Supporting Information

Electrochemically enabled Nickel-catalyzed controllable synthesis of monoaryl or diaryl amines from aryl halides and trimethylsilyl azides

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1. General considerations

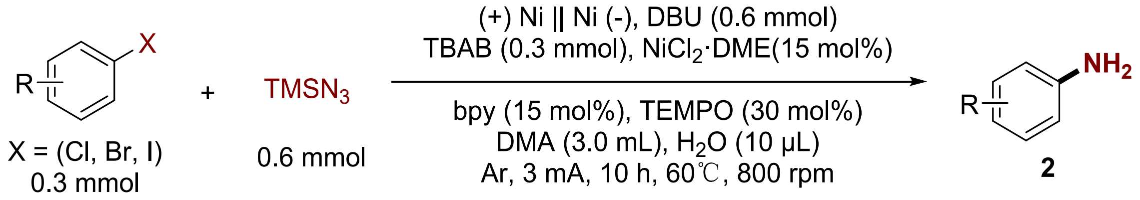
General. Unless otherwise noted, all reactions were carried out under an air atmosphere. Analytical thin-λayer chromatography (TLC) was performed on glass plates coated with 0.25 mm 230–400 mesh silica gel containing a fluorescent indicator. Visualization was accomplished by exposure to a UV lamp. All the products in this article are compatible with standard silica gel chromatography. Column chromatography was performed on silica gel (200–300 mesh) using standard methods.

Structural analysis. NMR spectra were measured on a Bruker Ascend 400 spectrometer and chemical shifts (*δ*) are reported in parts per million (ppm). ^{1}H NMR spectra were recorded at 400 MHz in NMR solvents and referenced internally to corresponding solvent resonance, and ^{13}C NMR spectra were recorded at 101 MHz and referenced to corresponding solvent resonance. Coupling constants are reported in Hz with multiplicities denoted as s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet) and br (broad). Infrared spectra were collected on a Thermo Fisher Nicolet 6700 FT-IR spectrometer using ATR (Attenuated Total Reflectance) method. Absorption maxima (v max) are reported in wavenumbers (cm^{-1}). High resolution mass spectra (HRMS) were acquired on Thermo Scientific LTQ Orbitrap XL with an APCI or ESI source.

Materials. Commercial reagents and solvent were purchased from Adamas, J&K, Energy, Sigma-Aldrich, Alfa Aesar, Acros Organics, TCI and used as received unless otherwise stated.

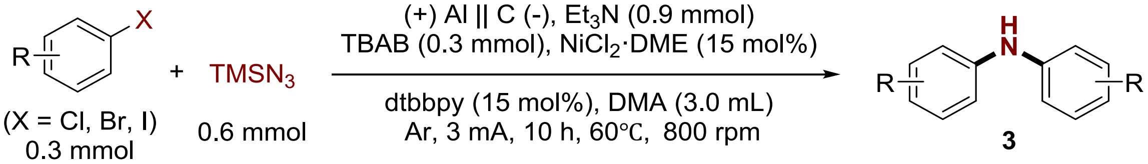
2. General procedure for amination of aryl halides

2.1 General procedure A for generating monoaryl amines



General Procedure A: aryl halides (0.30 mmol, 1.0 equiv.), $TMSN_3$ (0.60 mmol, 2.0 equiv.), $NiCl_2 \cdot DME$ (0.045 mmol, 15 mol%), bpy (0.045 mmol, 15 mol%), DBU (0.60 mmol, 2.0 equiv.), TEMPO (30 mol%), H_2O (10.0 μL), TBAB (0.30 mmol, 1.0 equiv.) and DMA (3.0 mL) were added to a dried 25 mL reaction tube, and electrolyze with Ni as anode and cathode at a constant current of 3 mA for 10 hours in an Ar atmosphere at 60 °C. After the reaction, the reaction mixture was diluted with 15 mL of water and then extracted with ethyl acetate (3 × 15 mL). The combined organic phases were dried over Na_2SO_4 and concentrated under vacuum to yield the crude product, which was subsequently purified by column chromatography on silica gel using a PE/EA (2:1) mixture as the eluent to obtain the desired products.

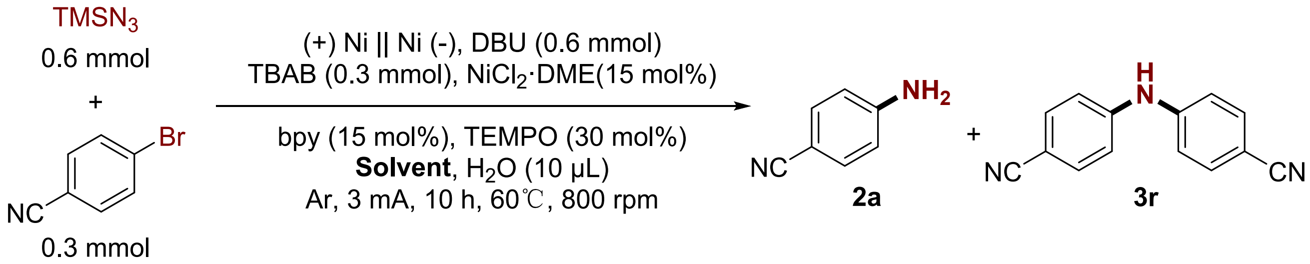
2.2 General procedure B for generating diaryl amines



General Procedure B: aryl halides (0.30 mmol, 1.0 equiv.), $TMSN_3$ (0.60 mmol, 2.0 equiv.), $NiCl_2 \cdot DME$ (0.045 mmol, 15 mol%), dtbbpy (0.045 mmol, 15 mol%), TEA (0.90 mmol, 3.0 equiv.), TBAB (0.30 mmol, 1.0 equiv.) and DMA (3.0 mL) were added to a dried 25 mL reaction tube, and electrolyze with Al as anode and Carbon as cathode at a constant current of 3 mA for 10 hours in an Ar atmosphere at 60 °C. After the reaction, the reaction mixture was diluted with 15 mL of water and then extracted with ethyl acetate (3 × 15 mL). The combined organic phases were dried over Na_2SO_4 and concentrated under vacuum to yield the crude product, which was subsequently purified by column chromatography on silica gel using a PE/EA (5:1) mixture as the eluent to obtain the desired products.

3. Optimization of nickel-catalyzed amination of aryl halides

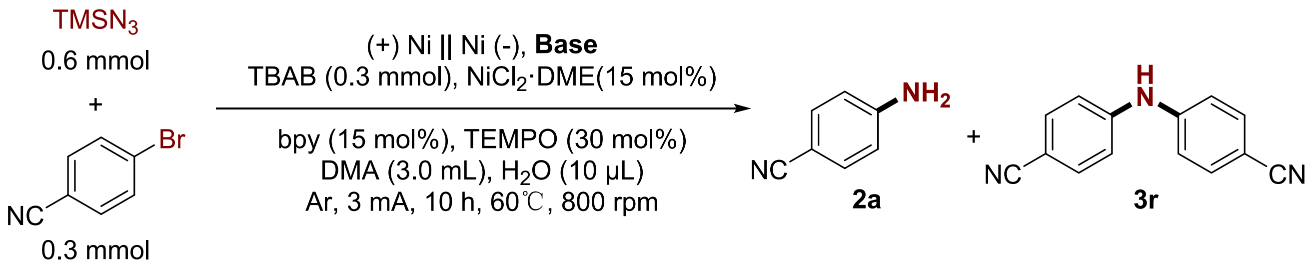
3.1 Optimization of solvent (Table SI-1)



Entry	Solvent (3.0 mL)	**2a** (%)	**3r** (%)
1	**DMA**	**70**	**10**
2	DMF	52	trace
3	MeCN	30	trace
4	DMSO	18	trace
5	MeOH	trace	trace
6	DCM	trace	trace

Reaction conditions: 4-Bromobenzonitrilel (1.0 equiv., 0.3 mmol), $TMSN_3$ (2.0 equiv., 0.6 mmol), $NiCl_2$·DME (15.0 mol%), bpy (15.0 mol%), DBU (2.0 equiv., 0.6 mmol), TBAB (1.0 equiv., 0.3 mmol), TEMPO (30 mol%), H_2O (10.0 μL), Solvent, Ar, 60°C, 800 rpm, Ni as Anode and cathode at 3 mA for 10h, isolated yields are shown.

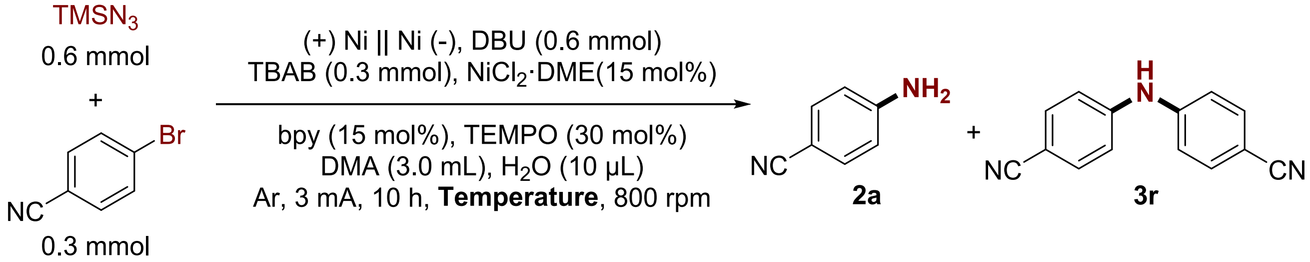
3.2 Optimization of base (Table SI-2)



Entry	Base (2.0 equiv.)	**2a** (%)	**3r** (%)
1	**DBU**	**70**	**10**
2	MTBD	53	13
3	TBD	33	19
4	DBN	48	7
4	TMG	62	15
5	$CsCO_3$	trace	trace
6	NaH_2PO_4	19	11
7	^{t}BuOK	trace	trace
8	TMEDA	24	22
9	DIPEA	27	14
10	DIPA	22	8
2	Et_3N	27	27

Reaction conditions: 4-Bromobenzonitrilel (1.0 equiv., 0.3 mmol), $TMSN_3$ (2.0 equiv., 0.6 mmol), $NiCl_2$·DME (15.0 mol%), bpy (15.0 mol%), Base, TBAB (1.0 equiv., 0.3 mmol), TEMPO (30 mol%), H_2O (10.0 µL), DMA (3.0 mL), Ar, 60°C, 800 rpm, Ni as Anode and cathode at 3 mA for 10h, isolated yields are shown.

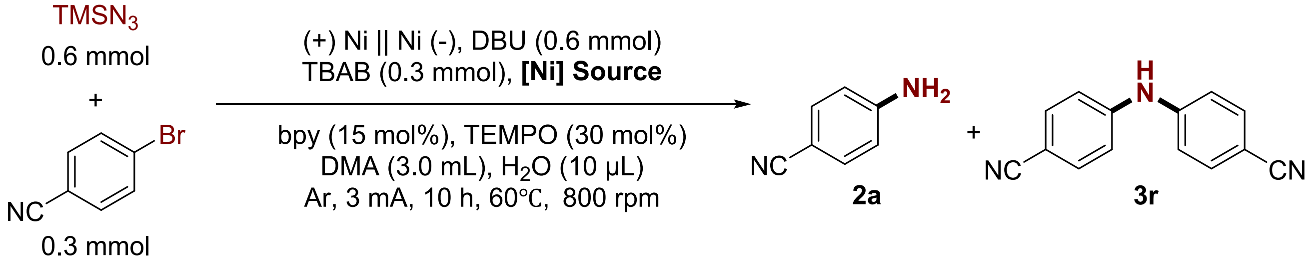
3.3 Optimization of temperature (Table SI-3)



Entry	Temperature	**2a** (%)	**3r** (%)
1	**60℃**	**70**	**10**
2	25℃	43	2
4	40℃	55	13
5	80℃	66	11

Reaction conditions: 4-Bromobenzonitrilel (1.0 equiv., 0.3 mmol), $TMSN_3$ (2.0 equiv., 0.6 mmol), $NiCl_2$·DME (15.0 mol%), bpy (15.0 mol%), DBU (2.0 equiv., 0.6 mmol), TBAB (1.0 equiv., 0.3 mmol), TEMPO (30 mol%), H_2O (10.0 μL), DMA (3.0 mL), Ar, Temperature, 800 rpm, Ni as Anode and cathode at 3 mA for 10h, isolated yields are shown.

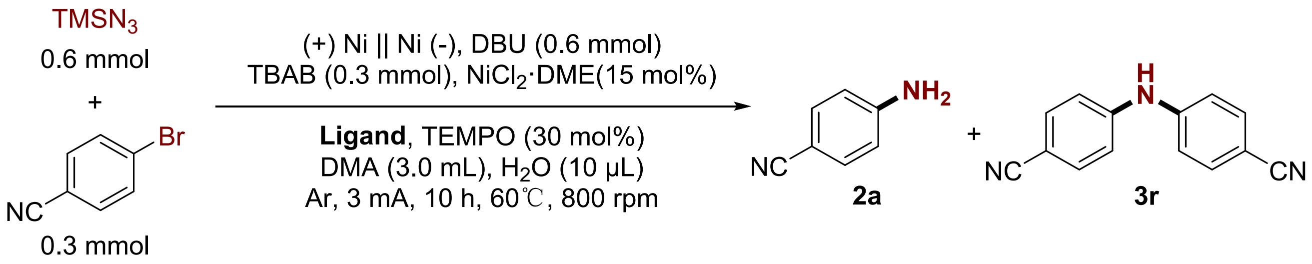
3.4 Optimization of [Ni] Source (Table SI-4)



Entry	[Ni] source (15 mol%)	**2a** (%)	**3r** (%)
1	**$NiCl_2 \cdot DME$**	**70**	**10**
2	$NiBr_2 \cdot DME$	64	6
3	$NiBr_2$	43	Trace
4	$NiCl_2$	40	Trace
5	NiI_2	28	Trace
6	$NiCl_2 \cdot 2PCy_3$	36	Trace
7	$NiCl_2 \cdot 2PPh_3$	27	Trace

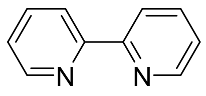
Reaction conditions: 4-Bromobenzonitrilel (1.0 equiv., 0.3 mmol), $TMSN_3$ (2.0 equiv., 0.6 mmol), [Ni] Source (15.0 mol%), bpy (15.0 mol%), DBU (2.0 equiv., 0.6 mmol), TBAB (1.0 equiv., 0.3 mmol), TEMPO (30 mol%), H_2O (10.0 μL), DMA (3.0 mL), Ar, 60℃, 800 rpm, Ni as Anode and cathode at 3 mA for 10h, isolated yields are shown.

3.5 Optimization of ligand (Table SI-5)

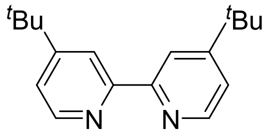


Entry	Ligand (15 mol%)	**2a** (%)	**3r** (%)
1	**L1**	**70**	**10**
2	L2	53	15
3	L3	50	12
4	L4	39	12
5	L5	33	14
6	L6	34	17
7	L7	48	15
8	L8	27	16
9	L9	41	trace
10	L10	38	trace
11	L11	66	trace
12	L12	62	8

Reaction conditions: 4-Bromobenzonitrilel (1.0 equiv., 0.3 mmol), $TMSN_3$ (2.0 equiv., 0.6 mmol), $NiCl_2$·DME (15.0 mol%), Ligand, DBU (2.0 equiv., 0.6 mmol), TBAB (1.0 equiv., 0.3 mmol), TEMPO (30 mol%), H_2O (10.0 μL), DMA (3.0 mL), Ar, 60°C, 800 rpm, Ni as Anode and cathode at 3 mA for 10h, isolated yields are shown.



L1



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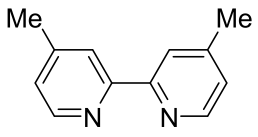
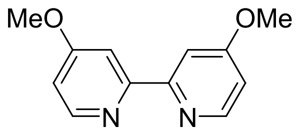


L3



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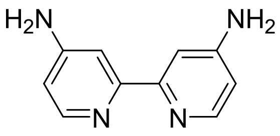

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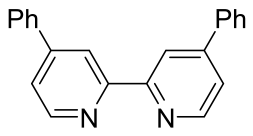

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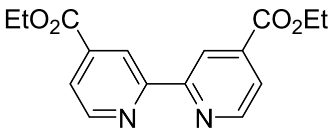

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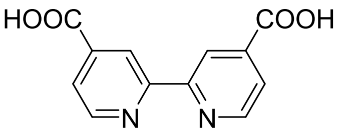

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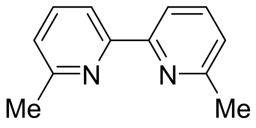

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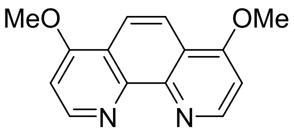

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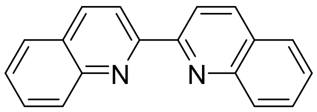

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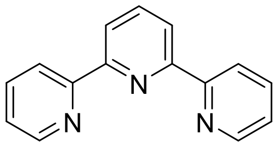
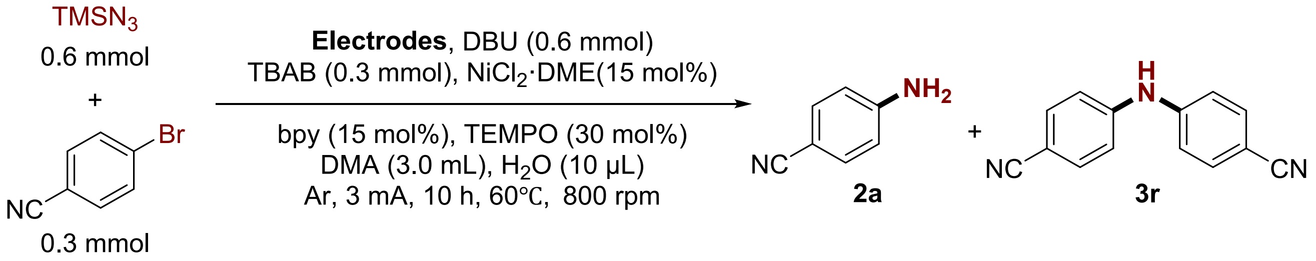


L12

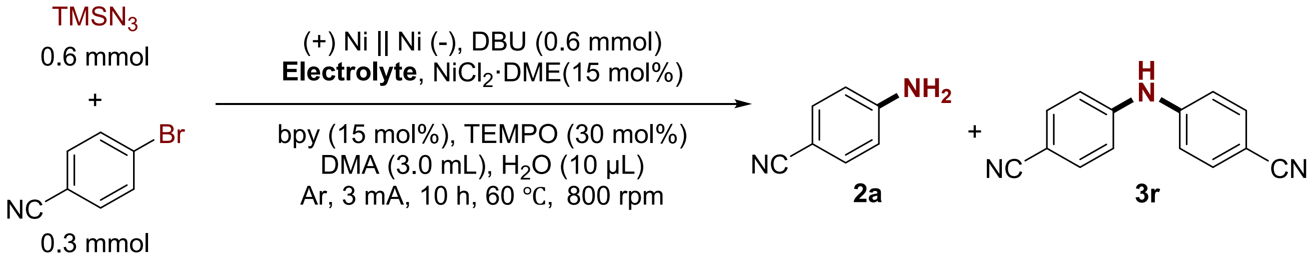
3.6 Optimization of electrodes (Table SI-6)



Entry	Eectrodes	**2a** (%)	**3r** (%)
1	**(+) Ni || Ni (-)**	**70**	**10**
2	(+) Ni || C (-)	63	12
3	(+) Al || C (-)	23	23
4	(+) Al || Ni (-)	27	14
5	(+) Fe || C (-)	31	11
6	(+) SS || C (-)	42	4
7	(+) Zn || C (-)	16	24

Reaction conditions: 4-Bromobenzonitrilel (1.0 equiv., 0.3 mmol), $TMSN_3$ (2.0 equiv., 0.6 mmol), $NiCl_2 \cdot DME$ (15.0 mol%), bpy (15.0 mol%), DBU (2.0 equiv., 0.6 mmol), TBAB (1.0 equiv., 0.3 mmol), TEMPO (30 mol%), H_2O (10.0 μL), DMA (3.0 mL), Ar, 60℃, 800 rpm, Eectrodes at 3 mA for 10h, isolated yields are shown.

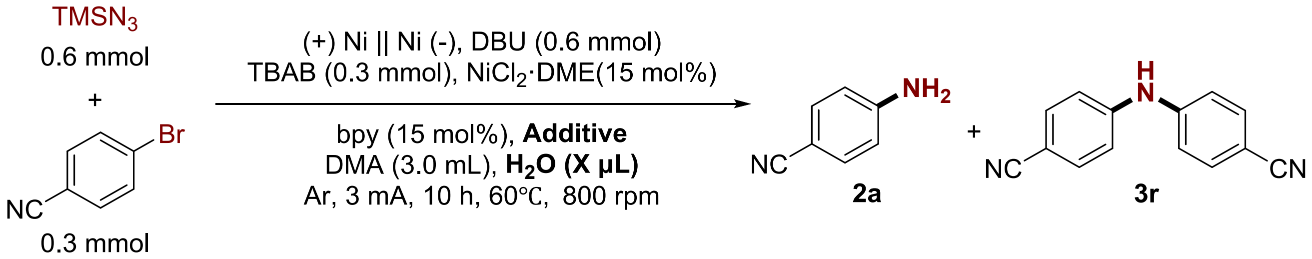
3.7 Optimization of electrolyte (Table SI-7)



Entry	Temperature (0.1 M)	**2a** (%)	**3r** (%)
1	**TBAB**	**70**	**10**
2	TBAI	43	6
4	TBACl	31	trace
5	NaI	33	trace
6	NaCl	24	trace
7	LiBr	50	10
8	*n*Bu$_4$NPF$_6$	54	7

Reaction conditions: 4-Bromobenzonitrilel (1.0 equiv., 0.3 mmol), TMSN$_3$ (2.0 equiv., 0.6 mmol), NiCl$_2$·DME (15.0 mol%), bpy (15.0 mol%), DBU (2.0 equiv., 0.6 mmol), electrolyte, TEMPO (30 mol%), H$_2$O (10.0 μL), DMA (3.0 mL), Ar, 60°C, 800 rpm, Ni as Anode and cathode at 3 mA for 10h, isolated yields are shown.

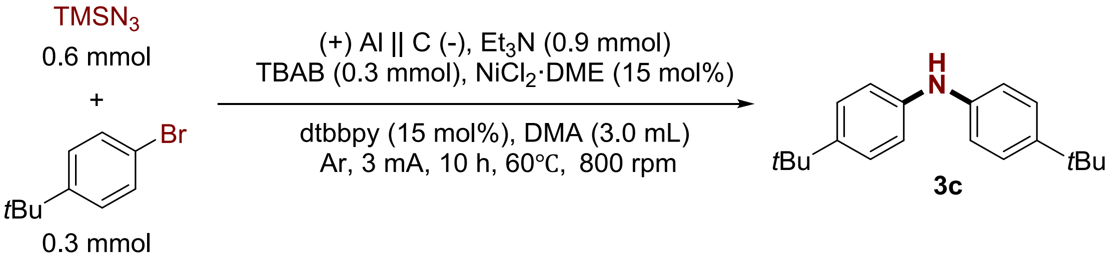
3.8 Optimization of additive (Table SI-8)



Entry	Additive	**2a** (%)	**3r** (%)
1	**TEMPO (30 mol%), H_2O (10 μL)**	**70**	**10**
3	TEMPO (20 mol%), H_2O (10 μL)	61	13
4	TEMPO (40 mol%), H_2O (10 μL)	57	11
5	TEMPO (50 mol%), H_2O (10 μL)	39	4
6	TEMPO (100 mol%), H_2O (10 μL)	22	Trace
7	TEMPO (0 mol%), H_2O (10 μL)	50	17
8	TEMPO (30 mol%), H_2O (0 μL)	58	16
9	TEMPO (30 mol%), H_2O (20 μL)	68	7
10	TEMPO (30 mol%), H_2O (30 μL)	62	8
11	TEMPO (30 mol%), H_2O (50 μL)	49	6
12	Without TEMPO and H_2O	44	18

Reaction conditions: 4-Bromobenzonitrilel (1.0 equiv., 0.3 mmol), $TMSN_3$ (2.0 equiv., 0.6 mmol), $NiCl_2$·DME (15.0 mol%), bpy (15.0 mol%), DBU (2.0 equiv., 0.6 mmol), TBAB (1.0 equiv., 0.3 mmol), Additive, H_2O (10.0 μL), DMA (3.0 mL), Ar, Temperature, 800 rpm, Ni as Anode and cathode at 3 mA for 10h, isolated yields are shown.

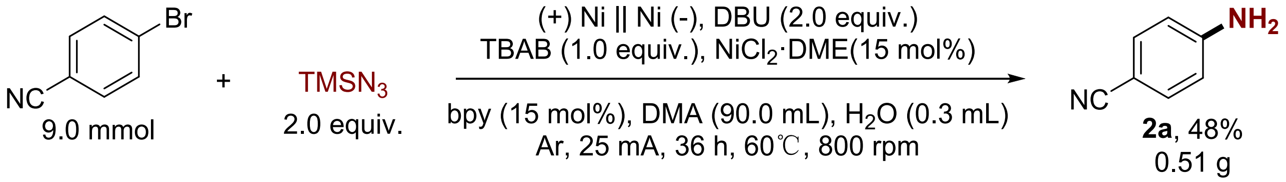
3.9 Optimization of diaryl amination



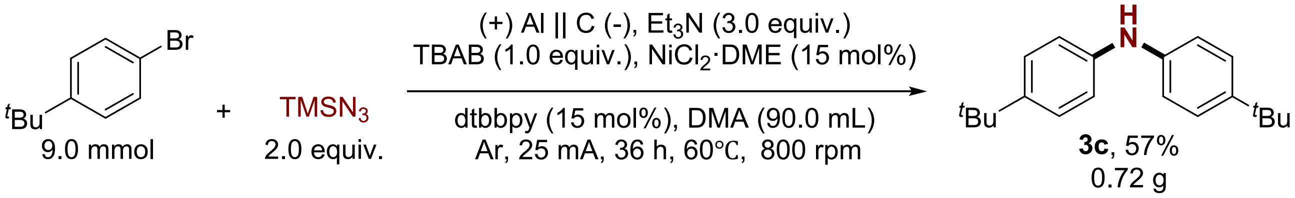
Entry	Variations from the ‘standard’ conditions	Yield **3c** (%)
1	**None**	**76**
2	Without electrolysis	N.R. [b]
3	Without dtbbpy	Trace
4	Without Et_3N	Trace
5	without $NiCl_2$·DME	Trace
6	DMF instead of DMA	66
7	MeCN instead of DMA	33
8	DBU instead of Et_3N	55
9	TMG instead of DBU	42
10	(+) Ni || C (-) as electrodes	60
11	(+) Al || Pt (-) as electrodes	27

Standard conditions B: aryl halides (1.0 equiv., 0.3 mmol), $TMSN_3$ (2.0 equiv., 0.6 mmol), Al (+)|| C (-), $NiCl_2$·DME (15.0 mol%, 0.045 mmol), dtbbpy (15.0 mol%, 0.045 mmol), TBAB (1.0 equiv., 0.3 mmol), Et_3N (3.0 equiv., 0.9 mmol), DMA (3.0 mL), 800 rpm, 60℃, constant current = 3 mA in Ar for 10h (3.7 F/mol), isolated yields are shown and in an undivided cell.

4. Gram-scale experiment

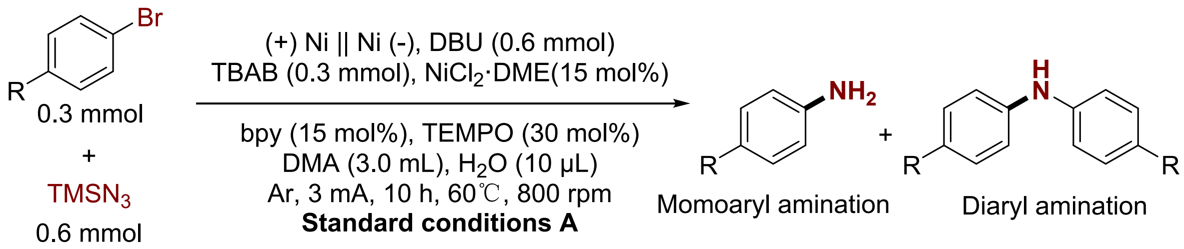


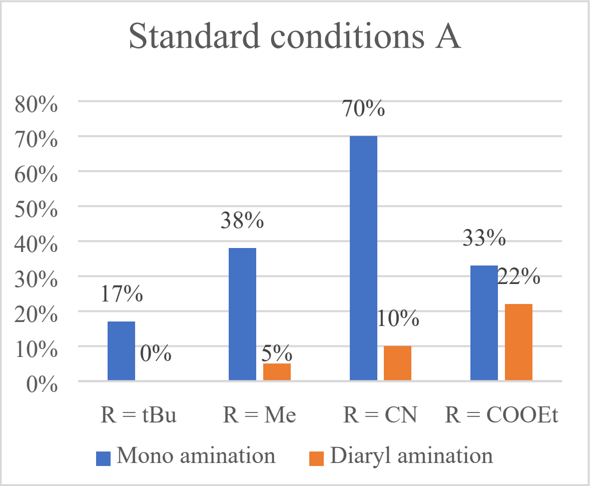
4-Bromobenzonitrile (9.0 mmol, 1.0 equiv.), $TMSN_3$ (18.0 mmol, 2.0 equiv.), $NiCl_2$·DME (1.35 mmol, 15 mol%), bpy (1.35 mmol, 15 mol%), DBU (18.0 mmol, 2.0 equiv.), H_2O (0.3 mL), TBAB (9.0 mmol, 1.0 equiv.) and DMA (90.0 mL) were added to a dried 250 mL reaction tube, and electrolyze with Ni as anode and cathode at a constant current of 25 mA for 36 hours in an Ar atmosphere at 60 °C. After the reaction, the reaction mixture was diluted with 200 mL of water and then extracted with ethyl acetate (3 × 200 mL). The combined organic phases were dried over Na_2SO_4 and concentrated under vacuum to yield the crude product, which was subsequently purified by column chromatography on silica gel using a PE/EA (2:1) mixture as the eluent to afford **2a** (0.51 g) with a yield of 48%.

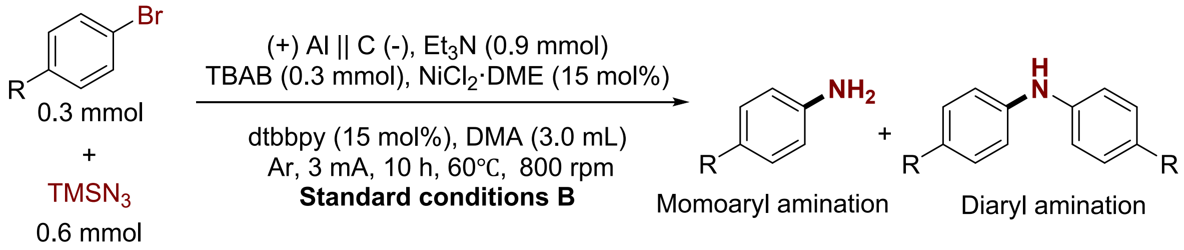


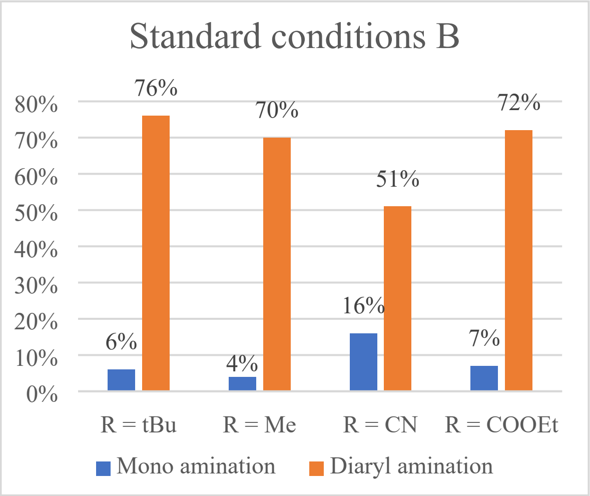
1-Bromo-4-(tert-butyl)benzene (9.0 mmol, 1.0 equiv.), $TMSN_3$ (18.0 mmol, 2.0 equiv.), $NiCl_2$·DME (1.35 mmol, 15 mol%), dtbbpy (1.35 mmol, 15 mol%), TEA (27.0 mmol, 3.0 equiv.), TBAB (9.0 mmol, 1.0 equiv.) and DMA (90.0 mL) were added to a dried 250 mL reaction tube, and electrolyze with Al as anode and Carbon as cathode at a constant current of 25 mA for 36 hours in an Ar atmosphere at 60 °C. After the reaction, the reaction mixture was diluted with 200 mL of water and then extracted with ethyl acetate (3 × 200 mL). The combined organic phases were dried over Na_2SO_4 and concentrated under vacuum to yield the crude product, which was subsequently purified by column chromatography on silica gel using a PE/EA (5:1) mixture as the eluent to afford **3a** (0.72 g) with a yield of 57%.

5. Comparison of standard condition A and standard condition B

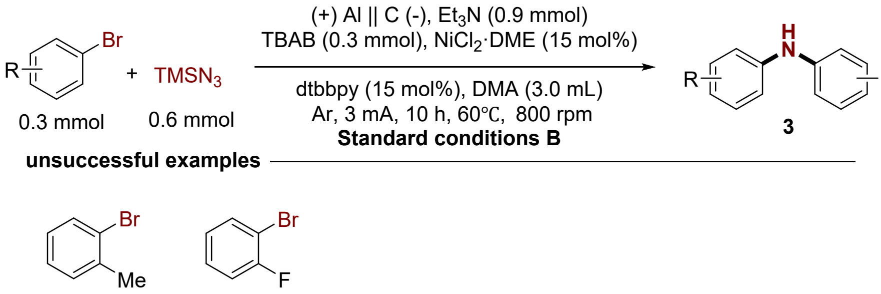




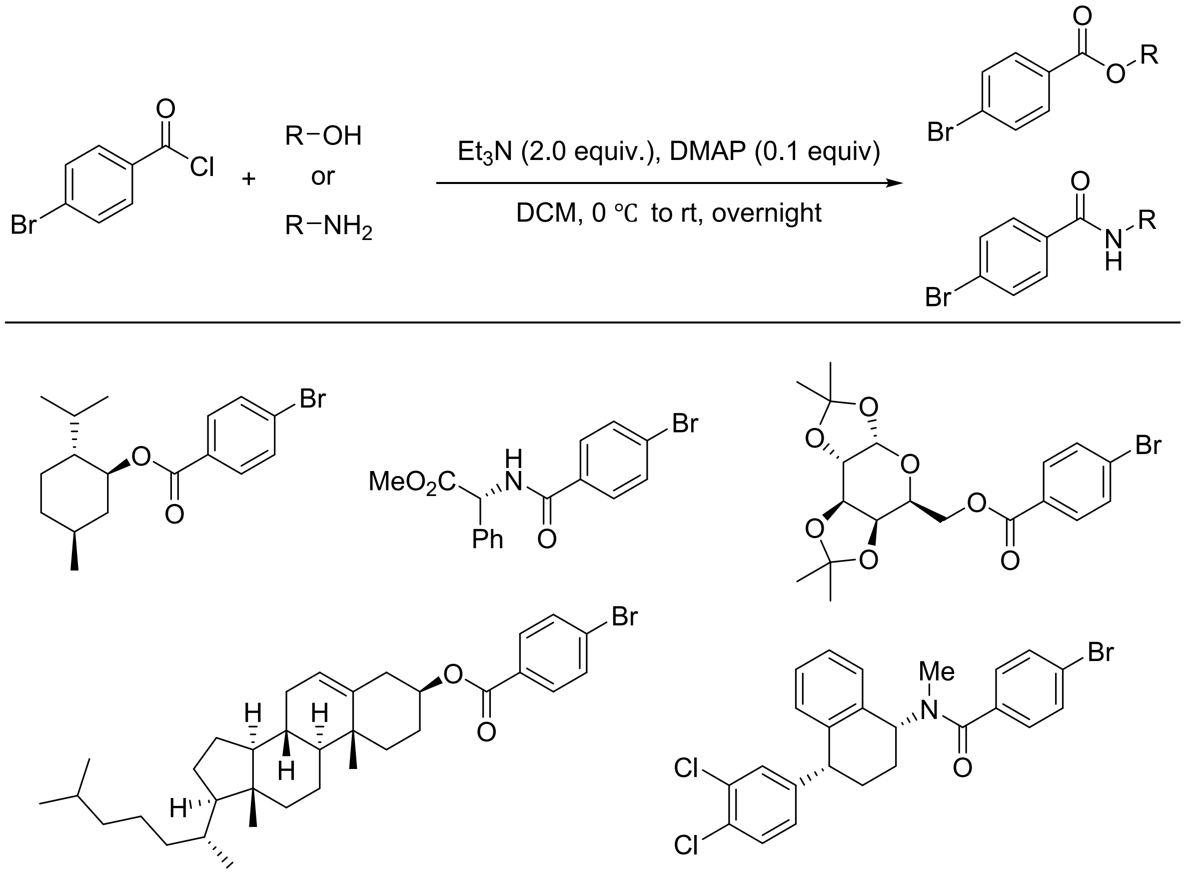




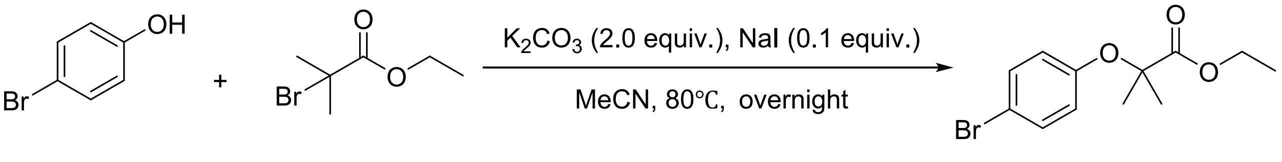
6. Unsuccessful substrate



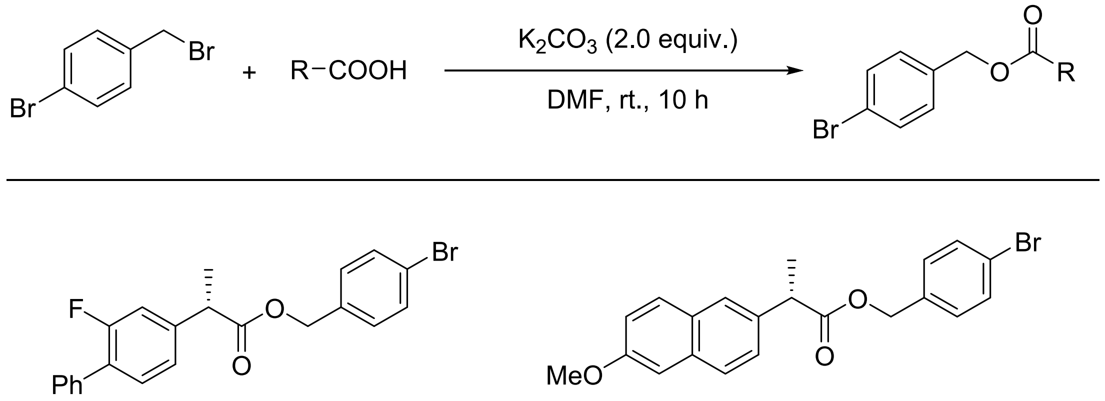
7. General procedure for the synthesis of aryl bromide drugs



To a solution of alcohol or amine (5.0 mmol, 1.0 equiv.), DMAP (0.5 mmol, 0.1 equiv.) and Et_3N (10 mmol, 2.0 equiv.) in DCM (10.0 mL) was added the solution of 4-bromobenzoylchloride (5.0 mmol, 1.0 equiv.) in DCM (10.0 mL) dropwise using syringe at 0 °C. After stirring for 30 minutes, the mixture was allowed to stir at room temperature overnight. Then the mixture was diluted with saturated NH_4Cl solution (20 mL), and extracted with DCM (3 × 10 mL). The organic layer was washed with brine, dried over $MgSO_4$ and evaporated. The residue was purified with flash column chromatography to give the desired aryl bromide.[1]



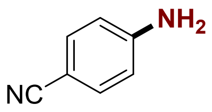
To a solution of 4-bromophenol (5.78 mmol, 1 equiv.), ethyl 2-bromoisobutyrate (5.78 mmol, 1 equiv.), K_2CO_3 (11.56 mmol, 2 equiv.) and NaI (0.58 mmol, 0.1 equiv.) in MeCN (30.0 mL) was heated at 80℃ overnight. The solvent was removed and the residue was partitioned between EtOAc and H_2O. The organic layer was washed with brine, dried over $MgSO_4$ and evaporated. The residue was purified with flash column chromatography to give the desired aryl bromide.[2]



To carboxylic acid (1.5 mmol) in DMF (10.0 mL) was added K_2CO_3 (2.0 mmol) and 4-bromobenzyl bromide (1.0 mmol). The resulting mixture was stirred at room temperature for 10 h, after which time the reaction mixture was diluted with H_2O and extracted with EtOAc (3 × 10 mL). The organic layer was washed with brine, dried over $MgSO_4$ and evaporated. The residue was purified with flash column chromatography to give the desired aryl bromide.[3]

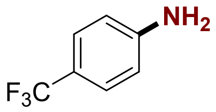
8. Characterization data of products

Preparation and Characterization Data for Isolated Products. **2a**,[4] **2b**,[4] **2c**,[5] **2d**,[4] **2e**,[6] **2f**,[7] **2g**,[8] **2h**,[7] **2i**,[6] **2j**,[9] **2k**,[8] **2l**,[7] **2m**,[10] **2n**,[4] **2o**,[11] **2p**,[12] **2q**,[13] **2r**,[4] **2s**,[6] **2t**,[7] **2u**,[7] **2v**,[14] **2w**,[4] **2x**,[4] **2y**,[15] **2za**,[4] **2zb**,[16] **2zc**,[17] **2zd**,[18] **2ze**,[19] **3a**,[20] **3b**,[21] **3c**,[22] **3d**,[21] **3e**,[22] **3f**,[20] **3g**,[20] **3h**,[20] **3i**,[20] **3j**,[20] **3k**,[20] **3l**,[20] **3m**,[20] **3n**,[20] **3o**,[23] **3r**,[20] **3t**,[22] **3u**,[22] **3v**,[24] **3x**,[22] **3zb**[24] and **4d**[25] are known compounds, and the characterization data were in accordance with the literature. ^{1}H/^{13}C/^{19}F NMR data for these compounds are provided here for completion's sake.



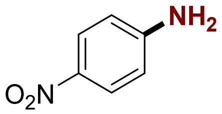
(2a) 4-aminobenzonitrile (CAS: 873-74-5)[4]: Following the General Procedure A with 4-bromobenzonitrile (54.6 mg, 0.3 mmol), **2a** was obtained as a yellow solid (24.8 mg, 70%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.40 (d, J = 8.4 Hz, 2H), 6.65 (d, J = 8.4 Hz, 2H), 4.22 (s, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 150.6, 133.8, 120.3, 114.5, 100.0.



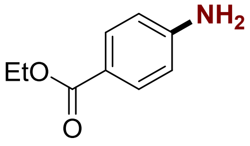
(2b) 4-(trifluoromethyl)aniline (CAS: 455-14-1)[4]: Following the General Procedure A with 1-bromo-4-(trifluoromethyl)benzene (67.5 mg, 0.3 mmol), **2b** was obtained as a yellow oil (30.5 mg, 63%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.38 (d, J = 8.8 Hz, 2H), 6.66 (d, J = 8.4 Hz, 2H), 3.92 (s, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 149.4, 126.7 (q, J = 3.8 Hz), 124.9 (q, J = 271.5 Hz), 120.1 (q, J = 32.6 Hz), 114.2. ^{19}F NMR (376 MHz, CDCl$_3$) δ -61.16.



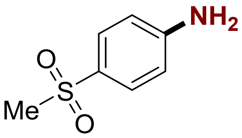
(2c) 4-nitroaniline (CAS: 100-01-6)[5]: Following the General Procedure A with 1-bromo-4-nitrobenzene (60.6 mg, 0.3 mmol), **2c** was obtained as a yellow solid (25.7 mg, 62%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, CDCl$_3$) δ 8.07 (d, J = 8.8 Hz, 2H), 6.63 (d, J = 8.8 Hz, 2H), 4.40 (s, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 152.5, 139.1, 126.34, 113.4.



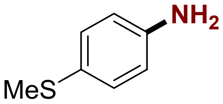
(2d) ethyl 4-aminobenzoate (CAS: 94-09-7)[4]: Following the General Procedure A with ethyl 4-bromobenzoate (68.7 mg, 0.3 mmol), **2d** was obtained as a white solid (16.3 mg, 33%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 – 7.80 (m, 2H), 6.67 – 6.59 (m, 2H), 4.31 (q, *J* = 7.2 Hz, 2H), 4.03 (s, 2H), 1.36 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.7, 150.8, 131.6, 120.1, 113.8, 60.3, 14.4.



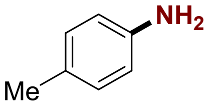
(2e) 4-(methylsulfonyl)aniline (CAS: 5470-49-5)[6]: Following the General Procedure A with 1-bromo-4-(methylsulfonyl)benzene (70.5 mg, 0.3 mmol), **2e** was obtained as a white solid (38.0 mg, 74%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 – 7.62 (m, 2H), 6.74 – 6.67 (m, 2H), 4.33 (s, 2H), 3.00 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.6, 129.4, 128.5, 114.1, 45.0.



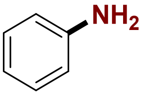
(2f) 4-(methylthio)aniline (CAS: 104-96-1)[7]: Following the General Procedure A with (4-bromophenyl)(methyl)sulfane (60.9 mg, 0.3 mmol), **2f** was obtained as a yellow oil (16.7 mg, 40%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 (d, *J* = 8.4 Hz, 2H), 6.63 (d, *J* = 8.4 Hz, 2H), 3.66 (s, 2H), 2.41 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.1, 131.0, 125.7, 115.7, 18.7.



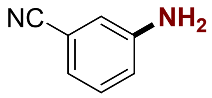
(2g) p-toluidine (CAS: 106-49-0)[8]: Following the General Procedure A with 1-bromo-4-methylbenzene (51.3 mg, 0.3 mmol), **2g** was obtained as a yellow oil (12.2 mg, 38%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.96 (d, *J* = 8.0 Hz, 2H), 6.59 (d, *J* = 8.4 Hz, 2H), 3.49 (s, 2H), 2.23 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.9, 129.8, 127.8, 115.3, 20.5.



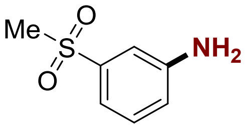
(2h) aniline (CAS: 62-53-3)[7]: Following the General Procedure A with bromobenzene (47.1 mg, 0.3 mmol), **2h** was obtained as a yellow oil (11.5 mg, 41%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 – 7.11 (m, 2H), 6.78 – 6.72 (m, 1H), 6.70 – 6.64 (m, 2H), 3.60 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.4, 129.3, 118.6, 115.1.



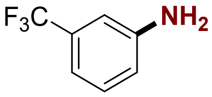
(2i) 3-aminobenzonitrile (CAS: 2237-30-1)[6]: Following the General Procedure A with 3-bromobenzonitrile (54.6 mg, 0.3 mmol), **2i** was obtained as a yellow solid (20.5 mg, 58%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, CDCl$_3$) *δ* 7.21 (t, *J* = 7.9 Hz, 1H), 7.01 (dt, *J* = 7.6, 1.2 Hz, 1H), 6.92 – 6.84 (m, 2H), 3.91 (s, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) *δ* 147.0, 130.1, 121.9, 119.24, 119.22, 117.4, 112.9.



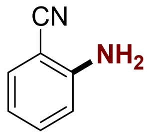
(2j) 3-(methylsulfonyl)aniline (CAS: 35216-39-8)[9]: Following the General Procedure A with 1-bromo-3-(methylsulfonyl)benzene (70.5 mg, 0.3 mmol), **2j** was obtained as a yellow solid (30.8 mg, 60%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, CDCl$_3$) *δ* 7.30 (q, *J* = 8.0 Hz), 7.27 (d, *J* = 1.6 Hz, 1H), 7.26 – 7.24 (m, 1H), 7.21 (t, *J* = 2.0 Hz, 1H), 6.92 – 6.87 (m, 1H), 4.04 (s, 2H), 3.03 (s, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) *δ* 147.5, 141.34, 130.3, 119.7, 116.6, 112.8, 44.4.



(2k) 3-(trifluoromethyl)aniline (CAS: 98-16-8)[8]: Following the General Procedure A with 1-bromo-3-(trifluoromethyl)benzene (67.5 mg, 0.3 mmol), **2k** was obtained as a yellow solid (29.0 mg, 60%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

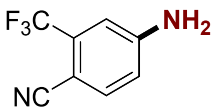
^{1}H NMR (400 MHz, CDCl$_3$) *δ* 7.23 (t, *J* = 8.0 Hz, 1H), 7.02 – 6.96 (m, 1H), 6.90 – 6.86 (m, 1H), 6.80 (dd, *J* = 8.4, 2.4 Hz, 1H), 3.81 (s, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) *δ* 146.7, 131.6 (q, *J* = 31.9 Hz), 129.8, 124.2 (q, *J* = 272.2 Hz), 118.0 (q, *J* = 1.6 Hz), 115.0 (q, *J* = 4.0 Hz), 111.3 (q, *J* = 3.9 Hz). ^{19}F NMR (376 MHz, CDCl$_3$) *δ* -62.95.



(2l) 2-aminobenzonitrile (CAS: 1885-29-6)[7]

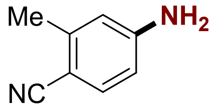
Following the General Procedure A with 2-bromobenzonitrile (54.6 mg, 0.3 mmol), **2l** was obtained as a yellow solid (17.4 mg, 49%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.38 – 7.28 (m, 2H), 6.77 – 6.68 (m, 2H), 4.45 (s, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 149.6, 133.9, 132.2, 117.8, 117.6, 115.1, 95.8.



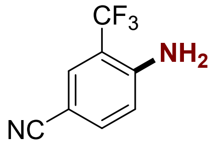
(2m) 4-amino-2-(trifluoromethyl)benzonitrile(CAS: 98-16-8)[10]: Following the General Procedure A with 4-bromo-2-(trifluoromethyl)benzonitrile (75.0 mg, 0.3 mmol), **2m** was obtained as a yellow solid (47.5 mg, 85%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.55 (d, J = 8.4 Hz, 1H), 6.95 (d, J = 2.0 Hz, 1H), 6.78 (dd, J = 8.4, 2.0 Hz, 1H), 4.45 (s, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 150.3, 136.3, 134.5 (q, J = 32.0 Hz), 122.4 (q, J = 273.7 Hz), 116.8, 116.3, 112.1 (q, J = 4.8 Hz). ^{19}F NMR (376 MHz, CDCl$_3$) δ -62.55.



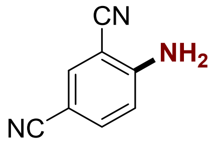
(2n) 4-amino-2-methylbenzonitrile (CAS: 72115-06-1)[4]: Following the General Procedure A with 4-bromo-2-methylbenzonitrile (58.8 mg, 0.3 mmol), **2n** was obtained as a yellow solid (23.8 mg, 60%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.34 (d, J = 8.4 Hz, 1H), 6.53 – 6.44 (m, 2H), 4.15 (s, 2H), 2.41 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 150.4, 143.5, 134.0, 119.4, 115.3, 112.0, 100.6, 20.4.



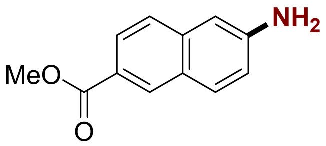
(2o) 4-amino-3-(trifluoromethyl)benzonitrile (CAS: 327-74-2)[11]: Following the General Procedure A with 4-bromo-3-(trifluoromethyl)benzonitrile (75.0 mg, 0.3 mmol), **2o** was obtained as a yellow solid (30.2 mg, 54%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.71 (d, J = 0.8 Hz, 1H), 7.52 (dd, J = 8.4, 1.6 Hz, 1H), 6.78 (d, J = 8.4 Hz, 1H), 4.78 (s, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 148.0, 136.2, 131.6 (q, J = 5.3 Hz), 123.7 (q, J = 272.4 Hz), 118.8, 117.2, 113.5 (q, J = 31.3 Hz), 99.8. ^{19}F NMR (376 MHz, CDCl$_3$) δ -63.63.



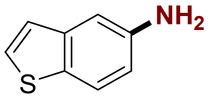
(2p) 4-aminoisophthalonitrile (CAS: 19619-22-8)[12]: Following the General Procedure A with 4-bromoisophthalonitrile (62.1 mg, 0.3 mmol), **2p** was obtained as a yellow solid (24.9 mg, 58%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, DMSO) δ 7.99 (d, *J* = 2.0 Hz, 1H), 7.63 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.06 (s, 2H), 6.85 (d, *J* = 8.8 Hz, 1H). ^{13}C NMR (101 MHz, DMSO) δ 154.8, 138.8, 137.1, 119.2, 116.8, 116.1, 97.3, 94.1.



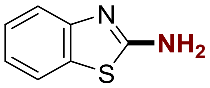
(2q) methyl 6-amino-2-naphthoate (CAS: 5159-59-1)[13]: Following the General Procedure A with methyl 6-bromo-2-naphthoate (79.5 mg, 0.3 mmol), **2q** was obtained as a yellow solid (38.6 mg, 64%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, DMSO) δ 8.34 (d, *J* = 1.2 Hz, 1H), 7.80 – 7.71 (m, 2H), 7.54 (d, *J* = 8.8 Hz, 1H), 7.01 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.84 (d, *J* = 2.0 Hz, 1H), 5.85 (s, 2H), 3.85 (s, 3H). ^{13}C NMR (101 MHz, DMSO) δ 167.2, 149.9, 138.1, 131.1, 131.0, 125.6, 125.5, 125.3, 121.9, 119.5, 105.6, 52.2.



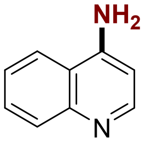
(2r) benzo[b]thiophen-5-amine (CAS: 20532-28-9)[4]: Following the General Procedure A with 5-bromobenzo[b]thiophene (63.9 mg, 0.3 mmol), **2r** was obtained as a yellow solid (17.0 mg, 38%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.61 (d, *J* = 8.4 Hz, 1H), 7.36 (d, *J* = 5.6 Hz, 1H), 7.13 (d, *J* = 5.6 Hz, 1H), 7.07 (d, *J* = 2.0 Hz, 1H), 6.75 (dd, *J* = 8.4, 2.4 Hz, 1H), 3.67 (s, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 143.5, 140.8, 130.4, 127.0, 123.00, 122.95, 114.8, 108.2.



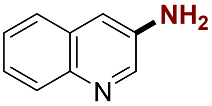
(2s) benzo[d]thiazol-2-amine (CAS: 136-95-8)[6]: Following the General Procedure A with 2-bromobenzo[d]thiazole (64.2 mg, 0.3 mmol), **2s** was obtained as a yellow solid (23.0 mg, 51%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.59 (d, *J* = 8.0 Hz, 1H), 7.54 (d, *J* = 8.4 Hz, 1H), 7.34 – 7.28 (m, 1H), 7.16 – 7.10 (m, 1H), 5.56 (s, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 165.9, 152.0, 131.6, 126.0, 122.3, 120.9, 119.2.



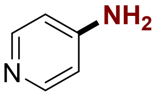
(2t) quinolin-4-amine (CAS: 578-68-7)[7]: Following the General Procedure A with 4-bromoquinoline (64.2 mg, 0.3 mmol), **2t** was obtained as a yellow solid (24.6 mg, 57%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, DMSO) δ 8.32 (d, *J* = 5.2 Hz, 1H), 8.19 – 8.12 (m, 1H), 7.79 – 7.74 (m, 1H), 7.62 – 7.55 (m, 1H), 7.42 – 7.34 (m, 1H), 6.79 (s, 2H), 6.56 (d, *J* = 5.2 Hz, 1H). ^{13}C NMR (101 MHz, DMSO) δ 151.9, 150.8, 149.3, 129.4, 129.3, 123.9, 122.8, 119.1, 102.8.



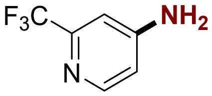
(2u) quinolin-3-amine (CAS: 578-68-7)[7]: Following the General Procedure A with 4-bromoquinoline (62.4 mg, 0.3 mmol), **2u** was obtained as a yellow solid (24.7mg, 57%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, *J* = 2.8 Hz, 1H), 7.99 – 7.93 (m, 1H), 7.61 – 7.56 (m, 1H), 7.48 – 7.39 (m, 2H), 7.23 (d, *J* = 2.4 Hz, 1H), 3.93 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.1, 142.8, 139.7, 129.10, 129.07, 126.9, 125.8, 125.6, 114.9.



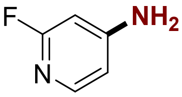
(2v) pyridin-4-amine (CAS: 504-24-5)[14]: Following the General Procedure A with 4-bromopyridine (47.4 mg, 0.3 mmol), **2v** was obtained as a white solid (14.7 mg, 52%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, DMSO) δ 7.95 (dd, *J* = 4.8, 1.5 Hz, 2H), 6.44 (dd, *J* = 4.8, 1.6 Hz, 2H), 5.95 (s, 2H). ^{13}C NMR (101 MHz, DMSO) δ 154.7, 150.0, 109.3.



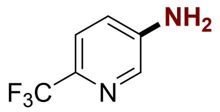
(2w) 2-(trifluoromethyl)pyridin-4-amine (CAS: 147149-98-2)[4]: Following the General Procedure A with 4-bromo-2-(trifluoromethyl)pyridine (67.8 mg, 0.3 mmol), **2w** was obtained as a yellow solid (44.3 mg, 91%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (s, 1H), 6.87 (s, 1H), 6.62 (d, *J* = 2.4 Hz, 1H), 4.64 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.93, 150.29, 148.93 (q, *J* = 33.7 Hz), 121.7 (q, *J* = 275.3 Hz), 111.13, 106.24 (q, *J* = 3.1 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -68.53.



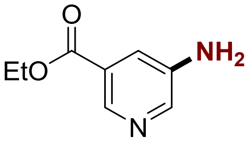
(2x) 2-fluoropyridin-4-amine (CAS: 18614-51-2)[4]: Following the General Procedure A with 4-bromo-2-fluoropyridine (52.8 mg, 0.3 mmol), **2x** was obtained as a yellow solid (20.9 mg, 62%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 5.6 Hz, 1H), 6.43 – 6.36 (m, 1H), 6.08 (d, *J* = 2.0 Hz, 1H), 4.61 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.44 (d, *J* = 232.2 Hz), 157.20 (d, *J* = 11.7 Hz), 147.50 (d, *J* = 18.6 Hz), 108.21 (d, *J* = 2.9 Hz), 92.78 (d, *J* = 41.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -69.93.



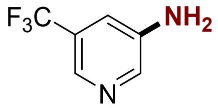
(2y) 6-(trifluoromethyl)pyridin-3-amine (CAS: 106877-33-2)[15]: Following the General Procedure A with 5-bromo-2-(trifluoromethyl)pyridine (67.8 mg, 0.3 mmol), **2y** was obtained as a yellow solid (31.1 mg, 64%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.1 (d, J = 2.8 Hz, 1H), 7.4 (d, J = 8.4 Hz, 1H), 7.03 – 6.98 (m, 1H), 4.07 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.8, 137.8 (q, J = 34.9 Hz), 136.9, 122.2 (q, J = 273.3 Hz), 121.2 (q, J = 2.8 Hz), 120.5. ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.63.



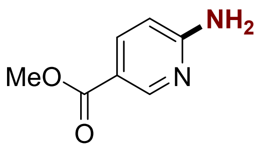
(2z) ethyl 5-aminonicotinate: Following the General Procedure A with ethyl 5-bromonicotinate (69.0 mg, 0.3 mmol), **2z** was obtained as a yellow solid (37.9 mg, 76%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.40 – 8.16 (m, 2H), 7.52 (s, 1H), 4.37 (q, J = 7.2 Hz, 2H), 3.86 (s, 2H), 1.38 (t, J = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.1, 143.7, 140.8, 129.9, 121.6, 116.1, 61.3, 14.3. HRMS（ESI）m/z calcd for $C_{19}H_{26}NO_7$ $(M+H)^+$ 380.17038, found 380.17043.



(2za) 5-(trifluoromethyl)pyridin-3-amine (CAS: 112110-07-3)[4]: Following the General Procedure A with 3-bromo-5-(trifluoromethyl)pyridine (67.8 mg, 0.3 mmol), **2za** was obtained as a yellow solid (34.1 mg, 70%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

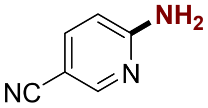
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 – 8.22 (m, 2H), 7.15 (t, J = 2.4 Hz, 1H), 3.99 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.3, 140.3 (q, J = 1.6 Hz), 136.1 (q, J = 4.3 Hz), 126.9 (q, J = 32.4 Hz), 123.6 (q, J = 273.5 Hz), 117.4 (q, J = 3.7 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.73.



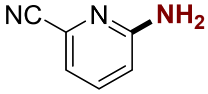
(2zb) methyl 6-aminonicotinate (CAS: 36052-24-1)[16]: Following the General Procedure A with methyl 6-bromonicotinate (64.8 mg, 0.3 mmol), **2zb** was obtained as a yellow solid (35.6 mg, 78%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, DMSO) δ 8.54 (s, 1H), 7.81 (dd, J = 8.8, 2.4 Hz, 1H), 6.82 (s, 2H), 6.47 (d, J = 8.8 Hz, 1H), 3.75 (s, 3H). ^{13}C NMR (101 MHz, DMSO) δ 166.2, 163.1, 151.5, 138.0, 113.8, 107.7, 51.8.

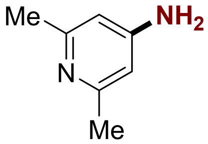
HRMS（ESI）m/z calcd for $C_7H_9N_2O_2$$(M+H)^+$ 153.06585, found 153.06573.



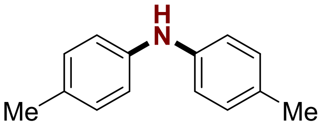
(2zc) 6-aminonicotinonitrile (CAS: 4214-73-7)[17]: Following the General Procedure A with 6-bromonicotinonitrile (54.9 mg, 0.3 mmol), **2zc** was obtained as a yellow solid (21.1 mg, 59%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (d, *J* = 1.6 Hz, 1H), 7.61 (dd, *J* = 8.4, 2.0 Hz, 1H), 6.50 (d, *J* = 8.8 Hz, 1H), 5.04 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.1, 153.12, 140.2, 118.1, 108.0, 98.5.



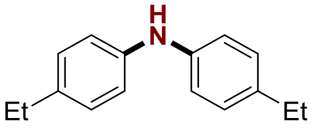
(2zd) 6-aminopicolinonitrile (CAS: 370556-44-8)[18]: Following the General Procedure A with 6-bromopicolinonitrile (54.9 mg, 0.3 mmol), **2zd** was obtained as a yellow solid (15.4 mg, 43%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 – 7.46 (m, 1H), 7.03 (dd, *J* = 7.2, 0.8 Hz, 1H), 6.68 (dd, *J* = 8.4, 0.8 Hz, 1H), 4.85 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.9, 138.2, 131.6, 119.0, 117.6, 112.8.



(2ze) 2,6-dimethylpyridin-4-amine (CAS: 3512-80-9)[19]: Following the General Procedure A with 4-bromo-2,6-dimethylpyridine (55.8 mg, 0.3 mmol), **2ze** was obtained as a yellow solid (17.2 mg, 47%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).
^{1}H NMR (400 MHz, $CDCl_3$) δ 6.24 (s, 2H), 3.98 (s, 2H), 2.39 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.3, 153.4, 106.3, 24.4.



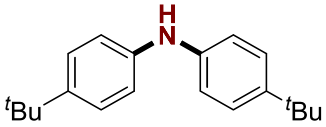
(3a) di-p-tolylamine (CAS: 620-93-9)[20]: Following the General Procedure B with 1-bromo-4-methylbenzene (51.3 mg, 0.3 mmol), **3a** was obtained as a yellow solid (29.6 mg, 70%). This target product was purified by column chromatography on silica gel (PE/EA = 5:1).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.05 (d, *J* = 8.0 Hz, 4H), 6.96 – 6.91 (m, 4H), 5.48 (s, 1H), 2.28 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.2, 130.2, 129.9, 117.9, 20.7.



(3b) bis(4-ethylphenyl)amine (CAS: 7268-62-4)[21]: Following the General Procedure B with 1-

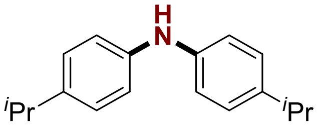
bromo-4-ethylbenzene (55.5 mg, 0.3 mmol), **3b** was obtained as a yellow solid (19.3 mg, 57%). This target product was purified by column chromatography on silica gel (PE/EA = 5:1).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.08 (d, J = 8.8 Hz, 4H), 7.01 – 6.94 (m, 4H), 5.52 (s, 1H), 2.59 (q, J = 7.6 Hz, 4H), 1.22 (t, J = 7.6 Hz, 6H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 141.3, 136.7, 128.7, 117.9, 28.2, 15.9.



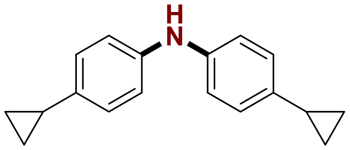
(3c) bis(4-(tert-butyl)phenyl)amine (CAS: 4627-22-9)[22]: Following the General Procedure B with 1-bromo-4-(tert-butyl)benzene (63.9 mg, 0.3 mmol), **3c** was obtained as a yellow solid (30.1 mg, 76%). This target product was purified by column chromatography on silica gel (PE/EA = 5:1).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.29 – 7.24 (m, 4H), 7.02 – 6.97 (m, 4H), 5.55 (s, 1H), 1.30 (s, 18H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 143.6, 141.0, 126.1, 117.4, 34.12, 31.5.



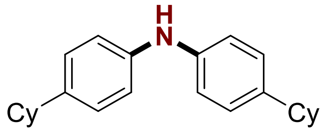
(3d) bis(4-isopropylphenyl)amine (CAS: 63451-41-2)[21]: Following the General Procedure B with 1-bromo-4-isopropylbenzene (59.7 mg, 0.3 mmol), **3d** was obtained as a yellow solid (28.9 mg, 76%). This target product was purified by column chromatography on silica gel (PE/EA = 5:1).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.11 (d, J = 8.4 Hz, 4H), 6.98 (d, J = 8.4 Hz, 4H), 5.53 (s, 1H), 2.91 – 2.78 (m, 2H), 1.23 (d, J = 6.8 Hz, 12H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 141.4, 128.8, 127.2, 117.8, 33.4, 24.2.



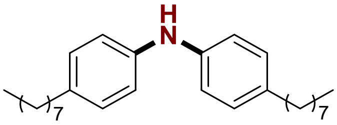
(3e) bis(4-cyclopropylphenyl)amine (CAS: 2722001-27-4)[22]: Following the General Procedure B with 1-bromo-4-cyclopropylbenzene (59.1 mg, 0.3 mmol), **3e** was obtained as a yellow solid (25.4 mg, 68%). This target product was purified by column chromatography on silica gel (PE/EA = 5:1).

^{1}H NMR (400 MHz, CDCl$_3$) δ 6.95 (q, J = 8.4 Hz, 8H), 5.50 (s, 1H), 1.89 – 1.78 (m, 2H), 0.97 – 0.82 (m, 4H), 0.68 – 0.54 (m, 4H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 141.2, 136.2, 126.7, 117.9, 14.8, 8.6.

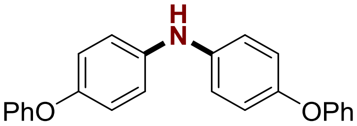


(3f) bis(4-cyclohexylphenyl)amine (CAS: 163687-39-6)[20]: Following the General Procedure

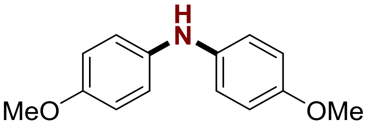
B with 1-bromo-4-cyclohexylbenzene (71.8 mg, 0.3 mmol), **3f** was obtained as a yellow solid (27.0 mg, 54%). This target product was purified by column chromatography on silica gel (PE/EA = 5:1).
^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.09 (d, *J* = 8.4 Hz, 4H), 6.97 (d, *J* = 8.4 Hz, 4H), 5.53 (s, 1H), 2.50 – 2.37 (m, 2H), 1.90 – 1.79 (m, 8H), 1.77 – 1.69 (m, 2H), 1.44 – 1.32 (m, 8H), 1.29 – 1.18 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) *δ* 141.4, 140.7, 127.5, 117.8, 43.8, 34.7, 27.0, 26.2.



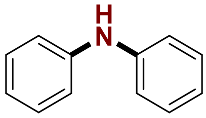
(3g) bis(4-octylphenyl)amine (CAS: 101-67-7)[20]: Following the General Procedure B with 1-bromo-4-octylbenzene (80.8 mg, 0.3 mmol), **3g** was obtained as a yellow solid (33.1 mg, 56%). This target product was purified by column chromatography on silica gel (PE/EA = 5:1).
^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.05 (d, *J* = 8.4 Hz, 4H), 6.96 (d, *J* = 8.4 Hz, 4H), 5.51 (s, 1H), 2.58 – 2.47 (m, 4H), 1.64 – 1.54 (m, 4H), 1.34 – 1.23 (m, 20H), 0.92 – 0.84 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) *δ* 141.3, 135.4, 129.2, 117.8, 35.3, 31.9, 31.8, 29.6, 29.4, 29.3, 22.7, 14.2.



(3h) bis(4-phenoxyphenyl)amine (CAS: 18162-30-6)[20]: Following the General Procedure B with 1-bromo-4-phenoxybenzene (74.7 mg, 0.3 mmol), **3h** was obtained as a yellow solid (29.7 mg, 56%). This target product was purified by column chromatography on silica gel (PE/EA = 5:1).
^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.34 – 7.27 (m, 4H), 7.07 – 6.93 (m, 14H), 5.55 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) *δ* 158.3, 150.8, 139.7, 129.7, 122.6, 120.7, 119.3, 117.8.

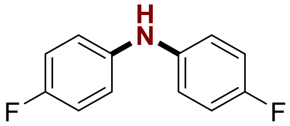


(3i) bis(4-methoxyphenyl)amine (CAS: 101-70-2)[20]: Following the General Procedure B with 1-bromo-4-methoxybenzene (56.1 mg, 0.3 mmol), **3i** was obtained as a yellow solid (16.5 mg, 48%). This target product was purified by column chromatography on silica gel (PE/EA = 5:1).
^{1}H NMR (400 MHz, $CDCl_3$) *δ* 6.94 (d, *J* = 8.8 Hz, 4H), 6.85 – 6.79 (m, 4H), 5.28 (s, 1H), 3.78 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) *δ* 154.3, 138.0, 119.6, 114.7, 55.7.

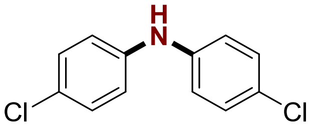


(3j) diphenylamine (CAS: 122-39-4)[20]: Following the General Procedure B with bromobenzene (47.1 mg, 0.3 mmol), **3j** was obtained as a yellow solid (17.3 mg, 68%). This target product was purified by column chromatography on silica gel (PE/EA = 5:1).

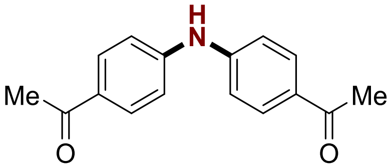
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.29 – 7.23 (m, 4H), 7.09 – 7.04 (m, 4H), 6.95 – 6.89 (m, 2H), 5.68 (s, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 143.2, 129.4, 121.0, 117.8.



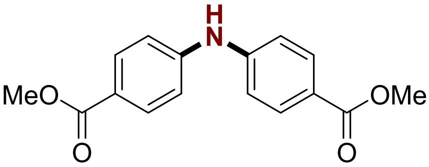
(3k) bis(4-fluorophenyl)amine (CAS: 330-91-6)[20]: Following the General Procedure B with 1-bromo-4-fluorobenzene (52.5 mg, 0.3 mmol), **3k** was obtained as a yellow solid (25.2 mg, 82%). This target product was purified by column chromatography on silica gel (PE/EA = 5:1).
^{1}H NMR (400 MHz, CDCl$_3$) δ 6.95 (d, J = 6.0 Hz, 8H), 5.46 (s, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 157.8 (d, J = 239.7 Hz), 139.8 (d, J = 2.4 Hz), 119.4 (d, J = 7.7 Hz), 116.0 (d, J = 22.5 Hz). ^{19}F NMR (376 MHz, CDCl$_3$) δ -122.63.



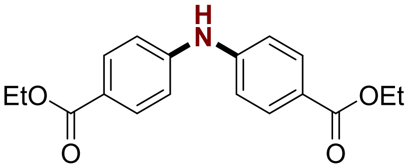
(3l) bis(4-chlorophenyl)amine (CAS: 6962-04-5)[20]: Following the General Procedure B with 1-bromo-4-chlorobenzene (57.4 mg, 0.3 mmol), **3l** was obtained as a yellow solid (24.6 mg, 69%). This target product was purified by column chromatography on silica gel (PE/EA = 5:1).
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.25 (d, J = 8.4 Hz, 4H), 6.99 (d, J = 8.8 Hz, 4H), 5.66 (s, 1H).^{13}C NMR (101 MHz, CDCl$_3$) δ 141.4, 129.4, 126.1, 119.1.



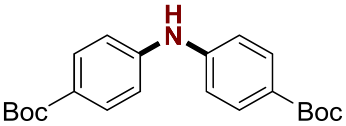
(3m) 1,1'-(azanediylbis(4,1-phenylene))bis(ethan-1-one) (CAS: 20255-76-9)[20]: Following the General Procedure B with 1-(4-bromophenyl)ethan-1-one (59.7 mg, 0.3 mmol), **3m** was obtained as a yellow solid (15.6 mg, 41%). This target product was purified by column chromatography on silica gel (PE/EA = 5:1).
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.94 (d, J = 8.4 Hz, 4H), 7.16 (d, J = 8.4 Hz, 4H), 6.36 (s, 1H), 2.57 (s, 6H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 196.4, 145.8, 131.0, 130.5, 117.0, 26.3.



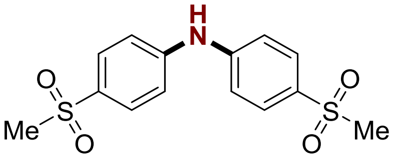
(3n) dimethyl 4,4'-azanediyldibenzoate (CAS: 17104-81-3)[20]: Following the General Procedure B with methyl 4-bromobenzoate (64.5 mg, 0.3 mmol), **3n** was obtained as a yellow solid (34.7 mg, 81%). This target product was purified by column chromatography on silica gel (PE/EA = 5:1).
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.98 (d, J = 8.4 Hz, 4H), 7.13 (d, J = 8.8 Hz, 4H), 6.44 (s, 1H), 3.89 (s, 6H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 166.8, 145.9, 131.5, 123.1, 116.9, 51.9.



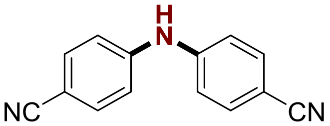
(3o) diethyl 4,4'-azanediyldibenzoate (CAS: 53884-32-5)[23]: Following the General Procedure B with ethyl 4-bromobenzoate (68.7 mg, 0.3 mmol), **3o** was obtained as a yellow solid (33.8 mg, 72%). This target product was purified by column chromatography on silica gel (PE/EA = 5:1).
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.98 (d, J = 8.8 Hz, 4H), 7.13 (d, J = 8.4 Hz, 4H), 6.44 (s, 1H), 4.36 (q, J = 7.2 Hz, 4H), 1.38 (t, J = 7.2 Hz, 6H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 166.3, 145.8, 131.4, 123.4, 116.9, 60.7, 14.4.



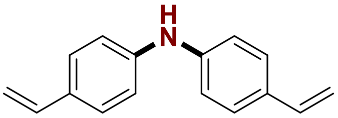
(3p) di-tert-butyl 4,4'-azanediyldibenzoate (CAS: 386218-10-6): Following the General Procedure B with tert-butyl 4-bromobenzoate (77.1 mg, 0.3 mmol), **3p** was obtained as a yellow solid (38.8 mg, 70%). This target product was purified by column chromatography on silica gel (PE/EA = 5:1).
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.92 (d, J = 8.8 Hz, 4H), 7.10 (d, J = 8.4 Hz, 4H), 6.40 (s, 1H), 1.59 (s, 18H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 165.5, 145.6, 131.24, 124.9, 116.7, 80.6, 28.3.



(3q) bis(4-(methylsulfonyl)phenyl)amine (CAS: 1140964-63-1): Following the General Procedure B with 1-bromo-4-(methylsulfonyl)benzene (70.5 mg, 0.3 mmol), **3q** was obtained as a yellow solid (28.8 mg, 59%). This target product was purified by column chromatography on silica gel (PE/EA = 5:1).
^{1}H NMR (400 MHz, DMSO) δ 9.45 (s, 1H), 7.82 (d, J = 8.8 Hz, 4H), 7.35 (d, J = 8.8 Hz, 4H), 3.16 (s, 6H). ^{13}C NMR (101 MHz, DMSO) δ 146.9, 132.4, 129.4, 117.3, 44.5. HRMS（ESI）m/z calcd for $C_{14}H_{15}NO_4S_2$ (M+H)$^+$ 326.05153, found 326.05096.

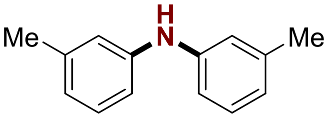


(3r) 4,4'-azanediyldibenzonitrile (CAS: 36602-05-8)[20]: Following the General Procedure B with 4-bromobenzonitrile (54.6 mg, 0.3 mmol), **3r** was obtained as a yellow solid (16.8 mg, 51%). This target product was purified by column chromatography on silica gel (PE/EA = 5:1).
^{1}H NMR (400 MHz, DMSO) δ 9.45 (s, 1H), 7.71 (d, J = 8.8 Hz, 4H), 7.27 (d, J = 8.8 Hz, 4H). ^{13}C NMR (101 MHz, DMSO) δ 146.2, 134.3, 119.9, 117.8, 102.6.



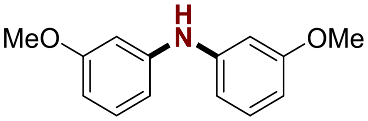
(3s) bis(4-vinylphenyl)amine (CAS: 852360-34-0): Following the General Procedure B with 1-bromo-4-vinylbenzene (54.9 mg, 0.3 mmol), **3s** was obtained as a yellow solid (14.3 mg, 43%). This target product was purified by column chromatography on silica gel (PE/EA = 5:1).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.33 (d, J = 8.4 Hz, 4H), 7.02 (d, J = 8.4 Hz, 4H), 6.66 (dd, J = 17.6, 10.8 Hz, 2H), 5.80 (s, 1H), 5.62 (d, J = 17.6 Hz, 2H), 5.12 (d, J = 11.2 Hz, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 142.5, 136.3, 130.7, 127.3, 117.7, 111.4.



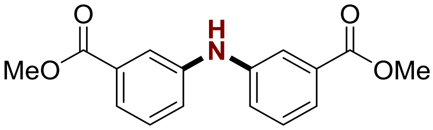
(3t) di-m-tolylamine (CAS: 626-13-1)[22]: Following the General Procedure B with 1-bromo-3-methylbenzene (51.3 mg, 0.3 mmol), **3t** was obtained as a yellow solid (18.6 mg, 63%). This target product was purified by column chromatography on silica gel (PE/EA = 5:1).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.18 – 7.10 (m, 2H), 6.91 – 6.84 (m, 4H), 6.74 (d, J = 7.6 Hz, 2H), 5.59 (s, 1H), 2.30 (s, 6H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 143.2, 139.2, 129.2, 121.8, 118.6, 115.0, 21.6.



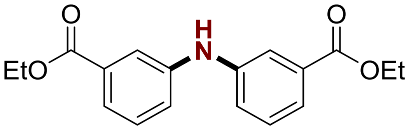
(3u) bis(3-methoxyphenyl)amine (CAS: 92248-06-1)[22]: Following the General Procedure B with 1-bromo-3-methoxybenzene (56.1 mg, 0.3 mmol), **3u** was obtained as a yellow solid (21.3 mg, 62%). This target product was purified by column chromatography on silica gel (PE/EA = 5:1).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.16 (t, J = 8.0 Hz, 2H), 6.70 – 6.62 (m, 4H), 6.52 – 6.45 (m, 2H), 5.72 (s, 1H), 3.77 (s, 6H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 160.7, 144.3, 130.1, 110.7, 106.5, 103.8, 55.2.



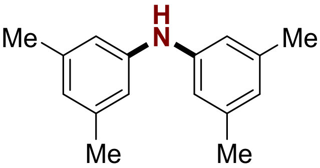
(3v) dimethyl 3,3'-azanediyldibenzoate (CAS: 1359968-14-1)[24]: Following the General Procedure B with methyl 3-bromobenzoate (64.5 mg, 0.3 mmol), **3v** was obtained as a yellow solid (24.0 mg, 56%). This target product was purified by column chromatography on silica gel (PE/EA = 5:1).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.72 (s, 2H), 7.62 (d, J = 7.6 Hz, 2H), 7.34 (t, J = 8.0 Hz, 2H), 7.31 – 7.27 (m, 2H), 5.99 (s, 1H), 3.91 (s, 6H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 167.0, 142.9, 131.5, 129.5, 122.5, 122.0, 118.9, 52.2.



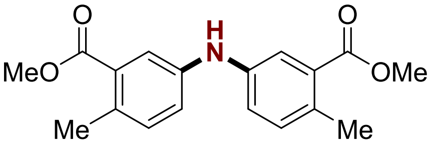
(3w) diethyl 3,3'-azanediyldibenzoate: Following the General Procedure B with ethyl 3-bromobenzoate (68.7 mg, 0.3 mmol), **3w** was obtained as a yellow solid (21.2 mg, 45%). This target product was purified by column chromatography on silica gel (PE/EA = 5:1).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.75 – 7.71 (m, 2H), 7.66 – 7.59 (m, 2H), 7.34 (t, J = 8.0 Hz, 2H), 7.30 – 7.26 (m, 2H), 5.99 (s, 1H), 4.37 (q, J = 7.2 Hz, 4H), 1.38 (t, J = 7.2 Hz, 6H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 166.5, 142.9, 131.9, 129.4, 122.5, 121.8, 118.9, 61.1, 14.3. HRMS（ESI）m/z calcd for $C_{18}H_{19}NO_4$ $(M+H)^+$ 314.13868, found 314.13803.



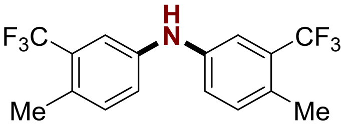
(3x) bis(3,5-dimethylphenyl)amine (CAS: 5369-25-5)[22]: Following the General Procedure B with 1-bromo-3,5-dimethylbenzene (55.5 mg, 0.3 mmol), **3x** was obtained as a yellow solid (24.6 mg, 73%). This target product was purified by column chromatography on silica gel (PE/EA = 5:1).

^{1}H NMR (400 MHz, CDCl$_3$) δ 6.68 (s, 4H), 6.57 (s, 2H), 5.49 (s, 1H), 2.26 (s, 12H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 143.3, 139.0, 122.7, 115.8, 21.5.



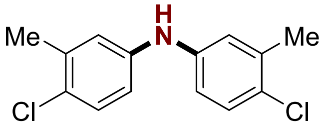
(3y) dimethyl 5,5'-azanediylbis(2-methylbenzoate): Following the General Procedure B with methyl 5-bromo-2-methylbenzoate (68.7 mg, 0.3 mmol), **3y** was obtained as a yellow solid (20.7 mg, 44%). This target product was purified by column chromatography on silica gel (PE/EA = 5:1).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.56 (d, J = 2.4 Hz, 2H), 7.17 – 7.06 (m, 4H), 5.68 (s, 1H), 3.87 (s, 6H), 2.52 (s, 6H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 167.9, 140.9, 132.6, 130.4, 121.4, 120.0, 51.9, 20.9. HRMS（ESI）m/z calcd for $C_{18}H_{19}NO_4$ $(M+H)^+$ 314.13868, found 314.13803.



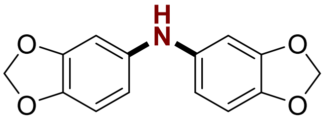
(3z) bis(4-methyl-3-(trifluoromethyl)phenyl)amine (CAS: 2732894-05-0): Following the General Procedure B with 4-bromo-1-methyl-2-(trifluoromethyl)benzene (71.7 mg, 0.3 mmol), **3z** was obtained as a yellow solid (31.0 mg, 62%). This target product was purified by column chromatography on silica gel (PE/EA = 5:1).

^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.25 (d, *J* = 2.4 Hz, 2H), 7.17 (d, *J* = 8.0 Hz, 2H), 7.11 – 7.06 (dm, 2H), 5.70 (s, 1H), 2.41 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) *δ* 140.7, 133.0, 129.9 (q, *J* = 29.9 Hz), 129.1 (d, *J* = 1.7 Hz), 124.3 (q, *J* = 274.8 Hz) 120.6, 115.5 (q, *J* = 5.8 Hz), 18.5 (d, *J* = 2.0 Hz).



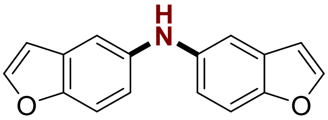
(3za) bis(4-chloro-3-methylphenyl)amine: Following the General Procedure B with 4-bromo-1-chloro-2-methylbenzene (61.7 mg, 0.3 mmol), **3za** was obtained as a yellow solid (26.8 mg, 67%). This target product was purified by column chromatography on silica gel (PE/EA = 5:1).

^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.20 (d, *J* = 8.4 Hz, 2H), 6.88 (d, *J* = 2.4 Hz, 2H), 6.80 (dd, *J* = 8.4, 2.4 Hz, 2H), 5.52 (s, 1H), 2.32 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) *δ* 141.6, 137.0, 129.7, 126.3, 120.3, 116.7, 20.3.



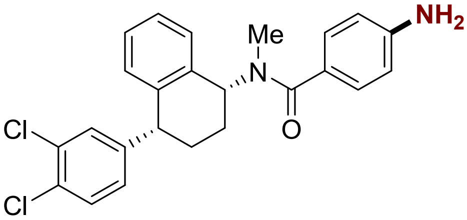
(3zb) bis(benzo[d][1,3]dioxol-5-yl)amine (CAS: 941689-87-8)[24]: Following the General Procedure B with 5-bromobenzo[d][1,3]dioxole (60.3 mg, 0.3 mmol), **3zb** was obtained as a yellow solid (16.2 mg, 42%). This target product was purified by column chromatography on silica gel (PE/EA = 5:1).

^{1}H NMR (400 MHz, $CDCl_3$) *δ* 6.70 (d, *J* = 8.4 Hz, 2H), 6.57 (d, *J* = 2.4 Hz, 2H), 6.42 (dd, *J* = 8.4, 2.4 Hz, 2H), 5.91 (s, 4H), 5.31 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) *δ* 148.3, 142.2, 139.1, 110.9, 108.6, 100.99, 100.95. HRMS（ESI）m/z calcd for $C_{14}H_{11}NO_4$ $(M+H)^+$ 252.07608, found 252.07556.



(3zc) di(benzofuran-5-yl)amine (CAS: 2254556-98-2): Following the General Procedure B with 5-bromobenzofuran (59.1 mg, 0.3 mmol), **3zc** was obtained as a yellow solid (21.3 mg, 57%). This target product was purified by column chromatography on silica gel (PE/EA = 5:1).

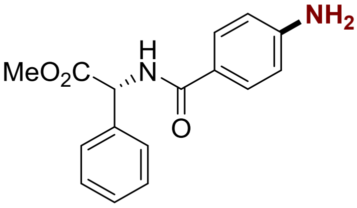
^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.58 (d, *J* = 2.0 Hz, 2H), 7.40 (d, *J* = 8.8 Hz, 2H), 7.24 (d, *J* = 2.4 Hz, 2H), 7.00 (dd, *J* = 8.8, 2.0 Hz, 2H), 6.66 (d, *J* = 1.2 Hz, 2H), 5.58 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) *δ* 150.7, 145.6, 140.2, 128.3, 117.0, 111.9, 109.8, 106.5.



(4a) 4-amino-N-((1R,4R)-4-(3,4-dichlorophenyl)-1,2,3,4-tetrahydronaphthalen-1-yl)-N-methylbenzamide: Following the General Procedure A with 4-bromo-N-((1R,4R)-4-(3,4-

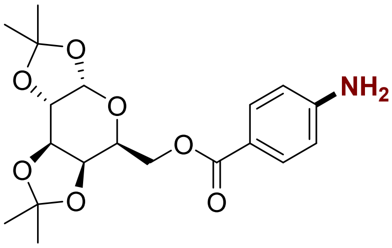
dichlorophenyl)-1,2,3,4-tetrahydronaphthalen-1-yl)-N-methylbenzamide (146.8 mg, 0.3 mmol), **4a** was obtained as a yellow solid (90.2 mg, 71%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.27 (m, 5H), 7.23 – 7.14 (m, 1H), 7.08 (d, J = 2.0 Hz, 1H), 6.96 (d, J = 7.6 Hz, 1H), 6.90 – 6.73 (m, 1H), 6.70 – 6.58 (m, 2H), 6.09 – 5.00 (m, 1H), 4.26 – 4.11 (m, 1H), 3.94 (s, 2H), 2.80 (d, J = 14.0 Hz, 3H), 2.40 – 1.71 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.2, 172.7, 148.1, 147.0, 146.8, 138.2, 137.7, 136.1, 132.2, 130.9, 130.7, 130.5, 130.0, 129.2, 128.1, 127.9, 127.6, 127.4, 127.2, 126.5, 125.6, 114.3, 114.0, 58.7, 52.9, 43.0, 42.7, 33.3, 23.0, 29.1, 22.4, 20.9, 14.1. HRMS（ESI）m/z calcd for $C_{24}H_{23}Cl_2N_2O$ $(M+H)^+$425.11820, found 425.11873.



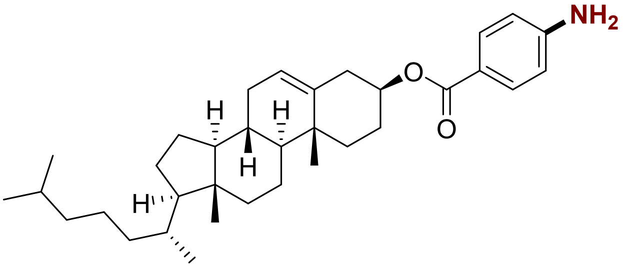
(4b) methyl (R)-2-(4-aminobenzamido)-2-phenylacetate: Following the General Procedure A with methyl (R)-2-(4-bromobenzamido)-2-phenylacetate (104.5 mg, 0.3 mmol), **4b** was obtained as a yellow solid (34.1 mg, 40%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.59 (m, 2H), 7.44 – 7.39 (m, 2H), 7.37 – 7.30 (m, 3H), 7.01 (d, J = 6.8 Hz, 1H), 6.62 – 6.58 (m, 2H), 5.74 (d, J = 6.8 Hz, 1H), 4.06 (s, 2H), 3.73 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.7, 166.3, 150.1, 136.8, 128.88, 128.86, 128.4, 127.3, 122.7, 113.9, 56.6, 52.7. HRMS（ESI）m/z calcd for $C_{16}H_{17}N_2O_3$ $(M+H)^+$ 285.12337, found 285.12361.



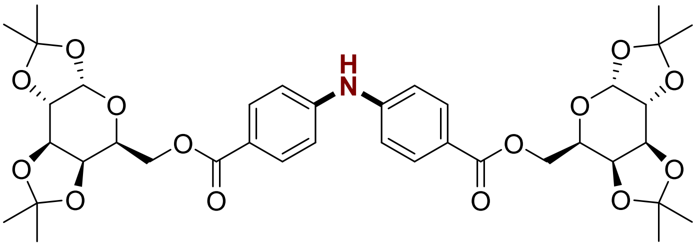
(4c) ((3aS,5aR,8aR,8bS)-2,2,7,7-tetramethyltetrahydro-5H-bis([1,3]dioxolo)[4,5-b:4',5'-d]pyran-5-yl)methyl 4-aminobenzoate: Following the General Procedure A with ((3aS,5aR,8aR,8bS)-2,2,7,7-tetramethyltetrahydro-5H-bis([1,3]dioxolo)[4,5-b:4',5'-d]pyran-5-yl)methyl 4-bromobenzoate (133.0 mg, 0.3 mmol), **4c** was obtained as a yellow solid (39.8 mg, 35%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 – 7.80 (m, 2H), 6.62 – 6.56 (m, 2H), 5.54 (d, J = 4.8 Hz, 1H), 4.62 (dd, J = 8.0, 2.4 Hz, 1H), 4.46 (dd, J = 11.2, 4.8 Hz, 1H), 4.38 – 4.27 (m, 3H), 4.17 – 4.07 (m, 3H), 1.49 (s, 3H), 1.45 (s, 3H), 1.33 (s, 3H), 1.31 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4, 151.0, 131.7, 119.3, 113.6, 109.5, 108.7, 96.2, 71.1, 70.6, 70.49, 66.2, 63.2, 26.0, 25.9, 24.9, 24.4. HRMS（ESI）m/z calcd for $C_{19}H_{26}NO_7$ $(M+H)^+$ 380.17038, found 380.17043.



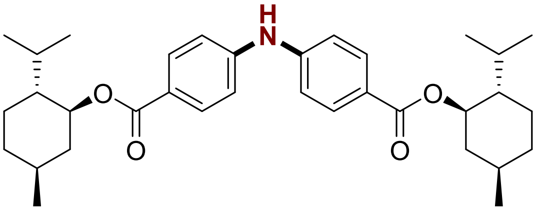
(4d) (8S,9S,10R,13R,14S,17R)-10,13-dimethyl-17-((R)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl4-aminobenzoate (CAS: 22575-25-3)[25]: Following the General Procedure A with (8S,9S,10R,13R,14S,17R)-10,13-dimethyl-17-((R)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren -3-yl 4-bromobenzoate (170.9 mg, 0.3 mmol), **4d** was obtained as a yellow solid (95.5 mg, 63%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.90 – 7.81 (m, 2H), 6.67 – 6.59 (m, 2H), 5.43 – 5.38 (m, 1H), 4.85 – 4.75 (m, 1H), 4.03 (s, 2H), 2.48 – 2.39 (m, 2H), 2.04 – 1.93 (m, 3H), 1.93 – 1.86 (m, 1H), 1.86 – 1.78 (m, 1H), 1.76 – 1.67 (m, 1H), 1.66 – 1.58 (m, 2H), 1.58 – 1.54 (m, 1H), 1.54 – 1.49 (m, 2H), 1.46 – 1.41 (m, 1H), 1.40 – 1.30 (m, 3H), 1.29 – 1.23 (m, 2H), 1.22 – 1.08 (m, 6H), 1.06 (s, 3H), 1.04 – 0.96 (m, 3H), 0.92 (d, J = 6.8 Hz, 3H), 0.87 (dd, J = 6.4, 1.6 Hz, 6H), 0.69 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 166.1, 150.6, 139.9, 131.6, 122.6, 120.5, 113.8, 73.9, 56.7, 56.2, 50.1, 42.3, 39.8, 39.5, 38.4, 37.1, 36.7, 36.2, 35.8, 32.0, 31.9, 28.3, 28.03, 27.99, 24.3, 23.9, 22.8, 22.6, 21.1, 19.4, 18.7, 11.9. HRMS（APCI）m/z calcd for $C_{34}H_{51}NO_2$ $(M+H)^+$ 506.39926, found 506.39862.



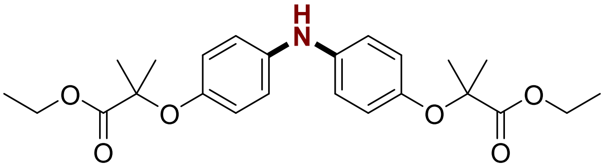
(4e) ((3aR,5aS,8aS,8bR)-2,2,7,7-tetramethyltetrahydro-5H-bis([1,3]dioxolo)[4,5-b:4',5'-d]pyran-5-yl)methyl 4-((4-((((3aS,5aR,8aR,8bS)-2,2,7,7-tetramethyltetrahydro-5H-bis([1,3]dioxolo)[4,5-b:4', 5'-d]pyran-5-yl)methoxy)carbonyl)phenyl)amino)benzoate: Following the General Procedure B with ((3aS,5aR,8aR,8bS)-2,2,7,7-tetramethyltetrahydro-5H-bis([1,3]dioxolo)[4,5-b:4',5'-d]pyran-5-yl)methyl 4-bromobenzoate (133.0 mg, 0.3 mmol), **4e** was obtained as a yellow solid (49.0 mg, 44%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.97 (d, J = 8.4 Hz, 4H), 7.13 (d, J = 8.8 Hz, 4H), 6.67 (s, 1H), 5.57 (d, J = 4.8 Hz, 2H), 4.66 (dd, J = 7.6, 2.4 Hz, 2H), 4.53 (d, J = 4.8 Hz, 1H), 4.50 (d, J = 4.8 Hz, 1H), 4.42 (d, J = 7.6 Hz, 1H), 4.40 (d, J = 7.6 Hz, 1H), 4.37 – 4.33 (m, 3H), 4.32 (d, J = 2.0 Hz, 1H), 4.22 – 4.16 (m, 2H), 1.50 (d, J = 18.4 Hz, 12H), 1.35 (d, J = 9.6 Hz, 12H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 166.1, 146.0, 131.6, 122.8, 116.9, 109.7, 108.8, 96.3, 71.2, 70.7, 70.6, 66.3, 63.7, 26.1, 26.0, 25.0, 24.5. HRMS（APCI）m/z calcd for $C_{42}H_{39}NO_6$ $(M-H)^-$ 740.29238, found 740.29297.



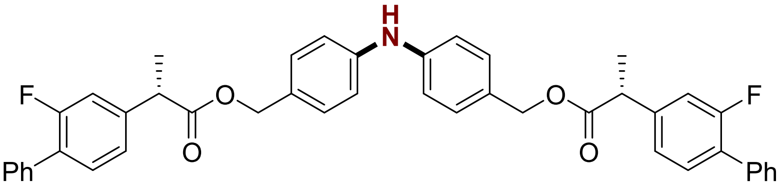
(4f) (1R,2S,5R)-2-isopropyl-5-methylcyclohexyl 4-((4-((((1S,2R,5S)-2-isopropyl-5-methylcyclohexyl) oxy)carbonyl)phenyl)amino)benzoate: Following the General Procedure B with (1S,2R,5S)-2-isopropyl-5-methylcyclohexyl 4-bromobenzoate (101.8 mg, 0.3 mmol), **4f** was obtained as a yellow solid (55.2 mg, 69%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.98 (d, J = 8.4 Hz, 4H), 7.14 (d, J = 8.4 Hz, 4H), 6.55 (s, 1H), 4.91 (td, J = 10.8, 4.4 Hz, 2H), 2.16 – 2.07 (m, 2H), 2.01 – 1.91 (m, 2H), 1.72 (d, J = 11.2 Hz, 4H), 1.60 – 1.48 (m, 4H), 1.19 – 1.04 (m, 4H), 0.98 – 0.86 (m, 14H), 0.80 (d, J = 7.2 Hz, 6H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 165.8, 145.8, 131.4, 123.7, 116.9, 74.5, 47.3, 41.1, 34.4, 31.5, 26.6, 23.7, 22.1, 20.8, 16.6. HRMS（APCI）m/z calcd for $C_{34}H_{47}NO_4$ $(M-H)^-$ 532.34323, found 532.34344.



(4g) diethyl 2,2'-((azanediylbis(4,1-phenylene))bis(oxy))bis(2-methylpropanoate): Following the General Procedure B with ethyl 2-(4-bromophenoxy)-2-methylpropanoate (86.1 mg, 0.3 mmol), **4g** was obtained as a yellow solid (21.3 mg, 33%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

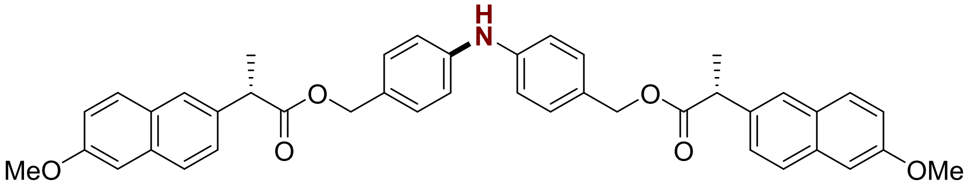
^{1}H NMR (400 MHz, CDCl$_3$) δ 6.90 – 6.85 (m, 4H), 6.82 – 6.77 (m, 4H), 5.40 (s, 1H), 4.24 (q, J = 7.2 Hz, 4H), 1.55 (s, 12H), 1.28 (t, J = 7.2 Hz, 6H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 174.4, 149.4, 139.0, 121.4, 118.6, 79.6, 61.3, 25.3, 14.1. HRMS（APCI）m/z calcd for $C_{24}H_{31}NO_6$ $(M+H)^+$ 430.22241, found 430.22192.



(4h) 4-((4-((((R)-2-(2-fluoro-[1,1'-biphenyl]-4-yl)propanoyl)oxy)methyl)phenyl)amino) benzyl (S)-2-(2-fluoro-[1,1'-biphenyl]-4-yl)propanoate: Following the General Procedure B with 4-bromobenzyl (S)-2-(2-fluoro-[1,1'-biphenyl]-4-yl)propanoate (124.0 mg, 0.3 mmol), **4h** was obtained as a yellow solid (35.8 mg, 35%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.55 – 7.49 (m, 4H), 7.45 – 7.39 (m, 4H), 7.39 – 7.32 (m, 4H), 7.20 – 7.07 (m, 8H), 7.03 – 6.97 (m, 4H), 5.77 (s, 1H), 5.06 (d, J = 23.2, 12.0 Hz, 4H), 3.78 (q, J = 7.2 Hz, 2H), 1.54 (d, J = 7.2 Hz, 6H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 173.9, 159.7 (d, J = 248.3

Hz), 142.9, 141.8 (d, J = 7.7 Hz), 135.5, 130.8 (d, J = 3.9 Hz), 129.8, 129.0 (d, J = 2.9 Hz), 128.5, 128.3, 127.8 (d, J = 13.6 Hz), 127.7, 123.6 (d, J = 3.3 Hz), 117.6, 115.3 (d, J = 23.7 Hz), 66.7, 45.1, 18.4. HRMS（APCI）m/z calcd for $C_{44}H_{37}F_2NO_4$ $(M+H)^+$ 682.27634, found 682.27539.



(4i) 4-((4-((((R)-2-(6-methoxynaphthalen-2-yl)propanoyl)oxy)methyl)phenyl)amino)benzyl (S)-2-(6-methoxynaphthalen-2-yl)propanoate: Following the General Procedure B with 4-bromobenzyl (S)-2-(6-methoxynaphthalen-2-yl)propanoate (119.8 mg, 0.3 mmol), **4i** was obtained as a yellow solid (41.2 mg, 42%). This target product was purified by column chromatography on silica gel (PE/EA = 2:1).

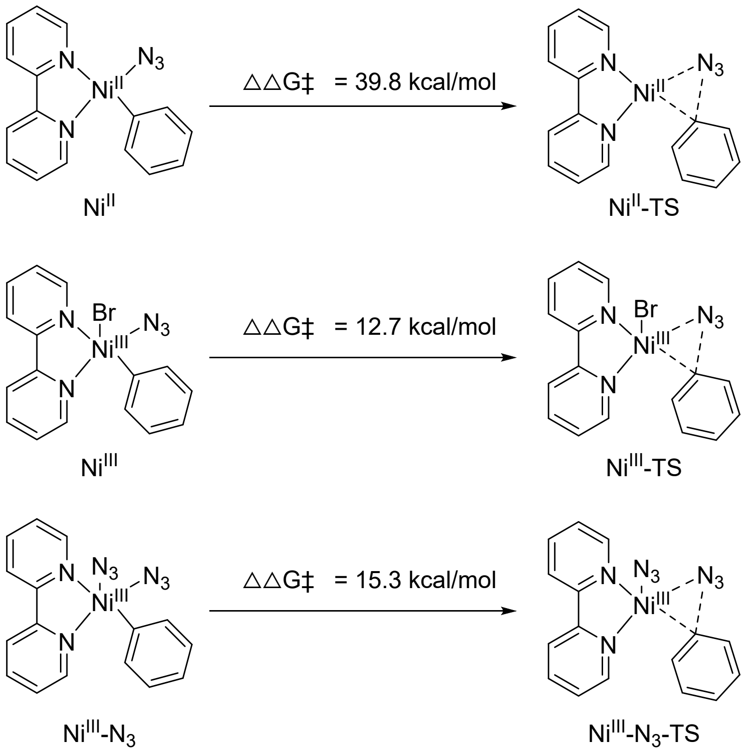
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 – 7.61 (m, 6H), 7.41 – 7.36 (m, 2H), 7.17 – 7.08 (m, 8H), 6.99 – 6.89 (m, 4H), 5.74 (s, 1H), 5.04 (dd, J = 28.8, 12.4 Hz, 4H), 3.89 (s, 6H), 1.58 (d, J = 7.2 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.6, 157.6, 142.8, 135.7, 133.7, 129.7, 129.3, 128.9, 128.5, 127.1, 126.3, 126.0, 119.0, 117.6, 105.6, 66.5, 55.3, 45.5, 18.6. HRMS（APCI）m/z calcd for $C_{42}H_{39}NO_6$ $(M+H)^+$ 654.28501, found 654.28418.

9. Computational methods and details

9.1 Computational Methods

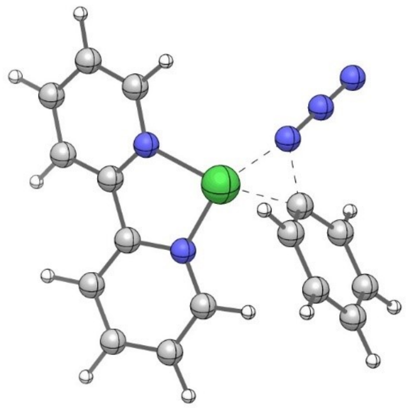
All calculations were carried out by using the Gaussian 16 suite of computational programs[26]. The obtained transition states were fully optimized at the DFT level using the B3LYP[[27]-D3(BJ) functional, which has been found reliable in calculating the configuration and energy barrier of the organic system.[28] The standard Def2SVP basis set[29] was applied for all atom.[30] Frequencies were analytically computed at the same level of theory to get the thermodynamic corrections and to confirm whether the structures are the corresponding transition states (only one imaginary frequency). All energies were reported in kcal/mol. The most stabilized conformation was reported herein, when several different conformations were obtained. Visualization was completed using CLYview20 software.[31]

9.2 Reductive Elimination Energy Barrier from Ni^{II} and Ni^{III}



10. Cartesian coordinates and energies of calculated structures

$\mathrm{Ni^{II}}$-TS

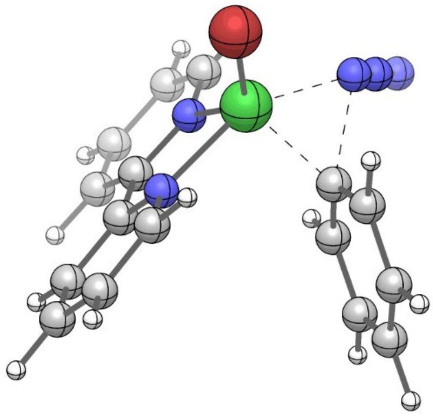


Zero-point correction= 0.262091
Thermal correction to Energy= 0.280111
Thermal correction to Enthalpy= 0.281055
Thermal correction to Gibbs Free Energy= 0.214887
Sum of electronic and thermal Free Energies= -2398.625504

C	-1.73006400	1.45484300	0.14410500
C	-2.26642000	2.74646000	0.23696100
C	-1.40972300	3.83238200	0.38819500
C	-0.02531800	3.60159000	0.42996300
C	0.44361400	2.29874200	0.31907200
N	-0.38199200	1.24152300	0.19808600
H	-1.80916300	4.84600600	0.46038600
H	-3.34493600	2.89581500	0.16970600
H	0.68274600	4.42270300	0.55372200
H	1.51086700	2.07003400	0.34427500
C	-2.51602200	0.22897000	-0.01865400
C	-3.89146700	0.11829900	0.23193400
N	-1.78338200	-0.84823400	-0.42855400
C	-4.52446300	-1.10654600	0.04765400
H	-4.45222000	0.98368000	0.58777900
C	-2.40035700	-2.03265900	-0.58875800
C	-3.76115500	-2.20778500	-0.37390800
H	-5.59416600	-1.21075200	0.24009300
H	-1.76261800	-2.85971600	-0.91246500
H	-4.21809700	-3.18500400	-0.53896300
Ni	0.14587600	-0.55564100	-0.25029100
C	2.06678300	-0.70532300	-0.13572300
C	2.82519400	-0.28477200	1.00091900
C	2.45416000	-0.23084600	-1.42695100
C	3.81167900	0.67680800	0.85112100

H	2.59288600	-0.69511500	1.98622300
C	3.43486800	0.75125100	-1.54012400
H	1.97841900	-0.65302400	-2.31416100
C	4.11728800	1.22406700	-0.41164200
H	4.35917700	1.01727100	1.73457900
H	3.69082500	1.13685400	-2.53099600
H	4.89951400	1.97874600	-0.51120300
N	1.31477600	-2.05076400	-0.16092300
N	1.55557700	-2.87062400	0.72089700
N	1.81082900	-3.66939200	1.50109400

Ni^{III}-Br-TS

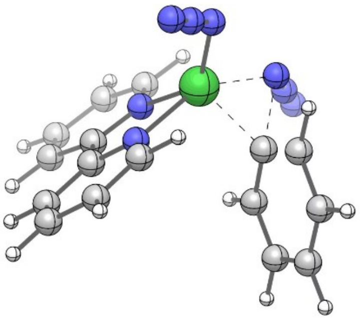


Zero-point correction= 0.276043
Thermal correction to Energy= 0.298145
Thermal correction to Enthalpy= 0.299089
Thermal correction to Gibbs Free Energy= 0.221383
Sum of electronic and thermal Free Energies= -2562.727774

C	-2.16513900	-0.79696100	0.38000000
C	-3.54832100	-0.99780700	0.30700000
C	-4.40568400	0.06870300	0.57597600
C	-3.86294300	1.30668000	0.92169100
C	-2.47473400	1.43172100	0.96973100
N	-1.65449200	0.41312000	0.69483500
H	-3.95338900	-1.97594100	0.04981500
H	-4.49541900	2.16631700	1.14691200
H	-2.00480400	2.38088600	1.23181900
C	-1.16390400	-1.86782300	0.15455500
C	-1.48521600	-3.18102500	-0.20814800
N	0.11503200	-1.49580700	0.34454000
C	-0.45315500	-4.10506300	-0.37266700
H	-2.52125100	-3.48148400	-0.36204900
C	1.10815600	-2.37467100	0.20057600

C	0.86590000	-3.70009100	-0.16216000
H	2.10929400	-1.98579300	0.40677300
H	1.69900100	-4.39551100	-0.27484700
Ni	0.42887200	0.50488500	0.63492500
C	0.75121100	0.88489100	-1.28751600
C	-0.28022700	0.77066000	-2.22561700
C	2.08006100	0.59672400	-1.62729500
C	0.01254700	0.25827500	-3.49343900
H	-1.30140500	1.06421900	-1.97493100
C	2.35114400	0.08057200	-2.89593900
H	2.87093000	0.75587800	-0.89261400
C	1.32231600	-0.09873400	-3.82999400
H	-0.79352900	0.14208800	-4.22283000
H	3.38144800	-0.17196300	-3.16013600
N	0.62584200	2.37225100	-0.06342300
H	1.54491700	-0.49440200	-4.82335400
H	-5.48756200	-0.06960700	0.52149000
H	-0.68037800	-5.13398300	-0.65974800
N	-0.25109200	3.09882300	-0.47989300
N	-1.05848600	3.80844200	-0.88787800
Br	2.32211500	0.28652600	2.10108600

Ni^{III}-N$_3$-TS



Zero-point correction= 0.263870 (Hartree/Particle)
Thermal correction to Energy= 0.284463
Thermal correction to Enthalpy= 0.285408
Thermal correction to Gibbs Free Energy= 0.211311
Sum of electronic and thermal Free Energies= -4972.570786

C	-1.92163500	-1.19716700	-0.24213400
C	-3.18038200	-1.65034500	-0.65561900
C	-4.30775700	-0.88044100	-0.37376200
C	-4.15389100	0.31986000	0.32159200
C	-2.86951800	0.70621100	0.70144500
N	-1.78666100	-0.02620000	0.41816900

H	-3.28201200	-2.59665000	-1.18569300
H	-5.00802700	0.95204800	0.56785300
H	-2.70166100	1.63598400	1.24692900
C	-0.66273200	-1.94617500	-0.47278500
C	-0.58807700	-3.14278700	-1.19401400
N	0.44152100	-1.38782200	0.06254900
C	0.65341200	-3.75853900	-1.35566600
H	-1.48167500	-3.58846500	-1.62984500
C	1.63398900	-1.96676600	-0.09762700
C	1.78531700	-3.16291500	-0.79995200
H	2.48987800	-1.46202700	0.35140300
H	2.77490300	-3.61028100	-0.90145200
Ni	0.16526500	0.41590400	0.99407900
C	0.93324800	1.48899000	-0.47560100
C	0.28871800	1.52154900	-1.71740900
C	2.33007400	1.56092000	-0.37907400
C	1.06299000	1.52425500	-2.88147000
H	-0.80153300	1.52705600	-1.78068700
C	3.08626000	1.55849500	-1.55285900
H	2.80065200	1.60221900	0.60427900
C	2.45996400	1.53192500	-2.80589700
H	0.56574800	1.52178900	-3.85512600
H	4.17695900	1.58950800	-1.48561600
N	0.06208600	2.42583700	0.95995100
H	3.05861600	1.53844900	-3.71931200
H	-5.29669900	-1.21852700	-0.69026200
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N	-0.80736100	3.10888400	0.46102900
N	-1.61070900	3.78220600	-0.01111000

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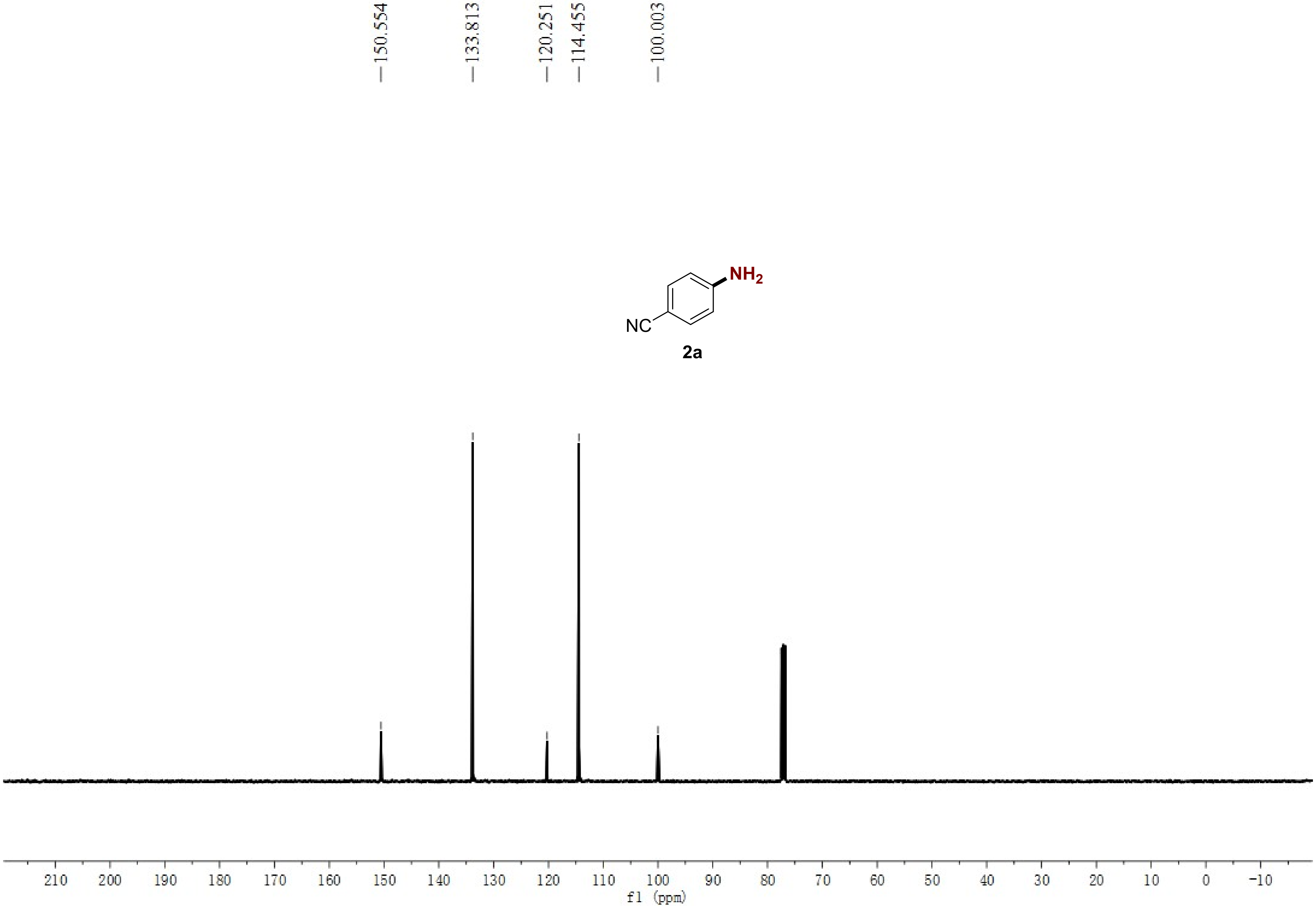
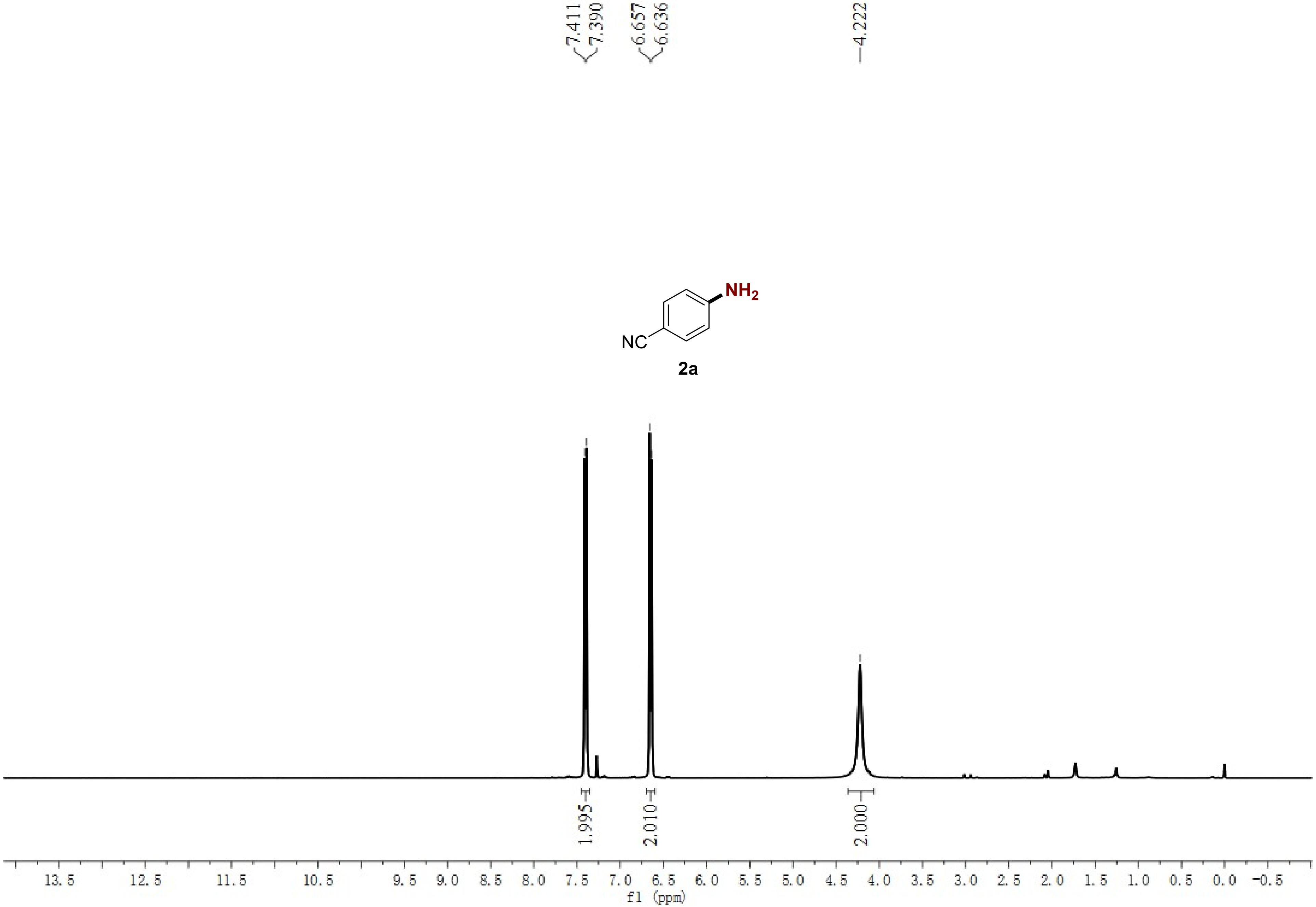
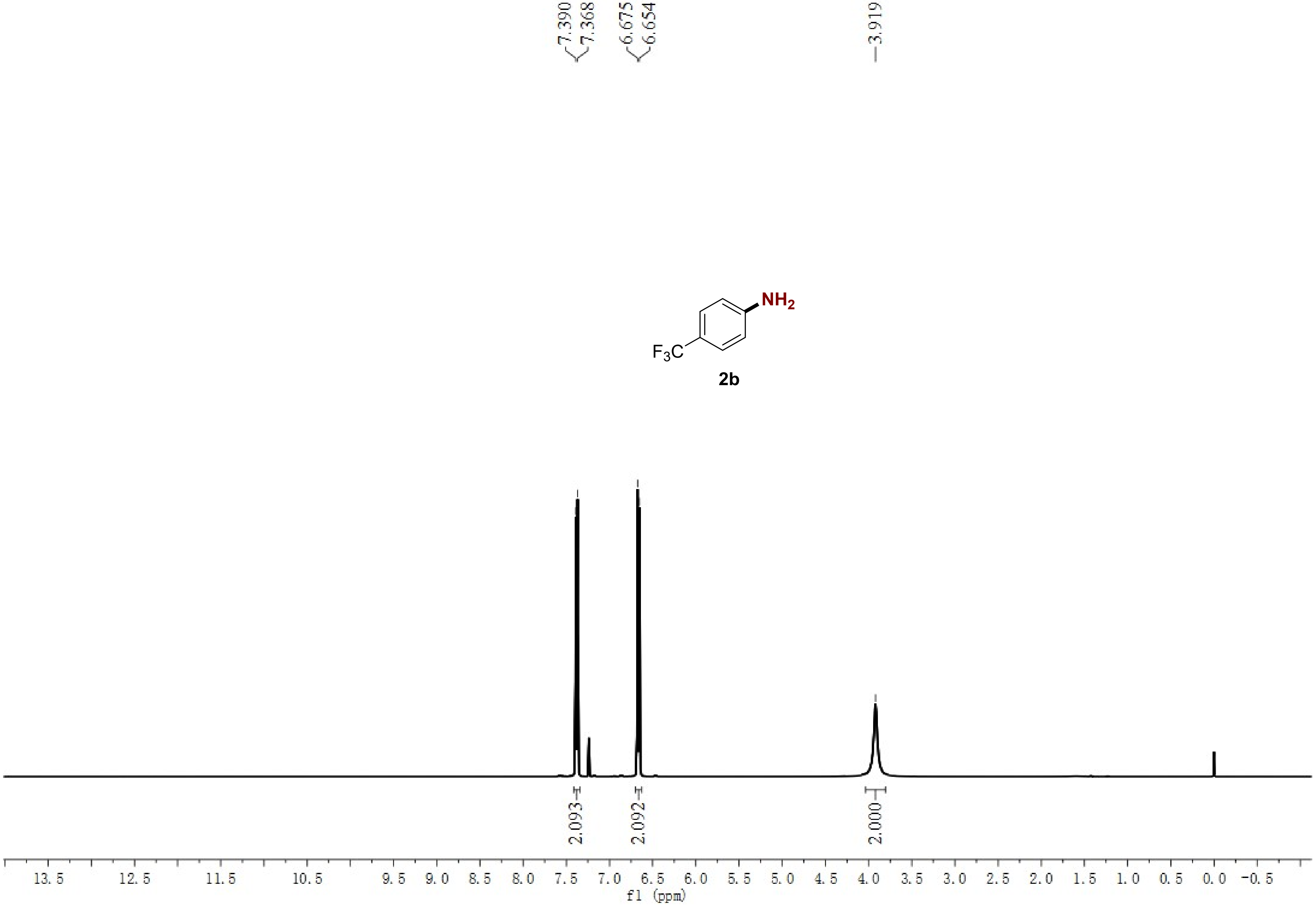
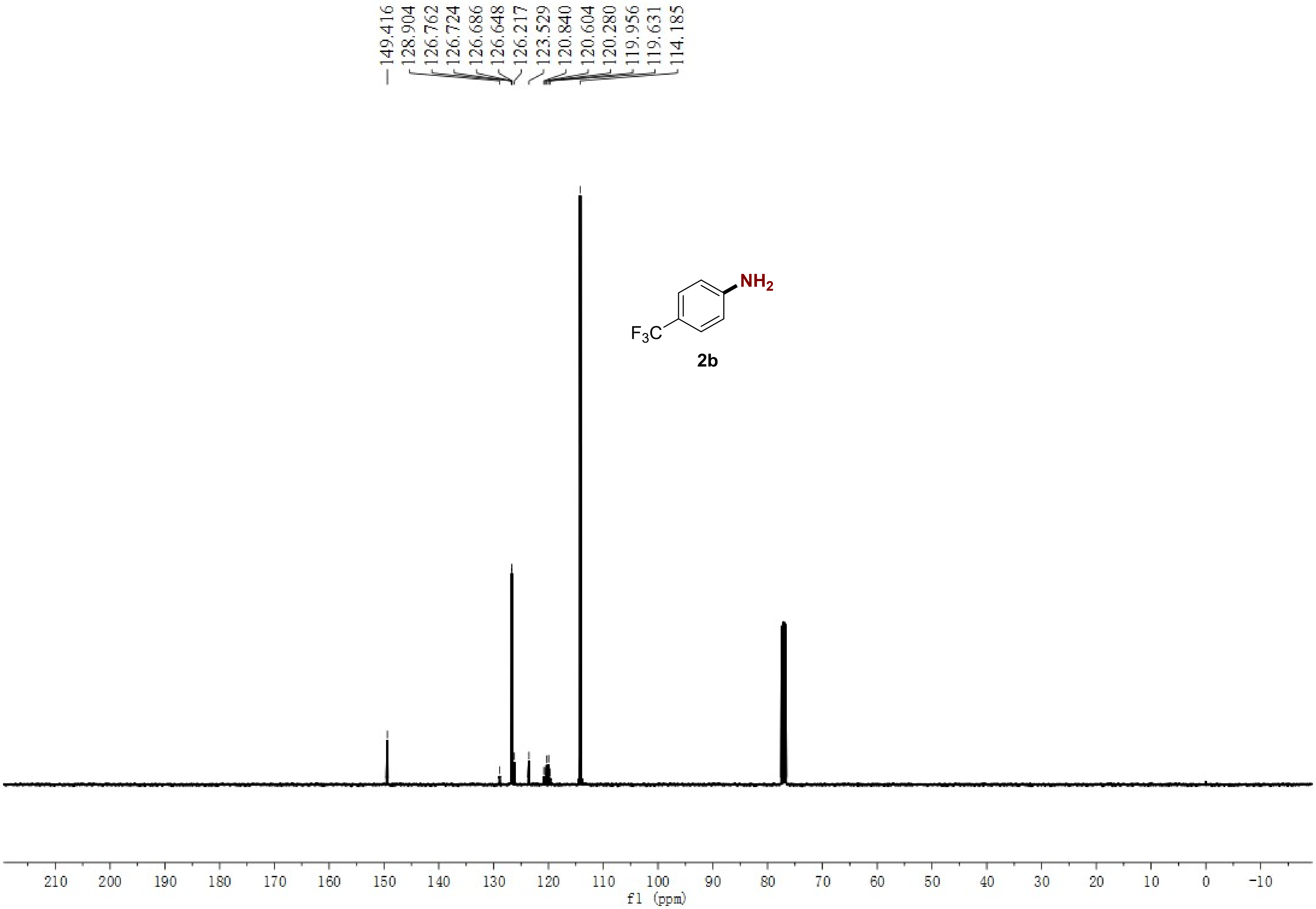
12. Copies of NMR spectra

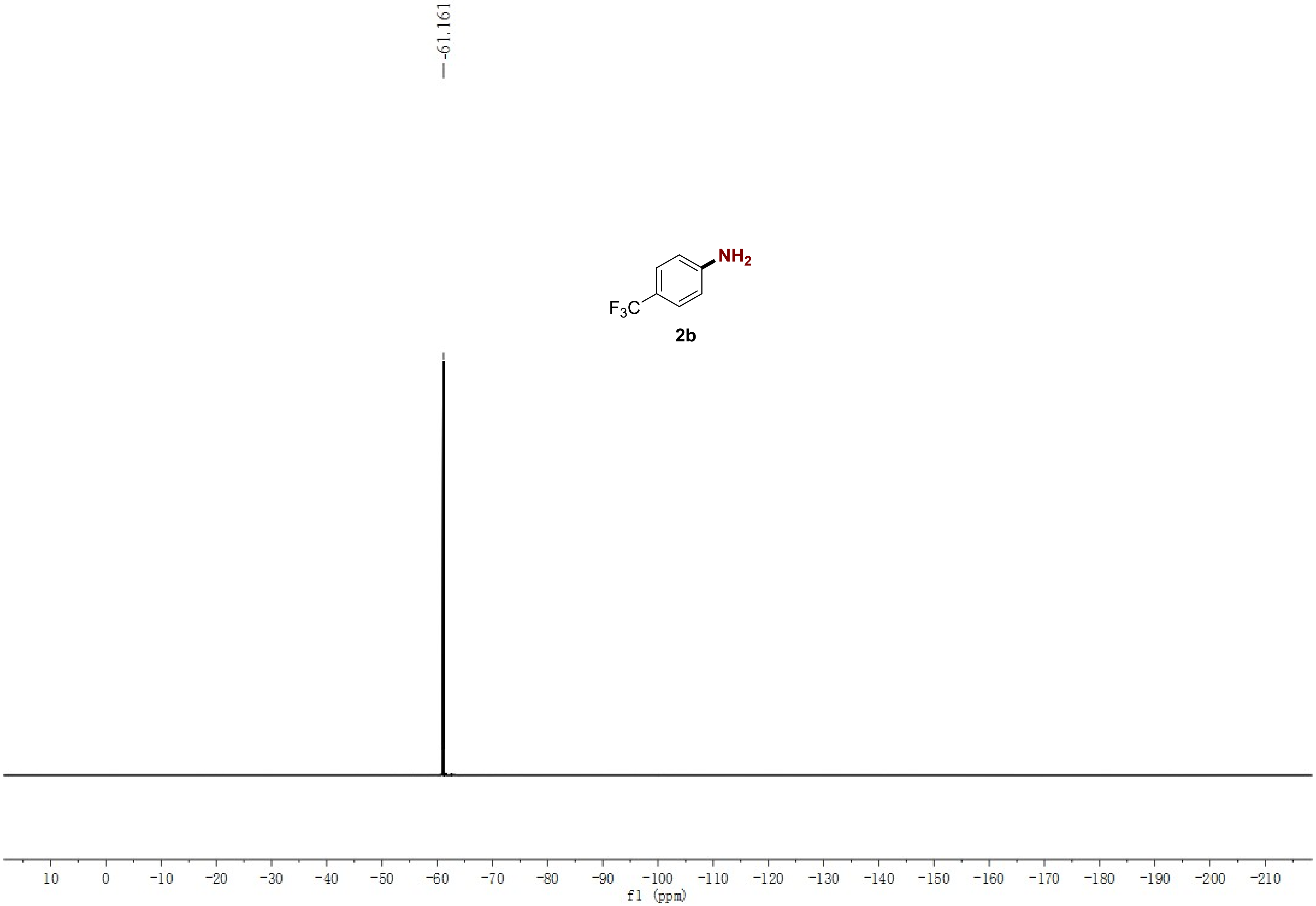

150.554
133.813
120.251
114.455
100.003
NH2
NC
2a
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

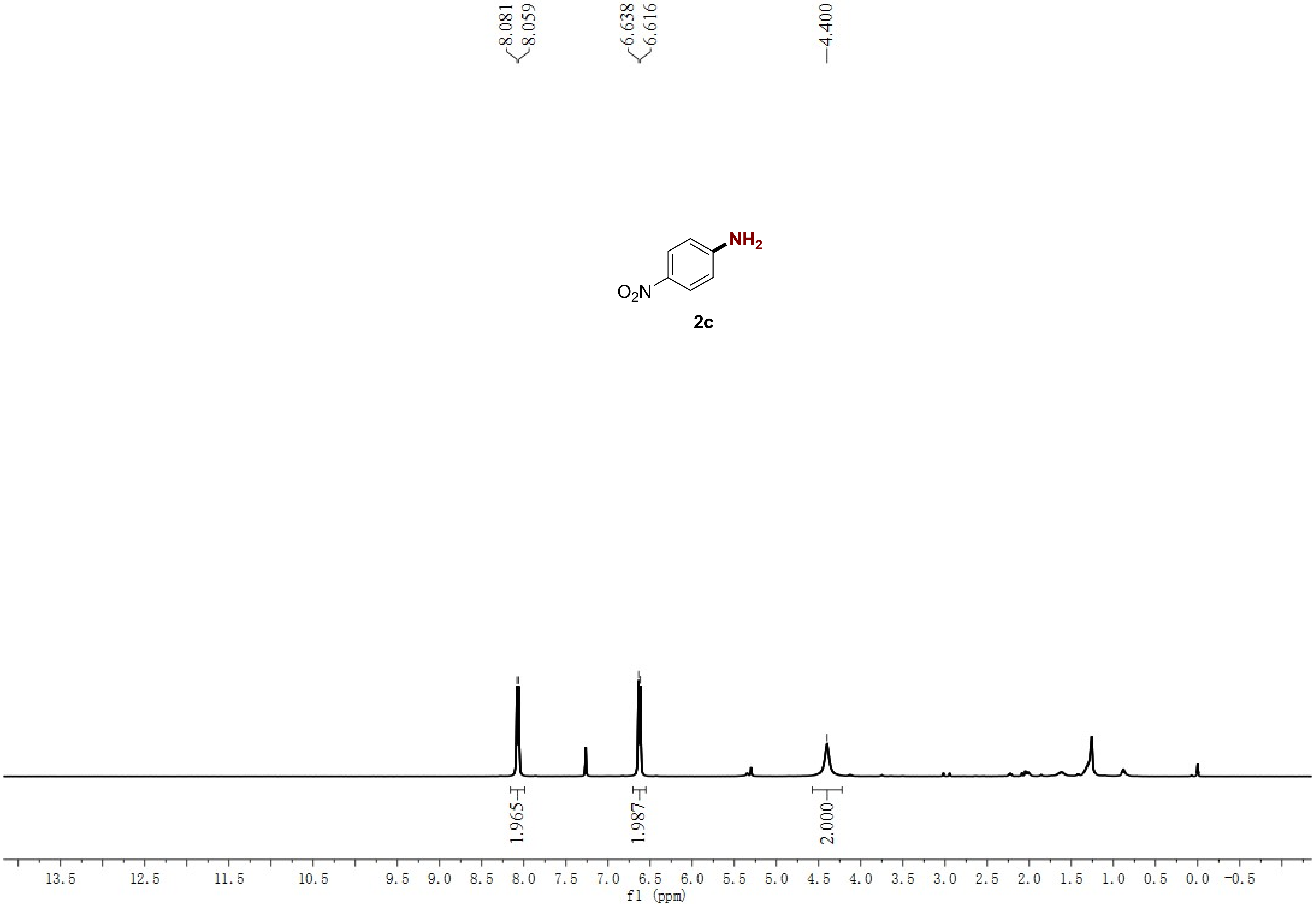

7.411
7.390
6.657
6.636
4.222
NH2
NC
2a
1.995
2.010
2.000
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

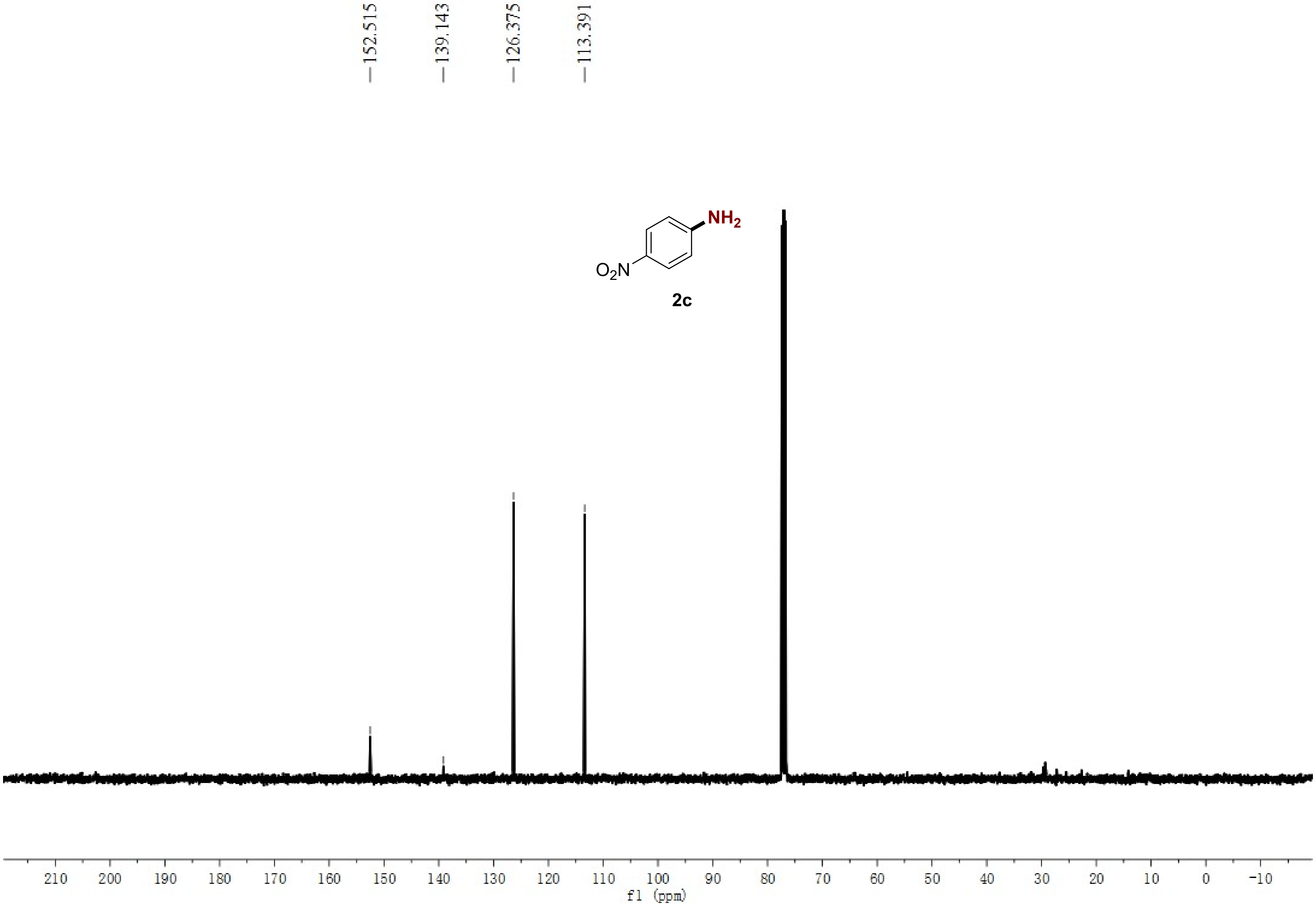

7.390
7.368
6.675
6.654
3.919
NH_2
F_3C
2b
2.093
2.092
2.000
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
f1 (ppm)


149.416
128.904
126.762
126.724
126.686
126.648
126.217
123.529
120.840
120.604
120.280
119.956
119.631
114.185
NH2
F3C
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)

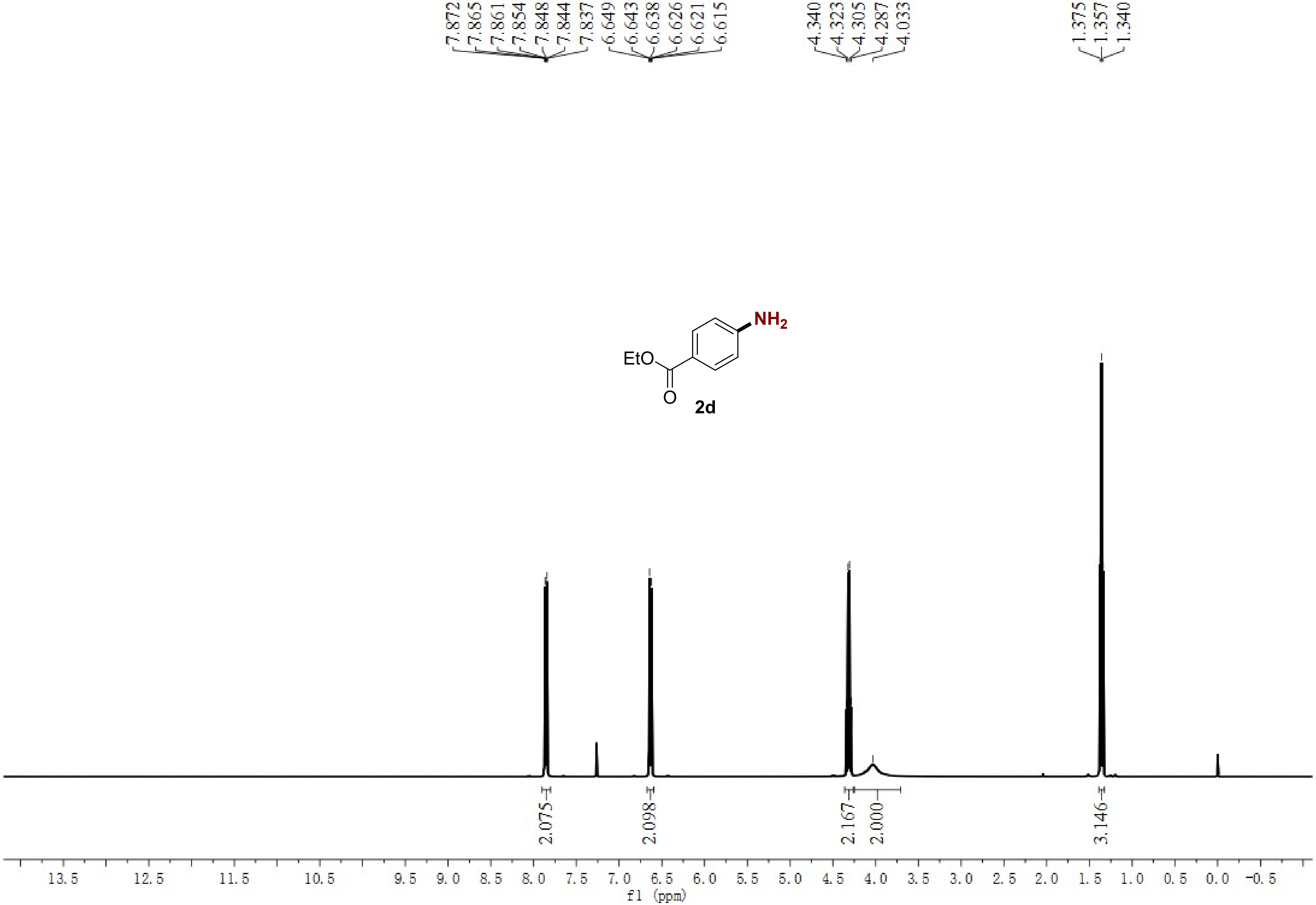
2b


-61.161
NH2
F3C
2b
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)

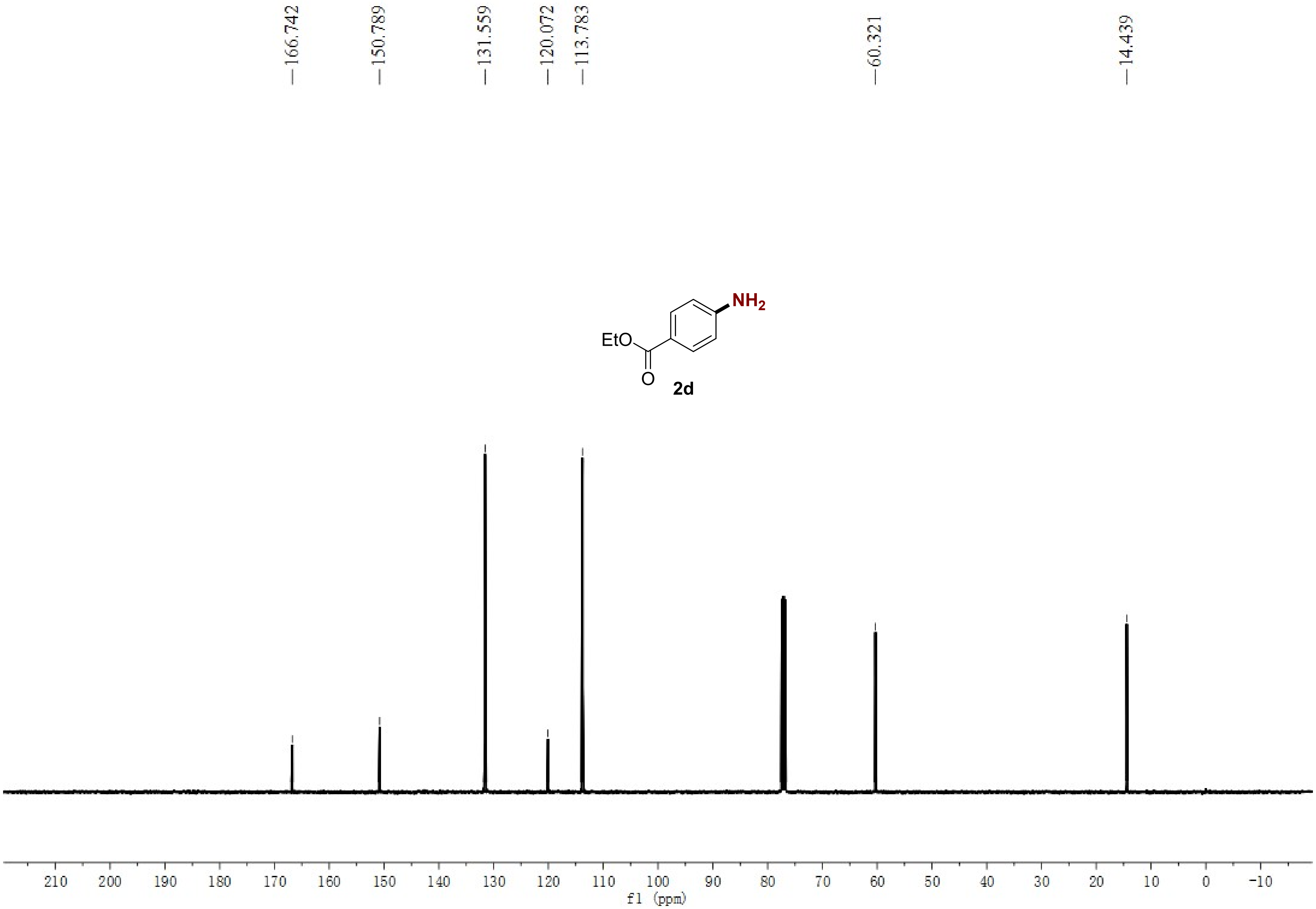

2c
8.081
8.059
6.638
6.616
4.400
NH2
O2N
1.965
1.987
2.000
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

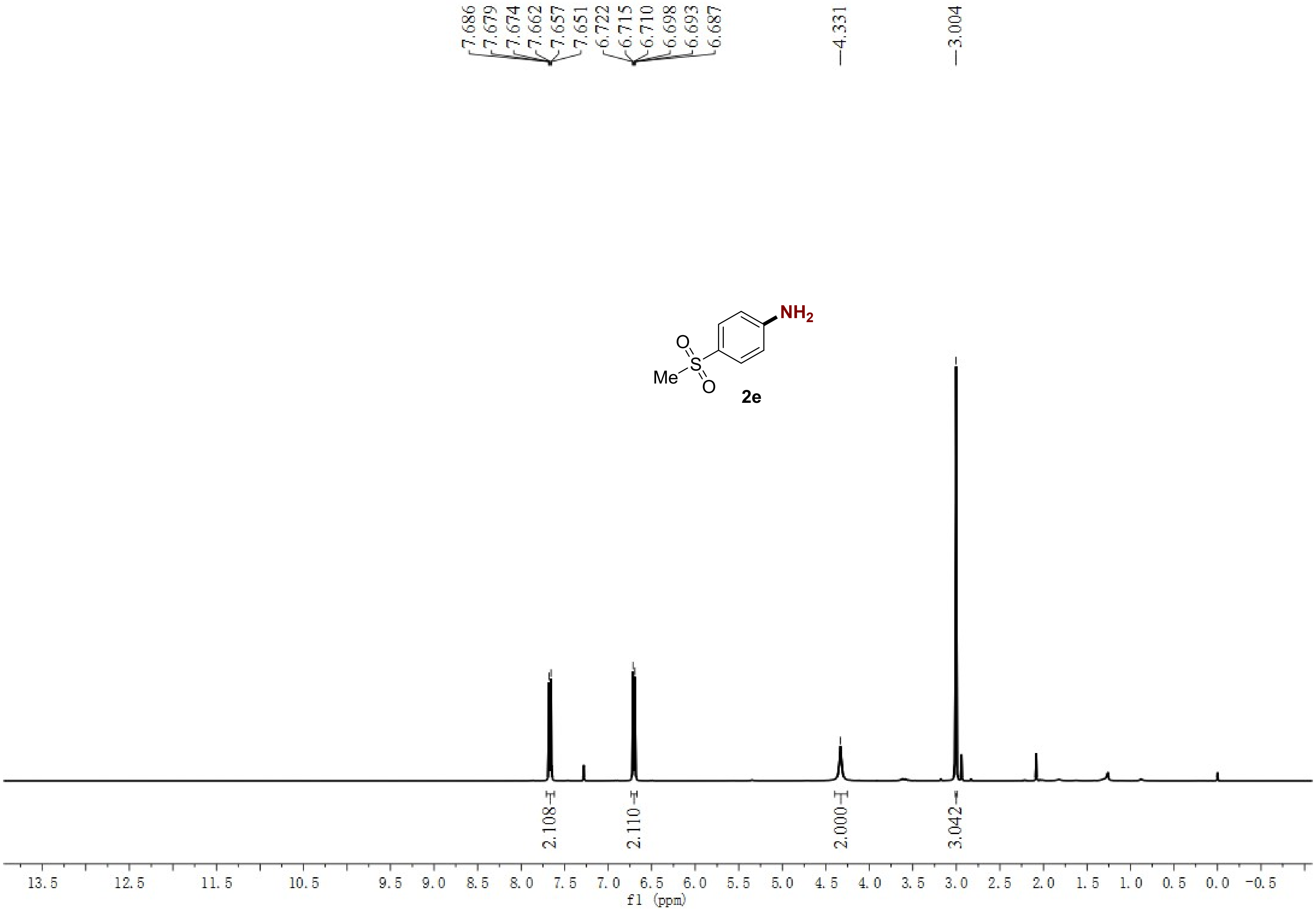

152.515
139.143
126.375
113.391
NH2
O2N
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

2c

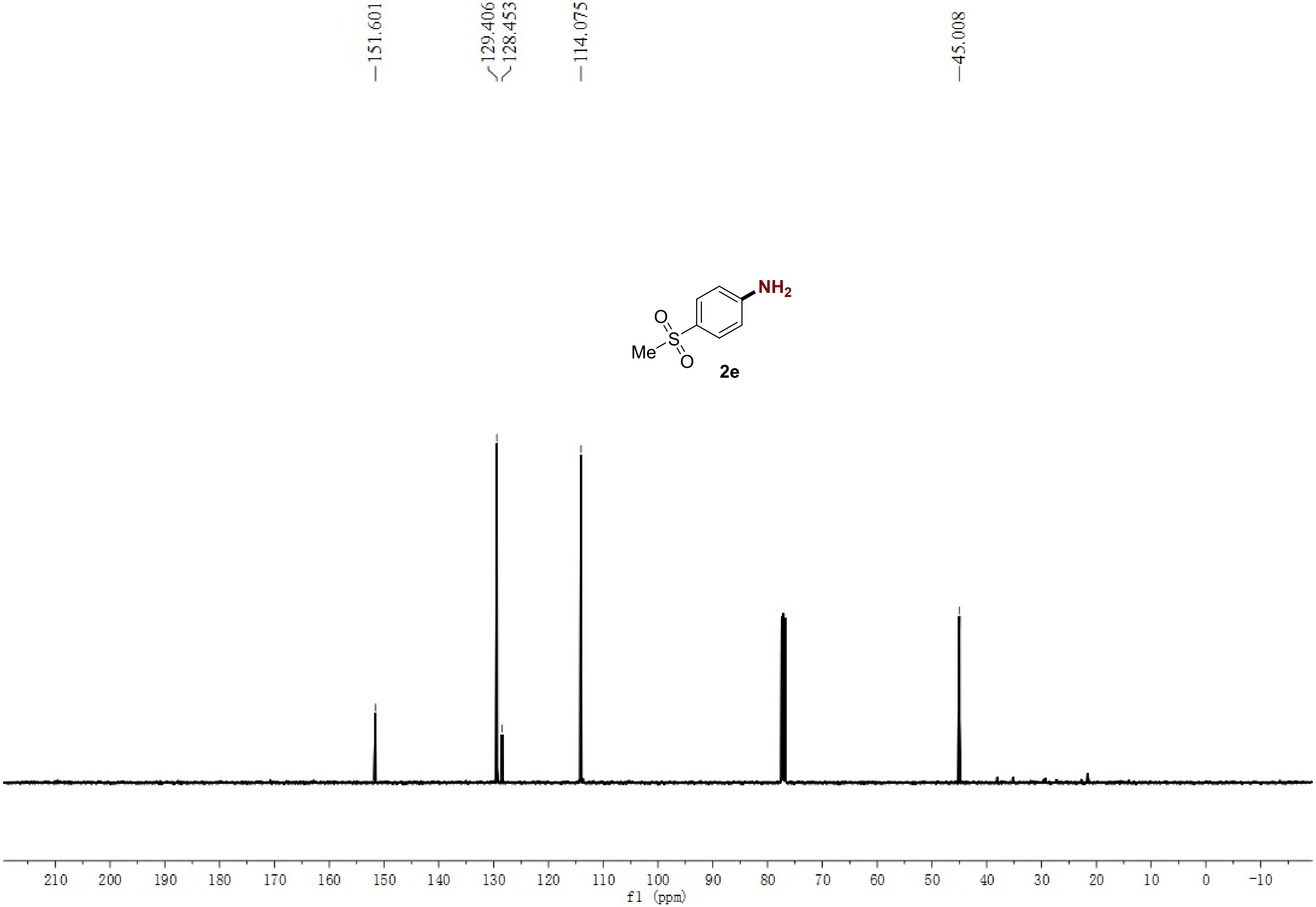

7.872
7.865
7.861
7.854
7.848
7.844
7.837
6.649
6.643
6.638
6.626
6.621
6.615
4.340
4.323
4.305
4.287
4.033
1.375
1.357
1.340
EtO
NH2
O
2.075
2.098
2.167
2.000
3.146
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
f1 (ppm)

2d

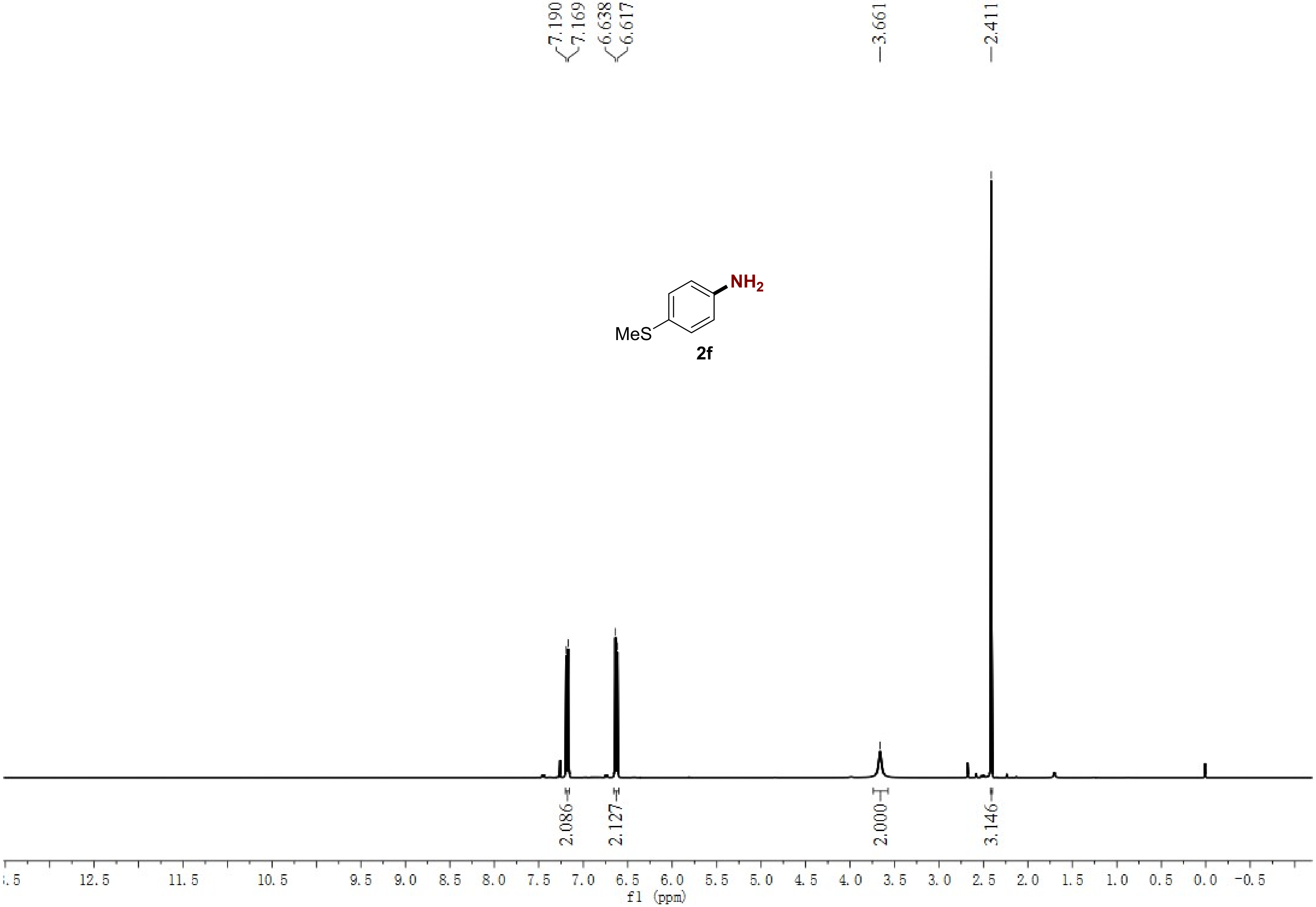

166.742
150.789
131.559
120.072
113.783
60.321
14.439
EtO
O
NH$_2$
2d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

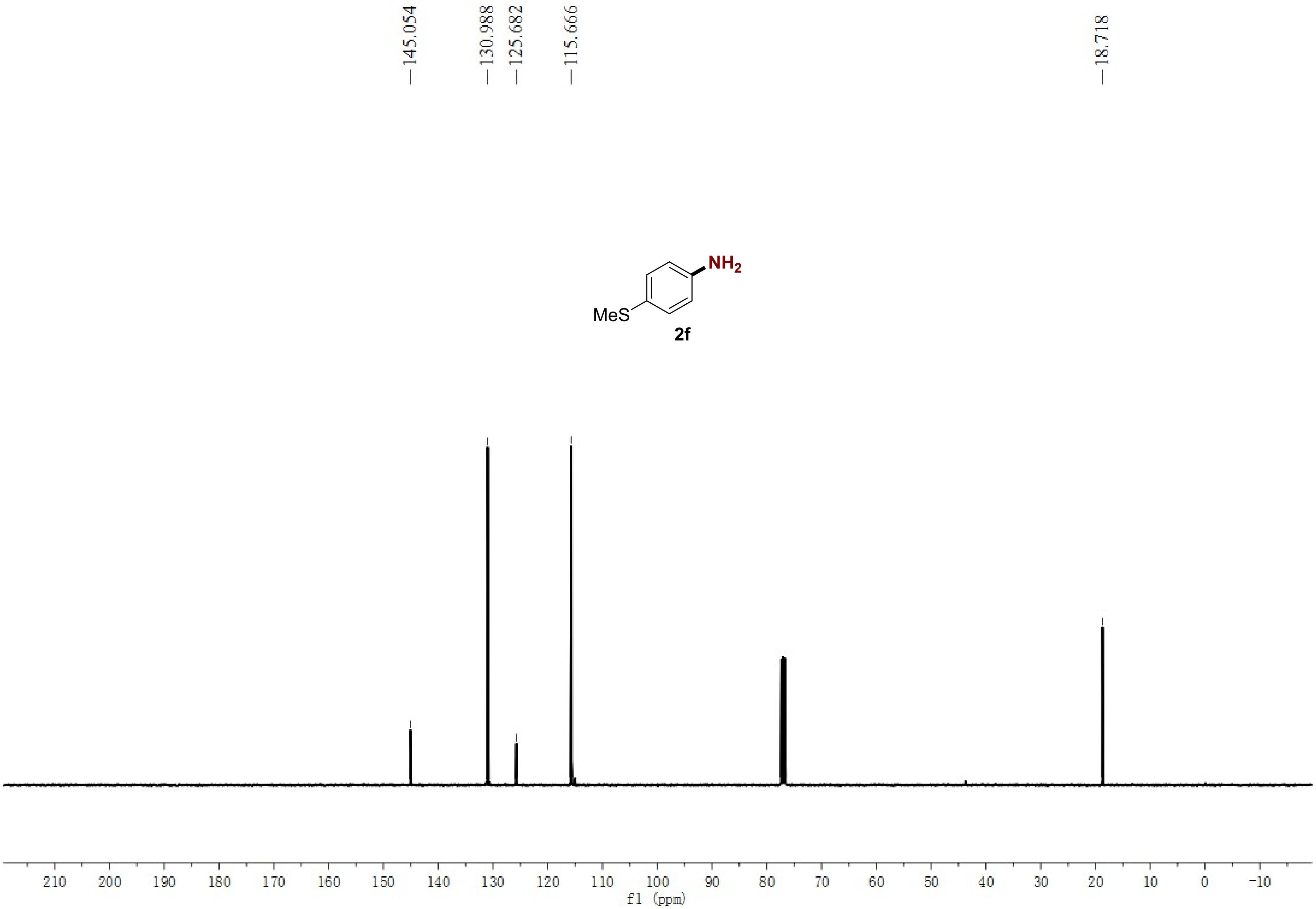

7.686
7.679
7.674
7.662
7.657
7.651
6.722
6.715
6.710
6.698
6.693
6.687
4.331
3.004
NH2
O
S
O
Me
2.108
2.110
2.000
3.042
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

2e


151.601
129.406
128.453
114.075
45.008
NH2
O
S
O
Me
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)

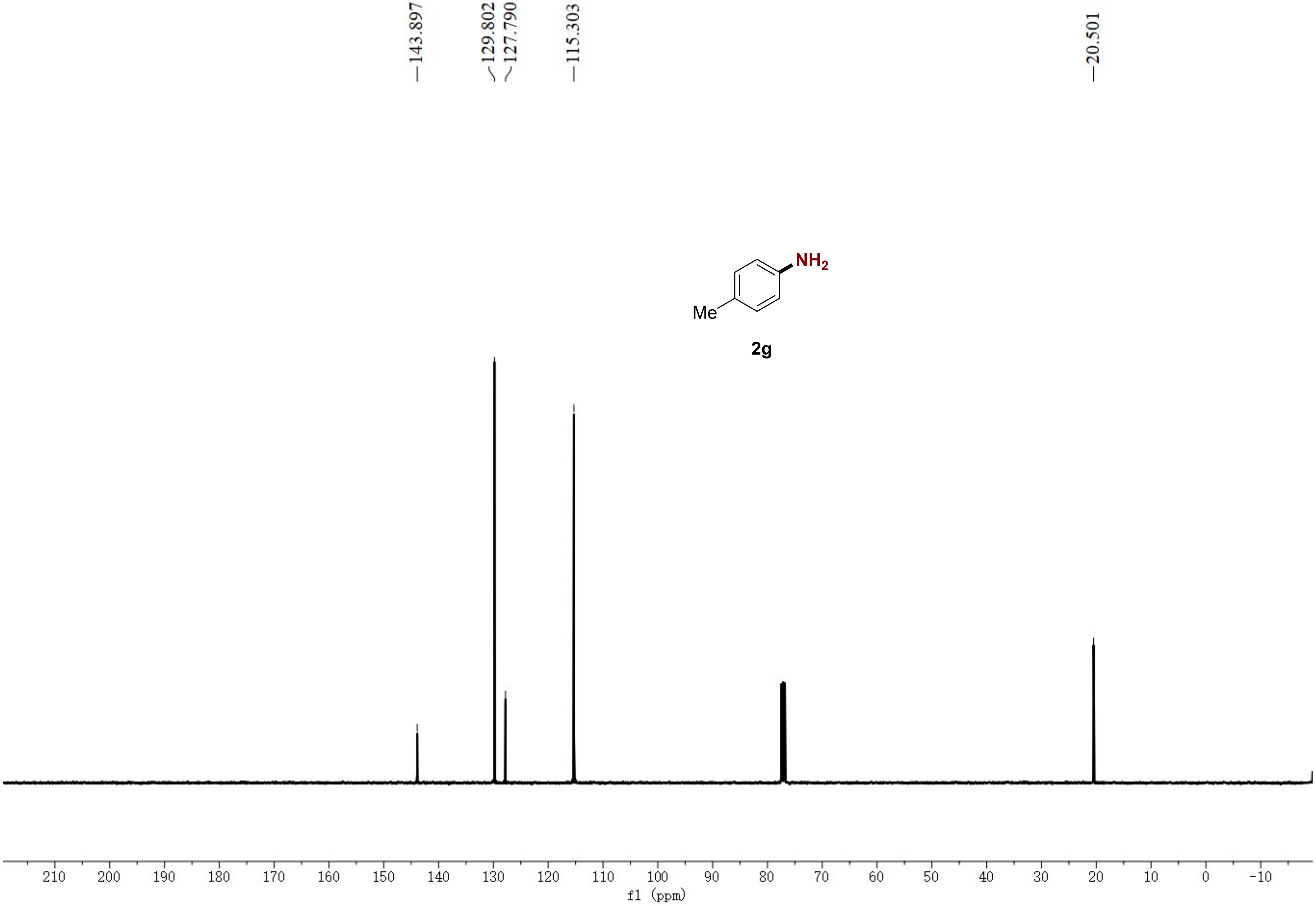
2e


7.190
7.169
6.638
6.617
3.661
2.411
NH$_2$
MeS
2f
2.086
2.127
2.000
3.146
.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

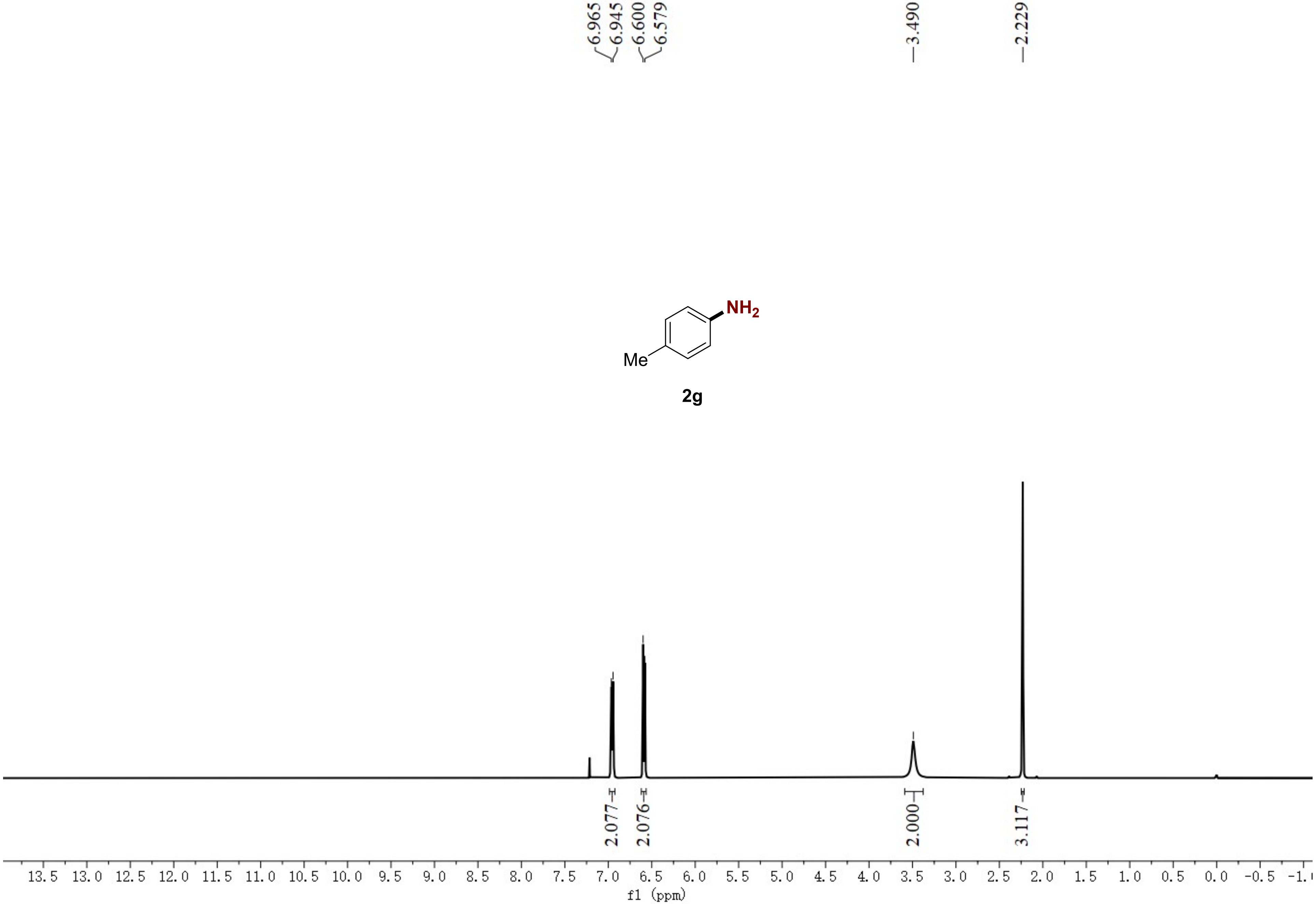


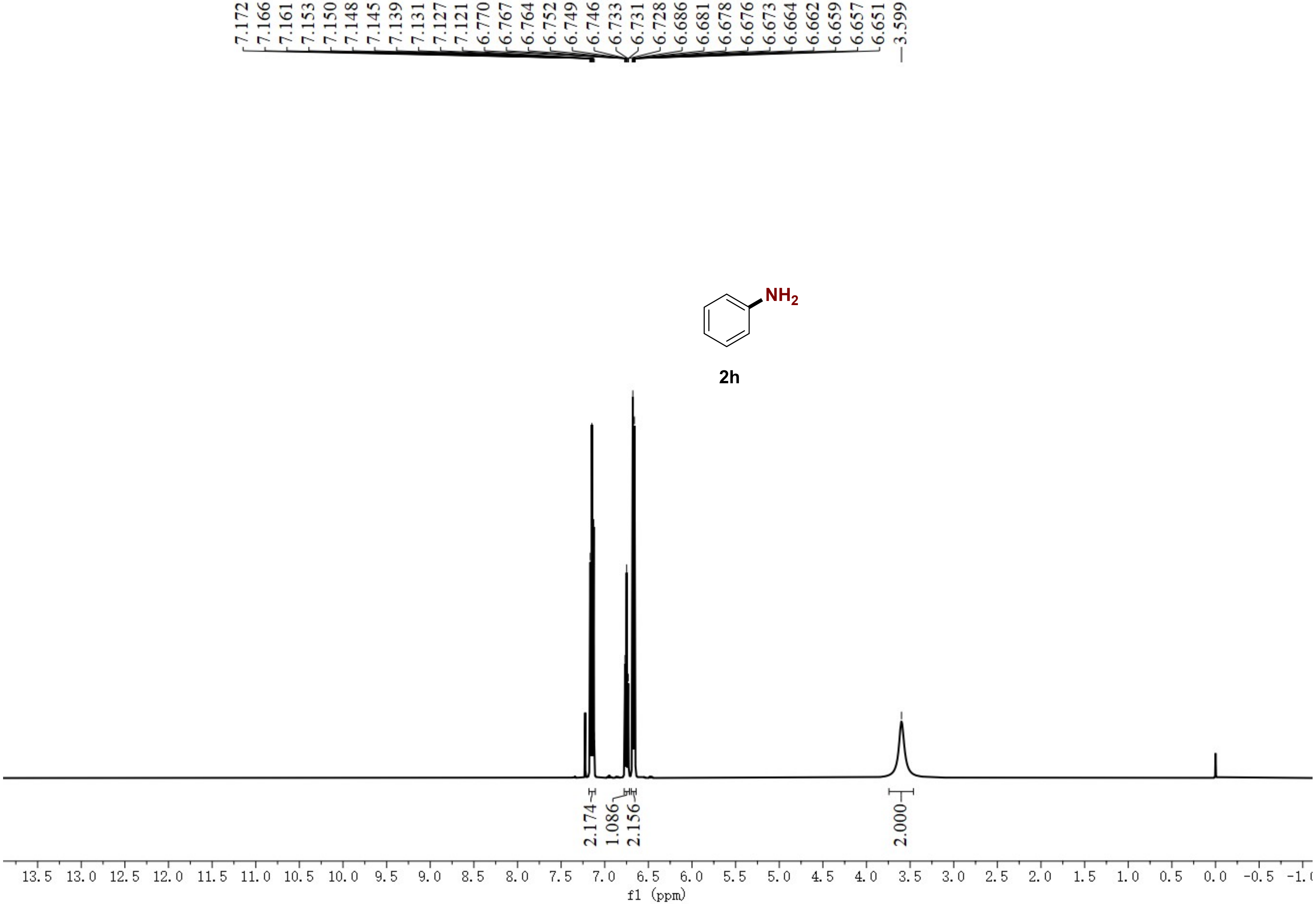
2f

145.054
130.988
125.682
115.666
18.718
NH2
MeS
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)

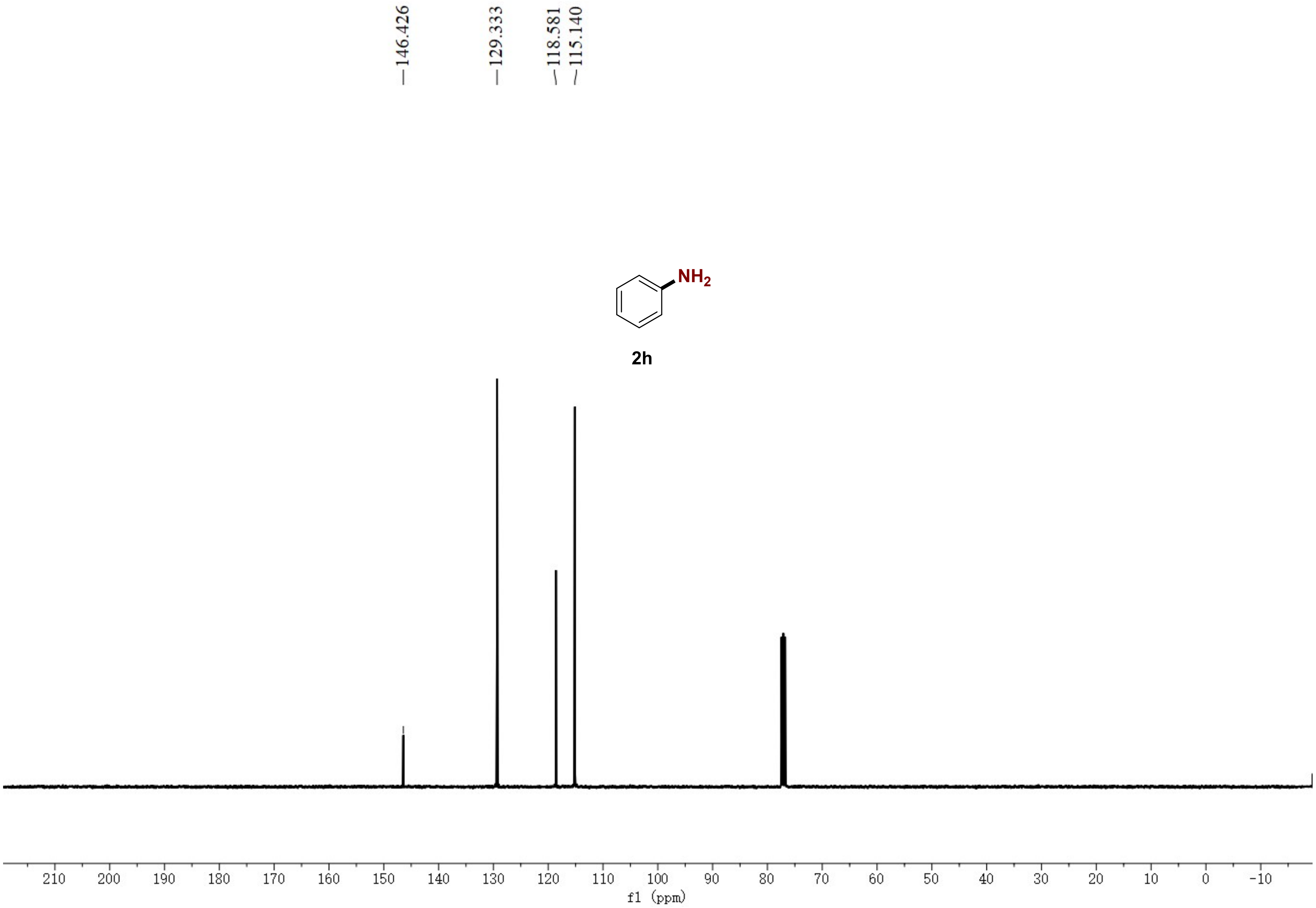

143.897
129.802
127.790
115.303
20.501
NH2
Me
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

2g

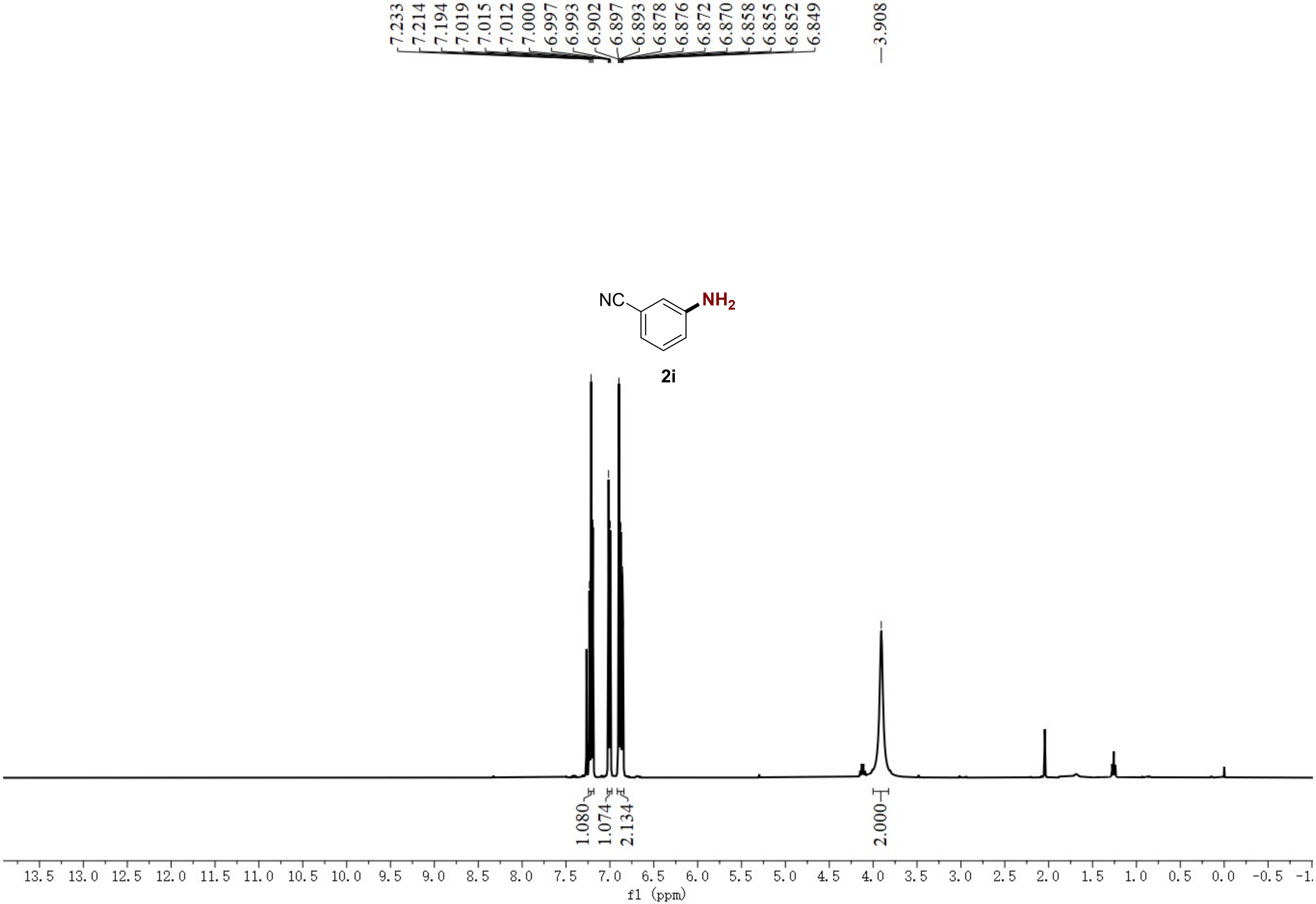

6.965
6.945
6.600
6.579
3.490
2.229
NH2
Me
2g
2.077
2.076
2.000
3.117
13.5
13.0
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.
f1 (ppm)


7.172
7.166
7.161
7.153
7.150
7.148
7.145
7.139
7.131
7.127
7.121
6.770
6.767
6.764
6.752
6.749
6.746
6.733
6.731
6.728
6.686
6.681
6.678
6.676
6.673
6.664
6.662
6.659
6.657
6.651
3.599
NH_2
2.174
1.086
2.156
2.000
13.5
13.0
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

2h

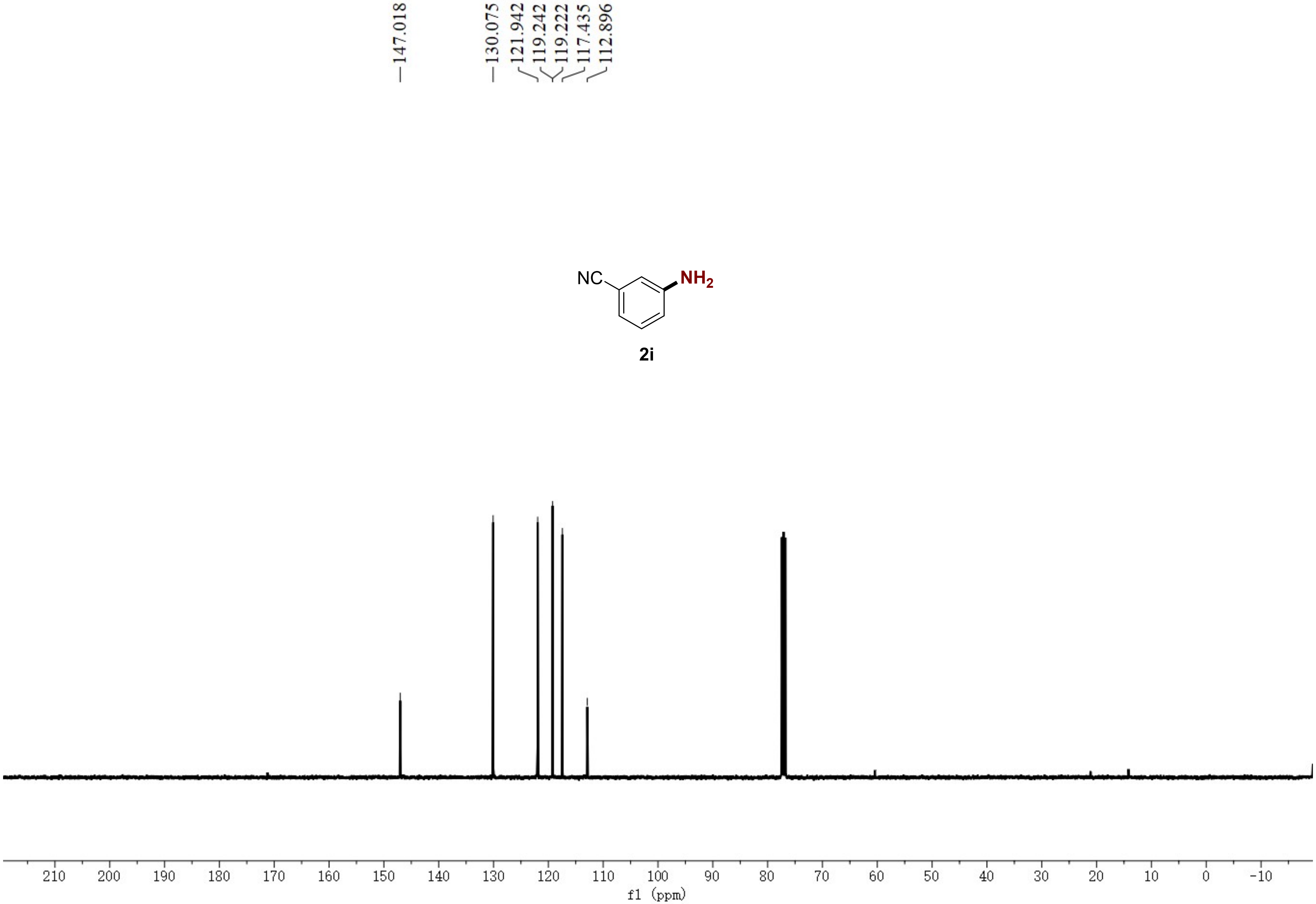

146.426
129.333
118.581
115.140
NH$_2$
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

2h

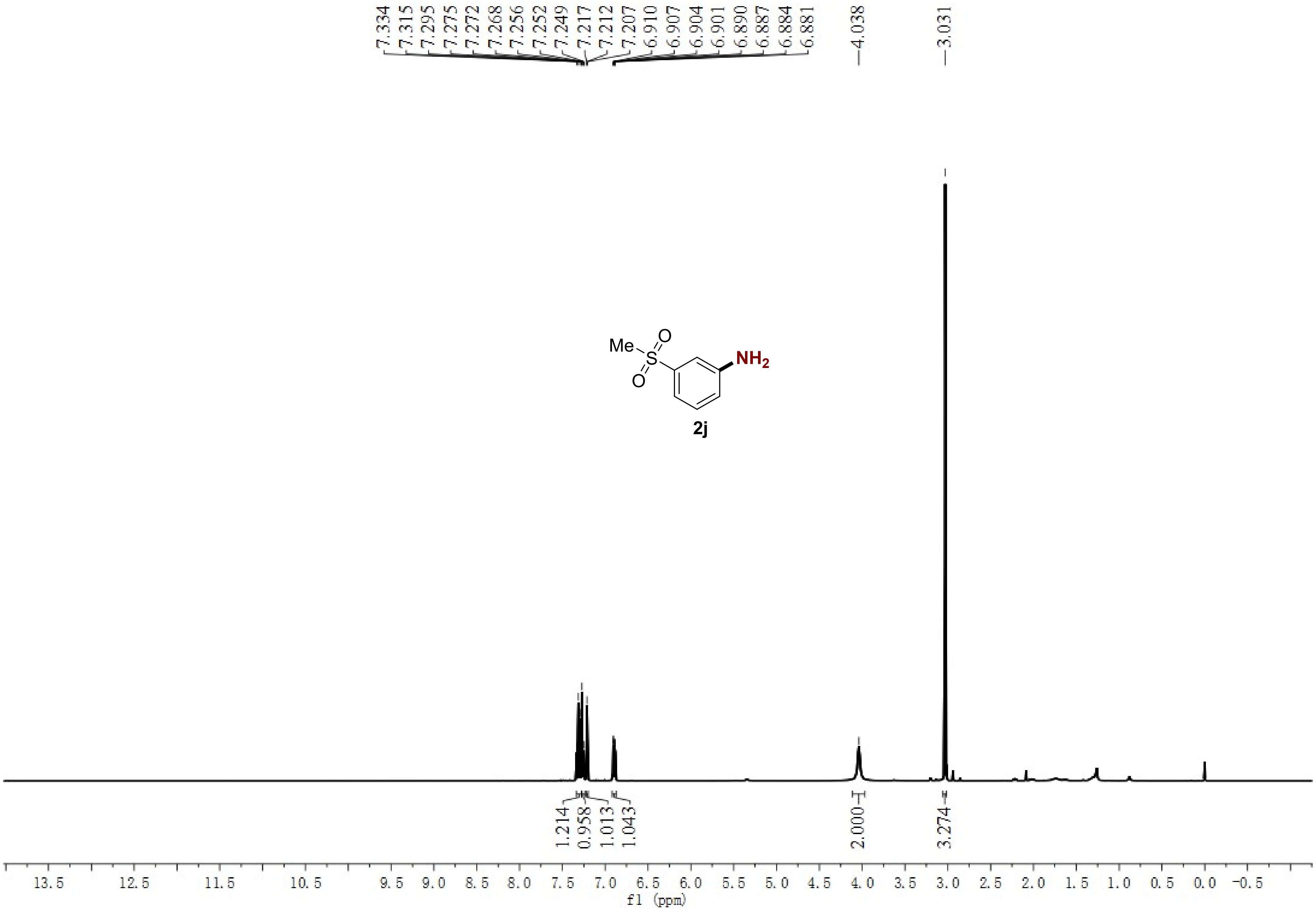


2i

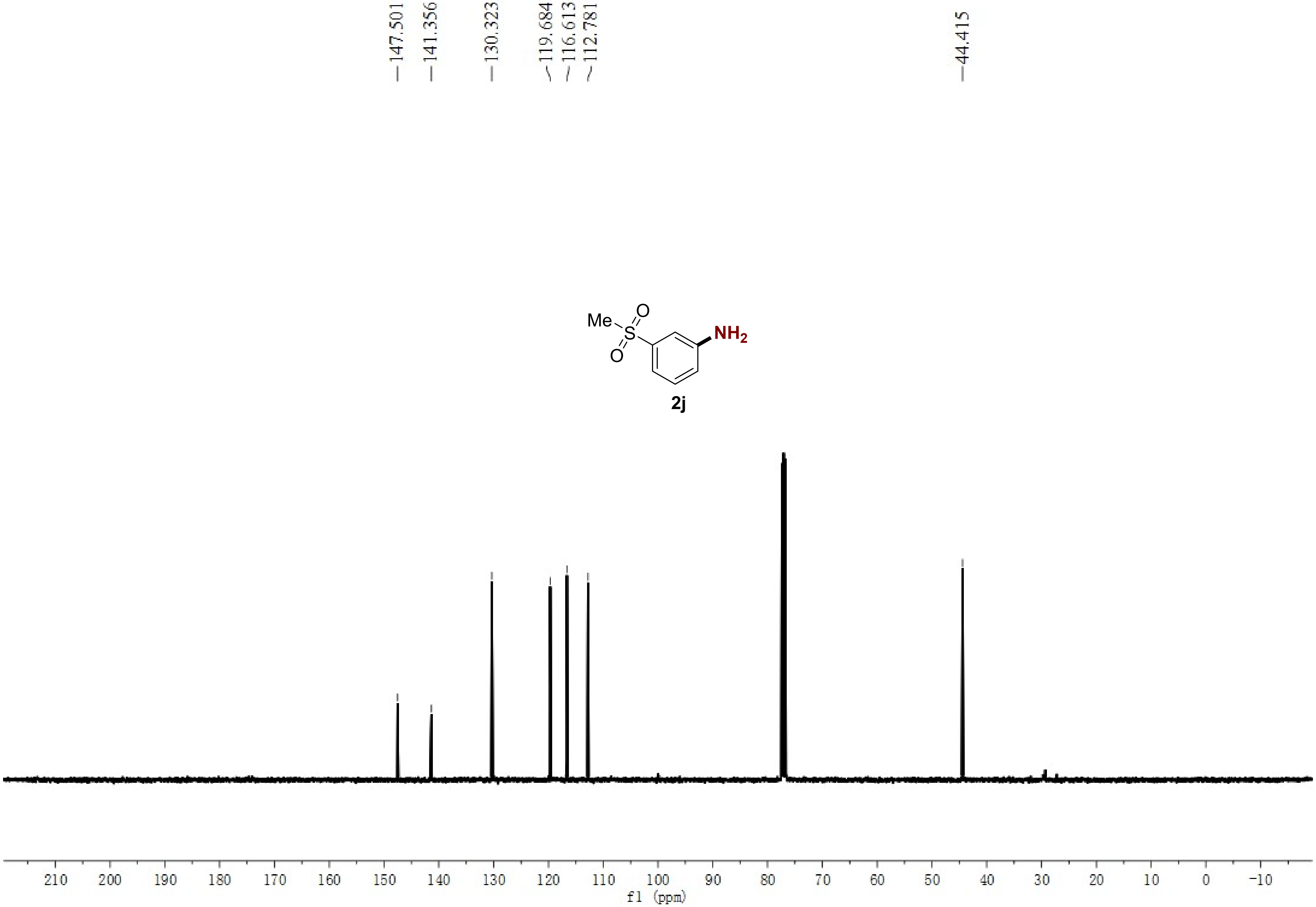
7.233
7.214
7.194
7.019
7.015
7.012
7.000
6.997
6.993
6.902
6.897
6.893
6.878
6.876
6.872
6.870
6.858
6.855
6.852
6.849
3.908
NC
NH2
1.080
1.074
2.134
2.000
13.5
13.0
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

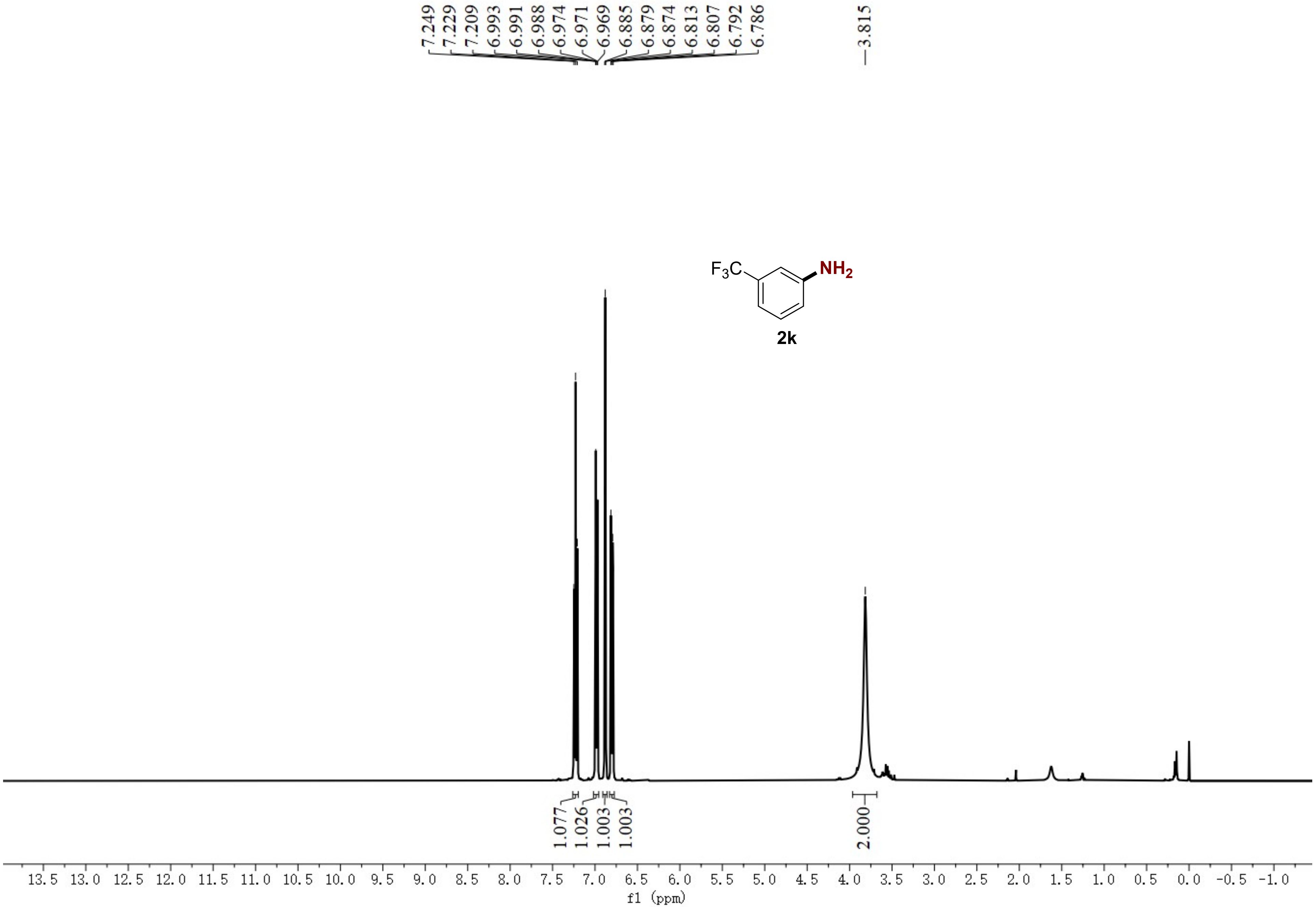

147.018
130.075
121.942
119.242
119.222
117.435
112.896
NC
NH2
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

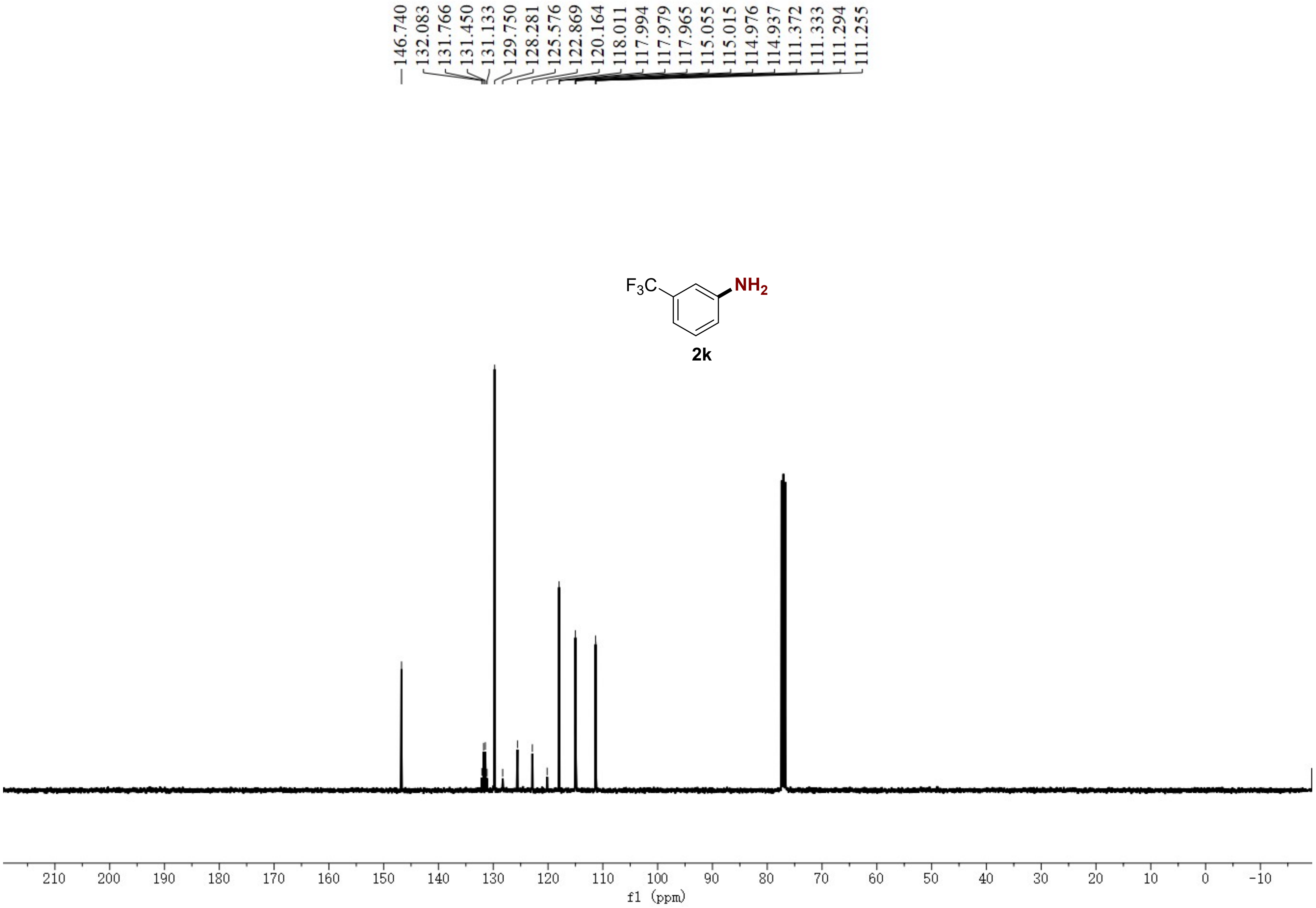
2i

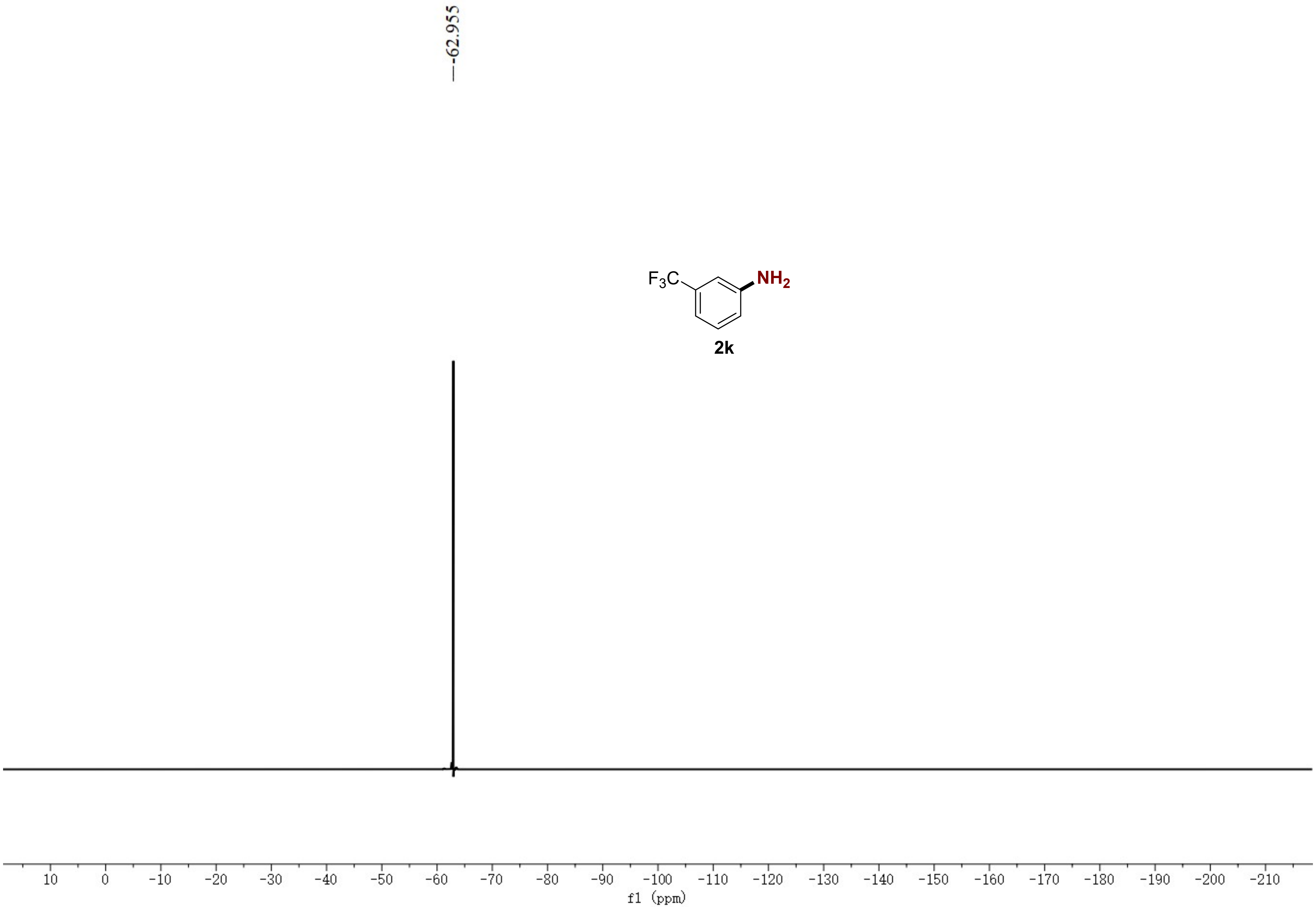


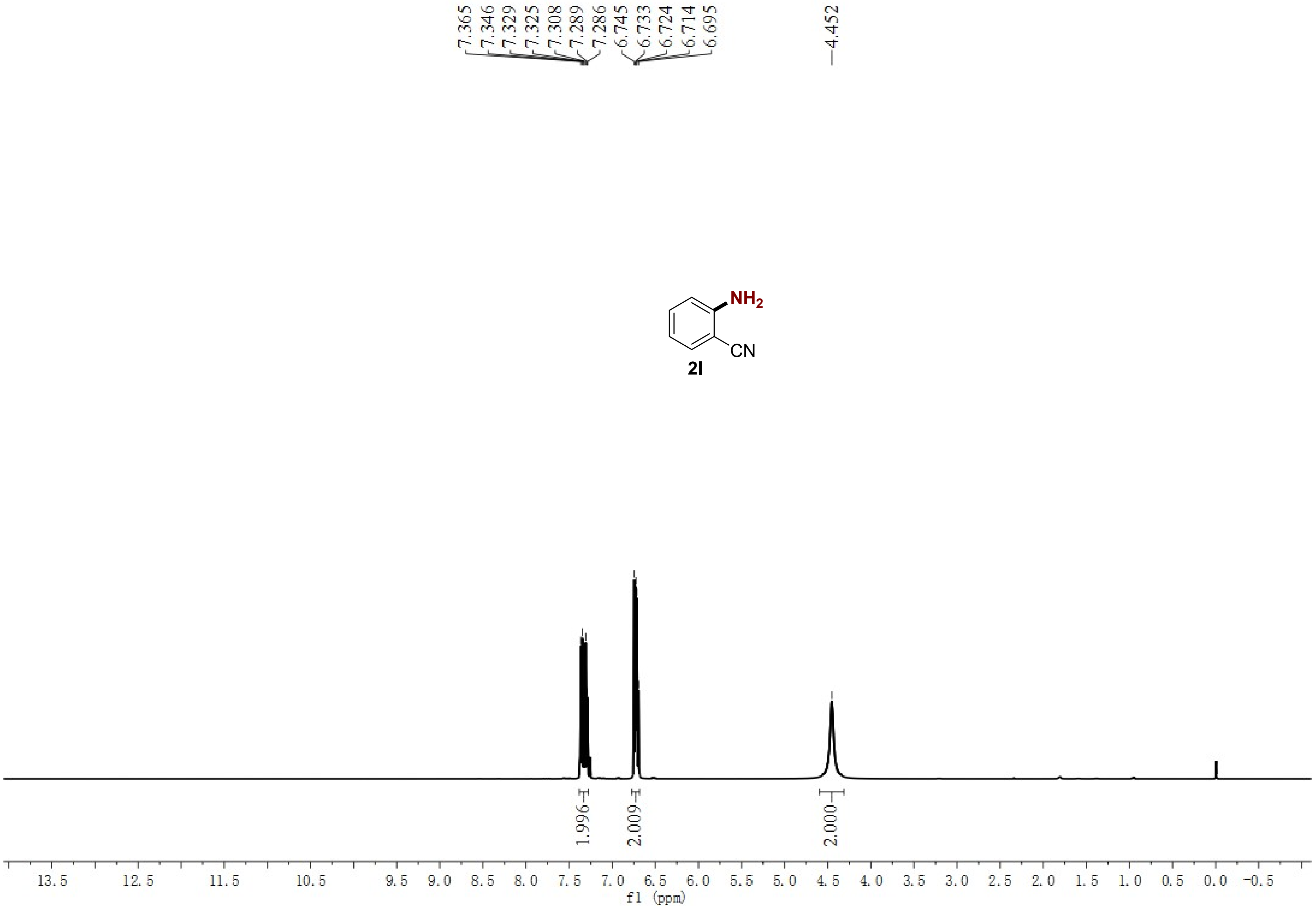
7.334
7.315
7.295
7.275
7.272
7.268
7.256
7.252
7.249
7.217
7.212
7.207
6.910
6.907
6.904
6.901
6.890
6.887
6.884
6.881
4.038
3.031
Me
S
O
O
NH2
2j
1.214
0.958
1.013
1.043
2.000
3.274
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
f1 (ppm)

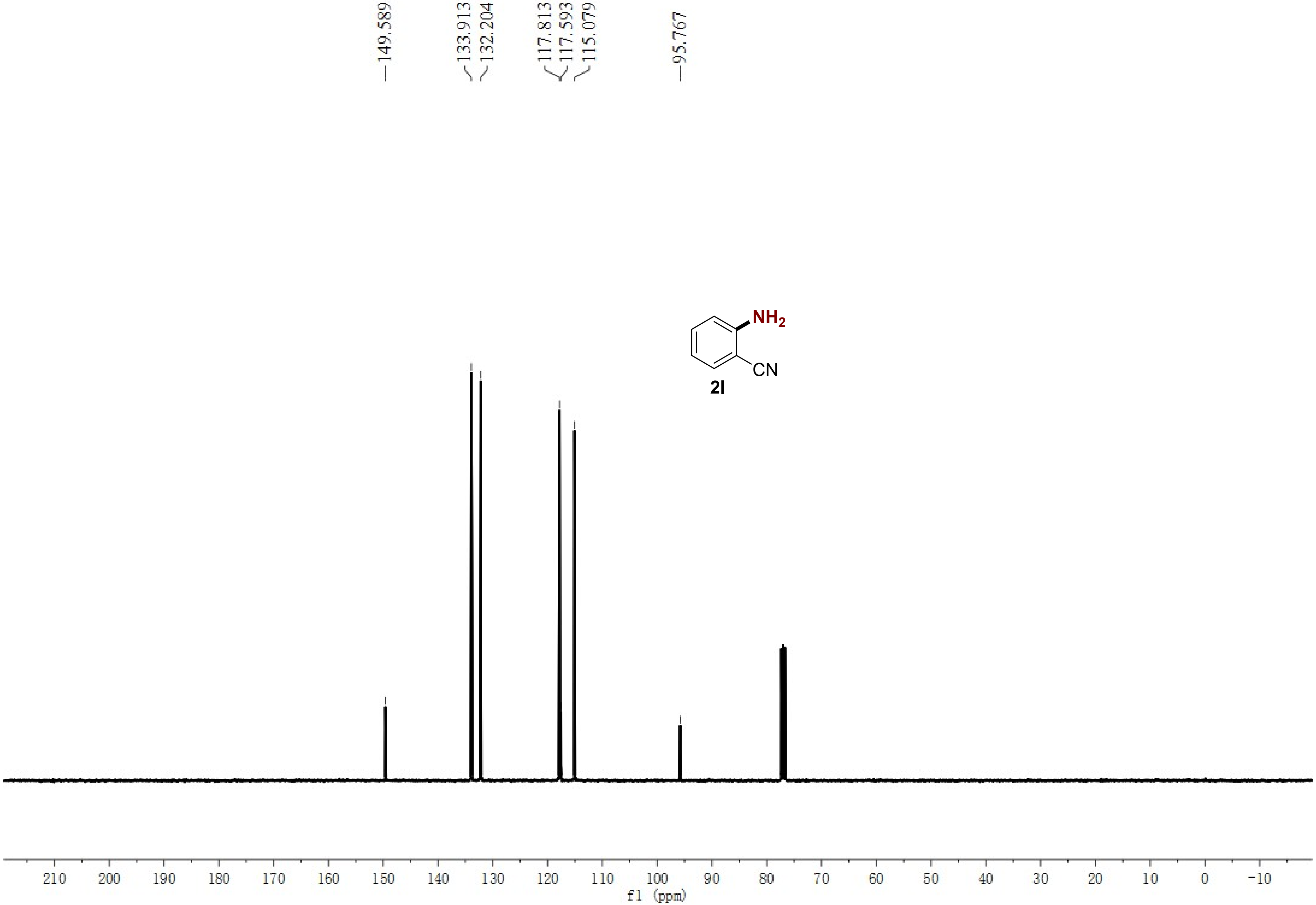

2j
147.501
141.356
130.323
119.684
116.613
112.781
44.415
Me
S
O
O
NH2
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


7.249
7.229
7.209
6.993
6.991
6.988
6.974
6.971
6.969
6.885
6.879
6.874
6.813
6.807
6.792
6.786
3.815
F_3C
NH_2
2k
1.077
1.026
1.003
1.003
2.000
13.5
13.0
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)


146.740
132.083
131.766
131.450
131.133
129.750
128.281
125.576
122.869
120.164
118.011
117.994
117.979
117.965
115.055
115.015
114.976
114.937
111.372
111.333
111.294
111.255
F3C
NH2
2k
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)

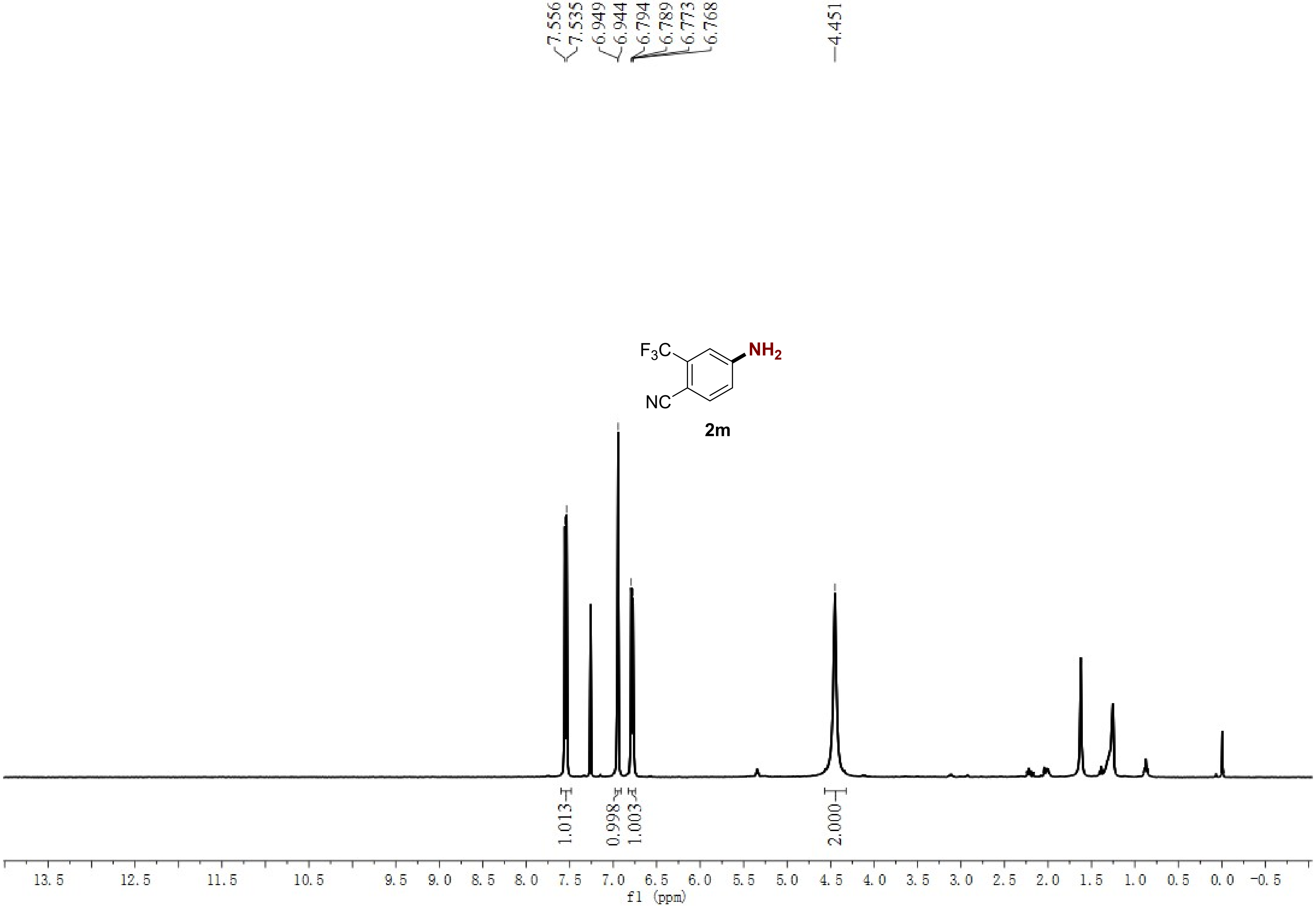

-62.955
F3C
NH2
2k
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

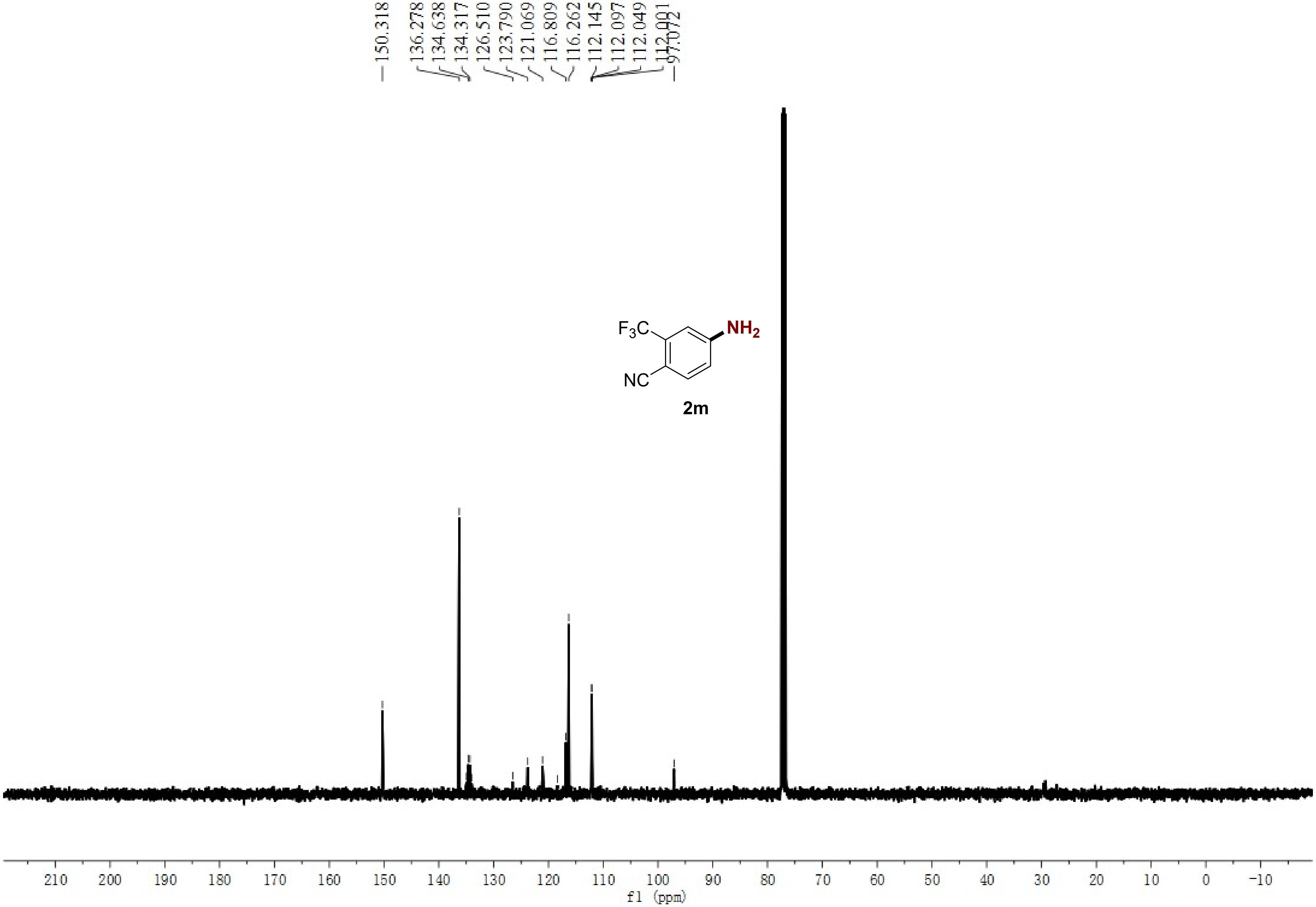

7.365
7.346
7.329
7.325
7.308
7.289
7.286
6.745
6.733
6.724
6.714
6.695
4.452
NH2
CN
2l
1.996
2.009
2.000
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)



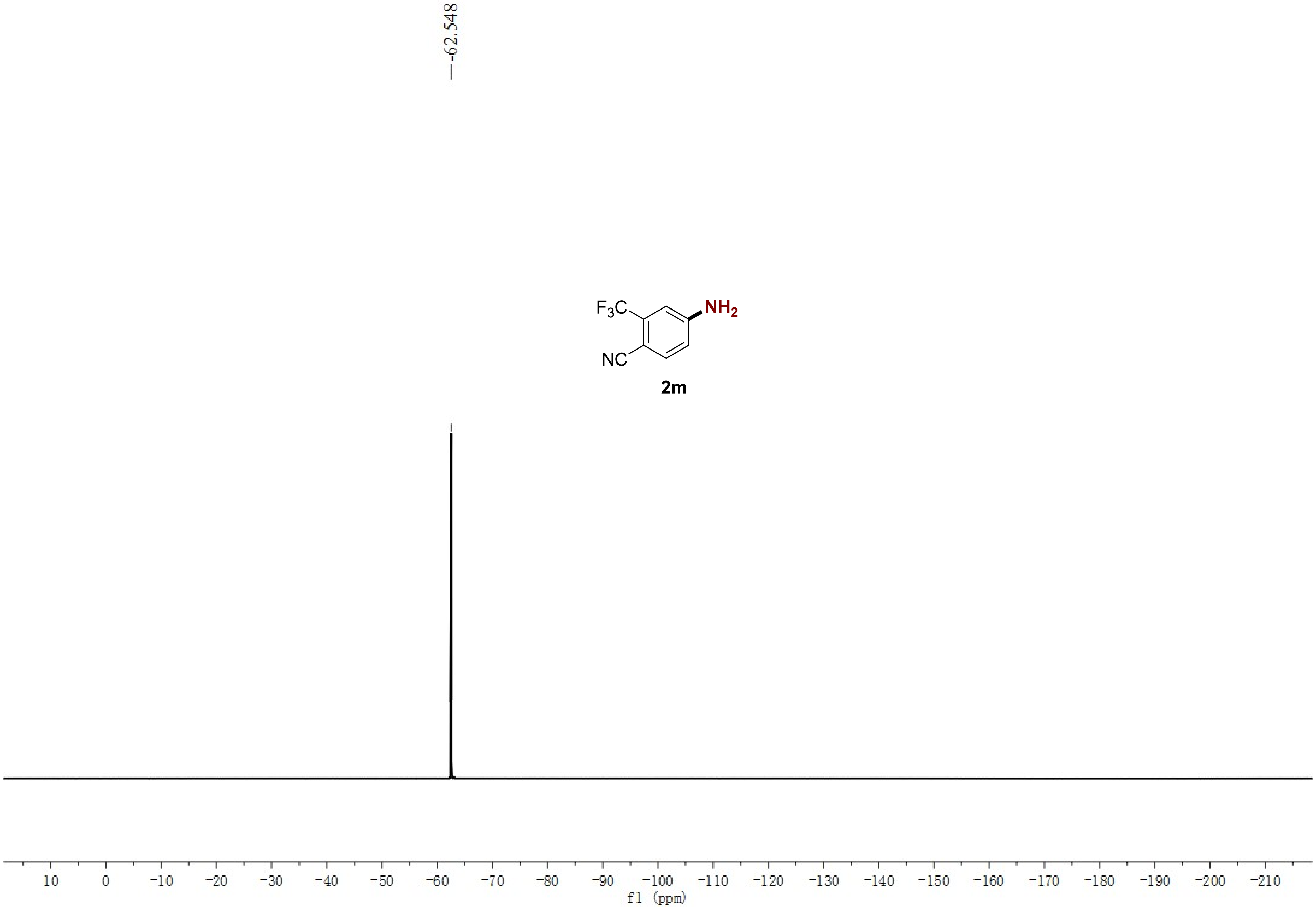
149.589
133.913
132.204
117.813
117.593
115.079
95.767
NH_2
CN
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

2l


7.556
7.535
6.949
6.944
6.794
6.789
6.773
6.768
4.451
F3C
NH2
NC
2m
1.013
0.998
1.003
2.000
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

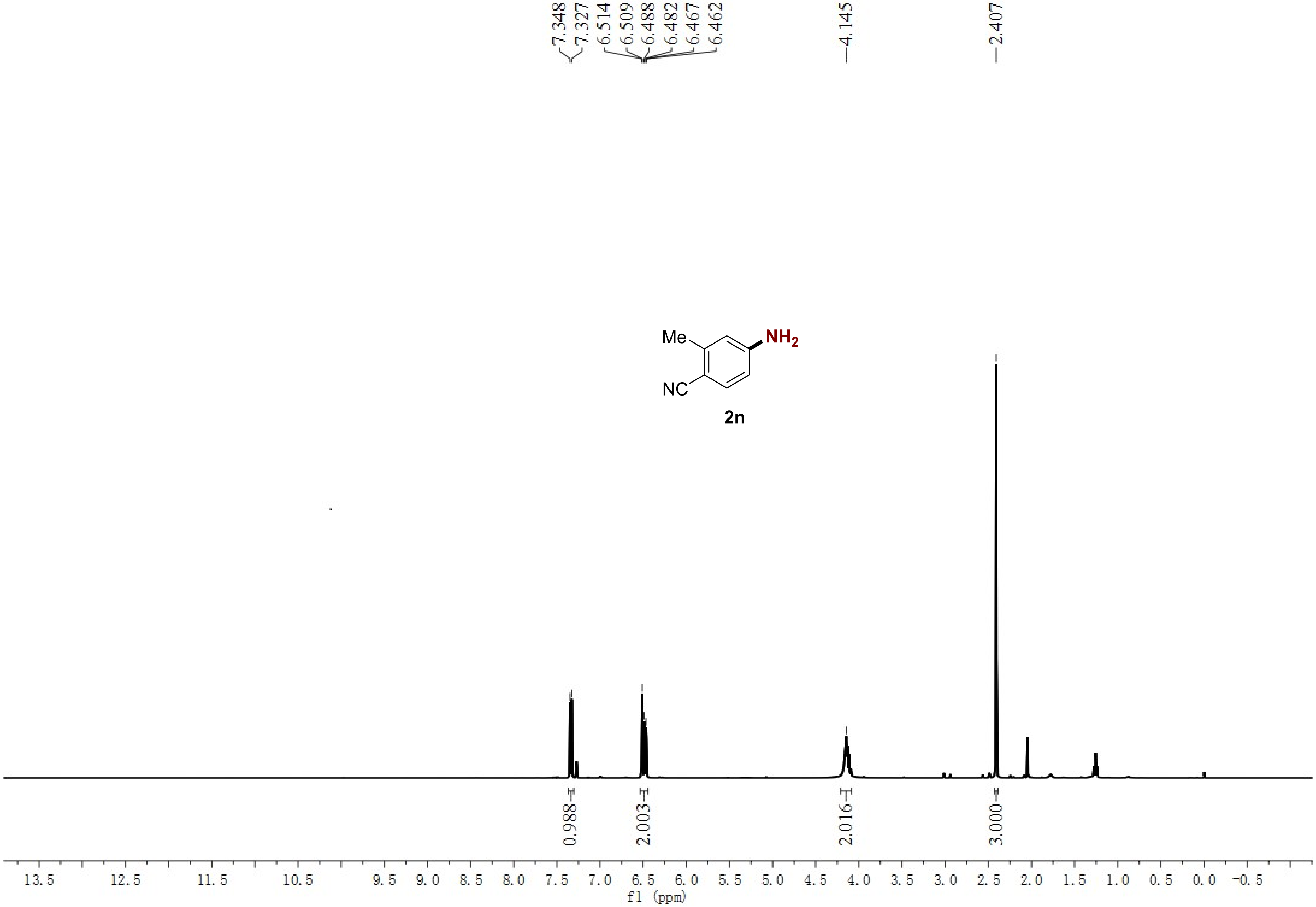

150.318
136.278
134.638
134.317
126.510
123.790
121.069
116.809
116.262
112.145
112.097
112.049
112.001
97.072
F$_3$C
NH$_2$
NC
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

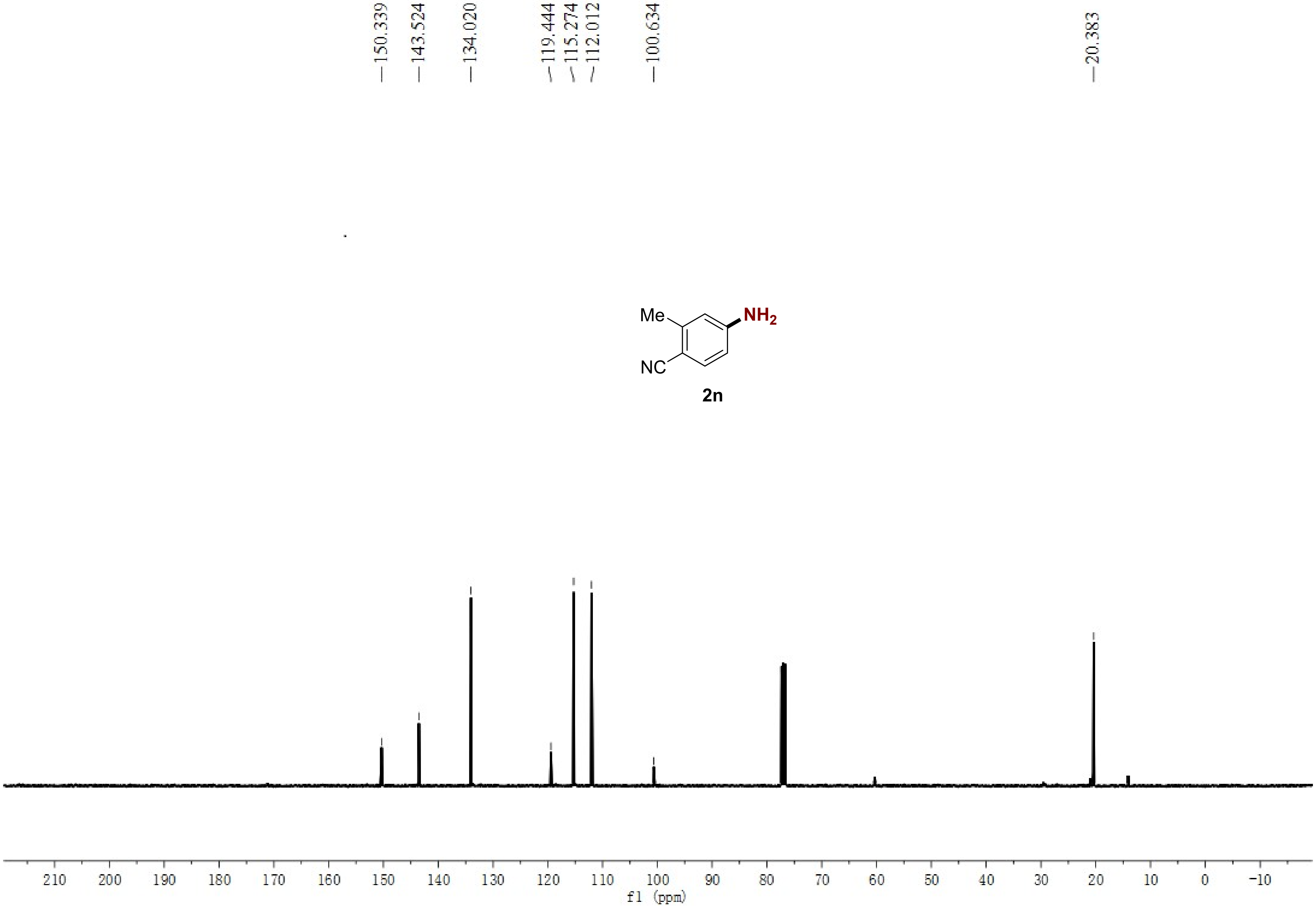
2m



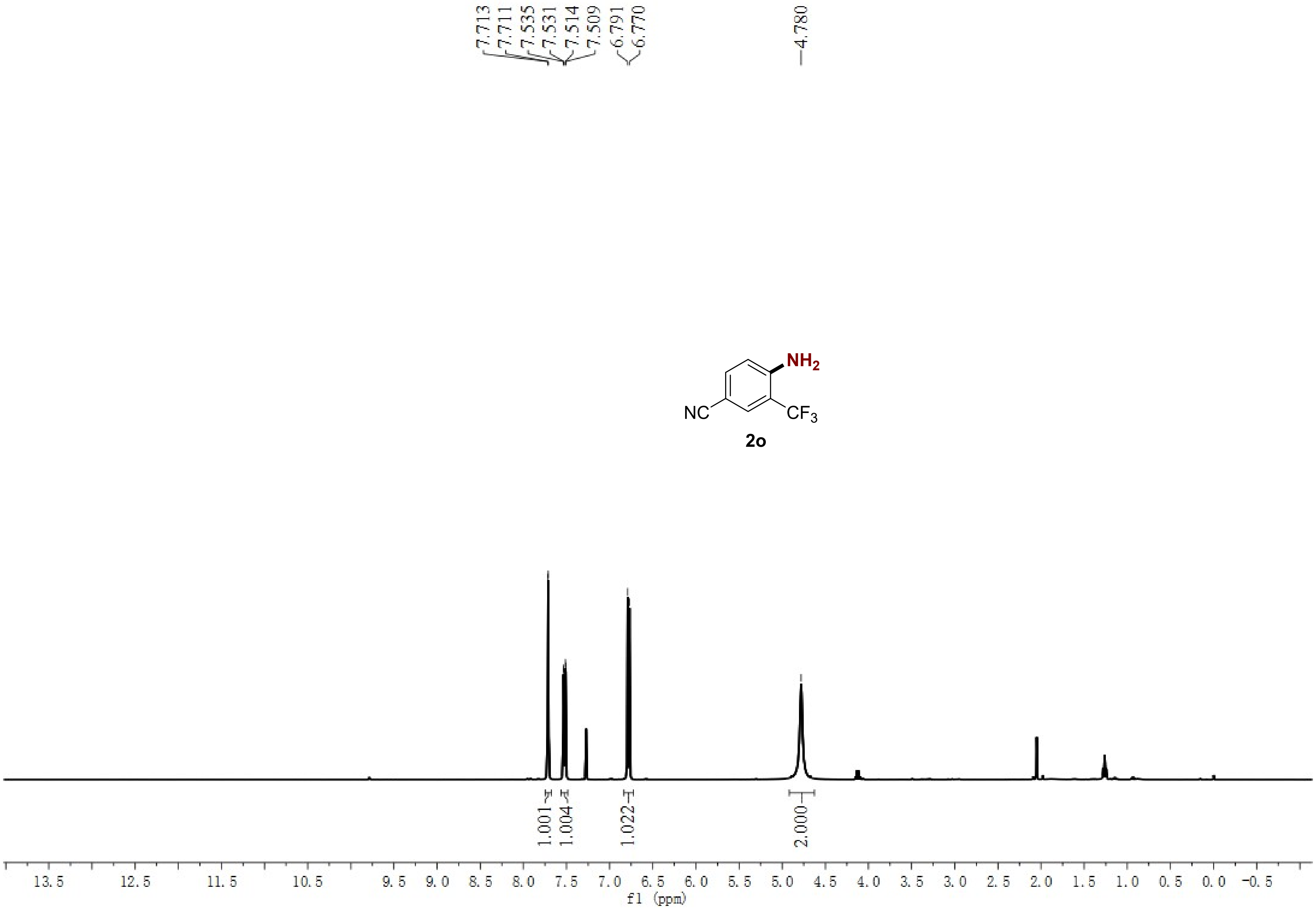
-62.548
F3C
NH2
NC
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
f1 (ppm)

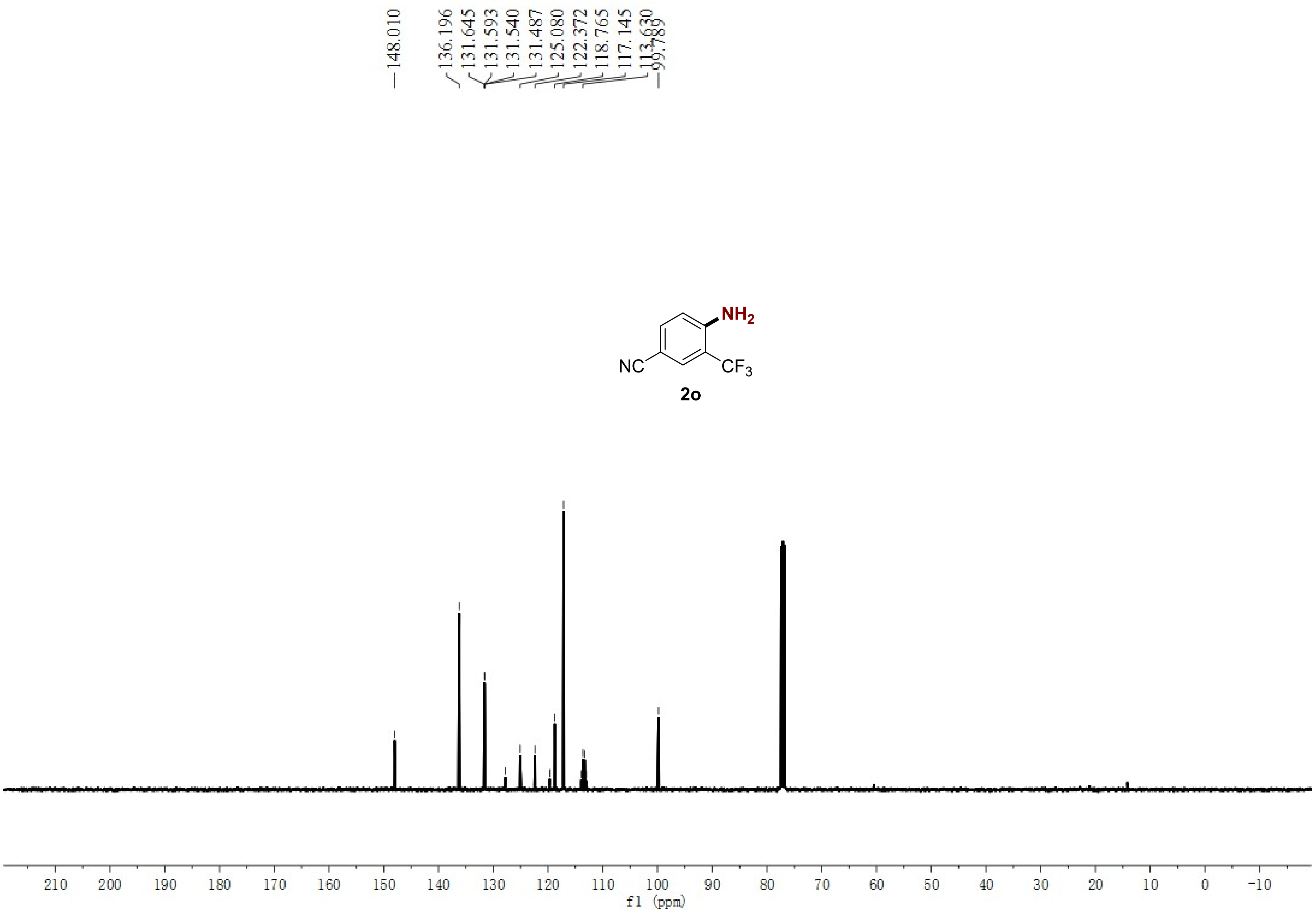
2m

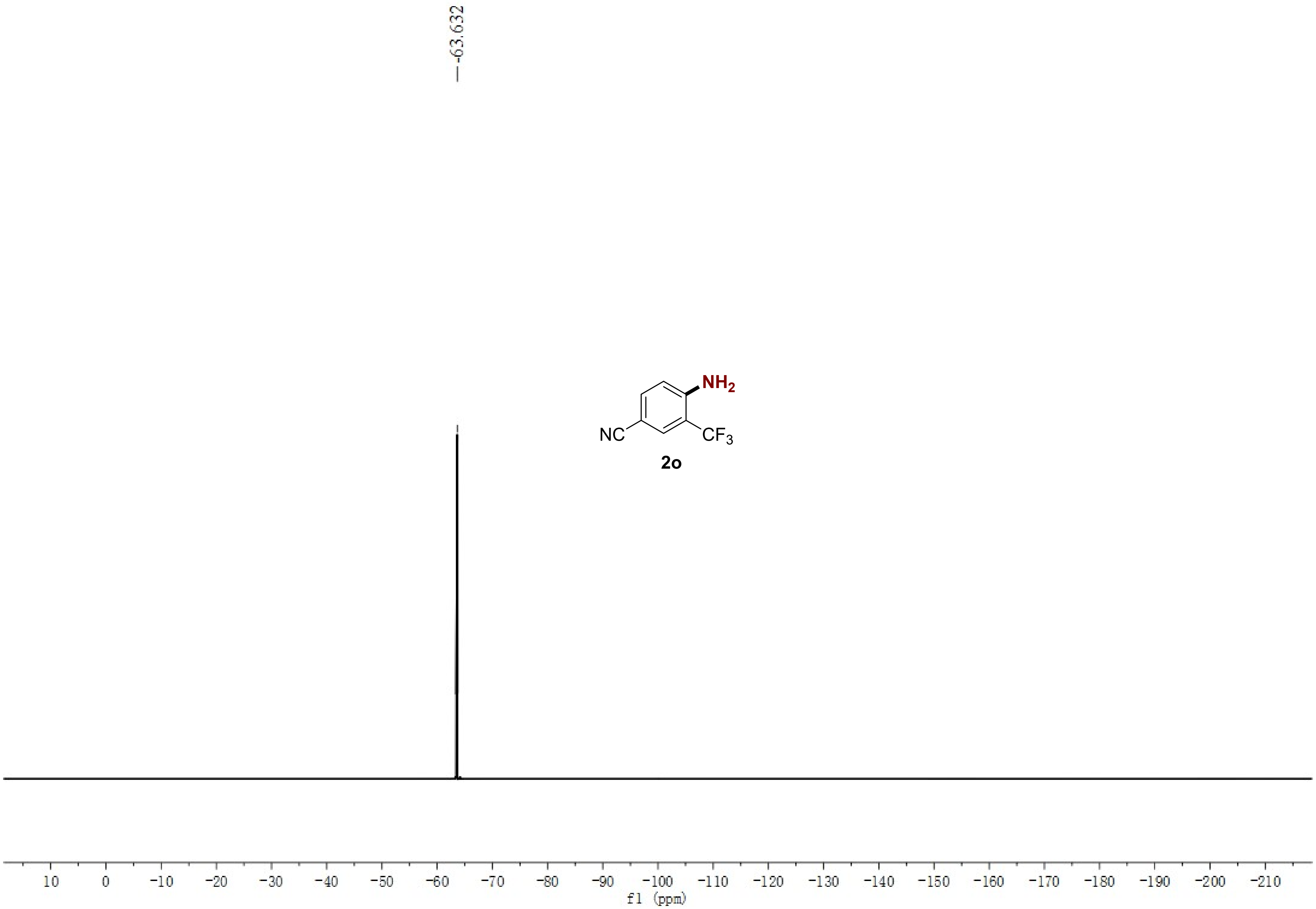

7.348
7.327
6.514
6.509
6.488
6.482
6.467
6.462
4.145
2.407
Me
NH2
NC
2n
0.988
2.003
2.016
3.000
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

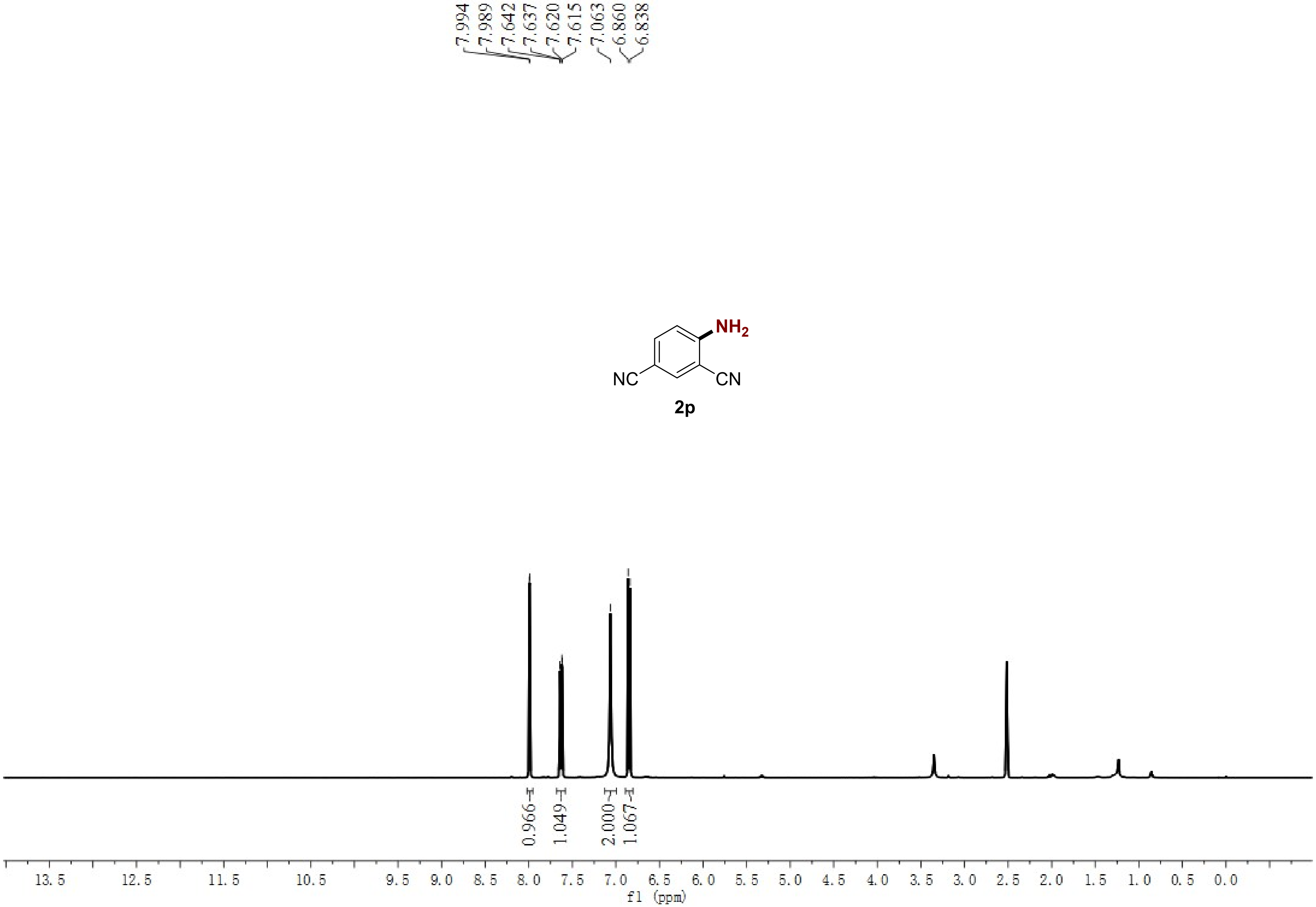

150.339
143.524
134.020
119.444
115.274
112.012
100.634
20.383
Me
NH2
NC
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

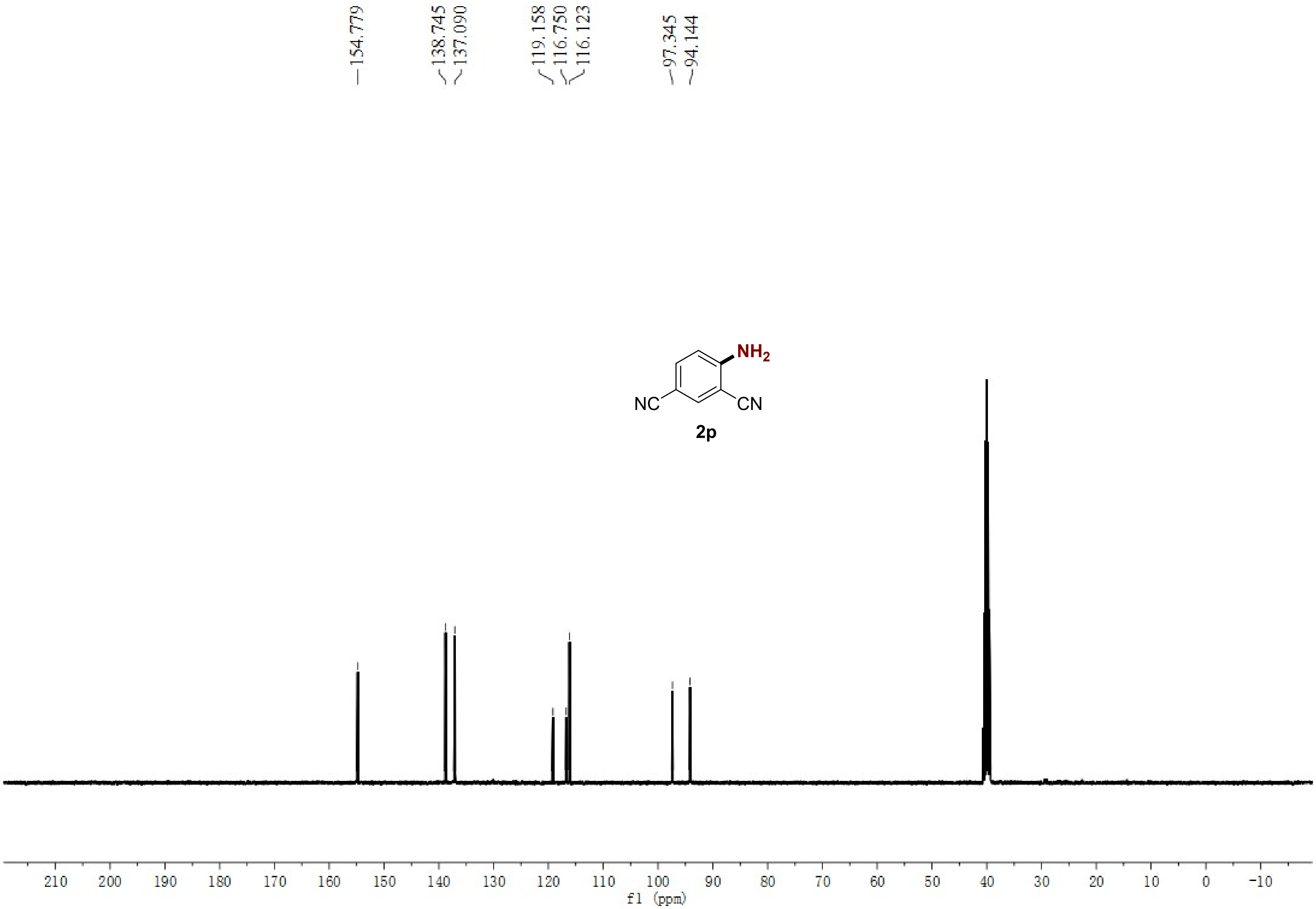
2n

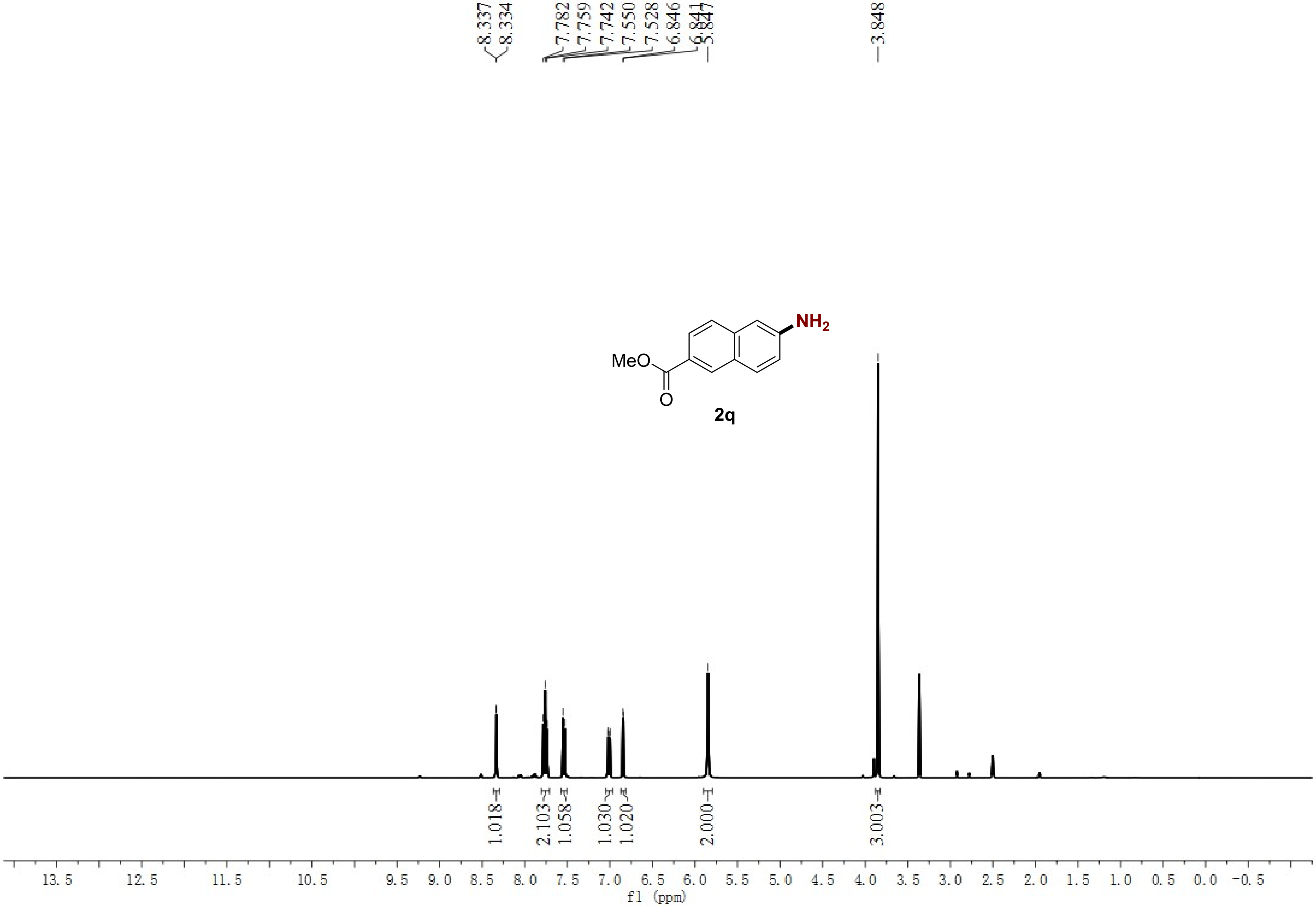

7.713
7.711
7.535
7.531
7.514
7.509
6.791
6.770
4.780
NH2
NC
CF3
2o
1.001
1.004
1.022
2.000
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
f1 (ppm)

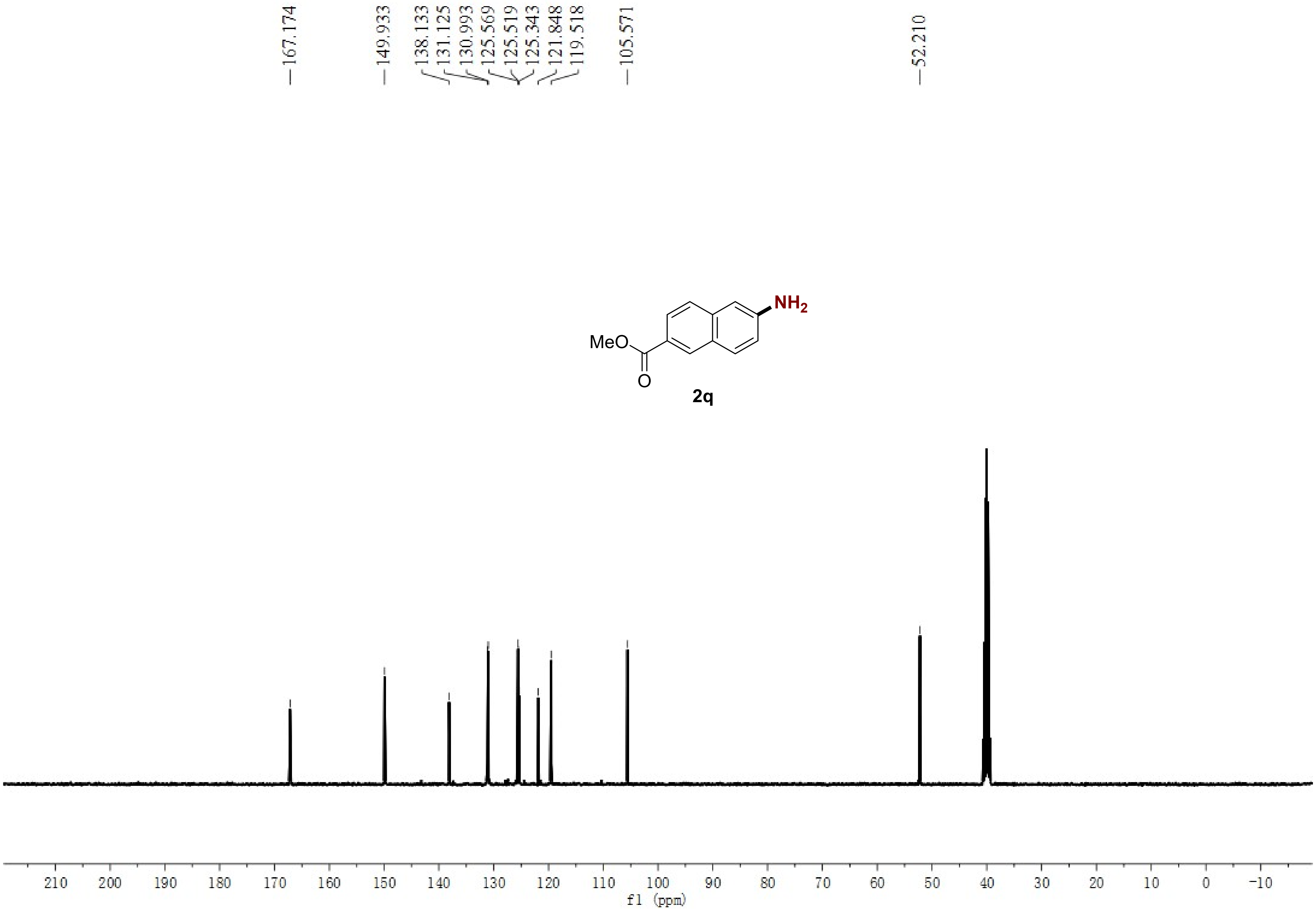

148.010
136.196
131.645
131.593
131.540
131.487
125.080
122.372
118.765
117.145
113.630
99.789
NH2
NC
CF3
2o
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

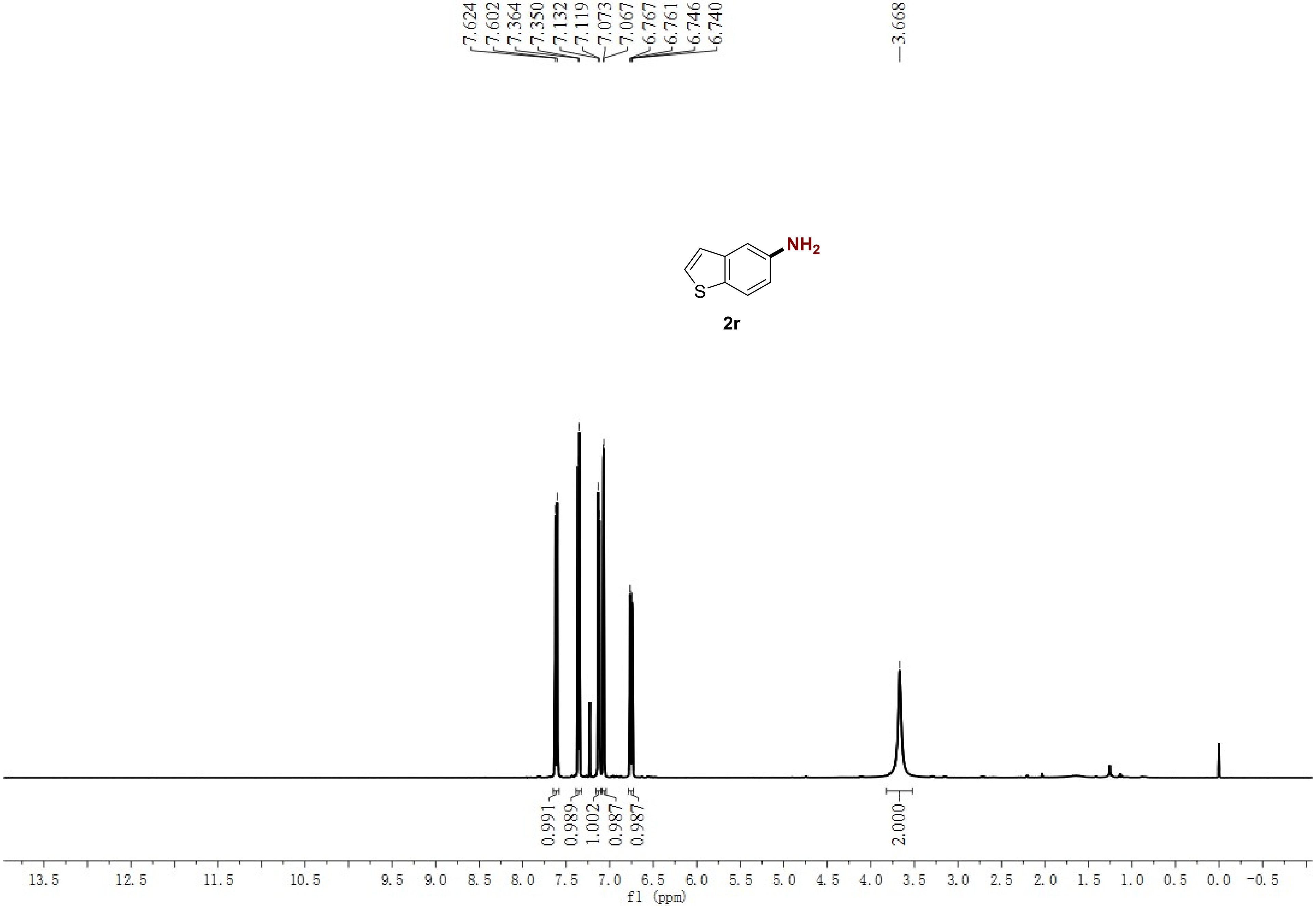

-63.632
NH2
NC
CF3
2o
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


7.994
7.989
7.642
7.637
7.620
7.615
7.063
6.860
6.838
NH2
NC
CN
2p
0.966
1.049
2.000
1.067
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

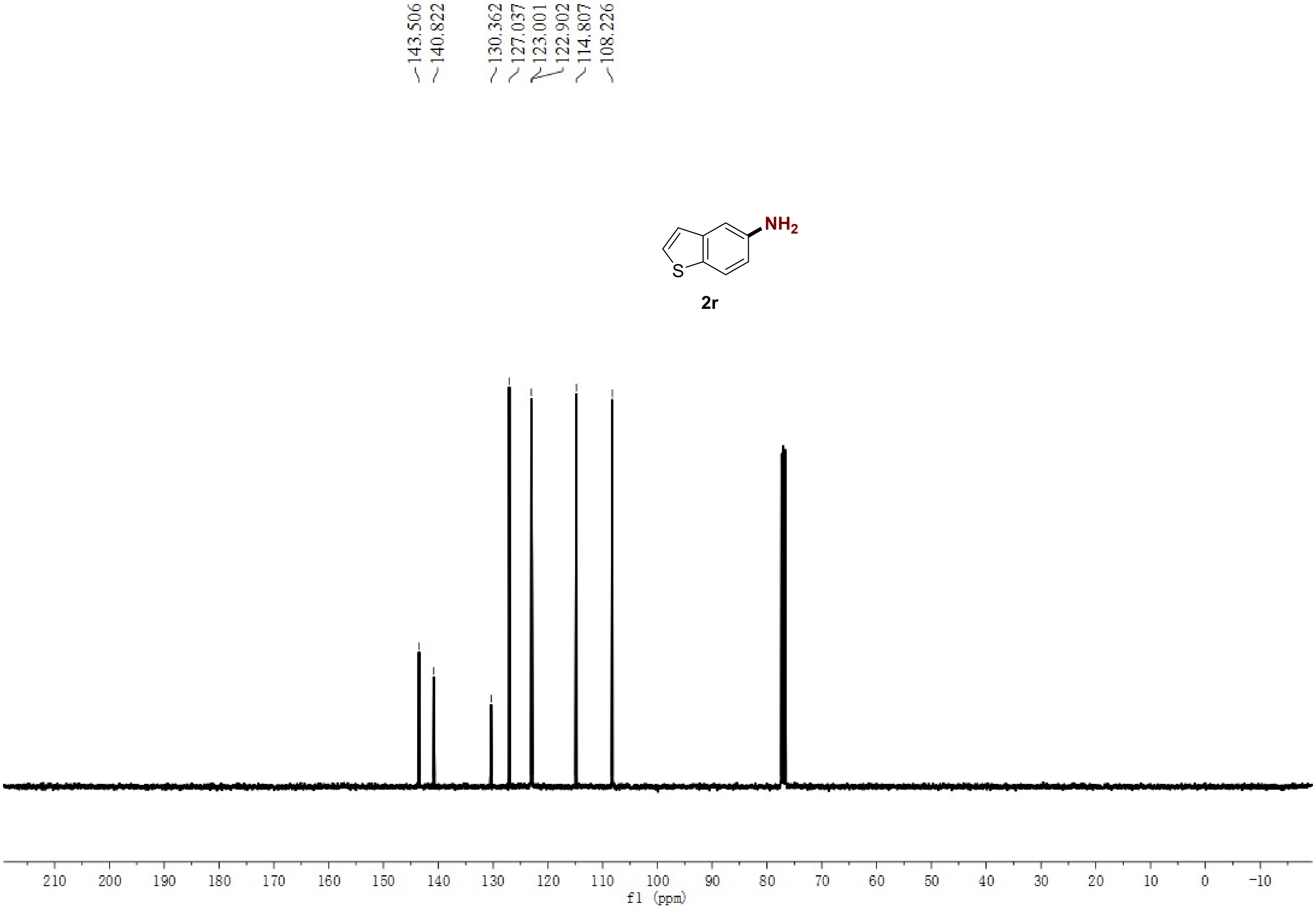

154.779
138.745
137.090
119.158
116.750
116.123
97.345
94.144
NH2
NC
CN
2p
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.337
8.334
7.782
7.759
7.742
7.550
7.528
6.846
6.841
5.847
3.848
MeO
O
NH2
2q
1.018
2.103
1.058
1.030
1.020
2.000
3.003
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


2q
167.174
149.933
138.133
131.125
130.993
125.569
125.519
125.343
121.848
119.518
105.571
52.210
MeO
O
NH2
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)

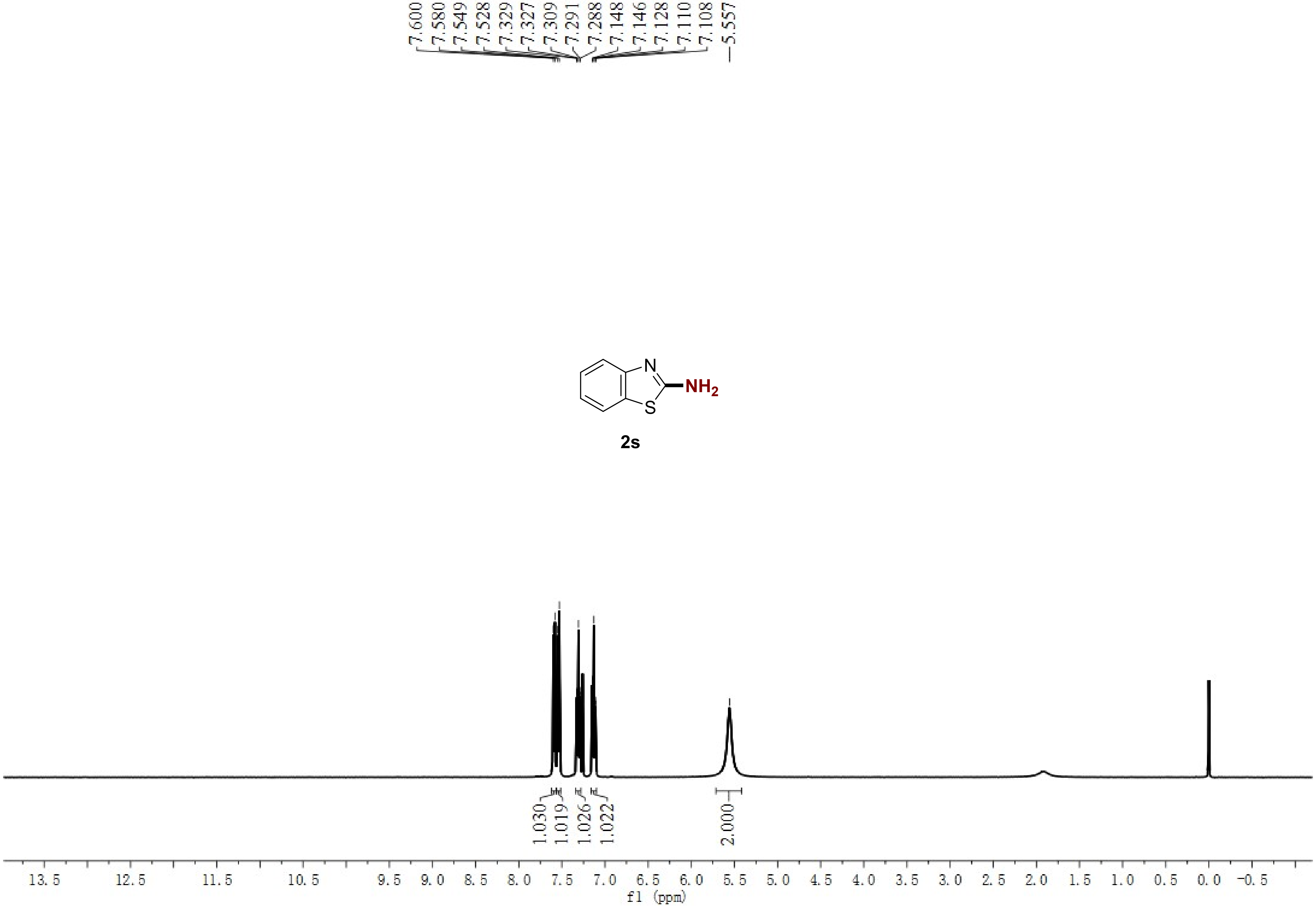

7.624
7.602
7.364
7.350
7.132
7.119
7.073
7.067
6.767
6.761
6.746
6.740
3.668
NH2
S
0.991
0.989
1.002
0.987
0.987
2.000
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

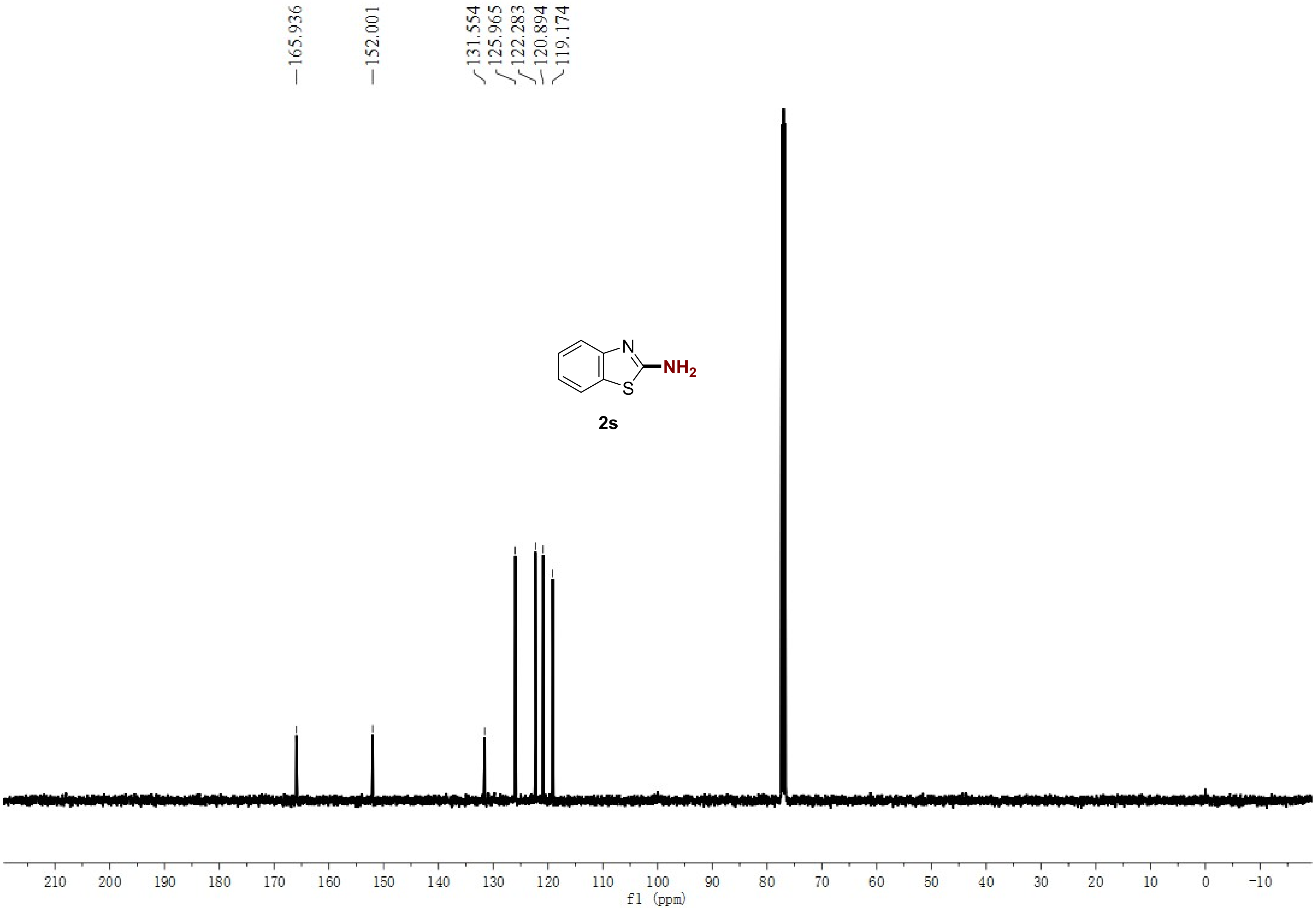
2r


143.506
140.822
130.362
127.037
123.001
122.902
114.807
108.226
NH2
S
2r
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)

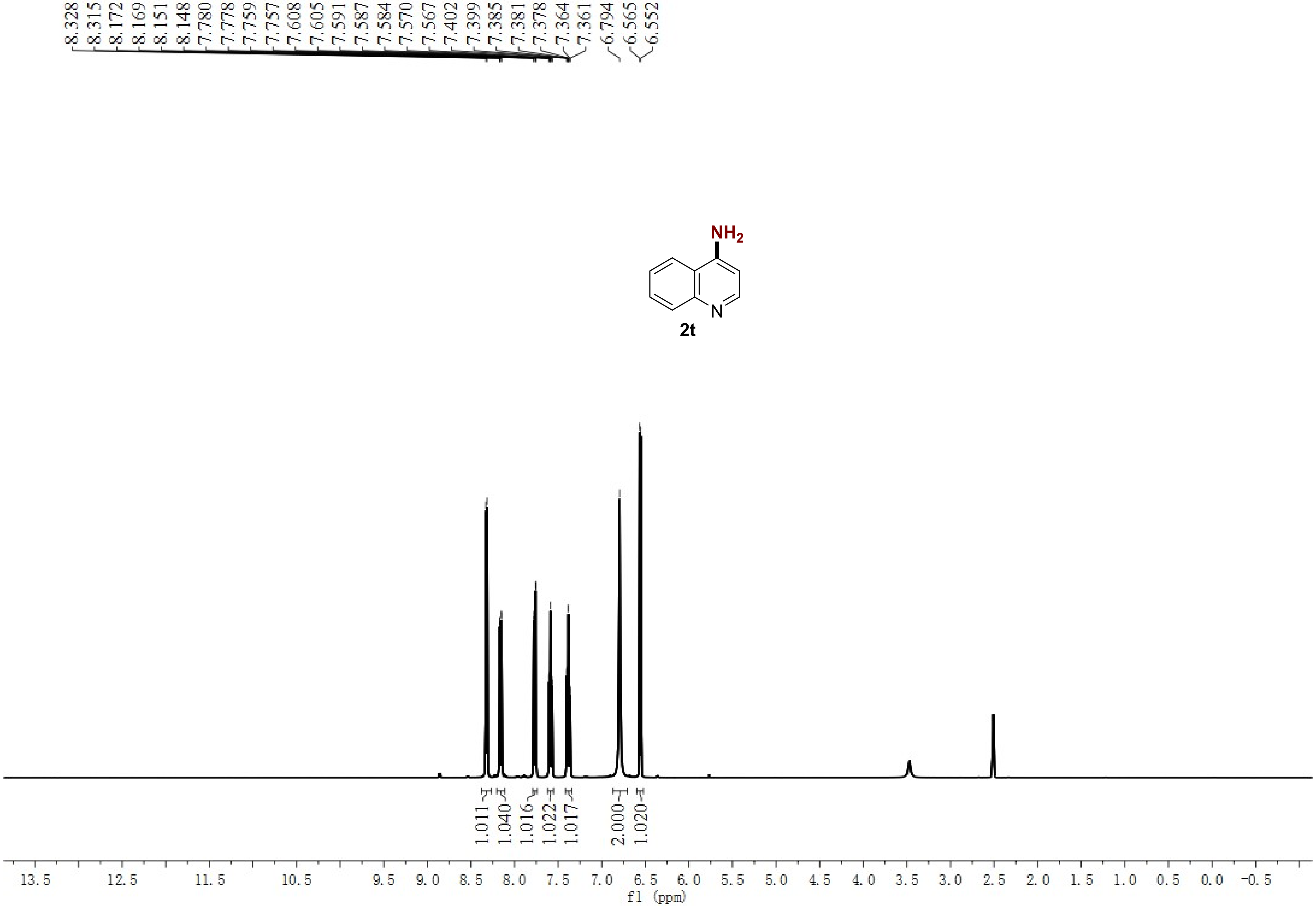
N
NH2
S

2s

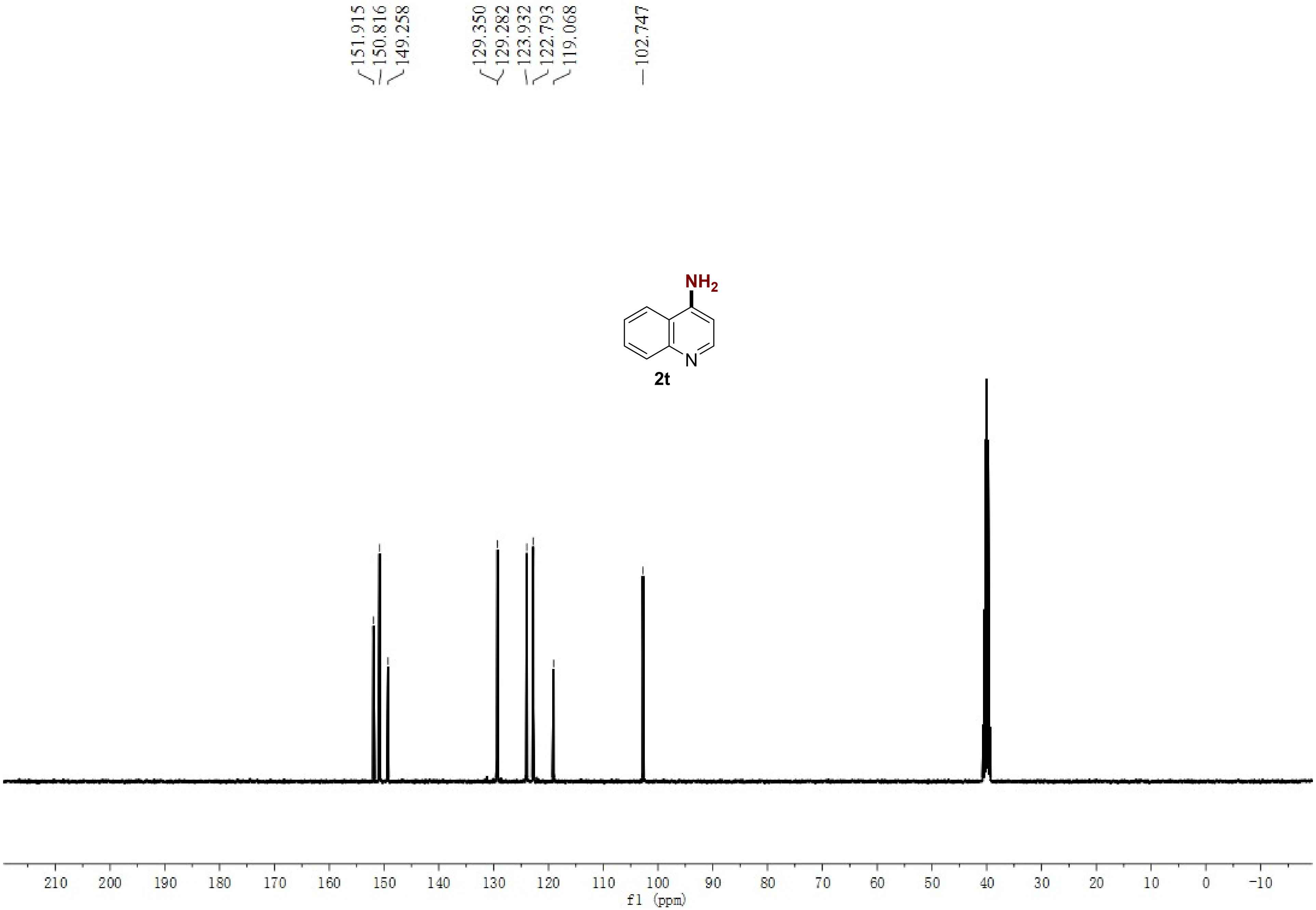

7.600
7.580
7.549
7.528
7.329
7.327
7.309
7.291
7.288
7.148
7.146
7.128
7.110
7.108
5.557
1.030
1.019
1.026
1.022
2.000
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

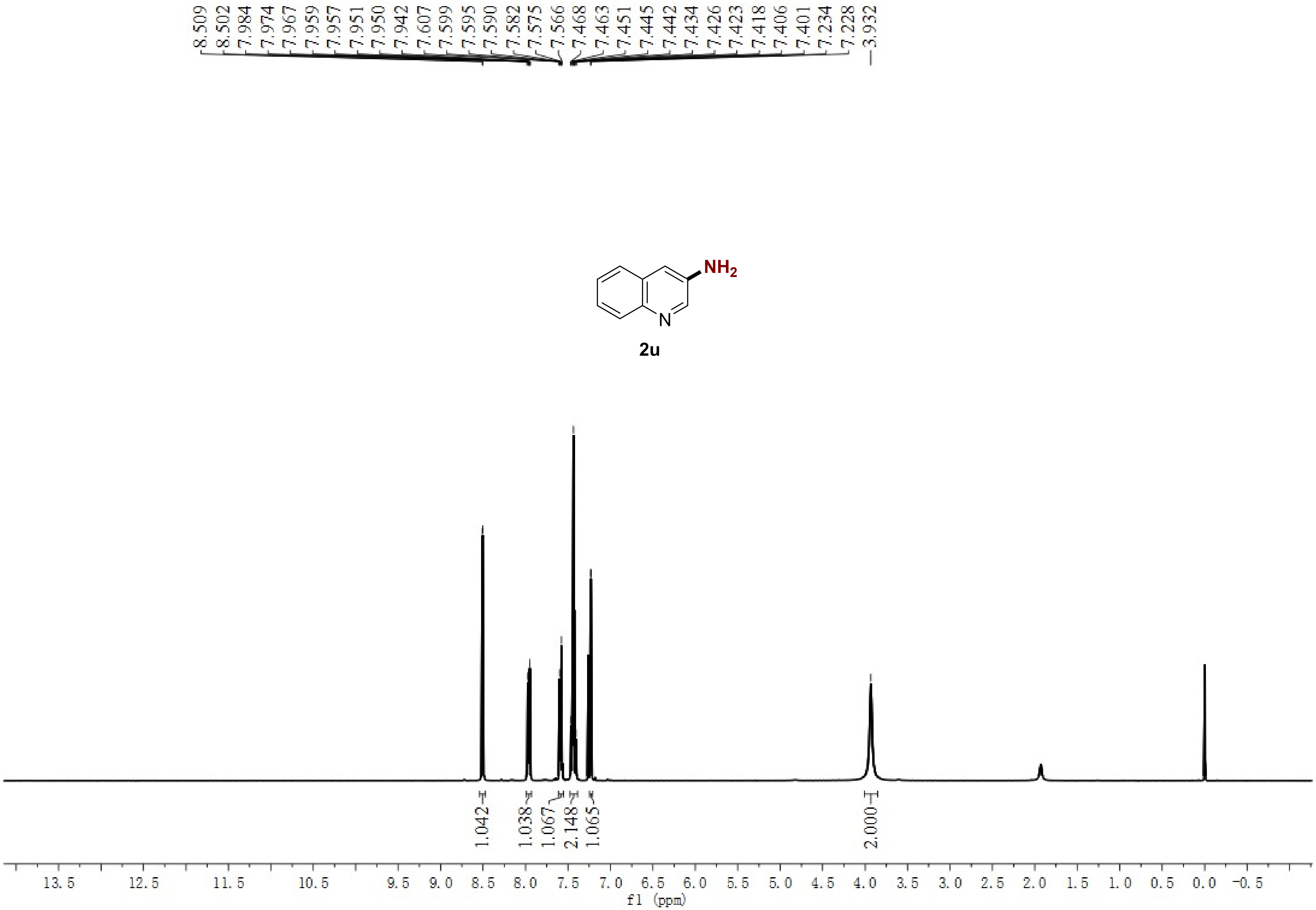

165.936
152.001
131.554
125.965
122.283
120.894
119.174
N
S
NH2
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

2s

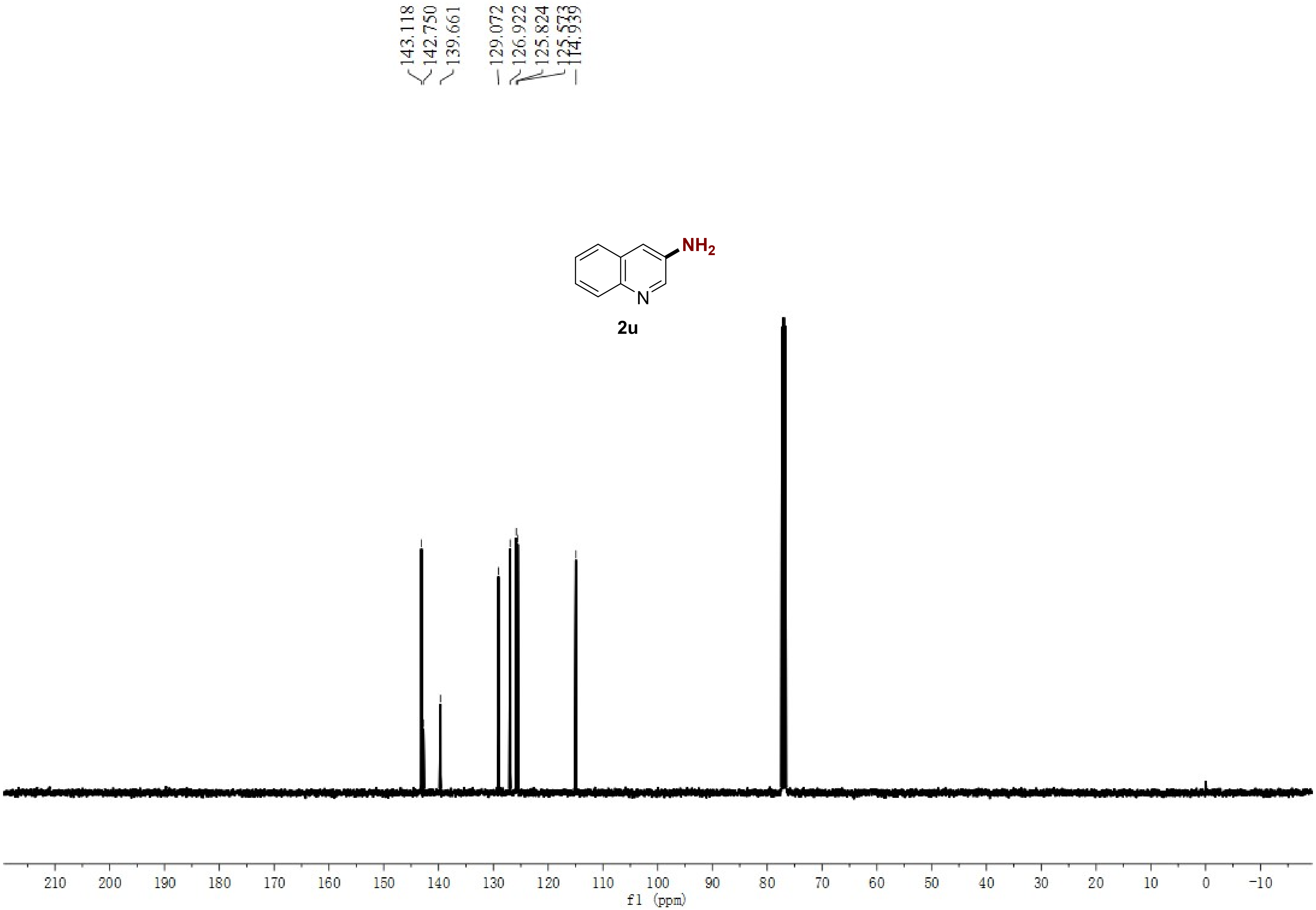

8.328
8.315
8.172
8.169
8.151
8.148
7.780
7.778
7.759
7.757
7.608
7.605
7.591
7.587
7.584
7.570
7.567
7.402
7.399
7.385
7.381
7.378
7.364
7.361
6.794
6.565
6.552
NH2
N
1.011
1.040
1.016
1.022
1.017
2.000
1.020
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
f1 (ppm)

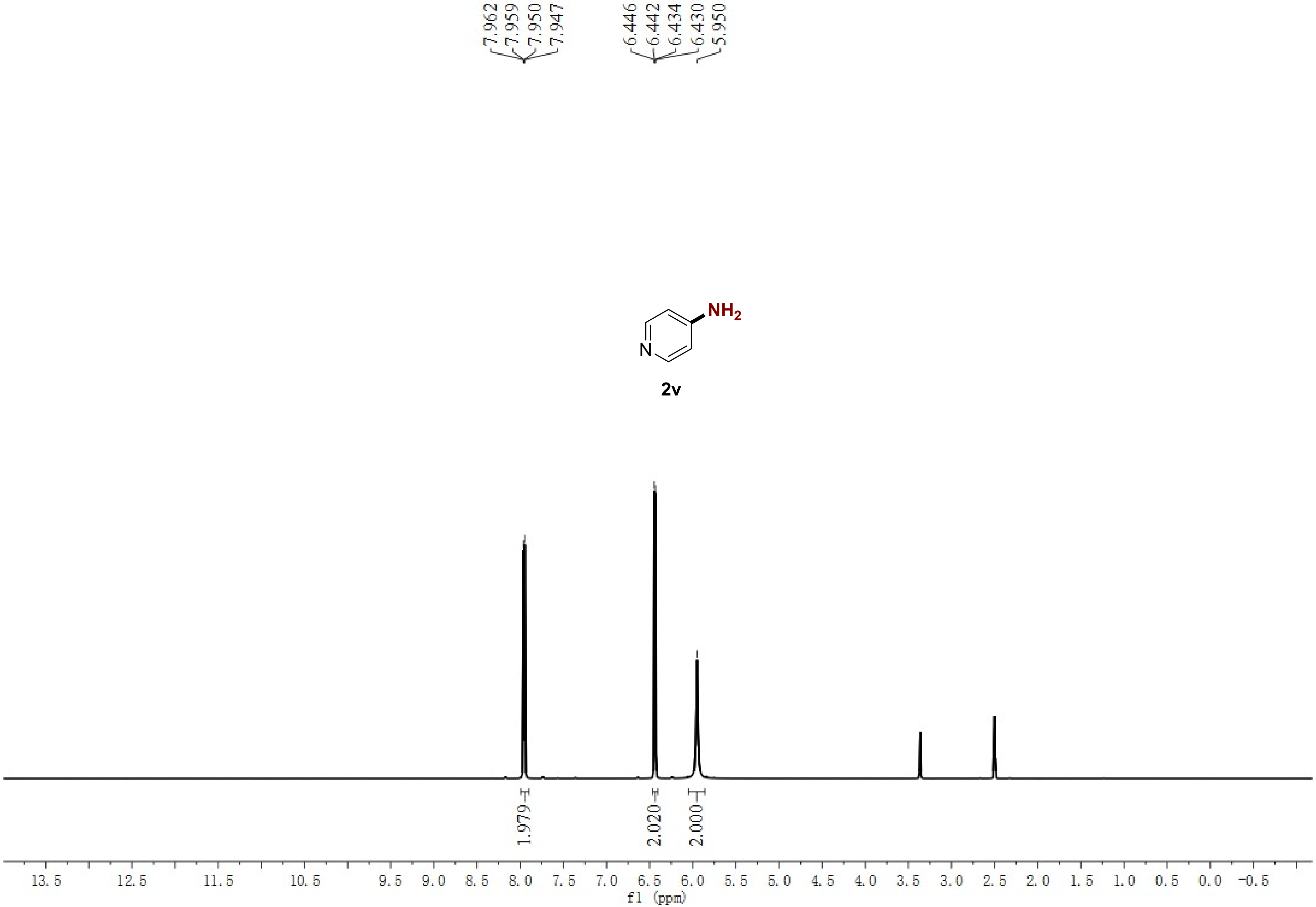
2t


151.915
150.816
149.258
129.350
129.282
123.932
122.793
119.068
102.747
NH2
N
2t
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)


8.509
8.502
7.984
7.974
7.967
7.959
7.957
7.951
7.950
7.942
7.607
7.599
7.595
7.590
7.582
7.575
7.566
7.468
7.463
7.451
7.445
7.442
7.434
7.426
7.423
7.418
7.406
7.401
7.234
7.228
3.932
NH2
N
1.042
1.038
1.067
2.148
1.065
2.000
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

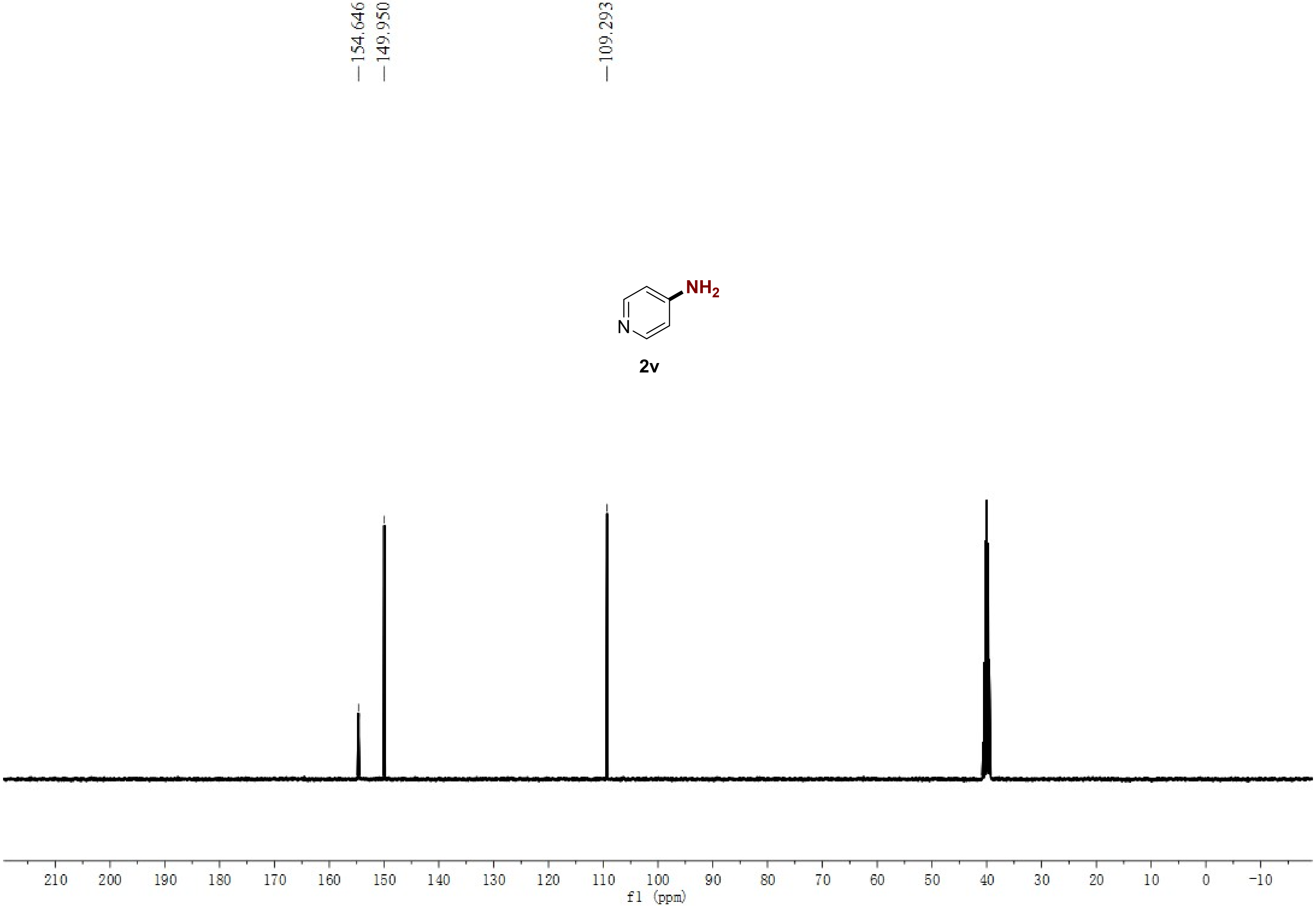
2u


143.118
142.750
139.661
129.072
126.922
125.824
125.573
114.939
NH2
N
2u
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)

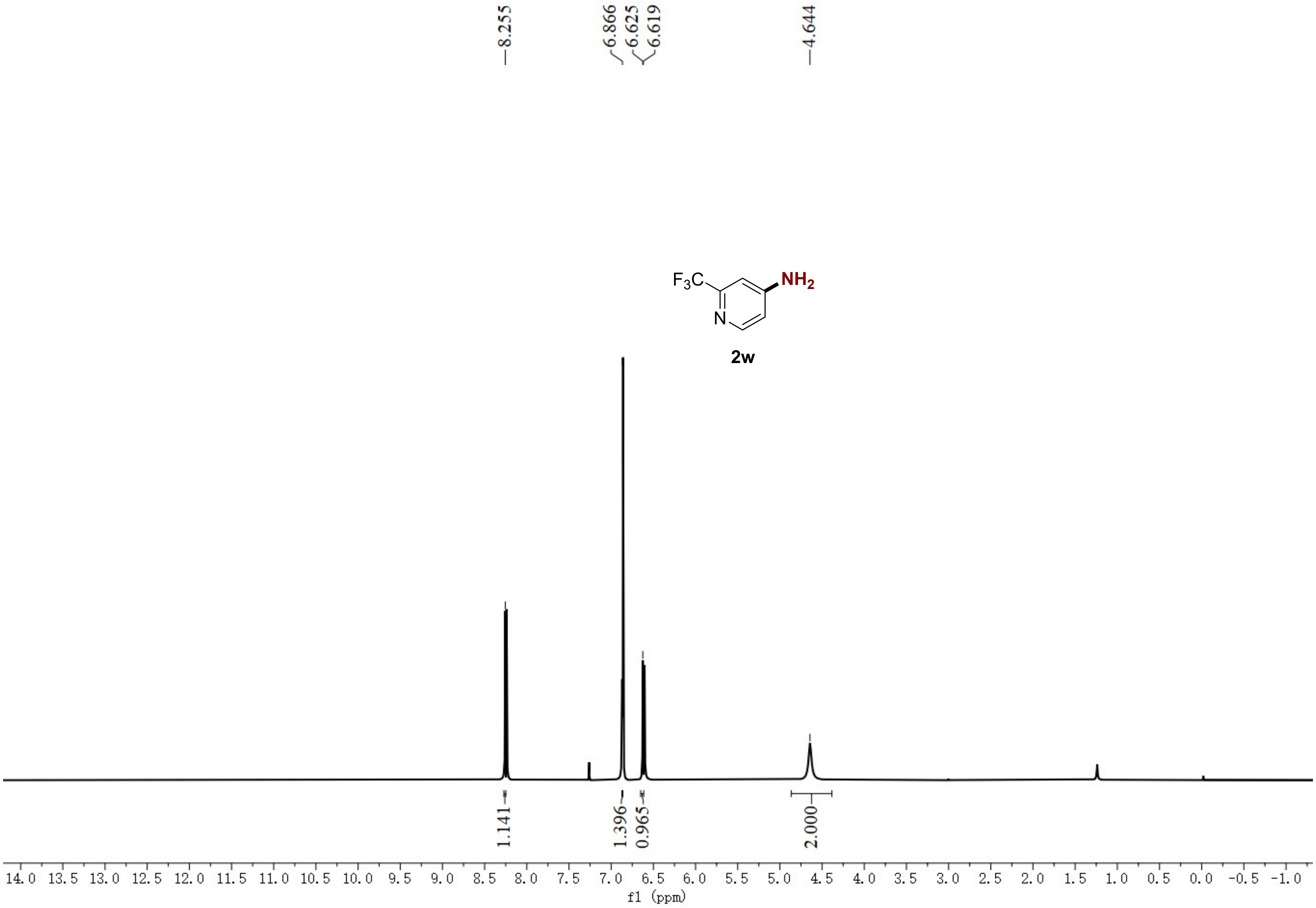


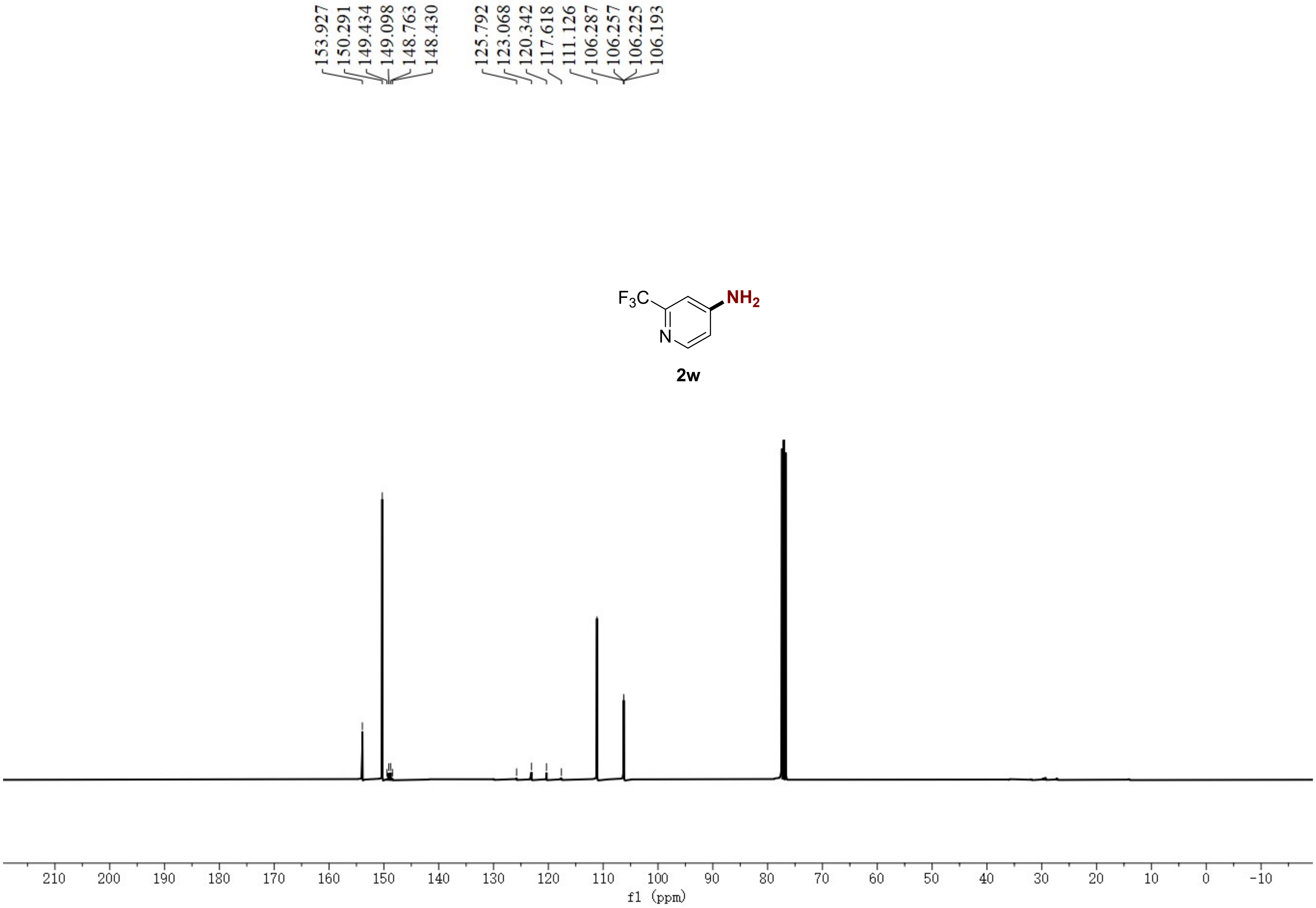
2v

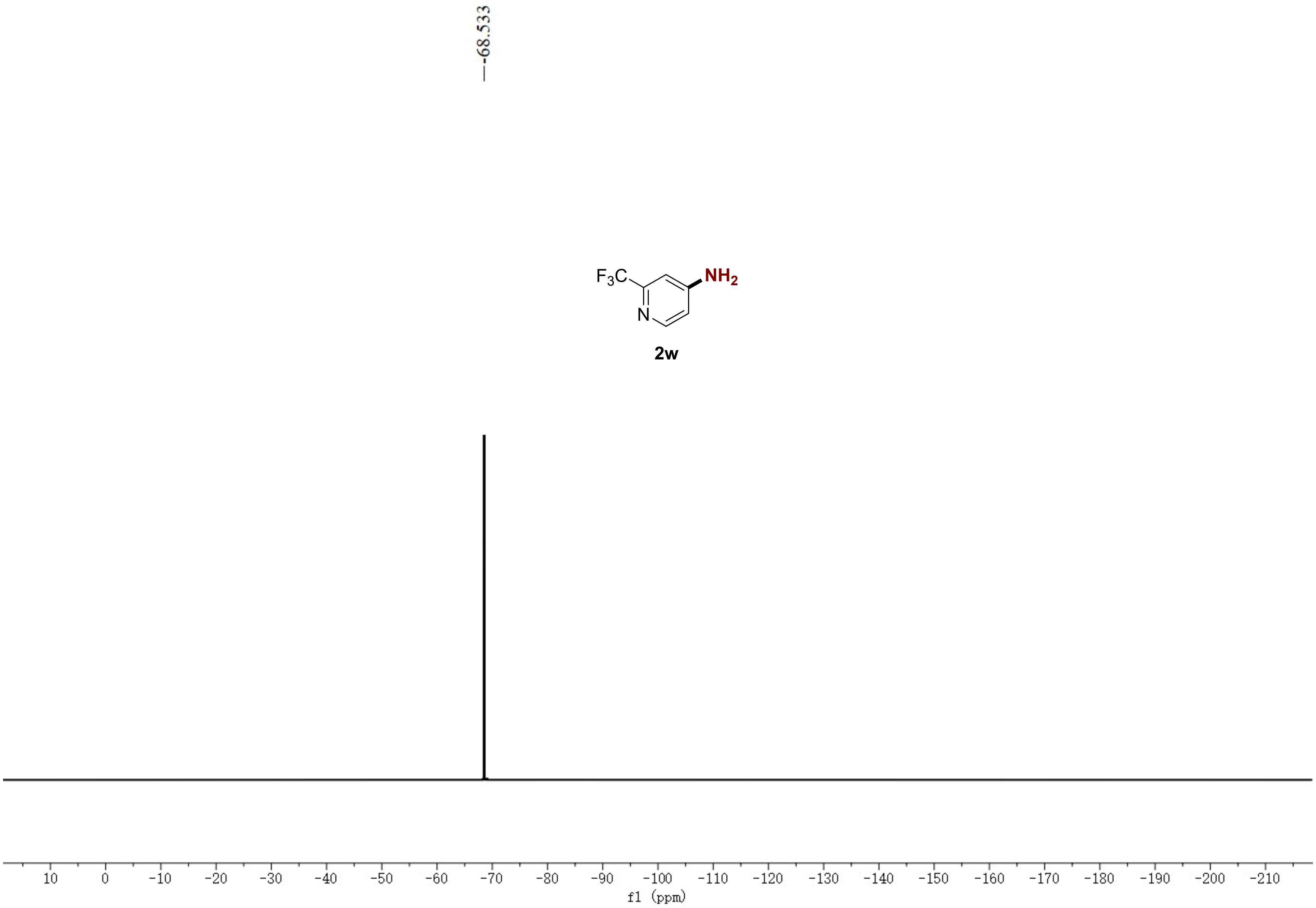
7.962
7.959
7.950
7.947
6.446
6.442
6.434
6.430
5.950
NH2
N
1.979
2.020
2.000
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

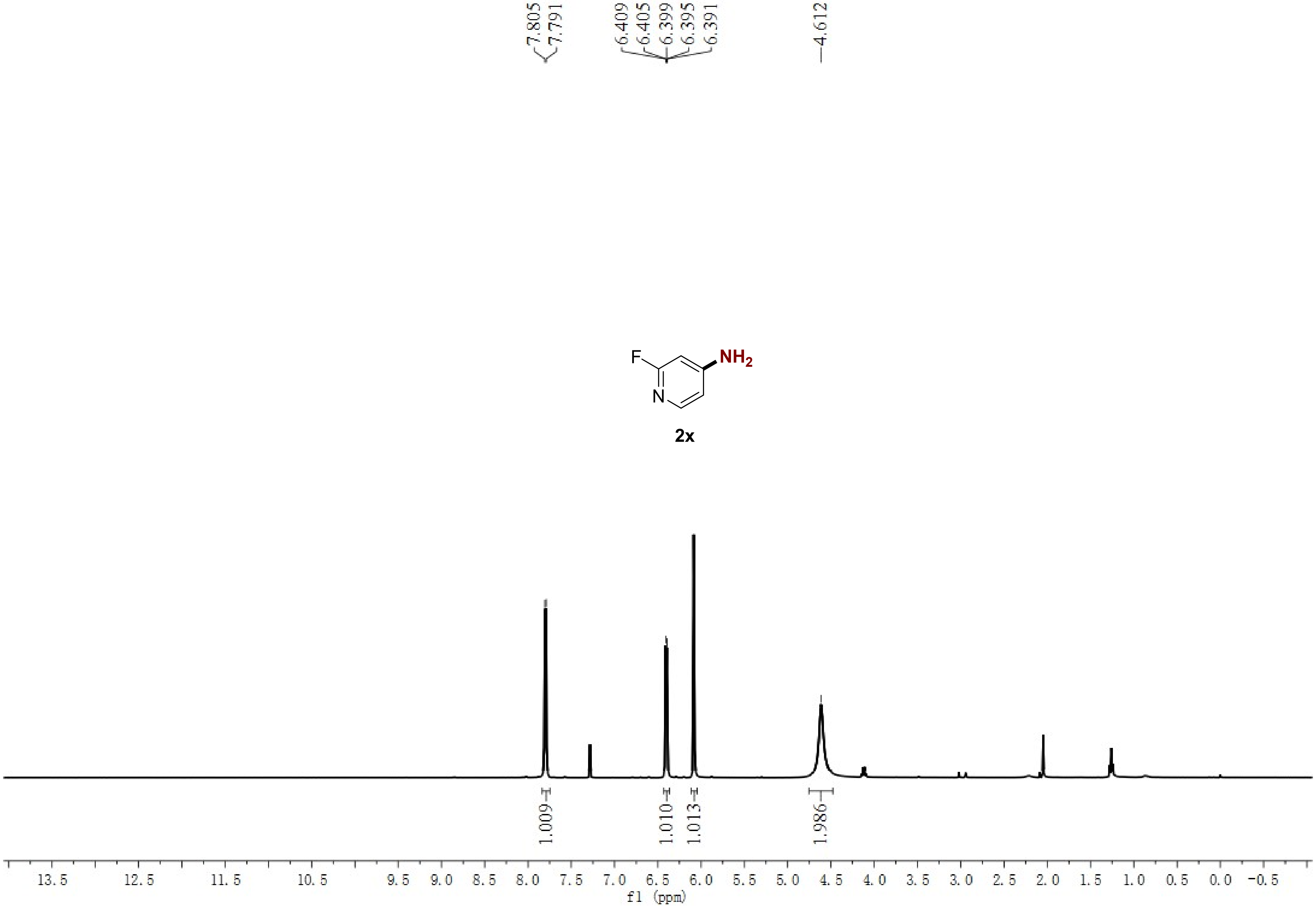

154.646
149.950
109.293
NH2
N
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

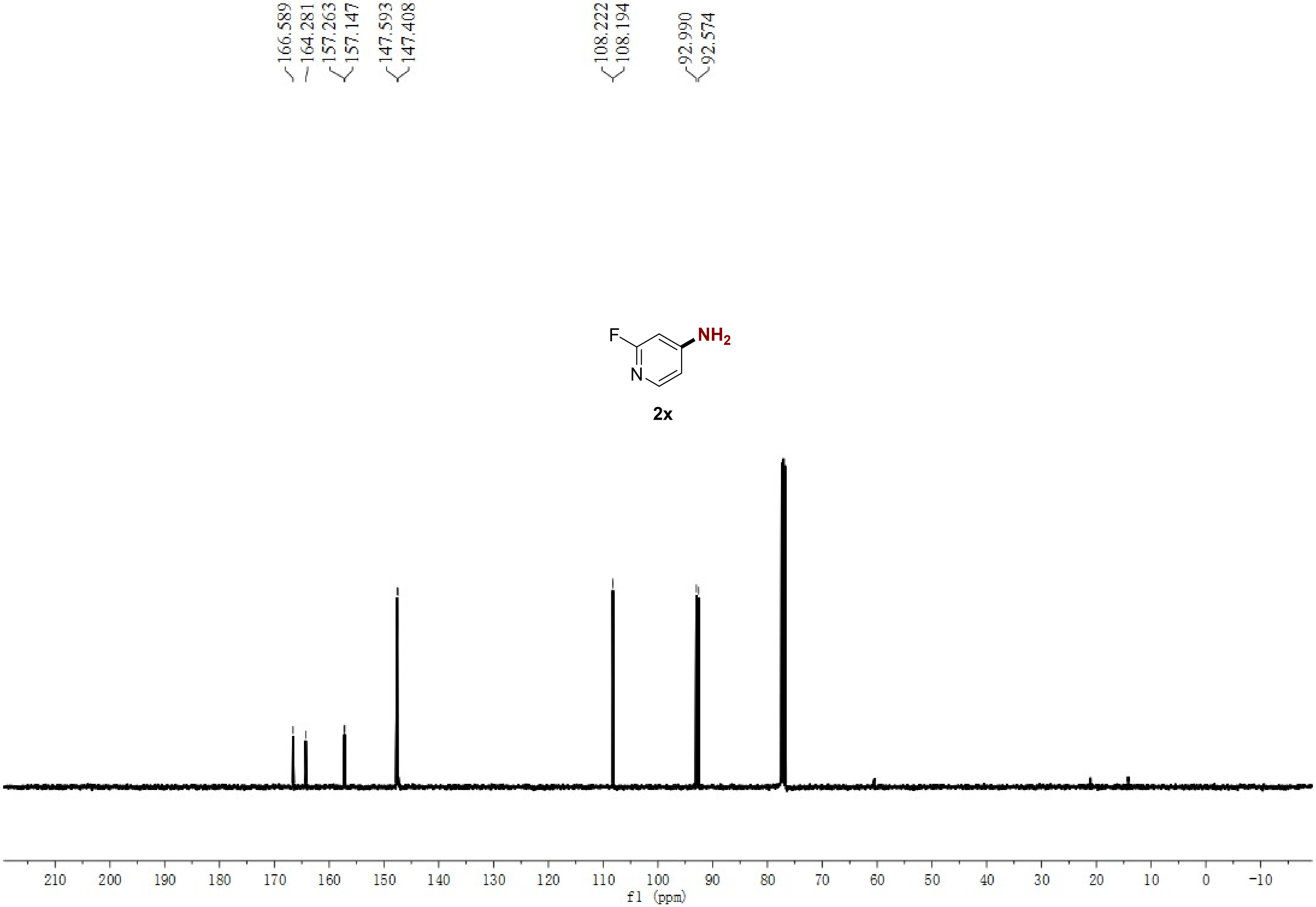
2v

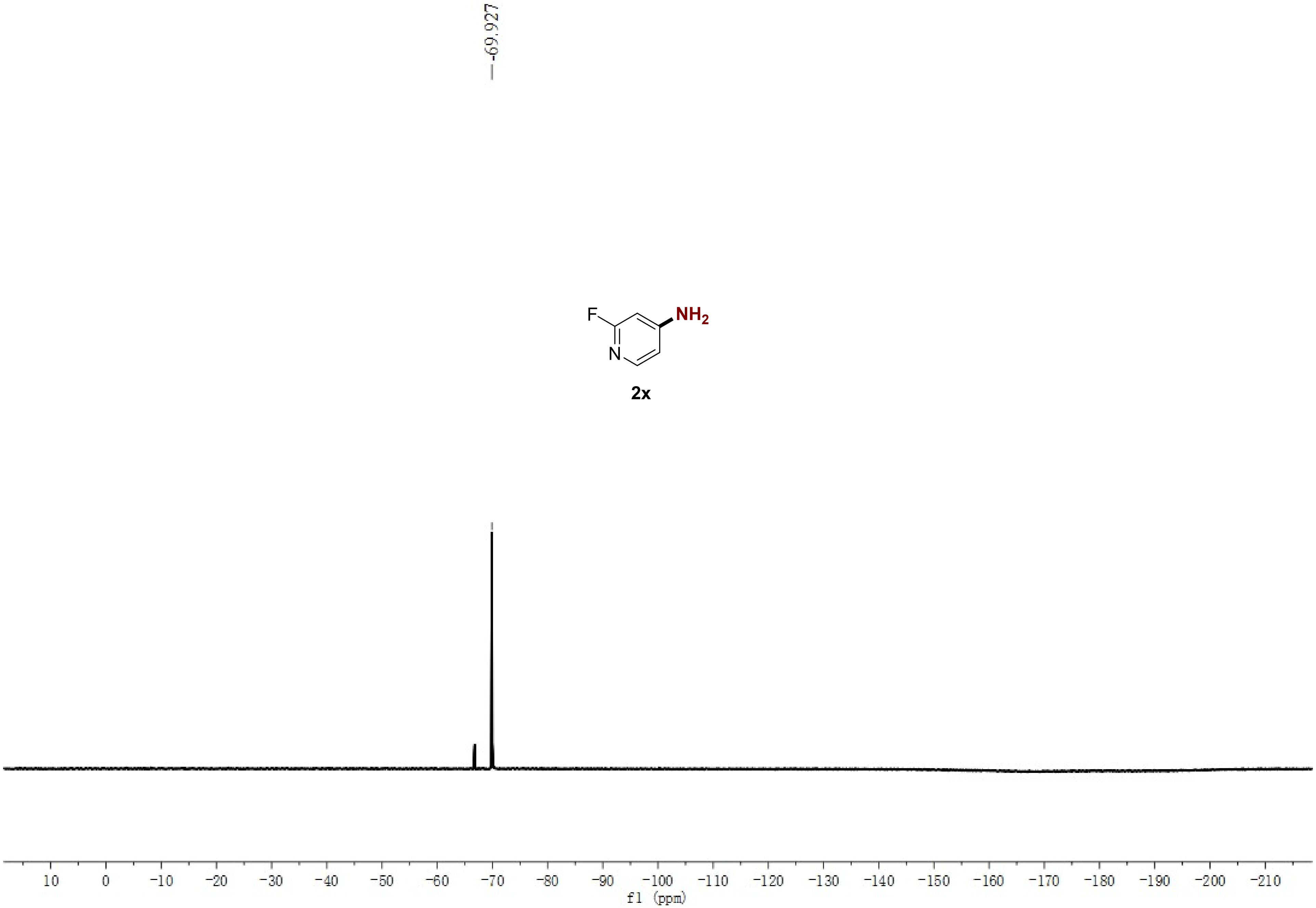

2w
8.255
6.866
6.625
6.619
4.644
F3C
NH2
N
1.141
1.396
0.965
2.000
14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

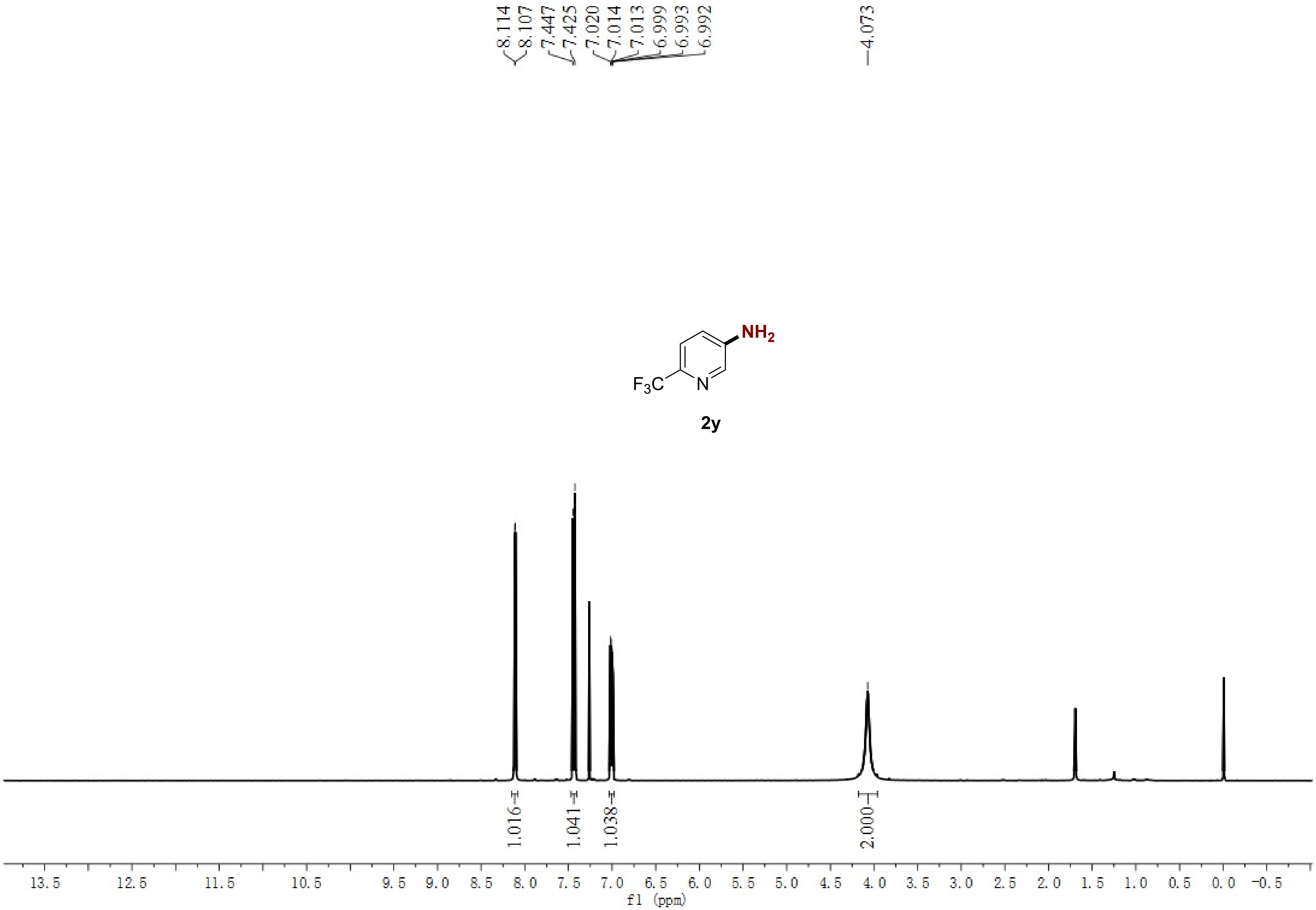

153.927
150.291
149.434
149.098
148.763
148.430
125.792
123.068
120.342
117.618
111.126
106.287
106.257
106.225
106.193
F3C
NH2
N
2w
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


-68.533
F3C
NH2
N
2w
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)

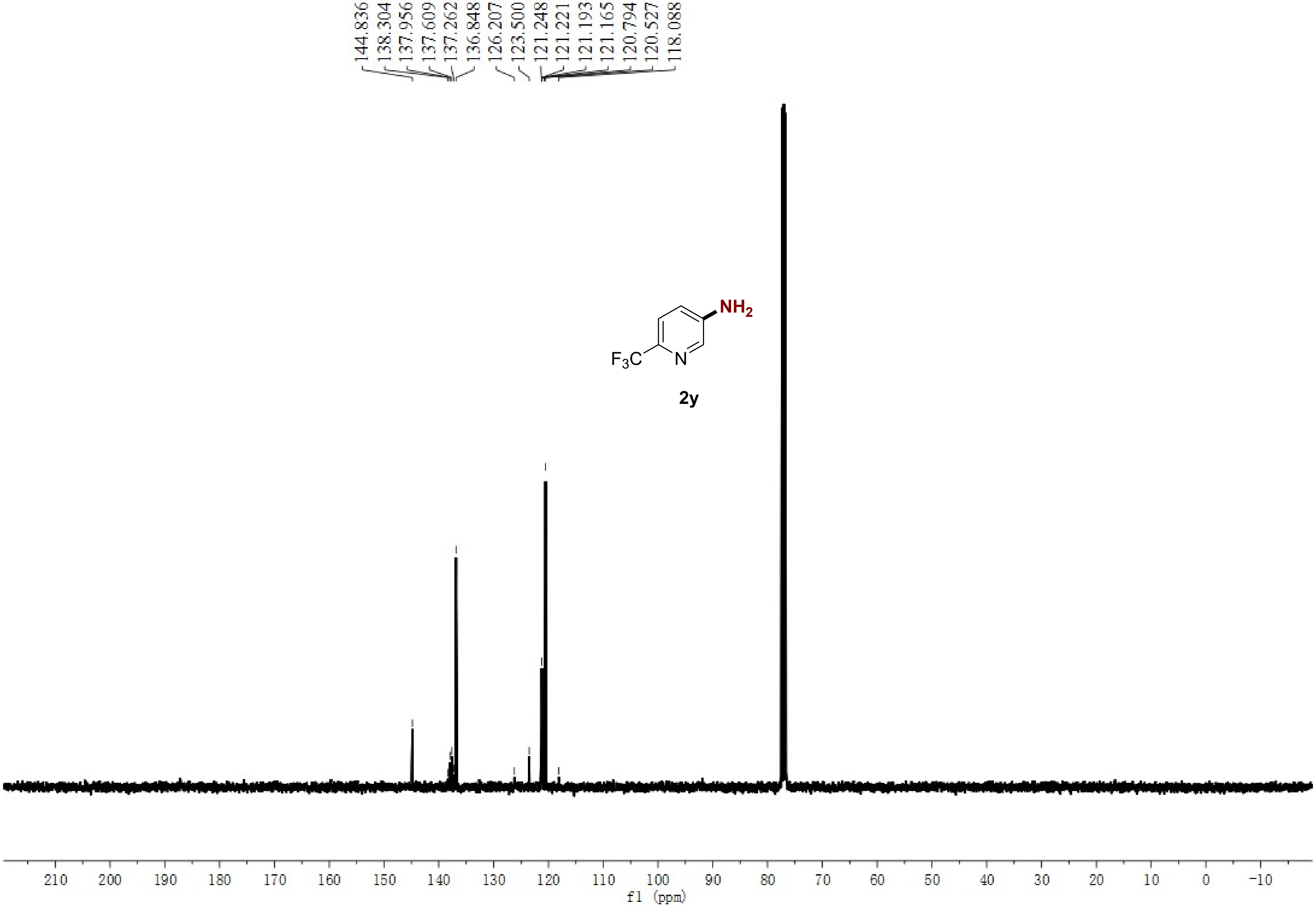

7.805
7.791
6.409
6.405
6.399
6.395
6.391
4.612
F
N
NH2
2x
1.009
1.010
1.013
1.986
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


166.589
164.281
157.263
157.147
147.593
147.408
108.222
108.194
92.990
92.574
F
NH$_2$
N
2x
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)

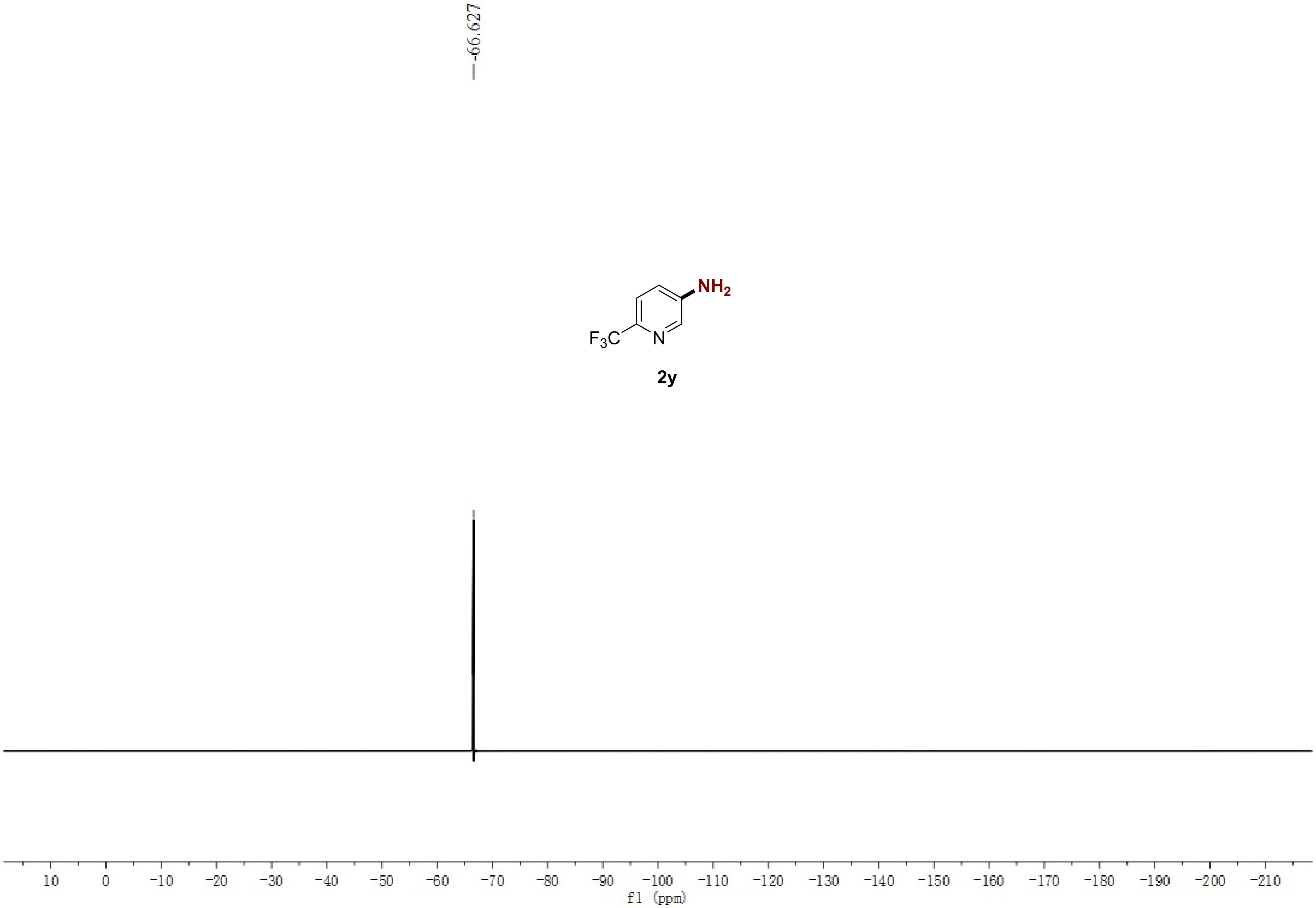

-69.927
F
N
NH2
2x
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

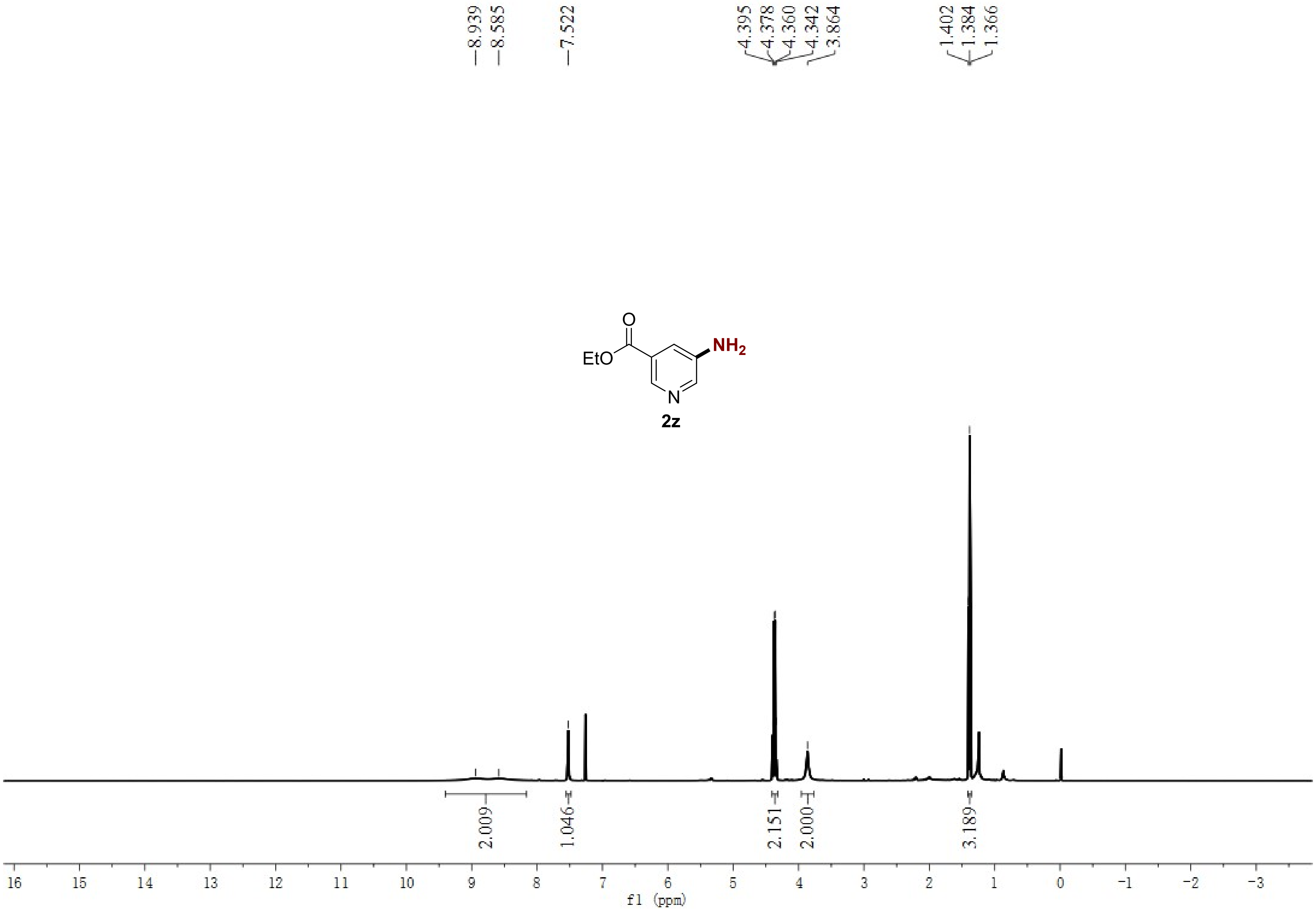

8.114
8.107
7.447
7.425
7.020
7.014
7.013
6.999
6.993
6.992
4.073
NH2
F3C
N
1.016
1.041
1.038
2.000
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
f1 (ppm)

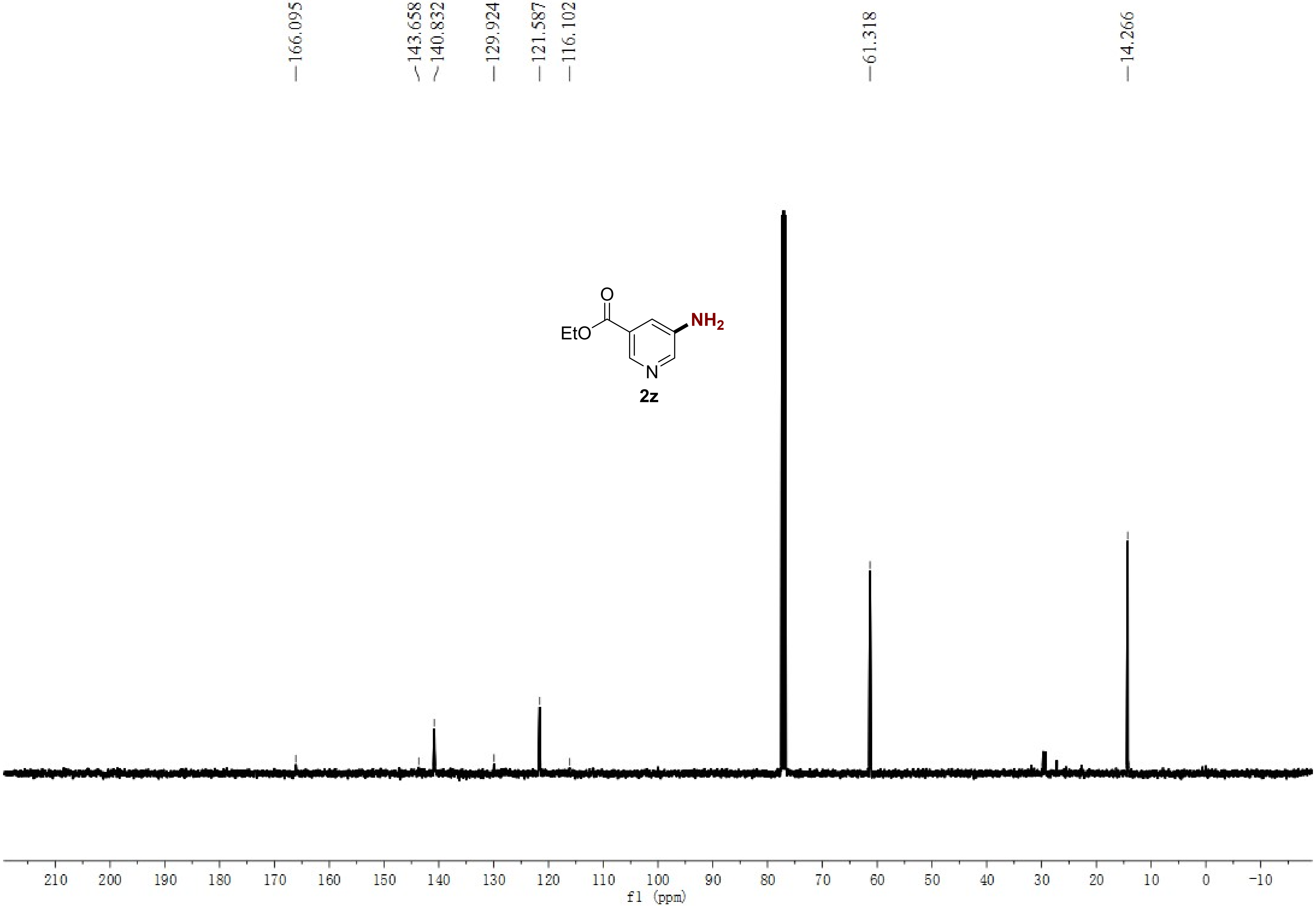
2y

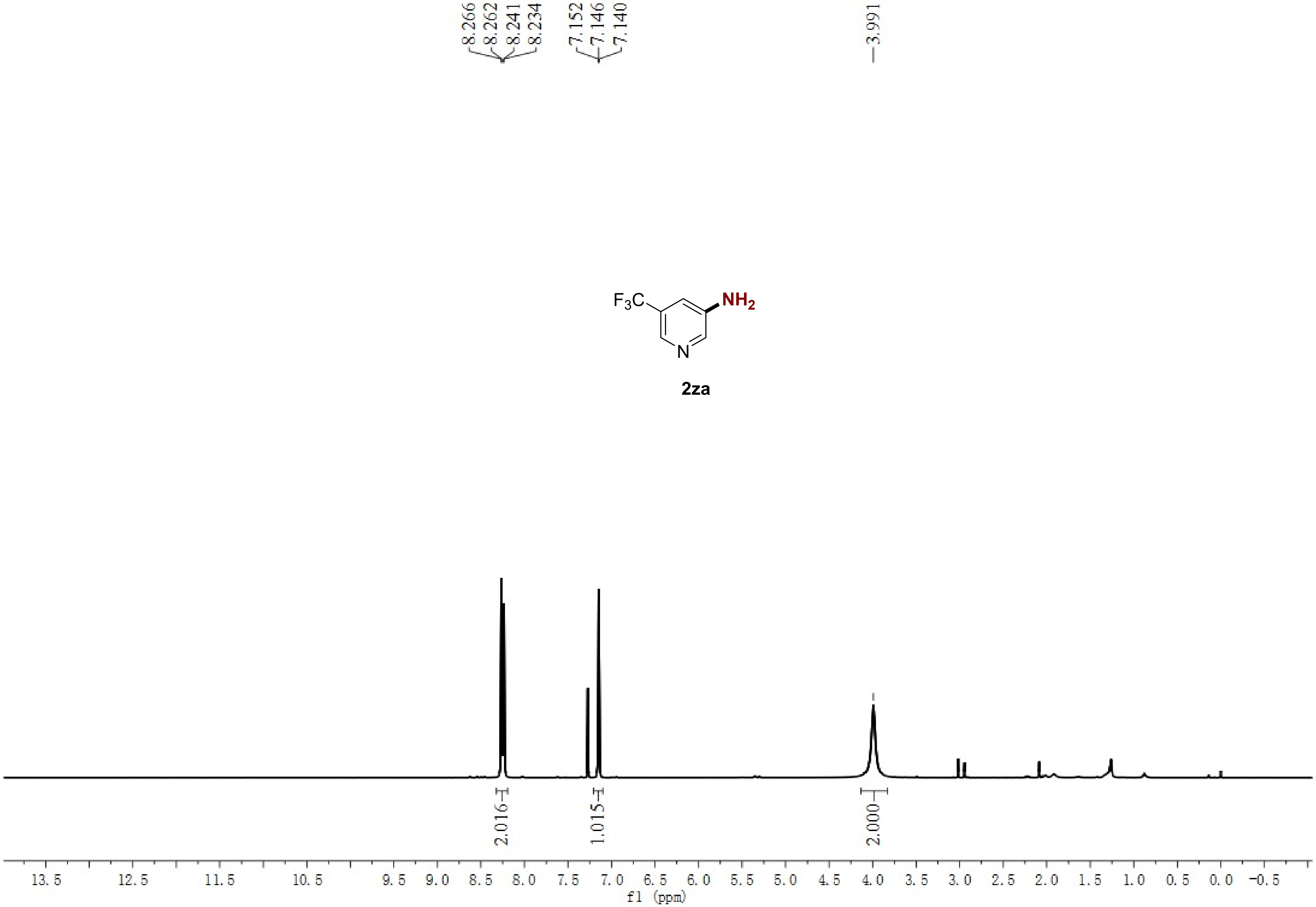

144.836
138.304
137.956
137.609
137.262
136.848
126.207
123.500
121.248
121.221
121.193
121.165
120.794
120.527
118.088
NH2
F3C
N
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

2y

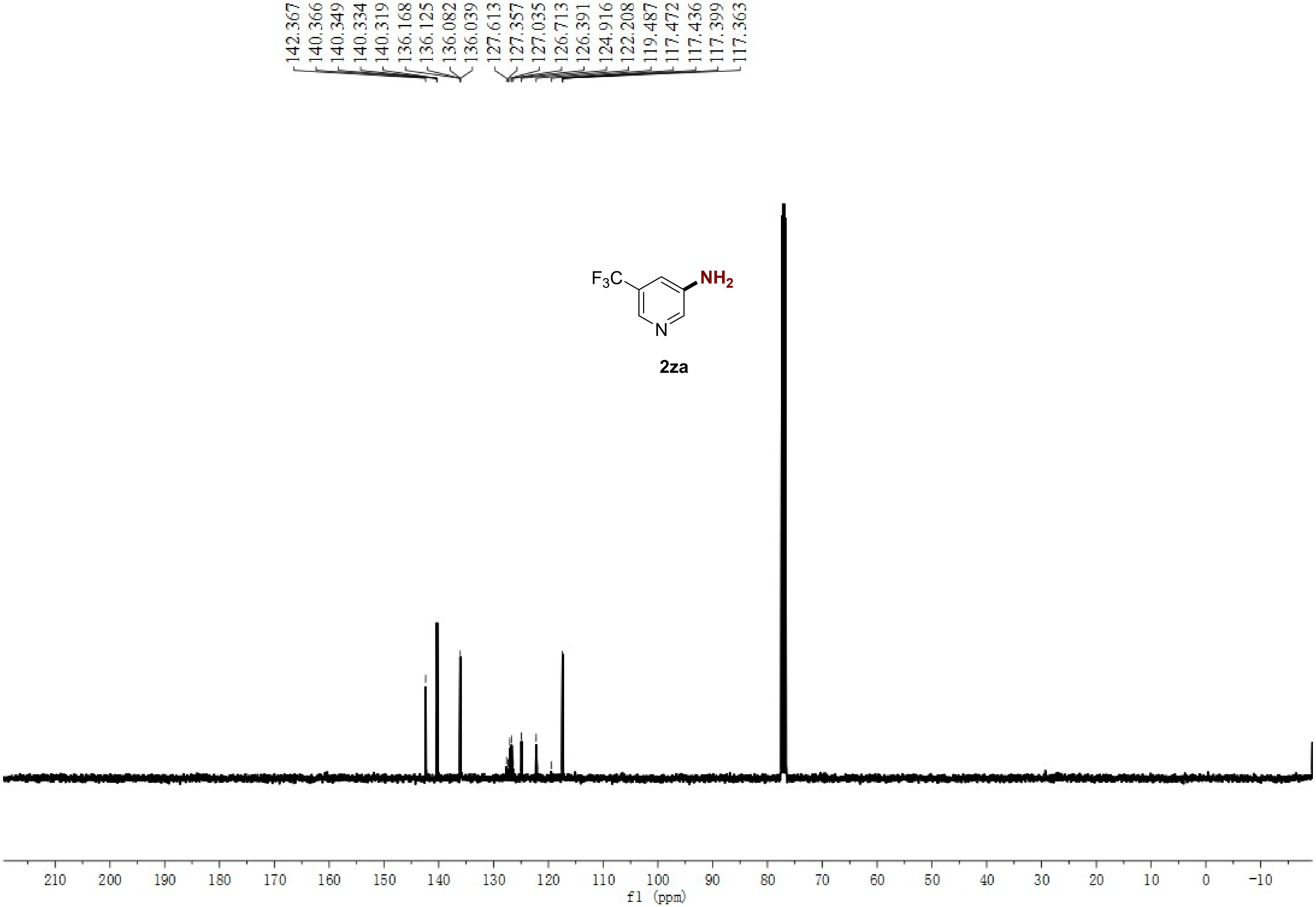

-66.627
NH2
F3C
N
2y
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

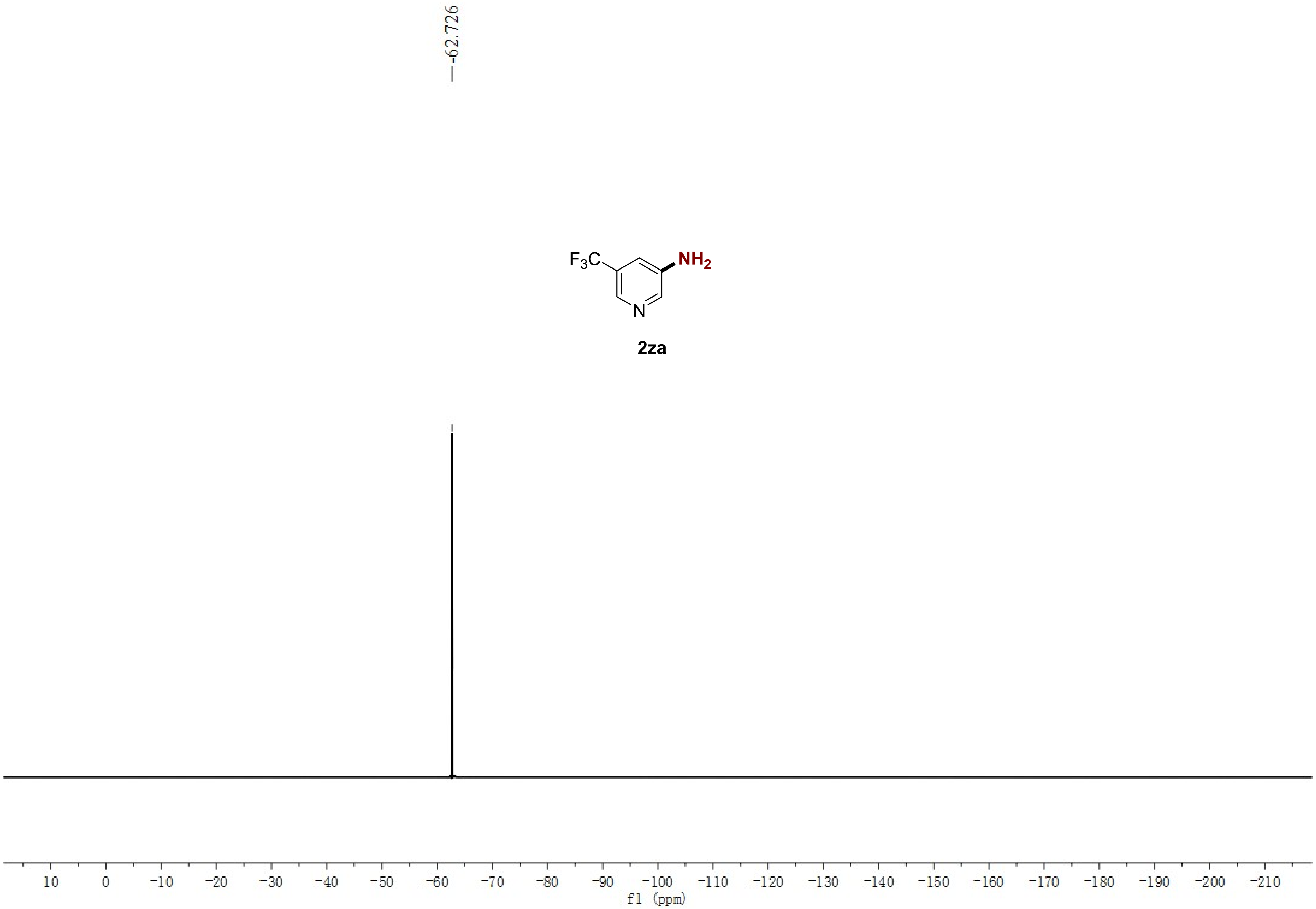

8.939
8.585
7.522
4.395
4.378
4.360
4.342
3.864
1.402
1.384
1.366
O
EtO
NH2
N
2z
2.009
1.046
2.151
2.000
3.189
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)


166.095
143.658
140.832
129.924
121.587
116.102
61.318
14.266
O
EtO
NH2
N
2z
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)

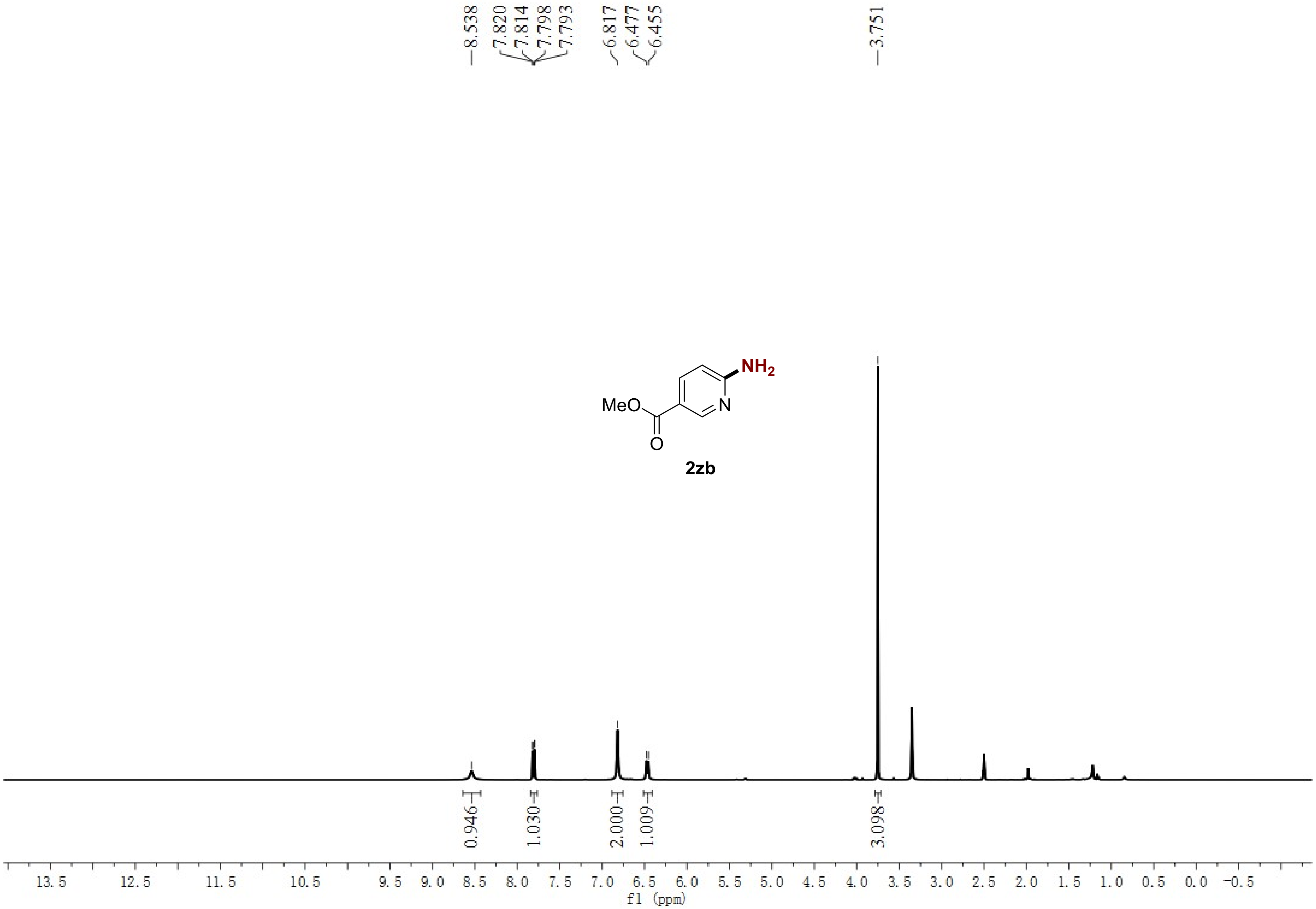

8.266
8.262
8.241
8.234
7.152
7.146
7.140
3.991
F3C
NH2
N
2.016
1.015
2.000
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

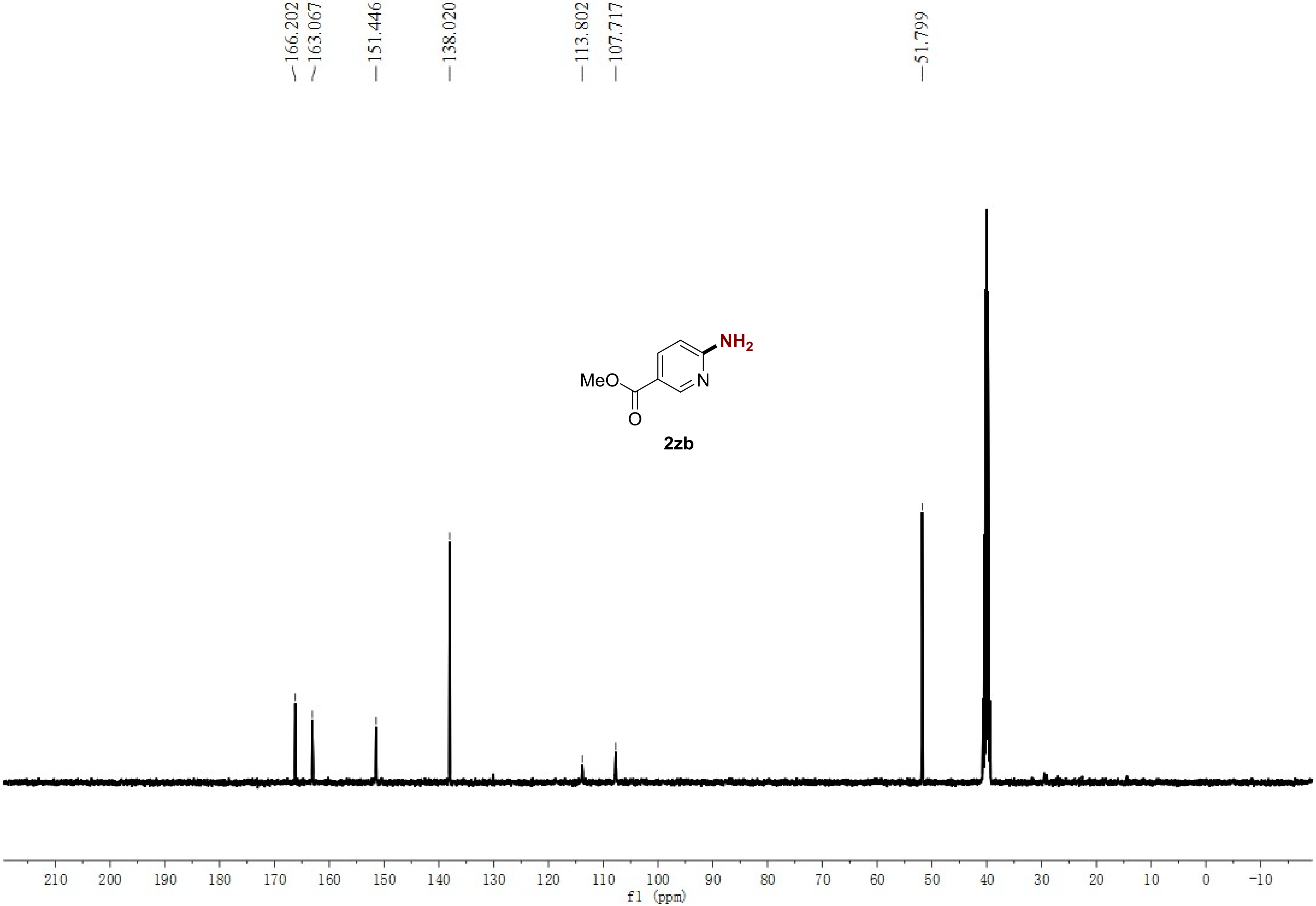
2za

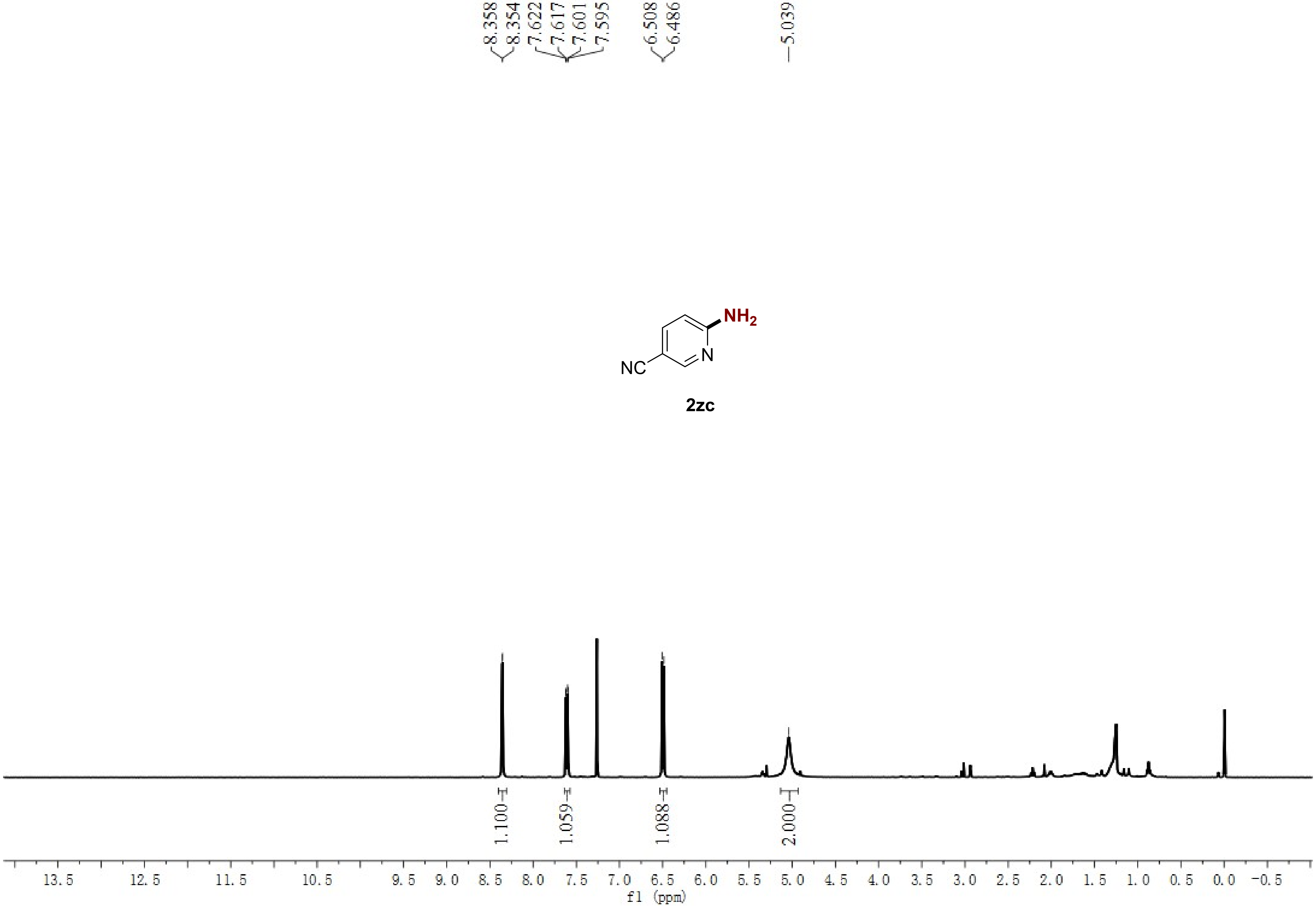

142.367
140.366
140.349
140.334
140.319
136.168
136.125
136.082
136.039
127.613
127.357
127.035
126.713
126.391
124.916
122.208
119.487
117.472
117.436
117.399
117.363
F_3C
NH_2
N
2za
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


-62.726
F3C
NH2
N
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)

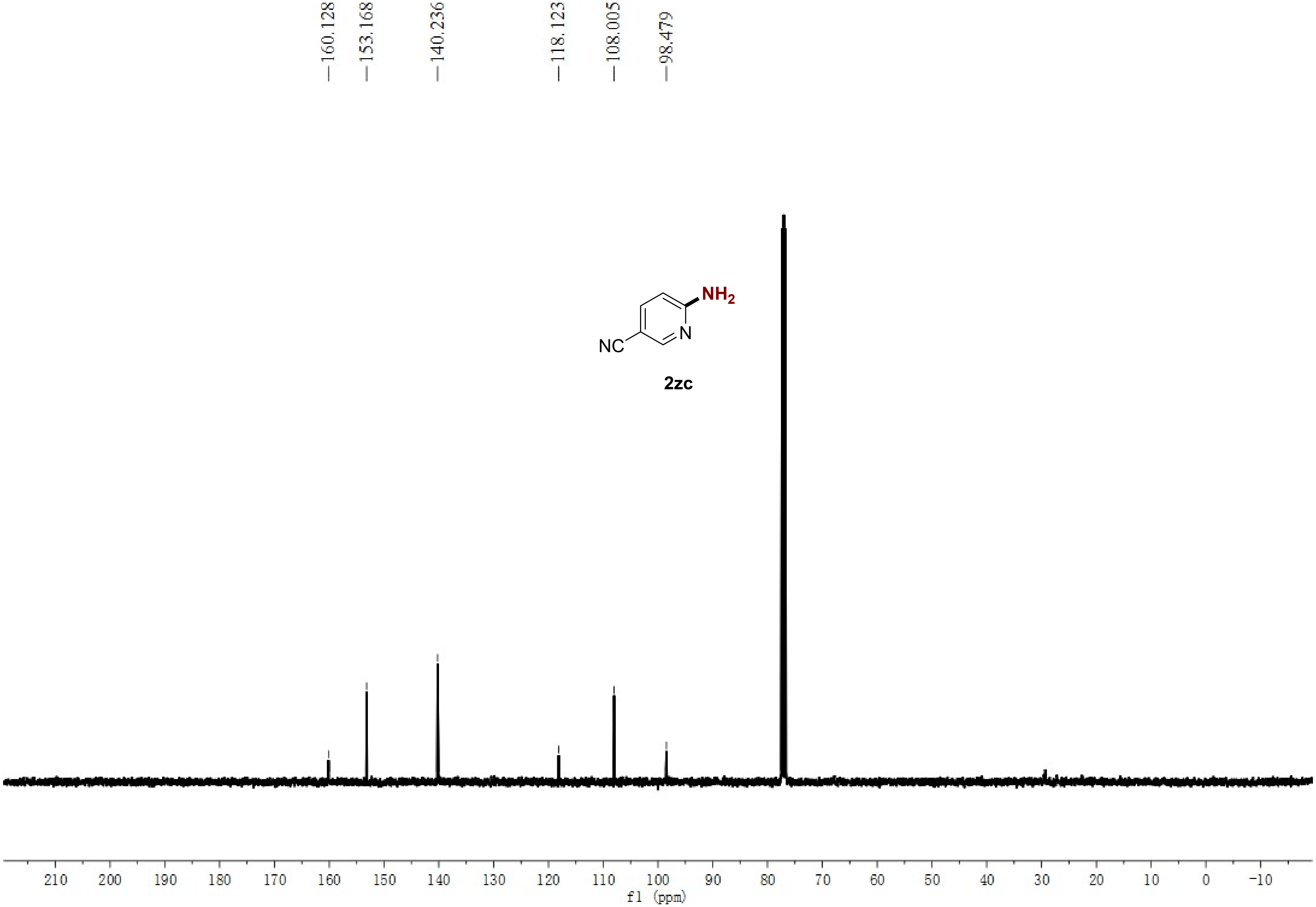
2za

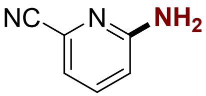

8.538
7.820
7.814
7.798
7.793
6.817
6.477
6.455
3.751
MeO
O
N
NH2
2zb
0.946
1.030
2.000
1.009
3.098
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


166.202
163.067
151.446
138.020
113.802
107.717
51.799
MeO
O
N
NH2
2zb
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)

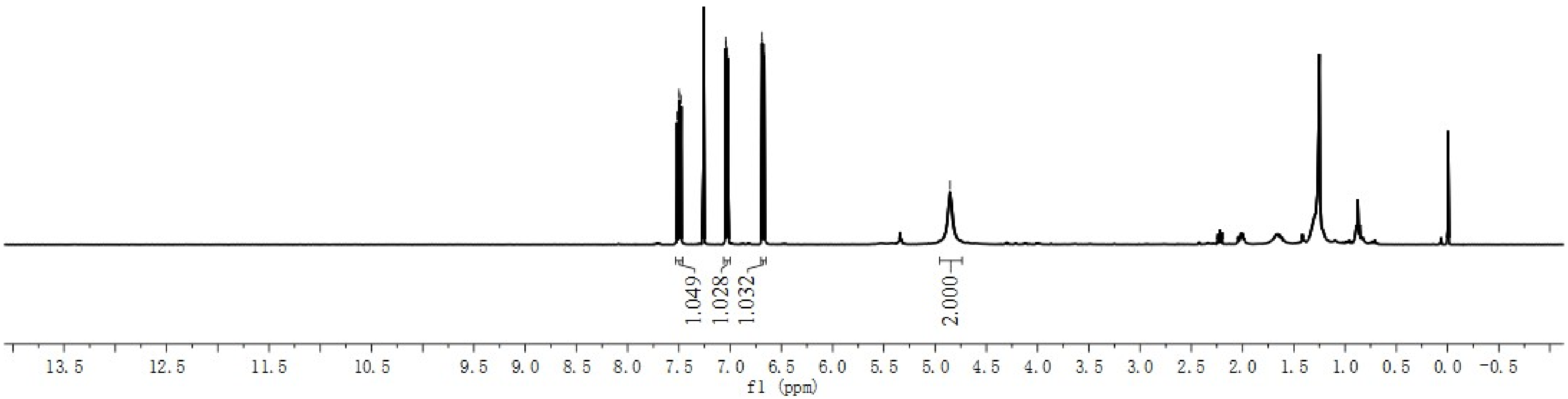

8.358
8.354
7.622
7.617
7.601
7.595
6.508
6.486
5.039
NH2
N
NC
1.100
1.059
1.088
2.000
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

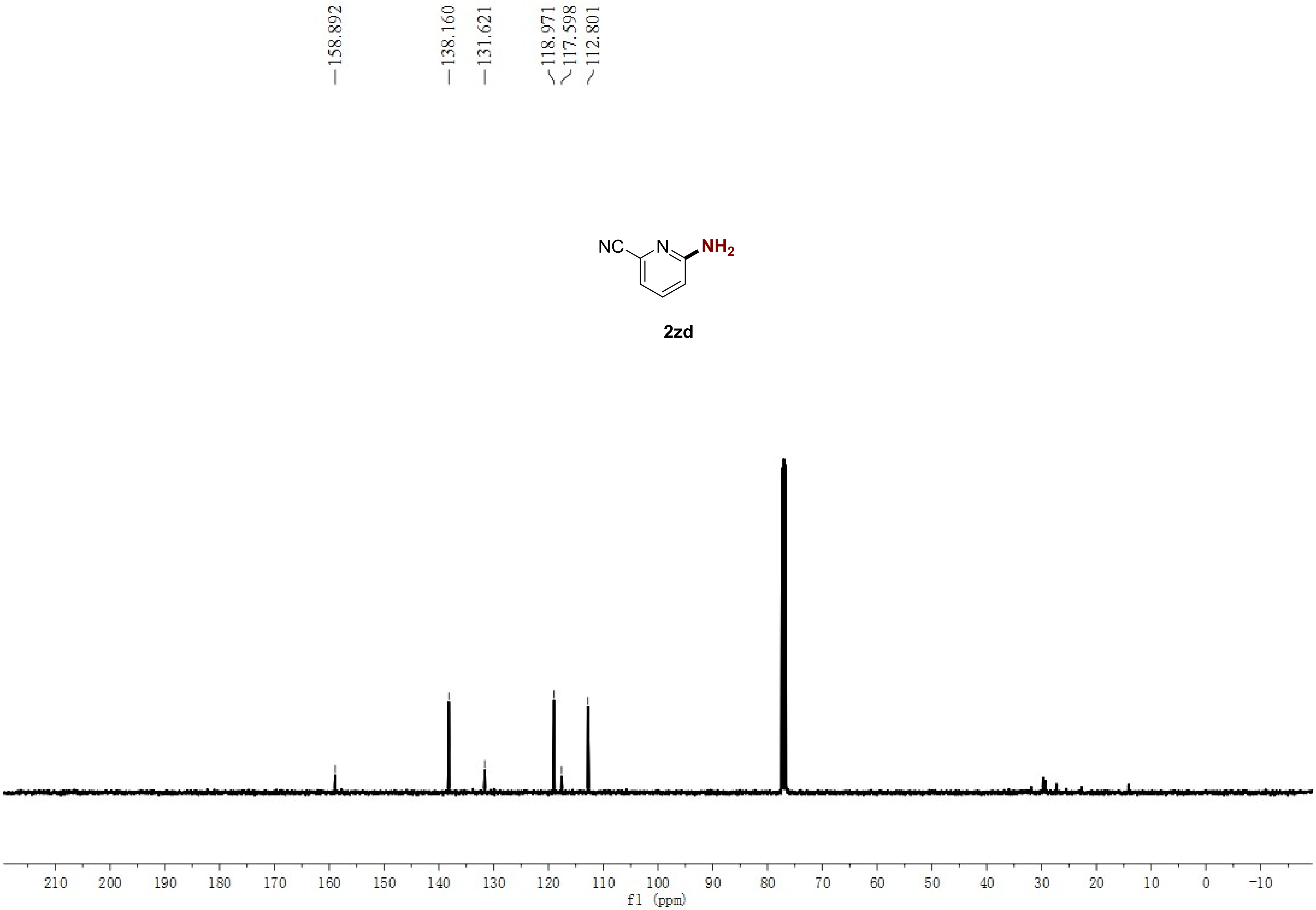
2zc


160.128
153.168
140.236
118.123
108.005
98.479
NH2
N
NC
2zc
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)



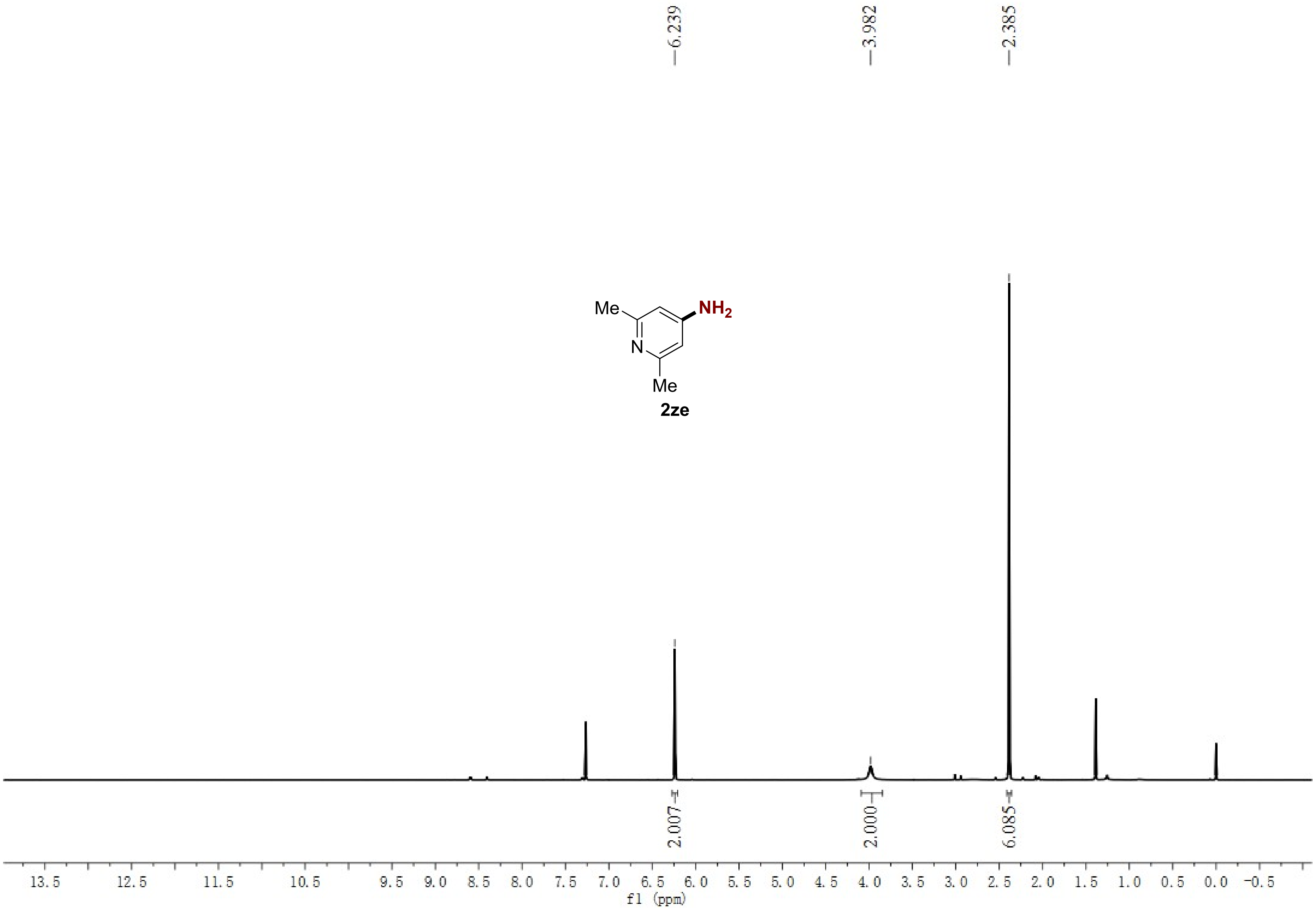
2zd


7.517
7.499
7.496
7.478
7.044
7.042
7.026
7.024
6.689
6.687
6.668
6.666
4.853
1.049
1.028
1.032
2.000
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)



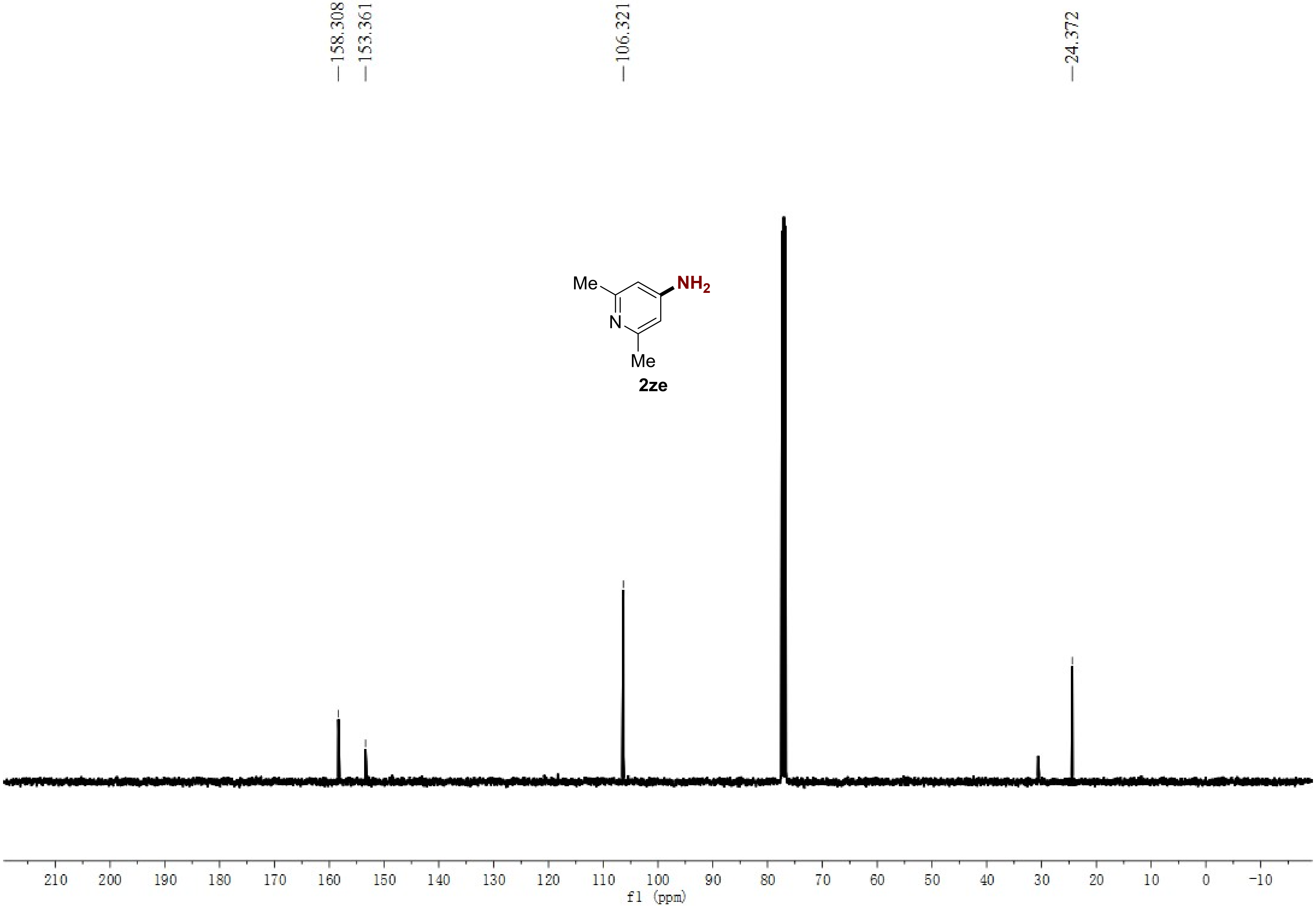
2zd

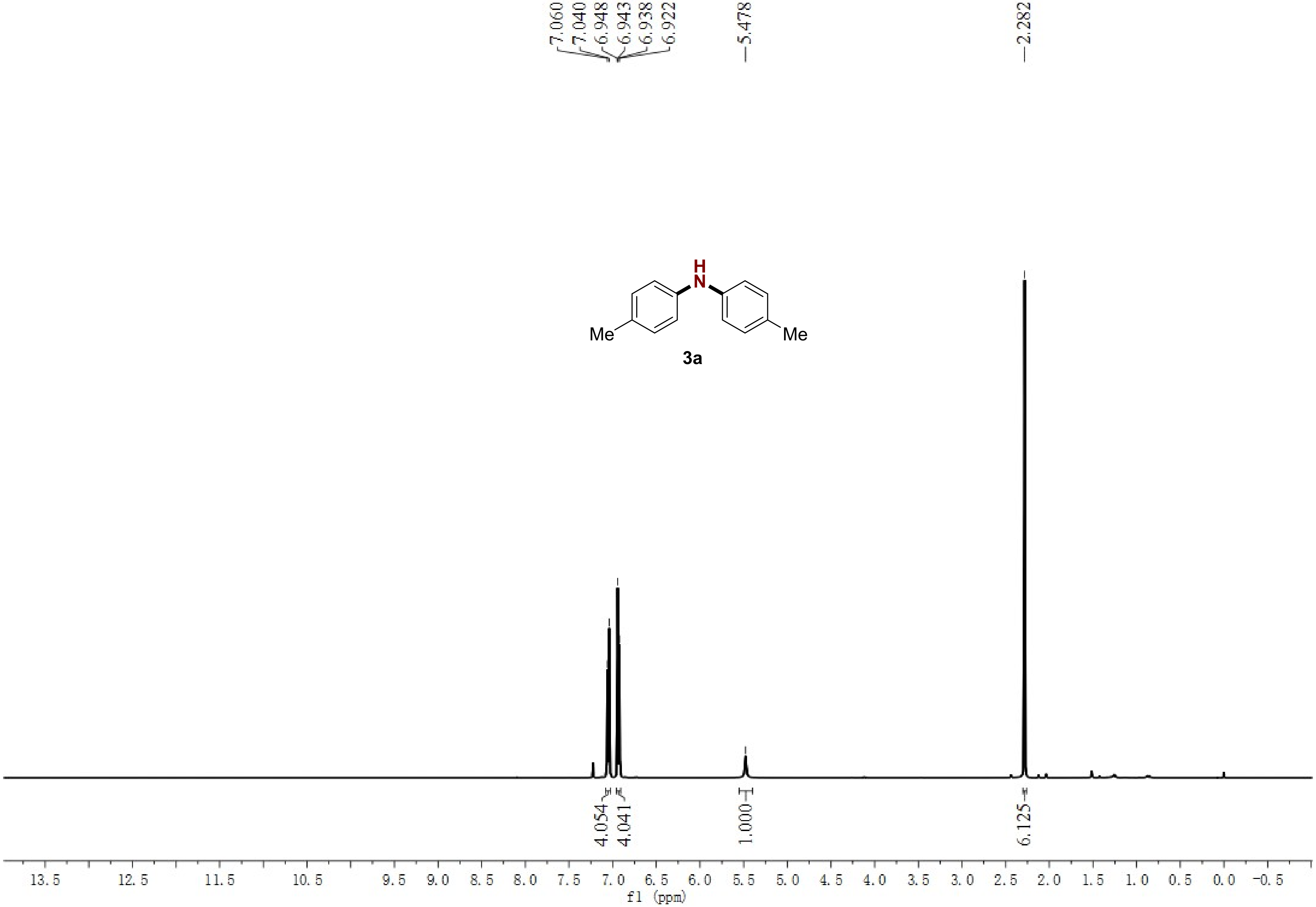
158.892
138.160
131.621
118.971
117.598
112.801
NC
N
NH2
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

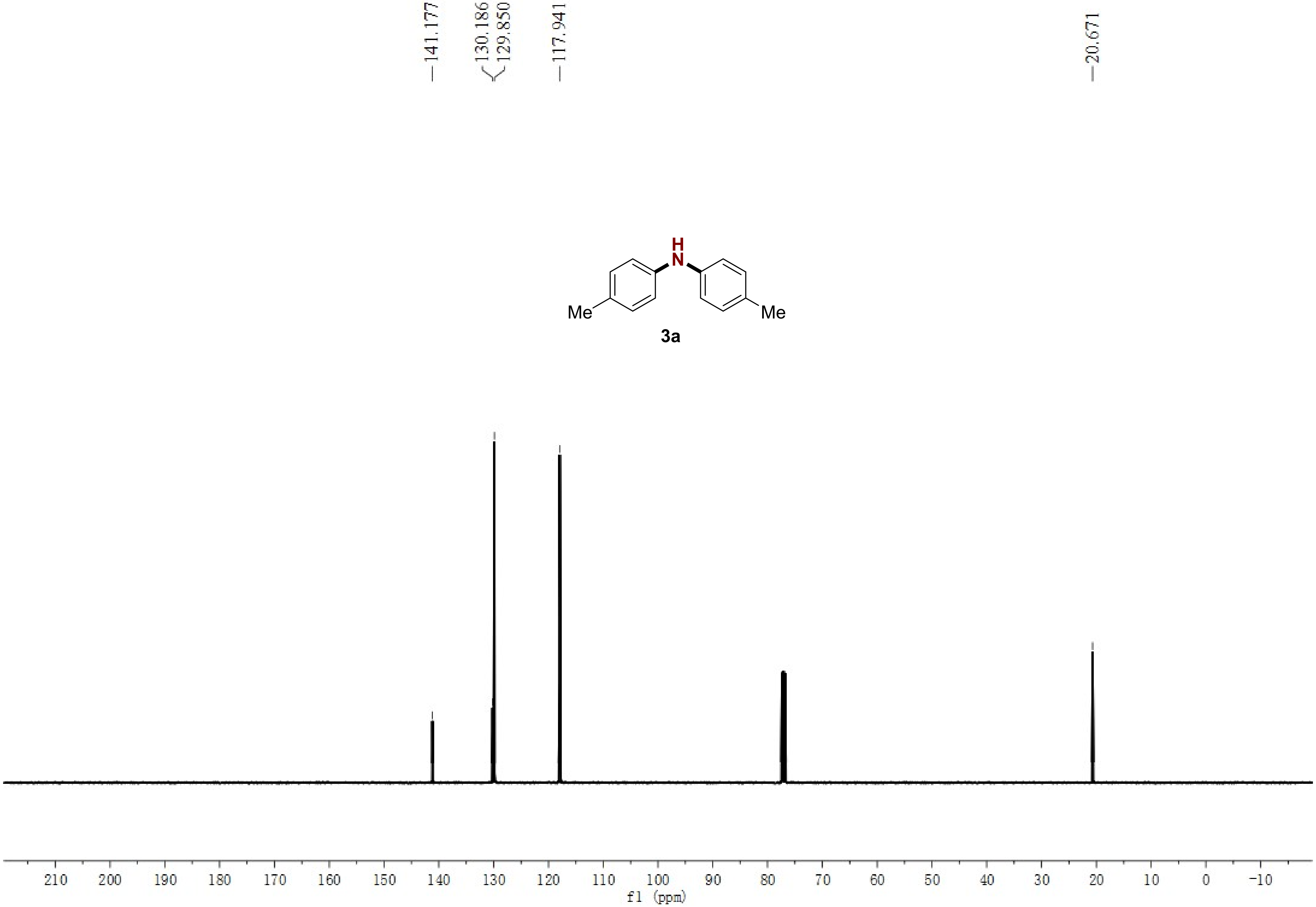


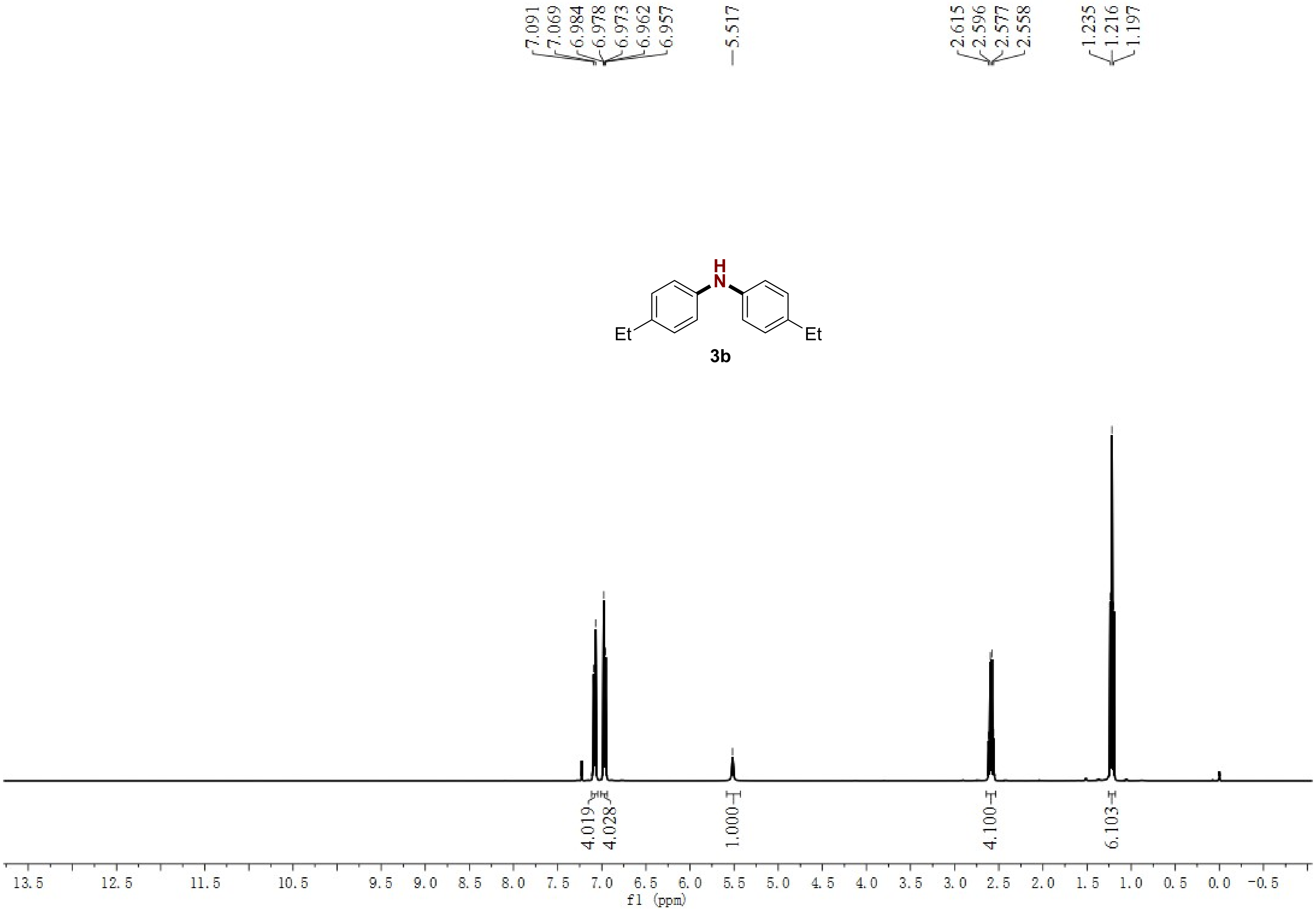
2ze

6.239
3.982
2.385
Me
NH2
N
Me
2.007
2.000
6.085
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


158.308
153.361
106.321
24.372
Me
NH2
N
Me
2ze
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)

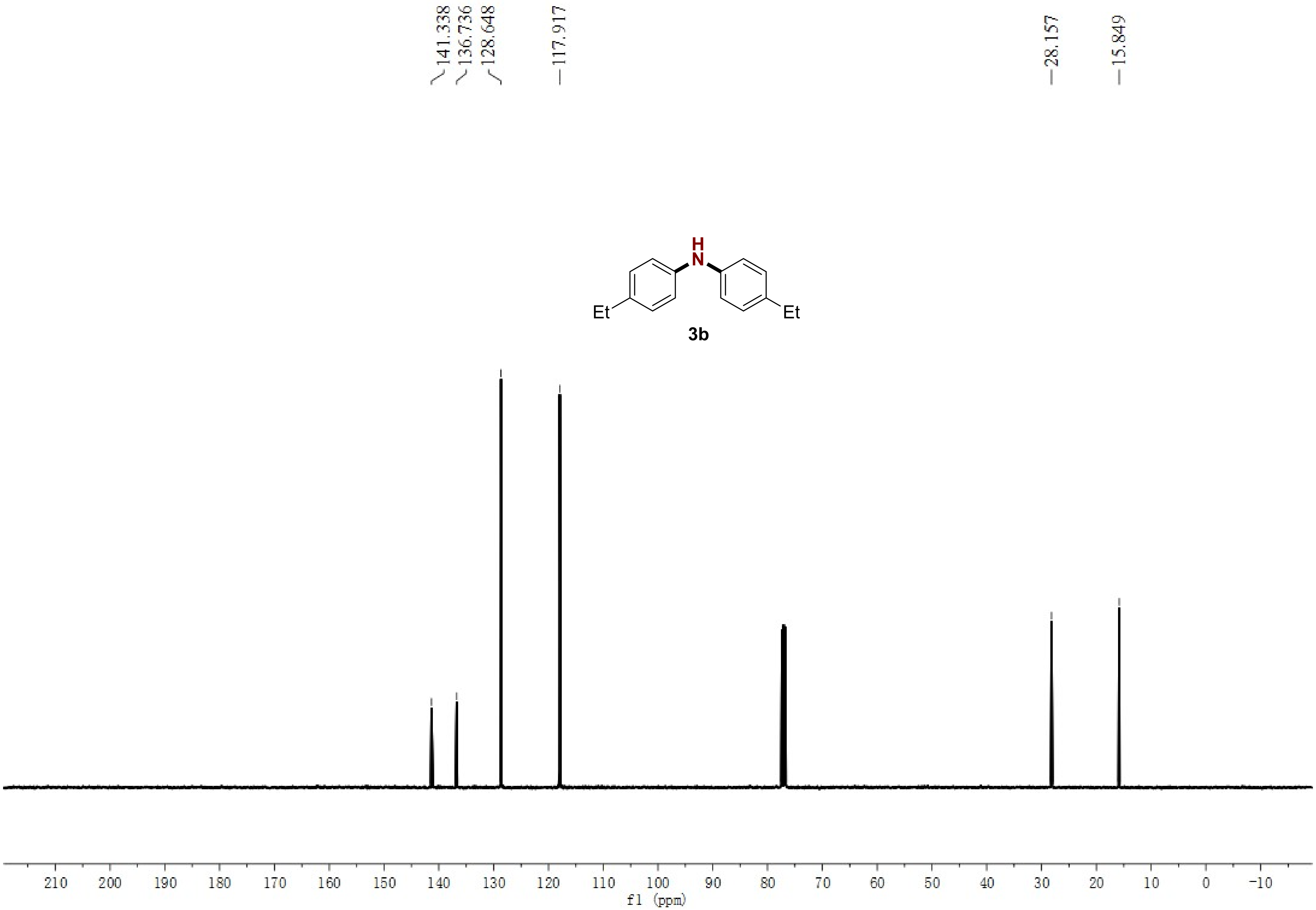

7.060
7.040
6.948
6.943
6.938
6.922
5.478
2.282
H
N
Me
Me
3a
4.054
4.041
1.000
6.125
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

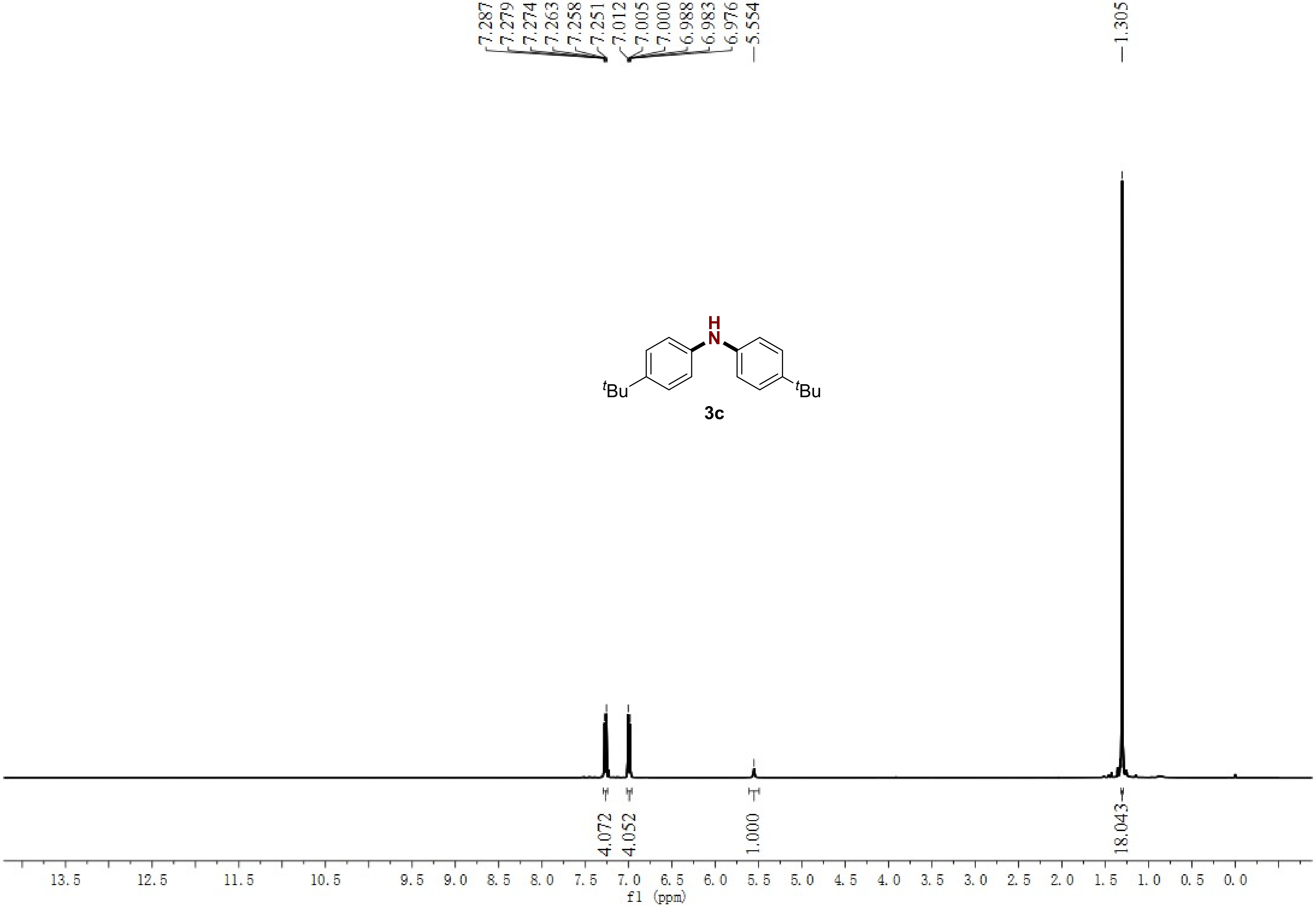

141.177
130.186
129.850
117.941
20.671
H
N
Me
Me
3a
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

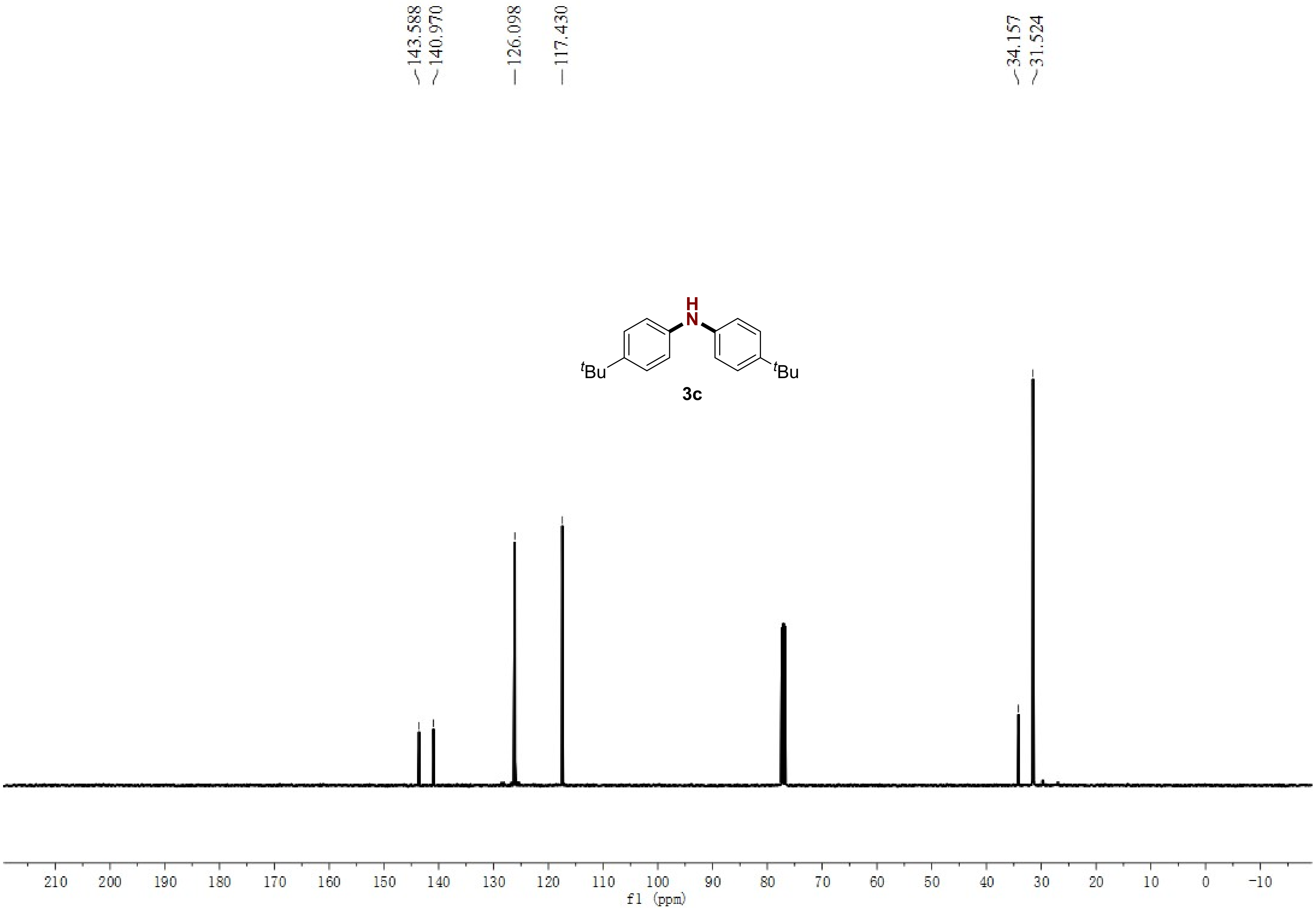


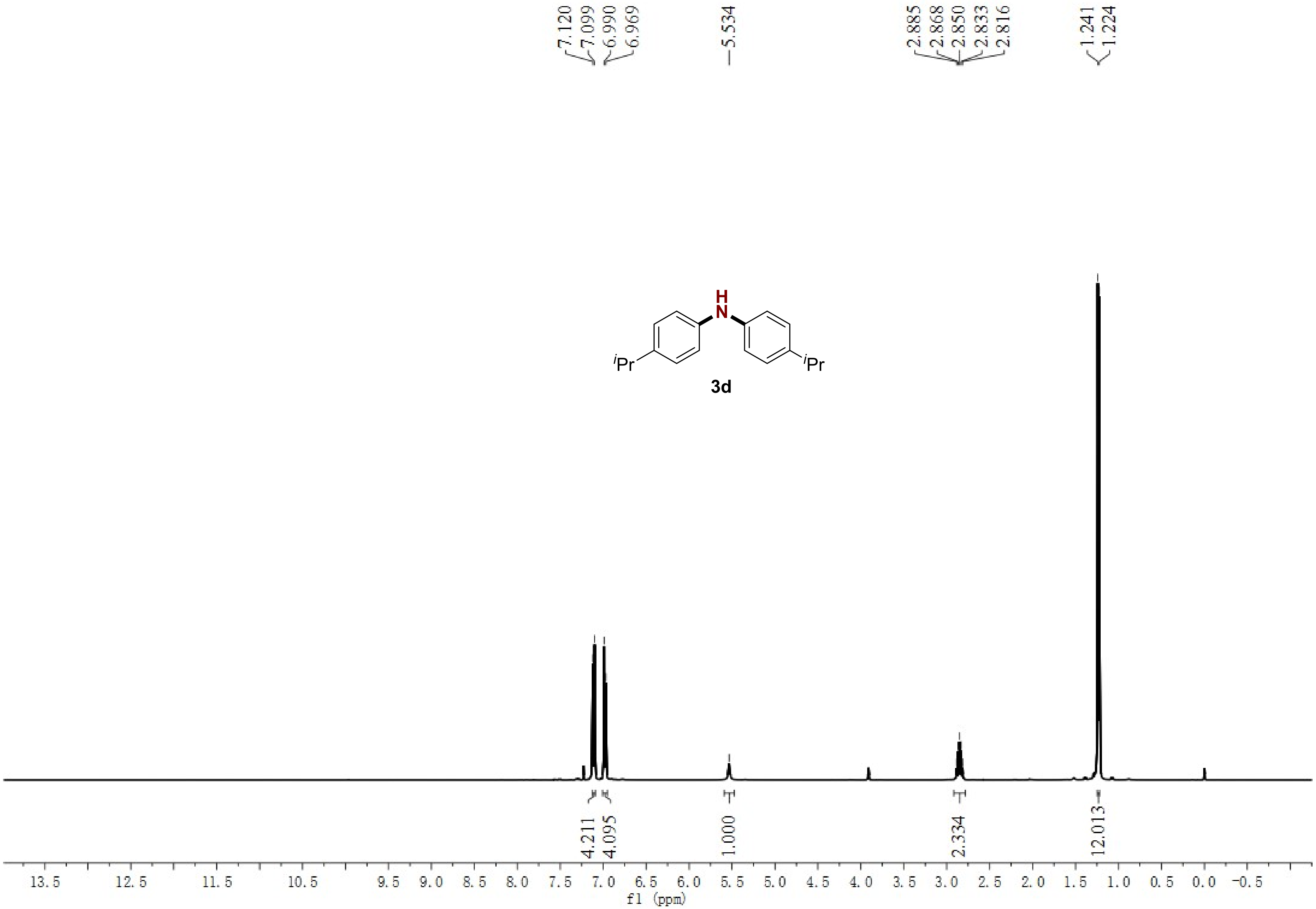
3b

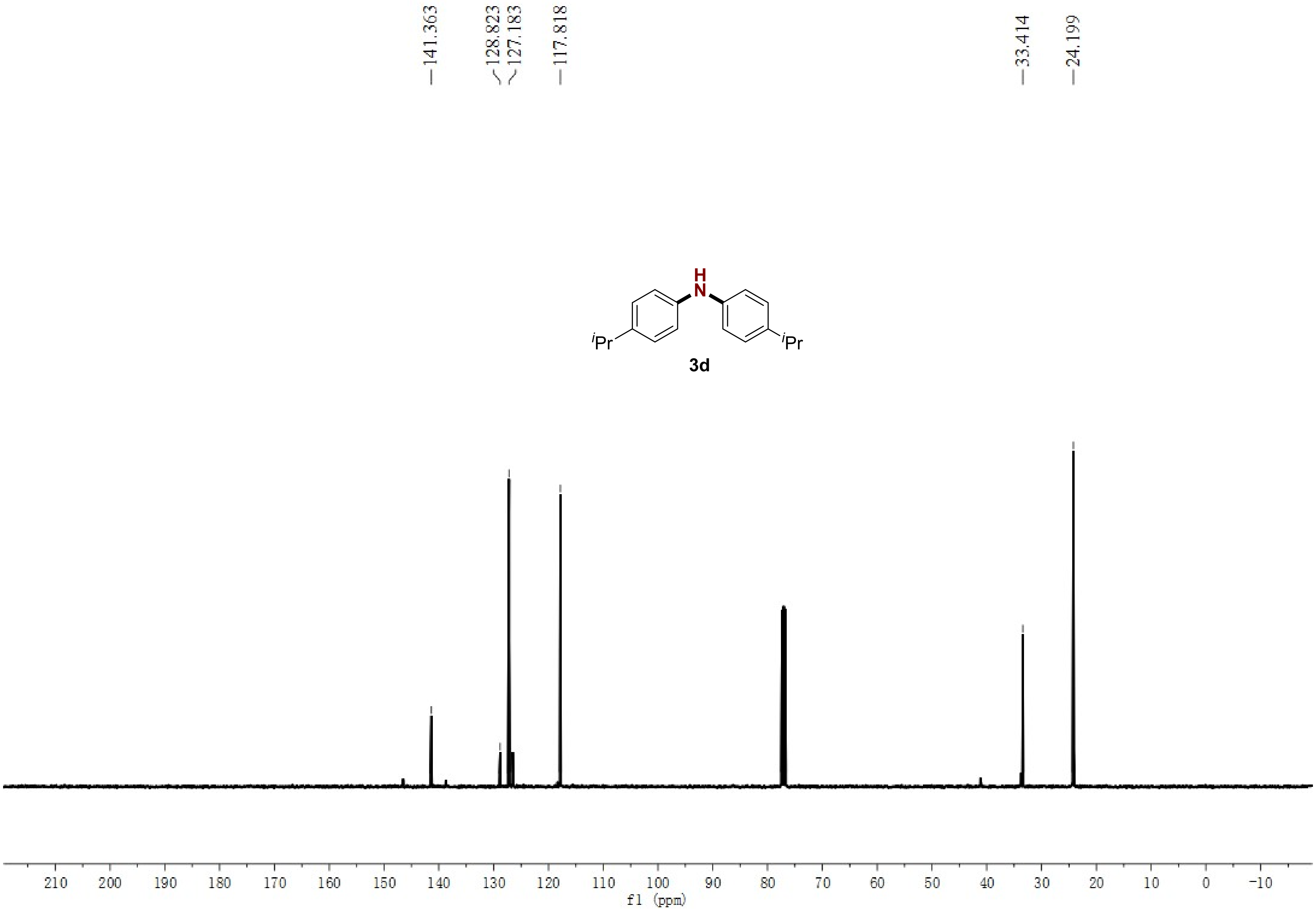
7.091
7.069
6.984
6.978
6.973
6.962
6.957
5.517
2.615
2.596
2.577
2.558
1.235
1.216
1.197
H
N
Et
Et
4.019
4.028
1.000
4.100
6.103
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

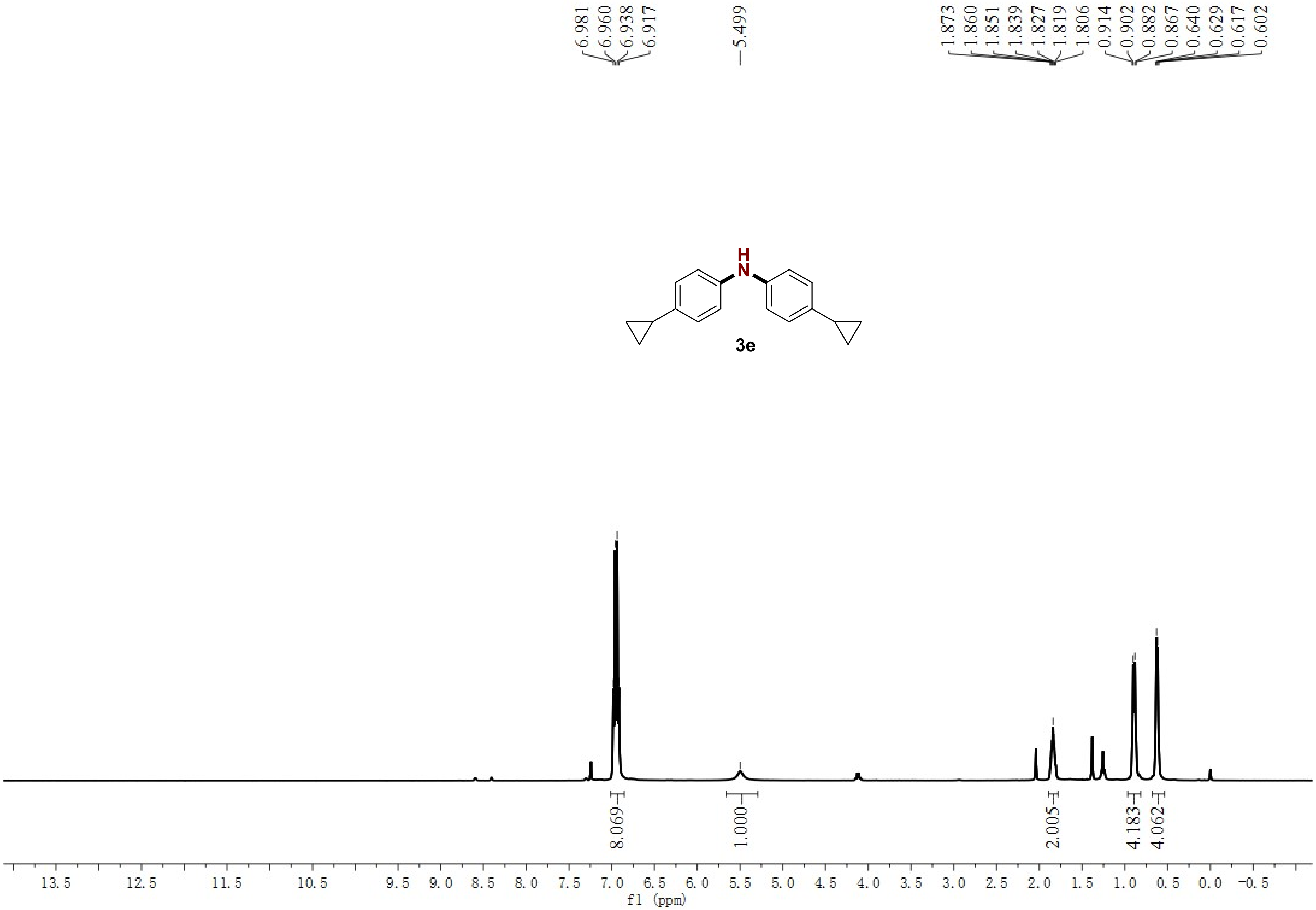

141.338
136.736
128.648
117.917
28.157
15.849
H
N
Et
Et
3b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

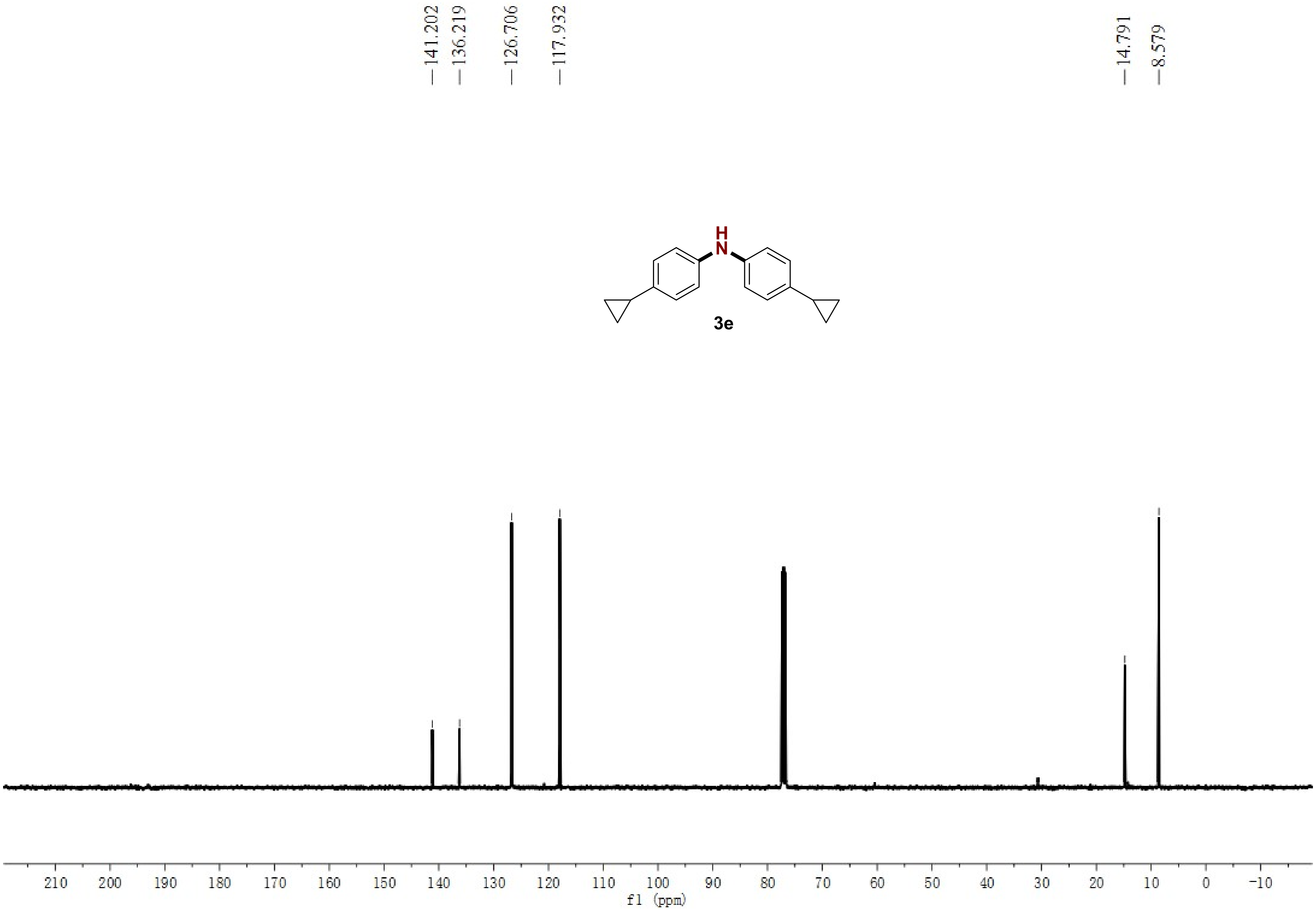

7.287
7.279
7.274
7.263
7.258
7.251
7.012
7.005
7.000
6.988
6.983
6.976
5.554
1.305
H
N
^{t}Bu
^{t}Bu
3c
4.072
4.052
1.000
18.043
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

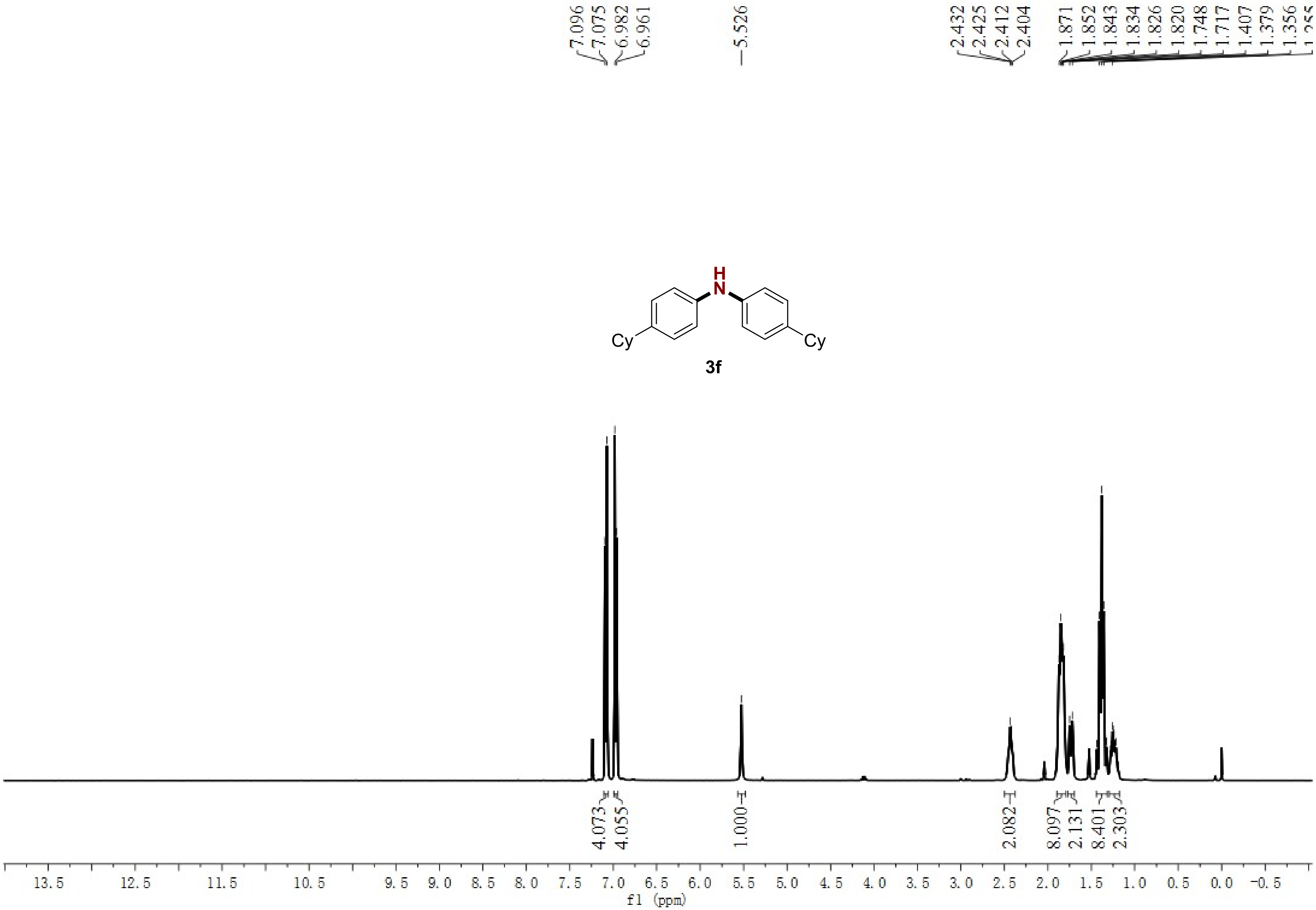

143.588
140.970
126.098
117.430
34.157
31.524
H
N
^{t}Bu
^{t}Bu
3c
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.120
7.099
6.990
6.969
5.534
2.885
2.868
2.850
2.833
2.816
1.241
1.224
H
N
^{i}Pr
^{i}Pr
3d
4.211
4.095
1.000
2.334
12.013
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
f1 (ppm)


141.363
128.823
127.183
117.818
33.414
24.199
H
N
iPr
iPr
3d
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)

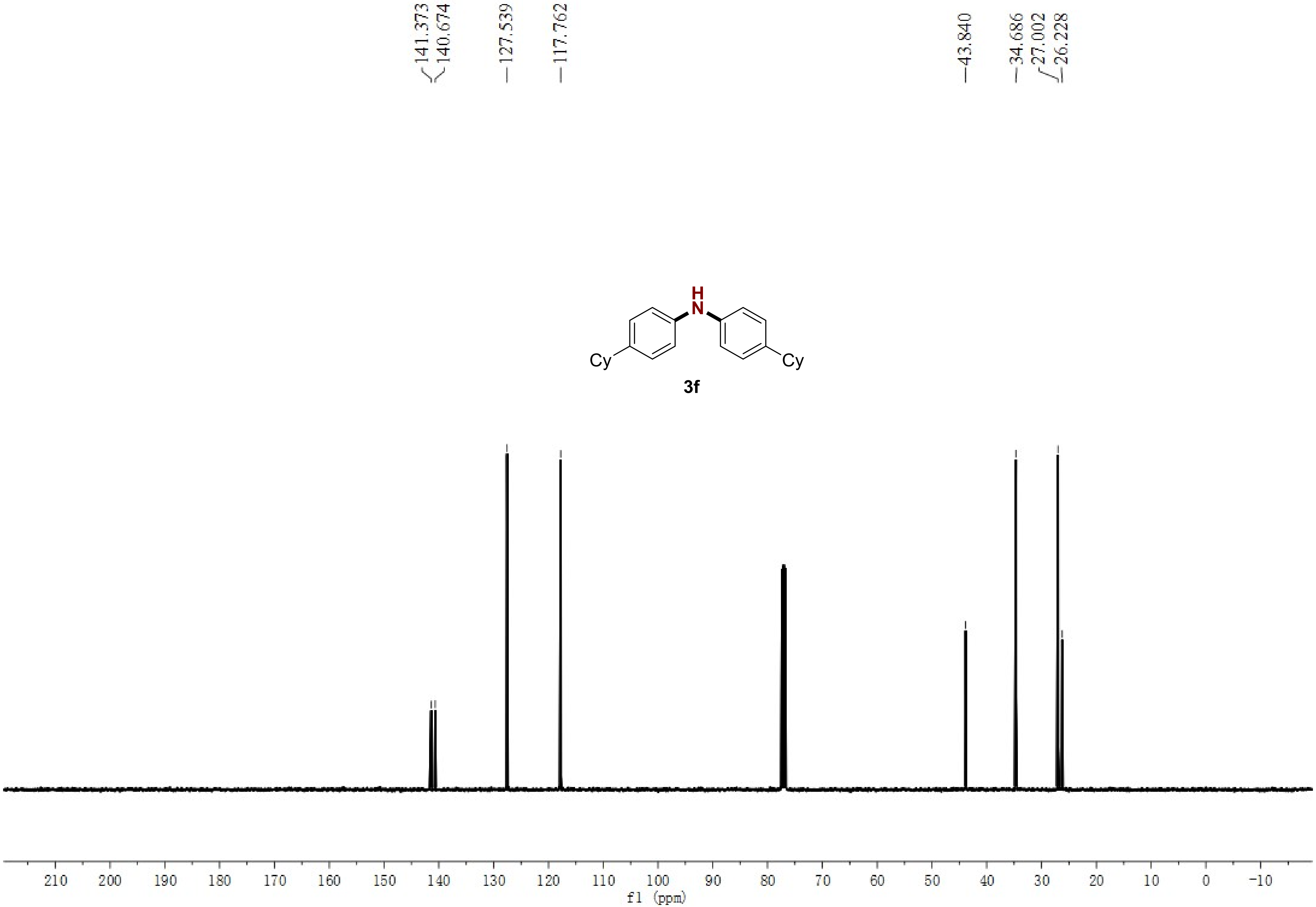

3e
6.981
6.960
6.938
6.917
5.499
1.873
1.860
1.851
1.839
1.827
1.819
1.806
0.914
0.902
0.882
0.867
0.640
0.629
0.617
0.602
H
N
8.069
1.000
2.005
4.183
4.062
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
f1 (ppm)

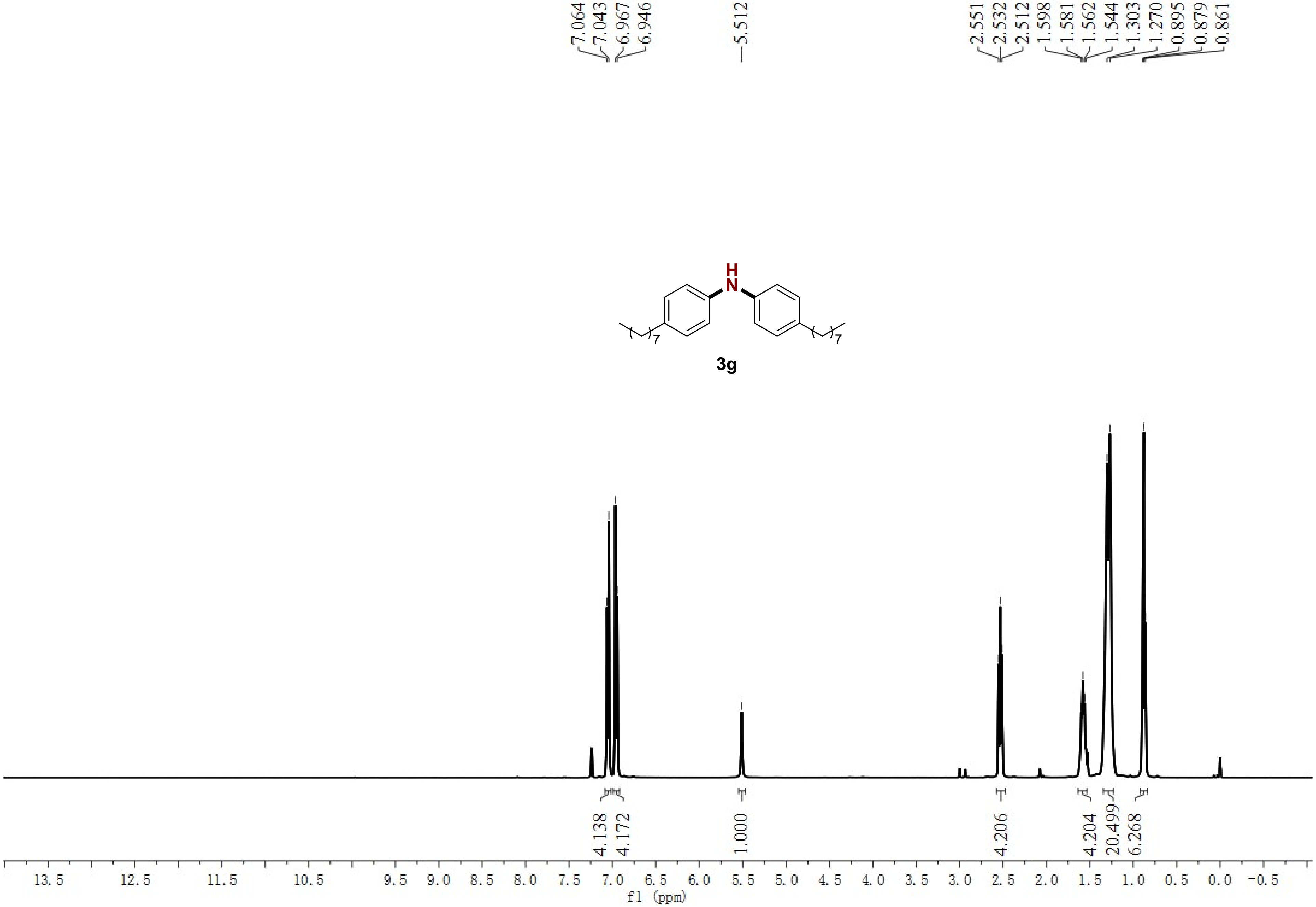

141.202
136.219
126.706
117.932
14.791
8.579
3e
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



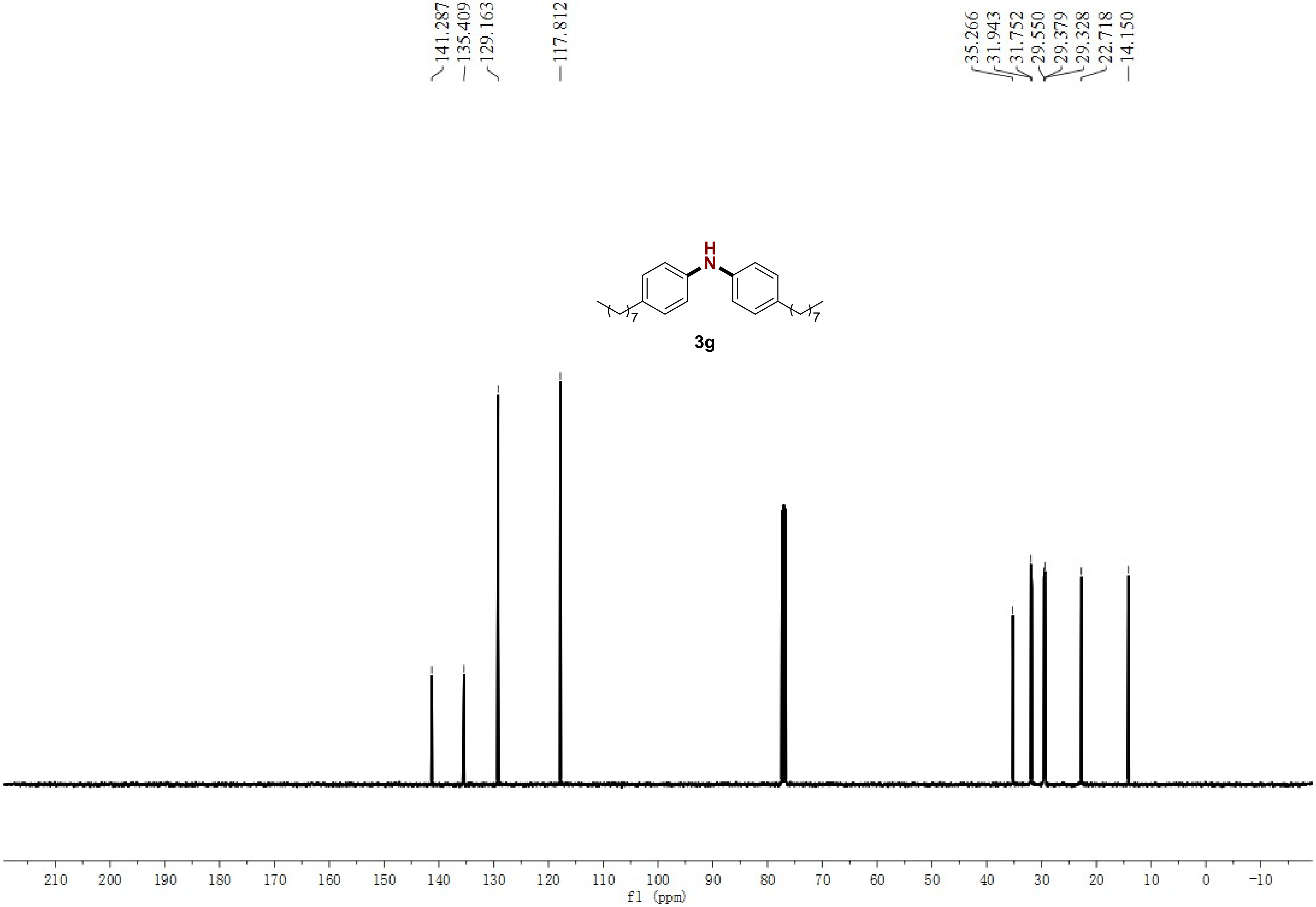
7.096
7.075
6.982
6.961
5.526
2.432
2.425
2.412
2.404
1.871
1.852
1.843
1.834
1.826
1.820
1.748
1.717
1.407
1.379
1.356
H
N
Cy
Cy
4.073
4.055
1.000
2.082
8.097
2.131
8.401
2.303
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
f1 (ppm)

3f


3f
141.373
140.674
127.539
117.762
43.840
34.686
27.002
26.228
H
N
Cy
Cy
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)

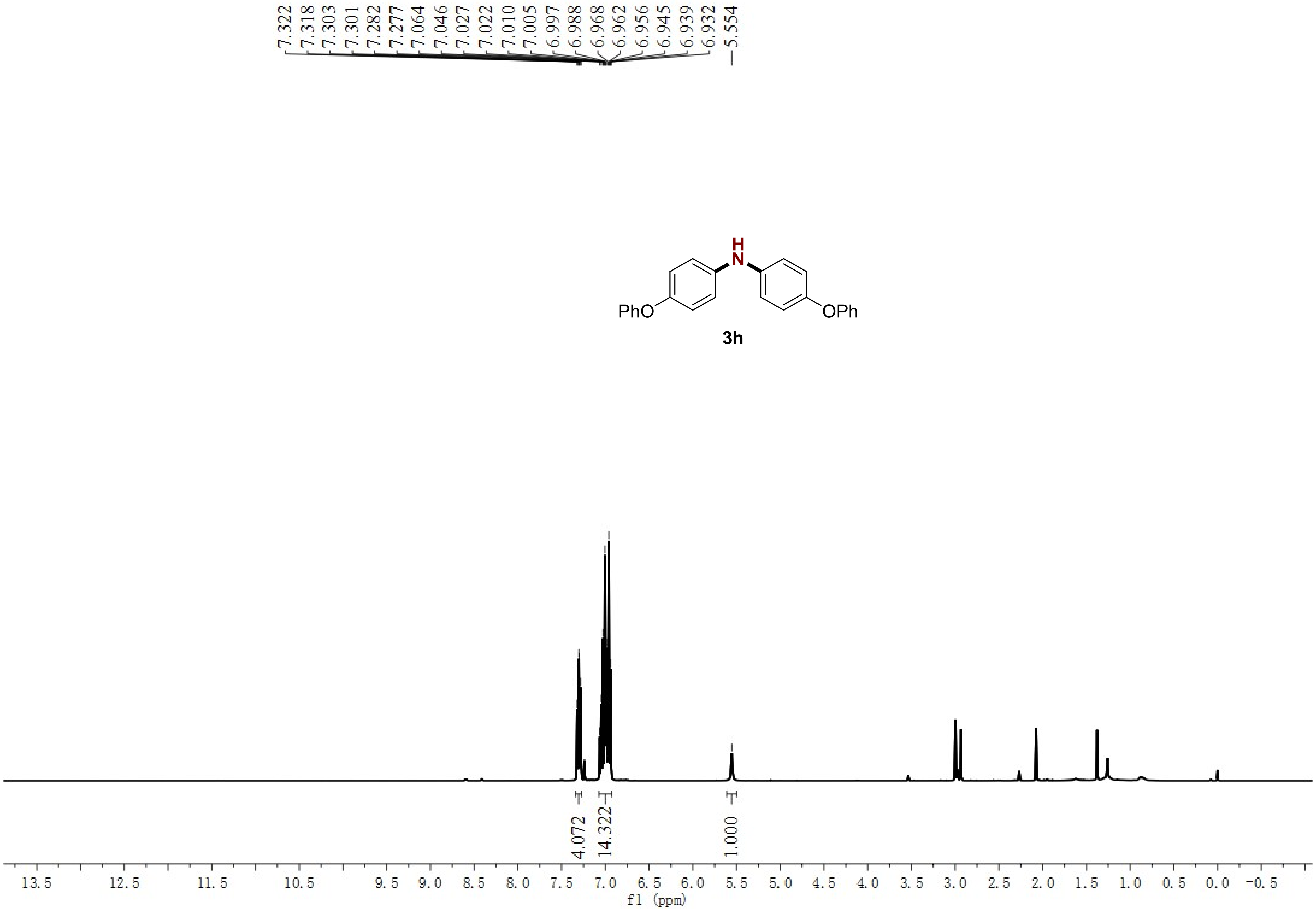

7.064
7.043
6.967
6.946
5.512
2.551
2.532
2.512
1.598
1.581
1.562
1.544
1.303
1.270
0.895
0.879
0.861
H
N
7
7
4.138
4.172
1.000
4.206
4.204
20.499
6.268
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

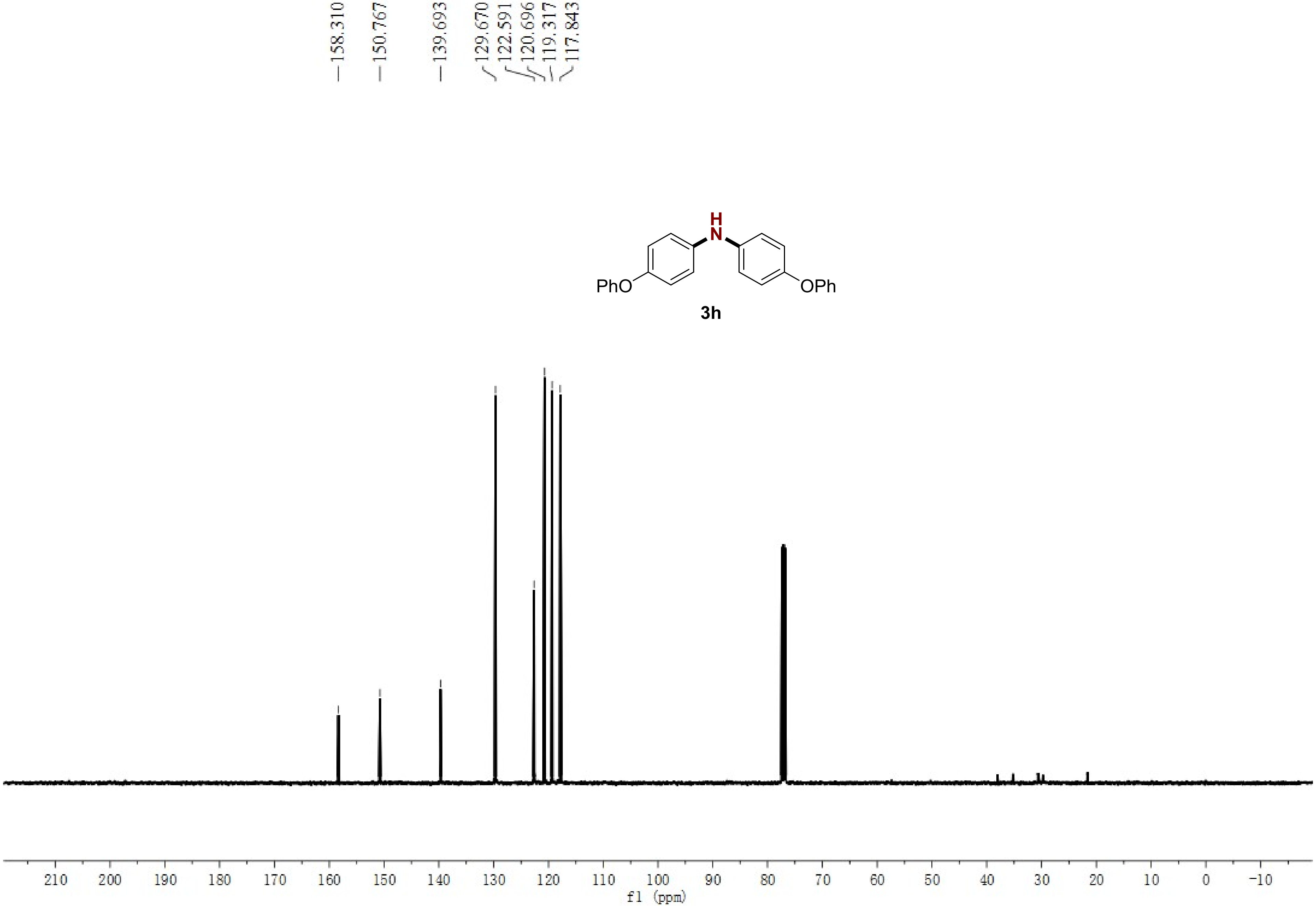
3g



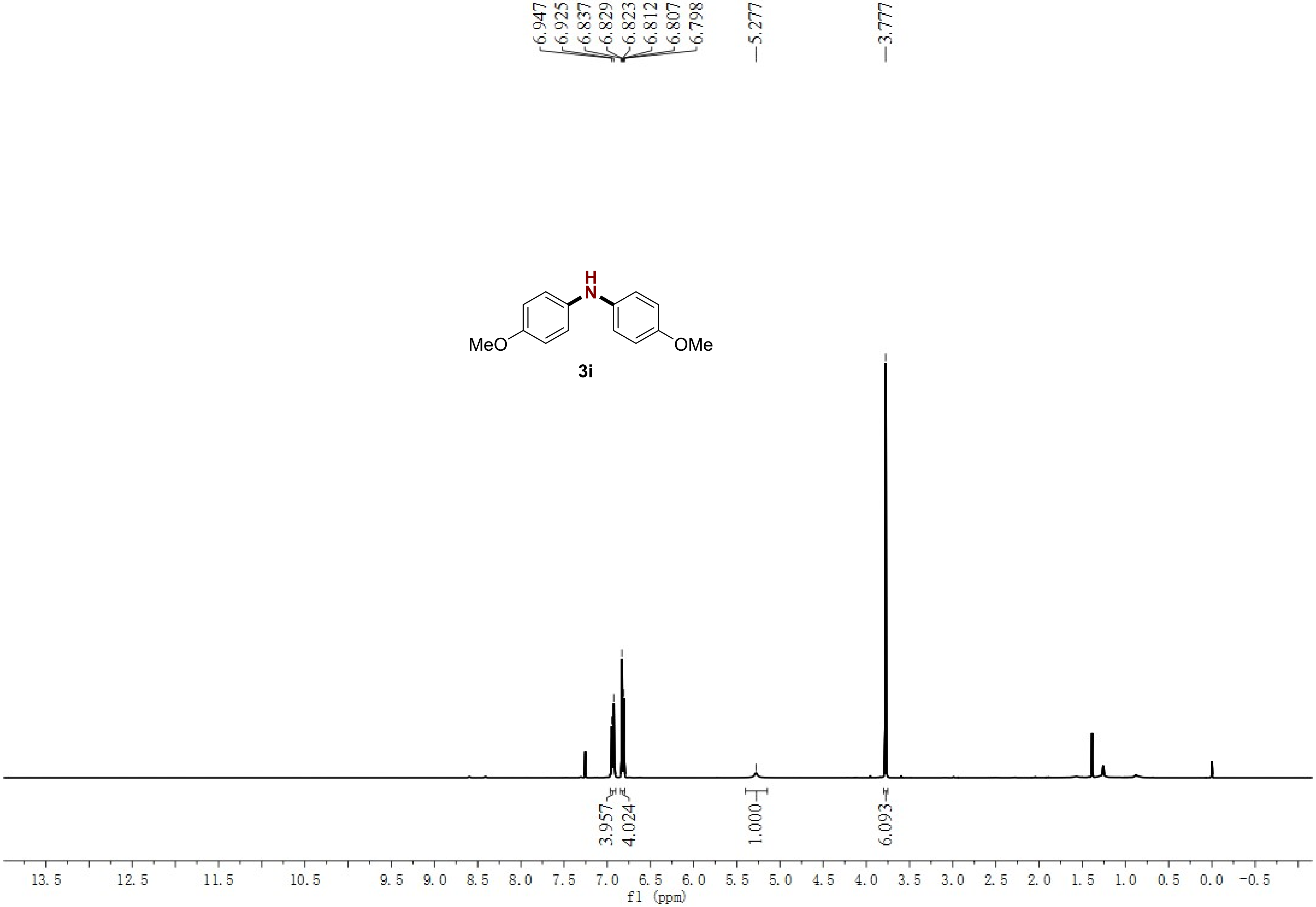
3g

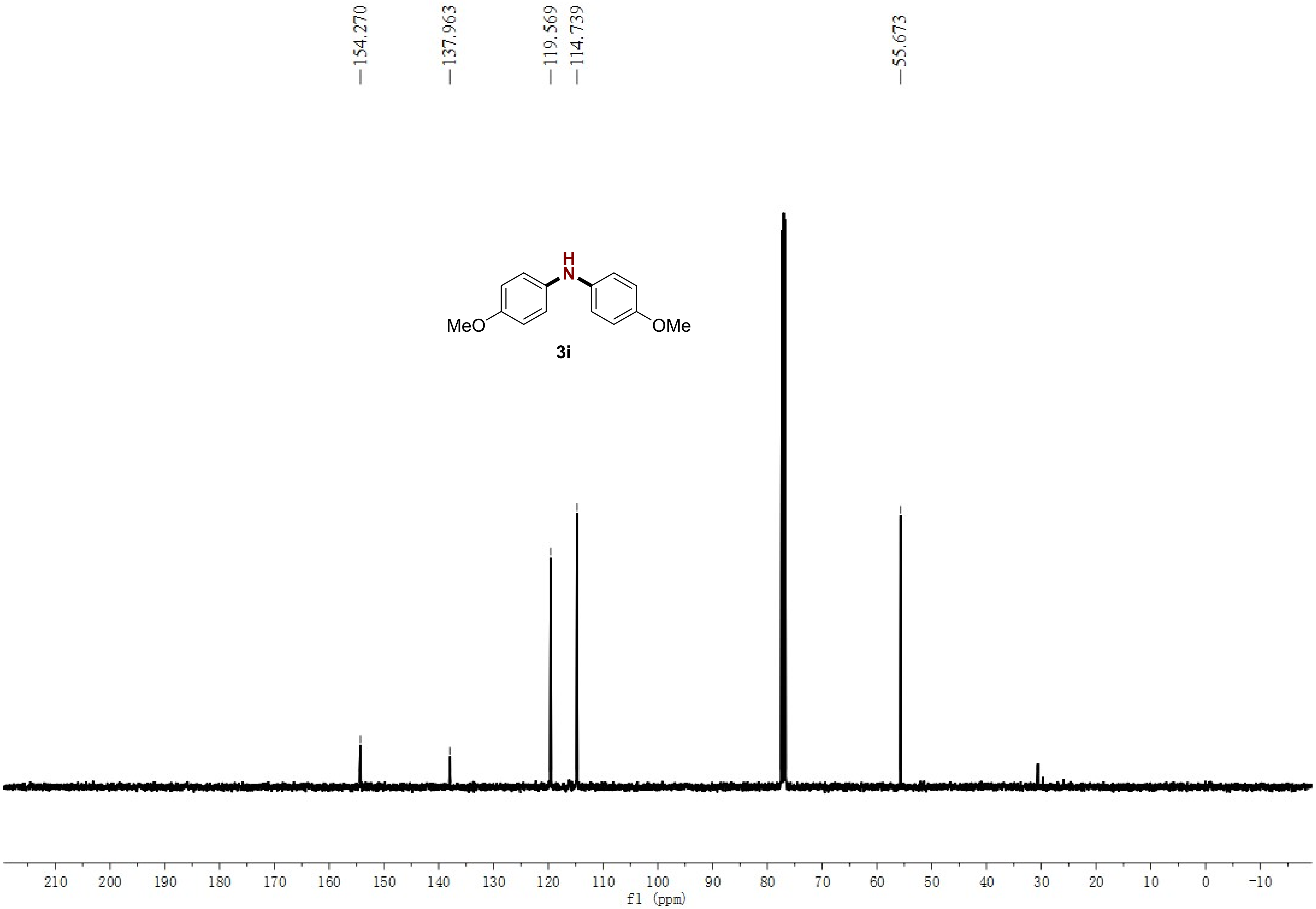
141.287
135.409
129.163
117.812
35.266
31.943
31.752
29.550
29.379
29.328
22.718
14.150
H
N
7
7
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.322
7.318
7.303
7.301
7.282
7.277
7.064
7.046
7.027
7.022
7.010
7.005
6.997
6.988
6.968
6.962
6.956
6.945
6.939
6.932
5.554
H
N
PhO
OPh
3h
4.072
14.322
1.000
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

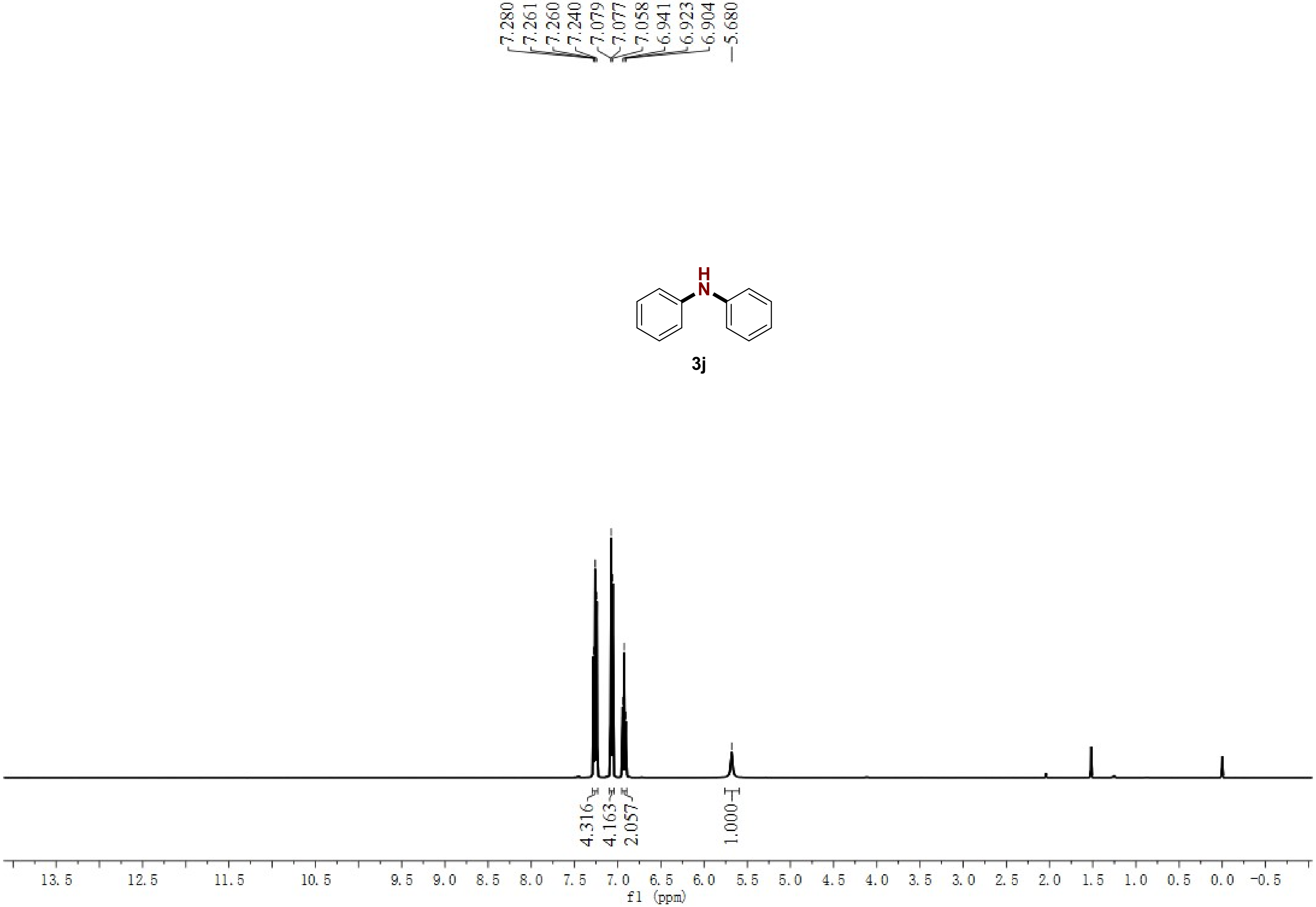

158.310
150.767
139.693
129.670
122.591
120.696
119.317
117.843
PhO
H
N
OPh
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

3h


6.947
6.925
6.837
6.829
6.823
6.812
6.807
6.798
5.277
3.777
H
N
MeO
OMe
3i
3.957
4.024
1.000
6.093
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

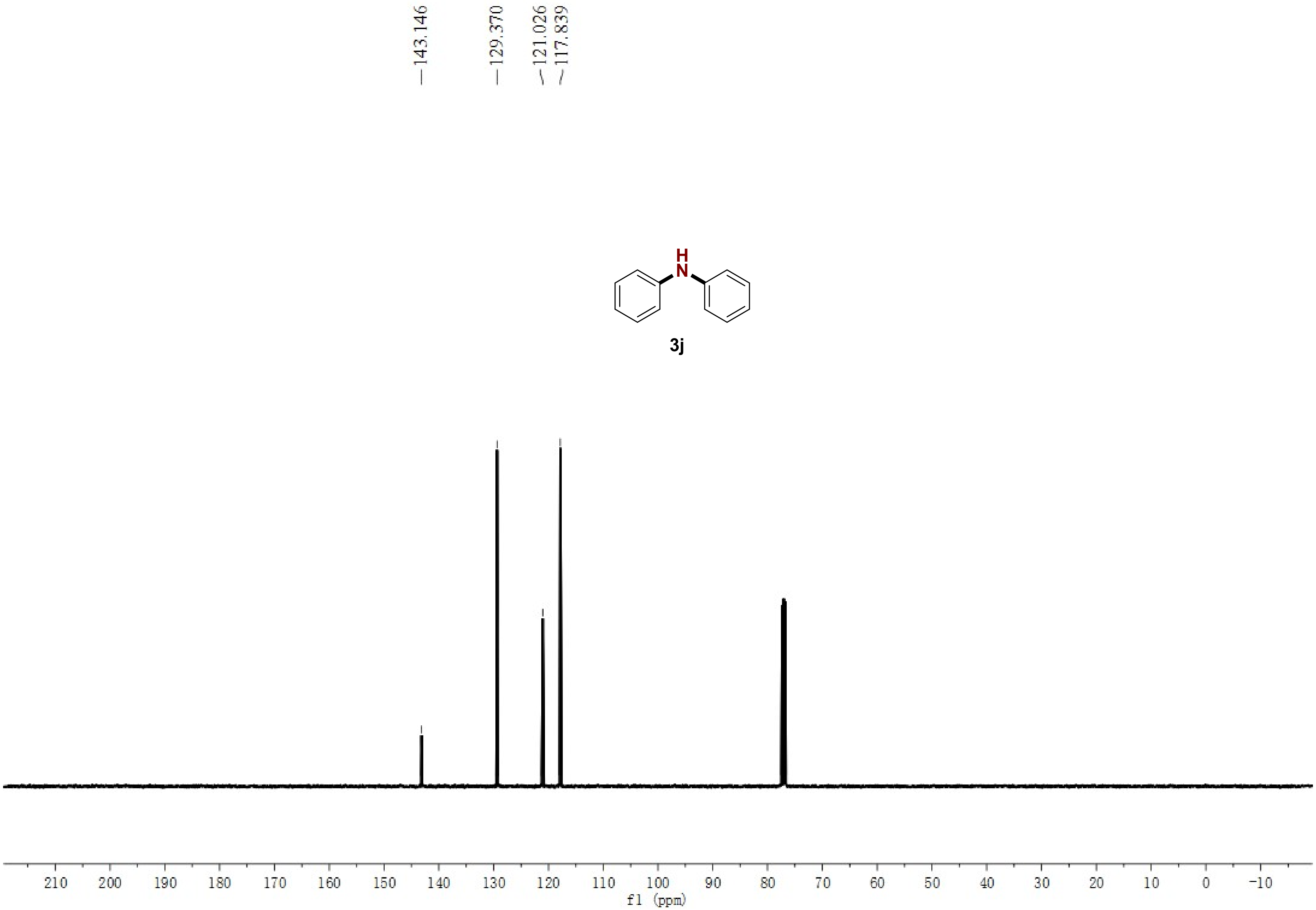

154.270
137.963
119.569
114.739
55.673
H
N
MeO
OMe
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3i

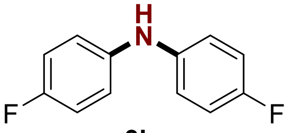


3j

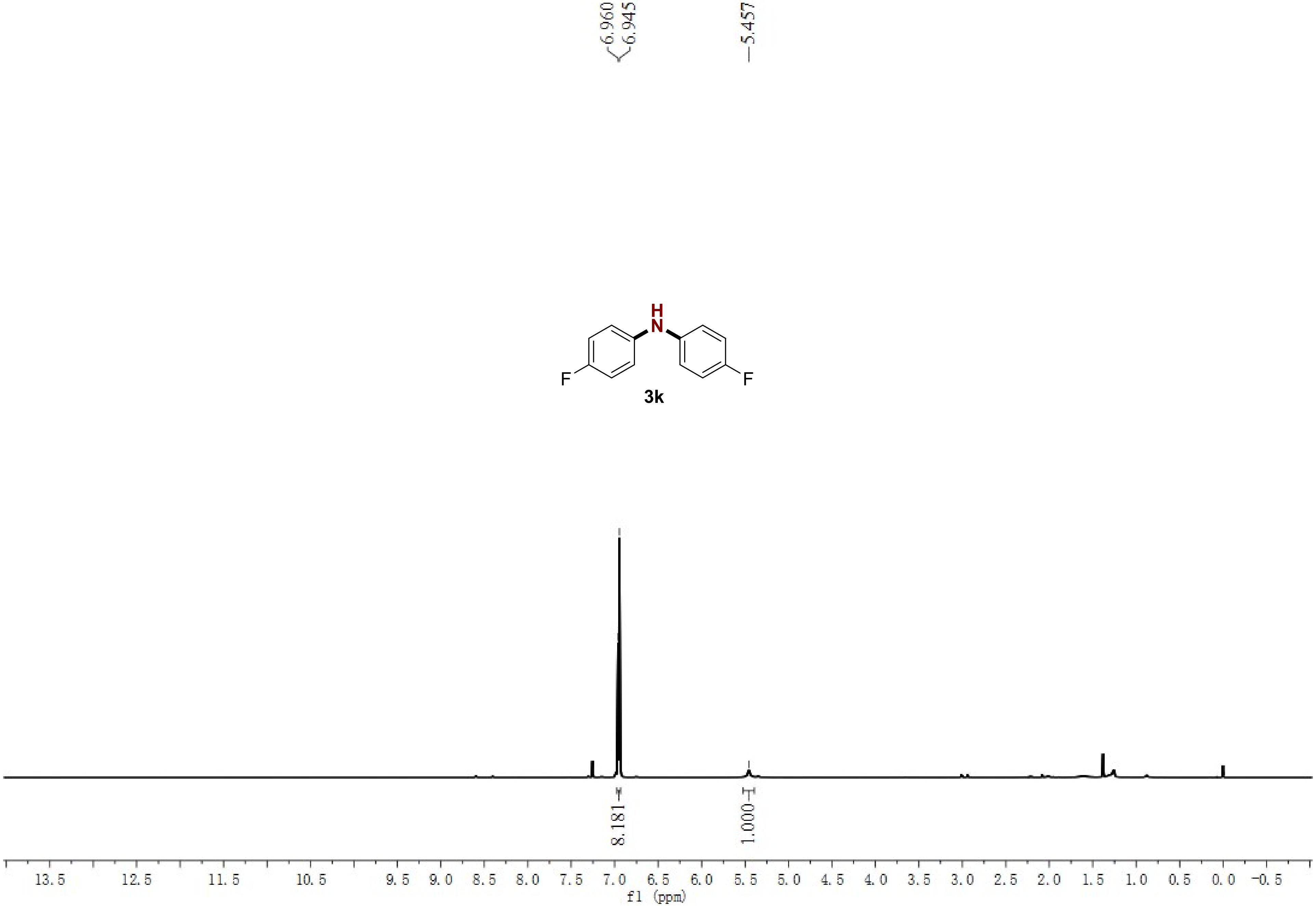
7.280
7.261
7.260
7.240
7.079
7.077
7.058
6.941
6.923
6.904
5.680
H
N
4.316
4.163
2.057
1.000
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

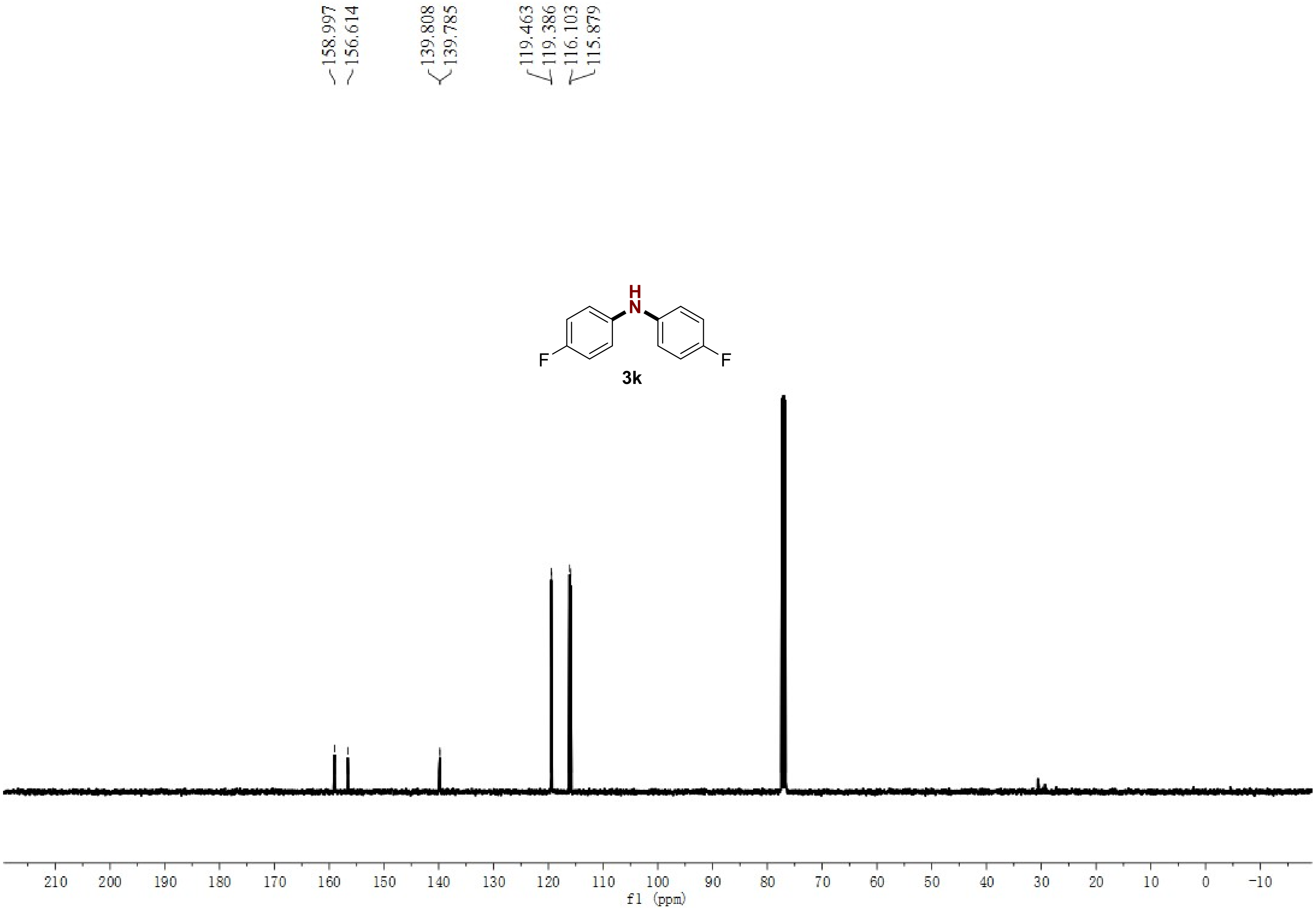

143.146
129.370
121.026
117.839
H
N
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

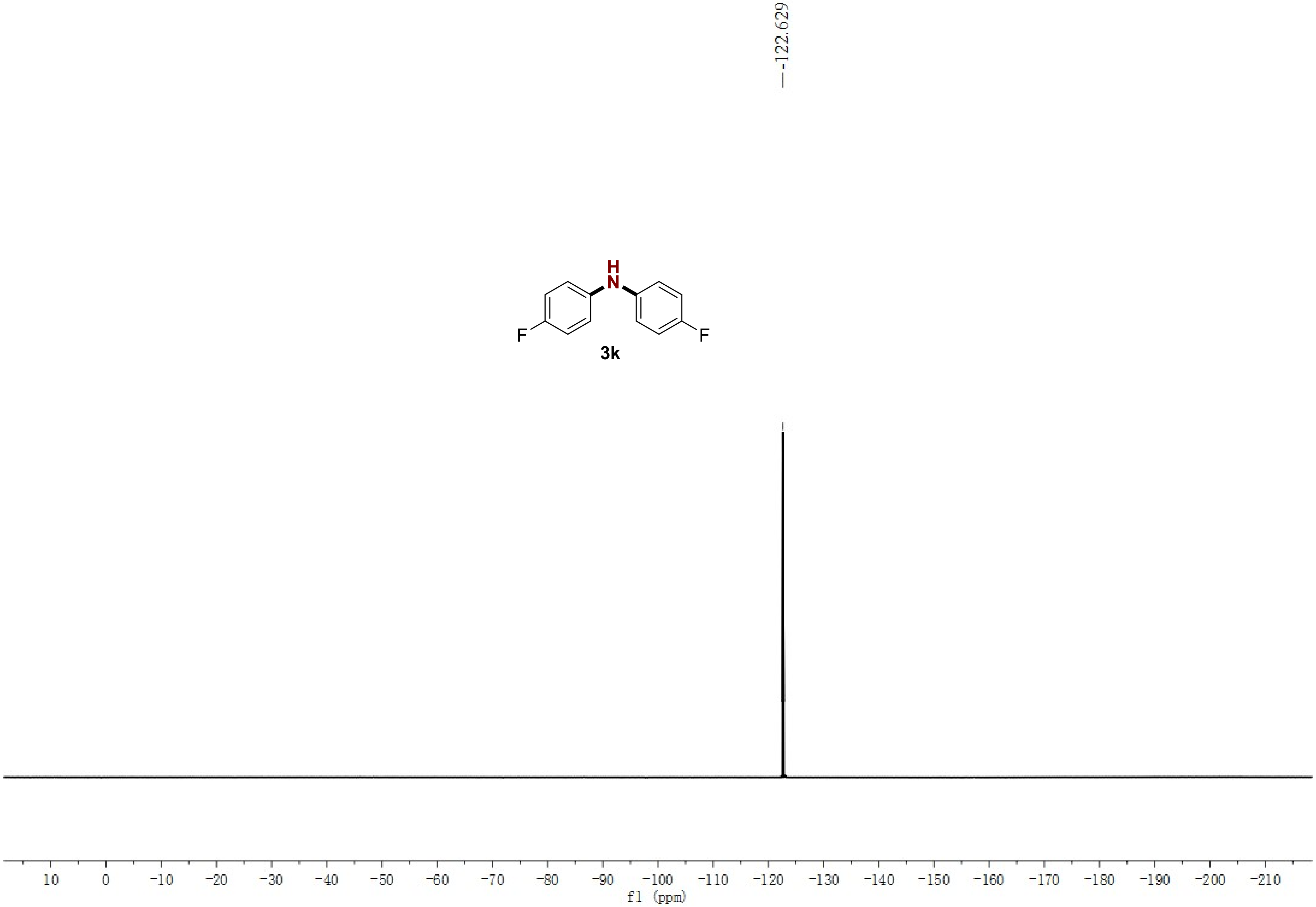
3j


H
N
F
F

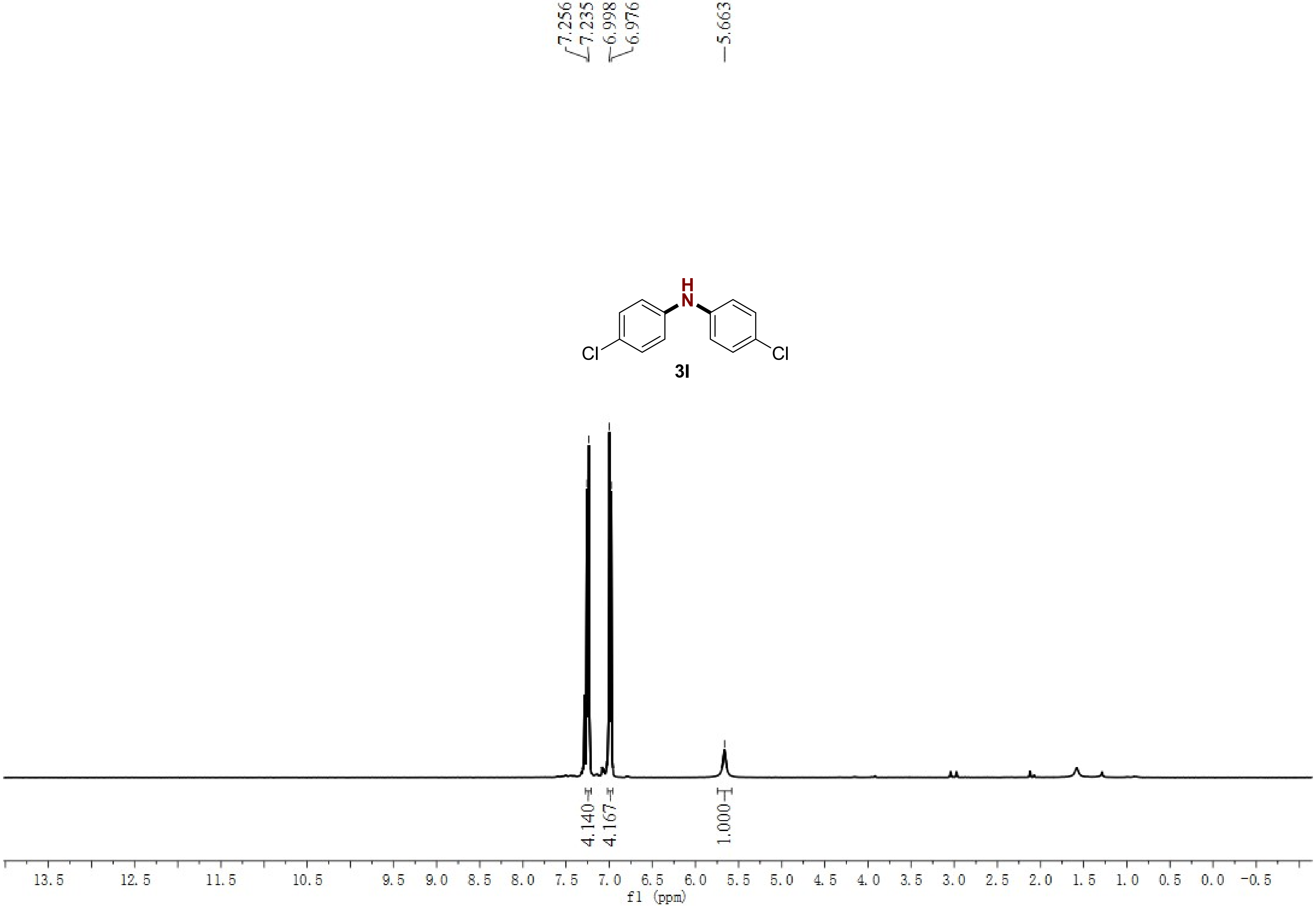
3k


6.960
6.945
5.457
8.181
1.000
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
f1 (ppm)

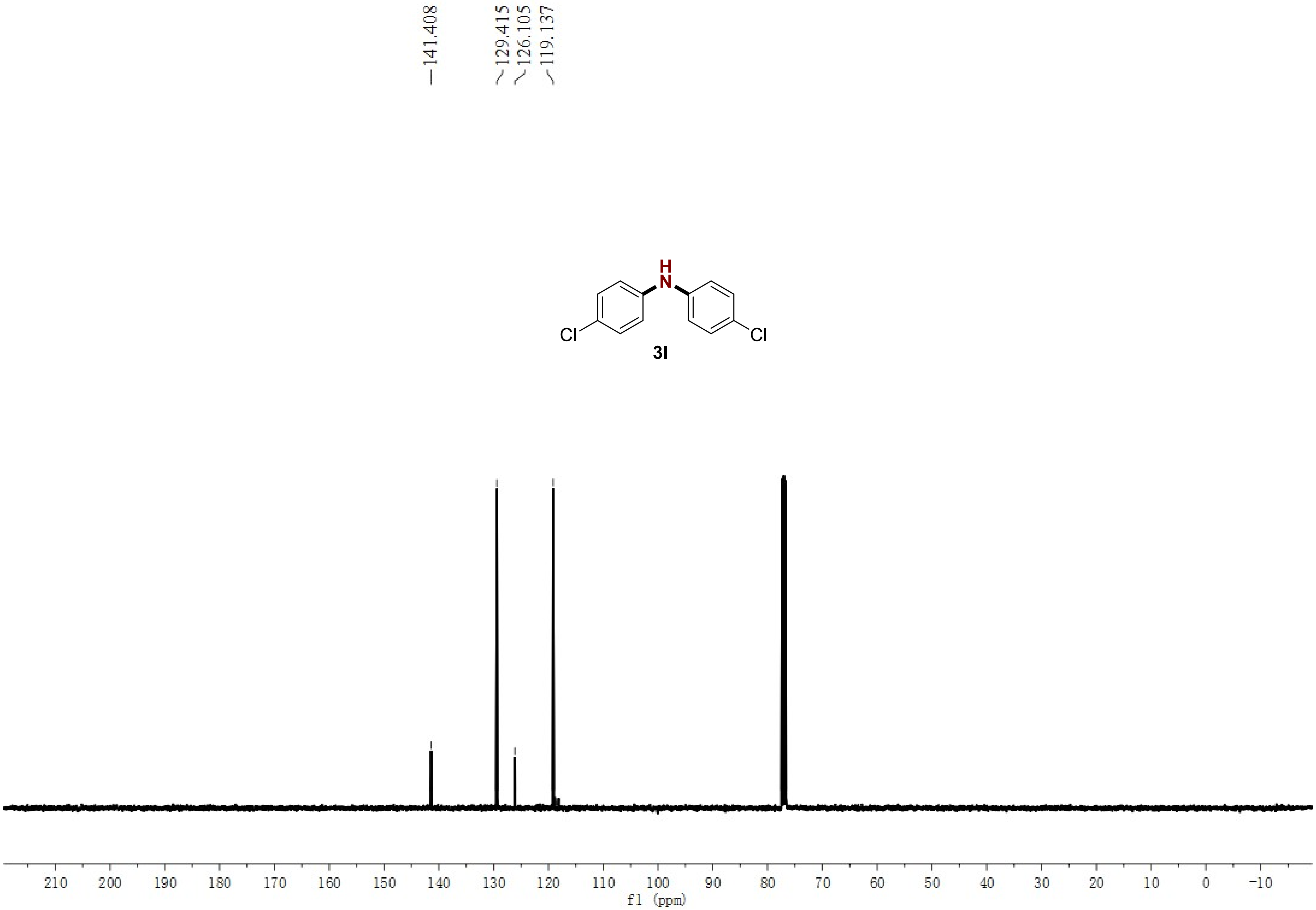

158.997
156.614
139.808
139.785
119.463
119.386
116.103
115.879
H
N
F
F
3k
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)


-122.629
H
N
F
F
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)

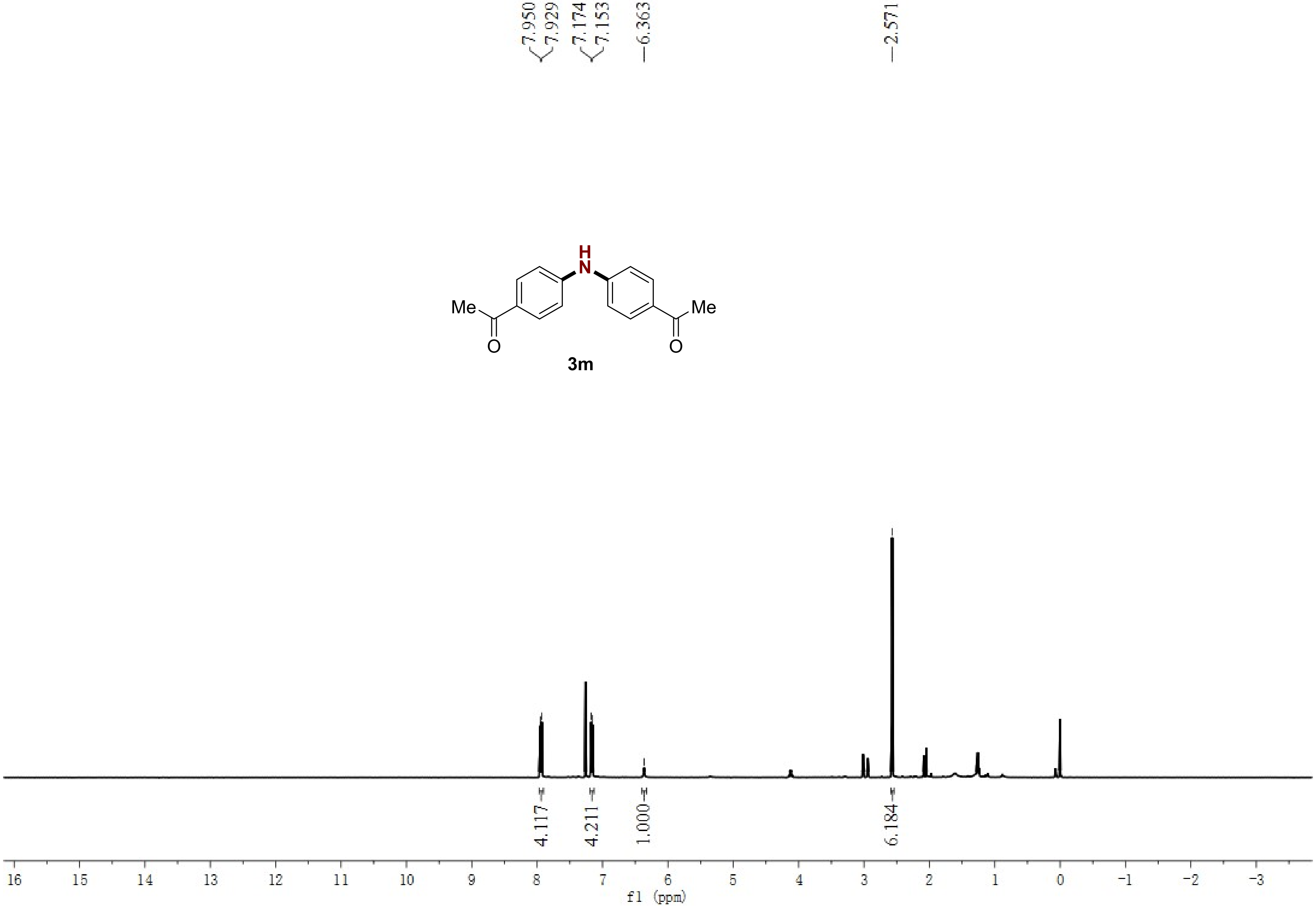
3k

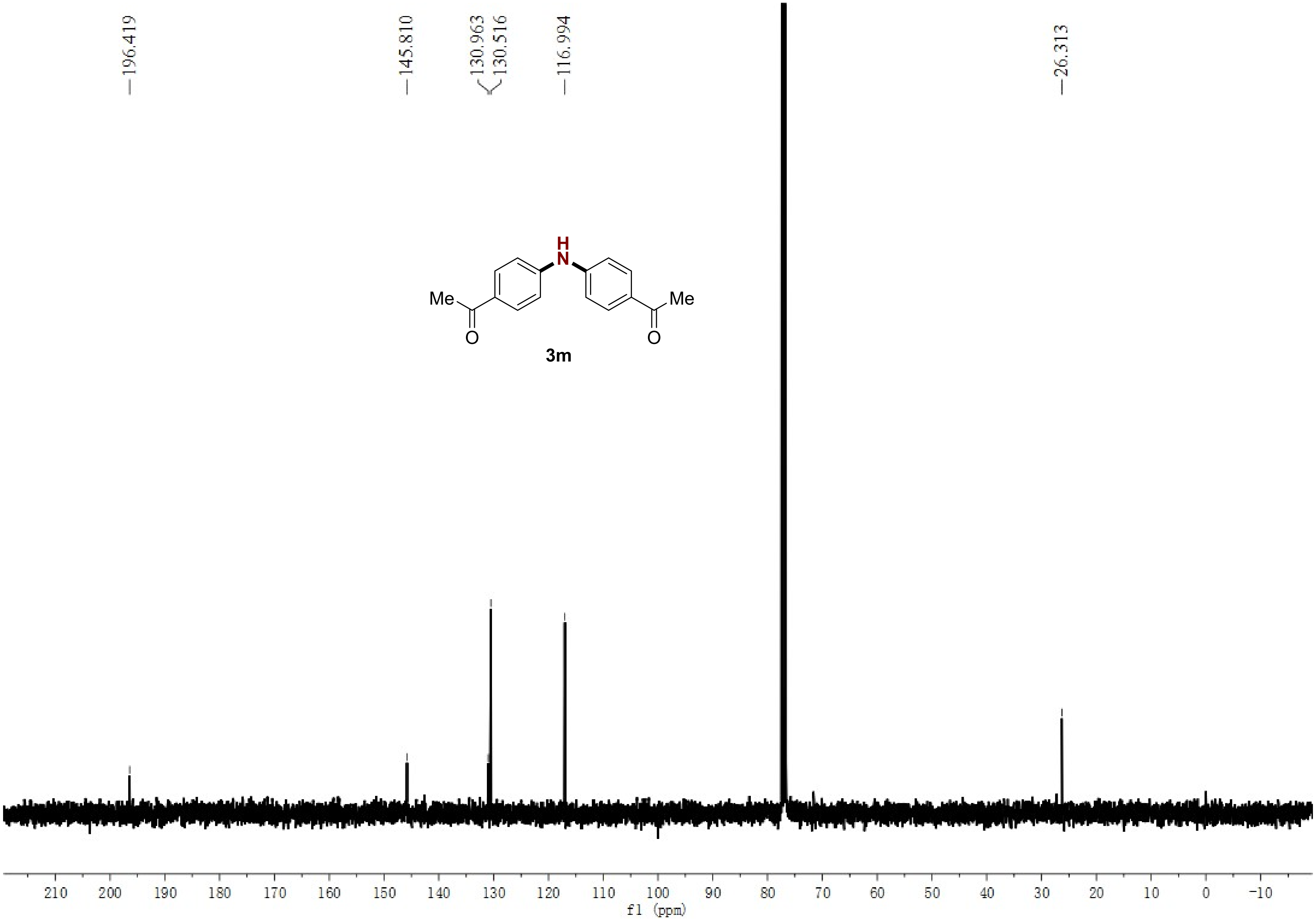

7.256
7.235
6.998
6.976
5.663
H
N
Cl
Cl
4.140
4.167
1.000
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

3l

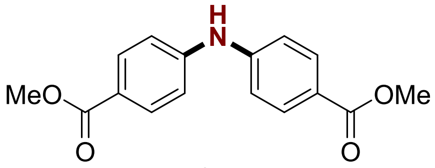

141.408
129.415
126.105
119.137
H
N
Cl
Cl
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

3l

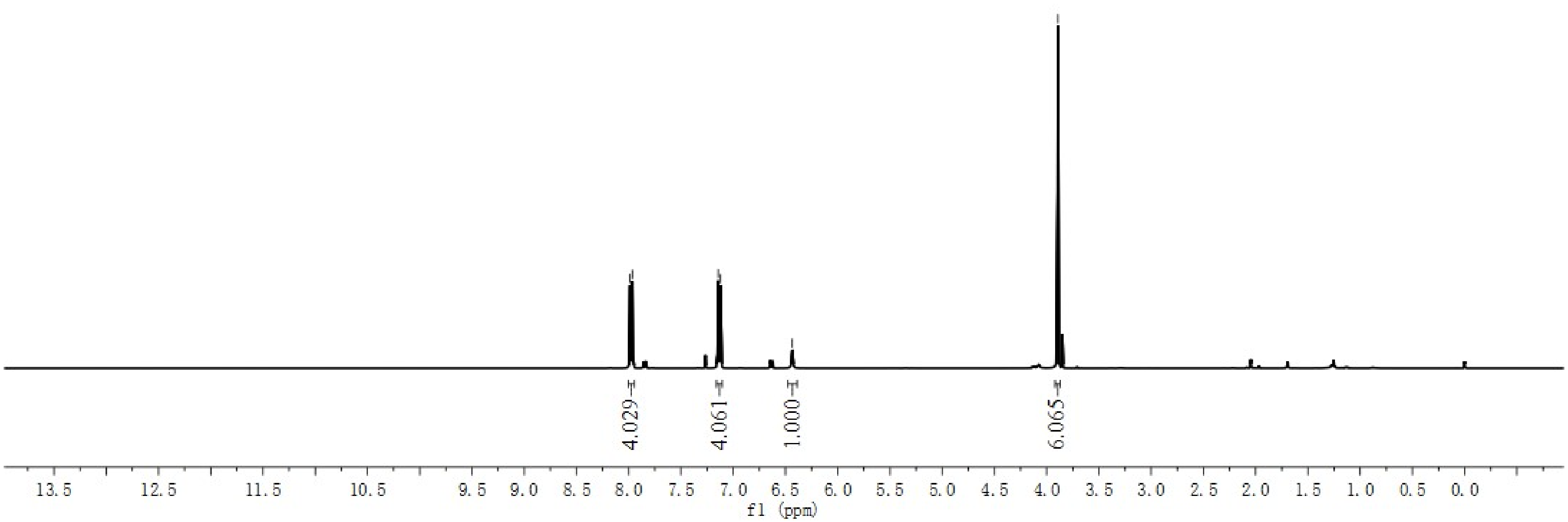

3m
7.950
7.929
7.174
7.153
6.363
2.571
H
N
Me
O
Me
O
4.117
4.211
1.000
6.184
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
−2
−3
f1 (ppm)

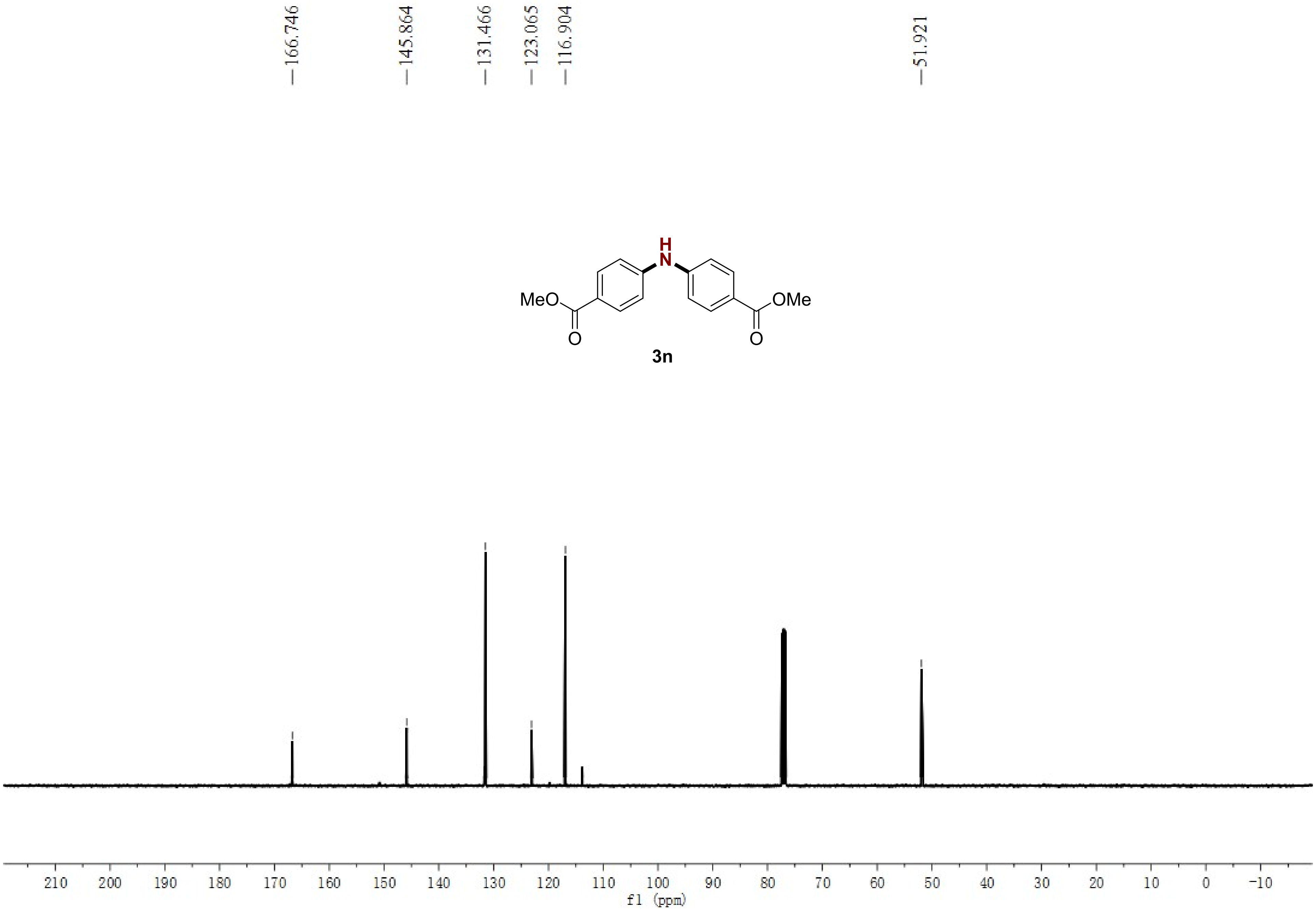

196.419
145.810
130.963
130.516
116.994
26.313
H
N
Me
O
Me
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

3m

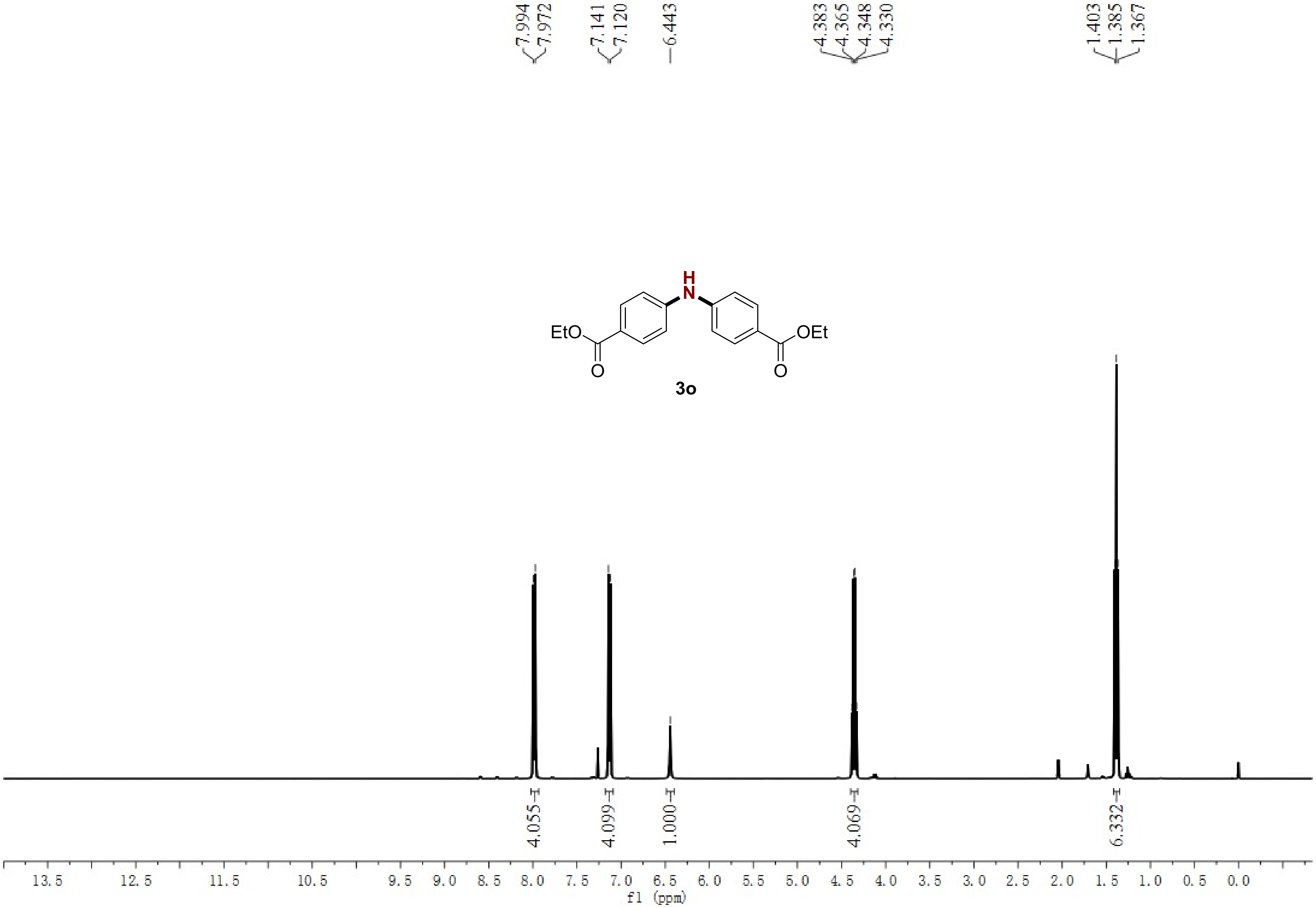

MeO
O
H
N
OMe
O

3n


7.987
7.966
7.144
7.122
6.435
3.894
4.029
4.061
1.000
6.065
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

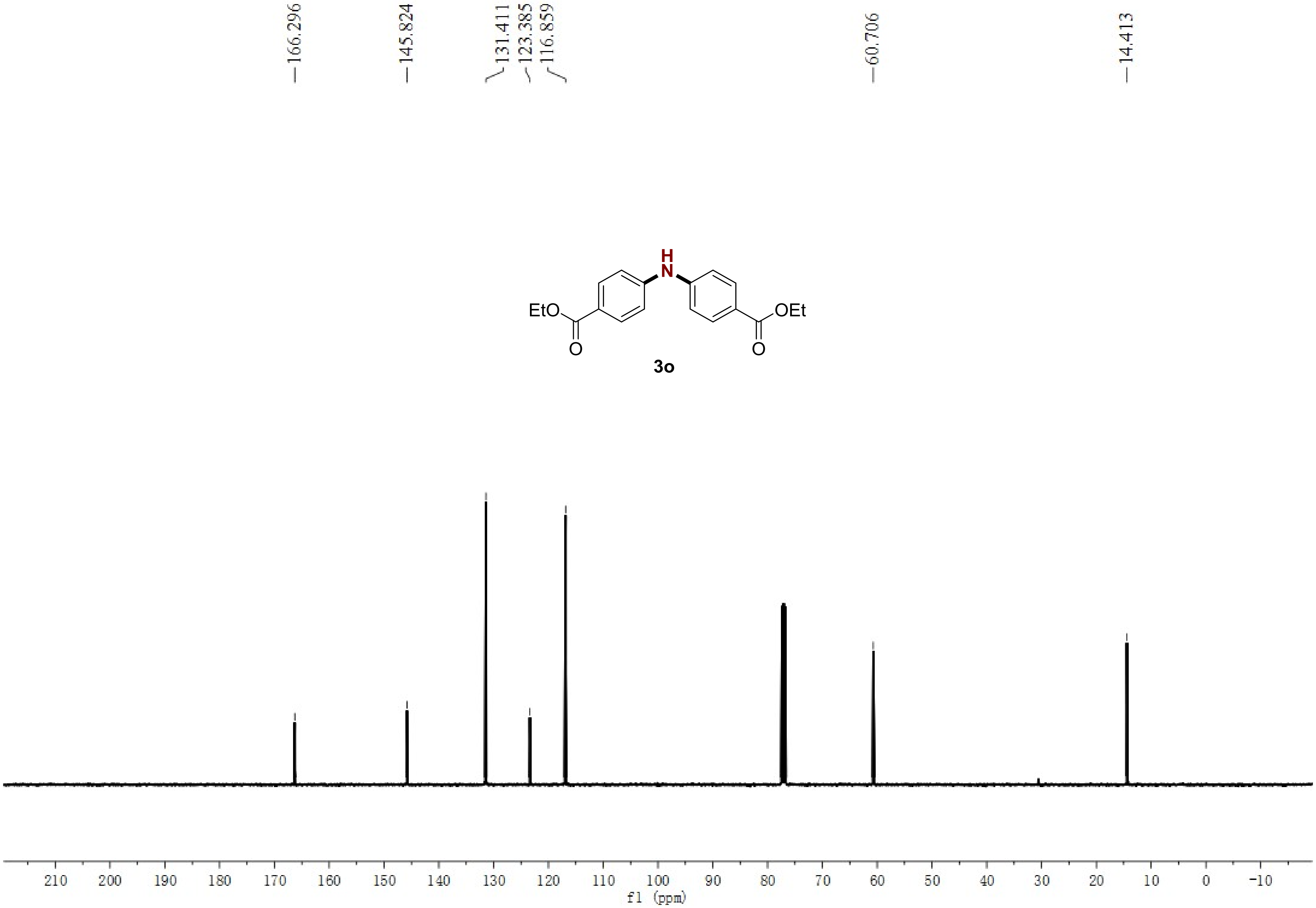

166.746
145.864
131.466
123.065
116.904
51.921
MeO
H
N
OMe
O
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

3n

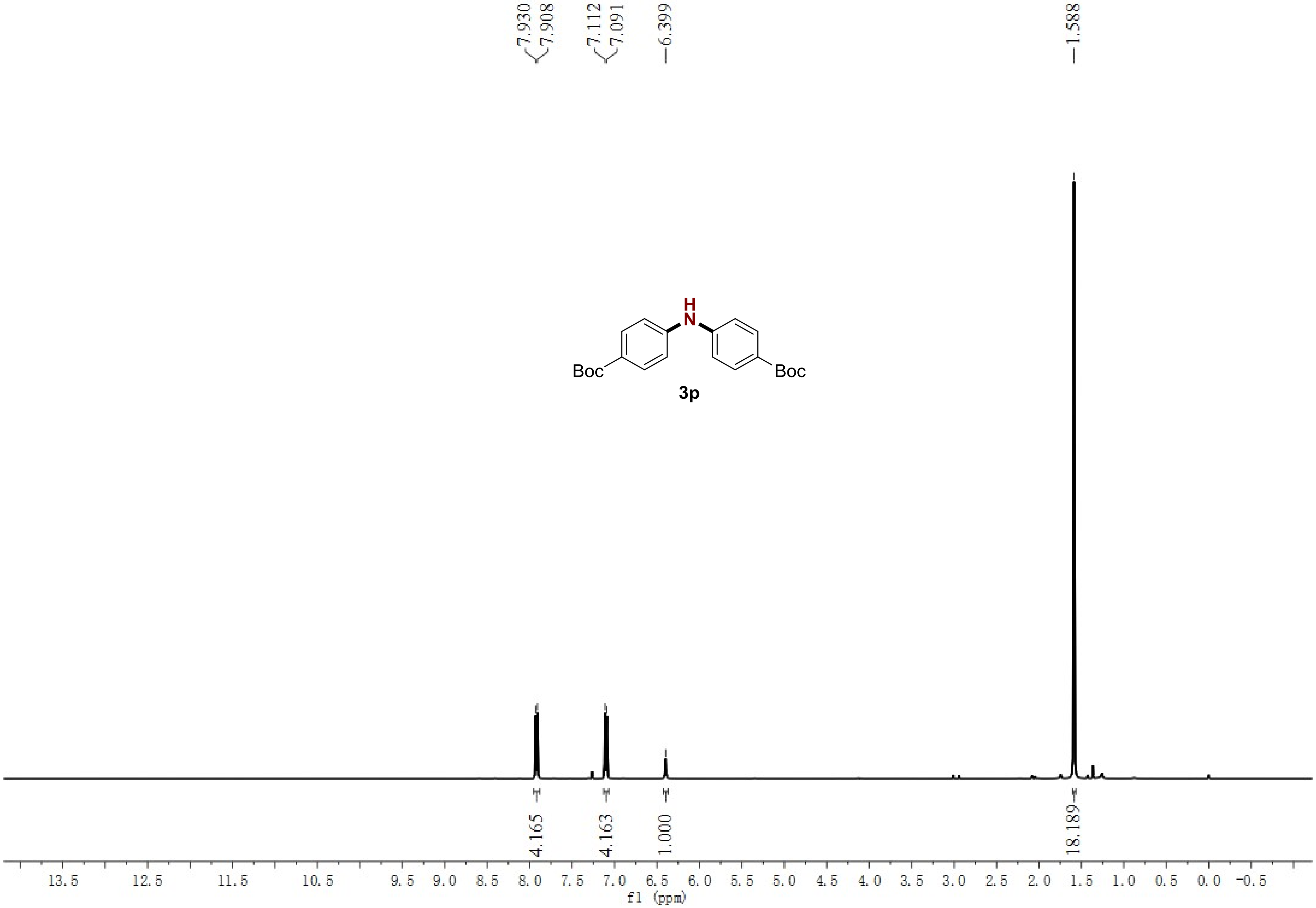


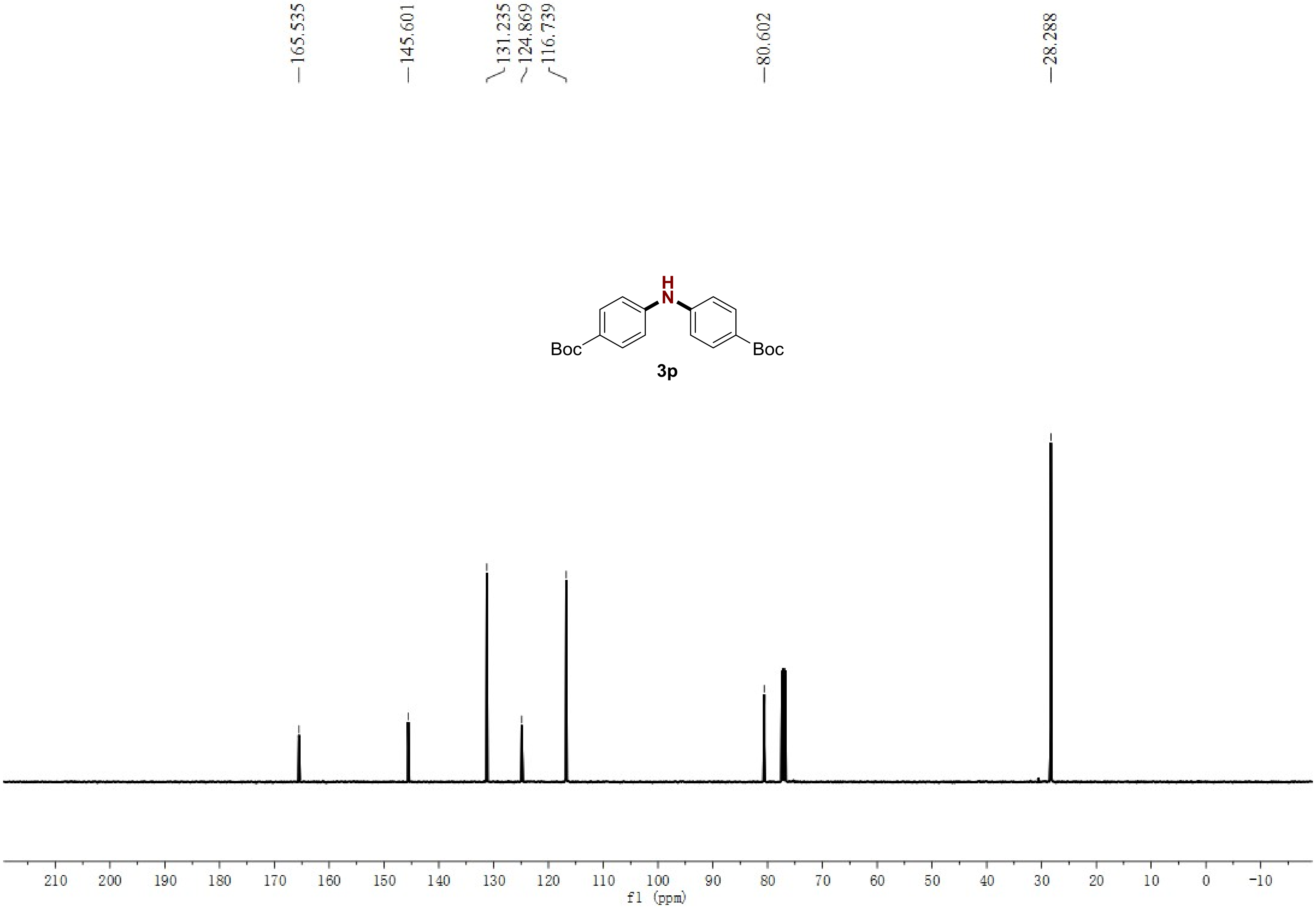
3o

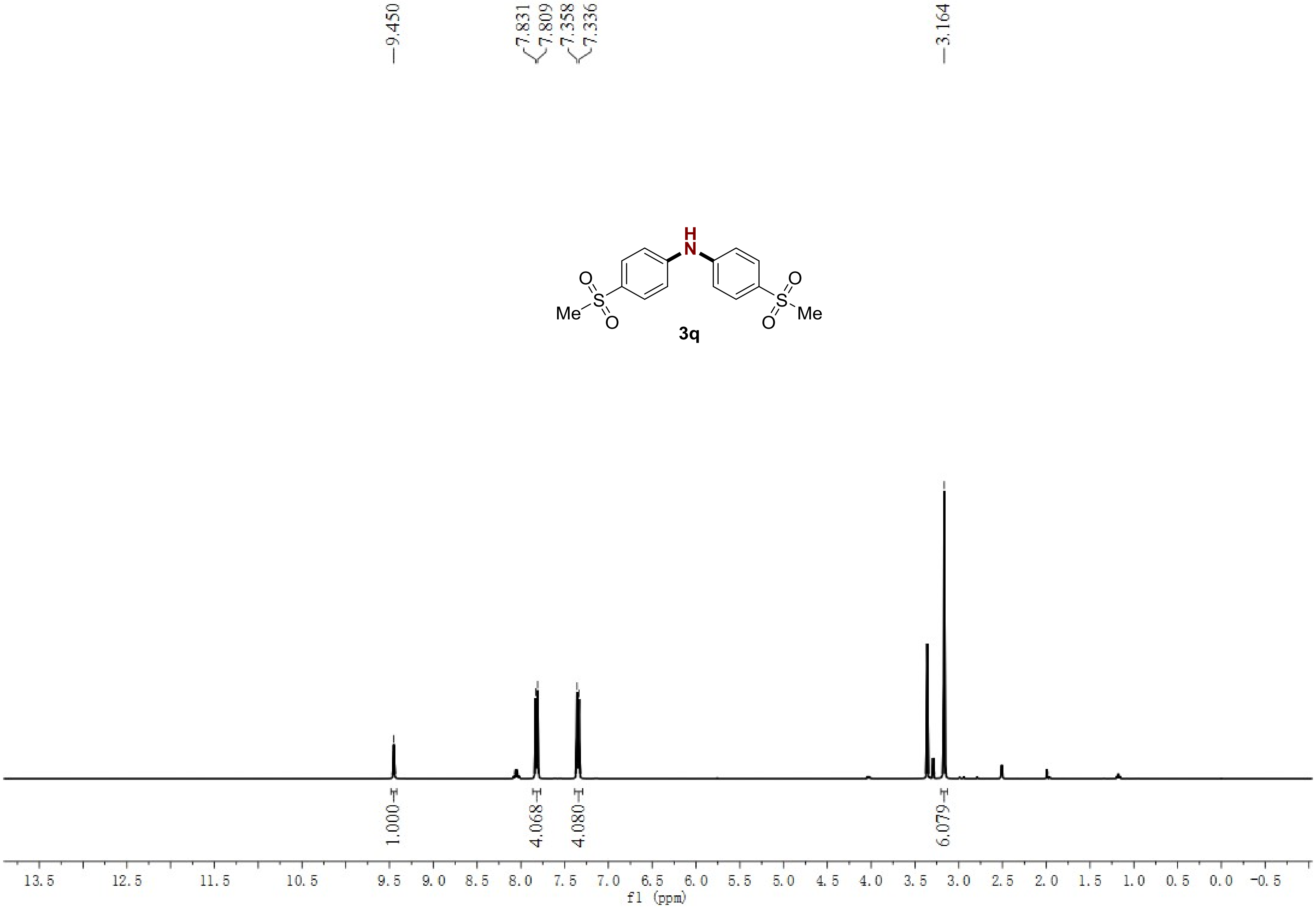
7.994
7.972
7.141
7.120
6.443
4.383
4.365
4.348
4.330
1.403
1.385
1.367
EtO
OEt
H
N
O
O
4.055
4.099
1.000
4.069
6.332
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


166.296
145.824
131.411
123.385
116.859
60.706
14.413
EtO
OEt
H
N
O
O
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)

3o

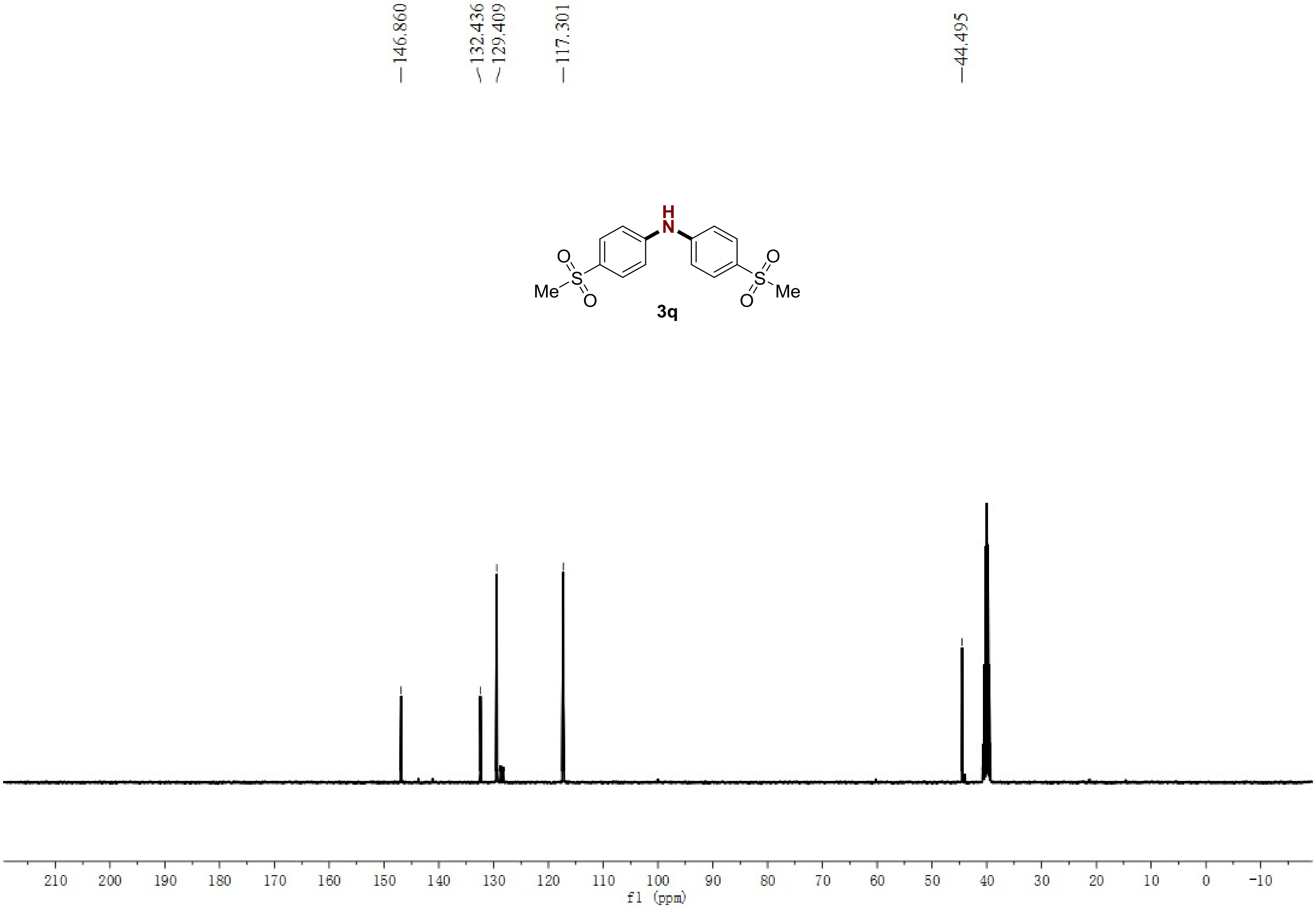

7.930
7.908
7.112
7.091
6.399
1.588
H
N
Boc
Boc
3p
4.165
4.163
1.000
18.189
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


165.535
145.601
131.235
124.869
116.739
80.602
28.288
H
N
Boc
Boc
3p
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)



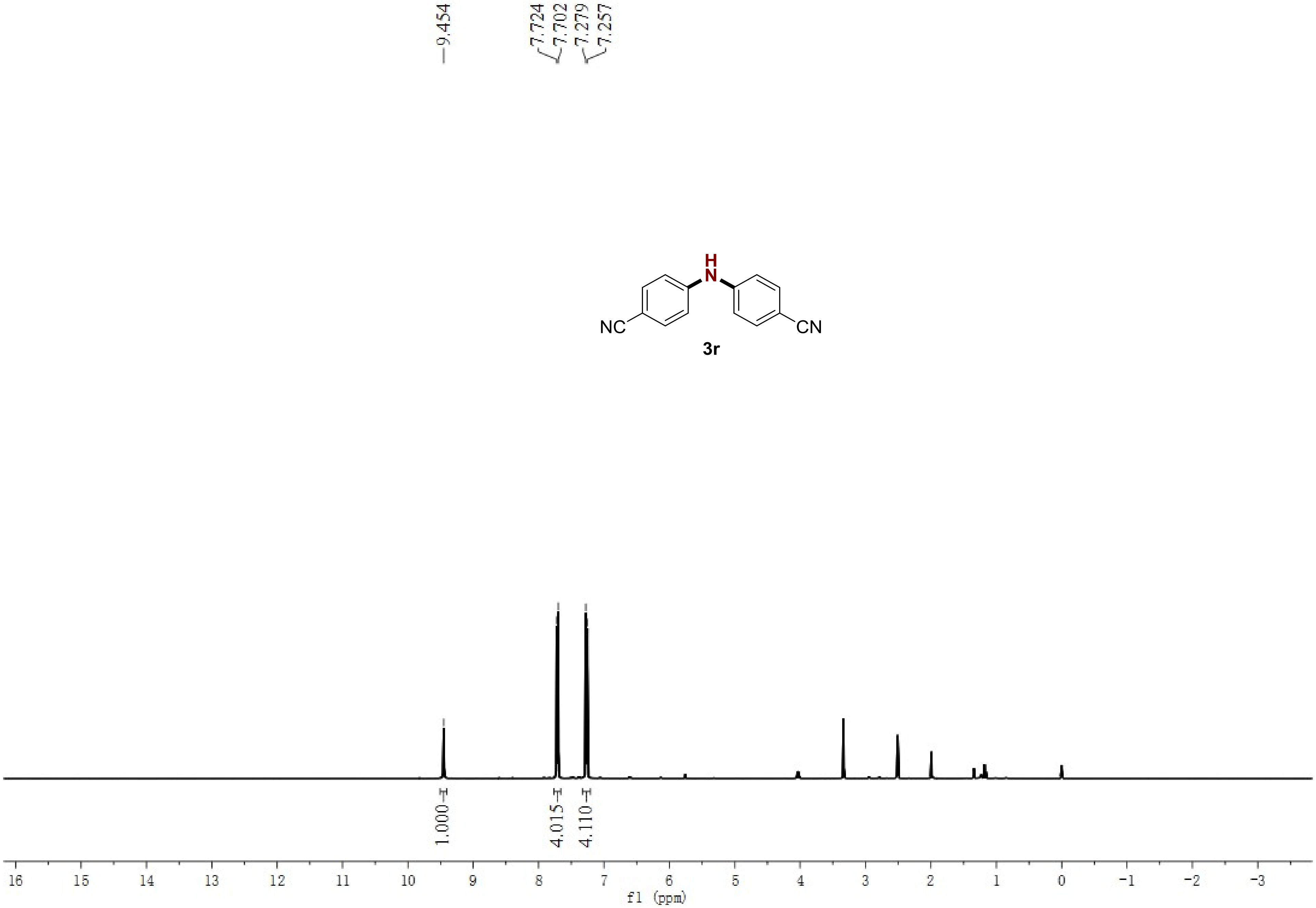
3q

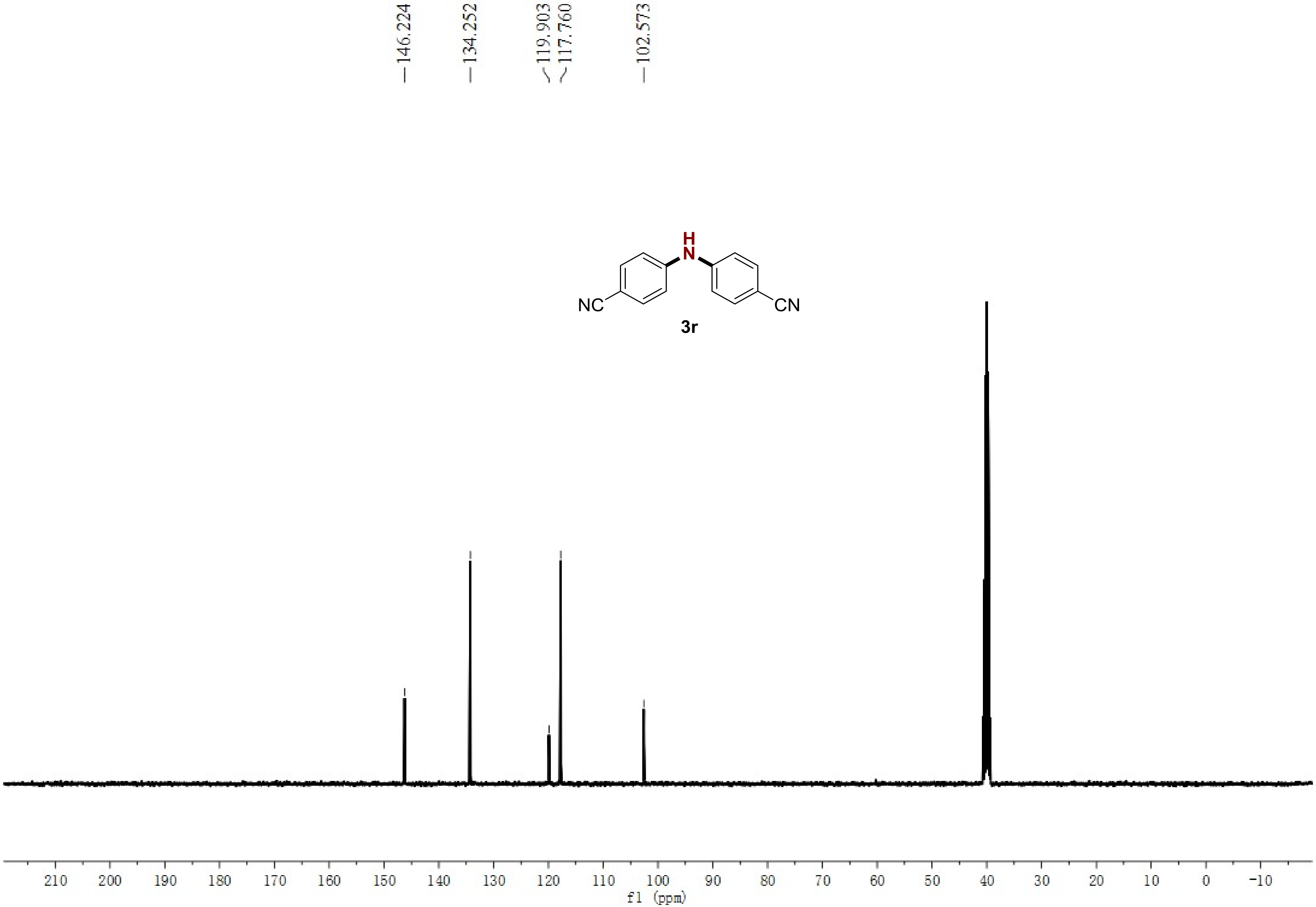
9.450
7.831
7.809
7.358
7.336
3.164
Me
S
O
O
N
H
Me
S
O
O
1.000
4.068
4.080
6.079
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

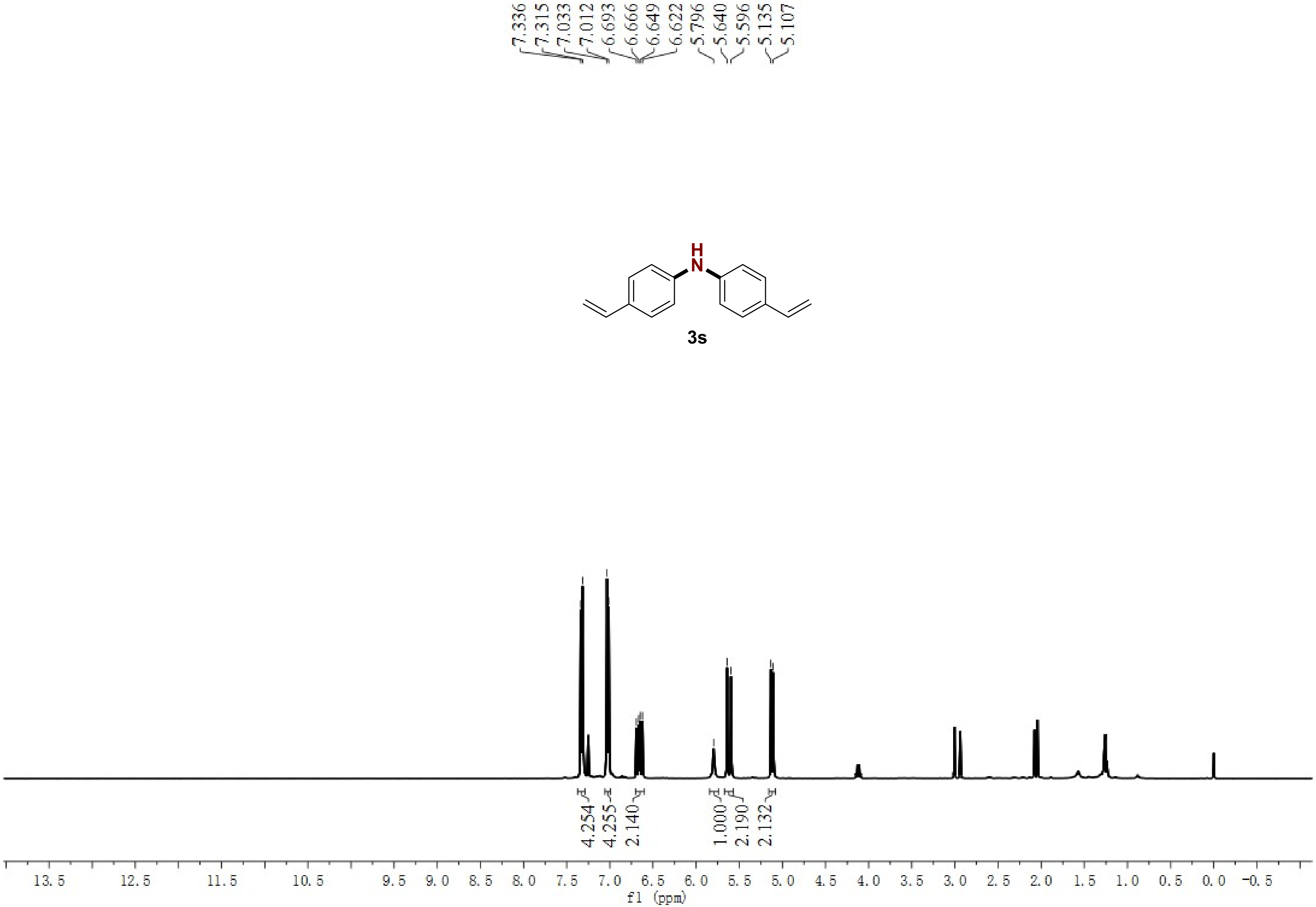


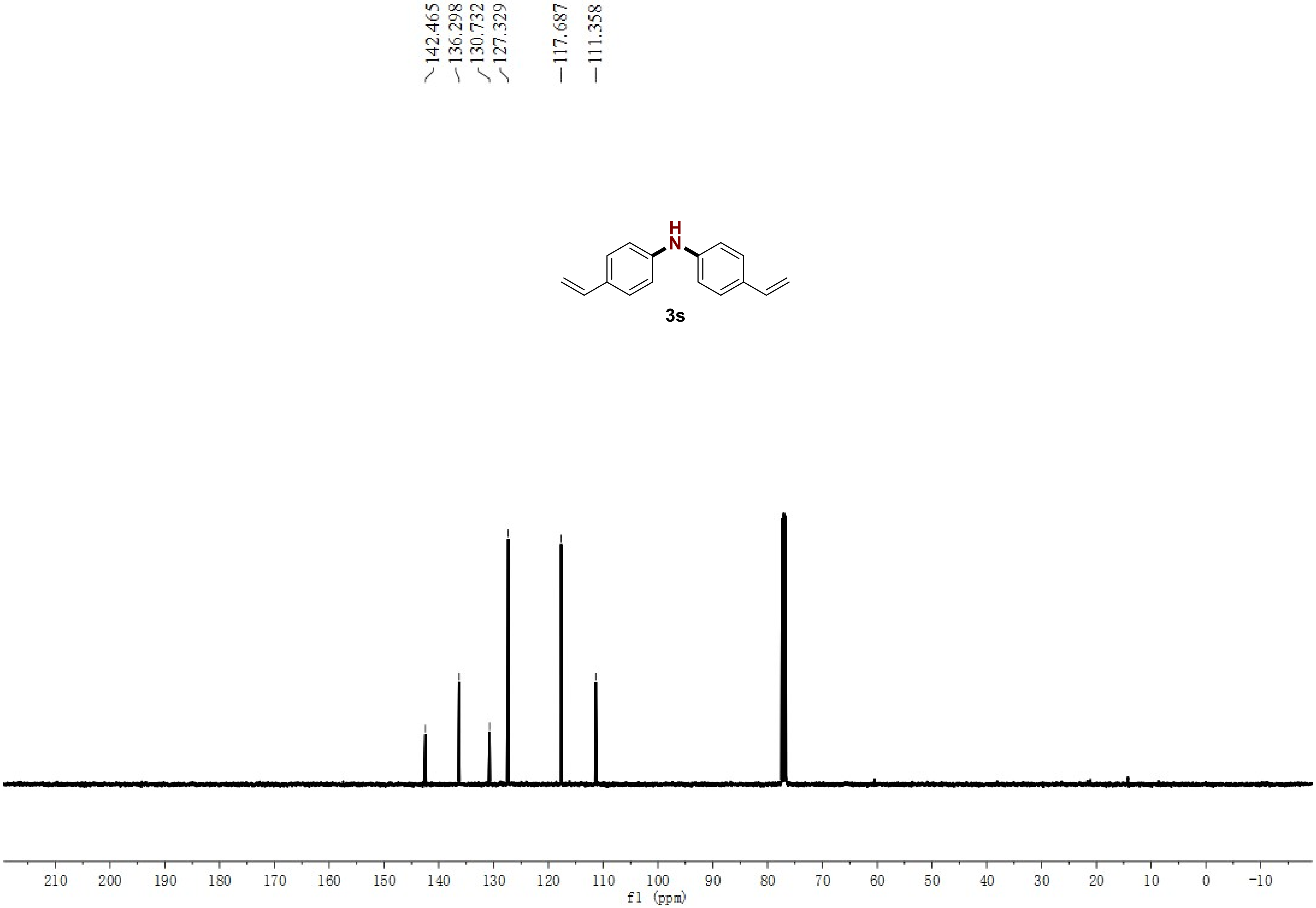
3q

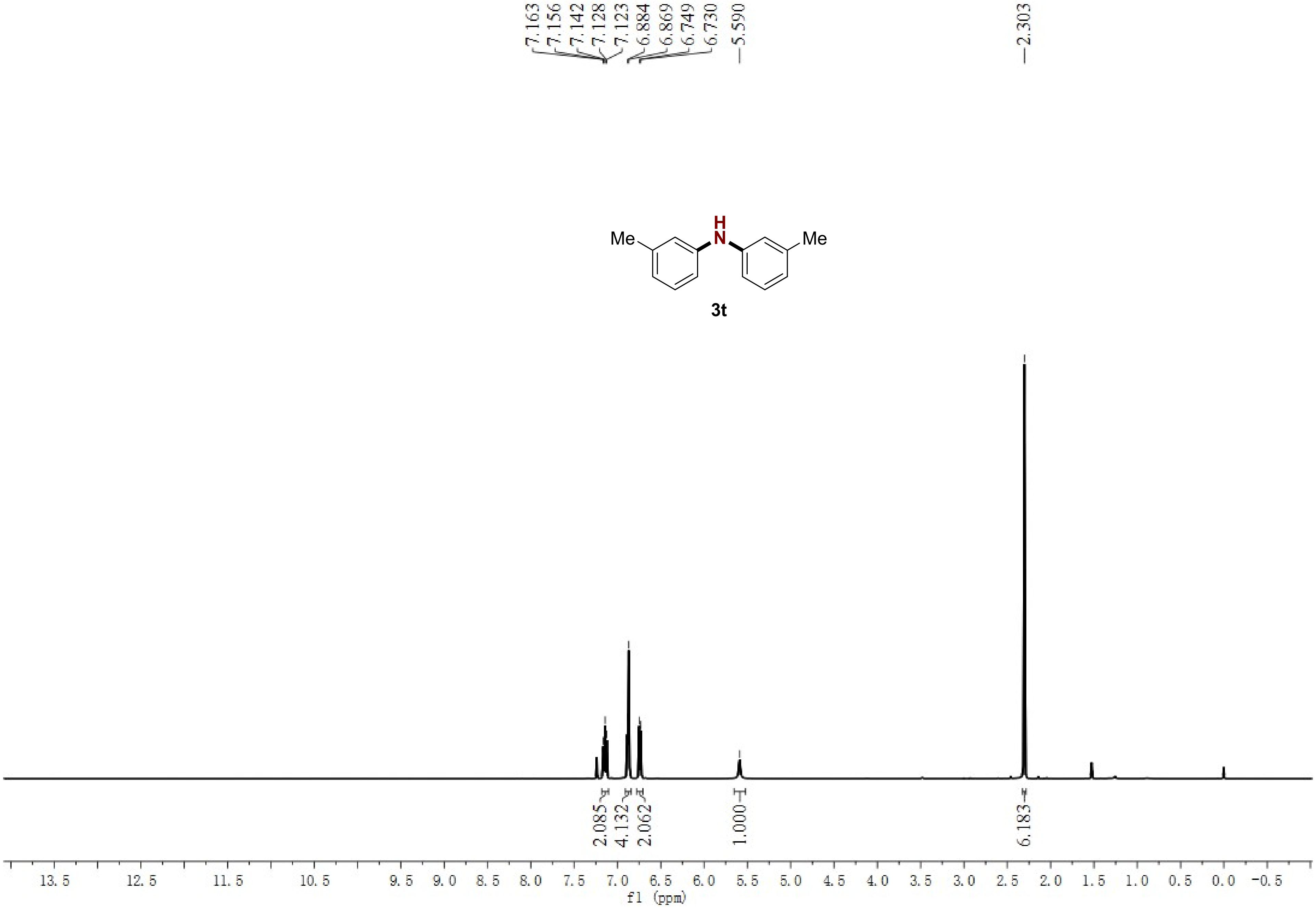
146.860
132.436
129.409
117.301
44.495
Me
S
O
O
H
N
O
O
S
Me
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

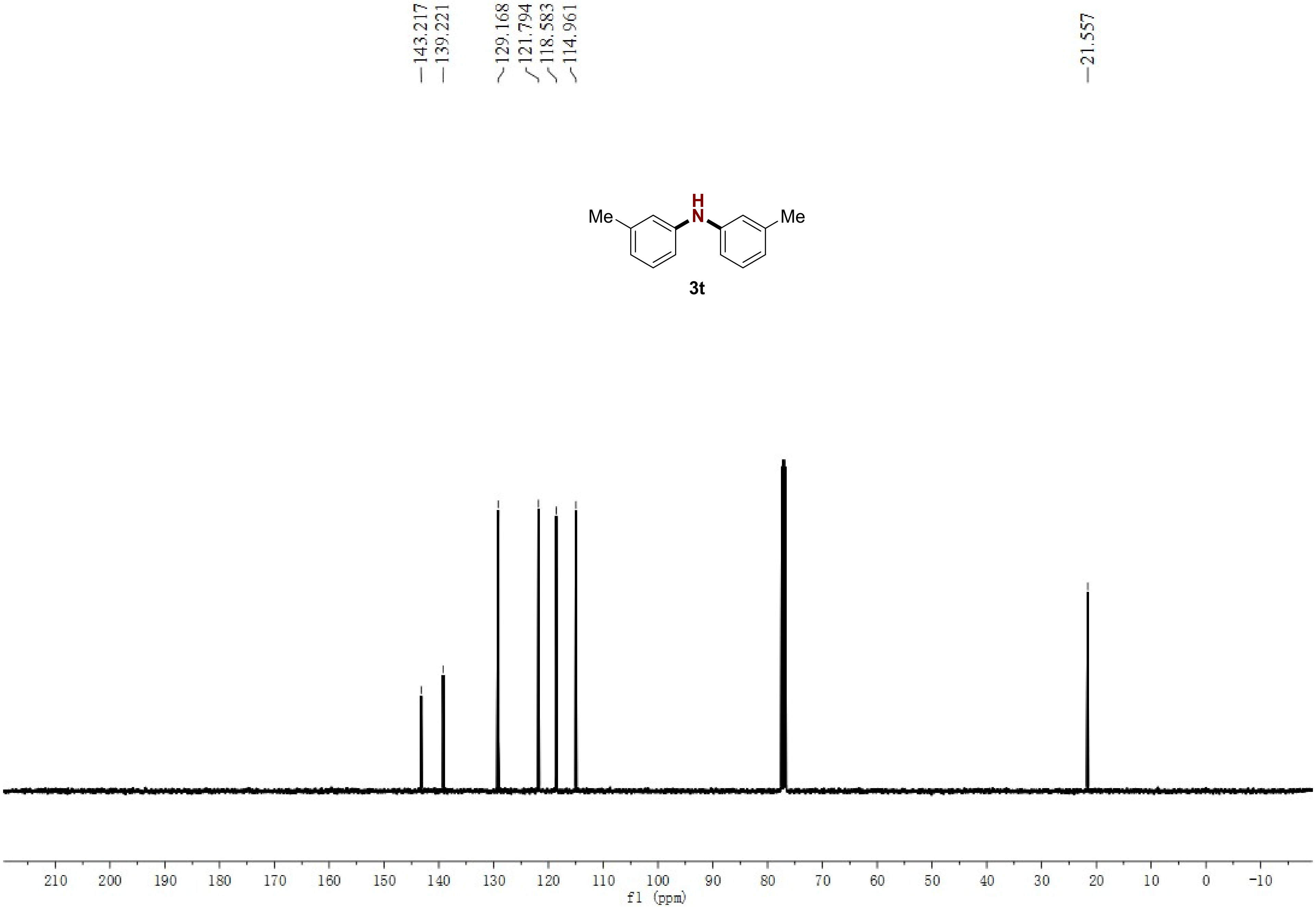

9.454
7.724
7.702
7.279
7.257
H
N
NC
CN
3r
1.000
4.015
4.110
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
−2
−3
f1 (ppm)

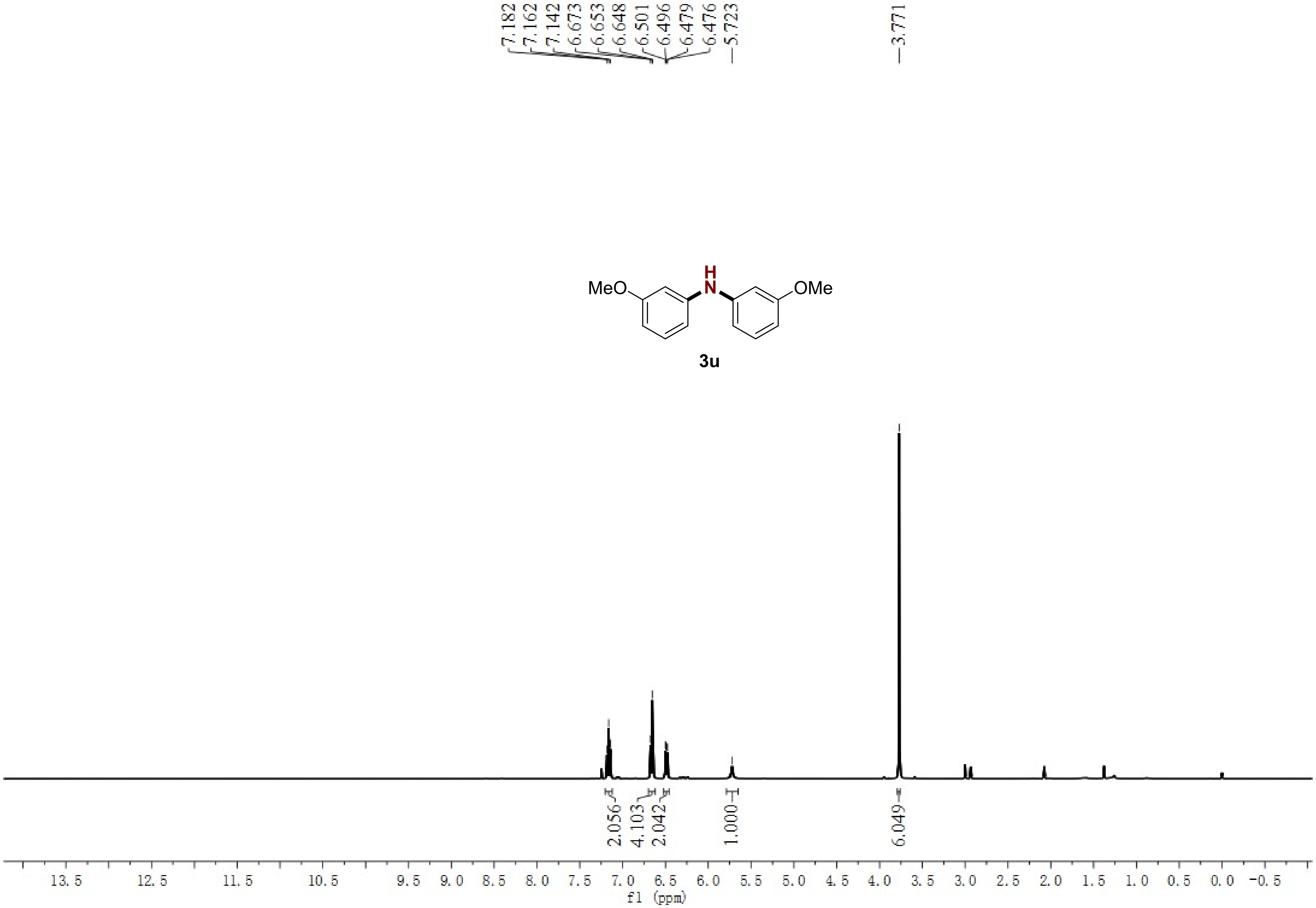

146.224
134.252
119.903
117.760
102.573
NC
H
N
CN
3r
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

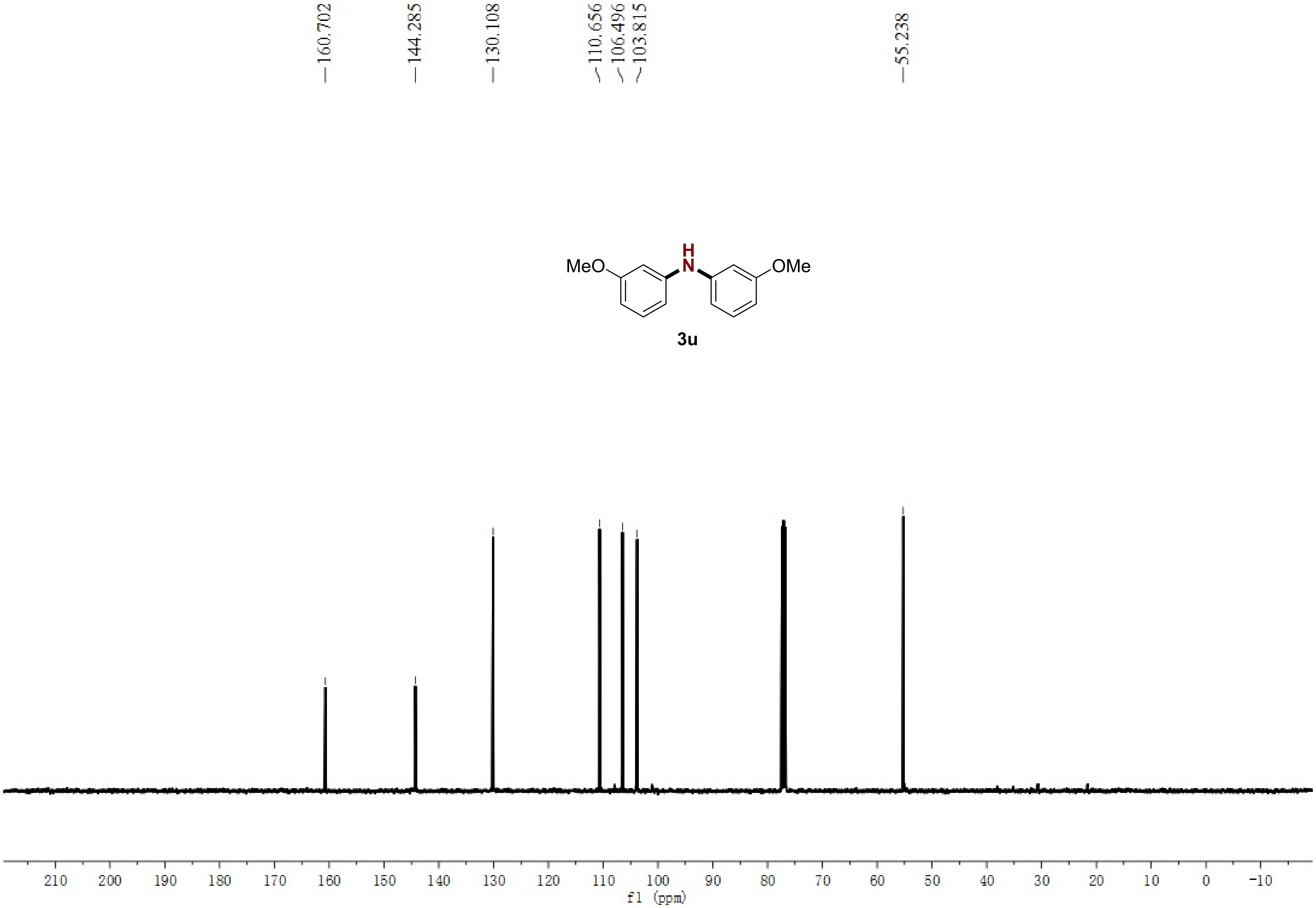

7.336
7.315
7.033
7.012
6.693
6.666
6.649
6.622
5.796
5.640
5.596
5.135
5.107
H
N
3s
4.254
4.255
2.140
1.000
2.190
2.132
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

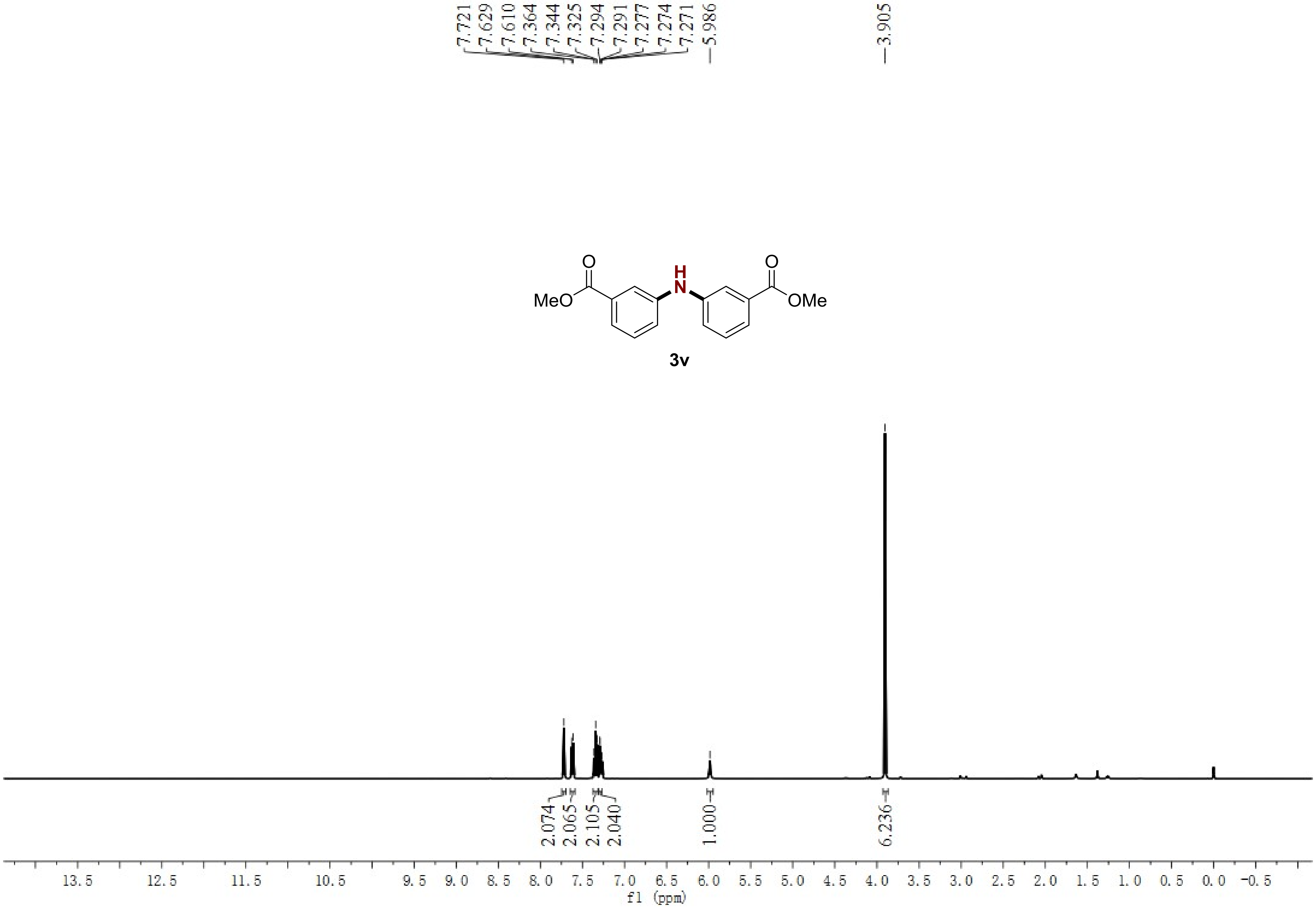

142.465
136.298
130.732
127.329
117.687
111.358
H
N
3s
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

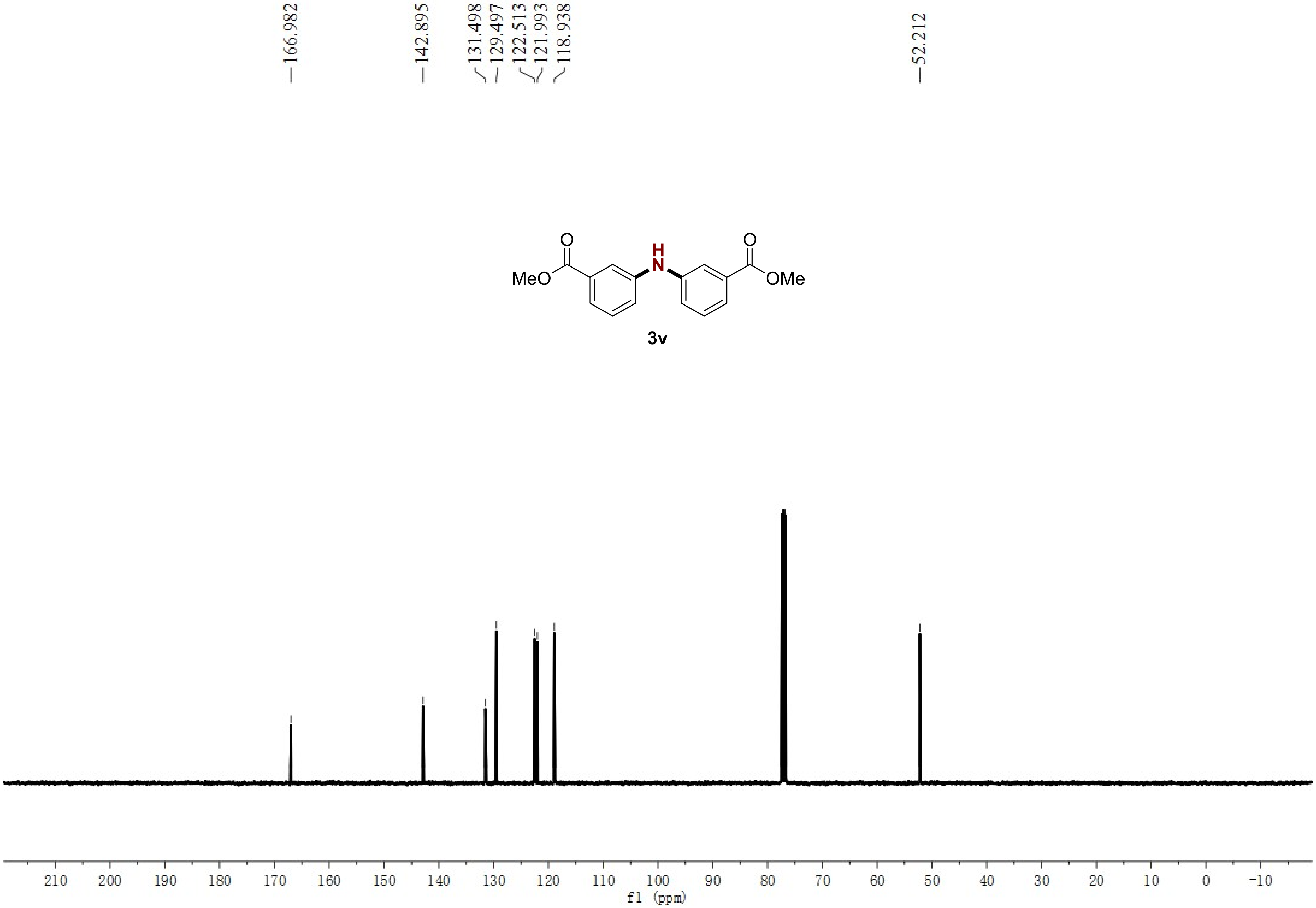

7.163
7.156
7.142
7.128
7.123
6.884
6.869
6.749
6.730
5.590
2.303
Me
H
N
Me
3t
2.085
4.132
2.062
1.000
6.183
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

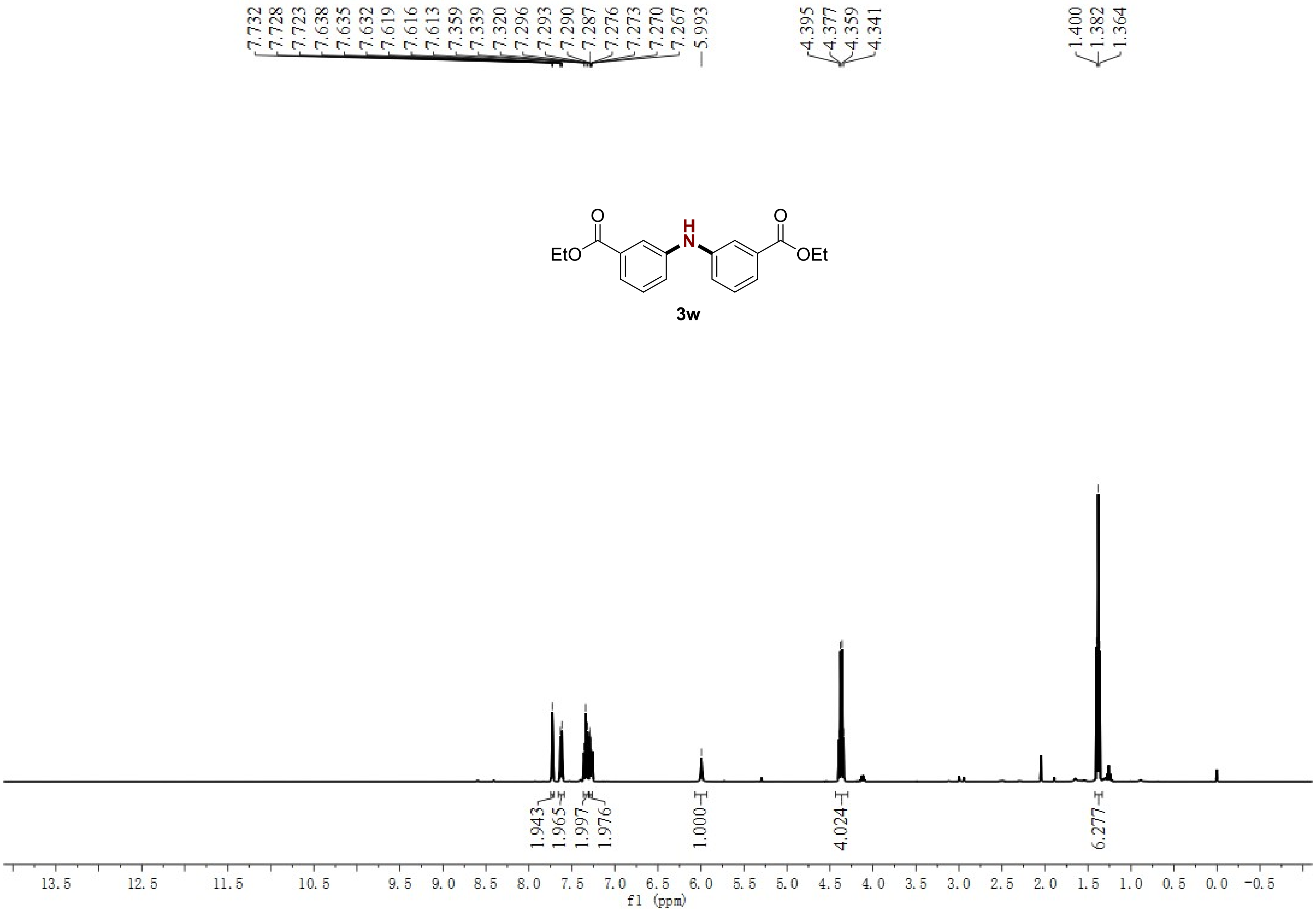

143.217
139.221
129.168
121.794
118.583
114.961
21.557
Me
H
N
Me
3t
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

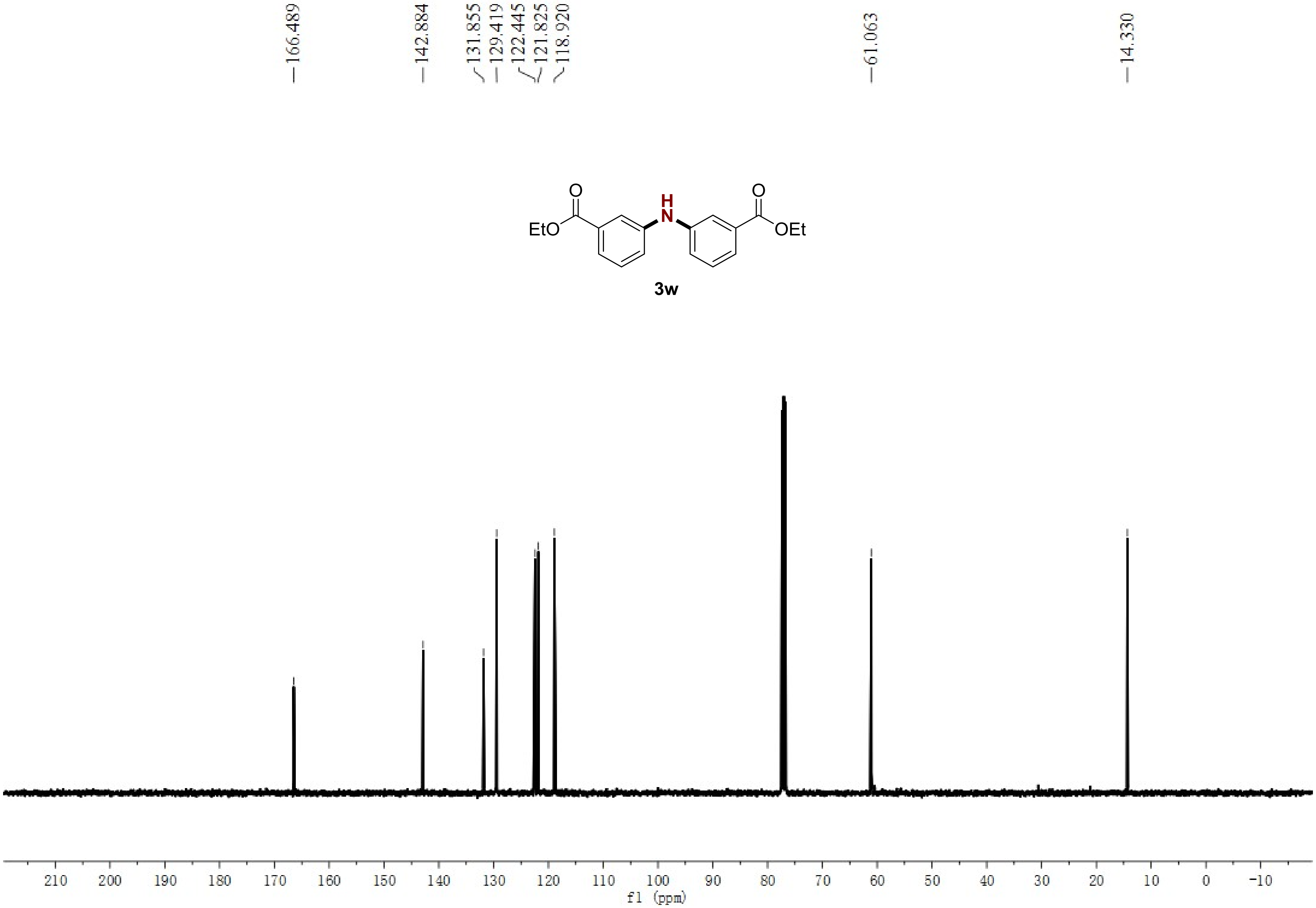

7.182
7.162
7.142
6.673
6.653
6.648
6.501
6.496
6.479
6.476
5.723
3.771
MeO
H
N
OMe
3u
2.056
4.103
2.042
1.000
6.049
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


160.702
144.285
130.108
110.656
106.496
103.815
55.238
MeO
H
N
OMe
3u
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)

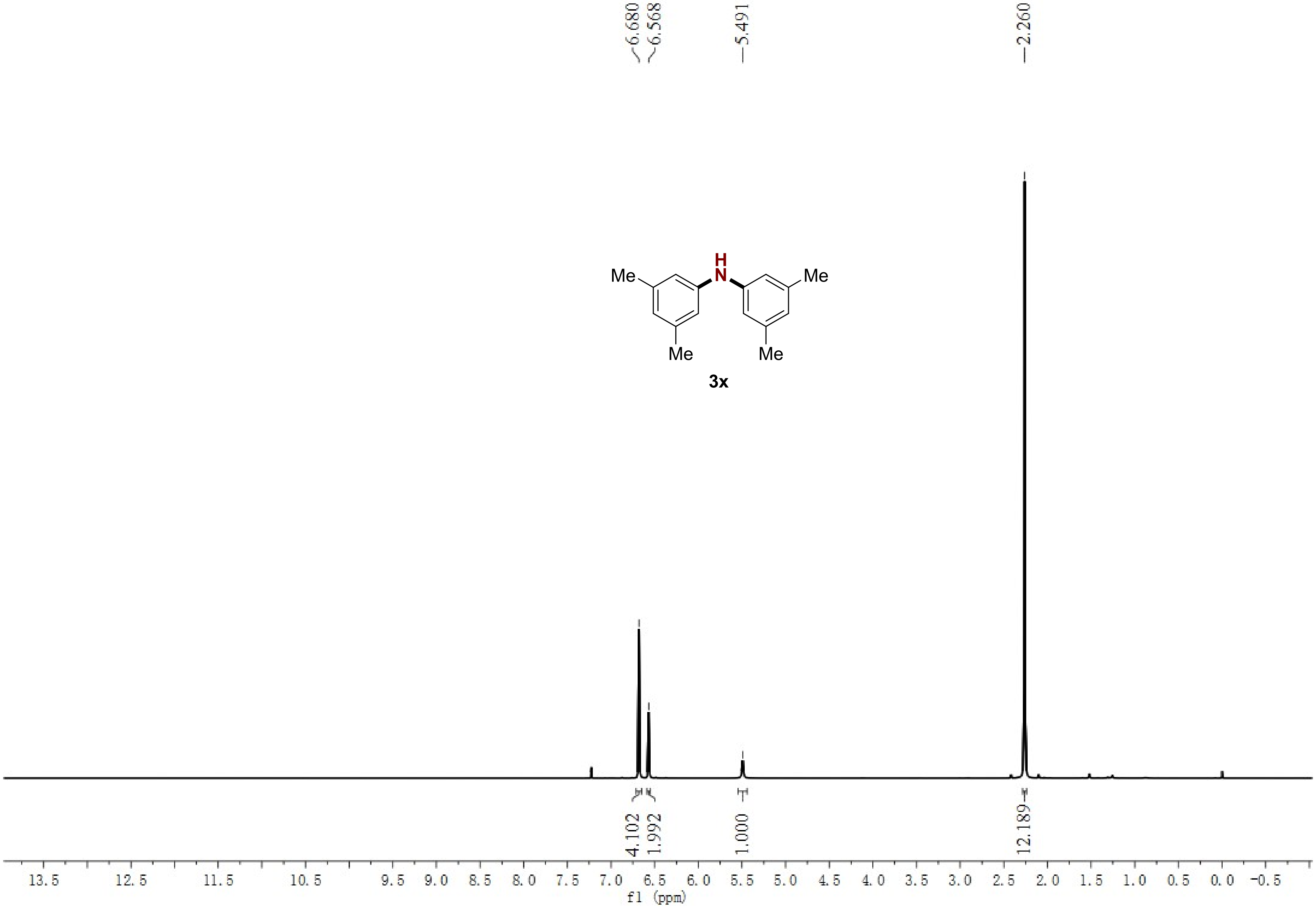

7.721
7.629
7.610
7.364
7.344
7.325
7.294
7.291
7.277
7.274
7.271
5.986
3.905
O
H
N
O
MeO
OMe
3v
2.074
2.065
2.105
2.040
1.000
6.236
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


166.982
142.895
131.498
129.497
122.513
121.993
118.938
52.212
MeO
O
H
N
O
OMe
3v
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)


7.732
7.728
7.723
7.638
7.635
7.632
7.619
7.616
7.613
7.359
7.339
7.320
7.296
7.293
7.290
7.287
7.276
7.273
7.270
7.267
5.993
4.395
4.377
4.359
4.341
1.400
1.382
1.364
O
H
N
O
EtO
OEt
3w
1.943
1.965
1.997
1.976
1.000
4.024
6.277
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
f1 (ppm)

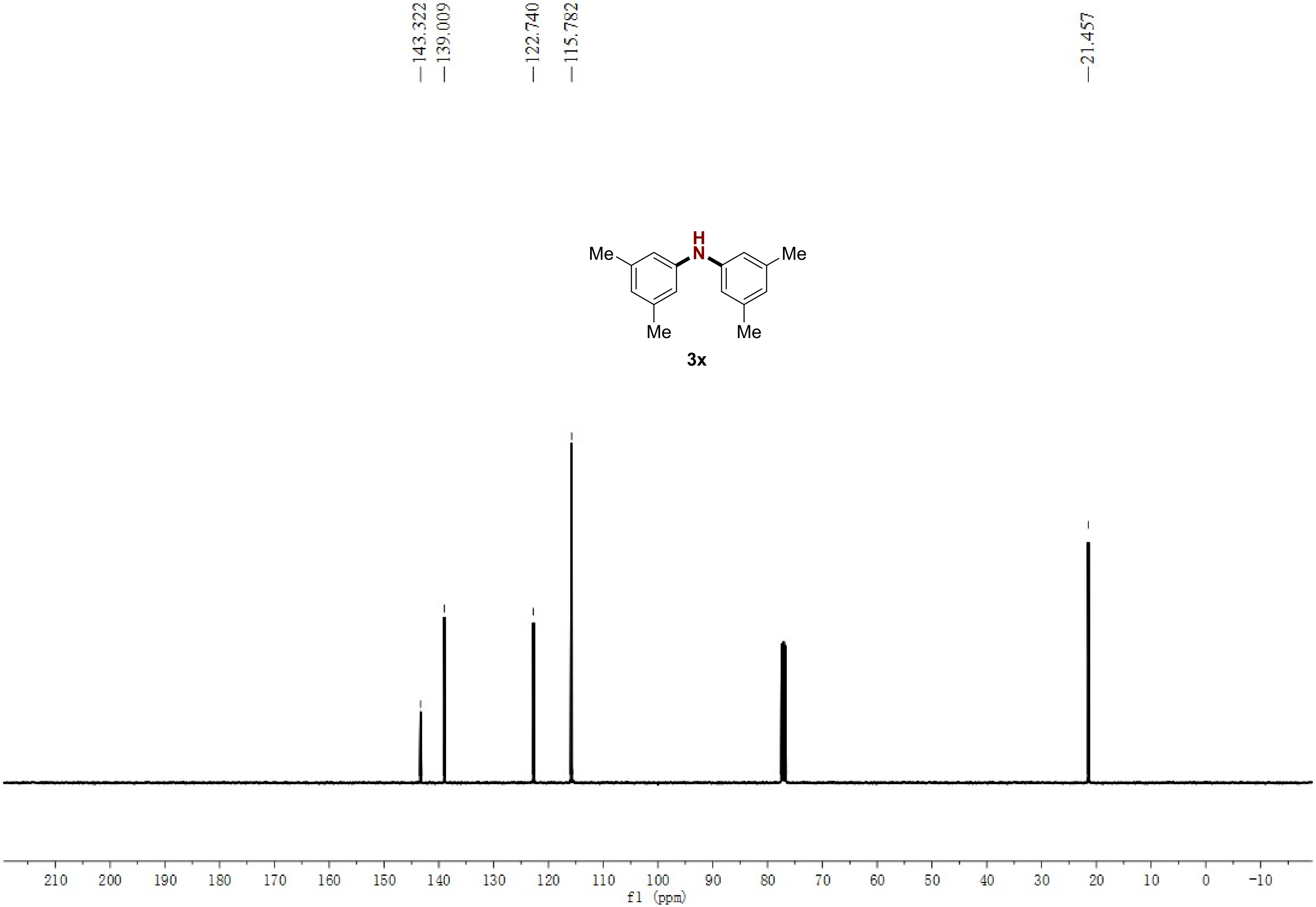

166.489
142.884
131.855
129.419
122.445
121.825
118.920
61.063
14.330
O
H
N
O
EtO
OEt
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

3w



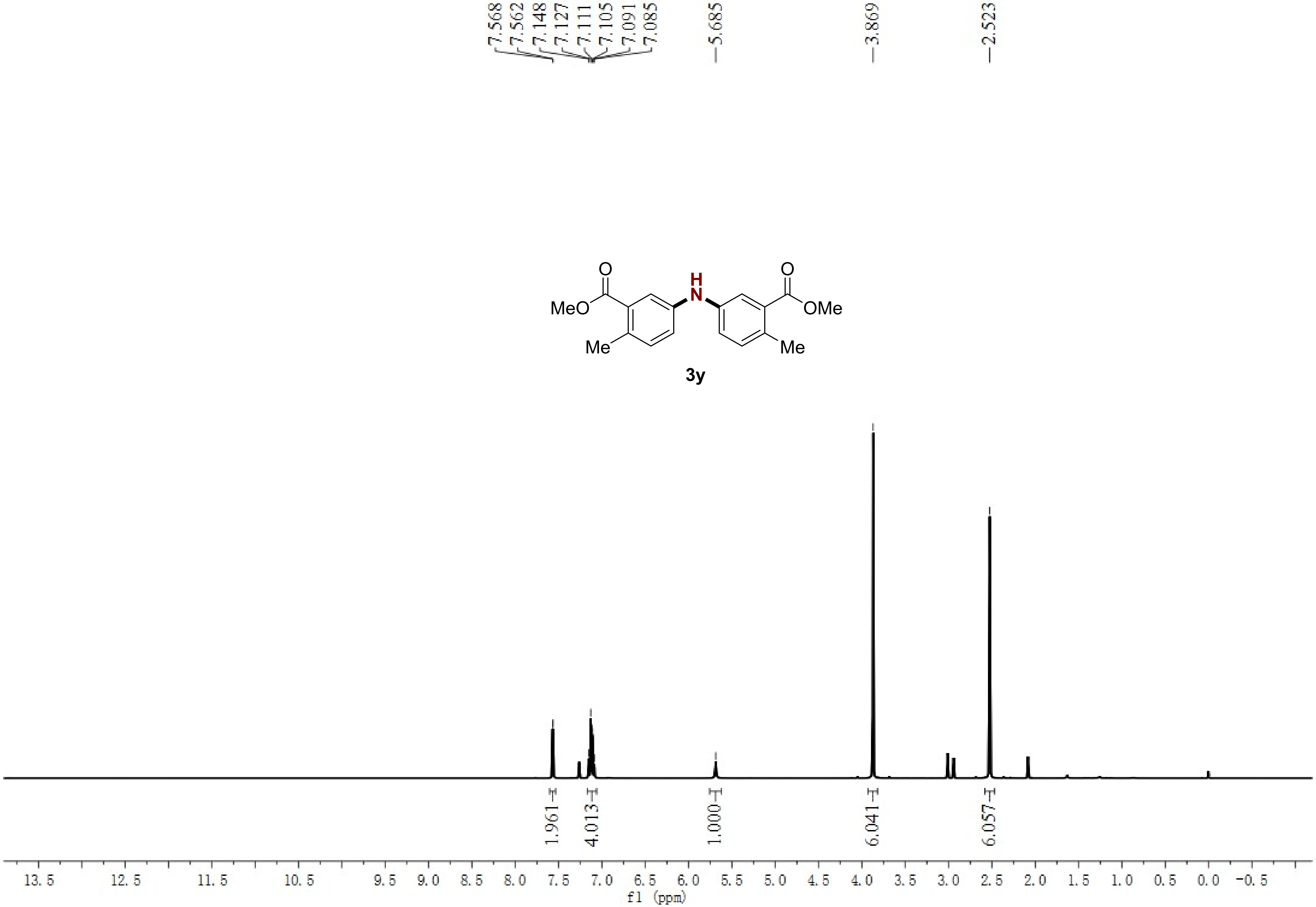
3x

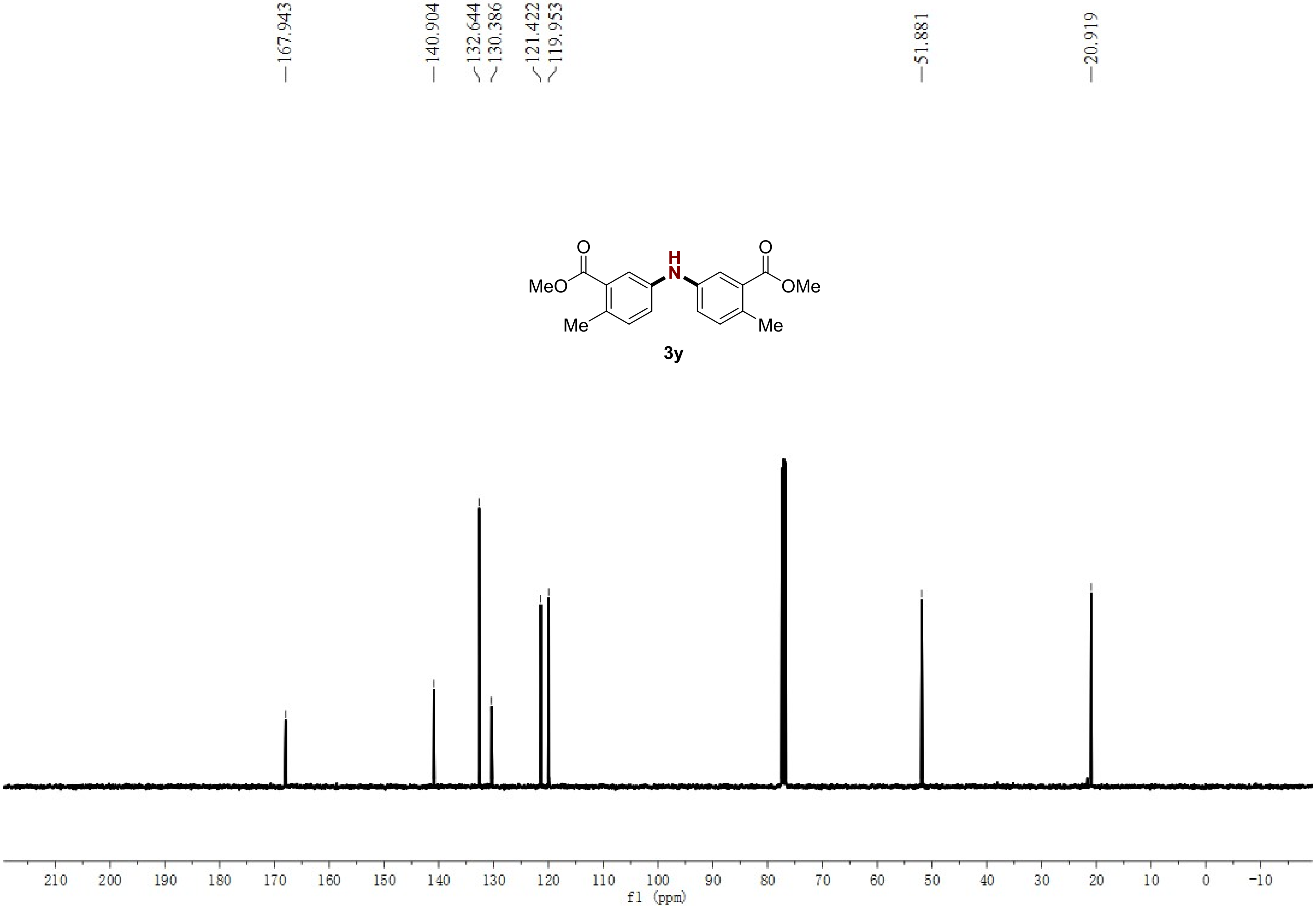
6.680
6.568
5.491
2.260
H
N
Me
Me
Me
Me
4.102
1.992
1.000
12.189
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)



3x

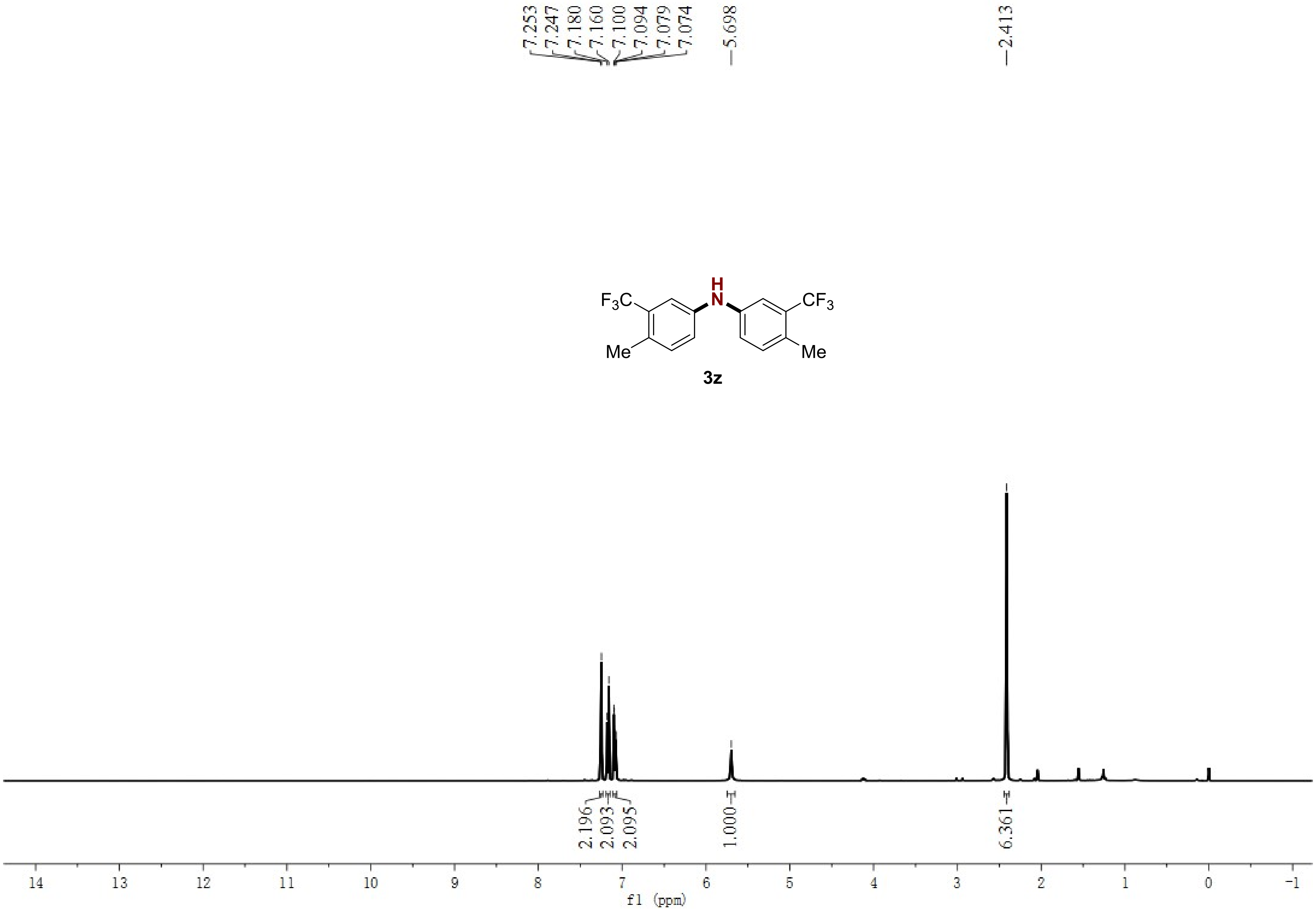
143.322
139.009
122.740
115.782
21.457
Me
H
N
Me
Me
Me
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)


7.568
7.562
7.148
7.127
7.111
7.105
7.091
7.085
5.685
3.869
2.523
O
MeO
H
N
O
OMe
Me
Me
3y
1.961
4.013
1.000
6.041
6.057
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

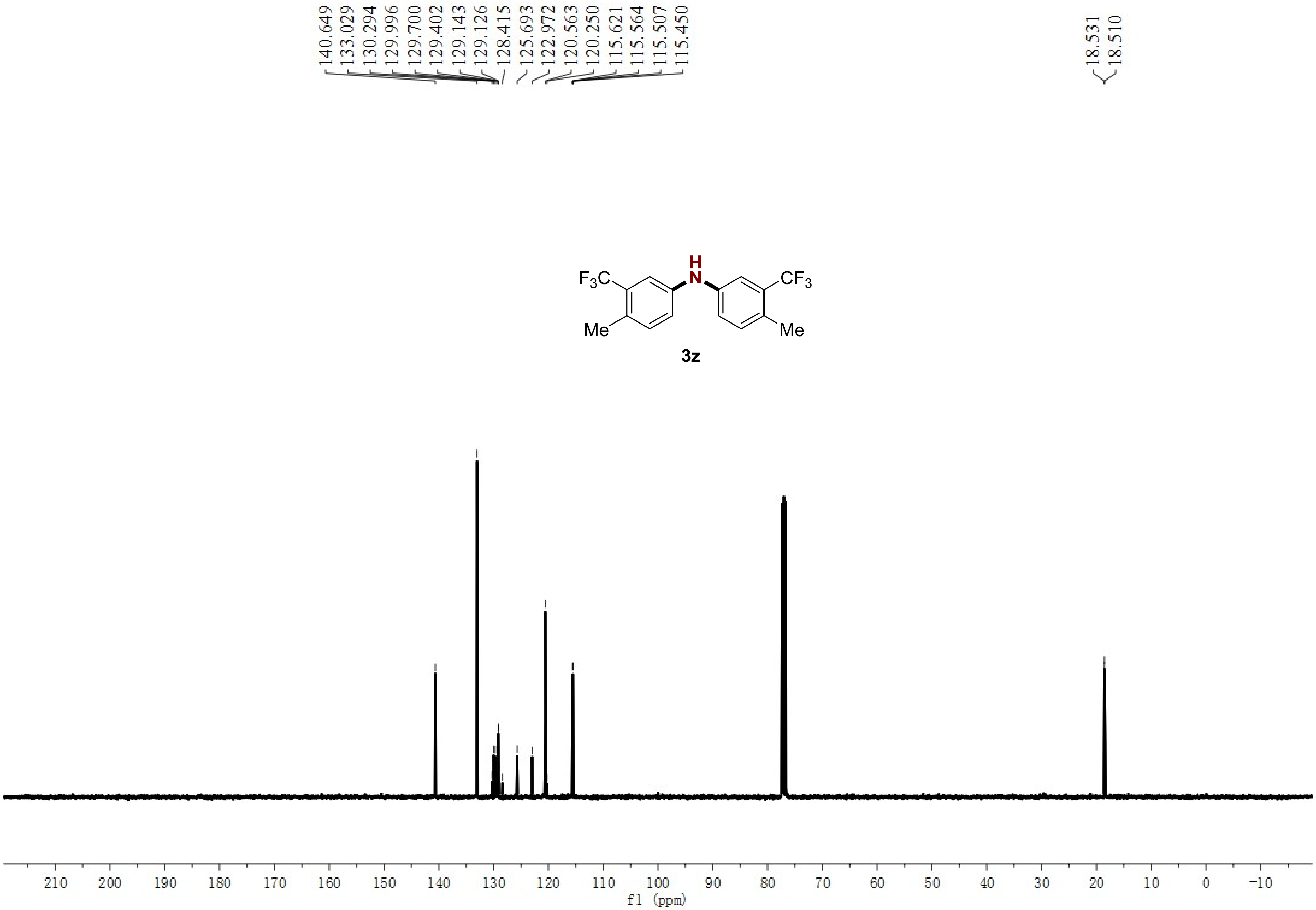


3y

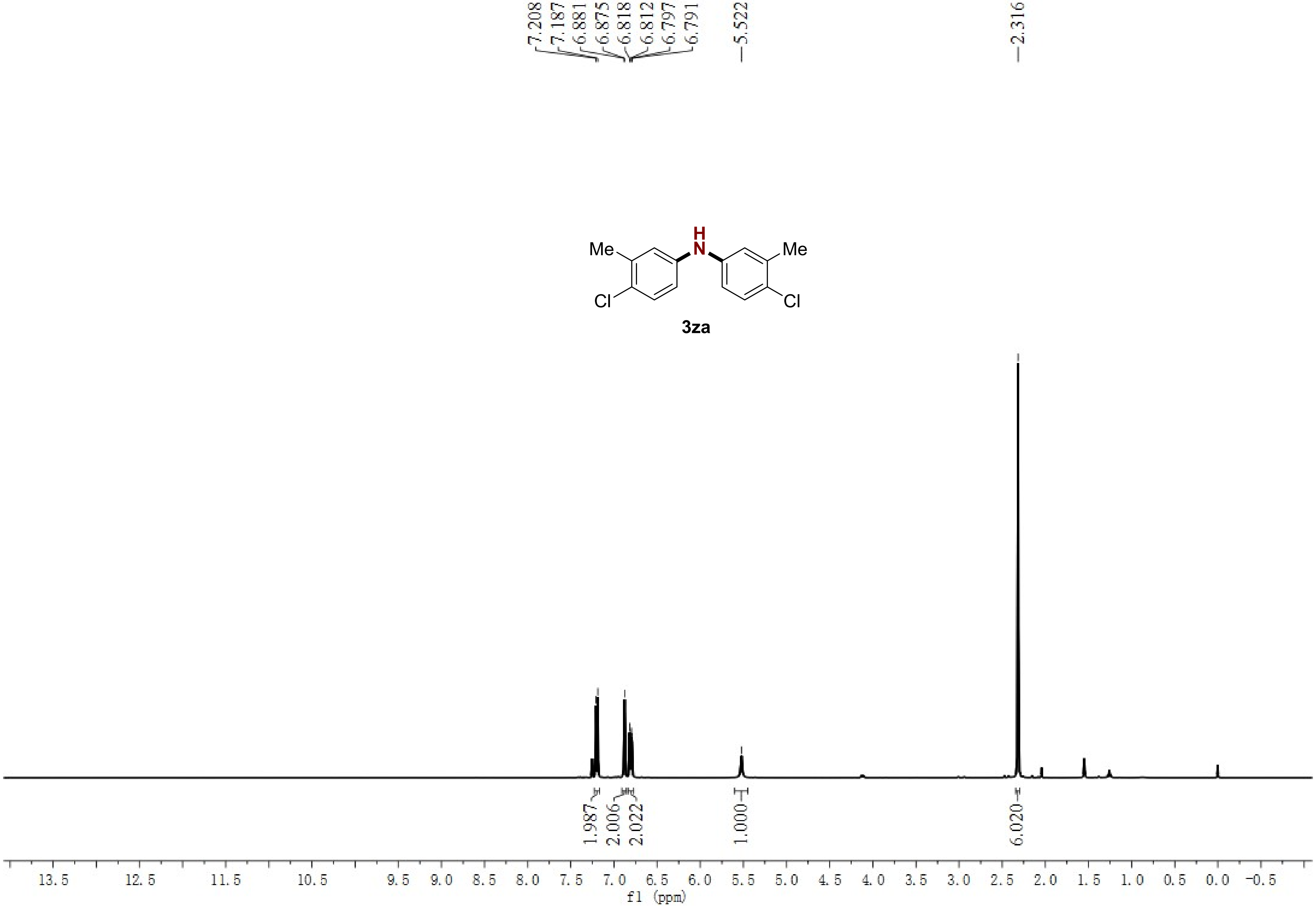
167.943
140.904
132.644
130.386
121.422
119.953
51.881
20.919
MeO
O
H
N
OMe
Me
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

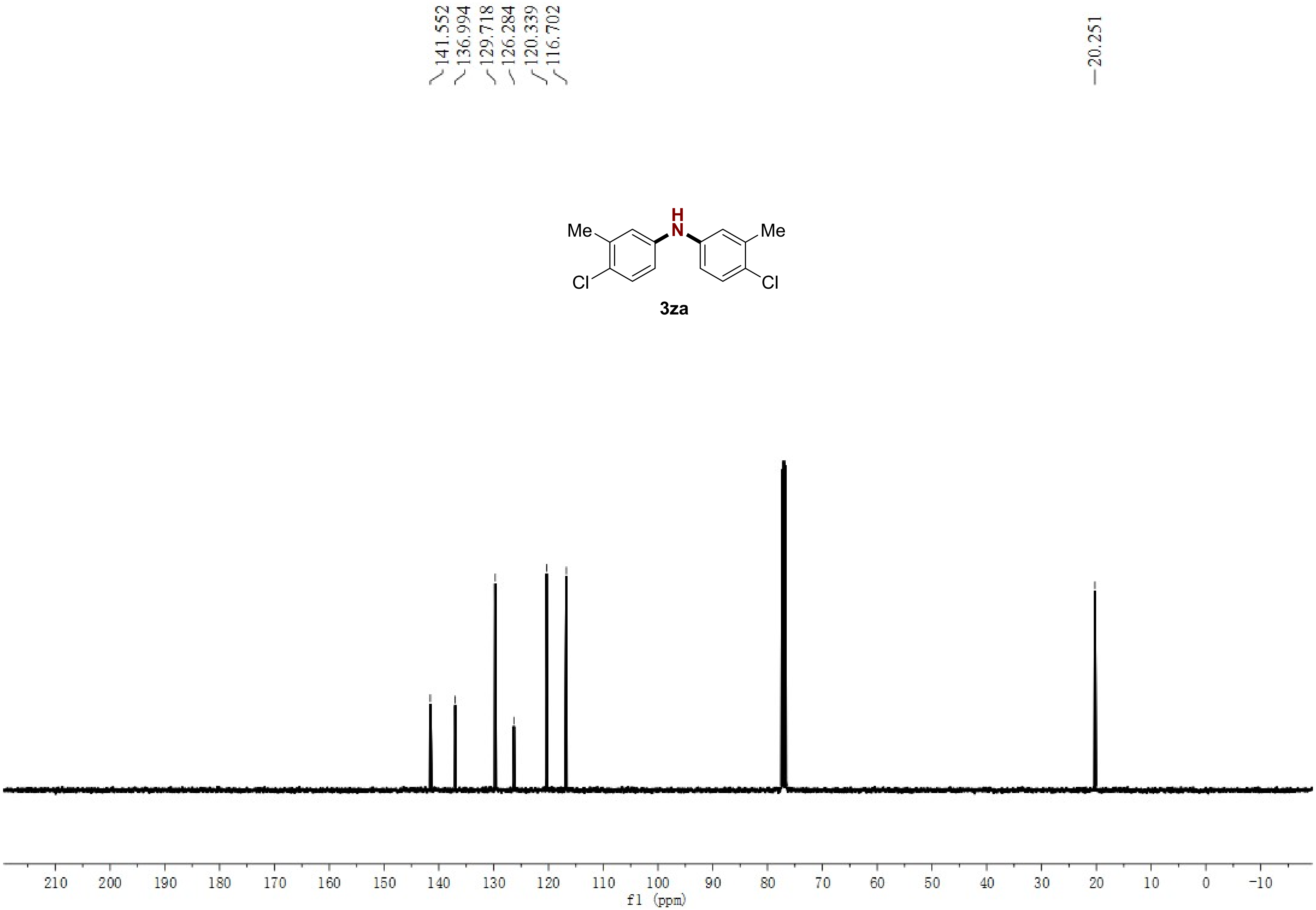

7.253
7.247
7.180
7.160
7.100
7.094
7.079
7.074
5.698
2.413
F3C
H
N
CF3
Me
Me
2.196
2.093
2.095
1.000
6.361
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
f1 (ppm)

3z

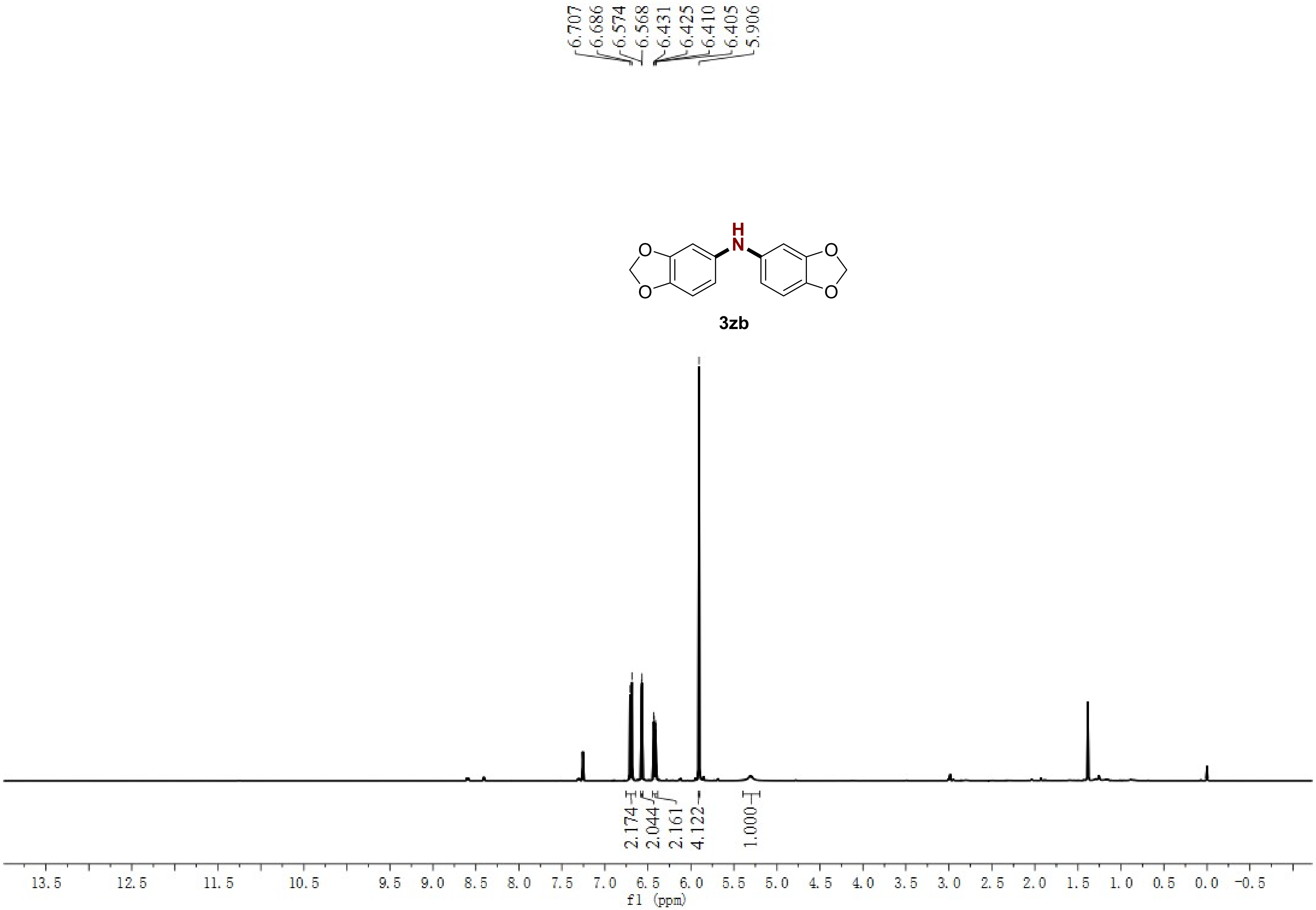

140.649
133.029
130.294
129.996
129.700
129.402
129.143
129.126
128.415
125.693
122.972
120.563
120.250
115.621
115.564
115.507
115.450
18.531
18.510
F$_3$C
H
N
CF$_3$
Me
Me
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

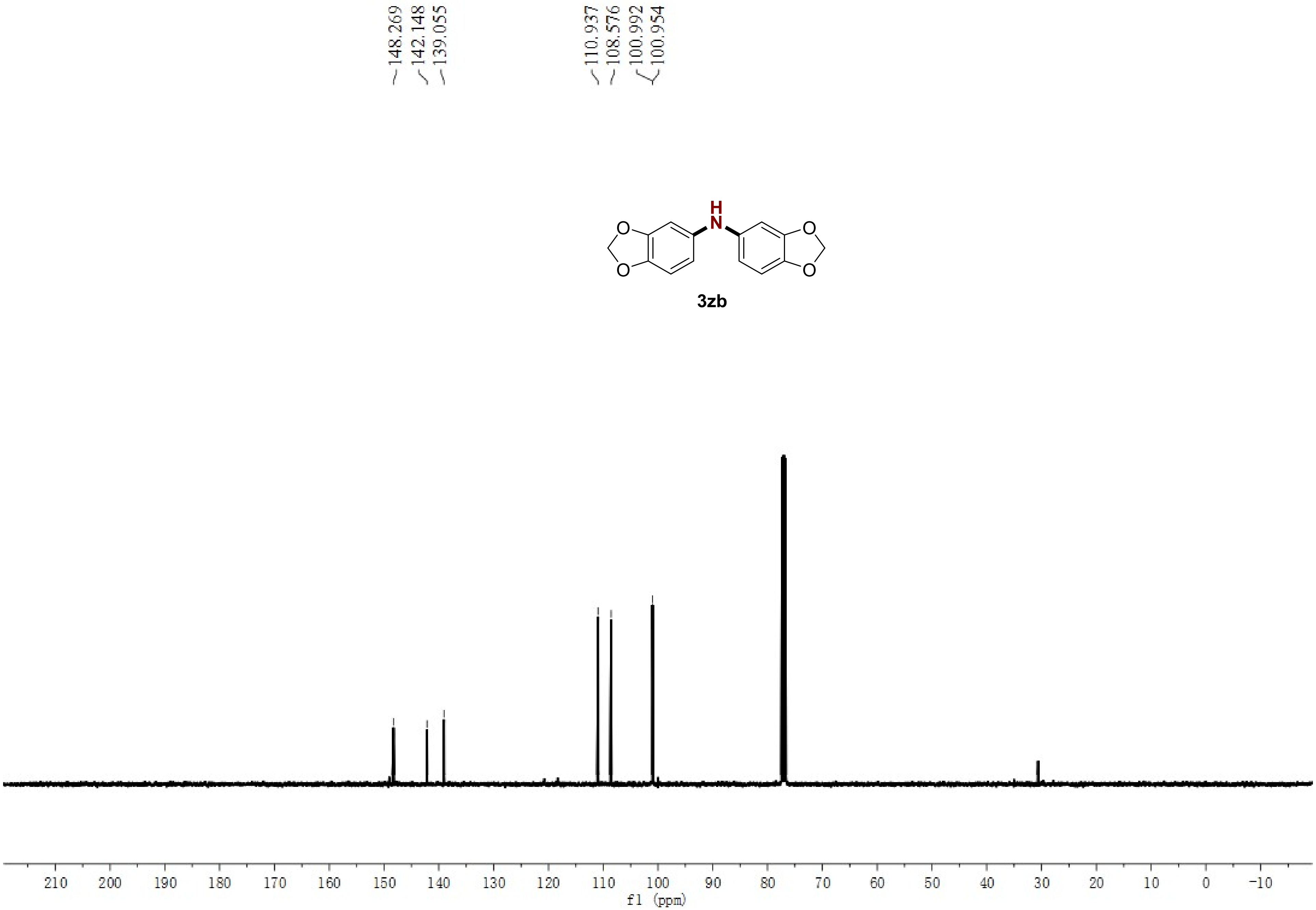
3z


7.208
7.187
6.881
6.875
6.818
6.812
6.797
6.791
5.522
2.316
Me
H
N
Me
Cl
Cl
3za
1.987
2.006
2.022
1.000
6.020
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

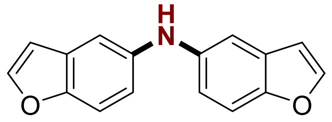

141.552
136.994
129.718
126.284
120.339
116.702
20.251
Me
H
N
Me
Cl
Cl
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

3za

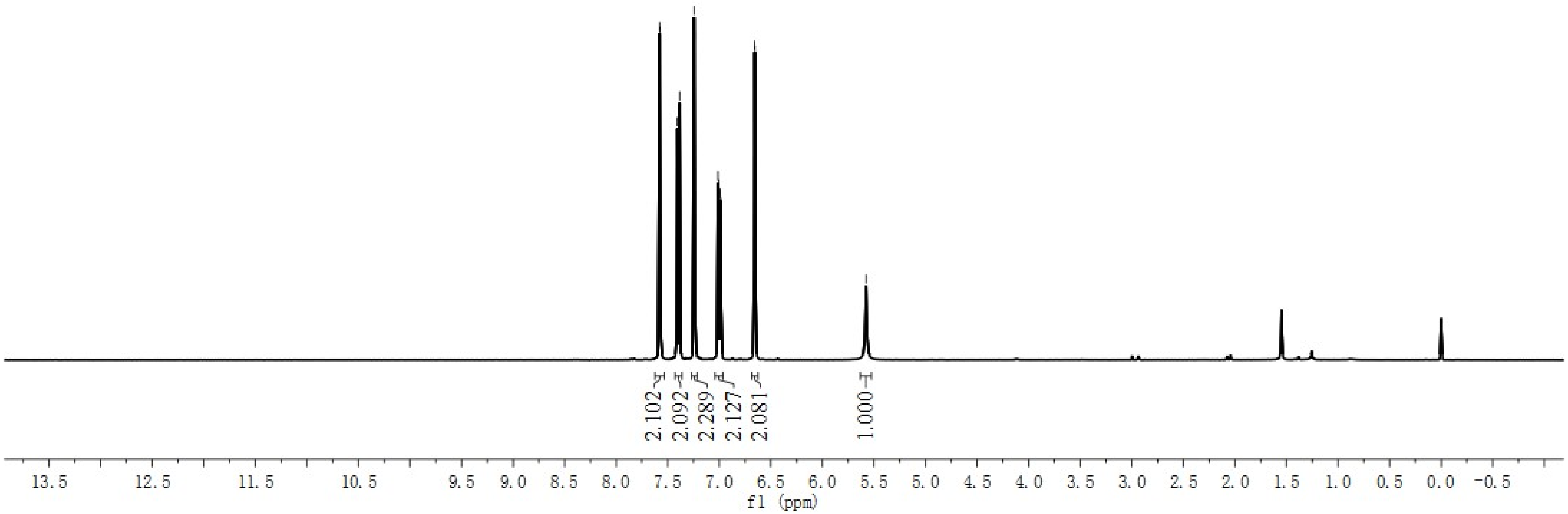

6.707
6.686
6.574
6.568
6.431
6.425
6.410
6.405
5.906
H
N
O
O
O
O
3zb
2.174
2.044
2.161
4.122
1.000
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
f1 (ppm)

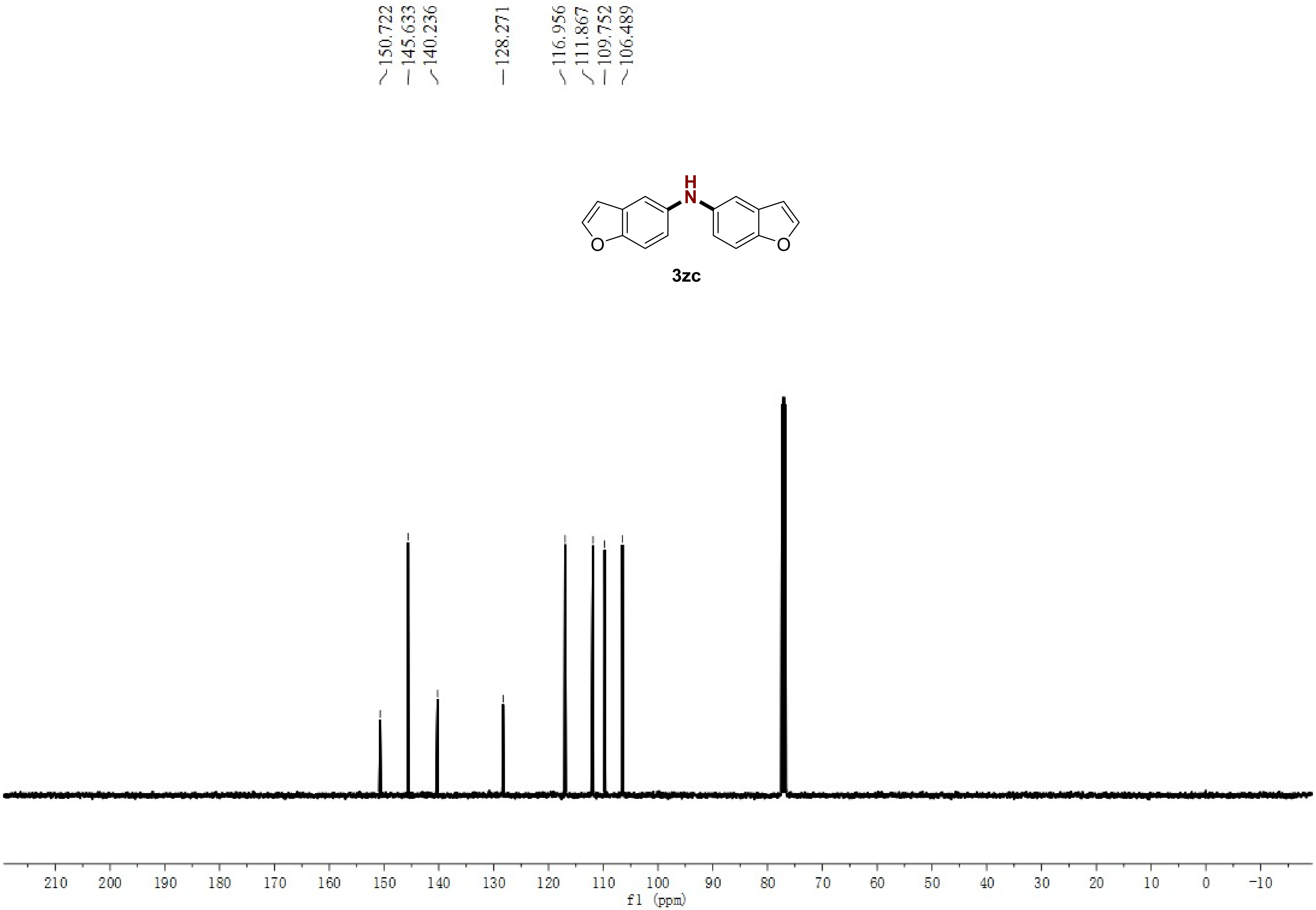

148.269
142.148
139.055
110.937
108.576
100.992
100.954
H
N
O
O
O
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

3zb

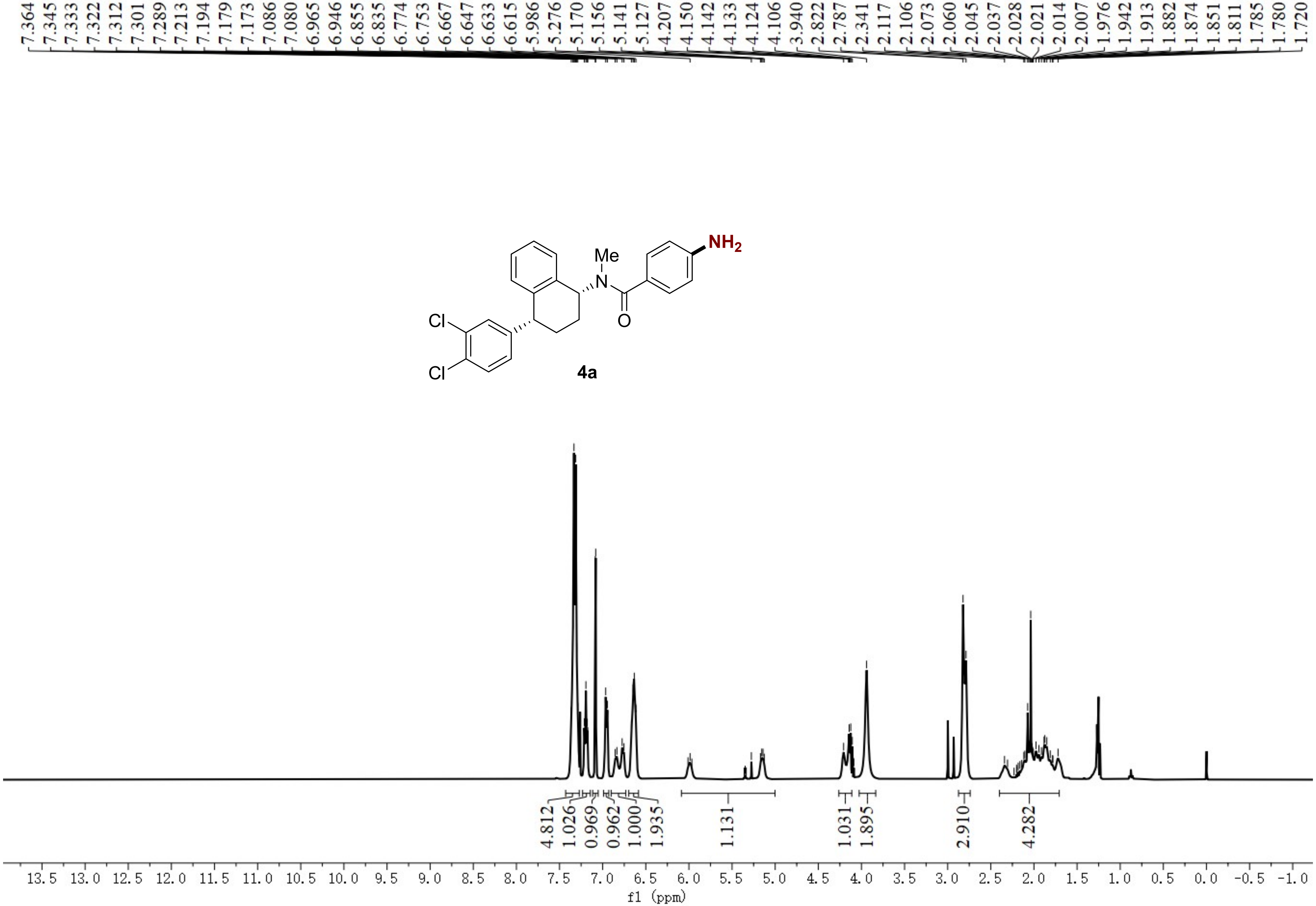


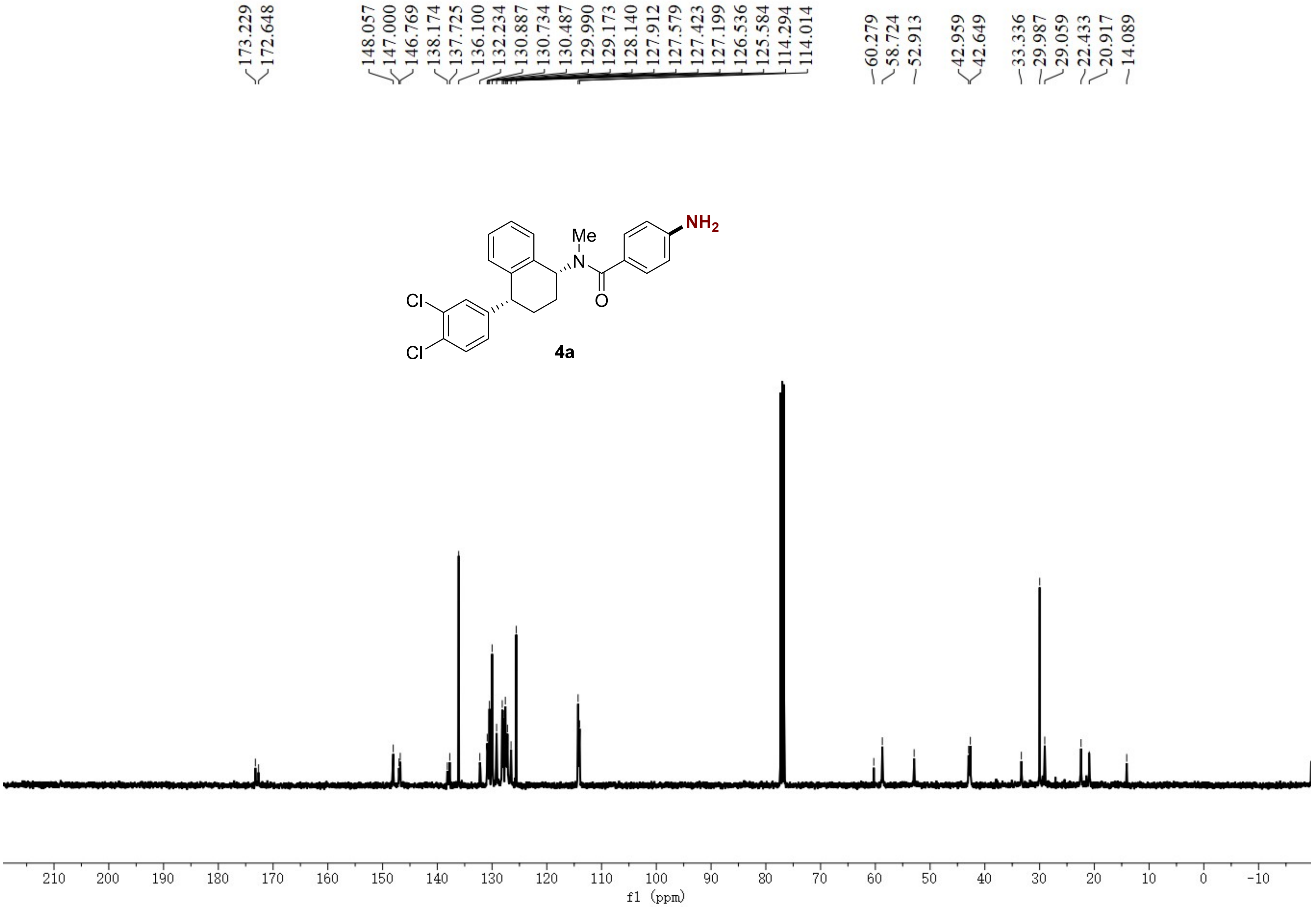
3zc


7.579
7.574
7.407
7.385
7.245
7.239
7.013
7.007
6.991
6.986
6.657
6.654
5.576
2.102
2.092
2.289
2.127
2.081
1.000
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

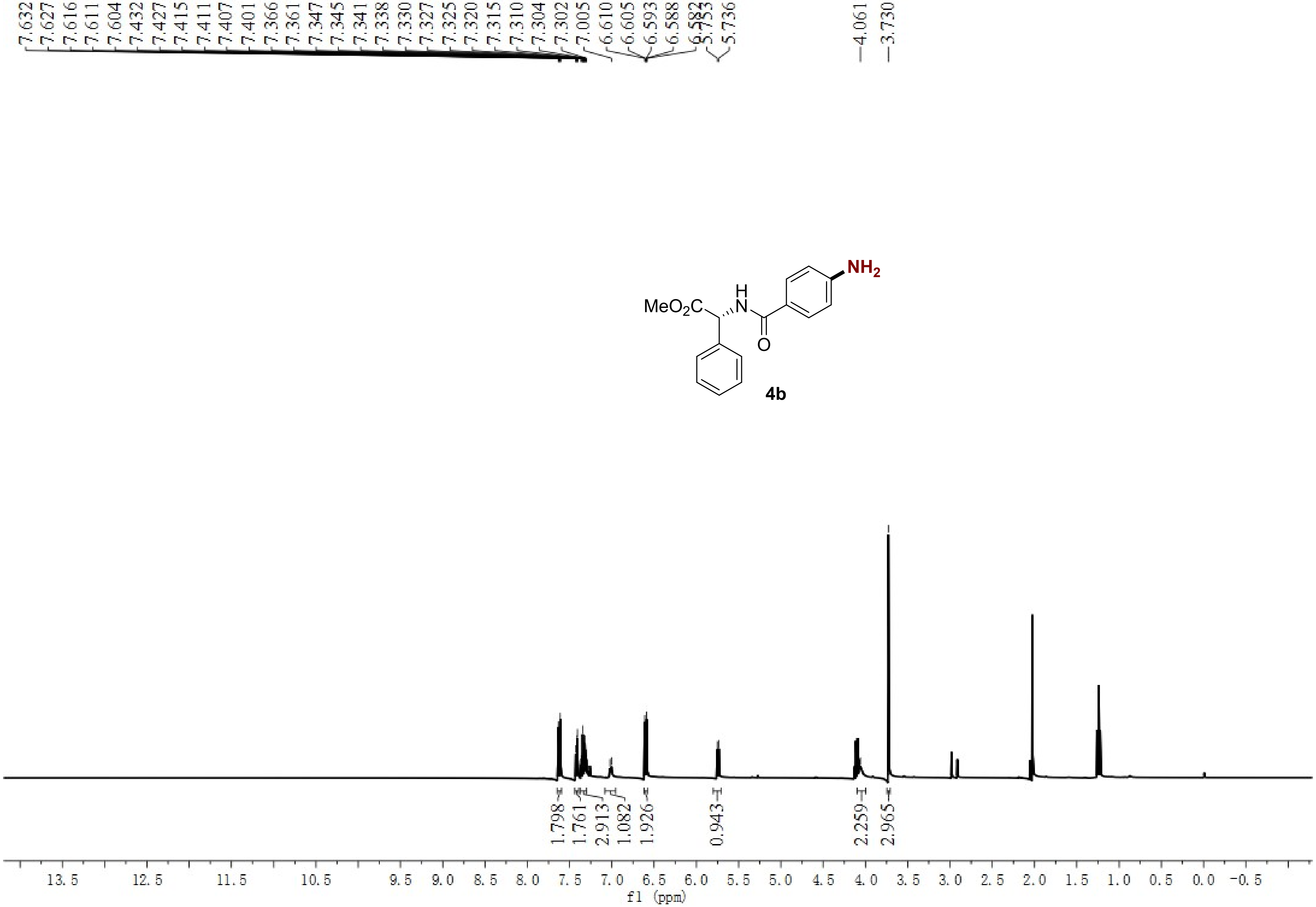

150.722
145.633
140.236
128.271
116.956
111.867
109.752
106.489
H
N
O
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

3zc

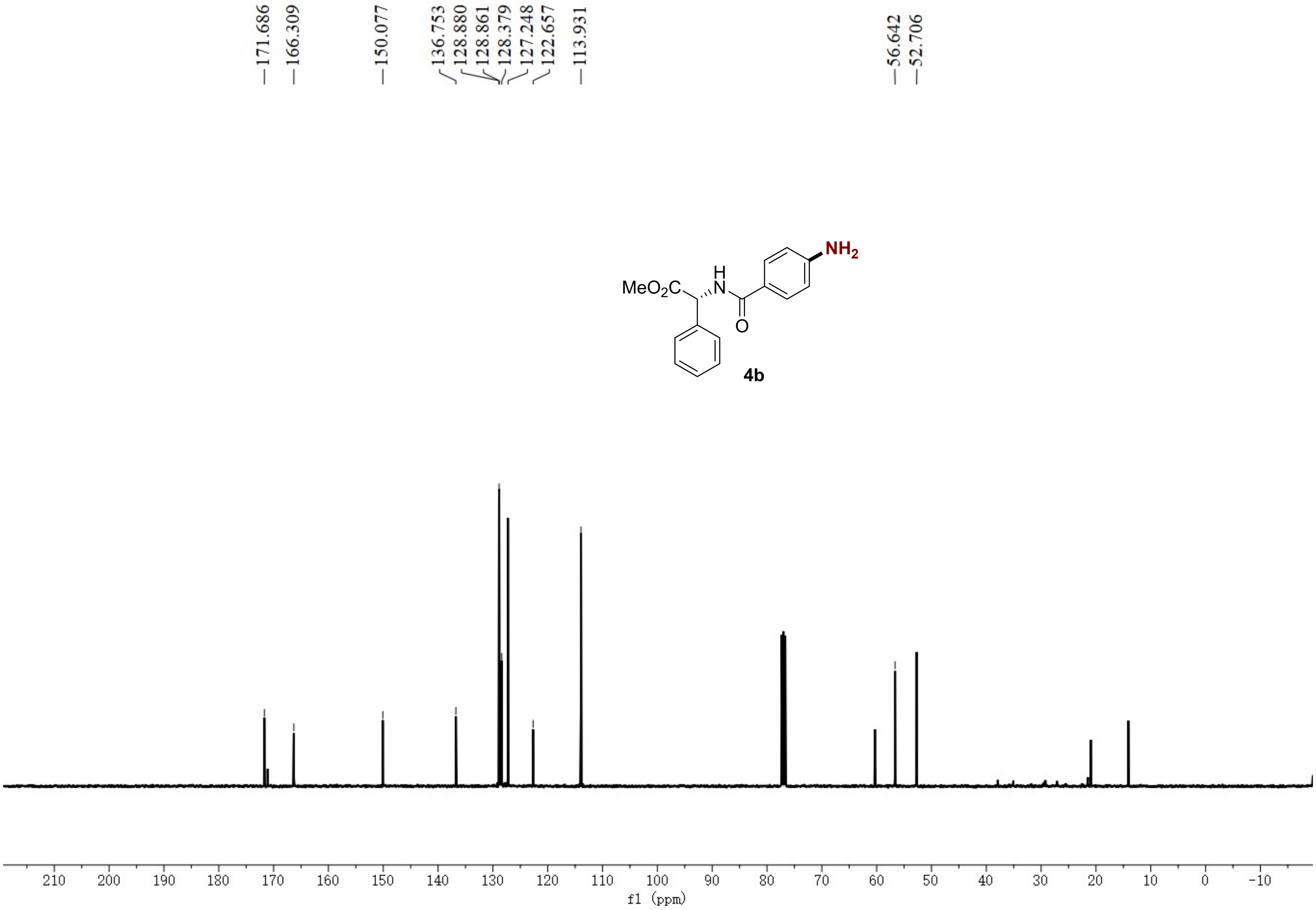

7.364
7.345
7.333
7.322
7.312
7.301
7.289
7.213
7.194
7.179
7.173
7.086
7.080
6.965
6.946
6.855
6.835
6.774
6.753
6.667
6.647
6.633
6.615
5.986
5.276
5.170
5.156
5.141
5.127
4.207
4.150
4.142
4.133
4.124
4.106
3.940
2.822
2.787
2.341
2.117
2.106
2.073
2.060
2.045
2.037
2.028
2.021
2.014
2.007
1.976
1.942
1.913
1.882
1.874
1.851
1.811
1.785
1.780
1.720
Me
N
NH2
O
Cl
Cl
4a
4.812
1.026
0.969
0.962
1.000
1.935
1.131
1.031
1.895
2.910
4.282
13.5
13.0
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)


173.229
172.648
148.057
147.000
146.769
138.174
137.725
136.100
132.234
130.887
130.734
130.487
129.990
129.173
128.140
127.912
127.579
127.423
127.199
126.536
125.584
114.294
114.014
60.279
58.724
52.913
42.959
42.649
33.336
29.987
29.059
22.433
20.917
14.089
Me
N
NH2
O
Cl
Cl
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)

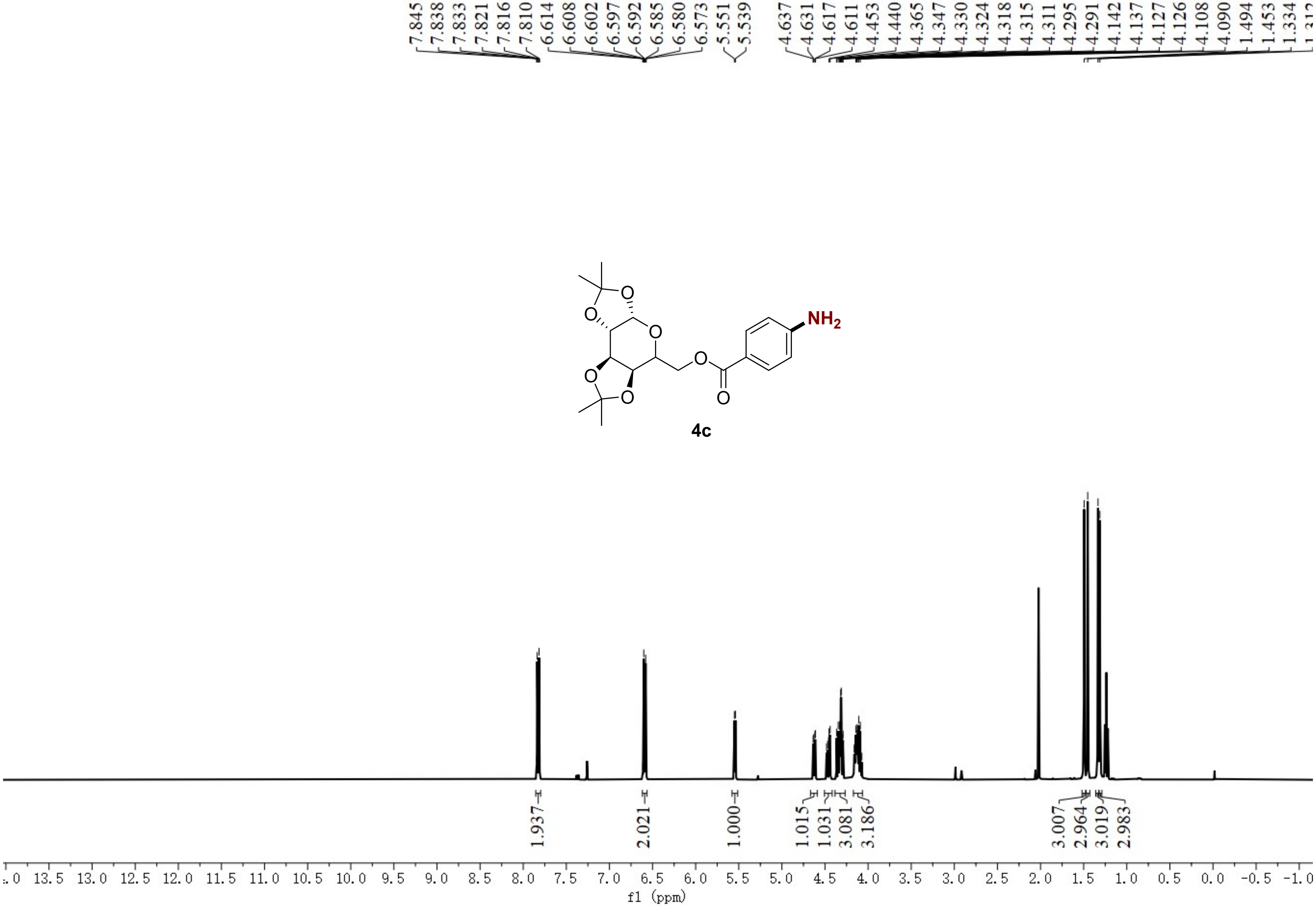
4a


7.632
7.627
7.616
7.611
7.604
7.432
7.427
7.415
7.411
7.407
7.401
7.366
7.361
7.347
7.345
7.341
7.338
7.330
7.327
7.325
7.320
7.315
7.310
7.304
7.302
7.005
6.610
6.605
6.593
6.588
6.582
5.753
5.736
4.061
3.730
NH2
H
N
MeO2C
O
1.798
1.761
2.913
1.082
1.926
0.943
2.259
2.965
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

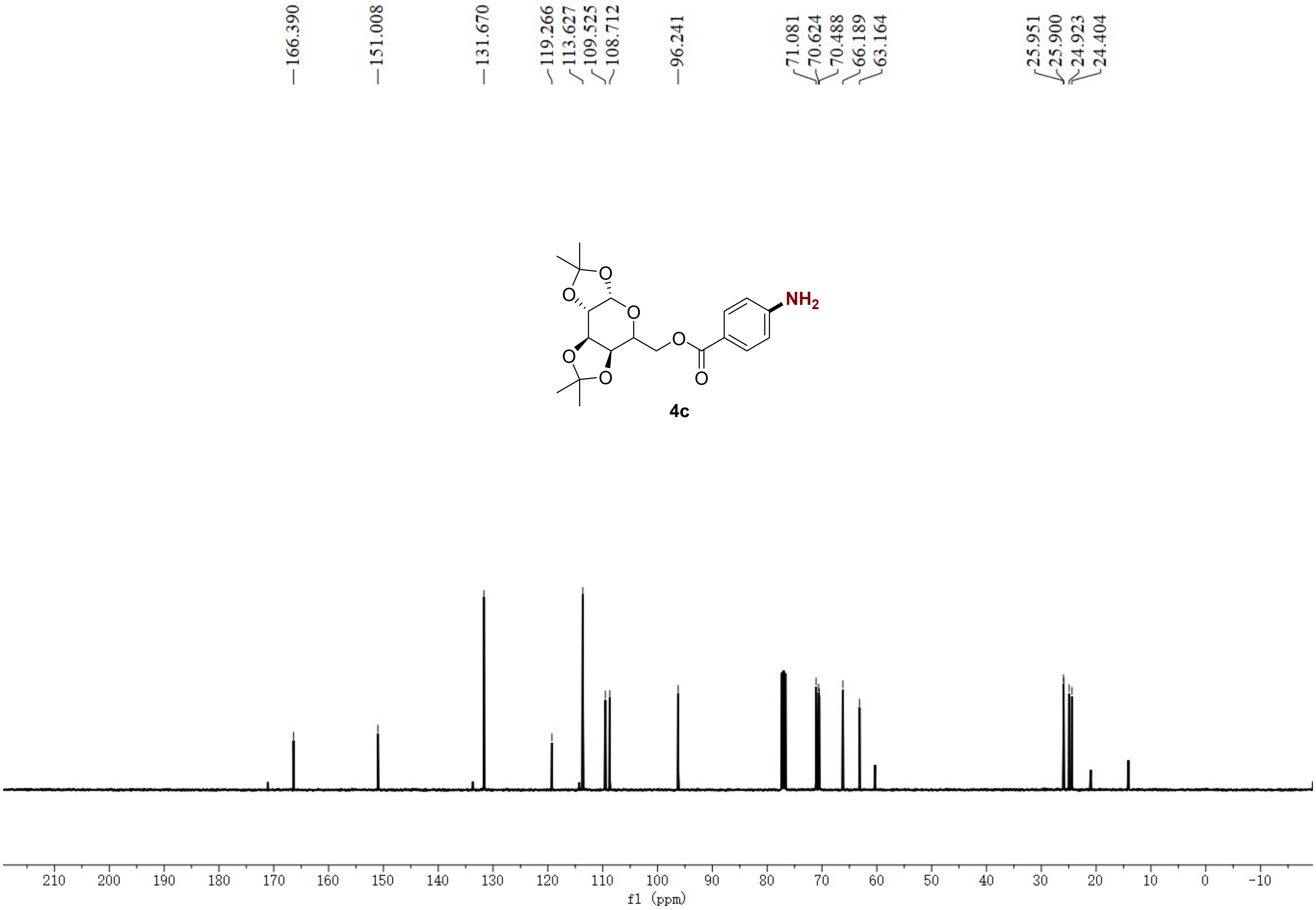
4b



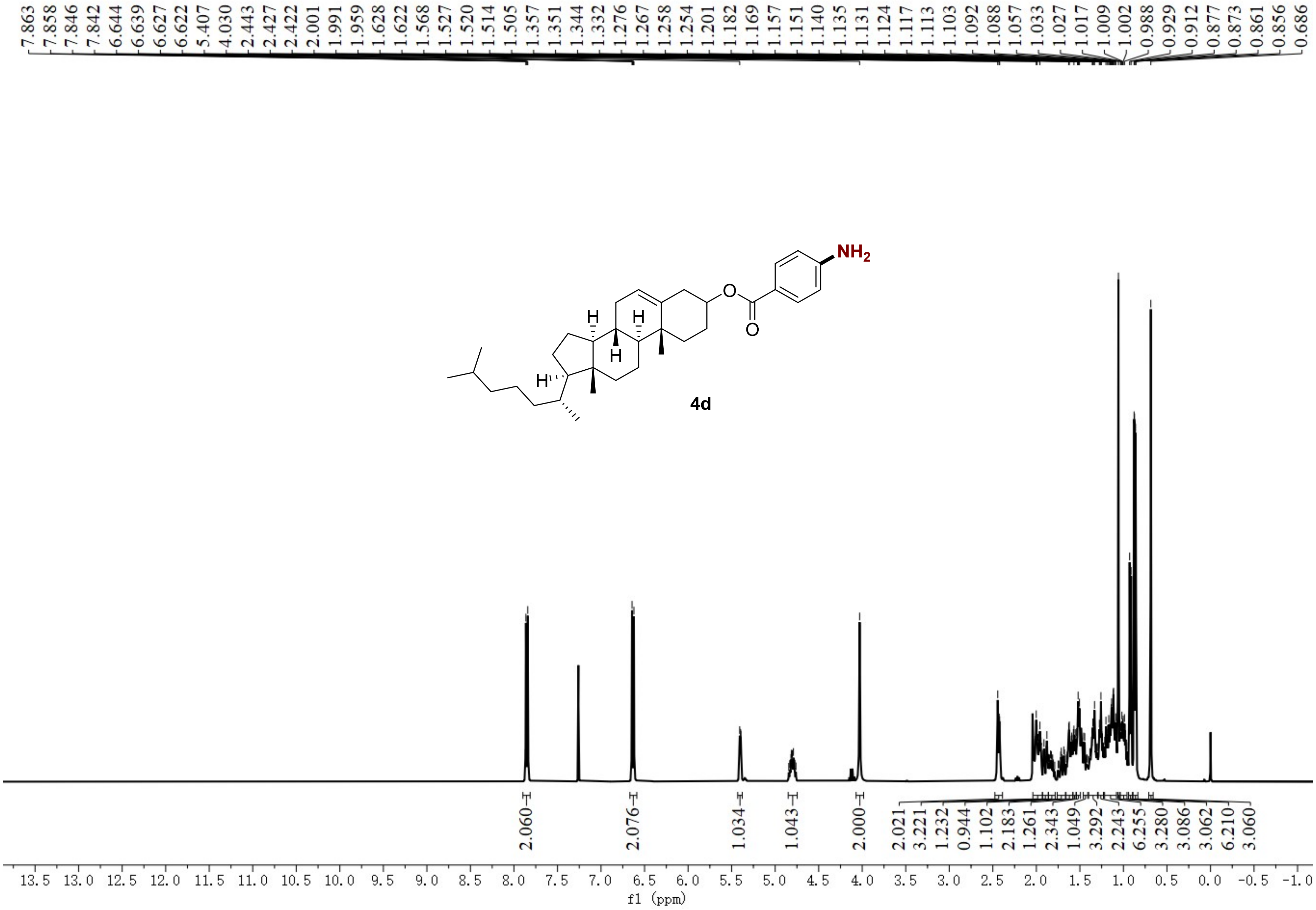
171.686
166.309
150.077
136.753
128.880
128.861
128.379
127.248
122.657
113.931
56.642
52.706
MeO$_2$C
H
N
O
NH$_2$
4b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

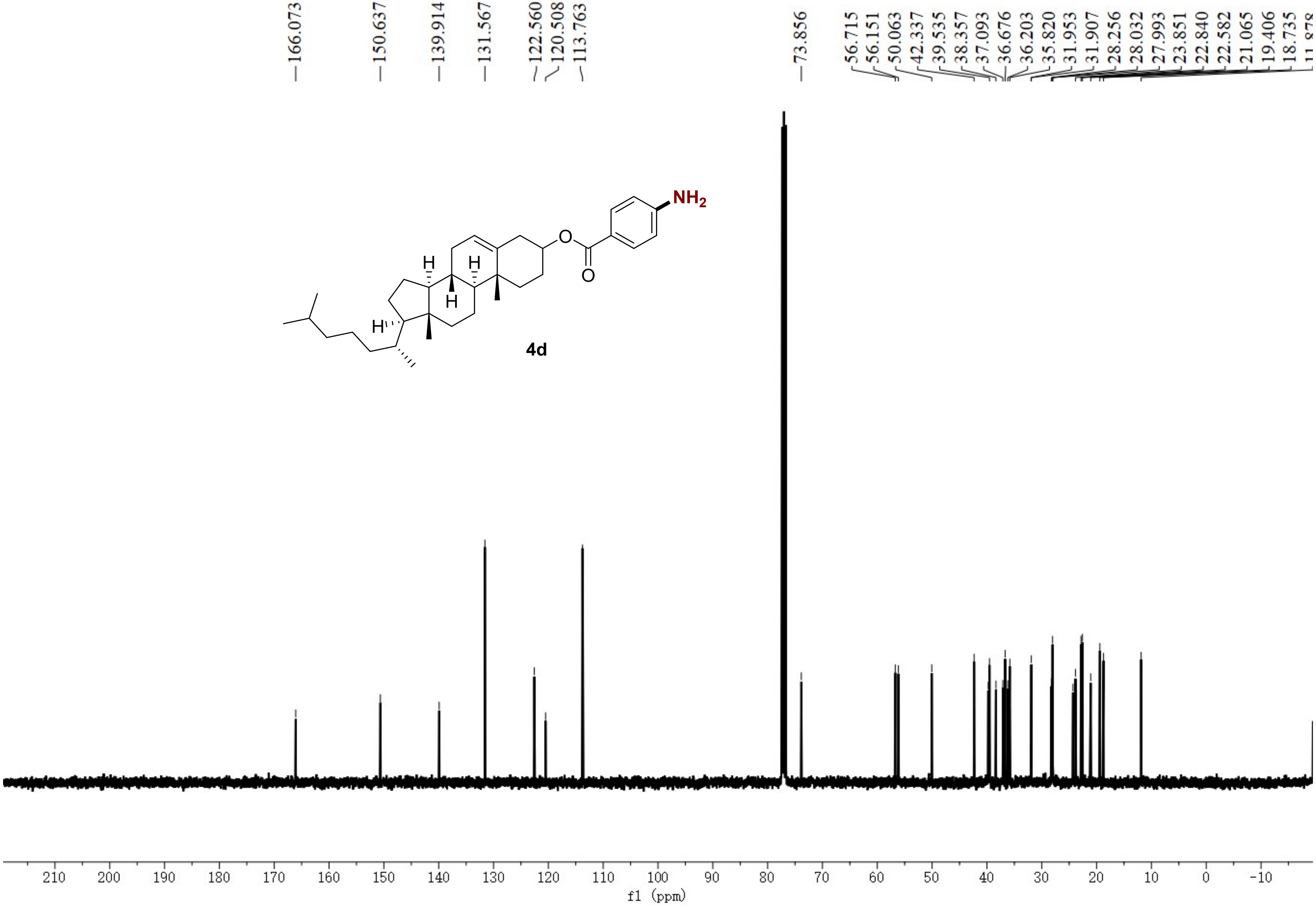
7.845
7.838
7.833
7.821
7.816
7.810
6.614
6.608
6.602
6.597
6.592
6.585
6.580
6.573
5.551
5.539
4.637
4.631
4.617
4.611
4.453
4.440
4.365
4.347
4.330
4.324
4.318
4.315
4.311
4.295
4.291
4.142
4.137
4.127
4.126
4.108
4.090
1.494
1.453
1.334
NH2
O
O
O
O
O
O
O
1.937
2.021
1.000
1.015
1.031
3.081
3.186
3.007
2.964
3.019
2.983
.0
13.5
13.0
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

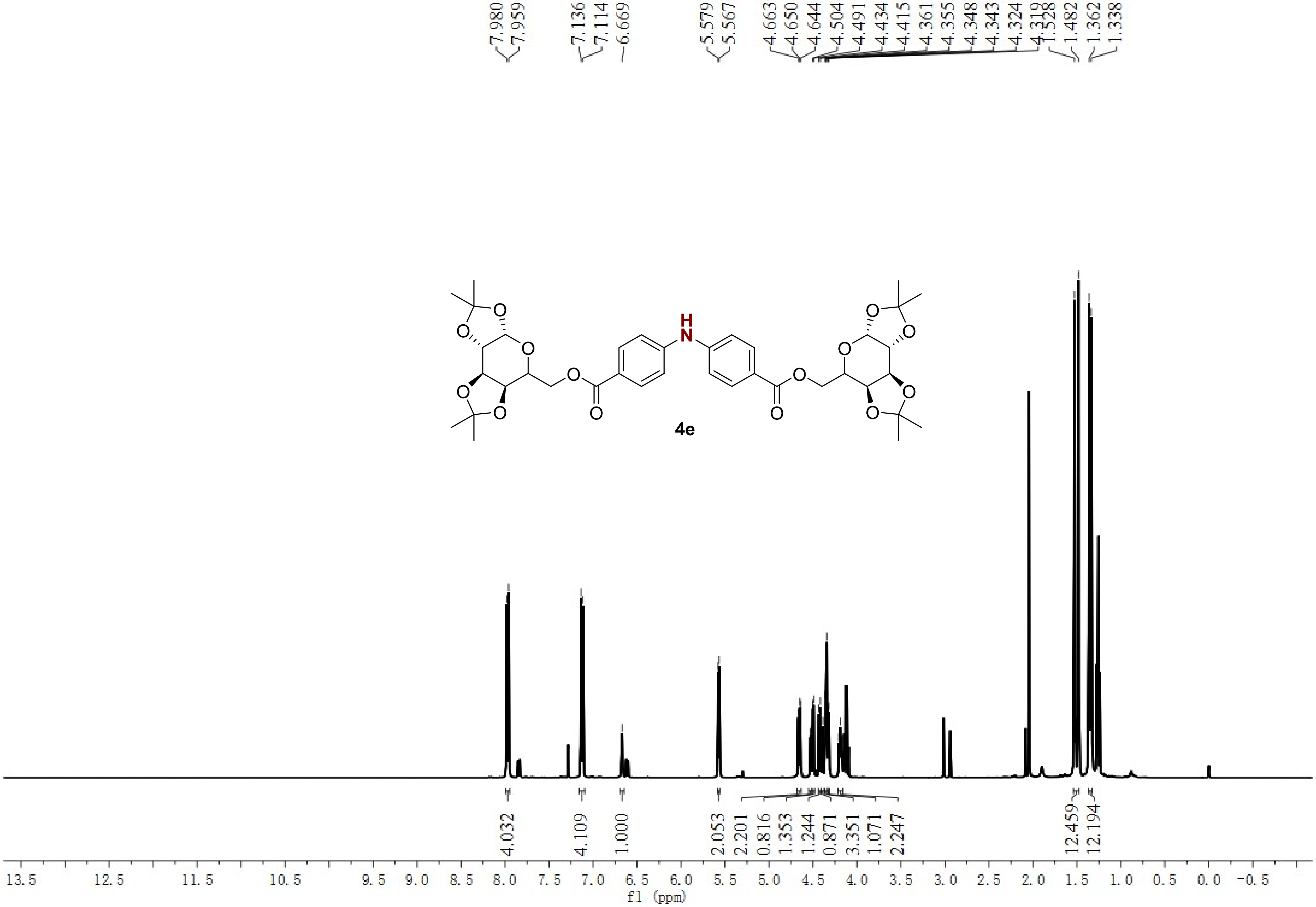
4c


166.390
151.008
131.670
119.266
113.627
109.525
108.712
96.241
71.081
70.624
70.488
66.189
63.164
25.951
25.900
24.923
24.404
NH_2
O
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)

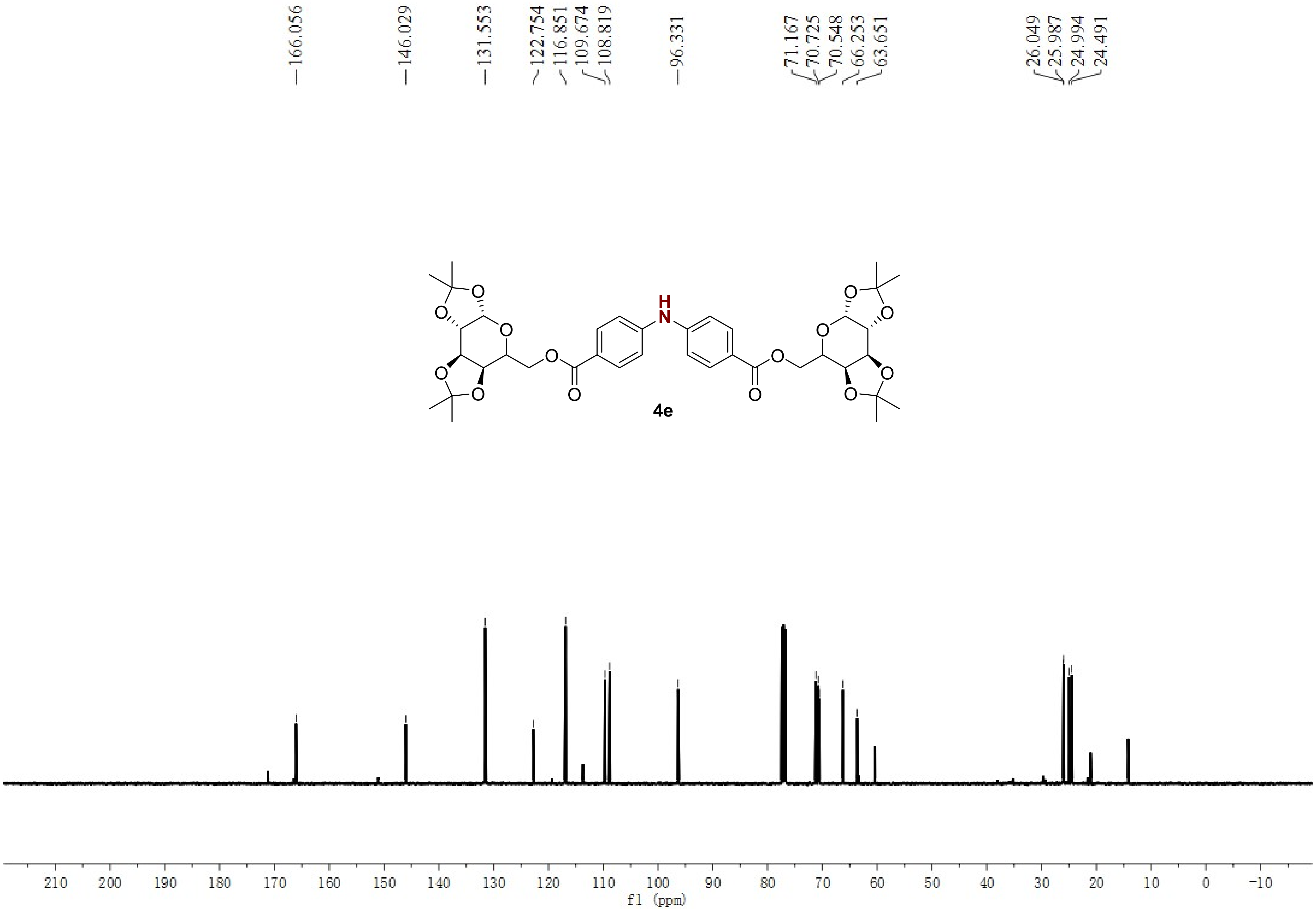
4c


7.863
7.858
7.846
7.842
6.644
6.639
6.627
6.622
5.407
4.030
2.443
2.427
2.422
2.001
1.991
1.959
1.628
1.622
1.568
1.527
1.520
1.514
1.505
1.357
1.351
1.344
1.332
1.276
1.267
1.258
1.254
1.201
1.182
1.169
1.157
1.151
1.140
1.135
1.131
1.124
1.117
1.113
1.103
1.092
1.088
1.057
1.033
1.027
1.017
1.009
1.002
0.988
0.929
0.912
0.877
0.873
0.861
0.856
0.686
NH2
O
O
H
H
H
H
4d
2.060
2.076
1.034
1.043
2.000
2.021
3.221
1.232
0.944
1.102
2.183
1.261
2.343
1.049
3.292
2.243
6.255
3.280
3.086
3.062
6.210
3.060
13.5
13.0
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)


166.073
150.637
139.914
131.567
122.560
120.508
113.763
73.856
56.715
56.151
50.063
42.337
39.535
38.357
37.093
36.676
36.203
35.820
31.953
31.907
28.256
28.032
27.993
23.851
22.840
22.582
21.065
19.406
18.735
11.878
NH_2
O
O
H
H
H
H
4d
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)

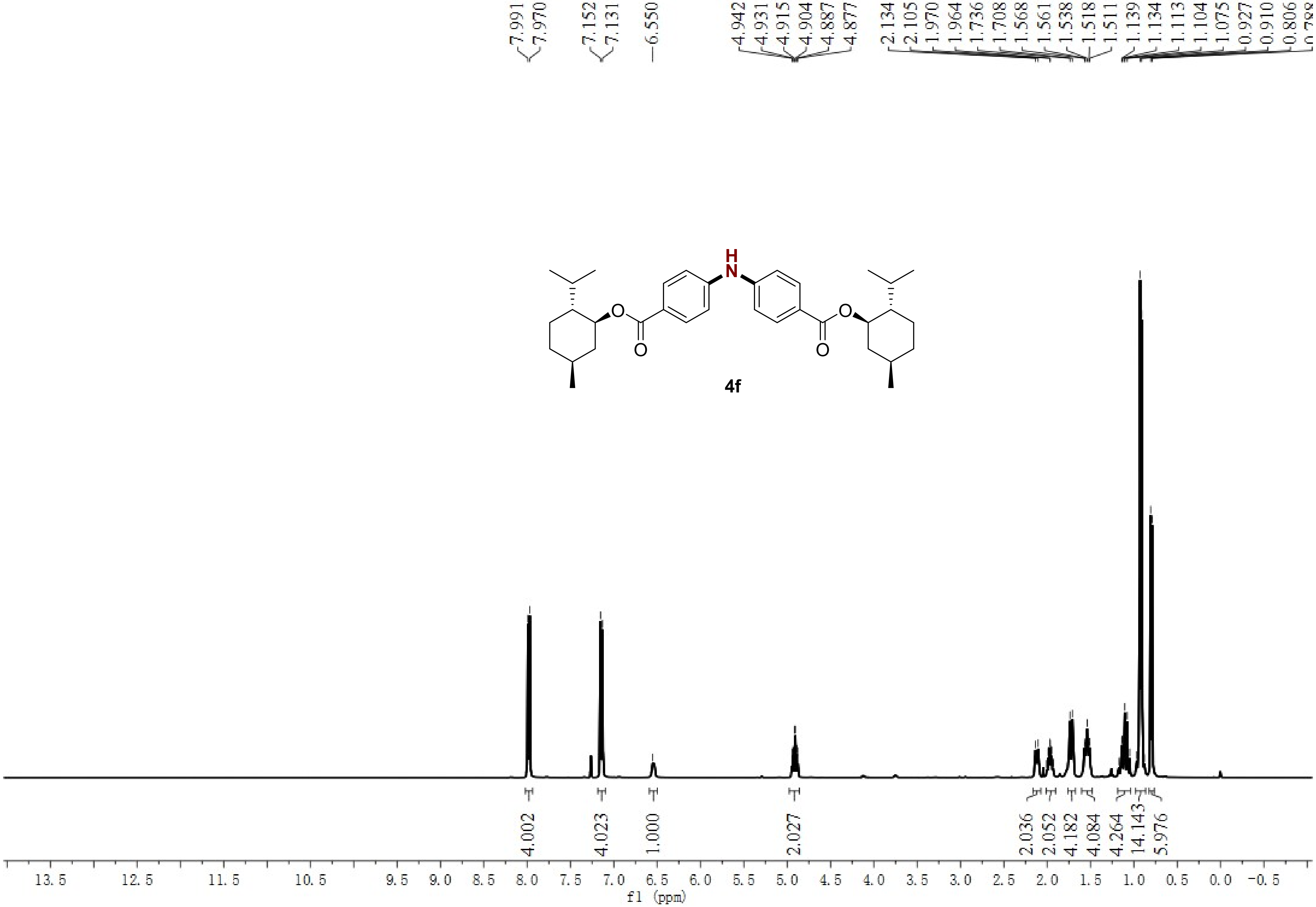

7.980
7.959
7.136
7.114
6.669
5.579
5.567
4.663
4.650
4.644
4.504
4.491
4.434
4.415
4.361
4.355
4.348
4.343
4.324
4.319
1.528
1.482
1.362
1.338
H
N
O
4.032
4.109
1.000
2.053
2.201
0.816
1.353
1.244
0.871
3.351
1.071
2.247
12.459
12.194
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

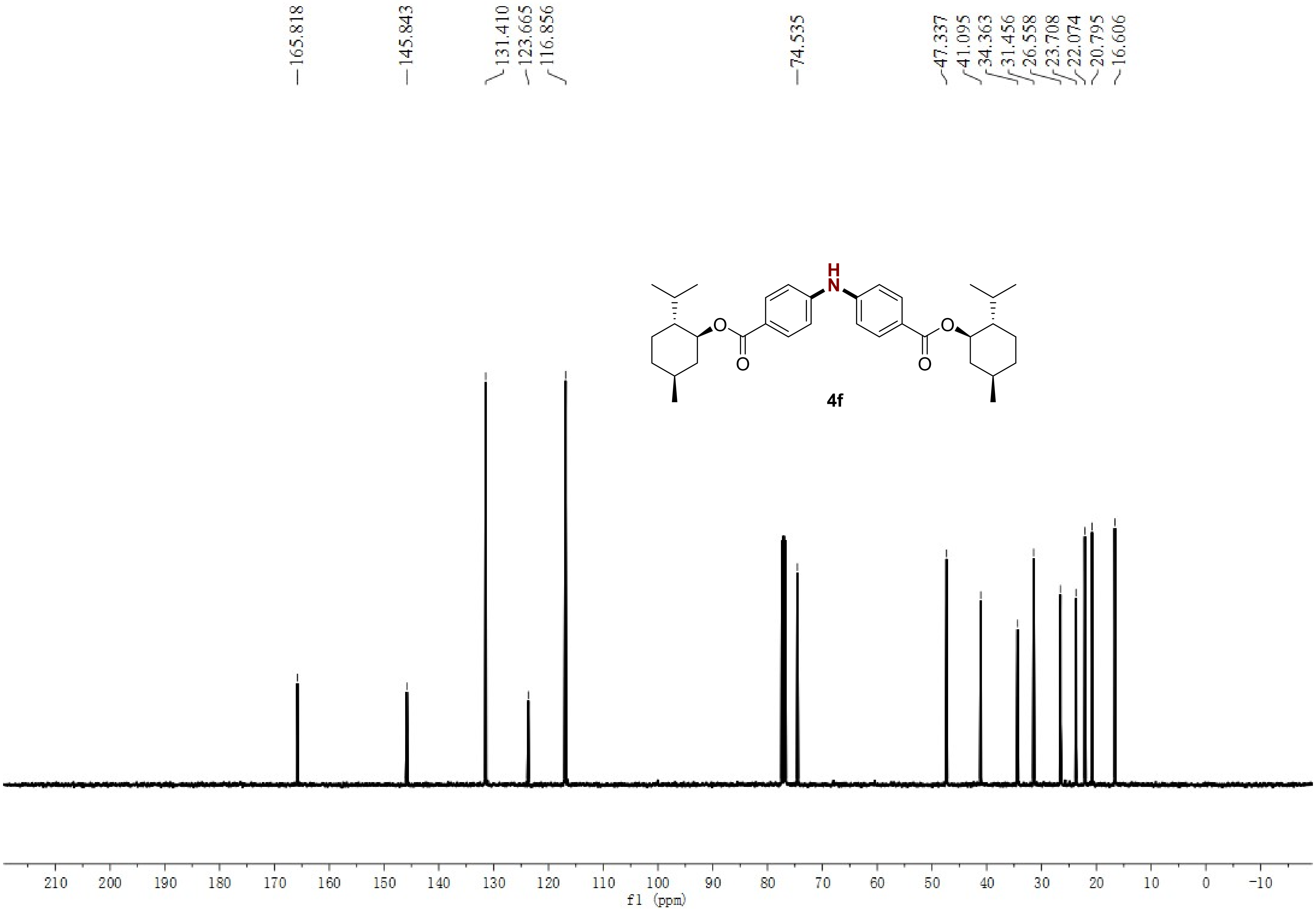
4e



4e

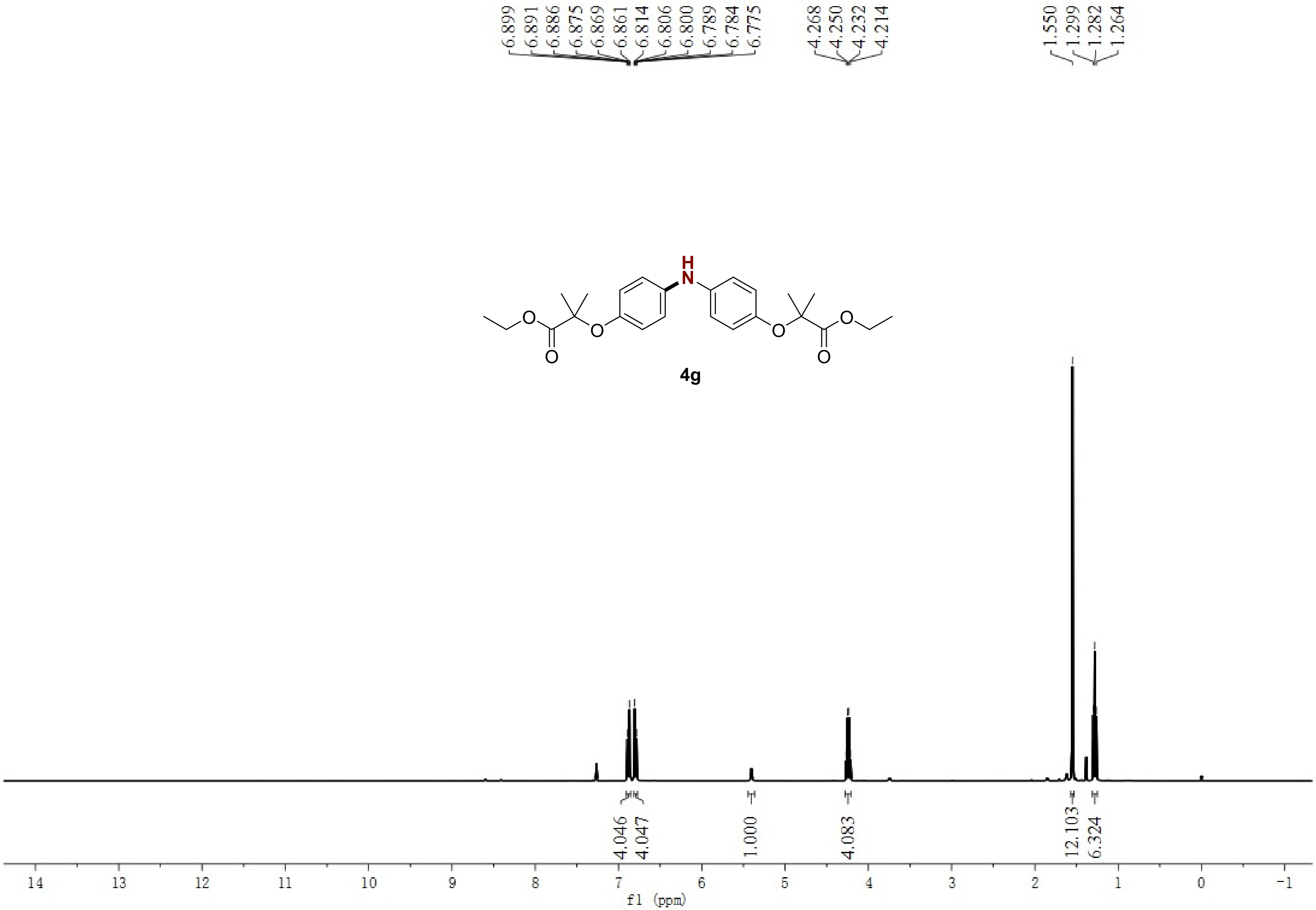
166.056
146.029
131.553
122.754
116.851
109.674
108.819
96.331
71.167
70.725
70.548
66.253
63.651
26.049
25.987
24.994
24.491
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

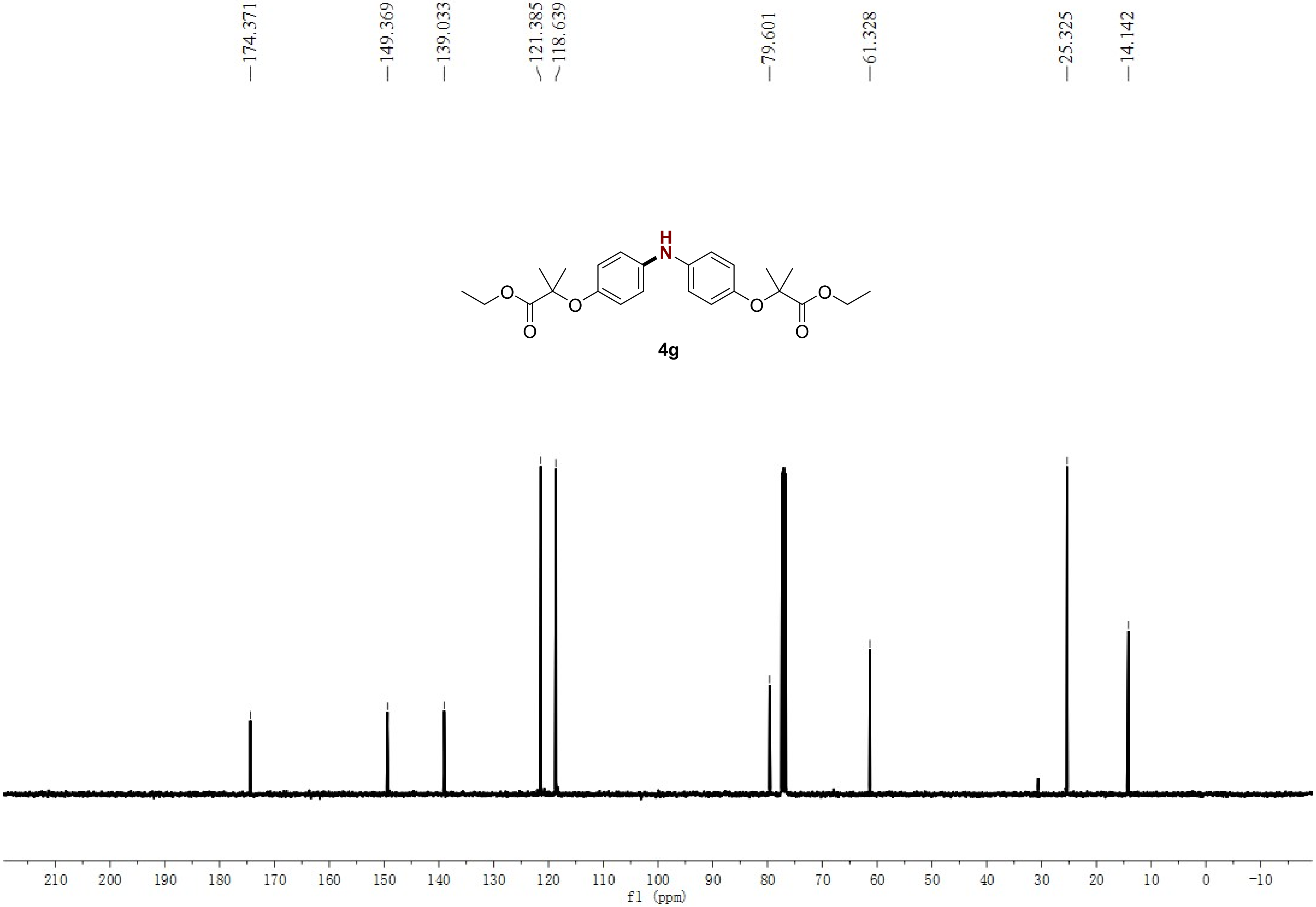

7.991
7.970
7.152
7.131
6.550
4.942
4.931
4.915
4.904
4.887
4.877
2.134
2.105
1.970
1.964
1.736
1.708
1.568
1.561
1.538
1.518
1.511
1.139
1.134
1.113
1.104
1.075
0.927
0.910
0.806
0.788
H
N
O
O
O
O
4f
4.002
4.023
1.000
2.027
2.036
2.052
4.182
4.084
4.264
14.143
5.976
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

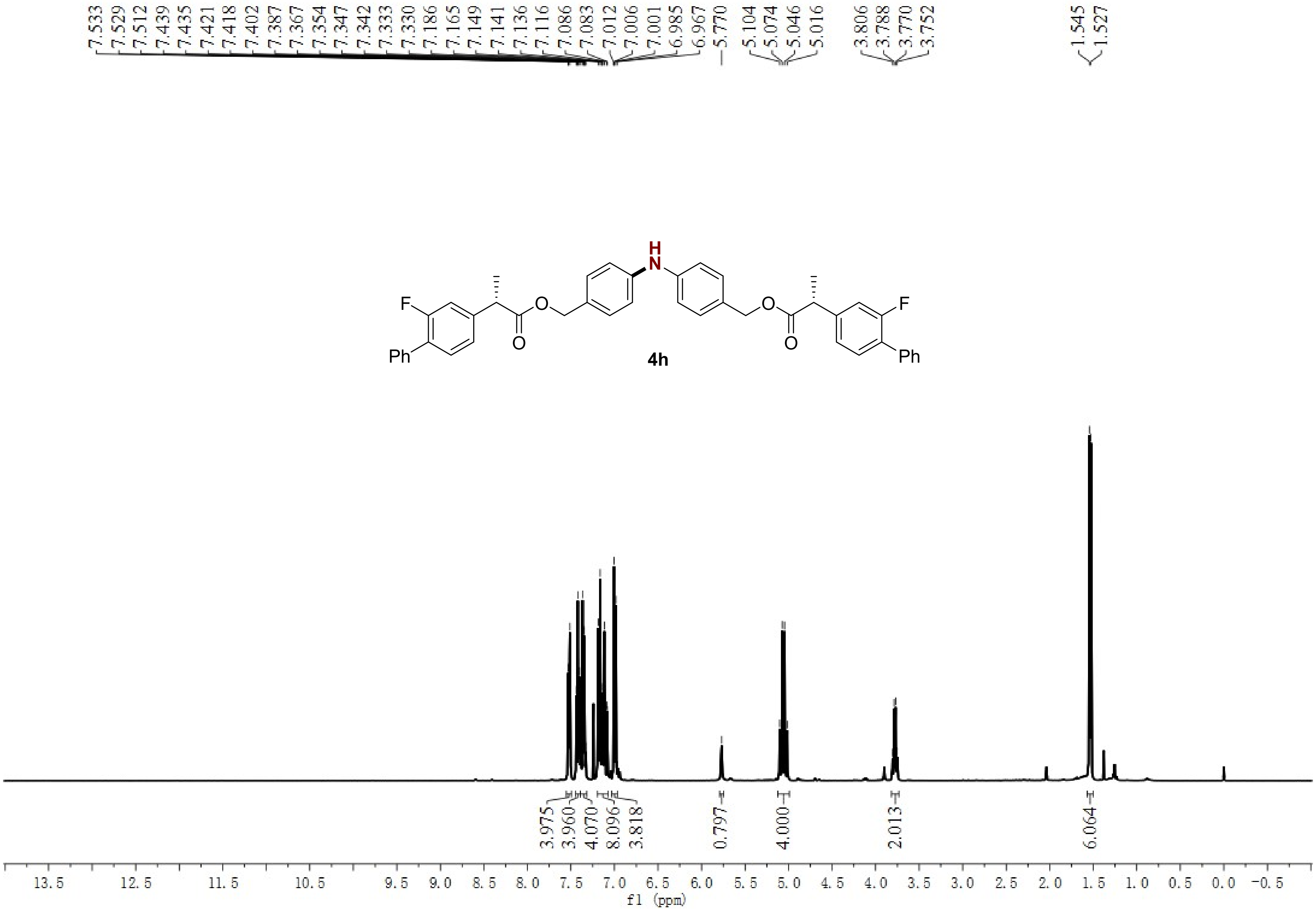


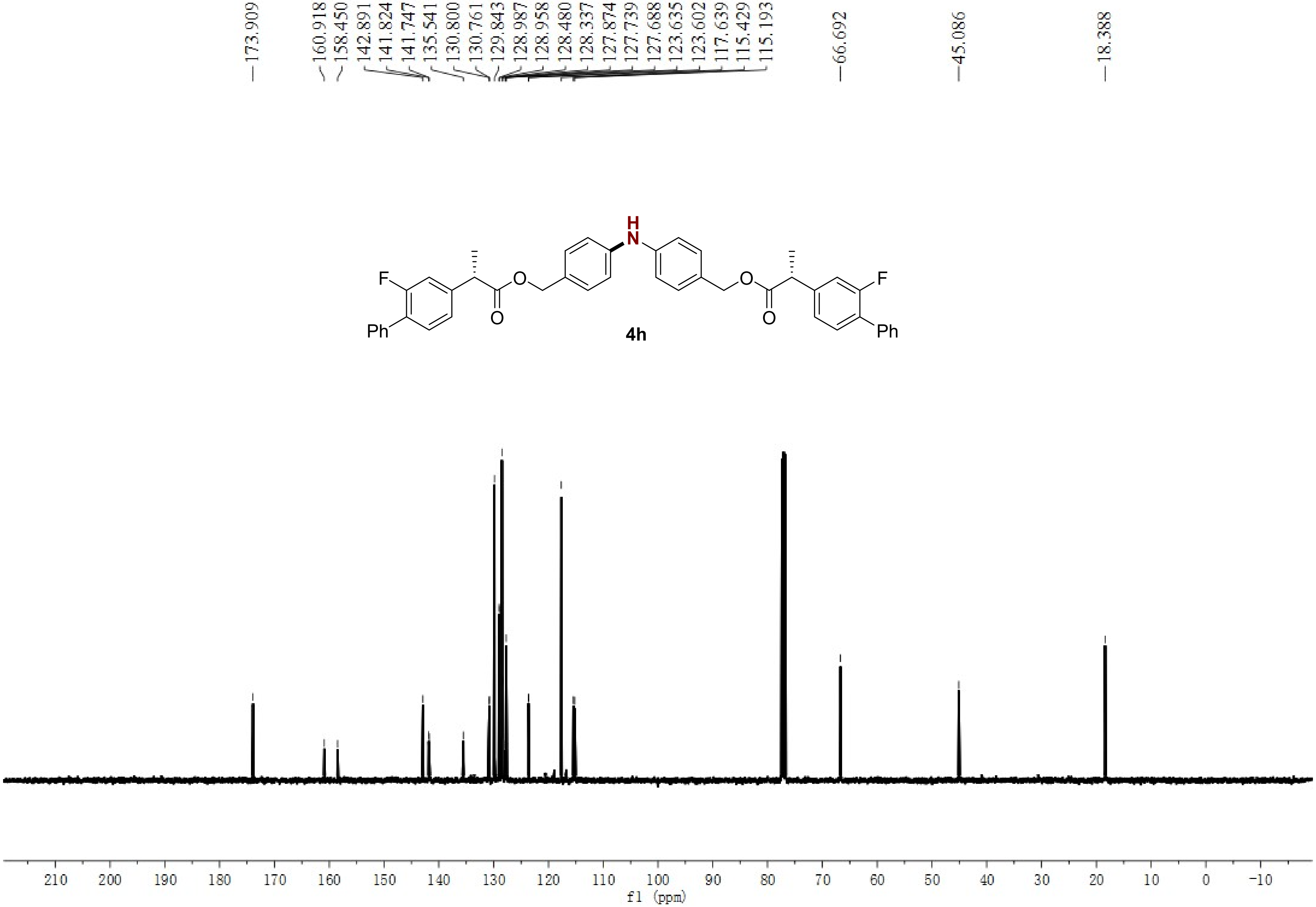
4f

165.818
145.843
131.410
123.665
116.856
74.535
47.337
41.095
34.363
31.456
26.558
23.708
22.074
20.795
16.606
H
N
O
O
O
O
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)

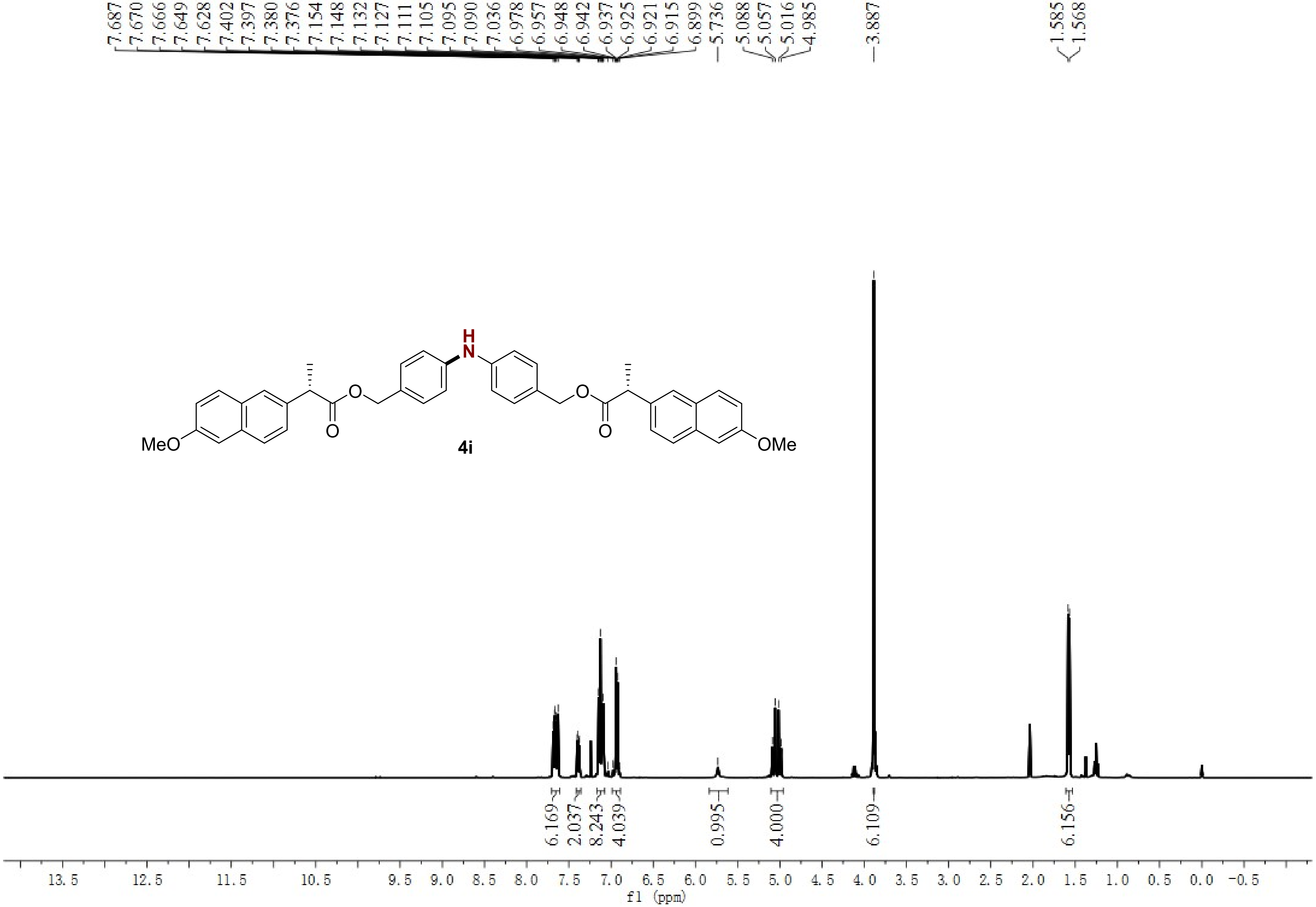

6.899
6.891
6.886
6.875
6.869
6.861
6.814
6.806
6.800
6.789
6.784
6.775
4.268
4.250
4.232
4.214
1.550
1.299
1.282
1.264
H
N
O
O
O
O
O
O
4g
4.046
4.047
1.000
4.083
12.103
6.324
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)

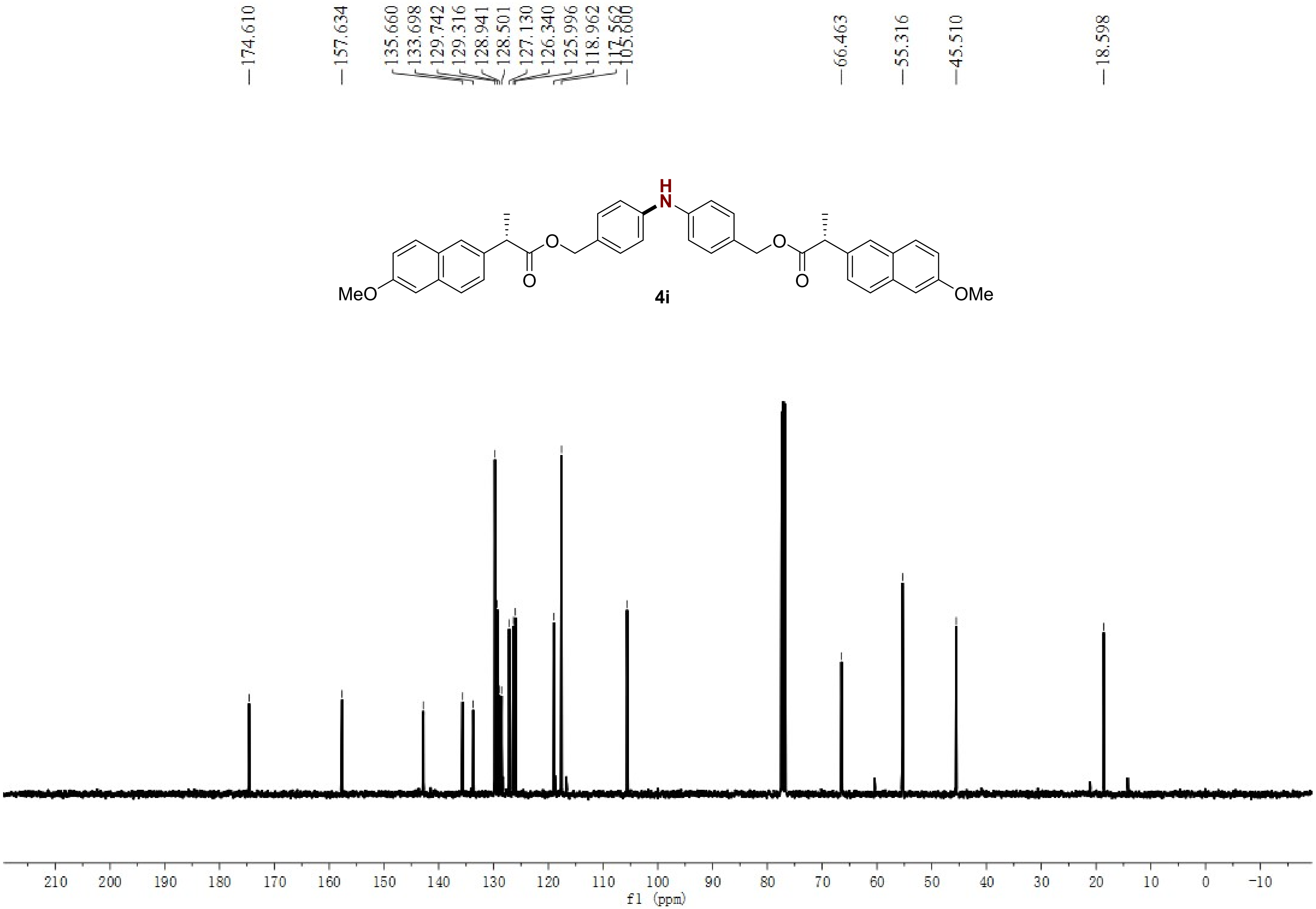

174.371
149.369
139.033
121.385
118.639
79.601
61.328
25.325
14.142
H
N
O
O
O
O
O
O
4g
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.533
7.529
7.512
7.439
7.435
7.421
7.418
7.402
7.387
7.367
7.354
7.347
7.342
7.333
7.330
7.186
7.165
7.149
7.141
7.136
7.116
7.086
7.083
7.012
7.006
7.001
6.985
6.967
5.770
5.104
5.074
5.046
5.016
3.806
3.788
3.770
3.752
1.545
1.527
H
N
F
O
O
Ph
4h
O
O
F
Ph
3.975
3.960
4.070
8.096
3.818
0.797
4.000
2.013
6.064
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


173.909
160.918
158.450
142.891
141.824
141.747
135.541
130.800
130.761
129.843
128.987
128.958
128.480
128.337
127.874
127.739
127.688
123.635
123.602
117.639
115.429
115.193
66.692
45.086
18.388
F
Ph
O
O
H
N
O
O
F
Ph
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)

4h


7.687
7.670
7.666
7.649
7.628
7.402
7.397
7.380
7.376
7.154
7.148
7.132
7.127
7.111
7.105
7.095
7.090
7.036
6.978
6.957
6.948
6.942
6.937
6.925
6.921
6.915
6.899
5.736
5.088
5.057
5.016
4.985
3.887
1.585
1.568
H
N
O
O
O
O
MeO
OMe
4i
6.169
2.037
8.243
4.039
0.995
4.000
6.109
6.156
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)



4i

174.610
157.634
135.660
133.698
129.742
129.316
128.941
128.501
127.130
126.340
125.996
118.962
117.562
105.600
66.463
55.316
45.510
18.598
H
N
O
O
O
O
MeO
OMe
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)