ as the internal standard.

3. Synthesis and Characterizations of Substrates



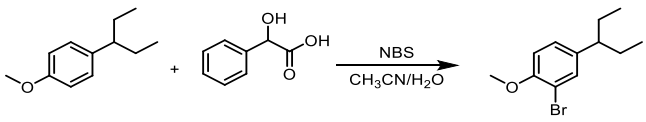
3.1: General procedure 1 for the synthesis of 1a-1p，1s-1ab，1ad-1af[2]



Step 1: Following a general procedure, to a flame-dried RBF fitted with a septum seal was added a solution of aryl halide (1.0 equiv) in THF (0.3 M). The mixture was cooled to -78°C, and a solution of n-BuLi (2.5 M in hexanes, 1.3 equiv) was added dropwise. The solution was left to stir for 30 min before adding a solution of the 3-Pentanone (10 mmol, 1.0 equiv) in THF (1.0 M) dropwise. The reaction mixture was left to stir for 1-3 h, while warming to rt. Water was added dropwise, followed by extraction with EtOAc (×3). The combined organics were dried Na_2SO_4, filtered, and concentrated under reduced pressure. The crude material was purified by silica gel chromatography to yield the desired product.

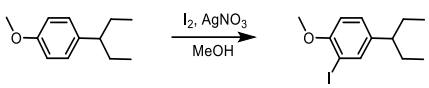
Step 2: Following a general procedure, a round-bottom flask was flame-dried and then cooled under argon. The tertiary alcohol (1.0 equiv) was added followed by dry DCM (0.25 M to the tertiary alcohol). Triethylsilane (2.0 equiv) was added, and then the reaction mixture was cooled to -78°C. Once the mixture was cooled, $BF_3 \cdot Et_2O$ (3.2 equiv) was added dropwise. The reaction mixture was stirred at -78°C for 30 minutes, and then was stirred at - 40°C for 30 minutes and then was stirred at 0°C for 60 minutes. The reaction mixture was slowly quenched by an equal volume of saturated sodium bicarbonate at 0°C. The layers were separated, and then the aqueous layer was extracted with DCM (×3). The combined organics were dried Na_2SO_4, filtered, and concentrated under reduced pressure. The crude material was purified by silica gel chromatography to yield the desired product**.**

3.2: General procedure 1 for the synthesis of 1q and 1ac[3]



Following a general procedure, to a flame-dried RBF was added NBS (1.2 equiv), mandelic acid (20 mol %), and an aromatic compound (1.0 equiv). MeCN / H_2O (1/1, 0.1 M) were then added. The reaction was then stirred at room temperature until completed, as judged by TLC. Upon completion, the reaction was diluted with ethyl acetate and added a saturated $NaHCO_3$ solution. The aqueous phase was extracted with ethyl acetate (×3) and the combined organic layers were dried over Na_2SO_4, filtered, and carefully concentrated in vacuo. The crude material was purified by silica gel chromatography to yield the desired product.

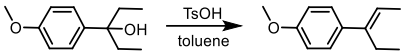
3.3: General procedure 1 for the synthesis of 1r[4]



Following a general procedure, to a mixture of I_2 (1.0 equiv) in methanol (1.8 M) at room temperature was added $AgNO_3$ (1.0 equiv). Aromatic compound (1.0 equiv) in methanol (1.8 M) was added and the mixture was stirred at room temperature 15 hours before being filtered over celite (rinsed with CH_2Cl_2). Water was added, followed by

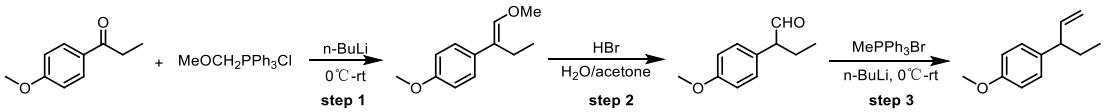
saturated $Na_2S_2O_3$ until discoloration, and the solution was extracted with DCM (×2). The combined organic layers were dried over Na_2SO_4, filtered and the filtrate was concentrated under reduced pressure. The crude material was purified by silica gel chromatography to yield the desired product**.**

3.4: General procedure 1 for the synthesis of 1D[5]



Following a general procedure, TsOH (0.1 equiv) was added to a solution of tertiary alcohol (1.0 equiv) in dry toluene (0.2 M) under argon atmosphere, and this solution was heated to reflux. After 4 hours, the reaction mixture was cooled to rt, the solution was washed with saturated $NaHCO_3$, and the organic layer was dried over Na_2SO_4, filtered and the filtrate was concentrated under reduced pressure. The crude material was purified by silica gel chromatography to yield the desired product.

3.5: General procedure 1 for the synthesis of 1D-T[6]



Step 1: Following a general procedure, (methoxymethyl)triphenylphosphonium chloride (1.6 equiv) was suspended in anhydrous THF (0.2 M) and the resultant mixture was cooled to 0˚C. Slowly by syringe, n-BuLi (2.5 M in hexanes, 1.6 equiv) was added to the stirring phosphonium chloride solution under an atmosphere of N_2. The reaction was allowed to stir under N_2 at 0˚C for 30 min, then at 23˚C for 30 min, at which point the solution turned deep red. Then, the mixture was recooled to 0˚C, and 4'-methoxyphenylacetone in minimal anhydrous THF (0.2 M) was added dropwise by syringe. After stirring under N_2 for 4 h, the reaction was quenched with H_2O. The layers were separated and the aqueous phase was extracted with ethyl acetate (×3) and the combined organic layers were dried over Na_2SO_4, filtered, and concentrated in vacuo. The crude material was purified by silica gel chromatography to yield the desired product.

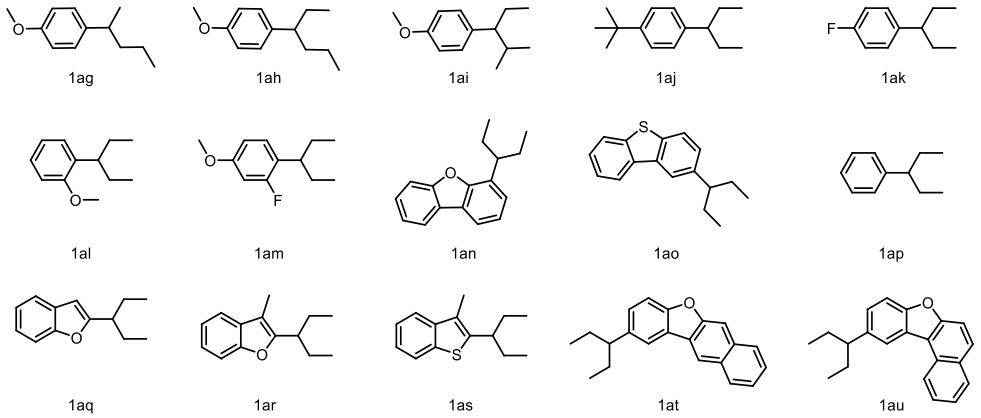
Step 2: Following a general procedure, enol ether (1.0 equiv) was dissolved in a 4:1 mixture of acetone and H_2O (0.9 M) and the resultant solution was cooled to 0˚C in an

ice bath. Conc. HBr (48%, 5.0 equiv) was added to the solution and the reaction mixture was stirred at 23˚C for 4 h. The aqueous was neutralized with saturated $NaHCO_3$ solution, as determined by pH paper. This aqueous solution was then extracted with DCM (×2). The combined organic layers were dried over Na_2SO_4, filtered and the filtrate was concentrated under reduced pressure. The crude material was purified by silica gel chromatography to yield the desired product**.**

Step 3: Following a general procedure, Methyltriphenylphosphonium bromide (1.6 equiv) was suspended in anhydrous THF (0.2 M) and the resultant mixture was cooled to 0˚C. Slowly by syringe, n-BuLi (2.5 M in hexanes, 1.6 equiv) was added to the stirring phosphonium chloride solution under an atmosphere of N_2. The reaction was allowed to stir under N_2 at 0˚C for 30 min, then at 23˚C for 30 min, at which point the solution turned deep red. Then, the mixture was recooled to 0˚C, and Aromatic aldehyde compound in minimal anhydrous THF (0.2M) was added dropwise by syringe. After stirring under N_2 for 4 h, the reaction was quenched with H_2O. The layers were separated and the aqueous phase was extracted with ethyl acetate (×3) and the combined organic layers were dried over Na_2SO_4, filtered, and concentrated in vacuo. The crude material was purified by silica gel chromatography to yield the desired product.

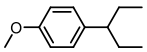
3.6：Unsuccessful substrates

The substrate **1ag-1ai** has been reported in the previous literature.[7-9] The structures of these unsuccessful substrates are listed below.



3.7: Characterization data of Substrates

1-methoxy-4-(pentan-3-yl) benzene (1a)



1a

Compound **1a** was isolated via column chromatography (PE) as colorless oil (1.44g, 75% yield).

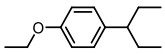
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.06 (d, *J* = 8.5 Hz, 2H), 6.85 (d, *J* = 8.6 Hz, 2H), 3.80 (s, 3H), 2.27 (m, 1H), 1.67 (m, 2H), 1.51 (m, 2H), 0.77 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.8, 138.0, 128.7, 113.6, 55.3, 49.0, 29.5, 12.3.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{12}H_{19}O$: 179.1431; Found: 179.1432.

Spectra are consistent with reported literature values.[10]

1-ethoxy-4-(pentan-3-yl) benzene (1b)



1b

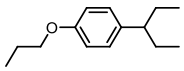
Compound **1b** was isolated via column chromatography (PE) as colorless oil (1.34g, 70% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.04 (d, *J* = 8.6 Hz, 2H), 6.84 (d, *J* = 8.6 Hz, 2H), 4.02 (q, *J* = 7.0 Hz, 2H), 2.26 (m, 1H), 1.67 (m, 2H), 1.59 – 1.45 (m, 2H), 1.41 (t, *J* = 7.0 Hz, 3H), 0.77 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.2, 137.9, 128.7, 114.2, 63.4, 49.0, 29.6, 15.1, 12.3.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{13}H_{21}O$: 193.1587; Found: 193.1584.

1-(pentan-3-yl)-4-propoxybenzene (1c)



1c

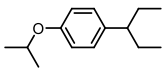
Compound **1a** was isolated via column chromatography (PE) as colorless oil (1.15g, 60% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.03 (d, *J* = 8.6 Hz, 2H), 6.83 (d, *J* = 8.6 Hz, 2H), 3.90 (t, *J* = 6.6 Hz, 2H), 2.32 – 2.14 (m, 1H), 1.86 – 1.74 (m, 2H), 1.66 (m, 2H), 1.54 – 1.41 (m, 2H), 1.03 (t, *J* = 7.4 Hz, 3H), 0.76 (t, *J* = 7.3 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.4, 137.8, 128.7, 114.2, 69.6, 49.0, 29.6, 22.8, 12.3, 10.7.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{14}H_{23}O$: 207.1744; Found: 207.1746.

1-isopropoxy-4-(pentan-3-yl) benzene (1d)



1d

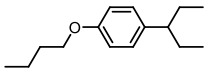
Compound **1d** was isolated via column chromatography (PE) as colorless oil (1.1g, 57% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.03 (d, *J* = 8.6 Hz, 2H), 6.82 (d, *J* = 8.6 Hz, 2H), 4.51 (m, 1H), 2.29 – 2.19 (m, 1H), 1.66 (m, 2H), 1.56 – 1.43 (m, 2H), 1.34 (d, *J* = 6.1 Hz, 6H), 0.77 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.1, 137.9, 128.7, 115.7, 69.9, 49.0, 29.5, 22.3, 12.3.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{14}H_{23}O$: 207.1744; Found: 207.1747.

1-butoxy-4-(pentan-3-yl) benzene (1e)



1e

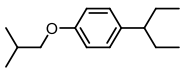
Compound **1e** was isolated via column chromatography (PE) as colorless oil (1.08g, 56% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.04 (d, *J* = 8.6 Hz, 2H), 6.83 (d, *J* = 8.6 Hz, 2H), 3.95 (t, *J* = 6.5 Hz, 2H), 2.26 (m, 1H), 1.77 (m, 2H), 1.66 (m, 2H), 1.55 – 1.43 (m, 4H), 0.98 (t, *J* = 7.4 Hz, 3H), 0.77 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.4, 137.8, 128.7, 114.2, 67.7, 49.0, 31.6, 29.6, 19.5, 14.0, 12.3.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{15}H_{25}O$: 221.1900; Found: 221.1904.

1-isobutoxy-4-(pentan-3-yl) benzene (1f)



1f

Compound **1f** was isolated via column chromatography (PE) as colorless oil (0.96g, 50%

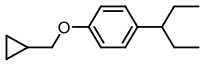
yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.03 (d, *J* = 8.6 Hz, 2H), 6.83 (d, *J* = 8.6 Hz, 2H), 3.70 (d, *J* = 6.5 Hz, 2H), 2.25 (m, 1H), 2.07 (m, 1H), 1.65 (m, 2H), 1.56 – 1.44 (m, 2H), 1.03 (d, *J* = 6.7 Hz, 6H), 0.77 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.51, 137.8, 128.7, 114.3, 74.5, 49.0, 29.6, 28.5, 19.5, 12.4.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{15}H_{25}O$: 221.1900; Found: 221.1905.

1-(cyclopropylmethoxy)-4-(pentan-3-yl) benzene (1g)



1g

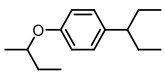
Compound **1g** was isolated via column chromatography (PE) as colorless oil (0.87g, 45% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.03 (d, *J* = 8.6 Hz, 2H), 6.83 (d, *J* = 8.6 Hz, 2H), 3.78 (d, *J* = 6.9 Hz, 2H), 2.25 (m, 1H), 1.72 – 1.59 (m, 2H), 1.49 (m, 2H), 1.33 – 1.20 (m, 1H), 0.76 (t, *J* = 7.4 Hz, 6H), 0.67 – 0.58 (m, 2H), 0.39 – 0.30 (m, 2H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.2, 137.9, 128.7, 114.3, 72.8, 49.0, 29.6, 12.3, 10.5, 3.3.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{15}H_{23}O$: 219.1744; Found: 219.1743.

1-(sec-butoxy)-4-(pentan-3-yl) benzene (1h)



1h

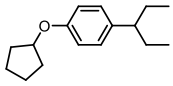
Compound **1h** was isolated via column chromatography (PE) as colorless oil (0.90g, 47% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.09 – 6.95 (m, 2H), 6.87 – 6.75 (m, 2H), 4.26 (m, 1H), 2.25 (m, 1H), 1.81 – 1.58 (m, 4H), 1.55 – 1.42 (m, 2H), 1.29 (d, *J* = 6.1 Hz, 3H), 0.98 (t, *J* = 7.5 Hz, 3H), 0.77 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.42, 137.8, 128.7, 115.8, 75.2, 49.0, 29.5, 29.4, 19.5, 12.4, 10.0.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{15}H_{25}O$: 221.1900; Found: 221.1900.

1-(cyclopentyloxy)-4-(pentan-3-yl) benzene (1i)



1i

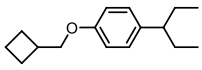
Compound **1i** was isolated via column chromatography (PE) as colorless oil (0.87g, 45% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.01 (d, *J* = 8.6 Hz, 2H), 6.80 (d, *J* = 8.7 Hz, 2H), 4.76 – 4.68 (m, 1H), 2.24 (m, 1H), 1.94 – 1.84 (m, 4H), 1.83 – 1.72 (m, 2H), 1.71 – 1.57 (m, 4H), 1.50 (m, 2H), 0.77 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.3, 137.5, 128.6, 115.3, 79.2, 48.9, 33.1, 29.5, 24.2, 12.4.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{16}H_{25}O$: 233.1900; Found: 233.1903.

1-(cyclobutylmethoxy)-4-(pentan-3-yl) benzene (1j)



1j

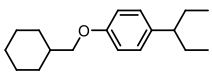
Compound **1j** was isolated via column chromatography (PE: EA=50:1) as colorless oil (0.95g, 49% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.04 (d, *J* = 8.6 Hz, 2H), 6.85 (d, *J* = 8.7 Hz, 2H), 3.92 (d, *J* = 6.7 Hz, 2H), 2.86 – 2.68 (m, 1H), 2.26 (m, 1H), 2.20 – 2.09 (m, 2H), 2.04 – 1.81 (m, 4H), 1.77 – 1.59 (m, 2H), 1.59 – 1.40 (m, 2H), 0.78 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.5, 137.8, 128.7, 114.3, 72.2, 49.0, 34.9, 29. 6, 25.1, 18.8, 12.3.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{16}H_{25}O$: 233.1900; Found: 233.1895.

1-(cyclohexylmethoxy)-4-(pentan-3-yl) benzene (1k)



1k

Compound **1k** was isolated via column chromatography (PE: EA=50:1) as colorless oil (0.95g, 49% yield).

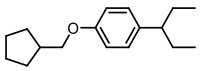
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.03 (d, *J* = 8.6 Hz, 2H), 6.82 (d, *J* = 8.6 Hz, 2H), 3.74 (d, *J* = 6.3 Hz, 2H), 2.25 (m, 1H), 1.93 – 1.83 (m, 2H), 1.83 – 1.59 (m, 6H), 1.57

– 1.44 (m, 2H), 1.37 – 1.17 (m, 3H), 1.06 (m, 2H), 0.77 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.6, 137.7, 128.7, 114.2, 73.6, 49.0, 38.0, 30.1, 29.6, 26.7, 26.0, 12.3.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{18}H_{28}NaO$: 283.2032; Found: 283.2030.

1-(cyclopentylmethoxy)-4-(pentan-3-yl) benzene (1l)



1l

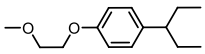
Compound **1l** was isolated via column chromatography (PE) as colorless oil (0.95g, 49% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.04 (d, *J* = 8.5 Hz, 2H), 6.84 (d, *J* = 8.5 Hz, 2H), 3.82 (d, *J* = 6.9 Hz, 2H), 2.36 (m, 1H), 2.26 (m, 1H), 1.94 – 1.77 (m, 2H), 1.73 – 1.57 (m, 6H), 1.51 (m, 2H), 1.44 – 1.30 (m, 2H), 0.77 (t, *J* = 7.3 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.5, 137.7, 128.7, 114.3, 72.3, 49.0, 39.3, 29.7, 29.6, 25.6, 12.3.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{17}H_{27}O$: 247.2057; Found: 247.2055.

1-(2-methoxyethoxy)-4-(pentan-3-yl) benzene (1m)



1m

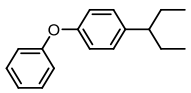
Compound **1m** was isolated via column chromatography (PE: EA=20:1) as yellow oil (1.16g, 60% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.07 – 6.96 (m, 2H), 6.92 – 6.79 (m, 2H), 4.11 (m, 2H), 3.80 – 3.70 (m, 2H), 3.45 (s, 3H), 2.25 (m, 1H), 1.76 – 1.58 (m, 2H), 1.58 – 1.43 (m, 2H), 0.85 – 0.69 (m, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.0, 138.2, 128.7, 114.3, 71.3, 67.3, 59.3, 49.0, 29.5, 12.3.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{14}H_{22}NaO_2$: 245.1512; Found: 245.1512.

1-(pentan-3-yl)-4-phenoxybenzene (1n)



1n

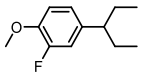
Compound **1n** was isolated via column chromatography (PE: EA=20:1) as yellow oil (1.02g, 53% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.33 (d, *J* = 8.6, 7.4 Hz, 2H), 7.14 – 7.05 (m, 3H), 7.04 – 6.92 (m, 4H), 2.38 – 2.26 (m, 1H), 1.78 – 1.63 (m, 2H), 1.62 – 1.47 (m, 2H), 0.81 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.9, 155.1, 141.0, 129.8, 129.0, 122.9, 119.0, 118.6, 49.2, 29.5, 12.3.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{17}H_{21}O$: 241.1587; Found: 241.1590.

2-fluoro-1-methoxy-4-(pentan-3-yl) benzene (1o)



1o

Compound **1o** was isolated via column chromatography (PE: EA=100:1) as colorless oil (1.06g, 55% yield).

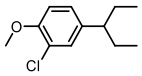
^{1}H NMR (400 MHz, Chloroform-*d*) δ 6.92 – 6.77 (m, 3H), 3.87 (s, 3H), 2.24 (m, 1H), 1.64 (m, 2H), 1.54 – 1.38 (m, 2H), 0.76 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.8, 151.3, 145.7, 145.6, 139.3, 139.2, 123.6, 123.5, 115.2, 115.0, 113.3, 113.3, 56.5, 49.0, 29.5, 12.2.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -136.0.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{12}H_{18}FO$: 197.1336; Found: 197.1332.

2-chloro-1-methoxy-4-(pentan-3-yl) benzene (1p)



1p

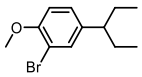
Compound **1p** was isolated via column chromatography (PE: EA=100:1) as colorless oil (1.00g, 52% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.14 (d, *J* = 2.2 Hz, 1H), 6.98 (d, *J* = 8.3, 2.2 Hz, 1H), 6.85 (d, *J* = 8.3 Hz, 1H), 3.88 (s, 3H), 2.24 (m, 1H), 1.65 (m, 2H), 1.55 – 1.38 (m, 2H), 0.76 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.1, 139.2, 129.4, 127.1, 122.1, 112.0, 56.3, 48.89, 29.4, 12.3.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{12}H_{18}ClO$: 213.1041; Found: 213.1040.

2-bromo-1-methoxy-4-(pentan-3-yl) benzene (1q)



1q

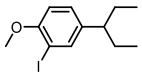
Compound **1q** was isolated via column chromatography (PE) as yellow oil (0.56g, 50% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.31 (d, *J* = 2.1 Hz, 1H), 7.02 (d, *J* = 8.4, 2.2 Hz, 1H), 6.83 (d, *J* = 8.3 Hz, 1H), 3.87 (s, 3H), 2.23 (m, 1H), 1.72 – 1.58 (m, 2H), 1.55 – 1.41 (m, 2H), 0.76 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.0, 139.7, 132.4, 127.9, 111.9, 111.5, 56.4, 48.83, 29.5, 12.3.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{12}H_{18}BrO$: 257.0536; Found: 257.0532.

2-iodo-1-methoxy-4-(pentan-3-yl) benzene (1r)



1r

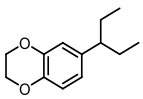
Compound **1r** was isolated via column chromatography (PE) as colorless oil (0.40g, 44% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.54 (d, *J* = 2.1 Hz, 1H), 7.06 (d, *J* = 8.4, 2.1 Hz, 1H), 6.75 (d, *J* = 8.4 Hz, 1H), 3.86 (s, 3H), 2.21 (m, 1H), 1.64 (m, 2H), 1.53 – 1.36 (m, 2H), 0.76 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.3, 140.3, 138.6, 128.9, 110.8, 86.0, 56.5, 48.7, 29.5, 12.3.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{12}H_{18}IO$: 305.0397; Found: 305.0396.

6-(pentan-3-yl)-2,3-dihydrobenzo[*b*] [1,4] dioxine (1s)



1s

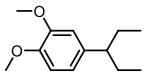
Compound **1s** was isolated via column chromatography (PE: EA=10:1) as colorless oil (0.98g, 51% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 6.78 (d, *J* = 8.2 Hz, 1H), 6.70 – 6.53 (m, 2H), 4.24 (m, 4H), 2.20 (m, 1H), 1.63 (m, 2H), 1.55 – 1.42 (m, 2H), 0.77 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 143.3, 141.6, 139.4, 120.9, 116.8, 116.3, 64.6, 64.45, 49.1, 29.5, 12.3.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{13}H_{19}O_2$: 207.1380; Found: 207.1379.

1,2-dimethoxy-4-(pentan-3-yl) benzene (1t)



1t

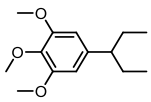
Compound **1t** was isolated via column chromatography (PE) as yellow oil (1.02g, 53% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 6.80 (d, *J* = 8.0 Hz, 1H), 6.71 – 6.59 (m, 2H), 3.87 (d, *J* = 5.6 Hz, 6H), 2.24 (m, 1H), 1.75 – 1.61 (m, 2H), 1.56 – 1.43 (m, 2H), 0.77 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 148.8, 147.2, 138.6, 119.9, 111.0, 110.9, 55.9, 55.9, 49.5, 29.5, 12.3.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{13}H_{21}O_2$: 209.1536; Found: 209.1538.

1,2,3-trimethoxy-5-(pentan-3-yl) benzene (1u)



1u

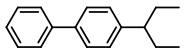
Compound **1u** was isolated via column chromatography (PE: EA=10:1) as colorless oil (0.93g, 48% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 6.34 (s, 2H), 3.84 (s, 6H), 3.83 (s, 3H), 2.22 (m, 1H), 1.76 – 1.58 (m, 3H), 1.58 – 1.40 (m, 2H), 0.79 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.1, 141.9, 136.1, 104.7, 61.0, 56.2, 50.3, 29.4, 12.4.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{14}H_{23}O_3$: 239.1642; Found: 239.1638.

4-(pentan-3-yl)-1,1'-biphenyl (1v)



1v

Compound **1v** was isolated via column chromatography (PE: EA=10:1) as white solid (0.90g, 47% yield).

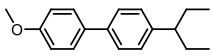
Melting Point: 61.1-61.6℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.62 – 7.57 (m, 2H), 7.55 – 7.49 (m, 2H), 7.45 – 7.39 (m, 2H), 7.35 – 7.28 (m, 1H), 7.24 – 7.17 (m, 2H), 2.36 (m, 1H), 1.71 (m, 2H), 1.65 – 1.56 (m, 2H), 0.81 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 145.1, 141.3, 138.8, 128.8, 128.4, 127.1, 127.0, 127.0, 49.5, 29.4, 12.4.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{17}H_{21}$: 225.1638; Found: 225.1633.

4-methoxy-4'-(pentan-3-yl)-1,1'-biphenyl (1w)



1w

Compound **1w** was isolated via column chromatography (PE: EA=10:1) as white solid (1.06g, 55% yield).

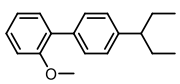
Melting Point: 89.2-90.3℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.54 (d, *J* = 8.8 Hz, 2H), 7.48 (d, *J* = 8.2 Hz, 2H), 7.18 (d, *J* = 8.2 Hz, 2H), 6.97 (d, *J* = 8.8 Hz, 2H), 3.85 (s, 3H), 2.42 – 2.27 (m, 1H), 1.77 – 1.66 (m, 2H), 1.65 – 1.55 (m, 2H), 0.81 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.0, 144.5, 138.4, 134.0, 128.3, 128.1, 126.6, 114.3, 55.5, 49.5, 29.4, 12.4.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{18}H_{23}O$: 255.1744; Found: 255.1745.

2-methoxy-4'-(pentan-3-yl)-1,1'-biphenyl (1x)



1x

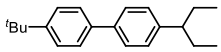
Compound **1x** was isolated via column chromatography (PE: EA=10:1) as colorless oil (1.00g, 52% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.47 (d, *J* = 8.2 Hz, 2H), 7.37 – 7.27 (m, 2H), 7.17 (d, *J* = 8.2 Hz, 2H), 7.06 – 6.94 (m, 2H), 3.82 (s, 3H), 2.43 – 2.28 (m, 1H), 1.72 (m, 2H), 1.66 – 1.55 (m, 2H), 0.83 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.6, 144.6, 136.0, 131.1, 130.8, 129.3, 128.4, 127.6, 120.9, 111.4, 55.7, 49.5, 29.3, 12.4.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{18}H_{23}O$: 255.1744; Found: 255.1745.

4-(tert-butyl)-4'-(pentan-3-yl)-1,1'-biphenyl (1y)



1y

Compound **1y** was isolated via column chromatography (PE: EA=10:1) as white solid (1.06g, 55% yield).

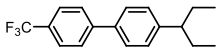
Melting Point: 52.6-53.1℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.58 – 7.48 (m, 4H), 7.45 (d, *J* = 8.4 Hz, 2H), 7.19 (d, *J* = 8.2 Hz, 2H), 2.35 (m, 1H), 1.71 (m, 2H), 1.65 – 1.55 (m, 2H), 1.36 (s, 9H), 0.81 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 150.0, 144.8, 138.6, 138.5, 128.3, 126.8, 126.7, 125.8, 49.5, 34.6, 31.5, 29.4, 12.4.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{21}H_{29}$: 281.2264; Found: 281.2260.

4-(pentan-3-yl)-4'-(trifluoromethyl)-1,1'-biphenyl (1z)



1z

Compound **1z** was isolated via column chromatography (PE: EA=10:1) as colorless oil (0.45g, 23% yield).

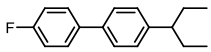
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.75 – 7.62 (m, 4H), 7.57 – 7.51 (m, 2H), 7.27 – 7.23 (m, 2H), 2.40 (m, 1H), 1.74 (m, 2H), 1.67 – 1.58 (m, 2H), 0.83 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 146.3, 144.9, 137.3, 128.6, 127.3, 127.2, 125.8, 125.8, 49.6, 29.4, 12.4.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.3.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{18}H_{20}F_3$: 293.1512; Found: 293.1510.

4-fluoro-4'-(pentan-3-yl)-1,1'-biphenyl (1aa)



1aa

Compound **1aa** was isolated via column chromatography (PE: EA=10:1) as white solid (0.42g, 22% yield).

Melting Point: 90.8-91.5℃.

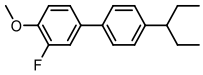
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.55 (dd, *J* = 8.8, 5.4 Hz, 2H), 7.47 (d, *J* = 8.2 Hz, 2H), 7.20 (d, *J* = 8.2 Hz, 2H), 7.11 (t, *J* = 8.7 Hz, 2H), 2.37 (m, 1H), 1.81 – 1.66 (m, 2H), 1.65 – 1.55 (m, 2H), 0.81 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 163.6, 161.2, 145.2, 137.8, 128.6, 128.4, 126.9, 115.8, 115.5, 49.5, 29.4, 12.4.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -116.4.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{17}H_{20}F$: 243.1544; Found: 243.1547.

3-fluoro-4-methoxy-4'-(pentan-3-yl)-1,1'-biphenyl (1ab)



1ab

Compound **1ab** was isolated via column chromatography (PE: EA=10:1) as yellow oil (0.68g, 35% yield).

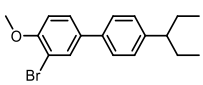
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.46 (d, *J* = 8.2 Hz, 2H), 7.38 – 7.28 (m, 2H), 7.22 – 7.15 (m, 2H), 7.02 (t, *J* = 8.3 Hz, 1H), 3.93 (s, 3H), 2.44 – 2.24 (m, 1H), 1.72 (m, 2H), 1.64 – 1.57 (m, 1H), 1.56 – 1.51 (m, 1H), 0.81 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.0, 151.5, 146.9, 146.8, 145.2, 137.3, 137.3, 134.7, 134.7, 128.4, 126.5, 122.5, 122.5, 114.8, 114.7, 113.8, 113.8, 56.5, 49.5, 29.4, 12.4.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -135.3.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{18}H_{22}FO$: 273.1649; Found: 273.1646.

3-bromo-4-methoxy-4'-(pentan-3-yl)-1,1'-biphenyl (1ac)



1ac

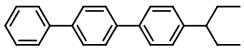
Compound **1ac** was isolated via column chromatography (PE: EA=10:1) as yellow oil (0.3g, 50% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.80 (d, *J* = 2.2 Hz, 1H), 7.50 (dd, *J* = 8.5, 2.3 Hz, 1H), 7.47 – 7.42 (m, 2H), 7.22 – 7.15 (m, 2H), 6.96 (d, *J* = 8.5 Hz, 1H), 3.93 (s, 3H), 2.36 (m, 1H), 1.79 – 1.65 (m, 2H), 1.64 – 1.52 (m, 3H), 0.81 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.2, 145.1, 137.0, 135.4, 131.9, 128.4, 126.9, 126.6, 112.2, 112.1, 56.5, 49.5, 29.4, 12.4.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{18}H_{22}BrO$: 333.0849; Found: 333.0846.

4-(pentan-3-yl)-1,1':4',1''-terphenyl (1ad)



1ad

Compound **1ad** was isolated via column chromatography (PE) as white solid (0.82g, 42% yield).

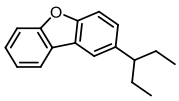
Melting Point: 195.3-196.5℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.73 – 7.65 (m, 6H), 7.62 – 7.58 (m, 2H), 7.49 (m, 2H), 7.42 – 7.35 (m, 1H), 7.25 (d, *J* = 8.2 Hz, 2H), 2.40 (m, 1H), 1.76 (m, 2H), 1.69 – 1.58 (m, 2H), 0.85 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 145.3, 141.0, 140.3, 139.9, 138.2, 128.9, 128.4, 127.6, 127.4, 127.4, 127.2, 126.9, 49.5, 29.4, 12.4.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{25}$: 301.1951; Found: 301.1950.

2-(pentan-3-yl)dibenzo[b,d]furan (1ae)



1ae

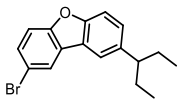
Compound **1ae** was isolated via column chromatography (PE) as colorless oil (1.50g, 52% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.00 – 7.93 (m, 1H), 7.74 (d, *J* = 1.8 Hz, 1H), 7.58 (m, 1H), 7.51 (d, *J* = 8.4 Hz, 1H), 7.45 (m, 1H), 7.35 (m, 1H), 7.28 – 7.23 (m, 1H), 2.50 (m, 1H), 1.86 – 1.74 (m, 2H), 1.72 – 1.61 (m, 2H), 0.83 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.6, 155.0, 140.5, 127.1, 127.0, 124.6, 124.2, 122.6, 120.7, 119.6, 111.8, 111.3, 49.9, 30.0, 12.4.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{17}H_{19}O$: 239.1431; Found: 239.1430.

2-bromo-8-(pentan-3-yl)dibenzo[b,d]furan (1af)



1af

Compound **1af** was isolated via column chromatography (PE) as colorless oil (0.93g, 48% yield).

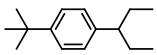
Melting Point: 39.5-40.2℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.07 (d, *J* = 2.0 Hz, 1H), 7.66 (d, *J* = 1.8 Hz, 1H), 7.54 – 7.45 (m, 2H), 7.42 (d, *J* = 8.7 Hz, 1H), 7.29 – 7.24 (m, 1H), 2.51 – 2.43 (m, 1H), 1.84 – 1.72 (m, 2H), 1.68 – 1.57 (m, 2H), 0.80 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.4, 155.3, 140.9, 129.7, 127.9, 126.6, 123.6, 123.2, 119.7, 115.5, 113.3, 111.5, 49.9, 29.9, 12.4.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{17}H_{18}BrO$: 317.0536; Found: 317.0536.

1-(tert-butyl)-4-(pentan-3-yl) benzene (1aj)



1aj

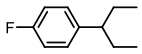
Compound **1aj** was isolated via column chromatography (PE) as colorless oil (1.03g, 67% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.34 – 7.27 (m, 2H), 7.11 – 7.04 (m, 2H), 2.30 (m, 1H), 1.69 (m, 2H), 1.63 – 1.48 (m, 2H), 1.33 (s, 9H), 0.80 (t, J = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 148.5, 142.8, 127.5, 125.1, 49.2, 34.5, 31.6, 29.3, 12.4.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{15}H_{25}$: 205.1951; Found: 205.1950.

1-fluoro-4-(pentan-3-yl) benzene (1ak)



1ak

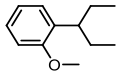
Compound **1ak** was isolated via column chromatography (PE) as colorless oil (1.50 g, 79% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.08 (m, 2H), 7.04 – 6.92 (m, 2H), 2.31 (m, 1H), 1.74 – 1.63 (m, 2H), 1.57 – 1.44 (m, 2H), 0.76 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 129.2, 129.1, 115.1, 114.9, 49.1, 29.6, 12.3.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -118.0.

1-methoxy-2-(pentan-3-yl) benzene (1al)



1al

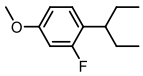
Compound **1al** was isolated via column chromatography (PE) as colorless oil (1.4 g, 73% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.20 – 7.09 (m, 2H), 6.97 – 6.83 (m, 2H), 3.81 (s, 3H), 2.94 (m, 1H), 1.73 – 1.51 (m, 4H), 0.78 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.0, 134.2, 127.6, 126.5, 120.6, 110.7, 55.6, 41.0, 28.1, 12.2.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{12}H_{19}O$: 179.1431; Found: 179.1428.

2-fluoro-4-methoxy-1-(pentan-3-yl) benzene (1am)



1am

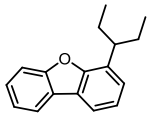
Compound **1am** was isolated via column chromatography (PE) as colorless oil (0.98 g, 49% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.05 (t, *J* = 8.5 Hz, 1H), 6.66 (m, 1H), 6.58 (dd, *J* = 12.0, 2.6 Hz, 1H), 3.78 (s, 3H), 2.68 (m, 1H), 1.76 – 1.62 (m, 2H), 1.61 – 1.47 (m, 2H), 0.79 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.8, 129.0, 128.9, 124.2, 124.0, 109.9, 109.9, 101.5, 101.2, 55.6, 41.5, 28.4, 28.4, 12.2.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{12}H_{18}FO$: 197.1336; Found: 197.1332.

4-(pentan-3-yl)dibenzo[b,d]furan (1an)



1an

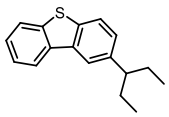
Compound **1an** was isolated via column chromatography (PE) as colorless oil (1.11 g, 39% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.94 (m, 1H), 7.78 (dd, *J* = 7.4, 1.6 Hz, 1H), 7.57 (dd, *J* = 8.2, 0.8 Hz, 1H), 7.43 (m, 1H), 7.35 – 7.21 (m, 3H), 3.05 (m, 1H), 1.93 – 1.74 (m, 4H), 0.82 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.1, 155.2, 130.0, 126.9, 126.0, 124.8, 123.9, 122.9, 122.6, 120.7, 118.0, 111.8, 44.0, 28.2, 12.4.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{12}H_{19}O$: 239.1431; Found: 239.1434.

2-(pentan-3-yl)dibenzo[b,d]thiophene (1ao)



1ao

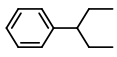
Compound **1ao** was isolated via column chromatography (PE) as colorless oil (1.04 g, 54% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.19 – 8.11 (m, 1H), 7.91 (d, *J* = 1.7 Hz, 1H), 7.87 – 7.80 (m, 1H), 7.76 (d, *J* = 8.3 Hz, 1H), 7.47 – 7.37 (m, 2H), 7.28 – 7.21 (m, 1H), 2.49 (m, 1H), 1.78 (m, 2H), 1.72 – 1.57 (m, 2H), 0.81 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 142.4, 139.9, 137.0, 135.8, 135.7, 127.0, 126.6, 124.3, 123.0, 122.6, 121.6, 120.9, 50.0, 29.8, 12.4.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{17}H_{19}S$: 255.1202; Found: 255.1206.

pentan-3-ylbenzene (1ap)



1ap

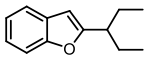
Compound **1ap** was isolated via column chromatography (PE) as colorless oil (0.73 g, 39% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.31 – 7.23 (m, 2H), 7.21 – 7.09 (m, 3H), 2.30 (m, 1H), 1.69 (m, 2H), 1.61 – 1.48 (m, 2H), 0.77 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 146.0, 128.3, 128.0, 125.9, 49.9, 29.4, 12.3.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{11}H_{17}$: 149.1325; Found: 149.1327.

2-(pentan-3-yl) benzofuran (1aq)



1aq

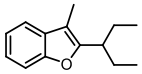
Compound **1aq** was isolated via column chromatography (PE) as colorless oil (1.27 g, 58% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.61 – 7.45 (m, 2H), 7.33 – 7.19 (m, 2H), 6.49 – 6.40 (m, 1H), 2.71 (m, 1H), 1.87 – 1.75 (m, 4H), 0.96 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.3, 154.8, 129.0, 123.0, 122.4, 120.3, 110.9, 102.4, 43.0, 26.5, 11.9.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{13}H_{17}O$: 189.1274; Found: 189.1275.

3-methyl-2-(pentan-3-yl) benzofuran (1ar)



1ar

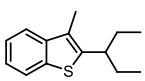
Compound **1ar** was isolated via column chromatography (PE) as colorless oil (1.30 g, 85% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.46 – 7.34 (m, 2H), 7.23 – 7.15 (m, 2H), 2.65 (m, 1H), 2.16 (s, 3H), 1.82 – 1.62 (m, 4H), 0.81 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.2, 154.1, 130.6, 123.0, 121.9, 118.7, 111.0, 110.7, 41.3, 27.2, 12.4, 8.1.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{14}H_{19}O$: 203.1431; Found: 203.1433.

3-methyl-2-(pentan-3-yl) benzo[b]thiophene (1as)



1as

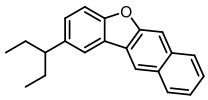
Compound **1as** was isolated via column chromatography (PE) as colorless oil (2.24 g, 76% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.80 (m, 1H), 7.65 (m, 1H), 7.37 (m, 1H), 7.31 – 7.25 (m, 1H), 2.95 (m, 1H), 2.35 (s, 3H), 1.86 – 1.75 (m, 2H), 1.69 – 1.58 (m, 2H), 0.88 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 144.9, 141.1, 138.4, 127.5, 123.7, 123.5, 122.4, 121.3, 43.3, 30.8, 12.4, 12.1.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{14}H_{19}S$: 219.1202; Found: 219.1205.

2-(pentan-3-yl) naphtho[2,3-b]benzofuran (1at)



1at

Compound **1at** was isolated via column chromatography (PE) as white solid (0.72 g, 74% yield).

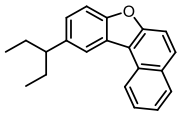
Melting Point: 79.6-80.3℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.41 (s, 1H), 8.03 (d, *J* = 8.0 Hz, 1H), 7.97 (d, *J* = 7.7 Hz, 1H), 7.91 (s, 1H), 7.84 (d, *J* = 1.9 Hz, 1H), 7.55 – 7.45 (m, 3H), 7.30 (m, 1H), 2.52 (m, 1H), 1.88 – 1.75 (m, 2H), 1.74 – 1.60 (m, 2H), 0.87 – 0.80 (m, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.4, 155.4, 140.6, 133.1, 130.3, 128.5, 128.3, 127.9, 125.9, 125.8, 124.3, 123.9, 120.3, 119.1, 111.2, 107.0, 49.9, 29.9, 12.5.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{21}H_{21}O$: 289.1587; Found: 289.1591.

10-(pentan-3-yl) naphtho[2,1-b]benzofuran (1au)



1au

Compound **1au** was isolated via column chromatography (PE) as white solid (0.61 g, 63% yield).

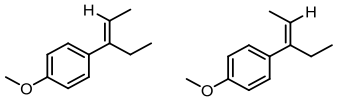
Melting Point: 59.1-61.2℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.65 (m, 1H), 8.15 (d, *J* = 1.7 Hz, 1H), 8.06 – 8.00 (m, 1H), 7.91 (d, *J* = 8.9 Hz, 1H), 7.79 – 7.71 (m, 2H), 7.63 (d, *J* = 8.5 Hz, 1H), 7.55 (m, 1H), 7.33 – 7.27 (m, 1H), 2.59 (m, 1H), 1.85 (m, 2H), 1.78 – 1.65 (m, 2H), 0.86 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.7, 154.7, 141.0, 130.6, 129.4, 129.3, 128.4, 127.2, 125.7, 125.0, 124.4, 123.7, 121.1, 117.6, 113.0, 111.5, 50.2, 30.1, 12.5.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{21}H_{21}O$: 289.1587; Found: 289.1589.

(*E*/*Z*)-1-methoxy-4-(pent-2-en-3-yl) benzene (1D(*E*)/ 1D(*Z*))



1D(*E*) **1D(*Z*)**

Compounds **1D(*E*)** and **1D(*Z*)** are mixture, and the compounds was isolated via column chromatography (PE) as colorless oil (2g, 60% yield).

1D(*E*) ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.27 (d, *J* = 8.8 Hz, 2H), 6.84 (d, *J* = 8.8 Hz, 2H), 5.65 (m, 1H), 3.80 (s, 3H), 2.56 – 2.38 (m, 2H), 1.78 (d, *J* = 6.9 Hz, 3H), 0.98 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.5, 141.8, 135.8, 127.3, 120.7, 113.7, 55.4, 22.8, 14.0, 13.4.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{12}H_{17}O$: 177.1274; Found: 177.1275.

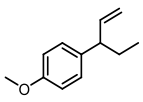
Spectra are consistent with reported literature values.[11]

1D(*Z*) ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.08 (d, *J* = 8.7 Hz, 2H), 6.88 (d, *J* = 8.7 Hz, 2H), 5.50 (m, 1H), 3.82 (s, 3H), 2.32 (m, 2H), 1.56 (d, *J* = 6.9 Hz, 3H), 0.95 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.2, 143.0, 133.7, 129.7, 119.6, 113.5, 55.3, 32.2, 14.8, 13.3.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{12}H_{17}O$: 177.1274; Found: 177.1275.

1-methoxy-4-(pent-1-en-3-yl) benzene (1D-T)



1D-T

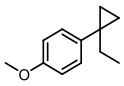
Compound **1D-T** was isolated via column chromatography (PE) as colorless oil (1g, 30% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.12 (d, *J* = 8.7 Hz, 2H), 6.86 (d, *J* = 8.7 Hz, 2H), 5.94 (m, 1H), 5.08 – 4.94 (m, 2H), 3.80 (s, 3H), 3.11 (q, *J* = 7.4 Hz, 1H), 1.80 – 1.63 (m, 2H), 0.88 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.1, 142.7, 136.7, 128.6, 113.9, 113.8, 55.4, 50.9, 28.5.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{12}H_{17}O$: 177.1274; Found: 177.1270.

1-(1-ethylcyclopropyl)-4-methoxybenzene (1D-C)



1D-C

Compound **1D-C** was isolated via column chromatography (PE) as colorless oil (0.78g, 56% yield).

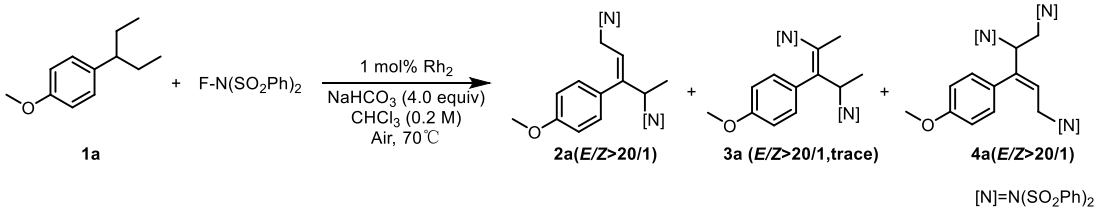
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.25 – 7.19 (dd, 2H), 6.86 – 6.80 (dd, 2H), 3.80 (s, 3H), 1.54 (q, *J* = 7.4 Hz, 2H), 0.84 (t, *J* = 7.3 Hz, 3H), 0.76 – 0.71 (m, 2H), 0.65 – 0.60(m, 2H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.8, 137.6, 130.3, 113.5, 55.4, 33.5, 26.3, 12.8, 11.5.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{12}H_{17}O$: 177.1274; Found: 177.1276.

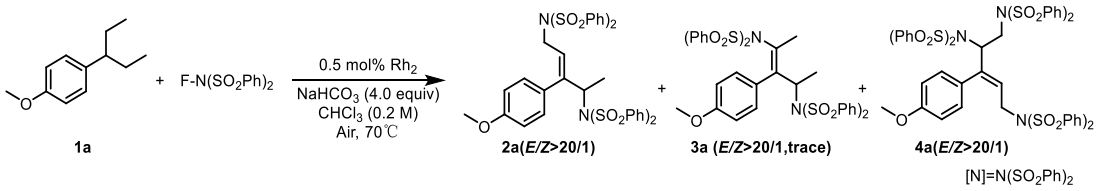
4. Synthesis and Characterizations of Products

4.1: General procedure for the synthesis of 1,4-diamines



To a reaction tube charged with NFSI (630 mg, 2.0 mmol), $NaHCO_3$ (135 mg, 1.6 mmol), $Rh_2(esp)_2$ (3 mg, 0.004 mmol) was added a solution of substrate **1a** (72 mg, 0.4 mmol) in $CHCl_3$ (2 mL). The mixture was stirred for 1 h at 70°C in oil bath. After the reaction was completed, the solvent was evaporated and the organic product purified by column chromatography (petroleum ether/EtOAc= 3/1, v/v), giving the expected product **2a** (200 mg, 65%) as a white solid.

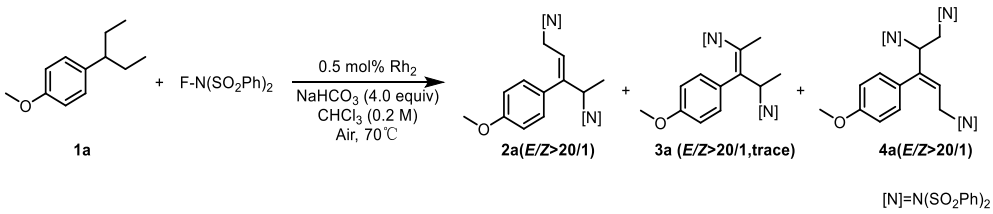
4.2: Gram-scale reaction



To a reaction tube charged with NFSI (6.3 g, 20 mmol), $NaHCO_3$ (1.35 g, 16 mmol), $Rh_2(esp)_2$ (15 mg, 0.02 mmol) was added a solution of substrate **1a** (0.72 g, 4 mmol) in $CHCl_3$ (20 mL). The mixture was stirred for 1 h at 70°C in oil bath. After the reaction was completed, the solvent was evaporated and the organic product purified by column chromatography (petroleum ether/EtOAc= 3/1, v/v), giving the expected product **2a** (1.72 g, 56%) as a white solid.

4.3: Mechanism Experiments

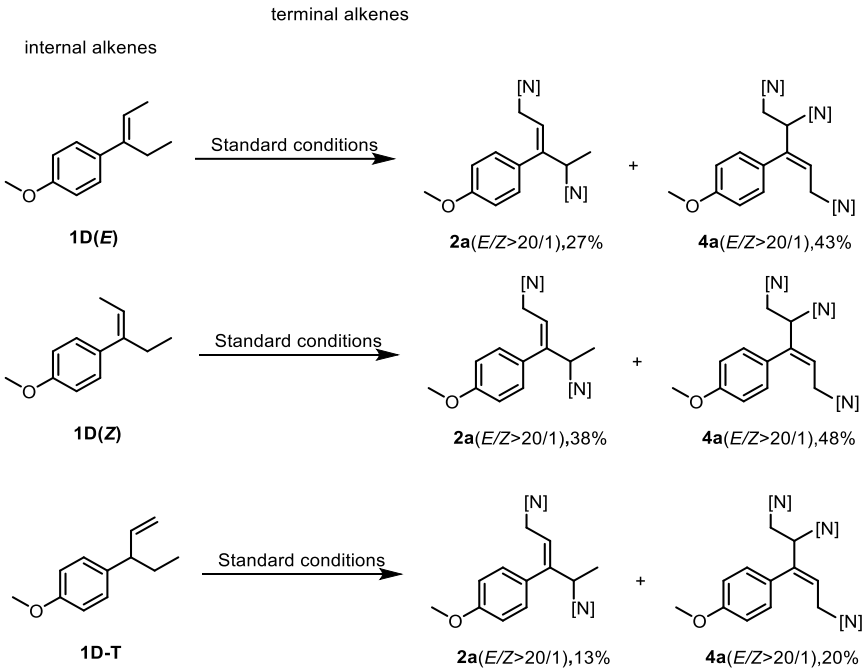
4.3.1: Radical inhibitor Experiments



Radical inhibitor (1 equiv)	Yield (%) of **2a**
Tempo	52%
BHT	30%

To a reaction tube charged with NFSI (630 mg, 2.0 mmol), $NaHCO_3$ (135 mg, 1.6 mmol), $Rh_2(esp)_2$ (3 mg, 0.004 mmol) was added a solution of substrate **1a** (72 mg, 0.4 mmol) in $CHCl_3$ (2 mL). Then TEMPO (63 mg, 0.4 mmol) or BHT (88 mg, 0.4 mmol) was added. The mixture was stirred for 1 h at 70°C in oil bath. After the reaction was completed, the solvent was evaporated and the organic product purified by column chromatography (petroleum ether/EtOAc= 3/1, v/v), giving the expected product **2a**. Compared with standard conditions, the yield of compound **2a** is significantly reduced.

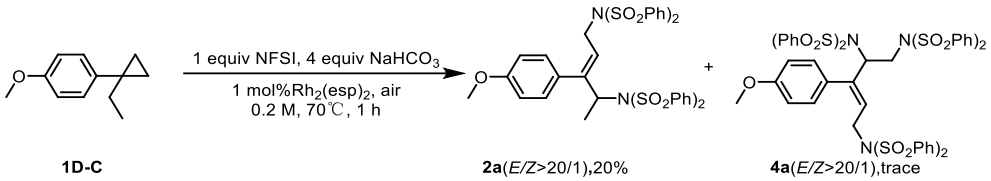
4.3.2: Possible olefin intermediate experiments



To a reaction tube charged with NFSI (315 mg, 1.0 mmol), $NaHCO_3$ (67 mg, 0.8 mmol), $Rh_2(esp)_2$ (1.5 mg, 0.002 mmol) was added a solution of substrate **1D(*E*)** (35 mg, 0.2 mmol) or **1D(*Z*)** (35 mg, 0.2 mmol) or **1D-T** (35 mg, 0.2 mmol) in $CHCl_3$ (2 mL), respectively. The mixture was stirred for 1 h at 70°C in oil bath. After the reaction was completed, the reaction mixture was quenched with triethylamine, extracted with dichloromethane. The combined organic extracts were dried over Na_2SO_4, concentrated in vacuum. The obtained residue was added with pyrazine as an internal standard, and

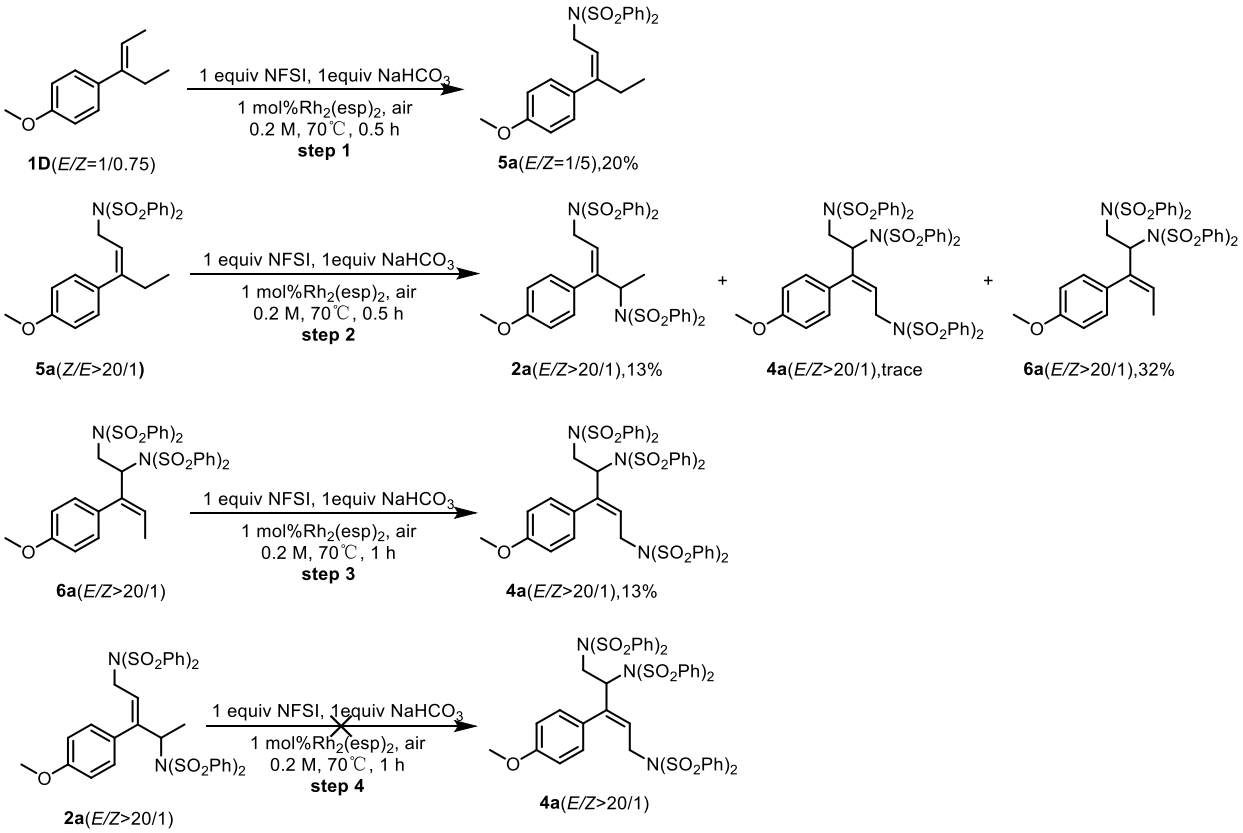
the yield of the product was checked by quantitative nuclear magnetic resonance.

4.3.3: cyclopropane intermediate experiments



To a reaction tube charged with NFSI (126 mg, 0.4 mmol), $NaHCO_3$ (135 mg, 1.6 mmol), $Rh_2(esp)_2$ (3 mg, 0.004 mmol) was added a solution of substrate **1D-C** (70 mg, 0.4 mmol) in $CHCl_3$ (2 mL). The mixture was stirred for 1 h at 70°C in oil bath. After the reaction was completed, the reaction mixture was quenched with triethylamine, extracted with dichloromethane. The combined organic extracts were dried over Na_2SO_4, concentrated in vacuum. The obtained residue was added with pyrazine as an internal standard, and the yield of the product was checked by quantitative nuclear magnetic resonance.

4.3.4: Intermediate verification experiments



Step 1: To a reaction tube charged with NFSI (63 mg, 0.2 mmol), $NaHCO_3$ (17 mg,

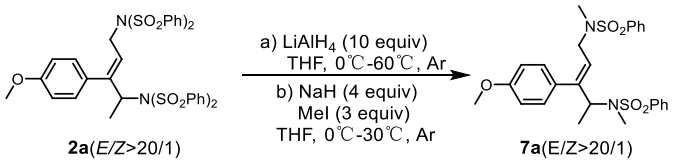
0.2 mmol), $Rh_2(esp)_2$ (1.5 mg, 0.002 mmol) was added a solution of substrate **1D** (35 mg, 0.2 mmol) in $CHCl_3$ (1 mL). The mixture was stirred for 0.5 h at 70°C in oil bath. After the reaction was completed, the solvent was evaporated and the organic product purified by column chromatography (petroleum ether/EtOAc= 3/1, v/v), giving the expected product **5a** (19 mg, 20%) as a white solid.

Step 2: To a reaction tube charged with NFSI (63 mg, 0.2 mmol), $NaHCO_3$ (17 mg, 0.2 mmol), $Rh_2(esp)_2$ (1.5 mg, 0.002 mmol) was added a solution of substrate **5a(***Z/E*>20/1**)** (94 mg, 0.2 mmol) in $CHCl_3$ (1 mL). The mixture was stirred for 0.5 h at 70°C in oil bath. After the reaction was completed, the reaction mixture was quenched with triethylamine, extracted with dichloromethane. The combined organic extracts were dried over Na_2SO_4, concentrated in vacuum. The obtained residue was added with pyrazine as an internal standard, and the yield of the product was checked by quantitative nuclear magnetic resonance.

Step 3: To a reaction tube charged with NFSI (63 mg, 0.2 mmol), $NaHCO_3$ (17 mg, 0.2 mmol), $Rh_2(esp)_2$ (1.5 mg, 0.002 mmol) was added a solution of substrate **6a** (153 mg, 0.2 mmol) in $CHCl_3$ (1 mL). The mixture was stirred for 1 h at 70°C in oil bath. After the reaction was completed, the solvent was evaporated and the organic product purified by column chromatography (petroleum ether/EtOAc= 3/1, v/v), giving the expected product **4a** (34 mg, 13%) as a white solid.

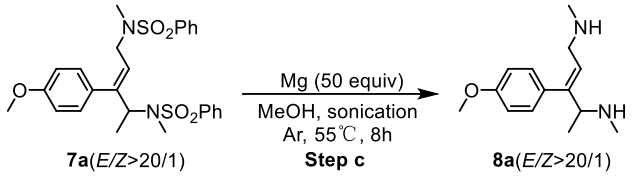
Step 4: To a reaction tube charged with NFSI (63 mg, 0.2 mmol), $NaHCO_3$ (17 mg, 0.2 mmol), $Rh_2(esp)_2$ (1.5 mg, 0.002 mmol) was added a solution of substrate **2a** (153 mg, 0.2 mmol) in $CHCl_3$ (1 mL). The mixture was stirred for 1 h at 70°C in oil bath. After the reaction was completed, the reaction mixture was quenched with triethylamine, extracted with dichloromethane. The combined organic extracts were dried over Na_2SO_4, concentrated in vacuum. The obtained residue was added with pyrazine as an internal standard, and the yield of the product was checked by quantitative nuclear magnetic resonance.

4.3.5: Synthetic applications



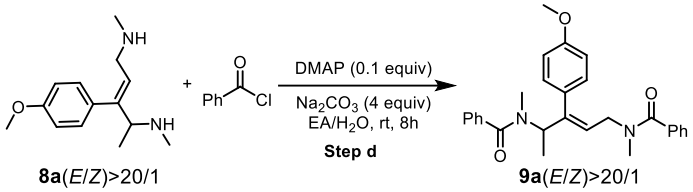
Step a: To a solution of **2a** (400 mg, 0.52 mmol) in dry THF (0.1 M) was added dropwise LAH (1 mol/L, 5.2 mL) at 0°C under Ar atmosphere. Then the reaction was stirred at 60℃ for about 6 h and the progress of the reaction was monitored by TLC. Upon completion, the reaction was quenched with THF/H_2O=10/1, and then 1 mol/L HCl was added until the system was a white emulsion. The product was extracted with EtOAc, and the combined organic layers removed under reduced pressure and the corresponding monoamination product was obtained after silica gel column chromatography (petroleum ether/ethyl acetate = 1/1).

Step b: The above product was dissolved in dry THF at 0 °C under Ar atmosphere, and NaH (4 eq) and MeI (3 eq) were added. The reaction was stirred at 30℃ for about 1 h and the progress of the reaction was monitored by TLC. Upon completion, Water was added dropwise, followed by extraction with EtOAc (×3). The combined organics were dried Na_2SO_4, filtered, and concentrated under reduced pressure. The crude material was purified by silica gel chromatography (petroleum ether/ethyl acetate = 3/1) to yield the desired product.



Step c: To a 50 mL tube charged with **7a** (100 mg), Mg powder (240 mg, 50 eq) was added. The tube was evacuated and backfilled with Ar atmosphere for three times. 5 mL MeOH was then added. After sonicated for 8 hours at 55℃, 1 M HCl was added to tune the mixture pH to 1. Then excess Na_2CO_3 was added to the reaction mixture until no gas evolution. The organic solvent was removed under reduced pressure, and the white solid residue was dissolved in EA/MeOH (1:1), and the mixture was filtered through a pad of Celite. The organic solvent was removed under vacuum, and the residue was purified by silica gel chromatography (DCM /MeOH = 10/1) to yield the

desired product.

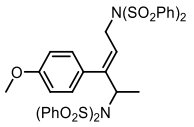


8a(*E*/*Z*)>20/1 **9a**(*E*/*Z*)>20/1

Step d: To a solution of **8a** (40 mg) in EtOAc (0.1 M) at room temperature was added DMAP (0.1 equiv), 15% sodium carbonate was then added under an air atmosphere. Finally, benzoyl chloride (3 equiv) was added. The reaction was stirred at room temperature for about 8h and the progress of the reaction was monitored by TLC. Upon completion, Water was added, followed by extraction with EtOAc (×3). The combined organics were dried Na_2SO_4, filtered, and concentrated under reduced pressure. The crude material was purified by silica gel chromatography (ethyl acetate) to yield the desired product **9a**.

4.4: Characterization data of products

(*E*)-*N*,*N*'-(3-(4-methoxyphenyl)pent-2-ene-1,4-diyl)bis(*N*-(phenylsulfonyl) benzenesulfonamide) (2a)



2a

Compound **2a** was isolated via column chromatography (PE: EA= 3: 1) as white solid (200 mg, 65% yield).

Melting Point: 135.1-136.0℃.

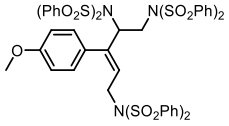
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.00 – 7.75 (m, 8H), 7.64 – 7.56 (m, 4H), 7.47 (m, 8H), 6.91 (d, *J* = 8.4 Hz, 2H), 6.74 (d, *J* = 8.4 Hz, 2H), 5.73 (m, 1H), 5.23 – 5.09 (m, 1H), 4.29 (m, 1H), 4.07 (dd, *J* = 17.4, 7.2 Hz, 1H), 3.81 (s, 3H), 1.36 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.2, 141.8, 139.9, 133.9, 133.7, 130.3, 129.2, 129.0, 128.8, 128.6, 128.3, 125.6, 113.7, 62.0, 55.3, 48.3, 18.6.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{36}H_{34}N_2NaO_9S_4$: 789.1039; Found: 789.1038.

(*E*)-*N*,*N*',*N*''-(3-(4-methoxyphenyl)pent-3-ene-1,2,5-triyl)tris(*N*-(phenylsulfonyl)

benzenesulfonamide) (4a)



4a

Compound **4a** was isolated via column chromatography (PE: EA= 2: 1) as white solid (25 mg, 6% yield).

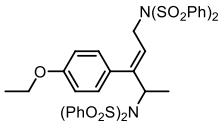
Melting Point: 134.7-135.6℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.18 – 8.03 (m, 6H), 7.95 – 7.88 (m, 4H), 7.72 – 7.62 (m, 5H), 7.57 (m, 6H), 7.51 – 7.39 (m, 7H), 7.28 – 7.21 (m, 2H), 6.74 – 6.62 (m, 2H), 6.31 (d, *J* = 8.2 Hz, 2H), 5.94 (m, *J* = 20.2, 7.5, 3.8 Hz, 2H), 4.60 (dd, *J* = 15.4, 7.1 Hz, 1H), 4.24 (m, 2H), 3.98 (dd, *J* = 17.7, 7.9 Hz, 1H), 3.78 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.4, 140.8, 139.8, 139.6, 138.4, 137.5, 134.4, 134.0, 134.0, 133.6, 130.5, 130.5, 130.0, 129.6, 129.5, 129.3, 129.2, 128.7, 128.6, 128.3, 113.6, 65.2, 55.3, 50.3, 48.1.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{48}H_{43}N_3NaO_{13}S_6$: 1084.1012; Found: 1084.1015.

(*E*)-*N*,*N*'-(3-(4-ethoxyphenyl)pent-2-ene-1,4-diyl)bis(*N*-(phenylsulfonyl) benzenesulfonamide) (2b)



2b

Compound **2b** was isolated via column chromatography (PE: EA= 3: 1) as white solid (200 mg, 64% yield).

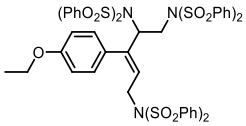
Melting Point: 126.7-127.4℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.04 – 7.69 (m, 8H), 7.66 – 7.54 (m, 4H), 7.54 – 7.36 (m, 8H), 6.90 (d, *J* = 8.7 Hz, 2H), 6.73 (d, *J* = 8.7 Hz, 2H), 5.73 (m, 1H), 5.17 (m, 1H), 4.29 (m, 1H), 4.13 – 3.96 (m, 3H), 1.45 (t, *J* = 7.0 Hz, 3H), 1.35 (d, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.7, 141.8, 139.9, 133.9, 133.7, 130.3, 129.2, 129.0, 128.7, 128.6, 128.4, 125.6, 114.2, 63.5, 62.0, 48.3, 18.7, 15.1.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{37}H_{36}N_2NaO_9S_4$: 803.1196; Found: 803.1200.

(*E*)-*N*,*N*',*N*''-(3-(4-ethoxyphenyl)pent-3-ene-1,2,5-triyl)tris(*N*-(phenylsulfonyl) benzenesulfonamide) (4b)



4b

Compound **4b** was isolated via column chromatography (PE: EA= 2: 1) as yellow solid (21 mg, 5% yield).

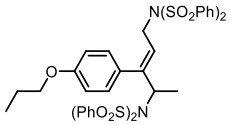
Melting Point: 128.9-129.5℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.22 – 8.03 (m, 6H), 7.95 – 7.88 (m, 4H), 7.72 – 7.62 (m, 5H), 7.58 (dd, *J* = 8.5, 7.3 Hz, 6H), 7.49 – 7.40 (m, 7H), 7.28 – 7.19 (m, 2H), 6.66 (d, *J* = 9.0 Hz, 2H), 6.25 (d, *J* = 8.2 Hz, 2H), 5.93 (m, 2H), 4.61 (dd, *J* = 15.4, 7.1 Hz, 1H), 4.23 (m, 2H), 4.04 – 3.91 (m, 3H), 1.41 (t, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.8, 140.8, 139.9, 139.6, 138.4, 137.5, 134.4, 134.0, 133.9, 133.6, 130.4, 130.4, 130.0, 129.5, 129.5, 129.2, 129.2, 128.7, 128.6, 128.3, 128.2, 114.1, 65.1, 63.4, 50.3, 48.1, 15.0.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{49}H_{45}N_3NaO_{13}S_6$: 1098.1169; Found: 1098.1165.

(*E*)-*N*,*N*'-(3-(4-propoxyphenyl)pent-2-ene-1,4-diyl)bis(*N*-(phenylsulfonyl) benzenesulfonamide) (2c)



2c

Compound **2c** was isolated via column chromatography (PE: EA= 3: 1) as white solid (170 mg, 53% yield).

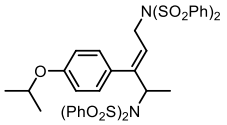
Melting Point: 133.1-133.8℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.03 – 7.70 (m, 8H), 7.65 – 7.54 (m, 4H), 7.54 – 7.37 (m, 8H), 6.89 (d, *J* = 8.7 Hz, 2H), 6.73 (d, *J* = 8.7 Hz, 2H), 5.72 (m, 1H), 5.18 (m, 1H), 4.29 (m, 1H), 4.08 (m, 1H), 3.91 (t, *J* = 6.5 Hz, 2H), 1.85 (m, 2H), 1.36 (d, *J* = 7.1 Hz, 3H), 1.08 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.9, 141.9, 139.9, 133.9, 133.7, 130.3, 129.2, 129.0, 128.7, 128.5, 128.4, 125.6, 114.2, 69.5, 62.0, 48.3, 22.8, 18.7, 10.8.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{38}H_{38}N_2NaO_9S_4$: 817.1352; Found: 817.1355.

(*E*)-*N*,*N*'-(3-(4-isopropoxyphenyl)pent-2-ene-1,4-diyl)bis(*N*-(phenylsulfonyl) benzenesulfonamide) (2d)



2d

Compound **2d** was isolated via column chromatography (PE: EA= 3: 1) as white solid (175 mg, 55% yield).

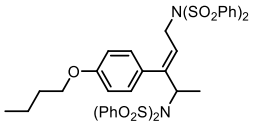
Melting Point: 155.4-156.3℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.00 – 7.75 (m, 8H), 7.59 (m, 4H), 7.47 (m, 8H), 6.90 (d, *J* = 8.6 Hz, 2H), 6.73 (d, *J* = 8.6 Hz, 2H), 5.73 (m, 1H), 5.24 – 5.12 (m, 1H), 4.54 (m, 1H), 4.29 (m, 1H), 4.09 (dd, *J* = 17.3, 7.2 Hz, 1H), 1.38 (d, *J* = 6.1 Hz, 6H), 1.34 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.7, 141.8, 139.9, 133.9, 133.7, 130.4, 129.2, 129.0, 128.7, 128.4, 128.4, 125.5, 115.3, 69.8, 61.9, 48.3, 22.3, 22.3, 18.7.

HRMS (ESI) m/z: [M+Na]+ Calcd for $C_{38}H_{38}N_2NaO_9S_4$: 817.1352; Found: 817.1355.

(*E*)-*N*,*N*'-(3-(4-butoxyphenyl)pent-2-ene-1,4-diyl)bis(*N*-(phenylsulfonyl) benzenesulfonamide) (2e)



2e

Compound **2e** was isolated via column chromatography (PE: EA= 3: 1) as white solid (182 mg, 56% yield).

Melting Point: 145.4-146.1℃.

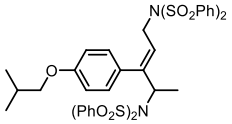
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.99 – 7.75 (m, 8H), 7.64 – 7.55 (m, 4H), 7.47 (m, 8H), 6.89 (d, *J* = 8.6 Hz, 2H), 6.73 (d, *J* = 8.7 Hz, 2H), 5.72 (m, 1H), 5.24 – 5.10 (m, 1H), 4.29 (m, 1H), 4.13 – 4.02 (m, 1H), 3.95 (t, *J* = 6.5 Hz, 2H), 1.85 – 1.75 (m, 2H), 1.57 (d, *J* = 4.1 Hz, 1H), 1.53 (d, *J* = 2.0 Hz, 1H), 1.35 (d, *J* = 7.1 Hz, 3H), 1.01

(t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.9, 141.9, 139.9, 133.9, 133.7, 130.3, 129.2, 129.0, 128.7, 128.5, 128.4, 125.6, 114.2, 67.7, 62.0, 48.3, 31.5, 19.5, 18.7, 14.0.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{39}H_{40}N_2NaO_9S_4$: 831.1509; Found: 831.1510.

(*E*)-*N*,*N*'-(3-(4-isobutoxyphenyl)pent-2-ene-1,4-diyl)bis(*N*-(phenylsulfonyl) benzenesulfonamide) (2f)



2f

Compound **2f** was isolated via column chromatography (PE: EA= 3: 1) as white solid (210 mg, 62% yield).

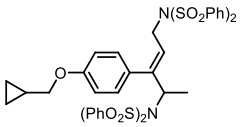
Melting Point: 161.1-162.0℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.04 – 7.72 (m, 8H), 7.65 – 7.54 (m, 4H), 7.54 – 7.35 (m, 8H), 6.89 (d, *J* = 8.6 Hz, 2H), 6.73 (d, *J* = 8.7 Hz, 2H), 5.72 (m, 1H), 5.17 (m, 1H), 4.29 (m, 1H), 4.07 (m, 1H), 3.71 (d, *J* = 6.5 Hz, 2H), 2.12 (m, 1H), 1.36 (d, *J* = 7.0 Hz, 3H), 1.07 (dd, *J* = 6.7, 0.9 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.0, 141.9, 139.9, 133.9, 133.7, 130.2, 129.2, 129.0, 128.6, 128.5, 128.3, 125.5, 114.2, 74.4, 62.0, 48.3, 28.4, 19.5, 18.6.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{39}H_{40}N_2NaO_9S_4$: 831.1509; Found: 831.1512.

(*E*)-*N*,*N*'-(3-(4-(cyclopropylmethoxy)phenyl)pent-2-ene-1,4-diyl)bis(*N*-(phenylsulfonyl)benzenesulfonamide) (2g)



2g

Compound **2g** was isolated via column chromatography (PE: EA= 3: 1) as white solid (155 mg, 48% yield).

Melting Point: 144.6-145.3℃.

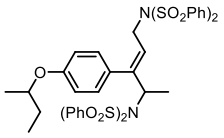
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.90 (dd, *J* = 36.4, 8.2 Hz, 8H), 7.60 (m, 4H), 7.48 (m, 8H), 6.89 (d, *J* = 8.3 Hz, 2H), 6.74 (d, *J* = 8.4 Hz, 2H), 5.73 (m, 1H), 5.18 (q, *J* = 7.1 Hz, 1H), 4.38 – 4.21 (m, 1H), 4.08 (dd, *J* = 17.3, 7.2 Hz, 1H), 3.80 (d, *J* = 6.9

Hz, 2H), 3.48 (s, 1H), 1.35 (d, *J* = 7.1 Hz, 3H), 0.72 – 0.65 (m, 2H), 0.38 (q, *J* = 5.3 Hz, 2H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.6, 141.7, 139.8, 133.8, 133.6, 130.2, 129.1, 128.9, 128.5, 128.2, 125.5, 114.2, 72.6, 61.9, 48.2, 18.5, 10.3, 3.3, 3.3.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{39}H_{38}N_2NaO_9S_4$: 829.1352; Found: 829.1355.

(*E*)-*N*,*N*'-(3-(4-(sec-butoxy)phenyl)pent-2-ene-1,4-diyl)bis(*N*-(phenylsulfonyl) benzenesulfonamide) (2h)



2h

Compound **2h** was isolated via column chromatography (PE: EA= 3: 1) as white solid (155 mg, 48% yield).

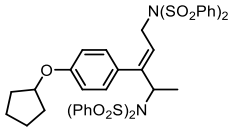
Melting Point: 150.6-151.4℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.07 – 7.71 (m, 8H), 7.71 – 7.36 (m, 13H), 6.91 (d, *J* = 8.3 Hz, 2H), 6.79 – 6.64 (m, 2H), 5.73 (m, 1H), 5.27 – 5.12 (m, 1H), 4.30 (m, 2H), 4.10 (m, 1H), 1.79 (m, 1H), 1.73 – 1.55 (m, 2H), 1.35 (m, 6H), 1.04 (m, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.0, 139.9, 133.9, 133.7, 130.3, 129.2, 128.9, 128.6, 128.3, 125.5, 115.3, 115.3, 74.9, 61.9, 48.2, 29.4, 29.4, 19.5, 18.6, 10.1.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{39}H_{40}N_2NaO_9S_4$: 831.1509; Found: 831.1512.

(*E*)-*N*,*N*'-(3-(4-(cyclopentyloxy)phenyl)pent-2-ene-1,4-diyl)bis(*N*-(phenylsulfonyl) benzenesulfonamide) (2i)



2i

Compound **2i** was isolated via column chromatography (PE: EA= 3: 1) as white solid (152 mg, 46% yield).

Melting Point: 146.2-147.3℃.

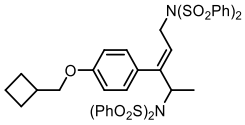
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.06 – 7.71 (m, 8H), 7.71 – 7.32 (m, 13H), 6.97

– 6.79 (m, 2H), 6.79 – 6.66 (m, 2H), 5.74 (m, 1H), 5.30 – 5.12 (m, 1H), 4.74 (m, 1H), 4.31 (m, 1H), 4.19 – 4.02 (m, 1H), 1.97 – 1.77 (m, 6H), 1.66 (m, 2H), 1.36 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.9, 141.8, 139.9, 133.9, 133.7, 130.2, 129.2, 128.9, 128.6, 128.3, 128.2, 125.4, 115.1, 79.2, 61.9, 48.3, 33.0, 33.0, 24.2, 18.6.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{40}H_{40}N_2NaO_9S_4$: 843.1509; Found: 843.1513.

(*E*)-*N*,*N*'-(3-(4-(cyclobutylmethoxy)phenyl)pent-2-ene-1,4-diyl)bis(*N*-(phenylsulfonyl)benzenesulfonamide) (2j)



2j

Compound **2j** was isolated via column chromatography (PE: EA= 3: 1) as white solid (140 mg, 43% yield).

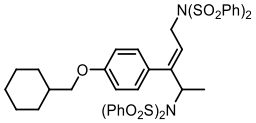
Melting Point: 152.7-153.1℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.02 – 7.74 (m, 8H), 7.64 – 7.54 (m, 4H), 7.54 – 7.39 (m, 8H), 6.89 (d, *J* = 8.7 Hz, 2H), 6.73 (d, *J* = 8.7 Hz, 2H), 5.73 (m, 1H), 5.17 (m, 1H), 4.29 (m, 1H), 4.08 (m, 1H), 3.92 (d, *J* = 6.6 Hz, 2H), 2.80 (m, 1H), 2.24 – 2.13 (m, 2H), 2.05 – 1.86 (m, 4H), 1.36 (d, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.0, 141.9, 139.9, 133.9, 133.7, 130.2, 129.2, 129.0, 128.6, 128.4, 125.6, 114.3, 72.1, 62.0, 48.3, 34.8, 25.0, 25.0, 18.8, 18.7.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{40}H_{40}N_2NaO_9S_4$: 843.1509; Found: 843.1513.

(*E*)-*N*,*N*'-(3-(4-(cyclohexylmethoxy)phenyl)pent-2-ene-1,4-diyl)bis(*N*-(phenylsulfonyl)benzenesulfonamide) (2k)



2k

Compound **2k** was isolated via column chromatography (PE: EA= 3: 1) as white solid (124 mg, 37% yield).

Melting Point: 133.5-134.5℃.

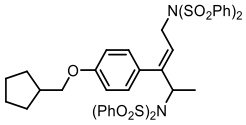
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.03 – 7.70 (m, 8H), 7.65 – 7.54 (m, 4H), 7.54 –

7.37 (m, 8H), 6.89 (d, *J* = 8.6 Hz, 2H), 6.72 (d, *J* = 8.7 Hz, 2H), 5.72 (m, 1H), 5.23 – 5.10 (m, 1H), 4.29 (m, 1H), 4.07 (m, 1H), 3.74 (d, *J* = 6.3 Hz, 2H), 1.95 – 1.86 (m, 2H), 1.86 – 1.68 (m, 4H), 1.36 (d, *J* = 7.1 Hz, 3H), 1.33 – 1.20 (m, 3H), 1.10 (m, 2H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.0, 141.9, 139.9, 133.9, 133.7, 130.2, 129.2, 128.9, 128.6, 128.3, 125.5, 114.2, 73.5, 62.0, 48.3, 37.9, 30.1, 30.1, 26.6, 25.9, 18.6.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{42}H_{44}N_2NaO_9S_4$: 871.1822; Found: 871.1825.

(*E*)-*N*,*N*'-(3-(4-(cyclopentylmethoxy)phenyl)pent-2-ene-1,4-diyl)bis(*N*-(phenylsulfonyl)benzenesulfonamide) (2l)



2l

Compound **2l** was isolated via column chromatography (PE: EA= 3: 1) as white solid (144 mg, 42% yield).

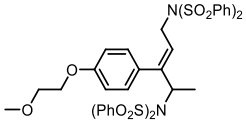
Melting Point: 131.3-132.2℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.99 – 7.71 (m, 8H), 7.65 – 7.54 (m, 4H), 7.47 (m, 8H), 6.92 – 6.83 (m, 2H), 6.73 (d, *J* = 8.5 Hz, 2H), 5.72 (m, 1H), 5.24 – 5.11 (m, 1H), 4.29 (m, 1H), 4.08 (dd, *J* = 17.4, 7.2 Hz, 1H), 3.82 (d, *J* = 6.9 Hz, 2H), 2.39 (m, 1H), 1.89 (m, 2H), 1.74 – 1.60 (m, 4H), 1.38 (dd, *J* = 15.9, 6.6 Hz, 5H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.0, 141.9, 139.9, 133.9, 133.7, 130.2, 129.2, 129.0, 128.6, 128.5, 128.4, 125.5, 114.2, 72.2, 62.0, 48.3, 39.2, 29.7, 29.6, 25.6, 18.7.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{41}H_{42}N_2NaO_9S_4$: 857.1665; Found: 857.1669.

(*E*)-*N*,*N*'-(3-(4-(2-methoxyethoxy)phenyl)pent-2-ene-1,4-diyl)bis(*N*-(phenylsulfonyl)benzenesulfonamide) (2m)



2m

Compound **2m** was isolated via column chromatography (PE: EA= 3: 1) as white solid (215 mg, 66% yield).

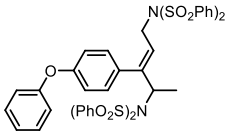
Melting Point: 128.5-129.4℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.01 – 7.71 (m, 8H), 7.59 (m, 4H), 7.47 (m, 8H), 6.90 (d, *J* = 8.6 Hz, 2H), 6.76 (d, *J* = 8.5 Hz, 2H), 5.74 (m, 1H), 5.17 (q, *J* = 7.2 Hz, 1H), 4.28 (m, 1H), 4.14 – 4.01 (m, 3H), 3.77 (dd, *J* = 5.6, 3.8 Hz, 2H), 3.47 (s, 3H), 1.36 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.5, 141.7, 139.9, 133.9, 133.7, 130.2, 129.2, 129.0, 128.6, 128.3, 125.6, 114.3, 71.1, 67.3, 61.9, 59.4, 48.2, 18.6.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{38}H_{38}N_2NaO_{10}S_4$: 833.1301; Found: 833.1305.

(*E*)-*N*,*N*'-(3-(4-phenoxyphenyl)pent-2-ene-1,4-diyl)bis(*N*-(phenylsulfonyl) benzenesulfonamide) (2n)



2n

Compound **2n** was isolated via column chromatography (PE: EA= 3: 1) as white solid (127 mg, 38% yield).

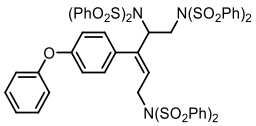
Melting Point: 144.7-145.6℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.04 – 7.79 (m, 8H), 7.61 (m, 4H), 7.50 (m, 8H), 7.38 (t, *J* = 7.9 Hz, 2H), 7.16 (t, *J* = 7.4 Hz, 1H), 7.06 (d, *J* = 8.0 Hz, 2H), 6.95 (d, *J* = 8.2 Hz, 2H), 6.85 (d, *J* = 8.3 Hz, 2H), 5.78 (m, 1H), 5.17 (q, *J* = 7.1 Hz, 1H), 4.29 (m, 1H), 4.10 (dd, *J* = 17.3, 7.2 Hz, 1H), 1.37 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.3, 156.6, 141.6, 139.9, 134.0, 133.8, 131.2, 130.5, 130.0, 129.2, 129.0, 128.7, 128.4, 126.0, 123.9, 119.5, 118.1, 61.8, 48.2, 18.7.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{41}H_{36}N_2NaO_9S_4$: 851.1196; Found: 851.1199.

(*E*)-*N*,*N*',*N*''-(3-(4-phenoxyphenyl)pent-3-ene-1,2,5-triyl)tris(*N*-(phenylsulfonyl) benzenesulfonamide) (4n)



4n

Compound **4n** was isolated via column chromatography (PE: EA= 2: 1) as white solid (22 mg, 5% yield).

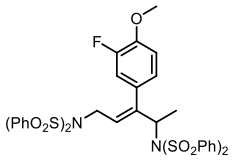
Melting Point: 130.2-131.0℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.17 (d, *J* = 7.8 Hz, 2H), 8.08 (d, *J* = 7.5 Hz, 4H), 7.95 (d, *J* = 7.2 Hz, 4H), 7.74 – 7.62 (m, 5H), 7.61 – 7.53 (m, 6H), 7.47 (dd, *J* = 14.7, 7.4 Hz, 7H), 7.35 (t, *J* = 7.9 Hz, 2H), 7.30 – 7.23 (m, 2H), 7.13 (t, *J* = 7.4 Hz, 1H), 7.02 (d, *J* = 8.0 Hz, 2H), 6.79 (d, *J* = 8.3 Hz, 2H), 6.34 (d, *J* = 8.1 Hz, 2H), 6.01 (dd, *J* = 7.9, 3.4 Hz, 1H), 5.90 (dd, *J* = 6.9, 4.3 Hz, 1H), 4.61 (dd, *J* = 15.4, 6.9 Hz, 1H), 4.26 (m, 2H), 4.01 (dd, *J* = 17.7, 7.9 Hz, 1H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.3, 156.7, 140.7, 139.8, 139.6, 138.4, 137.3, 134.4, 134.1, 134.0, 133.7, 130.9, 130.5, 130.3, 130.0, 129.5, 129.5, 129.3, 129.2, 128.7, 128.3, 123.7, 119.4, 118.2, 65.2, 50.3, 48.0.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{53}H_{45}N_3NaO_{13}S_6$: 1146.1169; Found: 1146.1172.

(*E*)-*N*,*N*'-(3-(3-fluoro-4-methoxyphenyl)pent-2-ene-1,4-diyl)bis(*N*-(phenylsulfonyl)benzenesulfonamide) (2o)



2o

Compound **2o** was isolated via column chromatography (PE: EA= 3: 1) as white solid (175 mg, 55% yield).

Melting Point: 142.3-143.1℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.01 – 7.75 (m, 8H), 7.65 – 7.57 (m, 4H), 7.49 (m, 8H), 6.85 – 6.72 (m, 2H), 6.53 (dd, *J* = 11.8, 1.8 Hz, 1H), 5.74 (m, 1H), 5.12 – 4.99 (m, 1H), 4.26 (m, 1H), 4.04 – 3.95 (m, 1H), 3.88 (s, 3H), 1.42 (d, *J* = 7.0 Hz, 3H).

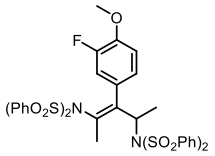
^{13}C NMR (101 MHz, Chloroform-*d*) δ 152.8, 150.4, 147.3, 147.2, 140.8, 139.8, 134.0, 133.8, 129.2, 129.0, 128.6, 128.3, 126.5, 125.3, 125.3, 116.8, 116.6, 112.9, 112.9, 62.0, 56.2, 48.1, 18.7.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -134.1.

HRMS (ESI) m/z: [M+H]+ Calcd for $C_{36}H_{34}FN_2O_9S_4$: 807.0945; Found: 807.0950.

(*E*)-*N*,*N*'-(3-(3-fluoro-4-methoxyphenyl)pent-2-ene-2,4-diyl)bis(*N*-(phenylsulfonyl)

benzenesulfonamide) (3o)



3o

Compound **3o** was isolated via column chromatography (PE: EA= 3: 1) as white solid (7 mg, 2% yield).

Melting Point: 113.3-114.2℃.

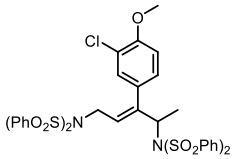
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.03 – 7.92 (m, 4H), 7.92 – 7.82 (m, 2H), 7.75 – 7.59 (m, 5H), 7.59 – 7.50 (m, 5H), 7.47 (t, *J* = 7.8 Hz, 2H), 7.35 (t, *J* = 7.8 Hz, 2H), 6.81 (s, 1H), 6.58 (d, *J* = 8.8 Hz, 1H), 6.31 (s, 1H), 5.59 (q, *J* = 7.3 Hz, 1H), 3.81 (s, 3H), 2.26 (s, 3H), 1.51 (d, *J* = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 151.9, 149.5, 147.0, 146.9, 146.6, 140.3, 139.6, 134.0, 134.0, 133.9, 130.9, 129.3, 129.1, 129.1, 128.8, 128.7, 126.8, 118.6, 118.4, 111.7, 60.4, 56.0, 21.2, 18.8.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -135.1.

HRMS (ESI) m/z: [M+H]+ Calcd for $C_{36}H_{34}FN_2O_9S_4$: 807.0945; Found: 807.0950.

(*E*)-*N*,*N*'-(3-(3-chloro-4-methoxyphenyl)pent-2-ene-1,4-diyl)bis(*N*-(phenylsulfonyl)benzenesulfonamide) (2p)



2p

Compound **2p** was isolated via column chromatography (PE: EA= 3: 1) as white solid (166 mg, 52% yield).

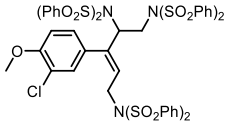
Melting Point: 125.6-126.4℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.00 – 7.80 (m, 8H), 7.65 – 7.57 (m, 4H), 7.55 – 7.43 (m, 8H), 6.99 (dd, *J* = 8.4, 2.2 Hz, 1H), 5.76 (m, 1H), 5.09 (m, 1H), 4.25 (m, 1H), 3.98 (m, 1H), 3.89 (s, 3H), 1.43 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.6, 140.5, 139.8, 134.0, 133.9, 130.6, 129.7, 129.2, 129.0, 129.0, 128.7, 128.3, 126.7, 122.1, 111.7, 62.0, 56.2, 48.0, 18.7.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{36}H_{33}ClN_2NaO_9S_4$: 823.0649; Found: 823.0650.

(*E*)-*N*,*N*',*N*''-(3-(3-chloro-4-methoxyphenyl)pent-3-ene-1,2,5-triyl)tris(*N*-(phenylsulfonyl)benzenesulfonamide) (4p)



4p

Compound **4p** was isolated via column chromatography (PE: EA= 3: 1) as yellow solid (13 mg, 3% yield).

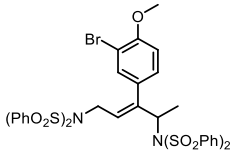
Melting Point: 169.3-170.1℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.14 (dd, *J* = 8.5, 1.2 Hz, 2H), 8.09 – 8.01 (m, 4H), 7.96 – 7.89 (m, 4H), 7.72 – 7.63 (m, 5H), 7.58 (m, 6H), 7.51 – 7.41 (m, 7H), 7.29 – 7.23 (m, 2H), 6.76 (d, *J* = 8.6 Hz, 1H), 6.61 (dd, *J* = 8.5, 2.2 Hz, 1H), 6.08 (dd, *J* = 7.7, 3.6 Hz, 1H), 6.02 (d, *J* = 2.2 Hz, 1H), 5.85 (t, *J* = 5.7 Hz, 1H), 4.53 (dd, *J* = 15.3, 6.5 Hz, 1H), 4.35 (dd, *J* = 15.4, 5.0 Hz, 1H), 4.24 (dd, *J* = 17.7, 3.7 Hz, 1H), 3.95 (dd, *J* = 17.7, 7.7 Hz, 1H), 3.87 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.8, 140.6, 139.5, 139.5, 138.4, 136.0, 134.4, 134.2, 134.1, 133.7, 131.6, 130.4, 130.3, 129.4, 129.4, 129.3, 129.2, 128.9, 128.7, 128.5, 128.3, 121.9, 111.8, 65.0, 56.2, 50.3, 47.8.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{48}H_{42}ClN_3NaO_{13}S_6$: 1118.0622; Found: 1118.0625.

(*E*)-*N*,*N*'-(3-(3-bromo-4-methoxyphenyl)pent-2-ene-1,4-diyl)bis(*N*-(phenylsulfonyl)benzenesulfonamide) (2q)



2q

Compound **2q** was isolated via column chromatography (PE: EA= 3: 1) as white solid (143 mg, 42% yield).

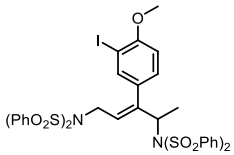
Melting Point: 116.5-117.3℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.98 – 7.83 (m, 8H), 7.60 (m, 4H), 7.54 – 7.43 (m, 8H), 7.06 – 6.97 (m, 2H), 6.72 (d, *J* = 8.4 Hz, 1H), 5.78 (m, 1H), 5.10 (m, 1H), 4.26 (m, 1H), 3.99 (m, 1H), 3.86 (s, 3H), 1.43 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.4, 140.4, 139.7, 134.0, 133.8, 133.5, 130.1, 129.4, 129.2, 129.1, 128.9, 128.3, 126.7, 111.5, 111.4, 62.0, 56.2, 47.9, 18.6.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{36}H_{33}BrN_2NaO_9S_4$: 867.0144; Found: 867.0146.

(*E*)-*N*,*N*'-(3-(3-iodo-4-methoxyphenyl)pent-2-ene-1,4-diyl)bis(*N*-(phenylsulfonyl) benzenesulfonamide) (2r)



2r

Compound **2r** was isolated via column chromatography (PE: EA= 3: 1) as white solid (167 mg, 47% yield).

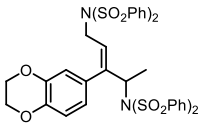
Melting Point: 119.2-120.4℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.00 – 7.78 (m, 8H), 7.65 – 7.57 (m, 4H), 7.50 (m, 8H), 7.24 (d, *J* = 2.1 Hz, 1H), 7.07 (dd, *J* = 8.4, 2.1 Hz, 1H), 6.64 (d, *J* = 8.4 Hz, 1H), 5.76 (m, 1H), 5.12 – 5.04 (m, 1H), 4.25 (m, 1H), 3.99 (dd, *J* = 17.3, 7.2 Hz, 1H), 3.87 (s, 3H), 1.42 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.7, 140.3, 139.8, 139.6, 134.0, 133.9, 130.8, 130.5, 129.3, 129.0, 128.4, 126.7, 110.5, 85.9, 62.1, 56.4, 48.0, 18.7.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{36}H_{33}IN_2NaO_9S_4$: 915.0006; Found: 915.0009.

(*E*)-*N*,*N*'-(3-(2,3-dihydrobenzo[*b*][1,4]dioxin-6-yl)pent-2-ene-1,4-diyl)bis(*N*-(phenylsulfonyl)benzenesulfonamide) (2s)



2s

Compound **2s** was isolated via column chromatography (PE: EA= 3: 1) as white solid (210 mg, 66% yield).

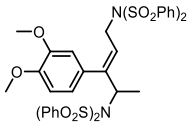
Melting Point: 147.0-148.1℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.05 – 7.76 (m, 8H), 7.64 – 7.56 (m, 4H), 7.55 – 7.40 (m, 8H), 6.71 (d, *J* = 8.7 Hz, 1H), 6.48 (dd, *J* = 4.4, 2.4 Hz, 2H), 5.71 (m, 1H), 5.20 – 5.05 (m, 1H), 4.35 – 4.17 (m, 5H), 4.11 (m, 1H), 1.33 (d, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 143.3, 141.3, 139.9, 133.9, 133.7, 129.8, 129.2, 128.9, 128.7, 128.4, 125.9, 122.2, 118.1, 117.2, 64.5, 64.4, 61.9, 48.3, 18.6.

HRMS (ESI) m/z: [M+Na]+ Calcd for $C_{37}H_{34}N_2NaO_{10}S_4$: 817.0988; Found: 817.0990.

(*E*)-*N*,*N*'-(3-(3,4-dimethoxyphenyl)pent-2-ene-1,4-diyl)bis(*N*-(phenylsulfonyl) benzenesulfonamide) (2t)



2t

Compound **2t** was isolated via column chromatography (PE: EA= 3: 1) as yellow solid (155 mg, 49% yield).

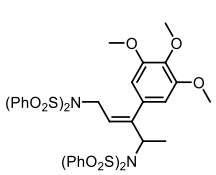
Melting Point: 113.2-114.1℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.02 – 7.73 (m, 8H), 7.64 – 7.55 (m, 4H), 7.54 – 7.38 (m, 8H), 6.68 (dd, *J* = 5.1, 3.2 Hz, 2H), 6.55 (dd, *J* = 8.1, 1.9 Hz, 1H), 5.77 – 5.69 (m, 1H), 5.12 (q, *J* = 7.2, 6.8 Hz, 1H), 4.28 (m, 1H), 4.05 (dd, *J* = 17.4, 6.8 Hz, 1H), 3.89 (s, 3H), 3.77 (s, 3H), 1.43 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 148.5, 148.5, 142.1, 139.8, 133.8, 133.6, 129.2, 129.1, 128.8, 128.5, 128.3, 125.5, 121.2, 112.3, 110.7, 62.3, 55.8, 55.8, 48.2, 18.6.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{37}H_{36}N_2NaO_{10}S_4$: 819.1145; Found: 819.1150.

(*E*)-*N*,*N*'-(3-(3,4,5-trimethoxyphenyl)pent-2-ene-1,4-diyl)bis(*N*-(phenylsulfonyl) benzenesulfonamide) (2u)



2u

Compound **2u** was isolated via column chromatography (PE: EA= 3: 1) as yellow solid (110 mg, 33% yield).

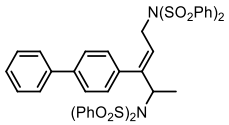
Melting Point: 125.4-126.6℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.05 – 7.71 (m, 8H), 7.66 – 7.56 (m, 4H), 7.56 – 7.36 (m, 8H), 6.36 (s, 2H), 5.79 – 5.70 (m, 1H), 5.12 – 5.02 (m, 1H), 4.29 (m, 1H), 4.05 – 3.96 (m, 1H), 3.87 (s, 3H), 3.76 (s, 6H), 1.49 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.0, 142.6, 139.9, 137.3, 134.0, 133.8, 132.3, 129.2, 128.9, 128.4, 125.6, 106.2, 62.3, 61.0, 56.2, 48.2, 18.7.

HRMS (ESI) m/z: [M+Na]+ Calcd for $C_{38}H_{38}N_2NaO_{11}S_4$: 849.1250; Found: 849.1251.

(*E*)-*N*,*N*'-(3-([1,1'-biphenyl]-4-yl)pent-2-ene-1,4-diyl)bis(*N*-(phenylsulfonyl) benzenesulfonamide) (2v)



2v

Compound **2v** was isolated via column chromatography (PE: EA= 3: 1) as white solid (109 mg, 60% yield).

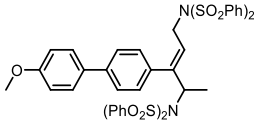
Melting Point: 148.5-149.9℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.00 – 7.73 (m, 8H), 7.64 – 7.58 (m, 4H), 7.56 – 7.46 (m, 10H), 7.41 (t, *J* = 7.4 Hz, 5H), 7.12 (d, *J* = 7.9 Hz, 2H), 5.80 (dd, *J* = 7.1, 4.9 Hz, 1H), 5.25 (q, *J* = 7.2 Hz, 1H), 4.34 (dd, *J* = 17.3, 4.8 Hz, 1H), 4.08 (dd, *J* = 17.4, 7.2 Hz, 1H), 1.43 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 142.0, 140.6, 140.5, 139.8, 135.8, 134.0, 133.7, 129.7, 129.2, 129.1, 129.0, 128.6, 128.4, 127.7, 127.0, 126.9, 125.8, 61.8, 48.1, 18.7.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{41}H_{36}N_2NaO_8S_4$: 835.1246; Found: 835.1250.

(*E*)-*N*,*N*'-(3-(4'-methoxy-[1,1'-biphenyl]-4-yl)pent-2-ene-1,4-diyl)bis(*N*-(phenylsulfonyl)benzenesulfonamide) (2w)



2w

Compound **2w** was isolated via column chromatography (PE: EA= 3: 1) as white solid (119 mg, 56% yield).

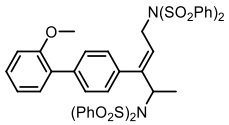
Melting Point: 146.7-147.8℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.01 – 7.68 (m, 8H), 7.63 – 7.45 (m, 10H), 7.45 – 7.32 (m, 6H), 7.08 (d, *J* = 8.1 Hz, 2H), 7.02 (d, *J* = 8.7 Hz, 2H), 5.78 (m, 1H), 5.25 (m, 1H), 4.34 (m, 1H), 4.09 (m, 1H), 3.88 (s, 3H), 1.42 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.5, 142.1, 140.2, 139.8, 135.1, 134.0, 133.7, 132.9, 129.7, 129.2, 129.0, 128.6, 128.4, 128.0, 126.4, 125.7, 114.5, 61.8, 55.5, 48.2, 18.7.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{42}H_{38}N_2NaO_9S_4$: 865.1352; Found: 865.1355.

(*E*)-*N*,*N*'-(3-(2'-methoxy-[1,1'-biphenyl]-4-yl)pent-2-ene-1,4-diyl)bis(*N*-(phenylsulfonyl)benzenesulfonamide) (2x)



2x

Compound **2x** was isolated via column chromatography (PE: EA= 3: 1) as white solid (58 mg, 53% yield).

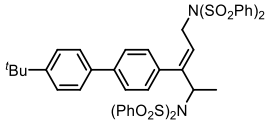
Melting Point: 145.4-146.3℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.00 – 7.70 (m, 8H), 7.63 – 7.34 (m, 16H), 7.12 – 7.02 (m, 4H), 5.81 (m, 1H), 5.31 (q, *J* = 8.1, 7.5 Hz, 1H), 4.34 (m, 1H), 4.13 (dd, *J* = 17.4, 7.1 Hz, 1H), 3.86 (s, 3H), 1.39 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.6, 142.1, 139.8, 138.2, 135.3, 133.9, 133.8, 131.0, 129.5, 129.2, 129.0, 128.9, 128.7, 128.4, 125.6, 121.1, 111.5, 61.6, 55.6, 48.1, 18.7.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{42}H_{38}N_2NaO_9S_4$: 865.1352; Found: 865.1355.

(*E*)-*N*,*N*'-(3-(4'-(tert-butyl)-[1,1'-biphenyl]-4-yl)pent-2-ene-1,4-diyl)bis(*N*-(phenylsulfonyl)benzenesulfonamide) (2y)



2y

Compound **2y** was isolated via column chromatography (PE: EA= 3: 1) as white solid (94 mg, 50% yield).

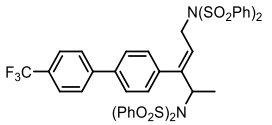
Melting Point: 160.0-161.6℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.99 – 7.74 (m, 8H), 7.64 – 7.44 (m, 15H), 7.41 (t, *J* = 7.6 Hz, 3H), 7.10 (d, *J* = 8.0 Hz, 2H), 5.79 (m, 1H), 5.30 – 5.20 (m, 1H), 4.33 (m, 1H), 4.09 (dd, *J* = 17.3, 7.2 Hz, 1H), 1.42 (d, *J* = 7.2 Hz, 3H), 1.40 (s, 9H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 150.8, 142.1, 140.5, 139.8, 137.6, 135.4, 134.0, 133.7, 129.6, 129.2, 129.0, 128.6, 128.4, 126.8, 126.7, 126.0, 125.8, 61.8, 48.2, 34.7, 31.5, 18.7.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{45}H_{44}N_2NaO_8S_4$: 891.1872; Found: 891.1875.

(*E*)-*N*,*N*'-(3-(4'-(trifluoromethyl)-[1,1'-biphenyl]-4-yl)pent-2-ene-1,4-diyl)bis(*N*-(phenylsulfonyl)benzenesulfonamide) (2z)



2z

Compound **2z** was isolated via column chromatography (PE: EA= 3: 1) as white solid (50 mg, 35% yield).

Melting Point: 168.2-169.4℃.

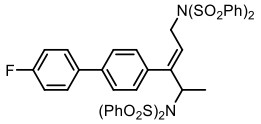
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.99 – 7.79 (m, 8H), 7.77 – 7.67 (m, 5H), 7.64 – 7.59 (m, 2H), 7.54 – 7.45 (m, 7H), 7.45 – 7.33 (m, 4H), 7.20 – 7.12 (m, 2H), 5.81 (m, 1H), 5.23 (m, 1H), 4.33 (m, 1H), 4.07 (m, 1H), 1.43 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 144.0 141.8, 139.8, 139.0, 136.8, 134.0, 133.8, 129.9, 129.2, 129.0, 128.6, 128.4, 127.3, 127.1, 126.1, 126.1, 126.0, 61.8, 48.1, 18.7.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.4.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{42}H_{35}F_3N_2NaO_8S_4$: 903.1120; Found: 903.1122.

(*E*)-*N*,*N*'-(3-(4'-fluoro-[1,1'-biphenyl]-4-yl)pent-2-ene-1,4-diyl)bis(*N*-(phenylsulfonyl)benzenesulfonamide) (2aa)



2aa

Compound **2aa** was isolated via column chromatography (PE: EA= 3: 1) as white solid (40 mg, 39% yield).

Melting Point: 154.1-155.4℃.

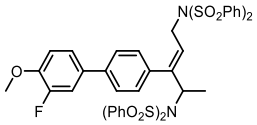
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.06 – 7.70 (m, 8H), 7.64 – 7.30 (m, 16H), 7.22 – 7.06 (m, 4H), 5.79 (m, 1H), 5.29 – 5.15 (m, 1H), 4.33 (m, 1H), 4.08 (dd, *J* = 17.3, 7.2 Hz, 1H), 1.41 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 164.0, 161.5, 142.0, 139.9, 135.8, 134.0, 133.7, 129.8, 129.2, 129.0, 128.7, 128.6, 128.5, 128.4, 126.8, 125.9, 116.1, 115.9, 61.8, 48.1, 18.7.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -115.2.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{41}H_{35}FN_2NaO_8S_4$: 853.1152; Found: 853.1153.

(*E*)-*N*,*N*'-(3-(3'-fluoro-4'-methoxy-[1,1'-biphenyl]-4-yl)pent-2-ene-1,4-diyl)bis(*N*-(phenylsulfonyl)benzenesulfonamide) (2ab)



2ab

Compound **2ab** was isolated via column chromatography (PE: EA= 3: 1) as white solid (94 mg, 50% yield).

Melting Point: 121.4-122.4℃.

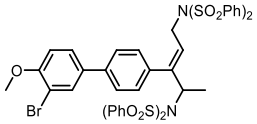
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.98 – 7.77 (m, 8H), 7.63 – 7.58 (m, 2H), 7.57 – 7.46 (m, 7H), 7.44 – 7.36 (m, 6H), 7.36 – 7.27 (m, 2H), 7.09 (d, *J* = 8.2 Hz, 2H), 5.80 (m, 1H), 5.23 (m, 1H), 4.34 (m, 1H), 4.18 – 4.02 (m, 1H), 3.95 (s, 3H), 1.43 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.9, 151.5, 147.4, 147.3, 141.9, 139.8, 139.0, 138.9, 135.6, 134.0, 133.7, 133.6, 133.5, 129.7, 129.2, 128.9, 128.6, 128.3, 126.4, 125.8, 122.6, 122.5, 114.6, 114.4, 113.9, 61.8, 56.4, 48.1, 18.7.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -134.6.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{42}H_{37}FN_2NaO_9S_4$: 883.1258; Found: 883.1260.

(*E*)-*N*,*N*'-(3-(3'-bromo-4'-methoxy-[1,1'-biphenyl]-4-yl)pent-2-ene-1,4-diyl)bis(*N*-(phenylsulfonyl)benzenesulfonamide) (2ac)



2ac

Compound **2ac** was isolated via column chromatography (PE: EA= 3: 1) as white solid (80 mg, 50% yield).

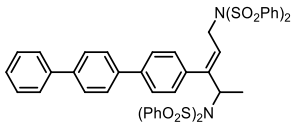
Melting Point: 115.0-115.7℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.97 – 7.78 (m, 8H), 7.61 (t, *J* = 7.4 Hz, 3H), 7.52 (m, 8H), 7.40 (dd, *J* = 15.6, 7.6 Hz, 5H), 7.08 (d, *J* = 7.9 Hz, 2H), 7.01 (d, *J* = 8.6 Hz, 1H), 5.78 (m, 1H), 5.28 – 5.11 (m, 1H), 4.32 (m, 1H), 4.06 (dd, *J* = 17.3, 7.2 Hz, 1H), 3.97 (s, 3H), 1.42 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.7, 142.0, 139.9, 138.8, 135.7, 134.4, 134.0, 133.7, 131.9, 129.7, 129.2, 129.1, 129.0, 128.6, 128.4, 126.9, 126.5, 125.9, 112.4, 61.9, 56.5, 48.1, 18.7.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{42}H_{37}BrN_2NaO_9S_4$: 943.0457; Found: 943.0460.

(*E*)-*N*,*N*'-(3-([1,1':4',1''-terphenyl]-4-yl)pent-2-ene-1,4-diyl)bis(*N*-(phenylsulfonyl)benzenesulfonamide) (2ad)



2ad

Compound **2ad** was isolated via column chromatography (PE: EA= 3: 1) as white solid (108 mg, 59% yield).

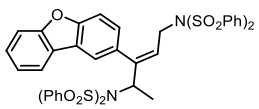
Melting Point: 160.2-160.8℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.05 – 7.80 (m, 8H), 7.78 – 7.64 (m, 7H), 7.61 (t, *J* = 7.5 Hz, 2H), 7.50 (m, 10H), 7.41 (m, 4H), 7.14 (d, *J* = 8.0 Hz, 2H), 5.81 (m, 1H), 5.31 – 5.20 (m, 1H), 4.35 (m, 1H), 4.10 (dd, *J* = 17.3, 7.2 Hz, 1H), 1.44 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 141.9, 140.5, 140.4, 139.9, 139.7, 139.2, 135.9, 135.8, 133.9, 133.7, 129.9, 129.7, 129.5, 129.1, 128.9, 128.9, 128.5, 128.3, 127.7, 127.5, 127.3, 127.1, 126.7, 125.7, 61.7, 48.0, 18.6.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{47}H_{40}N_2NaO_8S_4$: 911.1559; Found: 911.1560.

(*E*)-N,N'-(3-(dibenzo[b,d]furan-2-yl)pent-2-ene-1,4-diyl)bis(N-(phenylsulfonyl)benzenesulfonamide) (2ae)



2ae

Compound **2ae** was isolated via column chromatography (PE: EA= 3: 1) as white solid (180 mg, 54% yield).

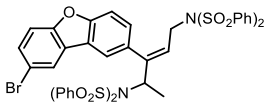
Melting Point: 113.6-114.6℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.02 – 7.79 (m, 9H), 7.62 – 7.55 (m, 4H), 7.53 – 7.43 (m, 8H), 7.37 (m, 4H), 7.19 (dd, *J* = 8.4, 1.8 Hz, 2H), 5.86 (m, 1H), 5.25 – 5.15 (m, 1H), 4.30 (m, 1H), 4.00 (dd, *J* = 17.3, 7.0 Hz, 1H), 1.56 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.5, 155.7, 142.1, 139.8, 134.0, 133.6, 131.4, 129.2, 129.0, 128.9, 128.3, 128.1, 127.6, 126.4, 124.1, 123.0, 121.3, 121.1, 111.8, 111.7, 62.8, 48.2, 18.9.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{41}H_{35}N_2O_9S_4$: 827.1220; Found: 827.1220.

(*E*)-N,N'-(3-(8-bromodibenzo[b,d]furan-2-yl)pent-2-ene-1,4-diyl)bis(N-(phenylsulfonyl)benzenesulfonamide) (2af)



2af

Compound **2af** was isolated via column chromatography (PE: EA= 3: 1) as white solid (140 mg, 52% yield).

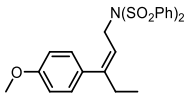
Melting Point: 118.1-119.3℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.09 – 7.72 (m, 10H), 7.63 – 7.56 (m, 4H), 7.52 – 7.35 (m, 10H), 7.21 (dd, *J* = 8.5, 1.8 Hz, 2H), 5.86 (m, 1H), 5.17 (m, 1H), 4.28 (m, 1H), 3.98 (m, 1H), 1.48 (d, *J* = 42.1 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.1, 155.2, 141.9, 139.9, 134.0, 133.6, 131.8, 130.4, 129.2, 128.9, 128.8, 128.4, 126.6, 124.0, 121.6, 115.9, 113.4, 111.9, 62.7, 48.2, 18.9.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{41}H_{34}BrN_2O_9S_4$: 905.0325; Found: 905.0327.

(*Z*)-*N*-(3-(4-methoxyphenyl)pent-2-en-1-yl)-*N*-(phenylsulfonyl) benzenesulfonamide (5a(*Z*))



5a(*Z*)

Compound **5a(Z)** was isolated via column chromatography (PE: EA= 10: 1) as white solid (40 mg, 20% yield).

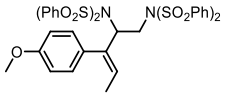
Melting Point: 122.3-123.3℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.06 (dd, *J* = 8.5, 1.3 Hz, 4H), 7.68 – 7.56 (m, 2H), 7.56 – 7.45 (m, 4H), 7.13 (d, *J* = 8.8 Hz, 2H), 6.83 (d, *J* = 8.7 Hz, 2H), 5.48 (t, *J* = 6.8 Hz, 1H), 4.58 (d, *J* = 6.9 Hz, 2H), 3.82 (s, 3H), 2.58 (q, *J* = 7.5 Hz, 2H), 1.00 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.2, 145.5, 140.4, 133.9, 133.7, 129.1, 128.3, 127.5, 120.7, 113.8, 55.4, 47.9, 23.0, 13.7.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{24}H_{25}NNaO_5S_2$: 494.1066; Found: 494.1069.

(*E*)-N,N'-(3-(4-methoxyphenyl)pent-3-ene-1,2-diyl)bis(*N*-(phenylsulfonyl) benzenesulfonamide) (6a)



6a

Compound **6a** was isolated via column chromatography (PE: EA= 3: 1) as white solid (50 mg, 32% yield).

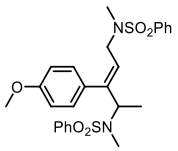
Melting Point: 138.2-139.3℃.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.05 – 7.97 (m, 4H), 7.92 (d, *J* = 7.9 Hz, 4H), 7.68 – 7.54 (m, 4H), 7.54 – 7.33 (m, 8H), 6.58 (d, *J* = 8.7 Hz, 2H), 6.51 – 6.39 (m, 1H), 6.25 – 6.13 (m, 2H), 5.99 (dd, *J* = 9.9, 3.9 Hz, 1H), 5.27 (dd, *J* = 15.3, 10.0 Hz, 1H), 3.97 (dd, *J* = 15.3, 3.9 Hz, 1H), 3.76 (s, 3H), 1.43 (dd, *J* = 6.9, 0.9 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.6, 139.2, 134.1, 133.7, 132.4, 131.3, 130.1, 129.9, 129.2, 128.8, 128.4, 113.3, 64.6, 55.2, 50.6, 15.2.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{36}H_{34}N_2NaO_9S_4$: 789.1039; Found: 789.1042.

(*E*)-*N*,*N*'-(3-(4-methoxyphenyl)pent-2-ene-1,4-diyl)bis(*N*-methyl benzenesulfonamide) (7a)



7a

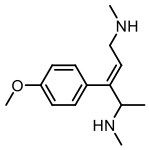
Compound **7a** was isolated via column chromatography (PE: EA= 3: 1) as colorless oil (145 mg, 55% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.71 (dd, *J* = 7.5, 1.7 Hz, 2H), 7.54 (d, *J* = 7.3 Hz, 1H), 7.52 – 7.40 (m, 5H), 7.32 (t, *J* = 7.7 Hz, 2H), 6.89 (d, *J* = 8.6 Hz, 2H), 6.78 (d, *J* = 8.6 Hz, 2H), 5.49 (m, 1H), 4.94 (q, *J* = 6.9 Hz, 1H), 3.80 (s, 3H), 3.75 (dd, *J* = 15.0, 5.8 Hz, 1H), 3.44 (dd, *J* = 15.0, 7.5 Hz, 1H), 2.58 (s, 3H), 2.53 (s, 3H), 1.14 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.2, 144.6, 139.8, 138.1, 132.7, 132.3, 129.9, 129.5, 129.2, 128.9, 127.4, 127.2, 124.0, 114.0, 57.3, 55.3, 48.8, 34.7, 28.3, 15.8.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{26}H_{30}N_2NaO_5S_2$: 537.1488; Found: 537.1486.

(*E*)-3-(4-methoxyphenyl)-*N*^{1},*N*^{4}-dimethylpent-2-ene-1,4-diamine (8a)



8a

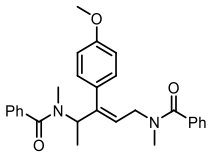
Compound **8a** was isolated via column chromatography (DCM: MeOH= 10: 1) as yellow oil (36 mg, 60% yield).

^{1}H NMR (400 MHz, Methanol-d_4) δ 7.07 (d, *J* = 8.7 Hz, 2H), 6.96 (d, *J* = 8.7 Hz, 2H), 5.66 (m, 1H), 3.82 (s, 3H), 3.09 (dd, *J* = 6.8, 2.7 Hz, 2H), 2.41 (s, 3H), 2.29 (s, 3H), 1.15 (d, *J* = 6.7 Hz, 3H).

^{13}C NMR (101 MHz, Methanol-d_4) δ 160.5, 146.8, 131.4, 131.1, 125.9, 114.8, 62.8, 55.7, 50.0, 35.2, 33.8, 20.6.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{14}H_{23}N_2O$: 235.1805; Found: 235.1805.

(*E*)-N,N'-(3-(4-methoxyphenyl)pent-2-ene-1,4-diyl)bis(N-methylbenzamide) (9a)



9a

Compound **9a** was isolated via column chromatography (EA) as colorless oil (57 mg, 76% yield).

^{1}H NMR (400 MHz, Methanol-d_4) δ 7.51 – 6.52 (m, 14H), 5.79 – 5.65 (m, 1H), 4.40 (m, 1H), 4.11 – 3.49 (m, 5H), 3.07 – 2.54 (m, 6H), 1.56 – 1.40 (m, 3H).

^{13}C NMR (101 MHz, Methanol-d_4) δ 174.5, 173.5, 160.9, 137.2, 131.0, 130.8, 130.7, 130.4, 129.6, 129.5, 129.4, 128.0, 127.7, 127.3, 125.4, 124.4, 115.1, 114.8, 60.5, 55.8, 49.4, 49.2, 49.0, 48.8, 48.6, 47.3, 33.4, 32.4, 28.1.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{28}H_{31}N_2O_3$: 443.2329; Found: 443.2328.

5. X-Ray Crystallographic Data

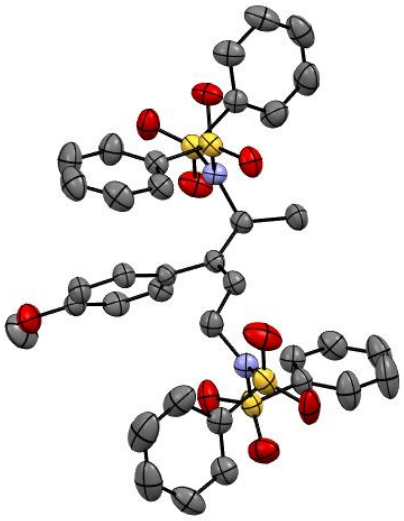
A solution of **2a** in $CHCl_3$ and MeOH (v/v = 1:1) was evaporated the solvent slowly at room temperature. A suitable crystal was selected and measured on a Bruker APEX-II CCD diffractometer. The crystal was kept at 302.0 K during data collection. Using Olex2, the structure was solved with the SHELXT structure solution program using Intrinsic Phasing and refined with the SHELXL refinement package using Least Squares minimization.

Crystal structure determination of (2a)

Crystal Data for $C_{36}H_{34}N_2O_9S_4$ (M =766.89 g/mol): triclinic, space group P-1 (no. 2), a = 11.2497(16) Å, b = 12.986(2) Å, c = 13.162(2) Å, α = 107.008(5)°, β = 94.207(5)°, γ = 101.192(5)°, V = 1786.4(5) Å^3, Z = 2, T = 302.0 K, μ(MoKα) = 0.324 mm^{-1}, *Dcalc* = 1.426 g/cm^3, 39078 reflections measured (3.888° ≤ 2Θ ≤ 49.998°), 6278 unique (R_{int} = 0.1139, R_{sigma} = 0.0782) which were used in all calculations. The final R_1 was 0.0518 (I > 2σ(I)) and wR_2 was 0.1506 (all data).

CCDC 2235969 (**2a**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif.

Crystal data and structure for 2a (thermal ellipsoids are shown at the 50% level).



Identification code	**2a**

Empirical formula	$C_{36}H_{34}N_2O_9S_4$
Formula weight	766.89
Temperature/K	302.0
Crystal system	Triclinic
Space group	P-1
a/Å	11.2497(16)
b/Å	12.986(2)
c/Å	13.162(2)
α/°	107.008(5)
β/°	94.207(5)
γ/°	101.192(5)
Volume/Å^3	1786.4(5)
Z	2
ρ_{calc}g/cm^3	1.426
μ/mm^{-1}	0.324
F(000)	800.0
Crystal size/mm^3	0.5 × 0.5 × 0.3
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.888 to 49.998
Index ranges	-13 ≤ h ≤ 13, -15 ≤ k ≤ 15, -15 ≤ l ≤ 15
Reflections collected	39078
Independent reflections	6278 [R_{int} = 0.1139, R_{sigma} = 0.0782]
Data/restraints/parameters	6278/0/462
Goodness-of-fit on F^2	1.021
Final R indexes [I>=2σ (I)]	R_1 = 0.0518, wR_2 = 0.1308
Final R indexes [all data]	R_1 = 0.0747, wR_2 = 0.1506
Largest diff. peak/hole / e Å^{-3}	0.33/-0.34

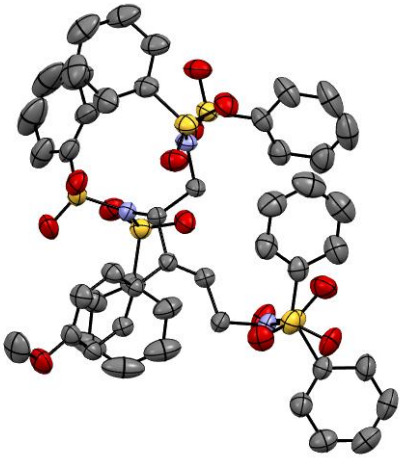
A solution of **4a** in $CHCl_3$ and MeOH ((v/v = 1:1)) was evaporated the solvent slowly at room temperature. A suitable crystal was selected and measured on a Bruker APEX-II CCD diffractometer. The crystal was kept at 281.0 K during data collection. Using Olex2, the structure was solved with the SHELXT structure solution program using Intrinsic Phasing and refined with the SHELXL refinement package using Least Squares minimization.

Crystal structure determination of (4a)

Crystal Data for $C_{48}H_{43}N_3O_{13}S_6$ (M =1062.21 g/mol): triclinic, space group P-1 (no. 2), a = 10.4451(10) Å, b = 12.2723(14) Å, c = 21.050(2) Å, α = 91.901(3)°, β = 97.835(3)°, γ = 114.482(3)°, V = 2420.7(5) Å^3, Z = 2, T = 281.0 K, μ(MoKα) = 0.351 mm^{-1}, *Dcalc* = 1.457 g/cm^3, 61377 reflections measured (3.926° ≤ 2Θ ≤ 50°), 8535 unique (R_{int} = 0.1279, R_{sigma} = 0.0740) which were used in all calculations. The final R_1 was 0.0451 (I > 2σ(I)) and wR_2 was 0.1252 (all data).

CCDC 2305251 (**4a**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif.

Crystal data and structure for 4a (thermal ellipsoids are shown at the 50% level).



Identification code	**4a**
Empirical formula	$C_{48}H_{43}N_3O_{13}S_6$
Formula weight	1062.21
Temperature/K	281.0
Crystal system	triclinic
Space group	P-1
a/Å	10.4451(10)

b/Å	12.2723(14)
c/Å	21.050(2)
α/°	91.901(3)
β/°	97.835(3)
γ/°	114.482(3)
Volume/Å^3	2420.7(5)
Z	2
ρ_{calc}g/cm^3	1.457
μ/mm^{-1}	0.351
F(000)	1104.0
Crystal size/mm^3	0.34 × 0.26 × 0.22
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.926 to 50
Index ranges	-12 ≤ h ≤ 11, -14 ≤ k ≤ 14, -25 ≤ l ≤ 25
Reflections collected	61377
Independent reflections	8535 [Rint = 0.1279, Rsigma = 0.0740]
Data/restraints/parameters	8535/0/632
Goodness-of-fit on F^2	1.015
Final R indexes [I>=2σ (I)]	R1 = 0.0451, wR2 = 0.1065
Final R indexes [all data]	R1 = 0.0781, wR2 = 0.1252
Largest diff. peak/hole / e Å^{-3}	0.23/-0.32

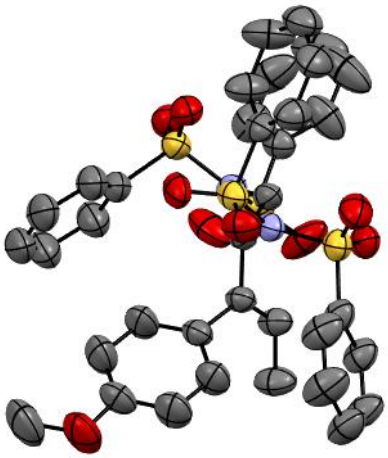
A solution of **6a** in $CHCl_3$ and MeOH ((v/v = 1:1)) was evaporated the solvent slowly at room temperature. A suitable crystal was selected and measured on a Bruker APEX-II CCD diffractometer. The crystal was kept at 303.0 K during data collection. Using Olex2, the structure was solved with the SHELXT structure solution program using Intrinsic Phasing and refined with the SHELXL refinement package using Least Squares minimization.

Crystal structure determination of (6a)

Crystal Data for $C_{36}H_{34}N_2O_9S_4$ (M =766.89 g/mol): monoclinic, space group $P2_1/n$ (no. 14), a = 11.2841(19) Å, b = 20.731(3) Å, c = 15.751(3) Å, β = 98.855(5)°, V = 3640.7(11) Å^3, Z = 4, T = 303.0 K, μ(MoKα) = 0.318 mm^{-1}, *Dcalc* = 1.399 g/cm^3, 124181 reflections measured (4.148° ≤ 2Θ ≤ 49.998°), 6407 unique (R_{int} = 0.1276, R_{sigma} = 0.0551) which were used in all calculations. The final R_1 was 0.0515 (I > 2σ(I)) and wR_2 was 0.1511 (all data).

CCDC 2235971 (**6a**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif.

Crystal data and structure for 6a (thermal ellipsoids are shown at the 50% level).



Identification code	**6a**
Empirical formula	$C_{36}H_{34}N_2O_9S_4$
Formula weight	766.89
Temperature/K	303.0
Crystal system	monoclinic
Space group	$P2_1/n$

a/Å	11.2841(19)
b/Å	20.731(3)
c/Å	15.751(3)
α/°	90
β/°	98.855(5)
γ/°	90
Volume/Å^3	3640.7(11)
Z	4
ρ_{calc}g/cm^3	1.399
μ/mm^{-1}	0.318
F(000)	1600.0
Crystal size/mm^3	0.5 × 0.46 × 0.45
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.148 to 49.998
Index ranges	-13 ≤ h ≤ 13, -24 ≤ k ≤ 24, -18 ≤ l ≤ 18
Reflections collected	124181
Independent reflections	6407 [R_{int} = 0.1276, R_{sigma} = 0.0551]
Data/restraints/parameters	6407/0/462
Goodness-of-fit on F^2	1.058
Final R indexes [I>=2σ (I)]	R_1 = 0.0515, wR_2 = 0.1285
Final R indexes [all data]	R_1 = 0.0752, wR_2 = 0.1511
Largest diff. peak/hole / e Å^{-3}	0.32/-0.30

6. Computational Data

Computational Details:

The present catalyst screening experiments found that $Rh_2(OAc)_4$ could also catalyze the reaction, and therefore $Rh_2(OAc)_4$ was used as the model in calculation to guarantee the calculation precision and reduce the computational cost, The geometric optimizations were conducted at the B3LYP[12, 13] combined with LANL2DZ[14-16] for Rh atoms and 6-31G(d)[17-20] for other atoms. The single point calculation was performed on the optimized geometries at the M06/def2-TZVP[21] level with the SMD ($CHCl_3$) solvent model.[22, 23] If other specified, the relative Gibbs free energies in the following decisions were the M06(SMD)/def2-TZVP single-point energies corrected by the B3LYP zero-Gibbs energies. NBO analysis was also used to probe the electron properties for the key species[24, 25]. All calculations were performed using Gaussian 09 software[26].

It should be emphasized that the triplet-state and singlet-state rection routes were in investigated the present simulation, respectively. The open-shell calculations were conducted for geometric optimization with Guess=MIX keyword. The spin contamination $<S^{**}>^2$ for triplet-state species in the range of 2.01~2.04 confirms those spin state species with two unpaired electrons in general; the $<S^{**}>^2$ for singlet-state species of zero means the full electron pairing properties for those state species except for s-TS1. This suggested the s-TS1 of some radical feature in the reaction.

Coordination of the optimized structures.

$Rh_2(OAc)_4$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-3.499709	-2.692406	-2.743666
2	45	0	-1.637752	-1.398325	-1.994297
3	8	0	-4.703474	-1.053727	-2.390073
4	8	0	-2.935953	0.173917	-1.677068
5	6	0	-4.169926	0.014517	-1.948070

6	6	0	-5.074516	1.210226	-1.757006
7	1	0	-6.101428	0.886208	-1.577366
8	1	0	-4.713855	1.829565	-0.932888
9	1	0	-5.057138	1.815543	-2.671093
10	8	0	-2.002372	-2.092797	-0.084906
11	6	0	-2.984373	-2.881615	0.103173
12	8	0	-3.775201	-3.314931	-0.795889
13	6	0	-3.251223	-3.316882	1.525832
14	1	0	-3.867629	-2.555404	2.018136
15	1	0	-3.793839	-4.263988	1.539734
16	1	0	-2.312215	-3.400393	2.077502
17	8	0	-3.134837	-1.998220	-4.653095
18	8	0	-1.362466	-0.775471	-3.942022
19	6	0	-2.153086	-1.209015	-4.841108
20	6	0	-1.886932	-0.773531	-6.263830
21	1	0	-1.281934	-1.541180	-6.760668
22	1	0	-2.827348	-0.678203	-6.811294
23	1	0	-1.333828	0.167422	-6.278031
24	8	0	-2.201719	-4.264858	-3.060601
25	8	0	-0.434064	-3.036934	-2.348420
26	6	0	-0.967712	-4.105317	-2.790158
27	6	0	-0.061985	-5.300230	-2.980801
28	1	0	0.955262	-4.973751	-3.206314
29	1	0	-0.039037	-5.877837	-2.049063
30	1	0	-0.446665	-5.945212	-3.773504

Thermal correction to Gibbs Free Energy= 0.155746
Sum of electronic and thermal Free Energies= -1132.957585
SCRF=-1135.13345485
<S**>2=0.000

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	4.252621	-0.026465	-0.928989
2	8	0	2.973192	1.702680	-0.209548
3	6	0	4.062623	1.192452	-0.630143
4	6	0	5.251660	2.121602	-0.758609
5	1	0	5.842439	1.852538	-1.637656
6	1	0	4.922883	3.160659	-0.821252
7	1	0	5.894572	2.004143	0.121933
8	45	0	2.678517	-1.354968	-0.752448
9	45	0	1.288776	0.481659	-0.019679

10	8	0	0.879762	0.826683	-2.034792
11	6	0	1.358545	0.039989	-2.916176
12	8	0	2.123336	-0.948940	-2.697816
13	6	0	0.978366	0.322739	-4.353727
14	1	0	1.366866	1.303945	-4.647768
15	1	0	1.384943	-0.442971	-5.015789
16	1	0	-0.111960	0.356217	-4.443349
17	8	0	3.156088	-1.699633	1.225966
18	8	0	1.825626	0.001208	1.920575
19	6	0	2.614911	-0.978523	2.120834
20	6	0	2.908537	-1.331570	3.562279
21	1	0	2.891977	-0.433543	4.183292
22	1	0	2.127548	-2.011013	3.923767
23	1	0	3.871109	-1.841307	3.639703
24	8	0	1.047920	-2.599930	-0.564770
25	8	0	-0.253564	-0.880002	0.134242
26	6	0	-0.052578	-2.098642	-0.168759
27	6	0	-1.242463	-3.024564	-0.051402
28	1	0	-0.950586	-4.055432	-0.257425
29	1	0	-1.670492	-2.945700	0.952556
30	1	0	-2.013992	-2.707523	-0.760865
31	7	0	-0.238931	2.160454	0.852071
32	16	0	-1.864037	2.435853	-0.161642
33	16	0	0.393888	3.744894	1.575985
34	6	0	-0.672546	3.738474	-2.256467
35	6	0	-0.435046	4.867191	-3.039085
36	6	0	-1.019698	6.092100	-2.705446
37	6	0	-1.843916	6.205648	-1.582741
38	6	0	-2.088770	5.093337	-0.779444
39	6	0	-1.497591	3.878802	-1.137252
40	6	0	0.770578	3.128348	4.219562
41	6	0	1.564694	2.805628	5.318095
42	6	0	2.932893	2.570333	5.148746
43	6	0	3.515280	2.645866	3.880665
44	6	0	2.734936	2.956490	2.766941
45	6	0	1.374223	3.197672	2.960798
46	9	0	-0.783761	1.504414	1.982219
47	1	0	-0.222939	2.778031	-2.487952
48	1	0	0.207953	4.789776	-3.910795
49	1	0	-0.830099	6.965329	-3.323573
50	1	0	-2.294212	7.160474	-1.328727
51	1	0	-2.712400	5.155596	0.104182
52	1	0	-0.286666	3.340109	4.330165
53	1	0	1.118228	2.748494	6.306274

54	1	0	3.548901	2.332140	6.011719
55	1	0	4.578904	2.463575	3.757316
56	1	0	3.154780	2.999486	1.769028
57	8	0	1.244432	4.270509	0.513864
58	8	0	-0.750605	4.493440	2.094795
59	8	0	-2.893685	2.730078	0.825783
60	8	0	-1.926305	1.263780	-1.020700

Thermal correction to Gibbs Free Energy= 0.343839
Sum of electronic and thermal Free Energies= -2847.689827
SCRF= -2849.98317440
<S**>2=0.000

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	8	0	2.545311	1.390163	-0.046487
3	6	0	3.739754	1.054900	-0.333514
4	6	0	4.781697	2.149504	-0.314358
5	1	0	4.645895	2.786727	-1.195626
6	1	0	4.642261	2.773398	0.572483
7	1	0	5.786342	1.724280	-0.332118
8	45	0	2.732132	-1.654380	-0.719804
9	45	0	1.026364	-0.014780	-0.063858
10	8	0	0.740517	0.359031	-2.099180
11	6	0	1.416805	-0.305022	-2.952518
12	8	0	2.302198	-1.181657	-2.700467
13	6	0	1.108672	-0.045349	-4.412151
14	1	0	0.834178	1.001082	-4.564235
15	1	0	1.961814	-0.315159	-5.037241
16	1	0	0.251983	-0.663450	-4.705455
17	8	0	3.044405	-2.017363	1.301106
18	8	0	1.455175	-0.507822	1.909365
19	6	0	2.348754	-1.380843	2.155448
20	6	0	2.590348	-1.702019	3.615279
21	1	0	2.666257	-0.773668	4.188105
22	1	0	1.732906	-2.262297	4.004518
23	1	0	3.495345	-2.299690	3.733880
24	8	0	1.240773	-3.080091	-0.743908
25	8	0	-0.329020	-1.568206	-0.151479
26	6	0	0.045819	-2.744382	-0.459552

27	6	0	-1.005247	-3.828666	-0.458711
28	1	0	-0.709303	-4.646104	-1.118976
29	1	0	-1.105168	-4.222111	0.559723
30	1	0	-1.971030	-3.416485	-0.758869
31	7	0	-0.621238	2.981318	1.264669
32	16	0	-2.075377	3.143373	0.147678
33	16	0	-0.611242	4.037056	2.708744
34	6	0	-0.535078	3.710868	-2.048867
35	6	0	-0.002726	4.580770	-3.000025
36	6	0	-0.292674	5.947509	-2.947515
37	6	0	-1.117307	6.460471	-1.943130
38	6	0	-1.658813	5.609122	-0.980265
39	6	0	-1.355887	4.248159	-1.052911
40	6	0	1.248046	2.769884	4.286969
41	6	0	2.545892	2.551596	4.749900
42	6	0	3.613954	3.274076	4.211754
43	6	0	3.394471	4.223380	3.208798
44	6	0	2.103894	4.452274	2.733162
45	6	0	1.049685	3.719721	3.283281
46	9	0	-0.704320	1.664104	1.783909
47	1	0	-0.323873	2.646148	-2.080123
48	1	0	0.637170	4.189348	-3.785577
49	1	0	0.125561	6.616324	-3.694834
50	1	0	-1.340341	7.522607	-1.907081
51	1	0	-2.293198	5.982787	-0.185128
52	1	0	0.402879	2.229331	4.697787
53	1	0	2.720575	1.824095	5.537240
54	1	0	4.621390	3.102710	4.580820
55	1	0	4.226456	4.792804	2.804501
56	1	0	1.908719	5.190307	1.962943
57	8	0	-0.683658	5.370360	2.110877
58	8	0	-1.555246	3.564345	3.713804
59	8	0	-3.185995	3.802741	0.827279
60	8	0	-2.189444	1.801963	-0.411469

Thermal correction to Gibbs Free Energy= 0.334359
Sum of electronic and thermal Free Energies= -2847.661809
SCRF= -2849.95599245
<S**>2=2.009

s-TS1

Center Atomic Atomic Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-4.407251	-1.457649	-1.122191
2	6	0	-5.224309	-2.316385	-0.351015
3	6	0	-6.370757	-1.852900	0.273547
4	6	0	-6.728124	-0.494756	0.182213
5	6	0	-5.917110	0.385419	-0.552918
6	6	0	-4.782197	-0.096871	-1.192710
7	6	0	-3.164865	-1.905185	-1.807342
8	6	0	-3.115206	-1.585362	-3.327731
9	6	0	-1.257356	-3.647911	-1.936791
10	6	0	-2.665951	-3.305971	-1.436283
11	6	0	-1.875292	-0.842867	-3.846540
12	1	0	-7.015226	-2.519470	0.838181
13	8	0	-7.858778	-0.139012	0.839406
14	1	0	-6.149189	1.442111	-0.612078
15	1	0	-4.136919	0.604708	-1.713149
16	1	0	-3.209731	-2.550916	-3.847654
17	1	0	-4.006428	-1.011006	-3.600269
18	1	0	-0.970907	-4.648561	-1.592600
19	1	0	-1.202969	-3.651289	-3.030775
20	1	0	-2.685013	-3.412094	-0.345194
21	1	0	-3.379131	-4.045034	-1.836318
22	1	0	-1.886430	-0.824788	-4.942951
23	1	0	-1.861798	0.189288	-3.490600
24	1	0	-0.941939	-1.306883	-3.519487
25	1	0	-4.977027	-3.369338	-0.268610
26	1	0	-0.526869	-2.926850	-1.556903
27	1	0	-2.325243	-1.160784	-1.315272
28	8	0	4.239878	-0.566102	1.888101
29	8	0	2.240096	0.502480	1.923282
30	6	0	3.356759	0.163916	2.433856
31	6	0	3.644081	0.656732	3.836753
32	1	0	3.400496	-0.138523	4.551556
33	1	0	4.707717	0.883755	3.942474
34	1	0	3.038500	1.535558	4.066183
35	45	0	3.881208	-1.303143	-0.007641
36	45	0	1.761217	-0.116191	-0.010040
37	8	0	2.842316	1.518462	-0.734006
38	6	0	4.081496	1.397174	-1.001064
39	8	0	4.785636	0.355987	-0.824769
40	6	0	4.773549	2.617058	-1.571031
41	1	0	5.789123	2.369633	-1.883563
42	1	0	4.199897	3.002847	-2.419003

43	1	0	4.811203	3.402483	-0.807744
44	8	0	2.902902	-2.932236	0.793522
45	8	0	0.905912	-1.859339	0.720527
46	6	0	1.645223	-2.868858	0.957202
47	6	0	0.951930	-4.120893	1.448658
48	1	0	0.072804	-3.860190	2.041011
49	1	0	0.622173	-4.702984	0.580061
50	1	0	1.644980	-4.733377	2.029332
51	8	0	3.467961	-1.970966	-1.908509
52	8	0	1.486842	-0.865543	-1.927502
53	6	0	2.382881	-1.595939	-2.456704
54	6	0	2.118648	-2.080419	-3.866063
55	1	0	1.721871	-1.260634	-4.470457
56	1	0	3.032972	-2.477635	-4.310135
57	1	0	1.361269	-2.871949	-3.838160
58	7	0	-0.294526	1.002174	-0.027580
59	16	0	-0.648444	2.151162	-1.395057
60	16	0	-1.229947	1.354870	1.446963
61	6	0	0.973259	4.169826	-0.461362
62	6	0	1.194487	5.440192	0.068691
63	6	0	0.115182	6.267266	0.391273
64	6	0	-1.196659	5.830786	0.189335
65	6	0	-1.439585	4.562287	-0.335431
66	6	0	-0.346285	3.753273	-0.653677
67	6	0	-2.561736	-0.954717	2.103726
68	6	0	-2.773759	-2.083312	2.894218
69	6	0	-1.845712	-2.435653	3.879144
70	6	0	-0.698048	-1.663222	4.076576
71	6	0	-0.467970	-0.534278	3.289416
72	6	0	-1.405098	-0.200797	2.311634
73	9	0	-1.435748	-0.377373	-0.756586
74	1	0	1.793138	3.503970	-0.708618
75	1	0	2.211871	5.784699	0.230917
76	1	0	0.297013	7.256147	0.803569
77	1	0	-2.032453	6.476745	0.442094
78	1	0	-2.446522	4.195282	-0.492329
79	1	0	-3.285968	-0.647389	1.360280
80	1	0	-3.673344	-2.674846	2.750630
81	1	0	-2.024226	-3.307826	4.502789
82	1	0	0.016139	-1.935048	4.848821
83	1	0	0.416027	0.078333	3.414647
84	8	0	-0.335902	2.222997	2.217637
85	8	0	-2.573358	1.812413	1.083967
86	8	0	-2.058015	2.085086	-1.780149

87	8	0	0.397290	1.863336	-2.367945
88	6	0	-8.268024	1.223770	0.806917
89	1	0	-8.474370	1.553971	-0.218698
90	1	0	-7.510864	1.878115	1.255802
91	1	0	-9.185481	1.271381	1.395362

Thermal correction to Gibbs Free Energy= 0.594880
Sum of electronic and thermal Free Energies= -3390.723094
SCRF=-3393.08100902
<S**>2=0.368

t-TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.109137	1.525506	5.336425
2	6	0	-3.634122	1.561020	6.652231
3	6	0	-3.760069	2.753202	7.337583
4	6	0	-3.329808	3.964457	6.741441
5	6	0	-2.785069	3.952738	5.442817
6	6	0	-2.689191	2.753865	4.759338
7	6	0	-2.988530	0.282549	4.512436
8	6	0	-4.117800	0.249308	3.429879
9	6	0	-1.743879	-1.963033	4.755384
10	6	0	-2.835346	-1.031438	5.309505
11	6	0	-3.918318	-0.809359	2.344340
12	1	0	-4.187877	2.795759	8.334221
13	8	0	-3.476940	5.065814	7.503398
14	1	0	-2.415701	4.855378	4.970776
15	1	0	-2.245355	2.736590	3.770630
16	1	0	-5.076096	0.097495	3.949658
17	1	0	-4.160775	1.232012	2.951414
18	1	0	-1.664647	-2.870920	5.365324
19	1	0	-1.947370	-2.263401	3.723942
20	1	0	-2.576924	-0.808844	6.352022
21	1	0	-3.794282	-1.568508	5.339408
22	1	0	-4.706925	-0.720526	1.587942
23	1	0	-2.955251	-0.660287	1.845560
24	1	0	-3.962026	-1.828343	2.747273
25	1	0	-3.975930	0.645022	7.123408
26	1	0	-0.769474	-1.461401	4.759941
27	1	0	-2.066848	0.446934	3.874423

28	8	0	3.873958	0.275576	-1.041473
29	8	0	2.611429	1.858677	-0.025596
30	6	0	3.683205	1.439120	-0.569054
31	6	0	4.834798	2.417211	-0.632969
32	1	0	5.298018	2.482677	0.358338
33	1	0	5.582735	2.079174	-1.352217
34	1	0	4.465535	3.411341	-0.897464
35	45	0	2.343205	-1.099548	-0.917063
36	45	0	0.971602	0.599760	0.142442
37	8	0	0.417578	1.133359	-1.798190
38	6	0	0.843470	0.474496	-2.799855
39	8	0	1.647866	-0.506636	-2.754932
40	6	0	0.349502	0.911446	-4.161190
41	1	0	0.698910	0.223451	-4.932406
42	1	0	-0.743941	0.952171	-4.158746
43	1	0	0.721475	1.919258	-4.376002
44	8	0	2.998780	-1.677952	0.937383
45	8	0	1.698275	-0.118878	1.939783
46	6	0	2.523203	-1.086488	1.957651
47	6	0	2.953844	-1.587240	3.317022
48	1	0	2.107017	-2.096677	3.790630
49	1	0	3.787157	-2.284949	3.219643
50	1	0	3.230004	-0.741639	3.951797
51	8	0	0.776242	-2.414451	-0.774019
52	8	0	-0.512850	-0.839321	0.222155
53	6	0	-0.310264	-1.998703	-0.252481
54	6	0	-1.475277	-2.960936	-0.218031
55	1	0	-2.035918	-2.837841	0.711265
56	1	0	-2.150755	-2.723260	-1.047849
57	1	0	-1.125151	-3.988966	-0.327996
58	7	0	-0.232520	2.273123	1.007115
59	16	0	-1.886833	2.567322	0.413018
60	16	0	0.474447	3.622107	1.863260
61	6	0	-1.160579	3.967060	-1.858055
62	6	0	-1.087023	5.121205	-2.636666
63	6	0	-1.571594	6.335642	-2.143469
64	6	0	-2.133336	6.404234	-0.866595
65	6	0	-2.212558	5.259602	-0.073553
66	6	0	-1.723381	4.055505	-0.583593
67	6	0	1.374885	2.136329	4.032926
68	6	0	2.356797	1.810668	4.968549
69	6	0	3.666255	2.275978	4.814559
70	6	0	4.006414	3.066584	3.714207
71	6	0	3.035175	3.406716	2.771415

72	6	0	1.732209	2.938043	2.947261
73	9	0	-1.048663	1.042922	2.712958
74	1	0	-0.780316	3.016182	-2.211889
75	1	0	-0.650958	5.073121	-3.630763
76	1	0	-1.510780	7.231089	-2.756345
77	1	0	-2.509449	7.349463	-0.485555
78	1	0	-2.637255	5.287343	0.922636
79	1	0	0.366941	1.746001	4.096012
80	1	0	2.096461	1.190585	5.822278
81	1	0	4.421995	2.023839	5.554151
82	1	0	5.023616	3.429807	3.595591
83	1	0	3.267298	4.032007	1.917879
84	8	0	1.146403	4.446944	0.851513
85	8	0	-0.544269	4.249472	2.717615
86	8	0	-2.808049	2.889119	1.503576
87	8	0	-2.157241	1.436260	-0.467752
88	6	0	-3.074676	6.331246	6.977436
89	1	0	-3.637533	6.575955	6.069798
90	1	0	-2.001160	6.342557	6.758392
91	1	0	-3.299371	7.058179	7.758526

Thermal correction to Gibbs Free Energy= 0.595778
Sum of electronic and thermal Free Energies= -3390.716884
SCRF= -3393.08016406
<S**>2=2.013

s-IM1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.995778	-0.269072	0.394868
2	6	0	3.756233	-0.485231	1.079459
3	6	0	3.618686	-1.438004	2.062096
4	6	0	4.735441	-2.218408	2.425015
5	6	0	5.990502	-2.022888	1.778534
6	6	0	6.114142	-1.084114	0.791599
7	6	0	5.080463	0.696005	-0.620208
8	6	0	3.907872	1.515071	-1.048642
9	6	0	7.124255	2.151487	-0.727690
10	6	0	6.354609	0.966944	-1.366862
11	6	0	3.059524	0.731931	-2.096479
12	1	0	2.646402	-1.542878	2.527960
13	8	0	4.721390	-3.162092	3.359982

14	1	0	6.826654	-2.640451	2.088531
15	1	0	7.078442	-0.958398	0.312965
16	1	0	3.257244	1.799488	-0.215987
17	1	0	6.505753	3.053105	-0.685467
18	1	0	7.444703	1.909603	0.290368
19	1	0	7.007048	0.091671	-1.412412
20	1	0	6.095996	1.233471	-2.398275
21	1	0	2.521385	-0.098284	-1.631399
22	1	0	2.321872	1.420425	-2.514370
23	1	0	3.680294	0.347584	-2.914486
24	1	0	2.877710	0.100561	0.848697
25	1	0	8.011978	2.373734	-1.327598
26	6	0	3.499206	-3.443402	4.066784
27	1	0	3.747350	-4.250414	4.755078
28	1	0	2.718930	-3.766391	3.371555
29	1	0	3.166019	-2.562384	4.623055
30	1	0	4.269427	2.434770	-1.520712
31	7	0	-0.584555	1.345851	0.368347
32	16	0	0.490519	1.238609	1.613624
33	16	0	-1.047322	2.891608	-0.110005
34	6	0	-1.372993	0.932755	3.618543
35	6	0	-1.979026	1.275055	4.827457
36	6	0	-1.537322	2.388451	5.548202
37	6	0	-0.487300	3.168676	5.059788
38	6	0	0.124524	2.841502	3.848603
39	6	0	-0.324980	1.725904	3.145449
40	6	0	0.068590	3.141368	-2.635263
41	6	0	0.966114	3.676937	-3.561632
42	6	0	1.971346	4.554375	-3.142358
43	6	0	2.081220	4.896721	-1.791593
44	6	0	1.187958	4.367073	-0.856858
45	6	0	0.192178	3.490093	-1.288636
46	1	0	-1.702615	0.071933	3.044578
47	1	0	-2.800274	0.672356	5.206543
48	1	0	-2.015803	2.650571	6.488429
49	1	0	-0.149174	4.038921	5.616068
50	1	0	0.930750	3.439829	3.441017
51	1	0	-0.719860	2.460322	-2.934254
52	1	0	0.871608	3.420732	-4.614061
53	1	0	2.657455	4.981884	-3.869655
54	1	0	2.850630	5.592792	-1.466360
55	1	0	1.244912	4.631694	0.192175
56	8	0	-2.283621	2.752718	-0.878295
57	8	0	1.656667	2.144115	1.430349

58	8	0	0.817684	-0.193262	1.774487
59	45	0	-2.592378	-2.522976	-1.535514
60	45	0	-1.539223	-0.562205	-0.545349
61	8	0	-4.421622	-1.604970	-1.282763
62	8	0	-3.446301	0.177850	-0.270391
63	6	0	-4.447806	-0.472812	-0.699288
64	6	0	-5.806312	0.153750	-0.464930
65	1	0	-6.143895	-0.094347	0.548405
66	1	0	-5.731442	1.240829	-0.540239
67	1	0	-6.534108	-0.237044	-1.179138
68	8	0	-1.777518	-1.517326	1.298698
69	6	0	-2.322031	-2.664767	1.344141
70	8	0	-2.739550	-3.344953	0.356201
71	6	0	-2.520152	-3.269692	2.720788
72	1	0	-3.506591	-2.976176	3.099268
73	1	0	-2.490450	-4.360183	2.662877
74	1	0	-1.761771	-2.898417	3.413757
75	8	0	-2.413612	-1.623827	-3.386491
76	8	0	-1.424206	0.207563	-2.481548
77	6	0	-1.892842	-0.468126	-3.452037
78	6	0	-1.837684	0.185063	-4.819163
79	1	0	-0.847211	0.617507	-4.989467
80	1	0	-2.072492	-0.539629	-5.600603
81	1	0	-2.568126	1.001332	-4.853388
82	8	0	-0.707976	-3.360280	-1.748166
83	8	0	0.308517	-1.508088	-0.909134
84	6	0	0.306650	-2.675547	-1.410125
85	6	0	1.662864	-3.313220	-1.658702
86	1	0	2.377549	-2.993720	-0.895966
87	1	0	1.574678	-4.401667	-1.669091
88	1	0	2.037190	-2.989857	-2.637515
89	8	0	-0.991379	3.817280	1.033971

Thermal correction to Gibbs Free Energy= 0.587645
Sum of electronic and thermal Free Energies= -3290.370457
SCRF= -3292.73224494
<S**>2=0.000

t-IM1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-3.836532	1.771164	5.183080
2	6	0	-4.033549	2.001239	6.575860
3	6	0	-3.954608	3.268480	7.145580
4	6	0	-3.677787	4.383924	6.342766
5	6	0	-3.478283	4.196546	4.962064
6	6	0	-3.552049	2.936213	4.399593
7	6	0	-3.916232	0.468526	4.605103
8	6	0	-3.633705	0.220749	3.143285
9	6	0	-3.073813	-1.435119	6.082190
10	6	0	-4.288596	-0.743845	5.424057
11	6	0	-4.889390	0.330627	2.249750
12	1	0	-4.112318	3.376369	8.213355
13	8	0	-3.579921	5.670278	6.792841
14	1	0	-3.265900	5.067808	4.349361
15	1	0	-3.387657	2.841580	3.331979
16	1	0	-2.867298	0.901271	2.758431
17	1	0	-3.220105	-0.792159	3.032495
18	1	0	-3.381545	-2.333774	6.630844
19	1	0	-2.337600	-1.735057	5.327511
20	1	0	-5.020048	-0.491153	6.201813
21	1	0	-4.787686	-1.471834	4.769666
22	1	0	-5.316385	1.338250	2.297740
23	1	0	-4.638145	0.117684	1.204166
24	1	0	-5.666667	-0.375776	2.565649
25	1	0	-4.247173	1.164338	7.232337
26	1	0	-2.571016	-0.760919	6.784354
27	8	0	4.494445	-0.003673	-1.949030
28	8	0	3.350011	1.792499	-1.190706
29	6	0	4.342927	1.246443	-1.769718
30	6	0	5.408137	2.176034	-2.298646
31	1	0	5.027392	2.682858	-3.192507
32	1	0	5.630353	2.942810	-1.552144
33	1	0	6.307334	1.615330	-2.558974
34	45	0	3.017572	-1.269153	-1.289558
35	45	0	1.846848	0.643483	-0.376488
36	8	0	0.910960	0.775749	-2.227744
37	6	0	1.164456	-0.074738	-3.142460
38	8	0	1.996608	-1.029593	-3.054350
39	6	0	0.410037	0.087140	-4.441496
40	1	0	0.726971	1.014278	-4.931624
41	1	0	0.605311	-0.758065	-5.102963
42	1	0	-0.660806	0.169154	-4.233834
43	8	0	4.000232	-1.480198	0.500350
44	8	0	2.933718	0.324681	1.354352

45	6	0	3.755707	-0.646947	1.426175
46	6	0	4.517842	-0.799562	2.721639
47	1	0	4.941056	-1.802864	2.793387
48	1	0	5.334592	-0.068559	2.740792
49	1	0	3.860561	-0.594962	3.569962
50	8	0	1.513444	-2.486594	-0.604646
51	8	0	0.469470	-0.716396	0.338370
52	6	0	0.572965	-1.955181	0.066999
53	6	0	-0.512030	-2.854485	0.607927
54	1	0	-1.490388	-2.416883	0.391777
55	1	0	-0.431463	-3.852379	0.174149
56	1	0	-0.411764	-2.920900	1.696888
57	7	0	0.808711	2.265745	0.484197
58	16	0	-0.882533	2.522087	0.154582
59	16	0	1.597373	3.400402	1.555027
60	6	0	-0.555782	3.773022	-2.274361
61	6	0	-0.654844	4.862306	-3.139160
62	6	0	-1.137724	6.088328	-2.673137
63	6	0	-1.521525	6.234729	-1.337529
64	6	0	-1.419388	5.158794	-0.456878
65	6	0	-0.938422	3.941059	-0.940523
66	6	0	0.231805	2.875210	3.917855
67	6	0	0.169561	2.439658	5.241526
68	6	0	1.302495	1.903084	5.858753
69	6	0	2.506784	1.800773	5.156946
70	6	0	2.580951	2.219581	3.828850
71	6	0	1.437006	2.745518	3.221538
72	1	0	-0.189792	2.810515	-2.614225
73	1	0	-0.359740	4.752867	-4.179015
74	1	0	-1.215102	6.932505	-3.353016
75	1	0	-1.895943	7.188864	-0.978310
76	1	0	-1.696258	5.251890	0.585768
77	1	0	-0.638120	3.299993	3.434841
78	1	0	-0.765926	2.528593	5.785026
79	1	0	1.249605	1.572219	6.892635
80	1	0	3.392009	1.403496	5.646506
81	1	0	3.502762	2.160313	3.265004
82	8	0	3.013488	3.357360	1.196890
83	8	0	0.853504	4.661435	1.487703
84	8	0	-1.573572	2.872104	1.403623
85	8	0	-1.316646	1.350000	-0.601105
86	6	0	-3.758084	5.909641	8.177518
87	1	0	-3.633578	6.985461	8.315962
88	1	0	-3.008439	5.378399	8.779887

89	1	0	-4.761421	5.615305	8.514474

Thermal correction to Gibbs Free Energy= 0.580333
Sum of electronic and thermal Free Energies= -3290.348230
SCRF= -3292.68202376
<S**>2=2.031

s-TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.418547	-0.642758	0.101152
2	6	0	3.878732	-0.952463	1.365691
3	6	0	4.275372	-2.083275	2.072880
4	6	0	5.239682	-2.947646	1.532068
5	6	0	5.777802	-2.666450	0.266752
6	6	0	5.366389	-1.542513	-0.433443
7	6	0	4.020472	0.576897	-0.633286
8	6	0	3.176591	1.581232	-0.034462
9	6	0	6.113223	1.552383	-1.664917
10	6	0	4.719911	0.945155	-1.928827
11	6	0	2.130643	0.733967	-0.816037
12	1	0	3.824958	-2.280198	3.038641
13	8	0	5.705891	-4.067328	2.141198
14	1	0	6.516420	-3.345799	-0.146481
15	1	0	5.803006	-1.362793	-1.409595
16	1	0	3.020608	1.580205	1.038865
17	1	0	6.034209	2.448022	-1.039247
18	1	0	6.778468	0.847334	-1.157848
19	1	0	4.805127	0.079936	-2.595001
20	1	0	4.112629	1.687365	-2.456166
21	1	0	1.921862	-0.289696	-0.518812
22	1	0	1.009580	1.229012	-0.301204
23	1	0	2.028904	0.923617	-1.880523
24	1	0	3.103357	-0.331982	1.803503
25	1	0	6.580707	1.841675	-2.612403
26	6	0	5.193953	-4.406741	3.424080
27	1	0	5.707668	-5.324167	3.715363
28	1	0	4.112704	-4.590307	3.388447
29	1	0	5.404998	-3.621132	4.160394
30	1	0	3.249780	2.590313	-0.434823

31	7	0	-0.206235	1.645662	0.289499
32	16	0	0.269019	1.914440	1.926147
33	16	0	-0.862617	3.012217	-0.552849
34	6	0	-1.952297	1.115791	3.360165
35	6	0	-3.029833	1.349550	4.216250
36	6	0	-3.314660	2.643875	4.656037
37	6	0	-2.520035	3.716870	4.244404
38	6	0	-1.443036	3.502271	3.385989
39	6	0	-1.178490	2.201962	2.951375
40	6	0	0.894868	3.535931	-2.616218
41	6	0	1.960316	4.205219	-3.221944
42	6	0	2.663132	5.186331	-2.516180
43	6	0	2.299135	5.504973	-1.204839
44	6	0	1.236809	4.841699	-0.587400
45	6	0	0.551941	3.854841	-1.299940
46	1	0	-1.720190	0.117223	3.009818
47	1	0	-3.645048	0.515340	4.542765
48	1	0	-4.154669	2.817273	5.323606
49	1	0	-2.739158	4.723435	4.589034
50	1	0	-0.818307	4.320367	3.051819
51	1	0	0.319958	2.786773	-3.149965
52	1	0	2.229667	3.972845	-4.248829
53	1	0	3.486581	5.711744	-2.992706
54	1	0	2.837777	6.276686	-0.661983
55	1	0	0.945025	5.073980	0.429138
56	8	0	-1.652794	2.495580	-1.666990
57	8	0	1.112592	3.121054	2.013514
58	8	0	0.862257	0.622111	2.307889
59	45	0	-2.417736	-2.618732	-1.226170
60	45	0	-1.275767	-0.679556	-0.338856
61	8	0	-4.177720	-1.547905	-1.150832
62	8	0	-3.099642	0.270857	-0.330764
63	6	0	-4.135521	-0.344817	-0.734419
64	6	0	-5.432124	0.432619	-0.704413
65	1	0	-5.695456	0.657405	0.334757
66	1	0	-5.291735	1.387204	-1.219867
67	1	0	-6.235543	-0.139105	-1.171561
68	8	0	-1.708617	-1.443080	1.551845
69	6	0	-2.309227	-2.560448	1.660074
70	8	0	-2.716366	-3.286645	0.701667
71	6	0	-2.585055	-3.053100	3.065006
72	1	0	-3.467823	-2.534281	3.457367
73	1	0	-2.785502	-4.125994	3.060256
74	1	0	-1.739802	-2.822784	3.718445

75	8	0	-2.086787	-1.884673	-3.122404
76	8	0	-0.855971	-0.165160	-2.306322
77	6	0	-1.377783	-0.837199	-3.250914
78	6	0	-1.138177	-0.327159	-4.655572
79	1	0	-0.065790	-0.180865	-4.819127
80	1	0	-1.536517	-1.024866	-5.393713
81	1	0	-1.626626	0.647002	-4.765809
82	8	0	-0.607623	-3.614299	-1.267648
83	8	0	0.468531	-1.839530	-0.355150
84	6	0	0.424417	-3.025219	-0.820106
85	6	0	1.730590	-3.789214	-0.864383
86	1	0	2.332617	-3.560265	0.018224
87	1	0	1.542154	-4.861913	-0.936809
88	1	0	2.299217	-3.473515	-1.747091
89	8	0	-1.458868	3.931794	0.422952

Thermal correction to Gibbs Free Energy= 0.583812
Sum of electronic and thermal Free Energies= -3290.340686
SCRF= -3292.68408655
<S**>2=0.000

t-TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.608439	-0.928988	-0.133967
2	6	0	4.697443	-0.656442	1.248247
3	6	0	5.341093	-1.524705	2.122672
4	6	0	5.928102	-2.703834	1.637571
5	6	0	5.841146	-3.000574	0.267605
6	6	0	5.187533	-2.134551	-0.593152
7	6	0	3.955131	0.004659	-1.064170
8	6	0	3.411520	1.264721	-0.625637
9	6	0	5.388374	0.152588	-3.139594
10	6	0	4.014022	-0.241714	-2.558597
11	6	0	2.102123	0.424172	-0.520673
12	1	0	5.375658	-1.275223	3.176640
13	8	0	6.584362	-3.611934	2.399749
14	1	0	6.291572	-3.919070	-0.094493
15	1	0	5.137329	-2.401078	-1.642908
16	1	0	3.706010	1.675445	0.336093
17	1	0	5.606630	1.208264	-2.945329

18	1	0	6.198968	-0.442411	-2.708579
19	1	0	3.791034	-1.286434	-2.799584
20	1	0	3.240927	0.360808	-3.045057
21	1	0	2.063275	-0.373737	0.213552
22	1	0	1.412358	1.320033	0.117109
23	1	0	1.555427	0.205882	-1.434806
24	1	0	4.226814	0.225996	1.669627
25	1	0	5.391704	0.000778	-4.224255
26	6	0	6.707910	-3.369103	3.796762
27	1	0	7.269040	-4.215313	4.195714
28	1	0	5.725622	-3.321092	4.282814
29	1	0	7.257891	-2.440640	3.993888
30	1	0	3.309148	2.037141	-1.387512
31	7	0	0.728025	2.245784	0.896536
32	16	0	1.328094	2.536932	2.415996
33	16	0	-0.599496	3.007228	0.251461
34	6	0	-0.454934	0.597583	3.290318
35	6	0	-1.309745	0.037482	4.239753
36	6	0	-1.548404	0.694181	5.450422
37	6	0	-0.937962	1.921766	5.714097
38	6	0	-0.083893	2.496284	4.771279
39	6	0	0.150281	1.824177	3.571477
40	6	0	0.120011	4.489282	-1.968642
41	6	0	0.575680	5.643771	-2.608411
42	6	0	0.907772	6.775085	-1.860308
43	6	0	0.782036	6.759040	-0.468276
44	6	0	0.324512	5.614828	0.184901
45	6	0	0.003257	4.488501	-0.577472
46	1	0	-0.287606	0.102714	2.339038
47	1	0	-1.797333	-0.910289	4.027670
48	1	0	-2.217384	0.252564	6.184306
49	1	0	-1.131790	2.438768	6.649792
50	1	0	0.385937	3.457396	4.948519
51	1	0	-0.161344	3.605223	-2.530313
52	1	0	0.663506	5.659579	-3.691400
53	1	0	1.260935	7.672207	-2.361902
54	1	0	1.038111	7.640674	0.112515
55	1	0	0.232080	5.586355	1.264351
56	8	0	-1.041575	2.098690	-0.829955
57	8	0	1.436509	3.970743	2.721924
58	8	0	2.556991	1.717811	2.462533
59	45	0	-2.832426	-2.581081	-1.391147
60	45	0	-1.869378	-0.344649	-0.987579
61	8	0	-4.178413	-1.705877	-2.685942

62	8	0	-3.287102	0.343067	-2.354544
63	6	0	-4.125505	-0.449567	-2.885502
64	6	0	-5.159325	0.153894	-3.808837
65	1	0	-5.959333	0.593963	-3.202210
66	1	0	-4.710947	0.954679	-4.401757
67	1	0	-5.589232	-0.612411	-4.456294
68	8	0	-3.244846	-0.151356	0.548231
69	6	0	-4.052615	-1.102142	0.799804
70	8	0	-4.123569	-2.219699	0.194292
71	6	0	-5.042652	-0.859394	1.919245
72	1	0	-5.872037	-0.256114	1.532139
73	1	0	-5.440261	-1.805140	2.292119
74	1	0	-4.566027	-0.292116	2.722370
75	8	0	-1.468677	-2.781603	-2.955353
76	8	0	-0.548794	-0.736535	-2.567334
77	6	0	-0.654173	-1.838332	-3.199565
78	6	0	0.265371	-2.030086	-4.389414
79	1	0	1.200666	-1.484761	-4.244182
80	1	0	0.458822	-3.092097	-4.553800
81	1	0	-0.227475	-1.628629	-5.282788
82	8	0	-1.433206	-3.347353	-0.068910
83	8	0	-0.549442	-1.309388	0.341224
84	6	0	-0.612020	-2.571338	0.508376
85	6	0	0.390851	-3.190988	1.457246
86	1	0	0.446599	-2.604443	2.378773
87	1	0	0.120744	-4.224292	1.680080
88	1	0	1.383924	-3.171244	0.993744
89	8	0	-1.534745	3.421489	1.299802

Thermal correction to Gibbs Free Energy= 0.574519
Sum of electronic and thermal Free Energies= -3290.321875
SCRF= -3292.66171135
<S**>2=2.013

s-IM2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.195486	2.124374	3.242738
2	6	0	-1.208782	1.654275	4.117236
3	6	0	-1.129308	2.099478	5.439900
4	6	0	-2.054909	3.036862	5.914002

5	6	0	-3.050409	3.516879	5.052213
6	6	0	-3.114520	3.062587	3.739265
7	6	0	-2.287272	1.593545	1.833727
8	6	0	-2.507481	2.576500	0.706645
9	6	0	-4.412531	0.172157	2.110409
10	6	0	-2.937106	0.212552	1.695975
11	6	0	-1.153273	1.918225	0.881266
12	1	0	-0.345377	1.714976	6.083307
13	8	0	-2.071676	3.542649	7.184825
14	1	0	-3.760801	4.244224	5.433427
15	1	0	-3.892906	3.444559	3.083628
16	1	0	-2.580385	3.634929	0.941119
17	1	0	-4.541406	0.454438	3.161059
18	1	0	-5.013419	0.861327	1.504425
19	1	0	-2.840460	-0.118371	0.653767
20	1	0	-2.361599	-0.504699	2.295311
21	1	0	-0.329177	2.528785	1.237658
22	1	0	-0.881218	1.181718	0.118892
23	1	0	-0.486566	0.925680	3.758077
24	1	0	-4.825472	-0.835000	1.980119
25	6	0	-1.090458	3.086475	8.098622
26	1	0	-1.286439	3.609392	9.036937
27	1	0	-0.074167	3.326117	7.757048
28	1	0	-1.164552	2.003228	8.266613
29	45	0	2.566041	-2.100966	0.430107
30	45	0	0.885032	-0.402103	0.548075
31	1	0	-3.123014	2.261645	-0.132519
32	8	0	3.950942	-0.688116	1.021266
33	8	0	2.357482	0.920597	1.144198
34	6	0	3.554330	0.499097	1.252707
35	6	0	4.590312	1.492324	1.728344
36	1	0	5.582163	1.207333	1.372005
37	1	0	4.332428	2.498767	1.391643
38	1	0	4.603290	1.492529	2.824713
39	8	0	1.291792	0.042438	-1.427049
40	6	0	2.188191	-0.626950	-2.036178
41	8	0	2.875456	-1.576562	-1.540445
42	6	0	2.482079	-0.236448	-3.466607
43	1	0	3.241512	0.554429	-3.467948
44	1	0	2.874818	-1.091413	-4.020536
45	1	0	1.581956	0.154768	-3.945485
46	8	0	2.174888	-2.548720	2.407874
47	8	0	0.573634	-0.948434	2.522924
48	6	0	1.275362	-1.888955	3.019228

49	6	0	1.035157	-2.244572	4.469294
50	1	0	0.960895	-3.330371	4.575839
51	1	0	1.892629	-1.913082	5.065667
52	1	0	0.128778	-1.763174	4.839698
53	8	0	1.101526	-3.431572	-0.160202
54	8	0	-0.490149	-1.819422	-0.064481
55	6	0	-0.093113	-3.010417	-0.280627
56	6	0	-1.144574	-4.017342	-0.688562
57	1	0	-0.681819	-4.875509	-1.179030
58	1	0	-1.669503	-4.365437	0.208747
59	1	0	-1.879875	-3.547434	-1.346110

Thermal correction to Gibbs Free Energy= 0.389960
Sum of electronic and thermal Free Energies= -1674.818828
SCRF= -1677.04360370
<S**>2=0.000

t-IM2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.345022	2.167062	3.321783
2	6	0	-1.401589	1.428087	4.044925
3	6	0	-1.157500	1.676292	5.399013
4	6	0	-1.868084	2.685455	6.059572
5	6	0	-2.816323	3.435392	5.350740
6	6	0	-3.046858	3.173959	4.004270
7	6	0	-2.621434	1.848090	1.873692
8	6	0	-2.707168	2.989408	0.883889
9	6	0	-4.969328	0.834490	2.160164
10	6	0	-3.541067	0.645254	1.636081
11	6	0	-1.507421	2.068151	0.870368
12	1	0	-0.413172	1.084660	5.921027
13	8	0	-1.709789	3.016550	7.377868
14	1	0	-3.358169	4.216611	5.875329
15	1	0	-3.784304	3.765822	3.467906
16	1	0	-2.559561	4.002885	1.246964
17	1	0	-4.975876	1.006955	3.241815
18	1	0	-5.454390	1.694395	1.682308
19	1	0	-3.574509	0.439039	0.557253
20	1	0	-3.091943	-0.241140	2.105317
21	1	0	-0.559665	2.459604	1.229199
22	1	0	-1.416434	1.366637	0.041795

23	1	0	-0.837013	0.645853	3.543331
24	1	0	-5.581081	-0.052104	1.956606
25	6	0	-0.766377	2.286466	8.140604
26	1	0	-0.804302	2.705289	9.148336
27	1	0	0.251463	2.396912	7.741835
28	1	0	-1.018534	1.217940	8.183961
29	45	0	2.898991	-1.951738	0.450383
30	45	0	0.863650	-0.585290	0.434524
31	1	0	-3.426096	2.908337	0.071831
32	8	0	3.930086	-0.234819	0.950984
33	8	0	2.057020	1.026367	0.934019
34	6	0	3.312096	0.870654	1.079001
35	6	0	4.130241	2.098464	1.400432
36	1	0	4.317598	2.650305	0.471910
37	1	0	3.573616	2.754275	2.074058
38	1	0	5.088229	1.815745	1.840077
39	8	0	1.229881	-0.229776	-1.578635
40	6	0	2.252829	-0.753712	-2.128168
41	8	0	3.119692	-1.496258	-1.563531
42	6	0	2.437500	-0.484785	-3.605961
43	1	0	2.163754	0.547881	-3.835614
44	1	0	3.466651	-0.687048	-3.907225
45	1	0	1.767360	-1.142363	-4.171825
46	8	0	2.537459	-2.315400	2.463695
47	8	0	0.649588	-1.048024	2.455123
48	6	0	1.517221	-1.793172	3.016794
49	6	0	1.335764	-2.065808	4.494662
50	1	0	1.627743	-3.093272	4.724563
51	1	0	1.994265	-1.396494	5.060704
52	1	0	0.302672	-1.882901	4.795603
53	8	0	1.704114	-3.559077	-0.051566
54	8	0	-0.171199	-2.300901	-0.066944
55	6	0	0.448999	-3.404680	-0.198411
56	6	0	-0.368624	-4.631734	-0.524183
57	1	0	0.212707	-5.319014	-1.142707
58	1	0	-0.620730	-5.145709	0.410837
59	1	0	-1.296138	-4.349280	-1.025622

Thermal correction to Gibbs Free Energy= 0.386158

Sum of electronic and thermal Free Energies= -1674.787795

SCRF= -1677.01997079

<S**>2=2.009

s-TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.624516	-0.636152	-0.066155
2	6	0	3.584447	-0.929492	0.828538
3	6	0	3.825726	-1.591960	2.032624
4	6	0	5.129172	-1.984108	2.362309
5	6	0	6.179036	-1.696119	1.477771
6	6	0	5.926210	-1.025853	0.286014
7	6	0	4.304011	0.108397	-1.333654
8	6	0	3.909637	-0.703206	-2.580267
9	6	0	3.659964	1.435060	-1.200287
10	1	0	2.989219	-1.774470	2.696647
11	8	0	5.478833	-2.636572	3.507621
12	1	0	7.186099	-1.995004	1.751795
13	1	0	6.762520	-0.790527	-0.366341
14	1	0	3.876745	-1.779540	-2.449818
15	1	0	3.114553	-0.292448	-3.197360
16	1	0	2.433598	1.222886	-0.858488
17	1	0	3.469965	1.913004	-2.167534
18	1	0	2.565725	-0.633750	0.601066
19	6	0	4.457553	-2.928598	4.449439
20	1	0	4.952205	-3.439206	5.277873
21	1	0	3.691058	-3.588241	4.021862
22	1	0	3.976940	-2.014001	4.820118
23	7	0	-0.533808	1.331875	0.342589
24	16	0	0.231669	1.445162	1.944832
25	16	0	-1.144187	2.882033	-0.302259
26	6	0	-1.996425	0.774494	3.443112
27	6	0	-2.963422	1.036806	4.414592
28	6	0	-3.008969	2.280969	5.047333
29	6	0	-2.086598	3.275924	4.711500
30	6	0	-1.122016	3.035559	3.735366
31	6	0	-1.092376	1.785386	3.112972
32	6	0	0.486669	3.459907	-2.439492
33	6	0	1.447324	4.219924	-3.105450
34	6	0	2.115422	5.251383	-2.436223
35	6	0	1.827069	5.525704	-1.097453
36	6	0	0.869007	4.770959	-0.416091
37	6	0	0.214415	3.747693	-1.100304
38	1	0	-1.942979	-0.185269	2.942525

39	1	0	-3.679727	0.264141	4.680079
40	1	0	-3.763075	2.476444	5.805083
41	1	0	-2.120733	4.242297	5.206322
42	1	0	-0.403483	3.794560	3.453154
43	1	0	-0.051714	2.659866	-2.935400
44	1	0	1.665379	4.017561	-4.150620
45	1	0	2.856002	5.847298	-2.962990
46	1	0	2.341175	6.332144	-0.582286
47	1	0	0.626333	4.969959	0.620435
48	8	0	-2.092838	2.537076	-1.353885
49	8	0	1.146982	2.591746	1.966036
50	8	0	0.724132	0.091542	2.196759
51	45	0	-2.518314	-2.515897	-1.481881
52	45	0	-1.439524	-0.590314	-0.469447
53	8	0	-4.335725	-1.563758	-1.280126
54	8	0	-3.340188	0.206205	-0.274303
55	6	0	-4.350796	-0.418781	-0.727130
56	6	0	-5.685005	0.279635	-0.588553
57	1	0	-5.875129	0.499544	0.466797
58	1	0	-5.644162	1.236601	-1.118441
59	1	0	-6.487565	-0.339600	-0.992135
60	8	0	-1.740140	-1.558868	1.356193
61	6	0	-2.296640	-2.705104	1.388658
62	8	0	-2.725511	-3.355909	0.388463
63	6	0	-2.486122	-3.330533	2.754413
64	1	0	-3.415140	-2.949365	3.195343
65	1	0	-2.568598	-4.415444	2.665046
66	1	0	-1.658219	-3.060326	3.414004
67	8	0	-2.284575	-1.634168	-3.326002
68	8	0	-1.181260	0.119894	-2.408214
69	6	0	-1.671963	-0.523485	-3.389006
70	6	0	-1.511999	0.106965	-4.756009
71	1	0	-0.454484	0.318363	-4.944182
72	1	0	-1.902937	-0.552779	-5.532019
73	1	0	-2.050151	1.060574	-4.774680
74	8	0	-0.674078	-3.412572	-1.638389
75	8	0	0.357537	-1.625396	-0.692493
76	6	0	0.344296	-2.796273	-1.189218
77	6	0	1.662654	-3.536344	-1.273723
78	1	0	2.425704	-3.044426	-0.669384
79	1	0	1.521704	-4.568664	-0.941481
80	1	0	1.986992	-3.571420	-2.320214
81	8	0	-1.570500	3.681134	0.852228
82	9	0	1.295025	1.244124	-0.493727

83	6	0	4.127357	2.397800	-0.132673
84	1	0	5.145833	2.739434	-0.377850
85	1	0	3.475019	3.272260	-0.084727
86	1	0	4.155381	1.929552	0.853182
87	6	0	5.234275	-0.035028	-2.570338
88	1	0	6.120857	-0.645395	-2.427814
89	1	0	5.390207	0.850850	-3.178326

Thermal correction to Gibbs Free Energy= 0.574116
Sum of electronic and thermal Free Energies= -3389.494807
SCRF= -3391.83716843
<S**>2=0.000

t-TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.757575	-0.559059	-0.074098
2	6	0	3.594452	-0.688578	0.714720
3	6	0	3.586684	-1.437544	1.885915
4	6	0	4.758305	-2.089056	2.302956
5	6	0	5.927007	-1.981818	1.524421
6	6	0	5.920655	-1.229334	0.360874
7	6	0	4.695260	0.262240	-1.322315
8	6	0	4.649207	-0.509408	-2.663659
9	6	0	3.897195	1.538919	-1.273099
10	1	0	2.665839	-1.485800	2.454072
11	8	0	4.867314	-2.836272	3.429550
12	1	0	6.826453	-2.483663	1.867130
13	1	0	6.845588	-1.141941	-0.199966
14	1	0	4.688698	-1.592661	-2.602114
15	1	0	3.969244	-0.117280	-3.415800
16	1	0	2.781272	1.304819	-1.083219
17	1	0	3.892661	2.004089	-2.267198
18	1	0	2.671305	-0.210954	0.404242
19	6	0	3.731149	-2.949169	4.280066
20	1	0	4.050728	-3.567218	5.120555
21	1	0	2.894133	-3.435204	3.763924
22	1	0	3.408509	-1.967100	4.645605
23	7	0	-0.749630	1.278761	0.397266
24	16	0	0.177531	1.355695	1.877113
25	16	0	-1.310310	2.829621	-0.223806

26	6	0	-1.918487	0.745560	3.587101
27	6	0	-2.780722	1.029306	4.646735
28	6	0	-2.722074	2.267200	5.291517
29	6	0	-1.800200	3.231874	4.877535
30	6	0	-0.939214	2.967256	3.813553
31	6	0	-1.010290	1.725202	3.180773
32	6	0	0.345455	3.272931	-2.377296
33	6	0	1.299357	4.005718	-3.080388
34	6	0	1.943719	5.088542	-2.472587
35	6	0	1.638156	5.442318	-1.156352
36	6	0	0.684745	4.716730	-0.439303
37	6	0	0.051002	3.644033	-1.063917
38	1	0	-1.947864	-0.209378	3.075677
39	1	0	-3.497144	0.279596	4.971830
40	1	0	-3.394936	2.480527	6.117880
41	1	0	-1.753959	4.194162	5.379474
42	1	0	-0.223374	3.703670	3.470229
43	1	0	-0.166218	2.428469	-2.822799
44	1	0	1.537325	3.736460	-4.105947
45	1	0	2.681087	5.661176	-3.029178
46	1	0	2.135213	6.287062	-0.687827
47	1	0	0.425930	4.977171	0.579473
48	8	0	-2.305906	2.513456	-1.244089
49	8	0	1.118422	2.478043	1.815982
50	8	0	0.653848	-0.011117	2.097915
51	45	0	-2.526797	-2.525946	-1.476937
52	45	0	-1.500252	-0.579213	-0.455844
53	8	0	-4.369623	-1.643695	-1.265979
54	8	0	-3.426831	0.143146	-0.251971
55	6	0	-4.422792	-0.502742	-0.705535
56	6	0	-5.773598	0.155686	-0.556938
57	1	0	-6.558146	-0.480610	-0.969197
58	1	0	-5.968088	0.354658	0.501695
59	1	0	-5.757826	1.121013	-1.072493
60	8	0	-1.785638	-1.555957	1.364959
61	6	0	-2.296452	-2.722814	1.391498
62	8	0	-2.695020	-3.385315	0.385168
63	6	0	-2.466876	-3.358964	2.753489
64	1	0	-3.403516	-3.001970	3.198082
65	1	0	-2.521675	-4.445062	2.658563
66	1	0	-1.644333	-3.069873	3.411658
67	8	0	-2.335971	-1.630350	-3.313940
68	8	0	-1.292113	0.150894	-2.384822
69	6	0	-1.763999	-0.496667	-3.371806

70	6	0	-1.627655	0.152147	-4.730325
71	1	0	-0.570714	0.348416	-4.937281
72	1	0	-2.044792	-0.491585	-5.506065
73	1	0	-2.149189	1.114662	-4.721695
74	8	0	-0.671633	-3.369928	-1.676864
75	8	0	0.296411	-1.580889	-0.682800
76	6	0	0.333521	-2.724422	-1.233152
77	6	0	1.693691	-3.360115	-1.402547
78	1	0	2.371540	-3.019484	-0.617707
79	1	0	1.603228	-4.448557	-1.398432
80	1	0	2.105613	-3.051941	-2.370846
81	8	0	-1.677737	3.649387	0.937229
82	9	0	1.348379	1.068852	-0.736734
83	6	0	4.312856	2.546367	-0.200225
84	1	0	5.360651	2.848083	-0.340106
85	1	0	3.684628	3.439044	-0.256710
86	1	0	4.205589	2.130561	0.804958
87	6	0	5.871647	0.261119	-2.313184
88	1	0	6.768209	-0.290001	-2.047631
89	1	0	6.065679	1.200339	-2.822810

Thermal correction to Gibbs Free Energy= 0.573588
Sum of electronic and thermal Free Energies= -3389.499258
SCRF= -3391.84939937
<S**>2=2.011

s-IM3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.353537	-0.179824	-0.150478
2	6	0	3.684560	-0.554856	1.021881
3	6	0	4.301699	-1.393137	1.954227
4	6	0	5.600207	-1.866383	1.722326
5	6	0	6.274496	-1.493339	0.546336
6	6	0	5.655202	-0.662859	-0.376406
7	6	0	3.723029	0.735507	-1.150798
8	6	0	2.107013	0.369722	-1.654059
9	6	0	3.787537	2.108531	-1.081464
10	1	0	3.754237	-1.665498	2.848770
11	8	0	6.288119	-2.683183	2.559515
12	1	0	7.278537	-1.870621	0.381253
13	1	0	6.187920	-0.383601	-1.282705

14	1	0	1.734670	-0.397772	-0.975936
15	1	0	1.465864	1.231171	-1.781847
16	1	0	3.288665	2.684742	-1.861234
17	1	0	2.668880	-0.217204	1.221710
18	6	0	5.657262	-3.111481	3.761572
19	1	0	6.382996	-3.752161	4.264526
20	1	0	4.746275	-3.685876	3.552620
21	1	0	5.410279	-2.261327	4.409513
22	7	0	-0.517079	1.549490	0.188666
23	16	0	-0.294875	1.475719	1.857382
24	16	0	-1.218999	2.900476	-0.502720
25	6	0	-0.156962	4.048846	2.933064
26	6	0	0.523783	5.142425	3.472373
27	6	0	1.918823	5.136915	3.554810
28	6	0	2.638980	4.025926	3.108553
29	6	0	1.966092	2.930359	2.560883
30	6	0	0.574206	2.958472	2.454021
31	6	0	0.475444	3.438837	-2.635693
32	6	0	1.493098	4.130662	-3.299570
33	6	0	2.202227	5.140851	-2.639185
34	6	0	1.887453	5.459537	-1.314467
35	6	0	0.870381	4.772649	-0.644550
36	6	0	0.177443	3.755782	-1.305792
37	1	0	-1.237172	4.032717	2.872684
38	1	0	-0.040021	5.994921	3.841089
39	1	0	2.441706	5.986482	3.986365
40	1	0	3.721343	4.001426	3.211540
41	1	0	2.504094	2.039547	2.256387
42	1	0	-0.113191	2.676761	-3.137426
43	1	0	1.709751	3.904550	-4.341025
44	1	0	2.976693	5.695211	-3.163444
45	1	0	2.415817	6.263267	-0.807930
46	1	0	0.594042	5.042303	0.368687
47	8	0	-2.062035	2.498409	-1.630037
48	8	0	0.679148	0.377056	2.027903
49	8	0	-1.554778	1.448899	2.604345
50	45	0	-2.337996	-2.680157	-1.443764
51	45	0	-1.379353	-0.629240	-0.558637
52	8	0	-4.101010	-1.677298	-1.764102
53	8	0	-3.262834	0.173565	-0.757479
54	6	0	-4.189478	-0.486000	-1.318024
55	6	0	-5.527118	0.208733	-1.442287
56	1	0	-6.051484	0.144037	-0.481782
57	1	0	-5.372447	1.265947	-1.670082

58	1	0	-6.137542	-0.271429	-2.209721
59	8	0	-1.970982	-1.287566	1.298903
60	6	0	-2.634925	-2.363069	1.409951
61	8	0	-2.956008	-3.153167	0.462827
62	6	0	-3.110473	-2.727209	2.799344
63	1	0	-4.168617	-2.456351	2.891966
64	1	0	-3.024668	-3.805754	2.955843
65	1	0	-2.540977	-2.176983	3.549946
66	8	0	-1.681392	-2.091754	-3.325258
67	8	0	-0.778722	-0.169040	-2.522977
68	6	0	-1.083936	-0.981333	-3.456246
69	6	0	-0.725412	-0.562734	-4.869165
70	1	0	0.213143	-0.001847	-4.879701
71	1	0	-0.656919	-1.434735	-5.522526
72	1	0	-1.514506	0.096742	-5.249077
73	8	0	-0.538582	-3.637814	-1.077400
74	8	0	0.428488	-1.716309	-0.363991
75	6	0	0.435333	-2.964119	-0.630312
76	6	0	1.736002	-3.715760	-0.420830
77	1	0	2.410880	-3.159595	0.231918
78	1	0	1.525121	-4.701414	0.001954
79	1	0	2.221749	-3.874211	-1.391476
80	8	0	-1.738860	3.845318	0.500324
81	6	0	4.467416	2.900965	-0.036275
82	1	0	5.139723	3.625854	-0.515975
83	1	0	3.715387	3.501900	0.496078
84	1	0	5.018924	2.285152	0.675125
85	6	0	3.216403	0.126437	-2.525965
86	1	0	3.586689	-0.890087	-2.626871
87	1	0	3.363996	0.762795	-3.394508

Thermal correction to Gibbs Free Energy= 0.564633
Sum of electronic and thermal Free Energies= -3289.126094
SCRF= -3291.50519695
<S**>2=0.000

t-IM3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.067416	-0.116855	-0.866735
2	6	0	3.775979	-0.216712	-0.337550

3	6	0	3.545652	-0.588926	0.992210
4	6	0	4.637961	-0.857439	1.829671
5	6	0	5.940688	-0.754364	1.317830
6	6	0	6.144679	-0.390472	-0.008470
7	6	0	5.288864	0.305063	-2.298771
8	6	0	4.705228	-0.582508	-3.396602
9	6	0	5.339819	1.757042	-2.574721
10	1	0	2.524790	-0.665352	1.350962
11	8	0	4.540185	-1.225503	3.137681
12	1	0	6.775426	-0.969714	1.978043
13	1	0	7.160406	-0.321571	-0.390434
14	1	0	4.128026	-1.447537	-3.081993
15	1	0	4.326220	-0.090525	-4.289322
16	1	0	5.372578	2.043808	-3.625703
17	1	0	2.918876	-0.007126	-0.973297
18	6	0	3.240355	-1.371995	3.698872
19	1	0	3.398691	-1.654444	4.741417
20	1	0	2.670234	-2.159328	3.189418
21	1	0	2.666228	-0.440368	3.651555
22	7	0	-1.105452	1.252785	0.687949
23	16	0	-0.568897	1.135614	2.339173
24	16	0	-1.632384	2.796654	0.080103
25	6	0	-0.091114	3.605446	3.468865
26	6	0	0.732110	4.670480	3.834843
27	6	0	2.071851	4.692204	3.437301
28	6	0	2.599114	3.647333	2.673933
29	6	0	1.789991	2.573058	2.304047
30	6	0	0.450294	2.571746	2.701583
31	6	0	0.646383	2.785583	-1.490343
32	6	0	1.802531	3.370392	-2.005584
33	6	0	2.176026	4.657999	-1.606768
34	6	0	1.400938	5.365267	-0.685528
35	6	0	0.252744	4.785039	-0.144541
36	6	0	-0.107041	3.500374	-0.552928
37	1	0	-1.132804	3.566465	3.762680
38	1	0	0.326667	5.480762	4.434003
39	1	0	2.708464	5.523505	3.728399
40	1	0	3.642123	3.661082	2.371516
41	1	0	2.195546	1.750423	1.725968
42	1	0	0.327865	1.797456	-1.805778
43	1	0	2.420866	2.819761	-2.708899
44	1	0	3.075690	5.109098	-2.016090
45	1	0	1.691995	6.366350	-0.380402
46	1	0	-0.353958	5.307169	0.586523

47	8	0	-2.507457	2.528662	-1.057300
48	8	0	0.326827	-0.027426	2.338807
49	8	0	-1.737039	1.176303	3.219261
50	45	0	-2.693872	-2.505989	-1.290858
51	45	0	-1.766173	-0.539353	-0.240485
52	8	0	-4.560238	-1.665283	-1.223337
53	8	0	-3.709301	0.149830	-0.182212
54	6	0	-4.668116	-0.518822	-0.682394
55	6	0	-6.034685	0.117097	-0.618225
56	1	0	-6.293891	0.314597	0.426671
57	1	0	-6.005424	1.081027	-1.135684
58	1	0	-6.781380	-0.535011	-1.073642
59	8	0	-2.144931	-1.469670	1.560130
60	6	0	-2.657547	-2.634509	1.587341
61	8	0	-2.980160	-3.327750	0.570769
62	6	0	-2.908322	-3.219972	2.956152
63	1	0	-3.717198	-2.660566	3.438536
64	1	0	-3.186342	-4.272057	2.877382
65	1	0	-2.014677	-3.101127	3.574750
66	8	0	-2.393973	-1.622790	-3.125431
67	8	0	-1.413093	0.171229	-2.158182
68	6	0	-1.820388	-0.490827	-3.168259
69	6	0	-1.593902	0.138890	-4.522163
70	1	0	-0.522215	0.302846	-4.674921
71	1	0	-1.986762	-0.502105	-5.312533
72	1	0	-2.084276	1.116956	-4.549217
73	8	0	-0.810551	-3.313669	-1.335483
74	8	0	0.077534	-1.473086	-0.367016
75	6	0	0.159232	-2.651350	-0.847565
76	6	0	1.506331	-3.330103	-0.809624
77	1	0	2.311352	-2.601207	-0.709378
78	1	0	1.532372	-3.998331	0.059380
79	1	0	1.638156	-3.941357	-1.705778
80	8	0	-2.103279	3.631343	1.190492
81	6	0	5.747353	2.777107	-1.561143
82	1	0	6.832281	2.748896	-1.350863
83	1	0	5.520335	3.791527	-1.908603
84	1	0	5.243940	2.622924	-0.599422
85	6	0	6.184925	-0.603469	-3.166711
86	1	0	6.616528	-1.478040	-2.686910
87	1	0	6.831588	-0.121066	-3.894434

Thermal correction to Gibbs Free Energy= 0.557795

Sum of electronic and thermal Free Energies= -3289.107501

SCRF= -3291.43413837

<S**>2=2.030

s-TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.325217	0.336955	-1.839021
2	6	0	4.440740	0.064771	-0.469110
3	6	0	5.164798	-1.039300	-0.004973
4	6	0	5.792225	-1.895510	-0.917279
5	6	0	5.687056	-1.635538	-2.292657
6	6	0	4.964154	-0.535868	-2.740503
7	6	0	3.545043	1.516025	-2.330949
8	6	0	1.223233	0.933757	-1.485002
9	6	0	4.078847	2.737103	-2.478689
10	1	0	5.236892	-1.208204	1.063577
11	8	0	6.526060	-2.994814	-0.578101
12	1	0	6.189233	-2.302550	-2.986706
13	1	0	4.906706	-0.336171	-3.808213
14	1	0	1.685794	0.774432	-0.525542
15	1	0	0.171131	1.161524	-1.531948
16	1	0	3.421837	3.539107	-2.816716
17	1	0	3.964474	0.723979	0.252320
18	6	0	6.686574	-3.297407	0.797876
19	1	0	7.307773	-4.194070	0.837338
20	1	0	5.722217	-3.504719	1.281557
21	1	0	7.189589	-2.482867	1.335497
22	7	0	0.939793	3.112754	-0.232330
23	16	0	0.710237	2.355747	1.200538
24	16	0	-0.246704	4.006274	-0.977847
25	6	0	-1.090688	3.721782	2.813505
26	6	0	-1.405770	4.646827	3.810446
27	6	0	-0.392977	5.362635	4.454504
28	6	0	0.945514	5.156054	4.109266
29	6	0	1.276724	4.234966	3.115488
30	6	0	0.251132	3.532177	2.478143
31	6	0	1.211905	6.094264	-2.068040
32	6	0	1.747328	7.383034	-2.062649
33	6	0	1.508819	8.236667	-0.982971
34	6	0	0.726367	7.806081	0.091493
35	6	0	0.185281	6.519884	0.096085
36	6	0	0.441803	5.671867	-0.983388

37	1	0	-1.859287	3.160507	2.297120
38	1	0	-2.444919	4.805937	4.084251
39	1	0	-0.646855	6.079636	5.230775
40	1	0	1.732438	5.706561	4.617179
41	1	0	2.309989	4.047353	2.844158
42	1	0	1.365386	5.425810	-2.908254
43	1	0	2.343979	7.722460	-2.905017
44	1	0	1.925295	9.240419	-0.982849
45	1	0	0.530214	8.474378	0.925437
46	1	0	-0.439477	6.180819	0.915242
47	8	0	-0.277158	3.562299	-2.386645
48	8	0	2.029256	1.800059	1.555314
49	8	0	-0.425697	1.375868	1.144690
50	45	0	-1.262230	-3.119224	-0.068774
51	45	0	-0.675776	-0.835482	0.460930
52	8	0	-2.776915	-2.377190	-1.264867
53	8	0	-2.212619	-0.233289	-0.781233
54	6	0	-2.928112	-1.116177	-1.356184
55	6	0	-4.077386	-0.613947	-2.200170
56	1	0	-3.823640	0.348272	-2.650180
57	1	0	-4.337720	-1.347155	-2.966170
58	1	0	-4.948978	-0.464236	-1.552054
59	8	0	-1.961917	-0.954742	2.030164
60	6	0	-2.601112	-2.037160	2.241640
61	8	0	-2.527778	-3.095917	1.542594
62	6	0	-3.504182	-2.058762	3.452564
63	1	0	-3.981241	-1.084667	3.582935
64	1	0	-4.253431	-2.846134	3.352478
65	1	0	-2.897363	-2.259524	4.343130
66	8	0	0.039050	-3.060893	-1.685536
67	8	0	0.626294	-0.932420	-1.294648
68	6	0	0.683467	-2.029319	-1.989878
69	6	0	1.553872	-2.085039	-3.218101
70	1	0	2.564377	-1.733955	-2.992089
71	1	0	1.588207	-3.111758	-3.584062
72	1	0	1.130908	-1.445411	-4.000973
73	8	0	0.285020	-3.734989	1.153118
74	8	0	0.841341	-1.590034	1.646783
75	6	0	0.994468	-2.850238	1.731561
76	6	0	2.146120	-3.331731	2.586126
77	1	0	2.150780	-2.793447	3.537830
78	1	0	2.078605	-4.407740	2.753876
79	1	0	3.086009	-3.101176	2.071509
80	8	0	-1.507101	4.060851	-0.218450

81	6	0	5.499173	3.138617	-2.208304
82	1	0	5.959105	3.574907	-3.105509
83	1	0	5.536468	3.911883	-1.429383
84	1	0	6.112332	2.294620	-1.882590
85	6	0	2.074152	1.299701	-2.653686
86	1	0	1.940521	0.543138	-3.438816
87	1	0	1.615091	2.211921	-3.057120

Thermal correction to Gibbs Free Energy= 0.563483
Sum of electronic and thermal Free Energies= -3289.141180
SCRF= -3291.46329483
<S**>2=0.000

t-TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.940647	1.092365	0.122194
2	6	0	4.421579	0.357955	1.196657
3	6	0	5.027492	-0.827855	1.627868
4	6	0	6.173145	-1.302257	0.977859
5	6	0	6.699489	-0.581572	-0.105092
6	6	0	6.089589	0.595434	-0.520785
7	6	0	4.301078	2.363611	-0.348231
8	6	0	2.069926	1.302611	-1.040905
9	6	0	4.742018	3.577683	0.020779
10	1	0	4.600782	-1.358146	2.471770
11	8	0	6.846506	-2.439857	1.316459
12	1	0	7.589684	-0.960672	-0.597597
13	1	0	6.514381	1.148421	-1.355116
14	1	0	2.030619	0.728506	-0.126387
15	1	0	1.369442	1.027696	-1.819658
16	1	0	4.226596	4.447871	-0.389616
17	1	0	3.530264	0.703340	1.713615
18	6	0	6.374207	-3.196767	2.419443
19	1	0	7.056884	-4.042952	2.516449
20	1	0	5.356084	-3.570923	2.247426
21	1	0	6.388452	-2.610530	3.347667
22	7	0	-0.314540	1.751179	0.006254
23	16	0	-0.121407	1.862862	1.715868
24	16	0	-1.317628	2.929882	-0.753697
25	6	0	-0.561442	4.393251	2.739917

26	6	0	-0.158063	5.659321	3.165388
27	6	0	1.175342	6.056379	3.028497
28	6	0	2.112838	5.184250	2.470031
29	6	0	1.721641	3.914092	2.042851
30	6	0	0.385020	3.536582	2.172527
31	6	0	0.210842	3.683361	-2.927780
32	6	0	1.057948	4.539336	-3.632912
33	6	0	1.529962	5.711081	-3.032992
34	6	0	1.149876	6.031238	-1.727374
35	6	0	0.298646	5.183767	-1.013023
36	6	0	-0.153844	4.010366	-1.618194
37	1	0	-1.588631	4.064475	2.833482
38	1	0	-0.885965	6.334069	3.607046
39	1	0	1.484508	7.042695	3.364584
40	1	0	3.151835	5.487344	2.373782
41	1	0	2.447838	3.230648	1.619247
42	1	0	-0.184615	2.779692	-3.380289
43	1	0	1.340020	4.298252	-4.654323
44	1	0	2.183863	6.379026	-3.587270
45	1	0	1.502564	6.949309	-1.265656
46	1	0	-0.028080	5.438705	-0.011383
47	8	0	-2.068182	2.250620	-1.811792
48	8	0	1.038681	0.991841	1.981044
49	8	0	-1.392191	1.615193	2.400869
50	45	0	-1.784870	-2.822324	-1.125313
51	45	0	-1.070157	-0.573645	-0.472331
52	8	0	-3.704043	-2.129393	-1.177398
53	8	0	-3.069183	-0.072404	-0.515842
54	6	0	-3.949278	-0.918278	-0.851034
55	6	0	-5.381998	-0.450323	-0.886826
56	1	0	-6.061826	-1.299817	-0.963556
57	1	0	-5.598783	0.138437	0.008855
58	1	0	-5.514191	0.209526	-1.751340
59	8	0	-1.336311	-1.188592	1.480969
60	6	0	-1.728391	-2.368199	1.733379
61	8	0	-1.993882	-3.275599	0.874813
62	6	0	-1.906570	-2.750332	3.184412
63	1	0	-1.357128	-3.676660	3.378475
64	1	0	-1.552173	-1.946951	3.829428
65	1	0	-2.964374	-2.952691	3.388508
66	8	0	-1.552640	-2.266558	-3.103561
67	8	0	-0.773471	-0.215794	-2.521303
68	6	0	-1.100402	-1.105490	-3.367614
69	6	0	-0.953295	-0.739491	-4.828640

70	1	0	0.041076	-0.319889	-5.007638
71	1	0	-1.115375	-1.611177	-5.464153
72	1	0	-1.687987	0.035329	-5.073851
73	8	0	0.177312	-3.403285	-1.041071
74	8	0	0.873454	-1.343214	-0.446896
75	6	0	1.082682	-2.565596	-0.720764
76	6	0	2.510955	-3.053561	-0.705333
77	1	0	2.540383	-4.105874	-0.415041
78	1	0	2.927558	-2.966952	-1.716017
79	1	0	3.117195	-2.445654	-0.030571
80	8	0	-2.024438	3.762404	0.230582
81	6	0	5.884329	3.879607	0.948017
82	1	0	6.651508	4.478456	0.438249
83	1	0	5.545975	4.475162	1.806934
84	1	0	6.356034	2.970676	1.329015
85	6	0	3.170173	2.239587	-1.356510
86	1	0	3.593323	1.900703	-2.324621
87	1	0	2.752486	3.230996	-1.599055

Thermal correction to Gibbs Free Energy= 0.557121
Sum of electronic and thermal Free Energies= -3289.080516
SCRF= -3291.40603947
<S**>2=2.014

G

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.754775	1.045367	-0.636695
2	6	0	5.642195	0.179276	0.017886
3	6	0	5.814407	-1.148073	-0.383870
4	6	0	5.080856	-1.642757	-1.467596
5	6	0	4.175975	-0.797778	-2.128142
6	6	0	4.014048	0.516121	-1.713262
7	6	0	4.572015	2.456738	-0.190638
8	6	0	2.436865	2.166423	1.148222
9	6	0	5.590521	3.306869	0.043752
10	1	0	6.507523	-1.780659	0.159025
11	8	0	5.164155	-2.916588	-1.949357
12	1	0	3.606157	-1.198163	-2.960745
13	1	0	3.301928	1.144258	-2.239826
14	1	0	2.979067	2.283475	2.089899

15	1	0	2.407193	1.096994	0.932782
16	1	0	5.328444	4.302201	0.405939
17	1	0	6.199429	0.541493	0.877028
18	6	0	6.044279	-3.821946	-1.304729
19	1	0	5.947274	-4.767839	-1.840960
20	1	0	5.769508	-3.972752	-0.252218
21	1	0	7.086955	-3.480749	-1.358632
22	7	0	1.045780	2.654472	1.383775
23	16	0	0.737596	3.431642	2.888000
24	16	0	-0.234684	1.790809	0.568896
25	6	0	0.990990	5.933625	1.748407
26	6	0	1.612681	7.169269	1.579748
27	6	0	2.773389	7.476035	2.297984
28	6	0	3.314608	6.550576	3.191939
29	6	0	2.702204	5.307847	3.370779
30	6	0	1.550932	5.013785	2.639930
31	6	0	-0.918398	3.756939	-1.232873
32	6	0	-1.772808	4.724240	-1.761287
33	6	0	-2.992791	4.998006	-1.135467
34	6	0	-3.365168	4.305442	0.018922
35	6	0	-2.518554	3.338237	0.562382
36	6	0	-1.300818	3.084070	-0.069308
37	1	0	0.086188	5.685138	1.203549
38	1	0	1.189882	7.895072	0.891114
39	1	0	3.252675	8.441616	2.162608
40	1	0	4.210771	6.794275	3.755141
41	1	0	3.097142	4.577816	4.068748
42	1	0	0.020005	3.514547	-1.719700
43	1	0	-1.491261	5.254845	-2.666321
44	1	0	-3.657471	5.748920	-1.553761
45	1	0	-4.315922	4.516244	0.499554
46	1	0	-2.782033	2.794306	1.461163
47	8	0	0.462113	1.177747	-0.565402
48	8	0	1.446674	2.736569	3.963142
49	8	0	-0.706994	3.648967	2.939912
50	8	0	-0.993629	0.974812	1.511208
51	6	0	7.060945	3.082981	-0.172903
52	1	0	7.494011	3.926195	-0.727455
53	1	0	7.606538	3.027060	0.780174
54	1	0	7.265026	2.165280	-0.730079
55	6	0	3.141901	2.929274	0.016616
56	1	0	2.556636	2.789162	-0.899946
57	1	0	3.135731	4.000768	0.242307

Thermal correction to Gibbs Free Energy= 0.384359
Sum of electronic and thermal Free Energies= -2156.272262
SCRF= -2156.39455394
<S**>2=0.000

2a(E)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.469808	5.117091	-0.348184
2	6	0	0.862679	3.776325	-0.313286
3	6	0	0.254844	2.858098	0.553686
4	6	0	-0.768297	3.325385	1.401104
5	6	0	-1.166911	4.656283	1.374850
6	6	0	-0.549366	5.563710	0.501187
7	8	0	-1.011742	6.847611	0.553897
8	6	0	0.702221	1.430841	0.586746
9	6	0	-0.076421	0.406006	0.213858
10	6	0	2.150662	1.253785	1.065505
11	6	0	2.250438	1.490975	2.582212
12	7	0	2.771759	-0.033994	0.599115
13	6	0	-1.426094	0.559258	-0.442025
14	7	0	-2.408206	-0.536803	-0.214452
15	1	0	0.958434	5.793970	-1.040144
16	1	0	1.639008	3.432338	-0.990841
17	1	0	-1.260219	2.631157	2.075806
18	1	0	-1.954715	5.019034	2.027969
19	6	0	-0.418448	7.809950	-0.301321
20	1	0	0.318475	-0.602674	0.244042
21	1	0	2.733699	2.046736	0.589352
22	1	0	3.284800	1.478232	2.927344
23	1	0	1.823001	2.478573	2.778520
24	1	0	1.669792	0.761183	3.150162
25	16	0	3.406544	-1.279151	1.624389
26	16	0	3.069244	-0.134287	-1.121610
27	1	0	-1.919597	1.484002	-0.147463
28	1	0	-1.297328	0.608360	-1.529797
29	16	0	-3.308734	-0.530844	1.273523
30	16	0	-2.195479	-2.035432	-1.048210
31	8	0	2.359297	-1.289336	-1.673128
32	8	0	2.765869	1.216829	-1.609332
33	8	0	3.899581	-2.290914	0.690680

34	8	0	4.312433	-0.669526	2.599513
35	8	0	-3.062012	-1.771453	2.003668
36	8	0	-2.998918	0.774357	1.862716
37	8	0	-0.909190	-2.641952	-0.698259
38	8	0	-3.443410	-2.773667	-0.850761
39	1	0	-0.928510	8.752319	-0.092417
40	1	0	0.654486	7.926184	-0.097390
41	1	0	-0.555870	7.551260	-1.359938
42	6	0	-5.025576	-0.496596	0.755010
43	6	0	-5.600314	0.735831	0.433024
44	6	0	-5.763733	-1.680674	0.739111
45	6	0	-6.945725	0.774905	0.068721
46	1	0	-5.009042	1.643551	0.485985
47	6	0	-7.109944	-1.624231	0.375857
48	1	0	-5.286660	-2.617773	0.997385
49	6	0	-7.697927	-0.402817	0.038936
50	1	0	-7.407567	1.725451	-0.182211
51	1	0	-7.698404	-2.536907	0.358412
52	1	0	-8.747048	-0.366712	-0.241617
53	6	0	-2.090251	-1.498685	-2.755114
54	6	0	-0.835230	-1.409218	-3.363410
55	6	0	-3.273925	-1.231266	-3.448570
56	6	0	-0.774145	-1.029112	-4.705787
57	1	0	0.067620	-1.626986	-2.800979
58	6	0	-3.192939	-0.856020	-4.788493
59	1	0	-4.231645	-1.330221	-2.948567
60	6	0	-1.946055	-0.753968	-5.413697
61	1	0	0.192618	-0.950086	-5.193781
62	1	0	-4.101852	-0.648455	-5.345756
63	1	0	-1.889780	-0.461288	-6.458570
64	6	0	4.834422	-0.373813	-1.345601
65	6	0	5.305743	-1.601024	-1.810636
66	6	0	5.686900	0.711045	-1.129962
67	6	0	6.670747	-1.742608	-2.058243
68	1	0	4.613961	-2.421269	-1.957710
69	6	0	7.051036	0.550568	-1.370555
70	1	0	5.291335	1.663023	-0.792998
71	6	0	7.540890	-0.672873	-1.834598
72	1	0	7.054348	-2.692516	-2.418792
73	1	0	7.728254	1.382692	-1.201743
74	1	0	8.604173	-0.791962	-2.023692
75	6	0	2.008000	-1.958202	2.508338
76	6	0	1.957848	-1.824685	3.898138
77	6	0	1.041731	-2.673894	1.798111

78	6	0	0.890860	-2.402842	4.586468
79	1	0	2.740521	-1.283568	4.417841
80	6	0	-0.026634	-3.231201	2.499244
81	1	0	1.107597	-2.783623	0.721692
82	6	0	-0.102074	-3.093790	3.887764
83	1	0	0.834274	-2.307079	5.667010
84	1	0	-0.804281	-3.752961	1.953170
85	1	0	-0.942141	-3.523822	4.425350

Thermal correction to Gibbs Free Energy= 0.563902
Sum of electronic and thermal Free Energies= -3770.639612
<S**>2=0.000

2a(Z)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.399288	-4.559333	-1.429237
2	6	0	-1.778665	-3.332808	-1.189478
3	6	0	-1.817596	-2.712291	0.068329
4	6	0	-2.541472	-3.368162	1.084292
5	6	0	-3.165595	-4.589373	0.861858
6	6	0	-3.096319	-5.199713	-0.398083
7	8	0	-3.741739	-6.396732	-0.517775
8	6	0	-1.113209	-1.417045	0.293866
9	6	0	0.093909	-1.221063	-0.266423
10	6	0	-1.826872	-0.419165	1.224944
11	6	0	-1.133929	-0.478037	2.603711
12	7	0	-1.905746	0.985127	0.644678
13	6	0	0.921057	0.034534	-0.266375
14	7	0	2.379006	-0.242057	-0.382121
15	1	0	-2.348416	-4.990489	-2.422644
16	1	0	-1.281669	-2.827691	-2.011189
17	1	0	-2.608795	-2.935593	2.078348
18	1	0	-3.711101	-5.093034	1.653973
19	6	0	-3.702300	-7.055687	-1.772873
20	1	0	0.515018	-2.024796	-0.864576
21	1	0	-2.857818	-0.760402	1.354000
22	1	0	-1.691110	0.055059	3.372515
23	1	0	-1.078593	-1.532804	2.888833
24	1	0	-0.106388	-0.110767	2.562105

25	16	0	-1.965269	2.400261	1.662660
26	16	0	-2.649523	1.152657	-0.951849
27	1	0	0.655986	0.665243	-1.122509
28	1	0	0.773767	0.643577	0.620092
29	16	0	3.096753	-0.170322	-1.937741
30	16	0	3.319186	-0.450880	1.049257
31	8	0	-1.866999	2.156769	-1.672087
32	8	0	-2.753378	-0.217226	-1.452685
33	8	0	-2.535152	3.454799	0.826555
34	8	0	-2.595968	2.054069	2.937474
35	8	0	4.405489	-0.807665	-1.822707
36	8	0	2.076822	-0.664158	-2.861842
37	8	0	4.542348	0.341064	0.926509
38	8	0	2.370163	-0.200857	2.137280
39	1	0	-4.262643	-7.983473	-1.642363
40	1	0	-4.175845	-6.454633	-2.560564
41	1	0	-2.672847	-7.292998	-2.072754
42	6	0	3.320606	1.580629	-2.257709
43	6	0	2.363995	2.255137	-3.020799
44	6	0	4.446238	2.229829	-1.742563
45	6	0	2.537146	3.619420	-3.262362
46	1	0	1.513243	1.717886	-3.425351
47	6	0	4.607026	3.591414	-1.998402
48	1	0	5.167991	1.678685	-1.151022
49	6	0	3.654867	4.284746	-2.753198
50	1	0	1.801923	4.156792	-3.853999
51	1	0	5.479552	4.110260	-1.611749
52	1	0	3.788868	5.344947	-2.950070
53	6	0	3.760099	-2.186669	1.087540
54	6	0	5.039078	-2.575867	0.688405
55	6	0	2.816606	-3.108108	1.549503
56	6	0	5.376625	-3.928052	0.753594
57	1	0	5.741767	-1.834047	0.329611
58	6	0	3.168304	-4.456107	1.603645
59	1	0	1.832472	-2.774904	1.860163
60	6	0	4.445047	-4.864363	1.207609
61	1	0	6.367833	-4.248251	0.446285
62	1	0	2.446098	-5.185606	1.958305
63	1	0	4.714001	-5.916067	1.253629
64	6	0	-4.341181	1.727857	-0.752280
65	6	0	-4.671794	3.045025	-1.071044
66	6	0	-5.309534	0.795061	-0.371451
67	6	0	-6.007242	3.437362	-0.989627
68	1	0	-3.894612	3.739345	-1.364281

69	6	0	-6.638832	1.207362	-0.279847
70	1	0	-5.033016	-0.235242	-0.175722
71	6	0	-6.986136	2.524821	-0.588005
72	1	0	-6.281313	4.459036	-1.235739
73	1	0	-7.402353	0.495643	0.020141
74	1	0	-8.023867	2.839691	-0.521091
75	6	0	-0.251973	2.829580	1.956343
76	6	0	0.272674	2.726827	3.244522
77	6	0	0.494587	3.345035	0.891466
78	6	0	1.590855	3.129132	3.464845
79	1	0	-0.342266	2.344254	4.051188
80	6	0	1.810266	3.738919	1.127619
81	1	0	0.052080	3.427130	-0.096218
82	6	0	2.357145	3.627581	2.410411
83	1	0	2.017989	3.047154	4.459692
84	1	0	2.409136	4.127776	0.309650
85	1	0	3.385906	3.928302	2.585926

Thermal correction to Gibbs Free Energy= 0.563712
Sum of electronic and thermal Free Energies= -3770.633274
<S**>2=0.000

4a(E)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.330211	4.265442	2.316749
2	6	0	0.332990	2.940705	1.878178
3	6	0	0.672384	2.607735	0.559832
4	6	0	1.000229	3.656834	-0.319563
5	6	0	0.995182	4.980196	0.101352
6	6	0	0.660318	5.294681	1.426297
7	8	0	0.685348	6.619971	1.744780
8	6	0	0.683361	1.180923	0.109782
9	6	0	1.793906	0.582899	-0.343509
10	6	0	-0.698624	0.510569	0.146129
11	6	0	-1.495129	1.066549	-1.067807
12	7	0	-0.698486	-0.979697	0.370305
13	6	0	3.141791	1.251083	-0.444929
14	7	0	4.280294	0.340368	-0.143571
15	1	0	0.074501	4.479718	3.347997
16	1	0	0.094582	2.149380	2.581985

17	1	0	1.246737	3.430191	-1.353861
18	1	0	1.240120	5.789412	-0.579283
19	6	0	0.339637	7.000720	3.066651
20	1	0	1.760824	-0.447946	-0.673438
21	1	0	-1.203351	0.892411	1.031784
22	1	0	-1.262572	2.135665	-1.104235
23	1	0	-1.136388	0.626606	-1.991824
24	16	0	-0.709664	-2.224080	-0.856258
25	16	0	-0.781666	-1.462935	2.030502
26	1	0	3.309287	1.625119	-1.460999
27	1	0	3.209413	2.108178	0.224716
28	16	0	5.115629	-0.356177	-1.461736
29	16	0	4.933645	0.319177	1.472803
30	8	0	-0.270934	-2.833277	2.077306
31	8	0	-0.122677	-0.397211	2.789948
32	8	0	-1.846254	-3.098331	-0.554869
33	8	0	-0.653373	-1.480107	-2.117471
34	8	0	5.955584	-1.419299	-0.916267
35	8	0	4.082283	-0.645462	-2.462612
36	8	0	6.386517	0.466789	1.381653
37	8	0	4.120160	1.299709	2.190099
38	1	0	0.417687	8.089224	3.094392
39	1	0	-0.687773	6.704356	3.316101
40	1	0	1.028754	6.569494	3.804896
41	6	0	6.158026	0.934775	-2.148049
42	6	0	5.751169	1.564101	-3.327716
43	6	0	7.360149	1.263937	-1.514215
44	6	0	6.564922	2.556240	-3.877035
45	1	0	4.827114	1.263660	-3.808593
46	6	0	8.160349	2.257248	-2.077062
47	1	0	7.648745	0.762963	-0.598014
48	6	0	7.764538	2.902546	-3.252358
49	1	0	6.262289	3.052006	-4.794822
50	1	0	9.096112	2.526265	-1.595915
51	1	0	8.395498	3.674712	-3.683837
52	6	0	4.563488	-1.309233	2.110099
53	6	0	5.571467	-2.274960	2.127475
54	6	0	3.283670	-1.559287	2.610974
55	6	0	5.280901	-3.529745	2.662155
56	1	0	6.551039	-2.042864	1.728078
57	6	0	3.007707	-2.823440	3.132102
58	1	0	2.521695	-0.787128	2.603546
59	6	0	4.003889	-3.802879	3.158750
60	1	0	6.053466	-4.292973	2.688496

61	1	0	2.011440	-3.037547	3.503765
62	1	0	3.783594	-4.784298	3.570312
63	6	0	-2.496886	-1.515101	2.571605
64	6	0	-3.304731	-2.594244	2.198295
65	6	0	-2.933261	-0.548509	3.479871
66	6	0	-4.577627	-2.700637	2.758250
67	1	0	-2.943339	-3.327072	1.487505
68	6	0	-4.208675	-0.672118	4.032909
69	1	0	-2.282305	0.272207	3.753543
70	6	0	-5.025562	-1.747538	3.678992
71	1	0	-5.213778	-3.537132	2.483397
72	1	0	-4.558402	0.071789	4.742276
73	1	0	-6.012640	-1.845495	4.122936
74	6	0	0.772805	-3.240174	-0.786885
75	6	0	1.872815	-2.876431	-1.567314
76	6	0	0.741825	-4.444598	-0.077835
77	6	0	2.987193	-3.716878	-1.593710
78	1	0	1.867716	-1.969362	-2.158386
79	6	0	1.856328	-5.278565	-0.126994
80	1	0	-0.132768	-4.713520	0.498407
81	6	0	2.979654	-4.911911	-0.873801
82	1	0	3.853542	-3.423828	-2.176411
83	1	0	1.845680	-6.216777	0.420312
84	1	0	3.848863	-5.563183	-0.899410
85	7	0	-2.986846	0.895825	-1.057006
86	16	0	-3.693855	0.805583	-2.695471
87	16	0	-3.742707	2.058277	0.035297
88	8	0	-3.631912	3.419863	-0.485885
89	8	0	-3.148066	1.739123	1.340806
90	8	0	-4.713933	1.850377	-2.795224
91	8	0	-2.572373	0.751122	-3.631381
92	6	0	-5.465391	1.578129	0.097731
93	6	0	-6.424768	2.470602	-0.383384
94	6	0	-5.814688	0.384950	0.732242
95	6	0	-7.773142	2.147912	-0.230873
96	1	0	-6.108921	3.383957	-0.873070
97	6	0	-7.167371	0.073315	0.870625
98	1	0	-5.049971	-0.284613	1.107560
99	6	0	-8.142781	0.952448	0.393033
100	1	0	-8.533729	2.829866	-0.599568
101	1	0	-7.455532	-0.853902	1.356934
102	1	0	-9.195074	0.707406	0.509497
103	6	0	-4.532402	-0.779216	-2.726194
104	6	0	-5.919321	-0.808500	-2.560948

105	6	0	-3.796554	-1.933182	-3.001182
106	6	0	-6.578411	-2.034406	-2.653709
107	1	0	-6.466028	0.109545	-2.381429
108	6	0	-4.471064	-3.151147	-3.084081
109	1	0	-2.724571	-1.876659	-3.145073
110	6	0	-5.856023	-3.202365	-2.910365
111	1	0	-7.657172	-2.073282	-2.532269
112	1	0	-3.909794	-4.058293	-3.285963
113	1	0	-6.375374	-4.154222	-2.982719

Thermal correction to Gibbs Free Energy= 0.742483
Sum of electronic and thermal Free Energies= -5385.007149
<S**>2=0.000

4a(Z)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	6	0	1.658409	2.596036	-2.447871
3	6	0	0.775787	2.574961	-1.359046
4	6	0	0.673802	3.745402	-0.581431
5	6	0	1.419184	4.879595	-0.877454
6	6	0	2.300991	4.879882	-1.968318
7	8	0	3.004132	6.033411	-2.166030
8	6	0	-0.041724	1.366892	-1.017404
9	6	0	-1.363065	1.532518	-0.851009
10	6	0	0.799740	0.094436	-0.813376
11	6	0	1.376009	0.212228	0.628728
12	7	0	0.151412	-1.199784	-1.268426
13	6	0	-2.406496	0.515713	-0.476119
14	7	0	-3.566044	1.107662	0.250935
15	1	0	3.075226	3.704138	-3.617454
16	1	0	1.742549	1.724090	-3.087024
17	1	0	0.008820	3.755007	0.277506
18	1	0	1.340552	5.777531	-0.272279
19	6	0	3.876476	6.105004	-3.283205
20	1	0	-1.762894	2.515522	-1.082066
21	1	0	1.666006	0.188514	-1.467537
22	1	0	1.709948	1.252618	0.705256
23	1	0	0.592276	0.079301	1.364874
24	16	0	-0.208329	-2.559276	-0.219054

25	16	0	0.337084	-1.478826	-2.975963
26	1	0	-2.799662	0.020173	-1.369030
27	1	0	-2.008481	-0.256636	0.177549
28	16	0	-4.728276	2.034607	-0.638764
29	16	0	-3.634271	0.970546	1.961276
30	8	0	-0.390427	-2.716388	-3.250942
31	8	0	-0.049560	-0.222672	-3.617833
32	8	0	0.799256	-3.600774	-0.431496
33	8	0	-0.370066	-1.920680	1.090463
34	8	0	-4.981880	3.282712	0.078489
35	8	0	-4.189738	2.036573	-1.999470
36	8	0	-4.973310	1.404748	2.350104
37	8	0	-3.161451	-0.380170	2.276277
38	1	0	4.314022	7.104712	-3.257834
39	1	0	4.678098	5.357025	-3.219725
40	1	0	3.333259	5.970828	-4.227768
41	6	0	-6.227497	1.051706	-0.644933
42	6	0	-6.374985	0.076697	-1.635383
43	6	0	-7.225799	1.303840	0.297429
44	6	0	-7.549643	-0.674494	-1.667119
45	1	0	-5.595512	-0.072366	-2.374521
46	6	0	-8.396031	0.546026	0.248997
47	1	0	-7.078148	2.067773	1.050238
48	6	0	-8.556260	-0.441329	-0.726320
49	1	0	-7.680931	-1.433588	-2.432812
50	1	0	-9.182848	0.729455	0.974773
51	1	0	-9.471230	-1.026592	-0.757723
52	6	0	-2.420380	2.127371	2.589484
53	6	0	-2.678938	3.499485	2.507894
54	6	0	-1.254003	1.624356	3.168835
55	6	0	-1.730202	4.384159	3.019236
56	1	0	-3.593308	3.858815	2.047378
57	6	0	-0.314074	2.525298	3.674064
58	1	0	-1.082927	0.555510	3.225735
59	6	0	-0.552386	3.899128	3.599761
60	1	0	-1.912838	5.453698	2.967145
61	1	0	0.598565	2.140536	4.118447
62	1	0	0.180153	4.597128	3.996080
63	6	0	2.081872	-1.740251	-3.326621
64	6	0	2.774128	-2.805252	-2.744597
65	6	0	2.678062	-0.908074	-4.277381
66	6	0	4.101548	-3.017619	-3.112511
67	1	0	2.293705	-3.436207	-2.006315
68	6	0	4.004930	-1.140777	-4.639613

69	1	0	2.104968	-0.106686	-4.729305
70	6	0	4.715963	-2.189665	-4.055308
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72	1	0	4.480079	-0.501135	-5.377794
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75	6	0	-2.921558	-2.881945	0.109743
76	6	0	-1.870995	-4.357545	-1.526409
77	6	0	-4.140367	-3.529093	-0.105506
78	1	0	-2.844749	-2.109952	0.865730
79	6	0	-3.093719	-4.995565	-1.722575
80	1	0	-0.985586	-4.677325	-2.057639
81	6	0	-4.229206	-4.575957	-1.023602
82	1	0	-5.012292	-3.216505	0.461324
83	1	0	-3.156296	-5.824899	-2.421022
84	1	0	-5.179270	-5.078862	-1.183201
85	7	0	2.495940	-0.684860	1.031797
86	16	0	2.467097	-1.219516	2.726772
87	16	0	4.057609	-0.346080	0.329379
88	8	0	3.756887	-0.047223	-1.072803
89	8	0	4.931901	-1.460793	0.682198
90	8	0	3.787693	-0.932453	3.286988
91	8	0	1.276896	-0.612502	3.328932
92	6	0	4.702383	1.170715	1.046092
93	6	0	4.353014	2.387399	0.450718
94	6	0	5.583632	1.107320	2.128758
95	6	0	4.877746	3.568866	0.976825
96	1	0	3.708567	2.410655	-0.420439
97	6	0	6.106900	2.296712	2.634196
98	1	0	5.841280	0.149702	2.561714
99	6	0	5.750404	3.523087	2.065929
100	1	0	4.607792	4.518524	0.524394
101	1	0	6.794947	2.263609	3.473894
102	1	0	6.161182	4.444819	2.469092
103	6	0	2.254728	-2.995578	2.678897
104	6	0	3.288744	-3.796072	2.187318
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111	1	0	3.928227	-5.820215	1.861136
112	1	0	0.071330	-5.362800	3.719772

113	1	0	1.876779	-6.823507	2.837952

Thermal correction to Gibbs Free Energy= 0.763910

Sum of electronic and thermal Free Energies= -5384.868213

<S**>2=0.000

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Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

8. NMR Spectra of Compounds

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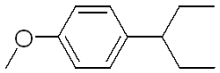

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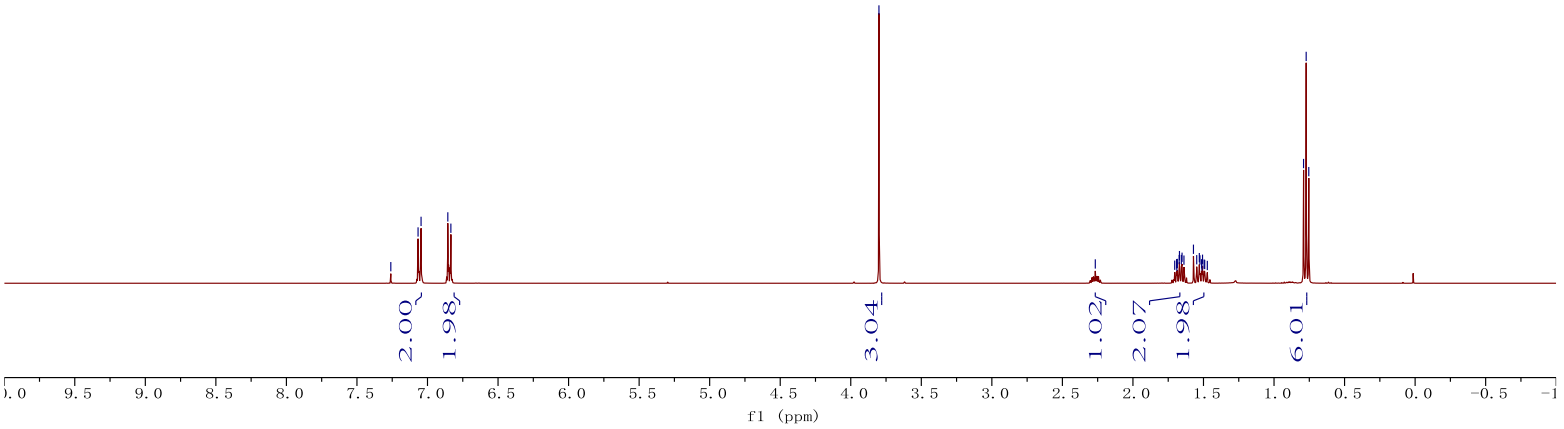
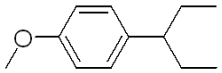


157.8
138.0
128.7
113.6
77.5
77.2
76.8
55.3
49.0
29.5
12.3

^{13}C NMR (101 MHz, $CDCl_3$)



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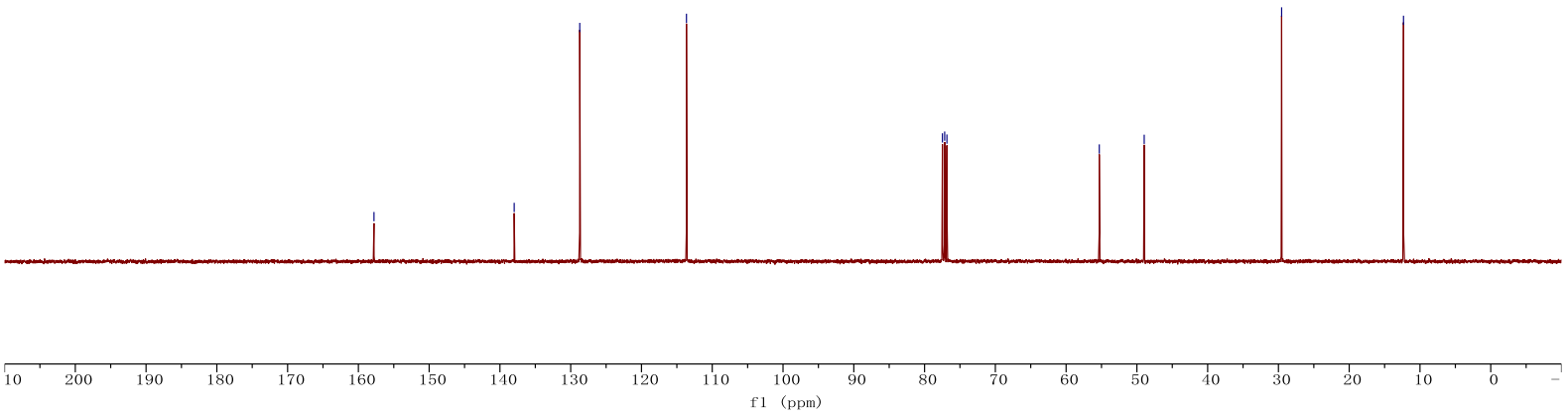

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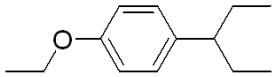

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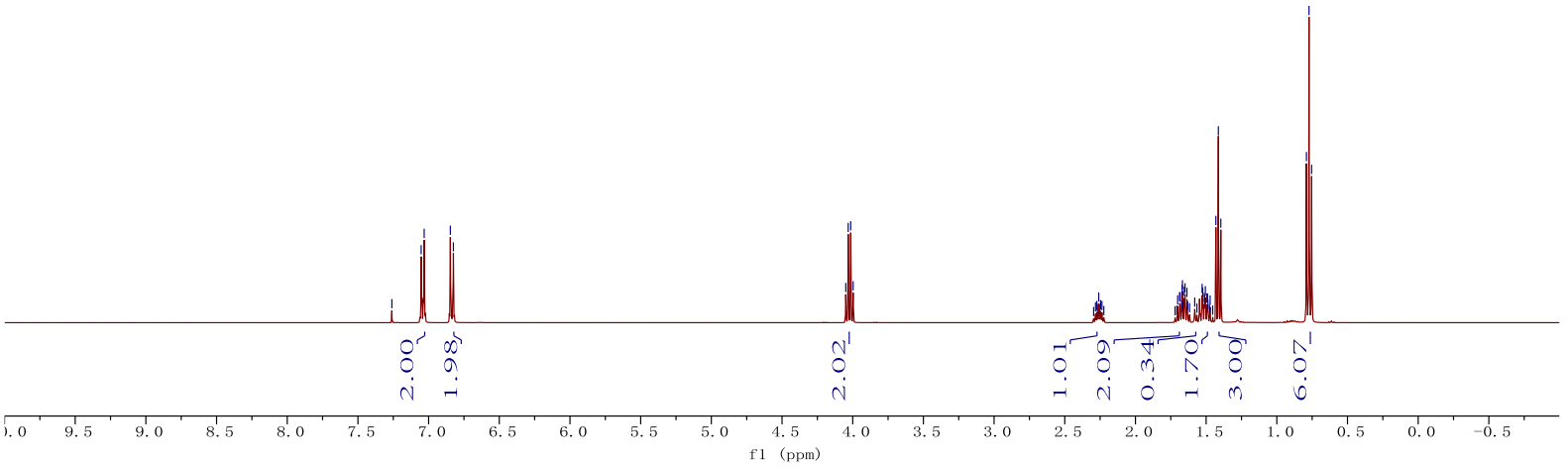

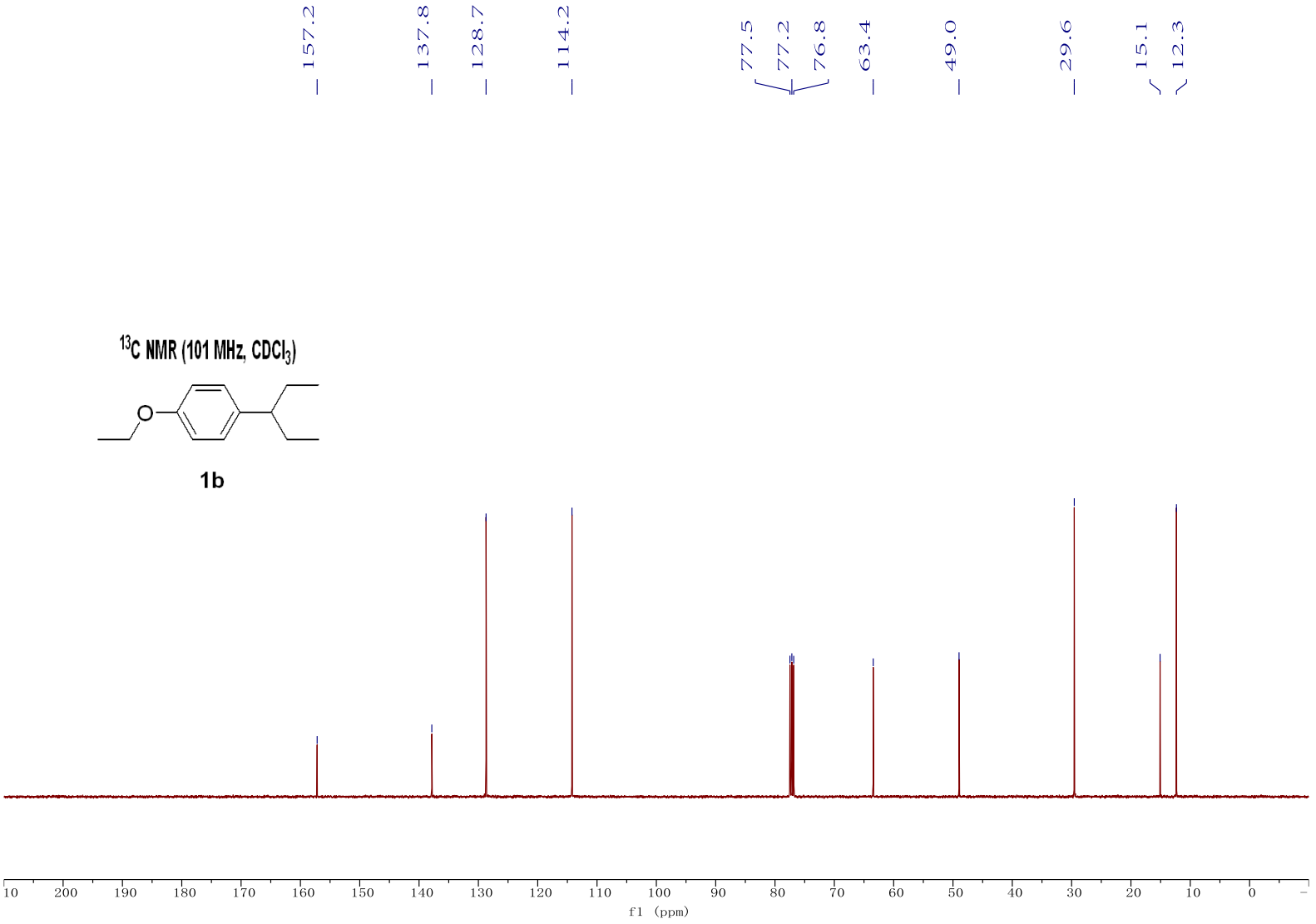
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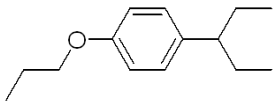
137.8
128.7
114.2
77.5
77.2
76.8
63.4
49.0
29.6
15.1
12.3
13C NMR (101 MHz, CDCl3)
O
1b
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

^{1}H NMR (400 MHz, $CDCl_3$)



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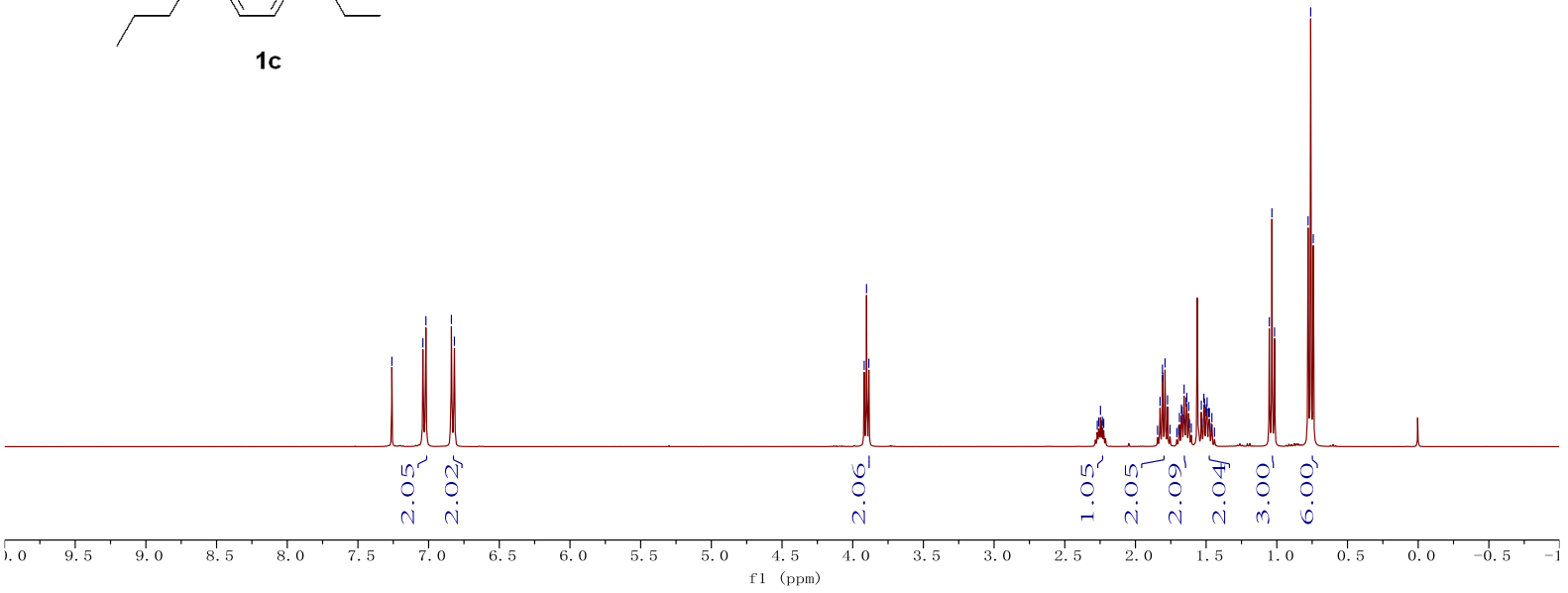

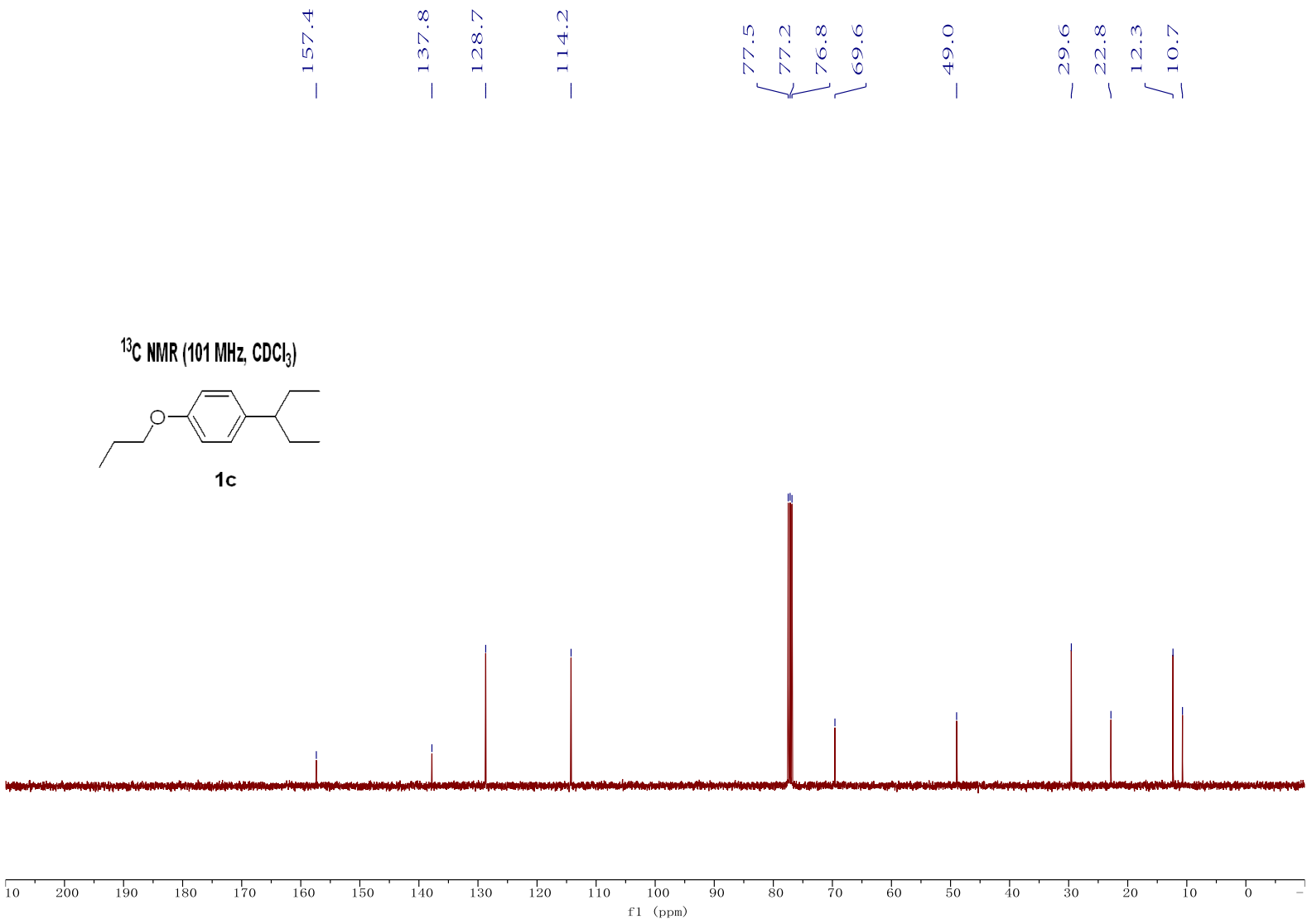
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137.8
128.7
114.2
77.5
77.2
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29.6
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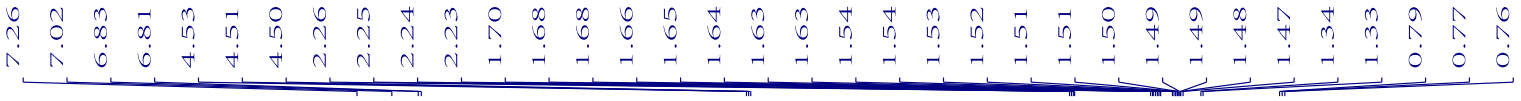
13C NMR (101 MHz, CDCl3)
1c
f1 (ppm)



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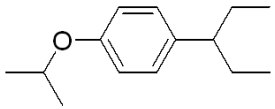
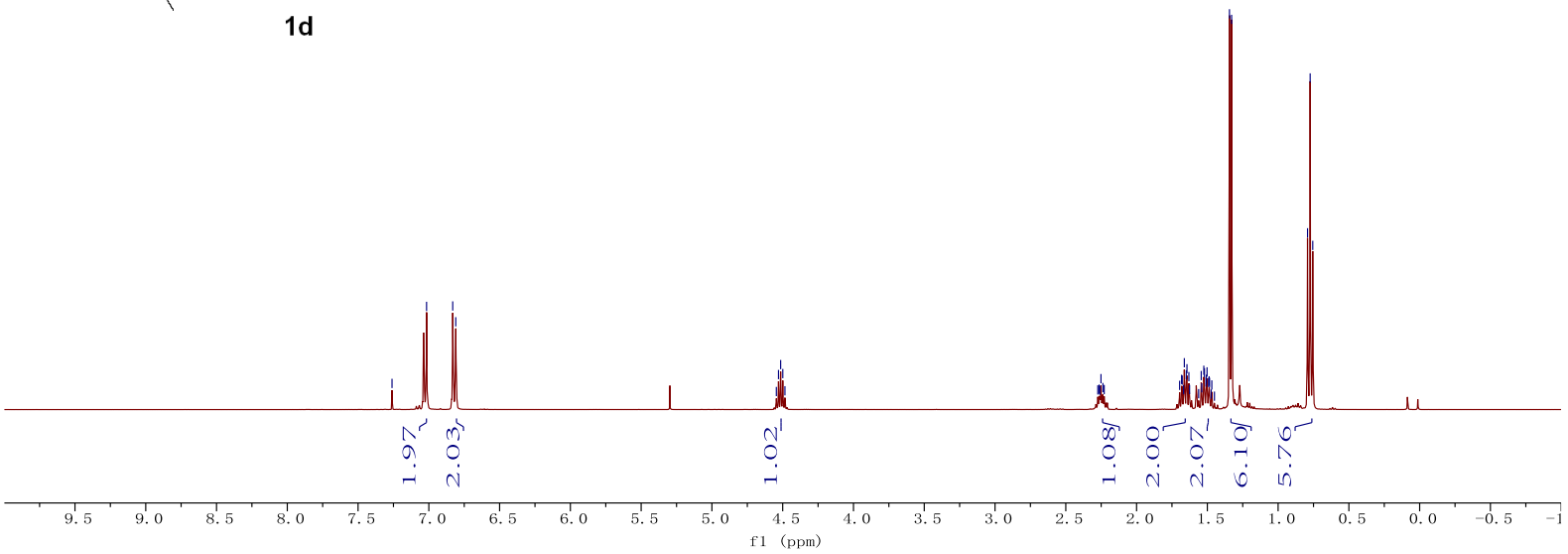
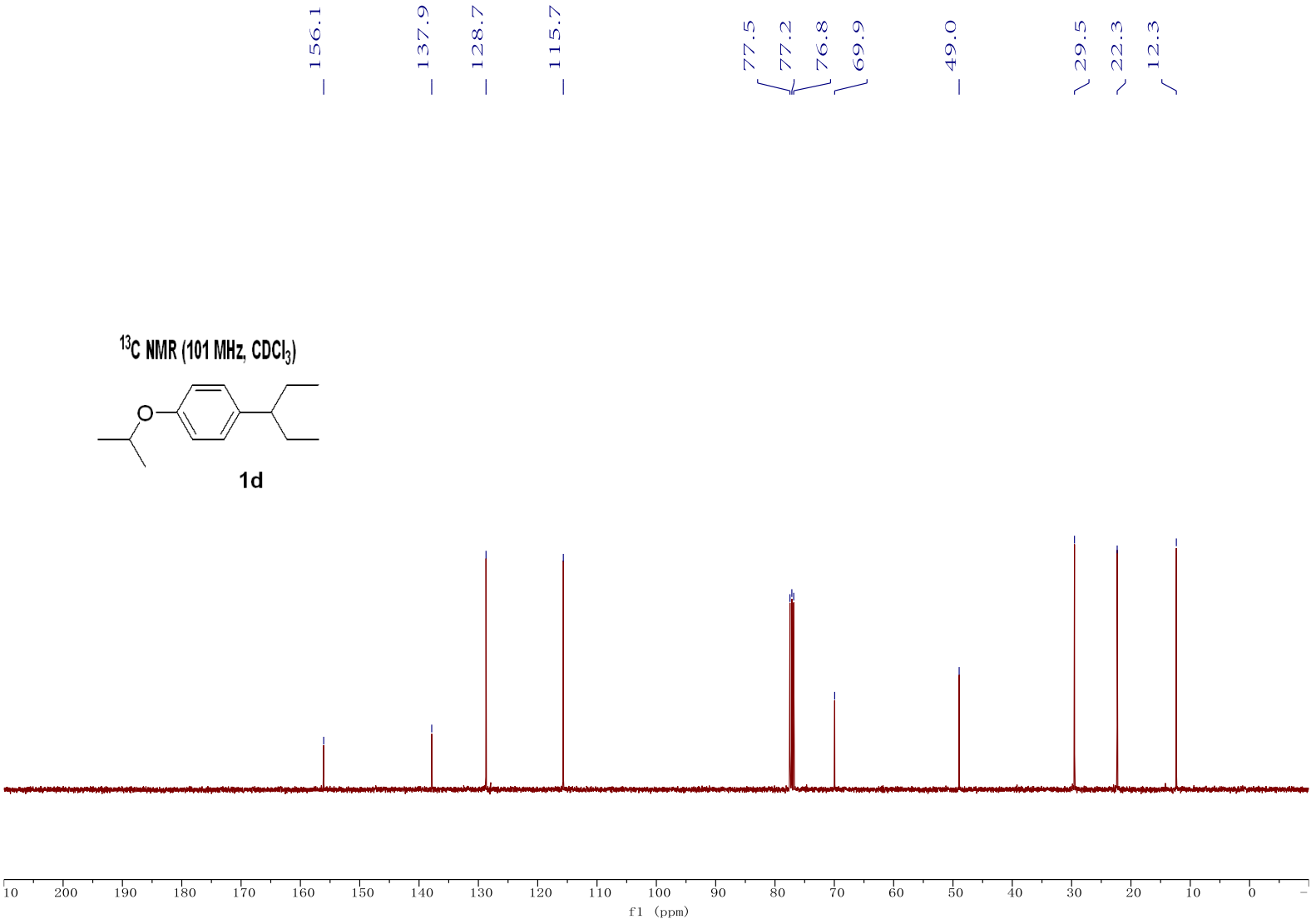
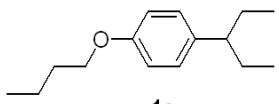


1d

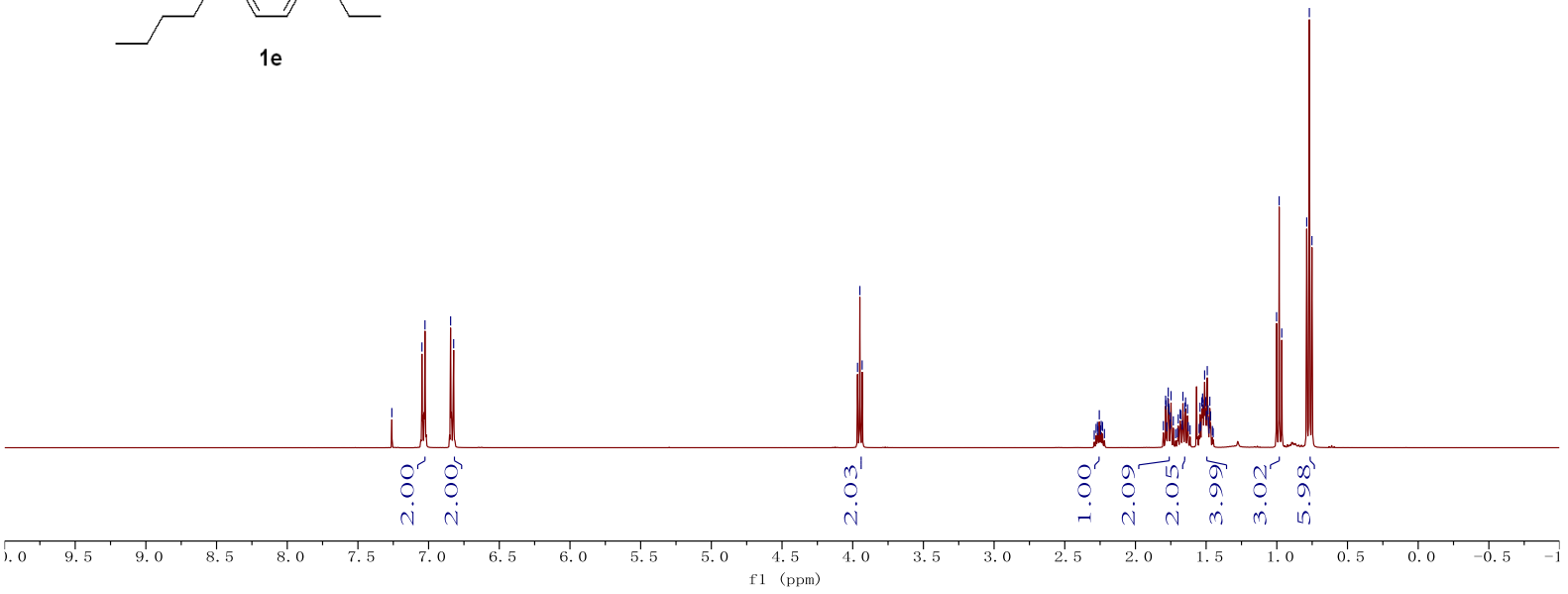



156.1
137.9
128.7
115.7
77.5
77.2
76.8
69.9
49.0
29.5
22.3
12.3
13C NMR (101 MHz, CDCl3)
O
1d
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

^{1}H NMR (400 MHz, $CDCl_3$)

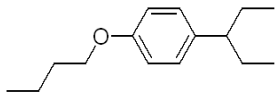


1e

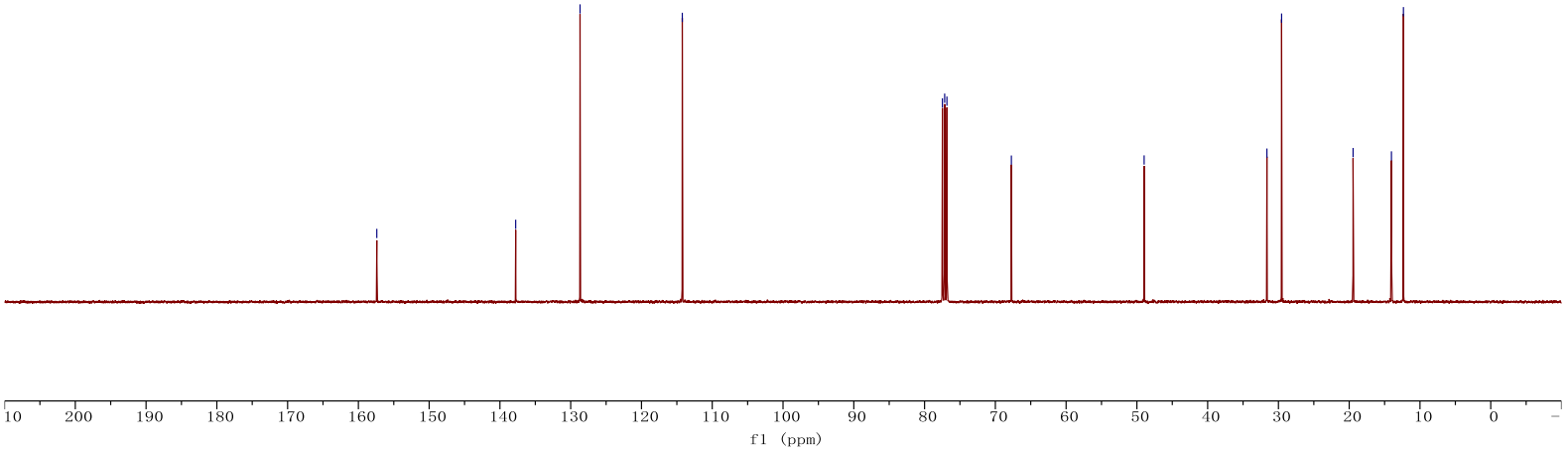


157.4
137.8
128.7
114.2
77.5
77.2
76.8
67.7
49.0
31.6
29.6
19.5
14.0
12.3

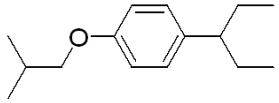
^{13}C NMR (101 MHz, $CDCl_3$)



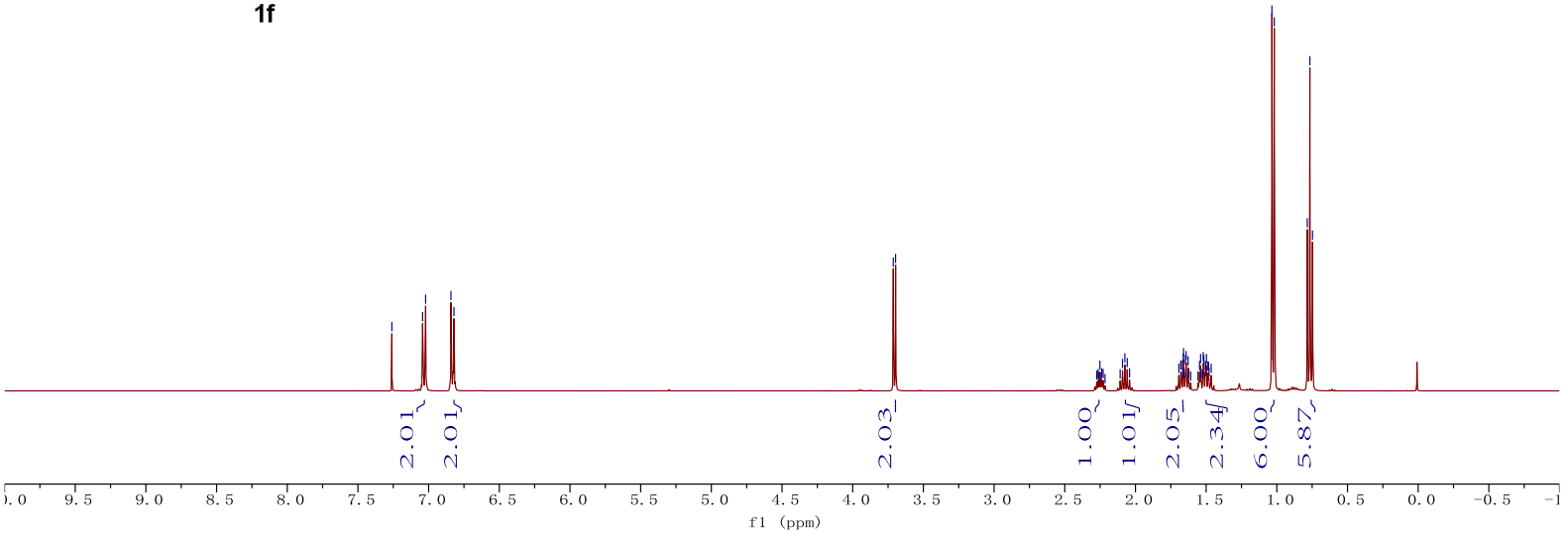
1e



^{1}H NMR (400 MHz, $CDCl_3$)

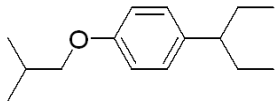


1f

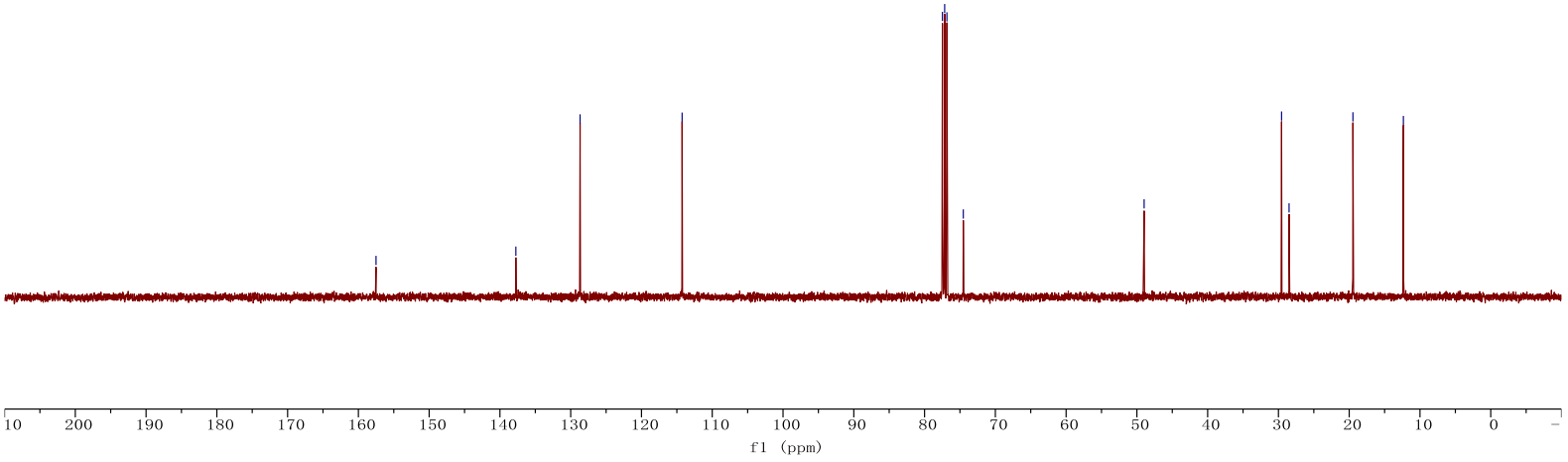


157.5
137.7
128.7
114.3
77.5
77.2
76.8
74.5
49.0
29.6
28.5
19.5
12.3

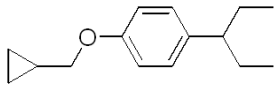
^{13}C NMR (101 MHz, $CDCl_3$)



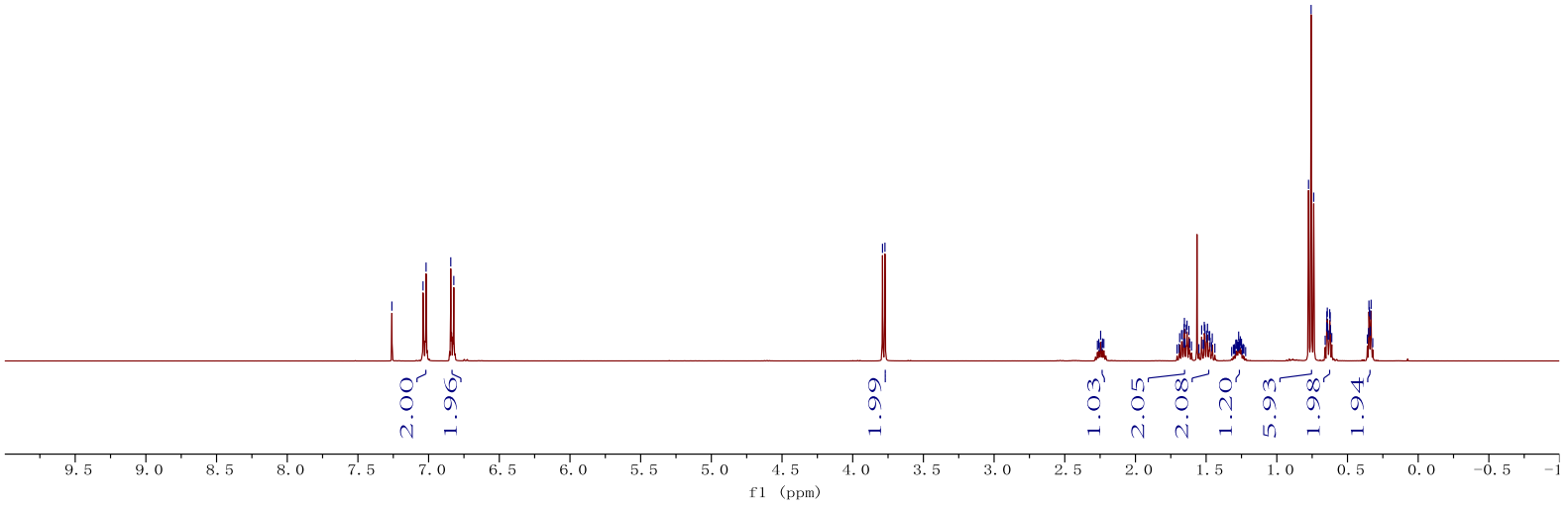
1f

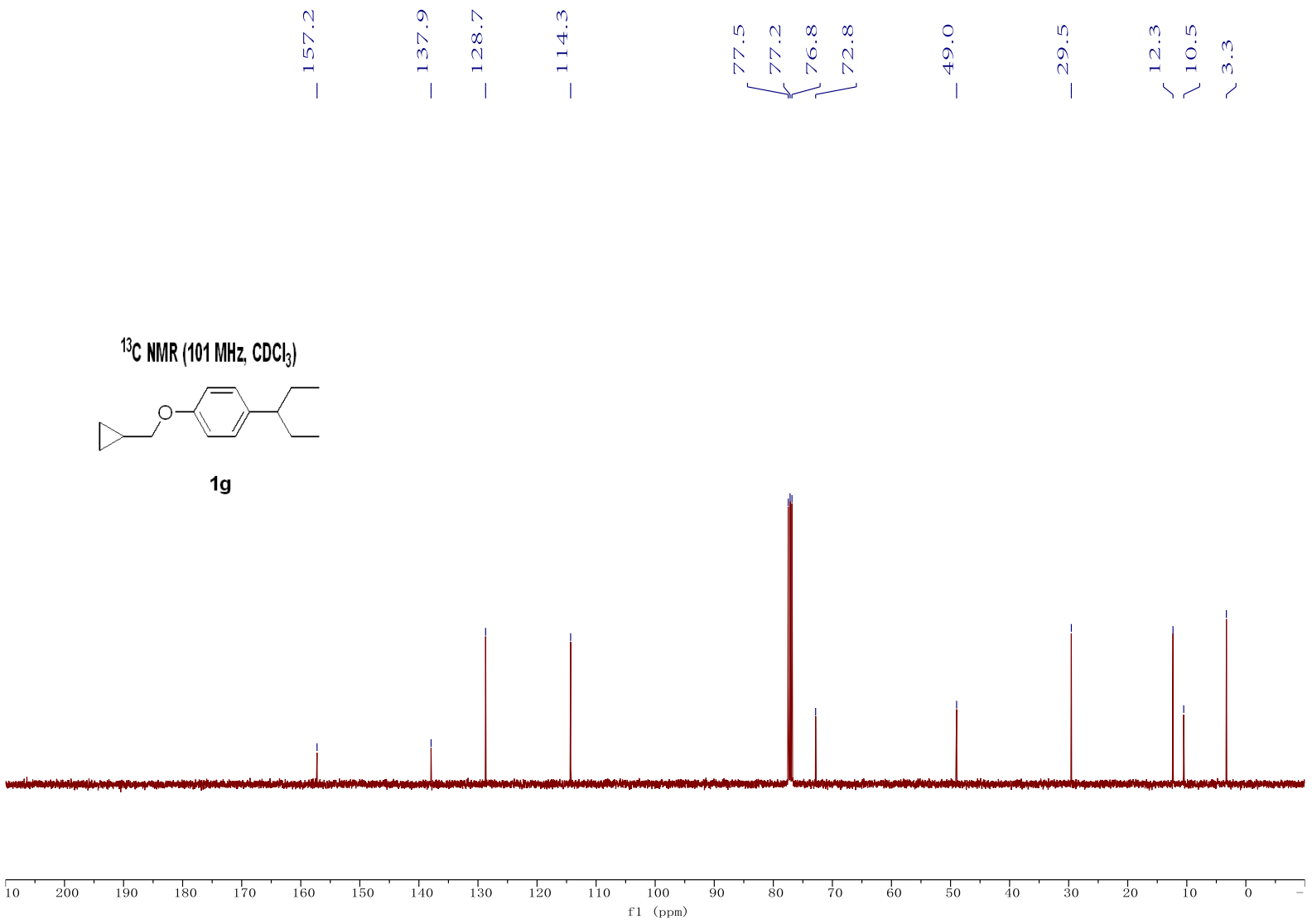


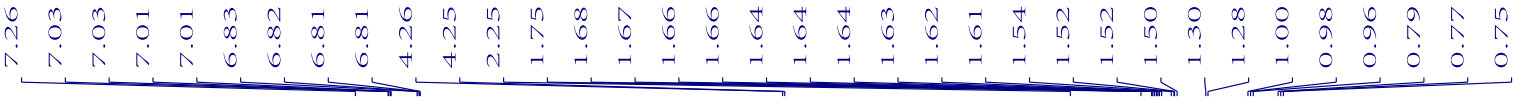
^{1}H NMR (400 MHz, $CDCl_3$)



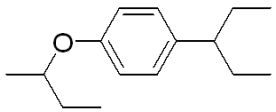
1g



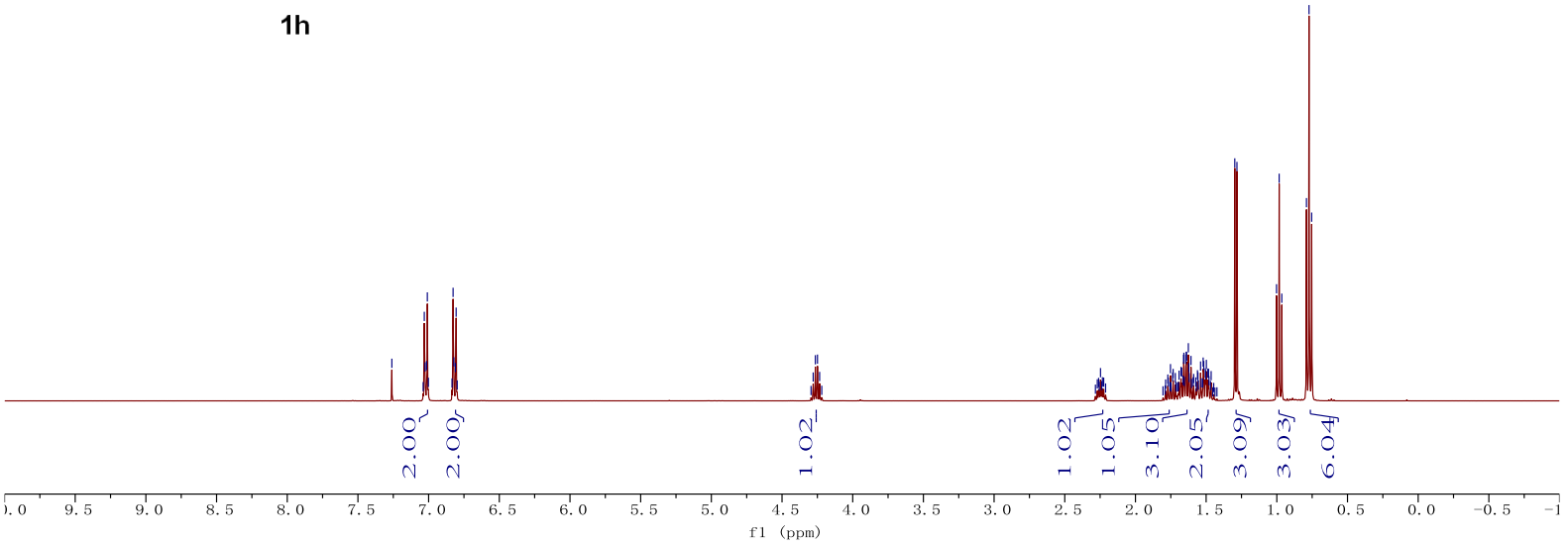

157.2
137.9
128.7
114.3
77.5
77.2
76.8
72.8
49.0
29.5
12.3
10.5
3.3
13C NMR (101 MHz, CDCl3)
1g
f1 (ppm)

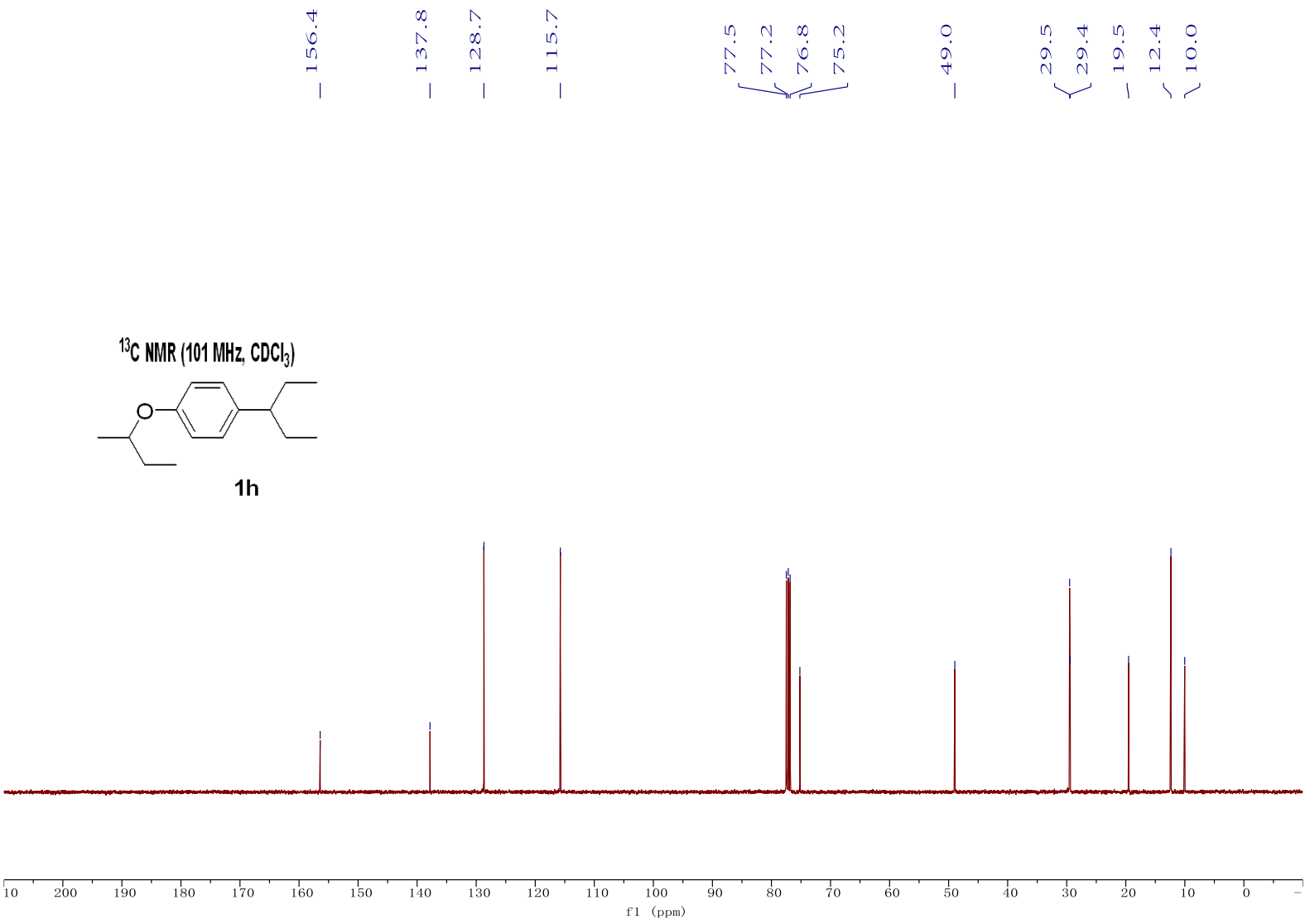


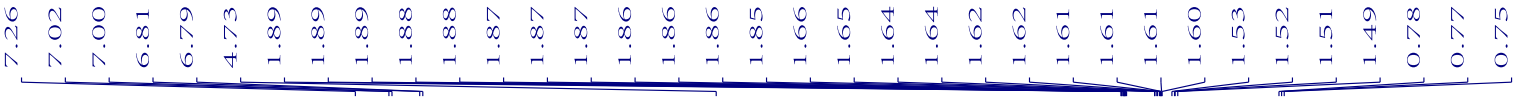
^{1}H NMR (400 MHz, $CDCl_3$)



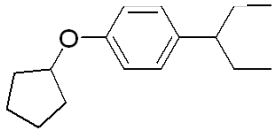
1h



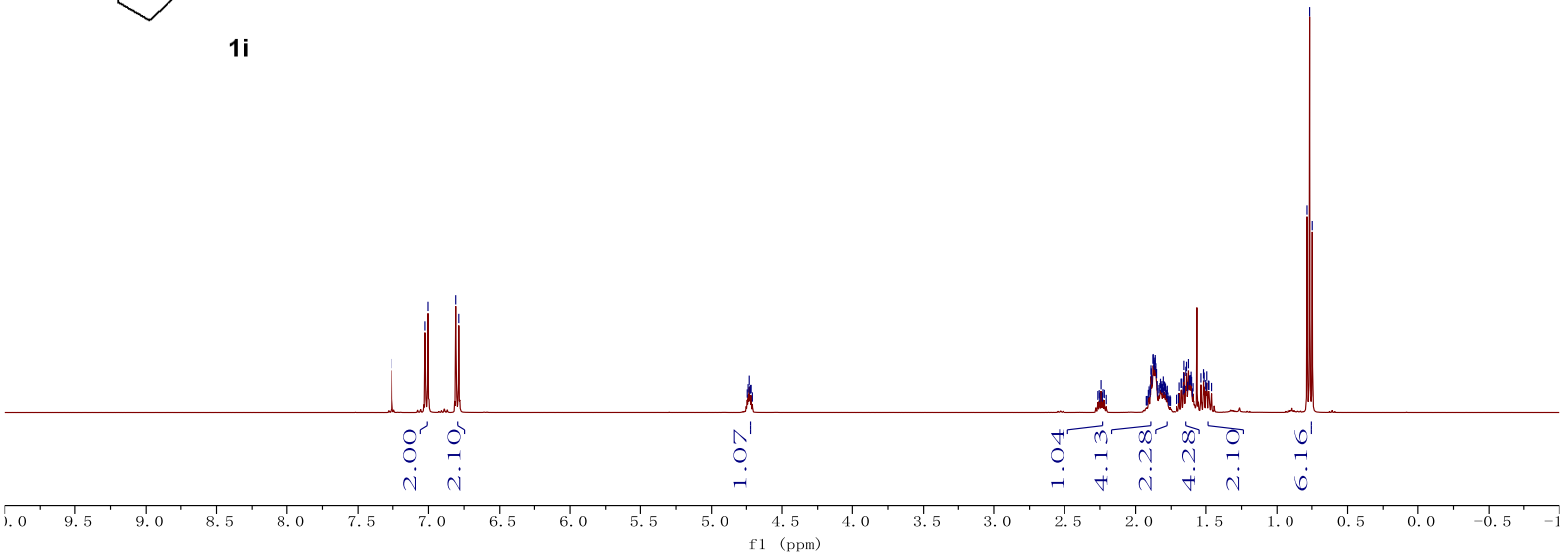

156.4
137.8
128.7
115.7
77.5
77.2
76.8
75.2
49.0
29.5
29.4
19.5
12.4
10.0
13C NMR (101 MHz, CDCl3)
O
1h
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

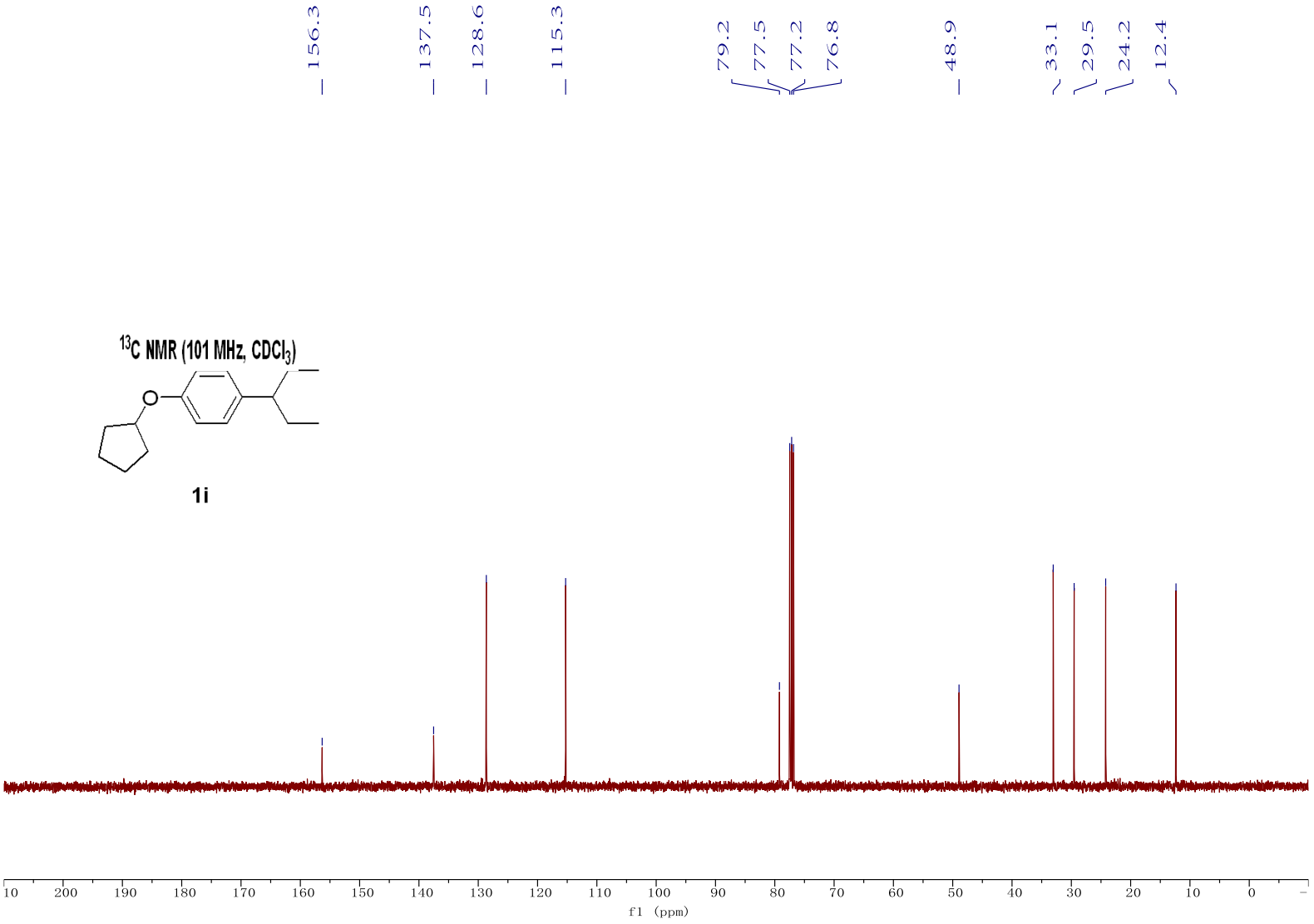


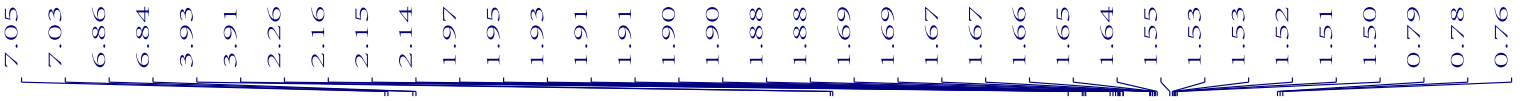
^{1}H NMR (400 MHz, $CDCl_3$)



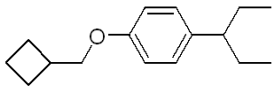
1i



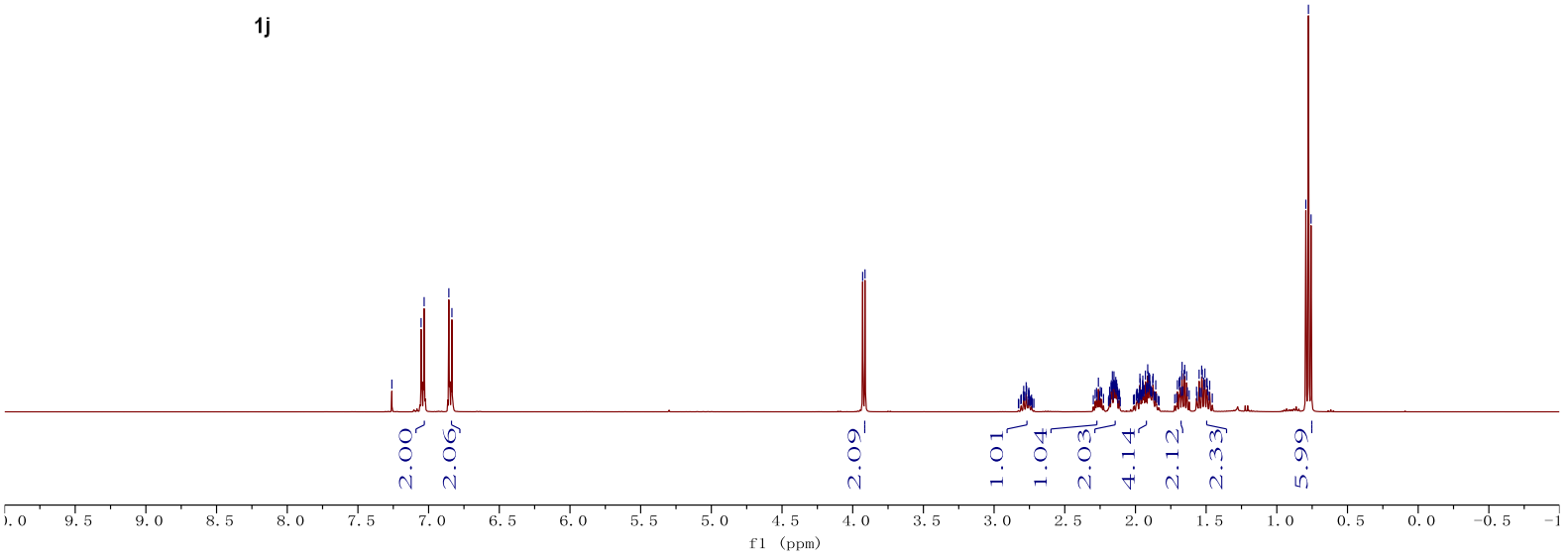

156.3
137.5
128.6
115.3
79.2
77.5
77.2
76.8
48.9
33.1
29.5
24.2
12.4
13C NMR (101 MHz, CDCl3)
1i
f1 (ppm)

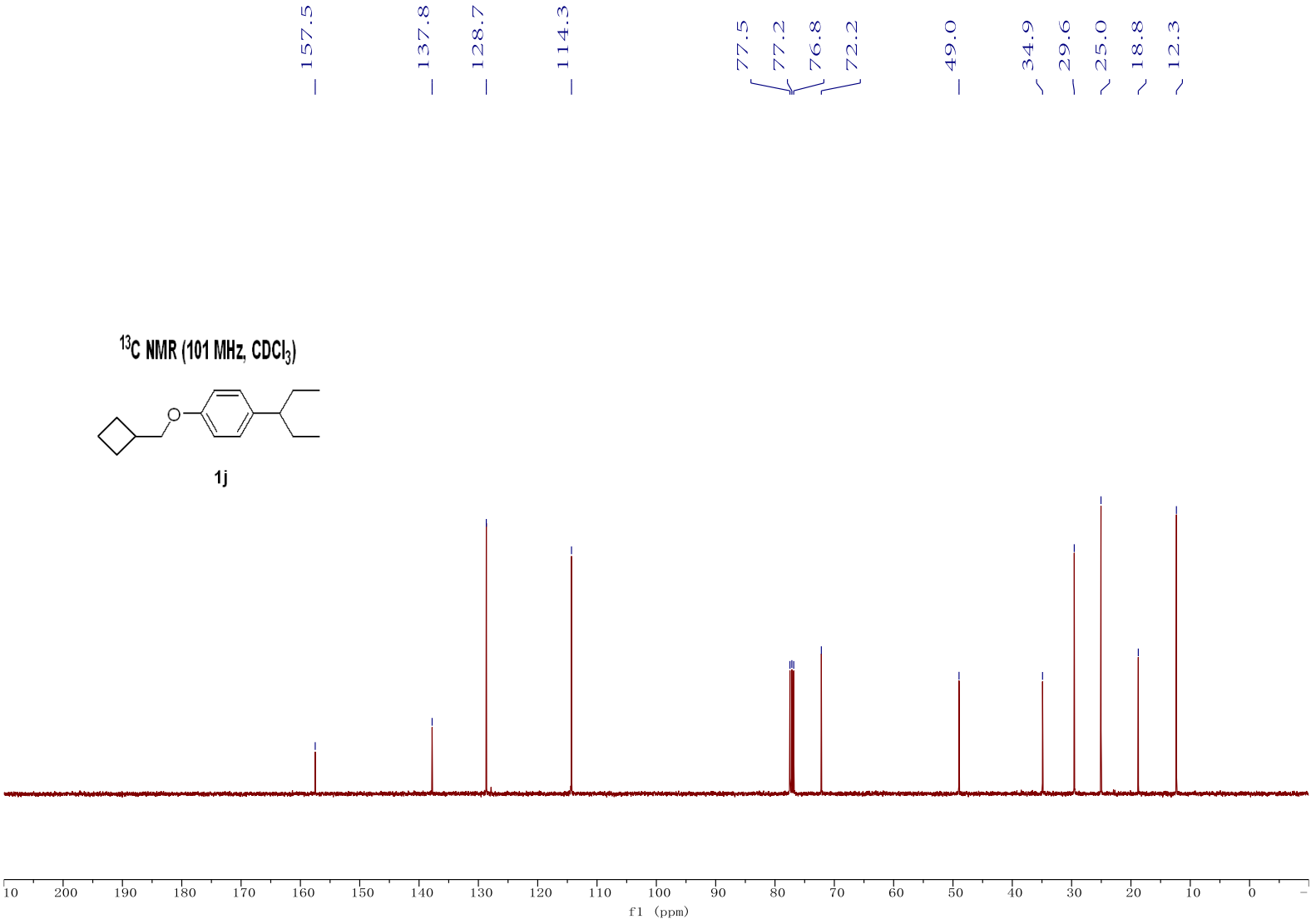


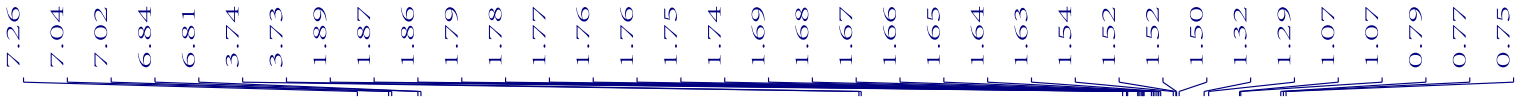
^{1}H NMR (400 MHz, $CDCl_3$)



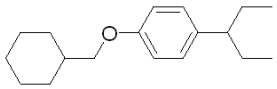
1j



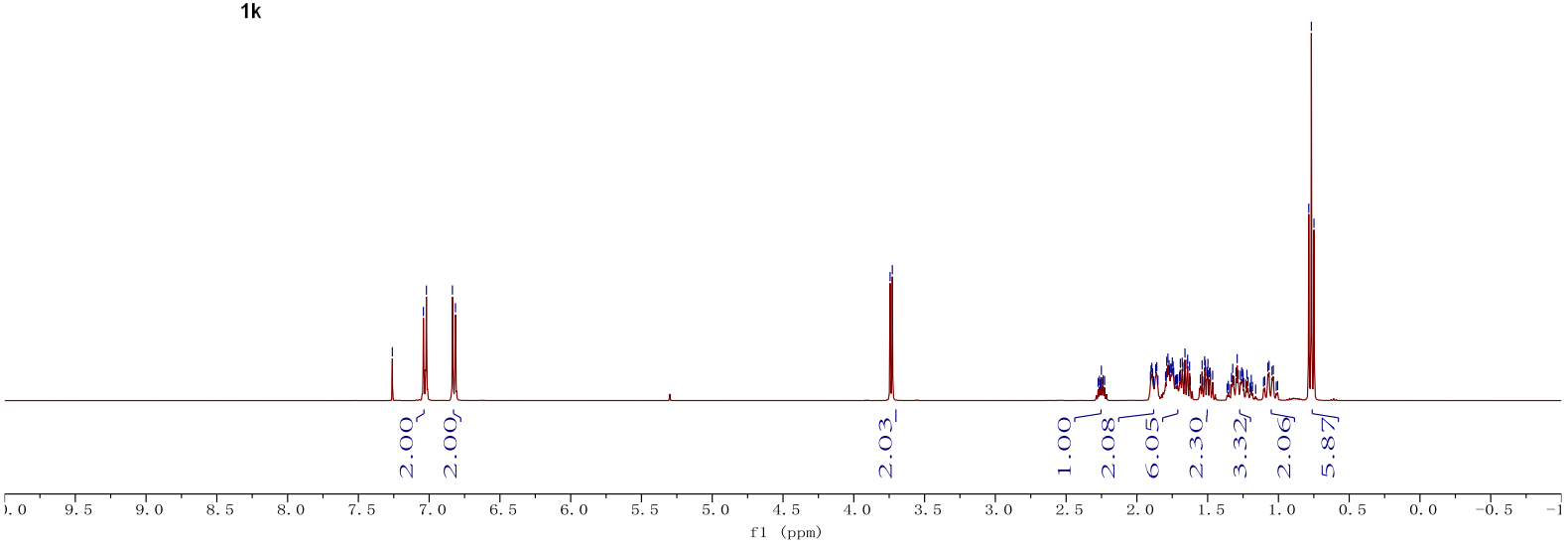

157.5
137.8
128.7
114.3
77.5
77.2
76.8
72.2
49.0
34.9
29.6
25.0
18.8
12.3
13C NMR (101 MHz, CDCl3)
1j
f1 (ppm)

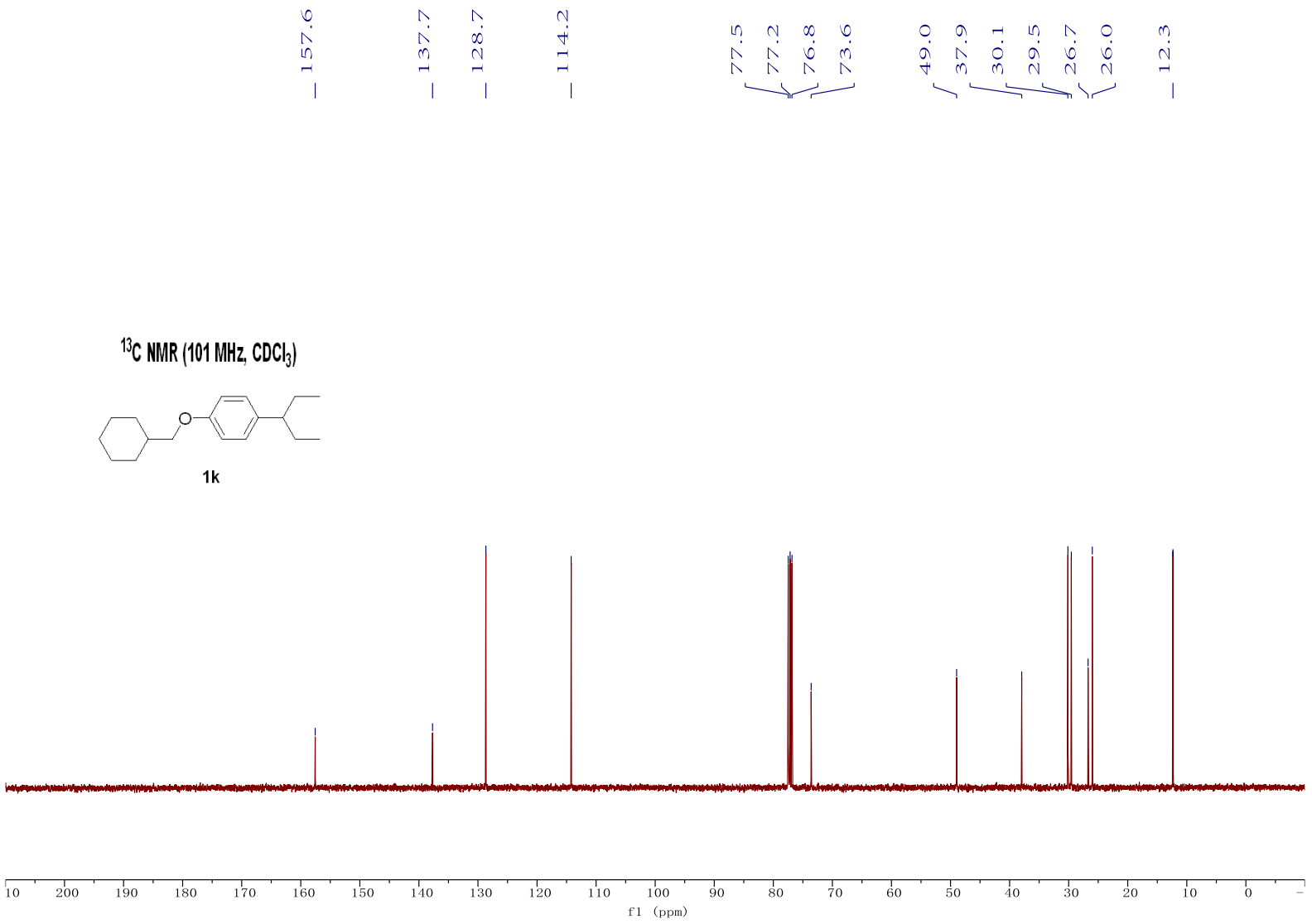


^{1}H NMR (400 MHz, $CDCl_3$)

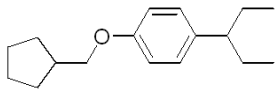


1k

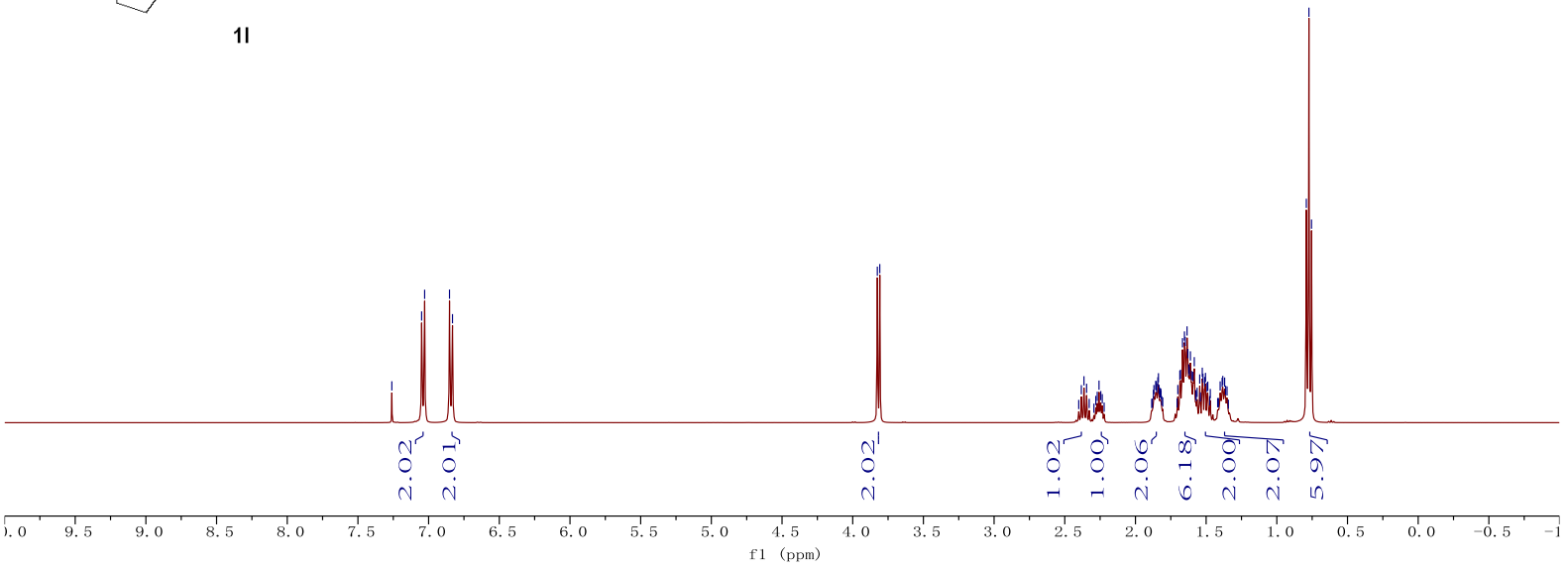


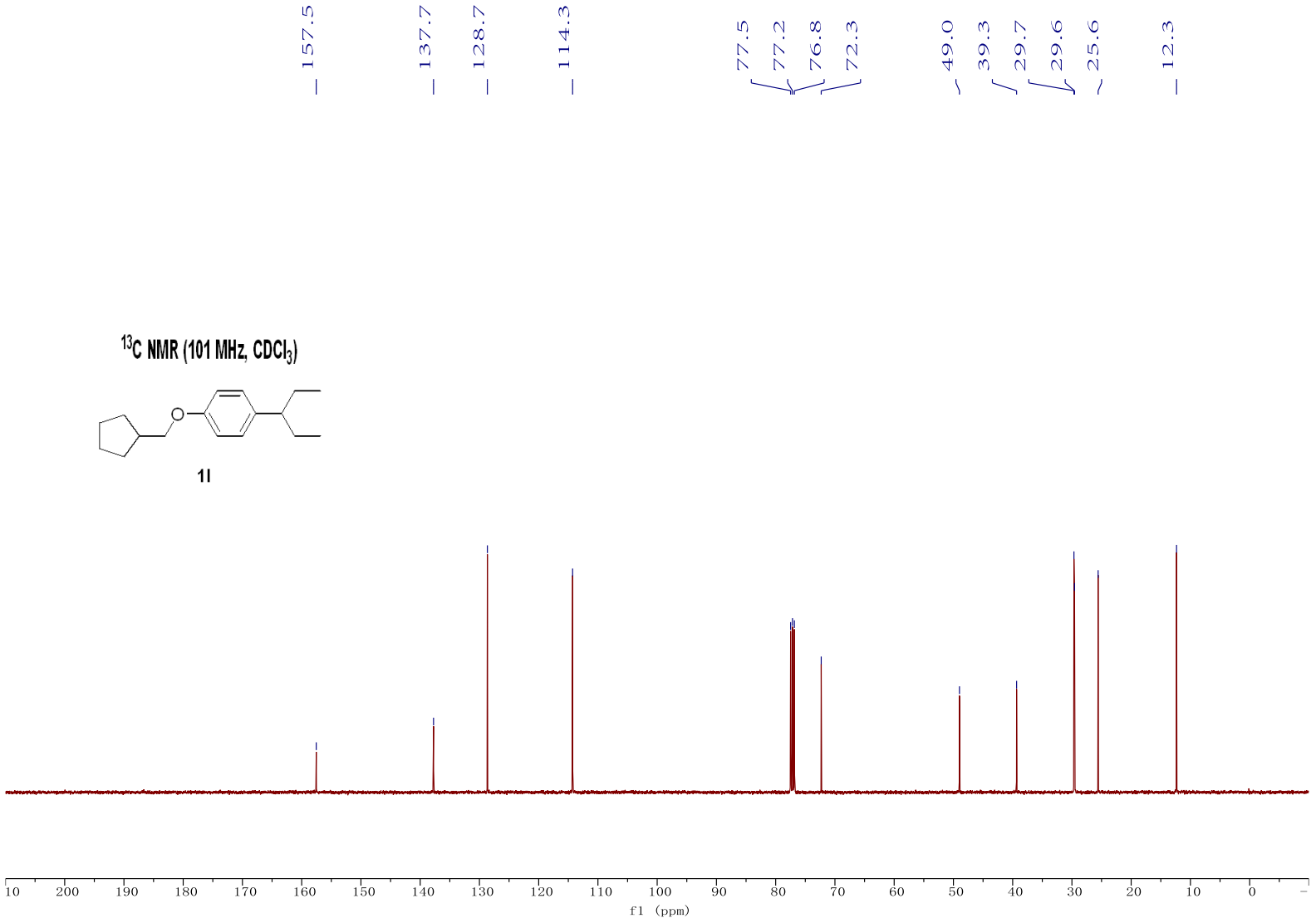

157.6
137.7
128.7
114.2
77.5
77.2
76.8
73.6
49.0
37.9
30.1
29.5
26.7
26.0
12.3
13C NMR (101 MHz, CDCl3)
1k
f1 (ppm)

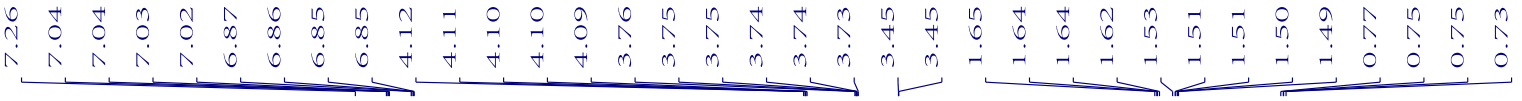
^{1}H NMR (400 MHz, $CDCl_3$)



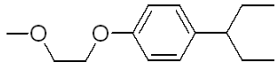
1l



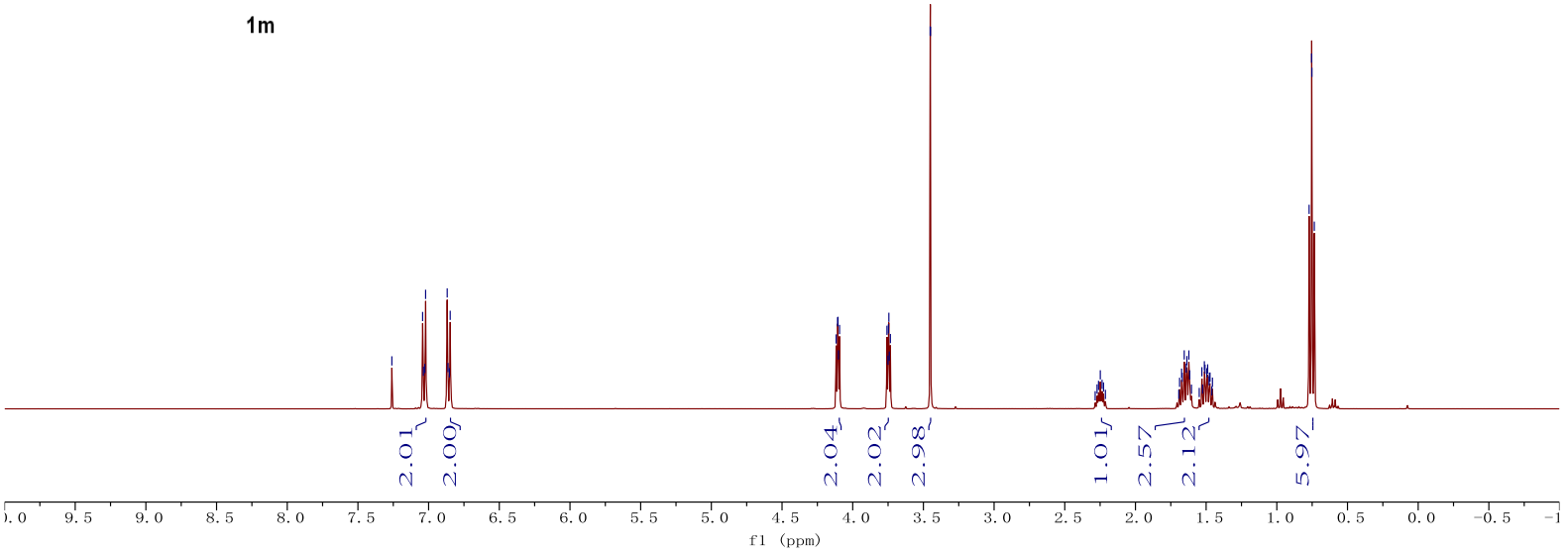

157.5
137.7
128.7
114.3
77.5
77.2
76.8
72.3
49.0
39.3
29.7
29.6
25.6
12.3
13C NMR (101 MHz, CDCl3)
1l
f1 (ppm)

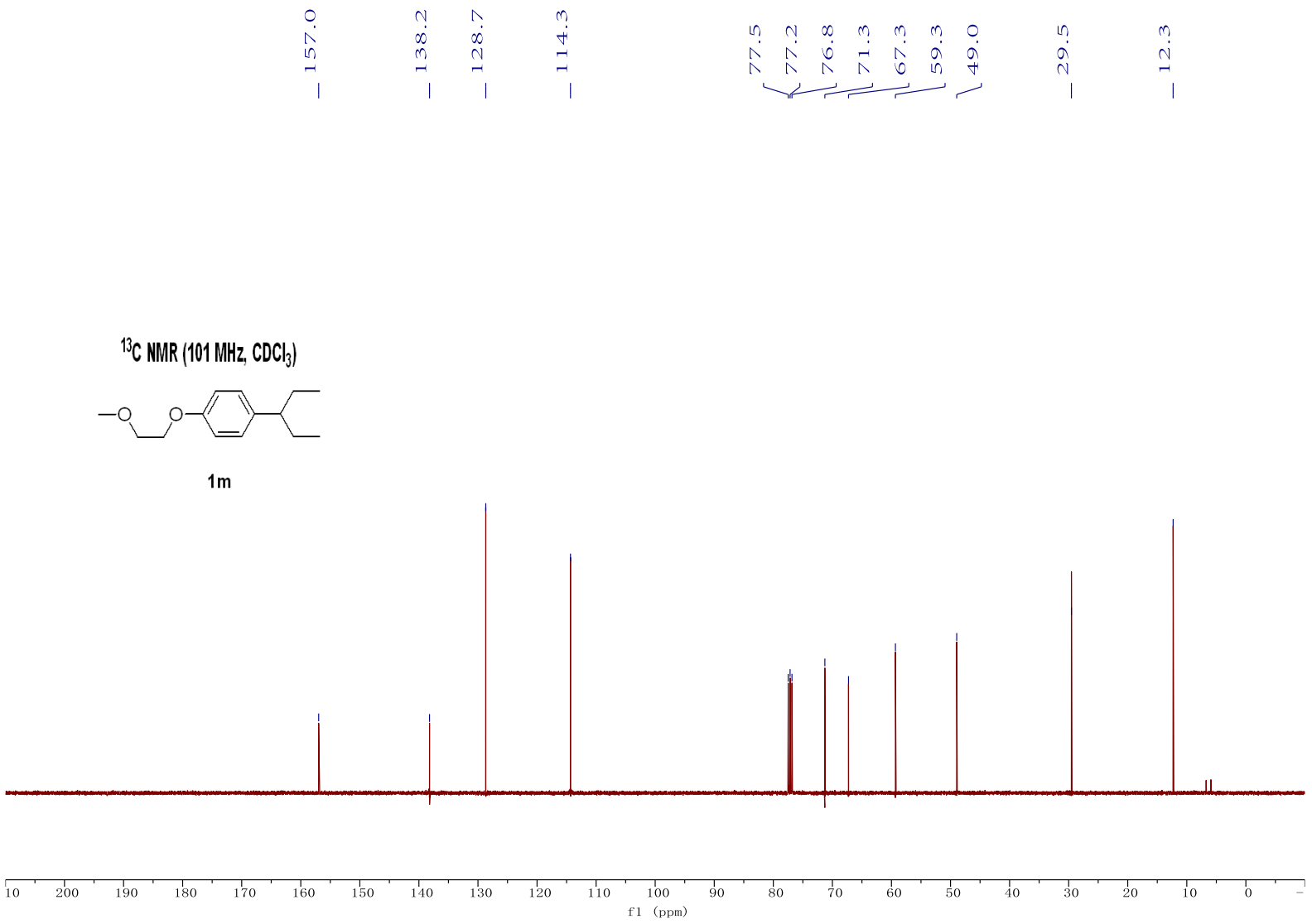


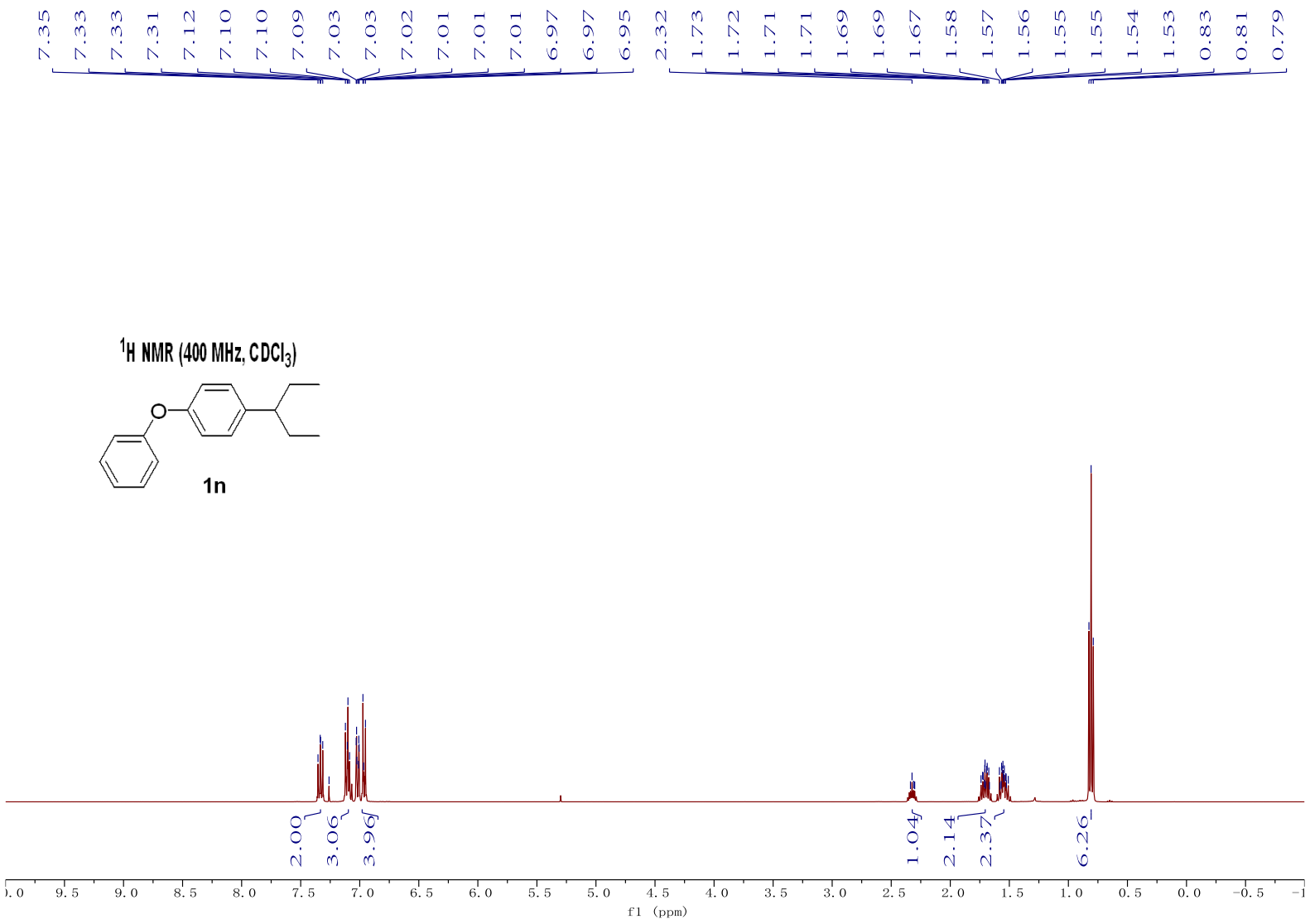
^{1}H NMR (400 MHz, $CDCl_3$)

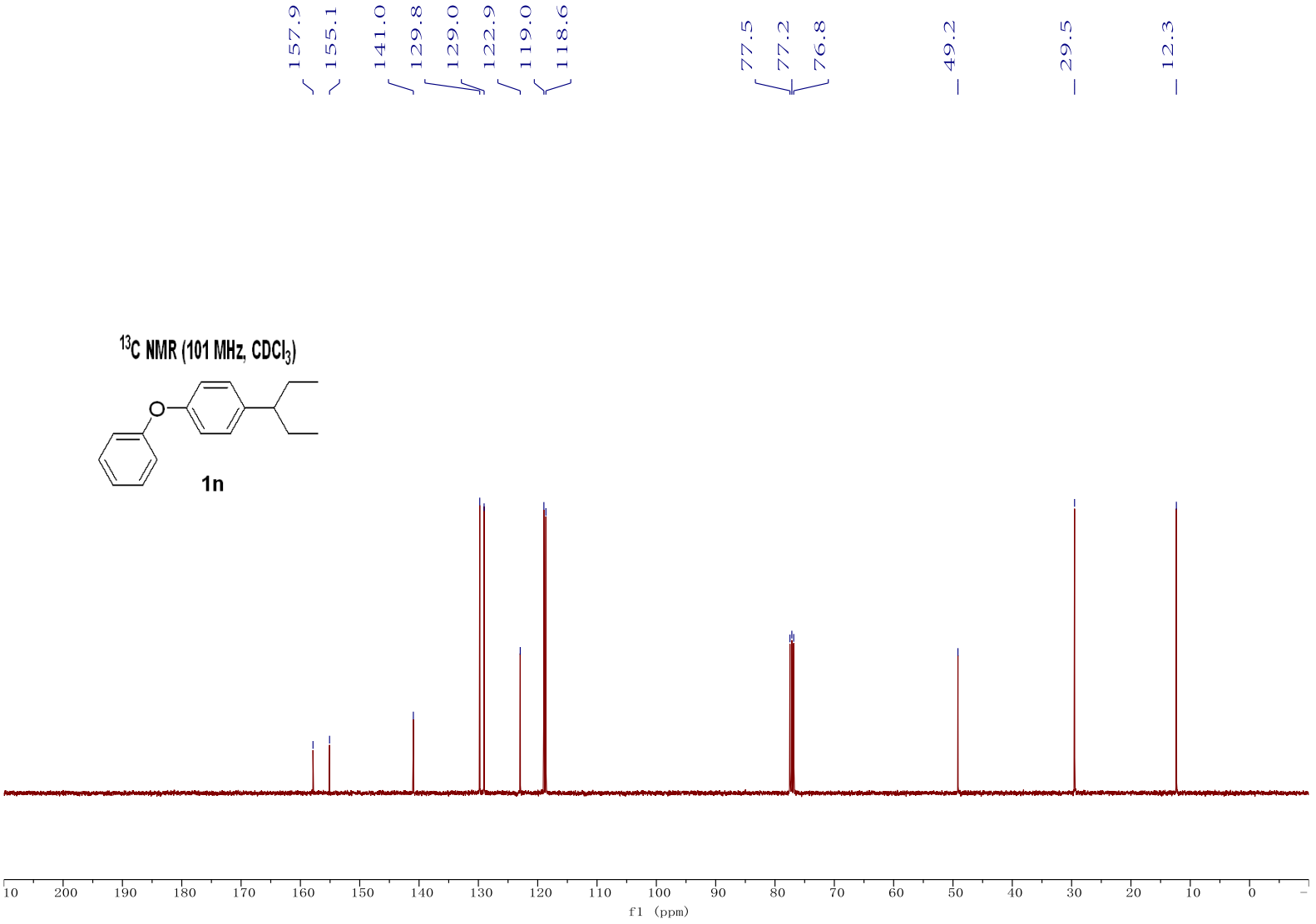


1m

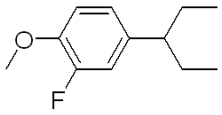



157.0
138.2
128.7
114.3
77.5
77.2
76.8
71.3
67.3
59.3
49.0
29.5
12.3
13C NMR (101 MHz, CDCl3)
1m
f1 (ppm)

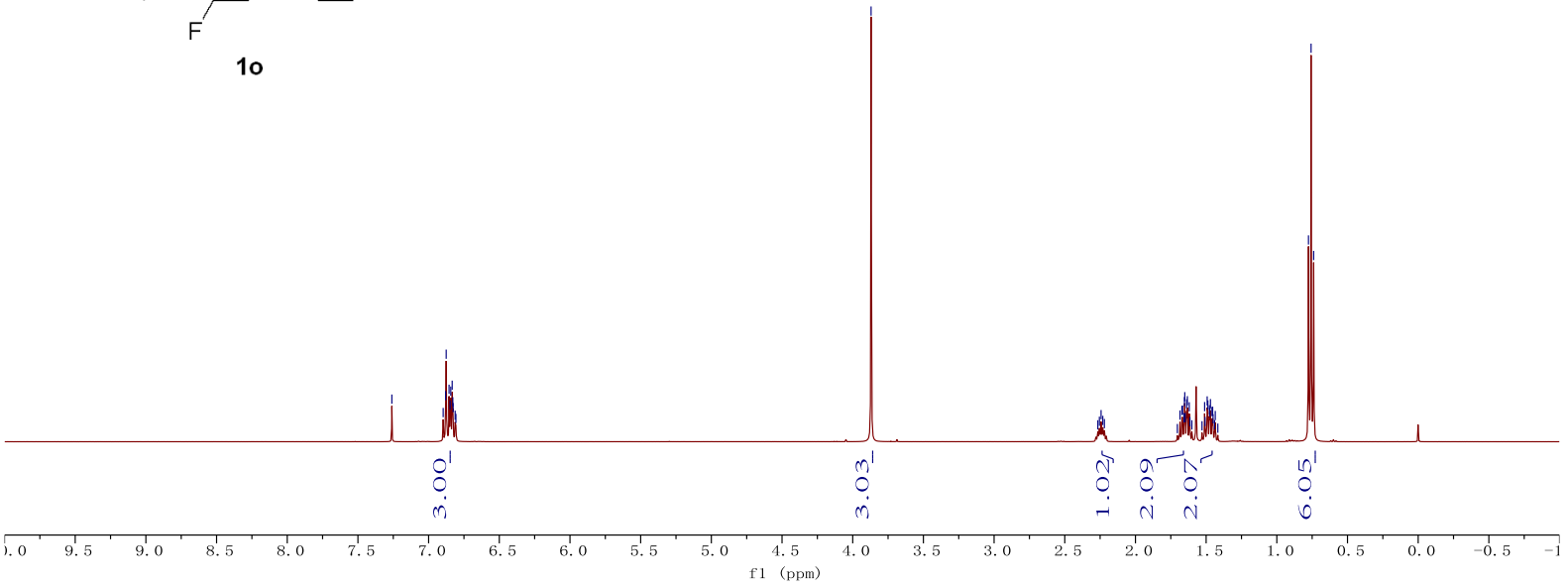

7.35
7.33
7.33
7.31
7.12
7.10
7.10
7.09
7.03
7.03
7.02
7.01
7.01
7.01
6.97
6.97
6.95
2.32
1.73
1.72
1.71
1.71
1.69
1.69
1.67
1.58
1.57
1.56
1.55
1.55
1.54
1.53
0.83
0.81
0.79
1H NMR (400 MHz, CDCl3)
1n
2.00
3.06
3.96
1.04
2.14
2.37
6.26
f1 (ppm)

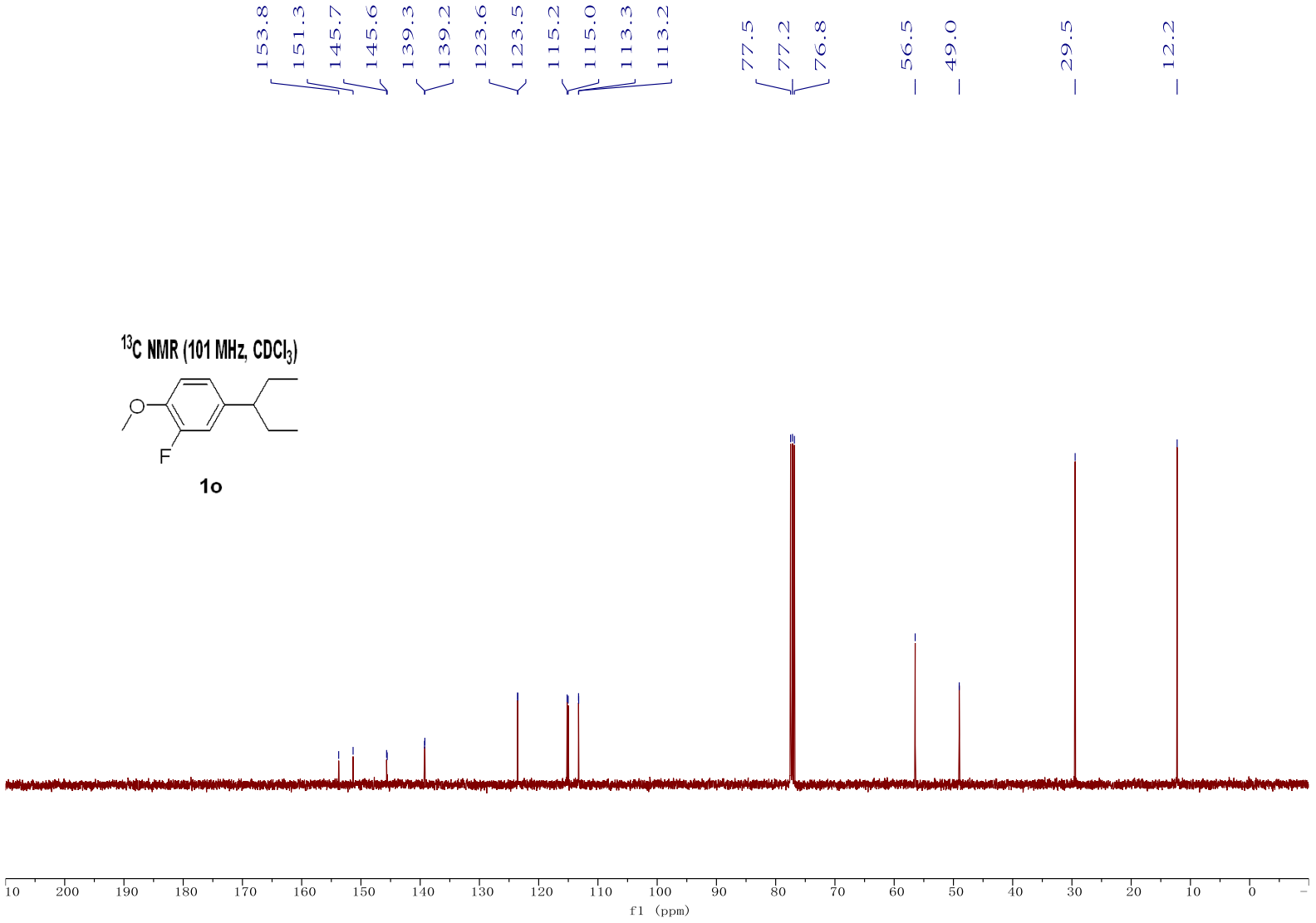

157.9
155.1
141.0
129.8
129.0
122.9
119.0
118.6
77.5
77.2
76.8
49.2
29.5
12.3
13C NMR (101 MHz, CDCl3)
1n
f1 (ppm)

^{1}H NMR (400 MHz, $CDCl_3$)

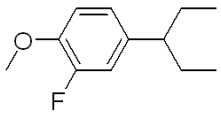


1o

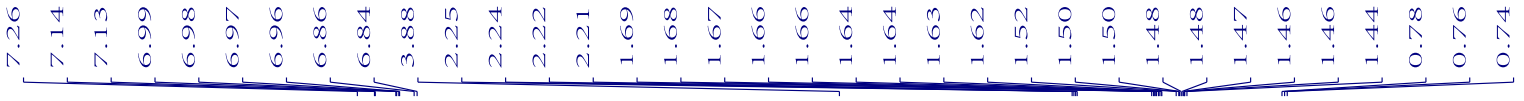



153.8
151.3
145.7
145.6
139.3
139.2
123.6
123.5
115.2
115.0
113.3
113.2
77.5
77.2
76.8
56.5
49.0
29.5
12.2
13C NMR (101 MHz, CDCl3)
O
F
1o
f1 (ppm)

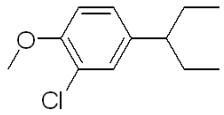
^{19}F NMR (376 MHz, $CDCl_3$)



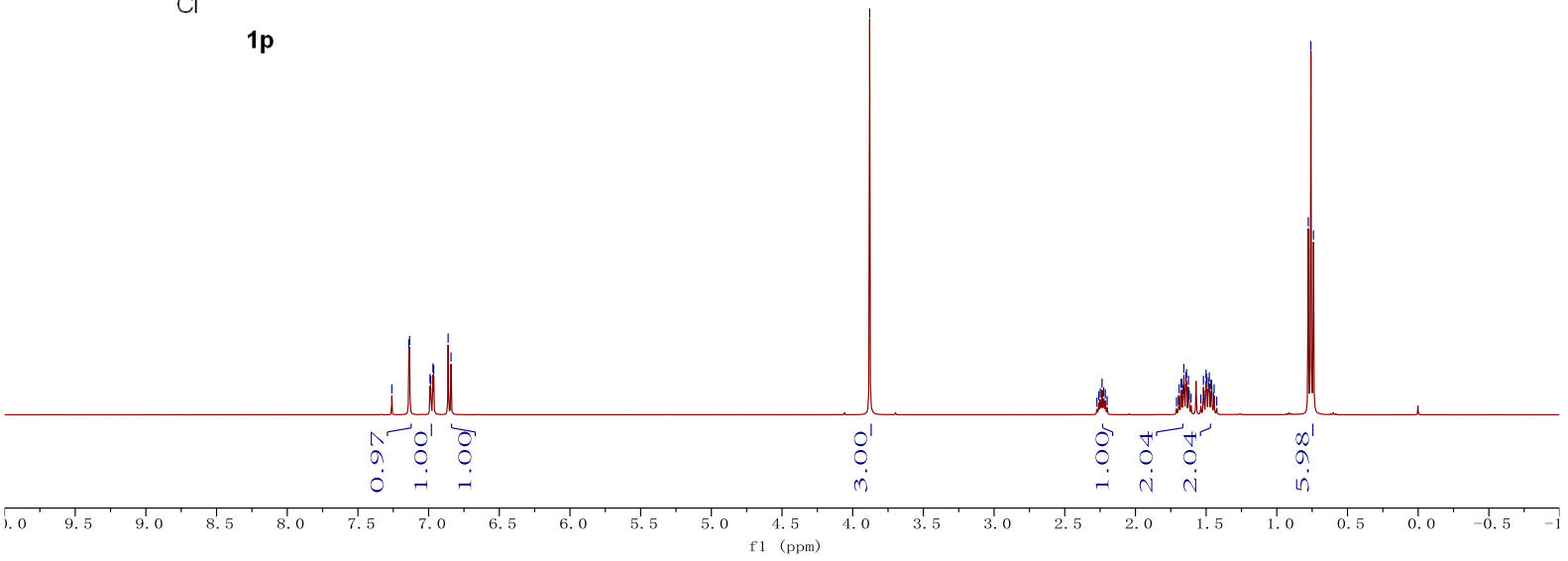
1o

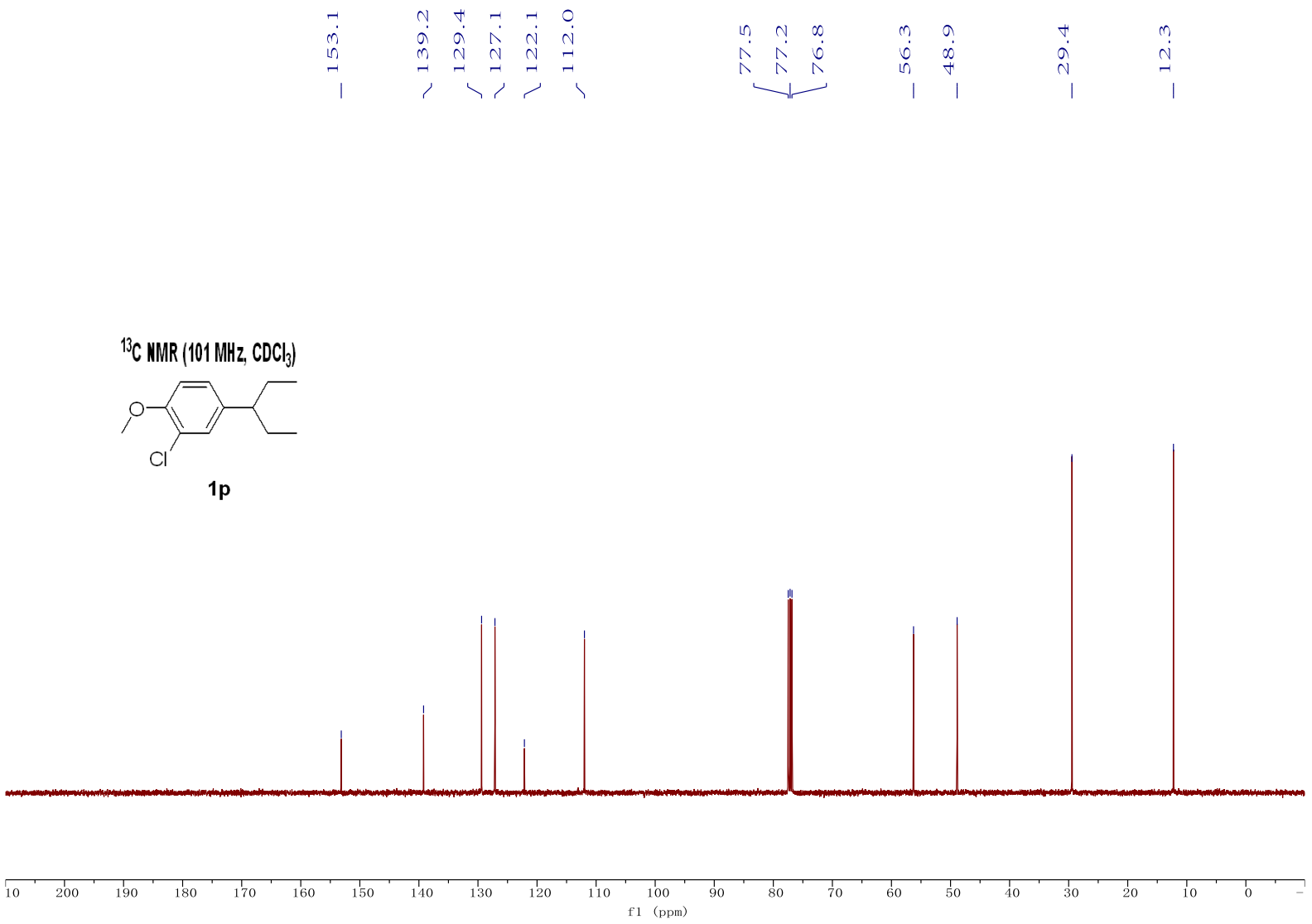


^{1}H NMR (400 MHz, $CDCl_3$)

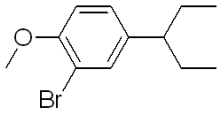


1p

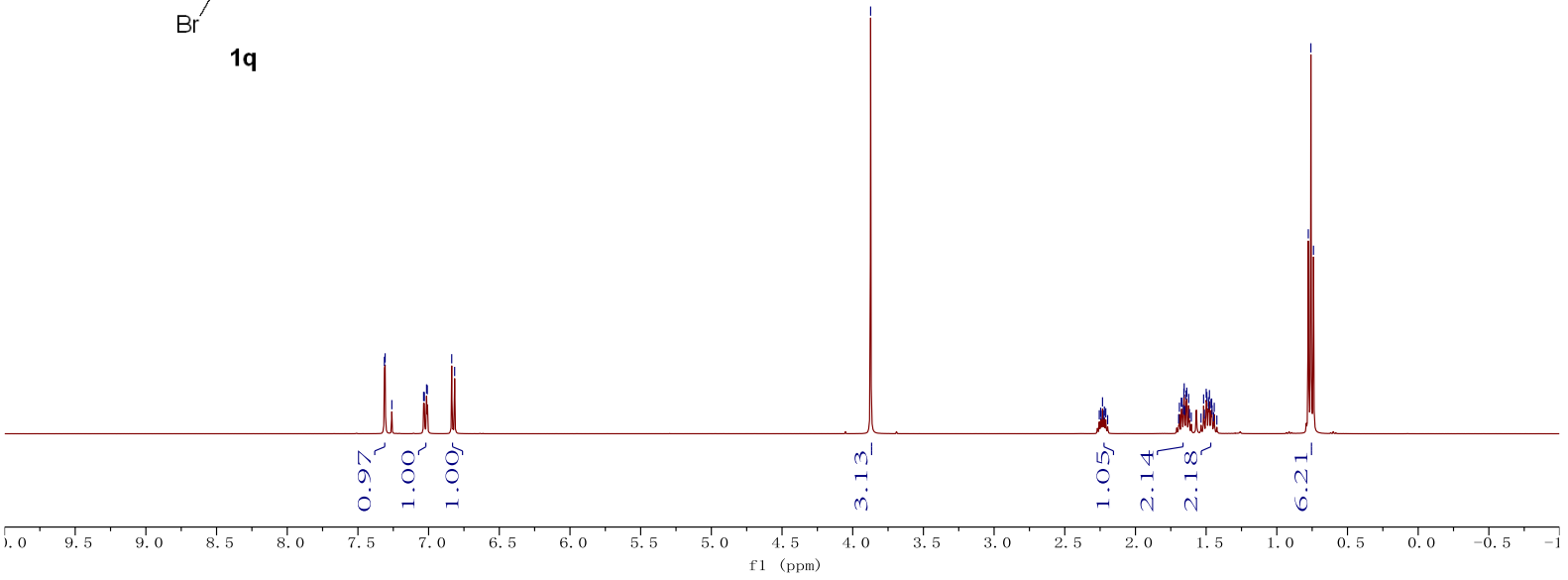


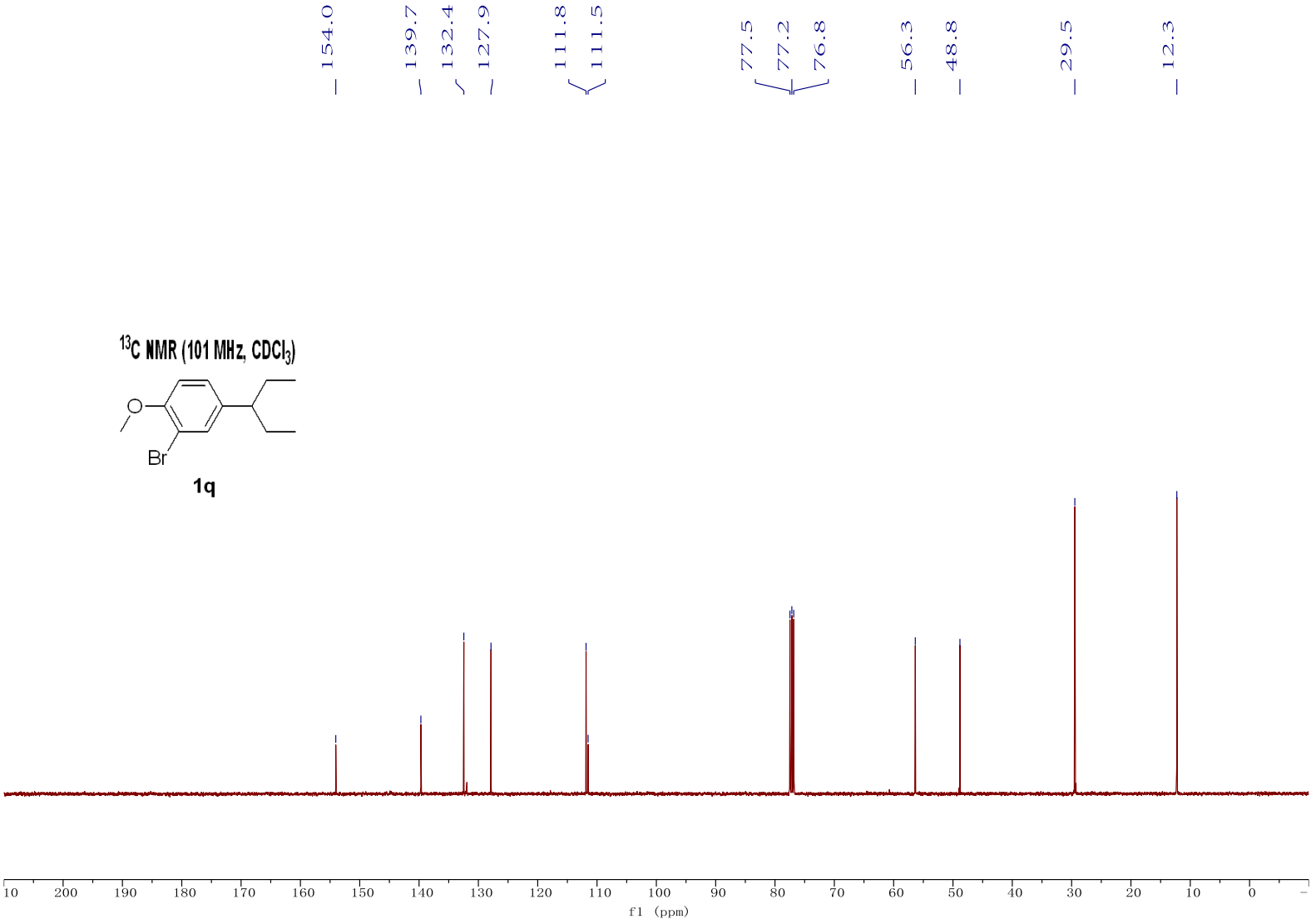

153.1
139.2
129.4
127.1
122.1
112.0
77.5
77.2
76.8
56.3
48.9
29.4
12.3
13C NMR (101 MHz, CDCl3)
O
Cl
1p
f1 (ppm)

^{1}H NMR (400 MHz, $CDCl_3$)

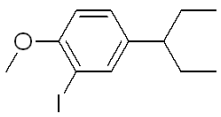


1q

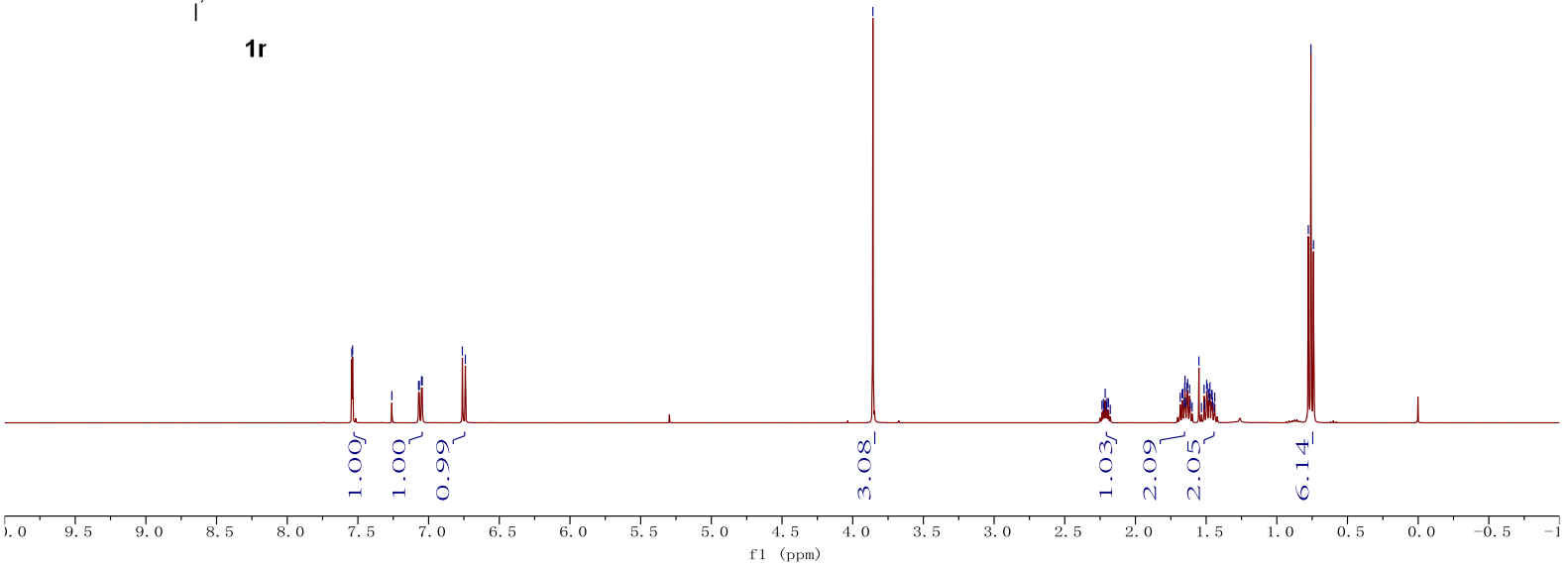


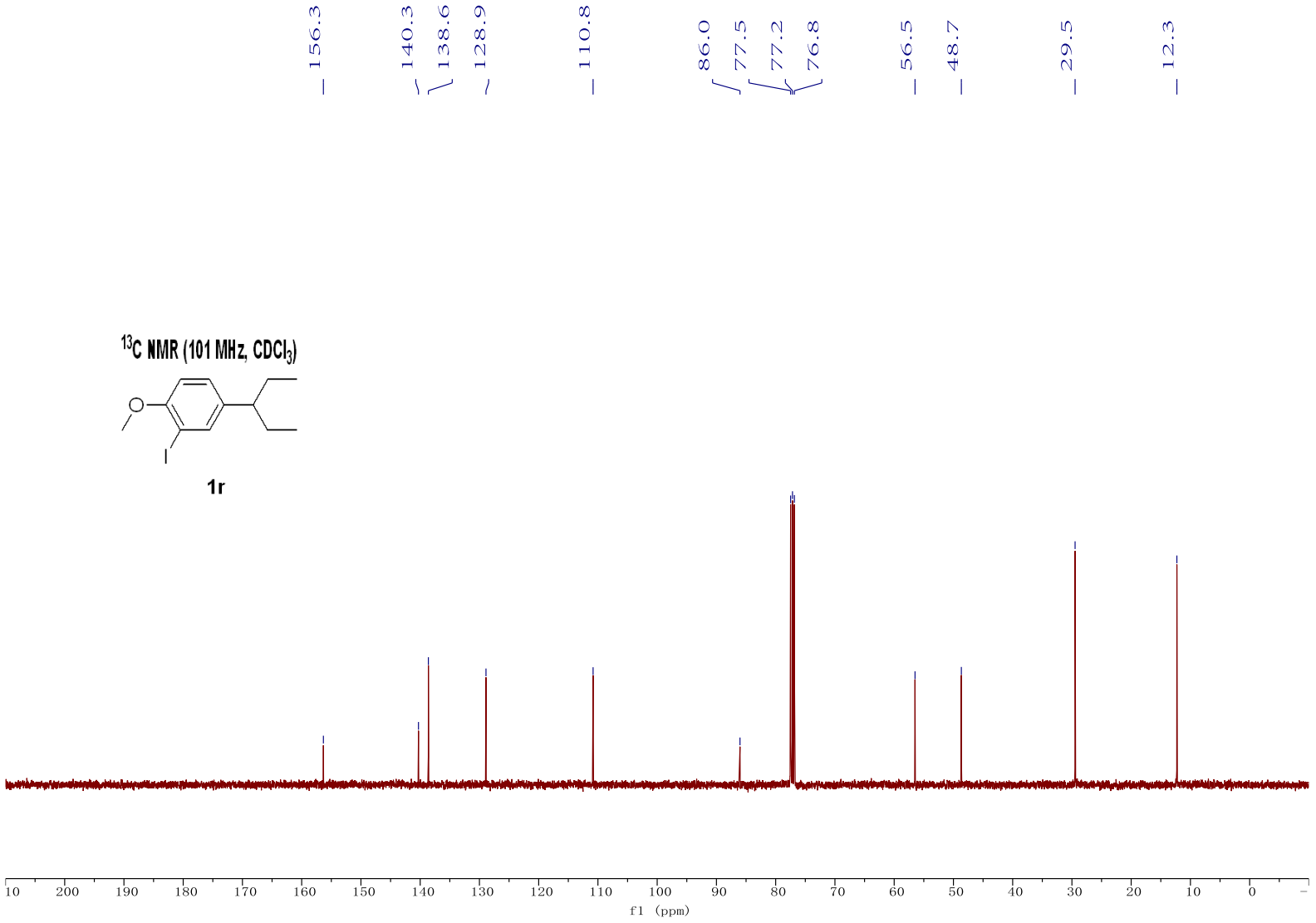

154.0
139.7
132.4
127.9
111.8
111.5
77.5
77.2
76.8
56.3
48.8
29.5
12.3
13C NMR (101 MHz, CDCl3)
O
Br
1q
f1 (ppm)

^{1}H NMR (400 MHz, $CDCl_3$)

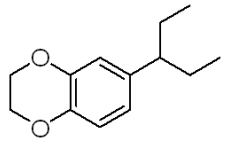


1r

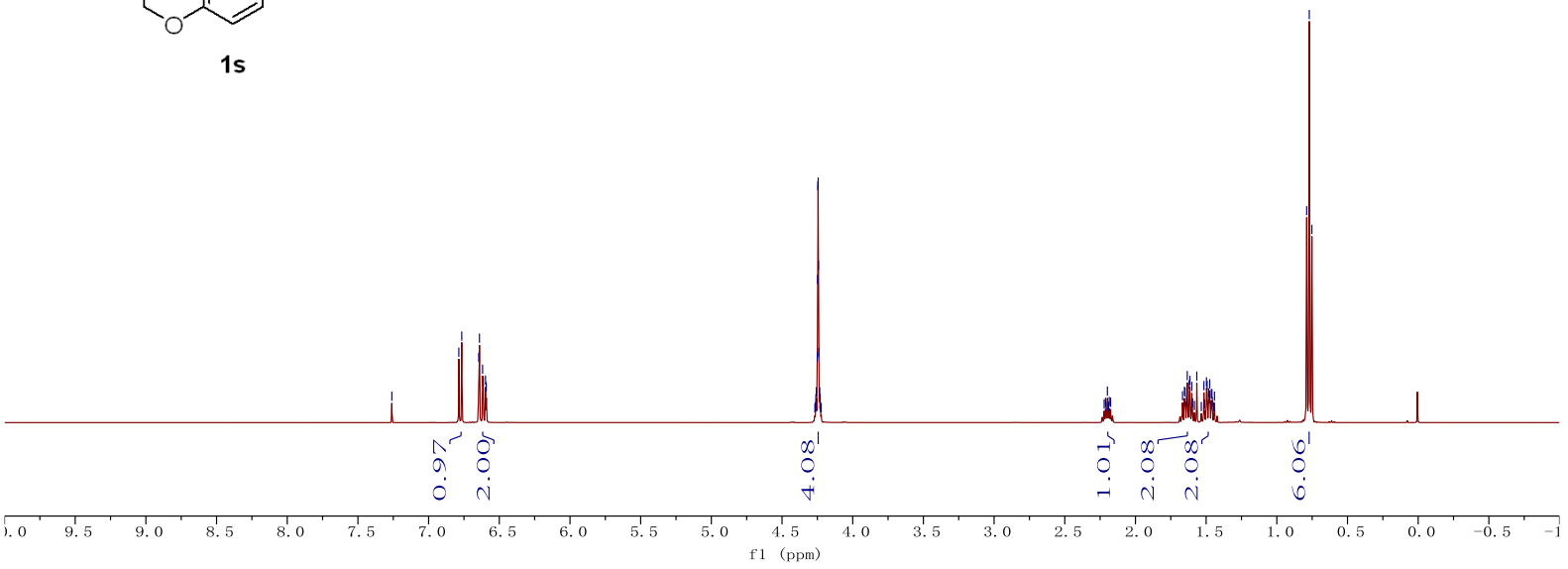


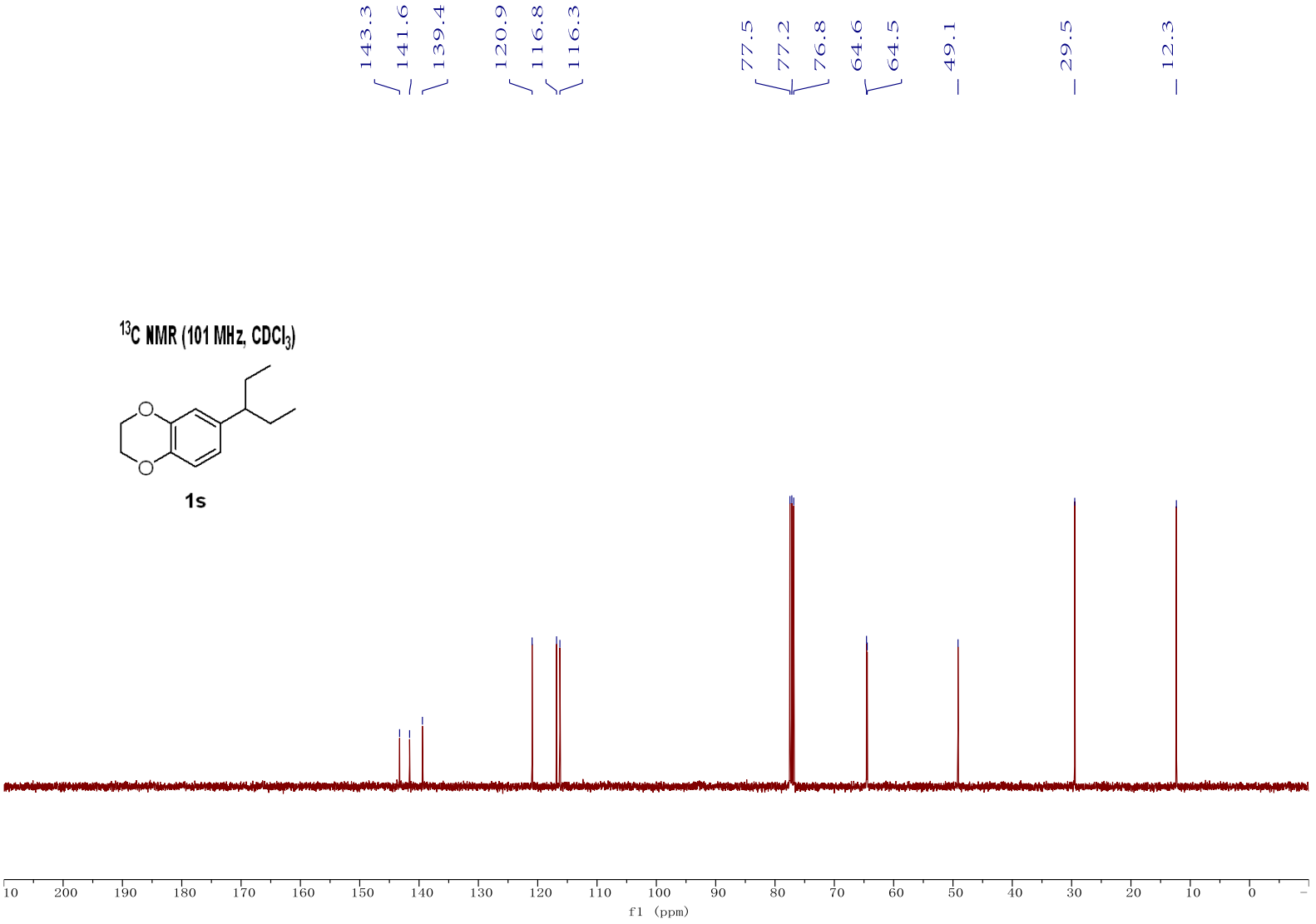

156.3
140.3
138.6
128.9
110.8
86.0
77.5
77.2
76.8
56.5
48.7
29.5
12.3
13C NMR (101 MHz, CDCl3)
1r
f1 (ppm)

^{1}H NMR (400 MHz, $CDCl_3$)



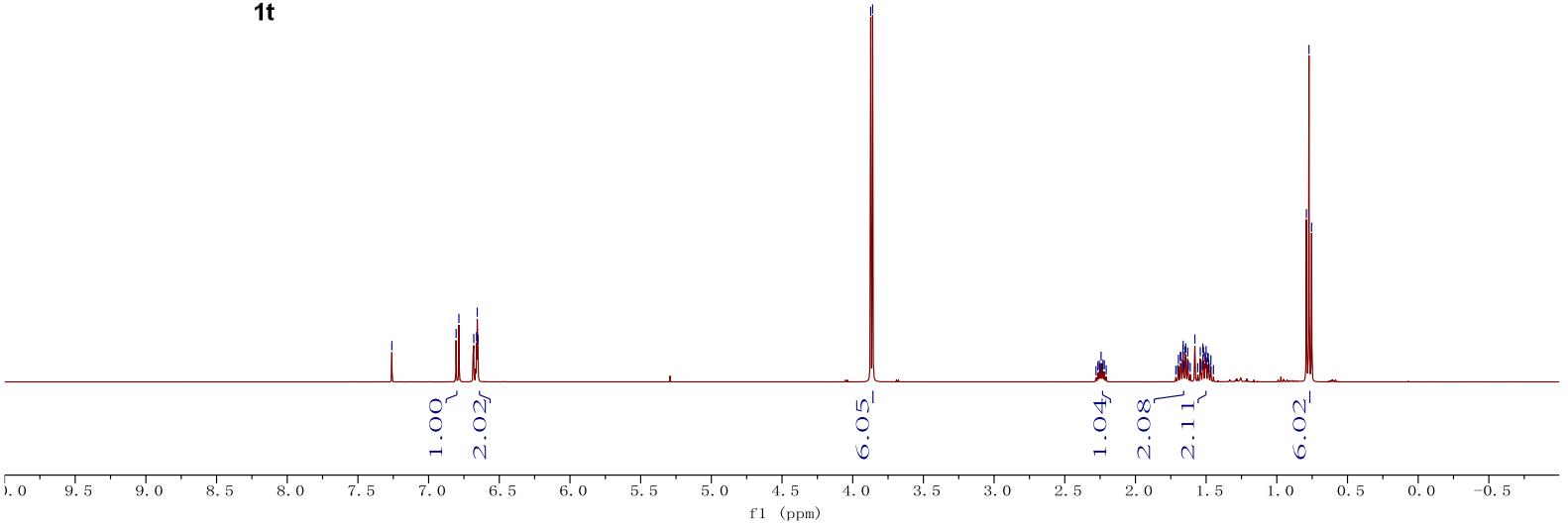
1s

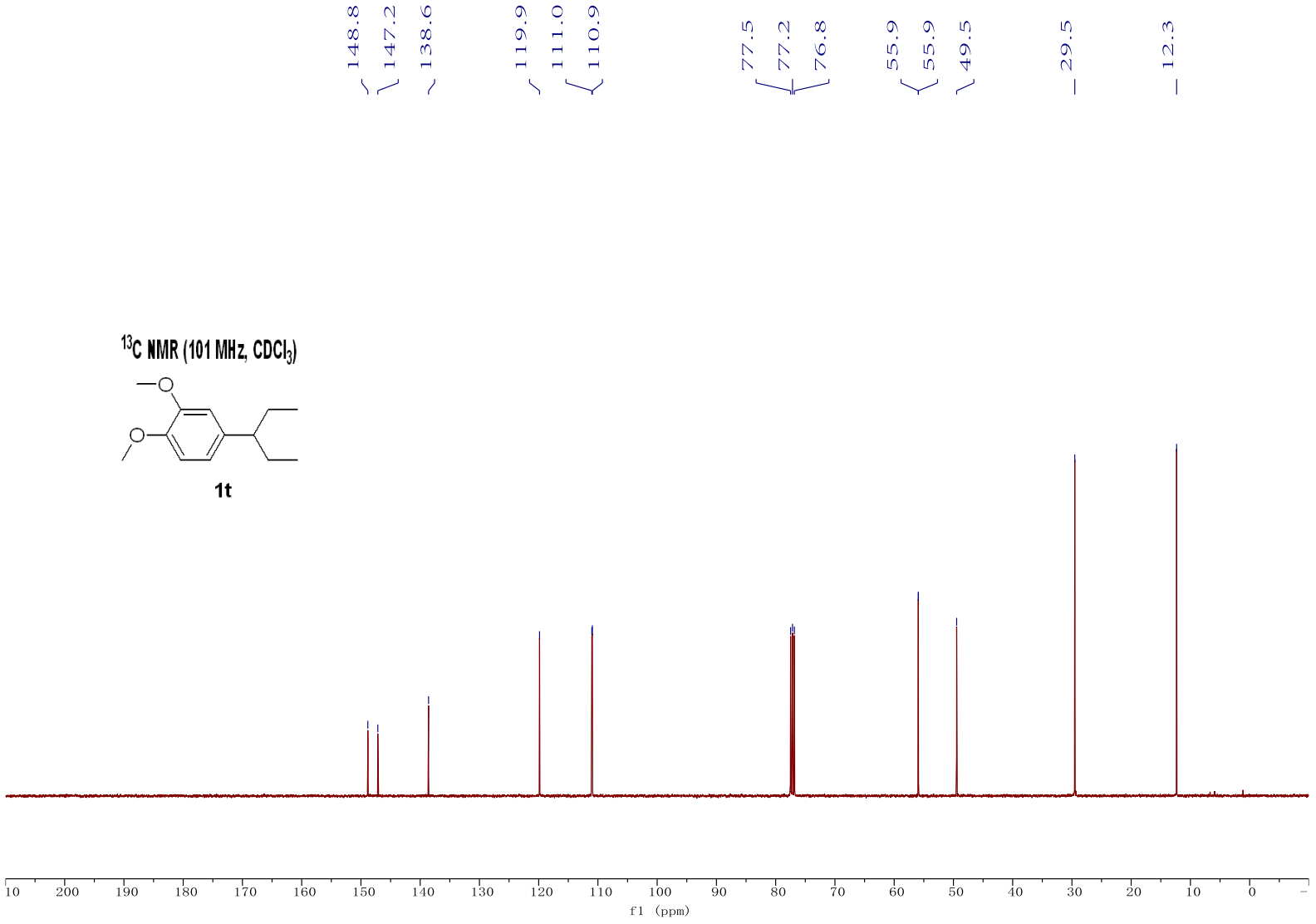



143.3
141.6
139.4
120.9
116.8
116.3
77.5
77.2
76.8
64.6
64.5
49.1
29.5
12.3
13C NMR (101 MHz, CDCl3)
1s
f1 (ppm)

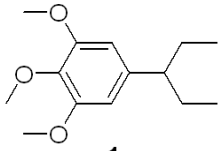
^{1}H NMR (400 MHz, $CDCl_3$)

1t

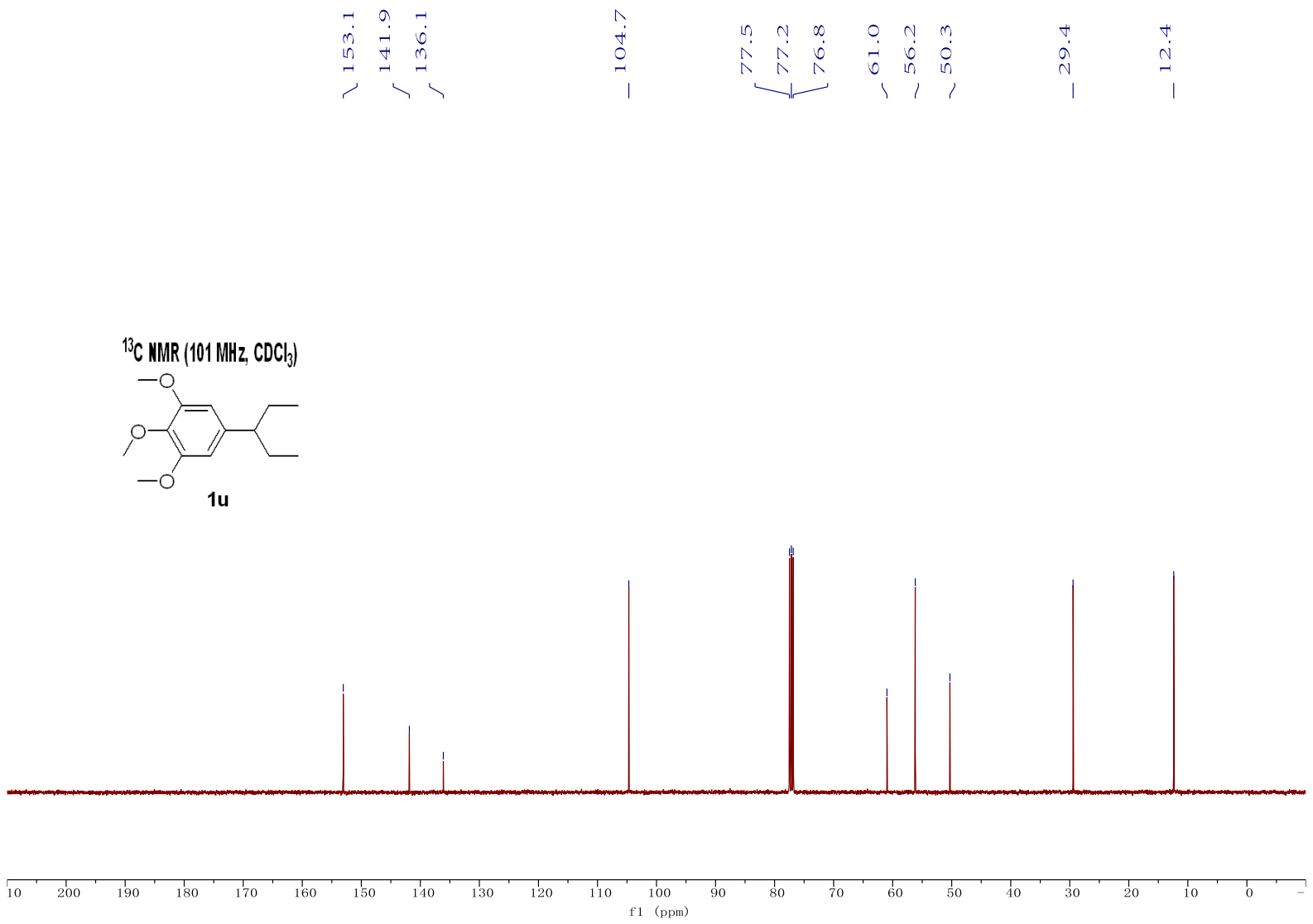


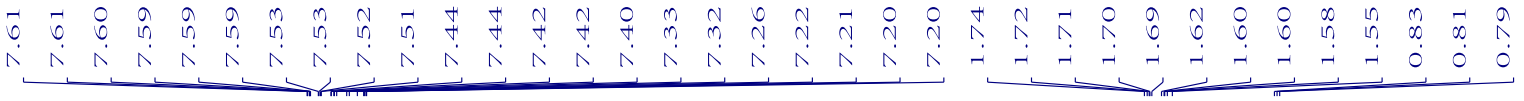

148.8
147.2
138.6
119.9
111.0
110.9
77.5
77.2
76.8
55.9
55.9
49.5
29.5
12.3
13C NMR (101 MHz, CDCl3)
1t
f1 (ppm)

^{1}H NMR (400 MHz, $CDCl_3$)

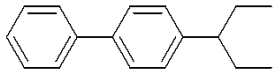


1u

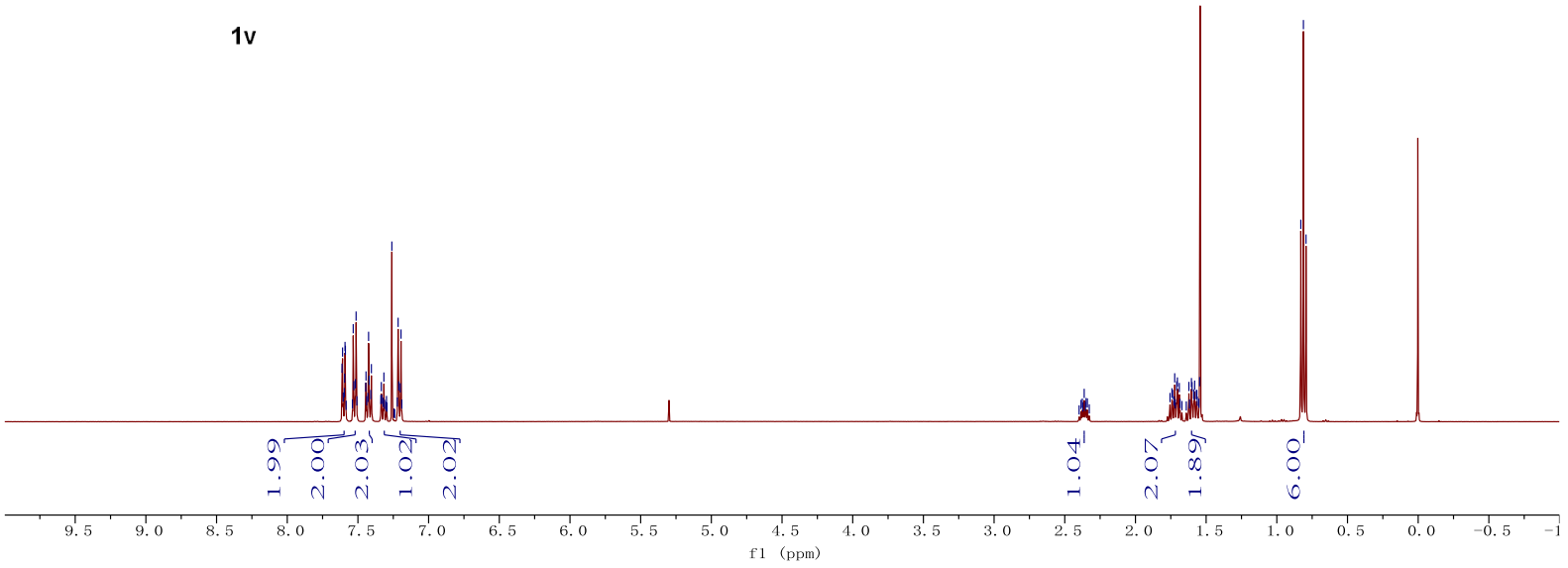

153.1
141.9
136.1
104.7
77.5
77.2
76.8
61.0
56.2
50.3
29.4
12.4
13C NMR (101 MHz, CDCl3)
1u
f1 (ppm)

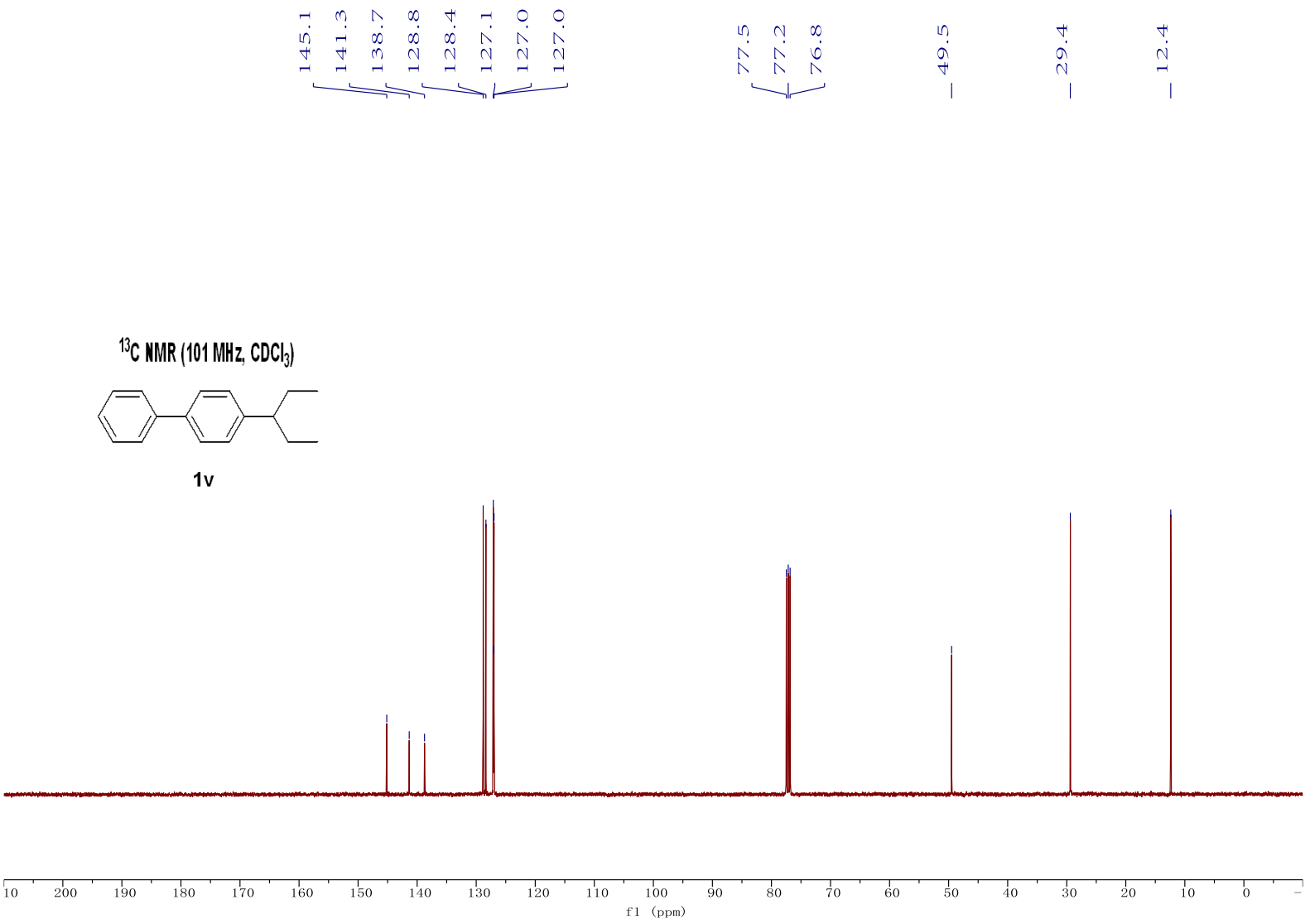


^{1}H NMR (400 MHz, $CDCl_3$)

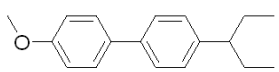


1v

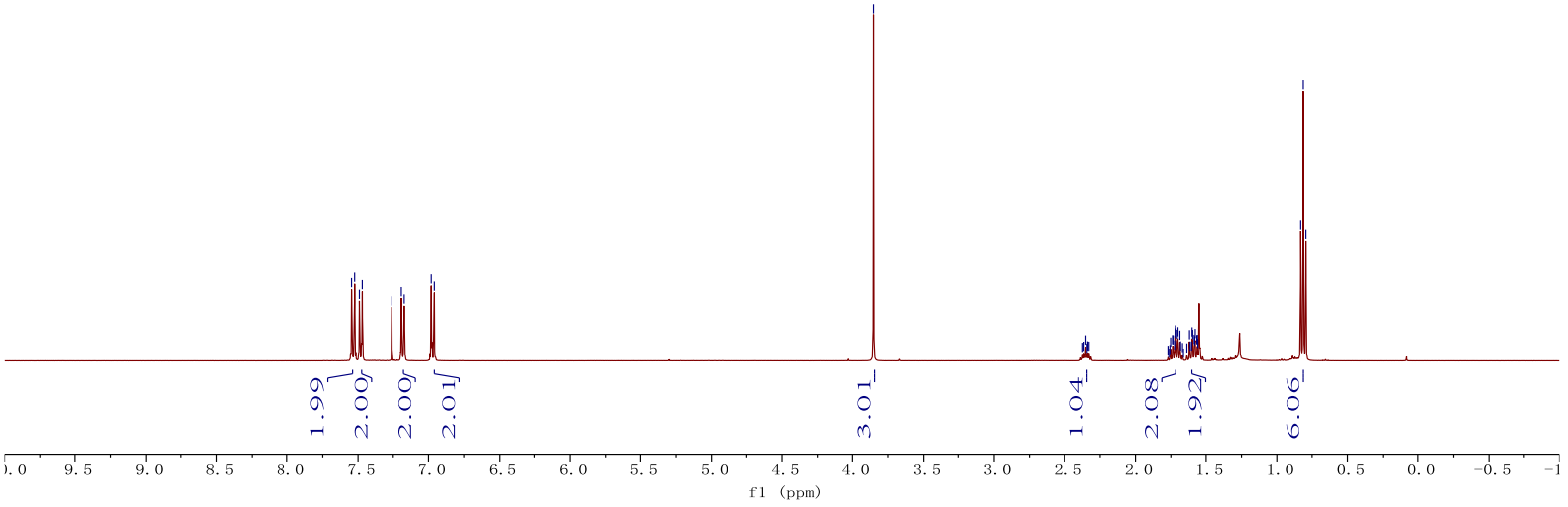


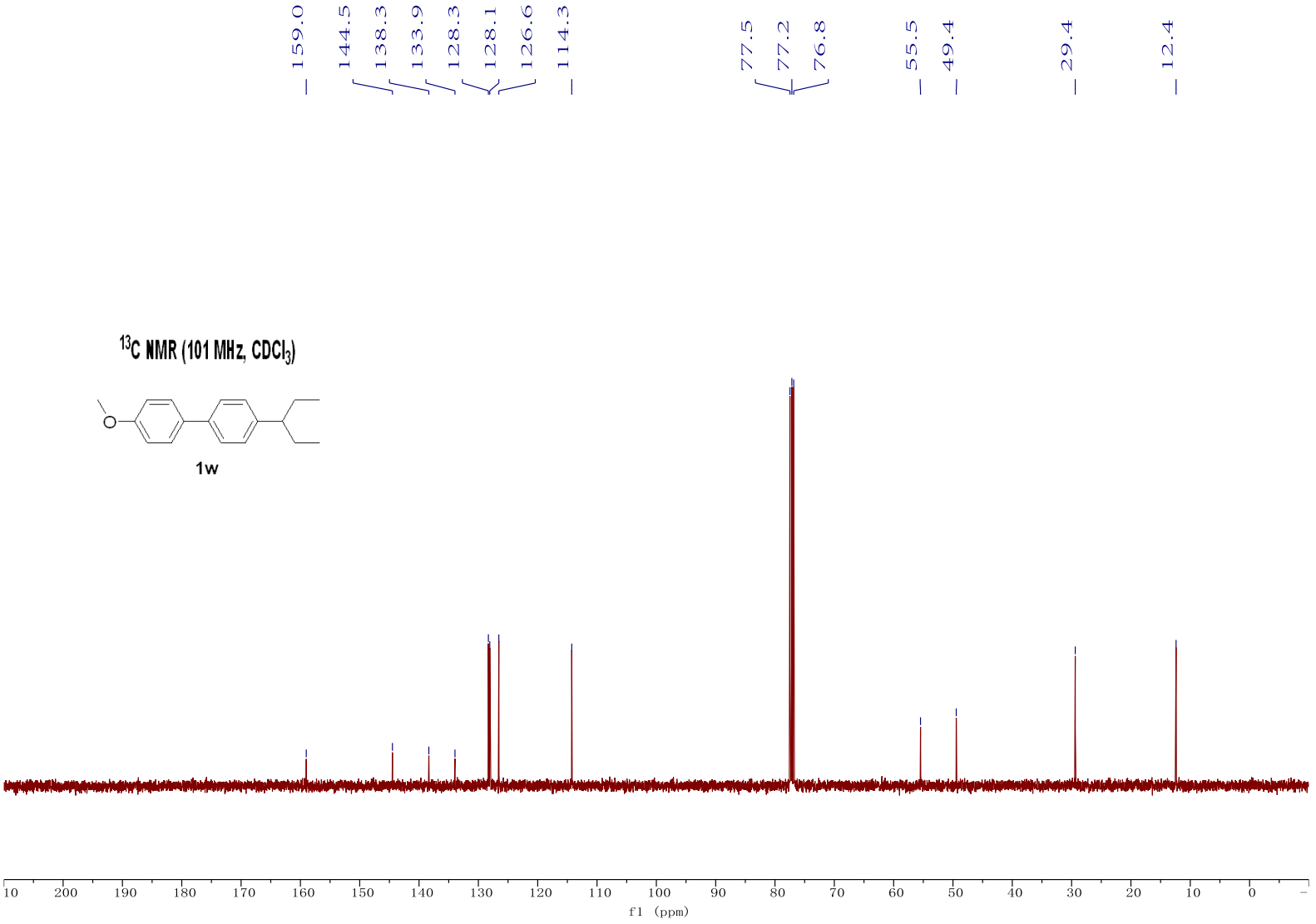

145.1
141.3
138.7
128.8
128.4
127.1
127.0
127.0
77.5
77.2
76.8
49.5
29.4
12.4
13C NMR (101 MHz, CDCl3)
1v
f1 (ppm)

^{1}H NMR (400 MHz, $CDCl_3$)



1w

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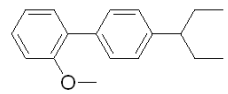
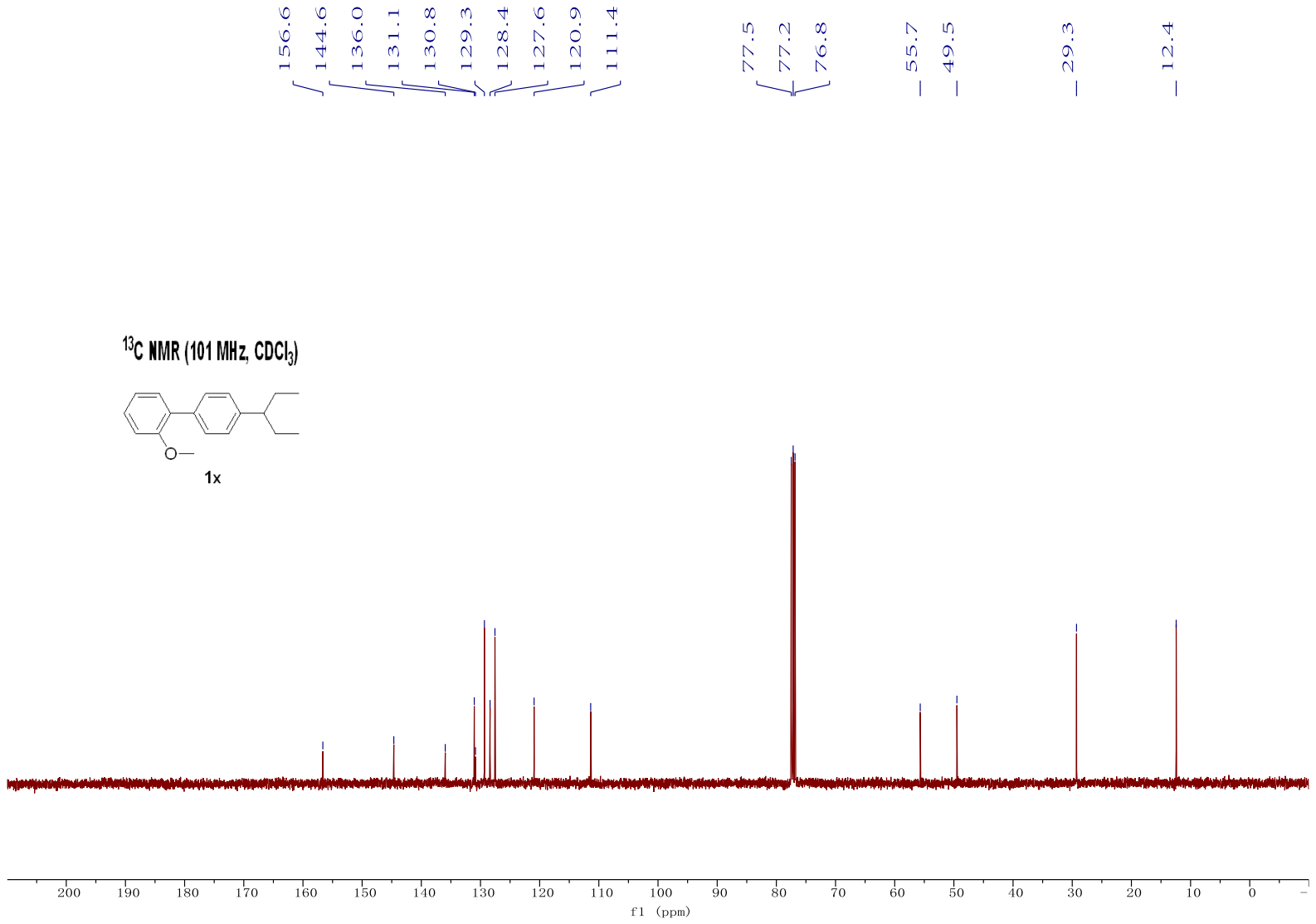
144.5
138.3
133.9
128.3
128.1
126.6
114.3
77.5
77.2
76.8
55.5
49.4
29.4
12.4
13C NMR (101 MHz, CDCl3)
1w
f1 (ppm)

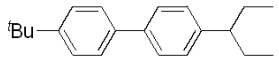
^{1}H NMR (400 MHz, $CDCl_3$)



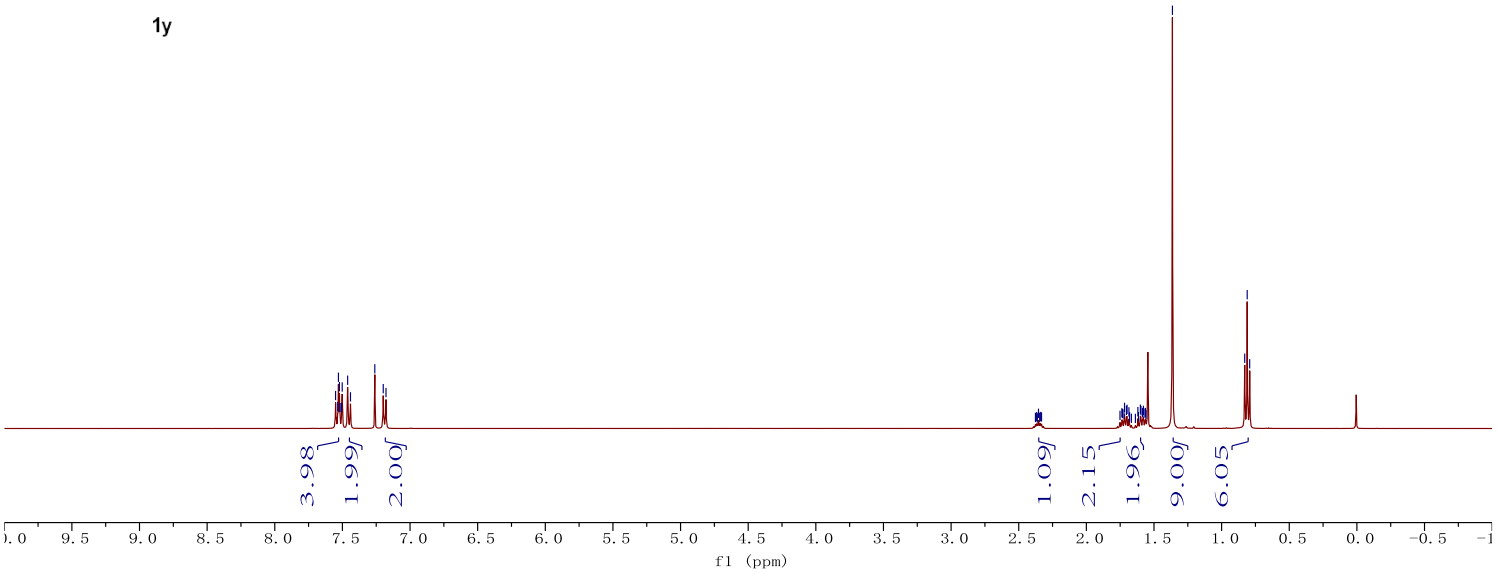
1x

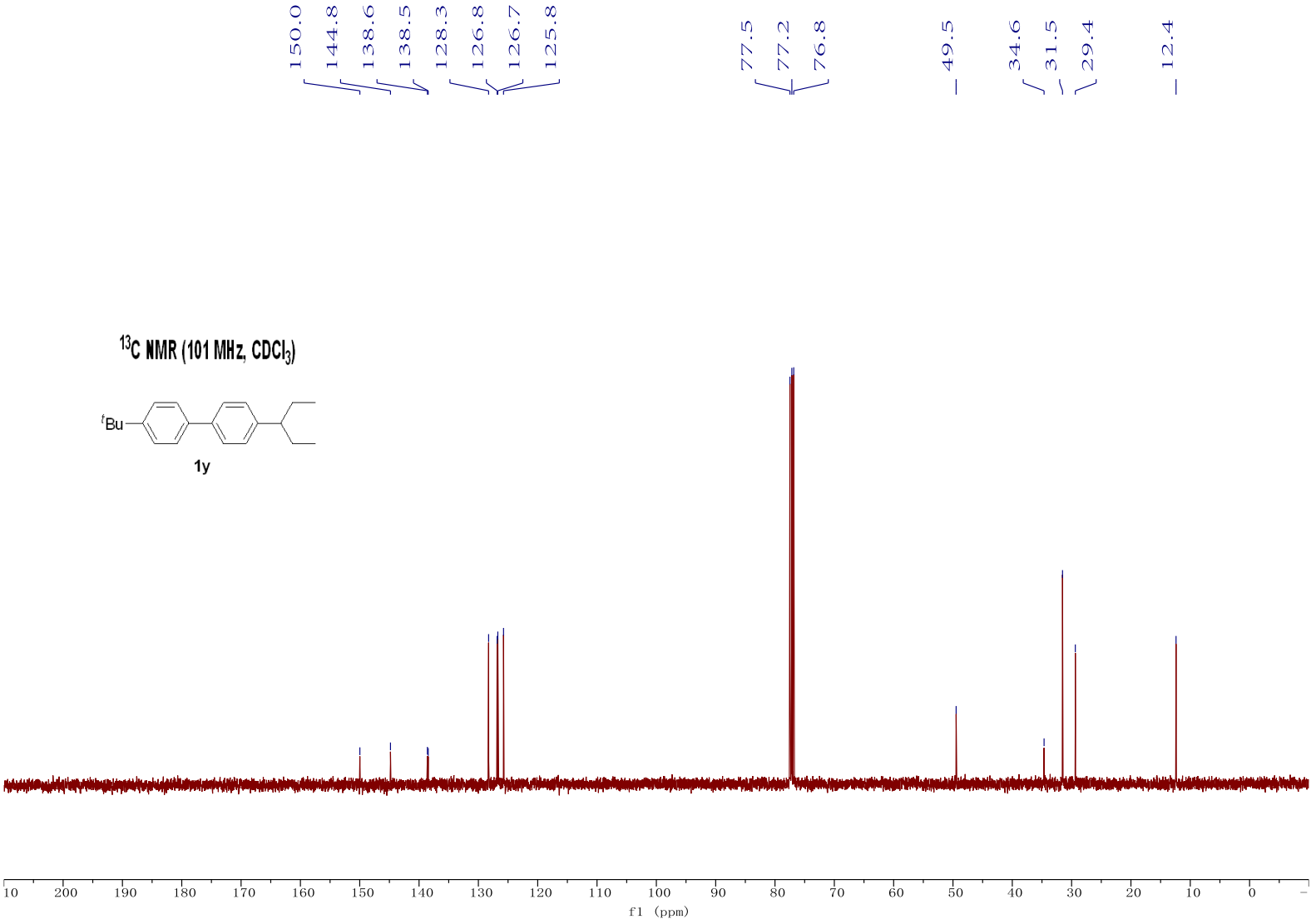

156.6
144.6
136.0
131.1
130.8
129.3
128.4
127.6
120.9
111.4
77.5
77.2
76.8
55.7
49.5
29.3
12.4
13C NMR (101 MHz, CDCl3)
O
1x
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

^{1}H NMR (400 MHz, $CDCl_3$)



1y

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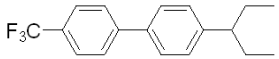
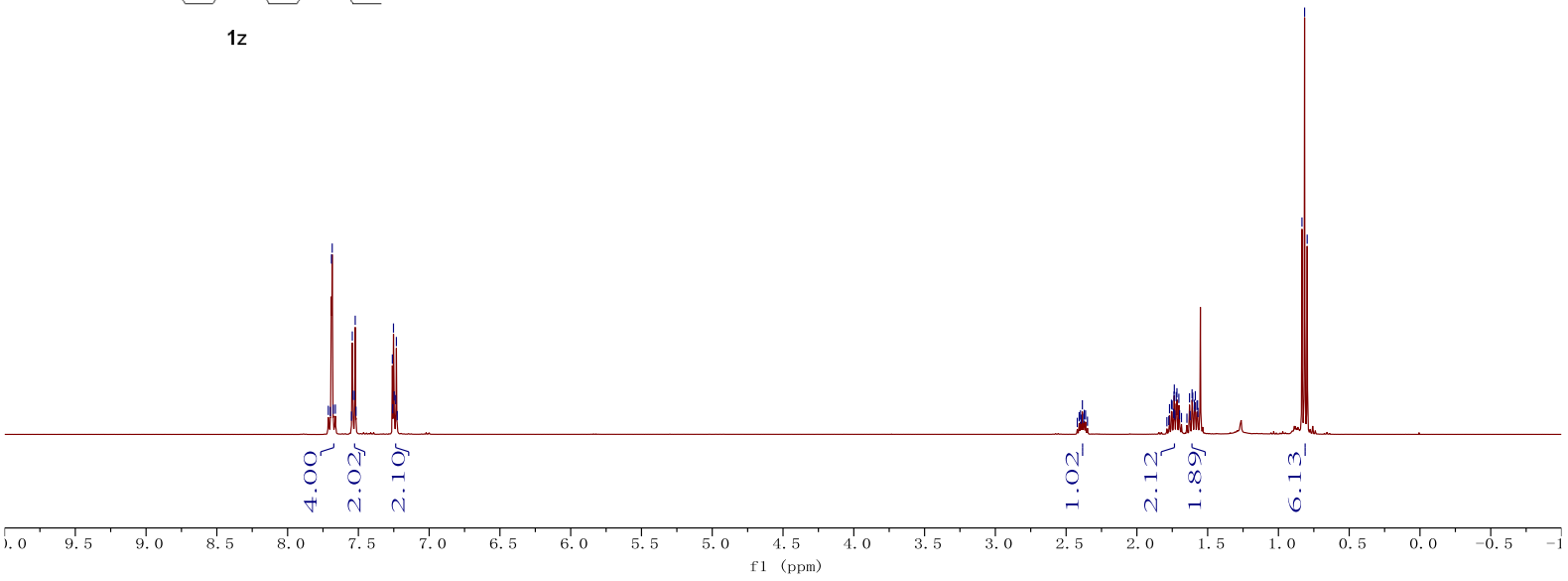
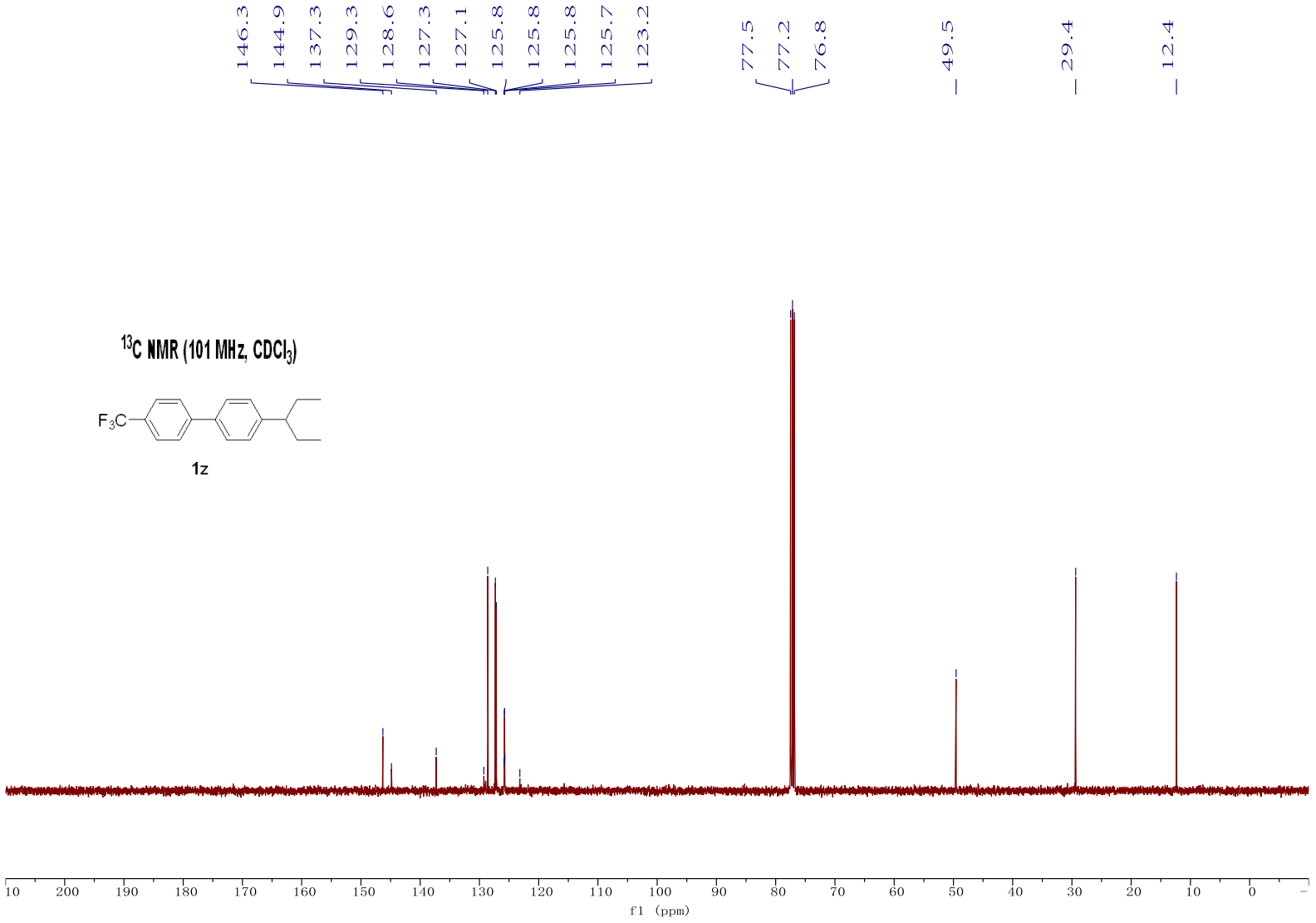
144.8
138.6
138.5
128.3
126.8
126.7
125.8
77.5
77.2
76.8
49.5
34.6
31.5
29.4
12.4
13C NMR (101 MHz, CDCl3)
tBu
1y
f1 (ppm)

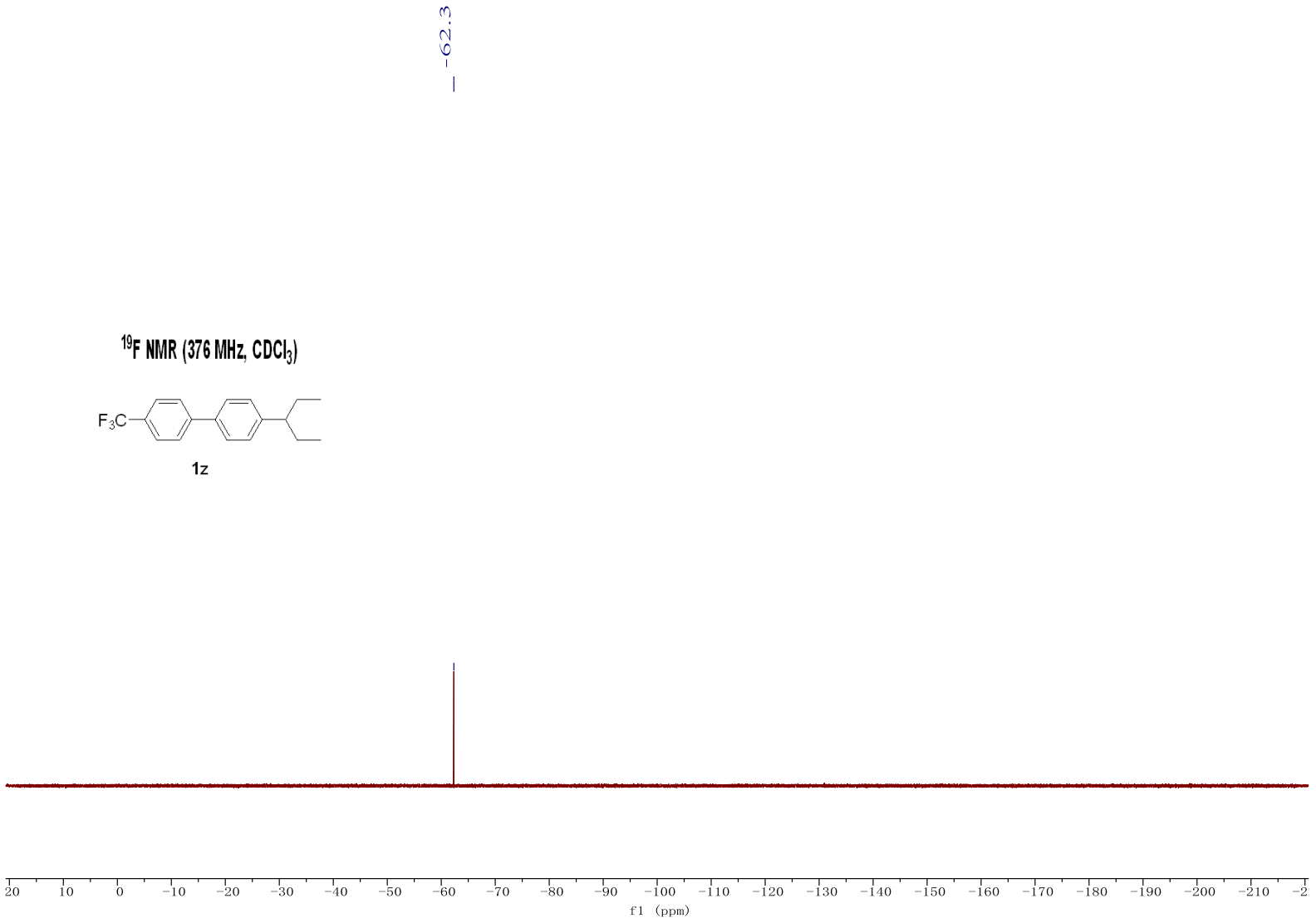
^{1}H NMR (400 MHz, $CDCl_3$)

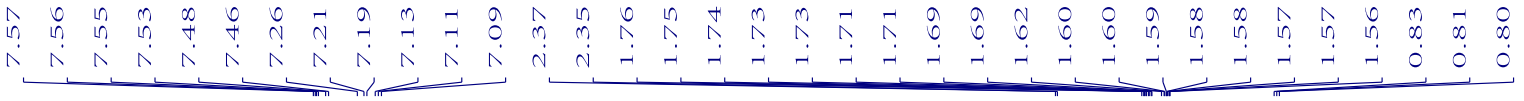


1z

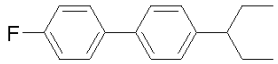



146.3
144.9
137.3
129.3
128.6
127.3
127.1
125.8
125.8
125.8
125.7
123.2
77.5
77.2
76.8
49.5
29.4
12.4
13C NMR (101 MHz, CDCl3)
F3C
1z
f1 (ppm)

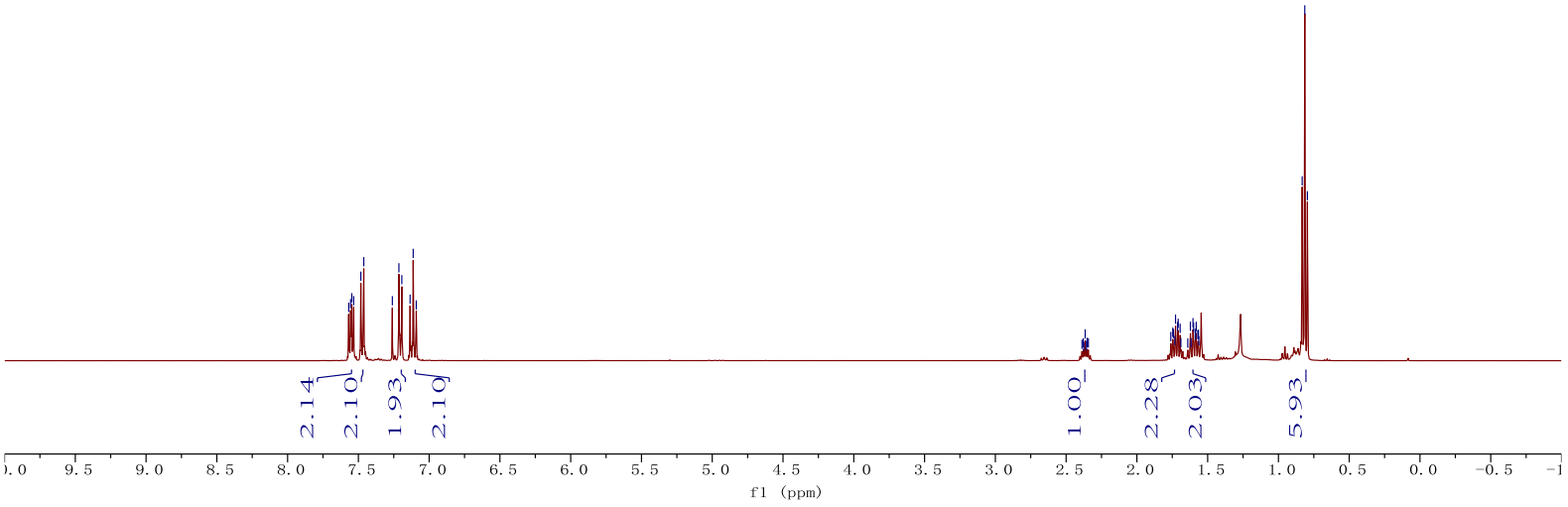

-62.3
19F NMR (376 MHz, CDCl3)
F3C
1z
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

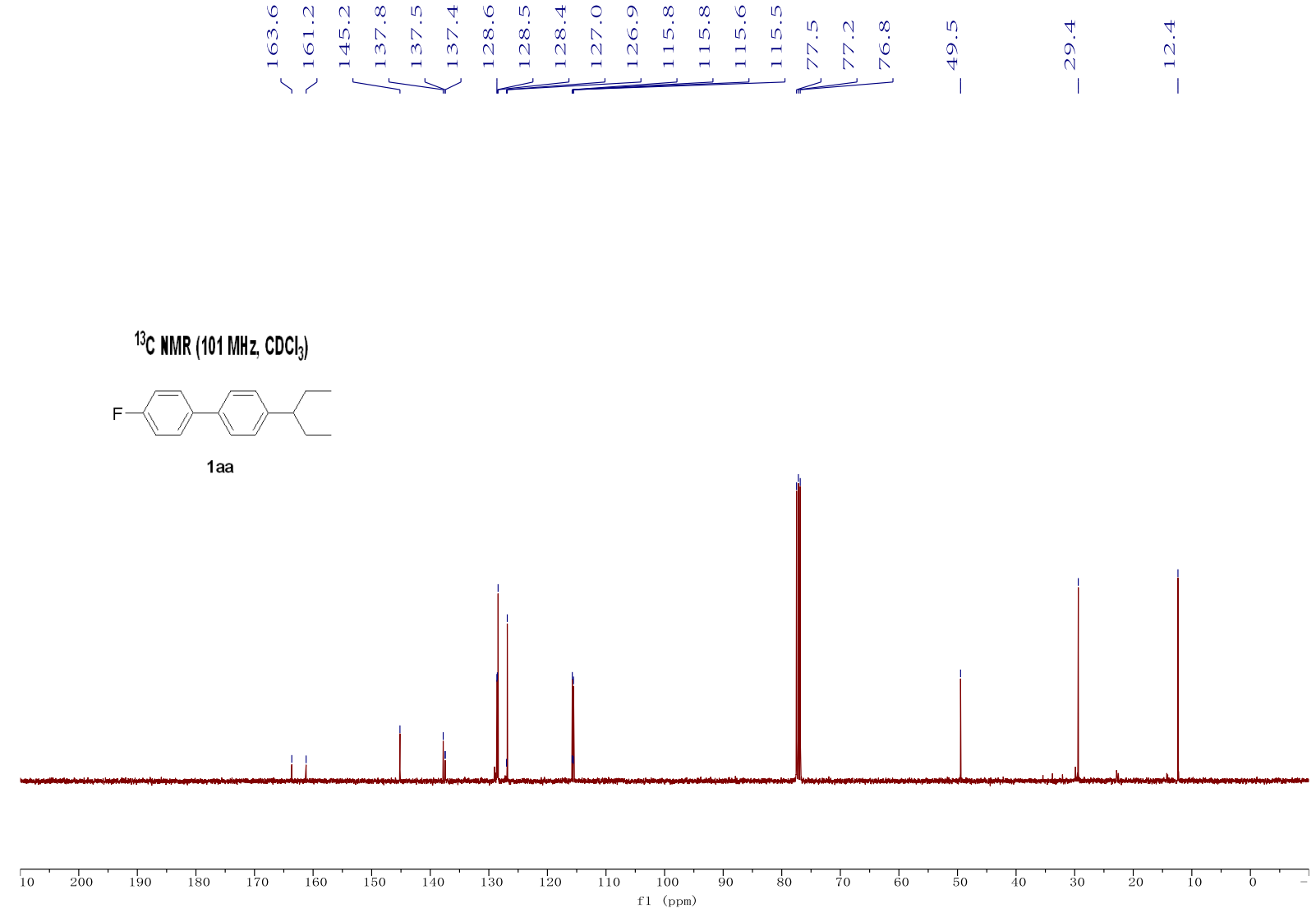


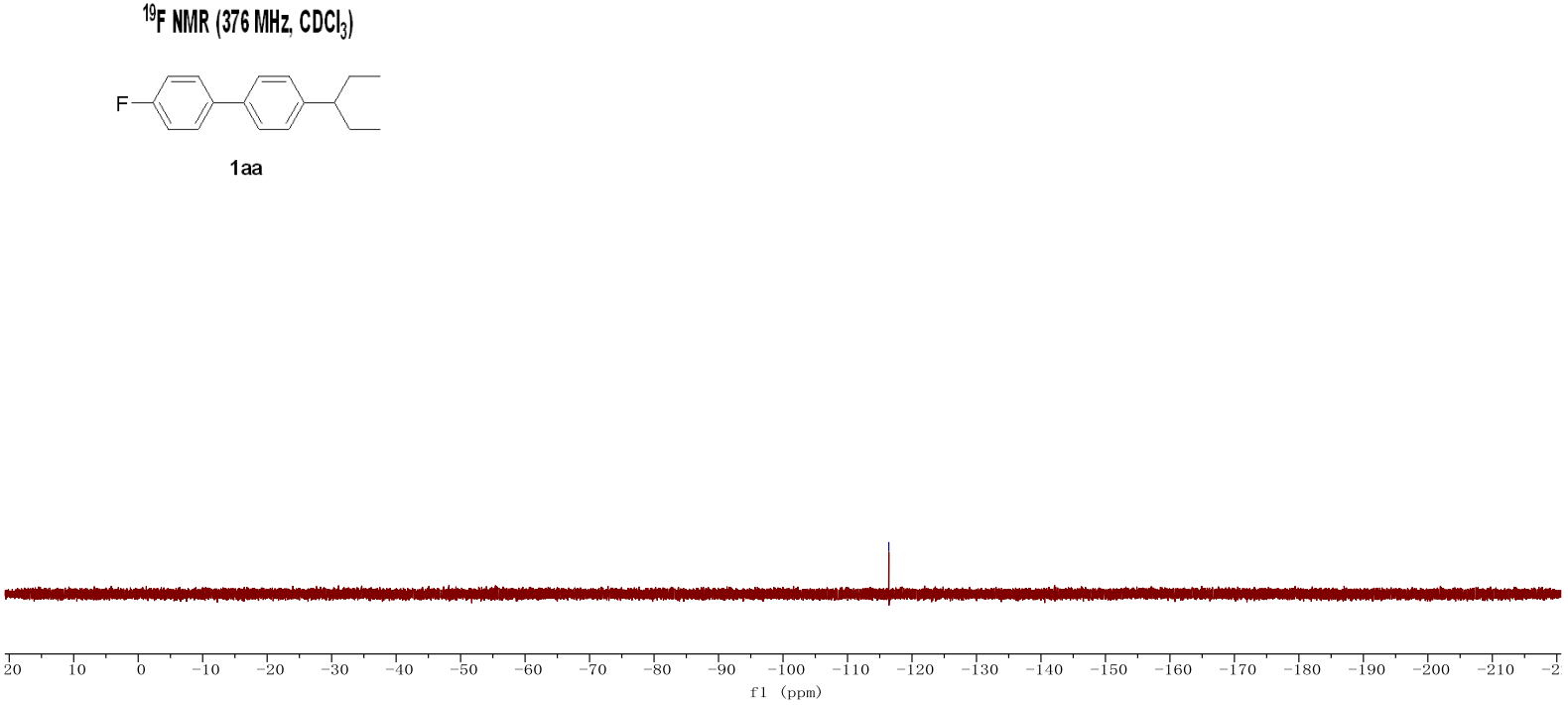
^{1}H NMR (400 MHz, $CDCl_3$)

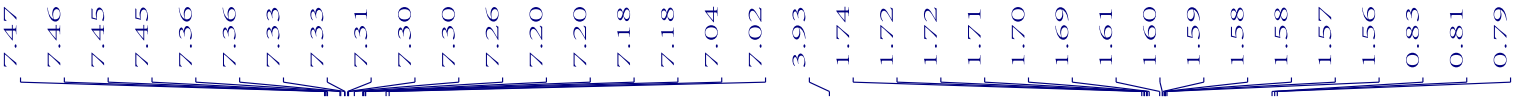


1aa

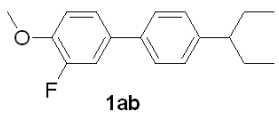



163.6
161.2
145.2
137.8
137.5
137.4
128.6
128.5
128.4
127.0
126.9
115.8
115.8
115.6
115.5
77.5
77.2
76.8
49.5
29.4
12.4
13C NMR (101 MHz, CDCl3)
F
1aa
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

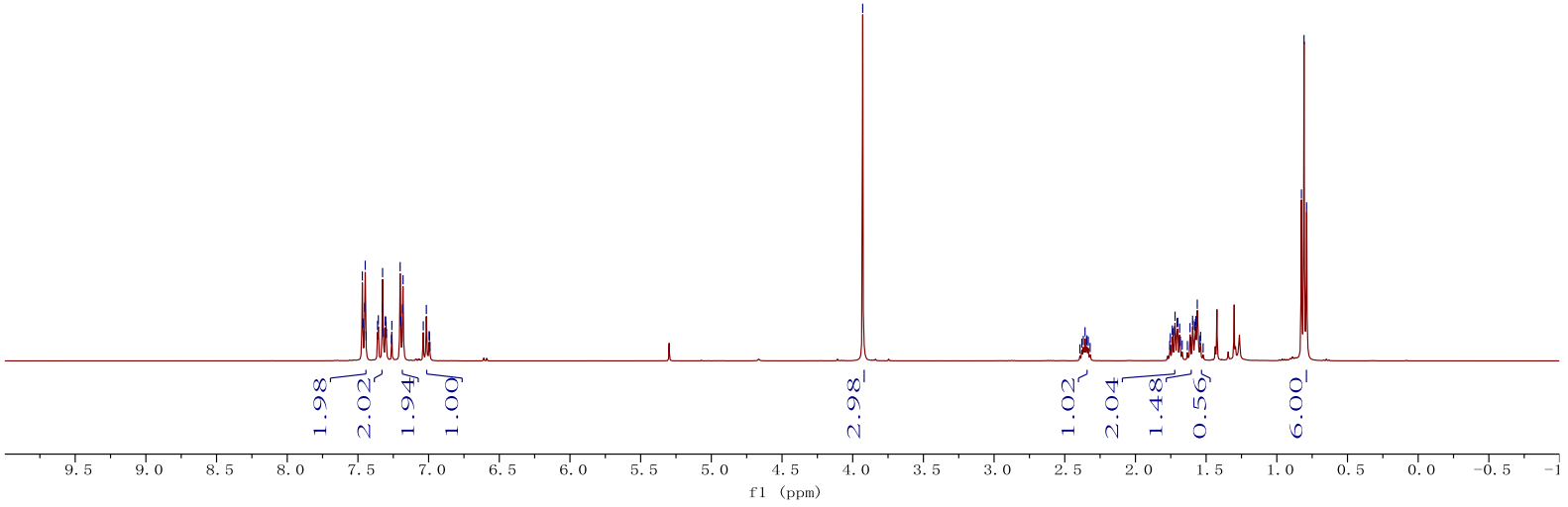

-116.4
19F NMR (376 MHz, CDCl3)
F
1aa
20 10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210 −2
f1 (ppm)

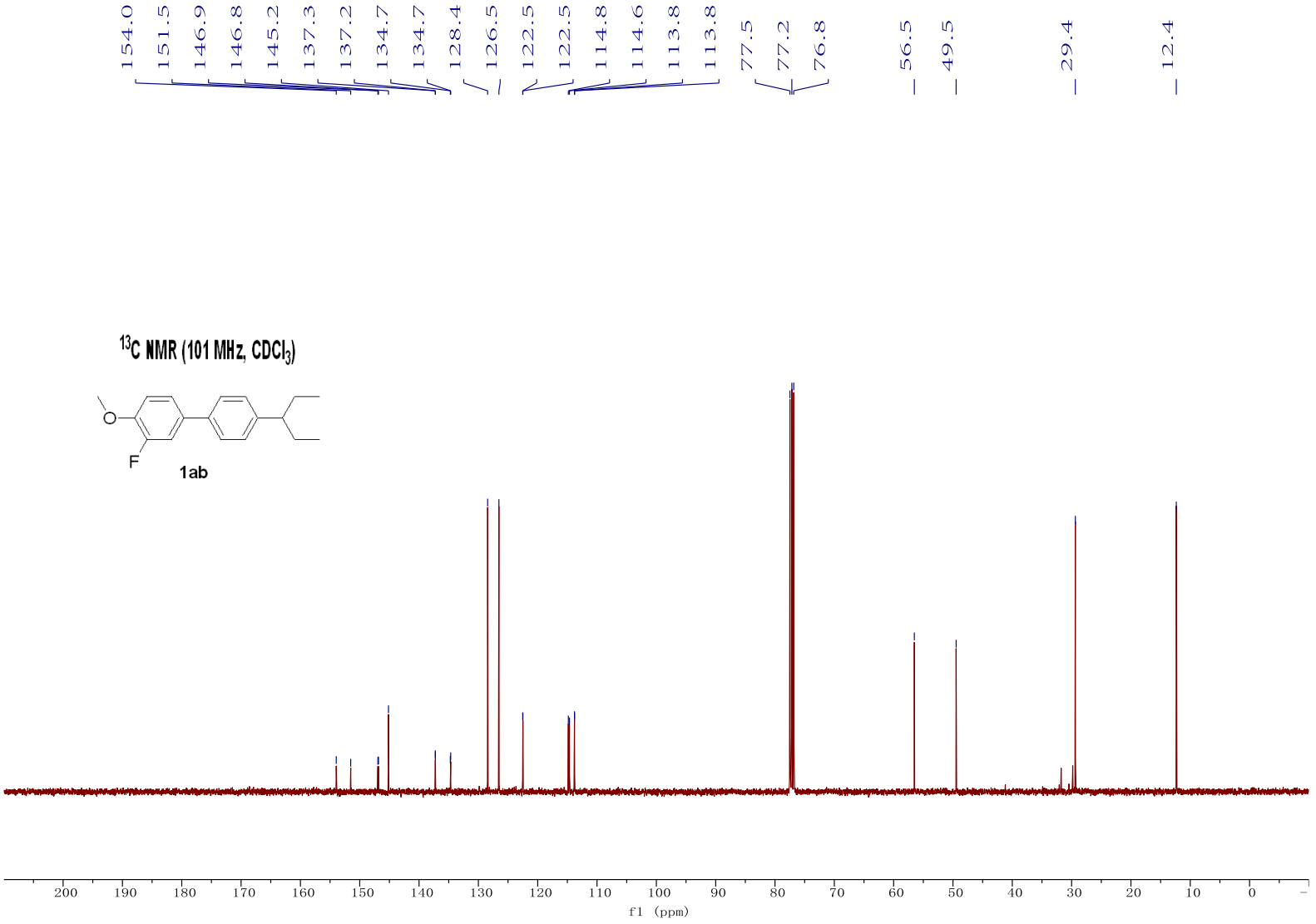


^{1}H NMR (400 MHz, $CDCl_3$)

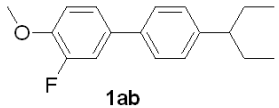


1ab



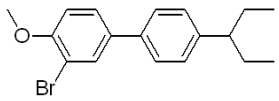

154.0
151.5
146.9
146.8
145.2
137.3
137.2
134.7
134.7
128.4
126.5
122.5
122.5
114.8
114.6
113.8
113.8
77.5
77.2
76.8
56.5
49.5
29.4
12.4
13C NMR (101 MHz, CDCl3)
O
F
1ab
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

^{19}F NMR (376 MHz, $CDCl_3$)

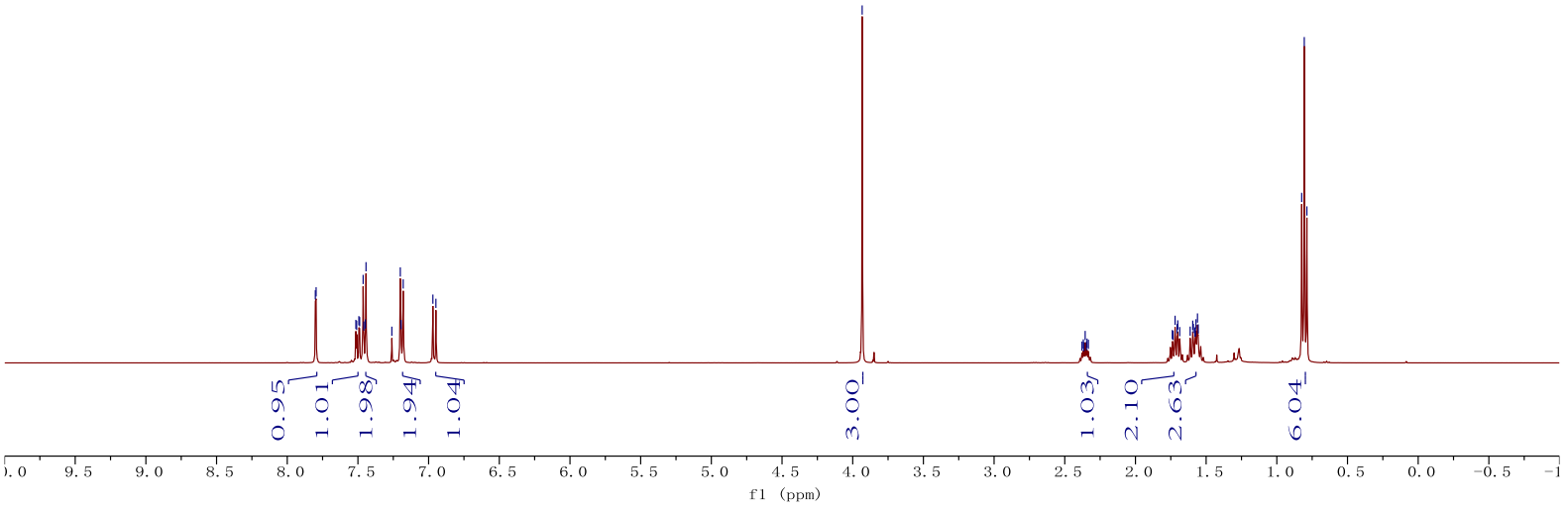


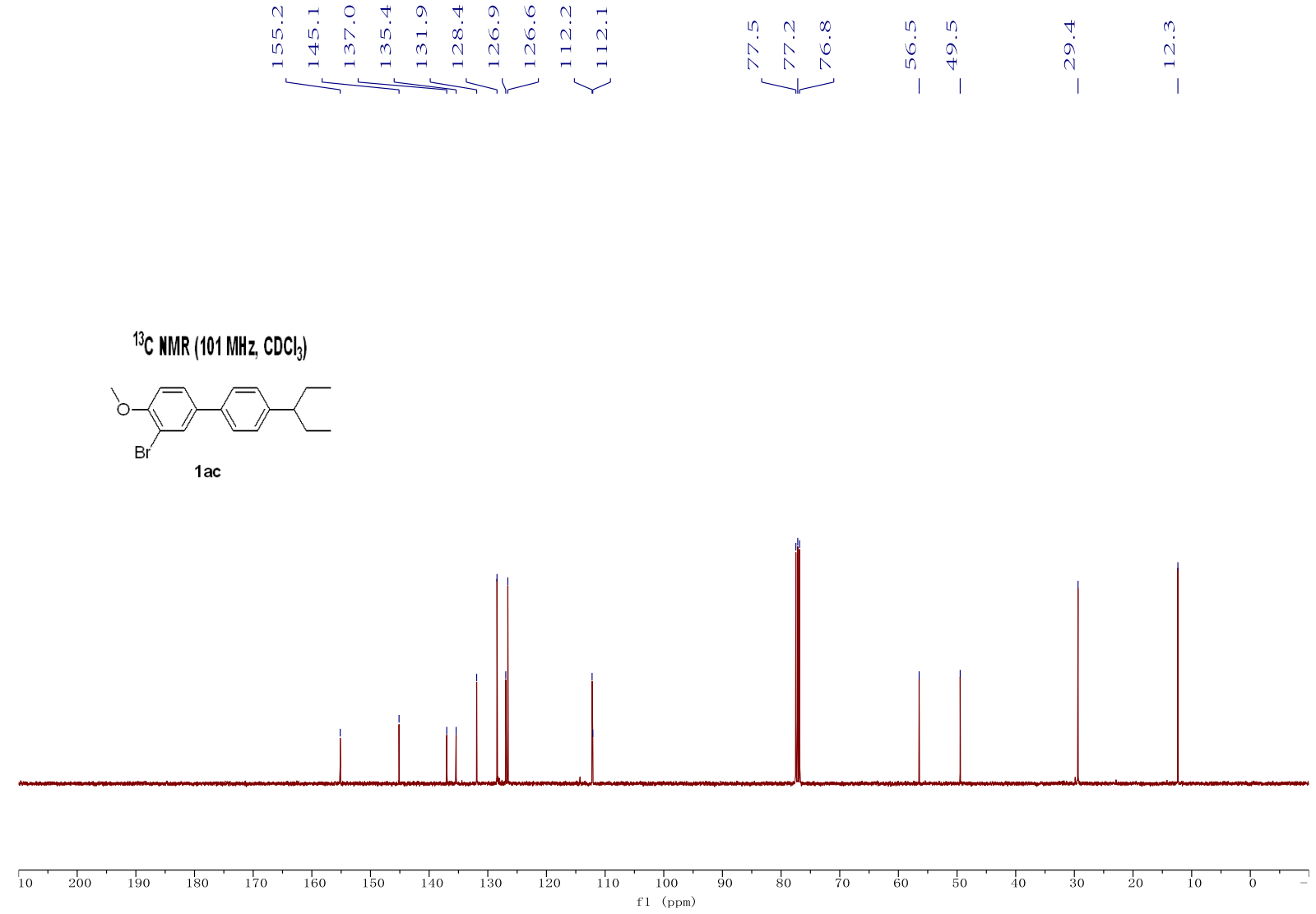
1ab

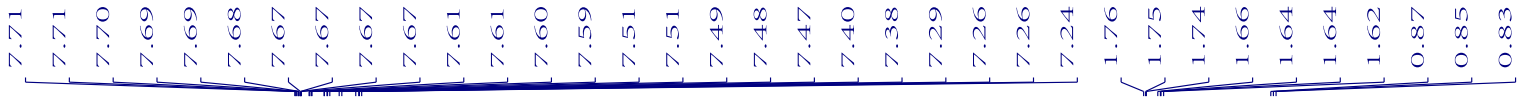
^{1}H NMR (400 MHz, $CDCl_3$)



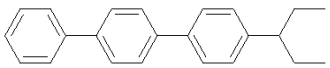
1ac



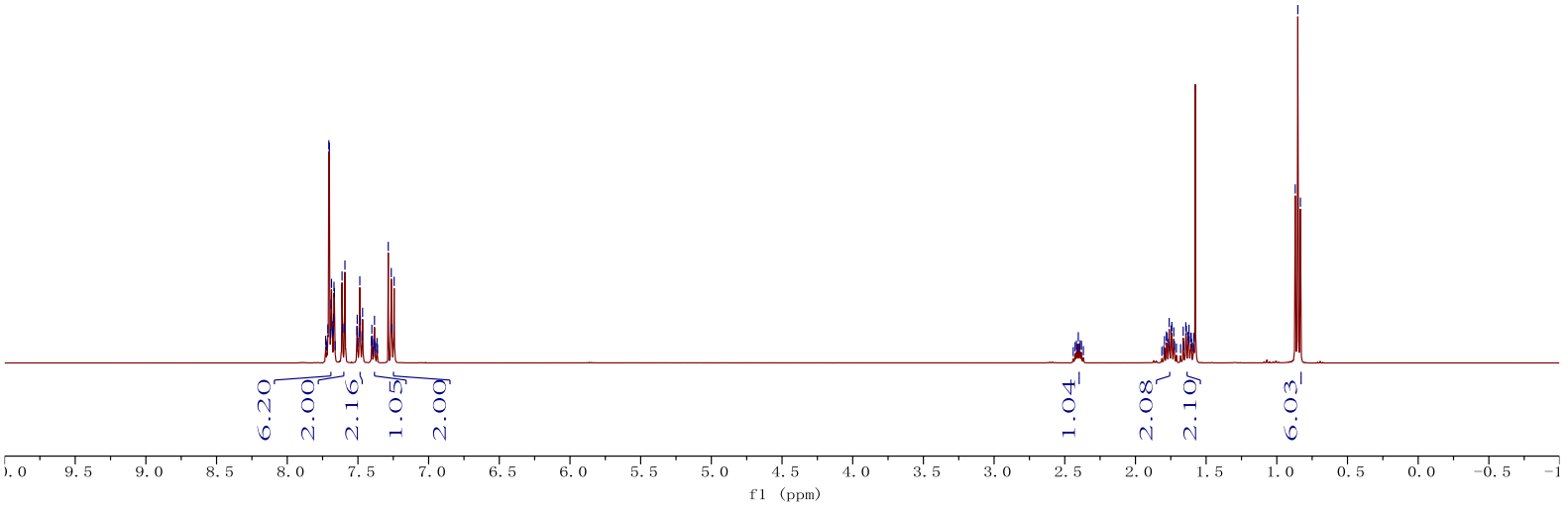

155.2
145.1
137.0
135.4
131.9
128.4
126.9
126.6
112.2
112.1
77.5
77.2
76.8
56.5
49.5
29.4
12.3
13C NMR (101 MHz, CDCl3)
O
Br
1ac
f1 (ppm)

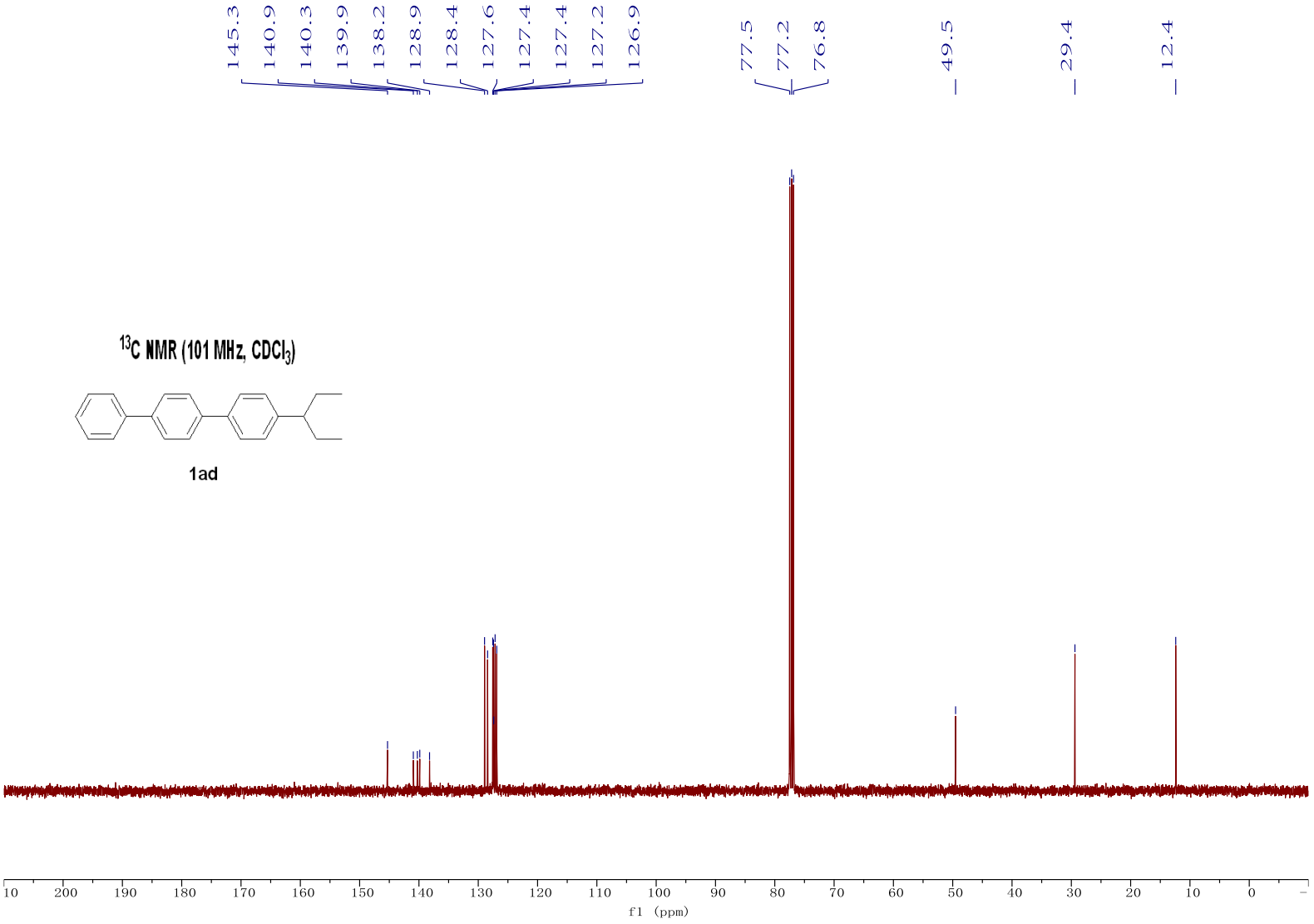


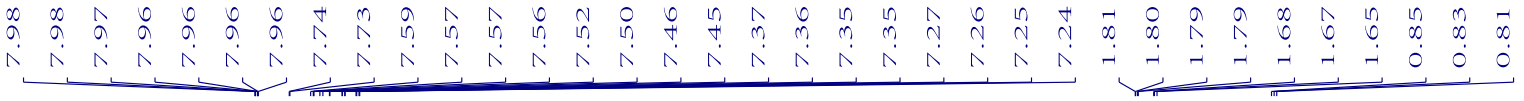
^{1}H NMR (400 MHz, $CDCl_3$)



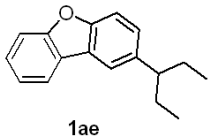
1ad



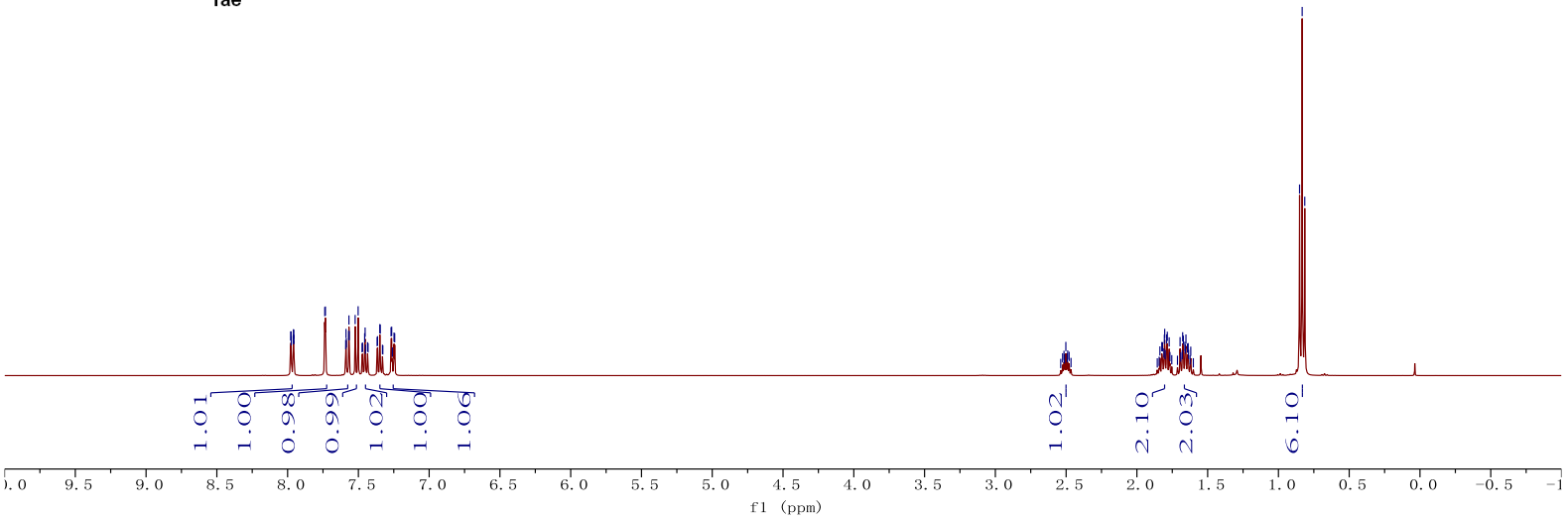

145.3
140.9
140.3
139.9
138.2
128.9
128.4
127.6
127.4
127.4
127.2
126.9
77.5
77.2
76.8
49.5
29.4
12.4
13C NMR (101 MHz, CDCl3)
1ad
f1 (ppm)



^{1}HNMR (400 MHz, $CDCl_3$)

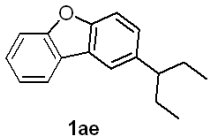


1ae

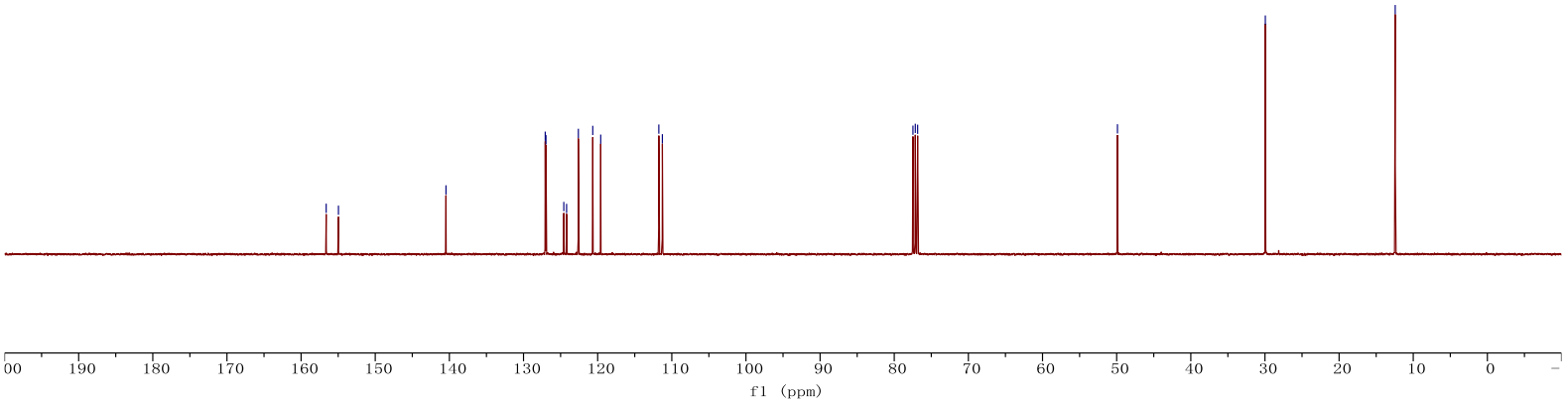


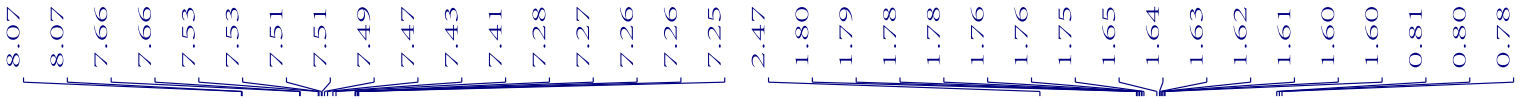
156.6
155.0
140.5
127.1
127.0
124.6
124.2
122.6
120.7
119.6
111.8
111.3
77.5
77.2
76.8
49.9
29.9
12.4

^{13}CNMR (101 MHz, $CDCl_3$)

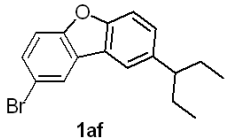


1ae

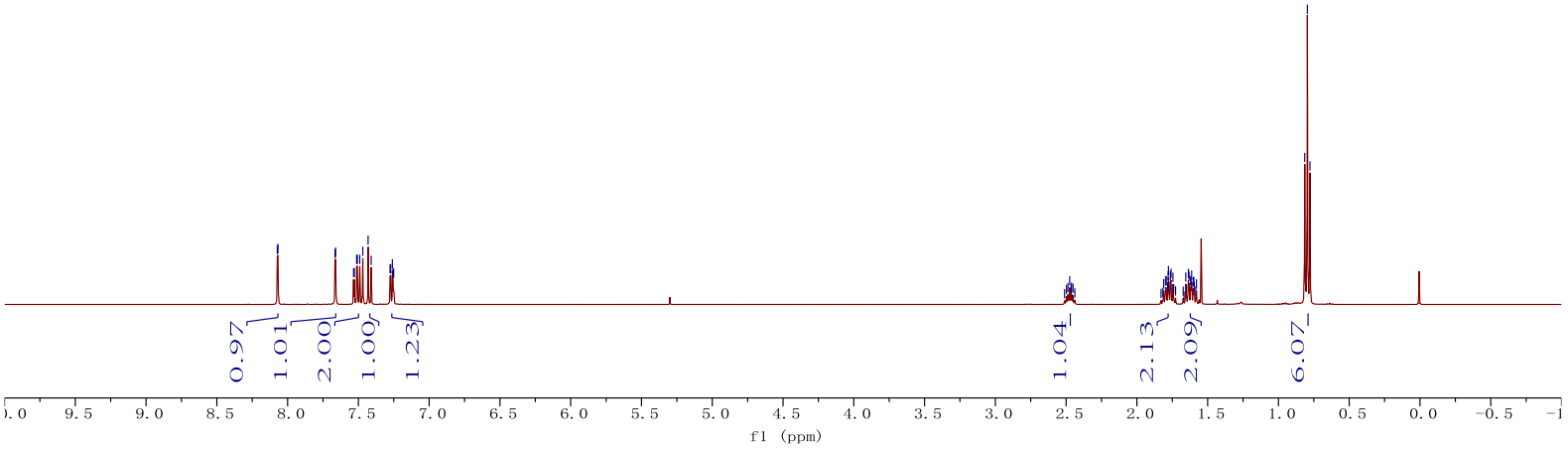




^{1}HNMR (400 MHz, $CDCl_3$)

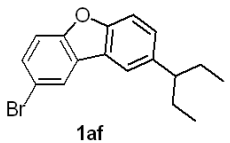


1af

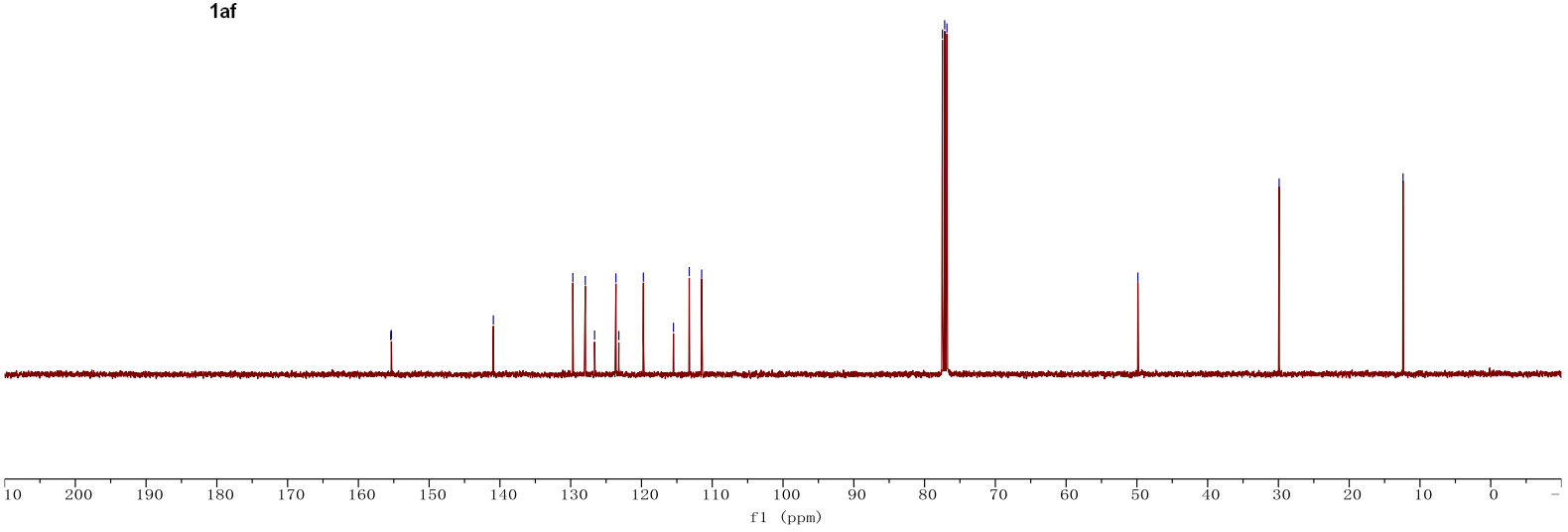


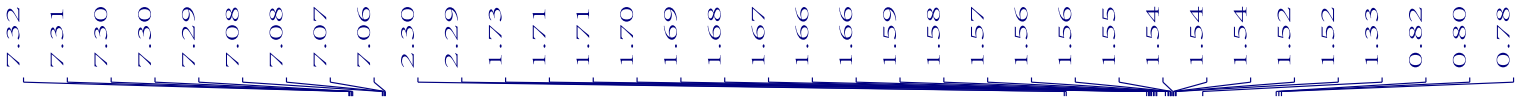
155.4
155.3
140.9
129.7
127.9
126.6
123.6
123.2
119.7
115.5
113.3
111.5
77.5
77.2
76.8
49.9
29.9
12.4

^{13}CNMR (101 MHz, $CDCl_3$)

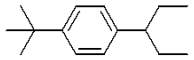


1af

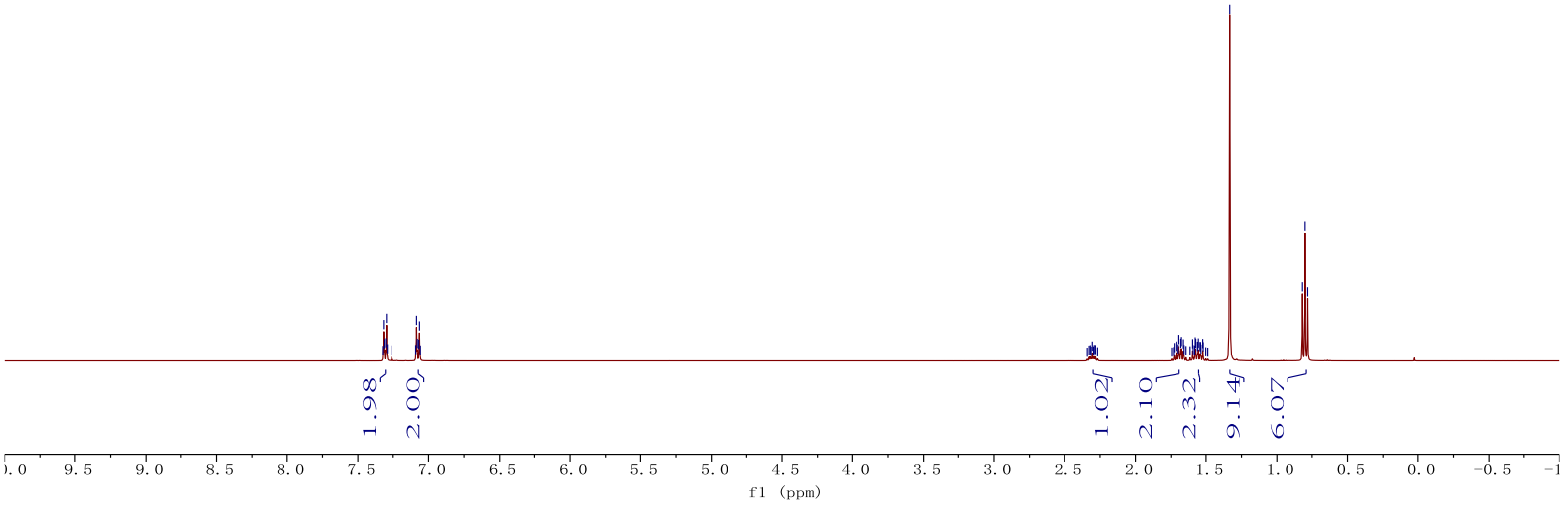




^{1}HNMR (400 MHz, $CDCl_3$)

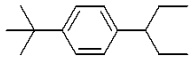


1aj

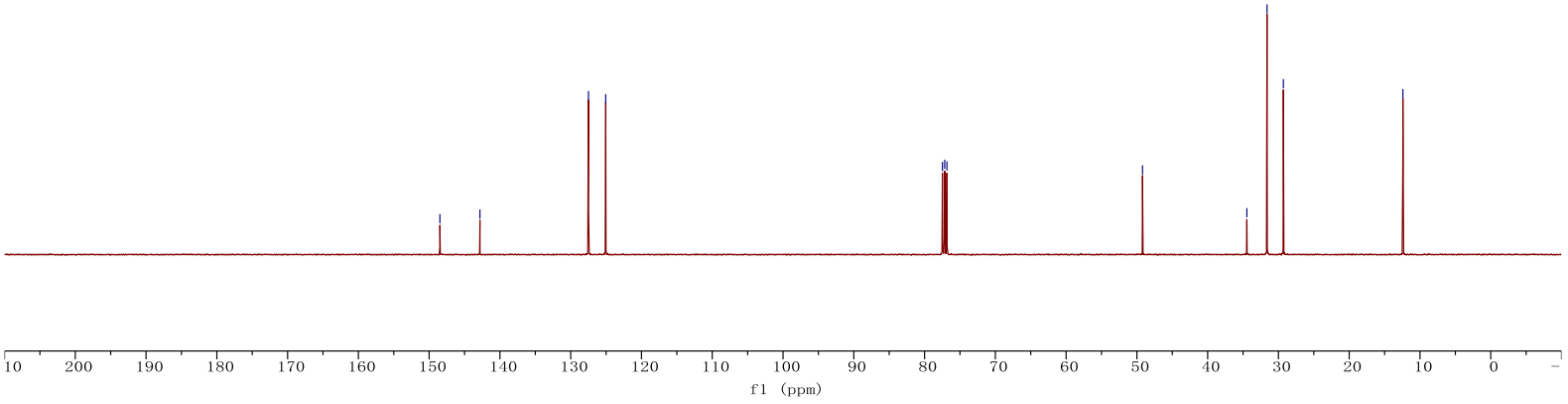


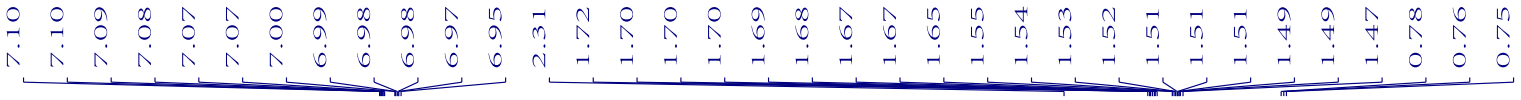
148.5
142.8
127.5
125.1
77.5
77.2
76.8
49.2
34.5
31.6
29.3
12.4

^{13}CNMR (101 MHz, $CDCl_3$)

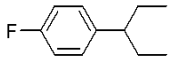


1aj

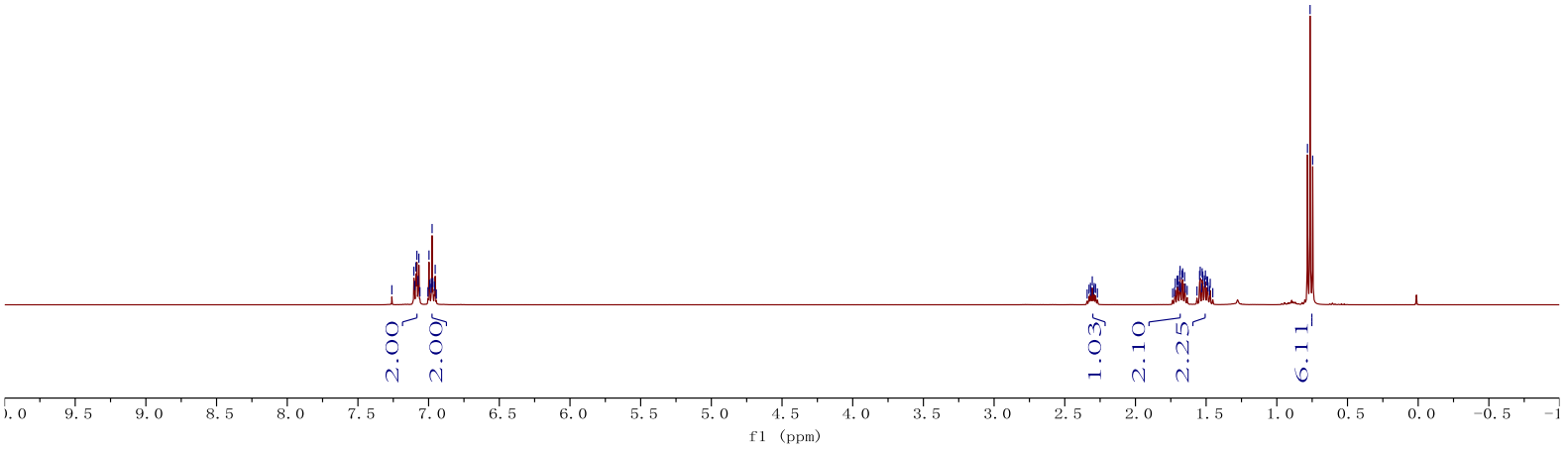


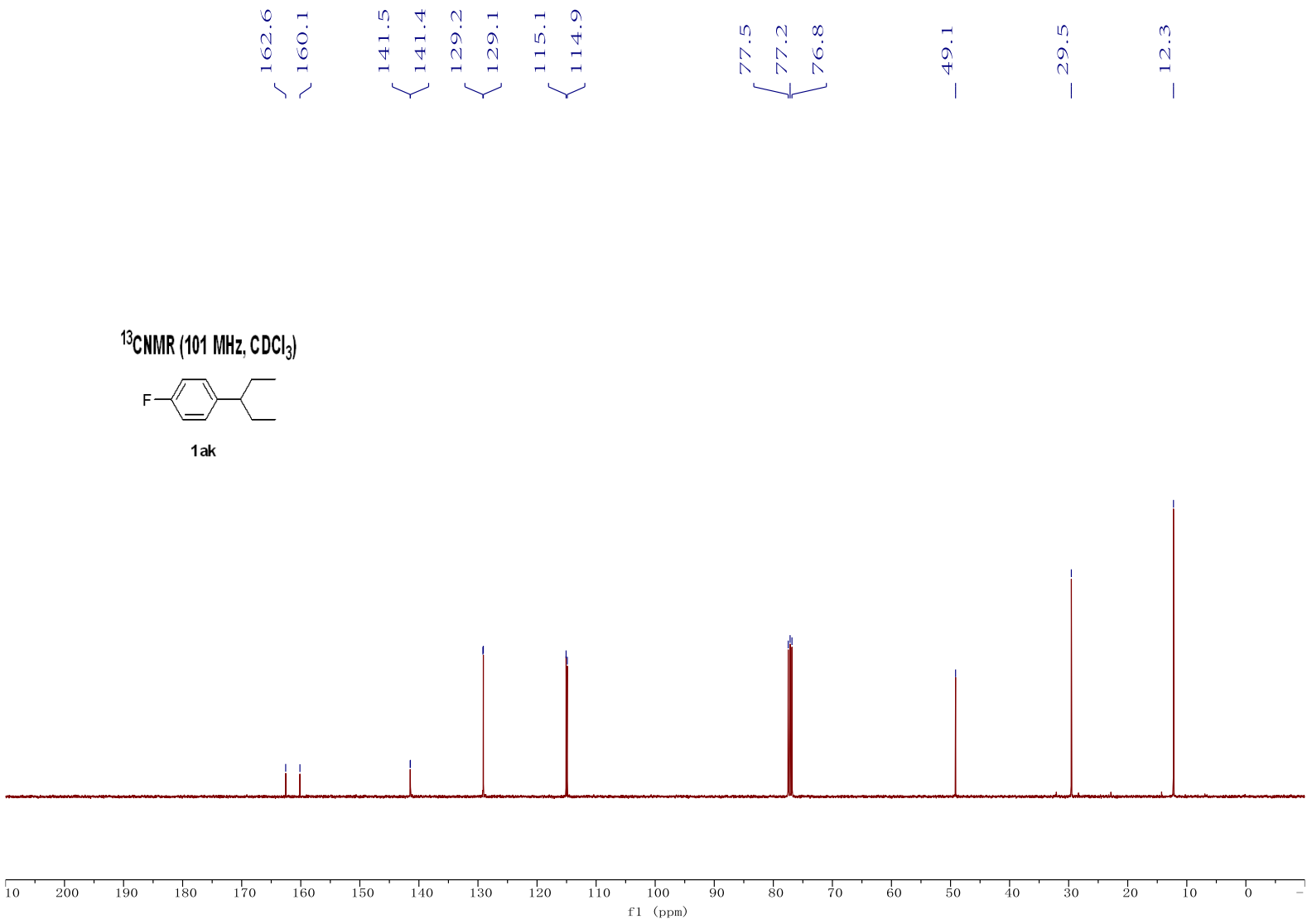


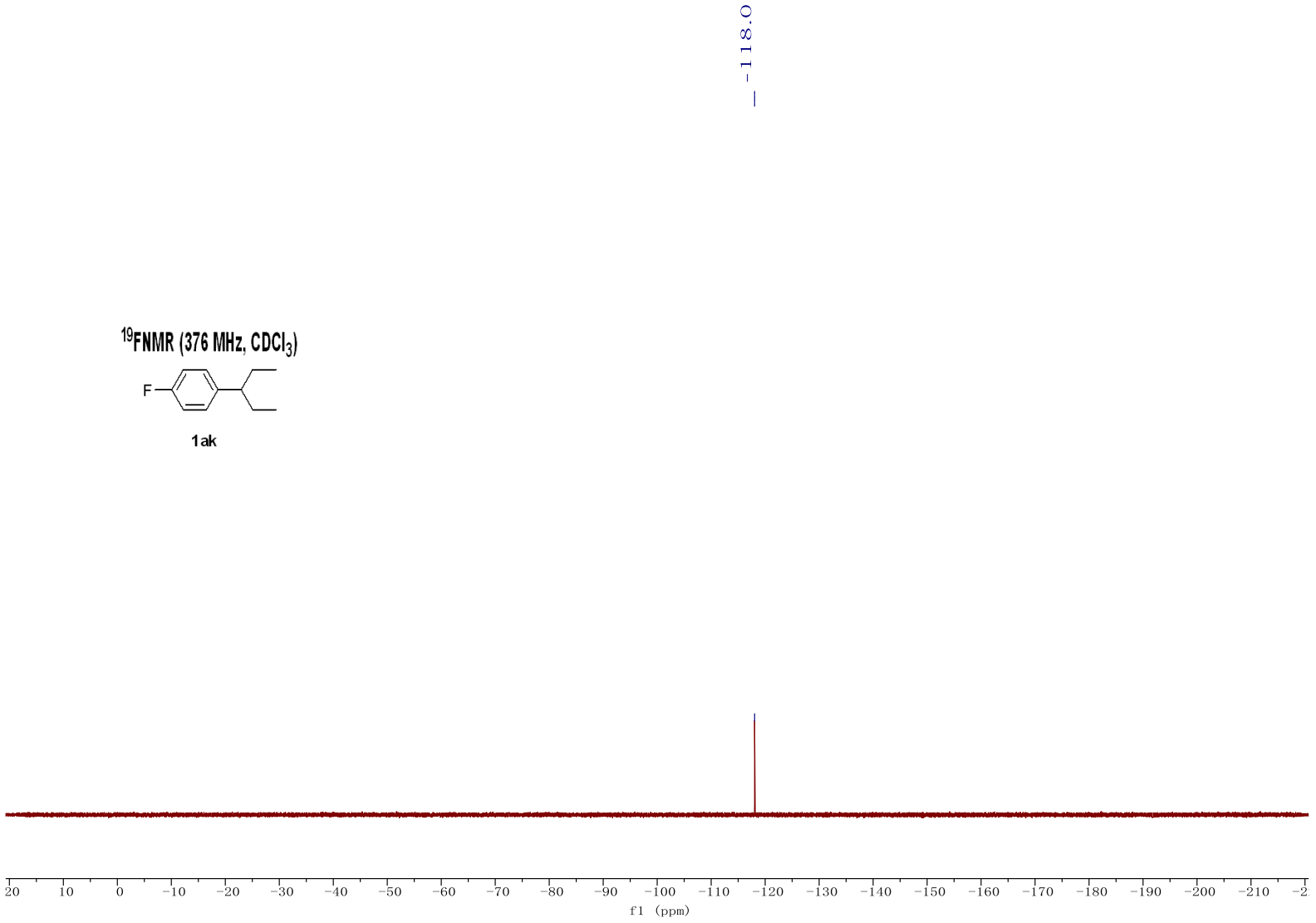
^{1}HNMR (400 MHz, $CDCl_3$)

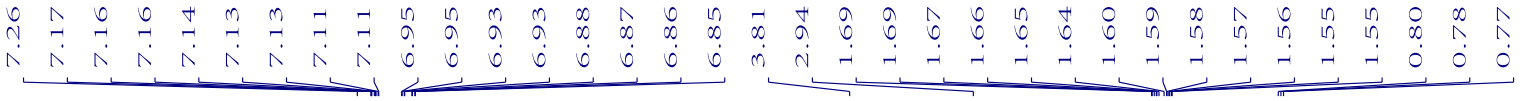


1ak

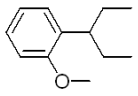



162.6
160.1
141.5
141.4
129.2
129.1
115.1
114.9
77.5
77.2
76.8
49.1
29.5
12.3
13CNMR (101 MHz, CDCl3)
F
1ak
f1 (ppm)

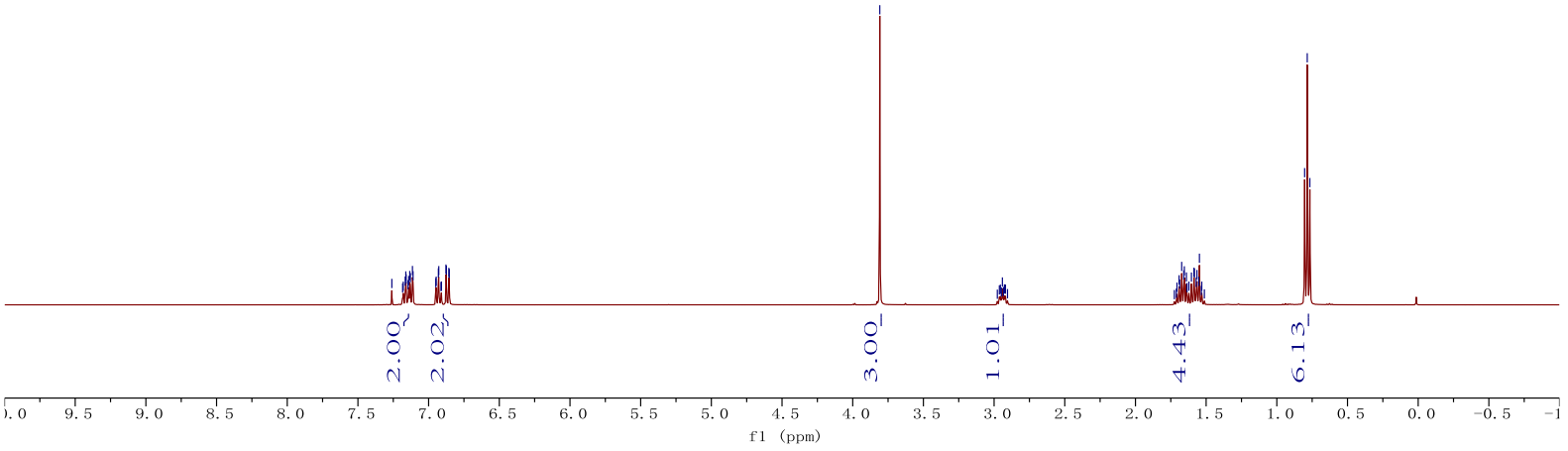

-118.0
19FNMR (376 MHz, CDCl3)
F
1ak
20 10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210 −2
f1 (ppm)

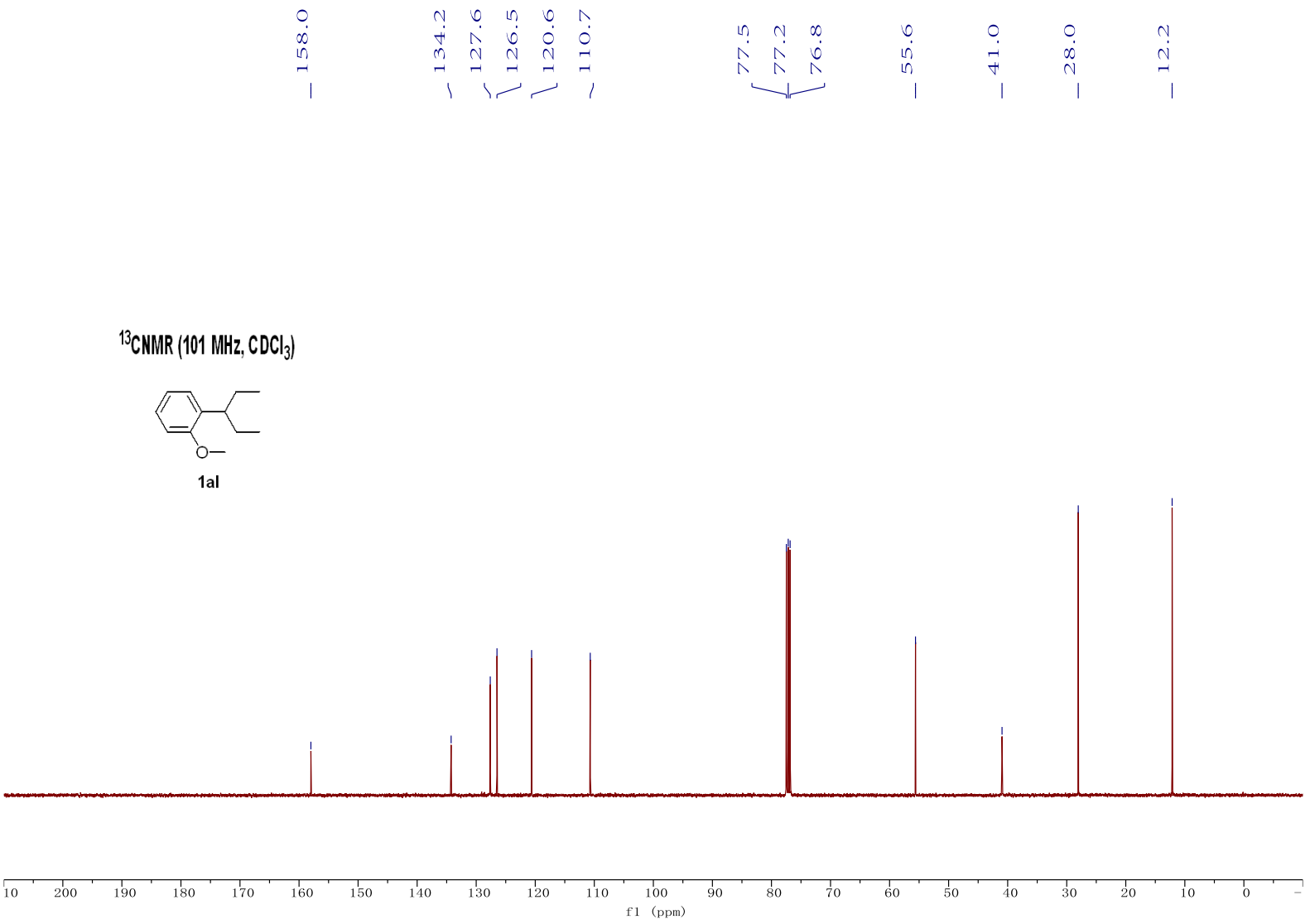


^{1}HNMR (400 MHz, $CDCl_3$)

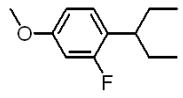


1al

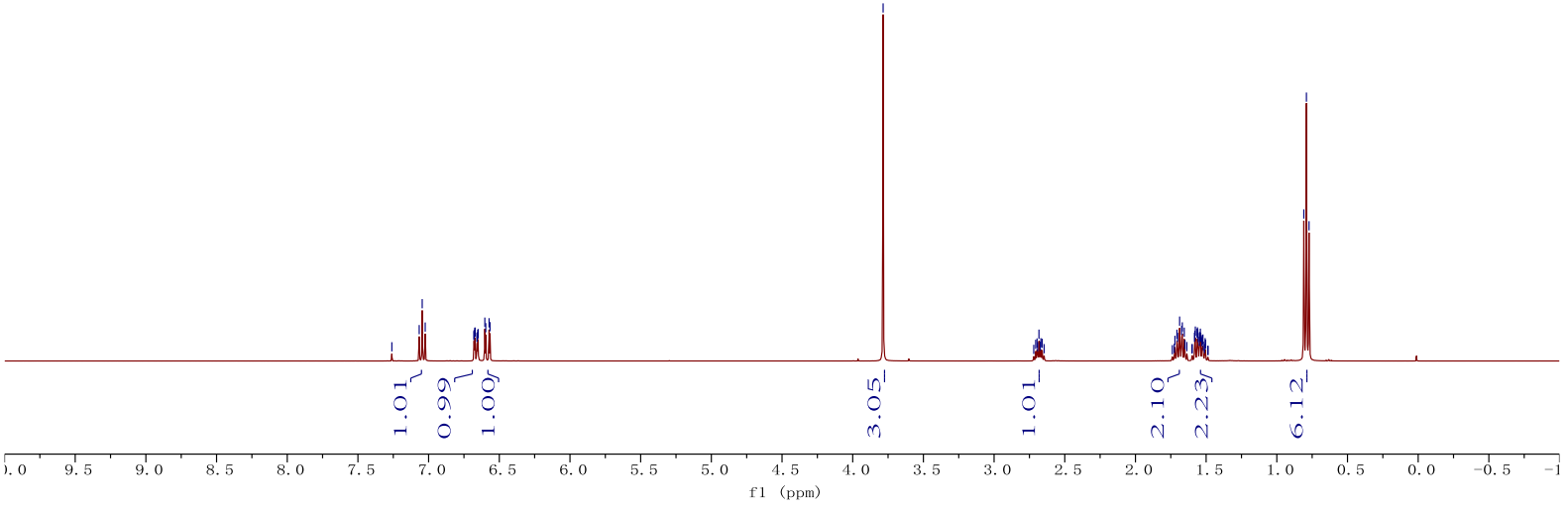


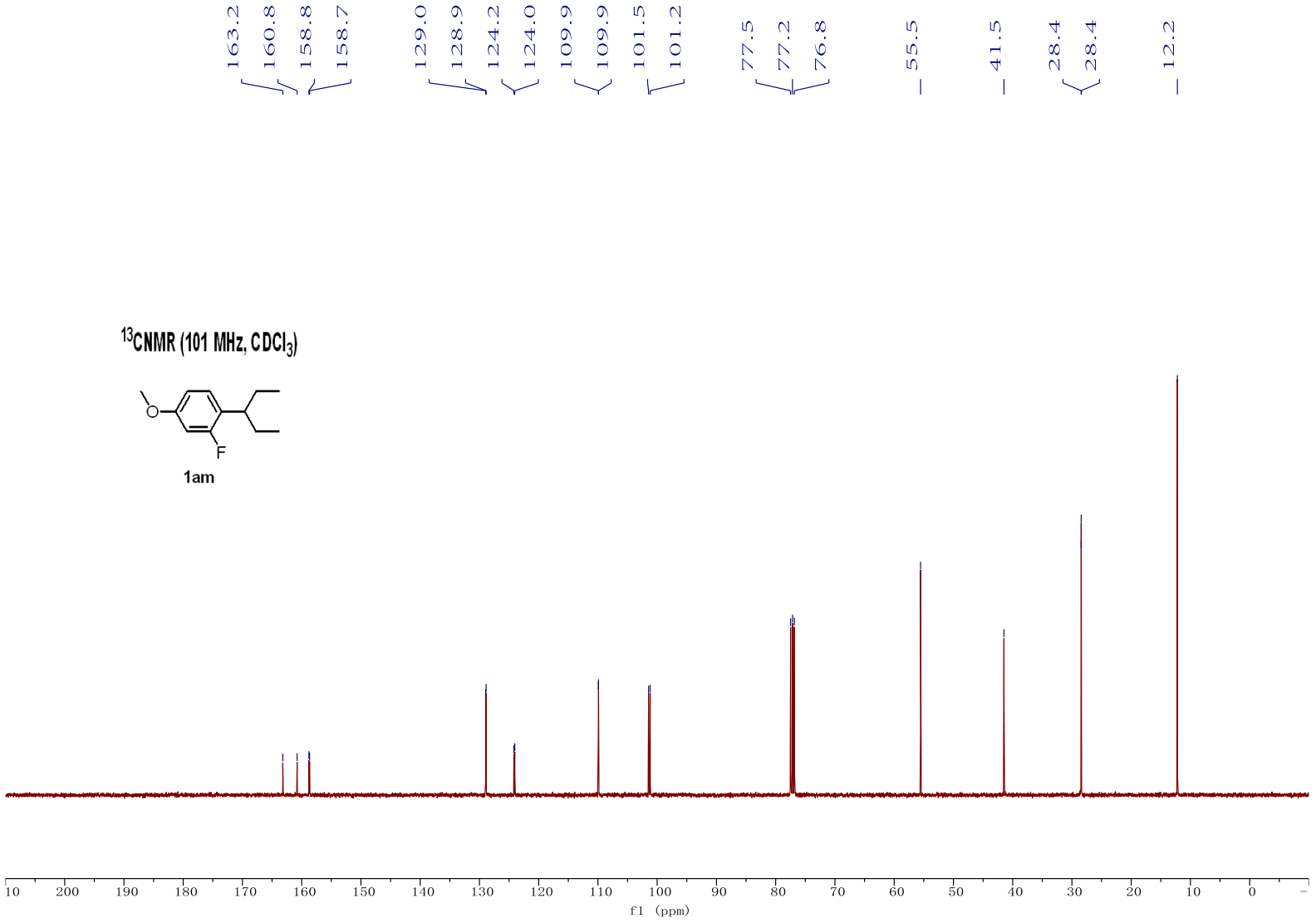

158.0
134.2
127.6
126.5
120.6
110.7
77.5
77.2
76.8
55.6
41.0
28.0
12.2
13CNMR (101 MHz, CDCl3)
1al
f1 (ppm)

^{1}HNMR (400 MHz, $CDCl_3$)

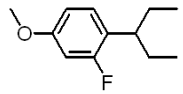


1am



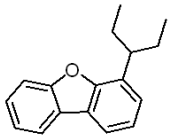

163.2
160.8
158.8
158.7
129.0
128.9
124.2
124.0
109.9
109.9
101.5
101.2
77.5
77.2
76.8
55.5
41.5
28.4
28.4
12.2
13CNMR (101 MHz, CDCl3)
O
F
1am
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

^{19}FNMR (376 MHz, $CDCl_3$)

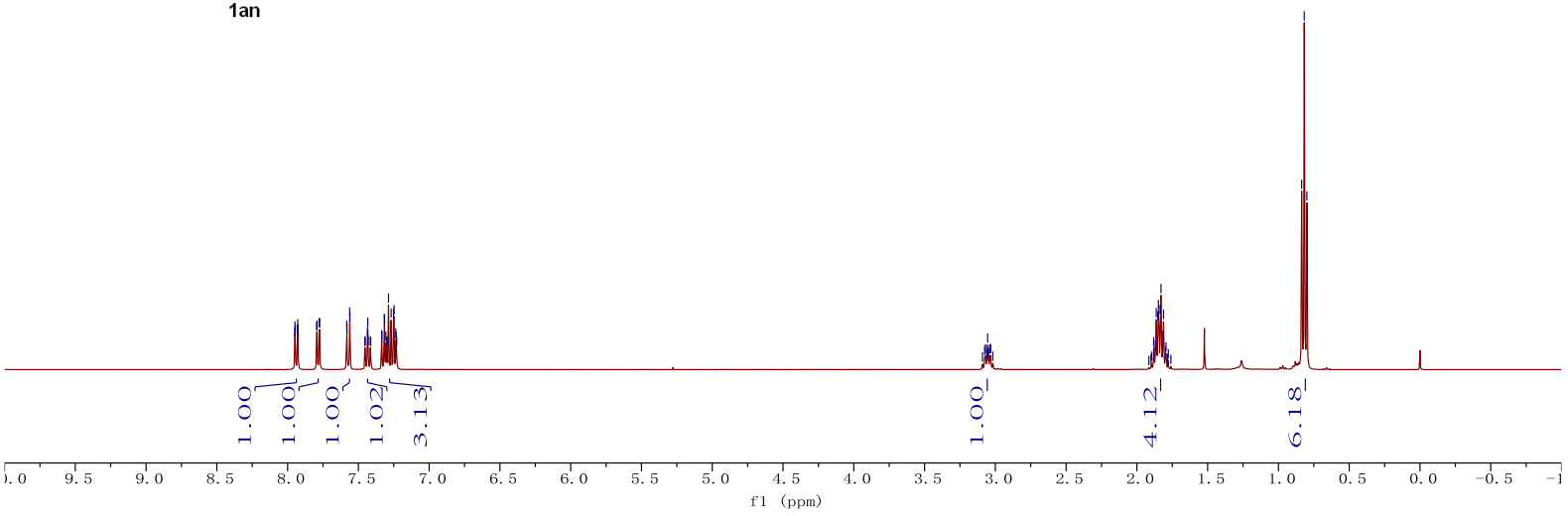


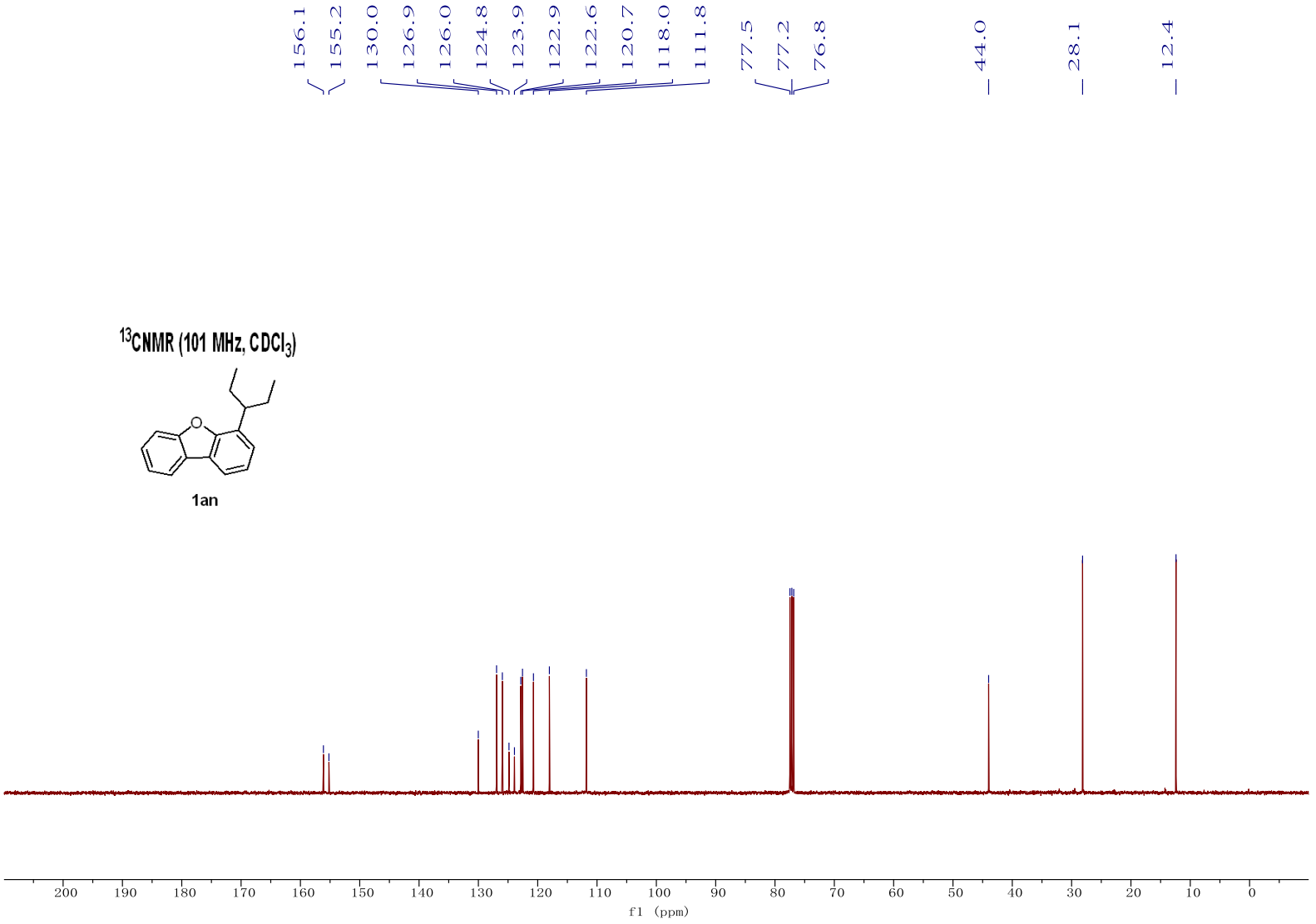
1am

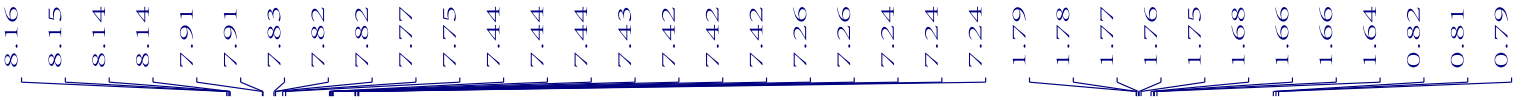
^{1}HNMR (400 MHz, $CDCl_3$)



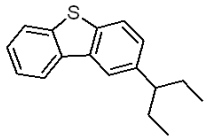
1an



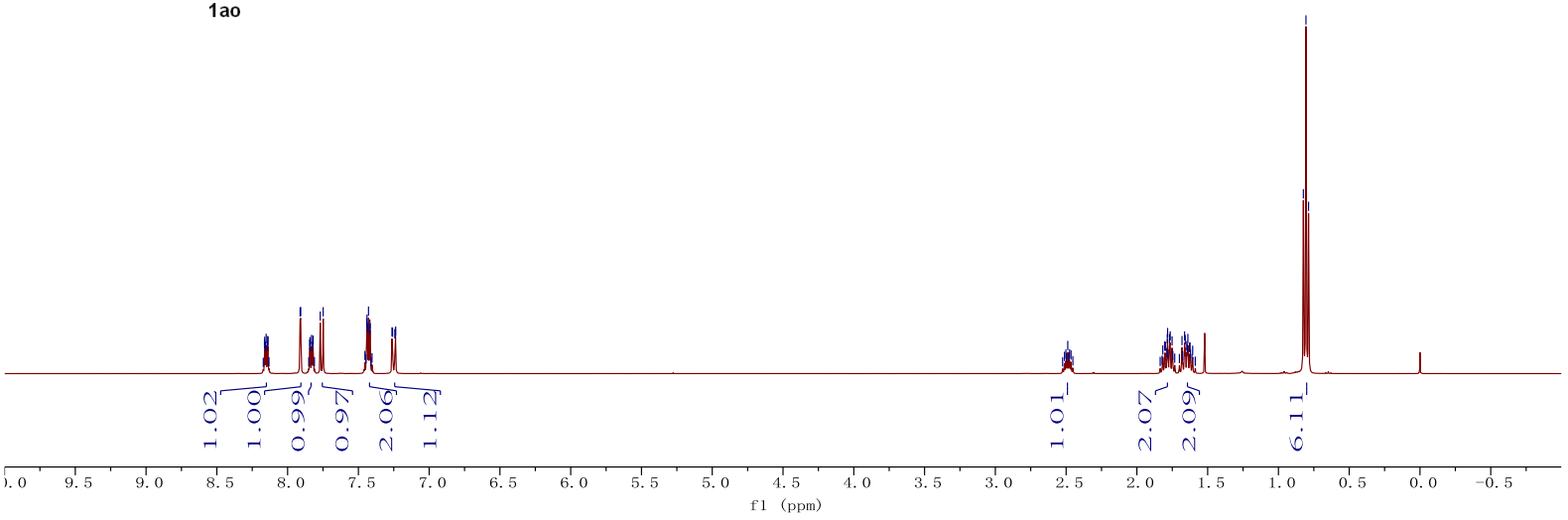

156.1
155.2
130.0
126.9
126.0
124.8
123.9
122.9
122.6
120.7
118.0
111.8
77.5
77.2
76.8
44.0
28.1
12.4
13CNMR (101 MHz, CDCl3)
1an
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



^{1}HNMR (400 MHz, $CDCl_3$)

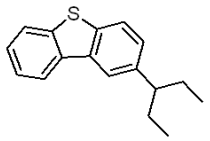


1ao

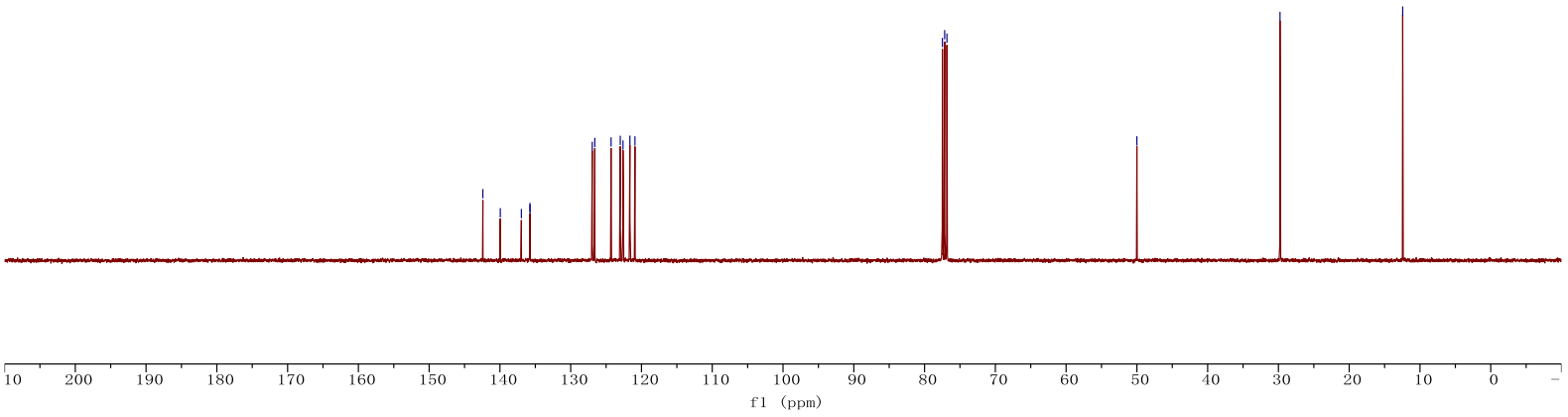


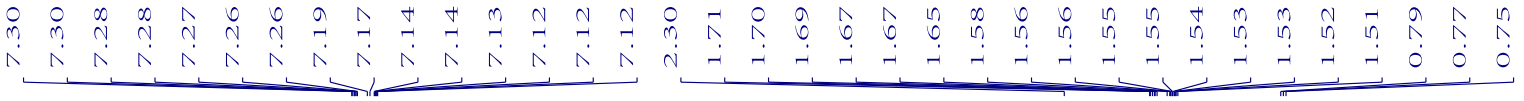
142.4
139.9
137.0
135.8
135.7
127.0
126.6
124.3
123.0
122.6
121.6
120.9
77.5
77.2
76.8
50.0
29.8
12.4

^{13}CNMR (101 MHz, $CDCl_3$)

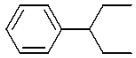


1ao

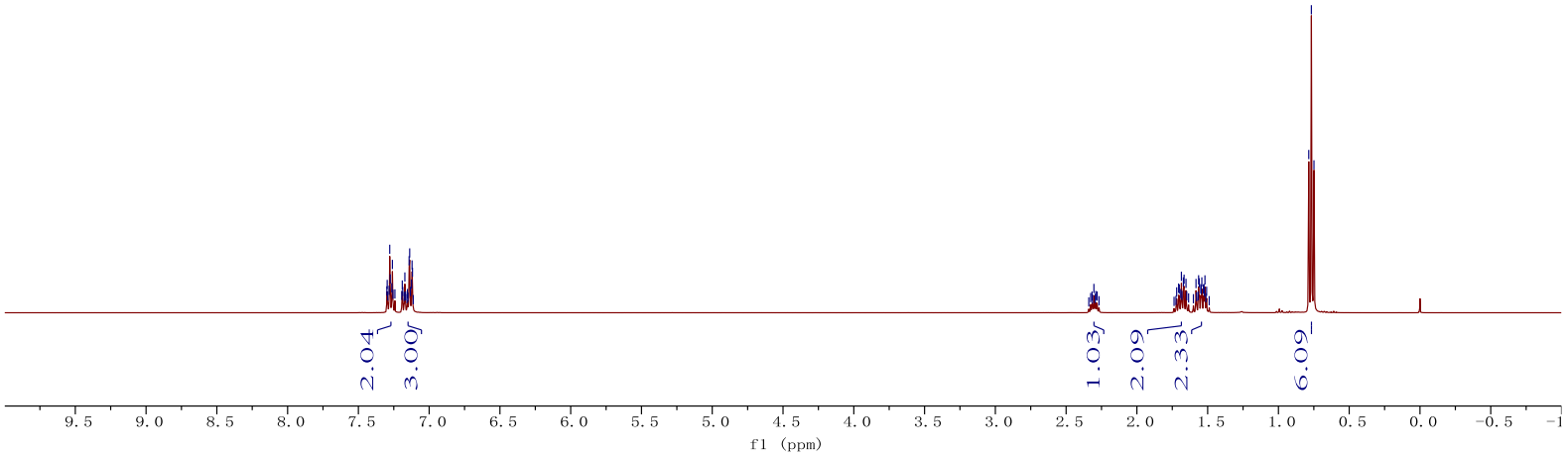


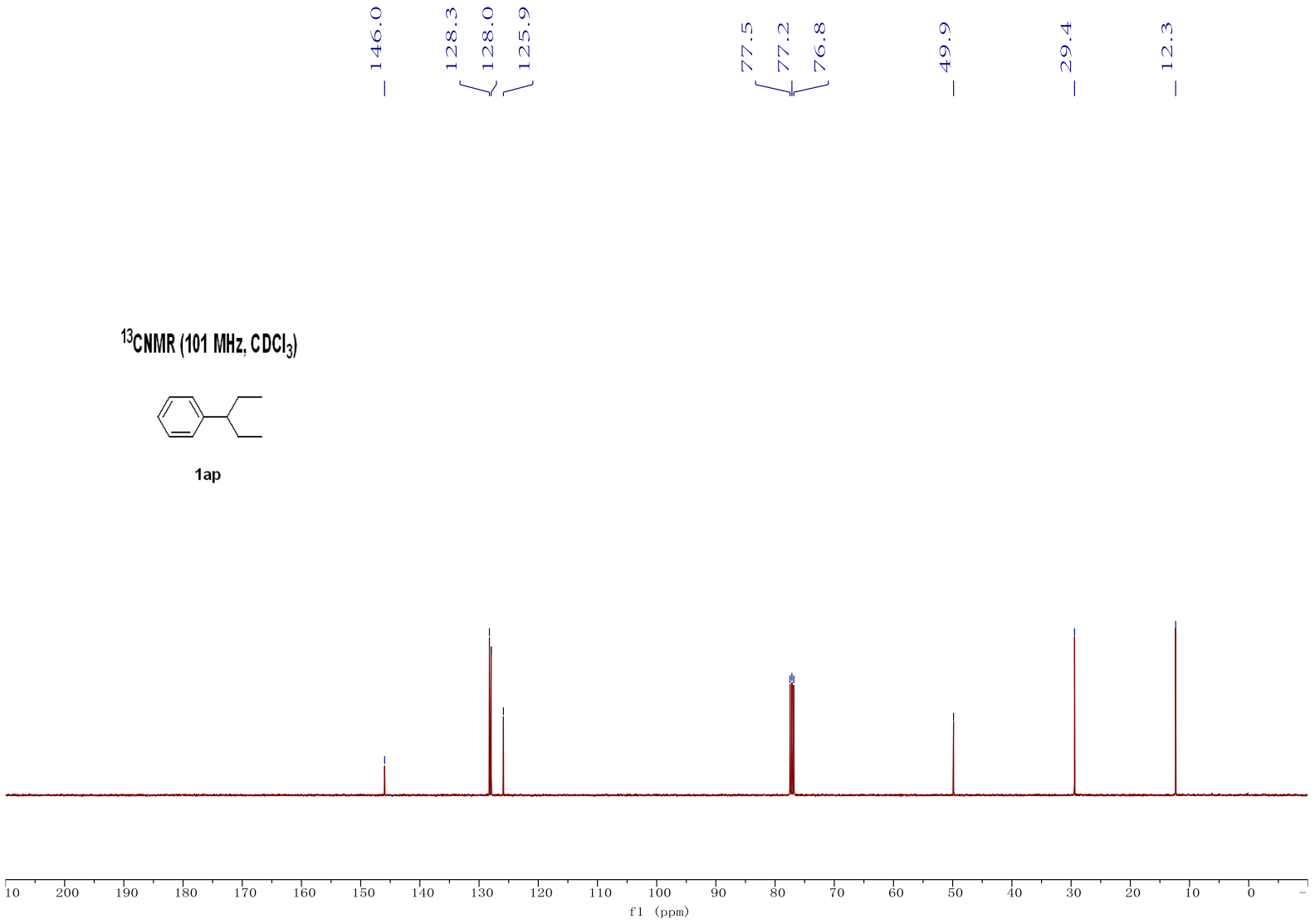


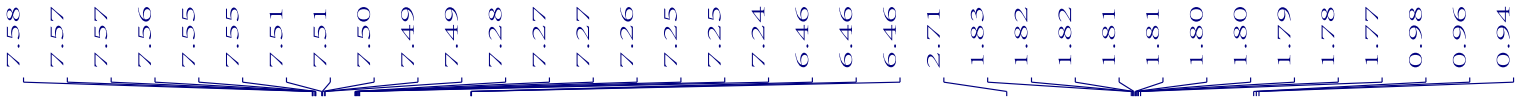
^{1}HNMR (400 MHz, $CDCl_3$)



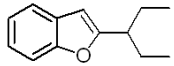
1ap



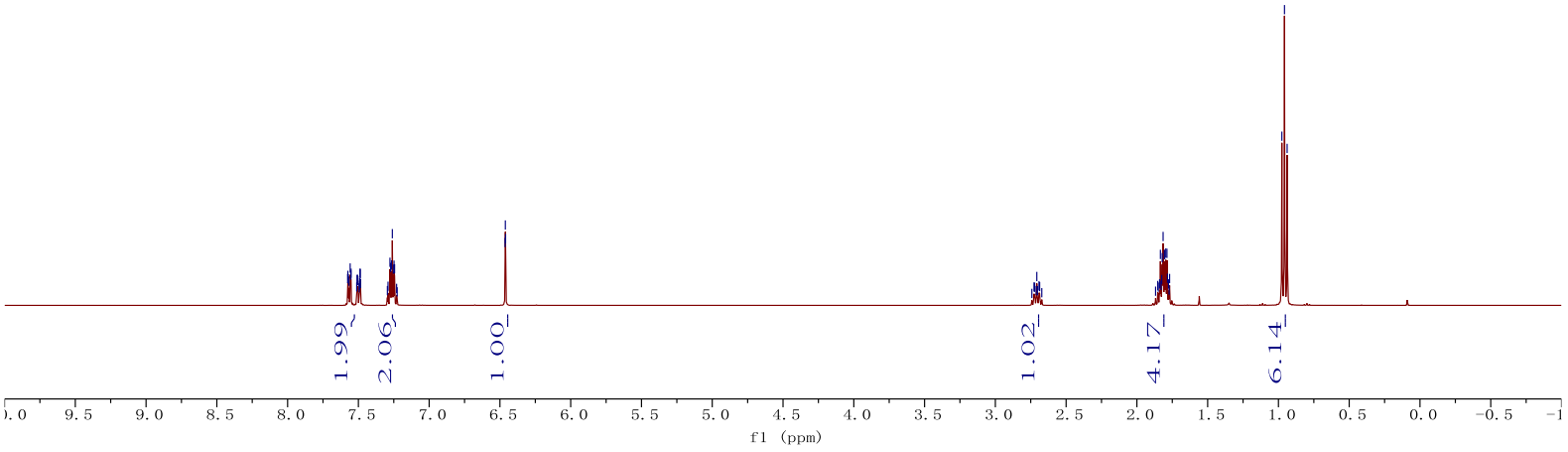

146.0
128.3
128.0
125.9
77.5
77.2
76.8
49.9
29.4
12.3
13CNMR (101 MHz, CDCl3)
1ap
f1 (ppm)

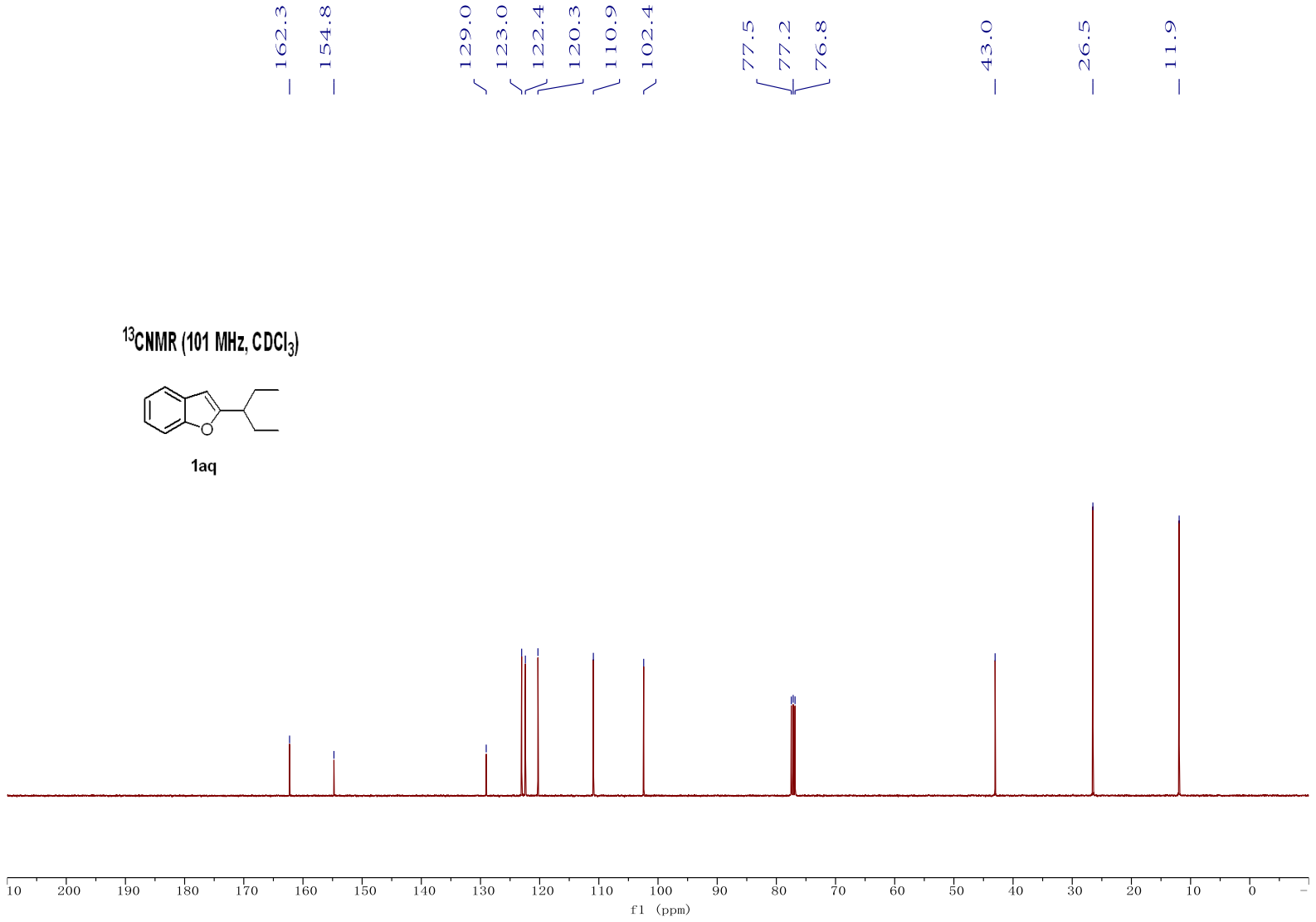


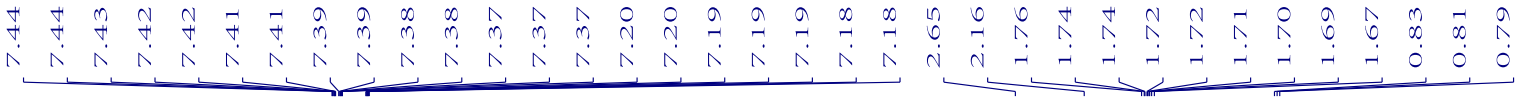
^{1}HNMR (400 MHz, $CDCl_3$)



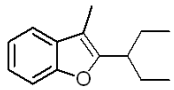
1aq



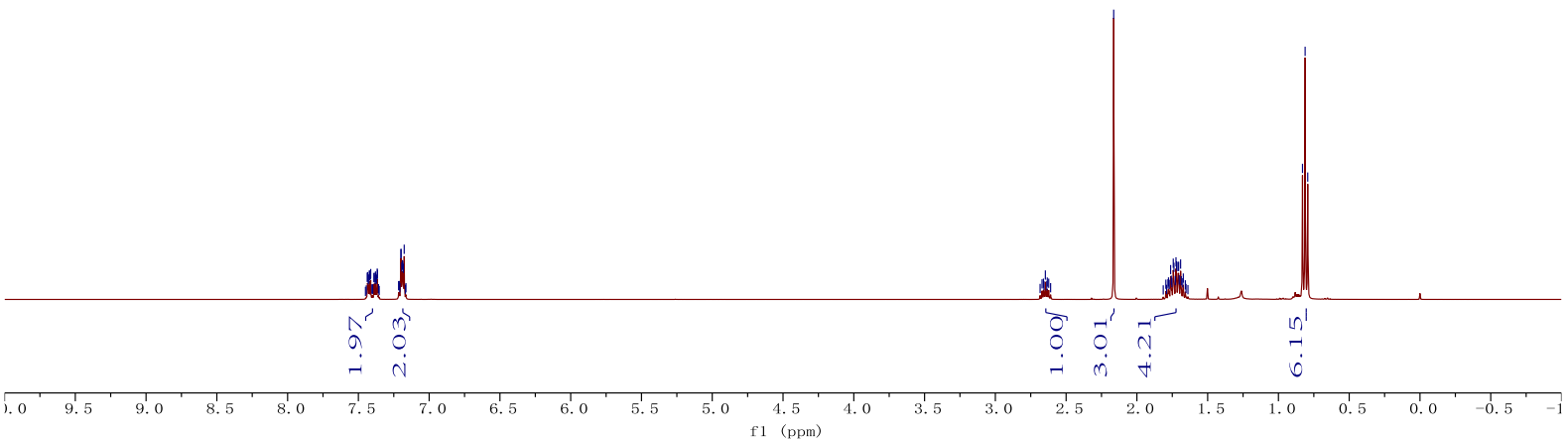

162.3
154.8
129.0
123.0
122.4
120.3
110.9
102.4
77.5
77.2
76.8
43.0
26.5
11.9
13CNMR (101 MHz, CDCl3)
1aq
f1 (ppm)



^{1}HNMR (400 MHz, $CDCl_3$)

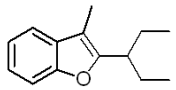


1ar

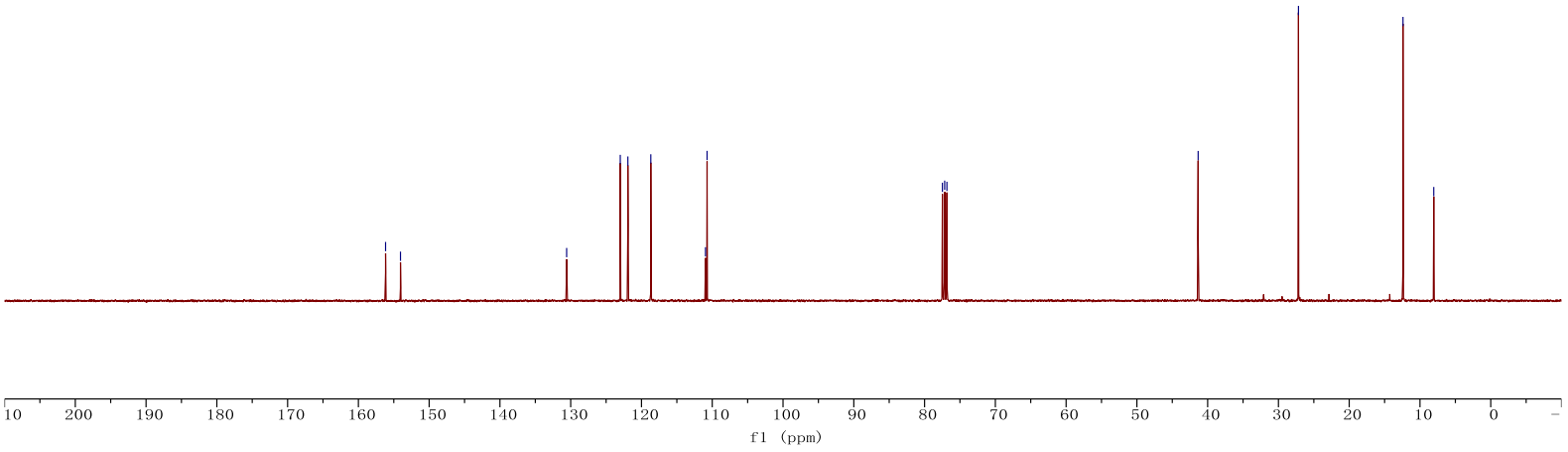


156.2
154.1
130.6
123.0
121.9
118.7
111.0
110.7
77.5
77.2
76.8
41.3
27.2
12.4
8.1

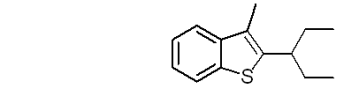
^{13}CNMR (101 MHz, $CDCl_3$)



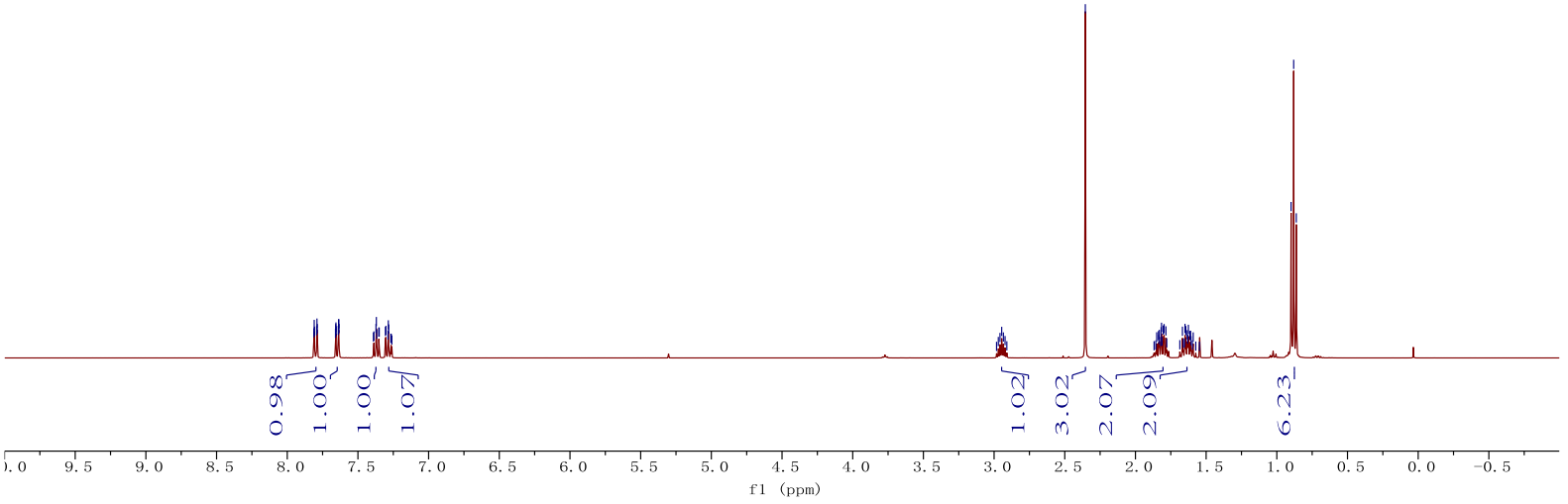
1ar



^{1}HNMR (400 MHz, $CDCl_3$)

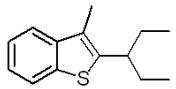


1as

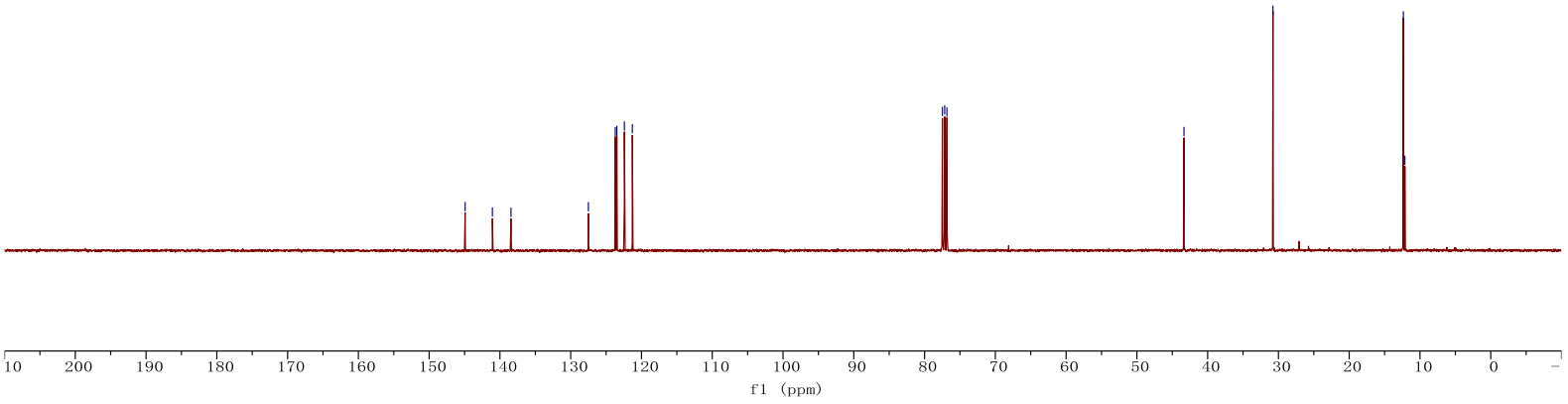


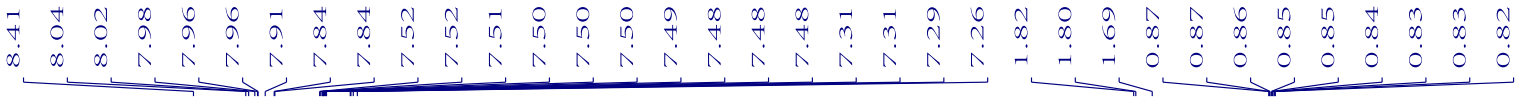
144.9
141.1
138.4
127.5
123.7
123.5
122.4
121.3
77.5
77.2
76.8
43.3
30.8
12.3
12.1

^{13}CNMR (101 MHz, $CDCl_3$)

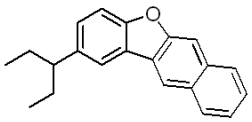


1as

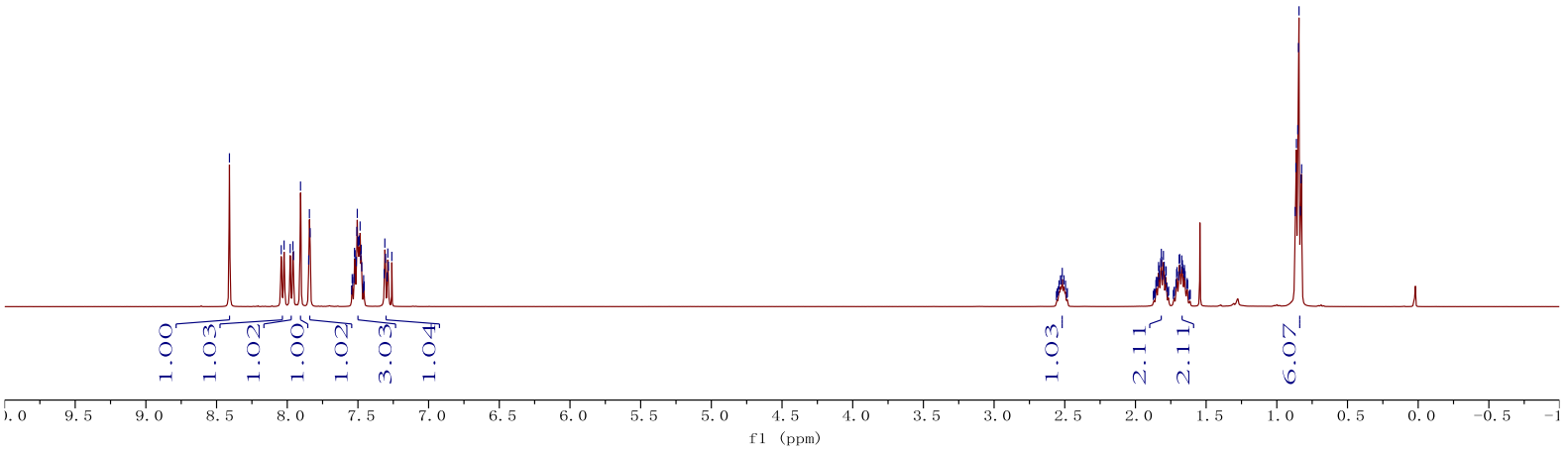




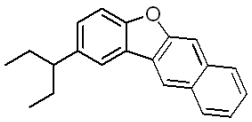
^{1}HNMR (400 MHz, $CDCl_3$)



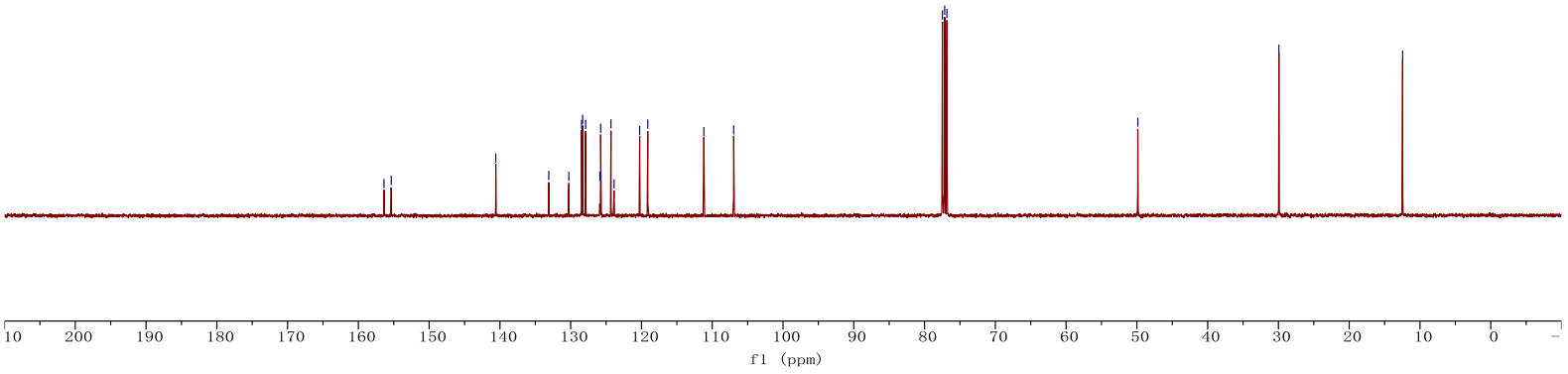
1at

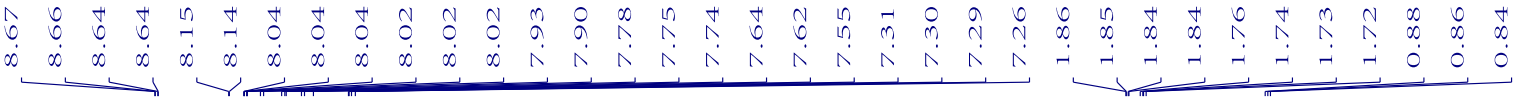


^{13}CNMR (101 MHz, $CDCl_3$)

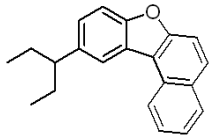


1at

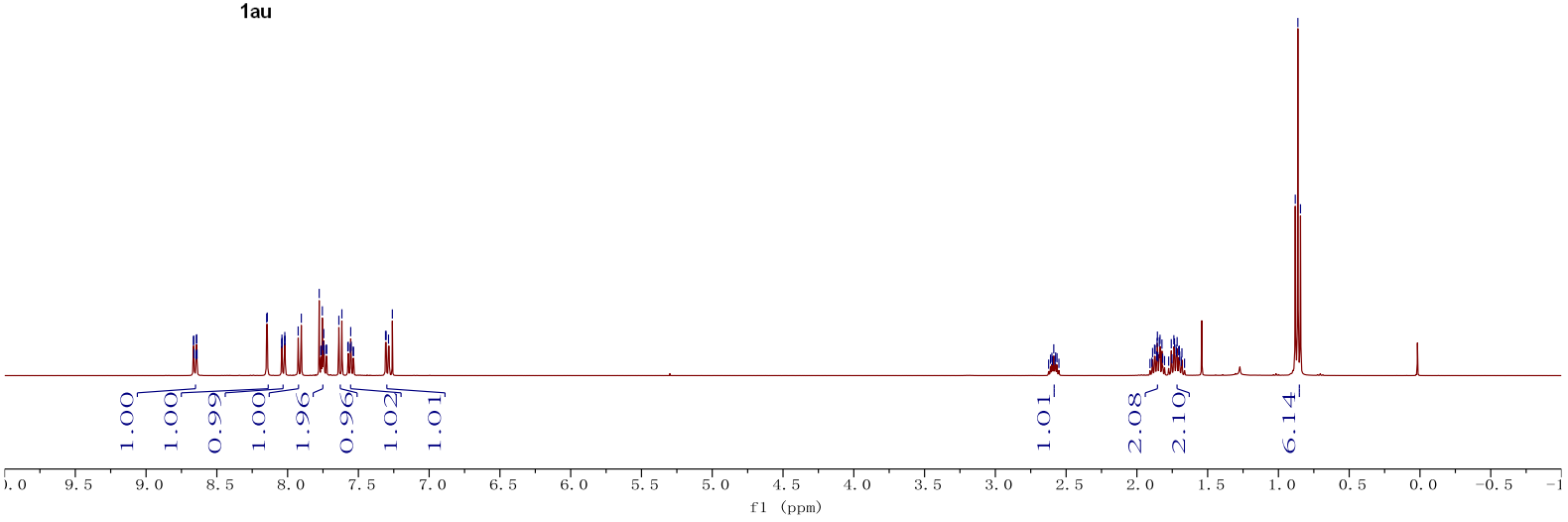




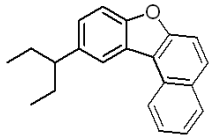
^{1}HNMR (400 MHz, $CDCl_3$)



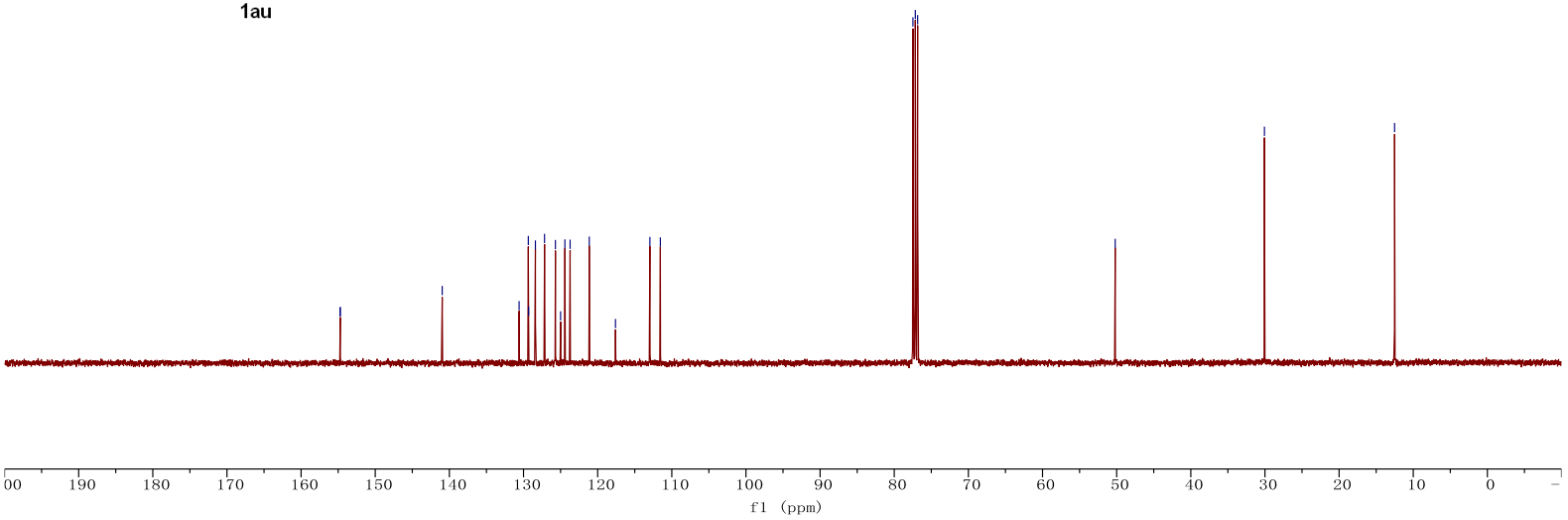
1au

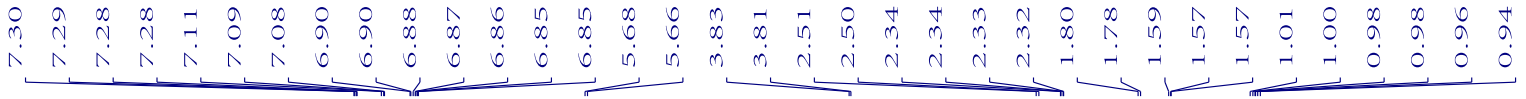


^{13}CNMR (101 MHz, $CDCl_3$)

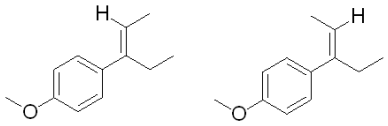


1au



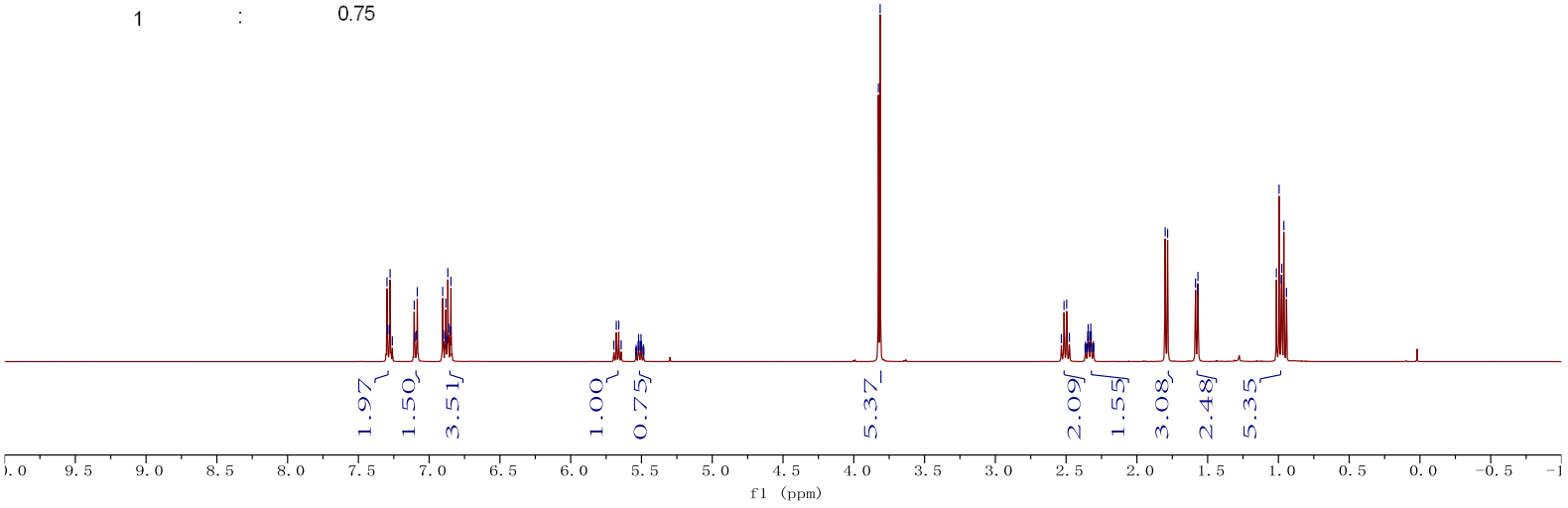


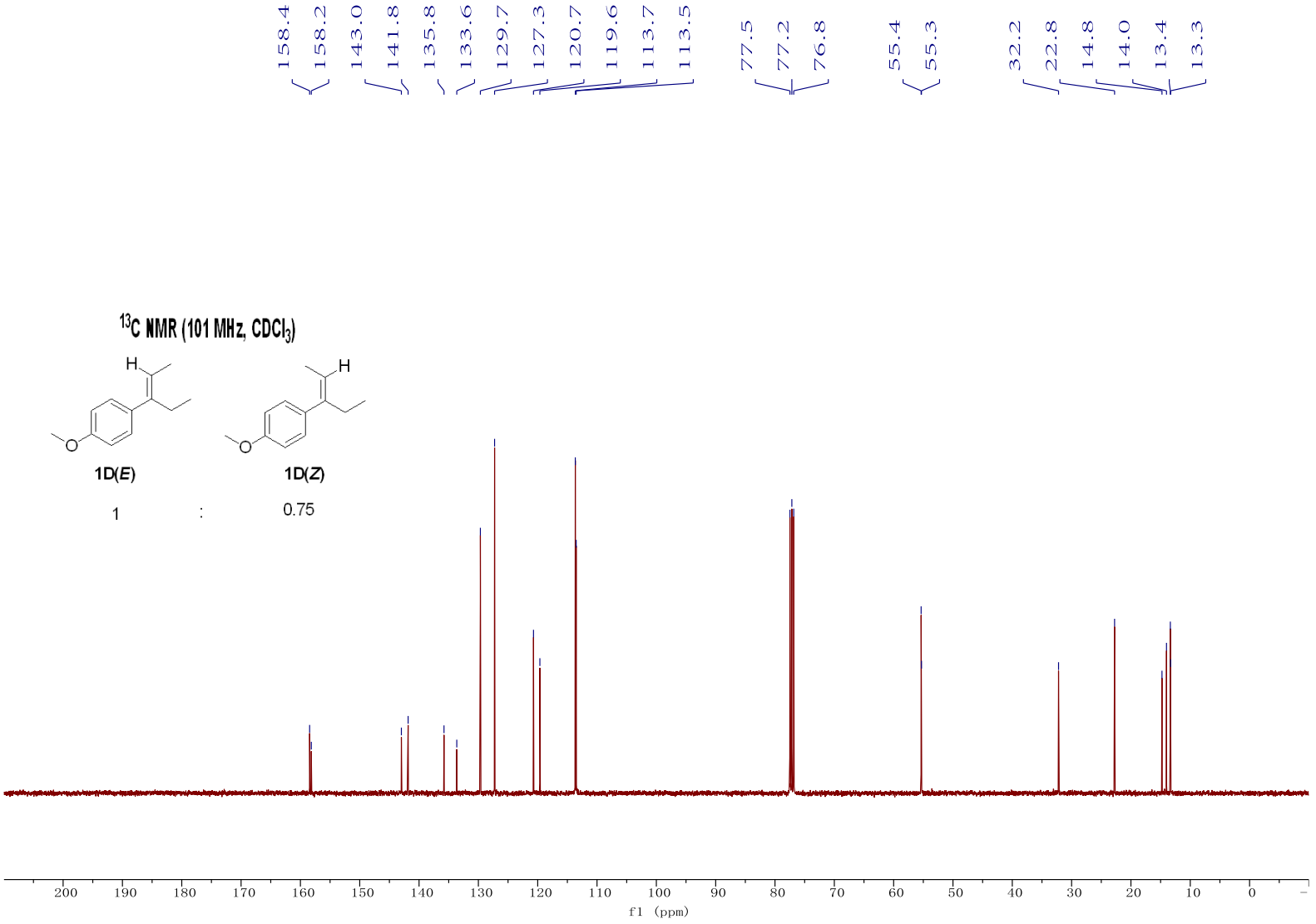
^{1}H NMR (400 MHz, $CDCl_3$)

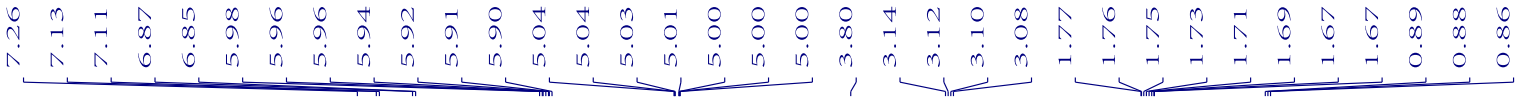


1D(*E*) **1D(*Z*)**

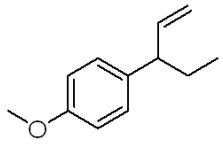
1 : 0.75



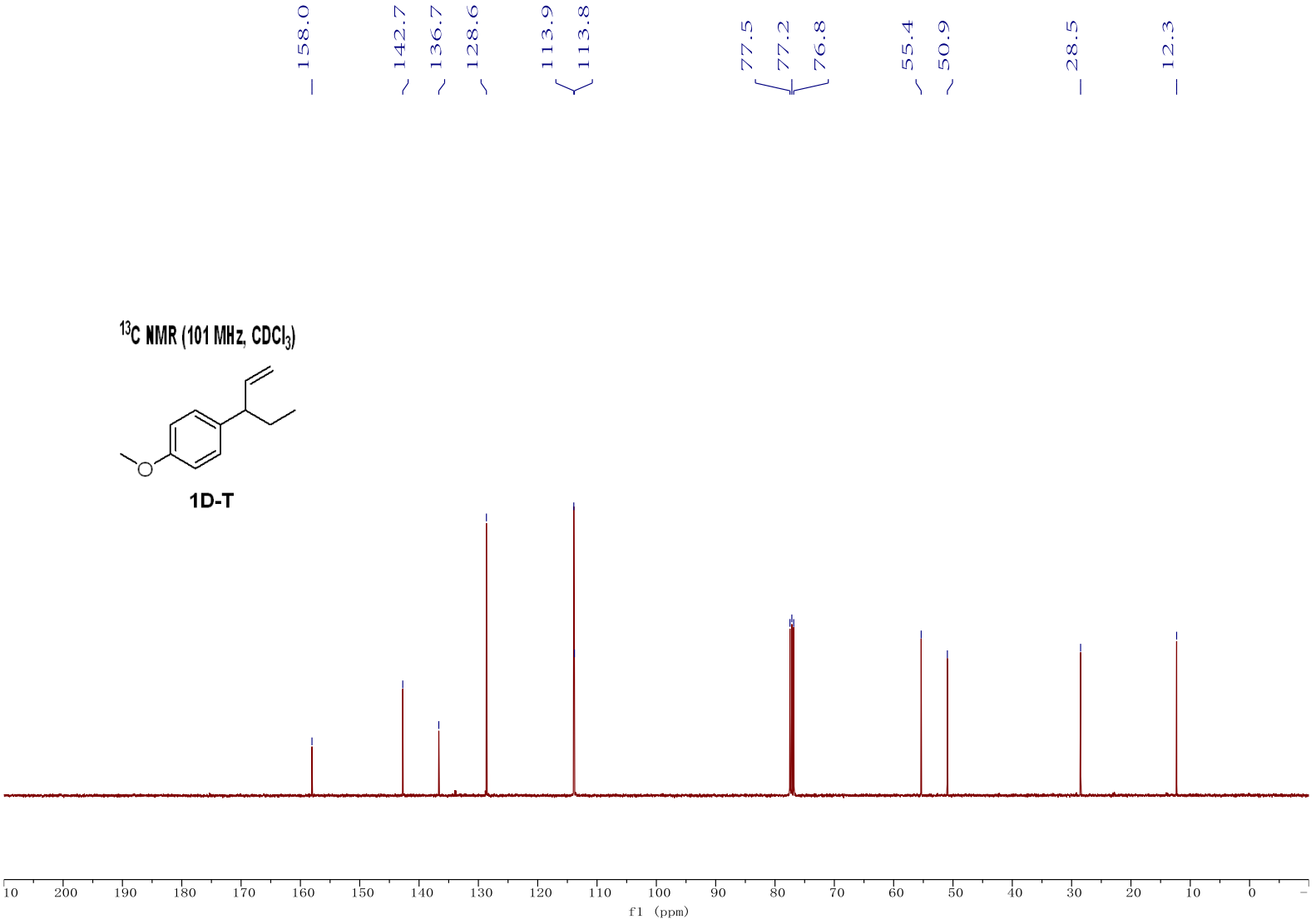

158.4
158.2
143.0
141.8
135.8
133.6
129.7
127.3
120.7
119.6
113.7
113.5
77.5
77.2
76.8
55.4
55.3
32.2
22.8
14.8
14.0
13.4
13.3
13C NMR (101 MHz, CDCl3)
1D(E)
1D(Z)
1 : 0.75
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



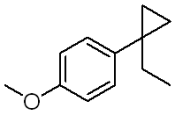
^{1}H NMR (400 MHz, $CDCl_3$)



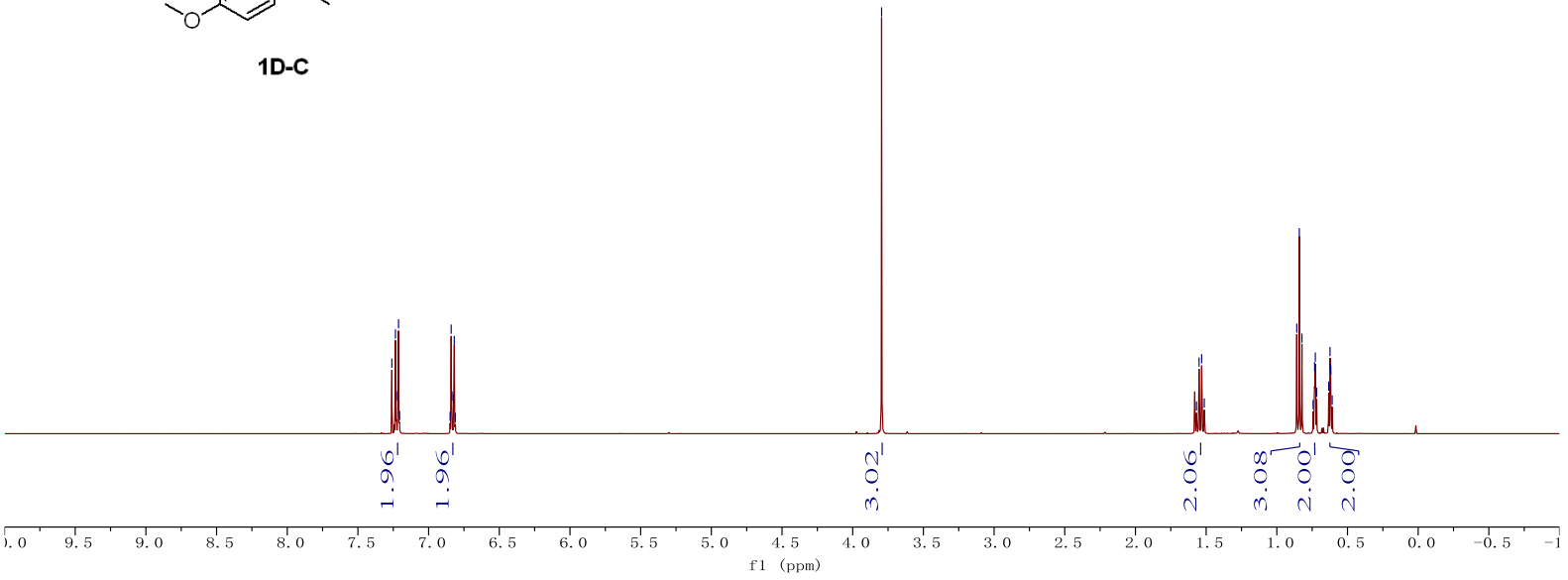
1D-T


158.0
142.7
136.7
128.6
113.9
113.8
77.5
77.2
76.8
55.4
50.9
28.5
12.3
13C NMR (101 MHz, CDCl3)
1D-T
f1 (ppm)

^{1}H NMR (400 MHz, $CDCl_3$)

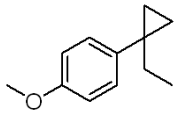


1D-C

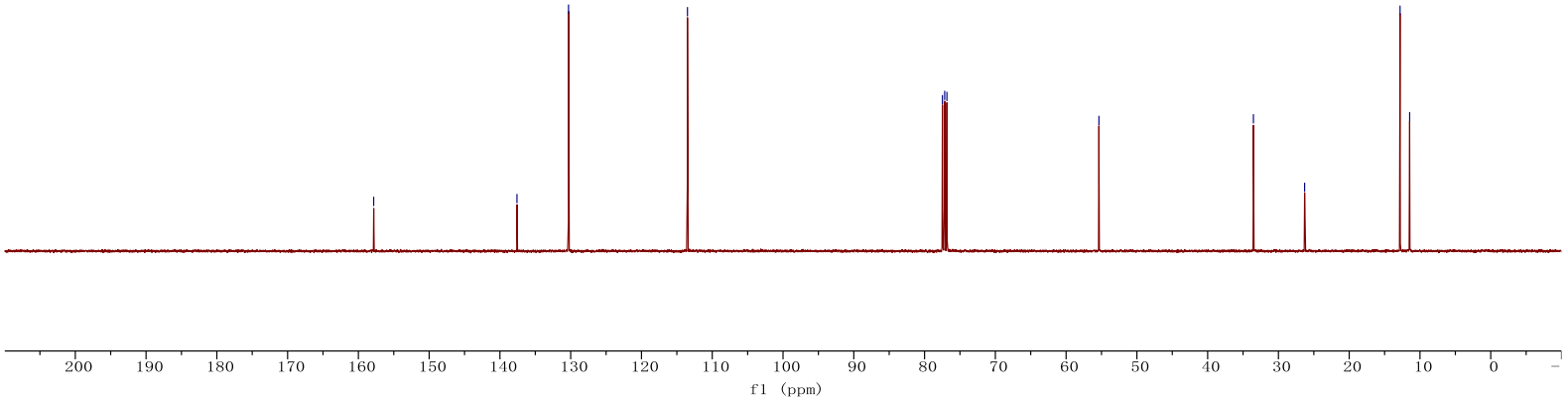


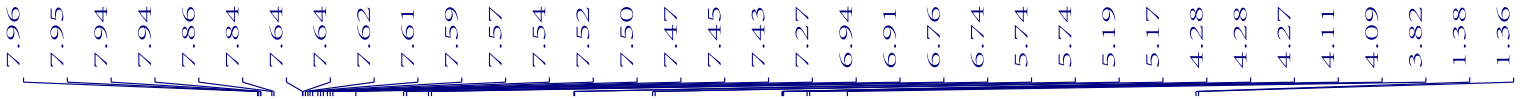
157.8
137.6
130.3
113.5
77.5
77.2
76.8
55.4
33.5
26.3
12.8
11.5

^{13}C NMR (101 MHz, $CDCl_3$)

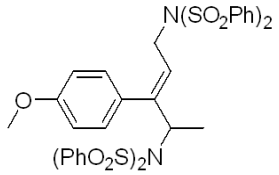


1D-C





^{1}H NMR (400 MHz, $CDCl_3$)



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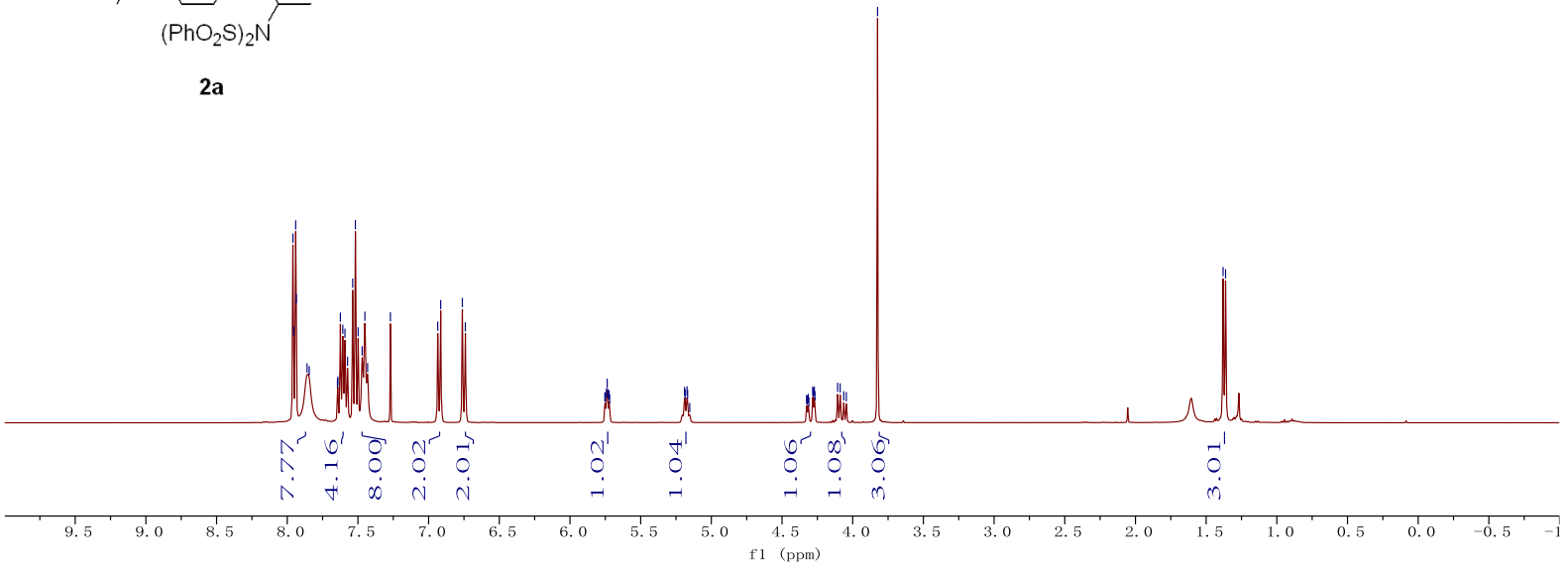

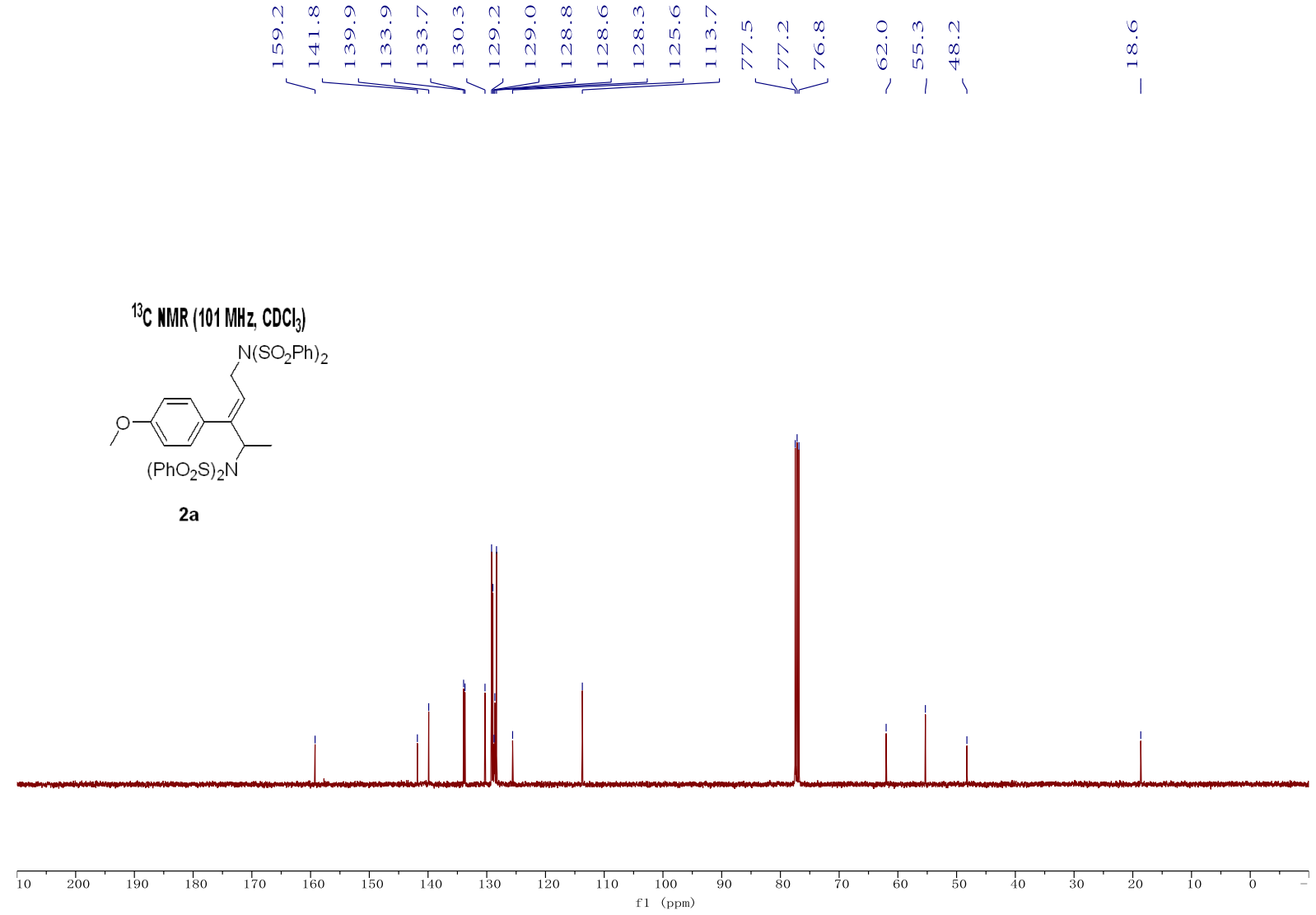
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133.9
133.7
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129.0
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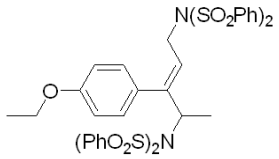
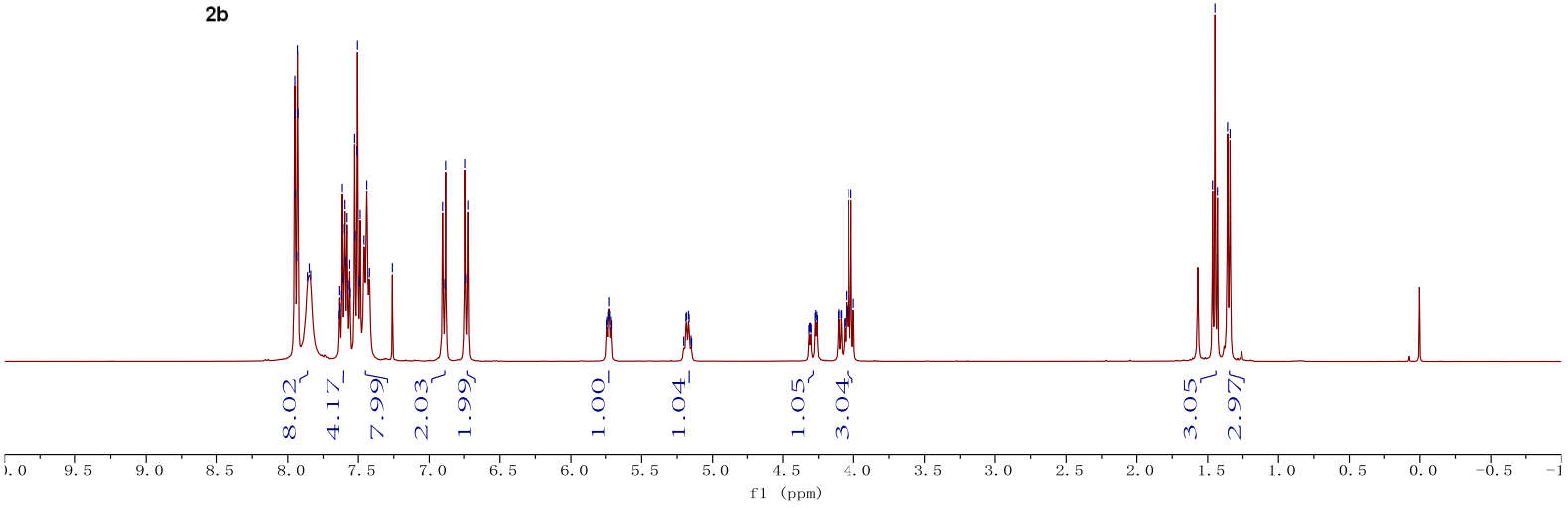
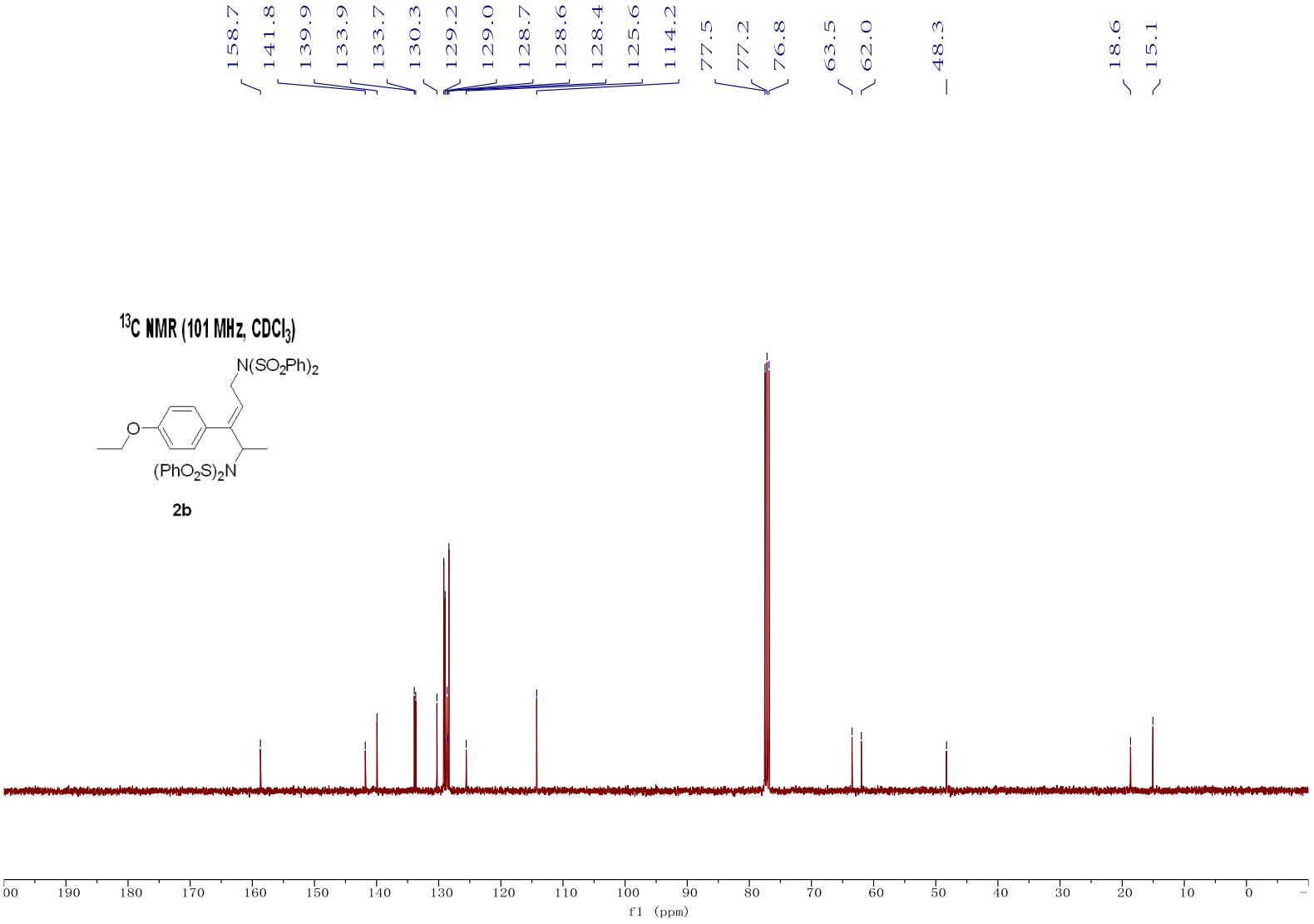
128.6
128.3
125.6
113.7
77.5
77.2
76.8
62.0
55.3
48.2
18.6
13C NMR (101 MHz, CDCl3)
N(SO2Ph)2
O
(PhO2S)2N
2a
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

^{1}H NMR (400 MHz, $CDCl_3$)



2b

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133.9
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129.0
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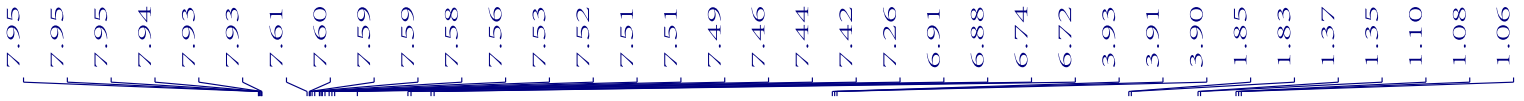
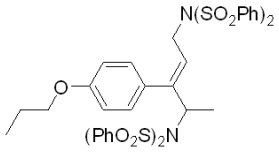
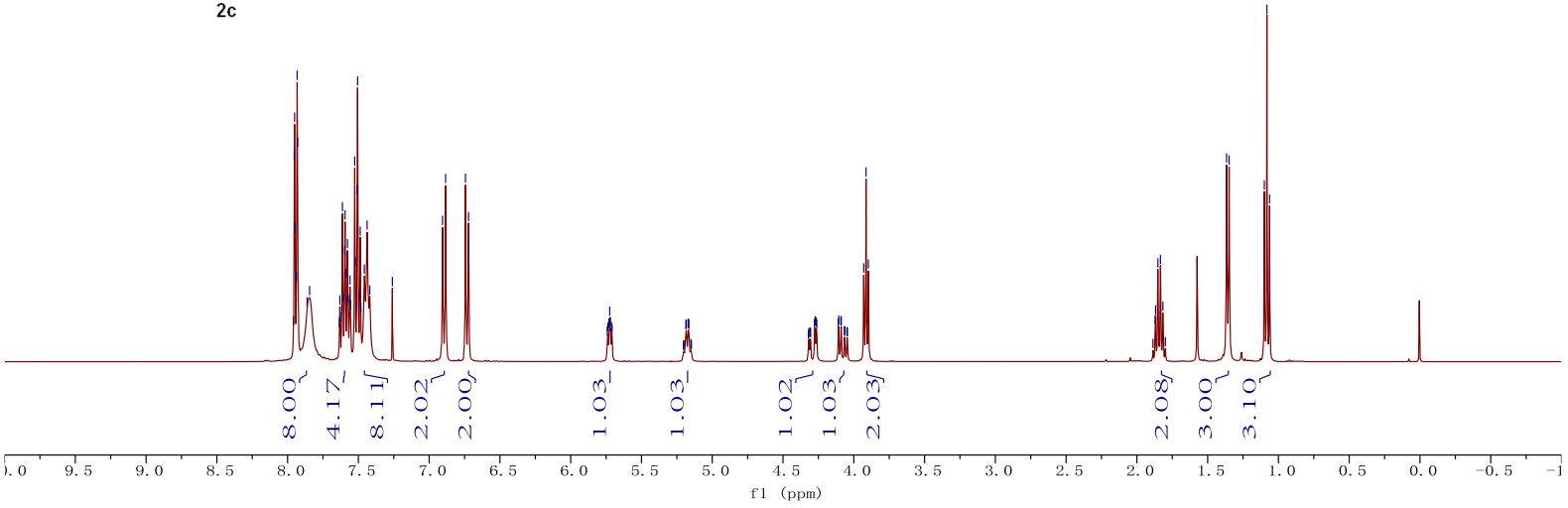
128.6
128.4
125.6
114.2
77.5
77.2
76.8
63.5
62.0
48.3
18.6
15.1
13C NMR (101 MHz, CDCl3)
N(SO2Ph)2
O
(PhO2S)2N
2b
f1 (ppm)

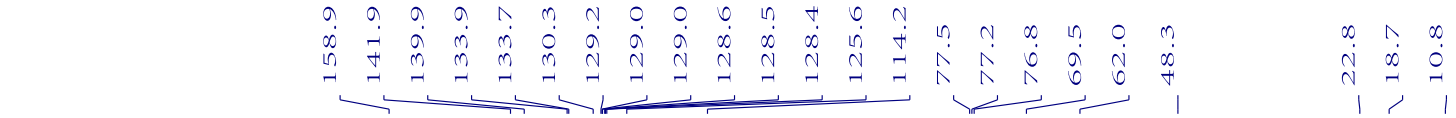


^{1}H NMR (400 MHz, $CDCl_3$)

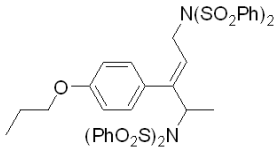


2c

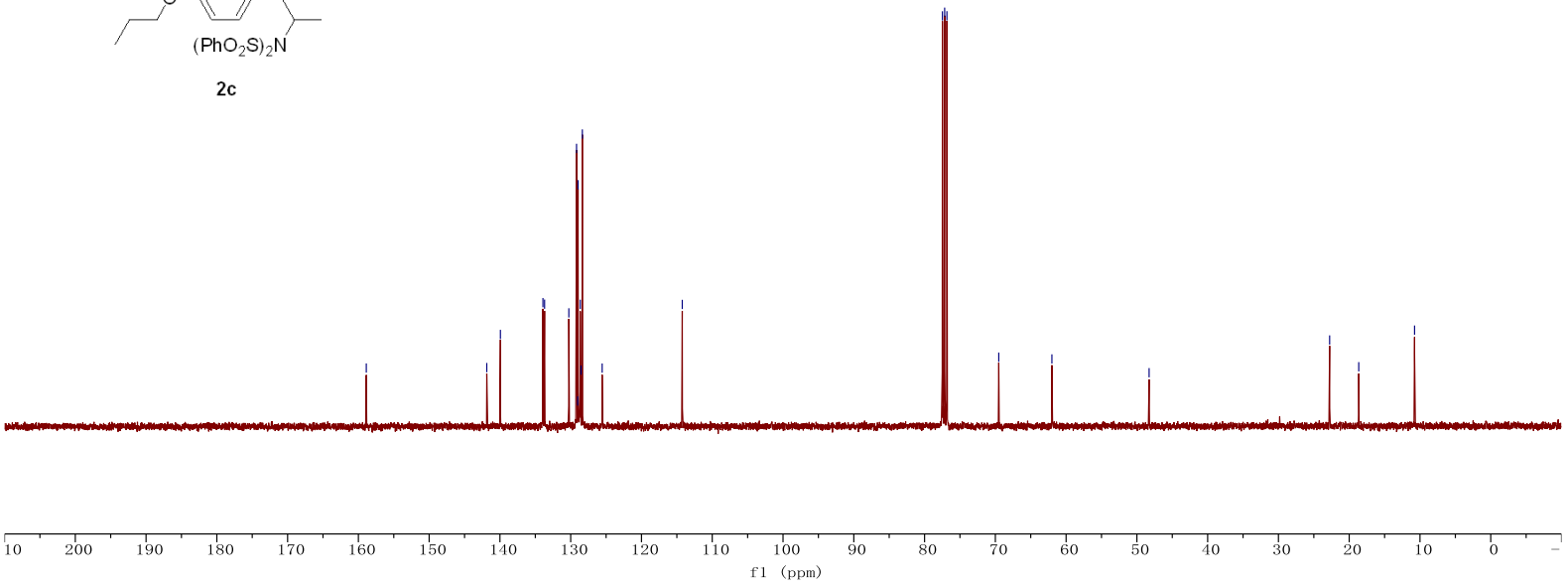




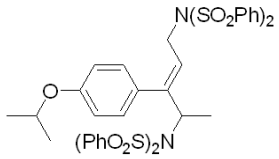
^{13}C NMR (101 MHz, $CDCl_3$)



2c



^{1}H NMR (400 MHz, $CDCl_3$)



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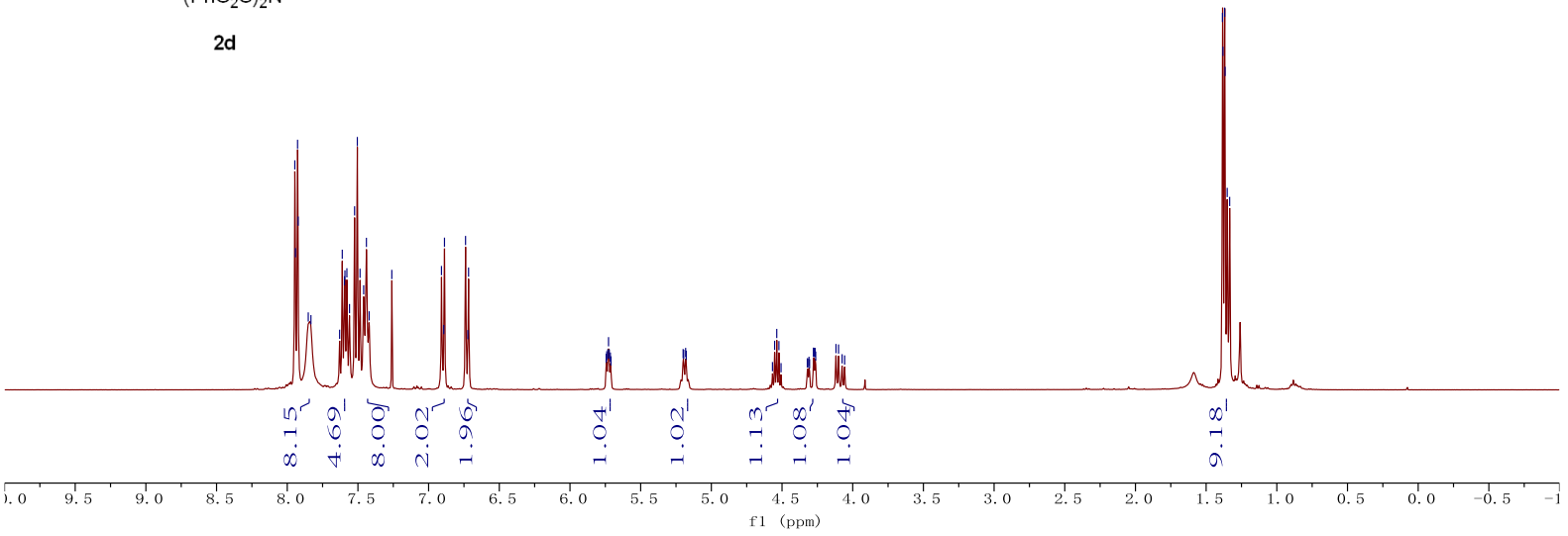

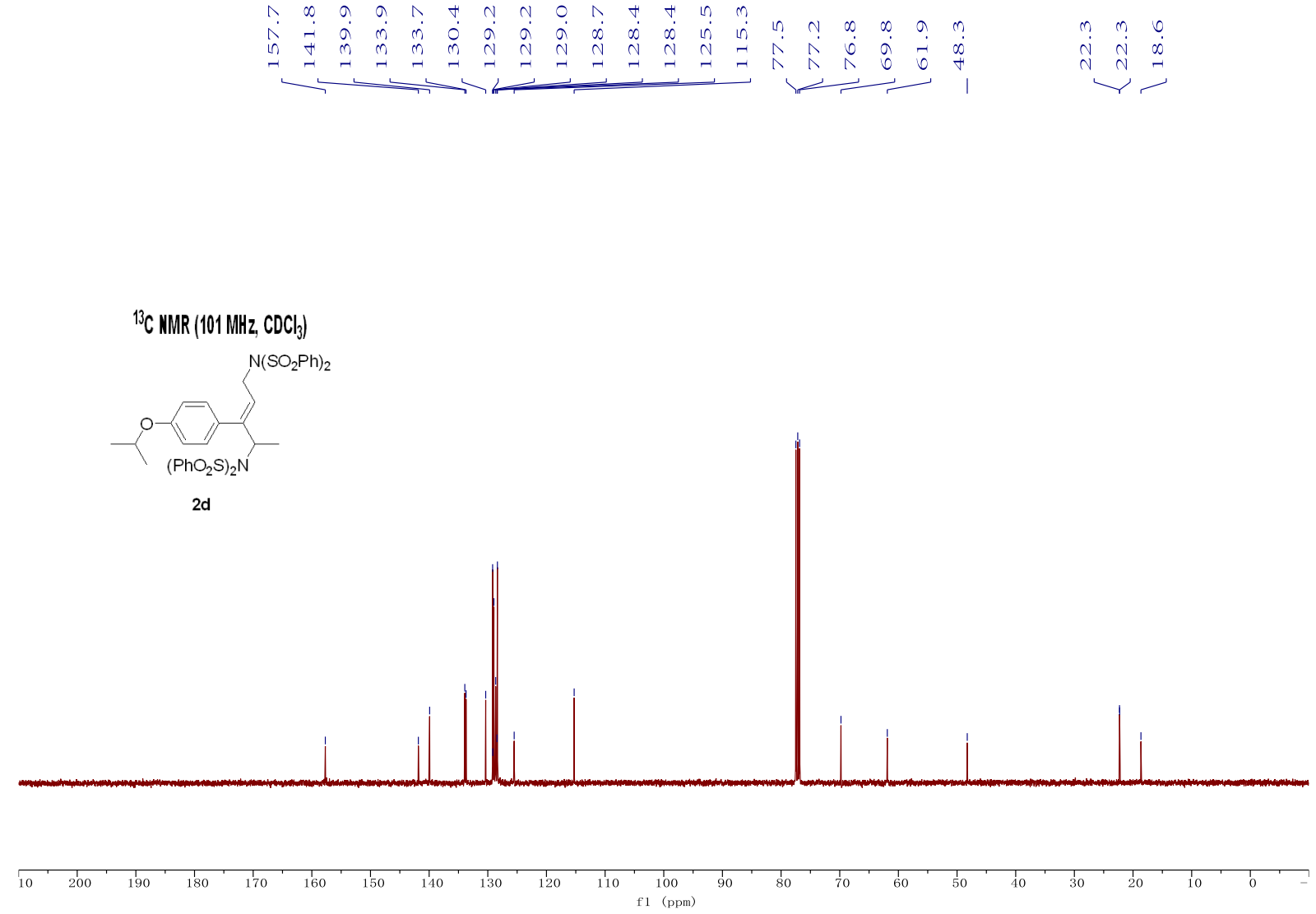
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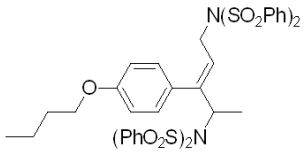
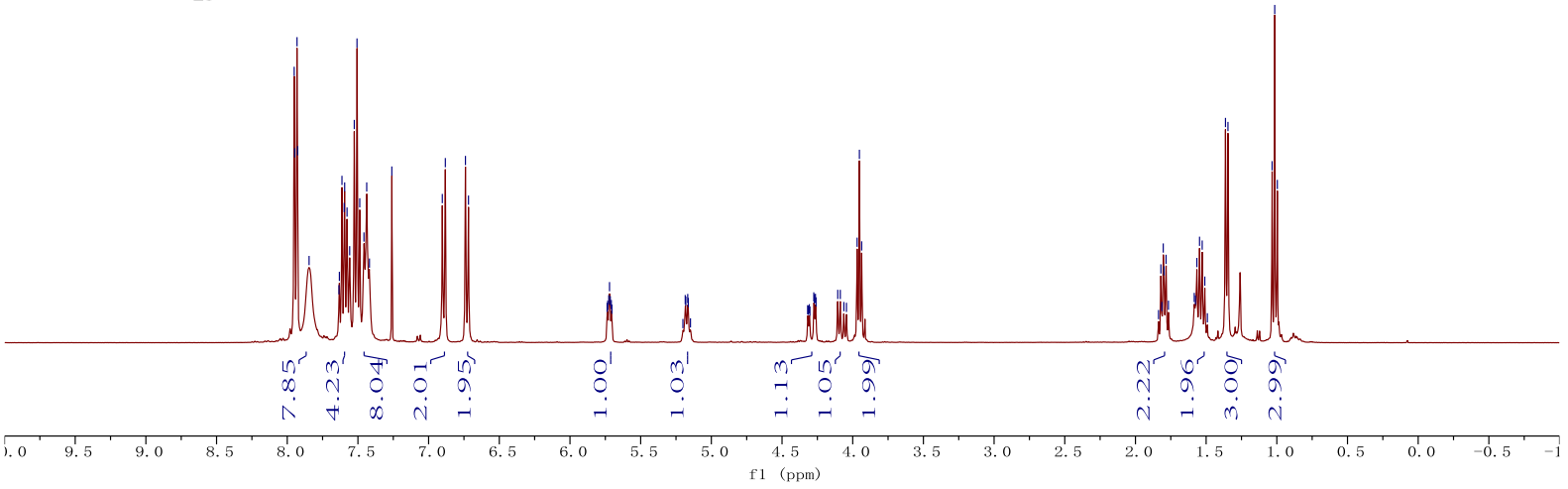
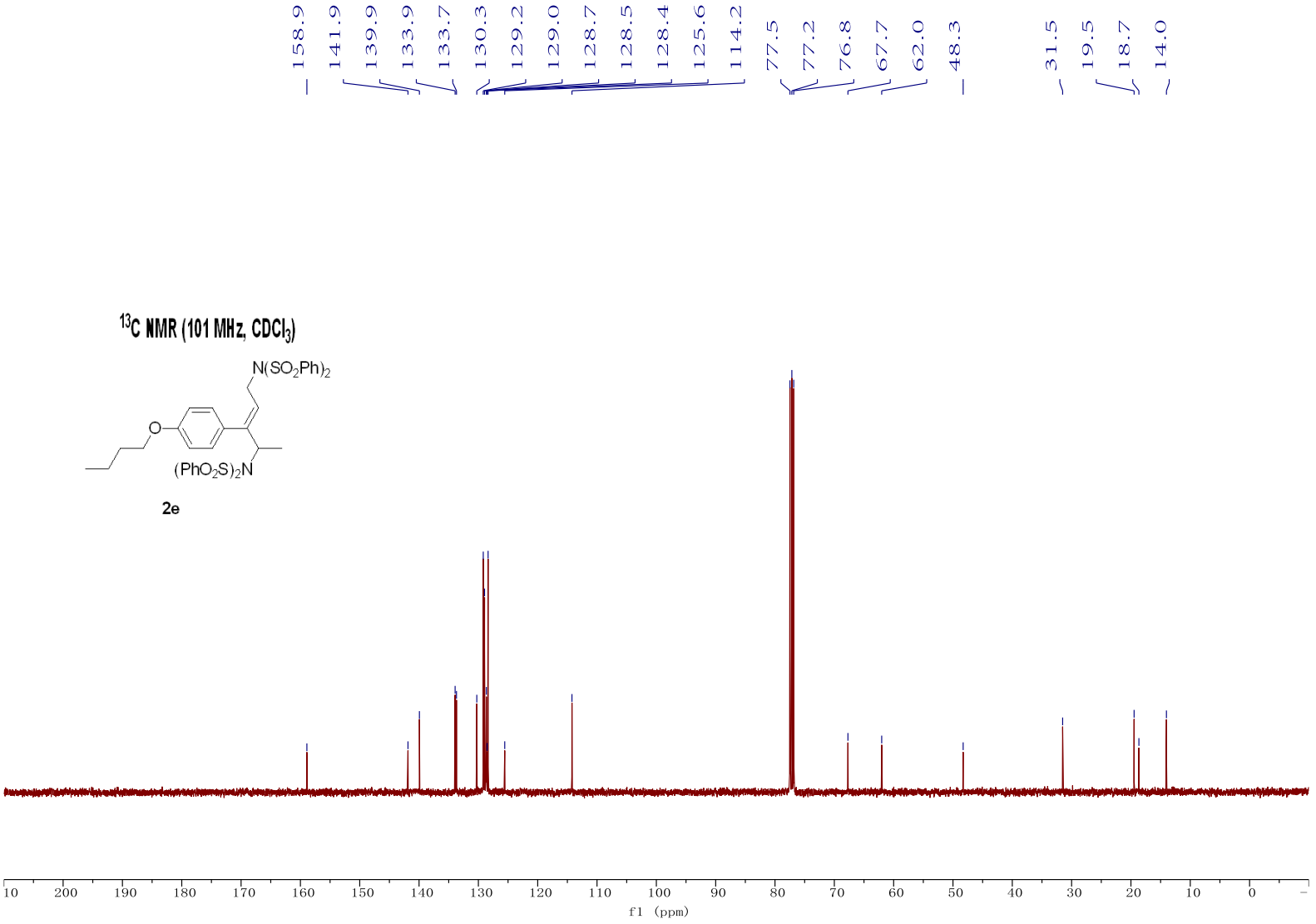
141.8
139.9
133.9
133.7
130.4
129.2
129.2
129.0
128.7
128.4
128.4
125.5
115.3
77.5
77.2
76.8
69.8
61.9
48.3
22.3
22.3
18.6
13C NMR (101 MHz, CDCl3)
N(SO2Ph)2
O
(PhO2S)2N
2d
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

^{1}H NMR (400 MHz, $CDCl_3$)

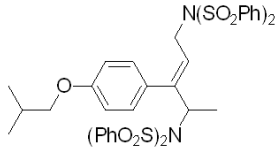


2e




158.9
141.9
139.9
133.9
133.7
130.3
129.2
129.0
128.7
128.5
128.4
125.6
114.2
77.5
77.2
76.8
67.7
62.0
48.3
31.5
19.5
18.7
14.0
13C NMR (101 MHz, CDCl3)
N(SO2Ph)2
O
(PhO2S)2N
2e
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

^{1}H NMR (400 MHz, $CDCl_3$)



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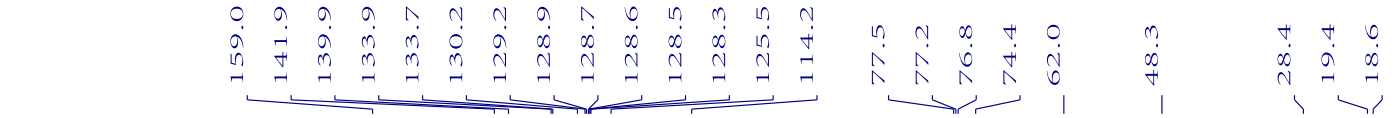
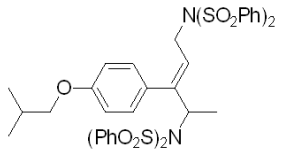


^{13}C NMR (101 MHz, $CDCl_3$)



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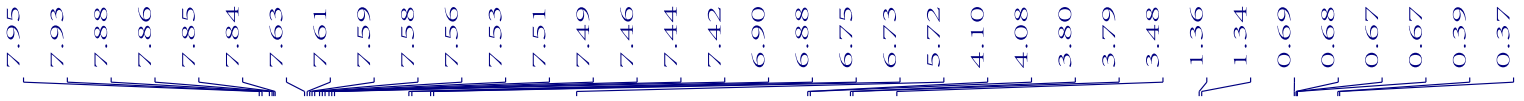
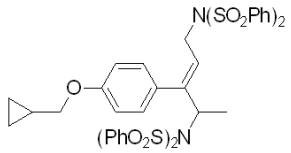


^{1}H NMR (400 MHz, $CDCl_3$)



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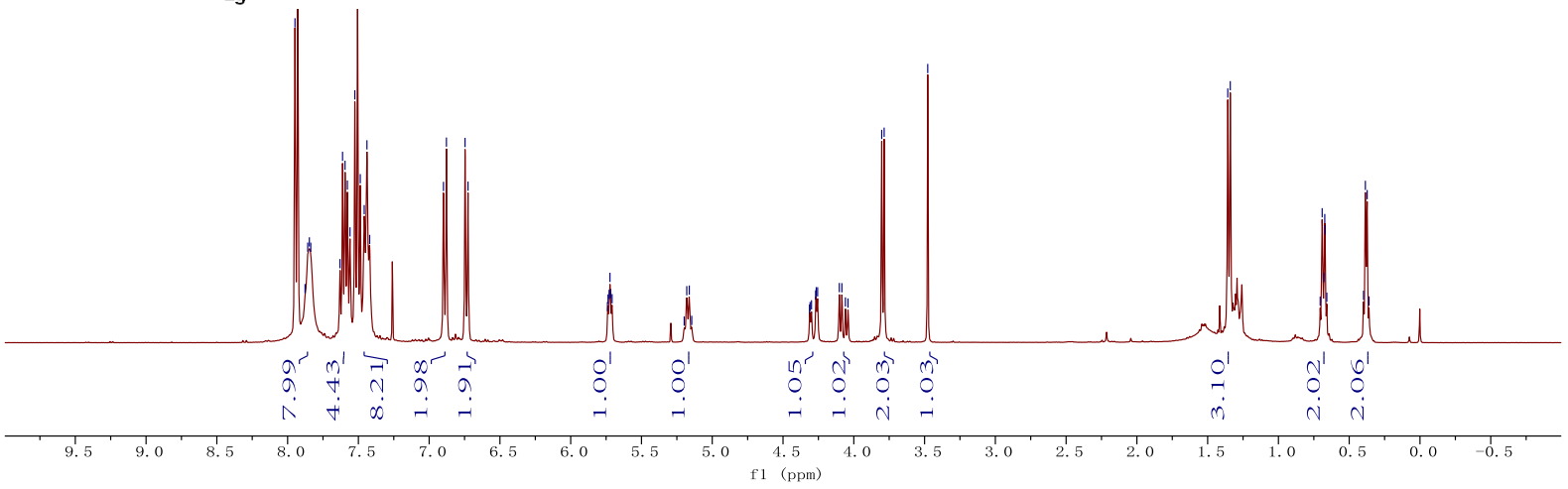

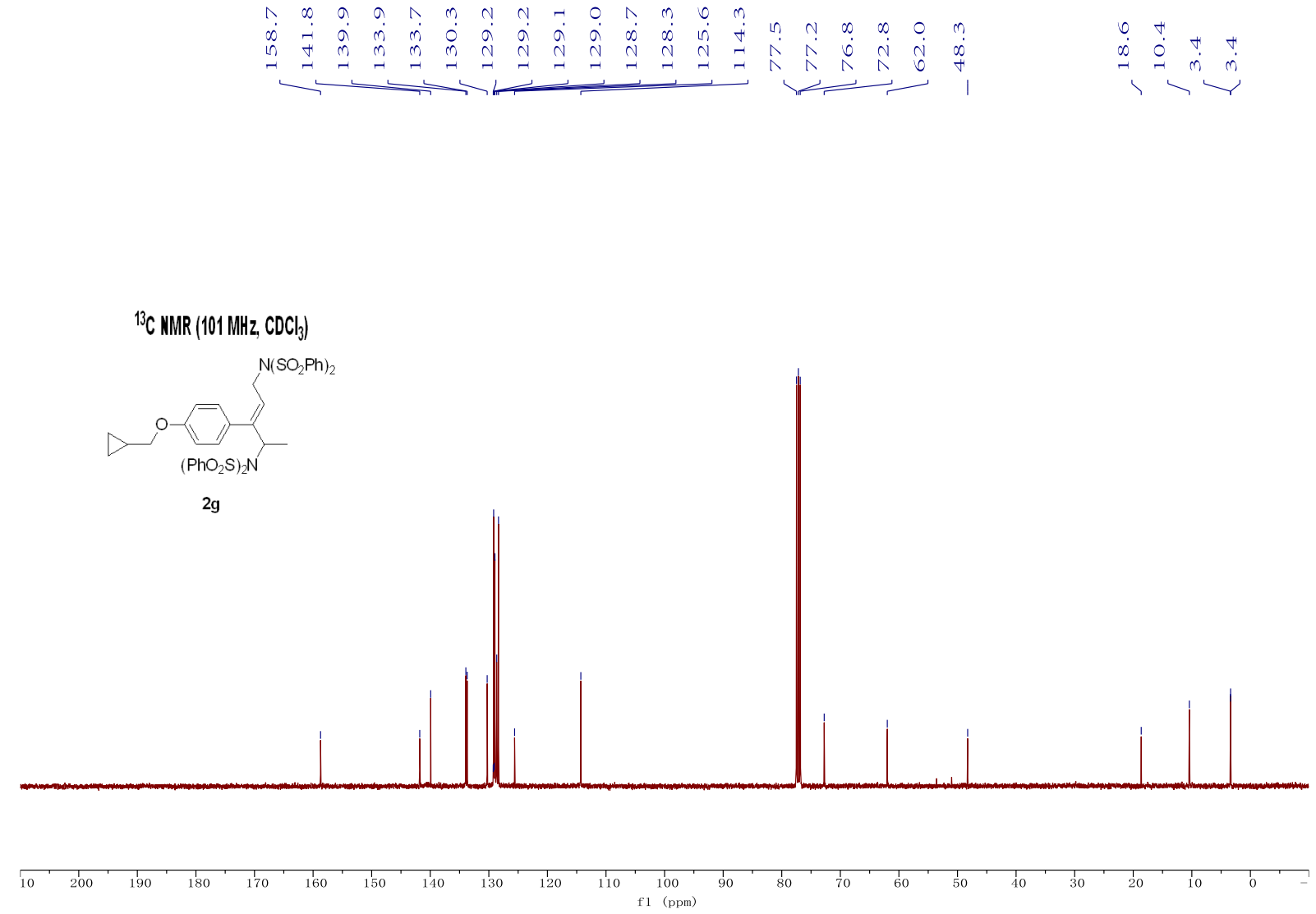
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133.9
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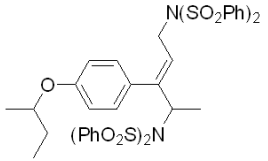
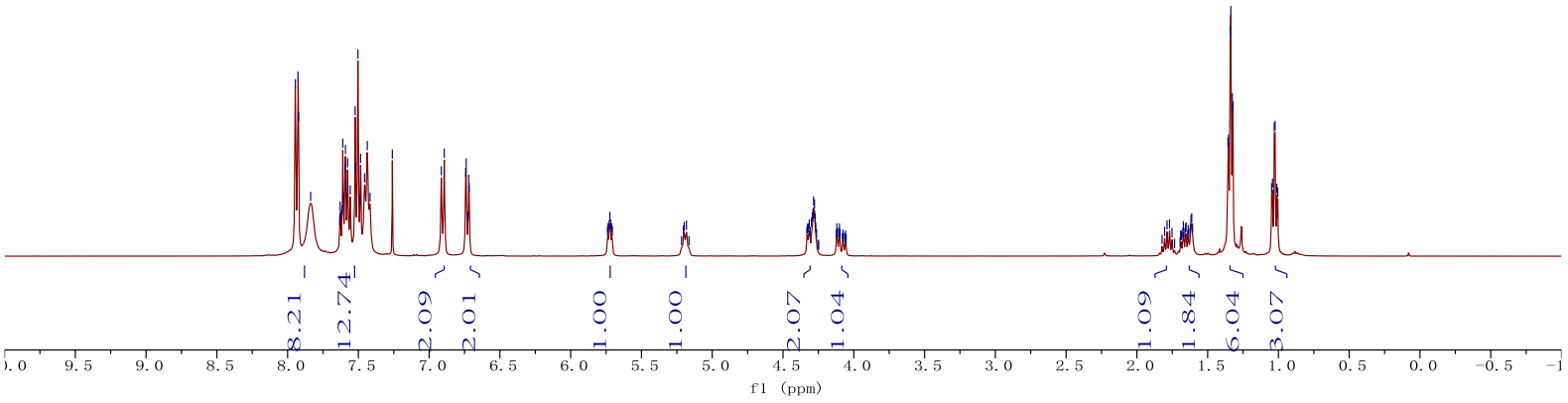
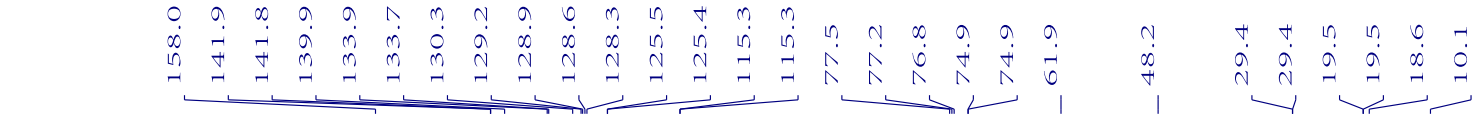
125.6
114.3
77.5
77.2
76.8
72.8
62.0
48.3
18.6
10.4
3.4
3.4
13C NMR (101 MHz, CDCl3)
N(SO2Ph)2
O
(PhO2S)2N
2g
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

^{1}H NMR (400 MHz, $CDCl_3$)

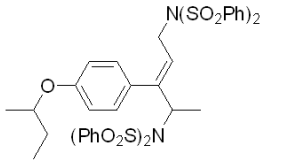


2h

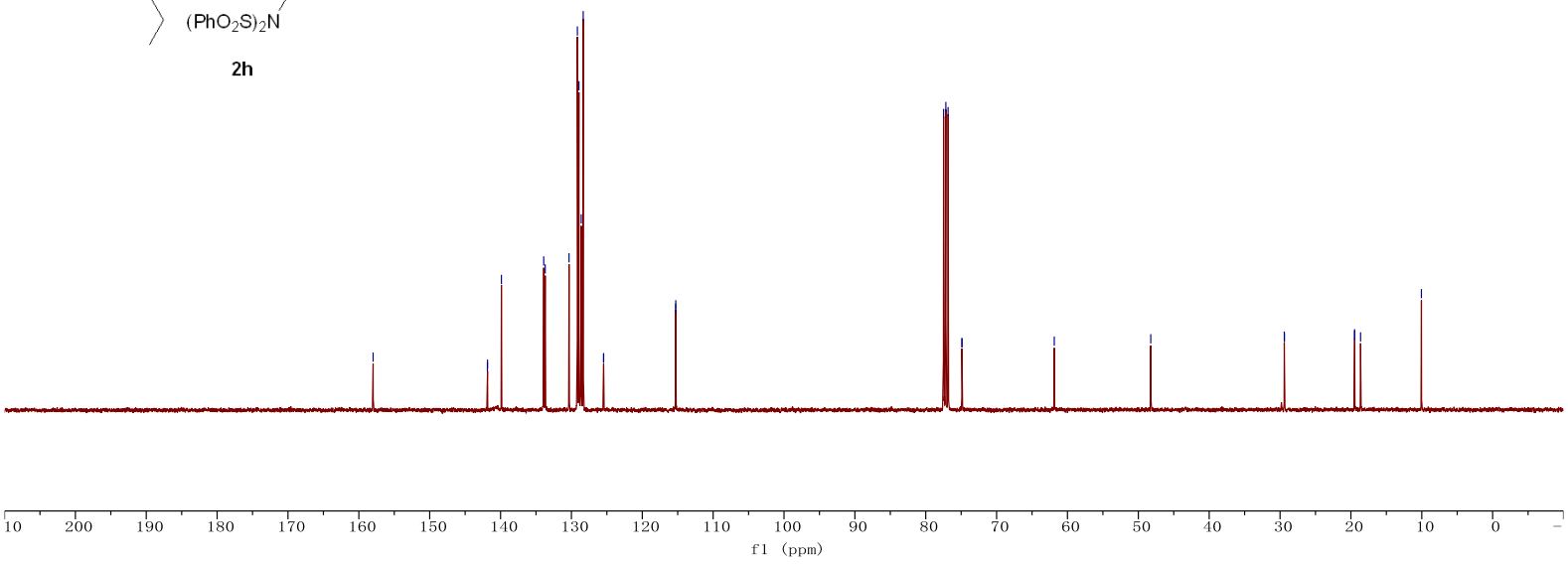




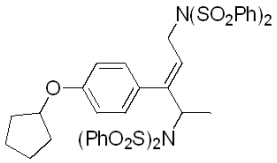
^{13}C NMR (101 MHz, $CDCl_3$)



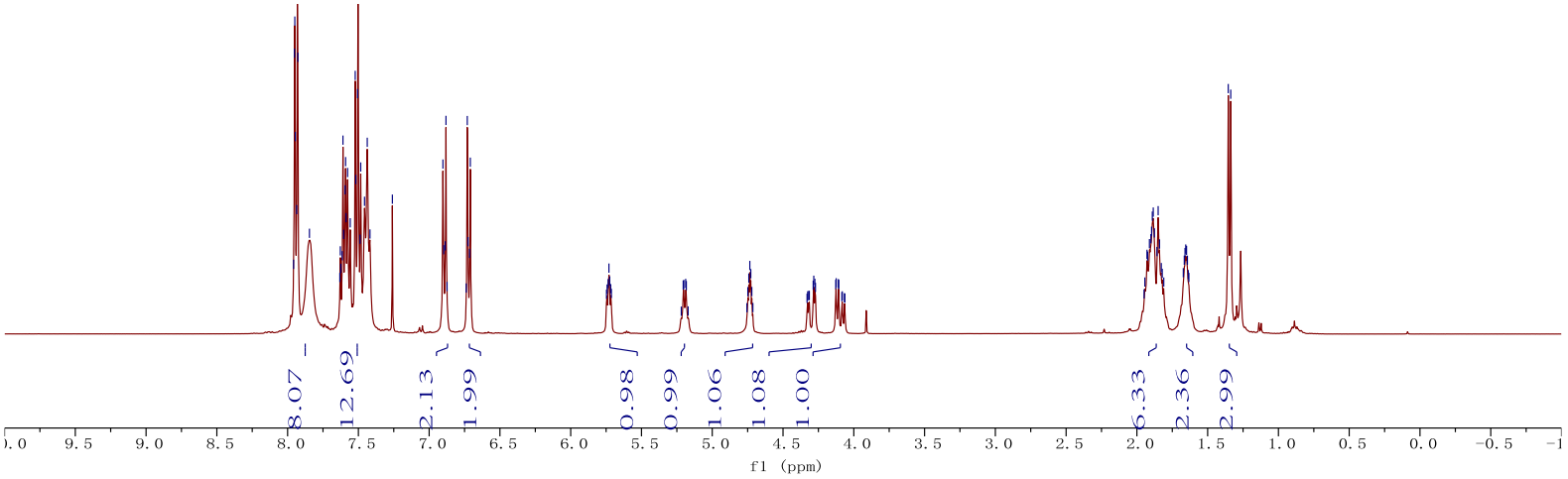
2h

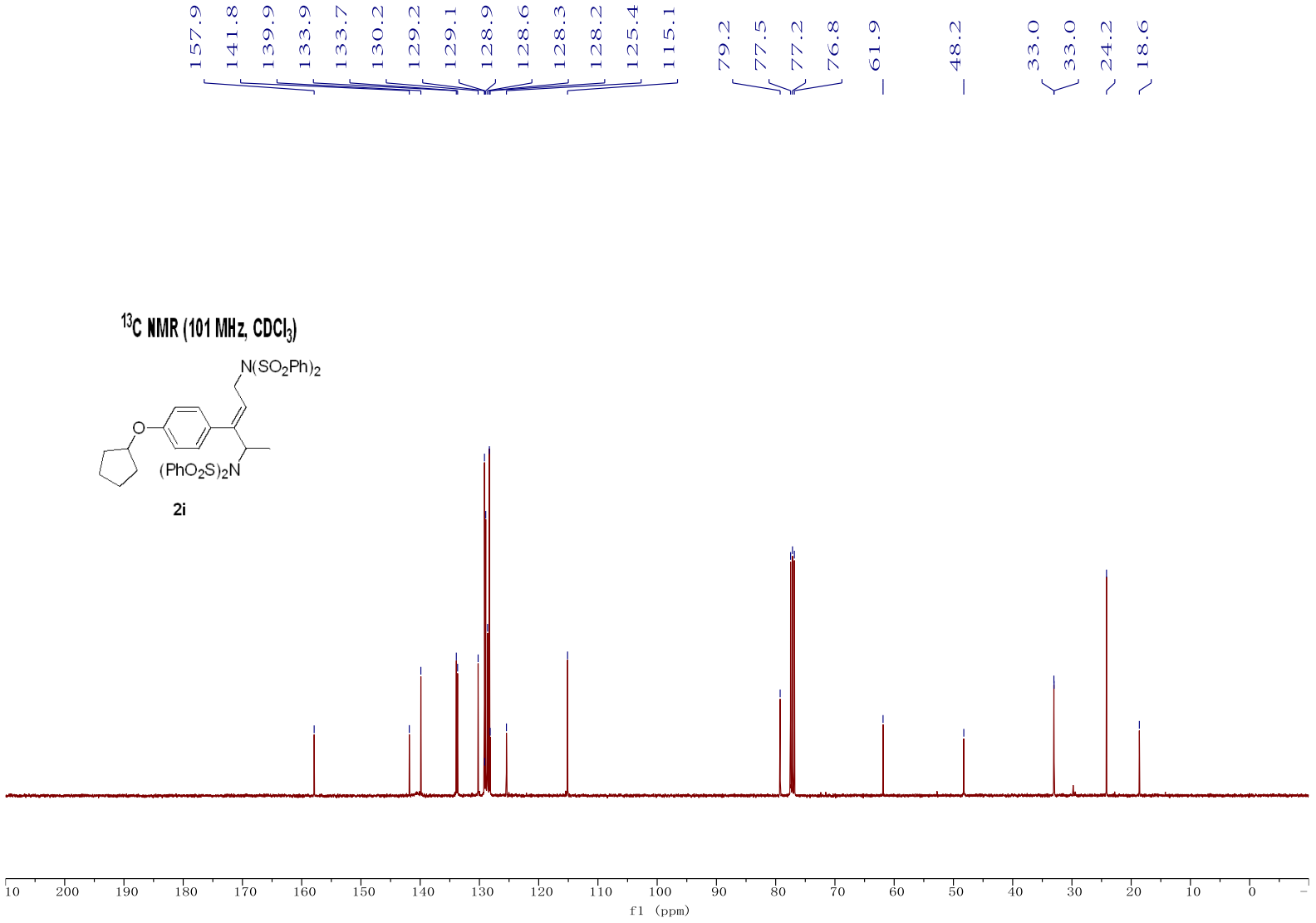


^{1}H NMR (400 MHz, $CDCl_3$)



2i

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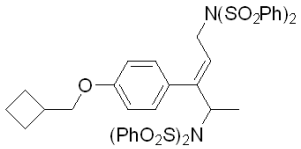
128.2
125.4
115.1
79.2
77.5
77.2
76.8
61.9
48.2
33.0
33.0
24.2
18.6
13C NMR (101 MHz, CDCl3)
N(SO2Ph)2
O
(PhO2S)2N
2i
f1 (ppm)

^{1}H NMR (400 MHz, $CDCl_3$)



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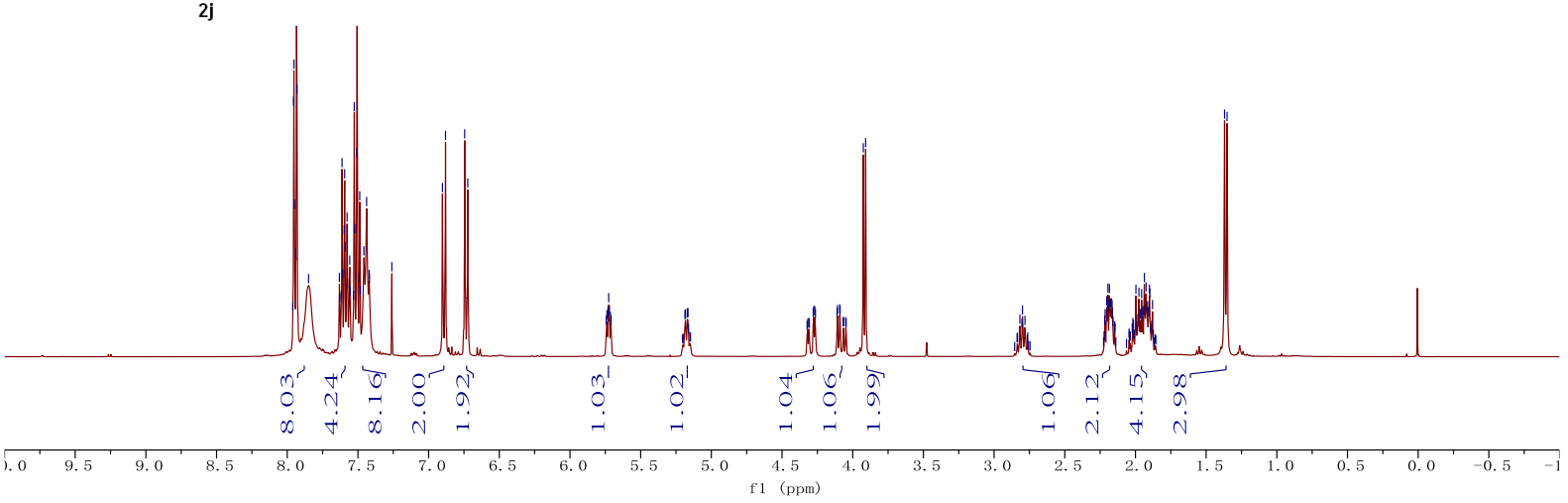
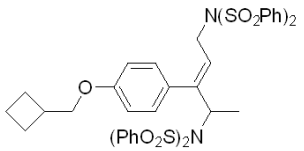
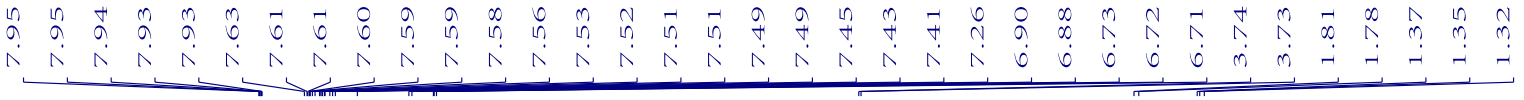


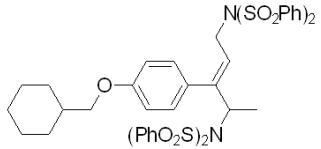
^{13}C NMR (101 MHz, $CDCl_3$)



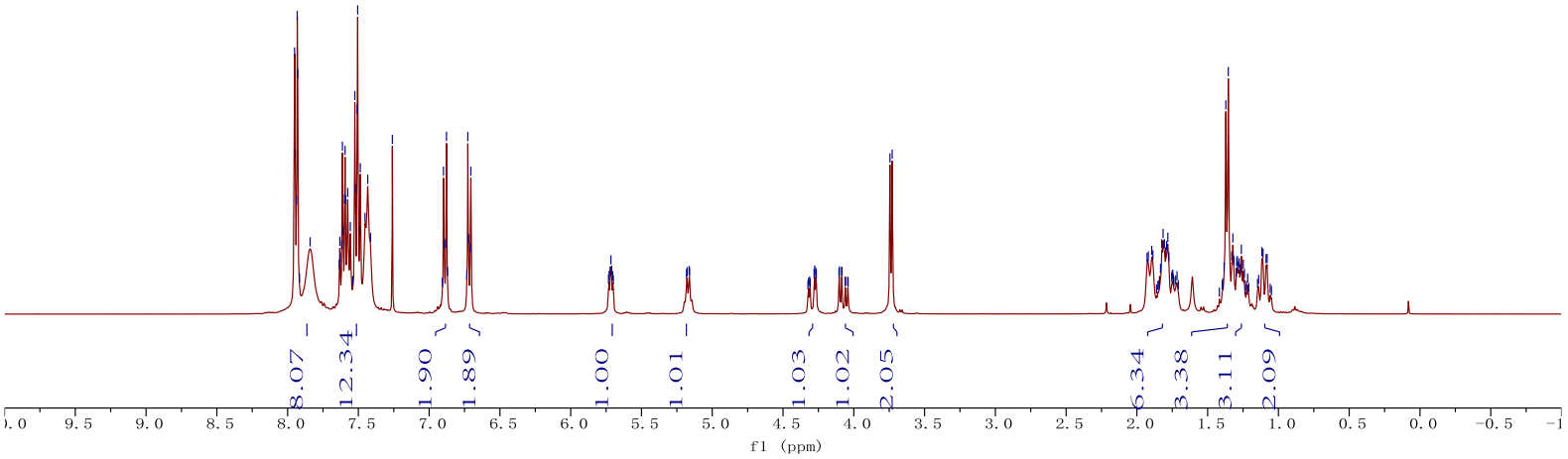
2j



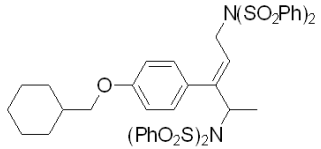
^{1}H NMR (400 MHz, $CDCl_3$)



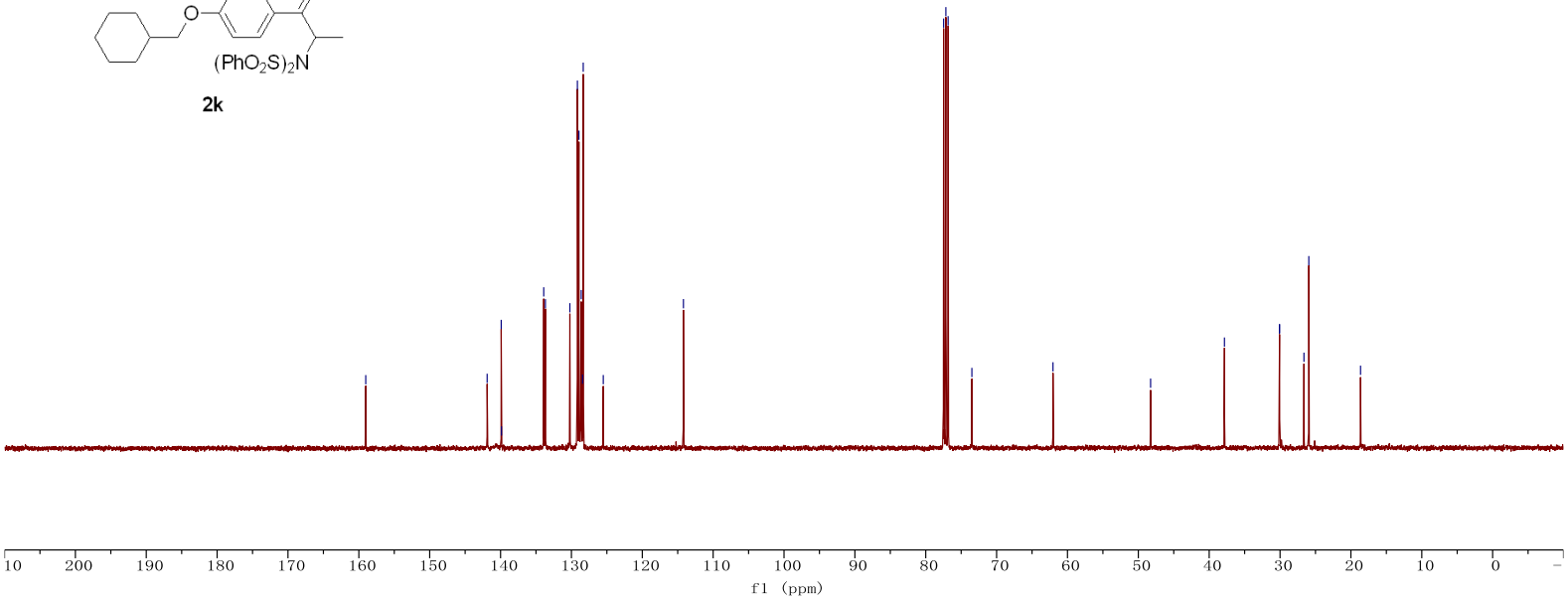
2k

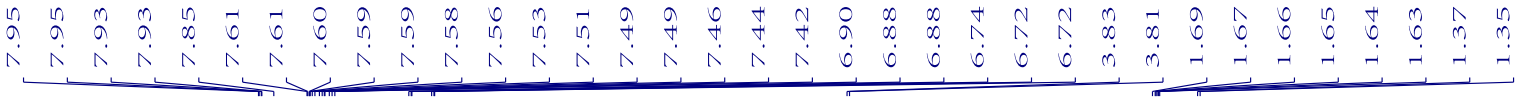


^{13}C NMR (101 MHz, $CDCl_3$)

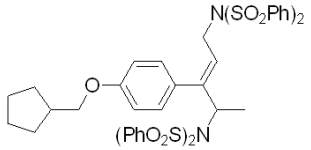


2k

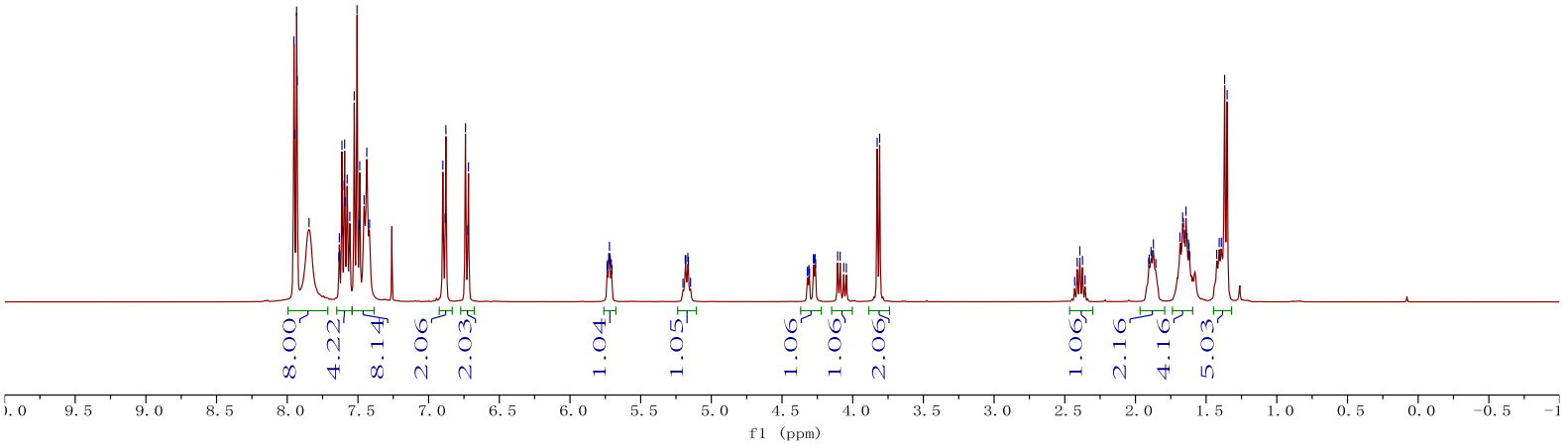


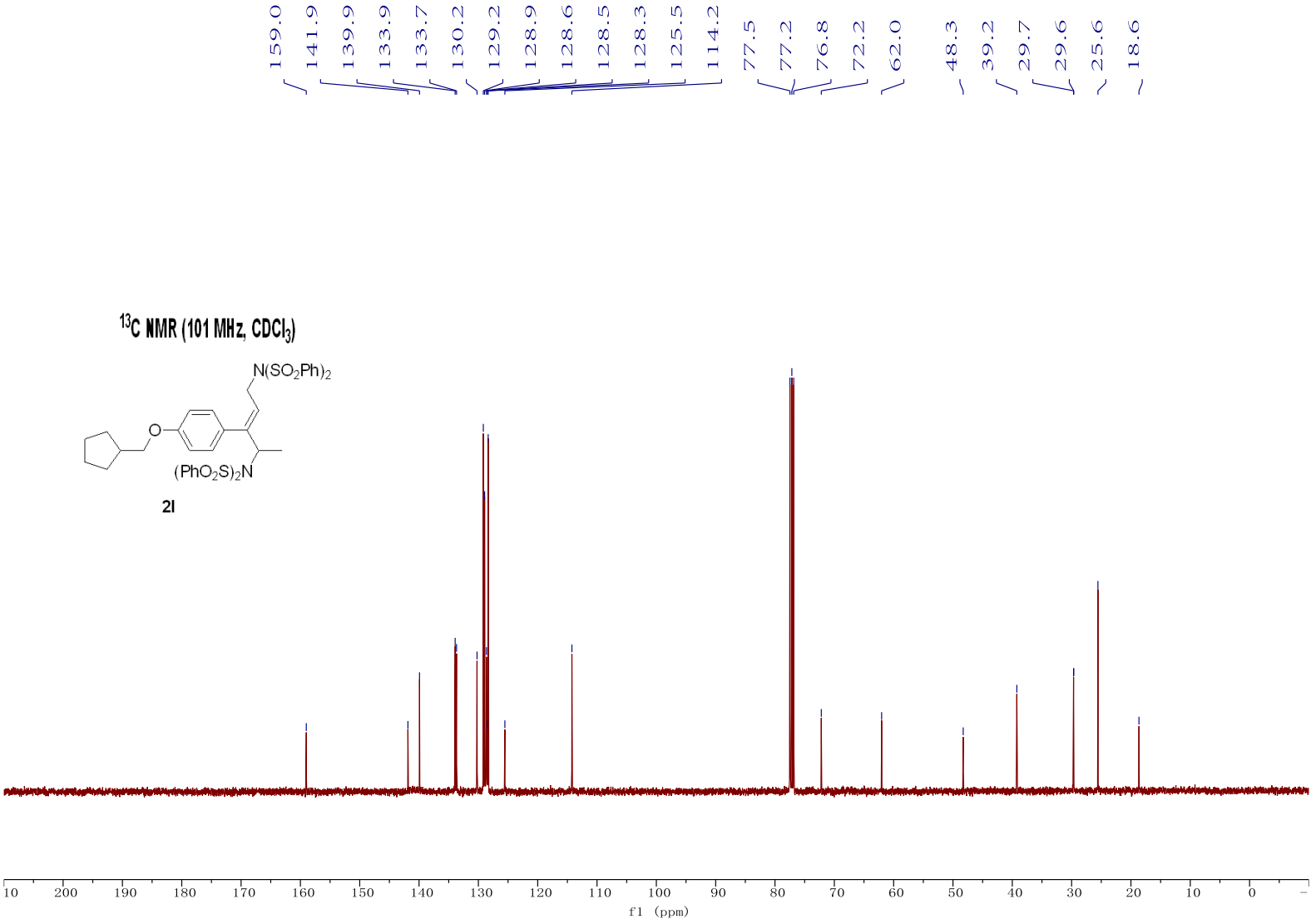


^{1}H NMR (400 MHz, $CDCl_3$)

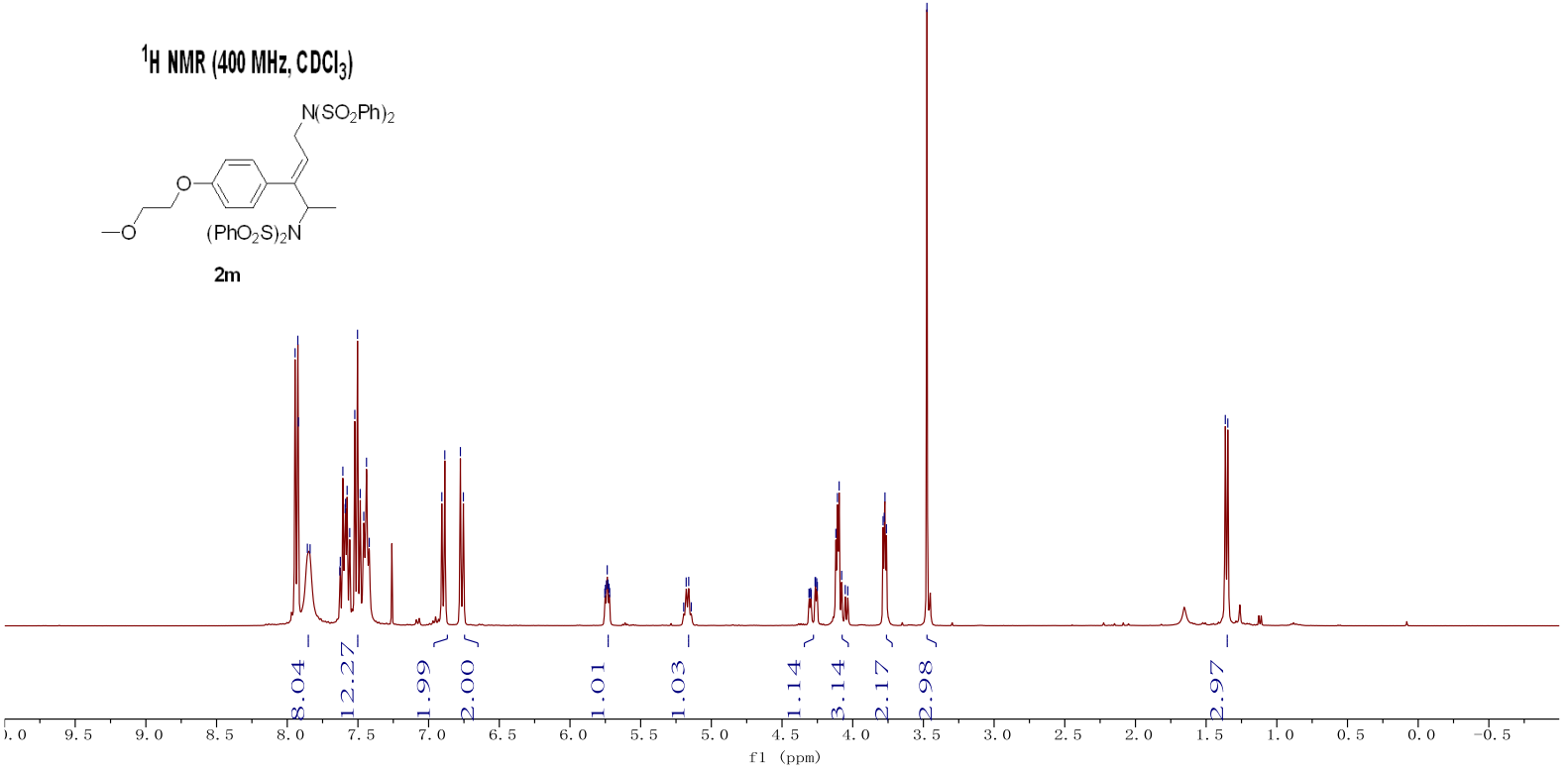


2l

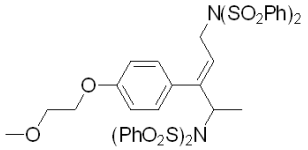



159.0
141.9
139.9
133.9
133.7
130.2
129.2
128.9
128.6
128.5
128.3
125.5
114.2
77.5
77.2
76.8
72.2
62.0
48.3
39.2
29.7
29.6
25.6
18.6
13C NMR (101 MHz, CDCl3)
N(SO2Ph)2
O
(PhO2S)2N
2l
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

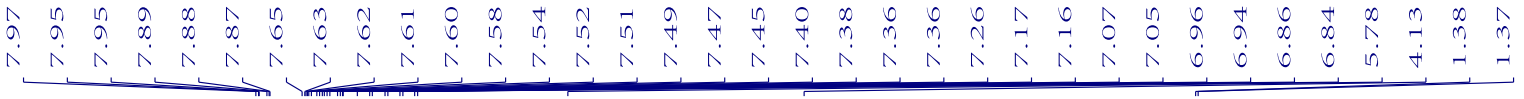

7.94
7.93
7.92
7.86
7.84
7.63
7.62
7.61
7.59
7.59
7.58
7.56
7.52
7.50
7.48
7.46
7.44
7.42
6.91
6.89
6.78
6.75
5.74
5.16
4.12
4.11
4.10
4.08
3.79
3.78
3.77
3.76
3.47
1.36
1.35


1H NMR (400 MHz, CDCl3)
N(SO2Ph)2
O
O
(PhO2S)2N
2m
8.04
12.27
1.99
2.00
1.01
1.03
1.14
3.14
2.17
2.98
2.97
f1 (ppm)

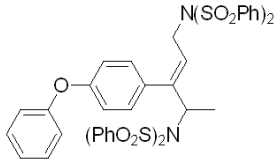
^{13}C NMR (101 MHz, $CDCl_3$)



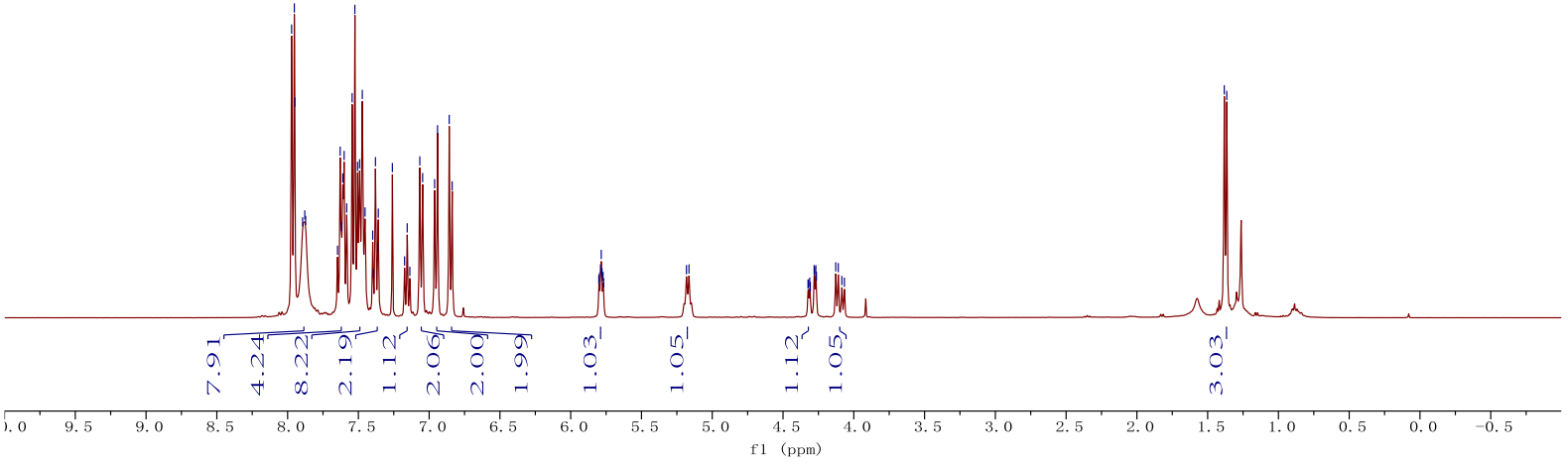
2m

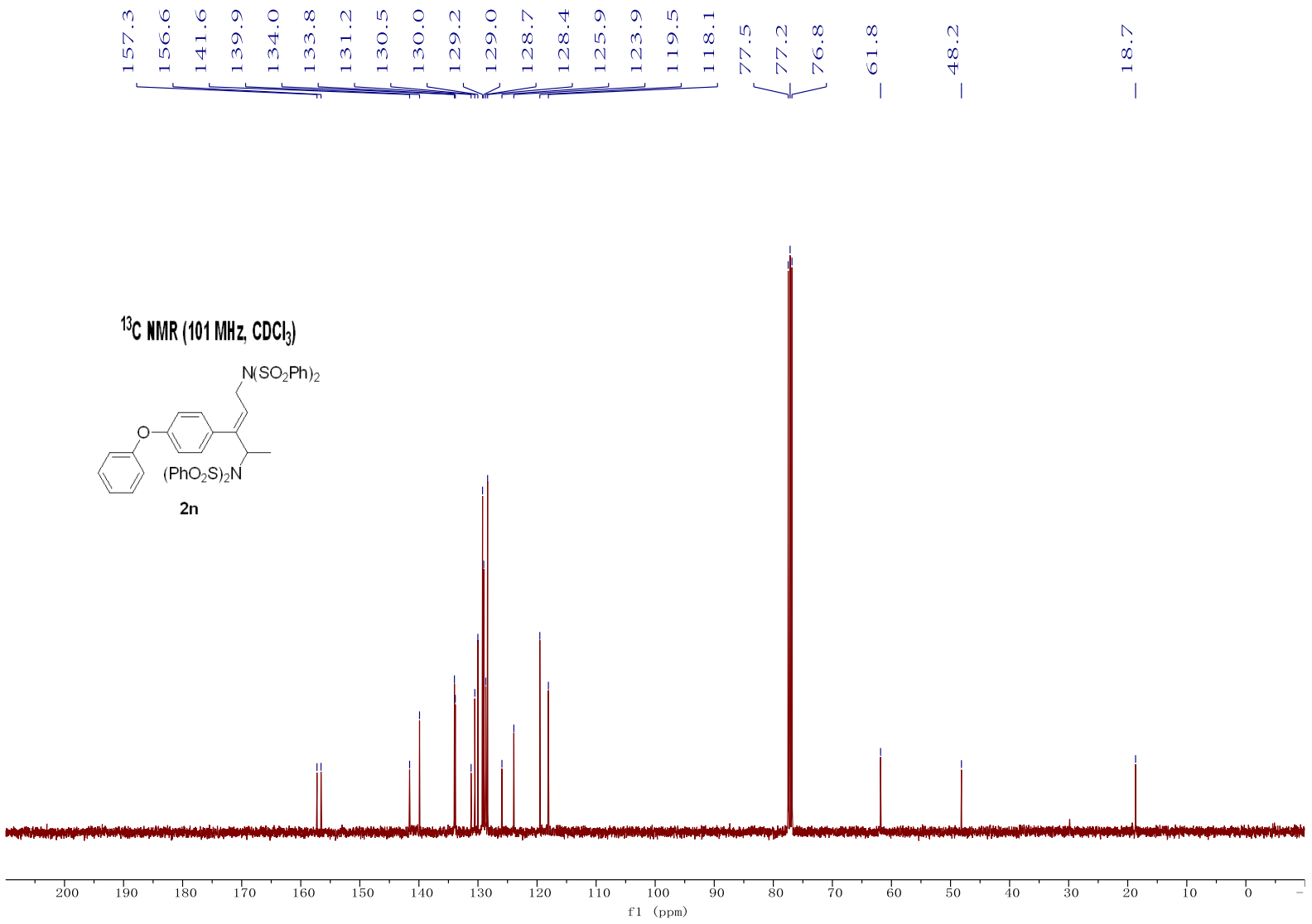


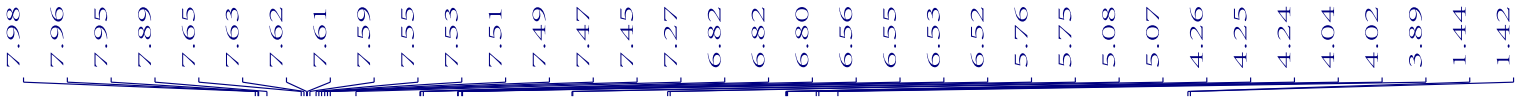
^{1}H NMR (400 MHz, $CDCl_3$)



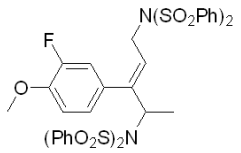
2n



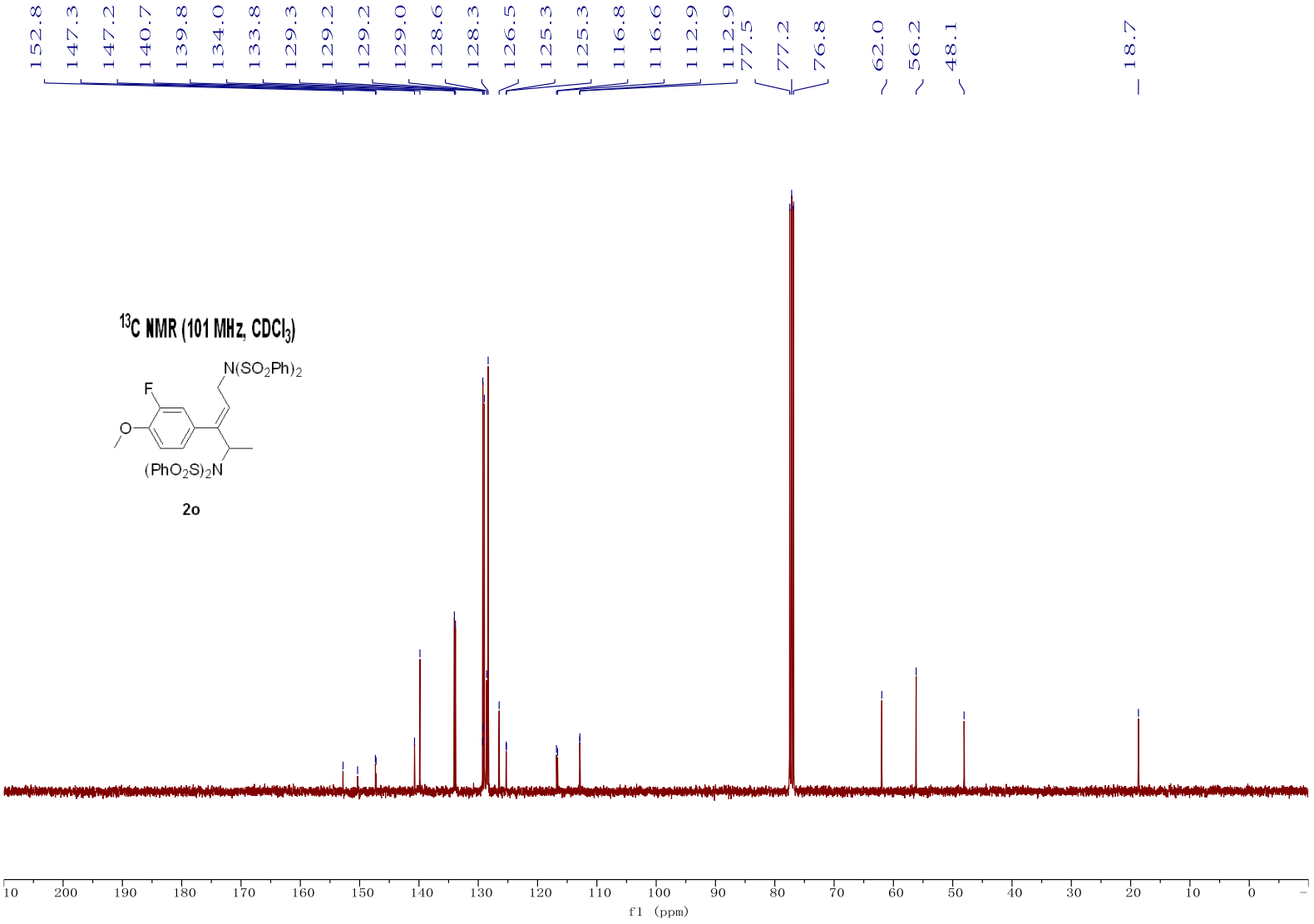

157.3
156.6
141.6
139.9
134.0
133.8
131.2
130.5
130.0
129.2
129.0
128.7
128.4
125.9
123.9
119.5
118.1
77.5
77.2
76.8
61.8
48.2
18.7
13C NMR (101 MHz, CDCl3)
N(SO2Ph)2
O
(PhO2S)2N
2n
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



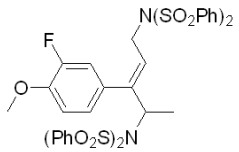
^{1}H NMR (400 MHz, $CDCl_3$)



2o

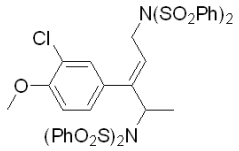

152.8
147.3
147.2
140.7
139.8
134.0
133.8
129.3
129.2
129.2
129.0
128.6
128.3
126.5
125.3
125.3
116.8
116.6
112.9
112.9
77.5
77.2
76.8
62.0
56.2
48.1
18.7
13C NMR (101 MHz, CDCl3)
N(SO2Ph)2
F
O
(PhO2S)2N
2o
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

^{19}F NMR (376 MHz, $CDCl_3$)

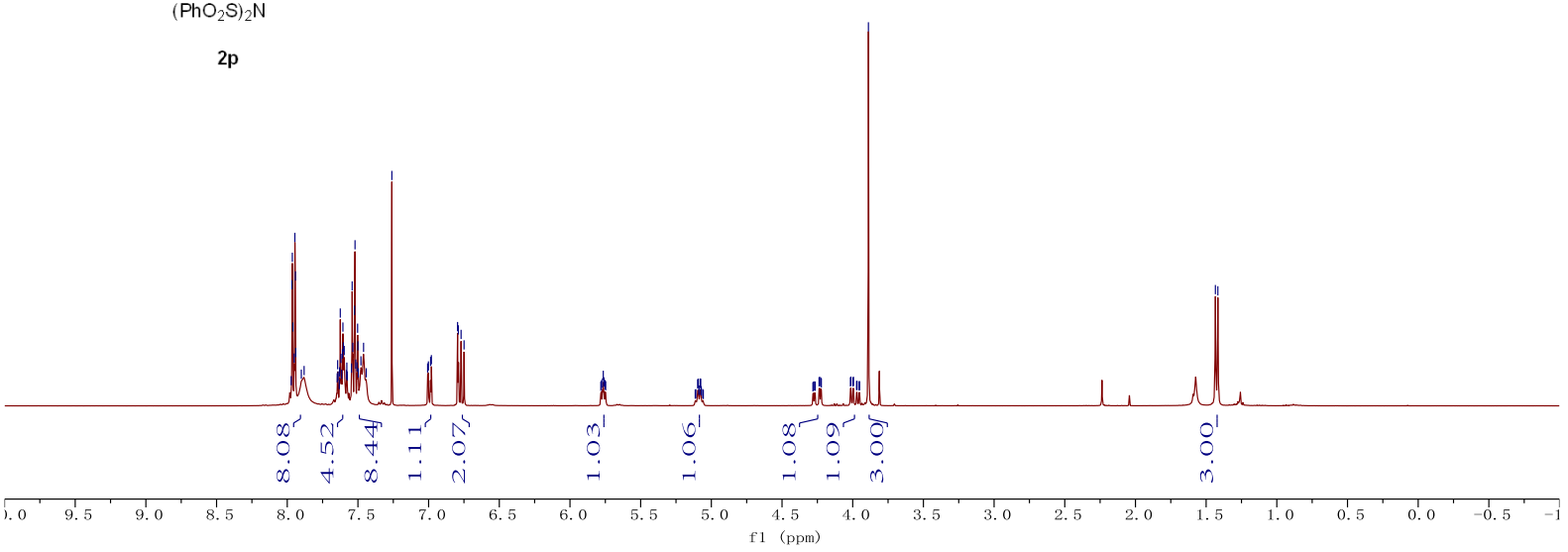


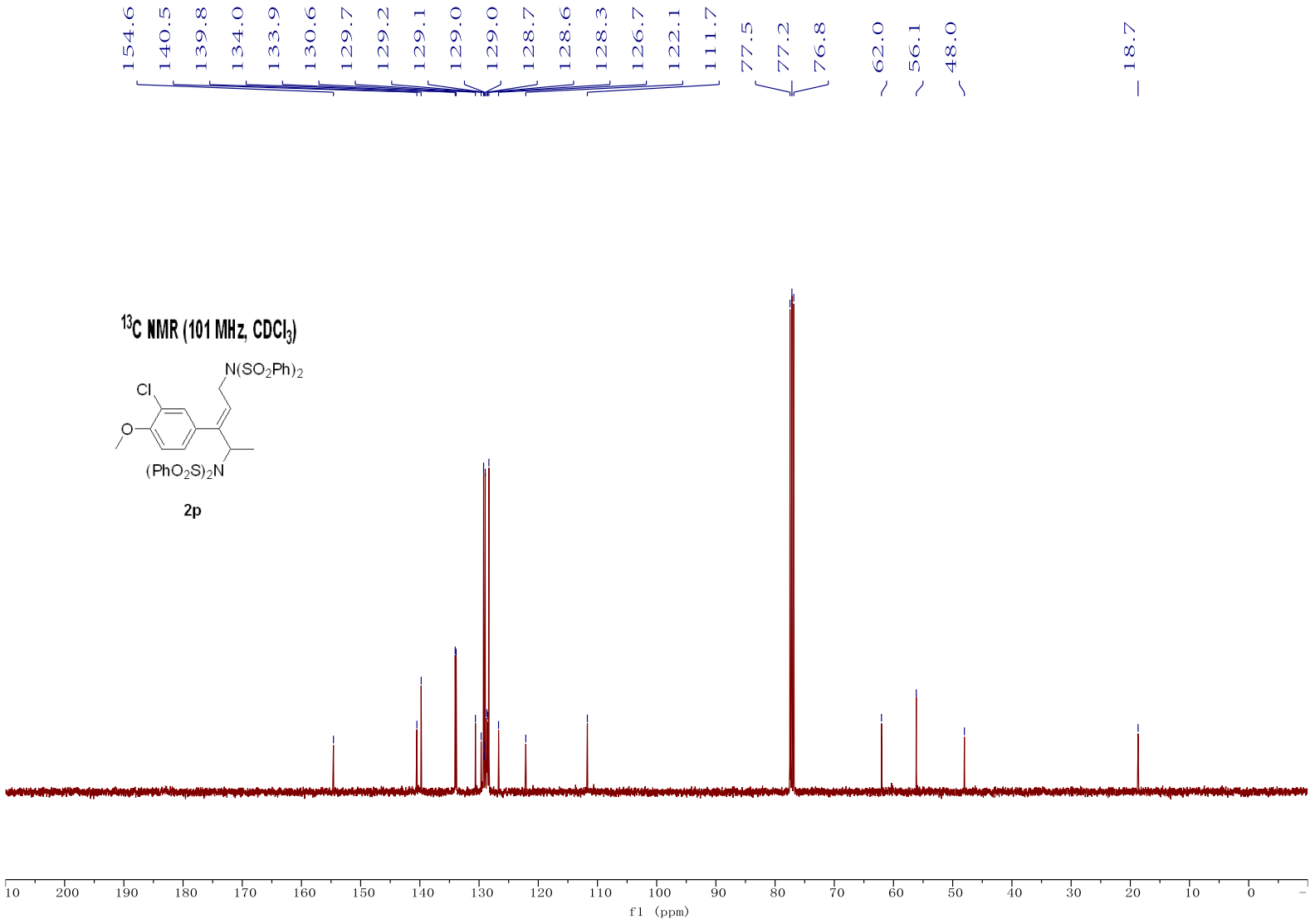
2o

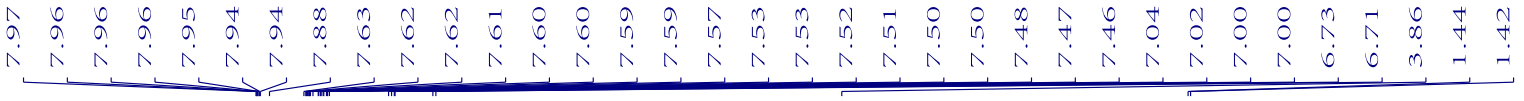
^{1}H NMR (400 MHz, $CDCl_3$)



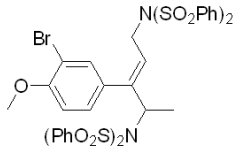
2p



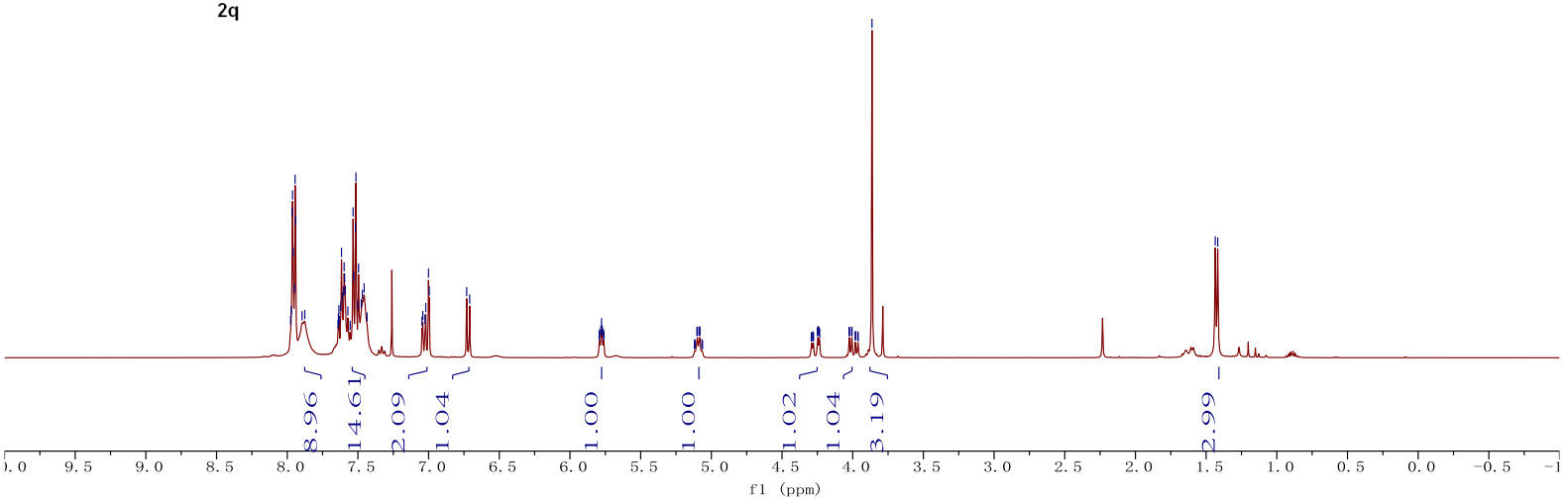

154.6
140.5
139.8
134.0
133.9
130.6
129.7
129.2
129.1
129.0
129.0
128.7
128.6
128.3
126.7
122.1
111.7
77.5
77.2
76.8
62.0
56.1
48.0
18.7
13C NMR (101 MHz, CDCl3)
N(SO2Ph)2
Cl
O
(PhO2S)2N
2p
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

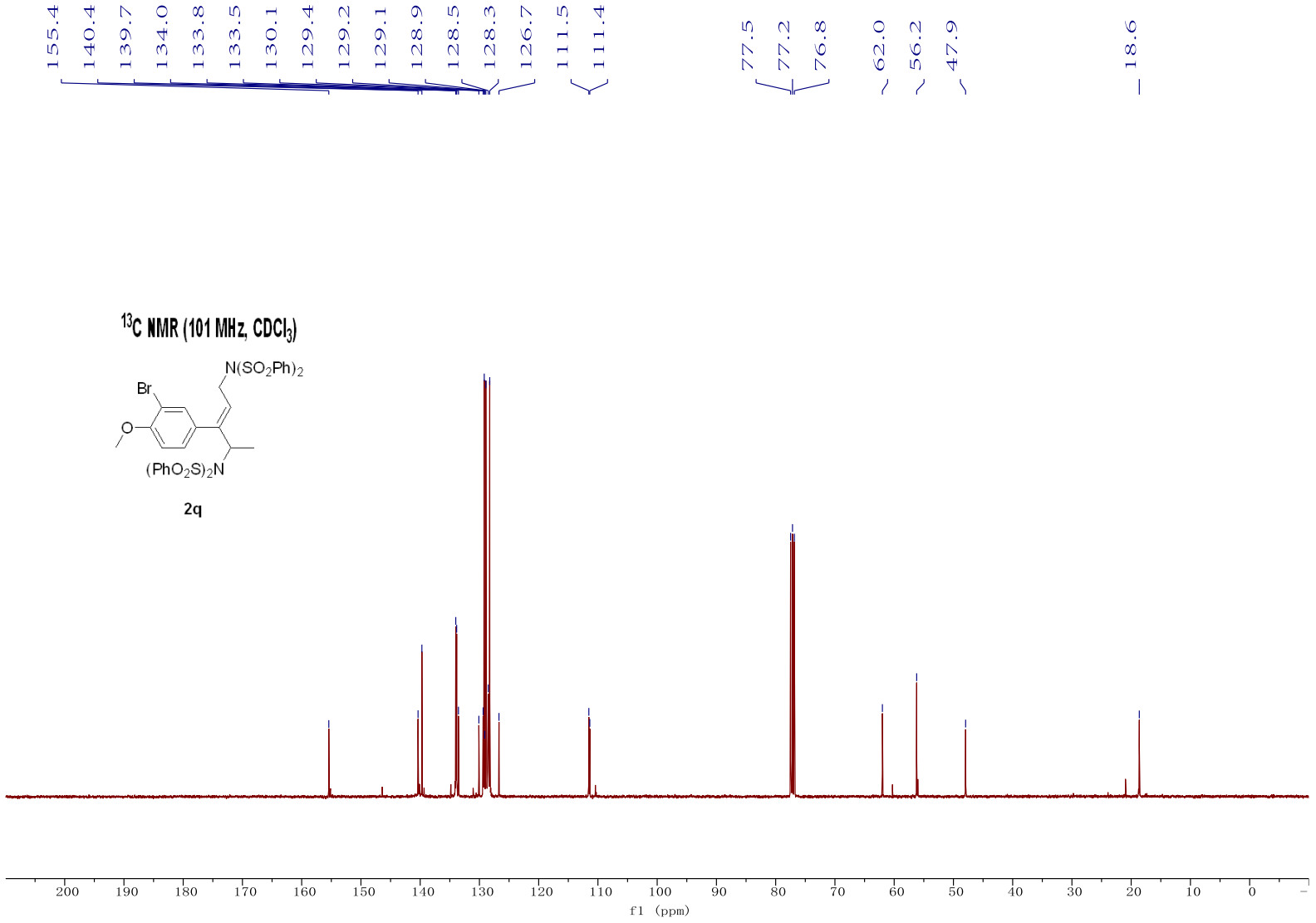


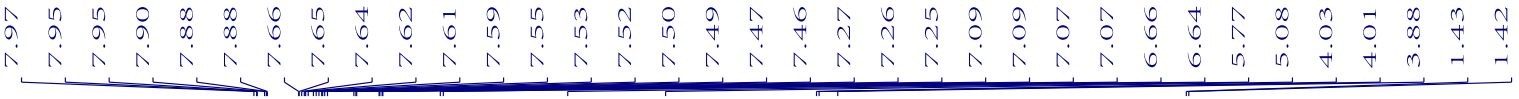
^{1}H NMR (400 MHz, $CDCl_3$)



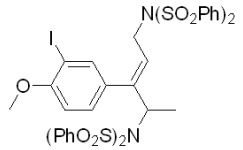
2q



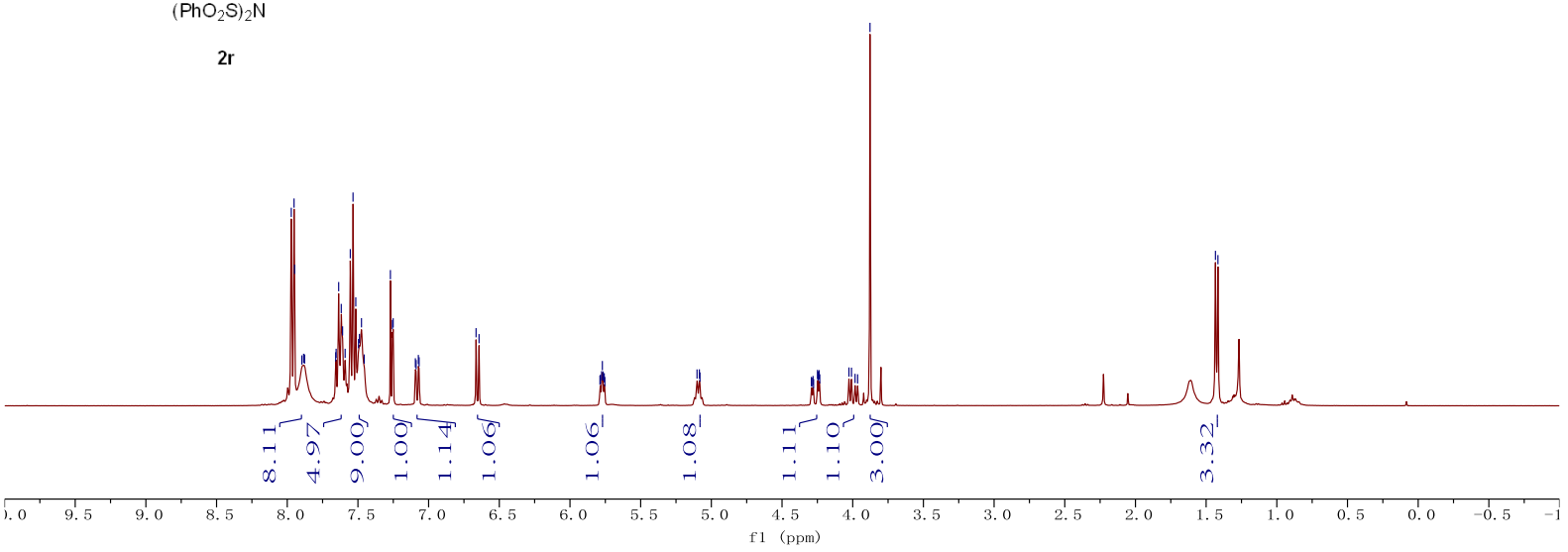

155.4
140.4
139.7
134.0
133.8
133.5
130.1
129.4
129.2
129.1
128.9
128.5
128.3
126.7
111.5
111.4
77.5
77.2
76.8
62.0
56.2
47.9
18.6
13C NMR (101 MHz, CDCl3)
N(SO2Ph)2
Br
O
(PhO2S)2N
2q
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

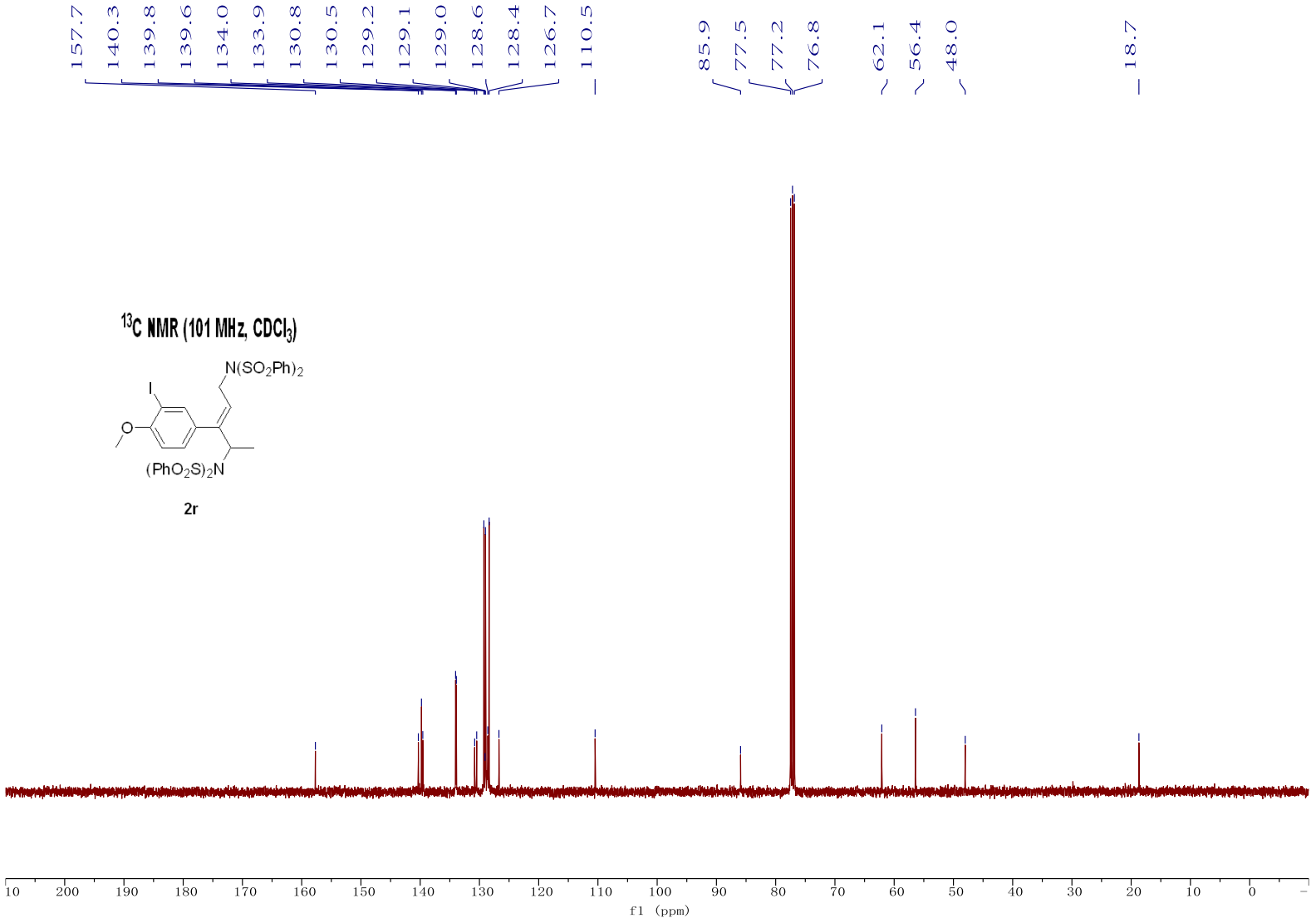


^{1}H NMR (400 MHz, $CDCl_3$)

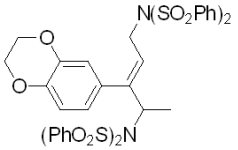


2r

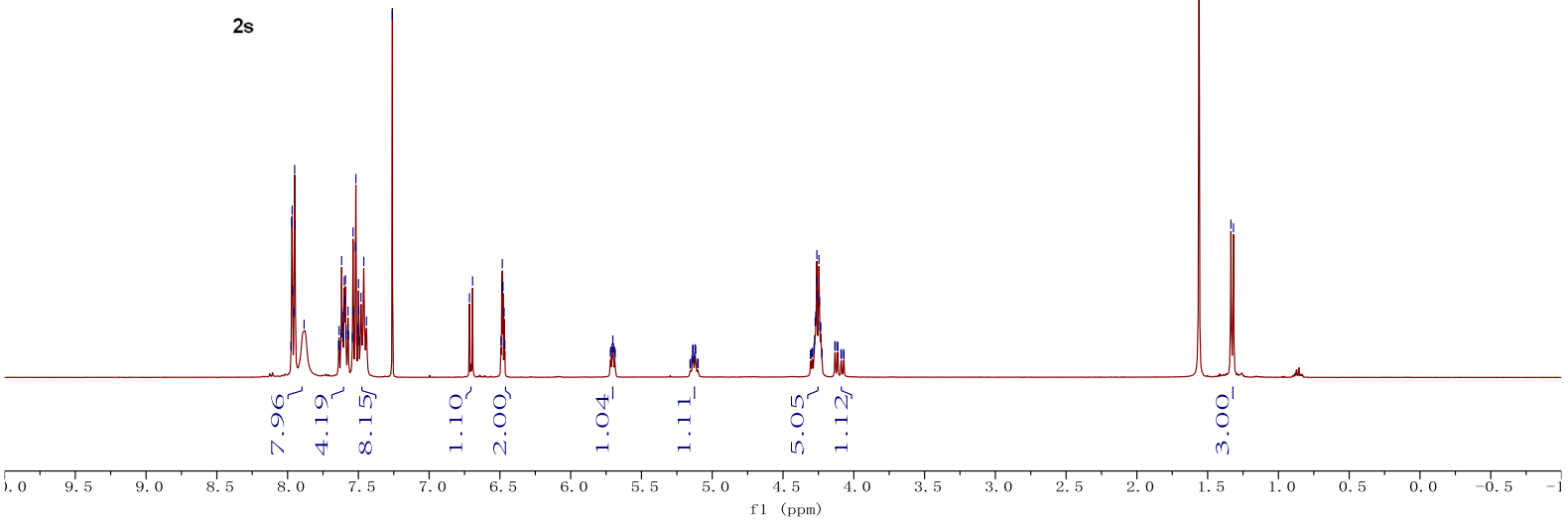



157.7
140.3
139.8
139.6
134.0
133.9
130.8
130.5
129.2
129.1
129.0
128.6
128.4
126.7
110.5
85.9
77.5
77.2
76.8
62.1
56.4
48.0
18.7
13C NMR (101 MHz, CDCl3)
N(SO2Ph)2
I
O
(PhO2S)2N
2r
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

^{1}H NMR (400 MHz, $CDCl_3$)

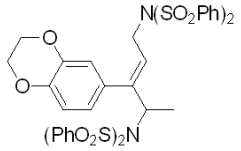


2s

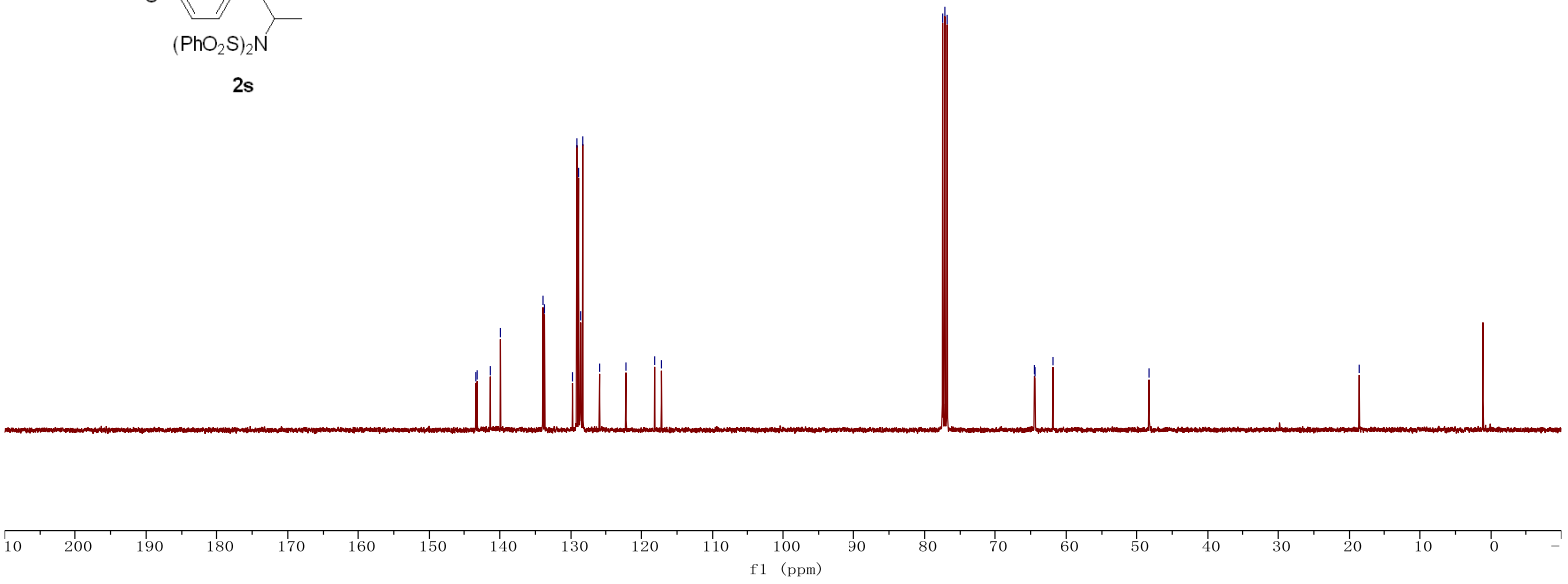


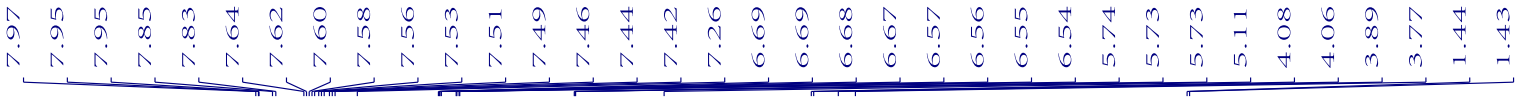
143.4
143.2
141.3
139.9
133.9
133.7
129.8
129.2
128.9
128.7
128.4
125.9
122.2
118.1
117.2
77.5
77.2
76.8
64.5
64.4
61.9
48.3
18.6

^{13}C NMR (101 MHz, $CDCl_3$)

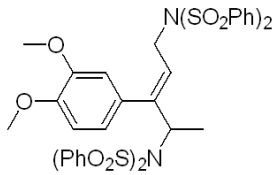


2s

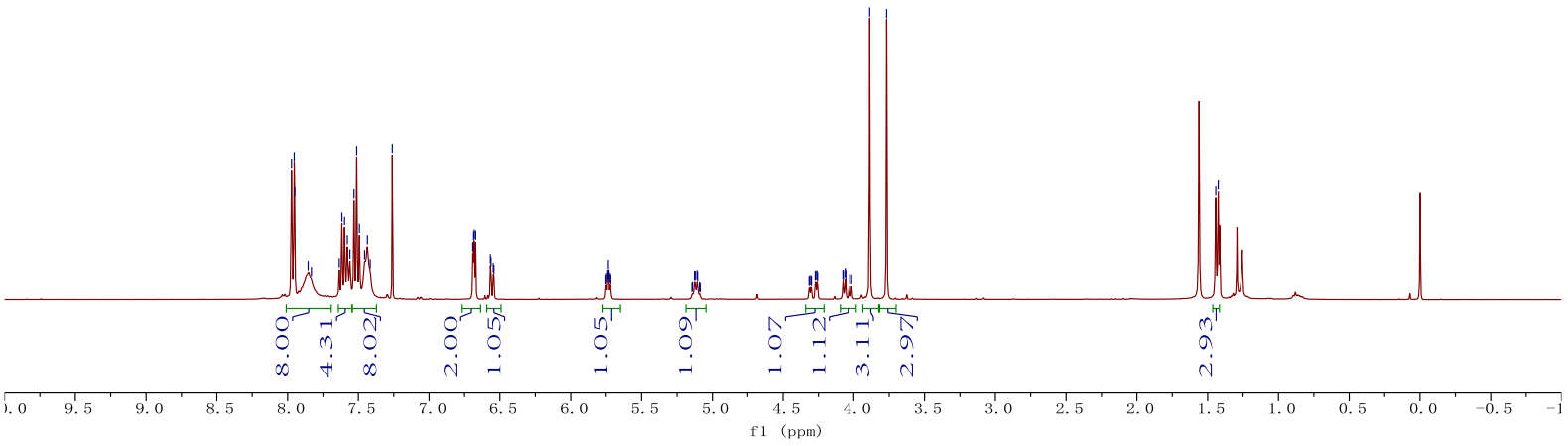


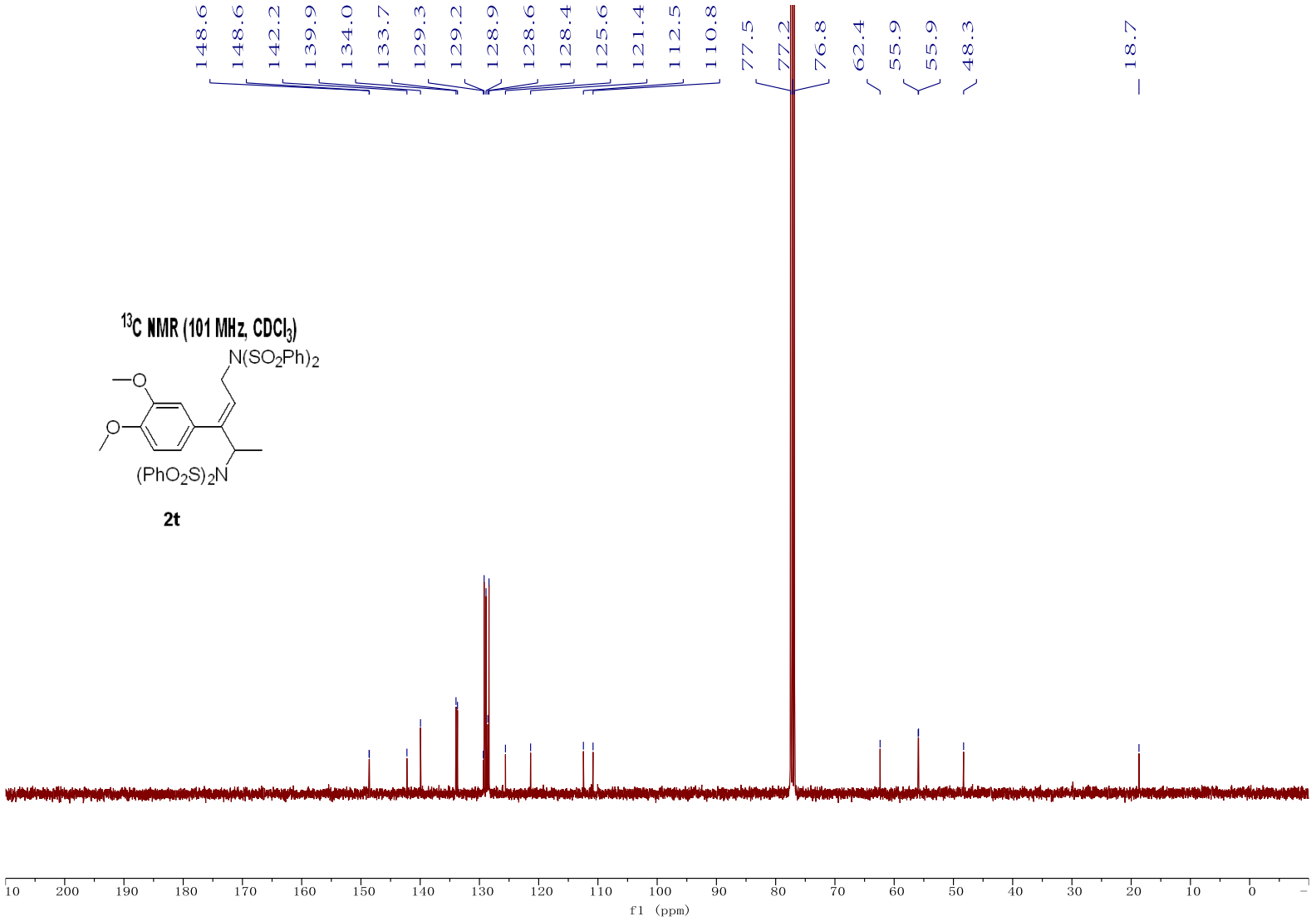


^{1}H NMR (400 MHz, $CDCl_3$)

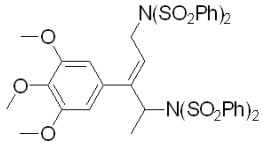


2t

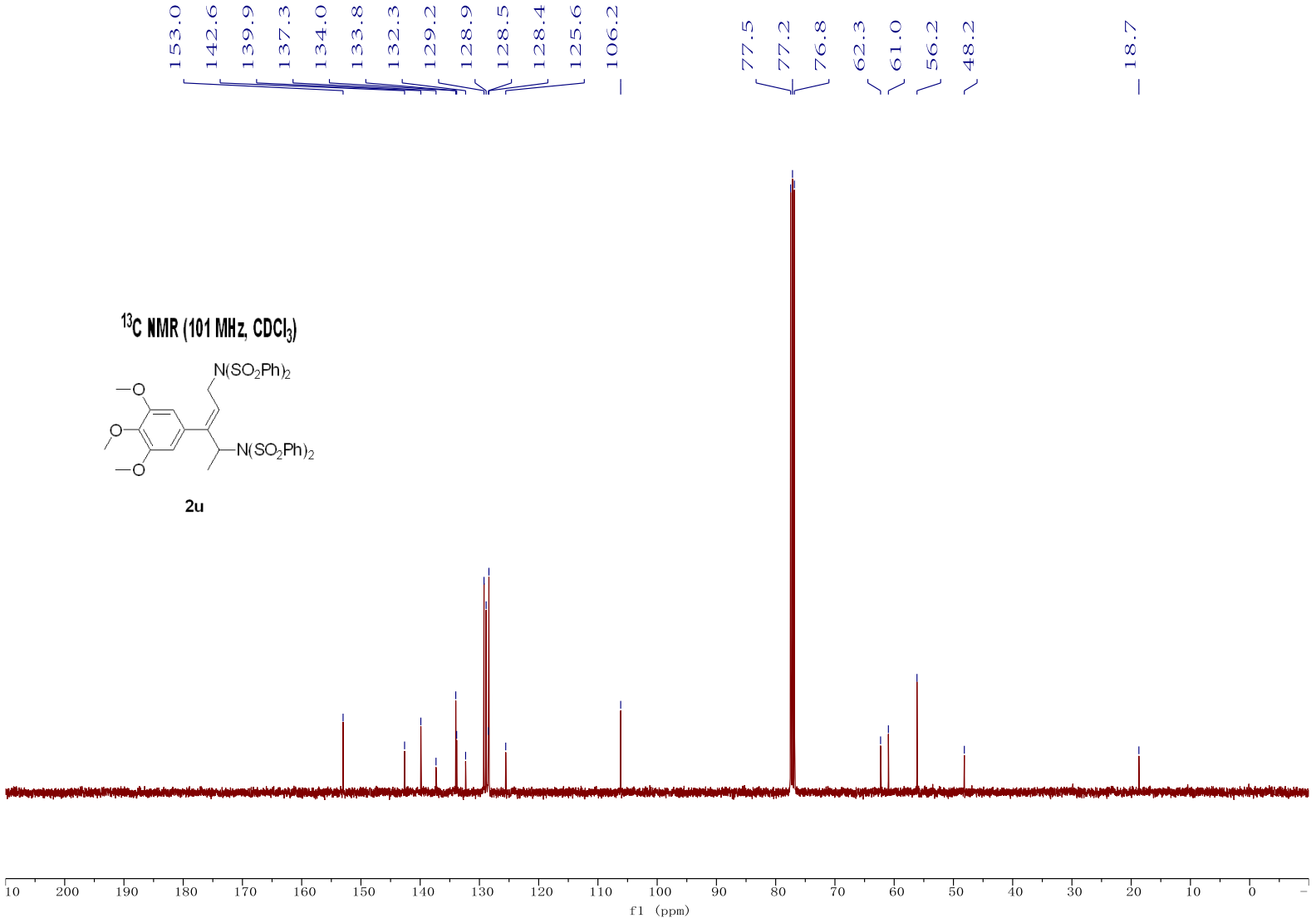


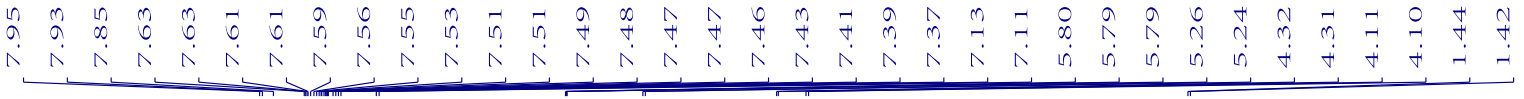

148.6
148.6
142.2
139.9
134.0
133.7
129.3
129.2
128.9
128.6
128.4
125.6
121.4
112.5
110.8
77.5
77.2
76.8
62.4
55.9
55.9
48.3
18.7
13C NMR (101 MHz, CDCl3)
N(SO2Ph)2
O
O
(PhO2S)2N
2t
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

^{1}H NMR (400 MHz, $CDCl_3$)

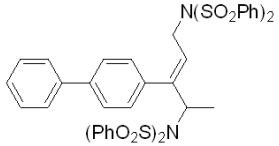


2u

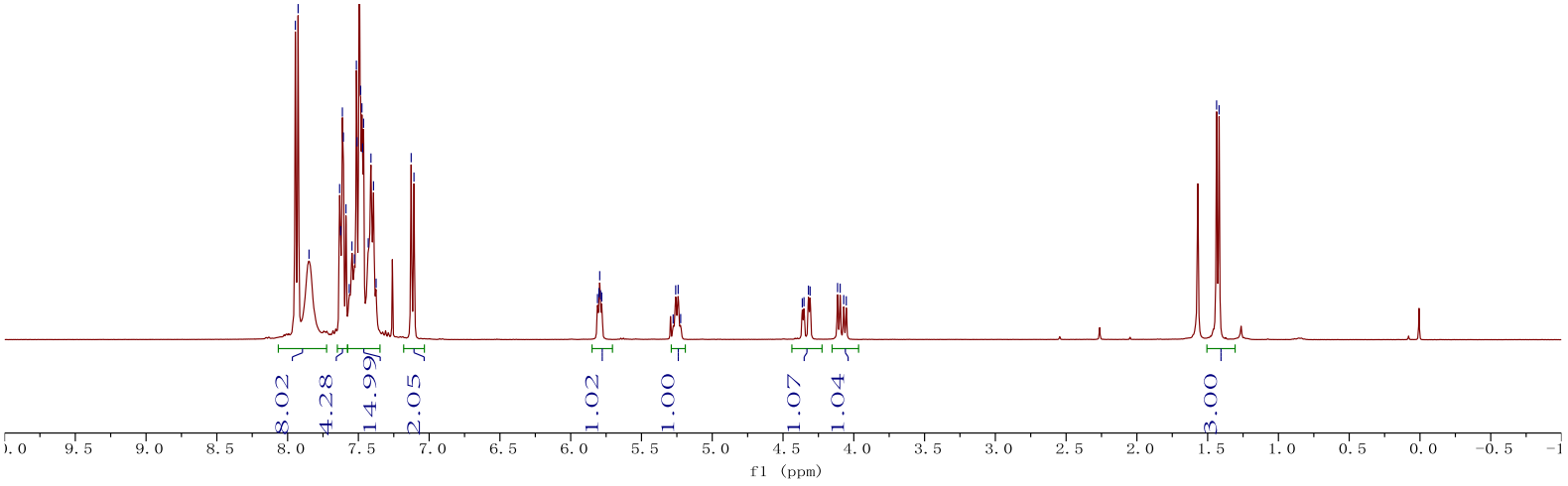

153.0
142.6
139.9
137.3
134.0
133.8
132.3
129.2
128.9
128.5
128.4
125.6
106.2
77.5
77.2
76.8
62.3
61.0
56.2
48.2
18.7
13C NMR (101 MHz, CDCl3)
N(SO2Ph)2
N(SO2Ph)2
2u
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



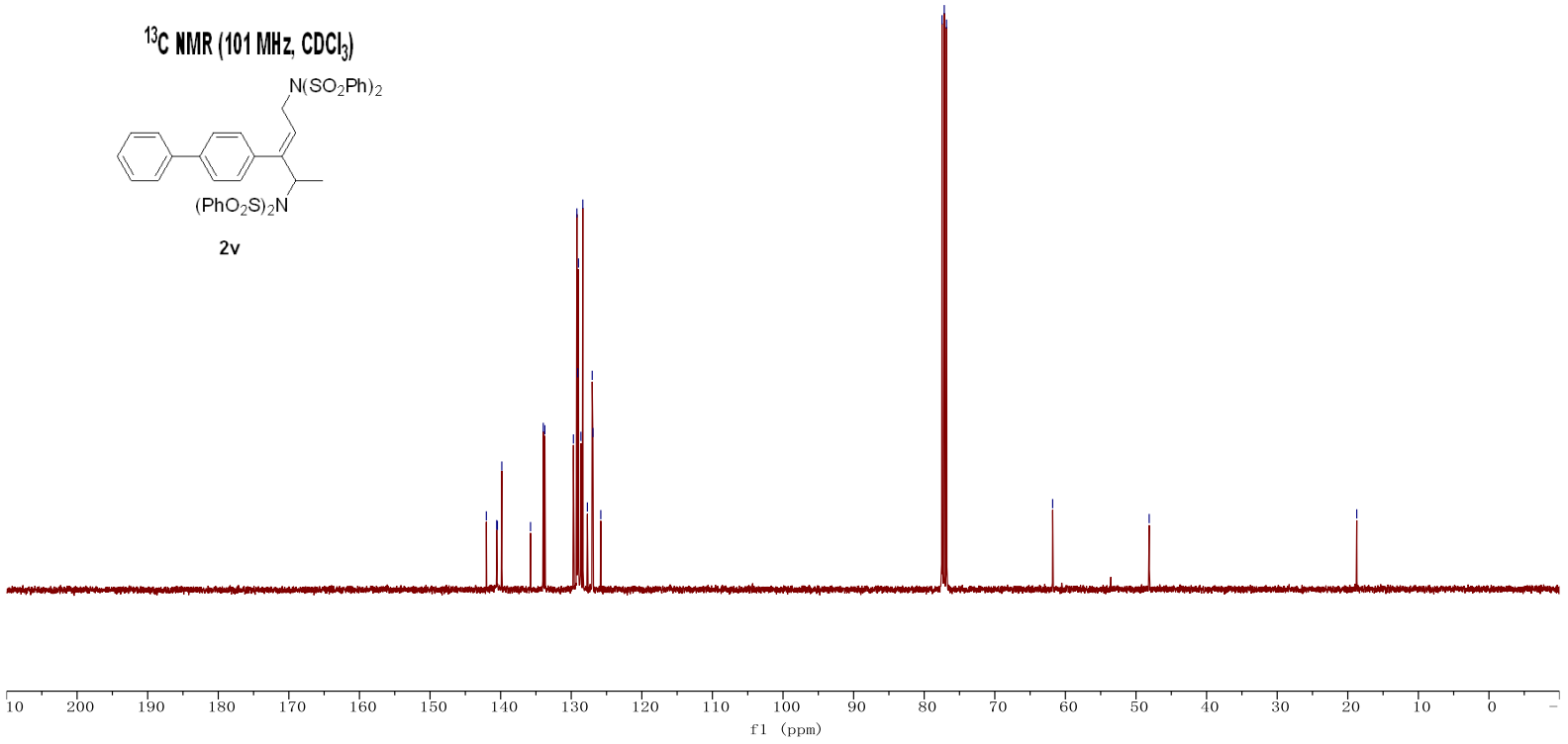
^{1}H NMR (400 MHz, $CDCl_3$)

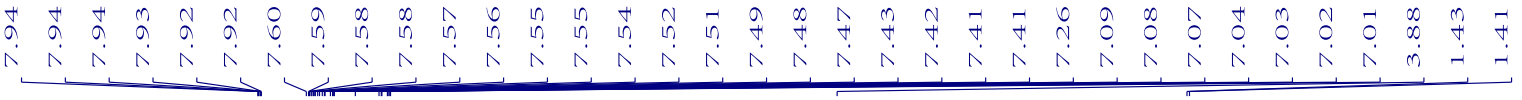


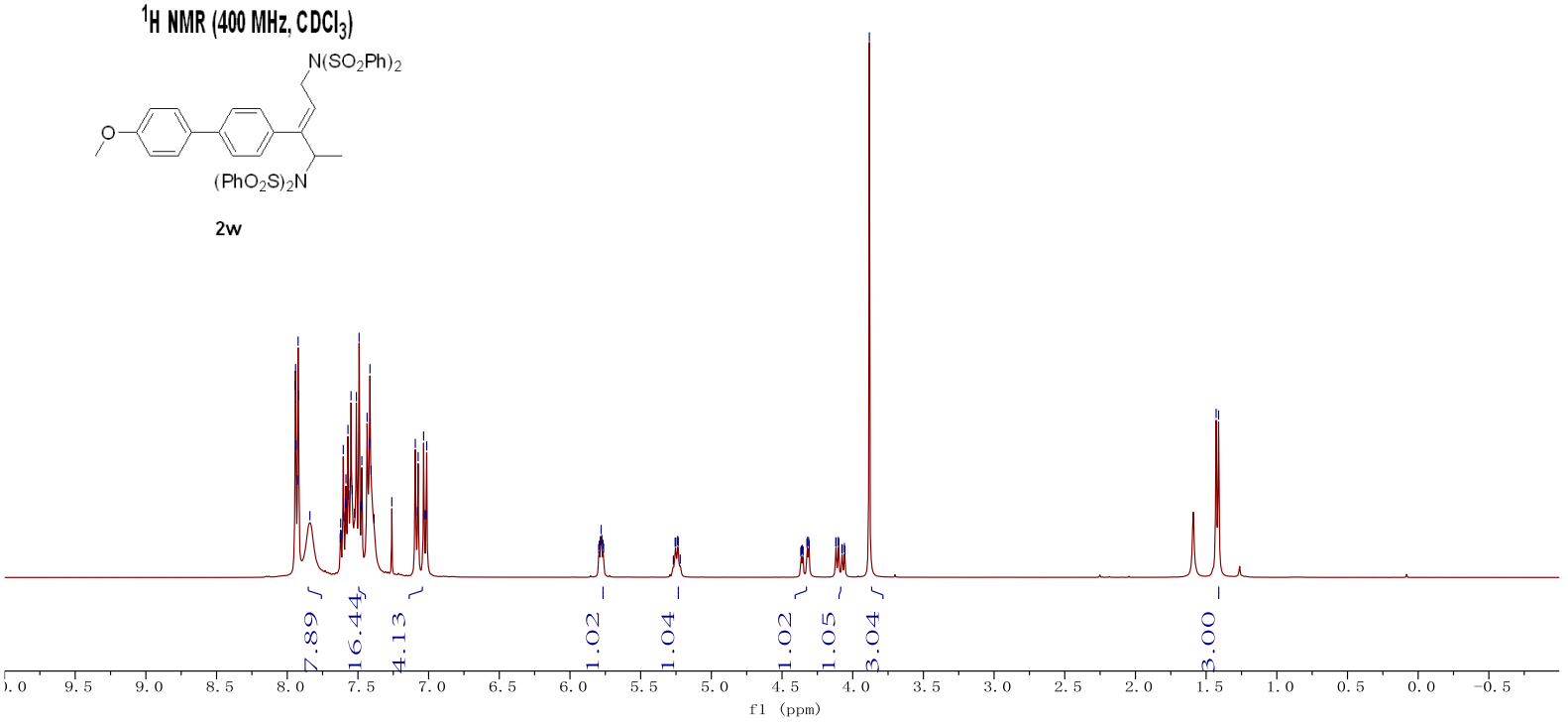
2v



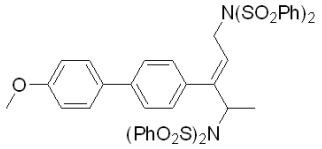

142.0
140.6
140.5
139.8
135.8
134.0
133.7
129.7
129.2
129.1
129.0
128.6
128.4
127.7
127.0
126.9
125.8
77.5
77.2
76.8
61.8
48.1
18.7


13C NMR (101 MHz, CDCl3)
N(SO2Ph)2
(PhO2S)2N
2v
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.94
7.94
7.94
7.93
7.92
7.92
7.60
7.59
7.58
7.58
7.57
7.56
7.55
7.55
7.54
7.52
7.51
7.49
7.48
7.47
7.43
7.42
7.41
7.41
7.26
7.09
7.08
7.07
7.04
7.03
7.02
7.01
3.88
1.43
1.41

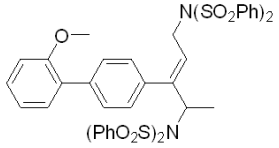

1H NMR (400 MHz, CDCl3)
N(SO2Ph)2
O
(PhO2S)2N
2w
7.89
16.44
4.13
1.02
1.04
1.02
1.05
3.04
3.00
f1 (ppm)

^{13}C NMR (101 MHz, $CDCl_3$)

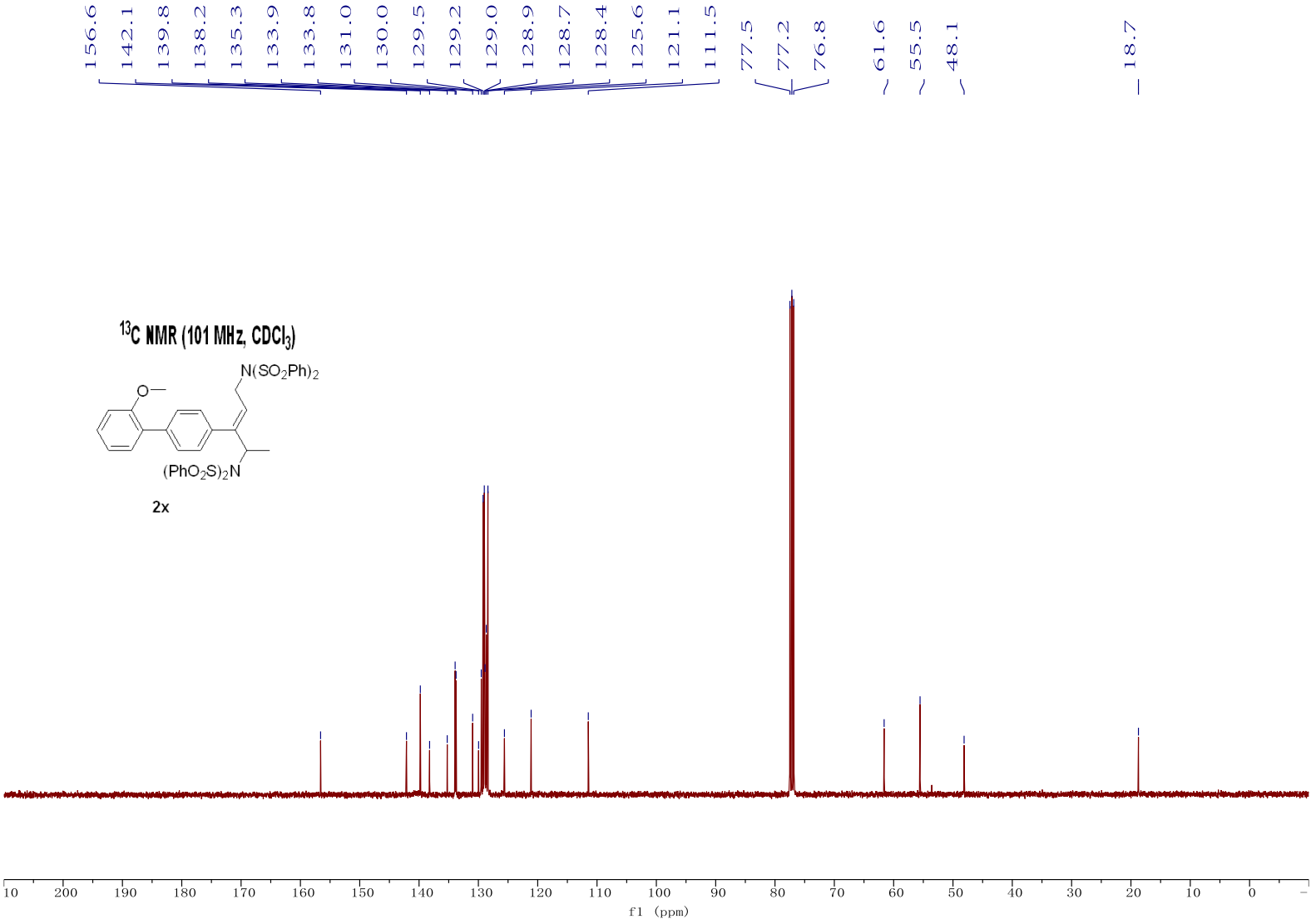


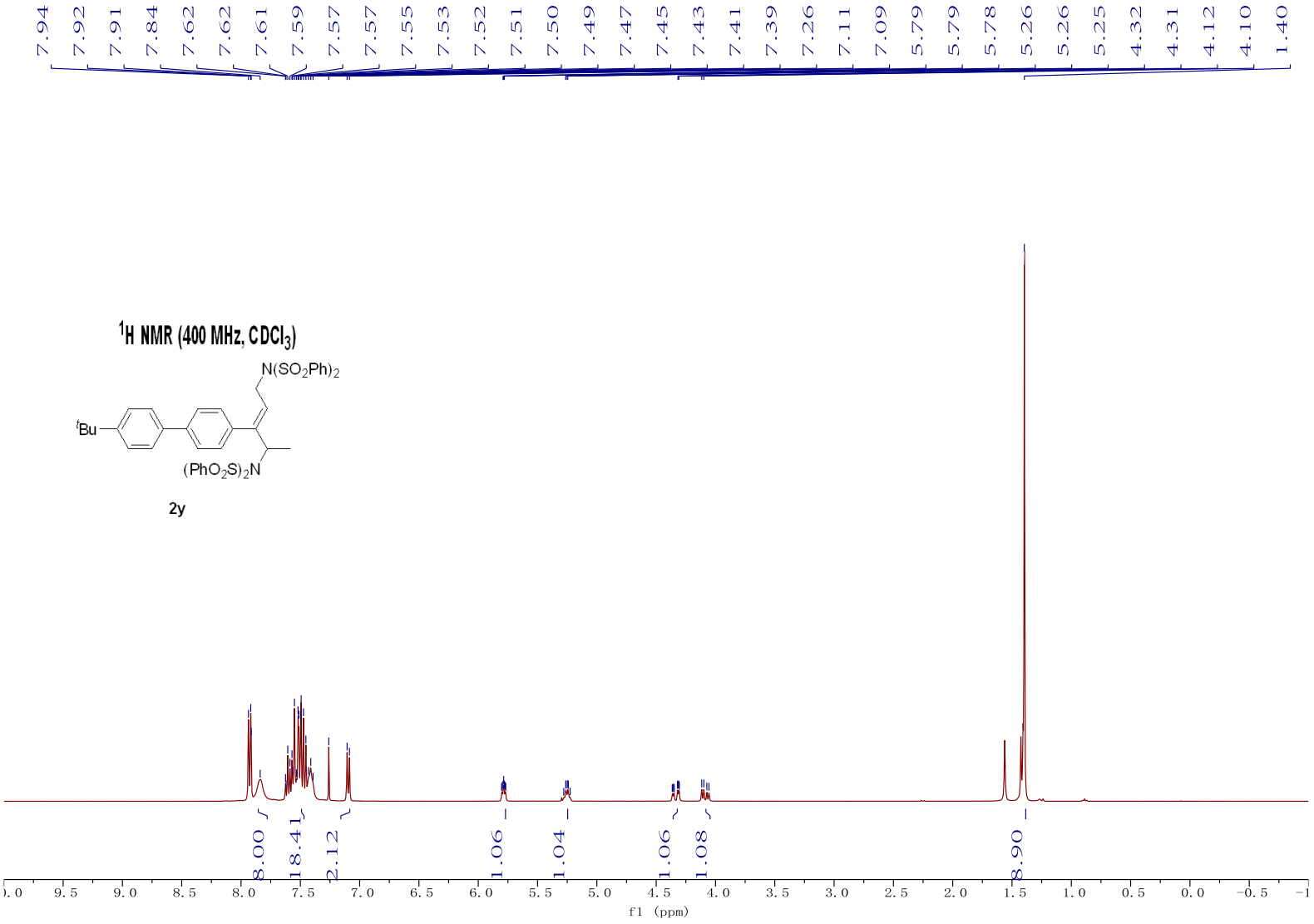
2w

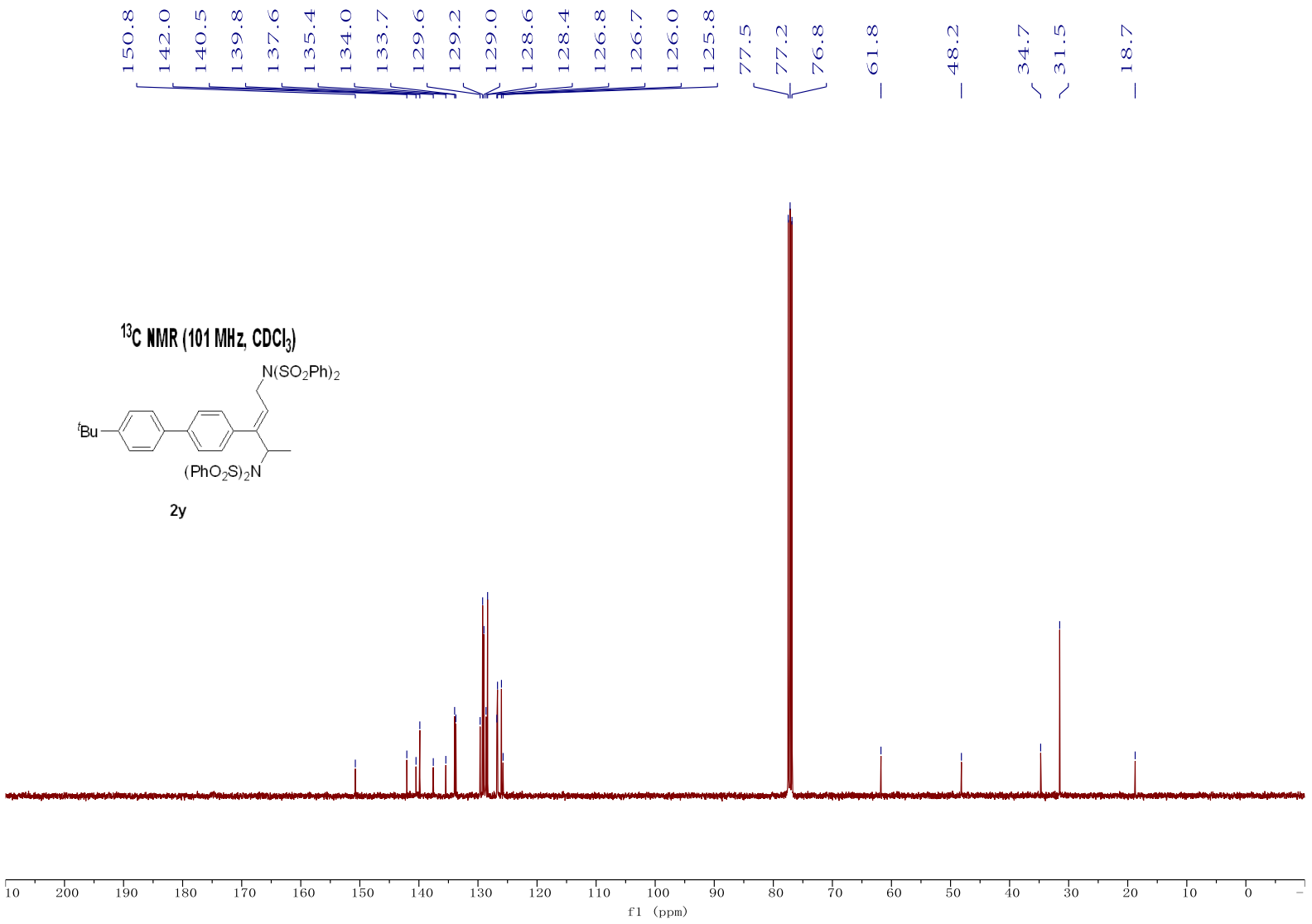
^{1}H NMR (400 MHz, $CDCl_3$)



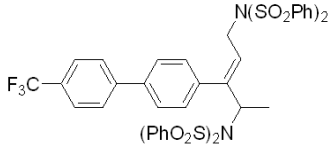
2x


156.6
142.1
139.8
138.2
135.3
133.9
133.8
131.0
130.0
129.5
129.2
129.0
128.9
128.7
128.4
125.6
121.1
111.5
77.5
77.2
76.8
61.6
55.5
48.1
18.7
13C NMR (101 MHz, CDCl3)
N(SO2Ph)2
O
(PhO2S)2N
2x
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

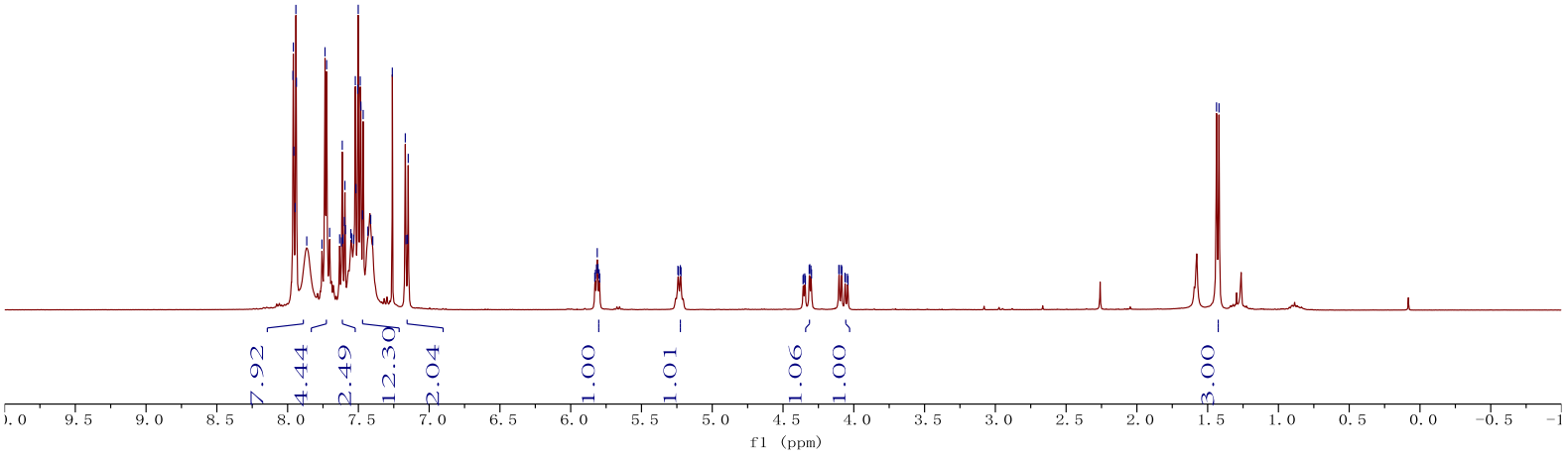

7.94
7.92
7.91
7.84
7.62
7.62
7.61
7.59
7.57
7.57
7.55
7.53
7.52
7.51
7.50
7.49
7.47
7.45
7.43
7.41
7.39
7.26
7.11
7.09
5.79
5.79
5.78
5.26
5.26
5.25
4.32
4.31
4.12
4.10
1.40
1H NMR (400 MHz, CDCl3)
N(SO2Ph)2
tBu
(PhO2S)2N
2y
8.00
18.41
2.12
1.06
1.04
1.06
1.08
8.90
f1 (ppm)

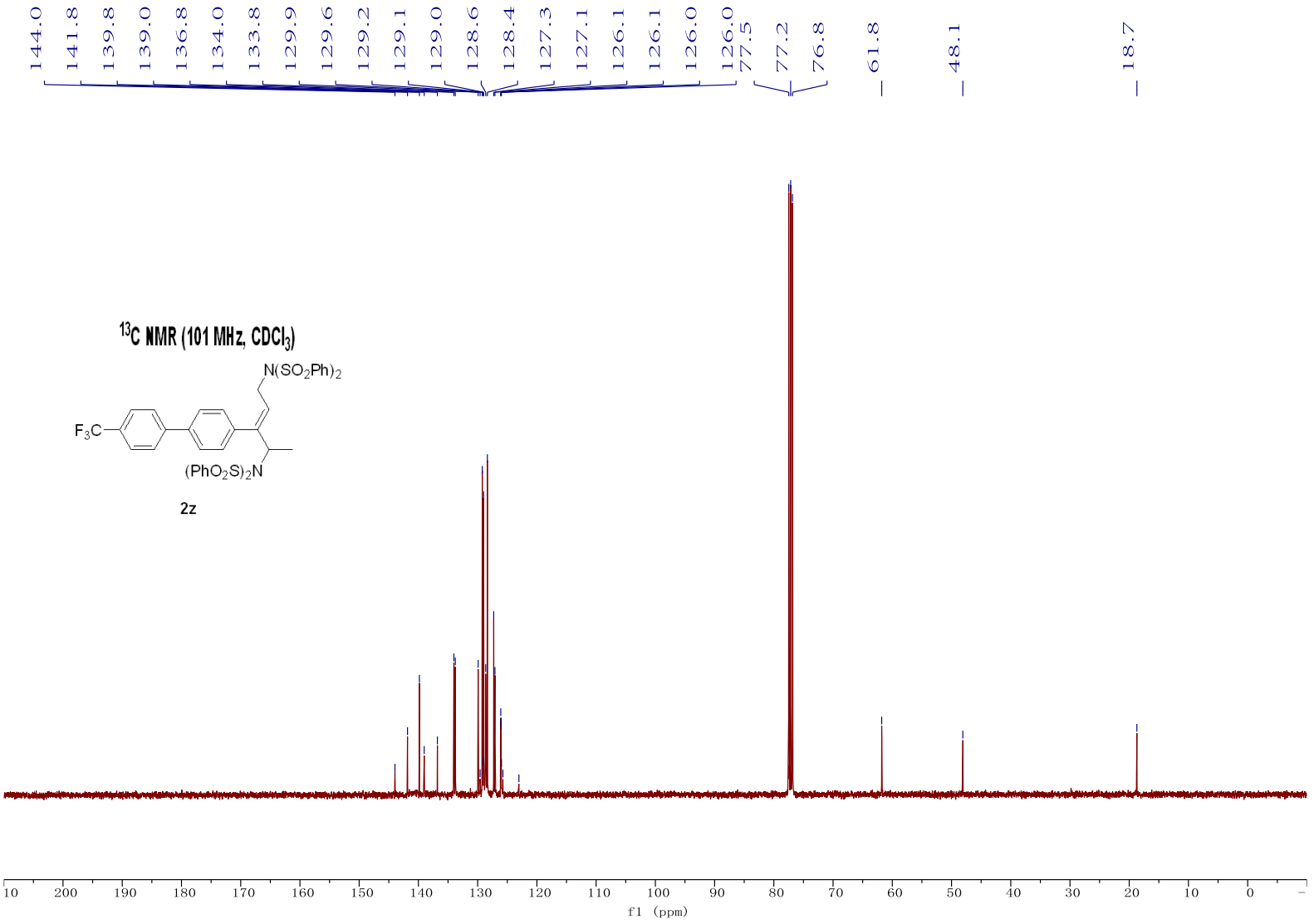

150.8
142.0
140.5
139.8
137.6
135.4
134.0
133.7
129.6
129.2
129.0
128.6
128.4
126.8
126.7
126.0
125.8
77.5
77.2
76.8
61.8
48.2
34.7
31.5
18.7
13C NMR (101 MHz, CDCl3)
N(SO2Ph)2
tBu
(PhO2S)2N
2y
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

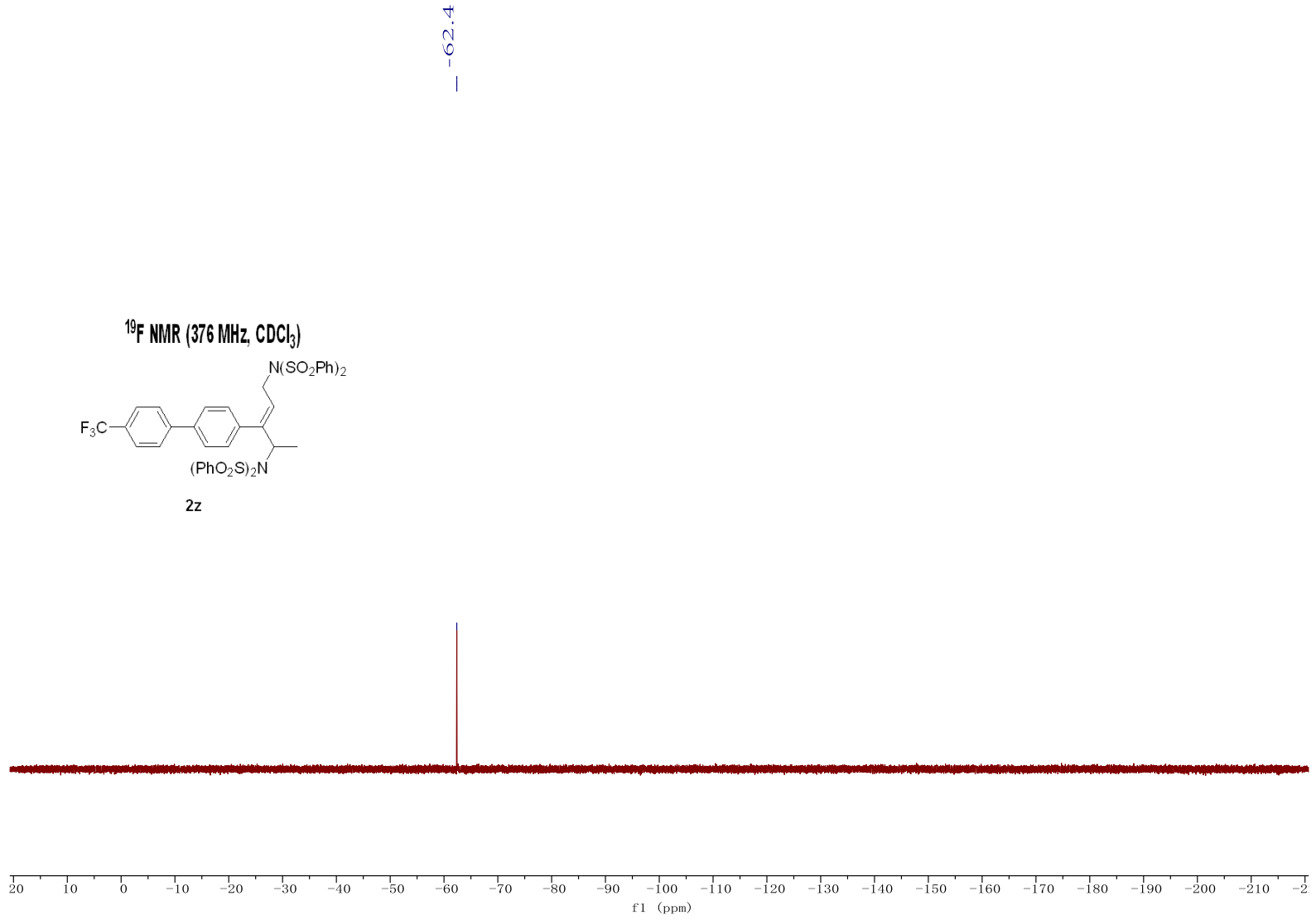
^{1}H NMR (400 MHz, $CDCl_3$)



2z




144.0
141.8
139.8
139.0
136.8
134.0
133.8
129.9
129.6
129.2
129.1
129.0
128.6
128.4
127.3
127.1
126.1
126.1
126.0
126.0
77.5
77.2
76.8
61.8
48.1
18.7
13C NMR (101 MHz, CDCl3)
N(SO2Ph)2
F3C
(PhO2S)2N
2z
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-62.4
19F NMR (376 MHz, CDCl3)
N(SO2Ph)2
F3C
(PhO2S)2N
2z
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
f1 (ppm)


7.95
7.93
7.85
7.63
7.61
7.59
7.58
7.57
7.56
7.56
7.55
7.53
7.52
7.50
7.48
7.43
7.41
7.39
7.26
7.19
7.17
7.16
7.15
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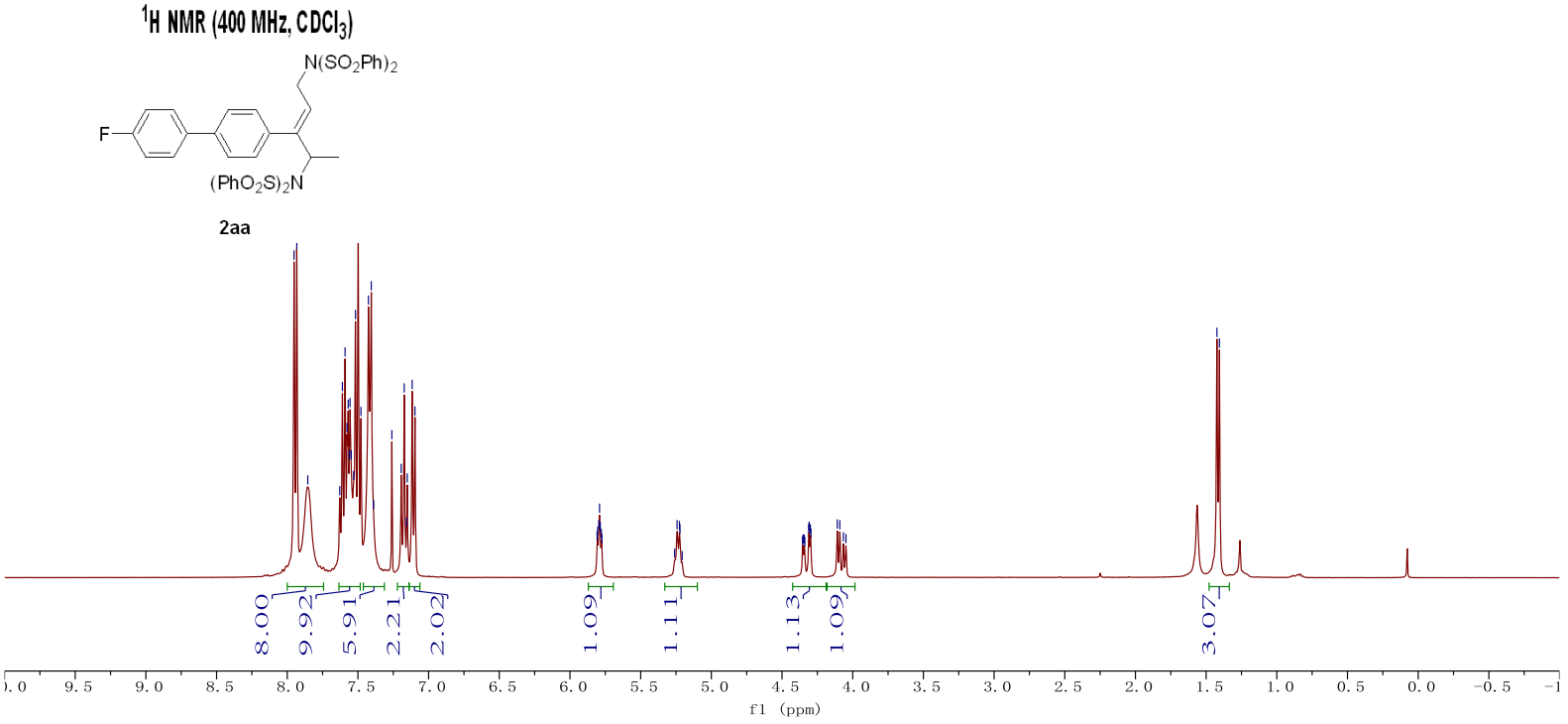
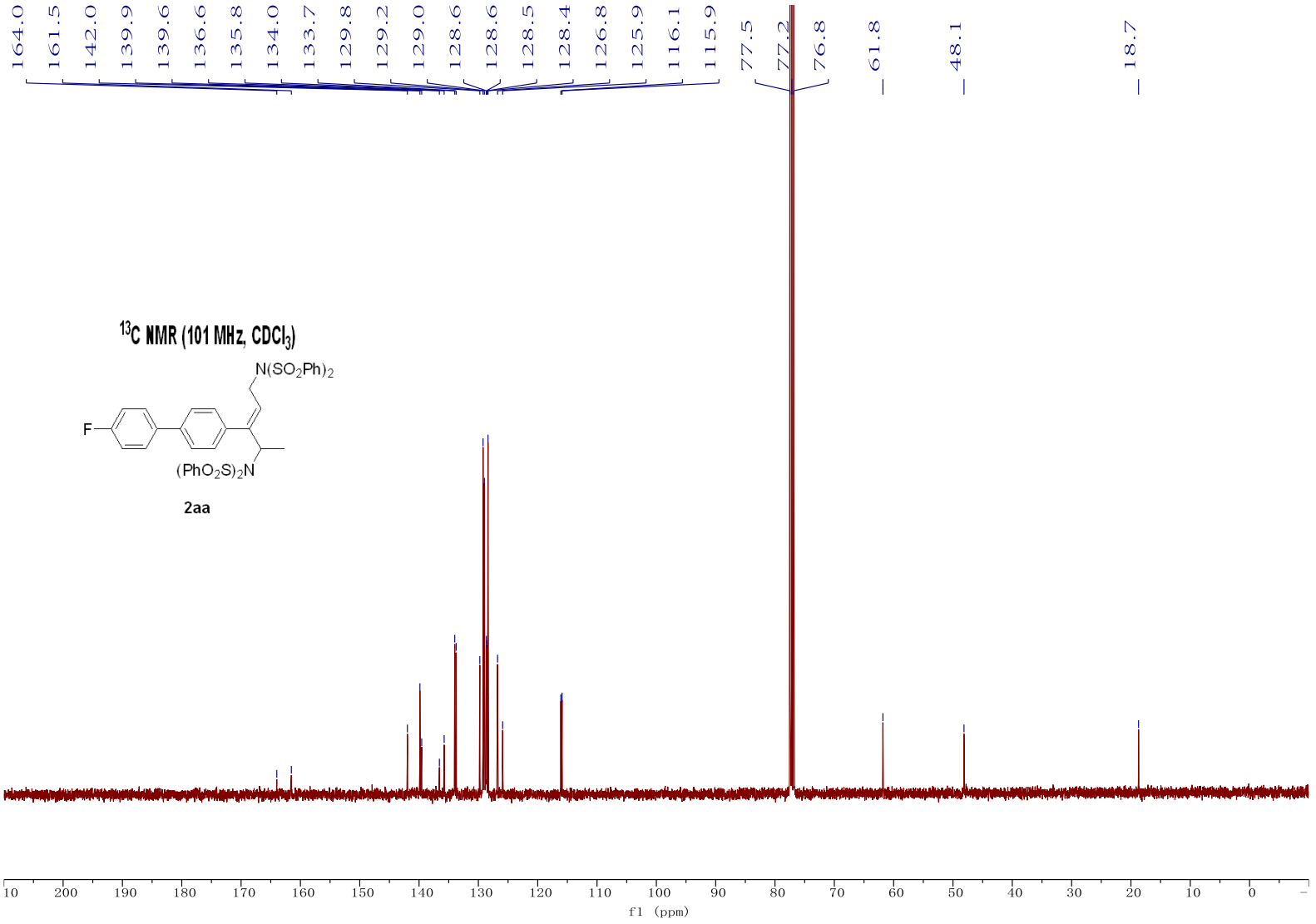
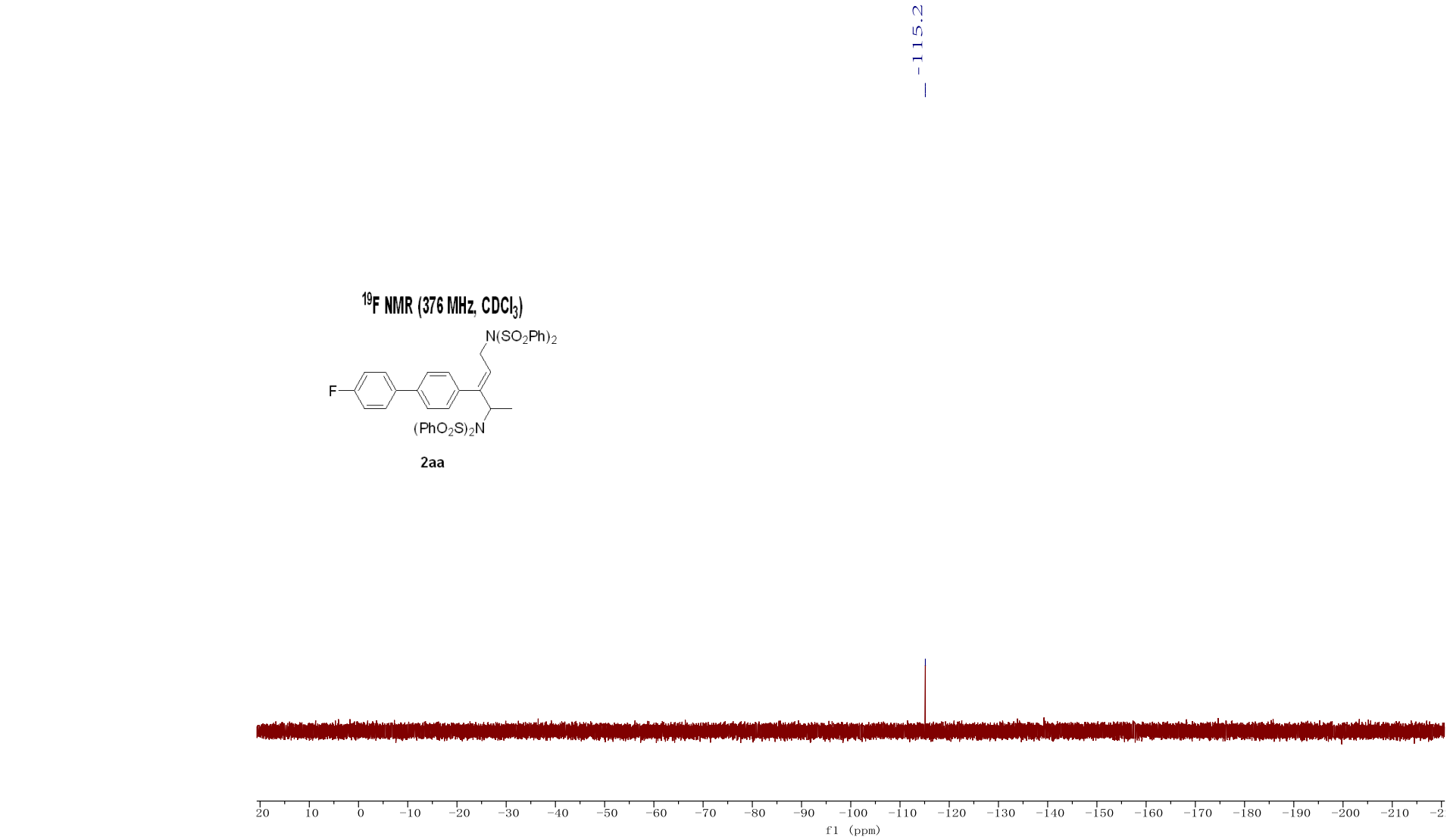
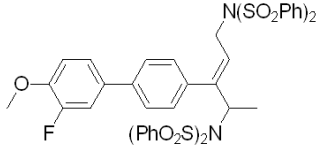
5.23
4.31
4.11
4.09
1.42
1.41


1H NMR (400 MHz, CDCl3)
N(SO2Ph)2
F
(PhO2S)2N
2aa
8.00
9.92
5.91
2.21
2.02
1.09
1.11
1.13
1.09
3.07
f1 (ppm)


164.0
161.5
142.0
139.9
139.6
136.6
135.8
134.0
133.7
129.8
129.2
129.0
128.6
128.6
128.5
128.4
126.8
125.9
116.1
115.9
77.5
77.2
76.8
61.8
48.1
18.7
13C NMR (101 MHz, CDCl3)
N(SO2Ph)2
F
(PhO2S)2N
2aa
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

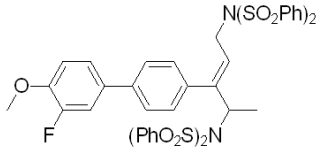

-115.2
19F NMR (376 MHz, CDCl3)
N(SO2Ph)2
F
(PhO2S)2N
2aa
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -2
f1 (ppm)

^{1}H NMR (400 MHz, $CDCl_3$)

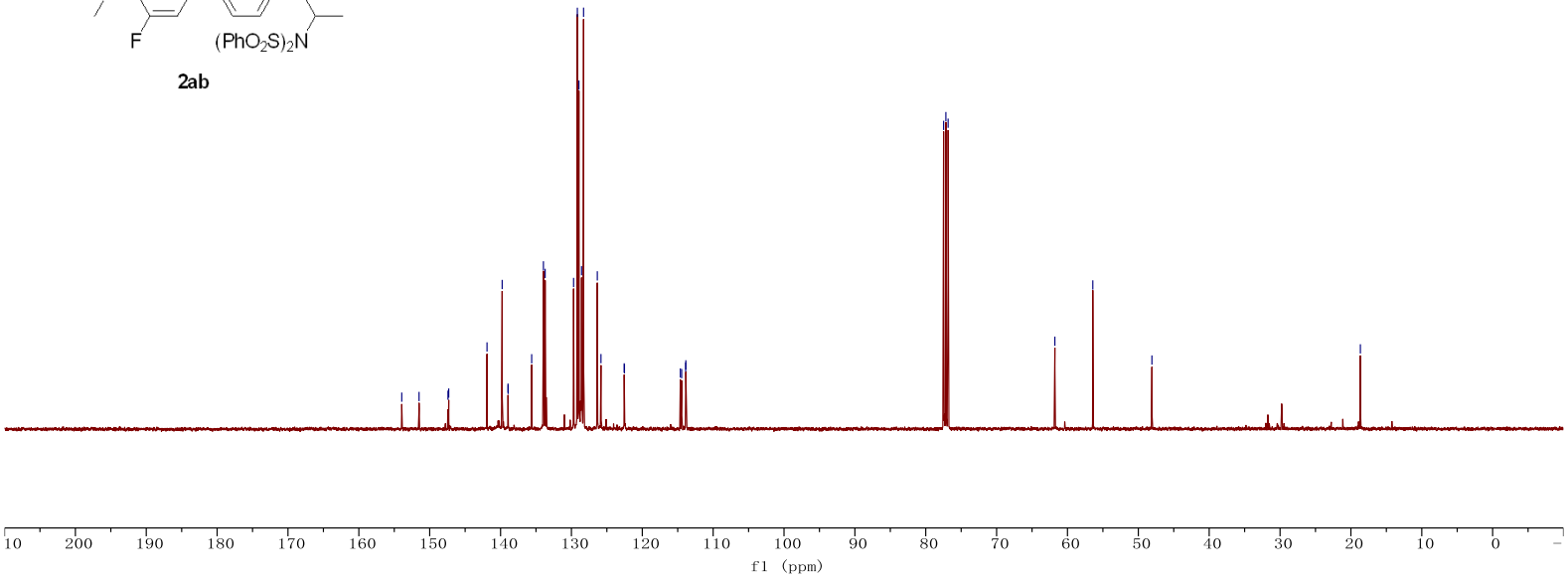


2ab

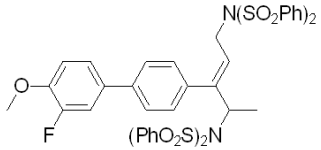
^{13}C NMR (101 MHz, $CDCl_3$)



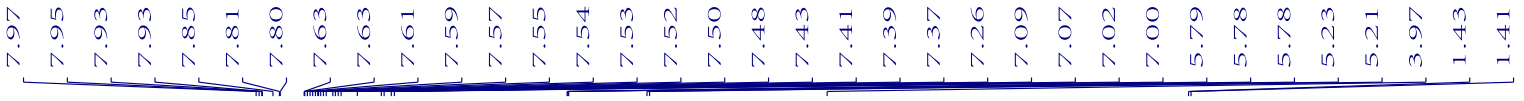
2ab



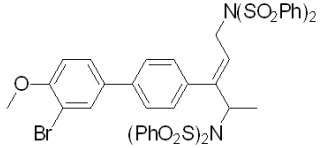
^{19}F NMR (376 MHz, $CDCl_3$)



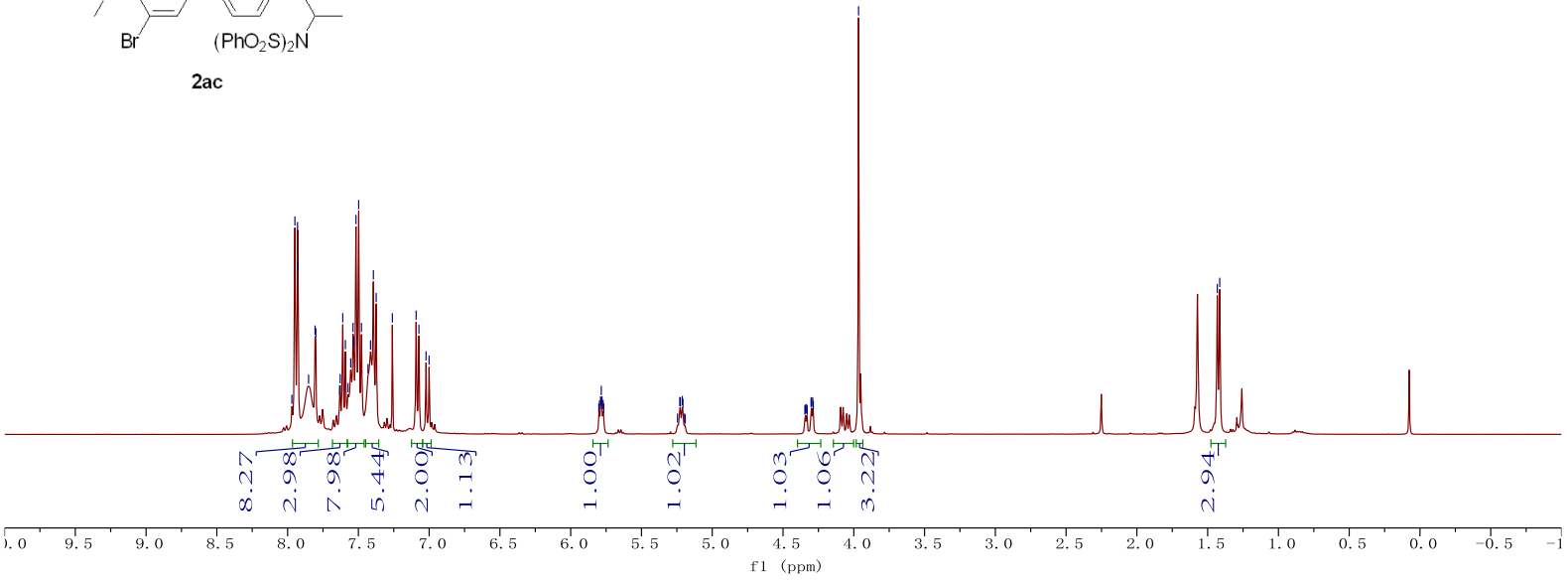
2ab

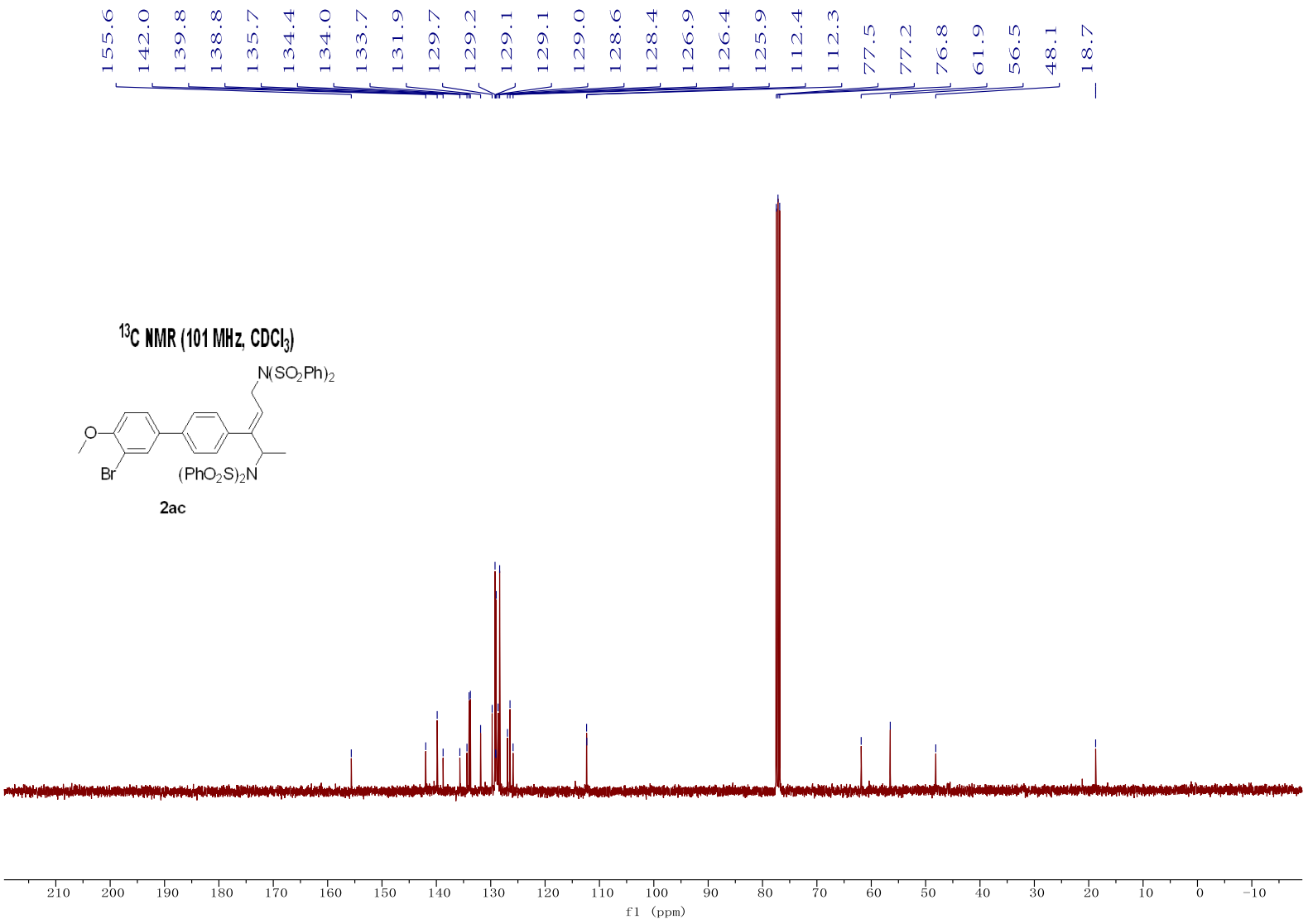


^{1}H NMR (400 MHz, $CDCl_3$)

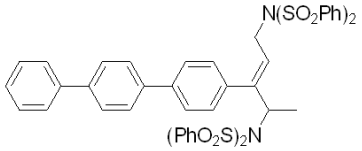


2ac

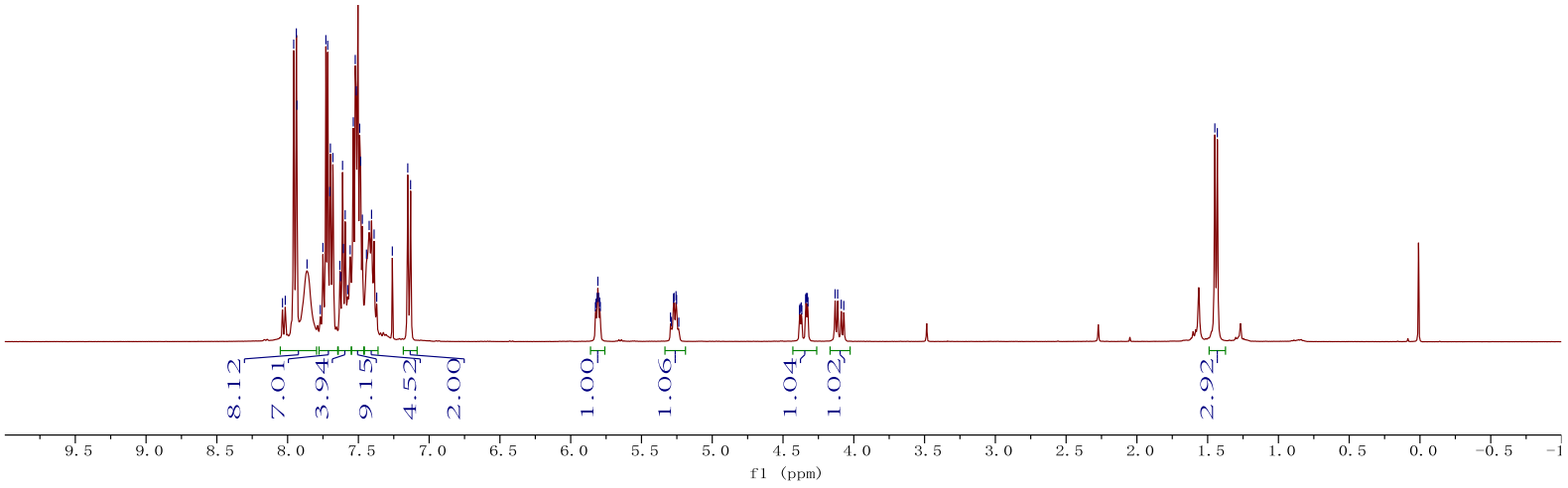


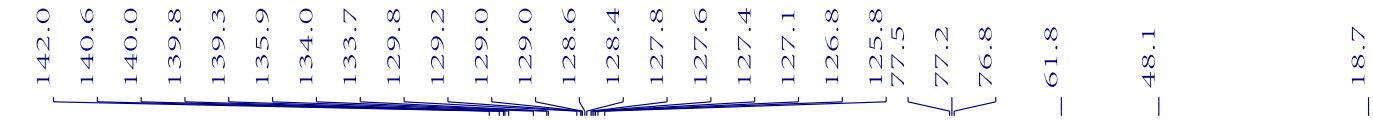

155.6
142.0
139.8
138.8
135.7
134.4
134.0
133.7
131.9
129.7
129.2
129.1
129.1
129.0
128.6
128.4
126.9
126.4
125.9
112.4
112.3
77.5
77.2
76.8
61.9
56.5
48.1
18.7
13C NMR (101 MHz, CDCl3)
N(SO2Ph)2
O
Br
(PhO2S)2N
2ac
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

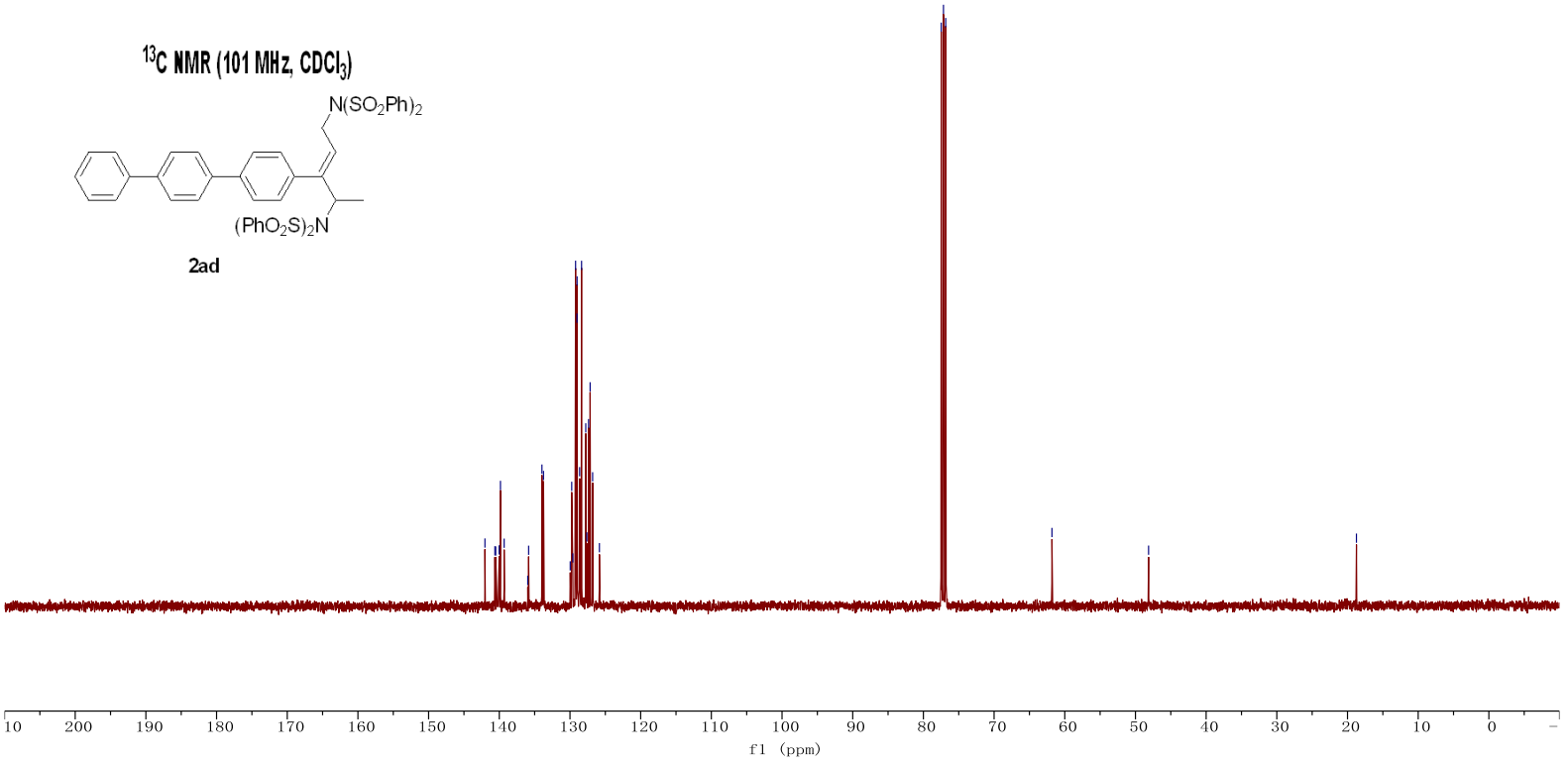
^{1}H NMR (400 MHz, $CDCl_3$)

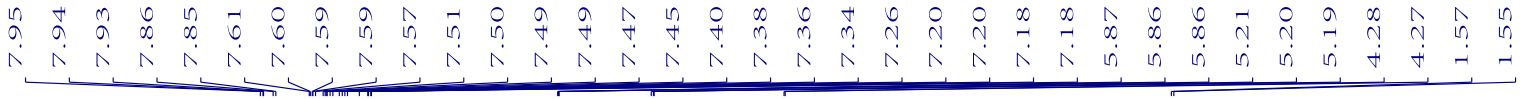


2ad

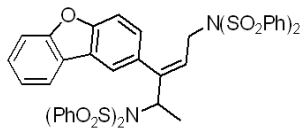



142.0
140.6
140.0
139.8
139.3
135.9
134.0
133.7
129.8
129.2
129.0
129.0
128.6
128.4
127.8
127.6
127.4
127.1
126.8
125.8
77.5
77.2
76.8
61.8
48.1
18.7

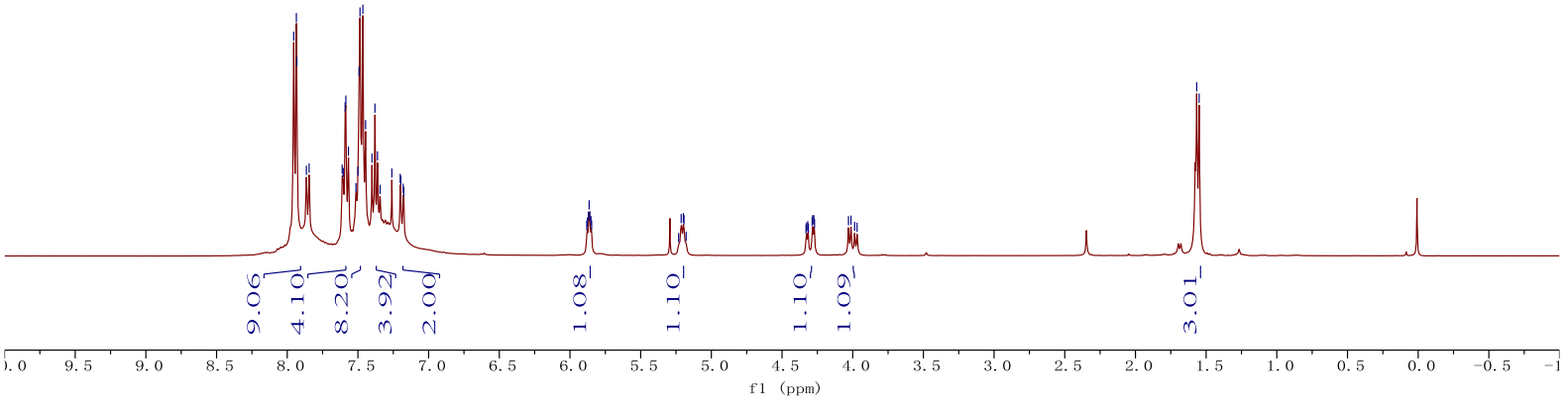

13C NMR (101 MHz, CDCl3)
N(SO2Ph)2
(PhO2S)2N
2ad
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

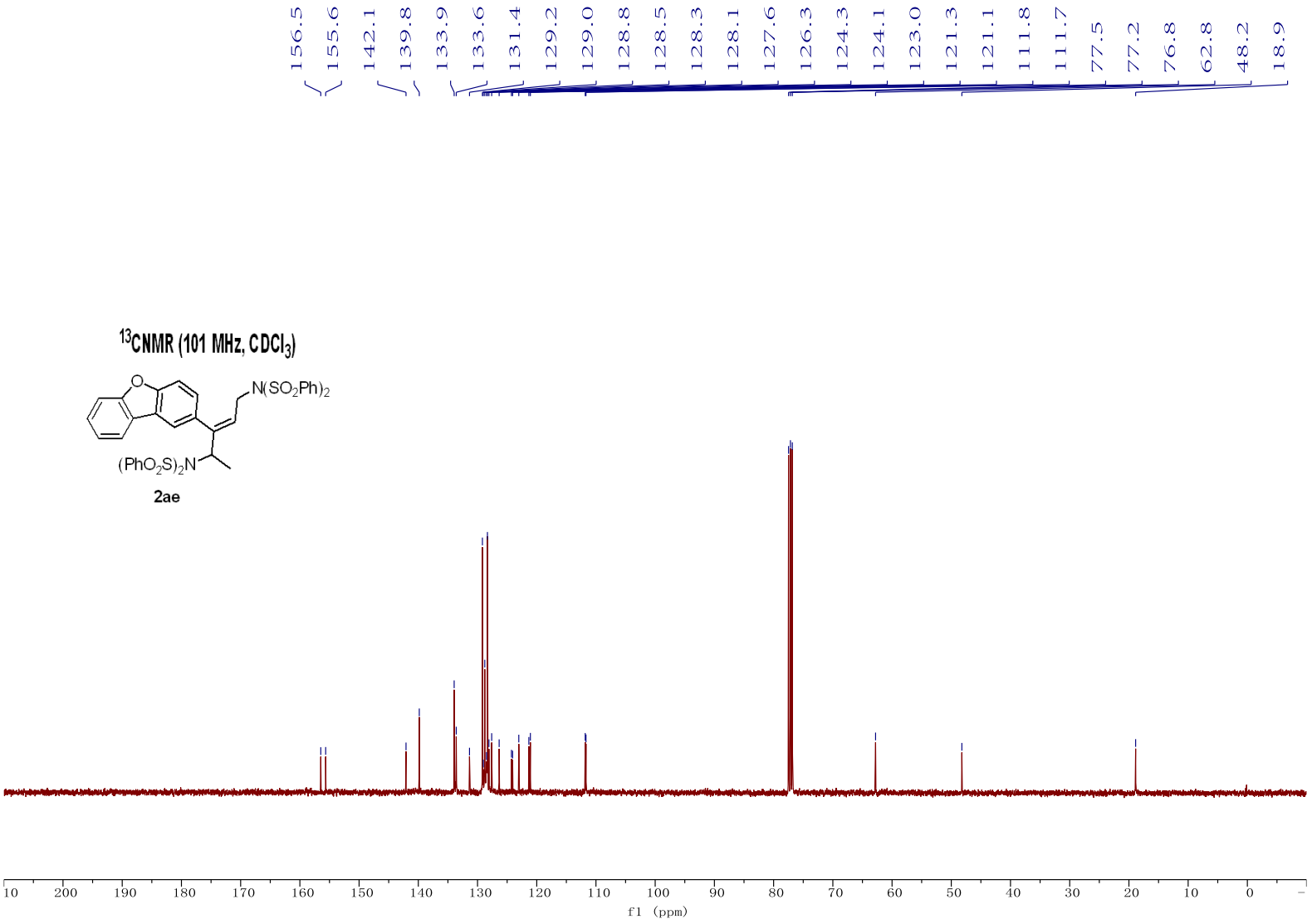


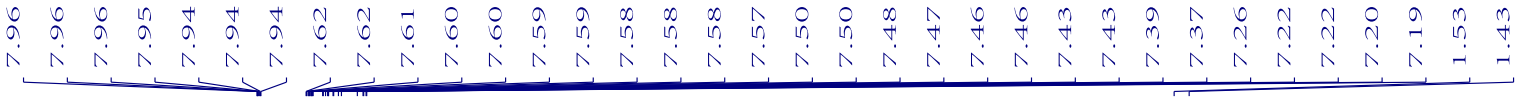
^{1}HNMR (400 MHz, $CDCl_3$)



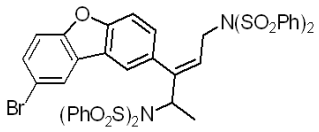
2ae



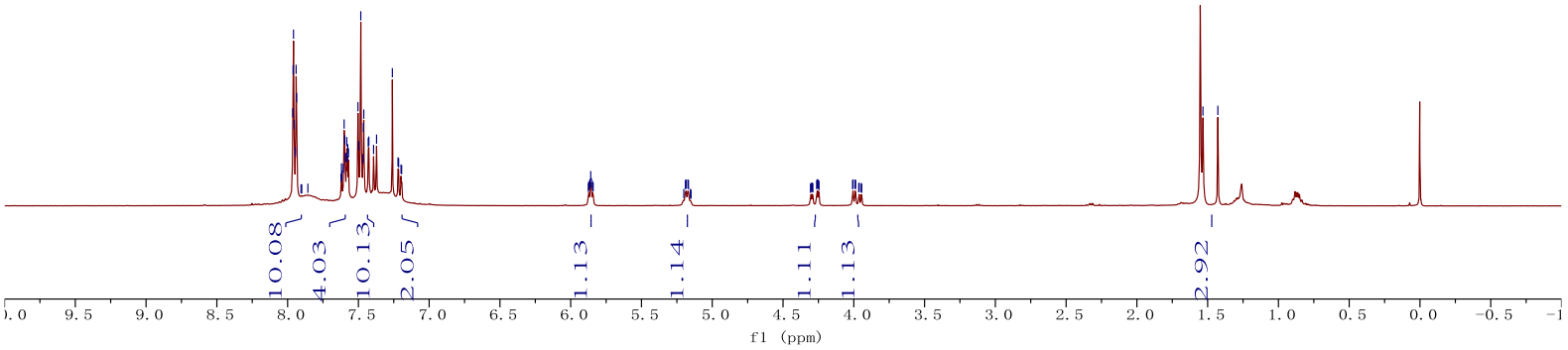

156.5
155.6
142.1
139.8
133.9
133.6
131.4
129.2
129.0
128.8
128.5
128.3
128.1
127.6
126.3
124.3
124.1
123.0
121.3
121.1
111.8
111.7
77.5
77.2
76.8
62.8
48.2
18.9
13CNMR (101 MHz, CDCl3)
N(SO2Ph)2
(PhO2S)2N
2ae
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

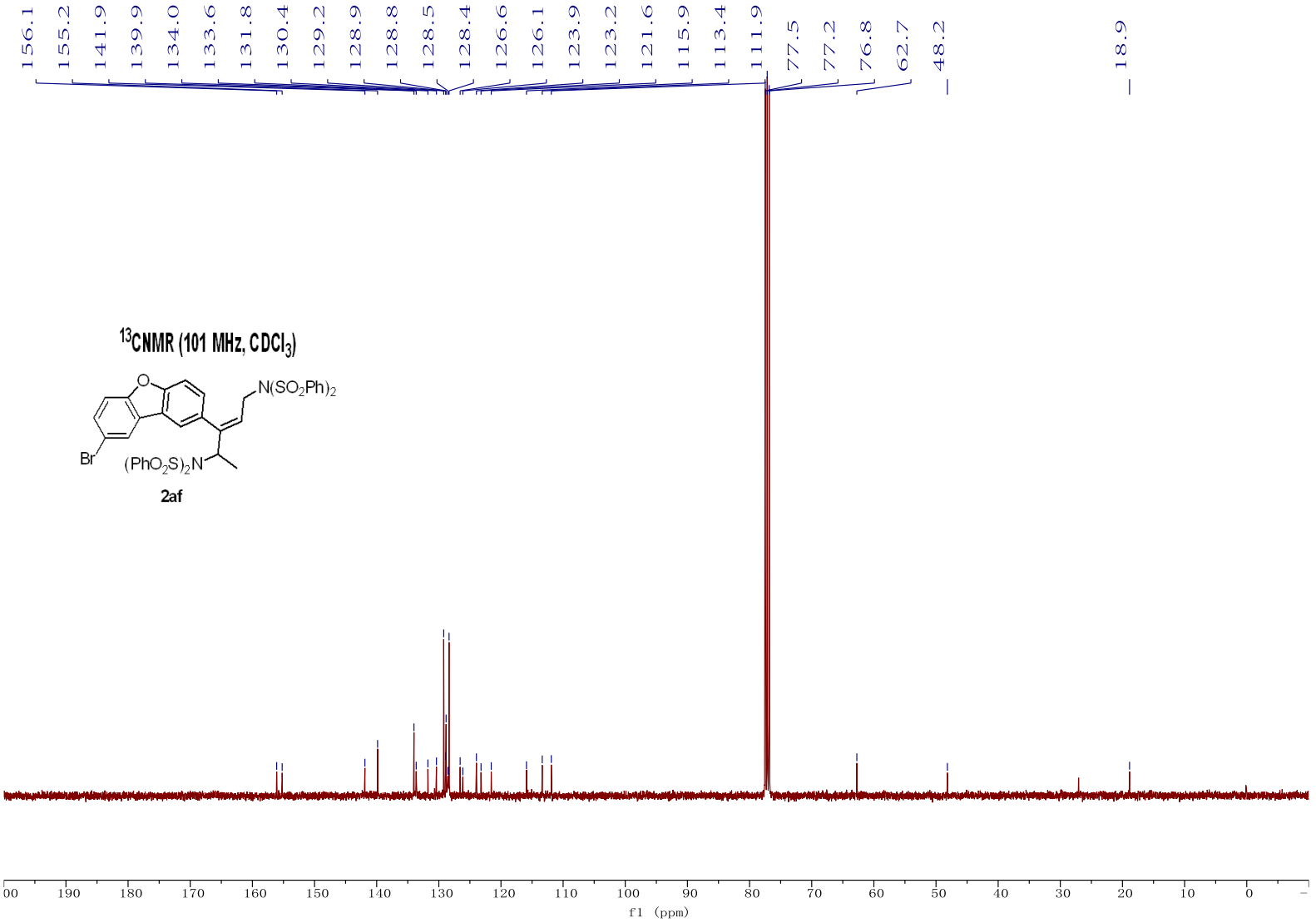


^{1}HNMR (400 MHz, $CDCl_3$)

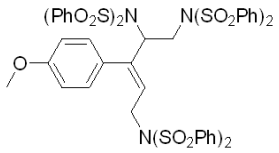


2af

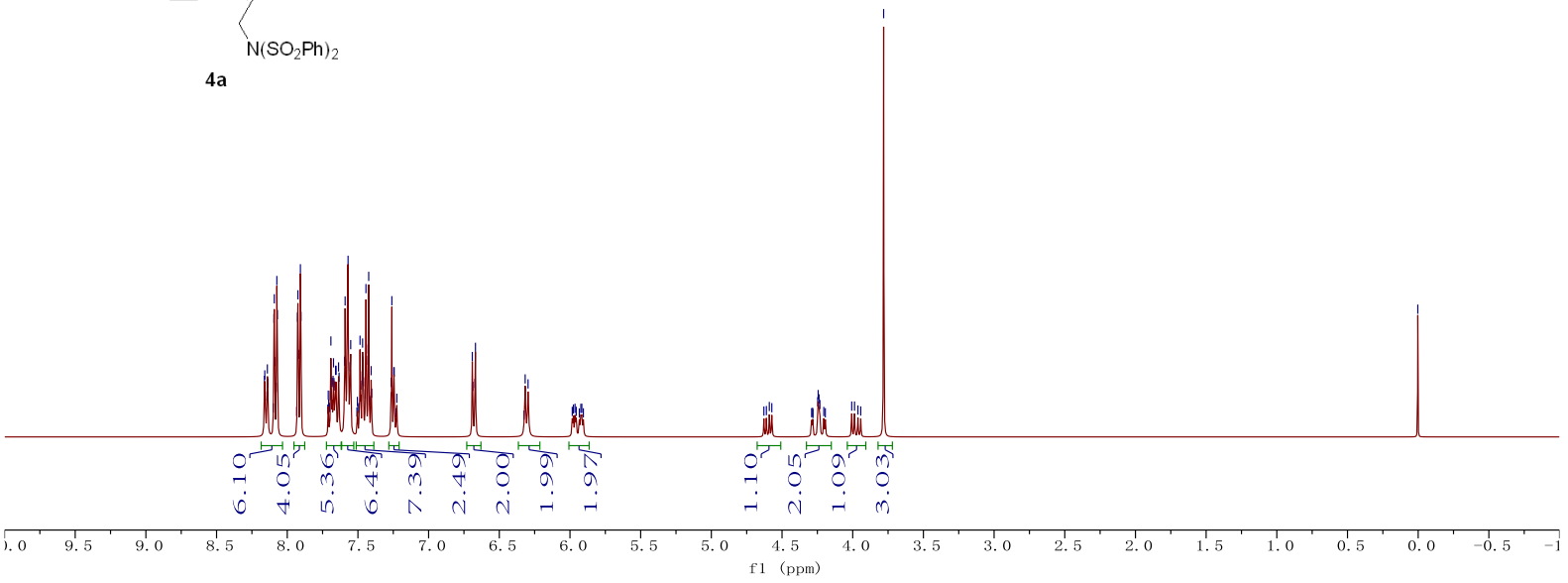


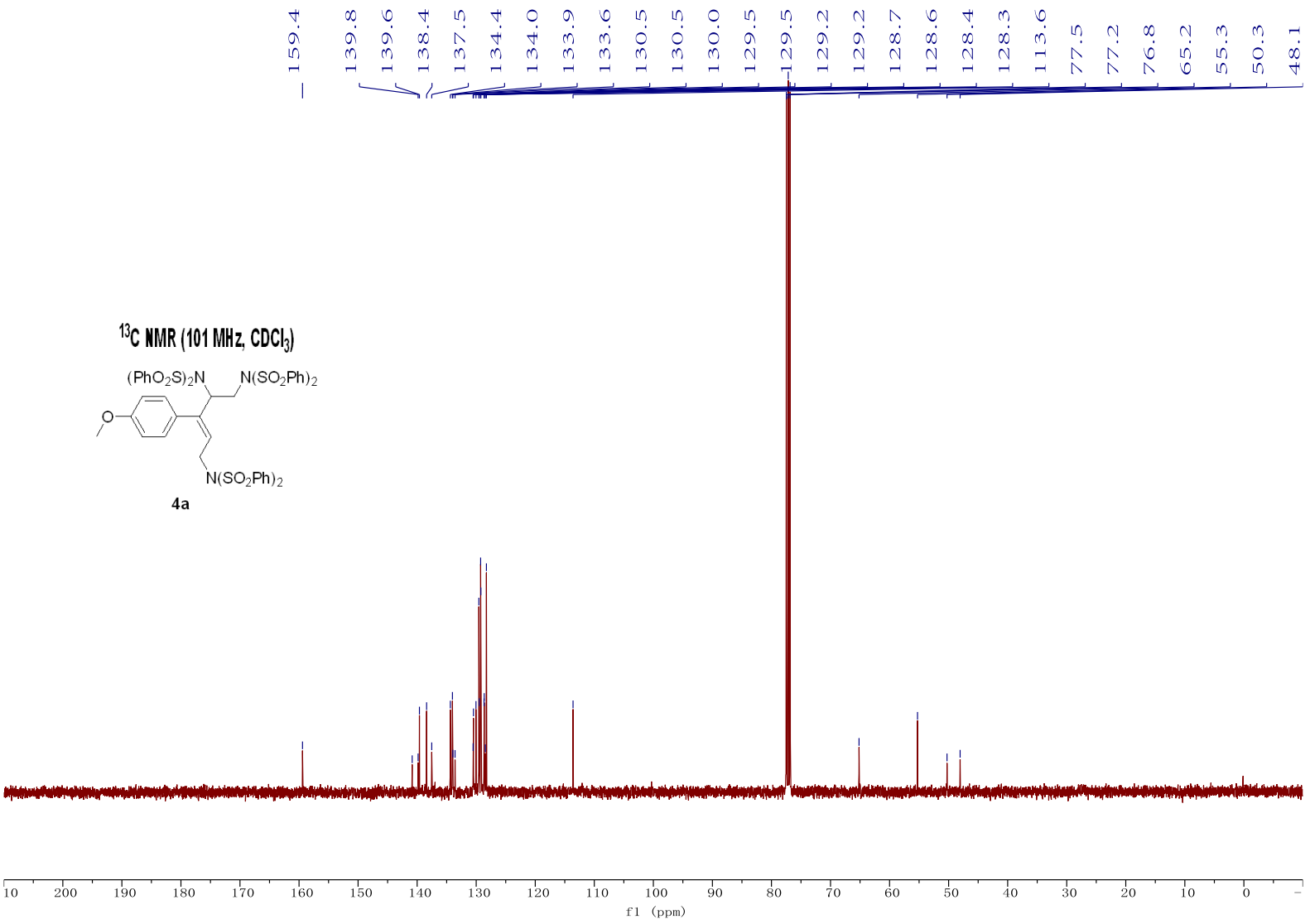

156.1
155.2
141.9
139.9
134.0
133.6
131.8
130.4
129.2
128.9
128.8
128.5
128.4
126.6
126.1
123.9
123.2
121.6
115.9
113.4
111.9
77.5
77.2
76.8
62.7
48.2
18.9
13CNMR (101 MHz, CDCl3)
N(SO2Ph)2
Br
(PhO2S)2N
2af
f1 (ppm)

^{1}H NMR (400 MHz, $CDCl_3$)

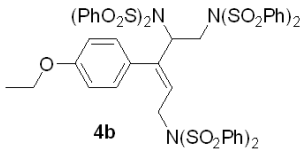


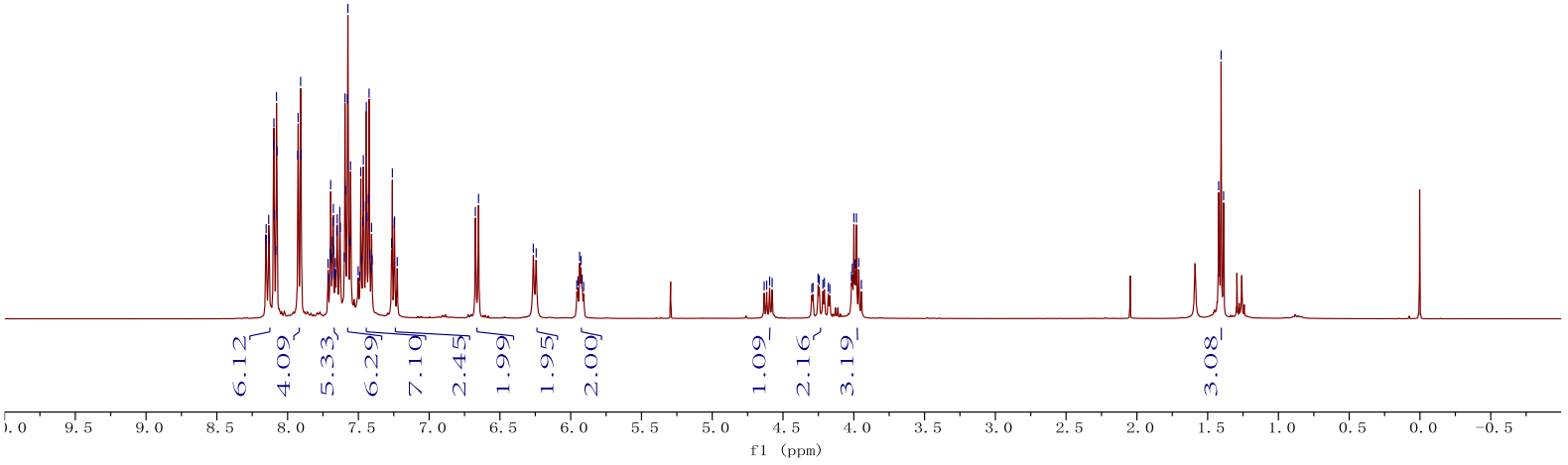
4a

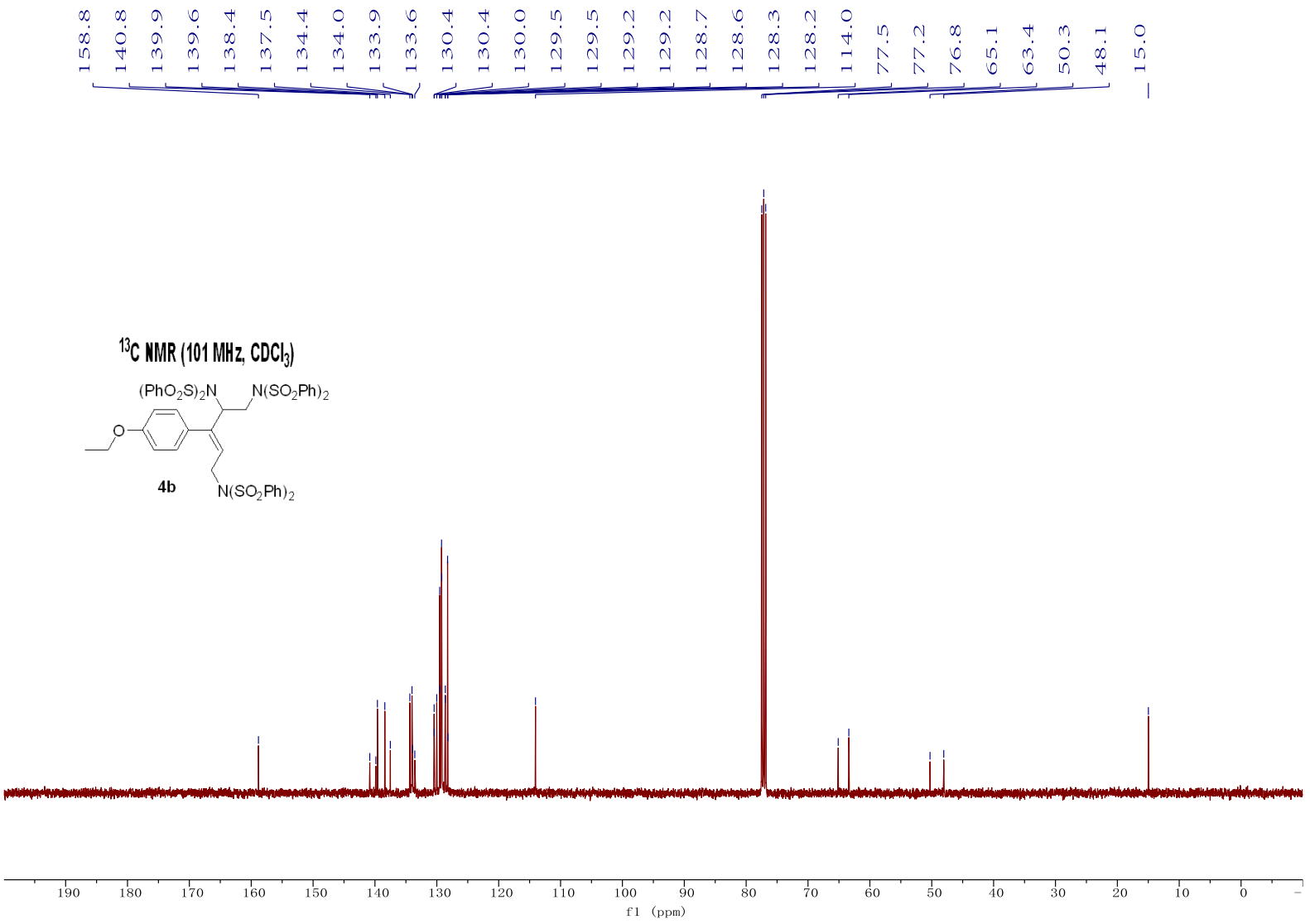



159.4
139.8
139.6
138.4
137.5
134.4
134.0
133.9
133.6
130.5
130.5
130.0
129.5
129.5
129.2
129.2
128.7
128.6
128.4
128.3
113.6
77.5
77.2
76.8
65.2
55.3
50.3
48.1
13C NMR (101 MHz, CDCl3)
(PhO2S)2N
N(SO2Ph)2
O
N(SO2Ph)2
4a
f1 (ppm)

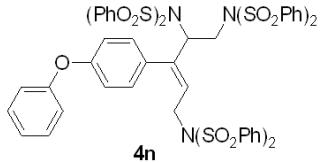
^{1}H NMR (400 MHz, $CDCl_3$)



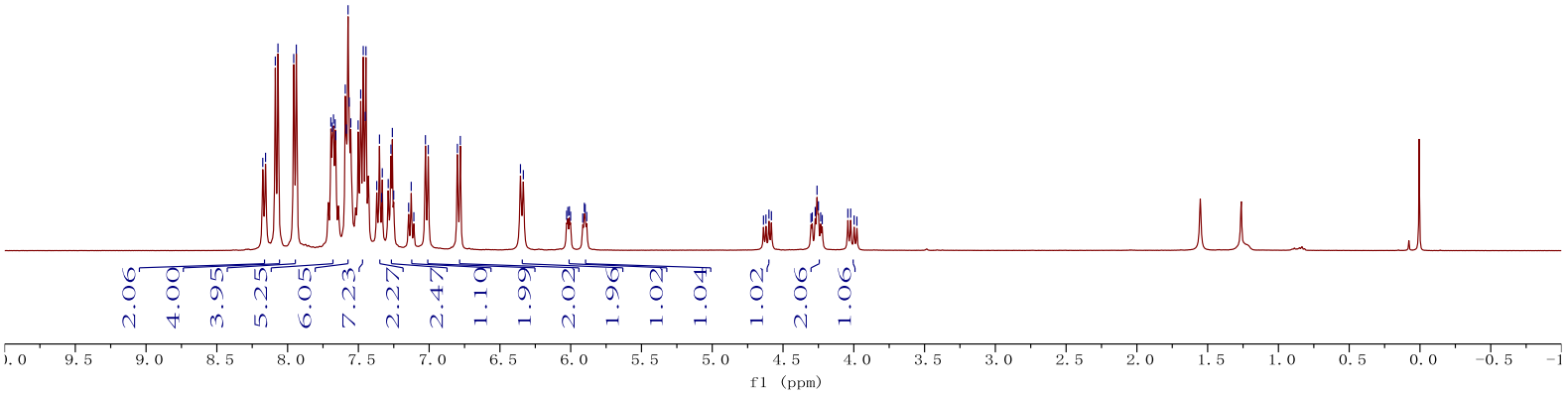


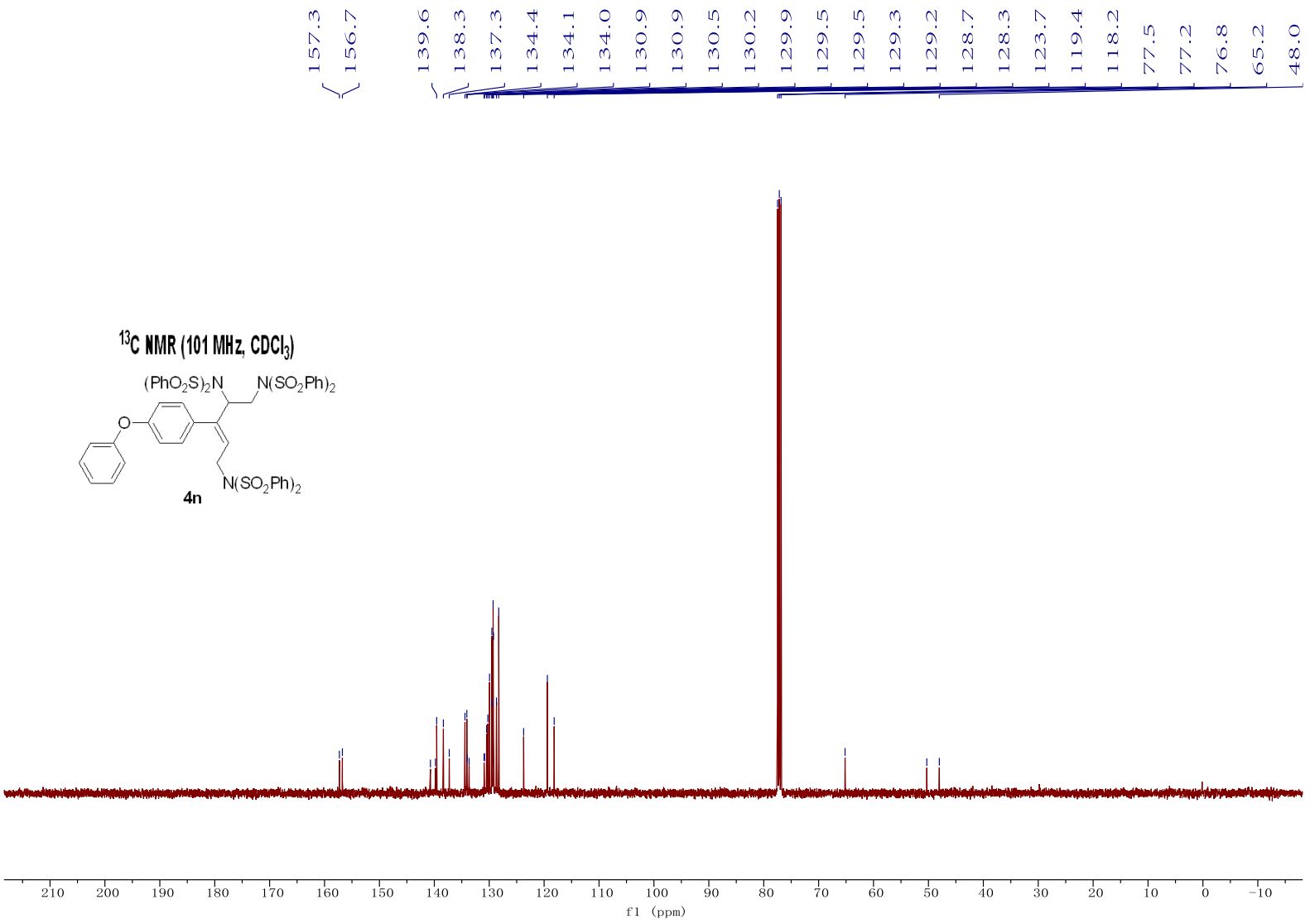

158.8
140.8
139.9
139.6
138.4
137.5
134.4
134.0
133.9
133.6
130.4
130.4
130.0
129.5
129.5
129.2
129.2
128.7
128.6
128.3
128.2
114.0
77.5
77.2
76.8
65.1
63.4
50.3
48.1
15.0
13C NMR (101 MHz, CDCl3)
(PhO2S)2N
N(SO2Ph)2
O
4b
N(SO2Ph)2
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

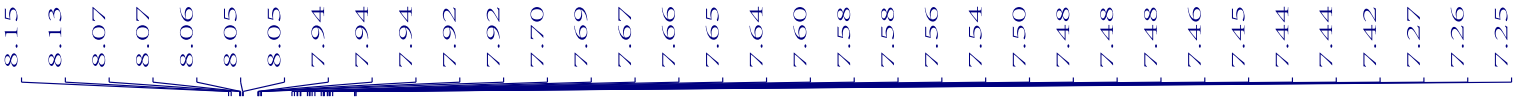
^{1}H NMR (400 MHz, $CDCl_3$)



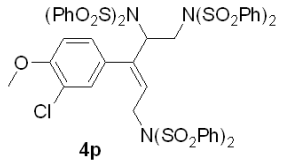
4n



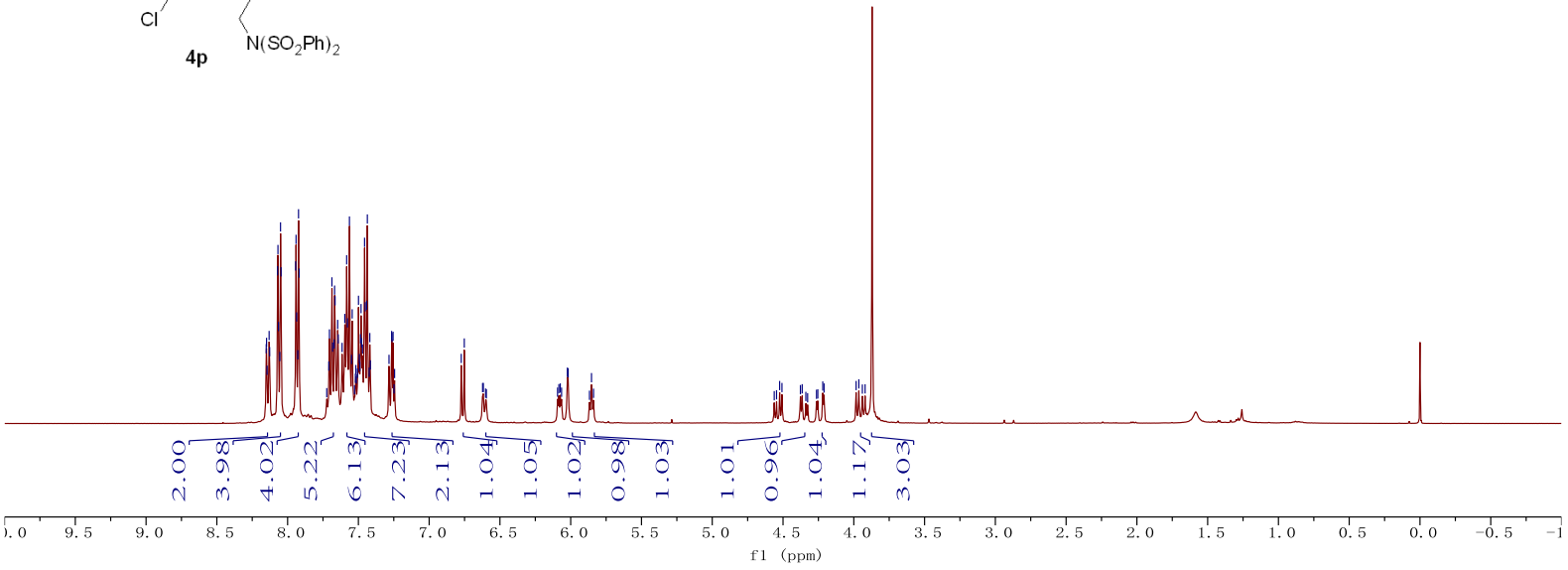

157.3
156.7
139.6
138.3
137.3
134.4
134.1
134.0
130.9
130.9
130.5
130.2
129.9
129.5
129.5
129.3
129.2
128.7
128.3
123.7
119.4
118.2
77.5
77.2
76.8
65.2
48.0
13C NMR (101 MHz, CDCl3)
(PhO2S)2N
N(SO2Ph)2
O
N(SO2Ph)2
4n
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

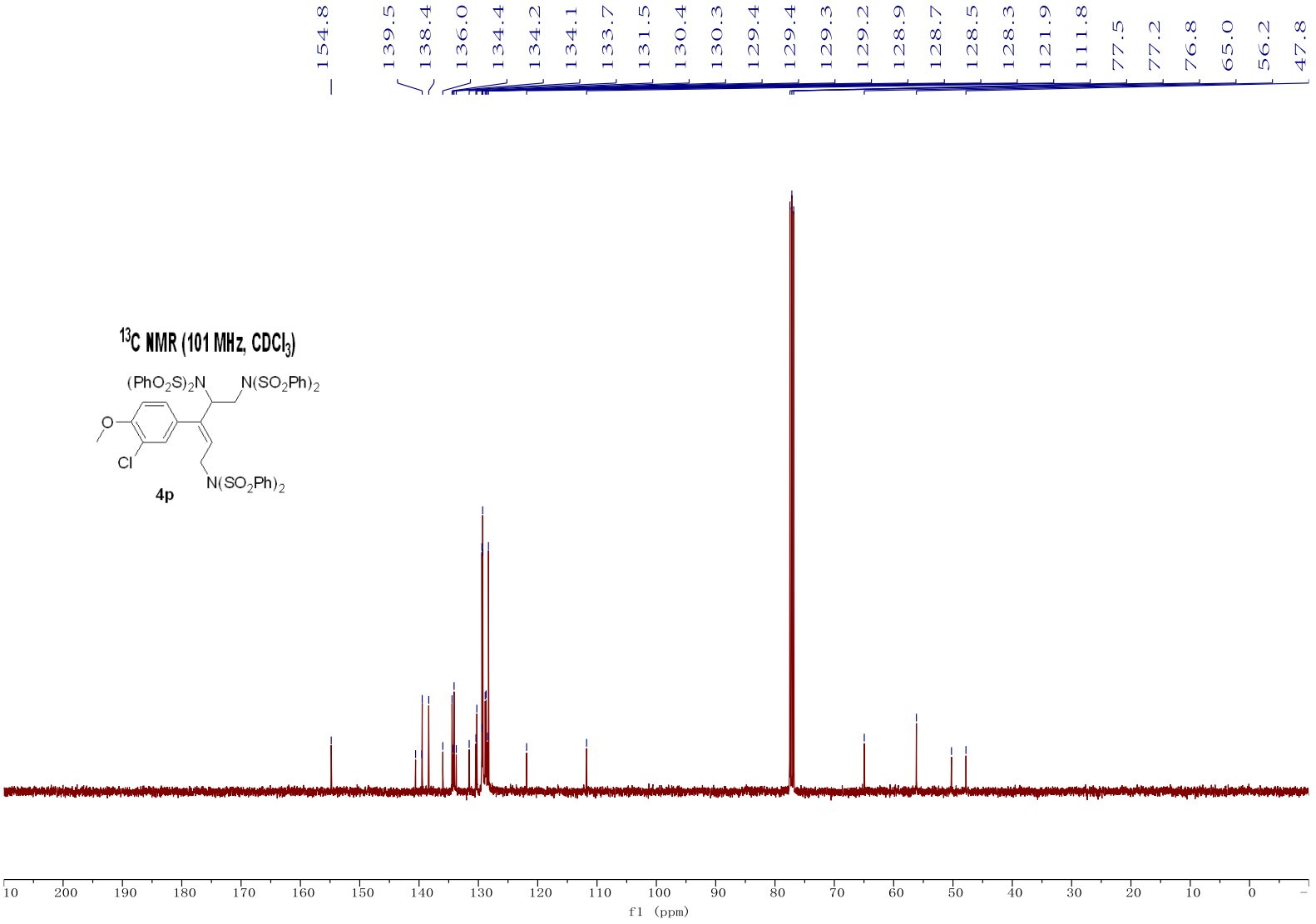


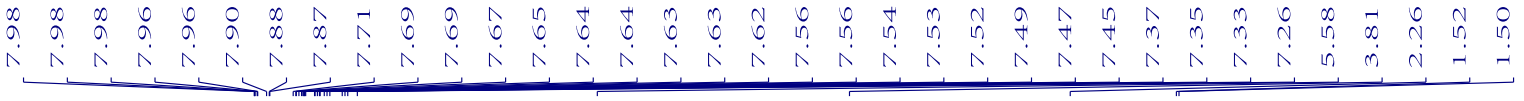
^{1}H NMR (400 MHz, $CDCl_3$)



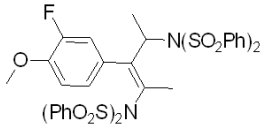
4p



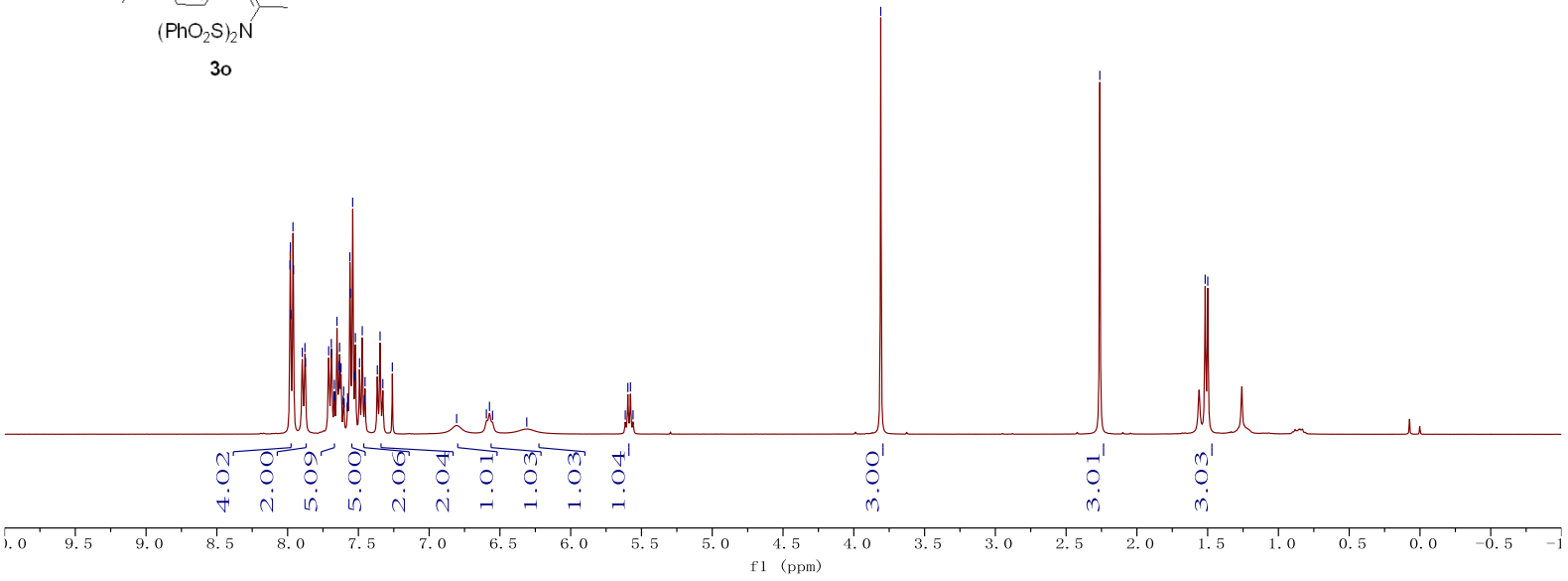

154.8
139.5
138.4
136.0
134.4
134.2
134.1
133.7
131.5
130.4
130.3
129.4
129.4
129.3
129.2
128.9
128.7
128.5
128.3
121.9
111.8
77.5
77.2
76.8
65.0
56.2
47.8
13C NMR (101 MHz, CDCl3)
(PhO2S)2N
N(SO2Ph)2
O
Cl
N(SO2Ph)2
4p
f1 (ppm)

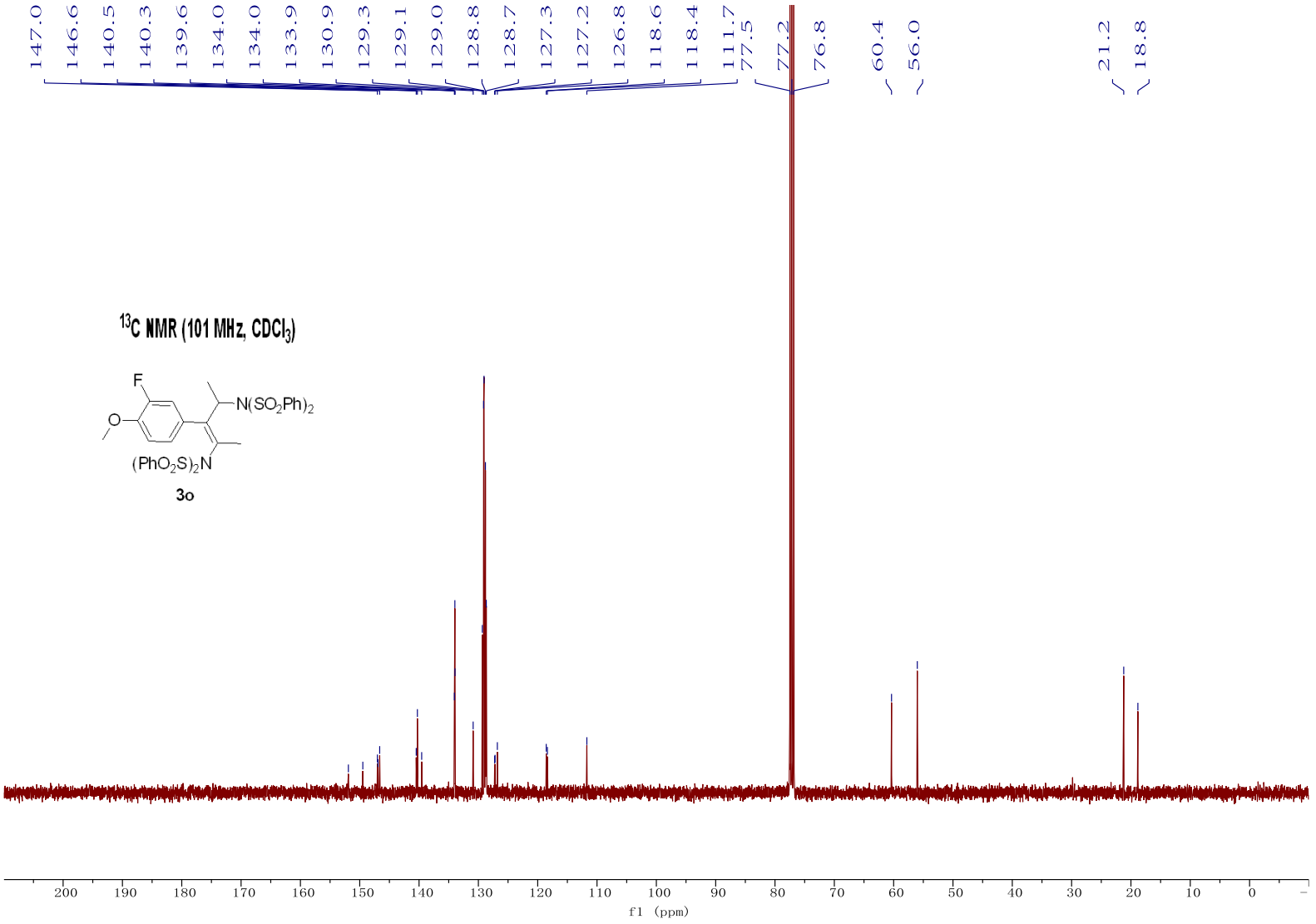


^{1}H NMR (400 MHz, $CDCl_3$)



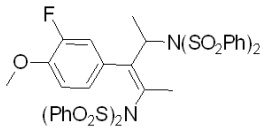
3o



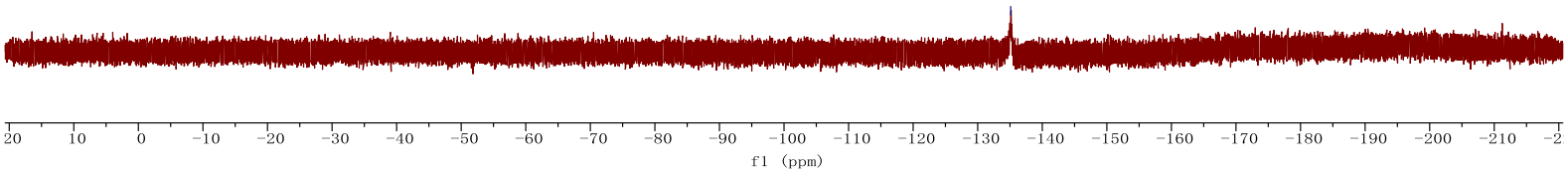

147.0
146.6
140.5
140.3
139.6
134.0
134.0
133.9
130.9
129.3
129.1
129.0
128.8
128.7
127.3
127.2
126.8
118.6
118.4
111.7
77.5
77.2
76.8
60.4
56.0
21.2
18.8
13C NMR (101 MHz, CDCl3)
F
O
N(SO2Ph)2
(PhO2S)2N
3o
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

-135.1

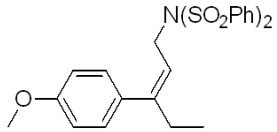
^{19}F NMR (376 MHz, $CDCl_3$)



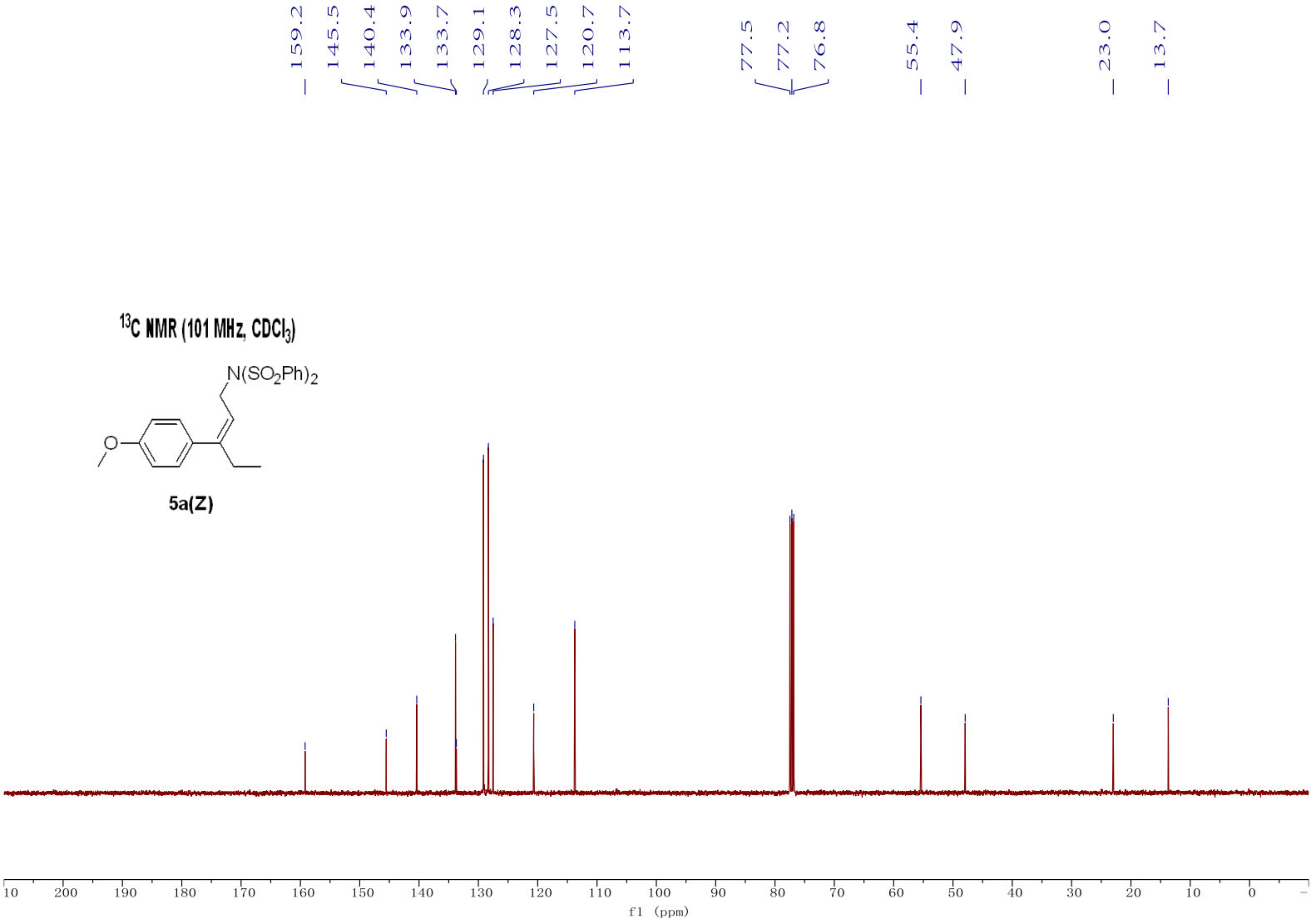
3o



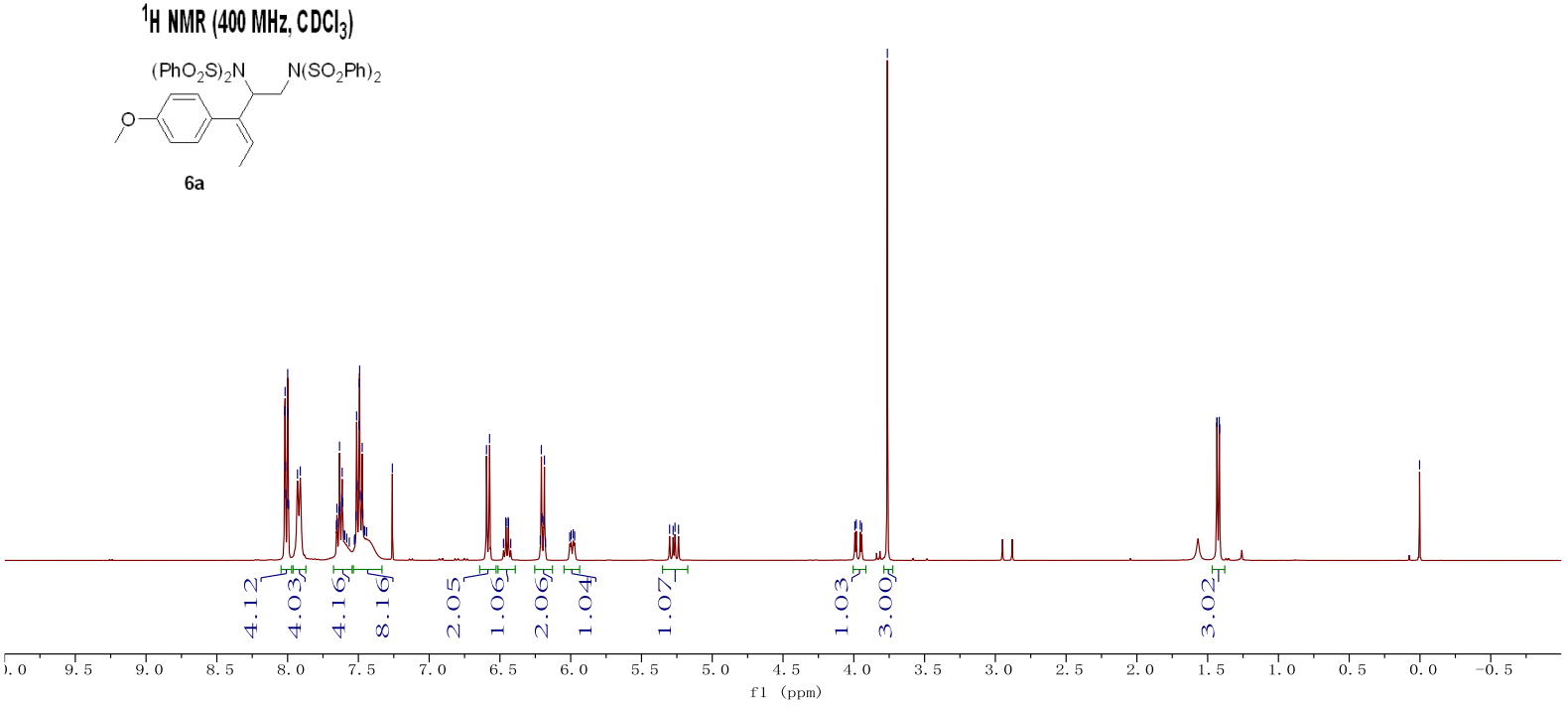
^{1}H NMR (400 MHz, $CDCl_3$)

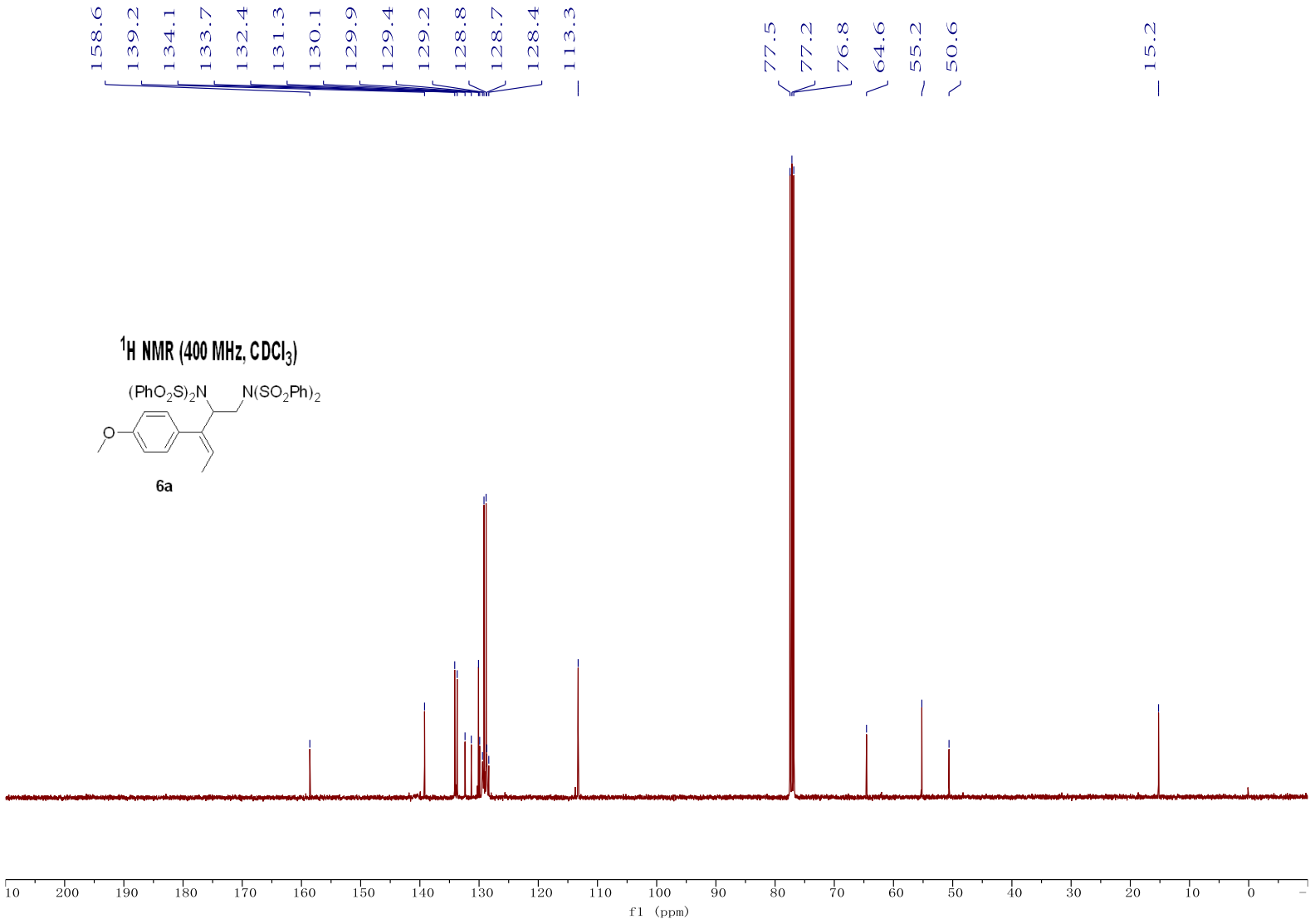


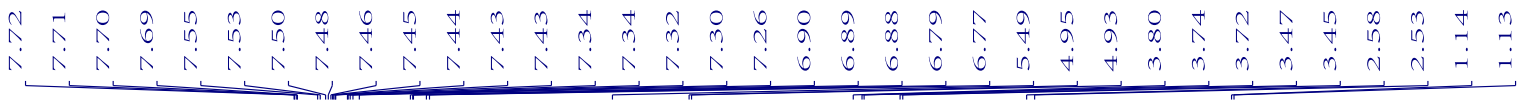
5a(Z)


159.2
145.5
140.4
133.9
133.7
129.1
128.3
127.5
120.7
113.7
77.5
77.2
76.8
55.4
47.9
23.0
13.7
13C NMR (101 MHz, CDCl3)
N(SO2Ph)2
O
5a(Z)
f1 (ppm)

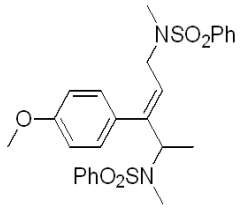

8.02
8.02
8.01
8.01
8.00
8.00
8.00
7.99
7.93
7.91
7.65
7.63
7.63
7.62
7.61
7.61
7.51
7.51
7.50
7.49
7.49
7.49
7.48
7.47
7.26
6.59
6.57
6.21
6.19
3.76
1.44
1.43
1.42
1.42
0.00


^{1}H NMR (400 MHz, CDCl$_3$)
(PhO$_2$S)$_2$N
N(SO$_2$Ph)$_2$
O
6a
4.12
4.03
4.16
8.16
2.05
1.06
2.06
1.04
1.07
1.03
3.00
3.02
f1 (ppm)

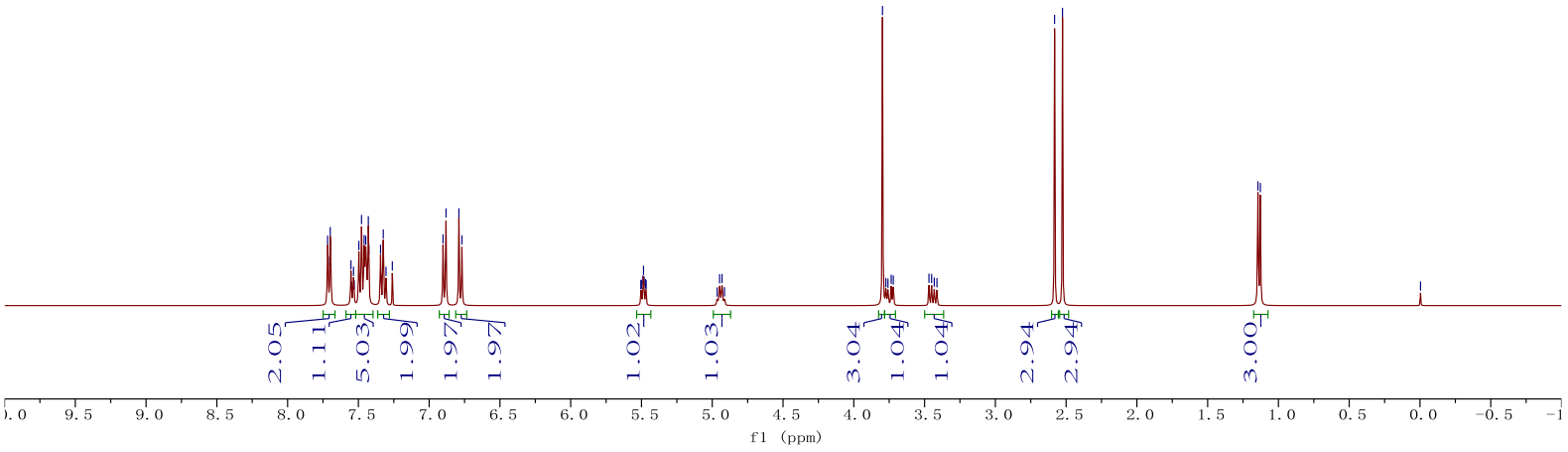

158.6
139.2
134.1
133.7
132.4
131.3
130.1
129.9
129.4
129.2
128.8
128.7
128.4
113.3
77.5
77.2
76.8
64.6
55.2
50.6
15.2
1H NMR (400 MHz, CDCl3)
(PhO2S)2N
N(SO2Ph)2
O
6a
f1 (ppm)

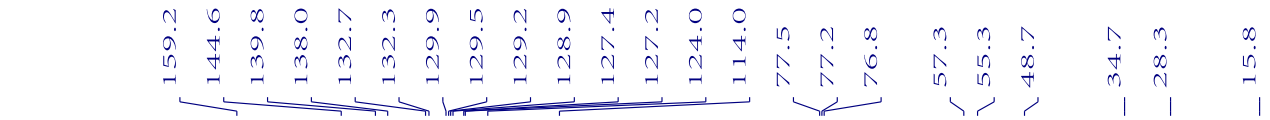


^{1}H NMR (400 MHz, $CDCl_3$)

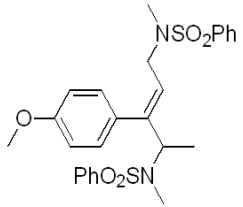


7a

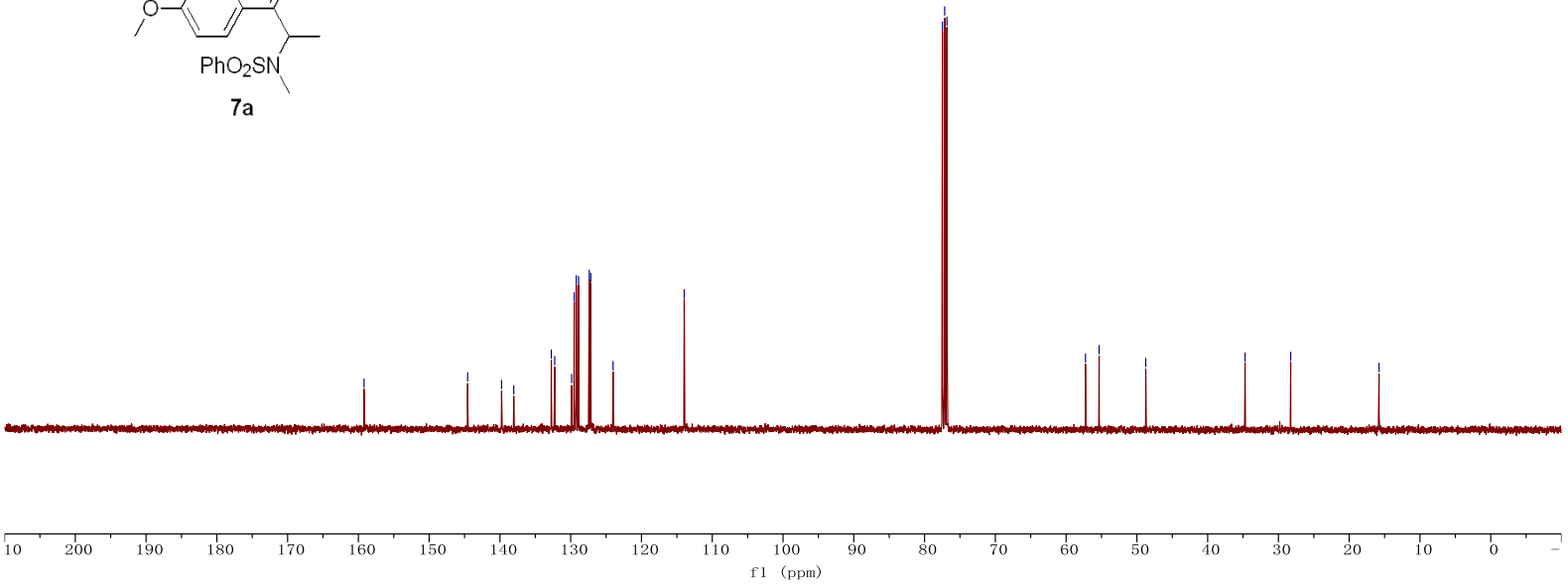


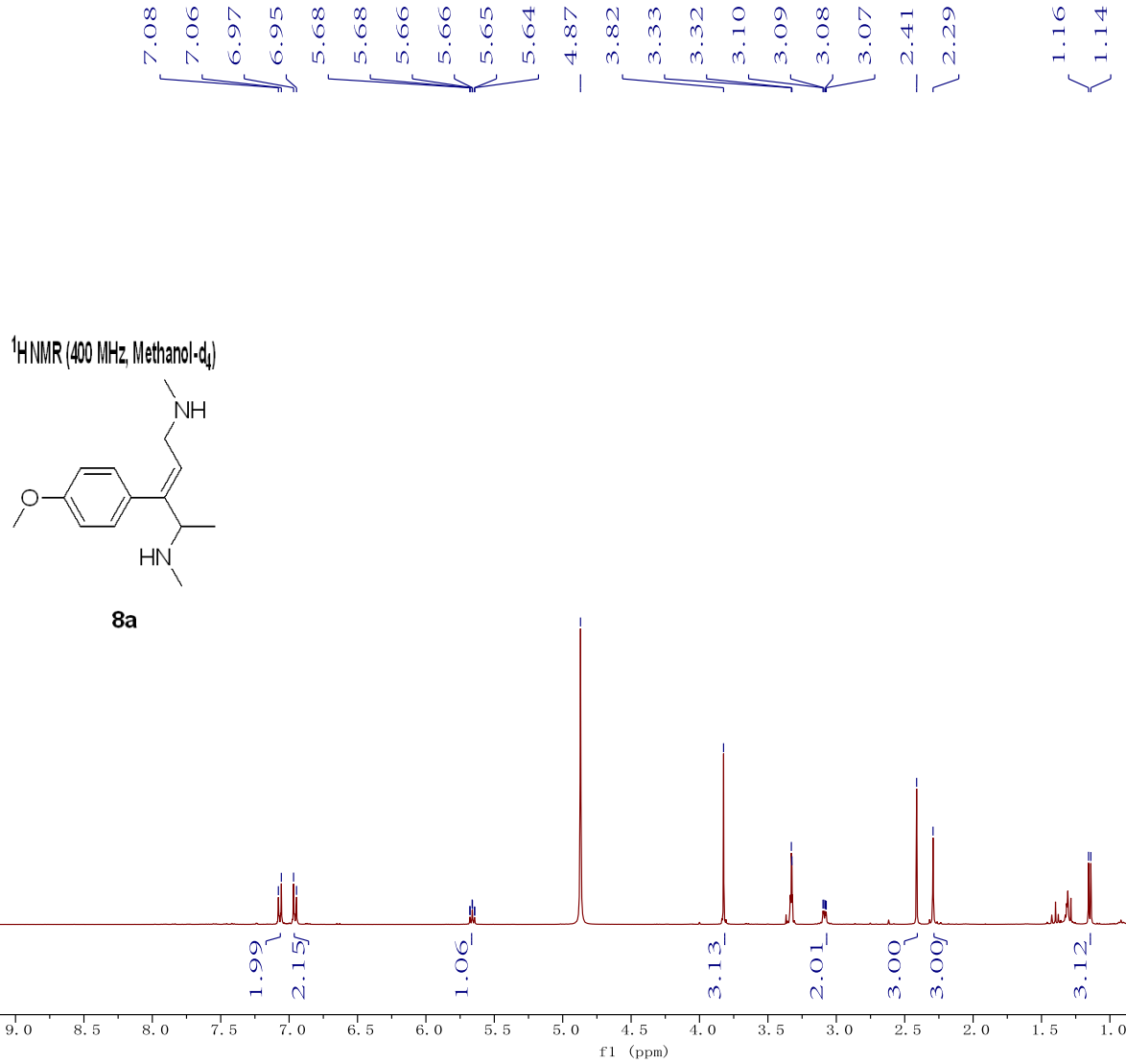


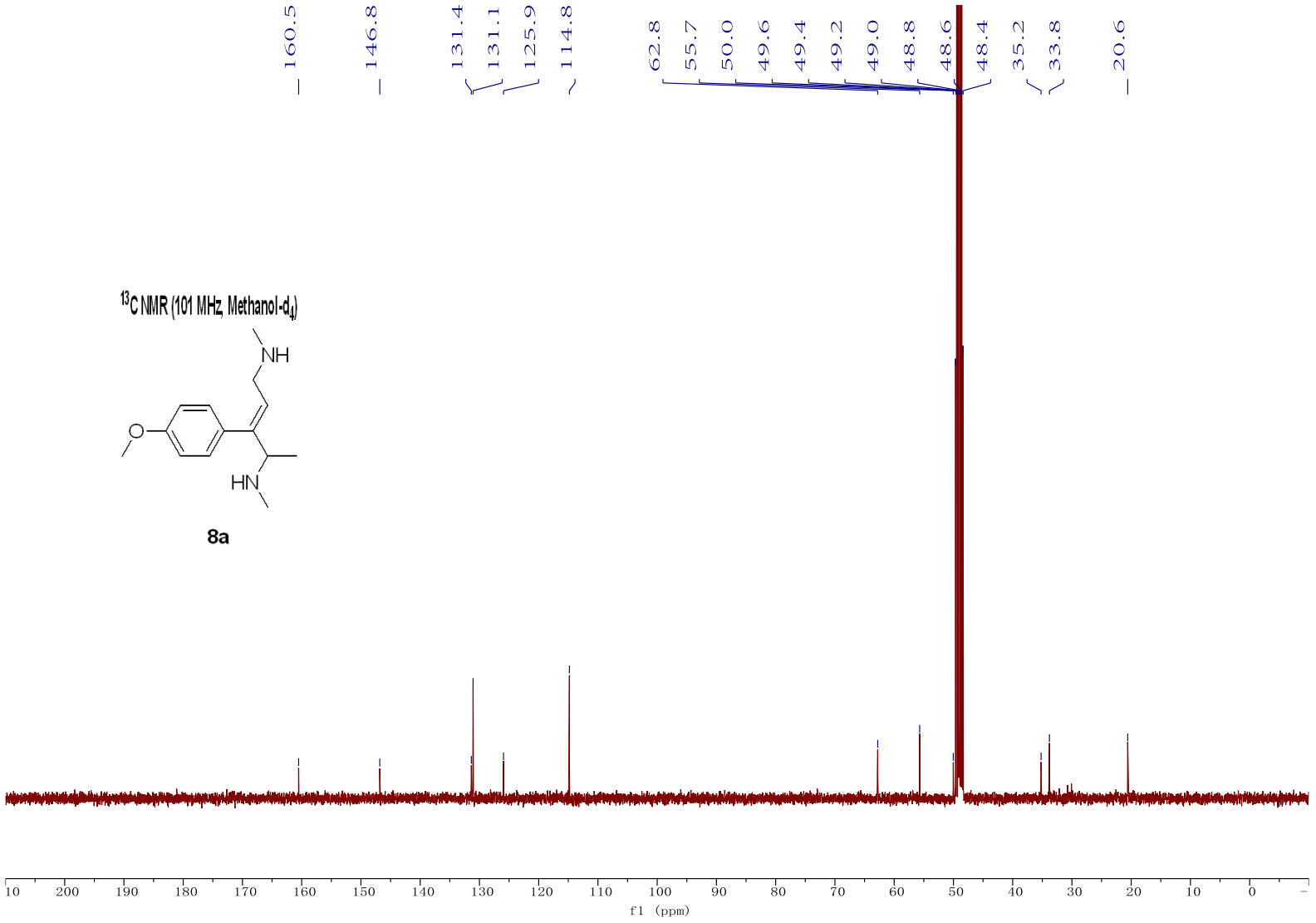
^{13}C NMR (101 MHz, $CDCl_3$)

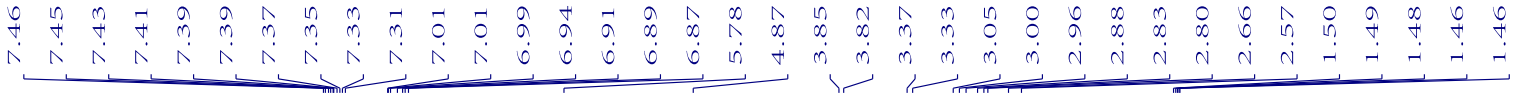


7a

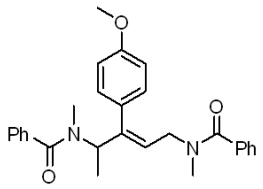



7.08
7.06
6.97
6.95
5.68
5.68
5.66
5.66
5.65
5.64
4.87
3.82
3.33
3.32
3.10
3.09
3.08
3.07
2.41
2.29
1.16
1.14
1H NMR (400 MHz, Methanol-d4)
NH
O
HN
8a
1.99
2.15
1.06
3.13
2.01
3.00
3.00
3.12
f1 (ppm)

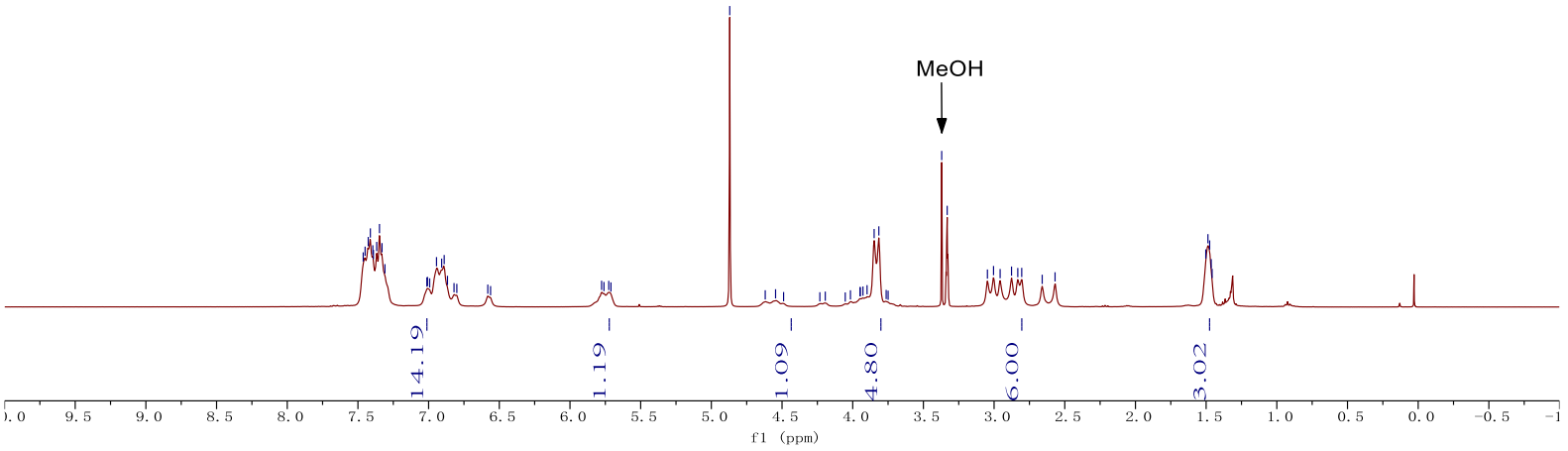

160.5
146.8
131.4
131.1
125.9
114.8
62.8
55.7
50.0
49.6
49.4
49.2
49.0
48.8
48.6
48.4
35.2
33.8
20.6
13C NMR (101 MHz, Methanol-d4)
NH
O
HN
8a
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

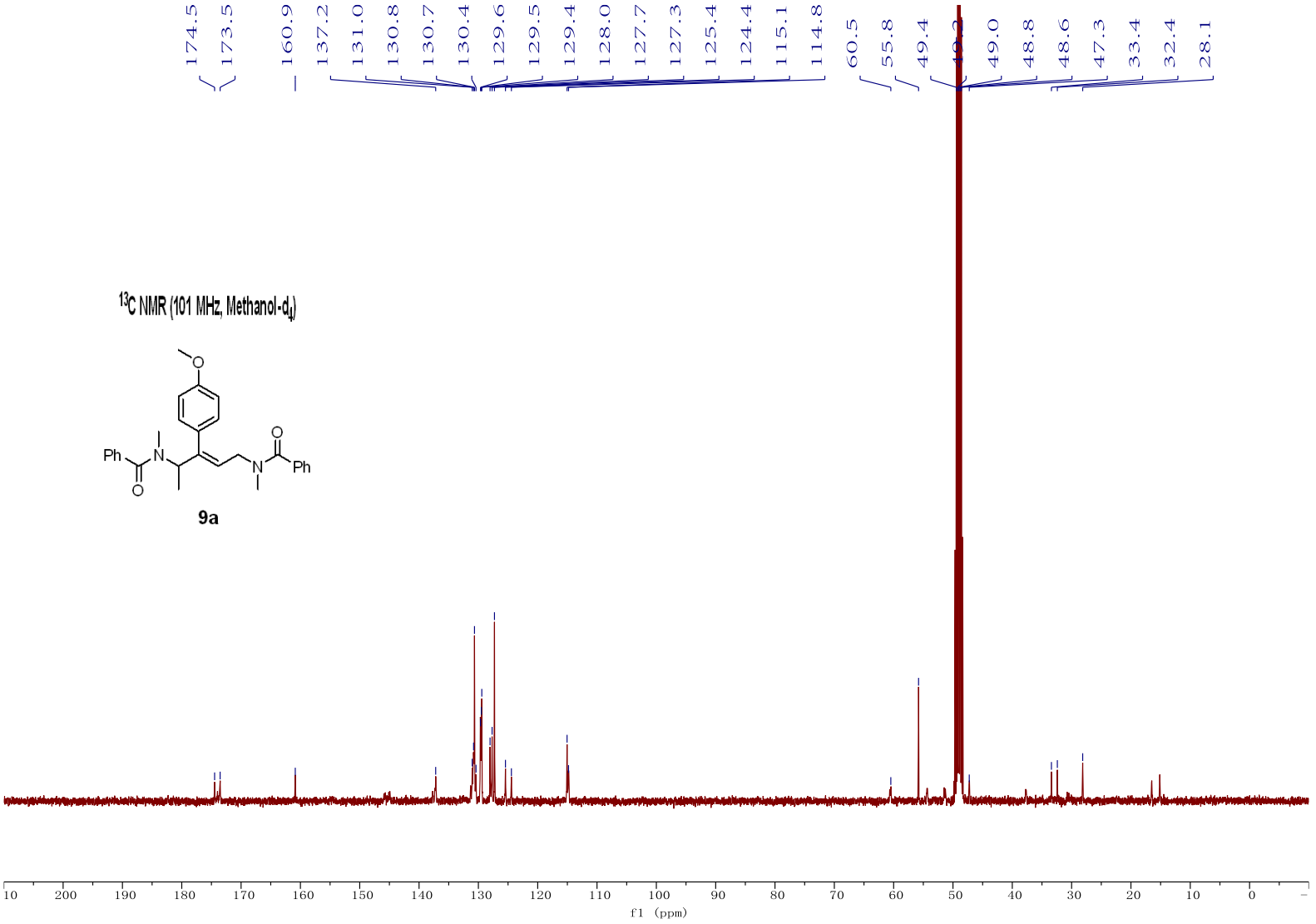


^{1}H NMR (400 MHz, Methanol-d_4)



9a




174.5
173.5
160.9
137.2
131.0
130.8
130.7
130.4
129.6
129.5
129.4
128.0
127.7
127.3
125.4
124.4
115.1
114.8
60.5
55.8
49.4
49.2
49.0
48.8
48.6
47.3
33.4
32.4
28.1
13C NMR (101 MHz, Methanol-d4)
Ph
N
O
O
N
Ph
9a
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)