Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Dual Aminoquinolate Diarylboron and Nickel Catalysed Metallaphotoredox Platform for Carbon–Oxygen Bond Construction

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Contents

1 General considerations

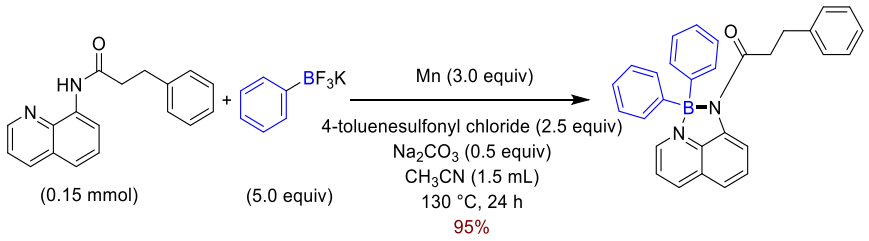
General. Unless otherwise noted, all reactions were carried out under an air atmosphere. Analytical thin-layer chromatography (TLC) was performed on glass plates coated with 0.25 mm 230–400 mesh silica gel containing a fluorescent indicator. Visualization was accomplished by exposure to a UV lamp. All 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 (ν max) are reported in wavenumbers (cm^{-1}). High resolution mass spectra (HRMS) were acquired on Thermo Scientific LTQ Orbitrap XL with an ESI source.

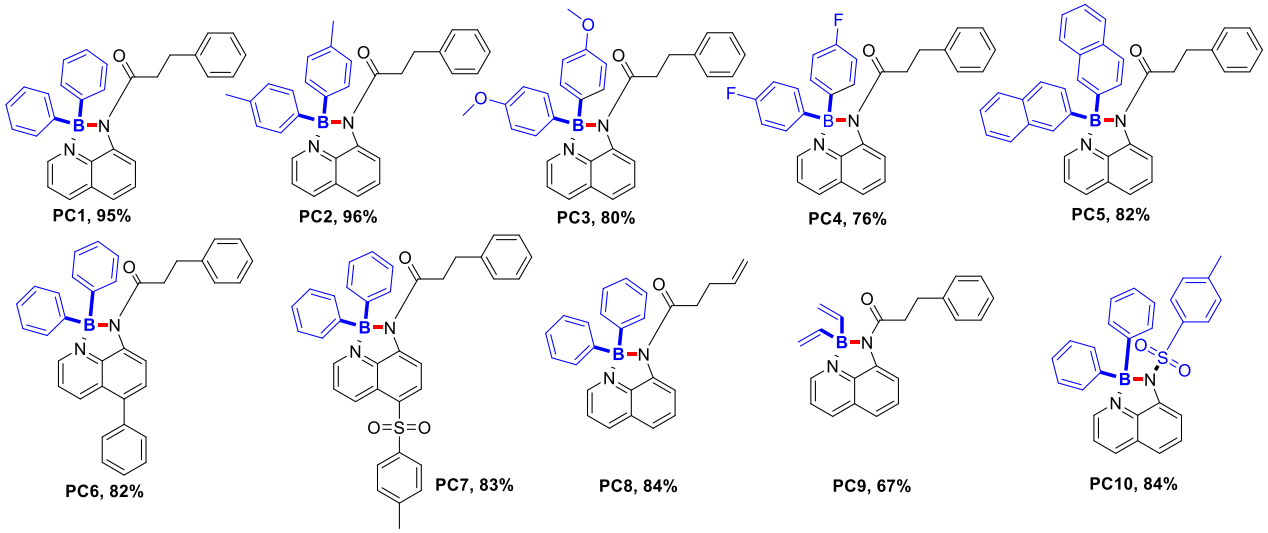
Materials. Commercial reagents and solvent were purchased from Adamas, J&K, Energy, Sigma-Aldrich, Alfa Aesar, Acros Organics, TCI and used as received unless otherwise stated.

2 Preparation of photocatalysts

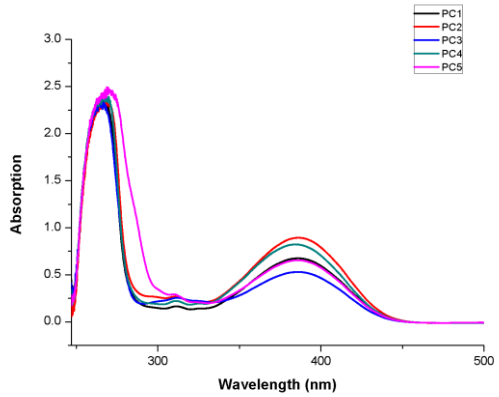
2.1 General procedure for synthesis of photocatalysts



General procedure A: A flame-dried 25 mL pressure column reaction tube was placed with a stirring bar. Then, 8-aminoquinoline derivative (0.15 mmol, 1.0 equiv), aryl or vinyl trifluoroborate (0.75 mmol, 5.0 equiv), Mn (24.7 mg, 0.45 mmol, 3.0 equiv), 4-toluenesulfonyl chloride (71.5 mg, 0.375 mmol, 2.5 equiv), Na_2CO_3 (7.9 mg, 0.075 mmol, 0.5 equiv) and CH_3CN (1.5 mL) were added. The resulting mixture was stirred 130 °C for 24 hours. The reaction mixture was filtered, concentrated and then purified by column chromatography on silica gel to give the target product.



2.2 Absorption and emission spectra of Photocatalysts



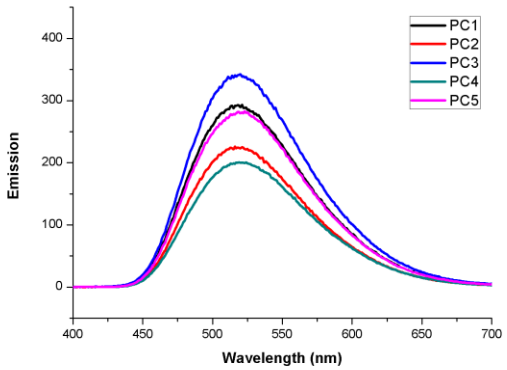
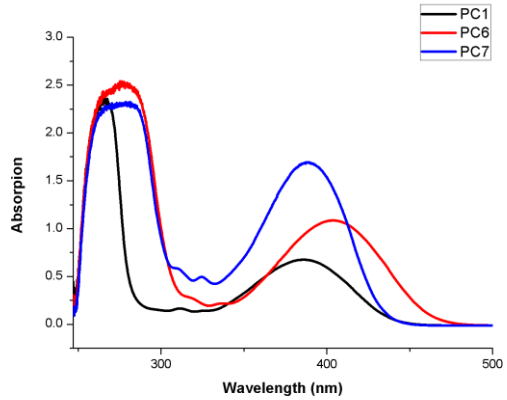


Figure 1a **Figure 1b**

Figure 1. a. UV−visible absorption spectra of PC1 - PC5 in DMSO at a concentration of 1.7 x 10^{-4} M;
b. Fluorescence emission spectra of PC1 - PC5 in DMSO at a concentration of 5 x 10^{-4} M.



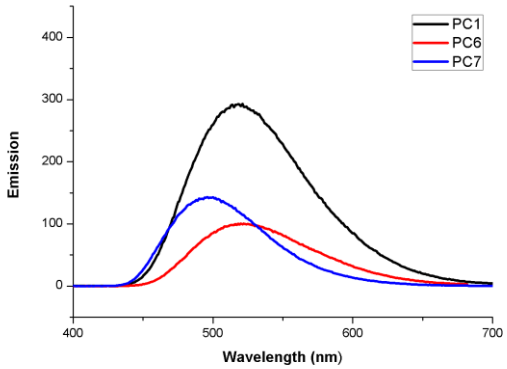
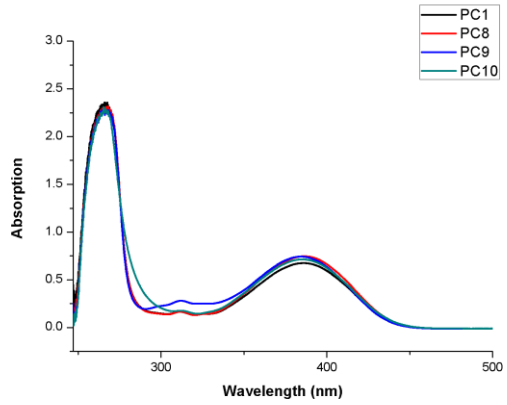


Figure 2a **Figure 2b**

Figure 2. a. UV−visible absorption spectra of PC1, PC6, PC7 in DMSO at a concentration of 1.7 x 10^{-4} M;
b. Fluorescence emission spectra of PC1, PC6, PC7 in DMSO at a concentration of 5 x 10^{-4} M.



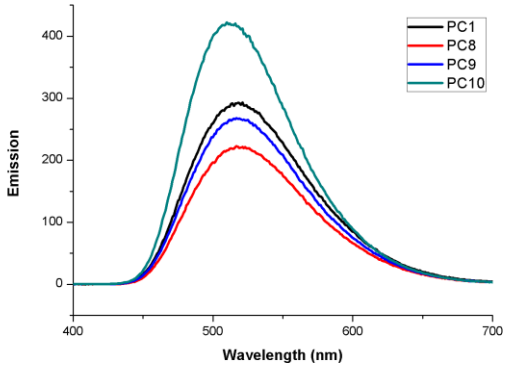


Figure 3a **Figure 3b**

Figure 3. a. UV−visible absorption spectra of PC1, PC8, PC9, PC10 in DMSO at a concentration of 1.7 x 10^{-4} M;
b. Fluorescence emission spectra of PC1, PC8, PC9, PC10 in DMSO at a concentration of 5 x 10^{-4} M.

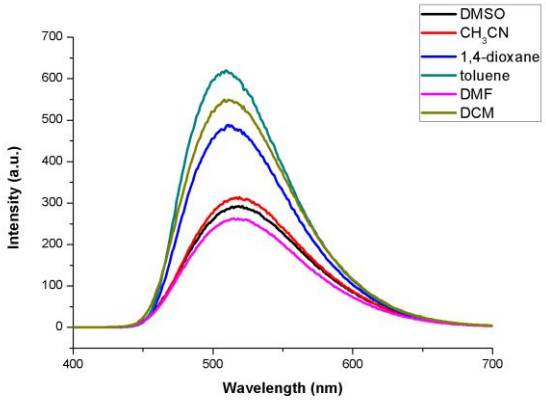


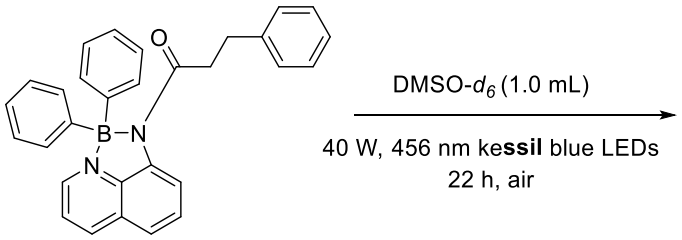
Figure 4. The fluorescence emission spectra of PC1 in DMSO, CH_3CN, 1,4-dioxane, toluene, DMF, DCM at a concentration of 5 x 10^{-4} M.

Table S1. **Summary of the measured photophysical properties of photocatalysts**

Entry	λ_{abs} (nm)	λ_{em} (nm) [a]	Quantum yield (%) [b]	Life time (ns) [b]
PC1	386	520	52.72	17.43
PC2	386	513	55.24	17.77
PC3	387	520	53.52	17.51
PC4	384	519	47.34	16.36
PC5	386	518	53.97	17.02
PC6	404	540	40.26	12.07
PC7	389	496	85.96	12.96
PC8	388	517	51.07	17.11
PC9	384	517	54.97	17.97
PC10	385	510	67.03	24.00

a. Excited at the longest absorption maximum wavelengths. b. The quantum yield and life time of PC in DMSO at a concentration of 5 x 10^{-4} M.

2.3 The test of photocatalyst stability



PC1 (0.1 mmol)

A flame-dried 25 mL quartz column reaction tube was placed with a magnetic stir bar. Then, **PC1**, and DMSO-d_6 (1.0 mL) were added. the reaction mixture was irradiated and stirred with two 40 W 456 nm Kessil blue LEDs. The reaction tube was placed at approximately 2 cm away from the light source (**Figure 6b**). A fan was used to cool down the tube during the irradiation. After stirring for 22 hours, 1,3,5-trimethoxybenzene was added to the reaction tube. Then, the DMSO-d_6 solution was transferred to an NMR tube and then characterized by ^{1}H NMR (**Figure 5a**), no obvious decomposition could be observed.

In addition, the photocatalyst was bench-stable and can be stored in the fume hood without further precaution at room temperature. **Figure 5b** showed the ^{1}H NMR characterization of **PC1** after one month's storage. Also, no obvious decomposition could be observed.

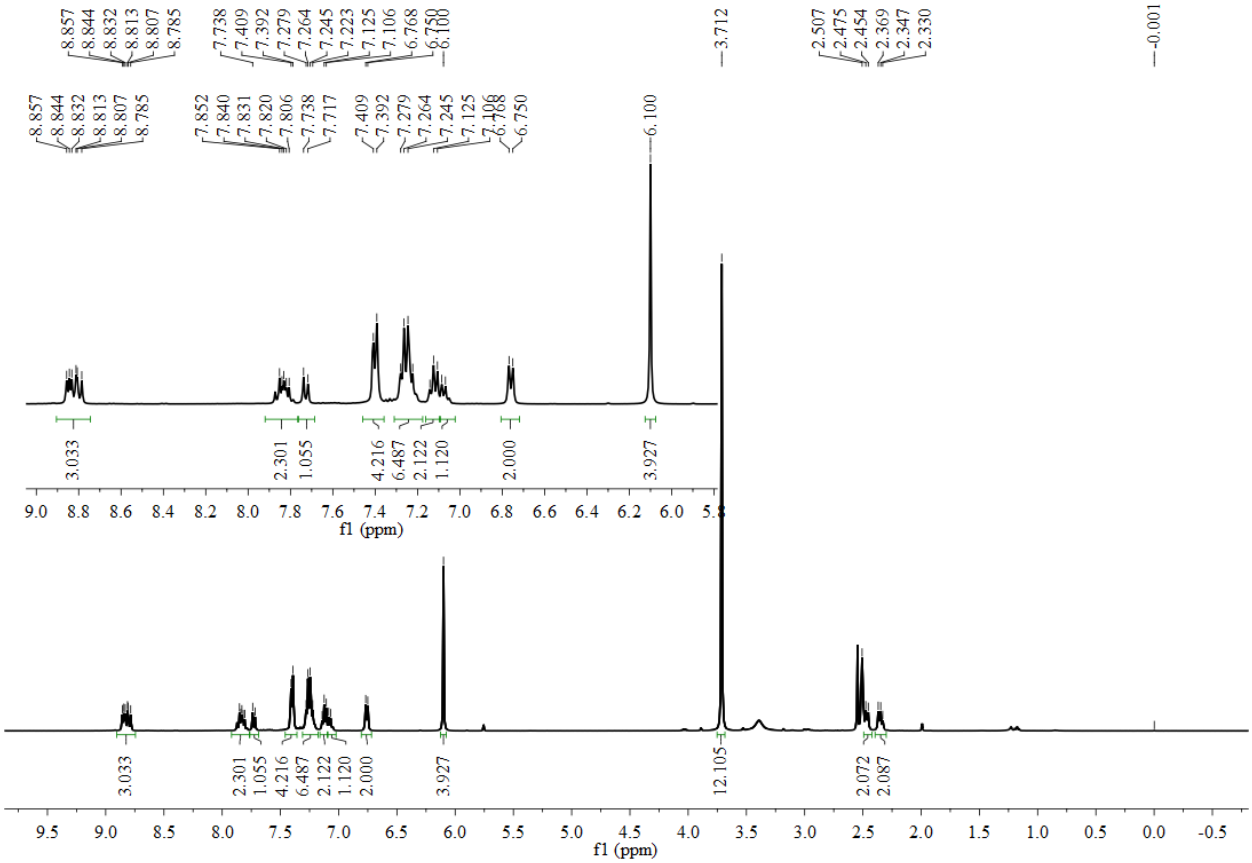


Figure 5a. The ^{1}H NMR characterization after 22 hours' irradiation

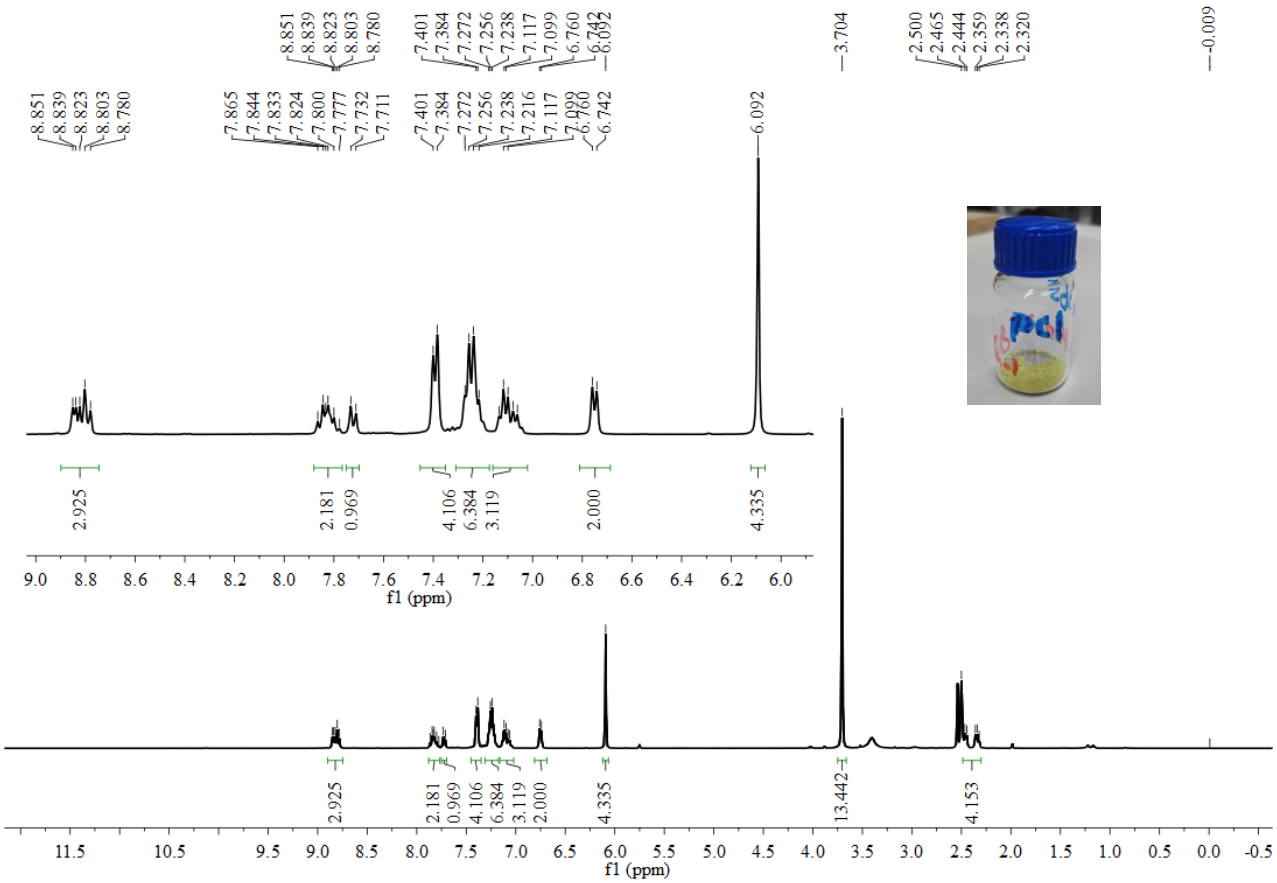
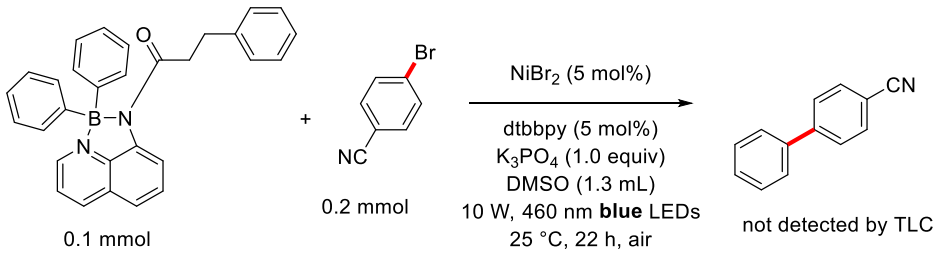


Figure 5b. The ^{1}H NMR characterization of **PC1** after one month's storage in the fume hood.

2.4 Test on the possibility of photocatalyst to participate in Suzuki-Miyaura cross-coupling as boronyl nucleophile

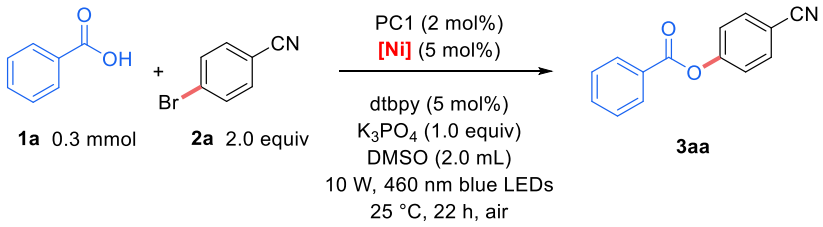


A flame-dried 25 mL quartz column reaction tube was placed with a magnetic stir bar. Then, **PC1** (44.0 mg, 0.1 mmol), 4-bromobenzonitrile (0.2 mmol), $NiBr_2$ (0.005 mmol), dtbpy (0.005 mmol), K_3PO_4 (0.1 mmol), and DMSO (1.3 mL) were added. The reaction tube was placed on a photocatalytic parallel reactor with a 460 nm blue LEDs light source (10 W) at the bottom (**Figure 6a**). Then the reaction mixture was irradiated with the 460 nm blue LEDs (at approximately 0.3 cm away from the light source). After stirring for 22 hours at 25 ℃, the assumed product of Suzuki-Miyaura reaction, [1,1'-biphenyl]-4-carbonitrile, was not detected by TLC, when compared to a standard sample.

3 Optimization of reaction conditions for synthesis of esters

3.1 Optimization tables for synthesis of ester

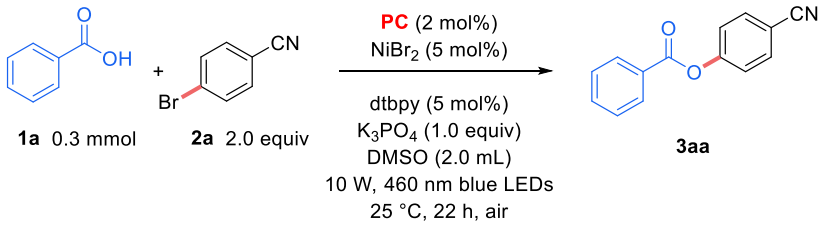
Table S2. The screening of nickel source[a]



Entry	[Ni] source	Yield (%)[a]
1	$NiBr_2$•DME	30
2	NiI_2	N. D.
3	$NiCl_2$	4
4	**$NiBr_2$**	**83**
5	$NiCl_2$•DME	84
6	$Ni(OAc)_2$•4H2O	72
7	$NiBr_2$•$3H_2O$	71
8	$Ni(acac)_2$	40
9	$NiCl_2(PCy_3)_2$	60
10	$NiCl_2(PPh_3)_2$	79

Reaction conditions: 1a (0.3 mmol, 1.0 equiv), 2a (0.6 mmol, 2.0 equiv), **PC1** (0.006 mmol, 2 mol%), **Ni source** (0.015 mmol, 5 mol%), dtbpy (4,4′-di-tert-butyl-2,2′-dipyridyl, 0.015 mmol, 5 mol%), K_3PO_4 (0.3 mmol, 1.0 equiv), DMSO (2.0 mL), 10 W 460 nm blue LEDs, 25 °C, air, 22 h. [a] Isolated yield. N. D. = not detected.

Table S3. The screening of photocatalysts[a]

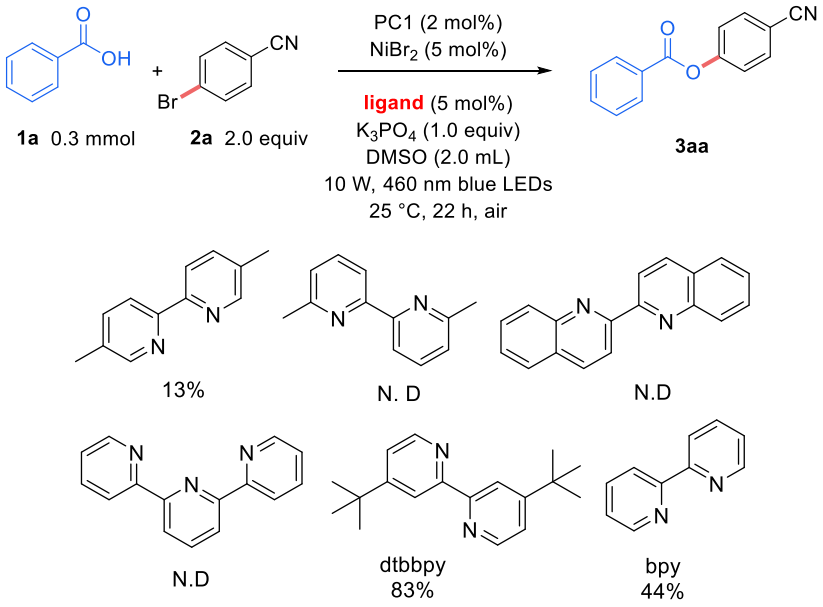


Entry	photocatalyst	Yield (%)[a]
1	**PC1**	**83**
2	PC2	55
3	PC3	50
4	PC4	72
5	PC5	57
6	PC6	62
7	PC7	45
8	PC8	73
9	PC9	51
10	PC10	71

Reaction conditions: 1a (0.3 mmol, 1.0 equiv), 2a (0.6 mmol, 2.0 equiv), **PC** (0.006 mmol, 2 mol%), $NiBr_2$ (0.015 mmol,

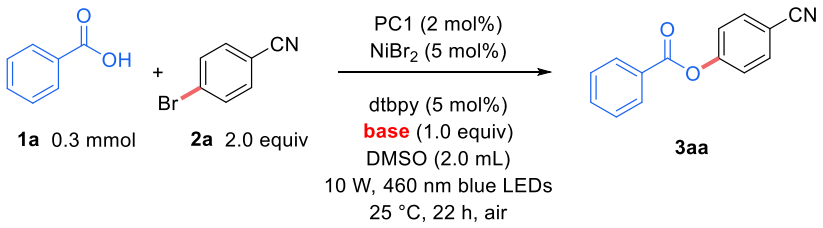
5 mol%), dtbpy (0.015 mmol, 5 mol%), K_3PO_4 (0.3 mmol, 1.0 equiv), DMSO (2.0 mL), 10 W 460 nm blue LEDs, 25 °C, air, 22 h. [a] Isolated yield. N. D. = not detected.

Table S4. The screening of ligands[a]



Reaction conditions: 1a (0.3 mmol, 1.0 equiv), 2a (0.6 mmol, 2.0 equiv), **PC1** (0.006 mmol, 2 mol%), $NiBr_2$ (0.015 mmol, 5 mol%), **ligand** (0.015 mmol, 5 mol%), K_3PO_4 (0.3 mmol, 1.0 equiv), DMSO (2.0 mL), 10 W 460 nm blue LEDs, 25 °C, air, 22 h. [a] Isolated yield. N. D. = not detected.

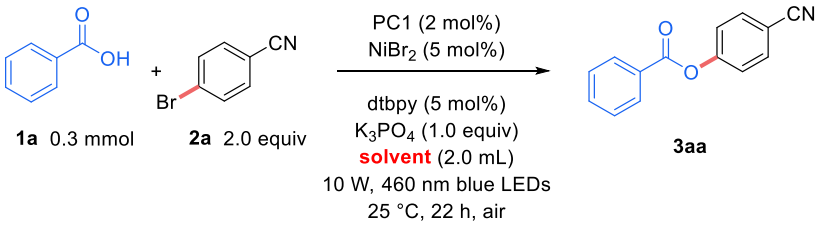
Table S5. The screening of bases[a]



Entry	base	Yield (%)[a]
1	*t*-BuONa	51
2	MeONa	7
3	K_2CO_3	53
4	K_2HPO_4	39
5	**K_3PO_4**	**83**
6	Triethylamine	13
7	DIPEA	33
8	Pyridine	trace
9	Diisopropylamine	26

Reaction conditions: 1a (0.3 mmol, 1.0 equiv), 2a (0.6 mmol, 2.0 equiv), **PC1** (0.006 mmol, 2 mol%), $NiBr_2$ (0.015 mmol, 5 mol%), dtbpy (0.015 mmol, 5 mol%), **base** (0.3 mmol, 1.0 equiv), DMSO (2.0 mL), 10 W 460 nm blue LEDs, 25 °C, air, 22 h. [a] Isolated yield. N. D. = not detected, DIPEA = *N*,*N*-diisopropylethylamine.

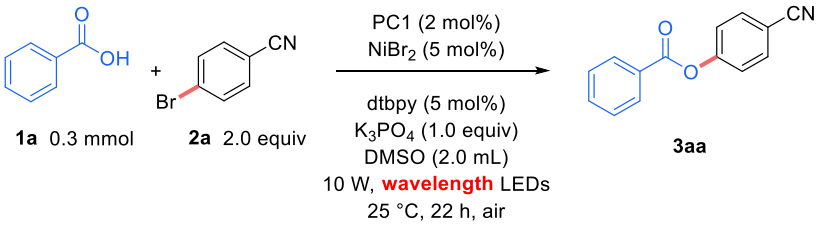
Table S6. The screening of solvents[a]



Entry	solvent	Yield (%)[a]
1	DMF	42
2	DMA	11
3	**DMSO**	**83**
4	CH_3CN	5
5	1,4-dioxane	trace
6	THF	18
7	DCM	trace
8	toluene	N. D.
9	isopropanol	N. D.

Reaction conditions: 1a (0.3 mmol, 1.0 equiv), 2a (0.6 mmol, 2.0 equiv), **PC1** (0.006 mmol, 2 mol%), $NiBr_2$ (0.015 mmol, 5 mol%), dtbpy (0.015 mmol, 5 mol%), K_3PO_4 (0.3 mmol, 1.0 equiv), **solvent** (2.0 mL), 10 W 460 nm blue LEDs, 25 °C, air, 22 h. [a] Isolated yield. N. D. = not detected.

Table S7. The screening of wavelengths[a]



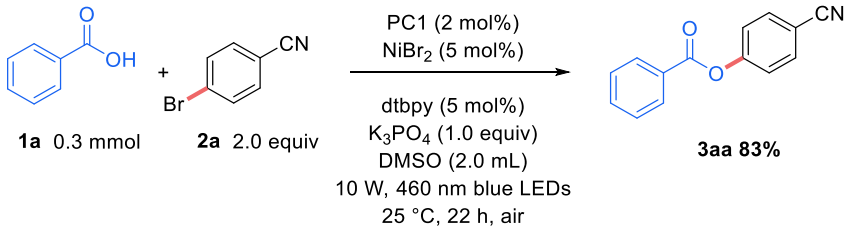
Entry	**Wavelength (nm)**	Yield (%)[a]
1	445	32
2	455	59
3	**460**	**83**
4	470	N. D.
5	white light	N. D.

Reaction conditions: 1a (0.3 mmol, 1.0 equiv), 2a (0.6 mmol, 2.0 equiv), **PC1** (0.006 mmol, 2 mol%), $NiBr_2$ (0.015 mmol, 5 mol%), dtbpy (0.015 mmol, 5 mol%), K_3PO_4 (0.3 mmol, 1.0 equiv), DMSO (2.0 mL), 10 W, LEDs, 25 °C, air, 22 h. [a] Isolated yield. N. D. = not detected.

4 General procedure for the synthesis of esters

4.1 Control experiments for the used reaction conditions in ester synthesis

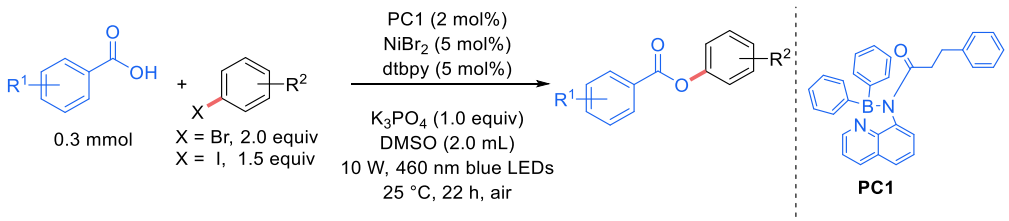
Table S8. The control experiments for the ester synthesis[a]



Entry	Variations from the 'standard' conditions	Yield (%)[a]
1	no **PC1**	N. D.
2	no $NiBr_2$	N. D.
3	no dtbpy	trace
4	no light	N. D.
5	no K_3PO_4	N. D.

Standard reaction conditions: 1a (0.3 mmol, 1.0 equiv), 2a (0.6 mmol, 2.0 equiv), **PC1** (0.006 mmol, 2 mol%), $NiBr_2$ (0.015 mmol, 5 mol%), dtbpy (0.015 mmol, 5 mol%), K_3PO_4 (0.3 mmol, 1.0 equiv), DMSO (2.0 mL), 10 W 460 nm blue LEDs, 25 °C, air, 22 h. [a] Isolated yield. N. D. = not detected.

4.2 General Procedure for the synthesis of esters

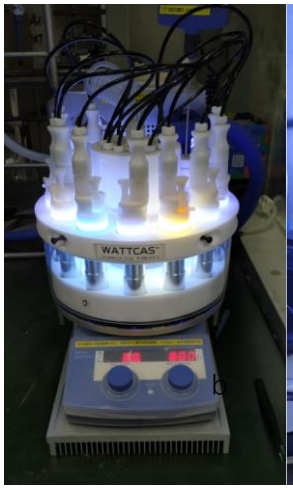


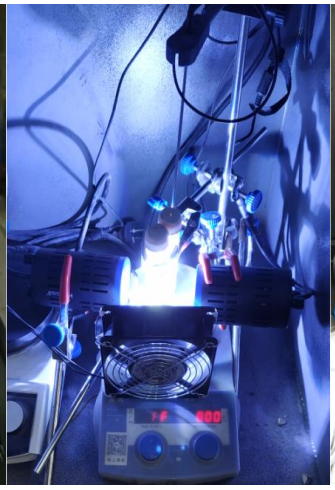
General Procedure B1: A flame-dried 25 mL quartz column reaction tube was placed with a magnetic stir bar. Then, aryl carboxylic acid (0.3 mmol, 1.0 equiv), aryl bromide (0.6 mmol, 2.0 equiv) / aryl iodine (0.45 mmol, 1.5 equiv), **PC1** (2.6 mg, 0.006 mmol, 2 mol%), $NiBr_2$ (3.3 mg, 0.015 mmol, 5 mol%), dtbpy (4.0 mg, 0.015 mmol, 5 mol%), K_3PO_4 (63.7 mg, 0.3 mmol, 1.0 equiv) and DMSO (2.0 mL) were added. The reaction tube was placed on a photocatalytic parallel reactor with a 460 nm blue LEDs light source (10 W) at the bottom (**Figure 6a**). Then the reaction mixture was irradiated with the 460 nm blue LEDs (at approximately 0.3 cm away from the light source). After stirring for 22 hours at 25 ℃, the reaction mixture was added 20 mL H_2O and then extracted with ethyl acetate (3 × 10 mL). The combined organic phase was washed with brine (2 × 5.0 mL), dried over anhydrous Na_2SO_4, and concentrated under vacuum to afford the crude product, which was purified by column chromatography on silica gel using petroleum ether/ethyl acetate as eluent to give the target products.

General Procedure B2: After addition of reagents and solvent, the reaction tube was placed on a photocatalytic parallel reactor with a 460 nm blue LEDs light source (10 W) at the bottom. Then, during the irradiation, the temperature of the reaction mixture was adjusted to 80 ℃. After stirring for 22 hours at 80 ℃, the same workup procedure with General procedure B1 was performed.

General Procedure B3: After addition of reagents and solvent, the reaction mixture was irradiated and stirred with two 40 W 456 nm Kessil blue LEDs. The reaction tube was placed at approximately 2 cm away from the light source

(**Figure 6b**). A fan was used to cool down the reaction tube and reaction mixture during the irradiation. After stirring for 22 hours, the same workup procedure with General procedure B1 was performed.





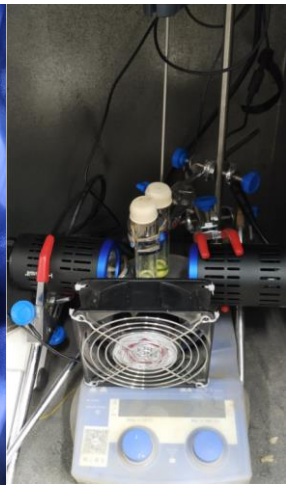
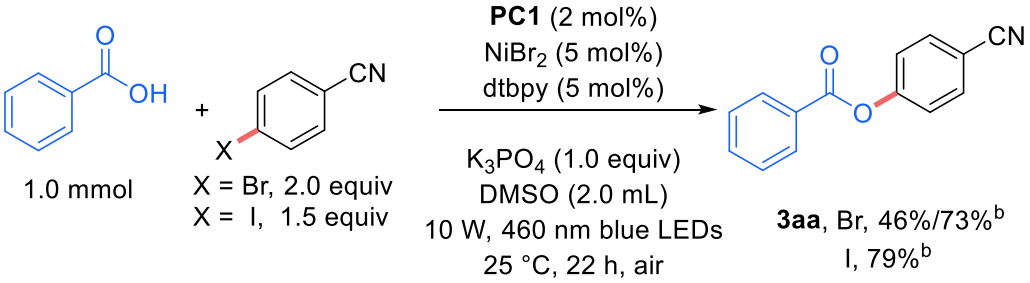
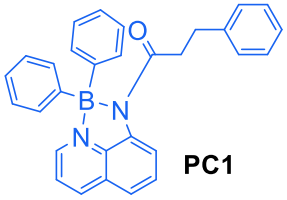


Figure 6a. WATTCAS parallel reactor Figure 6b. KESSIL Blue LEDs

Figure 6. picture of the reaction

4.3 The synthesis of 4-cyanophenyl benzoate on larger scale





	yield of **3aa**	recovery yield of **PC1**
X = Br,	46%/73%[b]	38%/42%[b]
X = I,	79%[b]	71%[b]

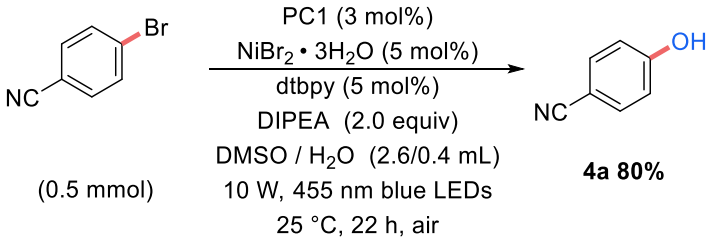
General Procedure B4: A flame-dried 25 mL quartz column reaction tube was placed with a magnetic stir bar. Then, benzoic acid (122.1 mg, 1.0 mmol, 1.0 equiv), 4-bromobenzonitrile (364.0 mg, 2.0 mmol, 2.0 equiv) / 4-iodobenzonitrile (343.5 mg, 1.5 mmol, 1.5 equiv), PC1 (8.8 mg, 0.02 mmol, 2 mol%), $NiBr_2$ (10.9 mg, 0.05 mmol, 5 mol%), dtbpy (13.4 mg, 0.05 mmol, 5 mol%), K_3PO_4 (212.3 mg, 1.0 mmol, 1.0 equiv), and DMSO (6.5 mL) were added. The reaction tube was placed on a photocatalytic parallel reactor with a 460 nm blue LEDs light source (10 W) at the bottom (**Figure 6a**). Then the reaction mixture was irradiated with the 460 nm blue LEDs (at approximately 0.3 cm away from the light source). After stirring for 22 hours at 25 °C, the reaction mixture was added 30 mL H_2O and then extracted with ethyl acetate (3 × 15 mL). The combined organic phase was washed with brine (2 × 5.0 mL), dried over anhydrous Na_2SO_4, and concentrated under vacuum to afford the crude product, which was purified by column chromatography on silica gel using petroleum ether/ethyl acetate as eluent to give the target product to recover the photocatalyst.

General Procedure B5: After addition of reagents and solvent, the reaction mixture was irradiated and stirred with two 40 W 456 nm Kessil blue LEDs. The reaction tube was placed, at approximately 2 cm away from the light source (**Figure 6b**). A fan was used to cool down the reaction tube and reaction mixture during the irradiation. After stirring for 22 hours, the same workup procedure with General procedure B4 was performed.

5 General procedure for the synthesis of phenol

5.1 Control experiments for the used reaction conditions in phenol synthesis

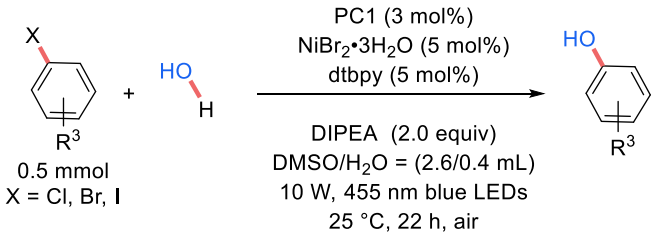
Table S9. The control experiments for the phenol synthesis [a]



Entry	Variations from the 'standard' conditions	Yield (%)[a]
1	no **PC1**	N. D.
2	no $NiBr_2 \cdot 3H_2O$	N. D.
3	no dtbpy	44
4	no light	N. D.
5	no DIPEA	N. D.

Standard reaction conditions: 4-bromobenzonitrile (0.5 mmol, 1.0 equiv), **PC1** (0.015 mmol, 3 mol%), $NiBr_2 \cdot 3H_2O$ (0.025 mmol, 5 mol%), dtbpy (0.025 mmol, 5 mol%), DIPEA (1.0 mmol, 2.0 equiv), and DMSO/ H_2O (2.6/0.4 mL), 10 W 455 nm blue LEDs, 25 °C, air, 22 h. [a] Isolated yield. N. D. = not detected.

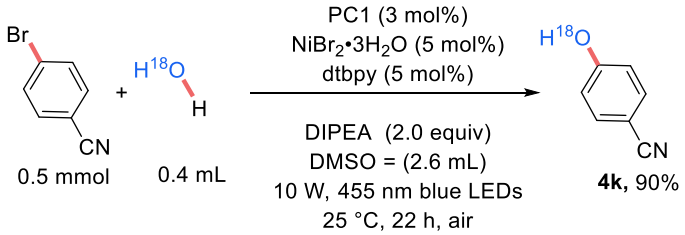
5.2 General procedure for the synthesis of phenol



General Procedure C1: A flame-dried 25 mL quartz column reaction tube was placed with a magnetic stir bar. Then, aryl bromide / aryl iodine / aryl chloride (0.5 mmol, 1.0 equiv), **PC1** (6.6 mg, 0.015 mmol, 3 mol%), $NiBr_2 \cdot 3H_2O$ (6.8 mg, 0.025 mmol, 5 mol%), dtbpy (6.7 mg, 0.025 mmol, 5 mol%), DIPEA (129.2 mg, 1.0 mmol, 2.0 equiv), and DMSO / H_2O (2.6/0.4 mL) were added. The reaction tube was placed on a photocatalytic parallel reactor with a 455 nm blue LEDs light source (10 W) at the bottom (**Figure 6a**). Then the reaction mixture was irradiated with the 455 nm blue LEDs (at approximately 0.3 cm away from the light source). After stirring for 22 hours at 25 ℃, the reaction mixture was acidified with 0.3 N HCl and then extracted with ethyl acetate (3 × 10 mL). The combined organic phase was washed with brine (2 × 5.0 mL), dried over anhydrous Na_2SO_4, and concentrated under vacuum to afford the crude product, which was purified by column chromatography on silica gel using petroleum ether/ethyl acetate as eluent to give the target products.

General Procedure C2: After addition of reagents and solvent, the reaction tube was placed on a photocatalytic parallel reactor with a 455 nm blue LEDs light source (10 W) at the bottom. Then, during the irradiation, the temperature of the reaction mixture was adjusted to 80 ℃. After stirring for 22 hours at 80 ℃, the same workup procedure with General procedure B1 was performed.

5.3 ^{18}O labelling experiment



General Procedure C3: A flame-dried 25 mL quartz column reaction tube was placed with a magnetic stir bar. Then, 4-bromobenzonitrile (91.0 mg, 0.5 mmol, 1.0 equiv), **PC1** (6.6 mg, 0.015 mmol, 3 mol%), $NiBr_2•3H_2O$ (6.8 mg, 0.025 mmol, 5 mol%), dtbpy (6.7 mg, 0.025 mmol, 5 mol%), DIPEA (129.2 mg, 1.0 mmol, 2.0 equiv), and DMSO/ $H_2{}^{18}O$ (2.6/0.4 mL) were added. The reaction tube was placed on a photocatalytic parallel reactor with a 455 nm blue LEDs light source (10 W) at the bottom (**Figure 6a**). Then the reaction mixture was irradiated with 455 nm the blue LEDs (at approximately 0.4 cm away from the light source). After stirring for 22 hours at 25 °C, the reaction mixture was acidified with 0.3 N HCl and then extracted with ethyl acetate (3 × 10 mL). The combined organic phase was washed with brine (2 × 5.0 mL), dried over anhydrous Na_2SO_4, and concentrated under vacuum to afford the crude product, which was purified by column chromatography on silica gel (PE/EA = 3:1) to give the target products **4k** in 90% yield, the products was determined by HRMS (**Figure 7**). The key peaks of ^{18}O labeled 4-(hydroxy)benzonitrile was observed.

HRMS (ESI) m/z calcd for $C_7H_6N^{18}O^+$ $(M+H)^+$ 122.0486, found 122.0485.

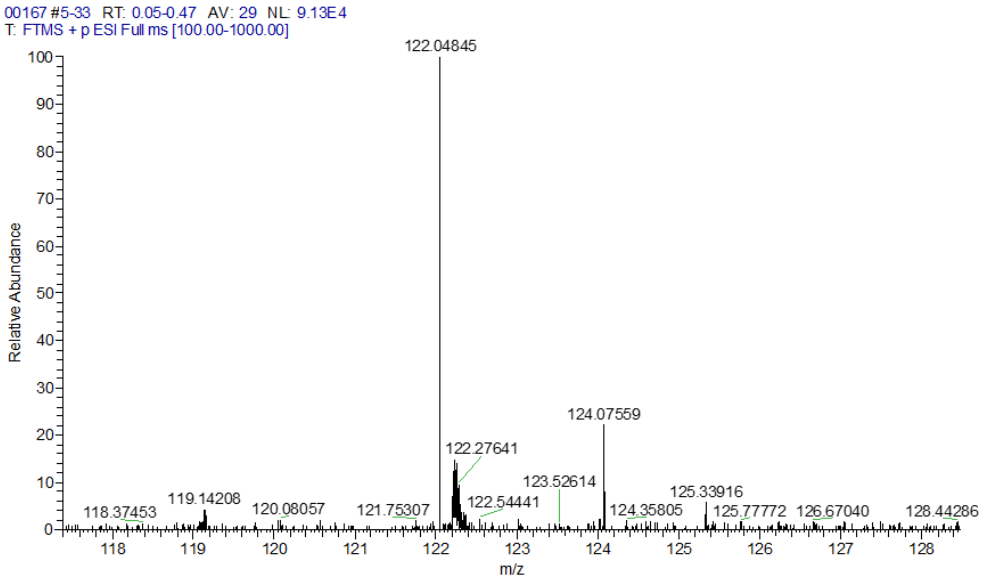
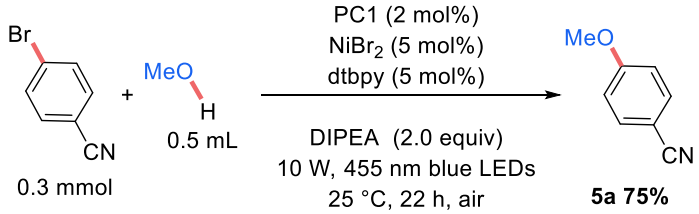


Figure 7. The HRMS spectra of **4k**

6 General procedure for the synthesis of ethers

6.1 Control experiments for the used reaction conditions in ether synthesis

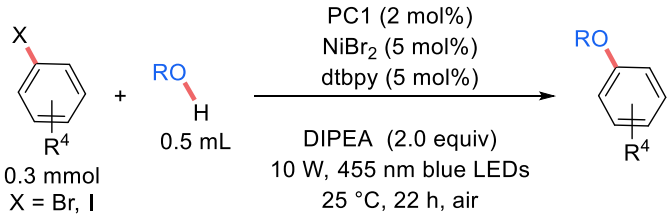
Table S10. The control experiments for the ether synthesis [a]



Entry	Variations from the 'standard' conditions	Yield (%)[a]
1	no **PC1**	13
2	no $NiBr_2$	trace
3	no dtbpy	15
4	no light	N. D.
5	no DIPEA	trace

Standard reaction conditions: 4-bromobenzonitrile (0.3 mmol, 1.0 equiv), **PC1** (0.006 mmol, 2 mol%), $NiBr_2$ (0.015 mmol, 5 mol%), dtbpy (0.015 mmol, 5 mol%), DIPEA (0.6 mmol, 2.0 equiv), and MeOH (0.5 mL), 10 W 455 nm blue LEDs, 25 °C, air, 22 h. [a] Isolated yield. N. D. = not detected.

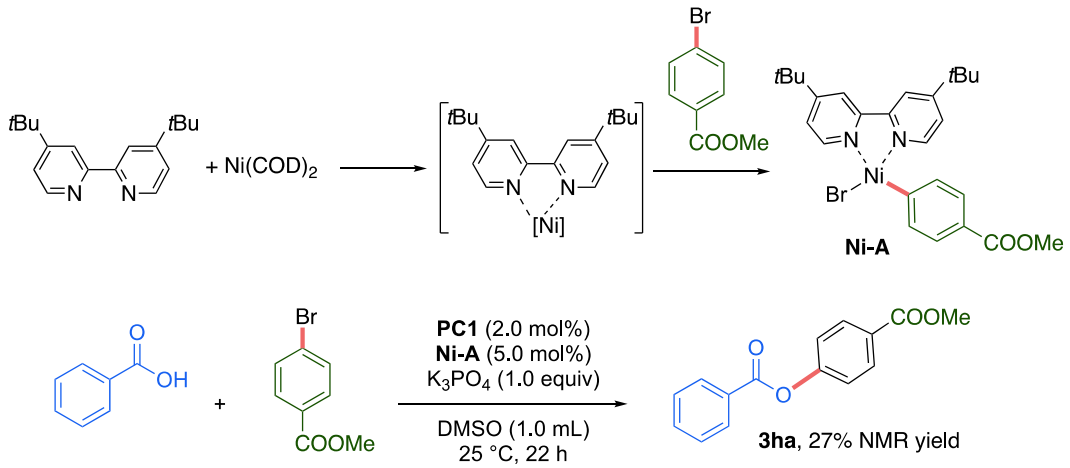
6.2 General procedure for the synthesis of ethers



General Procedure D: A flame-dried 25 mL quartz column reaction tube was placed with a magnetic stir bar. Then, aryl bromide /aryl iodine (0.3 mmol, 1.0 equiv), **PC1** (2.6 mg, 0.006 mmol, 2 mol%), $NiBr_2$ (3.3 mg, 0.015 mmol, 5 mol%), dtbpy (4.0 mg, 0.015 mmol, 5 mol%), DIPEA (77.5 mg, 0.6 mmol, 2.0 equiv), and alkyl alcohol (0.5 mL) were added. The reaction tube was placed on a photocatalytic parallel reactor with a 455 nm blue LEDs light source (10 W) at the bottom (**Figure 6a**). Then the reaction mixture was irradiated with the 455 nm blue LEDs (at approximately 0.3 cm away from the light source). After stirring for 22 hours at 25 ℃, the reaction mixture was filtered, and concentrated under vacuum to afford the crude product, which was purified by column chromatography on silica gel using petroleum ether/ethyl acetate as eluent to give the target products.

7 Proposed reaction mechanisms

7.1 The preparation and application of Ni-A species



Preparation: The **Ni-A** species was prepared according to known procedure (Chu *et al*, *Nat. Commun. 2018,* **9**, 4543).

In a nitrogen filled glove box, a 25 mL reaction tube containing a stirring bar was charged with $Ni(COD)_2$ (276.0 mg, 1.0 mmol, 1.0 equiv), 4,4'-di-tert-butyl-2,2'-bipyridine (268 mg, 1.0 mmol, 1.0 equiv) and THF (10.0 mL) giving a dark purple mixture which was stirred for 12 hours at room temperature. Methyl 4-bromobenzoate (2.2 g, 10.0 mmol, 10.0 equiv) was added and stirred for additional 4 hours. Dry pentane (60 mL) was added to the deep red colored mixture and filtered. The resulting precipitate was washed with pentane (20 mL × 3) and dried under vacuum to afford Ni(II)-aryl complex as a brown solid (531.1 mg). The product was used without further purification. The spectra data were also consistent with the literature. The complex was stored in a nitrogen filled glove box at -30 ºC. ^{1}H NMR (500 MHz, CD_2Cl_2) δ 9.22 (s, 1H), 7.84 (d, J = 14.0 Hz, 2H), 7.75-7.73 (br, 2H), 7.56-7.51 (m, 3H), 7.09 (d, J = 33.0 Hz, 2H), 3.84 (s, 3H), 1.41-1.34 (m, 18H).

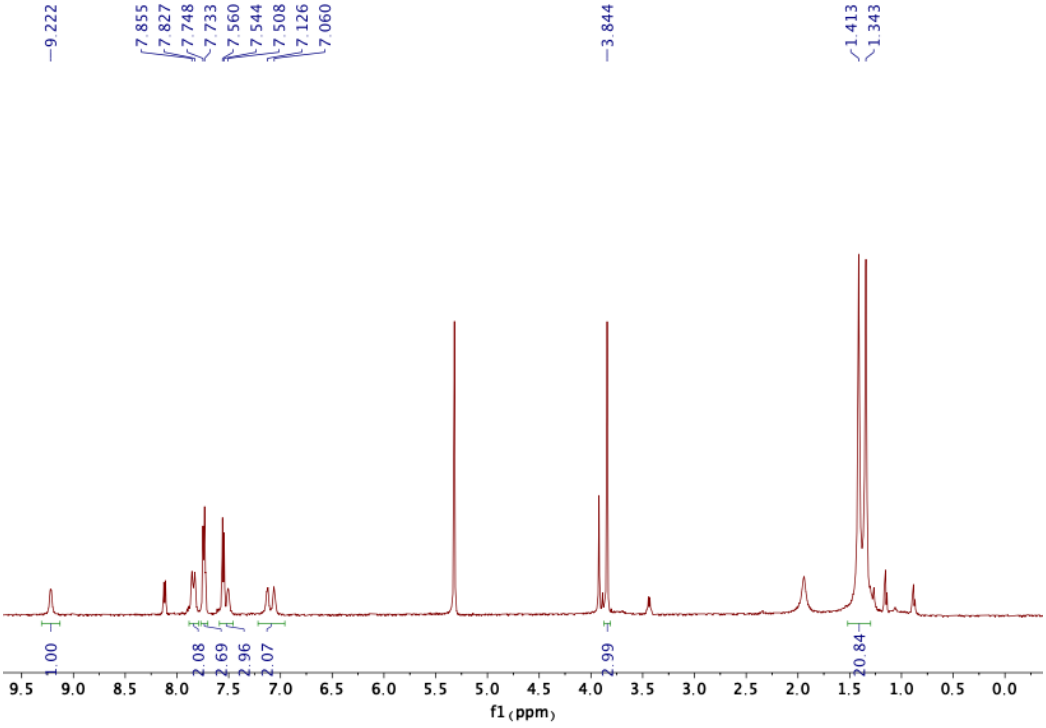


Figure 8. The copy of ^{1}H NMR spectra of **Ni-A**.

Application: A flame-dried reaction tube was placed with a magnetic stir bar. Then, benzoic acid (18.3 mg, 0.15 mmol, 1.0 equiv), methyl 4-bromobenzoate (48.4 mg, 0.225 mmol, 1.5 equiv), **PC1** (1.3 mg, 0.003 mmol, 2 mol%) and K_3PO_4 (31.8 mg, 0.15 mmol, 1.0 equiv) were added. The tube was then taken into the glovebox, where **Ni-A** (4.1 mg, 5 mol%) was added. After get out of the glovebox, 1.0 mL DMSO was injected into the tube. The reaction mixture was stirred and irradiated with four Kessil A160WE Tuna Blue LED Lights. A fan was used to cool down the reaction tube and reaction mixture during the irradiation. After stirring for 22 hours, the mixture was exposed to air. 1,3,5-Trimethoxybenzene (16.8 mg, 0.10 mmol), water, and ethyl acetate were added sequentially. A portion of organic layer was concentrated and analyzed by ^{1}H NMR to get the NMR yield (27%).

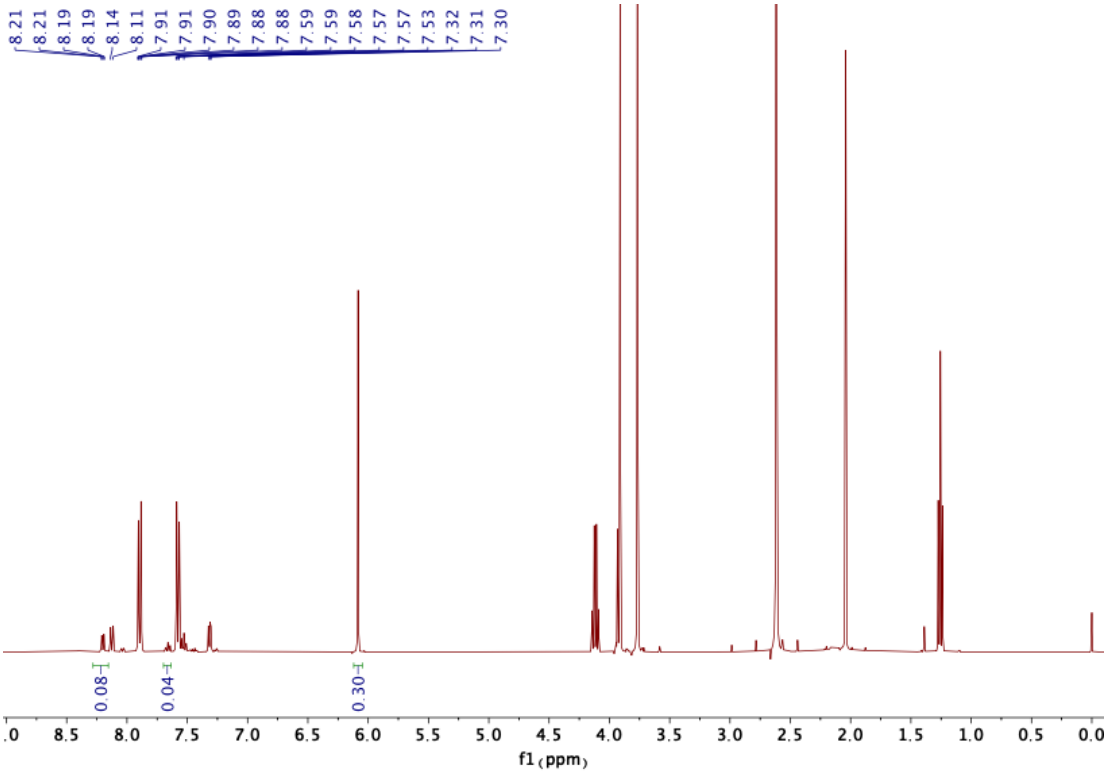


Figure 9. The copy of ^{1}H NMR spectra of the reaction mixture with 1,3,5-trimethoxybenzene as internal standard.

7.2 Proposed mechanisms

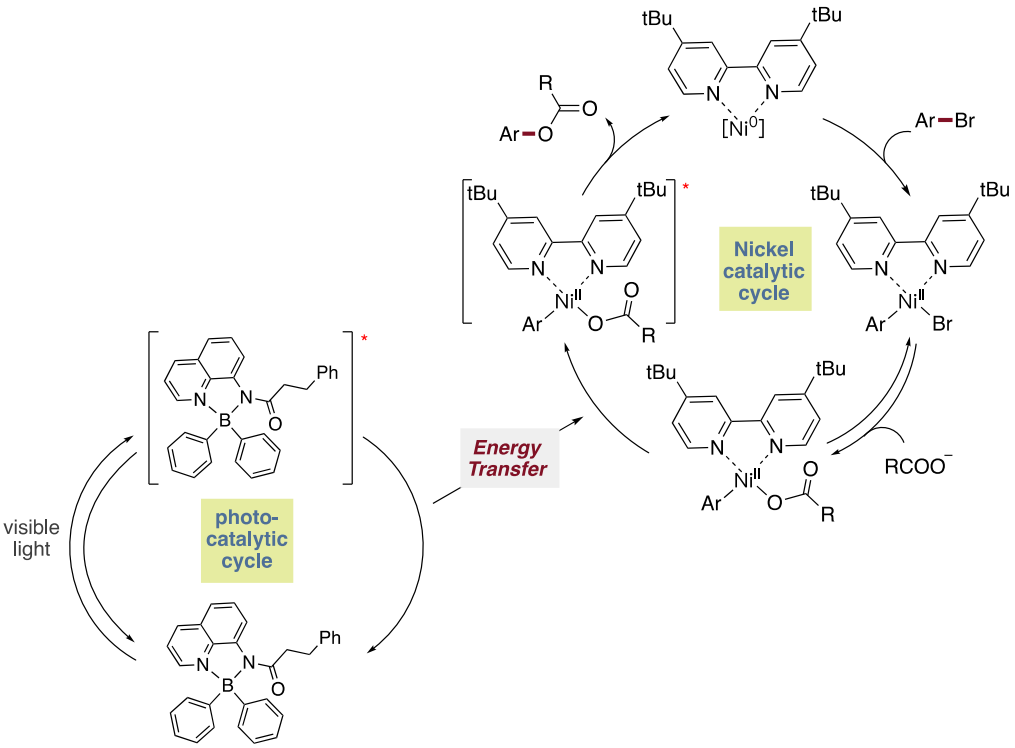
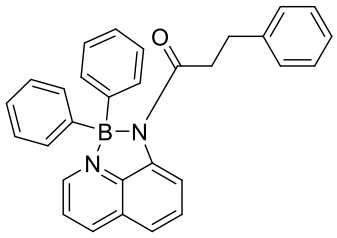


Figure 10. A proposed mechanism via energy transfer pathway, taking the synthesis of esters as an example.

8 Characterization data

(PC1) 1-(2,2-diphenyl-2 λ ⁴,3 λ ⁴-[1,3,2]diazaborolo[4,5,1-ij]quinolin-1(2H)-yl)-3-phenylpropan-1-one



1-(2,2-diphenyl-2λ⁴,3λ⁴-[1,3,2]diazaborolo[4,5,1-*ij*]quinolin-1(2*H*)-yl)-3-phenylpropan-1-one
Chemical Formula: $C_{30}H_{25}BN_2O$
Exact Mass: 440.2060
Molecular Weight: 440.3530

Following the General Procedure A with 3-phenyl-N-(quinolin-8-yl)propanamide (41.4 mg, 0.15 mmol), potassium phenyltrifluoroborate (138.0 mg, 0.75 mmol), **PC1** was obtained as yellow solid (62.7 mg, 95%).

This target product was purified by silica gel flash chromatography (PE: EA = 3:1).

Melting point (°C): 229.6 - 232.9.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.99 (d, J = 7.6 Hz, 1H), 8.43 (dd, J = 5.2, 0.8 Hz, 1H), 8.38 (d, J = 8.4 Hz, 1H), 7.80 (t, J = 8.4 Hz, 1H), 7.56 – 7.52 (m, 1H), 7.52 – 7.46 (m, 5H), 7.30 – 7.24 (m, 6H), 7.13 (t, J = 7.2 Hz, 2H), 7.10 – 7.03 (m, 1H), 6.83 (d, J = 6.8 Hz, 2H), 2.60 (dd, J = 9.5, 4.9 Hz, 2H), 2.57 – 2.49 (m, 2H).

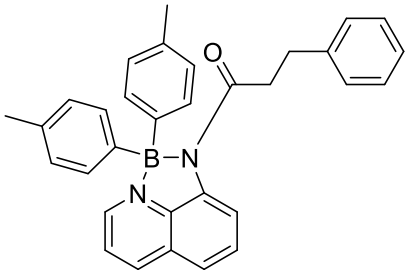
^{13}C NMR (101 MHz, $CDCl_3$) δ 176.2, 142.0, 141.5, 139.5, 139.1, 137.7, 133.5, 132.6, 128.5, 128.1, 127.9, 127.6, 127.2, 125.5, 122.5, 119.0, 117.2, 39.9, 31.5.

^{11}B NMR (128 MHz, $CDCl_3$) δ 5.50.

IR (cm^{-1}): 3065, 3009, 1634, 1512, 1399, 824, 693.

HRMS (ESI) m/z calcd for $C_{30}H_{26}BN_2O^+$ $(M+H)^+$ 441.2133, found 441.2141.

(PC2) 1-(2,2-di-p-tolyl-2 λ ⁴,3 λ ⁴-[1,3,2]diazaborolo[4,5,1-ij]quinolin-1(2H)-yl)-3-phenylpropan-1-one



1-(2,2-di-*p*-tolyl-2λ⁴,3λ⁴-[1,3,2]diazaborolo[4,5,1-*ij*]quinolin-1(2*H*)-yl)-3-phenylpropan-1-one
Chemical Formula: $C_{32}H_{29}BN_2O$
Exact Mass: 468.2373
Molecular Weight: 468.4070

Following the General Procedure A with 3-phenyl-N-(quinolin-8-yl)propanamide (41.4 mg, 0.15 mmol), potassium 4-tolyltrifluoroborate (148.5 mg, 0.75 mmol), **PC2** was obtained as yellow solid (67.7 mg, 96%).

This target product was purified by silica gel flash chromatography (PE: EA = 3:1).

Melting point (°C): 201.1 - 206.4.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.96 (d, J = 7.8 Hz, 1H), 8.38 (d, J = 5.2 Hz, 1H), 8.29 (d, J = 8.4 Hz, 1H), 7.75 (t, J = 8.0 Hz, 1H), 7.47 – 7.41 (m, 2H), 7.36 (d, J = 7.8 Hz, 4H), 7.13 – 7.03 (m, 7H), 6.81 (d, J = 7.0 Hz, 2H), 2.64 – 2.57 (m, 2H), 2.57 – 2.50 (m, 2H), 2.30 (s, 6H).

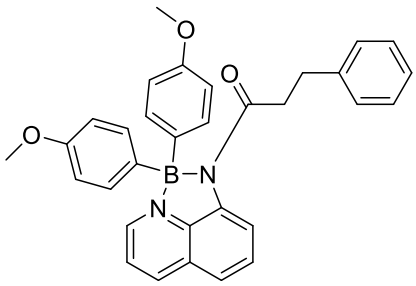
^{13}C NMR (101 MHz, $CDCl_3$) δ 176.3, 142.1, 141.6, 139.5, 139.0, 137.6, 136.7, 133.6, 132.6, 128.7, 128.5, 128.3, 127.6, 125.5, 122.4, 118.9, 117.1, 39.7, 31.5, 21.3.

^{11}B NMR (128 MHz, $CDCl_3$) δ 5.54.

IR (cm^{-1}): 3037, 2933, 1644, 1512, 1390, 1241, 1192, 1079, 834.

HRMS (ESI) m/z calcd for $C_{32}H_{30}BN_2O^+$ $(M+H)^+$ 469.2446, found 469.2455.

(PC3) 1-(2,2-bis(4-methoxyphenyl)-2l λ ⁴,3l λ ⁴-[1,3,2]diazaborolo[4,5,1-ij]quinolin-1(2H)-yl)-3-phenylpropan-1-one



1-(2,2-bis(4-methoxyphenyl)-2I^4,3I^4-[1,3,2]diazaborolo[4,5,1-*ij*]quinolin-1(2*H*)-yl)-3-phenylpropan-1-one
Chemical Formula: $C_{32}H_{29}BN_2O_3$
Exact Mass: 500.2271
Molecular Weight: 500.4050

Following the General Procedure A with 3-phenyl-N-(quinolin-8-yl)propenamide (41.4 mg, 0.15 mmol), potassium 4-methoxyphenyltrifluoroborate (160.5 mg, 0.75 mmol), **PC3** was obtained as yellow solid (59.7 mg, 80%).

This target product was purified by silica gel flash chromatography (PE: EA = 3:1).

Melting point (°C): 57.6 - 62.9.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.99 (d, J = 7.6 Hz, 1H), 8.40 (d, J = 5.2 Hz, 1H), 8.35 (d, J = 8.0 Hz, 1H), 7.79 (t, J = 8.0 Hz, 1H), 7.54 – 7.46 (m, 2H), 7.40 (d, J = 8.4 Hz, 4H), 7.15 (t, J = 7.2 Hz, 2H), 7.10 (d, J = 6.8 Hz, 1H), 6.88 (d, J = 7.2 Hz, 2H), 6.83 (d, J = 8.4 Hz, 4H), 3.78 (s, 6H), 2.69 - 2.63 (m, 2H), 2.59 - 2.53 (m, 2H).

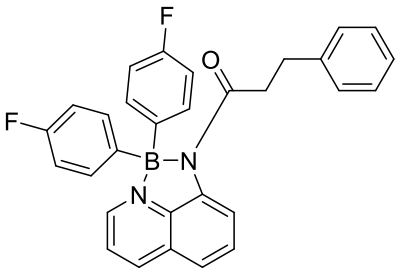
^{13}C NMR (101 MHz, $CDCl_3$) δ 176.3, 158.9, 142.0, 141.6, 139.5, 138.9, 137.5, 134.7, 132.6, 128.5, 128.1, 127.6, 125.5, 122.4, 118.9, 117.1, 113.4, 55.1, 39.6, 31.4.

^{11}B NMR (128 MHz, $CDCl_3$) δ 7.38.

IR (cm^{-1}): 3026, 2914, 2832, 1646, 1596, 1508, 1389, 1244, 1175, 1031, 831.

HRMS (ESI) m/z calcd for $C_{32}H_{30}BN_2O_3^+$ $(M+H)^+$ 501.2344, found 501.2352.

(PC4) 1-(2,2-bis(4-fluorophenyl)-2 λ ⁴,3 λ ⁴-[1,3,2]diazaborolo[4,5,1-ij]quinolin-1(2H)-yl)-3-phenylpropan-1-one



1-(2,2-bis(4-fluorophenyl)-2λ^4,3λ^4-[1,3,2]diazaborolo[4,5,1-*ij*]quinolin-1(2*H*)-yl)-3-phenylpropan-1-one
Chemical Formula: $C_{30}H_{23}BF_2N_2O$
Exact Mass: 476.1872
Molecular Weight: 476.3338

Following the General Procedure A with 3-phenyl-N-(quinolin-8-yl)propenamide (41.4 mg, 0.15 mmol), potassium 4-fluorophenyltrifluoroborate (151.5 mg, 0.75 mmol), **PC4** was obtained as yellow solid (54.1 mg, 76%).

This target product was purified by silica gel flash chromatography (PE: EA = 3:1).

Melting point (°C): 201.8 - 204.9.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.01 (d, J = 8.0 Hz, 1H), 8.42 (d, J = 8.0 Hz, 1H), 8.36 (d, J = 4.8 Hz, 1H), 7.82 (t, J = 8.0 Hz, 1H), 7.57 (dd, J = 8.4, 5.6 Hz, 1H), 7.53 (d, J = 8.4 Hz, 1H), 7.41 (dd, J = 8.4, 6.0 Hz, 4H), 7.17 (t, J = 7.2 Hz, 2H), 7.11 (dd, J = 8.5, 5.9 Hz, 1H), 6.96 (t, J = 8.8 Hz, 4H), 6.88 (d, J = 7.1 Hz, 2H), 2.74 – 2.64 (m, 2H), 2.54 – 2.46 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.9, 162.5 (d, J = 247 Hz), 141.8, 141.4, 139.4, 139.4, 137.5, 135.0 (d, J = 7 Hz), 132.8, 128.4, 128.2, 127.7, 125.7, 122.5, 119.1, 117.4, 114.8 (d, J = 19 Hz), 39.8, 31.3.

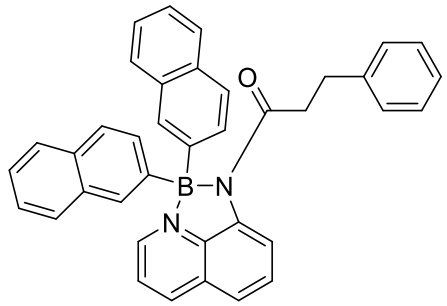
^{19}F NMR (376 MHz, $CDCl_3$) δ -115.33.

^{11}B NMR (128 MHz, $CDCl_3$) δ 4.88.

IR (cm^{-1}): 3027, 1653, 1587, 1512, 1390, 1324, 1173, 816, 693.

HRMS (ESI) m/z calcd for $C_{30}H_{24}BF_2N_2O^+$ $(M+H)^+$ 477.1944, found 477.1954.

(PC5) 1-(2,2-di(naphthalen-2-yl)-2 λ 4,3 λ 4-[1,3,2]diazaborolo[4,5,1-ij]quinolin-1(2H)-yl)-3-phenylpropan-1-one



1-(2,2-di(naphthalen-2-yl)-2λ^4,3λ^4-[1,3,2]diazaborolo[4,5,1-*ij*]quinolin-1(2*H*)-yl)-3-phenylpropan-1-one
Chemical Formula: $C_{38}H_{29}BN_2O$
Exact Mass: 540.2373
Molecular Weight: 540.4730

Following the General Procedure A with 3-phenyl-N-(quinolin-8-yl)propenamide (41.4 mg, 0.15 mmol), potassium 3-naphthyltrifluoroborate (175.5 mg, 0.75 mmol), **PC5** was obtained as yellow solid (66.7 mg, 82%).

This target product was purified by silica gel flash chromatography (PE: EA = 5:1).

Melting point (°C): 59.8 – 61.3.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.07 (d, J = 7.2 Hz, 1H), 8.41 (dd, J = 5.2, 0.8 Hz, 1H), 8.24 (dd, J = 8.4, 0.8 Hz, 1H), 8.06 (s, 2H), 7.85 – 7.75 (m, 4H), 7.75 - 7.69 (m, 3H), 7.59 (dd, J = 8.4, 1.2 Hz, 2H), 7.48 – 7.35 (m, 6H), 6.96 – 6.84 (m, 3H), 6.60 – 6.52 (m, 2H), 2.70 – 2.63 (m, 2H), 2.59 – 2.51 (m, 2H).

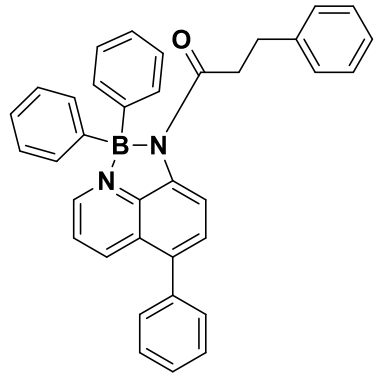
^{13}C NMR (101 MHz, $CDCl_3$) δ 176.4, 142.5, 141.2, 139.7, 139.3, 137.8, 133.5, 133.4, 133.0, 132.7, 131.0, 128.3, 128.3, 128.0, 127.7, 127.60, 127.4, 125.8, 125.7, 125.5, 122.5, 119.2, 117.4, 40.0, 31.5.

^{11}B NMR (128 MHz, $CDCl_3$) δ 5.25.

IR (cm^{-1}): 3056, 2924, 1644, 1503, 1399, 1173, 1070, 787.

HRMS (ESI) m/z calcd for $C_{38}H_{30}BN_2O^+$ $(M+H)^+$ 541.2446, found 541.2449.

(PC6) 3-phenyl-1-(2,2,7-triphenyl-2 λ 4,3 λ 4-[1,3,2]diazaborolo[4,5,1-ij]quinolin-1(2H)-yl)propan-1-one



3-phenyl-1-(2,2,7-triphenyl-2l^4,3l^4-[1,3,2]diazaborolo[4,5,1-*ij*]quinolin-1(2*H*)-yl)propan-1-one
Chemical Formula: $C_{36}H_{29}BN_2O$
Exact Mass: 516.2373
Molecular Weight: 516.4510

Following the General Procedure A with 3-phenyl-N-(5-phenylquinolin-8-yl)propanamide (52.8 mg, 0.15 mmol), potassium phenyltrifluoroborate (138.0 mg, 0.75 mmol), **PC6** was obtained as yellow solid (63.5 mg, 82%).

This target product was purified by silica gel flash chromatography (PE: EA: TEA= 3:1:0.3).

Melting point (°C): 180.8 – 184.2.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.06 (d, J = 8.0 Hz, 1H), 8.50 (dd, J = 8.8, 1.2 Hz, 1H), 8.43 (dd, J = 5.2, 1.2 Hz, 1H), 7.78 (d, J = 8.0 Hz, 1H), 7.58 – 7.49 (m, 6H), 7.49 – 7.42 (m, 4H), 7.32 – 7.22 (m, 6H), 7.19 – 7.10 (m, 2H), 7.10 – 7.04 (m, 1H), 6.89 – 6.81 (m, 2H), 2.68 – 2.60 (m, 2H), 2.59 – 2.53 (m, 2H).

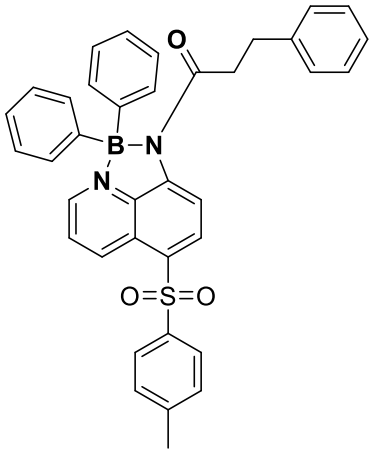
^{13}C NMR (101 MHz, $CDCl_3$) δ 176.2, 141.6, 141.4, 139.7, 138.1, 137.9, 137.7, 133.6, 132.8, 130.9, 129.8, 129.0, 128.5, 128.1, 128.0, 128.0, 127.2, 126.1, 125.6, 122.5, 118.8, 39.9, 31.5.

^{11}B NMR (128 MHz, $CDCl_3$) δ 5.92.

IR (cm^{-1}): 3084, 3018, 1653, 1503, 1399, 1182, 693.

HRMS (ESI) m/z calcd for $C_{36}H_{30}BN_2O^+$ $(M+H)^+$ 517.2446, found 517.2449.

(PC7) 1-(2,2-diphenyl-7-tosyl-2l^4,3l^4-[1,3,2]diazaborolo[4,5,1-ij]quinolin-1(2H)-yl)-3-phenylpropan-1-one



1-(2,2-diphenyl-7-tosyl-2l^4,3l^4-[1,3,2]diazaborolo[4,5,1-*ij*]quinolin-1(2*H*)-yl)-3-phenylpropan-1-one
Chemical Formula: $C_{37}H_{31}BN_2O_3S$
Exact Mass: 594.2148
Molecular Weight: 594.5360

Following the General Procedure A with 3-phenyl-N-(5-tosylquinolin-8-yl)propanamide (64.5 mg, 0.15 mmol), potassium phenyltrifluoroborate (138.0 mg, 0.75 mmol), **PC7** was obtained as yellow solid (74.0 mg, 83%).

This target product was purified by silica gel flash chromatography (PE: DCM: EA = 4:1:1).

Melting point (°C): 208.3 – 211.6.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.24 (d, J = 8.4 Hz, 1H), 9.01 (d, J = 8.4 Hz, 1H), 8.63 (d, J = 8.8 Hz, 1H), 8.47 (d, J = 4.8 Hz, 1H), 7.84 (d, J = 8.0 Hz, 2H), 7.65 (dd, J = 8.4, 5.2 Hz, 1H), 7.40 (dd, J = 6.8, 2.4 Hz, 4H), 7.31 – 7.21 (m, 8H), 7.31 - 7.23 (m, 3H), 6.81 (d, J = 6.8 Hz, 2H), 2.65 – 2.58 (m, 2H), 2.59 – 2.50 (m, 2H), 2.36 (s, 3H).

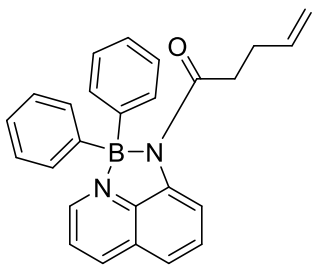
^{13}C NMR (101 MHz, $CDCl_3$) δ 176.9, 147.0, 144.6, 141.1, 140.5, 138.6, 137.7, 137.4, 136.9, 133.4, 130.2, 128.4, 128.1, 128.1, 127.6, 127.3, 126.3, 125.7, 124.4, 124.2, 116.5, 39.8, 31.1, 21.6.

^{11}B NMR (128 MHz, $CDCl_3$) δ 5.91.

IR (cm^{-1}): 3074, 2924, 1662, 1503, 1370, 1314, 1136, 712.

HRMS (ESI) m/z calcd for $C_{37}H_{32}BN_2O_3S^+$ $(M+H)^+$ 595.2221, found 595.2218.

(PC8) 1-(2,2-diphenyl-2 λ ^{4},3 λ ^{4}-[1,3,2]diazaborolo[4,5,1-ij]quinolin-1(2H)-yl)pent-4-en-1-one



1-(2,2-diphenyl-2λ^4,3λ^4-[1,3,2]diazaborolo[4,5,1-*ij*]quinolin-1(2*H*)-yl)pent-4-en-1-one
Chemical Formula: $C_{26}H_{23}BN_2O$
Exact Mass: 390.1903
Molecular Weight: 390.2930

Following the General Procedure A with N-(quinolin-8-yl)pent-4-enamide (33.9 mg, 0.15 mmol), potassium phenyltrifluoroborate (138.0 mg, 0.75 mmol), **PC8** was obtained as yellow solid (49.2 mg, 84%).

This target product was purified by silica gel flash chromatography (PE: EA = 3:1).

Melting point (°C): 196.5 – 198.4.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.97 (d, J = 7.6 Hz, 1H), 8.42 (dd, J = 5.2, 1.2 Hz, 1H), 8.37 (dd, J = 8.4, 1.2 Hz, 1H), 7.78 (t, J = 8.4 Hz, 1H), 7.54 – 7.46 (m, 6H), 7.30 – 7.22 (m, 6H), 5.58 – 5.45 (m, 1H), 4.79 – 4.66 (m, 2H), 2.32 - 2.24 (m, 2H), 2.05 – 1.97 (m, 2H).

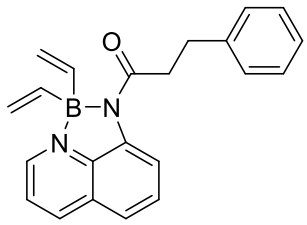
^{13}C NMR (101 MHz, $CDCl_3$) δ 176.4, 142.1, 139.5, 139.1, 137.8, 137.7, 133.5, 132.7, 127.8, 127.6, 127.1, 122.4, 118.9, 117.1, 114.4, 37.6, 29.3.

^{11}B NMR (128 MHz, $CDCl_3$) δ 5.25.

IR (cm^{-1}): 3070, 3020, 1659, 1508, 1389, 1326, 1163, 831.

HRMS (ESI) m/z calcd for $C_{26}H_{24}BN_2O^+$ $(M+H)^+$ 391.1976, found 391.1986.

(PC9) 1-(2,2-divinyl-2l^4,3l^4-[1,3,2]diazaborolo[4,5,1-ij]quinolin-1(2H)-yl)-3-phenylpropan-1-one



1-(2,2-divinyl-2l^4,3l^4-[1,3,2]diazaborolo[4,5,1-*ij*]quinolin-1(2*H*)-yl)-3-phenylpropan-1-one
Chemical Formula: $C_{22}H_{21}BN_2O$
Exact Mass: 340.1747
Molecular Weight: 340.2330

Following the General Procedure A with 3-phenyl-N-(quinolin-8-yl)propanamide (41.4 mg, 0.15 mmol), potassium vinyltrifluoroborate (100.5 mg, 0.75 mmol), **PC9** was obtained as yellow solid (33.5 mg, 66%).

This target product was purified by silica gel flash chromatography (PE: EA = 5:1).

Melting point (°C): 87.7 – 90.8.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.82 (d, J = 7.6 Hz, 1H), 8.39 (dd, J = 8.0, 0.4 Hz, 1H), 8.32 (d, J = 4.4 Hz, 1H), 7.72 (t, J = 8.0 Hz, 1H), 7.62 (dd, J = 8.4, 5.2 Hz, 1H), 7.44 (d, J = 8.0 Hz, 1H), 7.31 – 7.26 (m, 4H), 7.22 – 7.15 (m, 1H), 6.40 (dd, J = 19.6, 13.2 Hz, 2H), 5.58 (d, J = 3.6 Hz, 1H), 5.54 (d, J = 3.2 Hz, 1H), 5.32 (d, J = 3.6 Hz, 1H), 5.27 (d, J = 3.6 Hz, 1H), 3.11 - 3.04 (m, 2H), 2.97 – 2.87 (m, 2H).

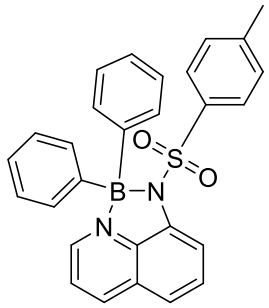
^{13}C NMR (101 MHz, $CDCl_3$) δ 175.7, 142.0, 141.7, 139.3, 138.8, 137.9, 132.5, 128.6, 128.5, 128.3, 127.8, 125.8, 123.8, 122.0, 118.4, 116.7, 39.2, 31.8.

^{11}B NMR (128 MHz, $CDCl_3$) δ 3.05.

IR (cm^{-1}): 3046, 2933, 1653, 1512, 1399, 1088, 947, 768.

HRMS (ESI) m/z calcd for $C_{22}H_{22}BN_2O^+$ $(M+H)^+$ 341.1820, found 341.1828.

(PC10) 2,2-diphenyl-1-tosyl-1,2-dihydro-2 λ ^{4},3 λ ^{4}-[1,3,2]diazaborolo[4,5,1-ij]quinoline



2,2-diphenyl-1-tosyl-1,2-dihydro-2λ^4,3λ^4-[1,3,2]diazaborolo[4,5,1-*ij*]quinoline
Chemical Formula: $C_{28}H_{23}BN_2O_2S$
Exact Mass: 462.1573
Molecular Weight: 462.3740

Following the General Procedure A with quinolin-8-amine (21.6 mg, 0.15 mmol), potassium phenyltrifluoroborate (138.0 mg, 0.75 mmol), 4-toluenesulfonyl chloride (57.2 mg, 0.3 mmol), **PC10** was obtained as yellow solid (58.2 mg, 84%).

This target product was purified by silica gel flash chromatography (PE: DCM: EA = 6:2:1).

Melting point (°C): 240.1 – 246.2.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (dd, J = 5.2, 1.2 Hz, 1H), 8.35 (dd, J = 8.4, 1.2 Hz, 1H), 7.84 (d, J = 7.2 Hz, 1H), 7.67 (t, J = 8.4 Hz, 1H), 7.56 (dd, J = 8.4, 5.2 Hz, 1H), 7.51 – 7.45 (m, 4H), 7.36 (d, J = 8.0 Hz, 1H), 7.31 - 7.26 (m, 6H), 6.97 (d, J = 8.4 Hz, 2H), 6.86 (d, J = 8.0 Hz, 2H), 2.22 (s, 3H).

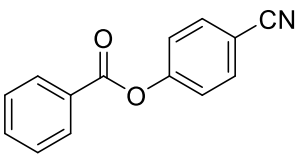
^{13}C NMR (101 MHz, $CDCl_3$) δ 142.4, 140.6, 140.3, 139.2, 137.6, 137.3, 134.1, 132.1, 128.7, 128.1, 127.5, 127.3, 127.0, 122.9, 115.8, 113.2, 21.3.

^{11}B NMR (128 MHz, $CDCl_3$) δ 8.77.

IR (cm^{-1}): 3056, 2999, 1512, 1390, 1324, 1154, 580.

HRMS (ESI) m/z calcd for $C_{28}H_{24}BN_2O_2S^+$ $(M+H)^+$ 463.16461, found 463.16498.

(3aa) 4-cyanophenyl benzoate (CAS: 16513-72-7) [1]



4-cyanophenyl benzoate
Chemical Formula: $C_{14}H_9NO_2$
Exact Mass: 223.0633
Molecular Weight: 223.2310

Following the General Procedure B1 with 4-bromobenzonitrile (109.2 mg, 0.6 mmol), benzoic acid (36.6 mg, 0.3 mmol), **3aa** was obtained as white solid (55.8 mg, 83%).

Following the General Procedure B3 with 4-bromobenzonitrile (109.2 mg, 0.6 mmol), benzoic acid (36.6 mg, 0.3 mmol), **3aa** was obtained as white solid (56.9 mg, 85%).

Following the General Procedure B1 with 4-iodinebenzonitrile (103.1 mg, 0.45 mmol), benzoic acid (36.6 mg, 0.3 mmol), **3aa** was obtained as white solid (60.3 mg, 90%).

Following the General Procedure B3 with 4-iodinebenzonitrile (103.1 mg, 0.45 mmol), benzoic acid (36.6 mg, 0.3 mmol), **3aa** was obtained as white solid (60.1 mg, 90%).

Following the General Procedure B4 with 4-bromobenzonitrile (364.0 mg, 2.0 mmol), benzoic acid (122.1 mg, 1.0 mmol), **3aa** was obtained as white solid (103.2 mg, 46%).

Following the General Procedure B5 with 4-bromobenzonitrile (364.0 mg, 2.0 mmol), benzoic acid (122.1 mg, 1.0 mmol), **3aa** was obtained as white solid (163.5 mg, 73%).

Following the General Procedure B5 with 4-iodobenzonitrile (343.5 mg, 1.5 mmol), benzoic acid (122.1 mg, 1.0 mmol), **3aa** was obtained as white solid (176.5 mg, 79%).

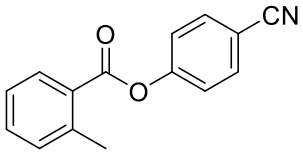
This target product was purified by silica gel flash chromatography (PE: EA = 10:1).

Melting point (°C): 87.9-89.9.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (dd, J = 8.4, 1.4 Hz, 2H), 7.77 – 7.72 (m, 2H), 7.68 (t, J = 7.4 Hz, 1H), 7.54 (t, J = 7.8 Hz, 2H), 7.38 (d, J = 8.8 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.3, 154.3, 134.2, 133.8, 130.3, 128.8, 128.7, 123.0, 118.3, 109.8.

(3ab) 4-cyanophenyl 2-methylbenzoate (CAS: 89013-79-6) [1]



4-cyanophenyl 2-methylbenzoate
Chemical Formula: $C_{15}H_{11}NO_2$
Exact Mass: 237.0790
Molecular Weight: 237.2580

Following the General Procedure B1 with 4-bromobenzonitrile (109.2 mg, 0.6 mmol), o-toluic acid (40.8 mg, 0.3 mmol), **3ab** was obtained as white solid (51.2 mg, 72%).

Following the General Procedure B1 with 4-iodinebenzonitrile (103.1 mg, 0.45 mmol), o-toluic acid (40.8 mg, 0.3 mmol), **3ab** was obtained as white solid (62.4 mg, 88%).

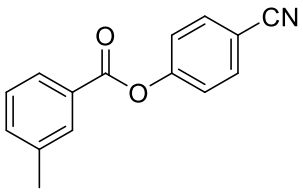
This target product was purified by silica gel flash chromatography (PE: EA = 10:1).

Melting point (°C): 88.3-89.7.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (dd, J = 8.0, 1.2 Hz, 1H), 7.78 – 7.69 (m, 2H), 7.56 – 7.48 (m, 1H), 7.38 – 7.31 (m, 4H), 2.67 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.7, 154.3, 141.8, 133.7, 133.4, 132.2, 131.3, 127.5, 126.1, 123.1, 118.4, 109.7, 22.0.

(3ac) 4-cyanophenyl 3-methylbenzoate (CAS: 89434-74-2) [1]



4-cyanophenyl 3-methylbenzoate
Chemical Formula: $C_{15}H_{11}NO_2$
Exact Mass: 237.0790
Molecular Weight: 237.2580

Following the General Procedure B1 with 4-bromobenzonitrile (109.2 mg, 0.6 mmol), m-toluic acid (40.8 mg, 0.3 mmol), **3ac** was obtained as white solid (21.9 mg, 31%).

Following the General Procedure B3 with 4-iodinebenzonitrile (103.1 mg, 0.45 mmol), m-toluic acid (40.8 mg, 0.3 mmol), **3ac** was obtained as white solid (64.1 mg, 90%).

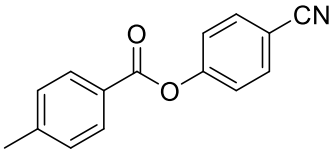
This target product was purified by silica gel flash chromatography (PE: EA = 10:1).

Melting point (°C): 76.7-78.5.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, J = 0.4 Hz, 1H), 7.98 (s, 1H), 7.78 – 7.71 (m, 2H), 7.48 (d, J = 8.0 Hz, 1H), 7.42 (t, J = 8.0 Hz, 1H), 7.39 – 7.34 (m, 2H), 2.45 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.5, 154.4, 138.7, 135.0, 133.7, 130.8, 128.7, 128.6, 127.5, 123.0, 118.3, 109.8, 21.3.

(3ad) 4-cyanophenyl 4-methylbenzoate (CAS: 32792-42-0) [2]



4-cyanophenyl 4-methylbenzoate
Chemical Formula: $C_{15}H_{11}NO_2$
Exact Mass: 237.0790
Molecular Weight: 237.2580

Following the General Procedure B1 with 4-bromobenzonitrile (109.2 mg, 0.6 mmol), p-toluic acid (40.8 mg, 0.3 mmol), **3ad** was obtained as white solid (50.5 mg, 71%).

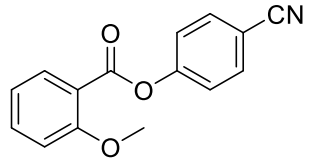
This target product was purified by silica gel flash chromatography (PE: EA = 10:1).

Melting point (°C): 144.0-145.5.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 – 8.05 (m, 2H), 7.76 – 7.70 (m, 2H), 7.39 – 7.34 (m, 2H), 7.33 (d, J = 8.0 Hz, 2H), 2.46 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.4, 154.4, 145.2, 133.7, 130.4, 129.52, 125.9, 123.0, 118.4, 109.7, 21.8.

(3ae) 4-cyanophenyl 2-methoxybenzoate (CAS: 849902-76-7)



4-cyanophenyl 2-methoxybenzoate
Chemical Formula: $C_{15}H_{11}NO_3$
Exact Mass: 253.0739
Molecular Weight: 253.2570

Following the General Procedure B1 with 4-bromobenzonitrile (109.2 mg, 0.6 mmol), o-Anisic acid (45.6 mg, 0.3 mmol), **3ae** was obtained as white solid (51.8 mg, 68%).

Following the General Procedure B1 with 4-iodinebenzonitrile (103.1 mg, 0.45 mmol), o-Anisic acid (45.6 mg, 0.3 mmol), **3ae** was obtained as white solid (66.3 mg, 87%).

This target product was purified by silica gel flash chromatography (PE: EA = 10:1).

Melting point (°C): 80.3-82.9.

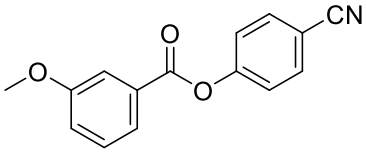
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (dd, J = 8.0, 1.8 Hz, 1H), 7.76 – 7.68 (m, 2H), 7.58 (ddd, J = 8.4, 7.6, 1.6 Hz, 1H), 7.42 – 7.32 (m, 2H), 7.10 – 7.02 (m, 2H), 3.94 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.3, 160.2, 154.4, 135.1, 133.6, 132.4, 123.1, 120.3, 118.4, 117.9, 112.3, 109.5, 56.1.

IR (cm^{-1}): 2970, 2845, 2229, 1746, 1596, 1495, 1202, 1031, 761, 554.

HRMS (ESI) m/z calcd for $C_{15}H_{12}NO_3^+$ $(M+H)^+$ 254.0812, found 254.0817.

(3af) 4-cyanophenyl 3-methoxybenzoate (CAS: 959295-26-2)



4-cyanophenyl 3-methoxybenzoate
Chemical Formula: $C_{15}H_{11}NO_3$
Exact Mass: 253.0739
Molecular Weight: 253.2570

Following the General Procedure B1 with 4-bromobenzonitrile (109.2 mg, 0.6 mmol), 3-methoxybenzoic acid (45.6 mg, 0.3 mmol), **3af** was obtained as white solid (45.3 mg, 60%).

Following the General Procedure B1 with 4-iodinebenzonitrile (103.1 mg, 0.45 mmol), 3-methoxybenzoic acid (45.6 mg, 0.3 mmol), **3af** was obtained as white solid (58.3 mg, 77%).

This target product was purified by silica gel flash chromatography (PE: EA = 10:1).

Melting point (°C): 89.4-92.3.

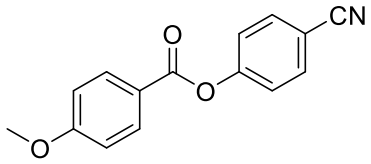
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 – 7.77 (m, 1H), 7.76 – 7.71 (m, 2H), 7.68 (dd, J = 2.4, 1.6 Hz, 1H), 7.43 (t, J = 8.0 Hz, 1H), 7.39 – 7.34 (m, 2H), 7.21 (ddd, J = 8.0, 3.2, 0.8 Hz, 1H), 3.88 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.2, 159.8, 154.3, 133.8, 129.9, 129.8, 123.0, 122.7, 120.6, 118.3, 114.7, 109.9, 55.6.

IR (cm^{-1}): 3018, 2227, 1738, 1587, 1277, 1211, 731, 542.

HRMS (ESI) m/z calcd for $C_{15}H_{12}NO_3^+$ $(M+H)^+$ 254.0812, found 254.0816.

(3ag) 4-cyanophenyl 4-methoxybenzoate (CAS: 74471-18-4) [1]



4-cyanophenyl 4-methoxybenzoate
Chemical Formula: $C_{15}H_{11}NO_3$
Exact Mass: 253.0739
Molecular Weight: 253.2570

Following the General Procedure B1 with 4-bromobenzonitrile (109.2 mg, 0.6 mmol), 4-methoxybenzoic acid (45.6 mg, 0.3 mmol), **3ag** was obtained as white solid (49.2 mg, 65%).

Following the General Procedure B1 with 4-iodinebenzonitrile (103.1 mg, 0.45 mmol), 4-methoxybenzoic acid (45.6 mg, 0.3 mmol), **3ag** was obtained as white solid (63.7 mg, 84%).

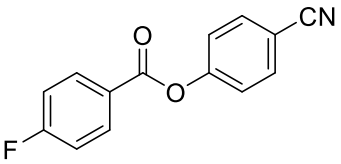
This target product was purified by silica gel flash chromatography (PE: EA = 10:1).

Melting point (°C): 89.3-91.2.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, J = 8.8 Hz, 2H), 7.72 (d, J = 8.8 Hz, 2H), 7.35 (d, J = 8.8 Hz, 2H), 6.99 (d, J = 8.8 Hz, 2H), 3.90 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.4, 164.0, 154.5, 133.7, 132.5, 123.0, 120.8, 118.4, 114.1, 109.6, 55.6.

(3ah) 4-cyanophenyl 4-fluorobenzoate (CAS: 32792-47-5) [1]



4-cyanophenyl 4-fluorobenzoate
Chemical Formula: $C_{14}H_8FNO_2$
Exact Mass: 241.0539
Molecular Weight: 241.2214

Following the General Procedure B1 with 4-bromobenzonitrile (109.2 mg, 0.6 mmol), 4-fluorobenzoic acid (42.0 mg, 0.3 mmol), **3h** was obtained as white solid (39.2 mg, 54%).

Following the General Procedure B3 with 4-iodinebenzonitrile (103.1 mg, 0.45 mmol), 4-fluorobenzoic acid (42.0 mg, 0.3 mmol), **3ah** was obtained as white solid (66.5 mg, 92%).

This target product was purified by silica gel flash chromatography (PE: EA = 10:1).

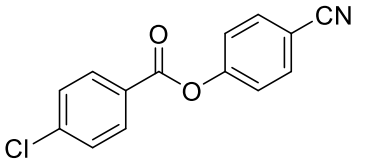
Melting point (°C): 98.2-100.0.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 – 8.17 (m, 2H), 7.77 – 7.71 (m, 2H), 7.41 – 7.33 (m, 2H), 7.25 – 7.16 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.5 (d, J = 257 Hz), 163.4, 154.1, 133.8, 133.01 (d, J = 10 Hz), 124.9 (d, J = 3 Hz), 122.9, 118.2, 116.1 (d, J = 22 Hz), 110.0.

^{19}F NMR (376 MHz, $CDCl_3$) δ -103.11.

(3ai) 4-cyanophenyl 4-chlorobenzoate (CAS: 32792-53-3) [1]



4-cyanophenyl 4-chlorobenzoate
Chemical Formula: $C_{14}H_8ClNO_2$
Exact Mass: 257.0244
Molecular Weight: 257.6730

Following the General Procedure B1 with 4-bromobenzonitrile (109.2 mg, 0.6 mmol), 4-chlorobenzoic acid (47.0 mg, 0.3 mmol), **3ai** was obtained as white solid (60.4 mg, 78%).

Following the General Procedure B3 with 4-iodinebenzonitrile (103.1 mg, 0.45 mmol), 4-chlorobenzoic acid (47.0 mg, 0.3 mmol), **3ai** was obtained as white solid (67.3 mg, 87%).

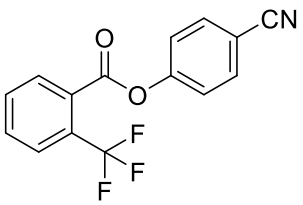
This target product was purified by silica gel flash chromatography (PE: EA = 10:1).

Melting point (°C): 115.3-117.1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 – 8.08 (m, 2H), 7.78 – 7.69 (m, 2H), 7.55 – 7.47 (m, 2H), 7.40 – 7.32 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.5, 154.0, 140.8, 133.8, 131.7, 129.2, 127.1, 122.9, 118.2, 110.0.

(3aj) 4-cyanophenyl 2-(trifluoromethyl)benzoate (CAS:) 849190-82-5



4-cyanophenyl 2-(trifluoromethyl)benzoate
Chemical Formula: $C_{15}H_8F_3NO_2$
Exact Mass: 291.0507
Molecular Weight: 291.2292

Following the General Procedure B1 with 4-bromobenzonitrile (109.2 mg, 0.6 mmol), 2-(trifluoromethyl)benzoic acid (57.0 mg, 0.3 mmol), **3aj** was obtained as white solid (66.9 mg, 77%).

Following the General Procedure B1 with 4-iodinebenzonitrile (103.1 mg, 0.45 mmol), 2-(trifluoromethyl)benzoic acid (57.0 mg, 0.3 mmol), **3aj** was obtained as white solid (77.3 mg, 89%).

his target product was purified by silica gel flash chromatography (PE: EA = 10:1).

Melting point (°C): 60.2-61.8.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 – 7.95 (m, 1H), 7.87 – 7.82 (m, 1H), 7.76 – 7.75 (m, 1H), 7.74 – 7.70 (m, 3H), 7.42 – 7.37 (m, 2H).

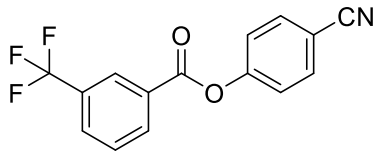
^{13}C NMR (101 MHz, $CDCl_3$) δ 164.3, 153.7, 133.8, 132.4, 132.1, 130.9, 129.4 (q, J = 2 Hz), 129.2 (q, J = 33 Hz), 127.1 (q, J = 5 Hz), 123.3 (q, J = 274 Hz), 122.6, 118.2, 110.3.

^{19}F NMR (376 MHz, $CDCl_3$) δ -59.17.

IR (cm^{-1}): 3074, 2227, 1775, 1503, 1414, 1173, 768, 552.

HRMS (ESI) m/z calcd for $C_{15}H_9F_3NO_2^+$ $(M+H)^+$ 292.0580, found 292.0584.

(3ak) 4-cyanophenyl 3-(trifluoromethyl)benzoate (CAS: 556016-47-8)



4-cyanophenyl 3-(trifluoromethyl)benzoate
Chemical Formula: $C_{15}H_8F_3NO_2$
Exact Mass: 291.0507
Molecular Weight: 291.2292

Following the General Procedure B1 with 4-bromobenzonitrile (109.2 mg, 0.6 mmol), 3-(trifluoromethyl)benzoic acid (57.0 mg, 0.3 mmol), **3ak** was obtained as white solid (57.6 mg, 66%).

his target product was purified by silica gel flash chromatography (PE: EA = 10:1).

Melting point (°C): 47.9-49.1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (s, 1H), 8.38 (d, J = 8.0 Hz, 1H), 7.93 (d, J = 8.0 Hz, 1H), 7.80 – 7.74 (m, 2H), 7.70 (t, J = 7.8 Hz, 1H), 7.43 – 7.36 (m, 2H).

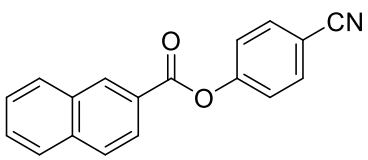
^{13}C NMR (101 MHz, $CDCl_3$) δ 163.1, 153.9, 133.9, 133.5 (q, J = 1 Hz), 131.6 (q, J = 33 Hz), 130.7 (q, J = 4 Hz), 129.6, 129.6, 127.2 (q, J = 4 Hz), 123.5 (q, J = 274 Hz), 122.8, 118.1, 110.3.

^{19}F NMR (376 MHz, $CDCl_3$) δ -62.85.

IR (cm^{-1}): 3102, 2227, 1738, 1503, 1333, 1239, 759, 562.

HRMS (ESI) m/z calcd for $C_{15}H_9F_3NO_2^+$ $(M+H)^+$ 292.0580, found 292.0578.

(3al) 4-cyanophenyl 2-naphthoate (CAS: 49583-89-3) [1]



4-cyanophenyl 2-naphthoate
Chemical Formula: $C_{18}H_{11}NO_2$
Exact Mass: 273.0790
Molecular Weight: 273.2910

Following the General Procedure B1 with 4-bromobenzonitrile (109.2 mg, 0.6 mmol), 2-naphthoic acid (51.7 mg, 0.3 mmol), **3al** was obtained as white solid (50.1 mg, 61%).

Following the General Procedure B1 with 4-iodinebenzonitrile (103.1 mg, 0.45 mmol), 2-naphthoic acid (51.7mg, 0.3 mmol), **3al** was obtained as white solid (58.1 mg, 71%).

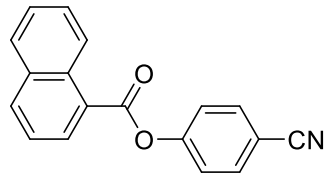
This target product was purified by silica gel flash chromatography (PE: EA = 10:1).

Melting point (°C): 115.3-117.5.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.78 (s, 1H), 8.17 (dd, J = 8.6, 1.8 Hz, 1H), 8.05 – 7.89 (m, 3H), 7.78 – 7.72 (m, 2H), 7.70 – 7.65 (m, 1H), 7.65 – 7.59 (m, 1H), 7.45 – 7.38 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.5, 154.4, 136.0, 133.8, 132.5, 132.3, 129.6, 129.1, 128.7, 127.9, 127.1, 125.8, 125.3, 123.0, 118.4, 109.8.

(3am) 4-cyanophenyl 1-naphthoate (CAS: 49583-90-6)



4-cyanophenyl 1-naphthoate
Chemical Formula: $C_{18}H_{11}NO_2$
Exact Mass: 273.0790
Molecular Weight: 273.2910

Following the General Procedure B1 with 4-bromobenzonitrile (109.2 mg, 0.6 mmol), 1-naphthoic acid (51.7 mg, 0.3 mmol), **3am** was obtained as white solid (54.5 mg, 67%).

Following the General Procedure B1 with 4-iodinebenzonitrile (103.1 mg, 0.45 mmol), 1-naphthoic acid (51.7 mg, 0.3 mmol), **3am** was obtained as white solid (68.3 mg, 83%).

This target product was purified by silica gel flash chromatography (PE: EA = 10:1).

Melting point (°C): 87.3-89.0.

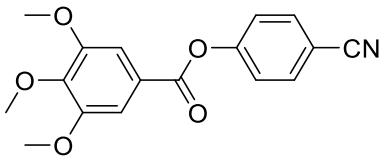
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.02 (d, J = 8.8 Hz, 1H), 8.48 (dd, J = 7.6, 1.2 Hz, 1H), 8.15 (d, J = 8.0 Hz, 1H), 7.95 (d, J = 8.0 Hz, 1H), 7.80 – 7.73 (m, 2H), 7.71 - 7.64 (m , 1H), 7.63 – 7.55 (m, 2H), 7.46 – 7.39 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.7, 154.3, 135.1, 134.0, 133.8, 131.8, 131.7, 128.9, 128.6, 126.7, 125.5, 124.7, 124.5, 123.2, 118.4, 109.8.

IR (cm^{-1}): 2232, 1707, 1502, 1195, 978, 888, 587.

HRMS (ESI) m/z calcd for $C_{18}H_{12}NO_2^+$ $(M+H)^+$ 274.0863, found 274.0871.

(3an) 4-cyanophenyl 3,4,5-trimethoxybenzoate (CAS: 284673-89-8)



4-cyanophenyl 3,4,5-trimethoxybenzoate
Chemical Formula: $C_{17}H_{15}NO_5$
Exact Mass: 313.0950
Molecular Weight: 313.3090

Following the General Procedure B1 with 4-bromobenzonitrile (109.2 mg, 0.6 mmol), 3,4,5-trimethoxybenzenoic acid (63.7 mg, 0.3 mmol), **3an** was obtained as white solid (30.1 mg, 32%).

Following the General Procedure B1 with 4-iodinebenzonitrile (103.1 mg, 0.45 mmol), 3,4,5-trimethbenzoic acid (63.7 mg, 0.3 mmol), **3an** was obtained as white solid (52.6 mg, 56%).

This target product was purified by silica gel flash chromatography (PE: EA = 3:1).

Melting point (°C): 96.3-98.9.

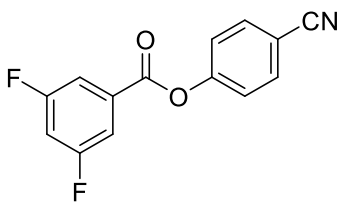
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 – 7.72 (m, 2H), 7.42 (s, 2H), 7.37 – 7.32 (m, 2H), 3.95 (s, 3H), 3.94 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.0, 154.3, 153.2, 143.4, 133.8, 123.4, 123.0, 118.3, 109.9, 107.6, 61.1, 56.4.

IR (cm^{-1}): 2945, 2229, 1727, 1596, 1420, 1226, 868, 755.

HRMS (ESI) m/z calcd for $C_{17}H_{16}NO_5^+$ $(M+H)^+$ 314.1023, found 314.1027.

(3ao) 4-cyanophenyl 3,5-difluorobenzoate (CAS: 849459-13-8)



4-cyanophenyl 3,5-difluorobenzoate
Chemical Formula: $C_{14}H_7F_2NO_2$
Exact Mass: 259.0445
Molecular Weight: 259.2118

Following the General Procedure B1 with 4-bromobenzonitrile (109.2 mg, 0.6 mmol), 3,5-difluorobenzoic acid (47.4 mg, 0.3 mmol), **3ao** was obtained as white solid (14.1 mg, 18%).

Following the General Procedure B1 with 4-iodinebenzonitrile (103.1 mg, 0.45 mmol), 3,5-difluorobenzoic acid (47.4 mg, 0.3 mmol), **3ao** was obtained as white solid (33.9 mg, 44%).

This target product was purified by silica gel flash chromatography (PE: EA = 10:1).

Melting point (°C): 138.4-139.2.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 – 7.74 (dt, J = 8.8 Hz, 2.0 Hz, 2H), 7.73 – 7.67 (m, 2H), 7.40 – 7.34 (dt, J = 8.8 Hz, 1.6 Hz, 2H), 7.13 (tt, J = 8.4, 2.4 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.0 (dd, J = 252 Hz, 12 Hz), 162.2 (t, J = 36 Hz), 153.7, 133.9, 131.8 (t, J = 9 Hz), 122.7,

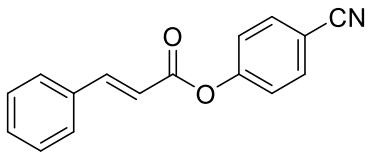
118.1, 113.4 (dd, J = 19 Hz, 8 Hz), 110.4, 109.7 (t, J = 24 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -107.41.

IR (cm^{-1}): 2235, 1746, 1602, 1332, 1207, 868.

HRMS (ESI) m/z calcd for $C_{14}H_8F_2NO_2^+$ $(M+H)^+$ 260.0518, found 260.0523.

(3ap) (*E*)-4-cyanophenyl cinnamate (CAS: 111864-03-0) [3]



4-cyanophenyl cinnamate
Chemical Formula: $C_{16}H_{11}NO_2$
Exact Mass: 249.0790
Molecular Weight: 249.2690

Following the General Procedure B1 with 4-bromobenzonitrile (109.2 mg, 0.6 mmol), trans-cinnamic acid (44.4 mg, 0.3 mmol), **3ap** was obtained as white solid (28.1 mg, 38%).

Following the General Procedure B1 with 4-iodinebenzonitrile (103.1 mg, 0.45 mmol), trans-cinnamic acid (44.4 mg, 0.3 mmol), **3ap** was obtained as white solid (49.8 mg, 67%).

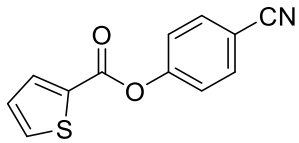
This target product was purified by silica gel flash chromatography (PE: EA = 10:1).

Melting point (°C): 101.6-102.9.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, J = 16.0 Hz, 1H), 7.71 (d, J = 8.8 Hz, 2H), 7.64 – 7.56 (m, 2H), 7.49 – 7.41 (m, 3H), 7.32 (d, J = 8.8 Hz, 2H), 6.62 (d, J = 16.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.5, 154.2, 147.9, 133.8, 133.7, 131.2, 129.1, 128.5, 122.8, 118.4, 116.3, 109.6.

(3aq) 4-cyanophenyl thiophene-2-carboxylate (CAS: 926557-71-3)



4-cyanophenyl thiophene-2-carboxylate
Chemical Formula: $C_{12}H_7NO_2S$
Exact Mass: 229.0197
Molecular Weight: 229.2530

Following the General Procedure B1 with 4-bromobenzonitrile (109.2 mg, 0.6 mmol), 2-thiophenecarboxylic acid (38.4 mg, 0.3 mmol), **3aq** was obtained as white solid (57.7 mg, 84%).

Following the General Procedure B1 with 4-iodinebenzonitrile (103.1 mg, 0.45 mmol), 2-thiophenecarboxylic acid (38.4 mg, 0.3 mmol), **3aq** was obtained as white solid (49.9 mg, 73%).

This target product was purified by silica gel flash chromatography (PE: EA = 10:1).

Melting point (°C): 117.1-118.2.

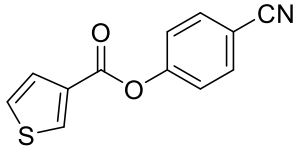
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (dd, J = 3.6, 1.2 Hz, 1H), 7.74 – 7.72 (m, 1H), 7.72 – 7.69 (m, 2H), 7.41 – 7.34 (m, 2H), 7.20 (dd, J = 5.0, 3.8 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 159.7, 153.9, 135.4, 134.5, 133.8, 131.8, 128.3, 122.9, 118.3, 109.9.

IR (cm^{-1}): 3112, 2227, 1737, 1503, 1408, 1257, 731, 542.

HRMS (ESI) m/z calcd for $C_{12}H_8NO_2S^+$ $(M+H)^+$ 230.0270, found 230.0273.

(3ar) 4-cyanophenyl thiophene-3-carboxylate (CAS: 1240742-51-1)



4-cyanophenyl thiophene-3-carboxylate
Chemical Formula: $C_{12}H_7NO_2S$
Exact Mass: 229.0197
Molecular Weight: 229.2530

Following the General Procedure B1 with 4-bromobenzonitrile (109.2 mg, 0.6 mmol), 3-thiophenecarboxylic acid (38.4 mg, 0.3 mmol), **3ar** was obtained as white solid (35.8 mg, 52%).

Following the General Procedure B3 with 4-iodinebenzonitrile (103.1 mg, 0.45 mmol), 3-thiophenecarboxylic acid (38.4 mg, 0.3 mmol), **3ar** was obtained as white solid (64.0 mg, 93%).

This target product was purified by silica gel flash chromatography (PE: EA =10:1).

Melting point (°C): 117.0-118.8.

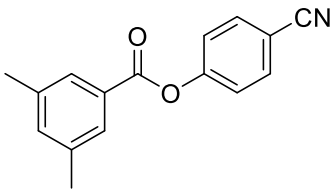
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (dd, J = 3.2, 1.2 Hz, 1H), 7.76 – 7.70 (m, 2H), 7.65 (dd, J = 5.2, 1.2 Hz, 1H), 7.41 (dd, J = 5.2, 3.2 Hz, 1H), 7.38 – 7.32 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.1, 154.0, 134.9, 133.7, 131.9, 128.2, 126.8, 122.9, 118.3, 109.8.

IR (cm^{-1}): 3102, 2229, 1746, 1508, 1481, 925, 736.

HRMS (ESI) m/z calcd for $C_{12}H_8NO_2S^+$ $(M+H)^+$ 230.0270, found 230.0275.

(3as) 4-cyanophenyl 3,5-dimethylbenzoate (CAS: 849610-41-9) [1]



4-cyanophenyl 3,5-dimethylbenzoate
Chemical Formula: $C_{16}H_{13}NO_2$
Exact Mass: 251.0946
Molecular Weight: 251.2850

Following the General Procedure B1 with 4-bromobenzonitrile (109.2 mg, 0.6 mmol), 3,5-dimethylbenzoic acid (45.1 mg, 0.3 mmol), **3as** was obtained as white solid (22.4 mg, 30%).

Following the General Procedure B3 with 4-iodinebenzonitrile (103.1 mg, 0.45 mmol), 3,5-dimethylbenzoic acid (45.1 mg, 0.3 mmol), **3as** was obtained as white solid (56.7 mg, 75%).

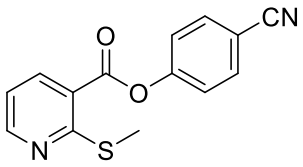
This target product was purified by silica gel flash chromatography (PE: EA =10:1).

Melting point (°C): 63.9-65.5.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (s, 2H), 7.77 – 7.71 (m, 2H), 7.38 – 7.33 (m, 2H), 7.30 (s, 1H), 2.41 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.7, 154.4, 138.5, 135.9, 133.7, 128.5, 128.0, 123.0, 118.3, 109.7, 21.2.

(3at) 4-cyanophenyl 2-(methylthio)nicotinate (CAS: 1061854-05-4)



4-cyanophenyl 2-(methylthio)nicotinate
Chemical Formula: $C_{14}H_{10}N_2O_2S$
Exact Mass: 270.0463
Molecular Weight: 270.3060

Following the General Procedure B1 with 4-bromobenzonitrile (109.2 mg, 0.6 mmol), 2-(methylthio)nicotinic acid (50.8 mg, 0.3 mmol), **3at** was obtained as white solid (24.1 mg, 30%).

Following the General Procedure B3 with 4-iodinebenzonitrile (103.1 mg, 0.45 mmol), 2-(methylthio)nicotinic acid (50.8 mg, 0.3 mmol), **3at** was obtained as white solid (41.2 mg, 51%).

This target product was purified by silica gel flash chromatography (PE: EA =10:1).

Melting point (°C): 167.9-169.5.

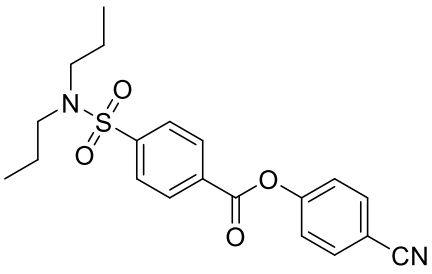
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (dd, J = 4.8, 1.6 Hz, 1H), 8.41 (dd, J = 7.8, 1.8 Hz, 1H), 7.78 – 7.71 (m, 2H), 7.42 – 7.34 (m, 2H), 7.15 (dd, J = 8.0, 4.8 Hz, 1H), 2.57 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.3, 162.9, 153.8, 153.0, 139.4, 133.8, 122.9, 121.3, 118.2, 118.1, 110.1, 14.0.

IR (cm^{-1}): 3093, 2924, 2227, 1738, 1559, 1229, 1032, 749.

HRMS (ESI) m/z calcd for $C_{14}H_{11}N_2O_2S^+$ $(M+H)^+$ 271.0536, found 271.0540.

(3au) 4-cyanophenyl 4-(N,N-dipropylsulfamoyl)benzoate (CAS: 2351103-21-2) [1]



4-cyanophenyl 4-(*N*,*N*-dipropylsulfamoyl)benzoate
Chemical Formula: $C_{20}H_{22}N_2O_4S$
Exact Mass: 386.1300
Molecular Weight: 386.4660

Following the General Procedure B1 with 4-bromobenzonitrile (109.2 mg, 0.6 mmol), probenecid (85.6 mg, 0.3 mmol), **3au** was obtained as white solid (58.5 mg, 51%).

Following the General Procedure B3 with 4-iodinebenzonitrile (103.1 mg, 0.45 mmol), probenecid (85.6 mg, 0.3 mmol), **3au** was obtained as white solid (67.6 mg, 58%).

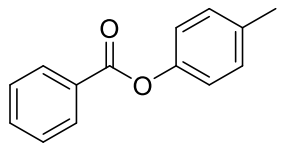
This target product was purified by silica gel flash chromatography (PE: EA =10:1).

Melting point (°C): 102.7-104.0.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 – 8.26 (m, 2H), 8.00 – 7.92 (m, 2H), 7.79 – 7.72 (m, 2H), 7.42 – 7.34 (m, 2H), 3.18 – 3.08 (m, 4H), 1.63 – 1.49 (m, 4H), 0.87 (t, J = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.1, 153.9, 145.5, 133.9, 131.9, 130.9, 127.3, 122.8, 118.1, 110.3, 49.9, 21.9, 11.2.

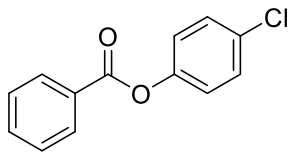
(3ba) p-tolyl benzoate (CAS: 614-34-6) [1]



p-tolyl benzoate
Chemical Formula: $C_{14}H_{12}O_2$
Exact Mass: 212.0837
Molecular Weight: 212.2480

Following the General Procedure B2 with 4-iodotoluene (98.1 mg, 0.45 mmol), benzoic acid (36.6 mg, 0.3 mmol), **3ba** was obtained as white solid (33.6 mg, 53%).
This target product was purified by silica gel flash chromatography (PE: EA = 50:1).
Melting point (°C): 70.6-72.1.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 – 8.20 (m, 2H), 7.64 (t, J = 7.4 Hz, 1H), 7.52 (t, J = 7.6 Hz, 2H), 7.24 (d, J = 8.0 Hz, 2H), 7.12 (d, J = 8.4 Hz, 2H), 2.39 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 165.4, 148.8, 135.5, 133.5, 130.2, 130.0, 129.7, 128.6, 121.4, 20.9.

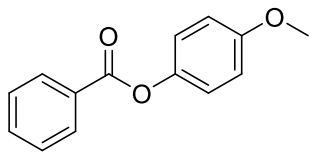
(3ca) 4-chlorophenyl benzoate (CAS: 2005-08-5) [4]



4-chlorophenyl benzoate
Chemical Formula: $C_{13}H_9ClO_2$
Exact Mass: 232.0291
Molecular Weight: 232.6630

Following the General Procedure B2 with 1-chloro-4-iodobenzene (107.3 mg, 0.45 mmol), benzoic acid (36.6 mg, 0.3 mmol), **3ca** was obtained as white solid (38.1 mg, 55%).
This target product was purified by silica gel flash chromatography (PE: EA = 40:1).
Melting point (°C): 82.4-83.8.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 – 8.16 (m, 2H), 7.69 – 7.63 (m, 1H), 7.56 – 7.48 (m, 2H), 7.43 – 7.36 (m, 2H), 7.21 – 7.14 (m, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 165.0, 149.5, 133.8, 131.3, 130.2, 129.6, 129.2, 128.7, 123.1.

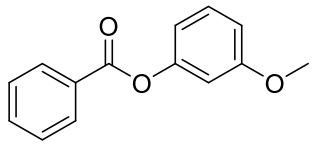
(3da) 4-methoxyphenyl benzoate (CAS: 1523-19-9) [4]



4-methoxyphenyl benzoate
Chemical Formula: $C_{14}H_{12}O_3$
Exact Mass: 228.0786
Molecular Weight: 228.2470

Following the General Procedure B2 with 1-iodo-4-methoxybenzene (105.3 mg, 0.45 mmol), benzoic acid (36.6 mg, 0.3 mmol), **3da** was obtained as white solid (26.1 mg, 40%).
This target product was purified by silica gel flash chromatography (PE: EA = 20:1).
Melting point (°C): 71.6-73.2.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (dd, J = 8.4, 1.2 Hz, 2H), 7.67 – 7.60 (m, 1H), 7.55 – 7.48 (m, 2H), 7.18 – 7.11 (m, 2H), 6.98 – 6.92 (m, 2H), 3.83 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 165.6, 157.4, 144.5, 133.5, 130.2, 129.7, 128.6, 122.5, 114.6, 55.6.

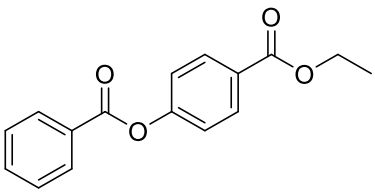
(3ea) 3-methoxyphenyl benzoate (CAS: 5554-24-5) [5]



3-methoxyphenyl benzoate
Chemical Formula: $C_{14}H_{12}O_3$
Exact Mass: 228.0786
Molecular Weight: 228.2470

Following the General Procedure B2 with 1-iodo-3-methoxybenzene (105.3 mg, 0.45 mmol), benzoic acid (36.6 mg, 0.3 mmol), **3ea** was obtained as colorless oil (39.4 mg, 58%).
This target product was purified by silica gel flash chromatography (PE: EA = 40:1).
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 – 8.19 (m, 2H), 7.68 – 7.62 (m, 1H), 7.56 – 7.49 (m, 2H), 7.34 (t, J = 8.2 Hz, 1H), 6.87 – 6.84 (m, 1H), 6.84 – 6.82 (m, 1H), 6.80 (t, J = 2.2 Hz, 1H), 3.83 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 165.1, 160.6, 152.0, 133.6, 130.2, 129.9, 129.6, 128.6, 113.9, 111.9, 107.7, 55.5.

(3fa) ethyl 4-(benzoyloxy)benzoate (CAS: 7471-31-0) [1]



ethyl 4-(benzoyloxy)benzoate
Chemical Formula: $C_{16}H_{14}O_4$
Exact Mass: 270.0892
Molecular Weight: 270.2840

Following the General Procedure B1 with ethyl 4-bromobenzoate (137.8 mg, 0.6 mmol), benzoic acid (36.6 mg, 0.3 mmol), **3aa** was obtained as corlorless solid (41.4 mg, 51%).

Following the General Procedure B1 with ethyl 4-iodobenzoate (124.2 mg, 0.45 mmol), benzoic acid (36.6 mg, 0.3 mmol), **3fa** was obtained as white solid (66.0 mg, 81%).

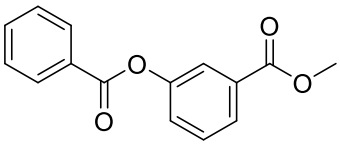
This target product was purified by silica gel flash chromatography (PE: EA = 20:1).

Melting point (°C): 85.1-86.5.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 – 8.18 (m, 2H), 8.16 – 8.10 (m, 2H), 7.69 – 7.62 (m, 1H), 7.55 – 7.47 (m, 2H), 7.34 – 7.28 (m, 2H), 4.39 (q, J = 7.2 Hz, 2H), 1.40 (t, J = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.9, 164.7, 154.6, 133.9, 131.2, 130.3, 129.2, 128.7, 128.2, 121.7, 61.1, 14.4.

(3ga) methyl 3-(benzoyloxy)benzoate (CAS: 108011-99-0)



methyl 3-(benzoyloxy)benzoate
Chemical Formula: $C_{15}H_{12}O_4$
Exact Mass: 256.0736
Molecular Weight: 256.2570

Following the General Procedure B3 with methyl 3-iodobenzoate (118.1 mg, 0.45 mmol), benzoic acid (36.6 mg, 0.3 mmol), **3ga** was obtained as white solid (45.8 mg, 60%).

This target product was purified by silica gel flash chromatography (PE: EA = 20:1).

Melting point (°C): 75.9-77.5.

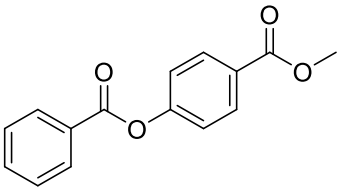
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (dd, J = 8.2, 1.0 Hz, 2H), 7.97 (dt, J = 7.6, 1.2 Hz, 1H), 7.93 – 7.88 (m, 1H), 7.70 – 7.62 (m, 1H), 7.57 – 7.48 (m,, 3H), 7.47 – 7.40 (m 1H), 3.93 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.2, 165.0, 150.9, 133.8, 131.8, 130.2, 129.5, 129.2, 128.7, 127.1, 126.5, 123.0, 52.3.

IR (cm^{-1}): 3093, 2952, 1728, 1436, 1249, 1060, 703.

HRMS (ESI) m/z calcd for $C_{15}H_{13}O_4^+$ $(M+H)^+$ 257.0808, found 257.0812.

(3ha) methyl 4-(benzoyloxy)benzoate (CAS: 75915-29-6) [1]



methyl 4-(benzoyloxy)benzoate
Chemical Formula: $C_{15}H_{12}O_4$
Exact Mass: 256.0736
Molecular Weight: 256.2570

Following the General Procedure B2 with methyl 4-bromobenzoate (129.0 mg, 0.6 mmol), benzoic acid (36.6 mg, 0.3 mmol), **3ha** was obtained as colorless solid (30.9 mg, 40%).

Following the General Procedure B1 with methyl 4-iodobenzoate (118.1 mg, 0.45 mmol), benzoic acid (36.6 mg, 0.3 mmol), **3ha** was obtained as white solid (38.7 mg, 50%).

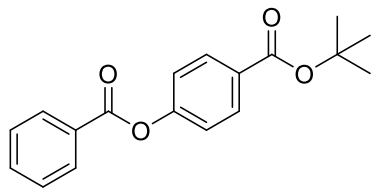
This target product was purified by silica gel flash chromatography (PE: EA = 20:1).

Melting point (°C): 131.0-131.9.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 – 8.18 (m, 2H), 8.16 – 8.09 (m, 2H), 7.70 – 7.62 (m, 1H), 7.52 (t, J = 7.8 Hz, 2H), 7.35 – 7.28 (m, 2H), 3.93 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4, 164.7, 154.6, 133.9, 131.3, 130.3, 129.1, 128.7, 127.8, 121.8, 52.2.

(3ia) tert-butyl 4-(benzoyloxy)benzoate



tert-butyl 4-(benzoyloxy)benzoate
Chemical Formula: $C_{18}H_{18}O_4$
Exact Mass: 298.1205
Molecular Weight: 298.3380

Following the General Procedure B3 with tert-butyl-4-bromobenzoate (154.3 mg, 0.6 mmol), benzoic acid (36.6 mg, 0.3 mmol), **3ia** was obtained as white solid (67.8 mg, 76%).

This target product was purified by silica gel flash chromatography (PE: EA = 20:1).

Melting point (°C): 95.4-97.9.

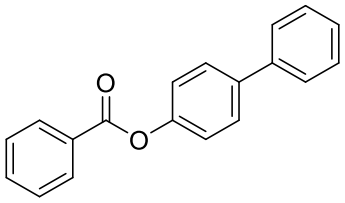
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 – 8.18 (m, 2H), 8.11 – 8.04 (m, 2H), 7.67 – 7.61 (m, 1H), 7.51 (t, J = 7.6 Hz, 2H), 7.30 – 7.25 (m, 2H), 1.60 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.0, 164.7, 154.3, 133.8, 131.1, 130.3, 129.7, 129.2, 128.7, 121.6, 81.2, 28.2.

IR (cm^{-1}): 2981, 1738, 1597, 1164, 1060, 683.

HRMS (ESI) m/z calcd for $C_{18}H_{19}O_4^+$ $(M+H)^+$ 299.1278, found 299.1277.

(3ja) [1,1'-biphenyl]-4-yl benzoate (CAS: 2170-13-0) [6]



[1,1'-biphenyl]-4-yl benzoate
Chemical Formula: $C_{19}H_{14}O_2$
Exact Mass: 274.0994
Molecular Weight: 274.3190

Following the General Procedure B2 with 4-bromobiphenyl (139.9 mg, 0.6 mmol), benzoic acid (36.6 mg, 0.3 mmol), **3ja** was obtained as white solid (32.6 mg, 40%).

Following the General Procedure B2 with 4-iodobiphenyl (126.1 mg, 0.45 mmol), benzoic acid (36.6 mg, 0.3 mmol), **3ja** was obtained as white solid (57.2 mg, 70%).

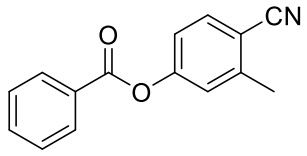
This target product was purified by silica gel flash chromatography (PE: EA = 20:1).

Melting point (°C): 146.5-147.9.

H NMR (400 MHz, $CDCl_3$) δ 8.28 – 8.23 (m, 2H), 7.69 – 7.64 (m, 3H), 7.64 – 7.58 (m, 2H), 7.58 – 7.51 (m, 2H), 7.50 – 7.44 (m, 2H), 7.41 – 7.35 (m, 1H), 7.34 – 7.29 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.3, 150.4, 140.4, 139.1, 133.7, 130.2, 129.6, 128.8, 128.6, 128.3, 127.4, 127.2, 122.0.

(3ka) 4-cyano-3-methylphenyl benzoate



4-cyano-3-methylphenyl benzoate
Chemical Formula: $C_{15}H_{11}NO_2$
Exact Mass: 237.0790
Molecular Weight: 237.2580

Following the General Procedure B3 with 4-bromo-2-methylbenzonitrile (177.6 mg, 0.6 mmol), benzoic acid (36.6 mg, 0.3 mmol), **3ka** was obtained as white solid (40.4 mg, 57%).

This target product was purified by silica gel flash chromatography (PE: EA = 20:1).

Melting point (°C): 79.3-80.6.

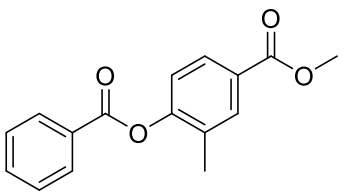
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 – 8.15 (m, 2H), 7.70 – 7.64 (m, 2H), 7.57 – 7.50 (m, 2H), 7.22 (d, J = 2.0 Hz, 1H), 7.17 (dd, J = 8.4, 2.0 Hz, 1H), 2.58 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.5, 154.1, 144.2, 134.1, 133.9, 130.3, 128.8, 123.8, 120.1, 117.6, 110.3, 20.6.

IR (cm^{-1}): 3093, 2227, 1747, 1229, 1060, 712, 590.

HRMS (ESI) m/z calcd for $C_{15}H_{12}NO_2^+$ $(M+H)^+$ 238.0863, found 238.0862.

(3la) methyl 4-(benzoyloxy)-3-methylbenzoate



methyl 4-(benzoyloxy)-3-methylbenzoate
Chemical Formula: $C_{16}H_{14}O_4$
Exact Mass: 270.0892
Molecular Weight: 270.2840

Following the General Procedure B2 with methyl 3-iodo-4-methylbenzoate (124.2 mg, 0.45 mmol), benzoic acid (36.6 mg, 0.3 mmol), **3la** was obtained as white solid (38.6 mg, 48%).

This target product was purified by silica gel flash chromatography (PE: EA = 20:1).

Melting point (°C): 42.4-45.3.

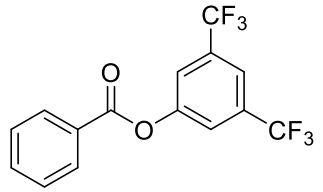
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 – 8.19 (m, 2H), 7.88 (dd, J = 7.8, 1.8 Hz, 1H), 7.83 (d, J = 1.6 Hz, 1H), 7.69 – 7.63 (m, 1H), 7.56 – 7.51 (m, 2H), 7.35 (d, J = 8.0 Hz, 1H), 3.90 (s, 3H), 2.29 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.3, 164.7, 149.4, 136.1, 133.8, 131.2, 130.2, 129.4, 129.1, 128.7, 127.3, 123.4, 52.2, 16.6.

IR (cm^{-1}): 3074, 2999, 2951, 1728, 1446, 1249, 1098, 712.

HRMS (ESI) m/z calcd for $C_{16}H_{15}O_4^+$ $(M+H)^+$ 271.0965, found 271.0970.

(3ma) 3,5-bis(trifluoromethyl)phenyl benzoate (CAS: 2076460-93-8) [1]



3,5-bis(trifluoromethyl)phenyl benzoate
Chemical Formula: $C_{15}H_8F_6O_2$
Exact Mass: 334.0428
Molecular Weight: 334.2174

Following the General Procedure B3 with 1,3-bis(trifluoromethyl)-5-bromobenzene (175.8 mg, 0.6 mmol), benzoic acid (36.6 mg, 0.3 mmol), **3ma** was obtained as colorless oil (65.8 mg, 66%).

Following the General Procedure B3 with 3,5-bis(trifluoromethyl)iodobenzene (153.0 mg, 0.45 mmol), benzoic acid (36.6 mg, 0.3 mmol), **3ma** was obtained as white solid (31.7 mg, 32%).

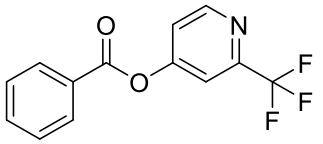
This target product was purified by silica gel flash chromatography (PE: EA = 20:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 – 8.17 (m, 2H), 7.81 (s, 1H), 7.75 (s, 2H), 7.69 (t, J = 7.4 Hz, 1H), 7.55 (t, J = 7.8 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.3, 151.5, 134.4, 133.0 (q, J = 34 Hz), 130.4, 128.8, 128.3, 122.8 (q, J = 273 Hz), 123.0 (q, J = 3 Hz), 119.8 (m).

^{19}F NMR (376 MHz, $CDCl_3$) δ -62.93.

(3na) 2-(trifluoromethyl)pyridin-4-yl benzoate (CAS: 2076460-92-7) [1]



2-(trifluoromethyl)pyridin-4-yl benzoate
Chemical Formula: $C_{13}H_8F_3NO_2$
Exact Mass: 267.0507
Molecular Weight: 267.2072

Following the General Procedure B1 with 2-(trifluoromethyl)-4-bromopyridine (135.6 mg, 0.6 mmol), benzoic acid (36.6 mg, 0.3 mmol), **3na** was obtained as colorless oil (43.9 mg, 55%).

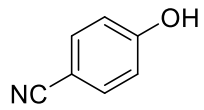
This target product was purified by silica gel flash chromatography (PE: EA = 20:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.78 (d, J = 5.6 Hz, 1H), 8.19 (dt, J = 8.0, 1.6 Hz, 2H), 7.74 – 7.67 (m, 1H), 7.66 (d, J = 2.0 Hz, 1H), 7.59 – 7.51 (m, 2H), 7.47 (dd, J = 5.2, 2.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.5, 158.8, 151.8, 150.2 (q, J = 35 Hz), 134.6, 130.4, 128.9, 128.1, 121.1 (q, J = 275 Hz), 119.6, 114.5 (q, J = 3 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -68.10.

(4a) 4-hydroxybenzonitrile (CAS: 767-00-0) [7]



4-hydroxybenzonitrile
Chemical Formula: C_7H_5NO
Exact Mass: 119.0371
Molecular Weight: 119.1230

Following the General Procedure C1 with 4-chlorobenzonitrile (68.8 mg, 0.5 mmol), H_2O (0.4 mL), **4a** was obtained as white solid (28.9 mg, 49%).

Following the General Procedure C2 with 4-chlorobenzonitrile (68.8 mg, 0.5 mmol), H_2O (0.4 mL), **4a** was obtained as white solid (42.3 mg, 71%).

Following the General Procedure C1 with 4-bromobenzonitrile (91.0 mg, 0.5 mmol), H_2O (0.4 mL), **4a** was obtained as white solid (47.4 mg, 80%).

Following the General Procedure C1 with 4-iodobenzonitrile (114.5 mg, 0.5 mmol), H_2O (0.4 mL), **4a** was obtained as white solid (48.6 mg, 82%).

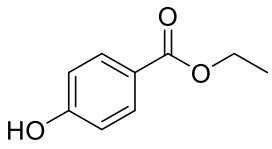
This target product was purified by silica gel flash chromatography (PE: EA = 5:1).

Melting point (°C): 100.7-103.2.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 – 7.51 (m, 2H), 7.02 – 6.87 (m, 2H), 6.41 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 159.9, 134.3, 119.2, 116.4, 103.5.

(4b) ethyl 4-hydroxybenzoate (CAS: 120-47-8) [7]



ethyl 4-hydroxybenzoate
Chemical Formula: $C_9H_{10}O_3$
Exact Mass: 166.0630
Molecular Weight: 166.1760

Following the General Procedure C1 with ethyl-4-bromobenzoate (114.5 mg, 0.5 mmol), H_2O (0.4 mL), **4b** was obtained as white solid (64.6 mg, 78%).

Following the General Procedure C1 with ethyl-4-iodobenzoate (138.0 mg, 0.5 mmol), H_2O (0.4 mL), **4b** was obtained as white solid (69.7 mg, 84%).

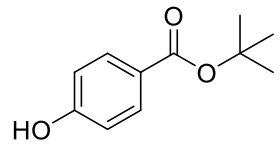
This target product was purified by silica gel flash chromatography (PE: EA = 5:1).

Melting point (°C): 116.6-117.7.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 – 7.93 (m, 2H), 6.94 – 6.85 (m, 3H), 4.36 (q, J = 7.2 Hz, 2H), 1.38 (t, J = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 167.1, 160.4, 131.9, 122.5, 115.3, 61.0, 14.3.

(4c) tert-butyl 4-hydroxybenzoate (CAS: 25804-49-3) [8]



tert-butyl 4-hydroxybenzoate
Chemical Formula: $C_{11}H_{14}O_3$
Exact Mass: 194.0943
Molecular Weight: 194.2300

Following the General Procedure C1 with tert-butyl-4-bromobenzoate (128.6 mg, 0.5 mmol), H_2O (0.4 mL), **4c** was obtained as white solid (69.5 mg, 72%).

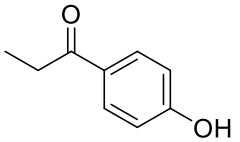
This target product was purified by silica gel flash chromatography (PE: EA = 5:1).

Melting point (°C): 114.7-115.9.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 – 7.85 (m, 2H), 7.04 (s, 1H), 6.91 – 6.83 (m, 2H), 1.59 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.6, 160.3, 131.8, 123.8, 115.2, 81.2, 28.3.

(4d) 1-(4-hydroxyphenyl)propan-1-one (CAS: 70-70-2) [9]



1-(4-hydroxyphenyl)propan-1-one
Chemical Formula: $C_9H_{10}O_2$
Exact Mass: 150.0681
Molecular Weight: 150.1770

Following the General Procedure C1 with 4'-bromopropiophenone (106.5 mg, 0.5 mmol), H_2O (0.4 mL), **4d** was obtained as white solid (60.1 mg, 80%).

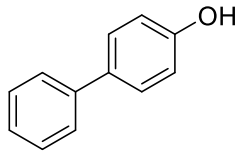
This target product was purified by silica gel flash chromatography (PE: EA = 5:1).

Melting point (°C): 147.0-148.6.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 – 7.89 (m, 2H), 6.92 – 6.85 (m, 2H), 5.77 (s, 1H), 2.96 (q, J = 7.2 Hz, 2H), 1.22 (t, J = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 199.03, 162.30, 130.77, 128.70, 115.62, 31.06, 8.86.

(4e) [1,1'-biphenyl]-4-ol (CAS: 92-69-3) [10]



[1,1'-biphenyl]-4-ol
Chemical Formula: $C_{12}H_{10}O$
Exact Mass: 170.0732
Molecular Weight: 170.2110

Following the General Procedure C1 with 4-bromobiphenyl (116.6 mg, 0.5 mmol), H_2O (0.4 mL), **4e** was obtained as white solid (36.5 mg, 43%).

Following the General Procedure C2 with 4-bromobiphenyl (116.6 mg, 0.5 mmol), H_2O (0.4 mL), **4e** was obtained as white solid (53.2 mg, 63%).

Following the General Procedure C1 with 4-iodobiphenyl (140.1 mg, 0.5 mmol), H_2O (0.4 mL), **4e** was obtained as white solid (51.0 mg, 60%).

Following the General Procedure C2 with 4-iodobiphenyl (140.1 mg, 0.5 mmol), H_2O (0.4 mL), **4e** was obtained as white solid (69.4 mg, 82%).

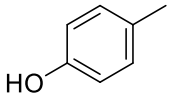
This target product was purified by silica gel flash chromatography (PE: EA = 5:1).

Melting point (°C): 162.4-163.1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 – 7.52 (m, 2H), 7.52 – 7.45 (m, 2H), 7.42 (t, J = 7.6 Hz, 2H), 7.31 (t, J = 7.2 Hz, 1H), 6.96 – 6.87 (m, 2H), 4.80 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.1, 140.8, 134.1, 128.7, 128.4, 126.7, 115.7.

(4f) p-cresol (CAS: 106-44-5) [7]



p-cresol
Chemical Formula: C_7H_8O
Exact Mass: 108.0575
Molecular Weight: 108.1400

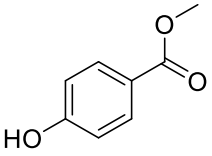
Following the General Procedure C2 with 4-bromotoluene (85.5 mg, 0.5 mmol), H_2O (0.4 mL), **4f** was obtained as yellow oil (35.6 mg, 65%).

This target product was purified by silica gel flash chromatography (PE: EA = 5:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.08 – 7.02 (m, 2H), 6.78 – 6.73 (m, 2H), 5.23 (s, 1H), 2.29 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 153.3, 130.1, 130.0, 115.1, 20.5.

(4g) methyl 4-hydroxybenzoate (CAS: 99-76-3) [7]



methyl 4-hydroxybenzoate
Chemical Formula: $C_8H_8O_3$
Exact Mass: 152.0473
Molecular Weight: 152.1490

Following the General Procedure C2 with methyl-4-chlorobenzoate (85.3 mg, 0.5 mmol), H_2O (0.4 mL), **4g** was obtained as white solid (27.3 mg, 36%).

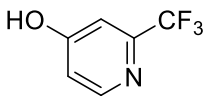
This target product was purified by silica gel flash chromatography (PE: EA = 5:1).

Melting point (°C): 121.8-123.9.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.89 (m, 2H), 6.93 – 6.85 (m, 2H), 6.52 (s, 1H), 3.90 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 167.4, 160.3, 132.0, 122.3, 115.3, 52.1.

(4h) 2-(trifluoromethyl)pyridin-4-ol (CAS: 170886-13-2)



2-(trifluoromethyl)pyridin-4-ol
Chemical Formula: $C_6H_4F_3NO$
Exact Mass: 163.0245
Molecular Weight: 163.0992

Following the General Procedure C2 with 2-(trifluoromethyl)-4-bromopyridine (113.0 mg, 0.5 mmol), H_2O (0.4 mL), **4h** was obtained as white solid (68.1 mg, 84%).

This target product was purified by silica gel flash chromatography (PE: EA = 5:1).

Melting point (°C): 121.1-124.1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 11.40 (s, 1H), 8.20 (d, J = 6.0 Hz, 1H), 7.19 (d, J = 2.4 Hz, 1H), 6.97 (dd, J = 6.0, 2.4 Hz, 1H).

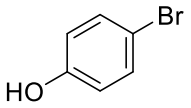
^{13}C NMR (101 MHz, $CDCl_3$) δ 170.2, 147.5, 146.5 (q, J = 35 Hz), 120.9 (d, J = 275 Hz), 115.6, 111.4 (d, J = 3 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -67.60.

IR (cm^{-1}): 2772, 1625, 1587, 1324, 1135, 1023, 853.

HRMS (ESI) m/z calcd for $C_6H_5F_3NO^+$ $(M+H)^+$ 164.0318, found 164.0319.

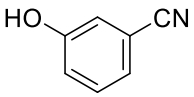
(4i) 4-bromophenol (CAS: 106-41-2) [7]



4-bromophenol
Chemical Formula: C_6H_5BrO
Exact Mass: 171.9524
Molecular Weight: 173.0090

Following the General Procedure C2 with 1,4-dibromobenzene (118.0 mg, 0.5 mmol), H_2O (0.4 mL), **4i** was obtained as brown solid (31.7 mg, 37%).
This target product was purified by silica gel flash chromatography (PE: EA = 5:1).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.29 (m, 2H), 6.77 – 6.68 (m, 2H), 5.09 (s, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 154.7, 132.5, 117.2, 112.9.

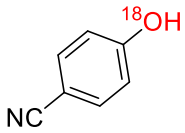
(4j) 3-hydroxybenzonitrile (CAS: 873-62-1) [7]



3-hydroxybenzonitrile
Chemical Formula: C_7H_5NO
Exact Mass: 119.0371
Molecular Weight: 119.1230

Following the General Procedure C2 with 3,5-dibromobenzonitrile (130.5 mg, 0.5 mmol), H_2O (0.4 mL), **4h** was obtained as white solid (30.0 mg, 50%).
This target product was purified by silica gel flash chromatography (PE: EA = 1:1).
Melting point (°C): 57.0-59.5.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (t, J = 8.0 Hz, 1H), 7.21 (d, J = 7.6 Hz, 1H), 7.14 (s, 1H), 7.11 (d, J = 8.4 Hz, 1H), 6.60 (s, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 156.4, 130.6, 124.4, 120.8, 118.8, 118.7, 112.7.

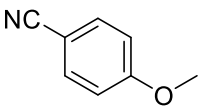
(4k) 4-(hydroxy)benzonitrile



4-(hydroxy)benzonitrile
Chemical Formula: $C_7H_5N^{18}O$
Exact Mass: 121.0414
Molecular Weight: 121.1232

Following the General Procedure C3 with 4-bromobenzonitrile (91.0 mg, 0.5 mmol), **$H_2{}^{18}O$** (0.4 mL), **4k** was obtained as white solid (54.6 mg, 90%).
This target product was purified by silica gel flash chromatography (PE: EA = 5:1).
Melting point (°C): 99.2-103.4.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, J = 8.8 Hz, 2H), 6.94 (d, J = 8.8 Hz, 2H), 6.86 (s, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 160.35, 134.37, 119.30, 116.52, 102.91.
IR (cm^{-1}): 3281, 2218, 1605, 1503, 834, 542.
HRMS (ESI) m/z calcd for $C_7H_6N_{18}O^+$ $(M+H)^+$ 122.0486, found 122.0485.

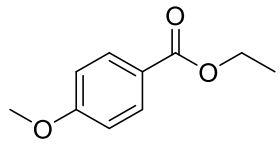
(5a) 4-methoxybenzonitrile (CAS: 874-90-8) [11]



4-methoxybenzonitrile
Chemical Formula: C_8H_7NO
Exact Mass: 133.0528
Molecular Weight: 133.1500

Following the General Procedure D with 4-bromobenzonitrile (54.6 mg, 0.3 mmol), MeOH (0.5 mL), **5a** was obtained as white solid (30.0 mg, 75%).
Following the General Procedure D with 4-iodobenzonitrile (68.8 mg, 0.3 mmol), MeOH (0.5 mL), **5a** was obtained as white solid (36.9 mg, 92%).
This target product was purified by silica gel flash chromatography (PE: EA = 10:1).
Melting point (°C): 54.2-56.0.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 – 7.55 (m, 2H), 6.97 – 6.92 (m, 2H), 3.85 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 162.9, 134.0, 119.3, 114.8, 104.0, 55.6.

(5b) ethyl 4-methoxybenzoate (CAS: 94-30-4) [11]



ethyl 4-methoxybenzoate
Chemical Formula: $C_{10}H_{12}O_3$
Exact Mass: 180.0786
Molecular Weight: 180.2030

Following the General Procedure D with ethyl-4-bromobenzoate (68.7 mg, 0.3 mmol), MeOH (0.5 mL), **5b** was obtained as colorless oil (36.3 mg, 67%).

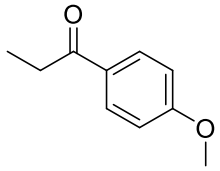
Following the General Procedure D with ethyl-4-iodobenzoate (82.8 mg, 0.3 mmol), MeOH (0.5 mL), **5b** was obtained as colorless oil (52.2 mg, 97%).

This target product was purified by silica gel flash chromatography (PE: EA = 10:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 – 7.97 (m, 2H), 6.95 – 6.87 (m, 2H), 4.34 (q, J = 7.2 Hz, 2H), 3.85 (s, 3H), 1.37 (t, J = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4, 163.3, 131.5, 123.0, 113.5, 60.6, 55.4, 14.4.

(5c) 1-(4-methoxyphenyl)propan-1-one (CAS: 121-97-1) [12]



1-(4-methoxyphenyl)propan-1-one
Chemical Formula: $C_{10}H_{12}O_2$
Exact Mass: 164.0837
Molecular Weight: 164.2040

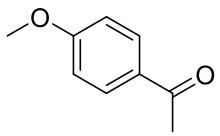
Following the General Procedure D with 4'-bromopropiophenone (63.9 mg, 0.3 mmol), MeOH (0.5 mL), **5c** was obtained as colorless oil (36.0 mg, 73%).

This target product was purified by silica gel flash chromatography (PE: EA = 20:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 – 7.90 (m, 2H), 6.94 – 6.88 (m, 2H), 3.84 (s, 3H), 2.93 (q, J = 7.3 Hz, 2H), 1.20 (t, J = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 199.5, 163.3, 130.2, 130.0, 113.7, 55.4, 31.4, 8.4.

(5d) 1-(4-methoxyphenyl)ethan-1-one (CAS: 100-06-1) [11]



1-(4-methoxyphenyl)ethan-1-one
Chemical Formula: $C_9H_{10}O_2$
Exact Mass: 150.0681
Molecular Weight: 150.1770

Following the General Procedure D with 4'-iodoacetophenone (73.8 mg, 0.3 mmol), MeOH (0.5 mL), **5d** was obtained as white solid (41.1 mg, 91%).

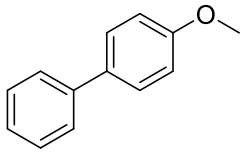
This target product was purified by silica gel flash chromatography (PE: EA = 20:1).

Melting point (°C): 32.0-34.4.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 – 7.89 (m, 2H), 6.95 – 6.87 (m, 2H), 3.85 (s, 3H), 2.54 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.8, 163.5, 130.6, 130.3, 113.7, 55.5, 26.3.

(5e) 4-methoxy-1,1'-biphenyl (CAS: 613-37-6) [11]



4-methoxy-1,1'-biphenyl
Chemical Formula: $C_{13}H_{12}O$
Exact Mass: 184.0888
Molecular Weight: 184.2380

Following the General Procedure D with 4-bromobiphenyl (69.9 mg, 0.3 mmol), MeOH (0.5 mL), **5e** was obtained as white solid (28.0 mg, 51%).

Following the General Procedure D with 4-iodobiphenyl (84.0 mg, 0.3 mmol), MeOH (0.5 mL), **5e** was obtained as white solid (29.1 mg, 53%).

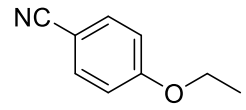
This target product was purified by silica gel flash chromatography (PE: EA = 10:1).

Melting point (°C): 84.1-87.4.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 – 7.53 (m, 4H), 7.48 – 7.41 (m, 2H), 7.37 – 7.30 (m, 1H), 7.05 – 6.98 (m, 2H), 3.87 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 159.2, 140.9, 133.8, 128.8, 128.2, 126.8, 126.7, 114.3, 55.4.

(5f) 4-ethoxybenzonitrile (CAS: 25117-74-2) [11]



4-ethoxybenzonitrile
Chemical Formula: C_9H_9NO
Exact Mass: 147.0684
Molecular Weight: 147.1770

Following the General Procedure D with 4-bromobenzonitrile (54.6 mg, 0.3 mmol), EtOH (0.5 mL), **5f** was obtained as white solid (29.0 mg, 66%%).

Following the General Procedure D with 4-iodobenzonitrile (68.8 mg, 0.3 mmol), EtOH (0.5 mL), **5f** was obtained as white solid (26.6 mg, 60%).

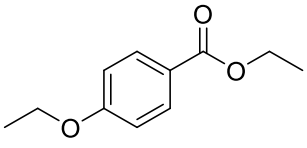
This target product was purified by silica gel flash chromatography (PE: EA = 10:1).

Melting point (°C): 57.4-59.4.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 – 7.52 (m, 2H), 6.95 – 6.88 (m, 2H), 4.07 (q, J = 7.1 Hz, 2H), 1.43 (t, J = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.3, 134.0, 119.3, 115.2, 103.7, 63.9, 14.6.

(5g) ethyl 4-ethoxybenzoate (CAS: 23676-09-7) [13]



ethyl 4-ethoxybenzoate
Chemical Formula: $C_{11}H_{14}O_3$
Exact Mass: 194.0943
Molecular Weight: 194.2300

Following the General Procedure D with ethyl 4-bromobenzoate (68.7 mg, 0.3 mmol), EtOH (0.5 mL), **5g** was obtained as colorless oil (33.9 mg, 58%).

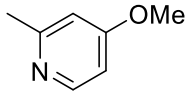
Following the General Procedure D with ethyl-4-iodobenzoate (82.8 mg, 0.3 mmol), EtOH (0.5 mL), **5g** was obtained as colorless oil (46.1 mg, 79%).

This target product was purified by silica gel flash chromatography (PE: EA = 20:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 – 7.95 (m, 2H), 6.94 – 6.86 (m, 2H), 4.34 (q, J = 7.2 Hz, 2H), 4.08 (q, J = 7.2 Hz, 2H), 1.43 (t, J = 7.0 Hz, 3H), 1.37 (t, J = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.5, 162.7, 131.5, 122.8, 114.0, 63.7, 60.6, 14.7, 14.4.

(5h) 4-methoxy-2-methylpyridine (CAS: 24103-75-1) [14]



4-methoxy-2-methylpyridine
Chemical Formula: C_7H_9NO
Exact Mass: 123.0684
Molecular Weight: 123.1550

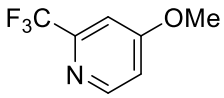
Following the General Procedure D with 4-bromo-2-methylpyridine (51.6 mg, 0.3 mmol), MeOH (0.5 mL), **5h** was obtained as white solid (19.3 mg, 52%).

This target product was purified by silica gel flash chromatography (PE: EA = 5:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (d, J = 6.0 Hz, 1H), 6.68 (d, J = 2.4 Hz, 1H), 6.65 (dd, J = 5.8, 2.2 Hz, 1H), 3.83 (s, 3H), 2.51 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.0, 159.9, 150.2, 109.0, 107.2, 55.0, 24.5.

(5i) 4-methoxy-2-(trifluoromethyl)pyridine (CAS: 1065103-97-0) [15]



4-methoxy-2-(trifluoromethyl)pyridine
Chemical Formula: $C_7H_6F_3NO$
Exact Mass: 177.0401
Molecular Weight: 177.1262

Following the General Procedure D with 2-(trifluoromethyl)-4-bromopyridine (67.8 mg, 0.3 mmol), MeOH (0.5 mL), **5i** was obtained as colorless oil (32.3 mg, 61%).

This target product was purified by silica gel flash chromatography (PE: EA = 5:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (d, J = 5.6 Hz, 1H), 7.19 (d, J = 2.4 Hz, 1H), 6.96 (dd, J = 5.6, 2.4 Hz, 1H), 3.91 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.6, 151.4, 149.8 (q, J = 34 Hz), 121.4 (q, J = 275 Hz), 111.8, 107.4 (q, J = 3 Hz), 55.6.

^{19}F NMR (376 MHz, $CDCl_3$) δ -68.31.

9 X-ray diffraction data of PC1 (CCDC: 1978990)

Table S11. Crystal data and structure refinement for PC1

Identification code	11_a
Crystal data	
Chemical formula	$C_{30}H_{25}BN_2O$
M_r	440.33
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	173
a, b, c (Å)	17.6430 (5), 8.5349 (3), 15.3612 (5)
β (°)	95.447 (1)
V (Å^3)	2302.66 (13)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.27 × 0.25 × 0.22
Data collection	
Diffractometer	Bruker D8 Venture
Absorption correction	Multi-scan *SADABS*
T_{min}, T_{max}	0.664, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	27450, 4885, 3976
R_{int}	0.060
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.633
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.102, 1.06
No. of reflections	4885
No. of parameters	307
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.23, −0.20

Table S12. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.17159 (6)	0.98532 (12)	0.34190 (8)	0.0441 (3)
N1	0.12901 (6)	0.45827 (13)	0.36799 (7)	0.0258 (2)
B1	0.20358 (8)	0.54879 (17)	0.33900 (10)	0.0245 (3)
C1	0.20407 (8)	0.85982 (16)	0.33286 (9)	0.0289 (3)
C2	0.28741 (8)	0.85992 (16)	0.31697 (9)	0.0298 (3)
H2A	0.293181	0.907274	0.259133	0.036*
H2AB	0.305914	0.750500	0.315863	0.036*
N2	0.16713 (6)	0.71959 (13)	0.33525 (7)	0.0253 (2)
C3	0.33608 (8)	0.95140 (18)	0.38763 (9)	0.0337 (3)
H3A	0.312942	1.055820	0.394488	0.040*
H3AB	0.335801	0.895399	0.444042	0.040*
C4	0.41736 (8)	0.97241 (17)	0.36699 (9)	0.0305 (3)
C5	0.47531 (9)	0.88216 (18)	0.40832 (10)	0.0384 (4)
H5	0.463526	0.804957	0.449503	0.046*
C7	0.56816 (9)	1.0139 (2)	0.33092 (11)	0.0443 (4)
H7	0.619522	1.027800	0.318707	0.053*
C6	0.55006 (9)	0.9027 (2)	0.39057 (12)	0.0440 (4)
H6	0.589085	0.839847	0.419614	0.053*
C8	0.51124 (10)	1.1051 (2)	0.28898 (12)	0.0498 (4)
H8	0.523360	1.182300	0.247956	0.060*
C9	0.43636 (9)	1.0839 (2)	0.30684 (11)	0.0420 (4)
H9	0.397428	1.146540	0.277471	0.050*
C10	0.11942 (9)	0.30889 (16)	0.38829 (9)	0.0307 (3)
H10	0.161618	0.239339	0.390924	0.037*
C11	0.04797 (9)	0.25248 (18)	0.40587 (10)	0.0367 (4)
H11	0.042321	0.145795	0.421662	0.044*
C12	−0.01371 (9)	0.35003 (19)	0.40045 (10)	0.0375 (4)
H12	−0.062237	0.310731	0.411564	0.045*
C13	−0.00530 (8)	0.50934 (18)	0.37830 (9)	0.0321 (3)
C14	0.06856 (7)	0.55806 (16)	0.36410 (8)	0.0263 (3)
C15	0.08860 (8)	0.71263 (16)	0.34425 (8)	0.0264 (3)
C16	0.03138 (8)	0.82278 (18)	0.33626 (10)	0.0336 (3)
H16	0.042097	0.928675	0.322834	0.040*
C17	−0.04382 (9)	0.7752 (2)	0.34844 (11)	0.0409 (4)
H17	−0.083184	0.851390	0.341917	0.049*
C18	−0.06264 (9)	0.6255 (2)	0.36908 (11)	0.0407 (4)
H18	−0.113865	0.599510	0.377172	0.049*

C19	0.21792 (7)	0.48326 (15)	0.24361 (9)	0.0245 (3)
C20	0.24159 (8)	0.32789 (16)	0.23284 (9)	0.0297 (3)
H20	0.250253	0.262744	0.282940	0.036*
C21	0.25271 (8)	0.26664 (18)	0.15158 (10)	0.0355 (3)
H21	0.269412	0.161429	0.146833	0.043*
C22	0.23968 (9)	0.3576 (2)	0.07758 (10)	0.0398 (4)
H22	0.247631	0.315835	0.021833	0.048*
C23	0.21491 (9)	0.51006 (19)	0.08528 (10)	0.0390 (4)
H23	0.204851	0.572954	0.034470	0.047*
C24	0.20463 (8)	0.57196 (17)	0.16723 (9)	0.0309 (3)
H24	0.188133	0.677436	0.171309	0.037*
C25	0.27183 (8)	0.53250 (15)	0.41598 (9)	0.0261 (3)
C26	0.26388 (9)	0.59968 (17)	0.49787 (9)	0.0328 (3)
H26	0.216829	0.647412	0.507830	0.039*
C27	0.32229 (10)	0.59879 (19)	0.56472 (10)	0.0412 (4)
H27	0.315724	0.649336	0.618587	0.049*
C28	0.38995 (10)	0.5246 (2)	0.55314 (11)	0.0445 (4)
H28	0.429850	0.522177	0.599219	0.053*
C29	0.39931 (9)	0.4540 (2)	0.47420 (11)	0.0430 (4)
H29	0.445490	0.401055	0.466159	0.052*
C30	0.34137 (8)	0.46007 (18)	0.40627 (10)	0.0343 (3)
H30	0.349389	0.413545	0.351715	0.041*

Table S13. Atomic displacement parameters (Å2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0398 (6)	0.0215 (5)	0.0714 (8)	0.0051 (5)	0.0068 (6)	−0.0018 (5)
N1	0.0259 (6)	0.0242 (6)	0.0275 (6)	0.0019 (5)	0.0033 (5)	−0.0029 (5)
B1	0.0237 (7)	0.0196 (7)	0.0305 (8)	0.0022 (6)	0.0038 (6)	−0.0010 (6)
C1	0.0334 (8)	0.0224 (7)	0.0307 (7)	0.0025 (6)	0.0022 (6)	−0.0004 (5)
C2	0.0330 (8)	0.0239 (7)	0.0333 (7)	−0.0011 (6)	0.0071 (6)	−0.0003 (6)
N2	0.0252 (6)	0.0206 (5)	0.0302 (6)	0.0030 (4)	0.0034 (5)	−0.0019 (4)
C3	0.0336 (8)	0.0365 (8)	0.0315 (7)	−0.0011 (6)	0.0060 (6)	−0.0029 (6)
C4	0.0321 (7)	0.0295 (7)	0.0302 (7)	−0.0015 (6)	0.0042 (6)	−0.0058 (6)
C5	0.0396 (9)	0.0347 (8)	0.0407 (8)	−0.0003 (7)	0.0030 (7)	0.0056 (7)
C7	0.0309 (8)	0.0506 (10)	0.0523 (10)	−0.0038 (7)	0.0089 (7)	−0.0020 (8)
C6	0.0345 (8)	0.0436 (9)	0.0528 (10)	0.0057 (7)	−0.0011 (7)	0.0044 (8)
C8	0.0411 (9)	0.0538 (11)	0.0559 (11)	−0.0042 (8)	0.0113 (8)	0.0189 (9)
C9	0.0356 (8)	0.0423 (9)	0.0484 (9)	0.0042 (7)	0.0047 (7)	0.0105 (8)
C10	0.0358 (8)	0.0231 (7)	0.0334 (7)	0.0002 (6)	0.0047 (6)	−0.0020 (6)
C11	0.0441 (9)	0.0296 (8)	0.0371 (8)	−0.0082 (7)	0.0083 (7)	−0.0029 (6)

C12	0.0328 (8)	0.0422 (9)	0.0385 (8)	−0.0103 (7)	0.0084 (6)	−0.0061 (7)
C13	0.0261 (7)	0.0396 (8)	0.0307 (7)	−0.0016 (6)	0.0032 (6)	−0.0072 (6)
C14	0.0237 (6)	0.0298 (7)	0.0251 (6)	0.0035 (6)	0.0010 (5)	−0.0041 (5)
C15	0.0257 (7)	0.0280 (7)	0.0251 (6)	0.0034 (6)	0.0005 (5)	−0.0047 (5)
C16	0.0328 (8)	0.0324 (8)	0.0348 (8)	0.0094 (6)	−0.0013 (6)	−0.0028 (6)
C17	0.0293 (8)	0.0477 (10)	0.0448 (9)	0.0152 (7)	−0.0017 (7)	−0.0048 (7)
C18	0.0239 (7)	0.0518 (10)	0.0464 (9)	0.0035 (7)	0.0038 (7)	−0.0073 (8)
C19	0.0182 (6)	0.0258 (7)	0.0294 (7)	−0.0013 (5)	0.0014 (5)	−0.0024 (5)
C20	0.0261 (7)	0.0268 (7)	0.0358 (7)	0.0012 (6)	0.0019 (6)	−0.0040 (6)
C21	0.0294 (8)	0.0320 (8)	0.0460 (9)	−0.0018 (6)	0.0078 (6)	−0.0143 (7)
C22	0.0383 (9)	0.0486 (10)	0.0339 (8)	−0.0122 (7)	0.0105 (7)	−0.0143 (7)
C23	0.0438 (9)	0.0435 (9)	0.0300 (8)	−0.0103 (7)	0.0043 (6)	0.0007 (7)
C24	0.0308 (7)	0.0277 (7)	0.0343 (7)	−0.0040 (6)	0.0031 (6)	−0.0009 (6)
C25	0.0280 (7)	0.0194 (6)	0.0309 (7)	−0.0015 (5)	0.0025 (5)	0.0025 (5)
C26	0.0387 (8)	0.0303 (7)	0.0299 (7)	−0.0015 (6)	0.0050 (6)	0.0019 (6)
C27	0.0554 (10)	0.0419 (9)	0.0256 (7)	−0.0115 (8)	0.0007 (7)	0.0042 (6)
C28	0.0423 (9)	0.0499 (10)	0.0381 (9)	−0.0126 (8)	−0.0122 (7)	0.0142 (7)
C29	0.0296 (8)	0.0481 (10)	0.0495 (10)	0.0031 (7)	−0.0052 (7)	0.0071 (8)
C30	0.0299 (7)	0.0351 (8)	0.0373 (8)	0.0023 (6)	−0.0009 (6)	−0.0011 (6)

Table S14. Geometric parameters (Å, °)

O1—C1	1.2287 (17)
N1—C10	1.3271 (18)
N1—C14	1.3618 (17)
N1—B1	1.6240 (18)
B1—N2	1.5921 (17)
B1—C19	1.611 (2)
B1—C25	1.612 (2)
C1—N2	1.3649 (17)
C1—C2	1.5133 (19)
C2—C3	1.532 (2)
C2—H2A	0.9900
C2—H2AB	0.9900
N2—C15	1.4067 (17)
C3—C4	1.509 (2)
C3—H3A	0.9900
C3—H3AB	0.9900
C4—C5	1.385 (2)
C4—C9	1.389 (2)
C5—C6	1.383 (2)
C5—H5	0.9500
C7—C6	1.378 (2)

C7—C8	1.381 (2)
C7—H7	0.9500
C6—H6	0.9500
C8—C9	1.386 (2)
C8—H8	0.9500
C9—H9	0.9500
C10—C11	1.399 (2)
C10—H10	0.9500
C11—C12	1.366 (2)
C11—H11	0.9500
C12—C13	1.413 (2)
C12—H12	0.9500
C13—C14	1.4045 (19)
C13—C18	1.414 (2)
C14—C15	1.4067 (19)
C15—C16	1.3764 (19)
C16—C17	1.417 (2)
C16—H16	0.9500
C17—C18	1.365 (2)
C17—H17	0.9500
C18—H18	0.9500
C19—C24	1.3973 (19)
C19—C20	1.4048 (19)
C20—C21	1.384 (2)
C20—H20	0.9500
C21—C22	1.378 (2)
C21—H21	0.9500
C22—C23	1.382 (2)
C22—H22	0.9500
C23—C24	1.393 (2)
C23—H23	0.9500
C24—H24	0.9500
C25—C30	1.394 (2)
C25—C26	1.4016 (19)
C26—C27	1.384 (2)
C26—H26	0.9500
C27—C28	1.378 (2)
C27—H27	0.9500
C28—C29	1.378 (2)
C28—H28	0.9500
C29—C30	1.391 (2)
C29—H29	0.9500
C30—H30	0.9500
C10—N1—C14	119.63 (12)
C10—N1—B1	130.25 (11)

C14—N1—B1	109.99 (11)
N2—B1—C19	112.51 (11)
N2—B1—C25	112.12 (11)
C19—B1—C25	117.81 (11)
N2—B1—N1	96.35 (10)
C19—B1—N1	106.59 (10)
C25—B1—N1	109.03 (11)
O1—C1—N2	122.17 (13)
O1—C1—C2	119.23 (13)
N2—C1—C2	118.59 (12)
C1—C2—C3	111.94 (11)
C1—C2—H2A	109.2
C3—C2—H2A	109.2
C1—C2—H2AB	109.2
C3—C2—H2AB	109.2
H2A—C2—H2AB	107.9
C1—N2—C15	121.13 (11)
C1—N2—B1	127.71 (11)
C15—N2—B1	110.85 (10)
C4—C3—C2	113.05 (12)
C4—C3—H3A	109.0
C2—C3—H3A	109.0
C4—C3—H3AB	109.0
C2—C3—H3AB	109.0
H3A—C3—H3AB	107.8
C5—C4—C9	118.13 (14)
C5—C4—C3	120.84 (14)
C9—C4—C3	121.03 (13)
C6—C5—C4	121.02 (15)
C6—C5—H5	119.5
C4—C5—H5	119.5
C6—C7—C8	119.63 (15)
C6—C7—H7	120.2
C8—C7—H7	120.2
C7—C6—C5	120.27 (15)
C7—C6—H6	119.9
C5—C6—H6	119.9
C7—C8—C9	119.91 (16)
C7—C8—H8	120.0
C9—C8—H8	120.0
C8—C9—C4	121.05 (15)
C8—C9—H9	119.5
C4—C9—H9	119.5
N1—C10—C11	120.87 (14)
N1—C10—H10	119.6
C11—C10—H10	119.6

C12—C11—C10	120.36 (14)
C12—C11—H11	119.8
C10—C11—H11	119.8
C11—C12—C13	119.99 (14)
C11—C12—H12	120.0
C13—C12—H12	120.0
C14—C13—C12	116.27 (13)
C14—C13—C18	116.27 (14)
C12—C13—C18	127.47 (14)
N1—C14—C13	122.84 (13)
N1—C14—C15	112.59 (12)
C13—C14—C15	124.57 (13)
C16—C15—N2	133.10 (13)
C16—C15—C14	117.55 (13)
N2—C15—C14	109.34 (11)
C15—C16—C17	118.71 (14)
C15—C16—H16	120.6
C17—C16—H16	120.6
C18—C17—C16	123.42 (14)
C18—C17—H17	118.3
C16—C17—H17	118.3
C17—C18—C13	119.46 (14)
C17—C18—H18	120.3
C13—C18—H18	120.3
C24—C19—C20	116.14 (13)
C24—C19—B1	123.19 (12)
C20—C19—B1	120.60 (12)
C21—C20—C19	122.13 (14)
C21—C20—H20	118.9
C19—C20—H20	118.9
C22—C21—C20	120.30 (14)
C22—C21—H21	119.9
C20—C21—H21	119.9
C21—C22—C23	119.30 (14)
C21—C22—H22	120.4
C23—C22—H22	120.4
C22—C23—C24	120.27 (15)
C22—C23—H23	119.9
C24—C23—H23	119.9
C23—C24—C19	121.84 (14)
C23—C24—H24	119.1
C19—C24—H24	119.1
C30—C25—C26	116.19 (13)
C30—C25—B1	124.29 (12)
C26—C25—B1	119.46 (12)
C27—C26—C25	122.19 (15)

C27—C26—H26	118.9
C25—C26—H26	118.9
C28—C27—C26	120.00 (15)
C28—C27—H27	120.0
C26—C27—H27	120.0
C27—C28—C29	119.49 (14)
C27—C28—H28	120.3
C29—C28—H28	120.3
C28—C29—C30	120.20 (15)
C28—C29—H29	119.9
C30—C29—H29	119.9
C29—C30—C25	121.85 (15)
C29—C30—H30	119.1
C25—C30—H30	119.1

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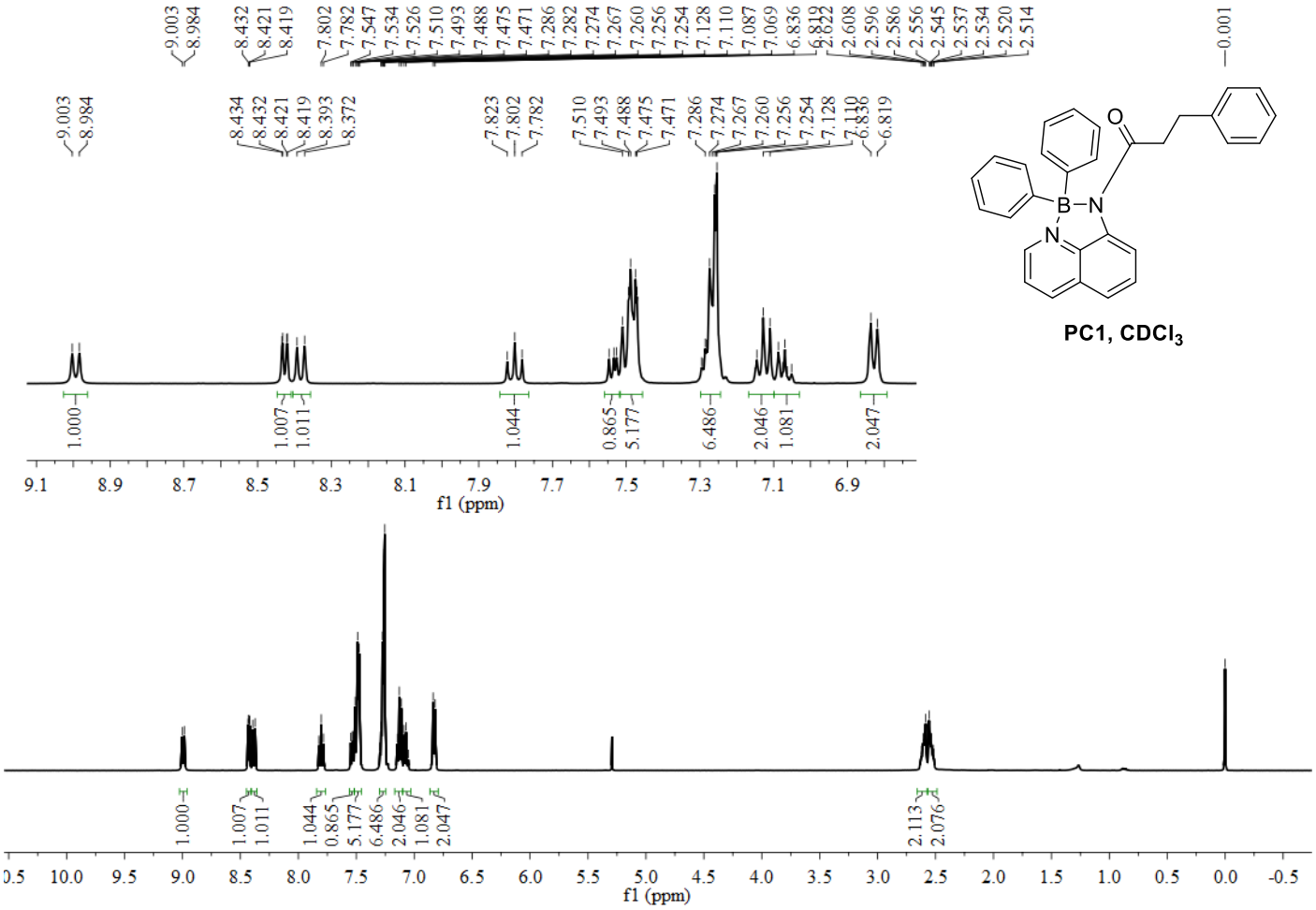
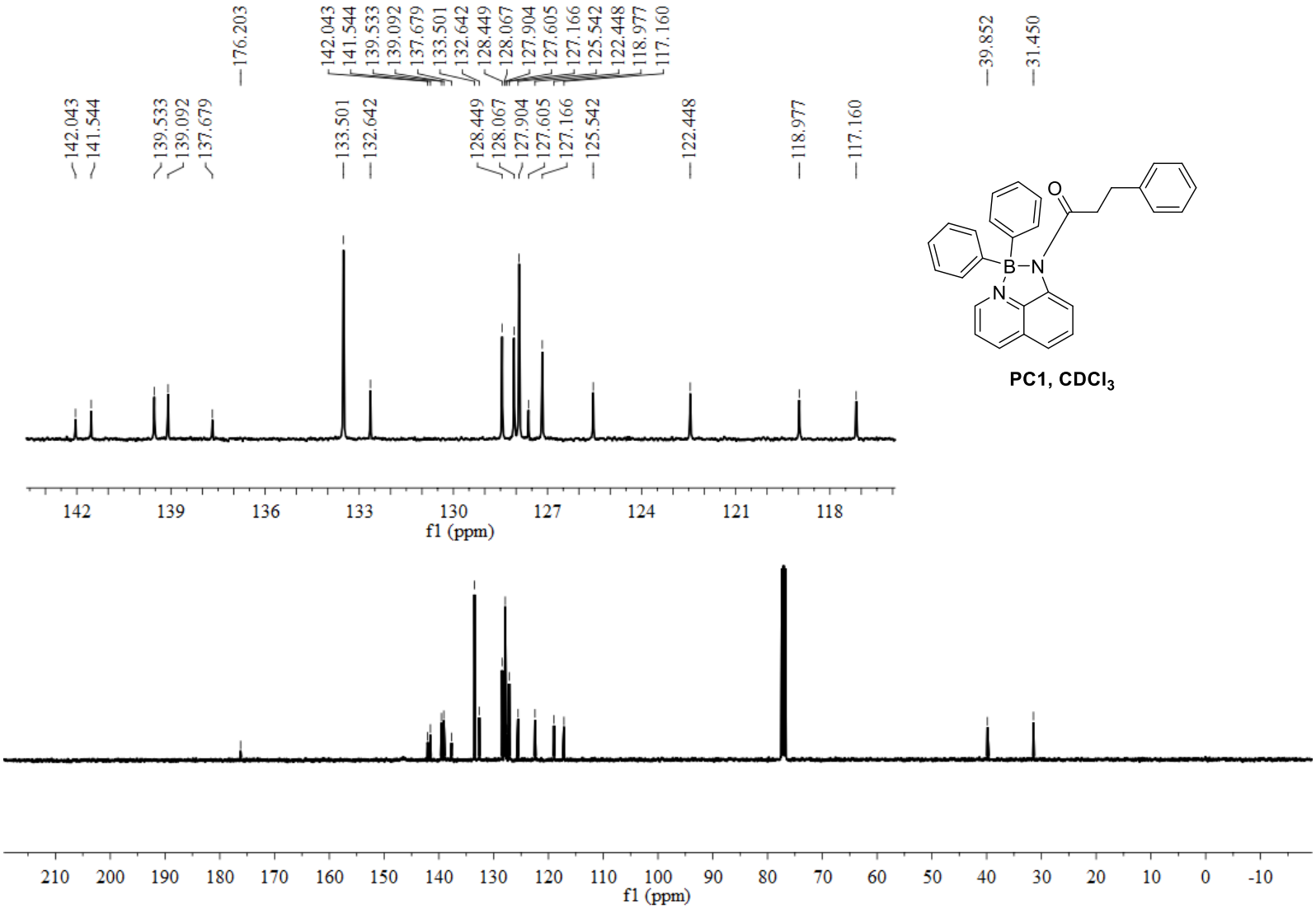
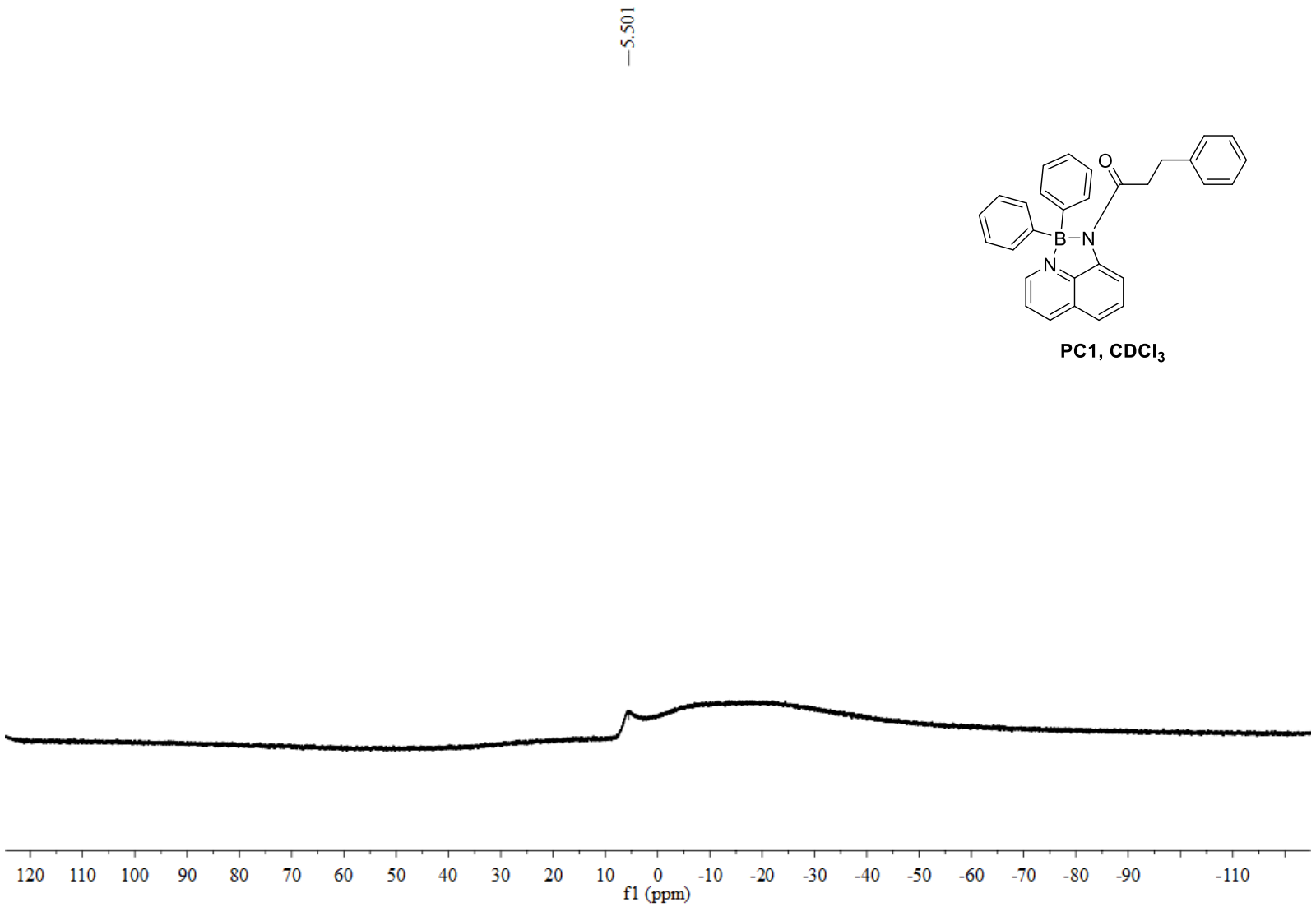
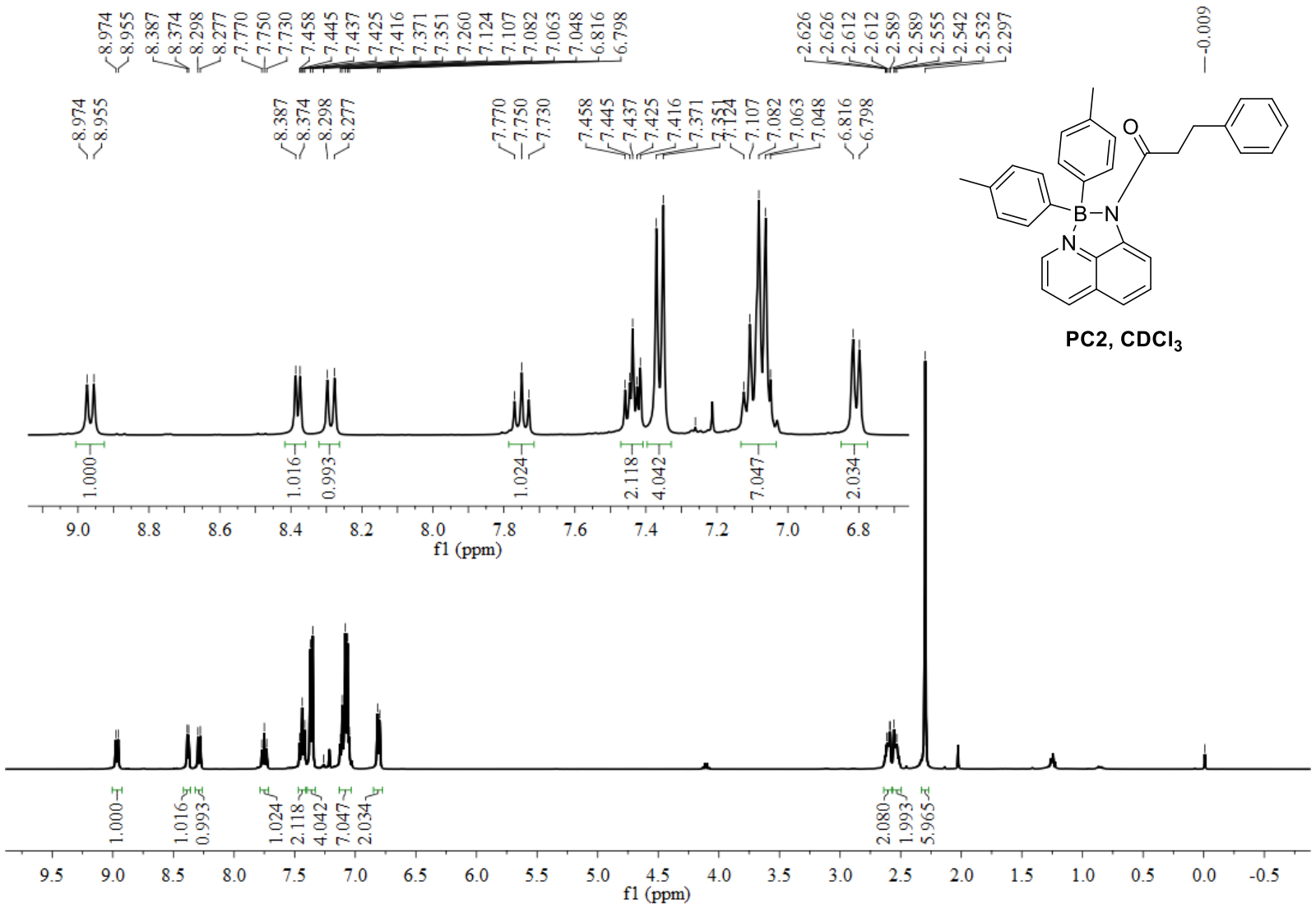
11 NMR spectra



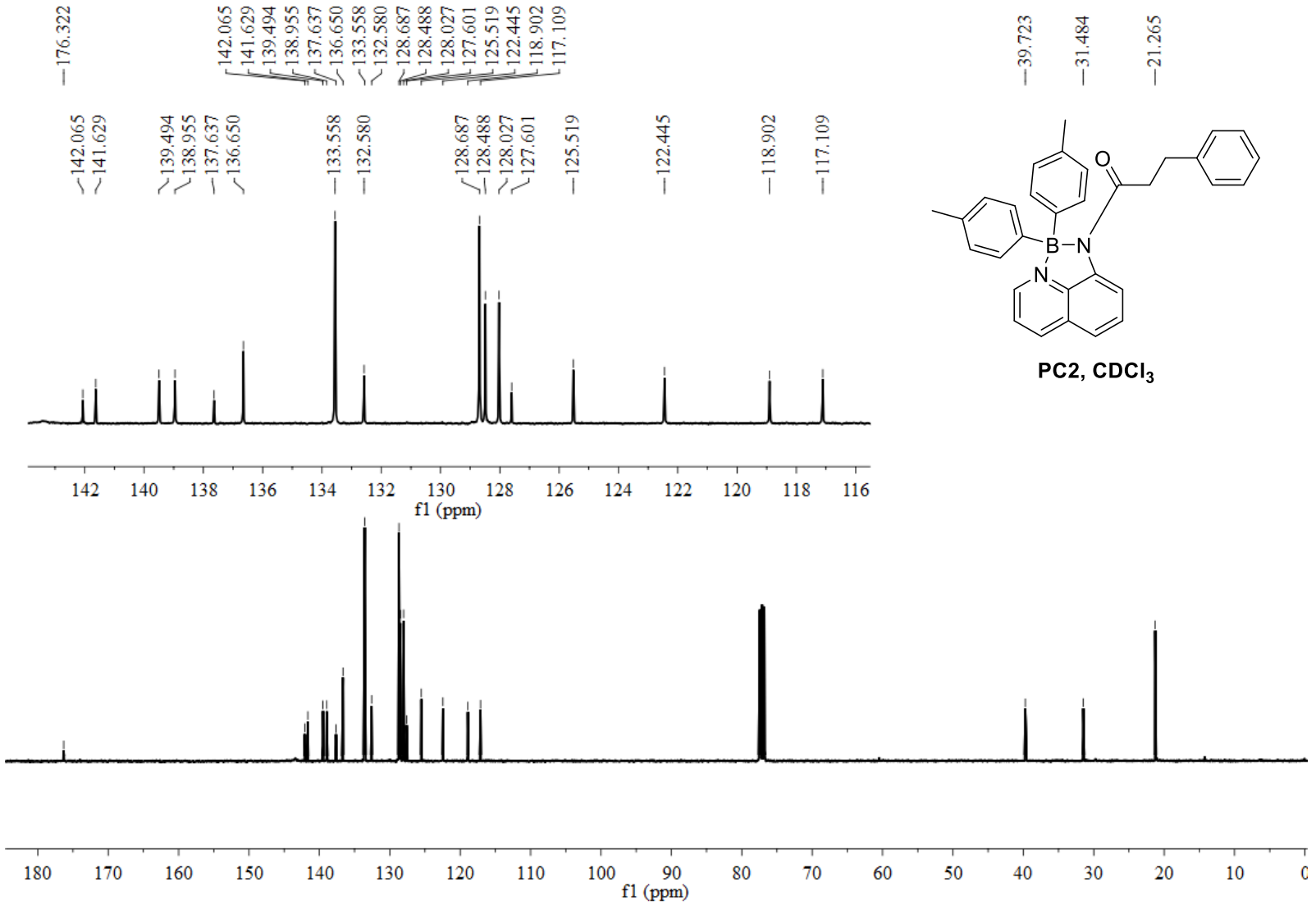

176.203
142.043
141.544
139.533
139.092
137.679
133.501
132.642
128.449
128.067
127.904
127.605
127.166
125.542
122.448
118.977
117.160
39.852
31.450
O
B
N
N
f1 (ppm)
f1 (ppm)

PC1, $CDCl_3$

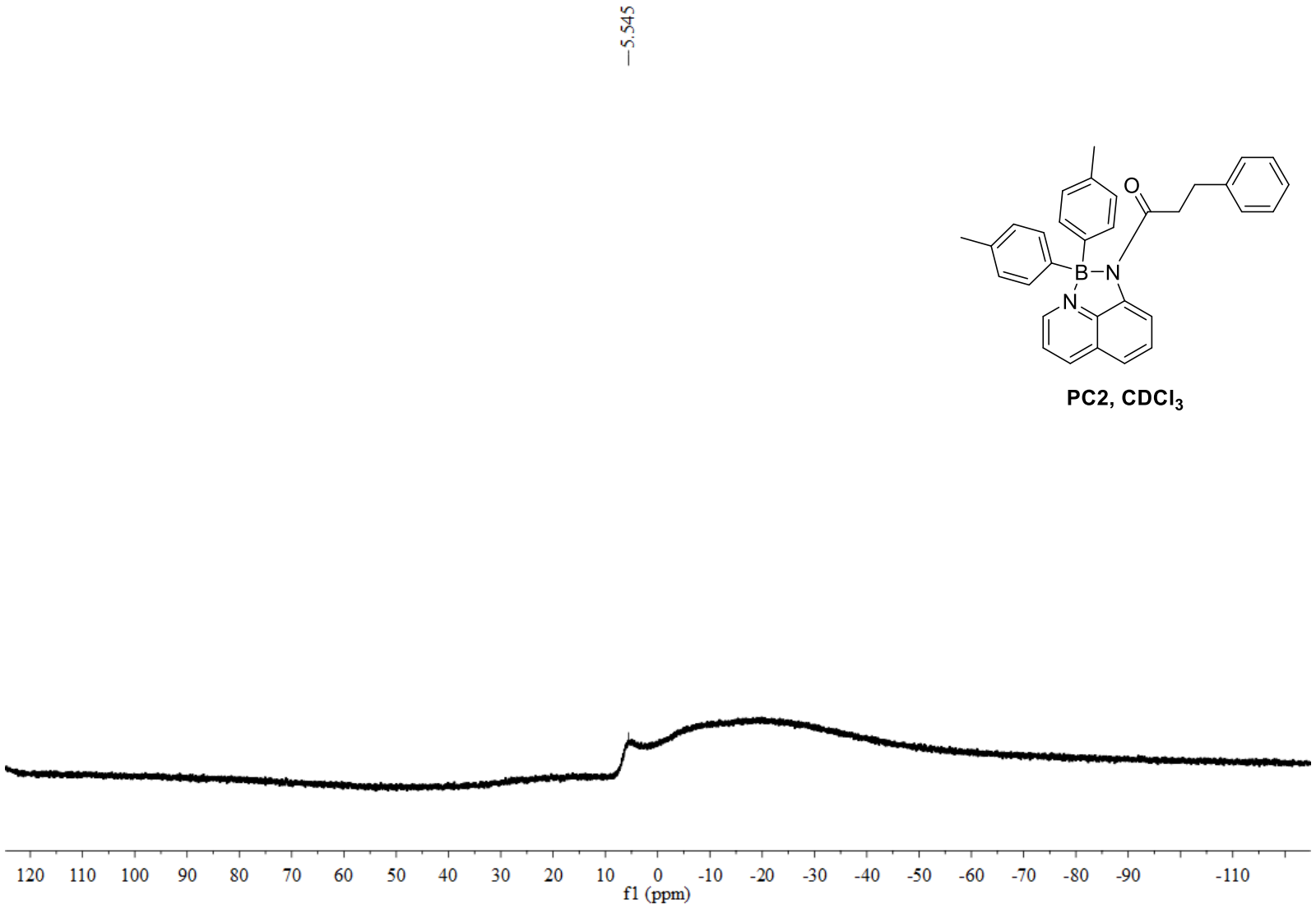

5.501
O
B
N
N
PC1, CDCl3
120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110
f1 (ppm)


8.974
8.955
8.387
8.374
8.298
8.277
7.770
7.750
7.730
7.458
7.445
7.437
7.425
7.416
7.371
7.351
7.260
7.124
7.107
7.082
7.063
7.048
6.816
6.798
2.626
2.626
2.612
2.612
2.589
2.589
2.555
2.542
2.532
2.297
-0.009
O
B
N
N
1.000
1.016
0.993
1.024
2.118
4.042
7.047
2.034
f1 (ppm)
2.080
1.993
5.965

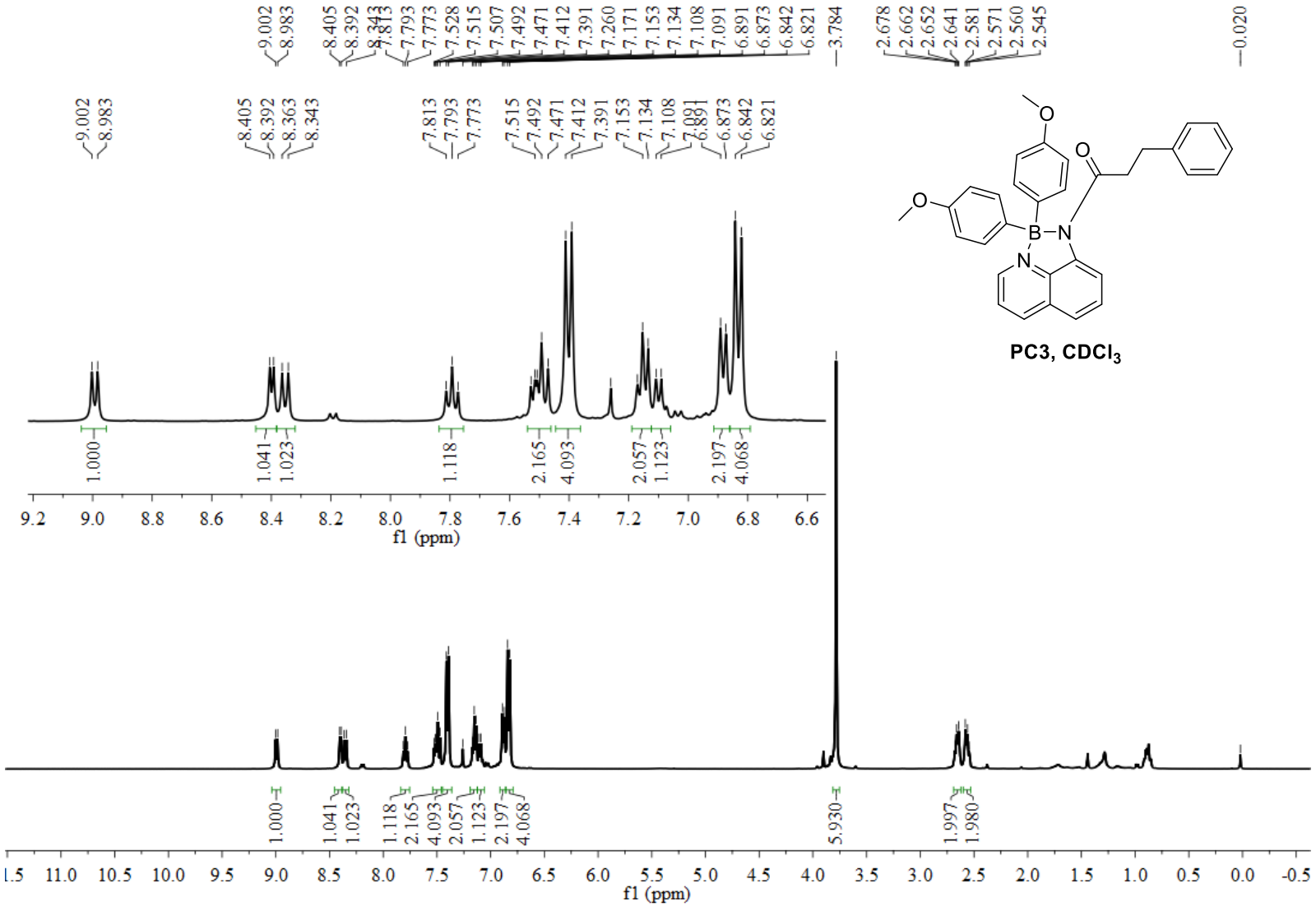
PC2, $CDCl_3$

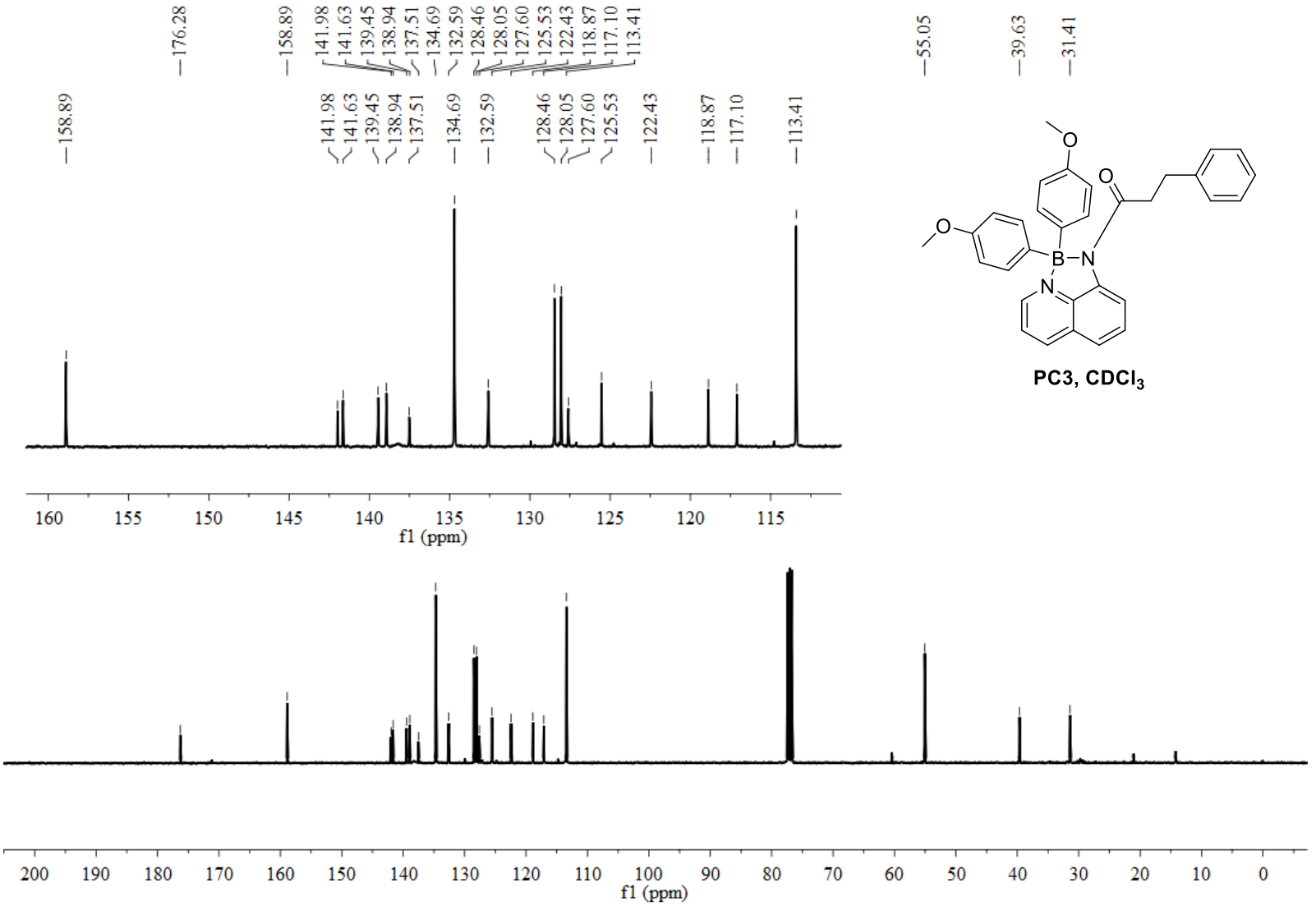

176.322
142.065
141.629
139.494
138.955
137.637
136.650
133.558
132.580
128.687
128.488
128.027
127.601
125.519
122.445
118.902
117.109
39.723
31.484
21.265
O
B
N
N
f1 (ppm)
f1 (ppm)

PC2, $CDCl_3$

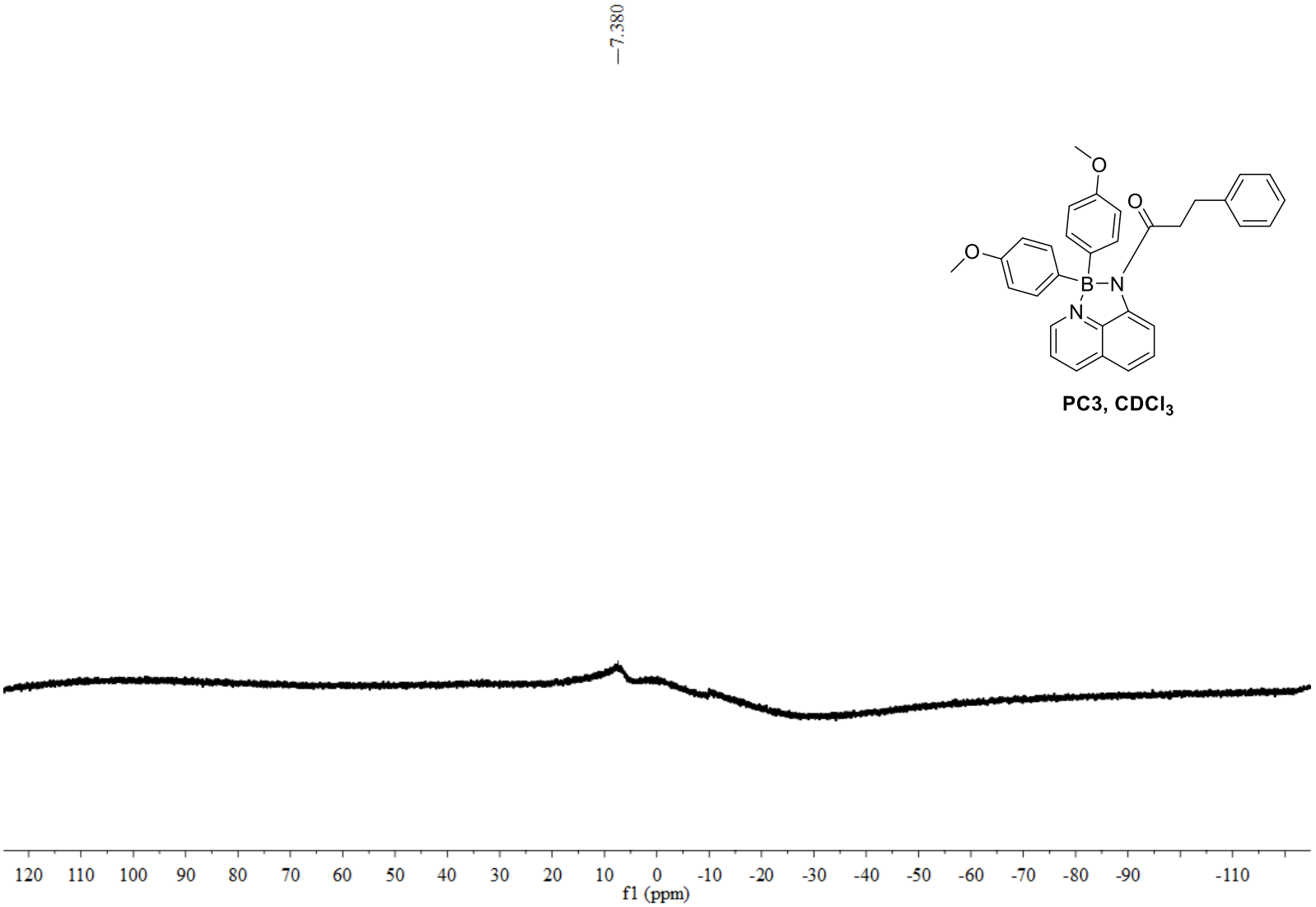

5.545
O
B
N
N
120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110
f1 (ppm)

PC2, $CDCl_3$

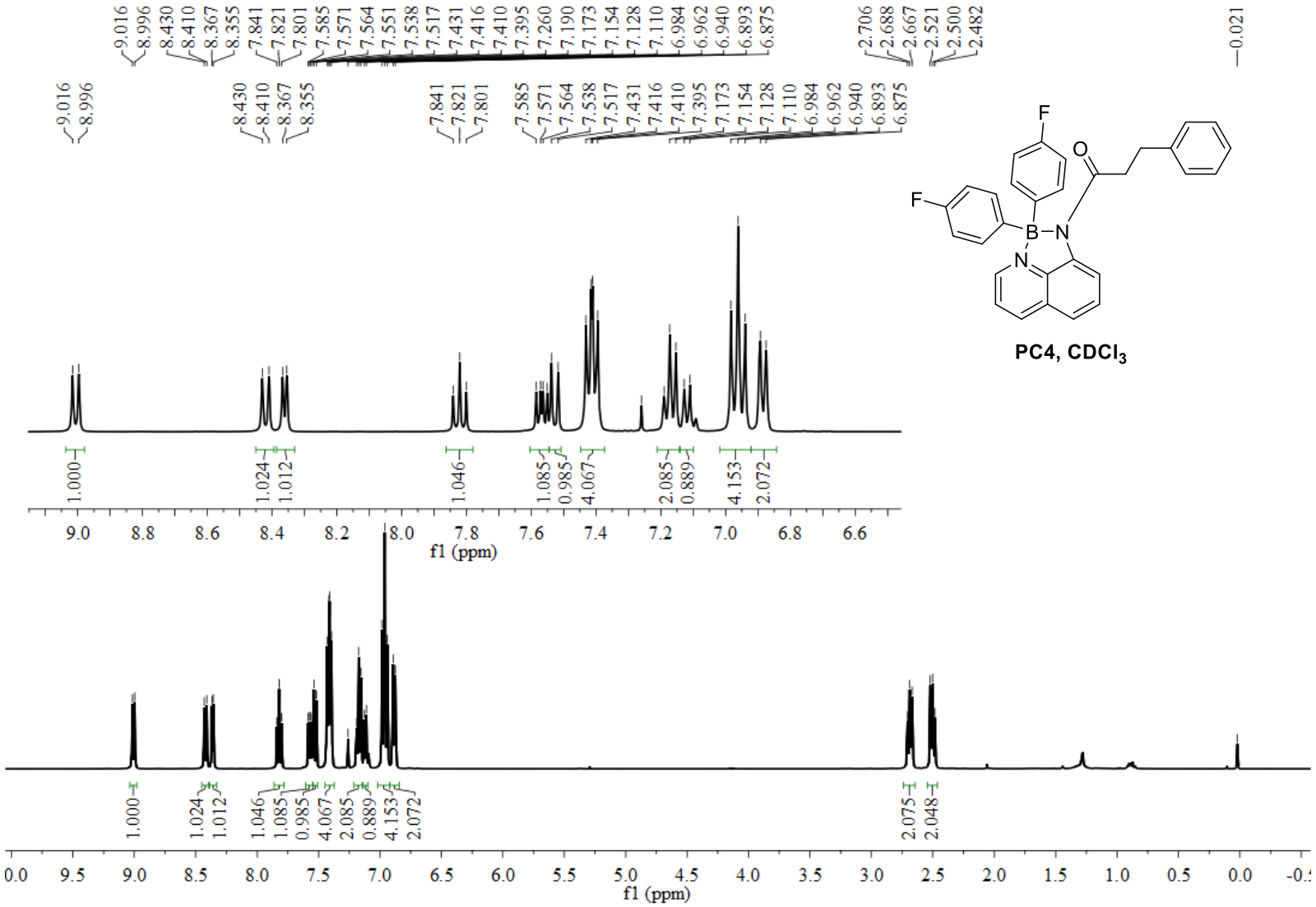

9.002
8.983
8.405
8.392
8.343
7.813
7.793
7.773
7.528
7.515
7.507
7.492
7.471
7.412
7.391
7.260
7.171
7.153
7.134
7.108
7.091
6.891
6.873
6.842
6.821
3.784
2.678
2.662
2.652
2.641
2.581
2.571
2.560
2.545
0.020
O
O
O
B
N
N
PC3, CDCl3
1.000
1.041
1.023
1.118
2.165
4.093
2.057
1.123
2.197
4.068
5.930
1.997
1.980
f1 (ppm)

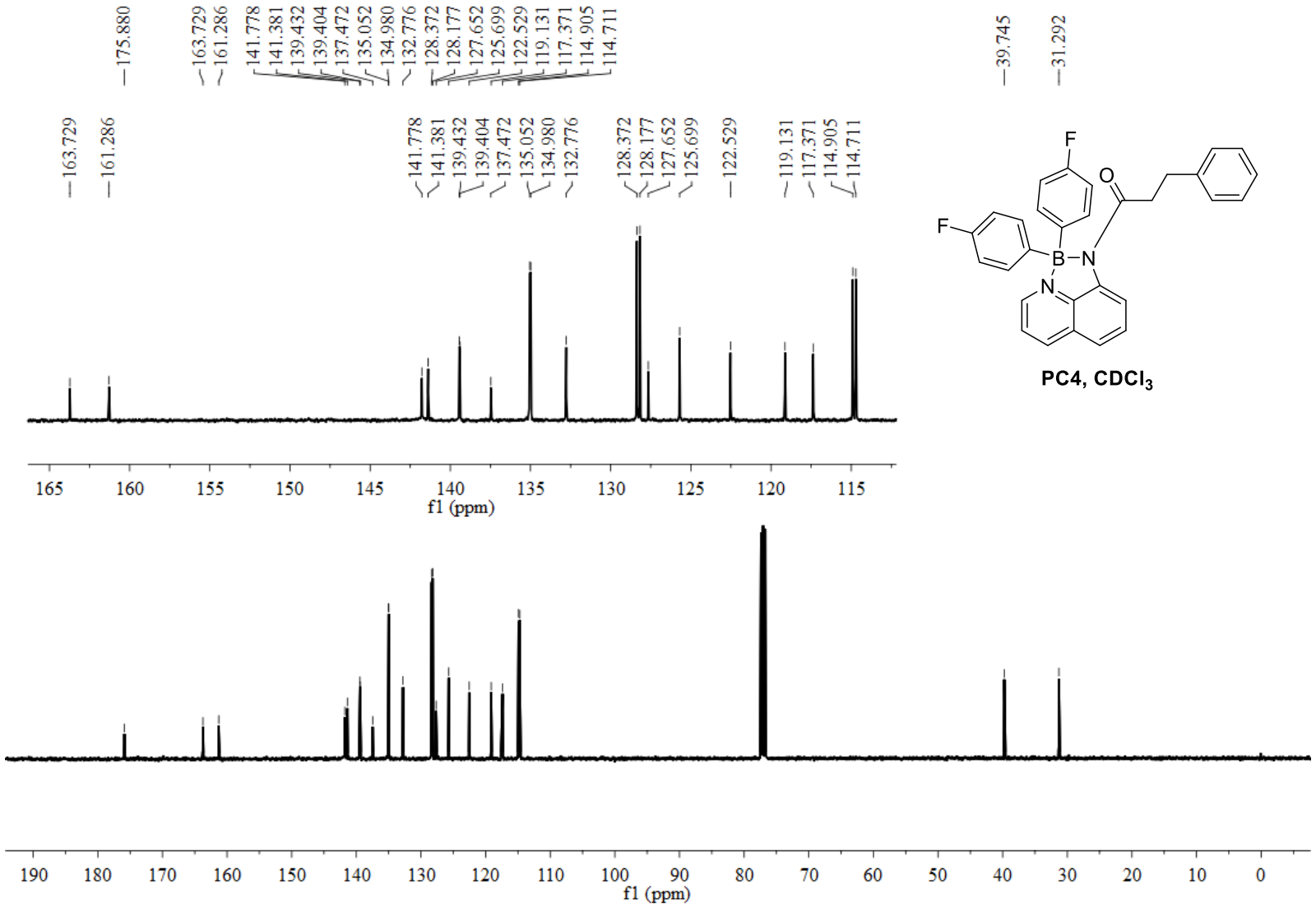

176.28
158.89
141.98
141.63
139.45
138.94
137.51
134.69
132.59
128.46
128.05
127.60
125.53
122.43
118.87
117.10
113.41
55.05
39.63
31.41
O
O
O
B
N
N
160
155
150
145
140
135
130
125
120
115
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

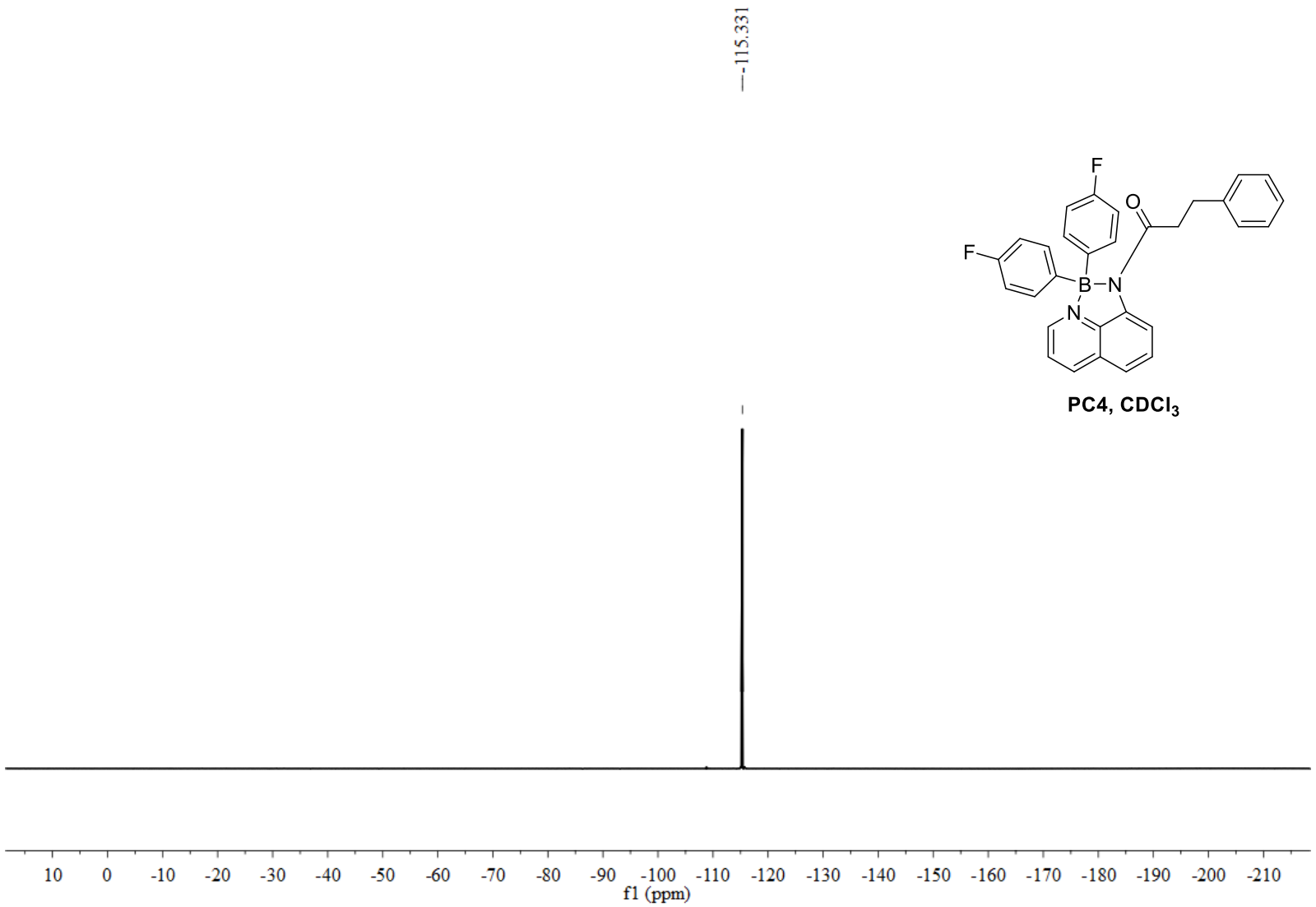
PC3, $CDCl_3$


7.380
O
O
O
B
N
N
120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110
f1 (ppm)

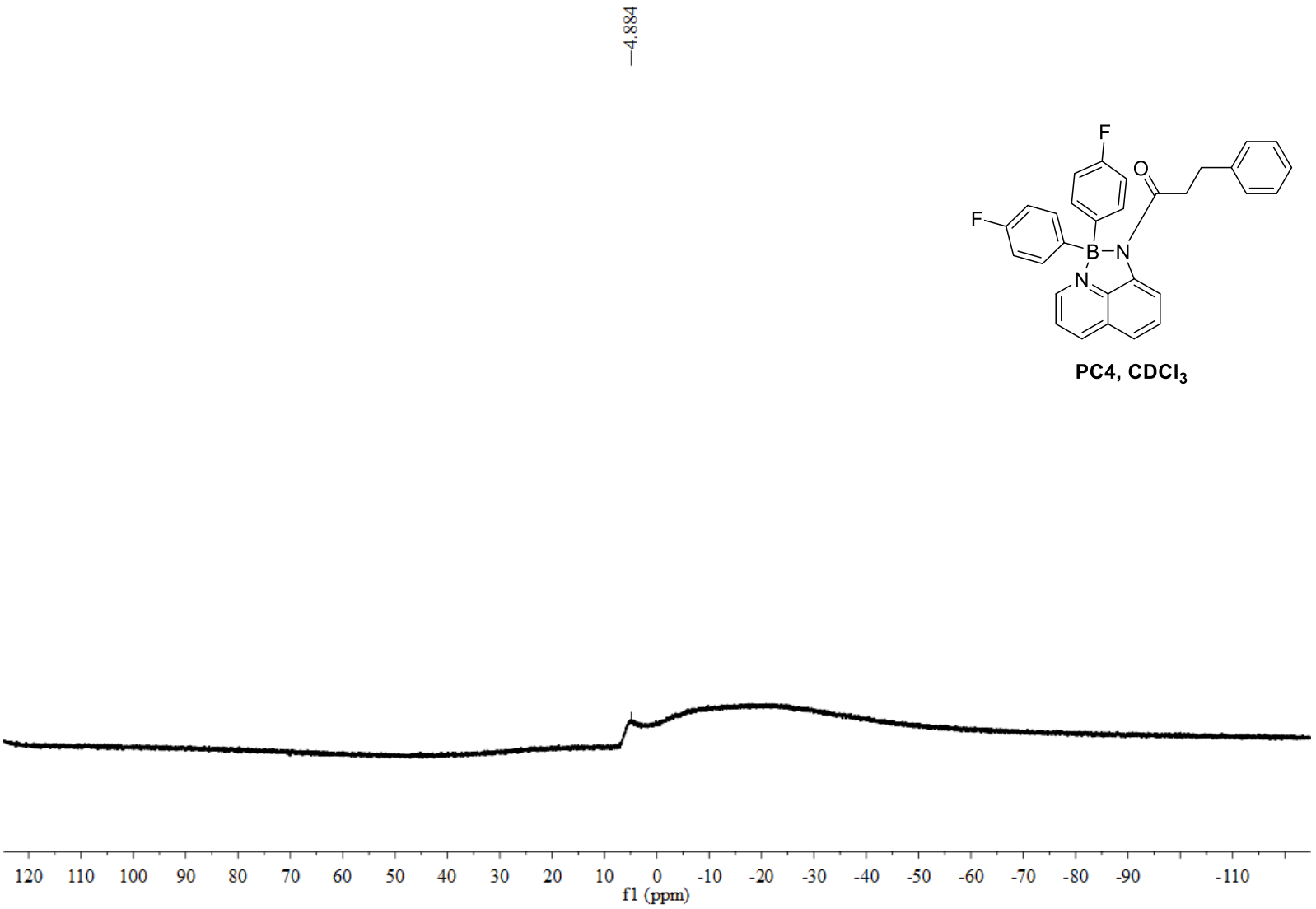
PC3, $CDCl_3$


9.016
8.996
8.430
8.410
8.367
8.355
7.841
7.821
7.801
7.585
7.571
7.564
7.551
7.538
7.517
7.431
7.416
7.410
7.395
7.260
7.190
7.173
7.154
7.128
7.110
6.984
6.962
6.940
6.893
6.875
2.706
2.688
2.667
2.521
2.500
2.482
-0.021
F
O
F
B
N
N
PC4, CDCl3
1.000
1.024
1.012
1.046
1.085
0.985
4.067
2.085
0.889
4.153
2.072
2.075
2.048
f1 (ppm)

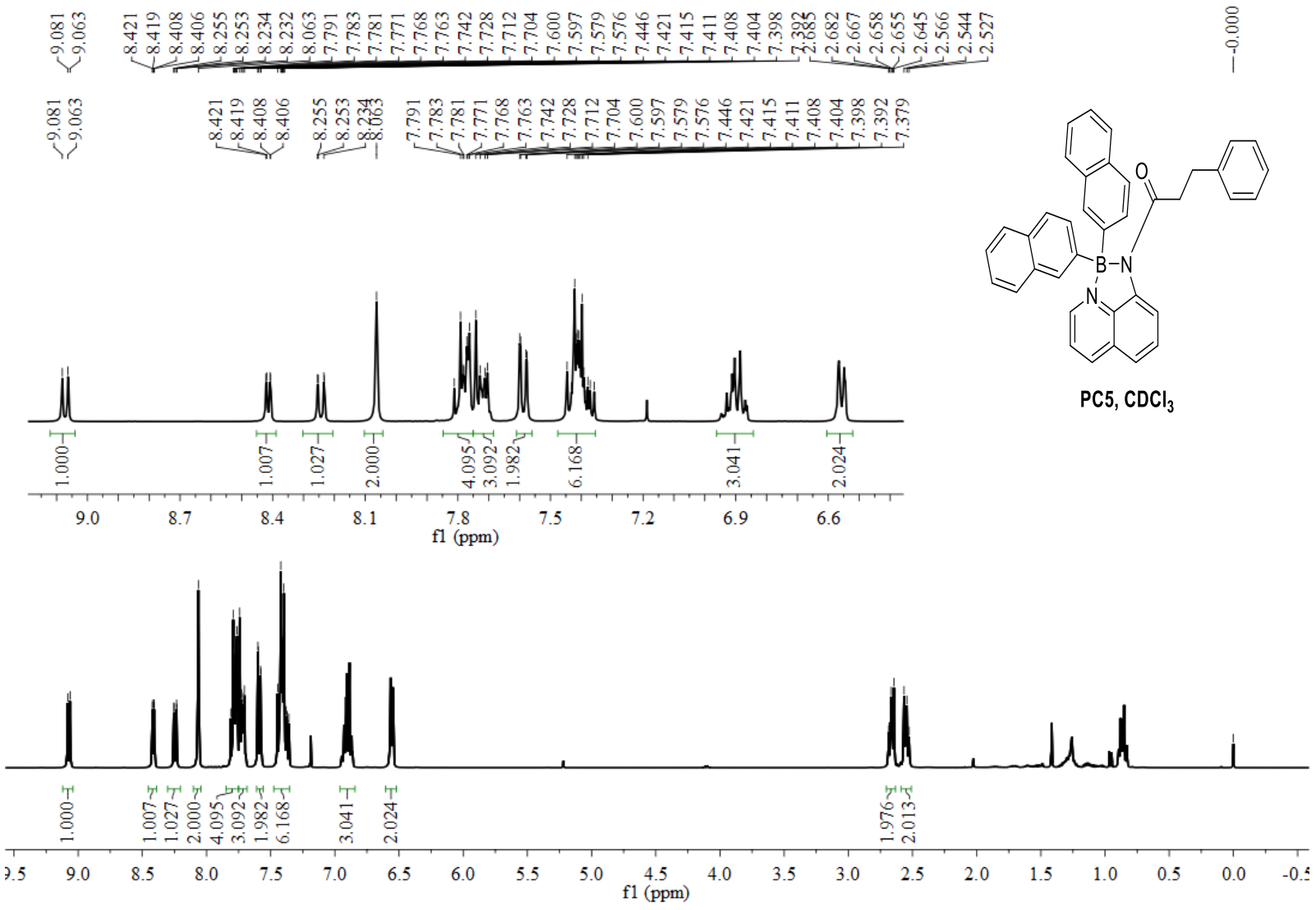

175.880
163.729
161.286
141.778
141.381
139.432
139.404
137.472
135.052
134.980
132.776
128.372
128.177
127.652
125.699
122.529
119.131
117.371
114.905
114.711
39.745
31.292
f1 (ppm)
f1 (ppm)
F
F
O
B
N
N
PC4, CDCl3

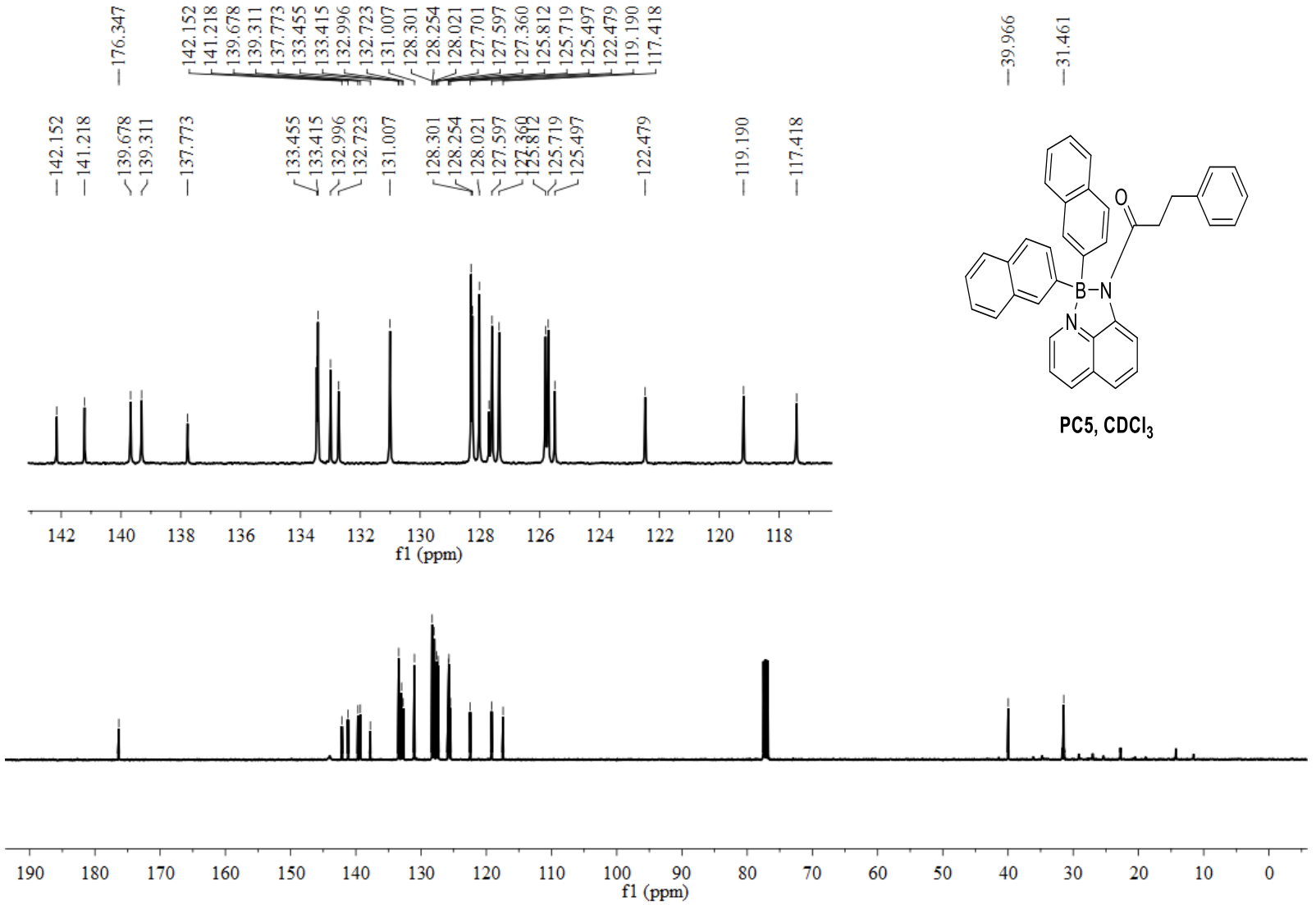

-115.331
F
O
F
B
N
N
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

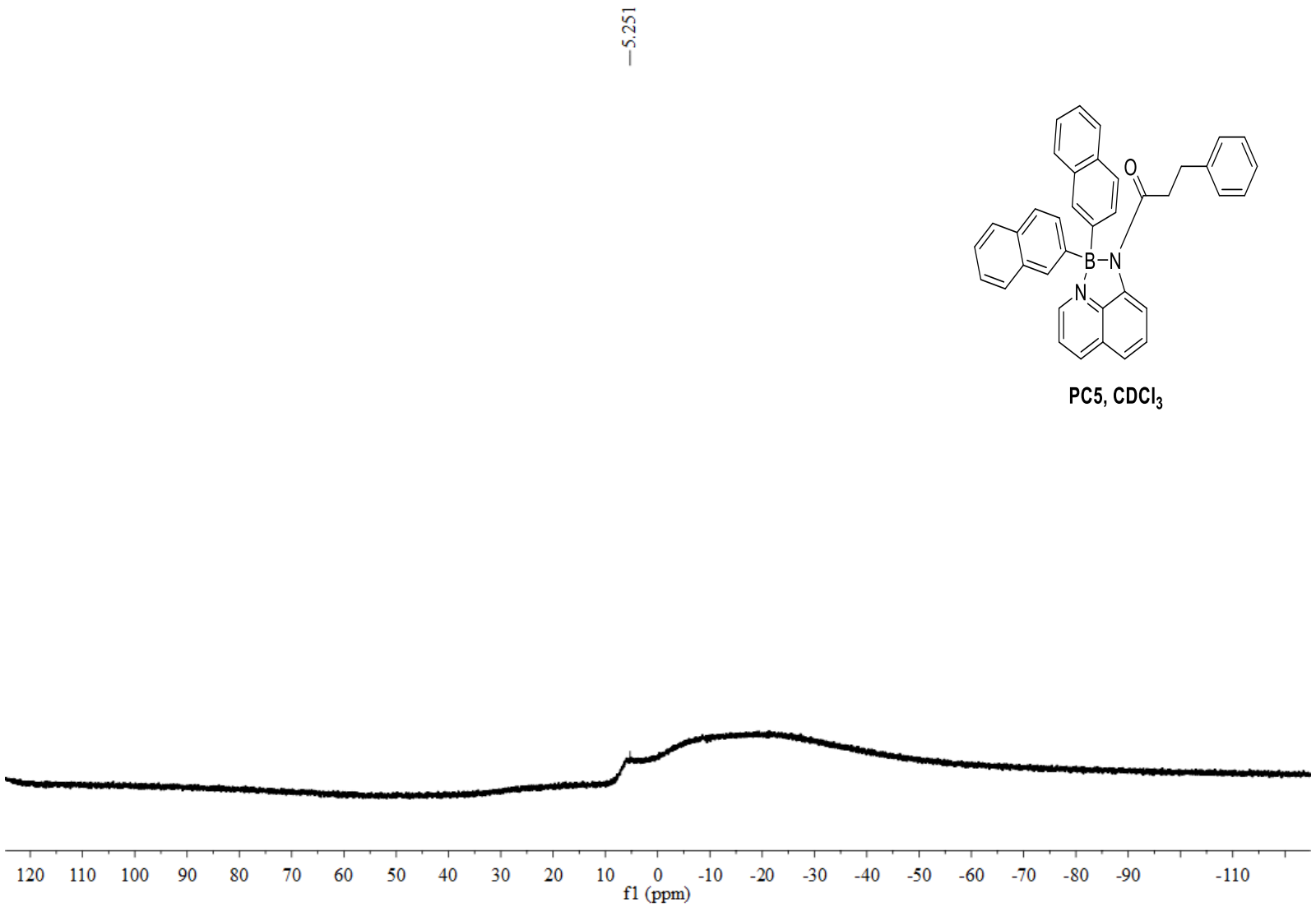
PC4, $CDCl_3$


4.884
F
O
F
B
N
N
120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110
f1 (ppm)

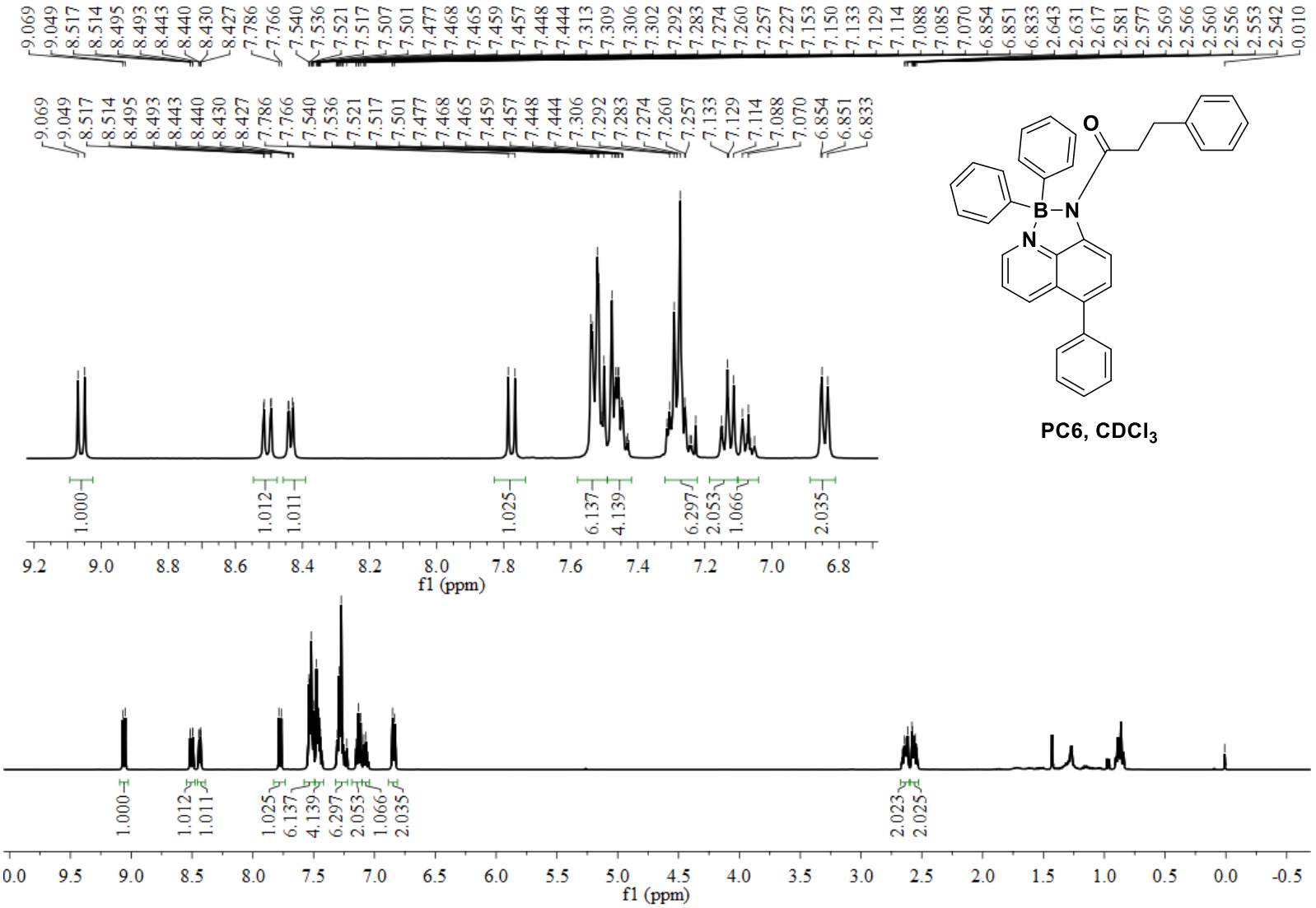
PC4, $CDCl_3$

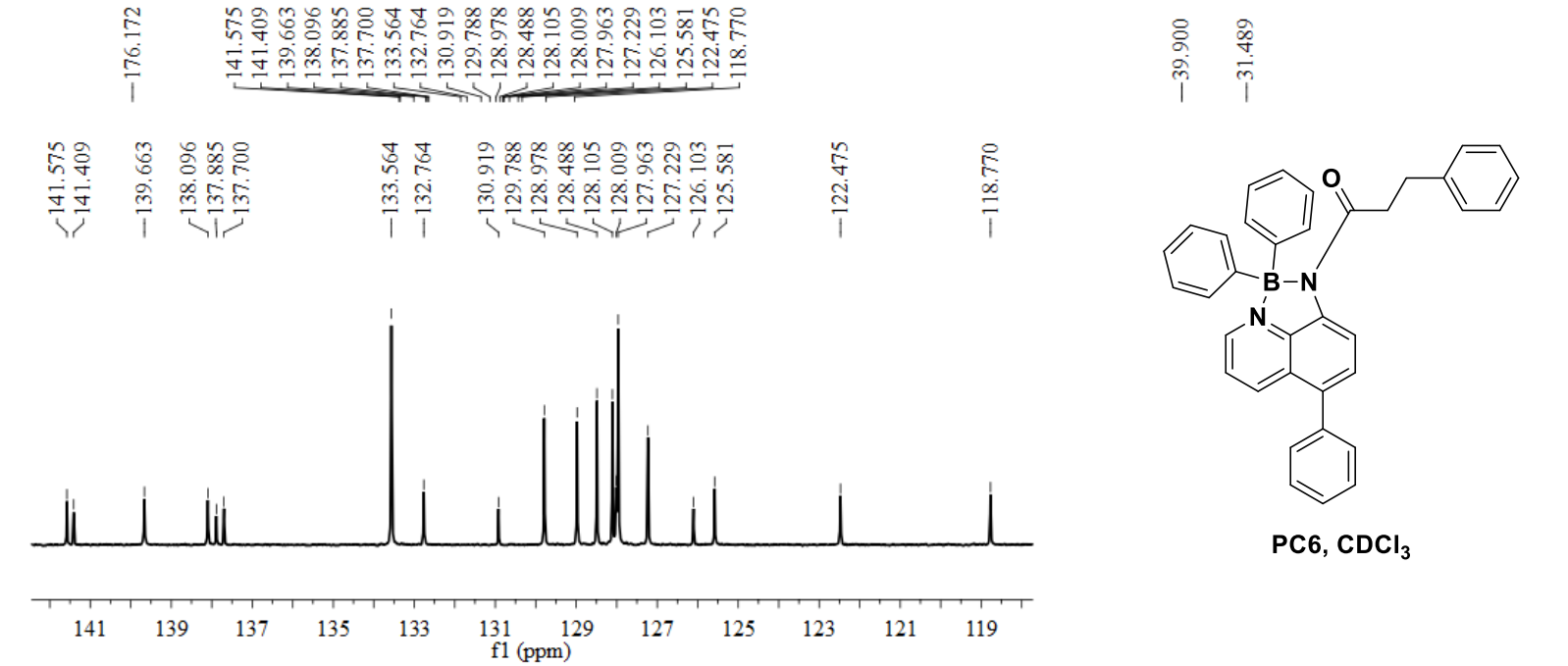

9.081
9.063
8.421
8.419
8.408
8.406
8.255
8.253
8.234
8.232
8.063
7.791
7.783
7.781
7.771
7.768
7.763
7.742
7.728
7.712
7.704
7.600
7.597
7.579
7.576
7.446
7.421
7.415
7.411
7.408
7.404
7.398
2.682
2.667
2.658
2.655
2.645
2.566
2.544
2.527
-0.000
7.392
7.379
O
B–N
N
PC5, CDCl3
1.000
1.007
1.027
2.000
4.095
3.092
1.982
6.168
3.041
2.024
1.976
2.013
f1 (ppm)


176.347
142.152
141.218
139.678
139.311
137.773
133.455
133.415
132.996
132.723
131.007
128.301
128.254
128.021
127.701
127.597
127.360
125.812
125.719
125.497
122.479
119.190
117.418
39.966
31.461
O
B
N
N
PC5, CDCl3
f1 (ppm)
f1 (ppm)

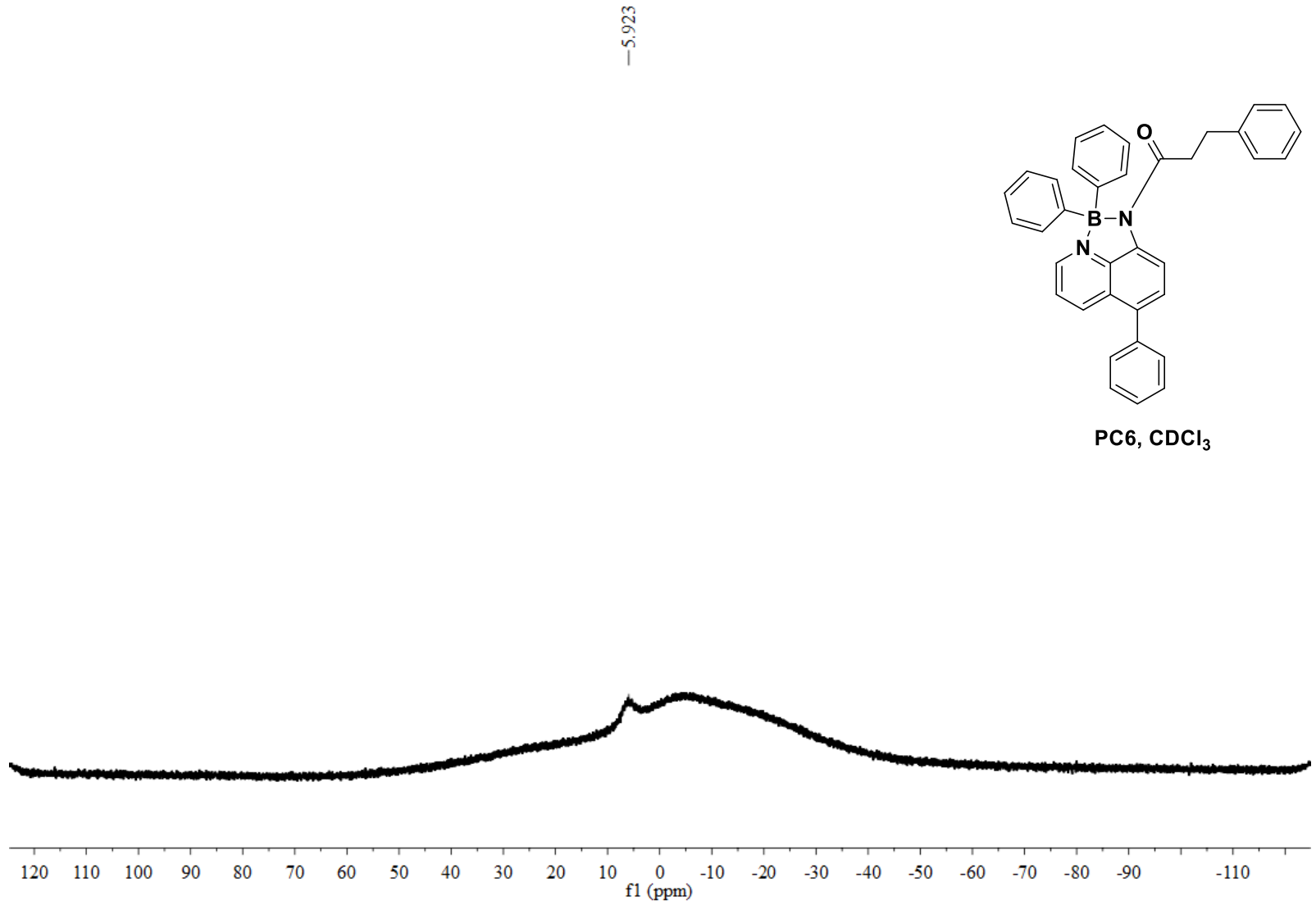

5.251
O
B
N
N
120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110
f1 (ppm)

PC5, $CDCl_3$

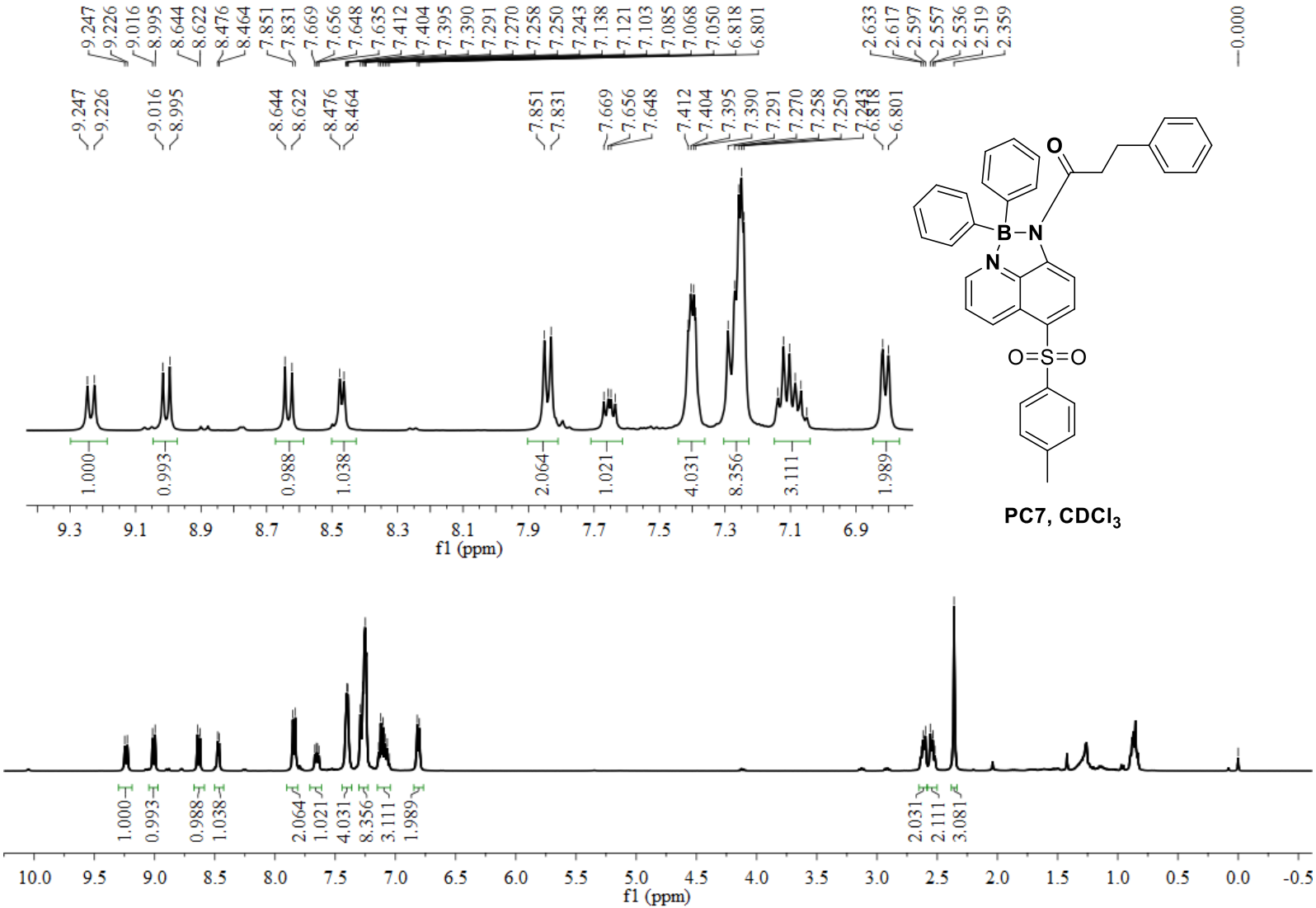

9.069 9.049 8.517 8.514 8.495 8.493 8.443 8.440 8.430 8.427 7.786 7.766 7.540 7.536 7.521 7.517 7.507 7.501 7.477 7.468 7.465 7.459 7.457 7.448 7.444 7.313 7.309 7.306 7.302 7.292 7.283 7.274 7.260 7.257 7.227 7.153 7.150 7.133 7.129 7.114 7.088 7.085 7.070 6.854 6.851 6.833 2.643 2.631 2.617 2.581 2.577 2.569 2.566 2.560 2.556 2.553 2.542 0.010
1.000 1.012 1.011 1.025 6.137 4.139 6.297 2.053 1.066 2.035
f1 (ppm)
2.023 2.025
O
B
N
N
PC6, CDCl3

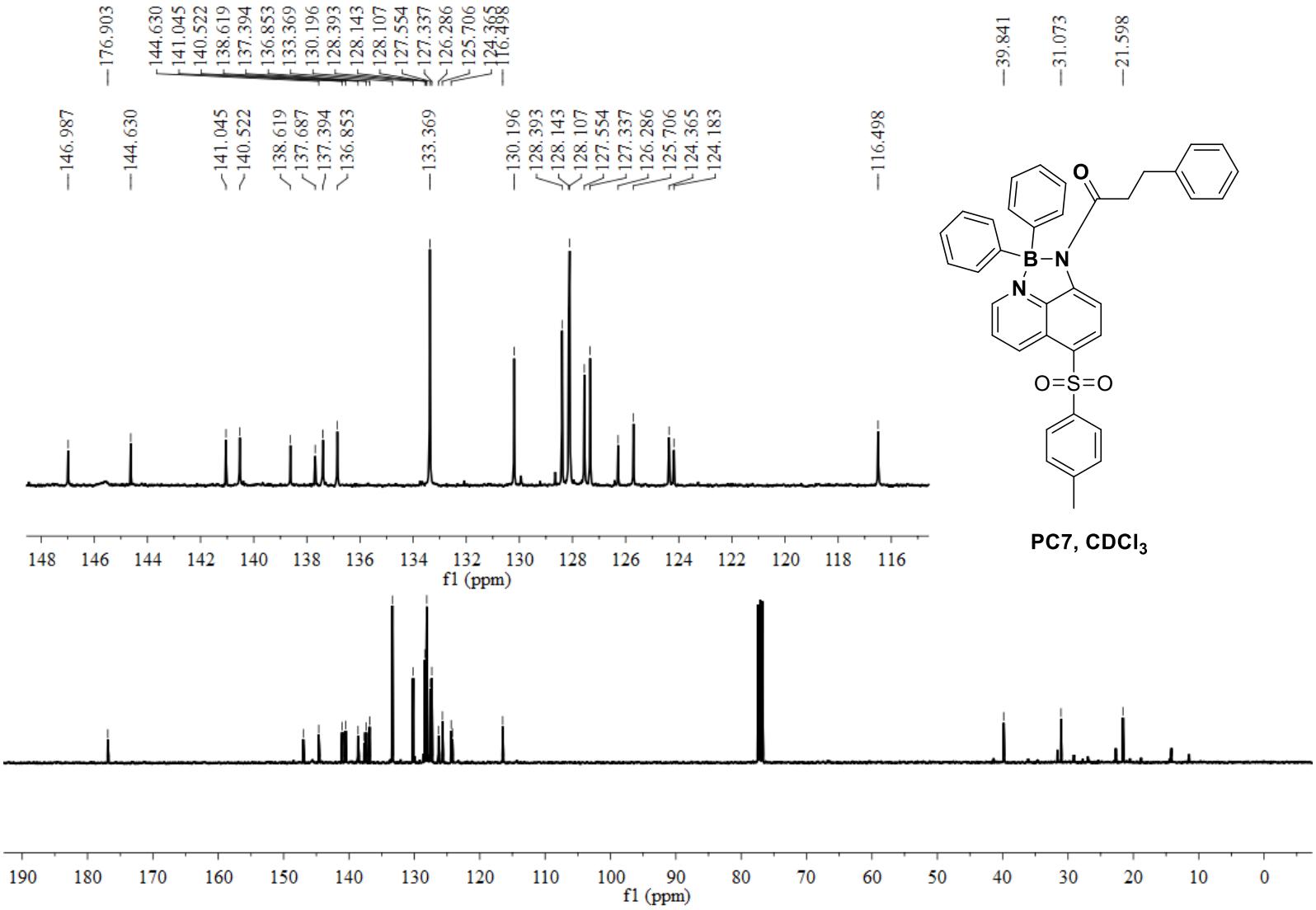

176.172
141.575
141.409
139.663
138.096
137.885
137.700
133.564
132.764
130.919
129.788
128.978
128.488
128.105
128.009
127.963
127.229
126.103
125.581
122.475
118.770
39.900
31.489
O
B
N
N
141
139
137
135
133
131
129
127
125
123
121
119
f1 (ppm)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

PC6, $CDCl_3$

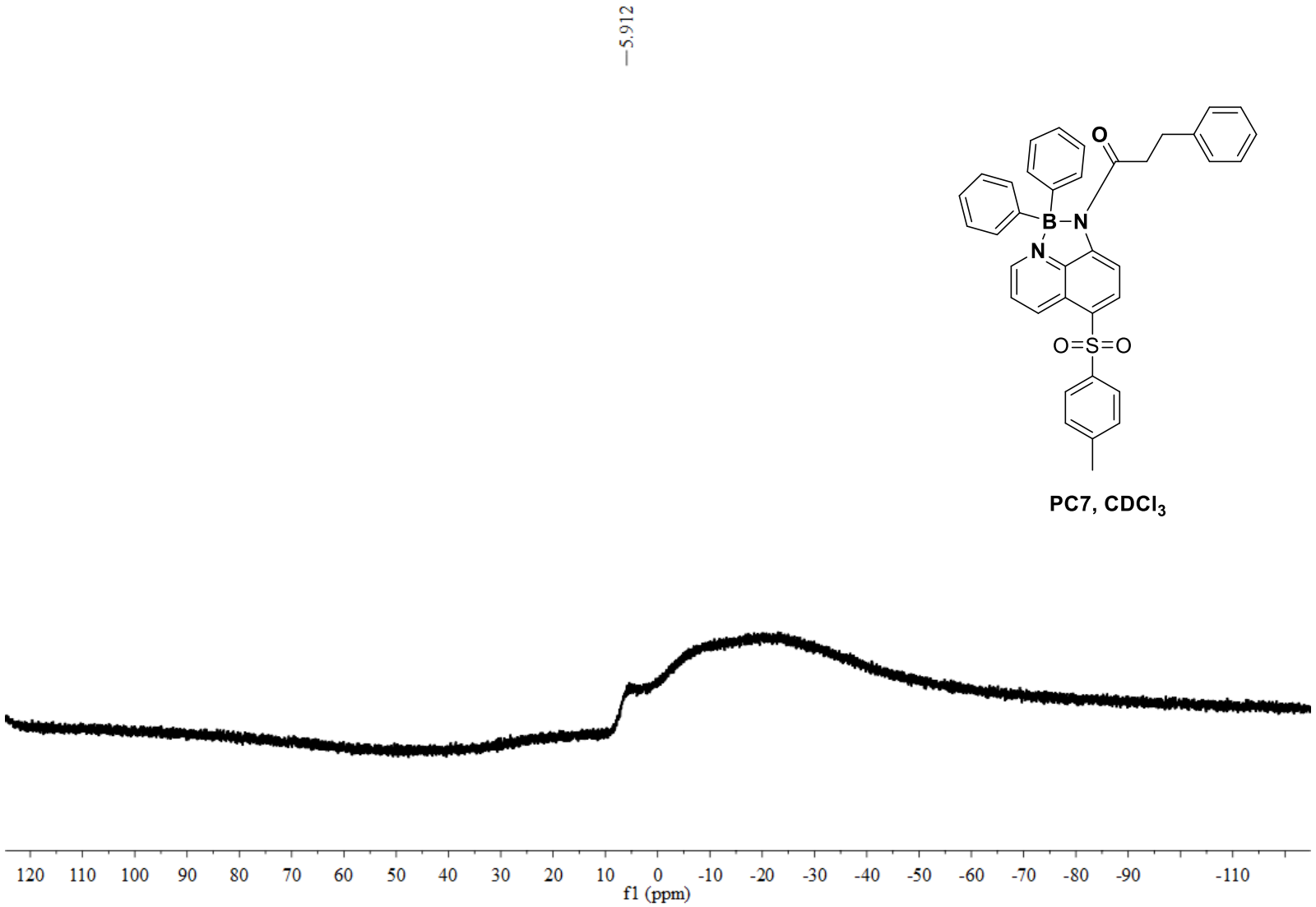

5.923
O
B
N
N
120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110
f1 (ppm)

PC6, $CDCl_3$

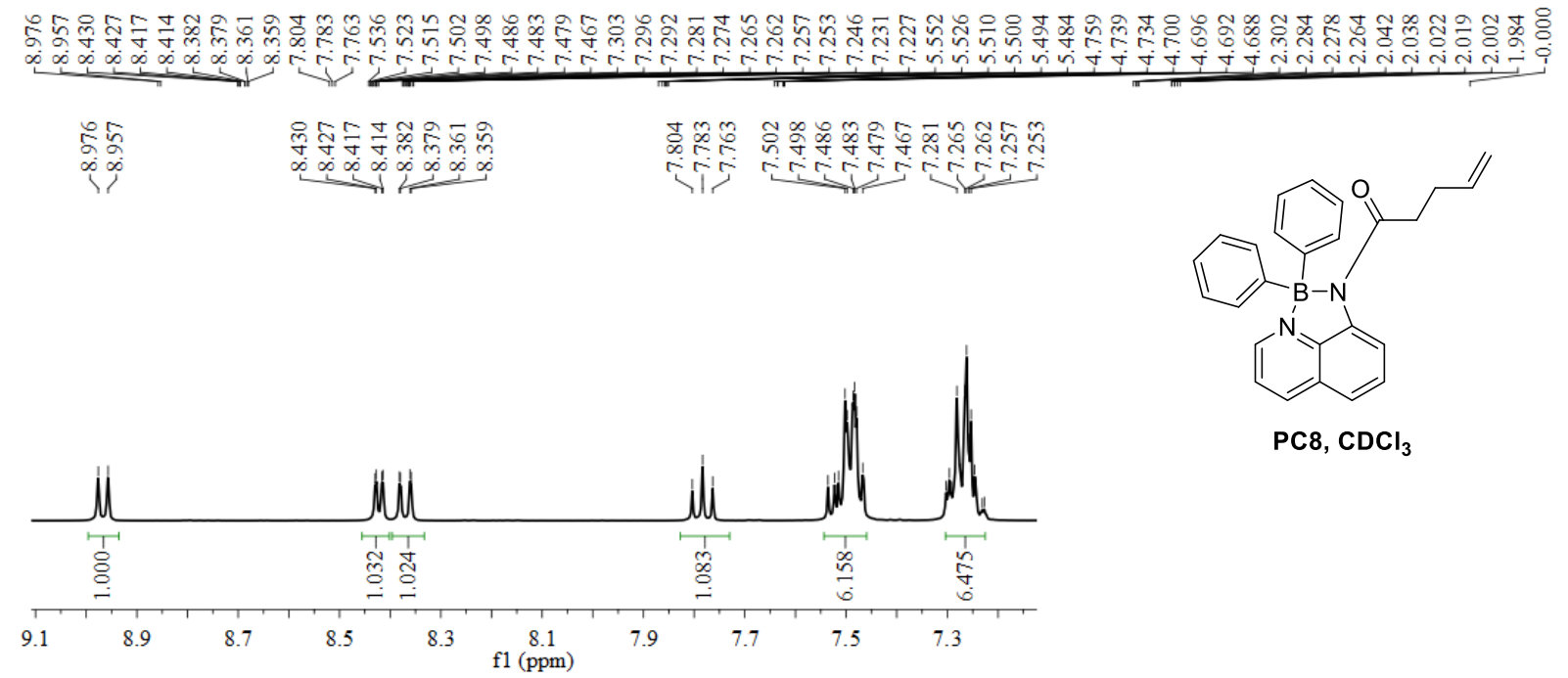

9.247
9.226
9.016
8.995
8.644
8.622
8.476
8.464
7.851
7.831
7.669
7.656
7.648
7.635
7.412
7.404
7.395
7.390
7.291
7.270
7.258
7.250
7.243
7.138
7.121
7.103
7.085
7.068
7.050
6.818
6.801
2.633
2.617
2.597
2.557
2.536
2.519
2.359
0.000
1.000
0.993
0.988
1.038
2.064
1.021
4.031
8.356
3.111
1.989
f1 (ppm)
2.031
2.111
3.081
O
B
N
N
O=S=O
PC7, CDCl3


176.903
144.630
141.045
140.522
138.619
137.394
136.853
133.369
130.196
128.393
128.143
128.107
127.554
127.337
126.286
125.706
124.365
116.498
39.841
31.073
21.598
146.987
144.630
141.045
140.522
138.619
137.687
137.394
136.853
133.369
130.196
128.393
128.143
128.107
127.554
127.337
126.286
125.706
124.365
124.183
116.498
O
B–N
N
O=S=O
148 146 144 142 140 138 136 134 132 130 128 126 124 122 120 118 116
f1 (ppm)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

PC7, $CDCl_3$

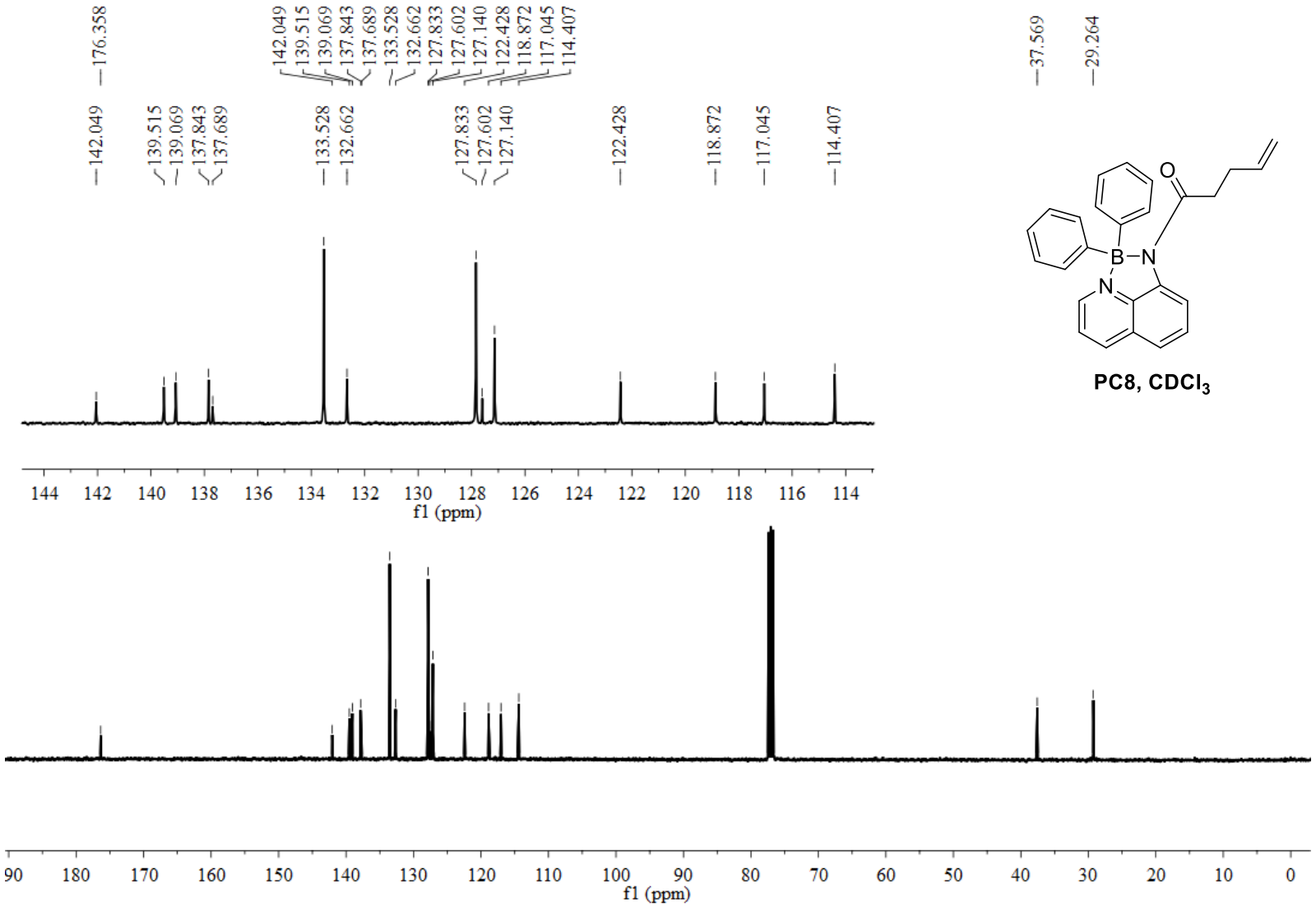

5.912
O
B
N
N
O=S=O
120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110
f1 (ppm)

PC7, $CDCl_3$

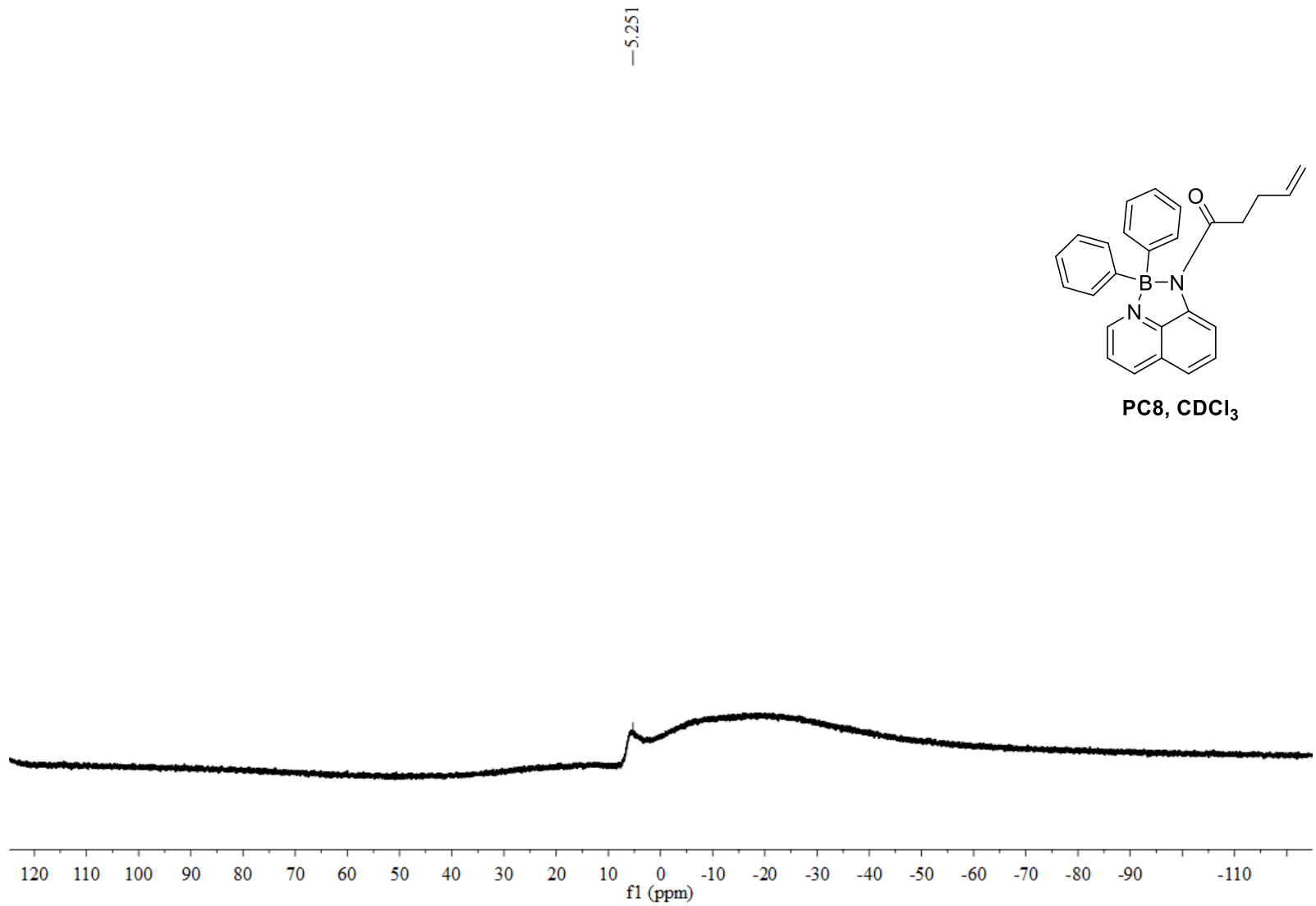

8.976
8.957
8.430
8.427
8.417
8.414
8.382
8.379
8.361
8.359
7.804
7.783
7.763
7.536
7.523
7.515
7.502
7.498
7.486
7.483
7.479
7.467
7.303
7.296
7.292
7.281
7.274
7.265
7.262
7.257
7.253
7.246
7.231
7.227
5.552
5.526
5.510
5.500
5.494
5.484
4.759
4.739
4.734
4.700
4.696
4.692
4.688
2.302
2.284
2.278
2.264
2.042
2.038
2.022
2.019
2.002
1.984
0.000
1.000
1.032
1.024
1.083
6.158
6.475
f1 (ppm)
1.011
2.054
2.056
2.350

O
B
N
N

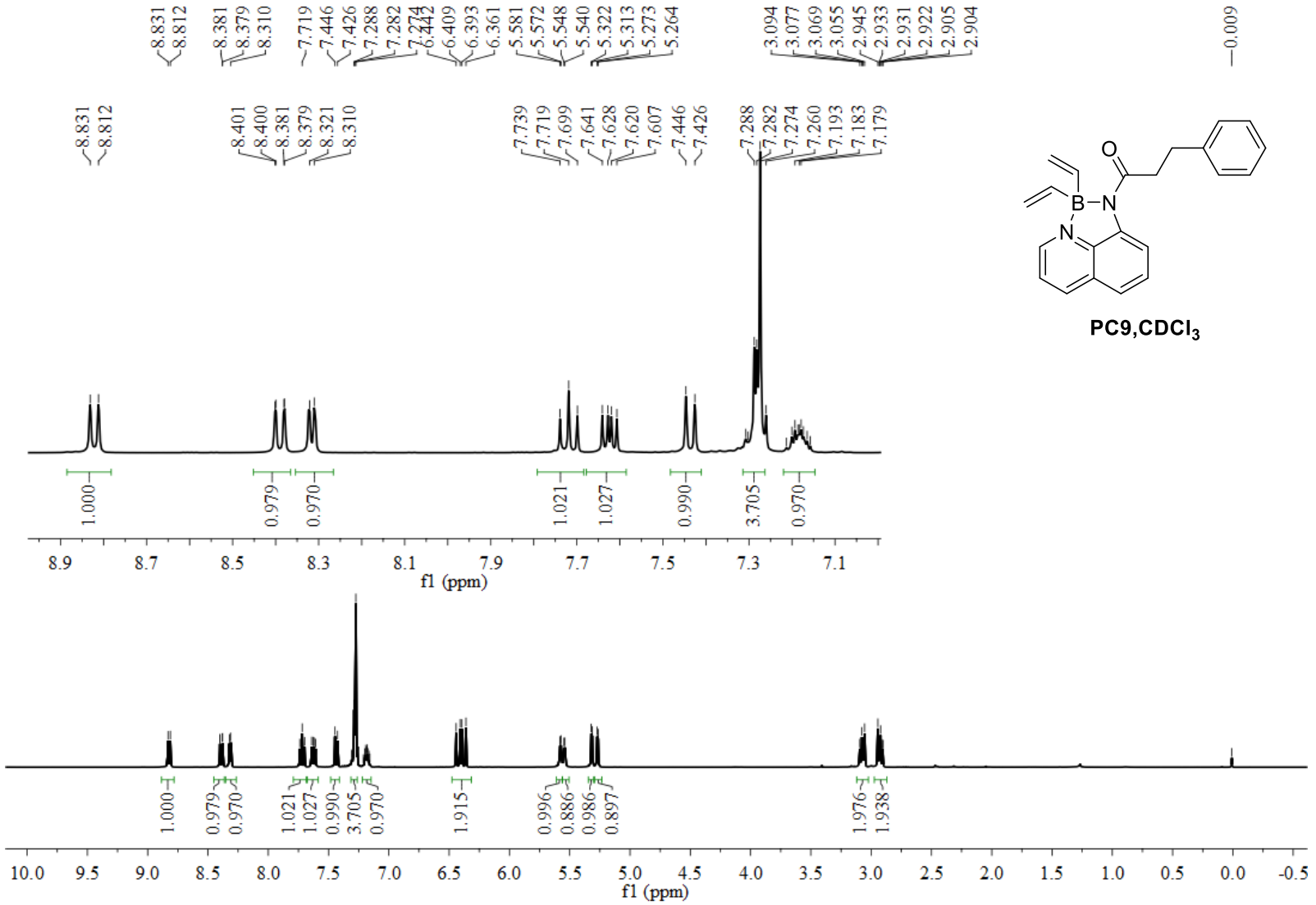
PC8, $CDCl_3$

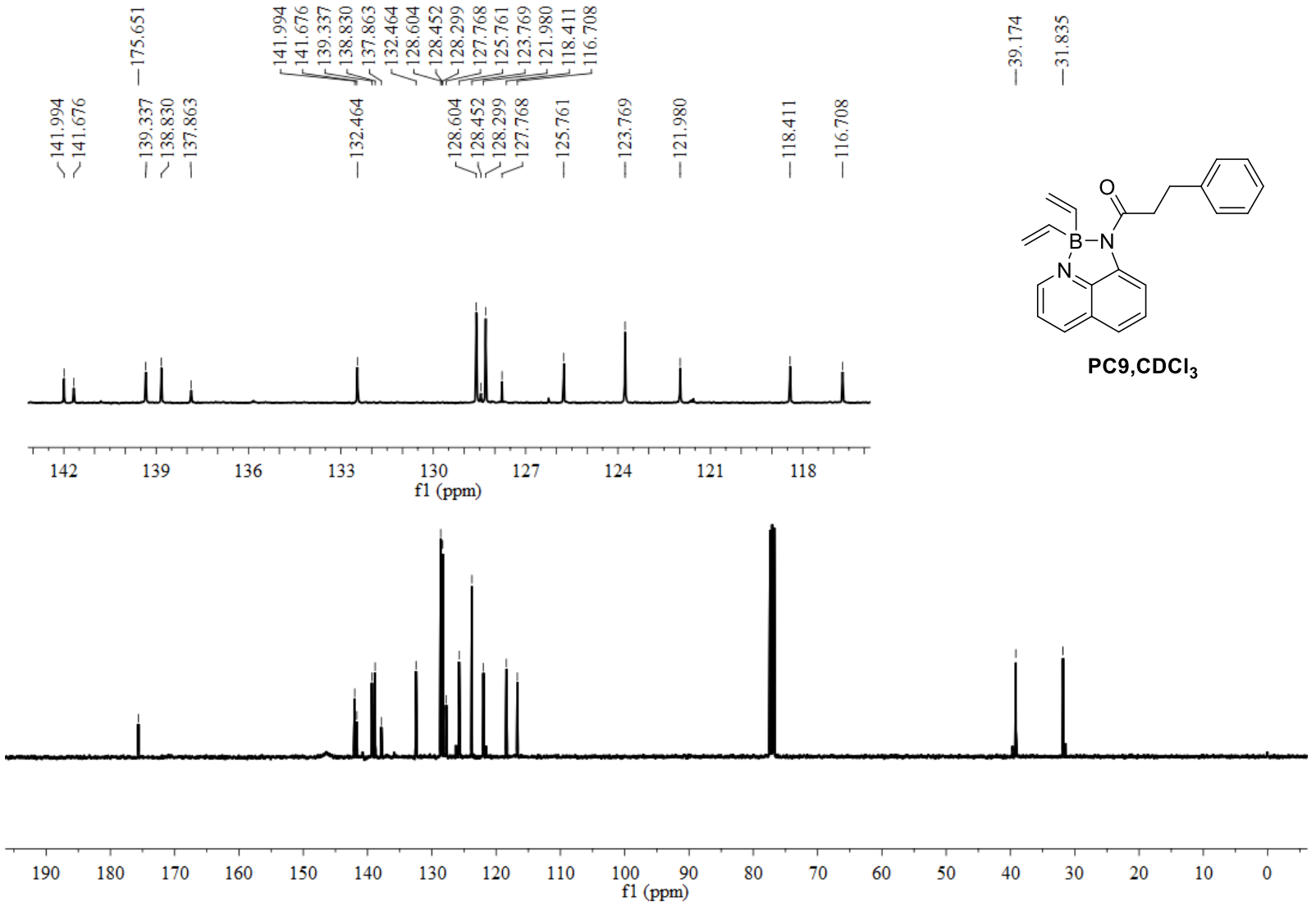

176.358
142.049
139.515
139.069
137.843
137.689
133.528
132.662
127.833
127.602
127.140
122.428
118.872
117.045
114.407
37.569
29.264
O
B
N
N
f1 (ppm)
f1 (ppm)

PC8, $CDCl_3$

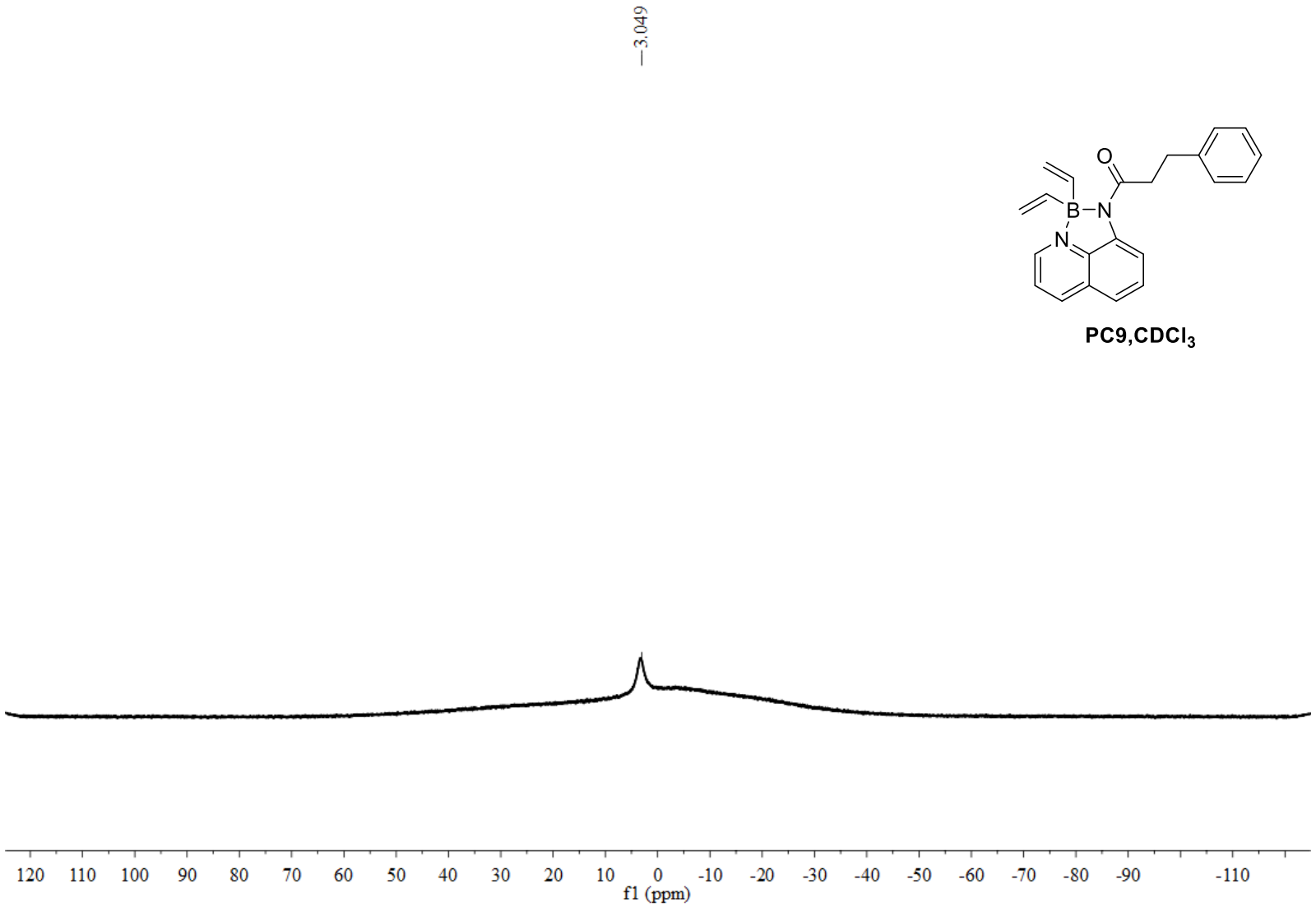

5.251
O
B
N
N
120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110
f1 (ppm)

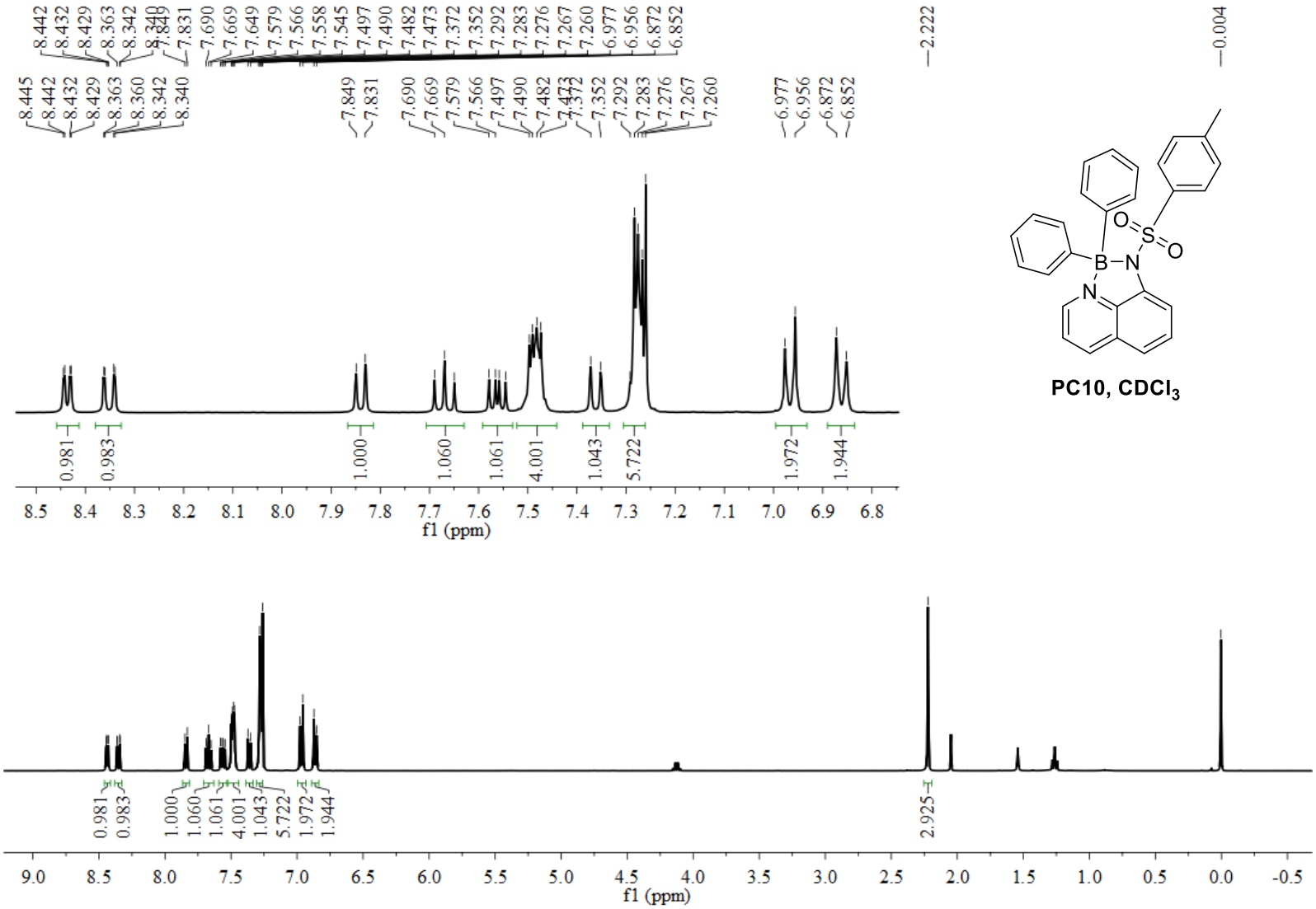
PC8, $CDCl_3$

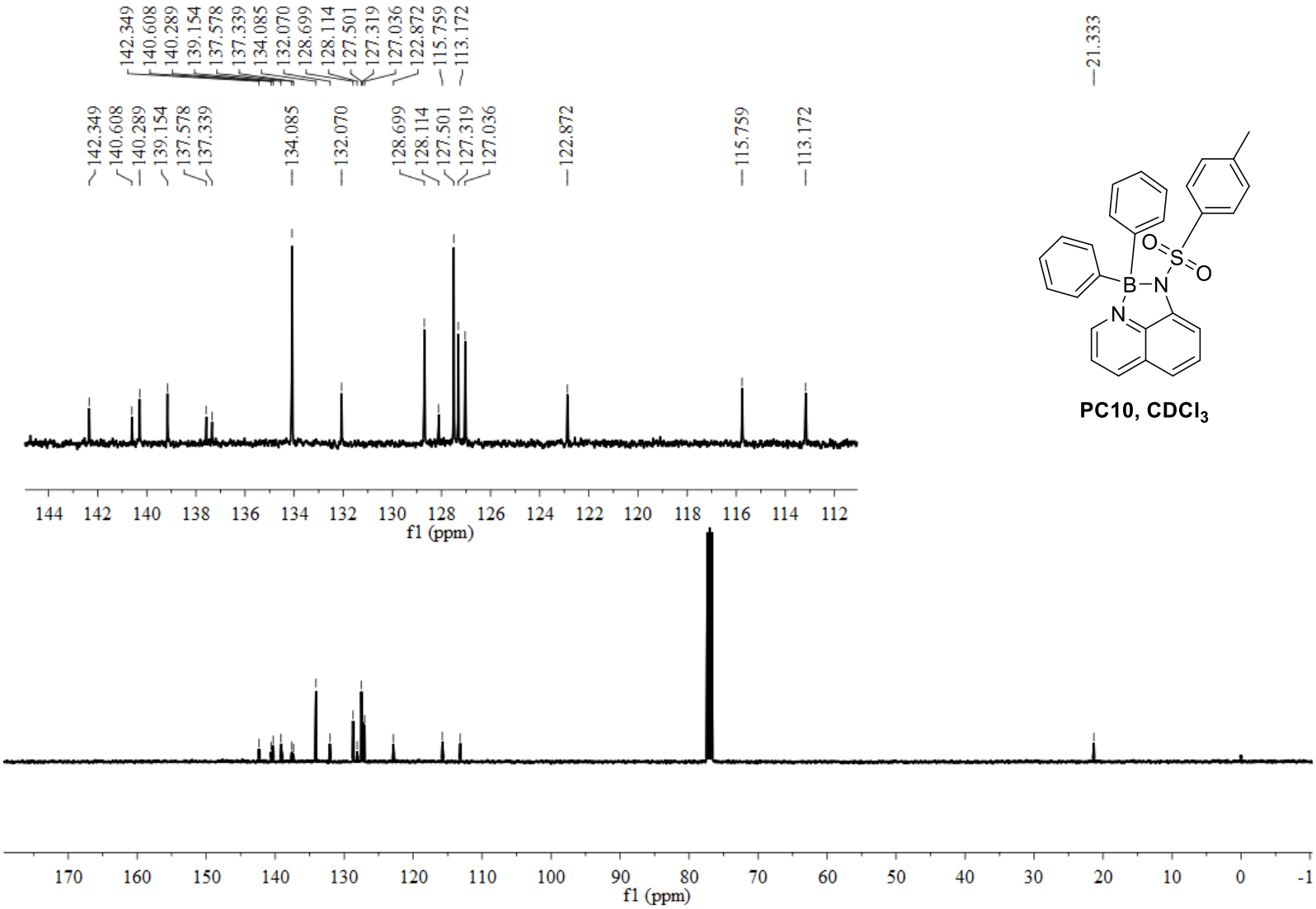

8.831
8.812
8.381
8.379
8.310
7.719
7.446
7.426
7.288
7.282
7.274
6.442
6.409
6.393
6.361
5.581
5.572
5.548
5.540
5.322
5.313
5.273
5.264
3.094
3.077
3.069
3.055
2.945
2.933
2.931
2.922
2.905
2.904
0.009
8.401
8.400
8.381
8.379
8.321
8.310
7.739
7.719
7.699
7.641
7.628
7.620
7.607
7.446
7.426
7.288
7.282
7.274
7.260
7.193
7.183
7.179
1.000
0.979
0.970
1.021
1.027
0.990
3.705
0.970
f1 (ppm)
1.000
0.979
0.970
1.021
1.027
0.990
3.705
0.970
1.915
0.996
0.886
0.986
0.897
1.976
1.938
f1 (ppm)
O
B
N
N
PC9,CDCl3


141.994
141.676
139.337
138.830
137.863
132.464
128.604
128.452
128.299
127.768
125.761
123.769
121.980
118.411
116.708
175.651
39.174
31.835
O
B
N
N
142
139
136
133
130
127
124
121
118
f1 (ppm)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

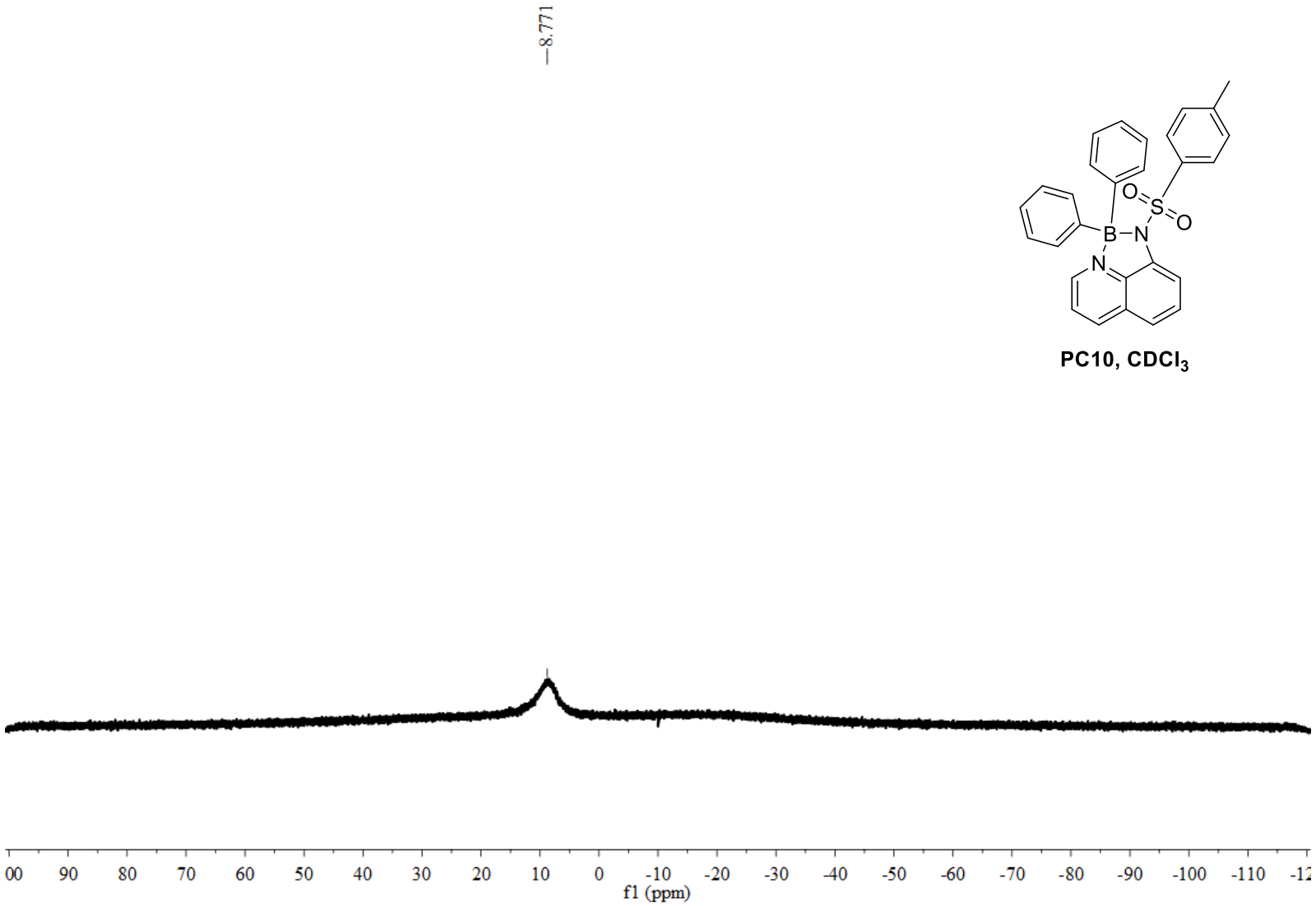
PC9,CDCl$_3$


3.049
O
B
N
N
PC9,CDCl3
120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110
f1 (ppm)

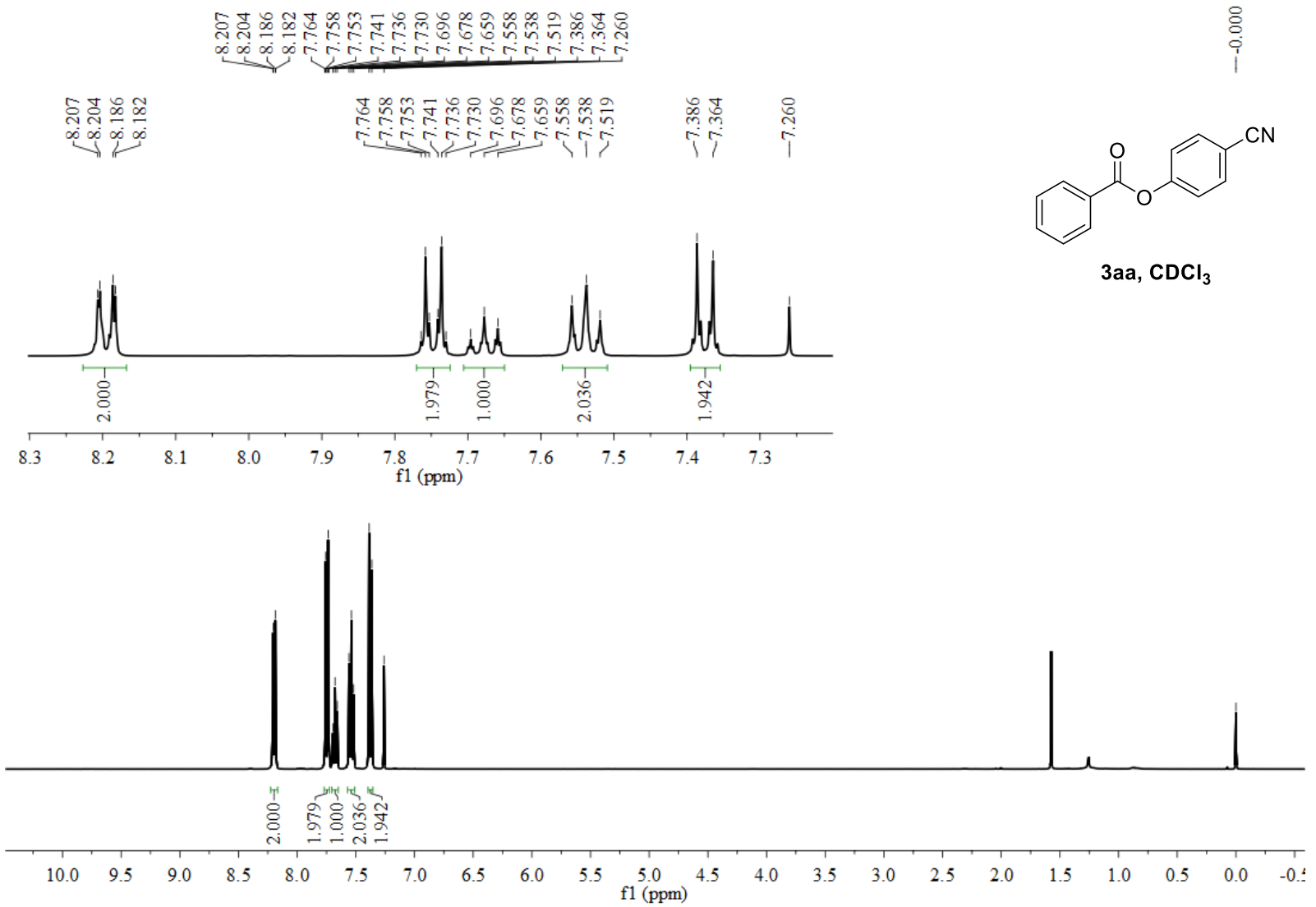

8.442
8.432
8.429
8.363
8.342
7.831
7.690
7.669
7.649
7.579
7.566
7.558
7.545
7.497
7.490
7.482
7.473
7.372
7.352
7.292
7.283
7.276
7.267
7.260
6.977
6.956
6.872
6.852
2.222
0.004
0.981
0.983
1.000
1.060
1.061
4.001
1.043
5.722
1.972
1.944
2.925
f1 (ppm)
PC10, CDCl3

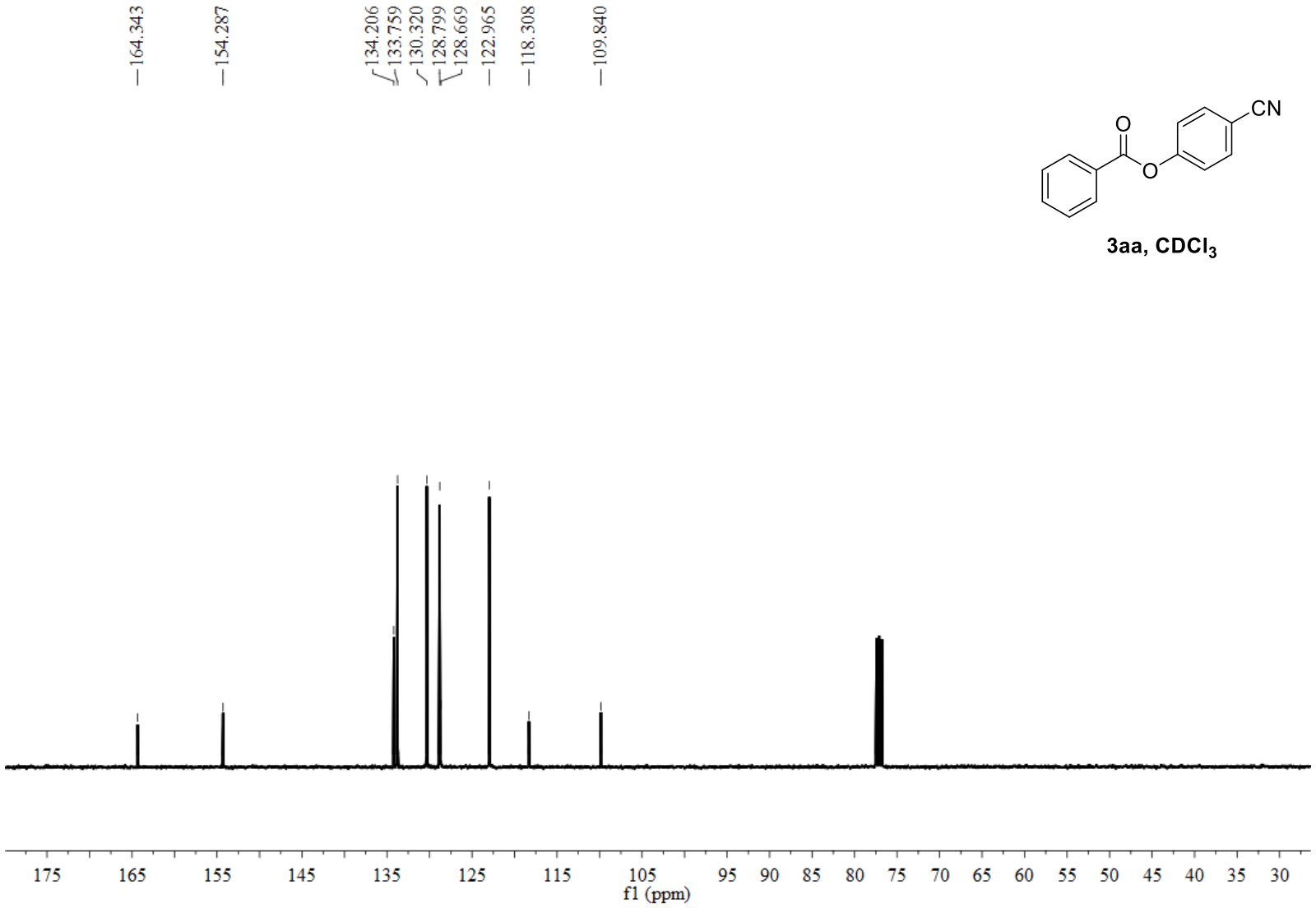

142.349
140.608
140.289
139.154
137.578
137.339
134.085
132.070
128.699
128.114
127.501
127.319
127.036
122.872
115.759
113.172
21.333
O
S
O
B
N
N
144 142 140 138 136 134 132 130 128 126 124 122 120 118 116 114 112
f1 (ppm)
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

PC10, $CDCl_3$

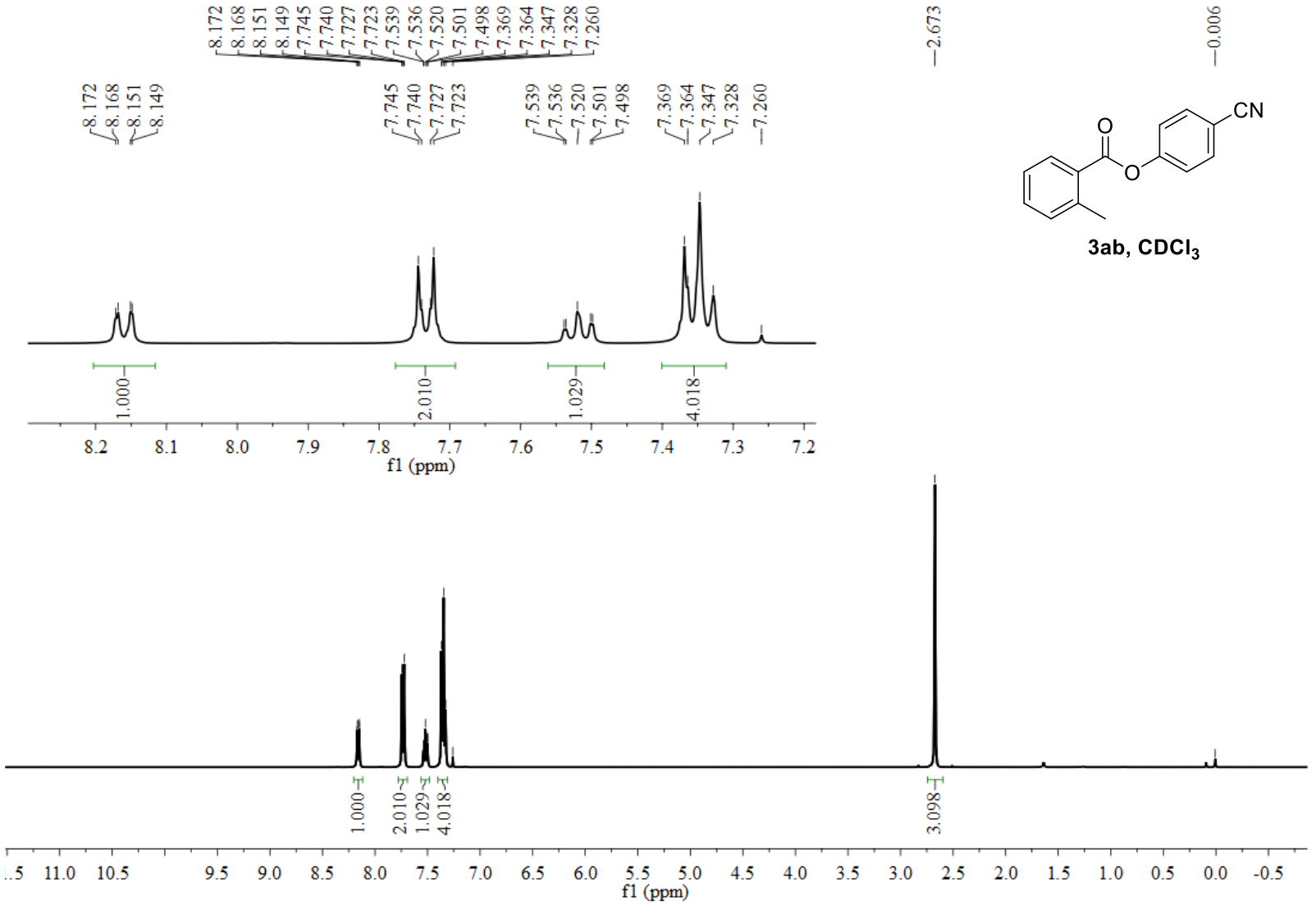

8.771
O
S
O
B
N
N
00 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -12
f1 (ppm)

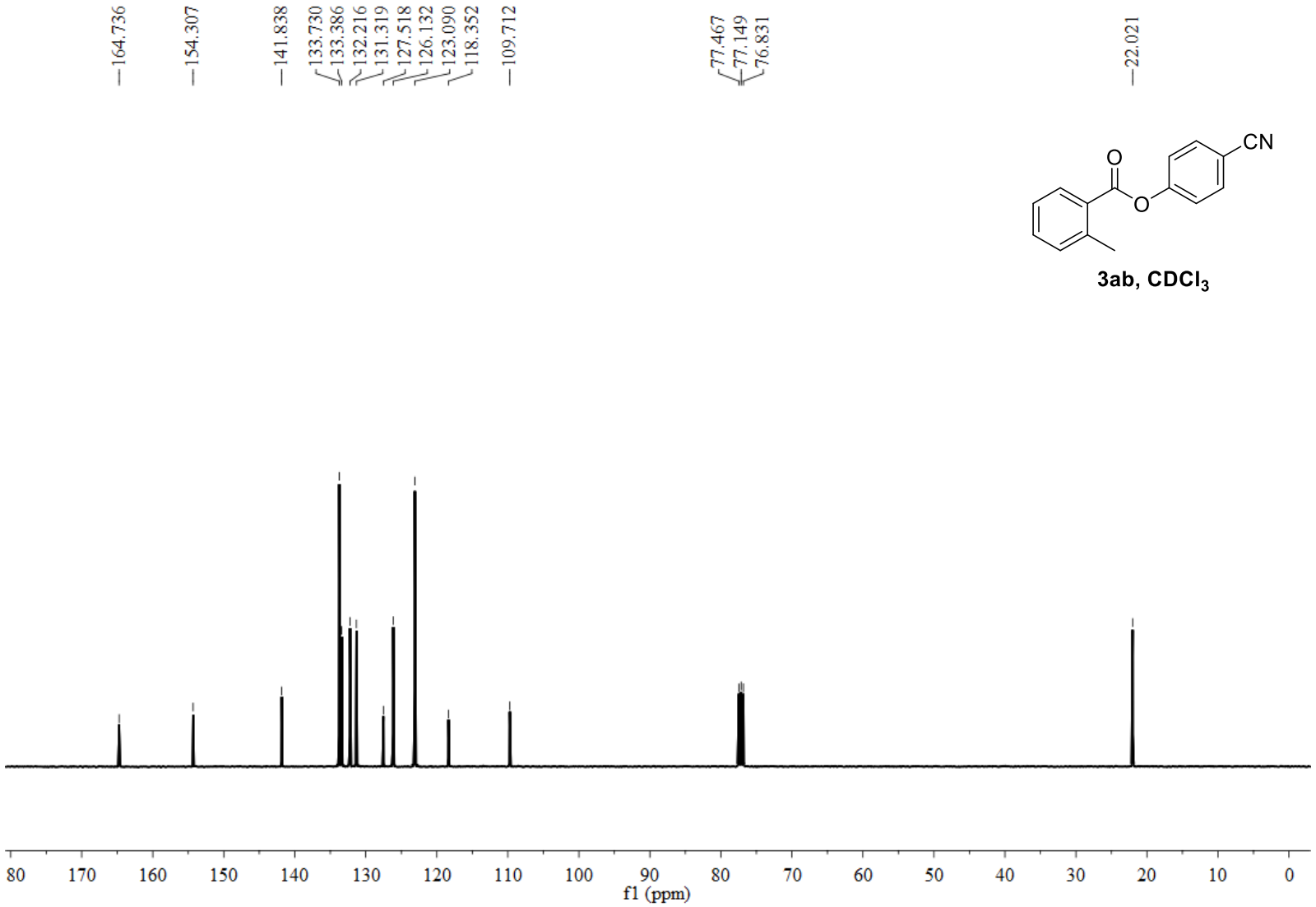
PC10, $CDCl_3$


8.207
8.204
8.186
8.182
7.764
7.758
7.753
7.741
7.736
7.730
7.696
7.678
7.659
7.558
7.538
7.519
7.386
7.364
7.260
-0.000
CN
O
O
3aa, CDCl3
2.000
1.979
1.000
2.036
1.942
f1 (ppm)

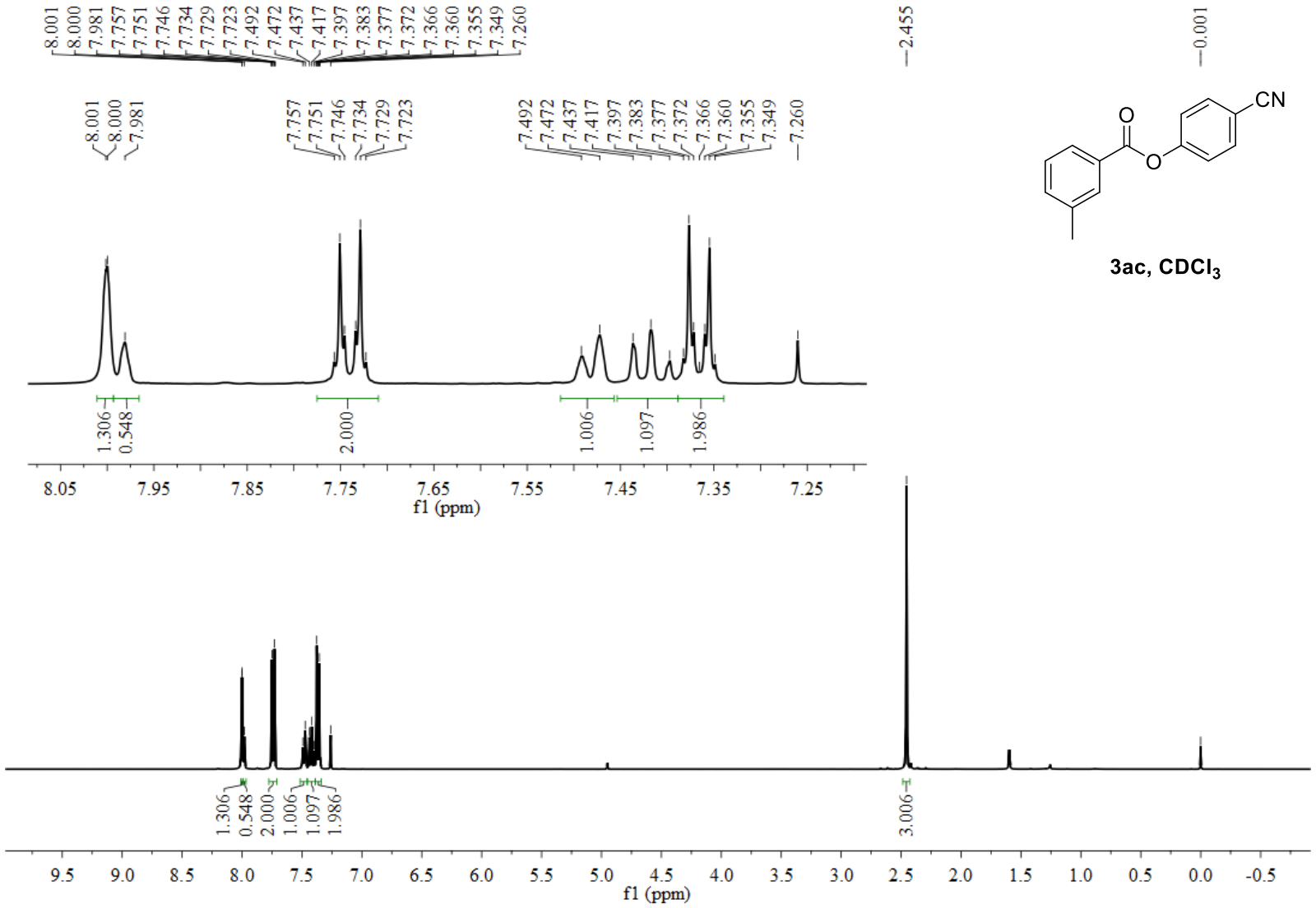

164.343
154.287
134.206
133.759
130.320
128.799
128.669
122.965
118.308
109.840
O
O
CN
175
165
155
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
f1 (ppm)

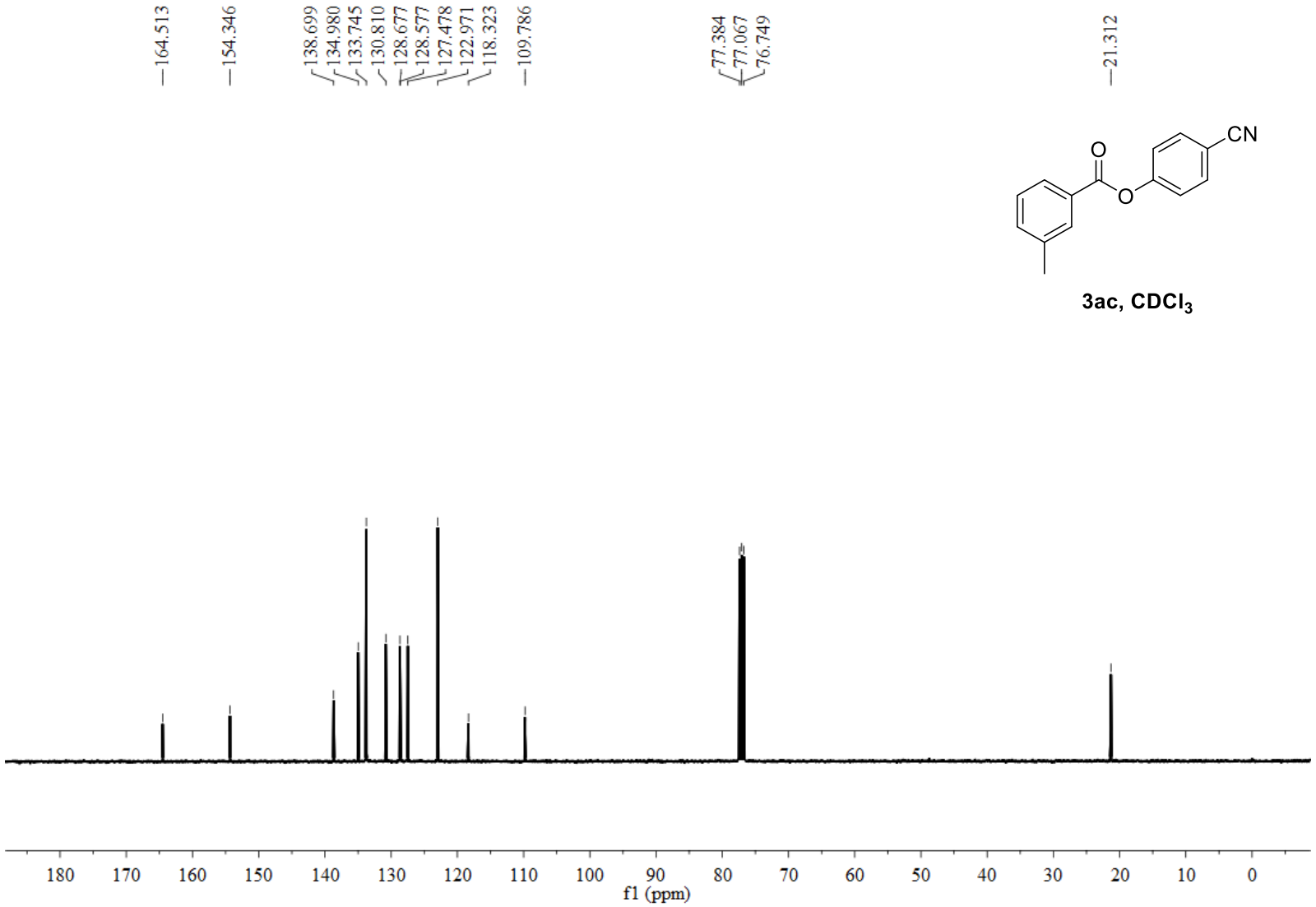
3aa, $CDCl_3$


8.172
8.168
8.151
8.149
7.745
7.740
7.727
7.723
7.539
7.536
7.520
7.501
7.498
7.369
7.364
7.347
7.328
7.260
2.673
0.006
CN
O
O
3ab, CDCl3
1.000
2.010
1.029
4.018
3.098
f1 (ppm)

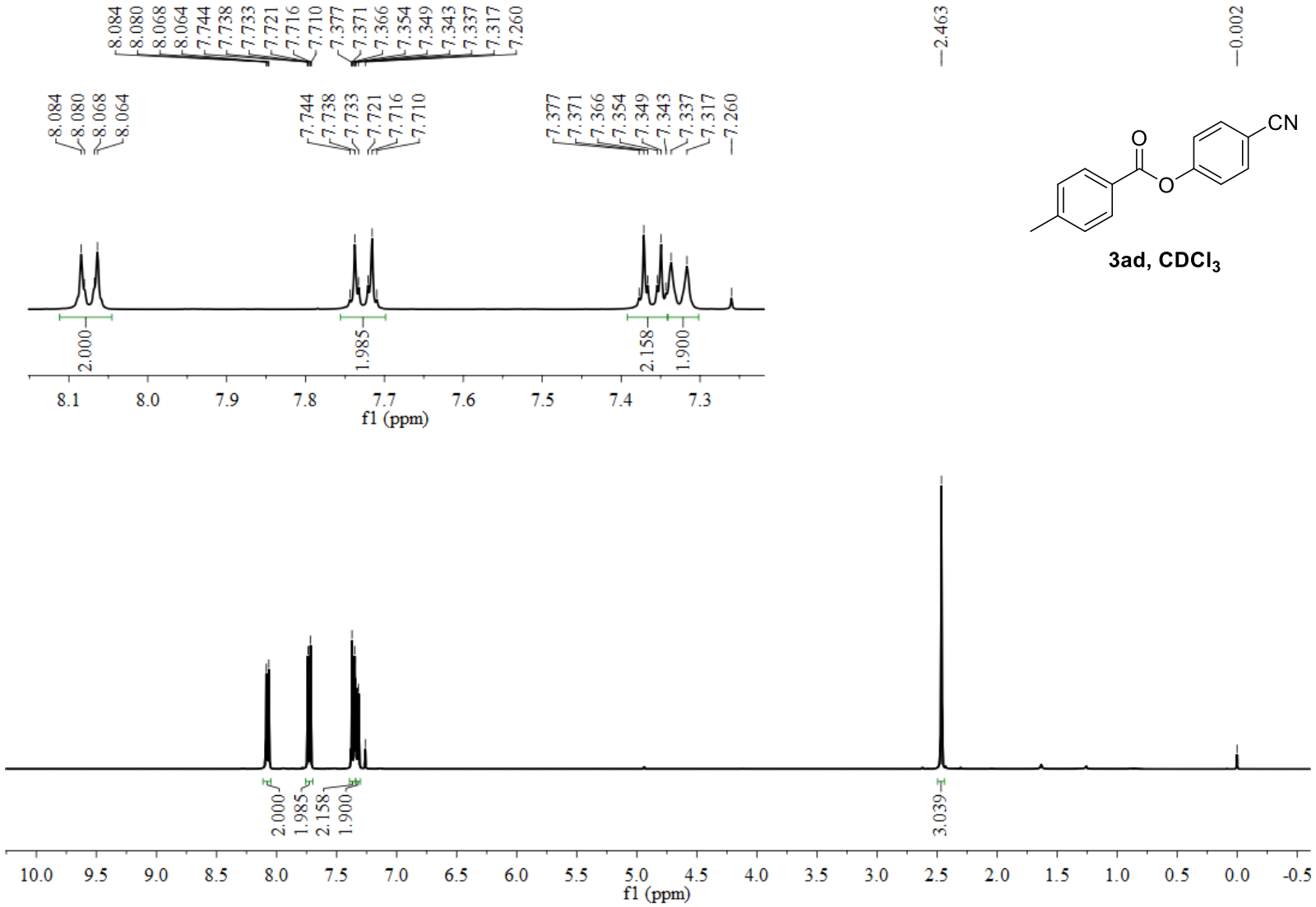

164.736
154.307
141.838
133.730
133.386
132.216
131.319
127.518
126.132
123.090
118.352
109.712
77.467
77.149
76.831
22.021
CN
O
O
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

3ab, $CDCl_3$

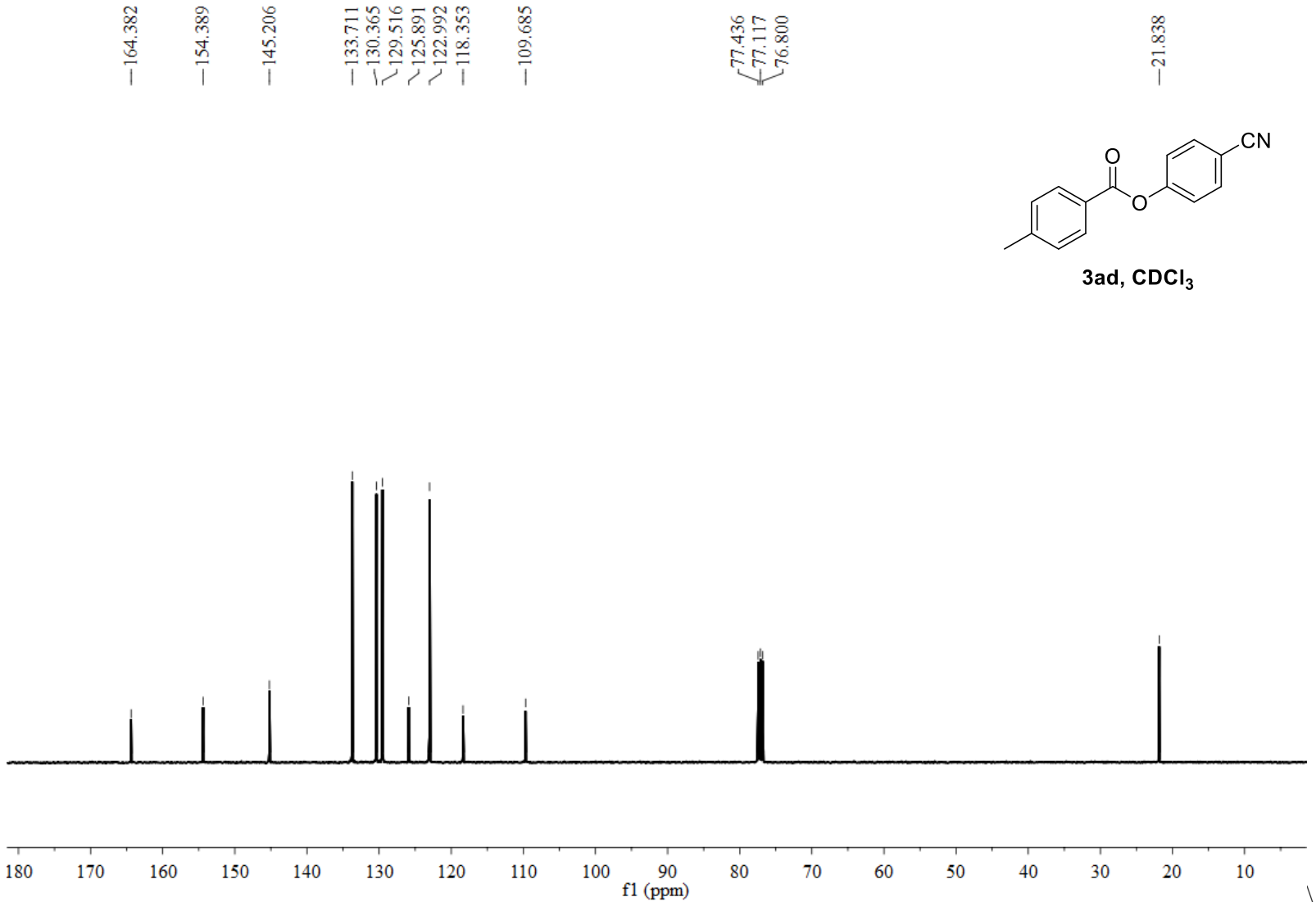

8.001
8.000
7.981
7.757
7.751
7.746
7.734
7.729
7.723
7.492
7.472
7.437
7.417
7.397
7.383
7.377
7.372
7.366
7.360
7.355
7.349
7.260
2.455
0.001
CN
O
O
3ac, CDCl3
1.306
0.548
2.000
1.006
1.097
1.986
3.006
f1 (ppm)


164.513
154.346
138.699
134.980
133.745
130.810
128.677
128.577
127.478
122.971
118.323
109.786
77.384
77.067
76.749
21.312
O
O
CN
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

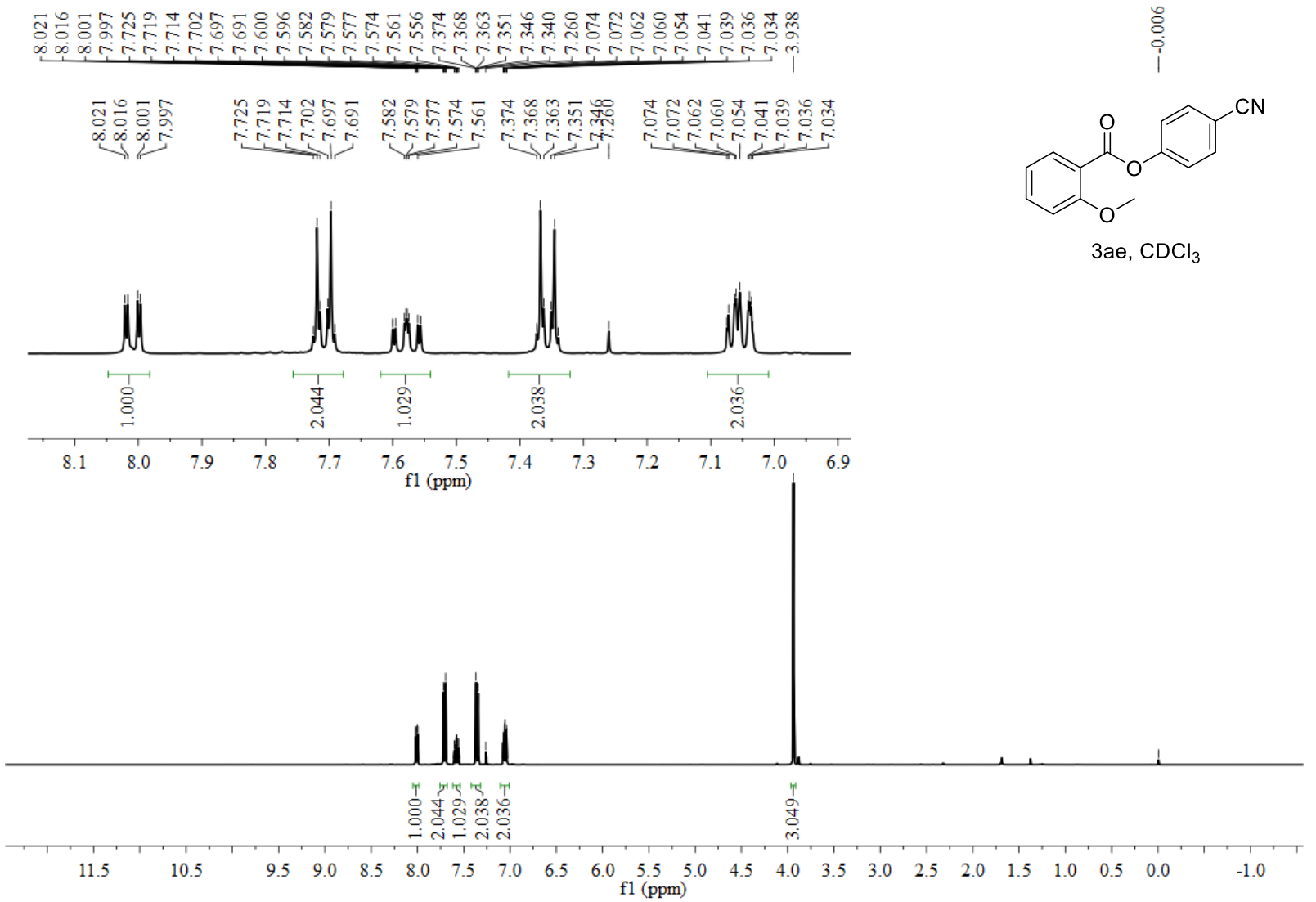
3ac, $CDCl_3$


8.084
8.080
8.068
8.064
7.744
7.738
7.733
7.721
7.716
7.710
7.377
7.371
7.366
7.354
7.349
7.343
7.337
7.317
7.260
2.463
0.002
CN
O
O
2.000
1.985
2.158
1.900
3.039
f1 (ppm)
f1 (ppm)

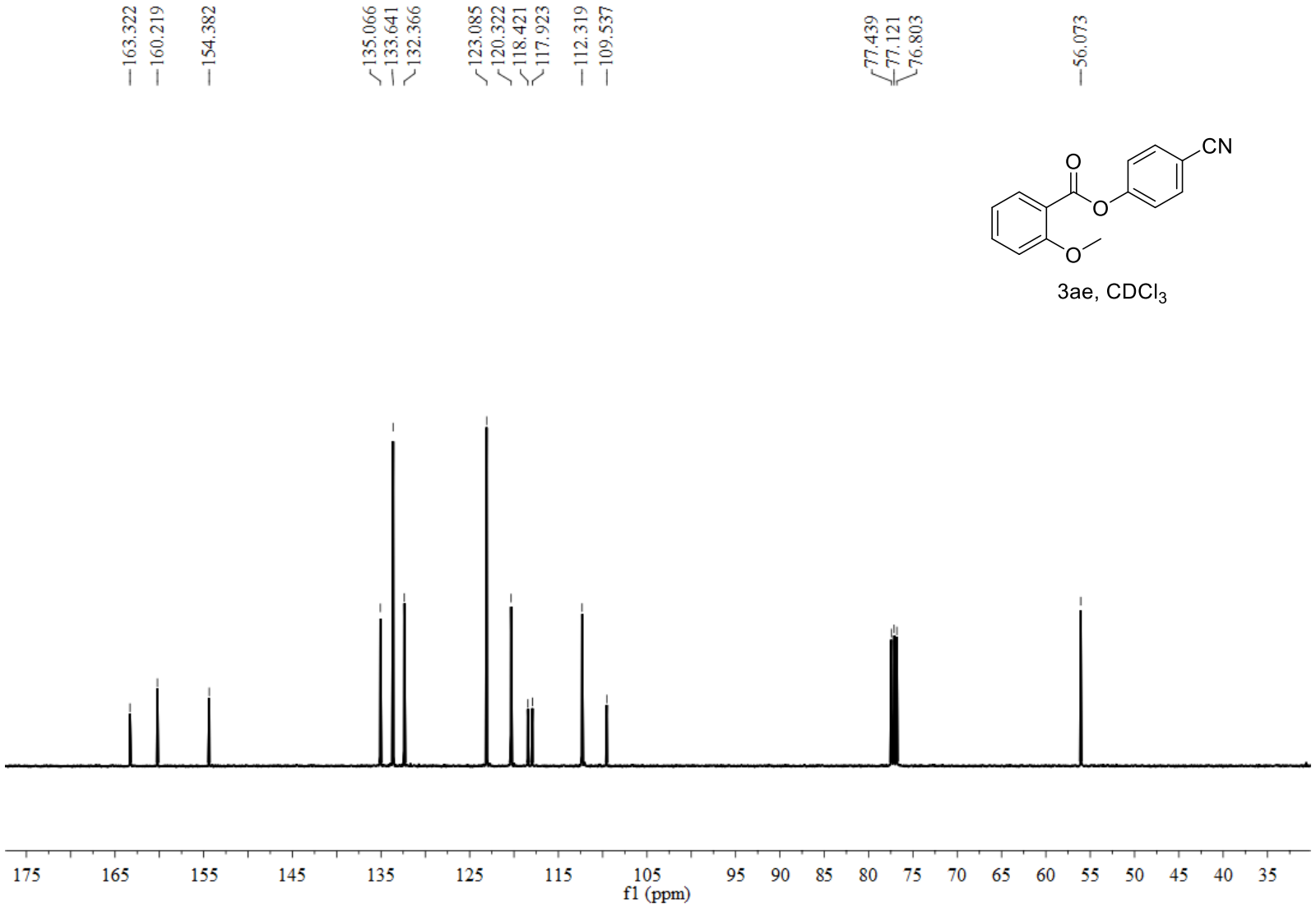
3ad, $CDCl_3$

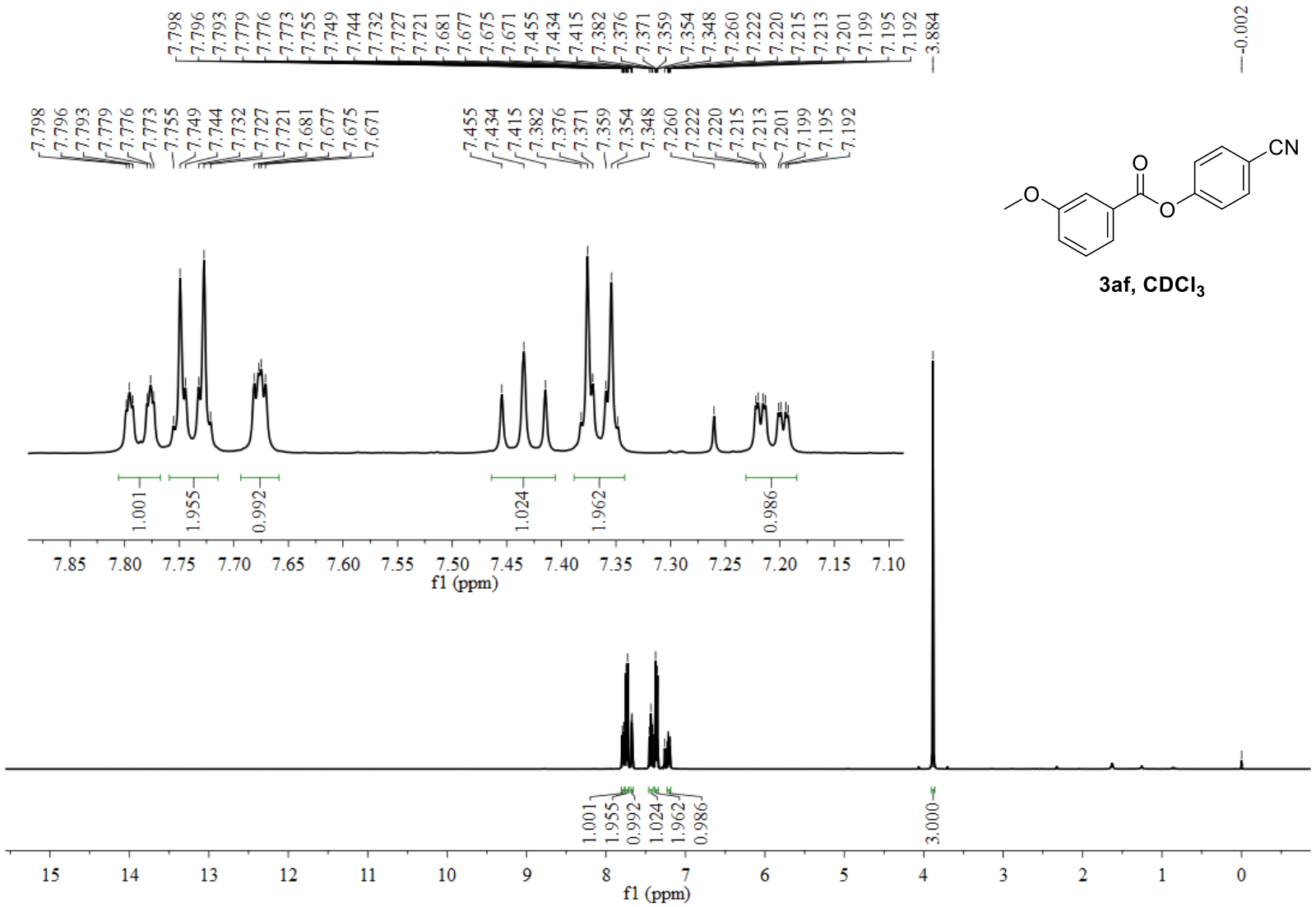

164.382
154.389
145.206
133.711
130.365
129.516
125.891
122.992
118.353
109.685
77.436
77.117
76.800
21.838
O
O
CN
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

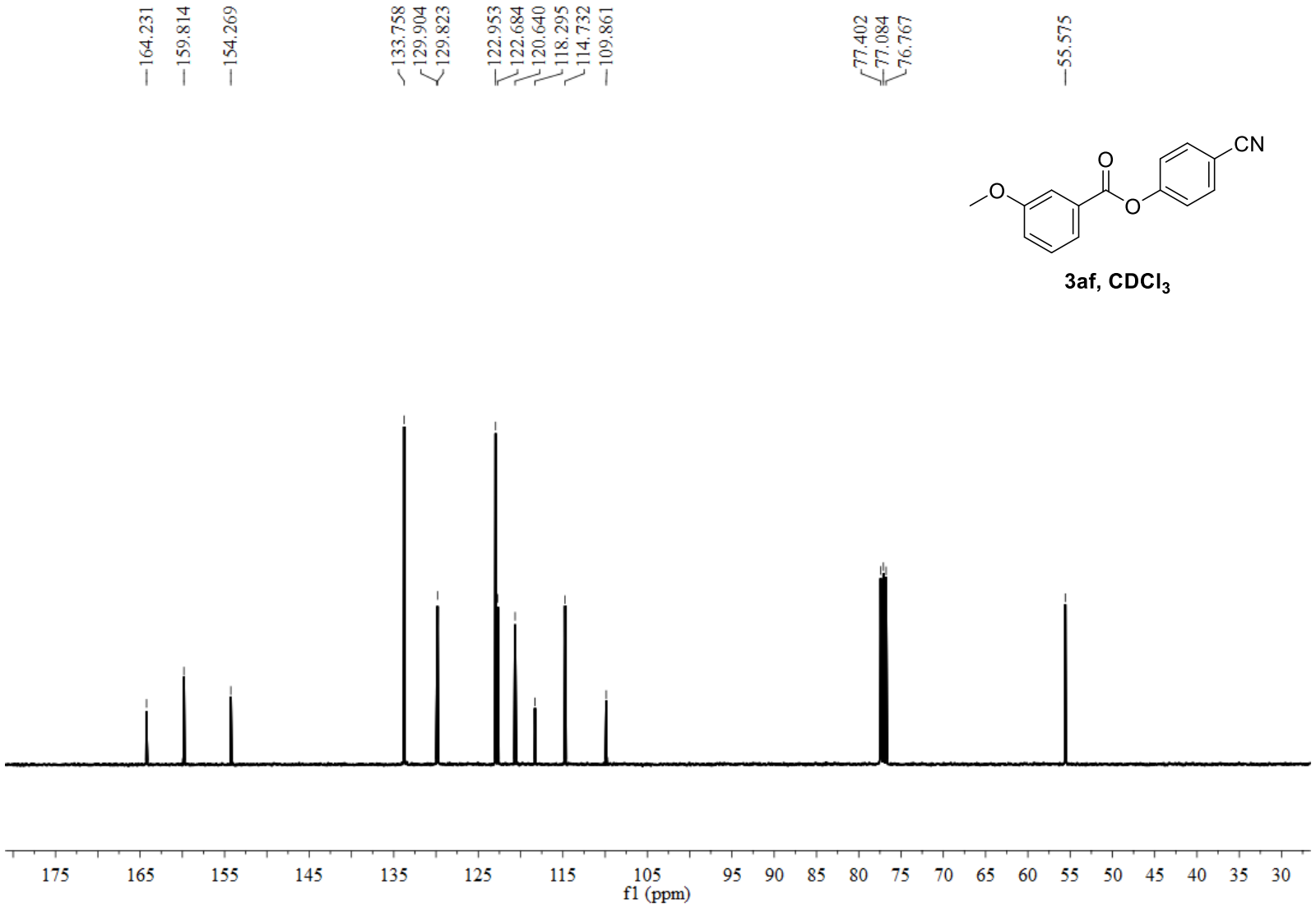
3ad, $CDCl_3$


8.021
8.016
8.001
7.997
7.725
7.719
7.714
7.702
7.697
7.691
7.600
7.596
7.582
7.579
7.577
7.574
7.561
7.556
7.374
7.368
7.363
7.351
7.346
7.340
7.260
7.074
7.072
7.062
7.060
7.054
7.041
7.039
7.036
7.034
3.938
-0.006
O
O
O
CN
1.000
2.044
1.029
2.038
2.036
f1 (ppm)
3.049
f1 (ppm)

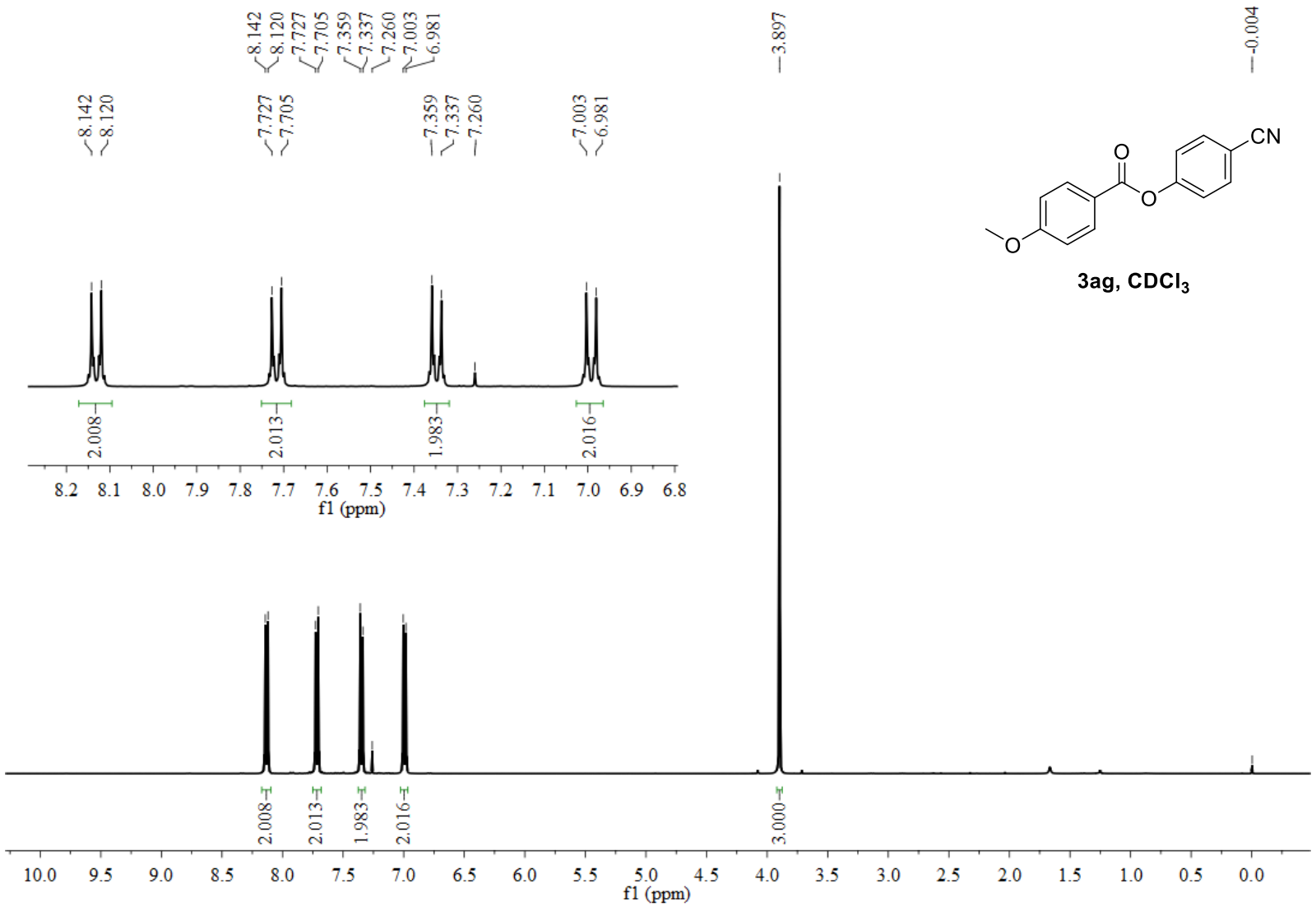
3ae, $CDCl_3$

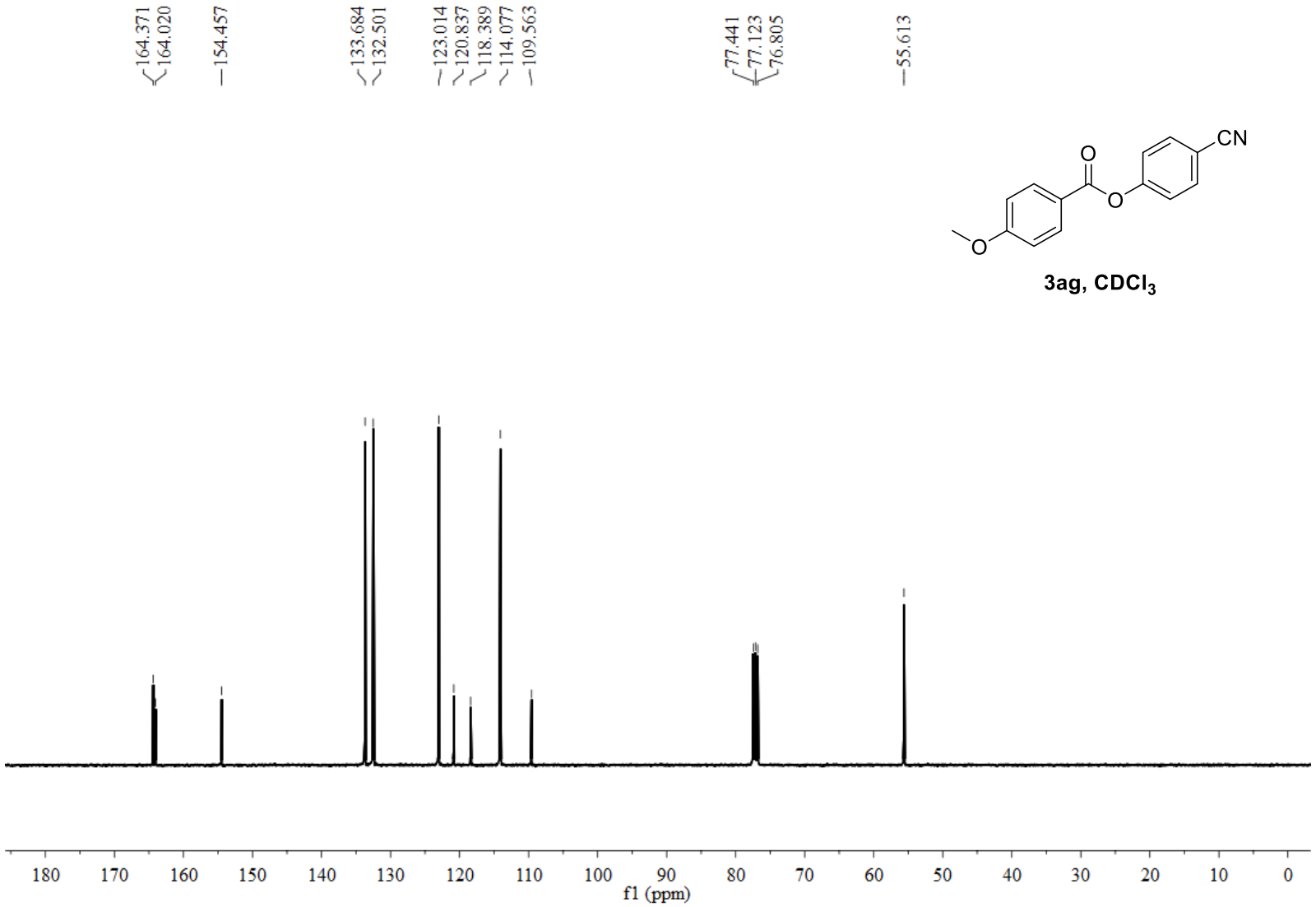

163.322
160.219
154.382
135.066
133.641
132.366
123.085
120.322
118.421
117.923
112.319
109.537
77.439
77.121
76.803
56.073
CN
O
O
O
3ae, CDCl3
175
165
155
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
f1 (ppm)

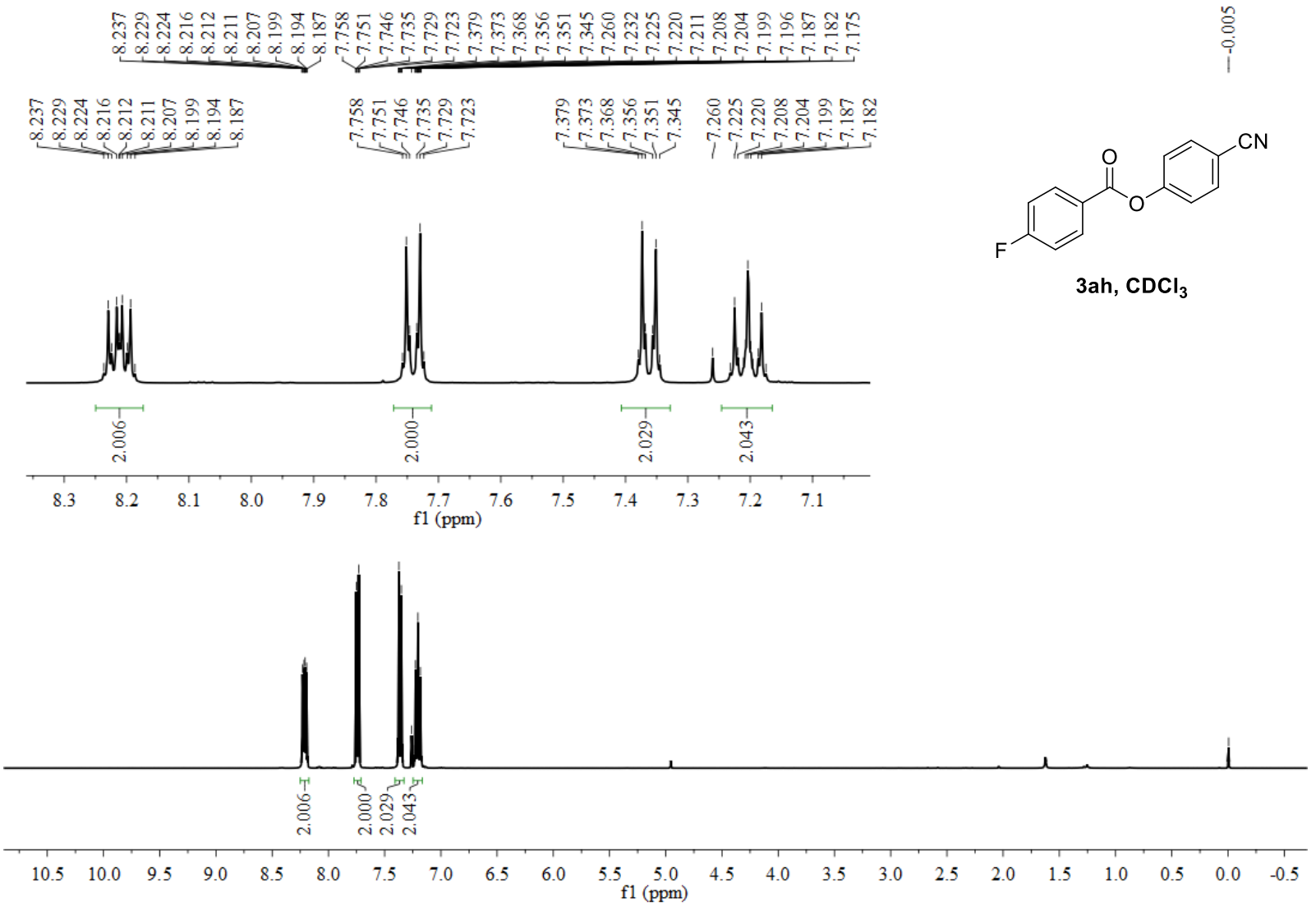

7.798
7.796
7.793
7.779
7.776
7.773
7.755
7.749
7.744
7.732
7.727
7.721
7.681
7.677
7.675
7.671
7.455
7.434
7.415
7.382
7.376
7.371
7.359
7.354
7.348
7.260
7.222
7.220
7.215
7.213
7.201
7.199
7.195
7.192
3.884
0.002
O
O
O
CN
3af, CDCl3
1.001
1.955
0.992
1.024
1.962
0.986
3.000
f1 (ppm)

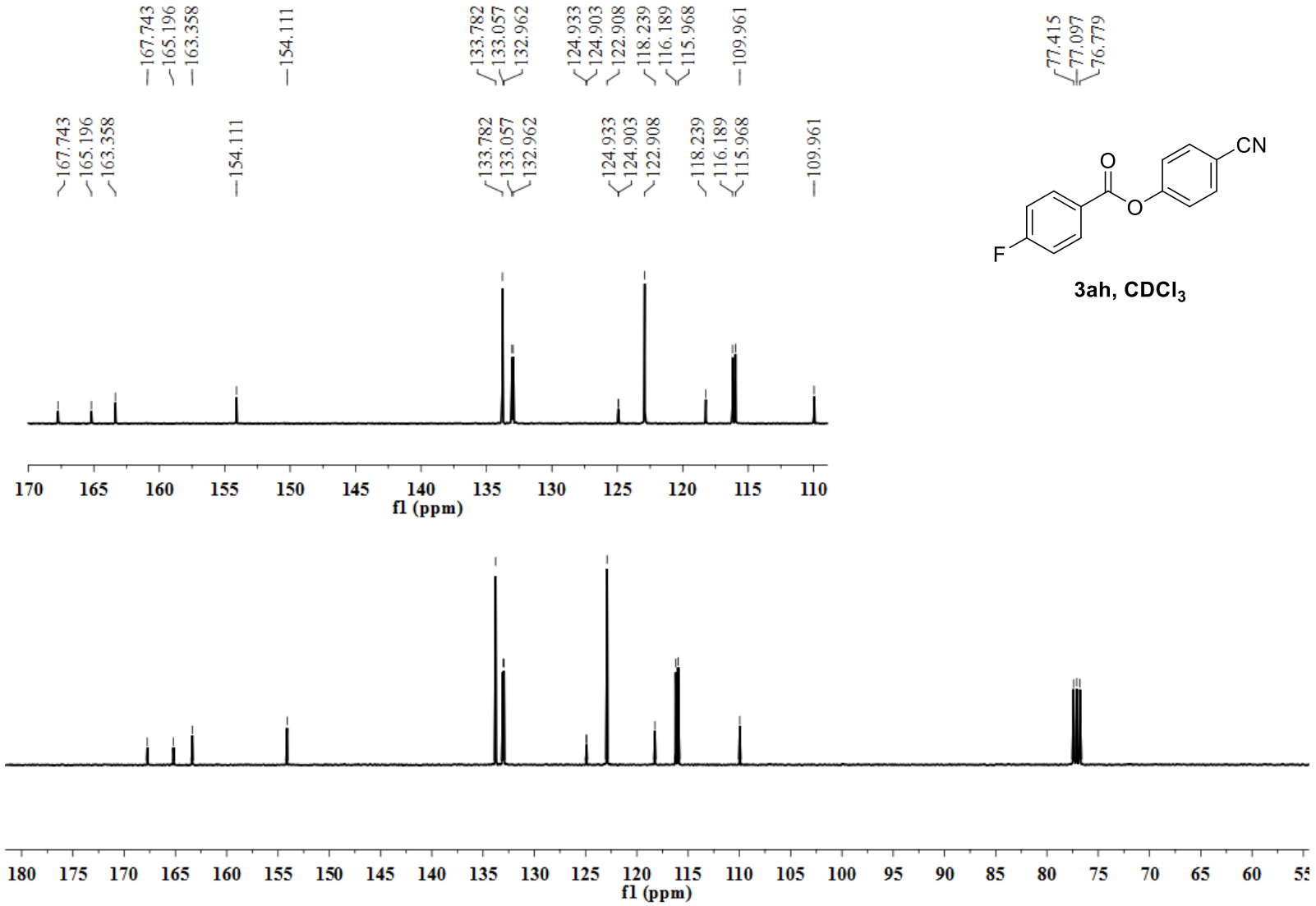

164.231
159.814
154.269
133.758
129.904
129.823
122.953
122.684
120.640
118.295
114.732
109.861
77.402
77.084
76.767
55.575
O
O
O
CN
175
165
155
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
f1 (ppm)

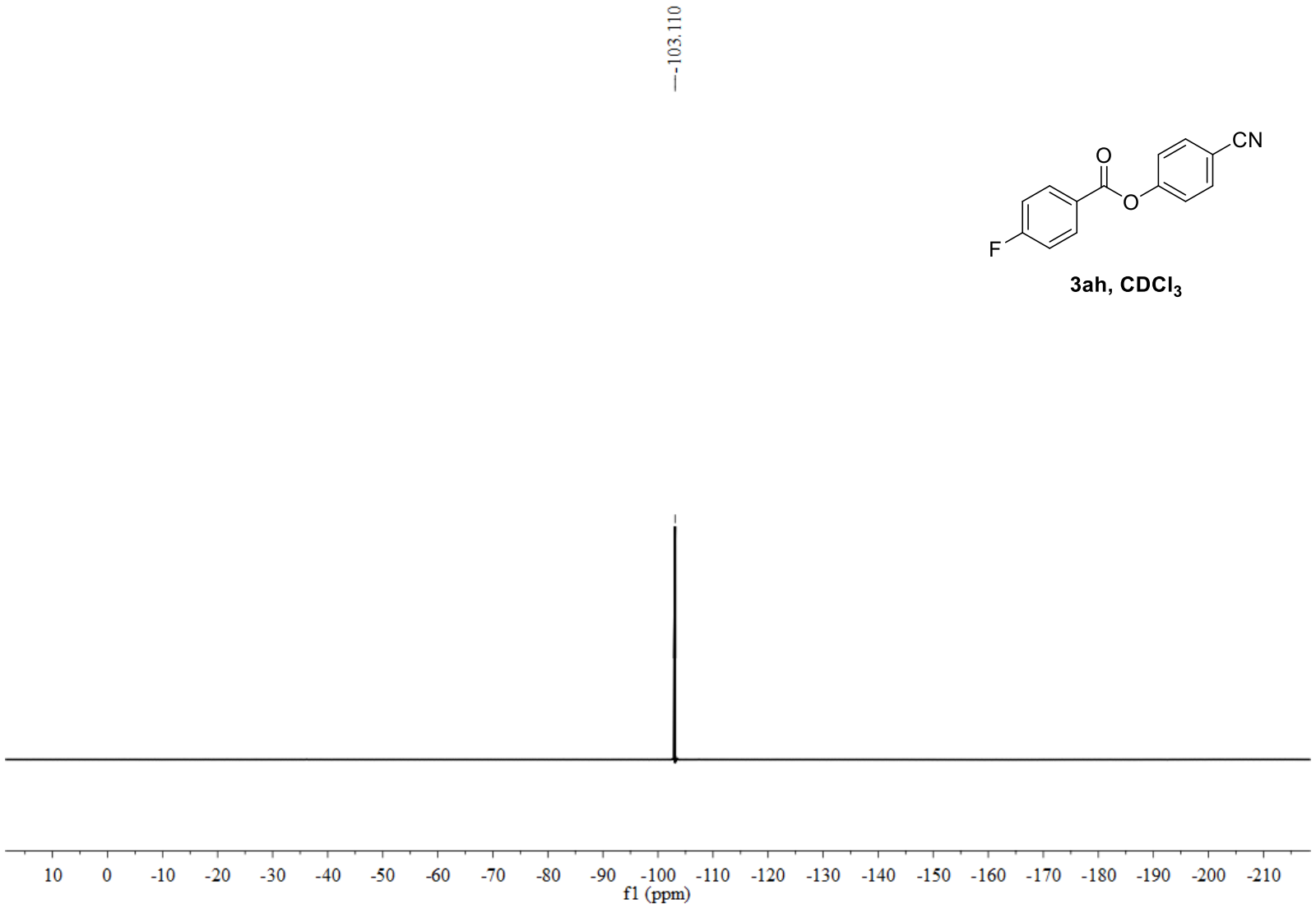
3af, $CDCl_3$


8.142
8.120
7.727
7.705
7.359
7.337
7.260
7.003
6.981
3.897
-0.004
2.008
2.013
1.983
2.016
3.000
f1 (ppm)
CN
O
O
O
3ag, CDCl3

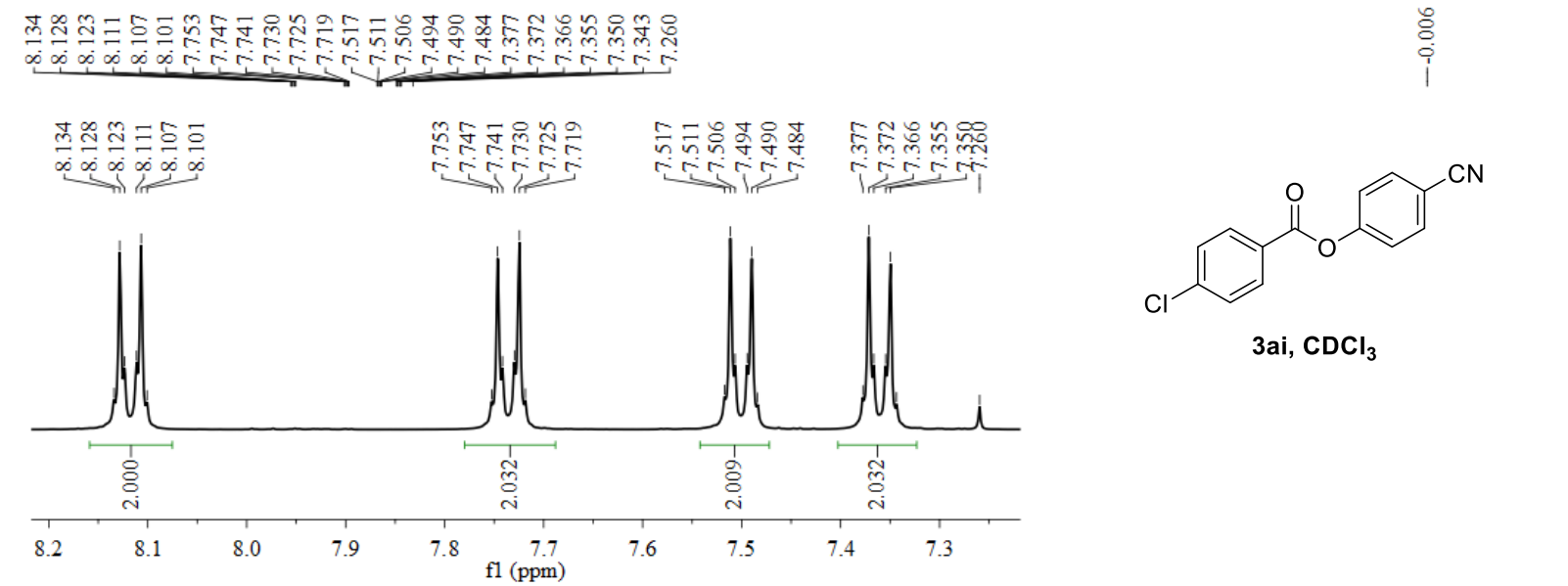

164.371
164.020
154.457
133.684
132.501
123.014
120.837
118.389
114.077
109.563
77.441
77.123
76.805
55.613
O
O
O
CN
3ag, CDCl3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

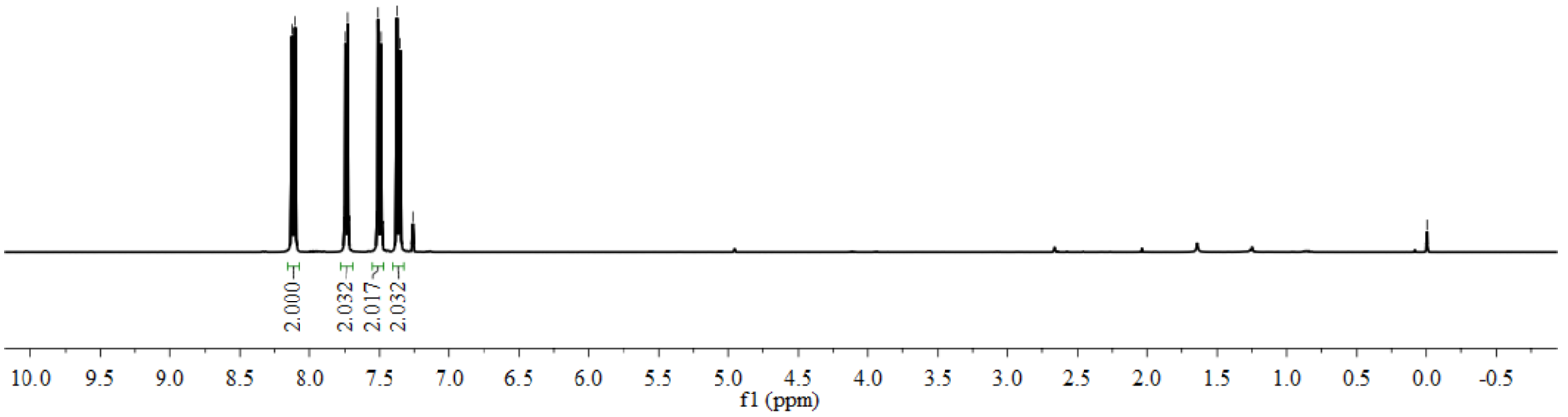

8.237
8.229
8.224
8.216
8.212
8.211
8.207
8.199
8.194
8.187
7.758
7.751
7.746
7.735
7.729
7.723
7.379
7.373
7.368
7.356
7.351
7.345
7.260
7.232
7.225
7.220
7.211
7.208
7.204
7.199
7.196
7.187
7.182
7.175
-0.005
2.006
2.000
2.029
2.043
f1 (ppm)
O
O
CN
F
3ah, CDCl3

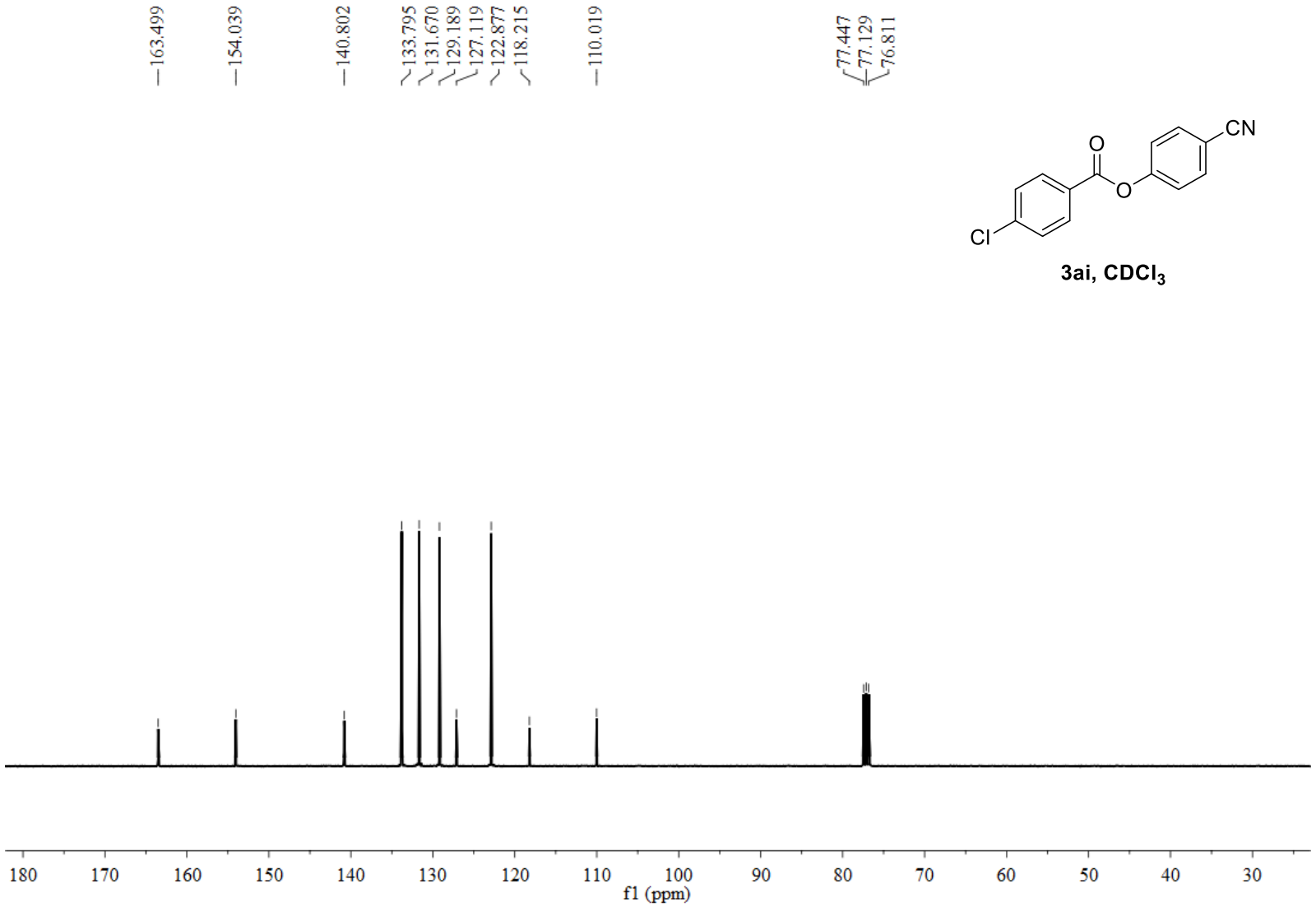

167.743
165.196
163.358
154.111
133.782
133.057
132.962
124.933
124.903
122.908
118.239
116.189
115.968
109.961
77.415
77.097
76.779
O
O
CN
F
3ah, CDCl3
fl (ppm)
fl (ppm)

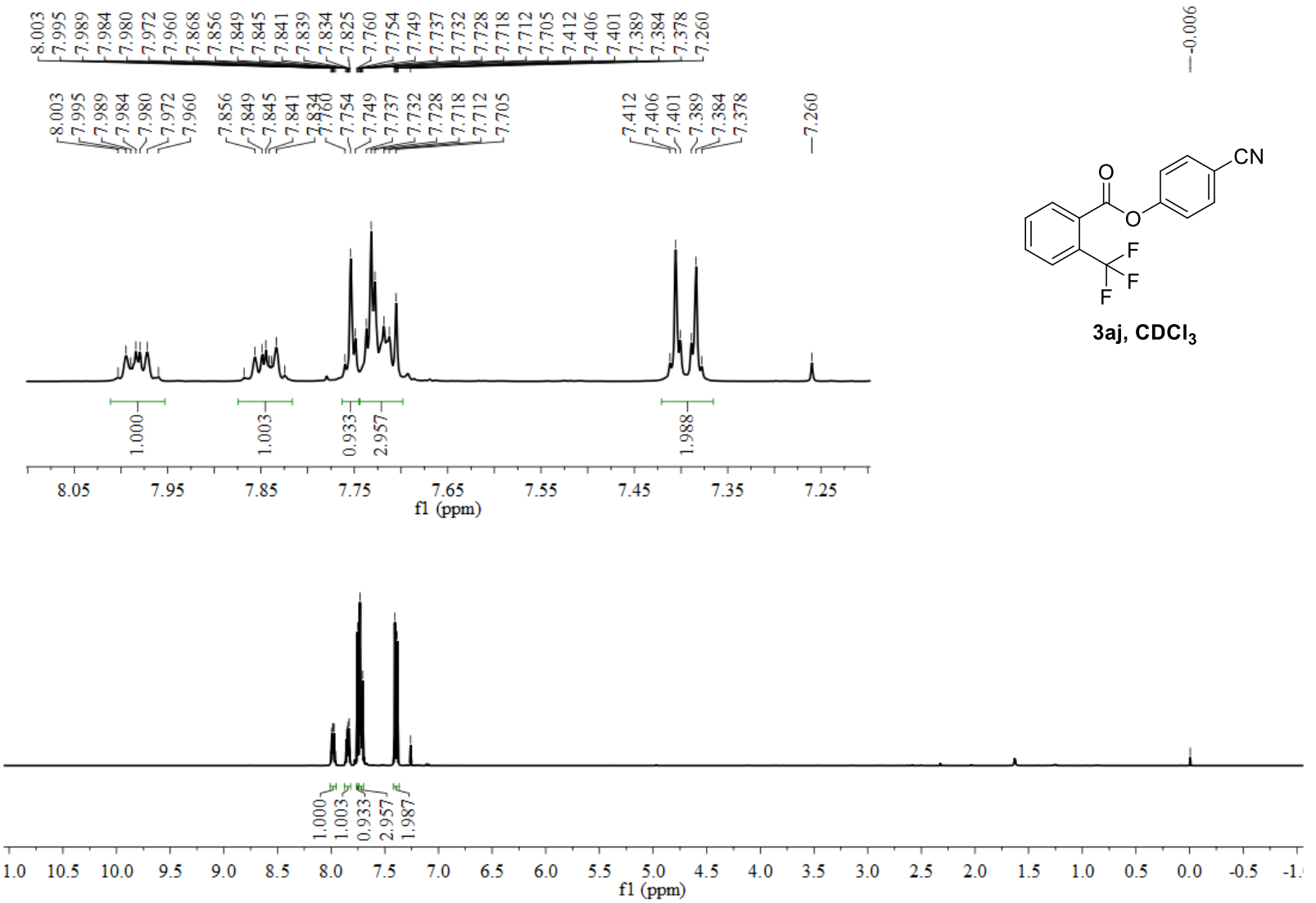

-103.110
CN
O
O
F
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

3ah, $CDCl_3$

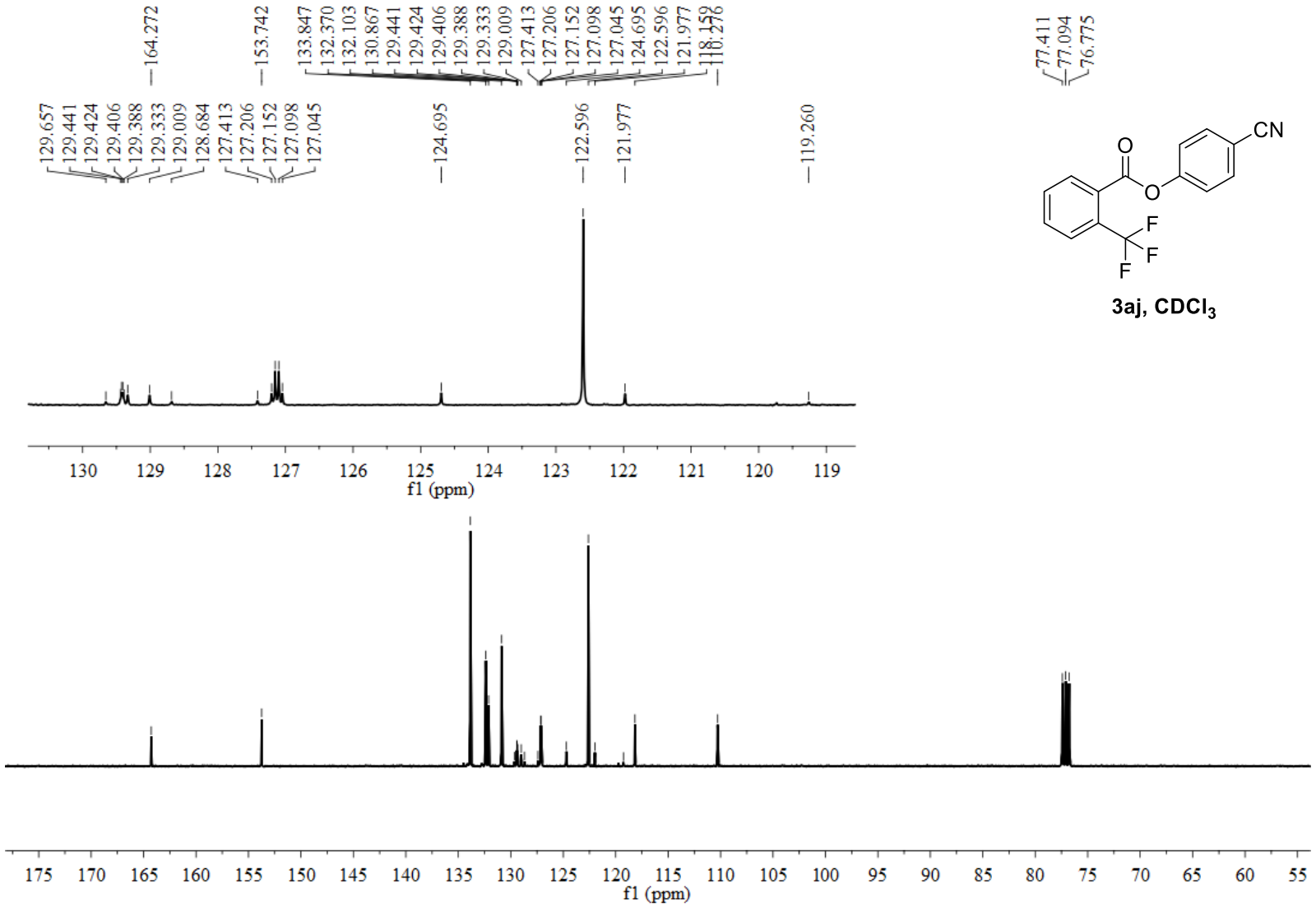

8.134
8.128
8.123
8.111
8.107
8.101
7.753
7.747
7.741
7.730
7.725
7.719
7.517
7.511
7.506
7.494
7.490
7.484
7.377
7.372
7.366
7.355
7.350
7.343
7.260
-0.006
2.000
2.032
2.009
2.032
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
f1 (ppm)
O
O
CN
Cl
3ai, CDCl3

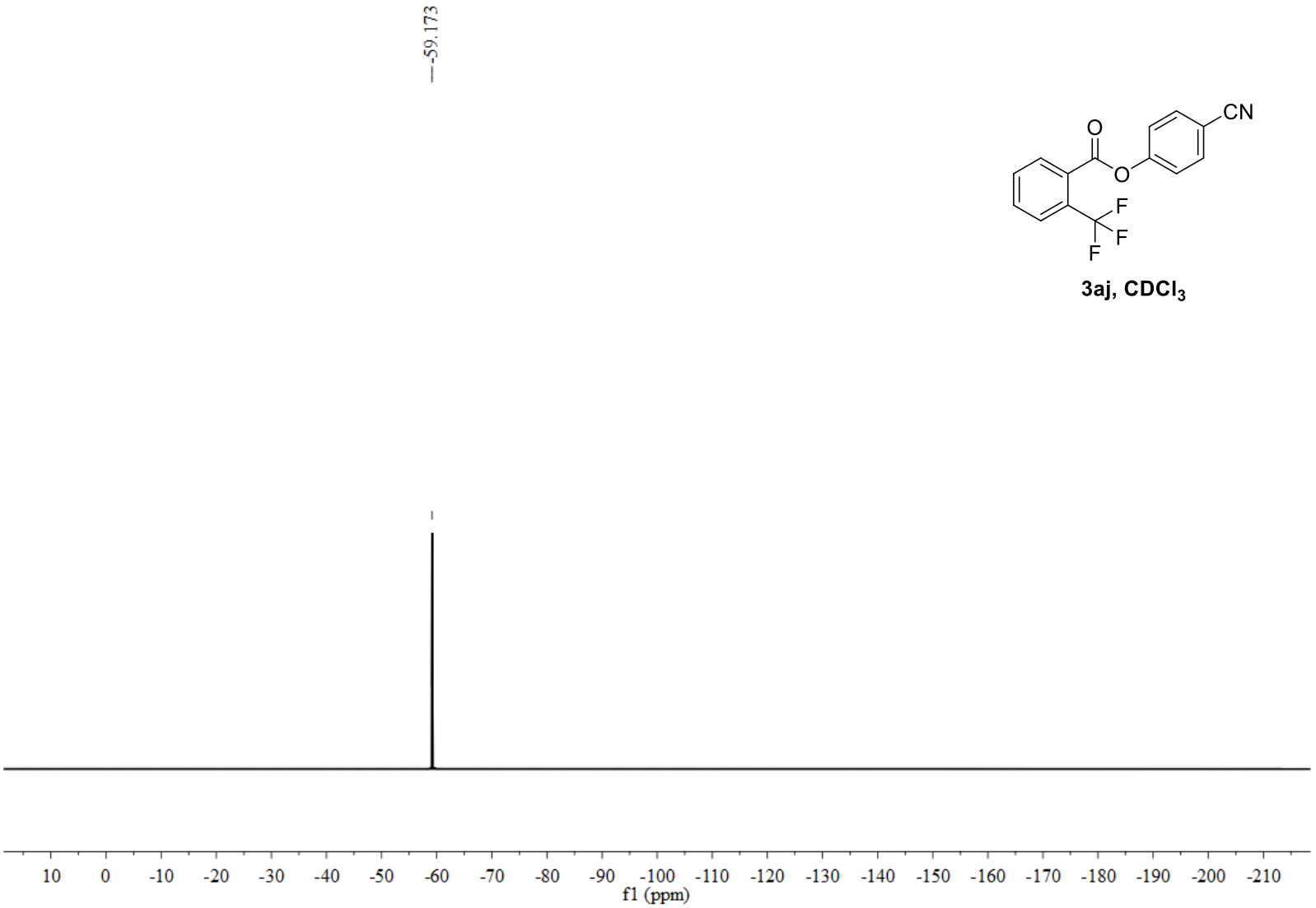

2.000
2.032
2.017
2.032
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


163.499
154.039
140.802
133.795
131.670
129.189
127.119
122.877
118.215
110.019
77.447
77.129
76.811
O
O
CN
Cl
3ai, CDCl3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
f1 (ppm)

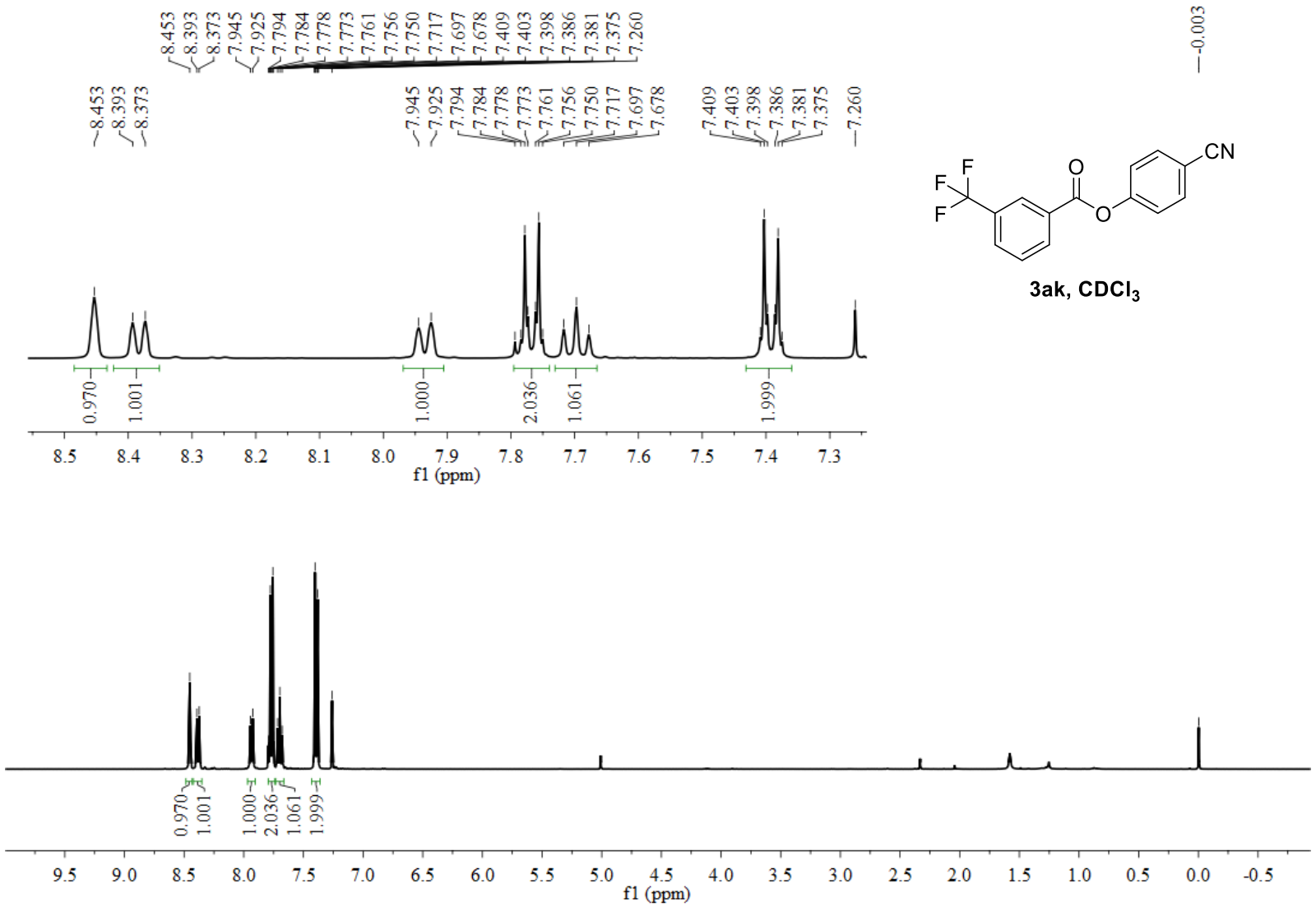

8.003
7.995
7.989
7.984
7.980
7.972
7.960
7.868
7.856
7.849
7.845
7.841
7.839
7.834
7.825
7.760
7.754
7.749
7.737
7.732
7.728
7.718
7.712
7.705
7.412
7.406
7.401
7.389
7.384
7.378
7.260
-0.006
1.000
1.003
0.933
2.957
1.988
8.05
7.95
7.85
7.75
7.65
7.55
7.45
7.35
7.25
f1 (ppm)
1.000
1.003
0.933
2.957
1.987
1.0
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)
O
O
CN
F
F
F

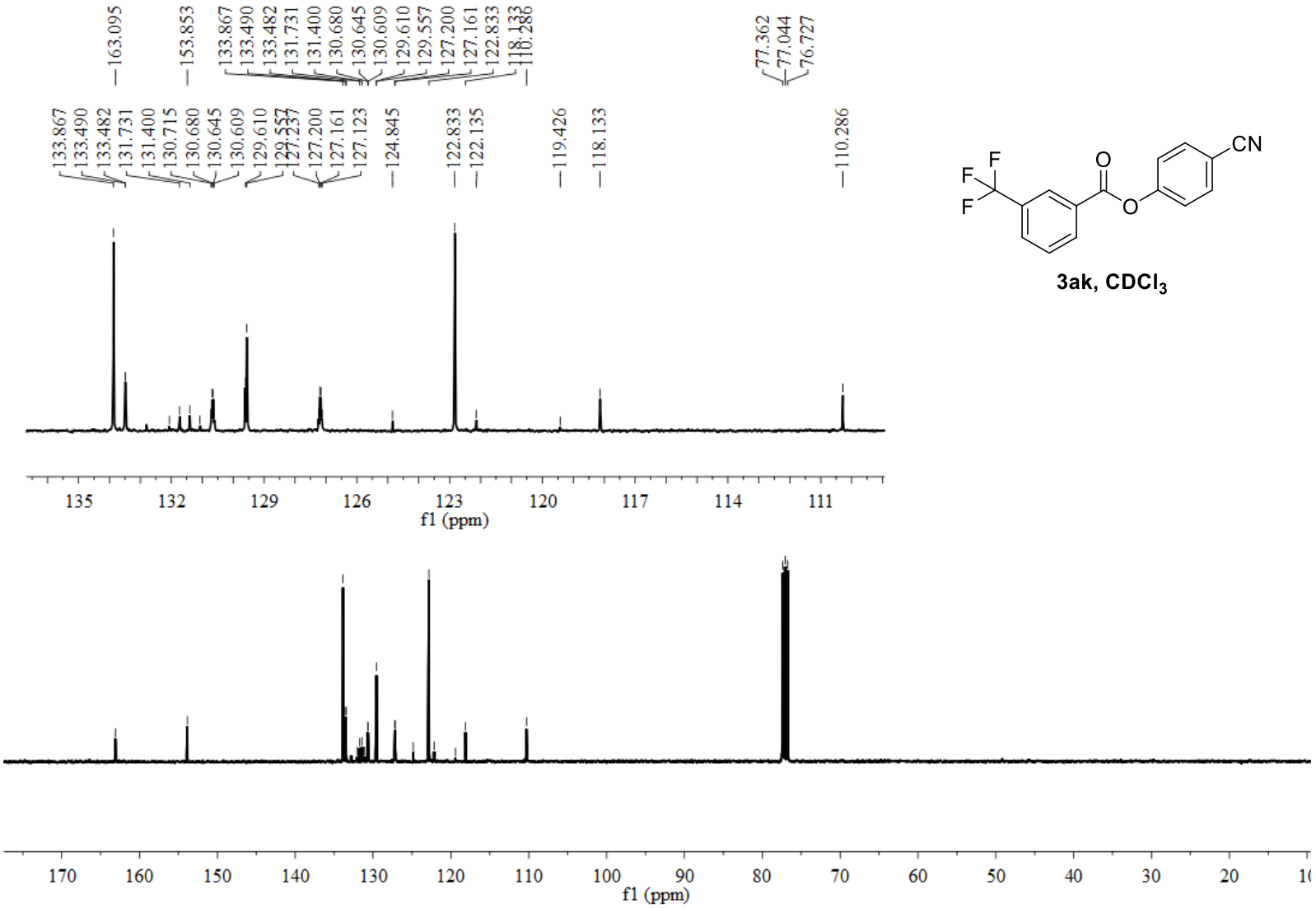
3aj, $CDCl_3$


164.272
153.742
133.847
132.370
132.103
130.867
129.441
129.424
129.406
129.388
129.333
129.009
127.413
127.206
127.152
127.098
127.045
124.695
122.596
121.977
119.260
77.411
77.094
76.775
129.657
129.441
129.424
129.406
129.388
129.333
129.009
128.684
127.413
127.206
127.152
127.098
127.045
CN
O
O
F
F
F
3aj, CDCl3
f1 (ppm)
f1 (ppm)


-59.173
CN
O
O
F
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)

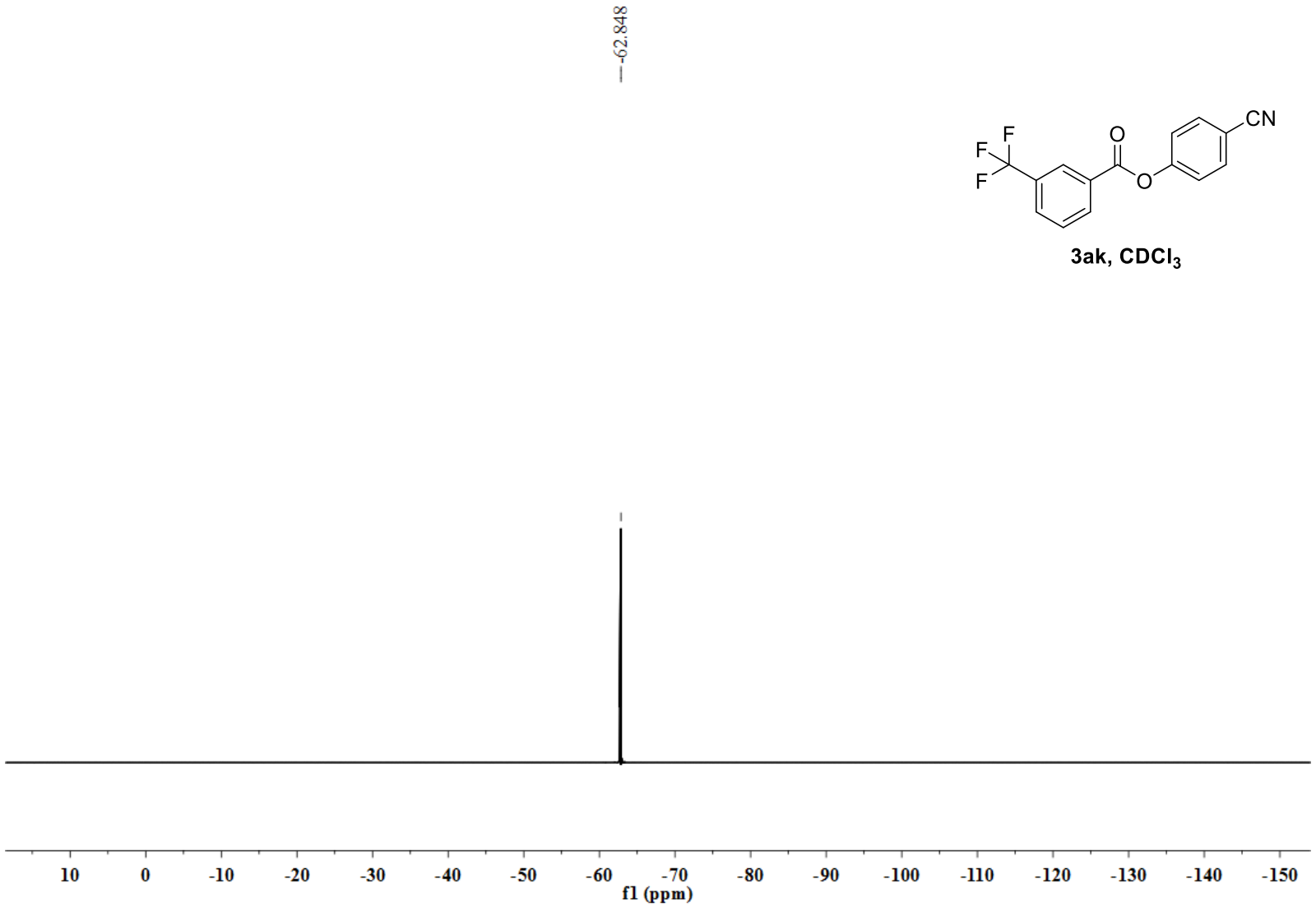
3aj, $CDCl_3$


8.453
8.393
8.373
7.945
7.925
7.794
7.784
7.778
7.773
7.761
7.756
7.750
7.717
7.697
7.678
7.409
7.403
7.398
7.386
7.381
7.375
7.260
-0.003
0.970
1.001
1.000
2.036
1.061
1.999
f1 (ppm)
F
F
F
O
O
CN
3ak, CDCl3

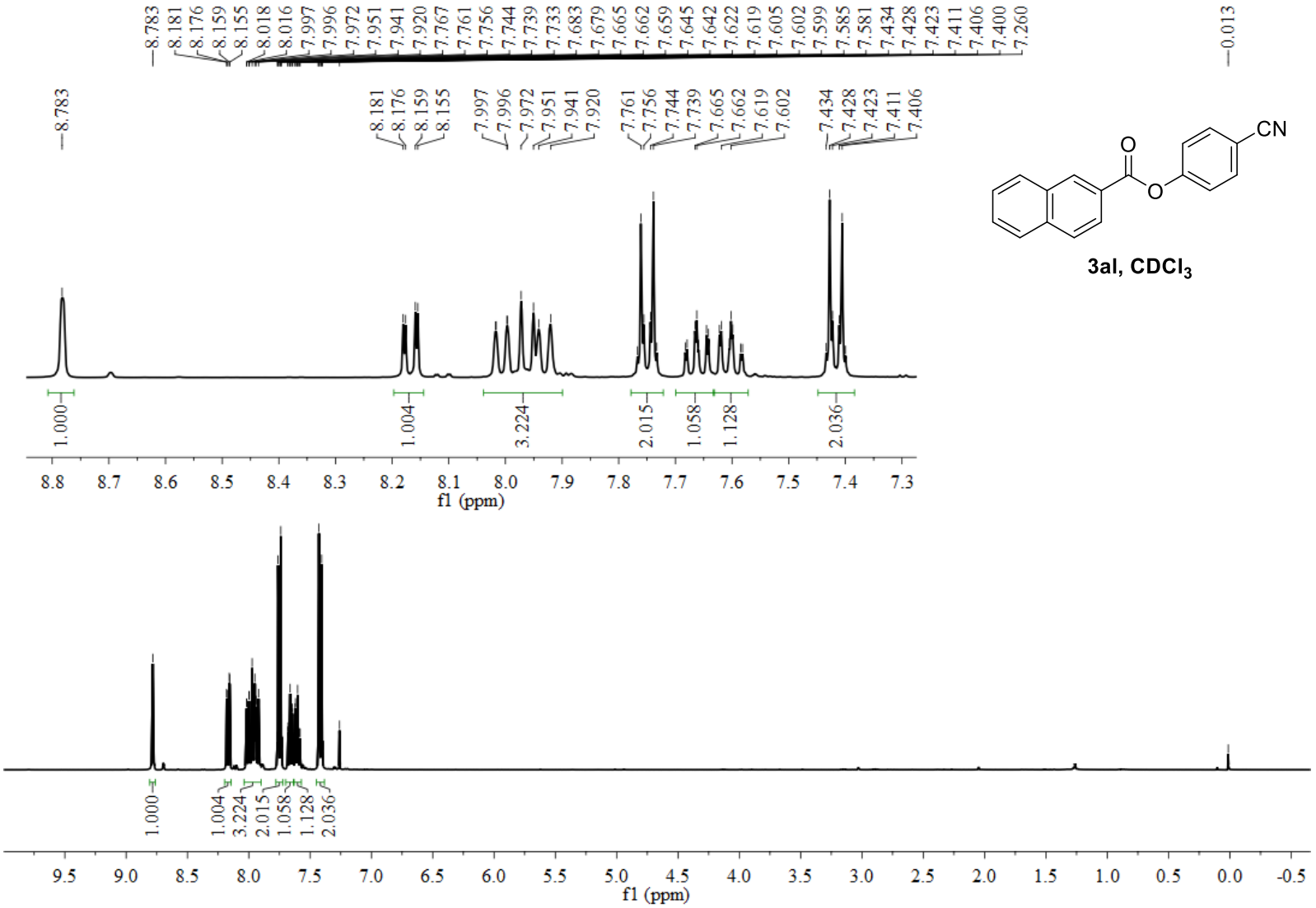

163.095
153.853
133.867
133.490
133.482
131.731
131.400
130.680
130.645
130.609
129.610
129.557
127.200
127.161
122.833
118.133
110.286
77.362
77.044
76.727
124.845
119.426
f1 (ppm)
f1 (ppm)

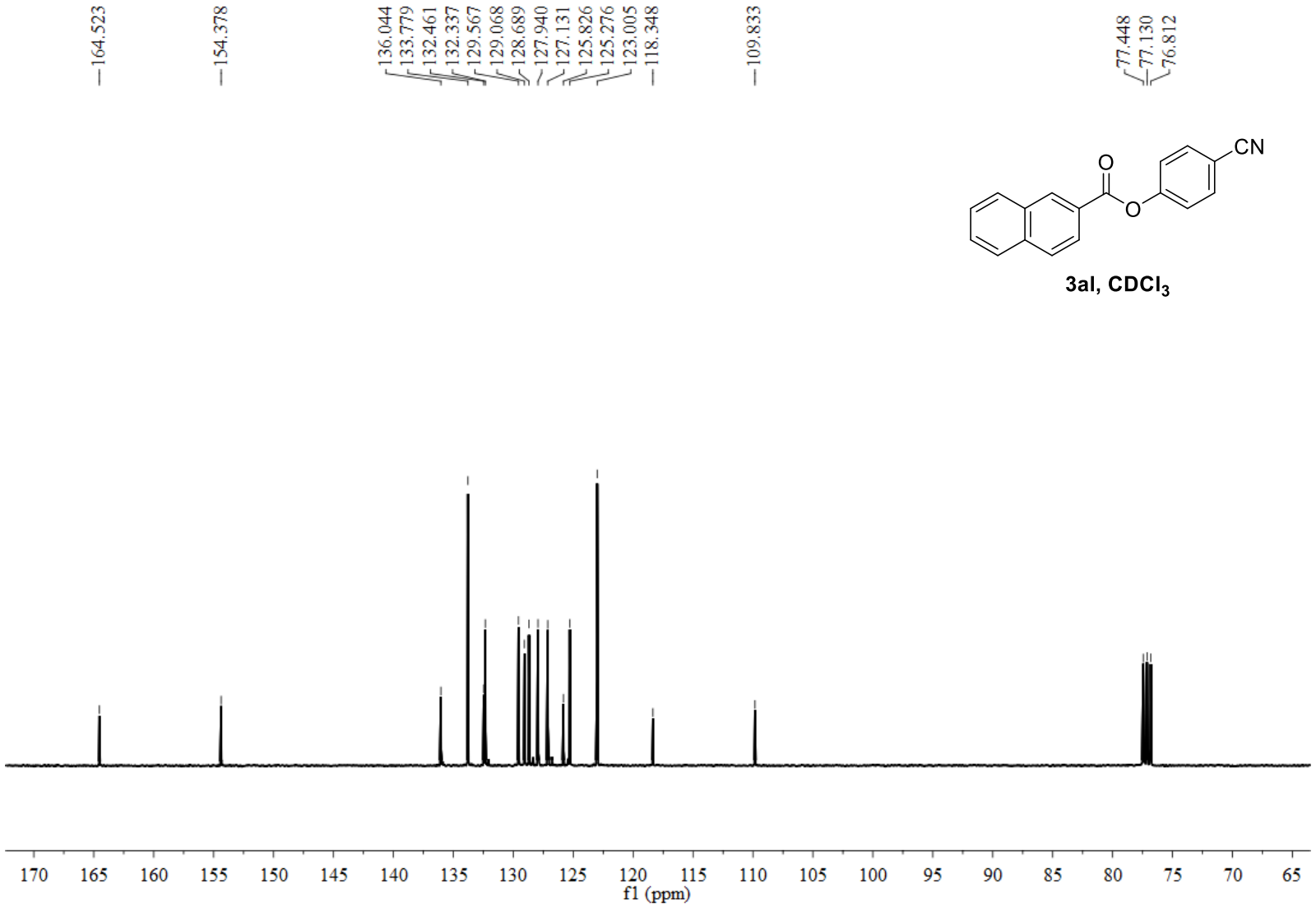
F
F
F
O
O
CN

3ak, $CDCl_3$

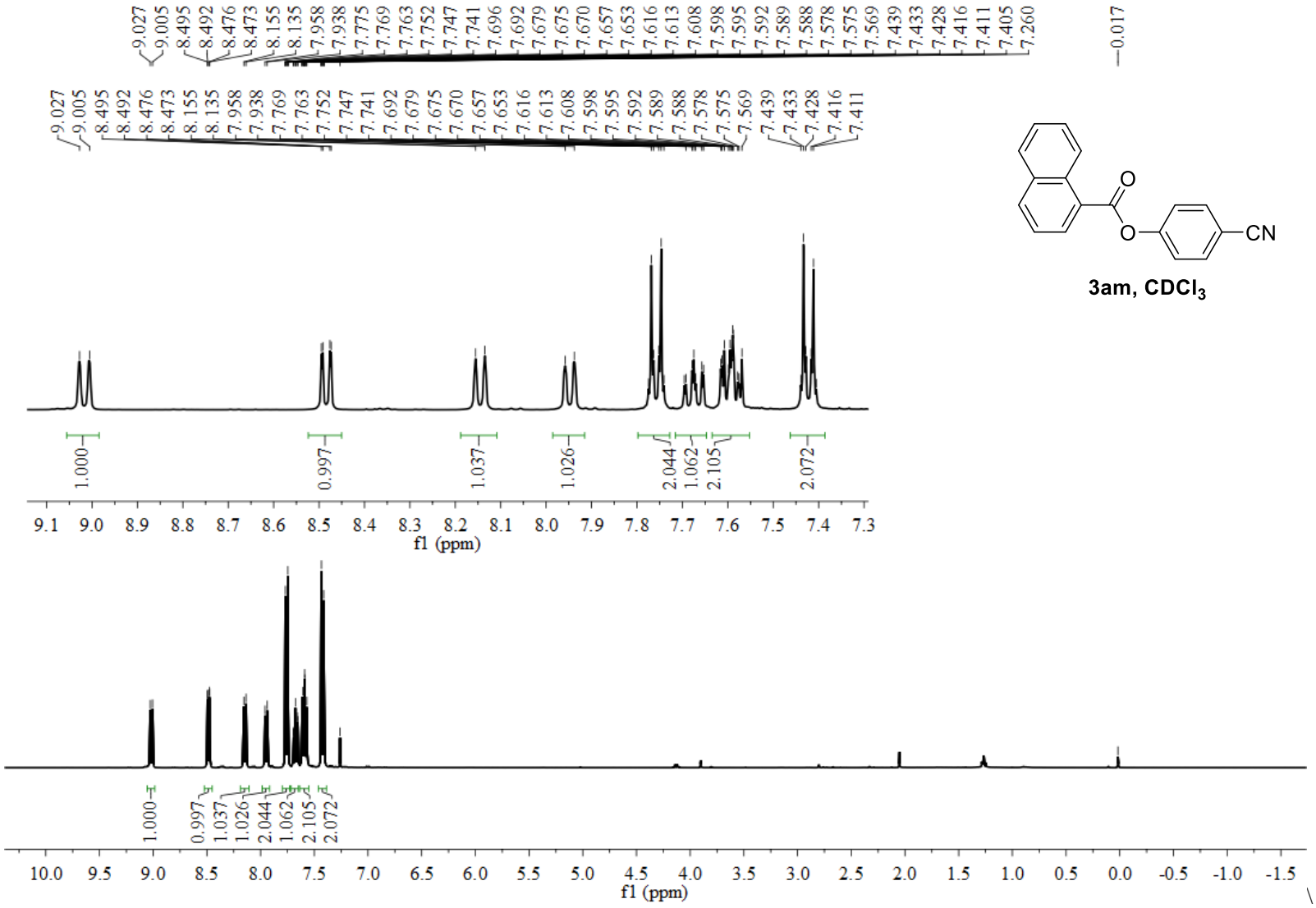

-62.848
F
F
F
O
O
CN
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
f1 (ppm)

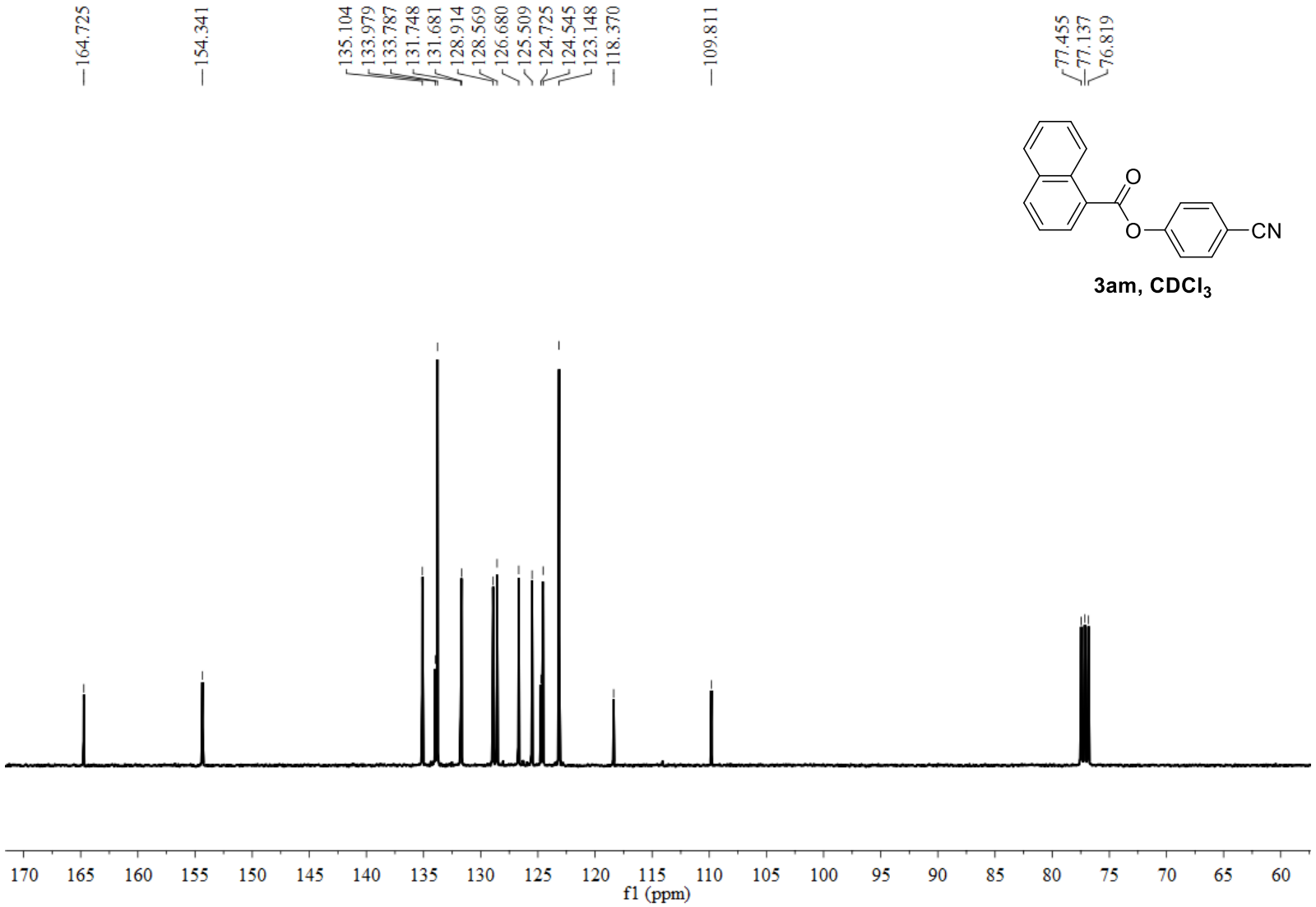
3ak, $CDCl_3$

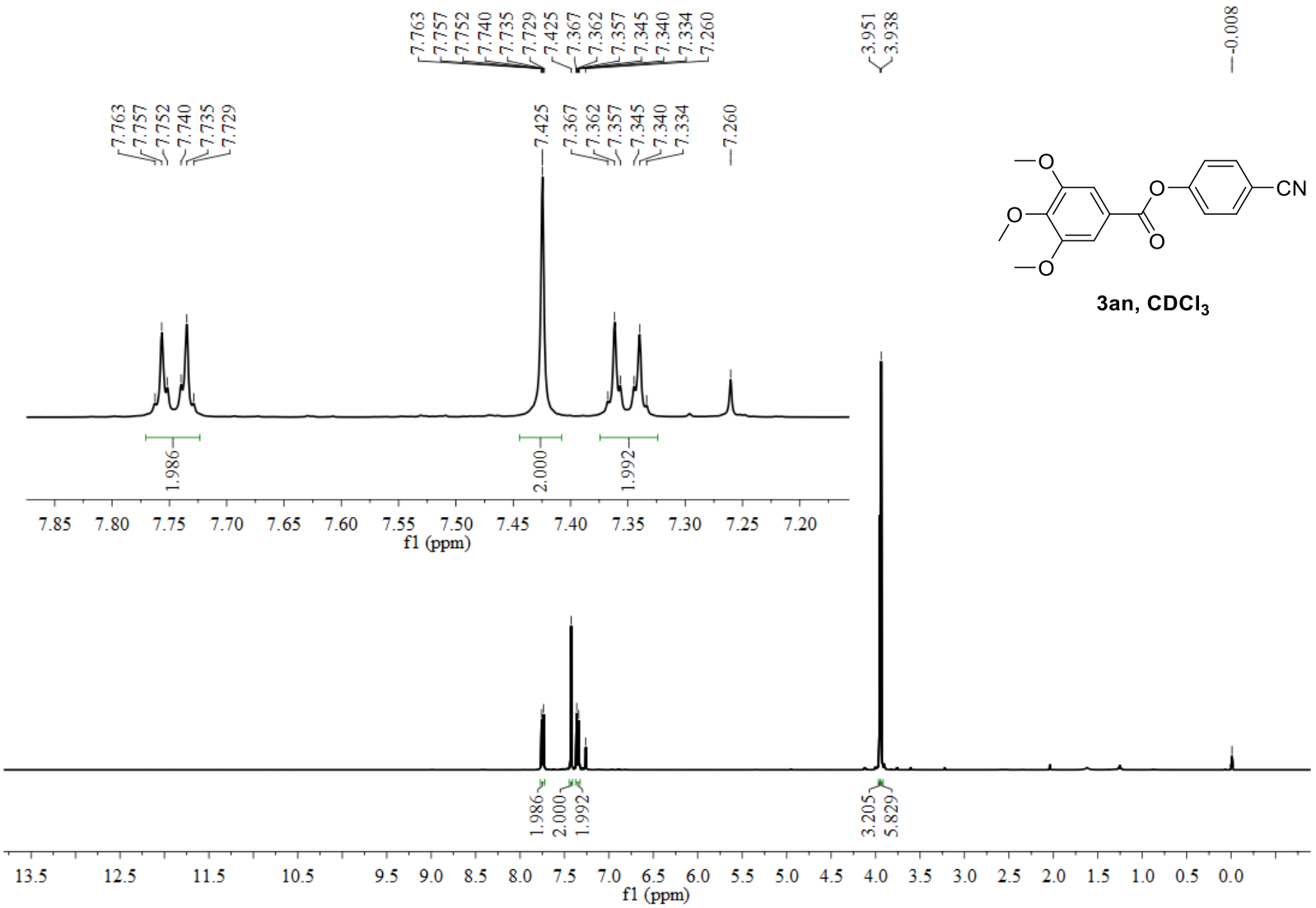

8.783
8.181
8.176
8.159
8.155
8.018
8.016
7.997
7.996
7.972
7.951
7.941
7.920
7.767
7.761
7.756
7.744
7.739
7.733
7.683
7.679
7.665
7.662
7.659
7.645
7.642
7.622
7.619
7.605
7.602
7.599
7.585
7.581
7.434
7.428
7.423
7.411
7.406
7.400
7.260
0.013
1.000
1.004
3.224
2.015
1.058
1.128
2.036
f1 (ppm)
O
O
CN
3al, CDCl3

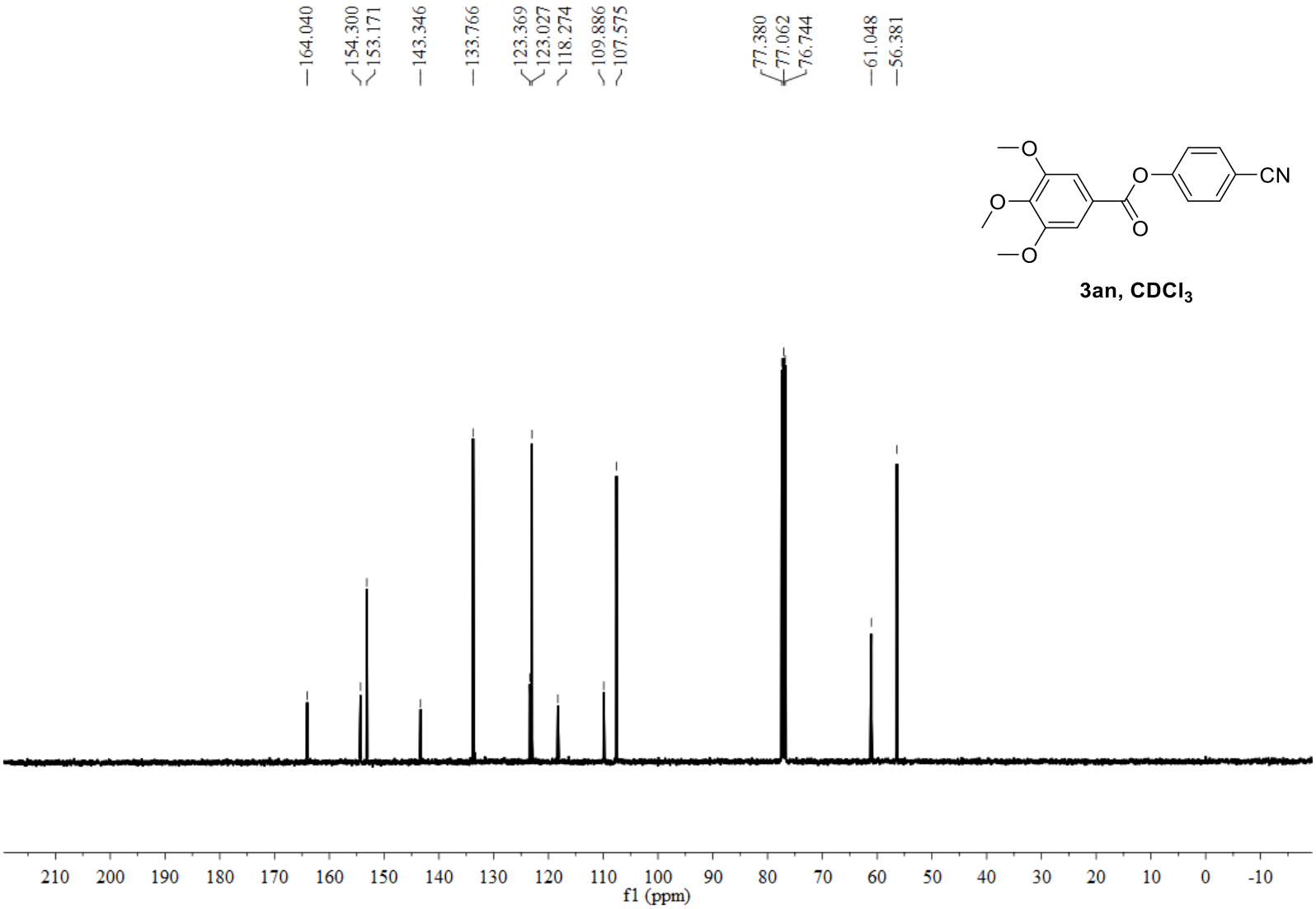

164.523
154.378
136.044
133.779
132.461
132.337
129.567
129.068
128.689
127.940
127.131
125.826
125.276
123.005
118.348
109.833
77.448
77.130
76.812
O
O
CN
170
165
160
155
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
f1 (ppm)

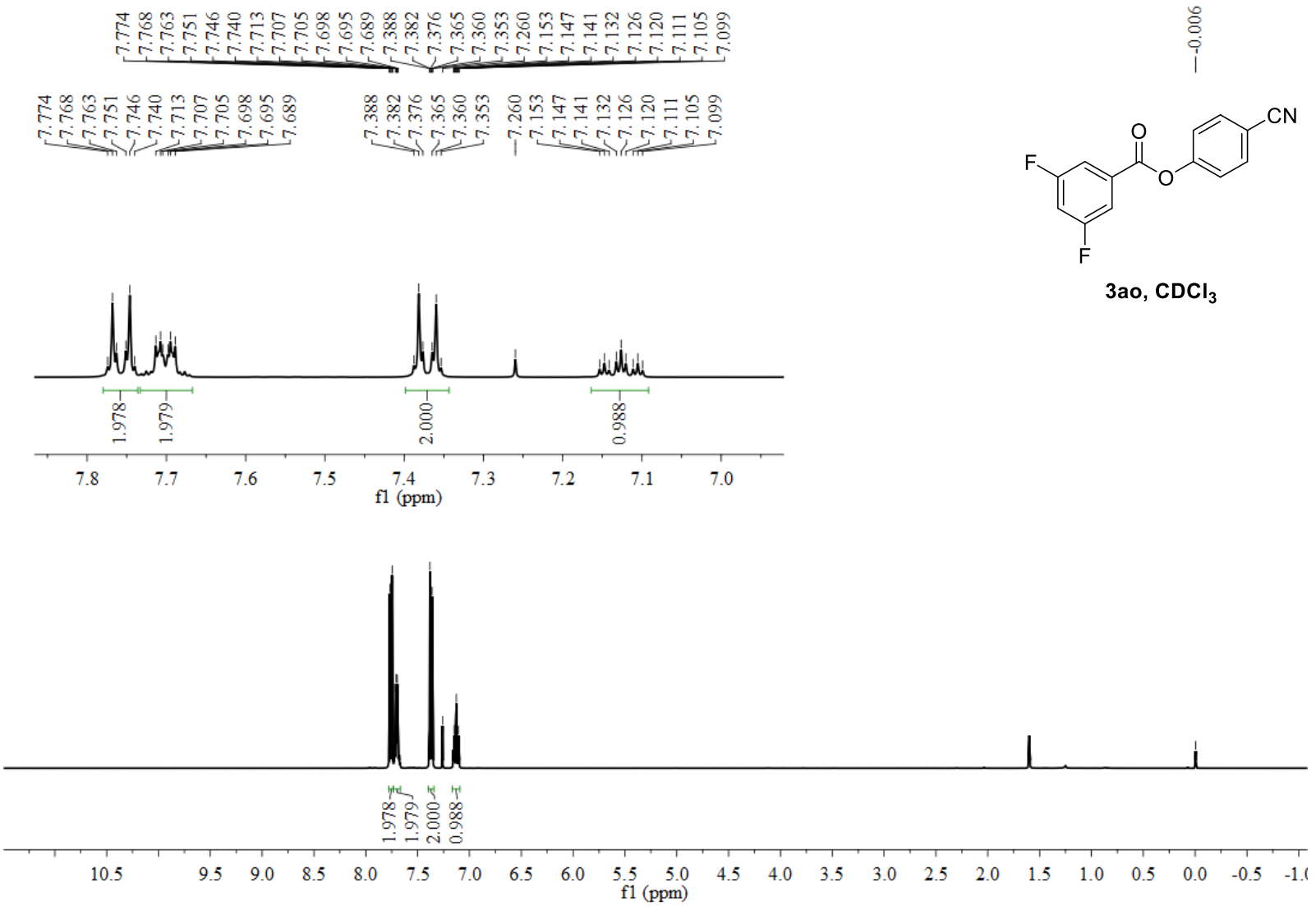
3al, $CDCl_3$


9.027
9.005
8.495
8.492
8.476
8.473
8.155
8.135
7.958
7.938
7.775
7.769
7.763
7.752
7.747
7.741
7.696
7.692
7.679
7.675
7.670
7.657
7.653
7.616
7.613
7.608
7.598
7.595
7.592
7.589
7.588
7.578
7.575
7.569
7.439
7.433
7.428
7.416
7.411
7.405
7.260
0.017
O
O
CN
3am, CDCl3
1.000
0.997
1.037
1.026
2.044
1.062
2.105
2.072
f1 (ppm)

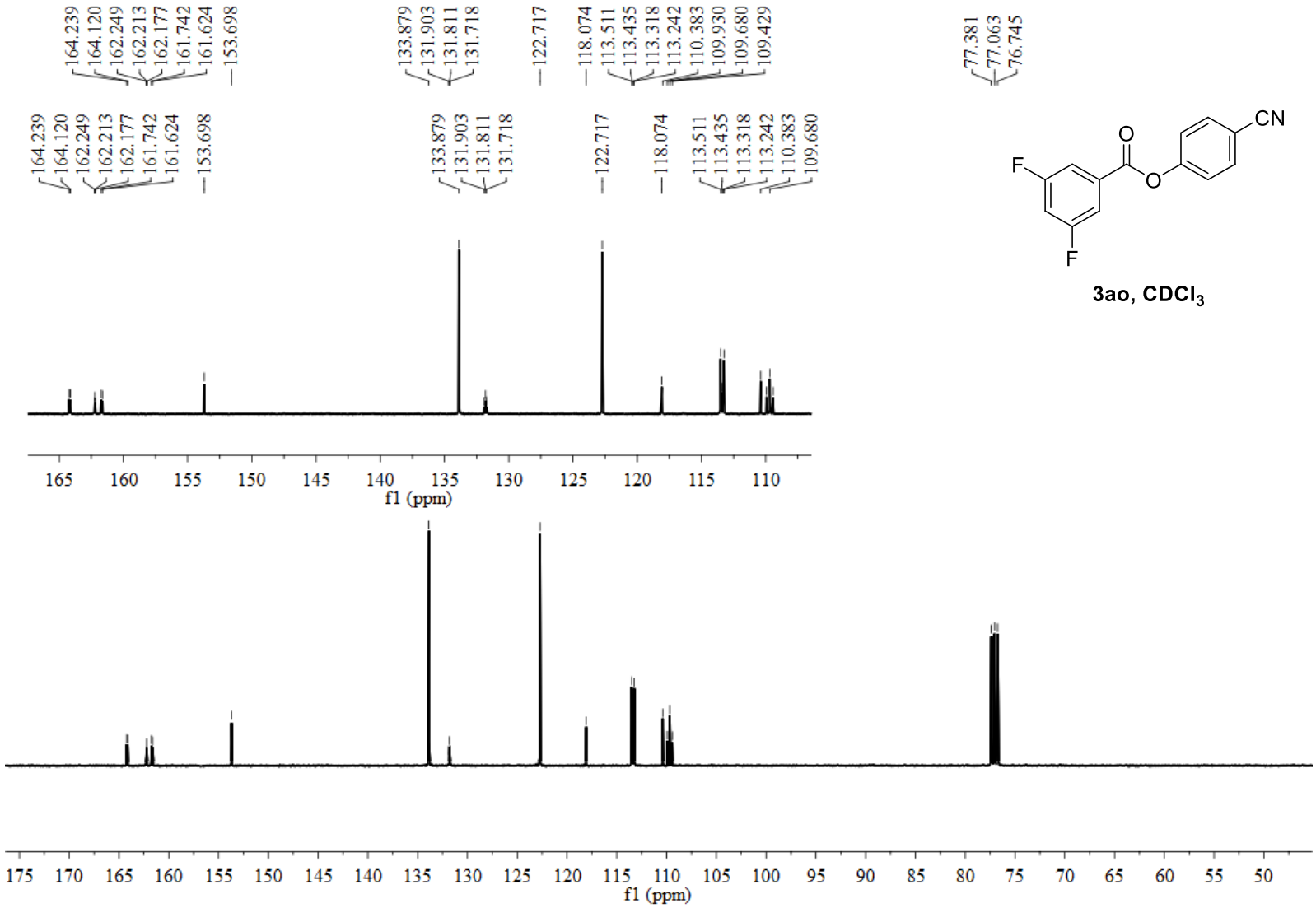

164.725
154.341
135.104
133.979
133.787
131.748
131.681
128.914
128.569
126.680
125.509
124.725
124.545
123.148
118.370
109.811
77.455
77.137
76.819
O
O
CN
3am, CDCl3
170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60
f1 (ppm)

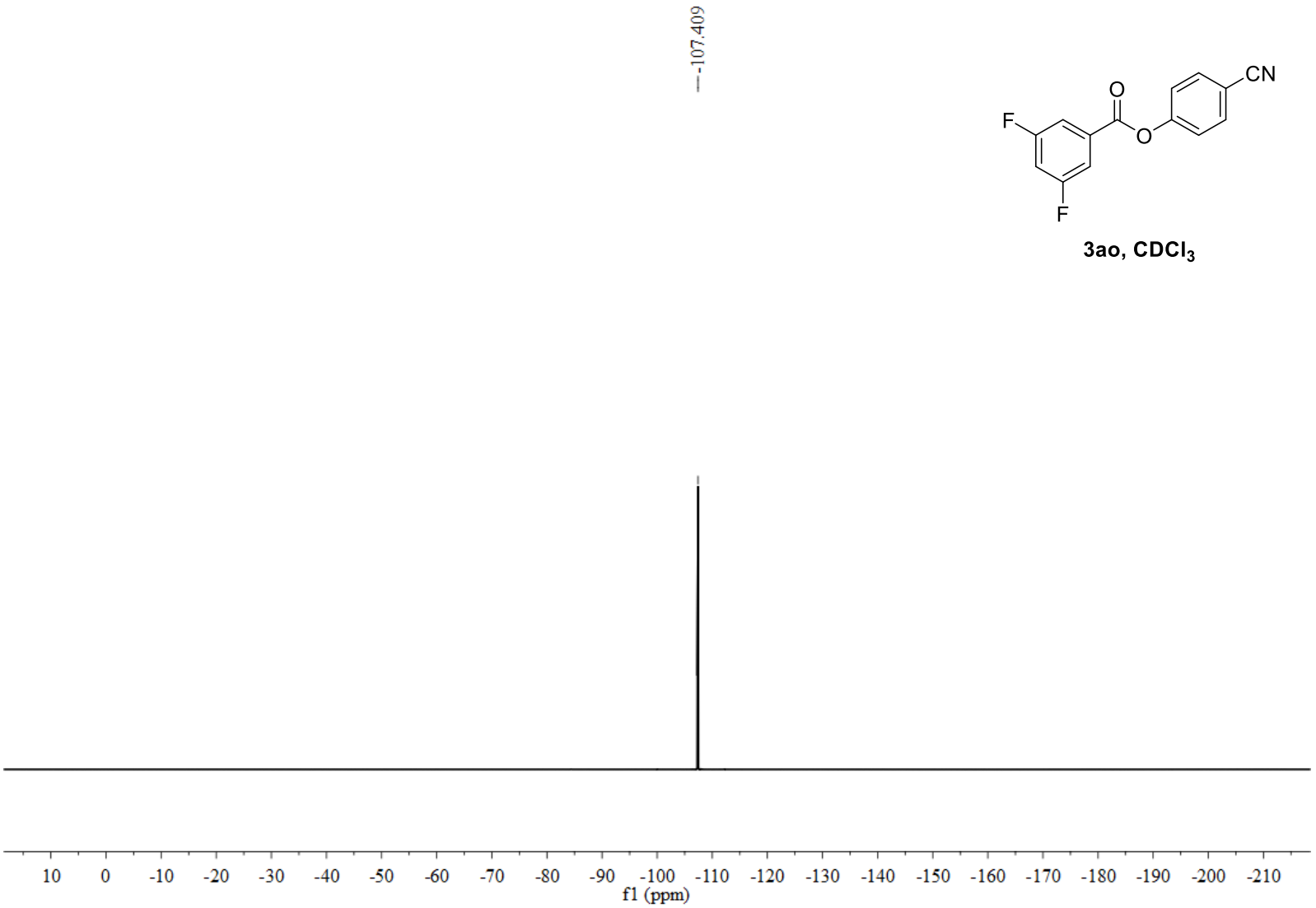

7.763
7.757
7.752
7.740
7.735
7.729
7.425
7.367
7.362
7.357
7.345
7.340
7.334
7.260
3.951
3.938
-0.008
1.986
2.000
1.992
3.205
5.829
f1 (ppm)
O
O
O
O
O
CN
3an, CDCl3


164.040
154.300
153.171
143.346
133.766
123.369
123.027
118.274
109.886
107.575
77.380
77.062
76.744
61.048
56.381
O
O
O
O
O
CN
3an, CDCl3
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)

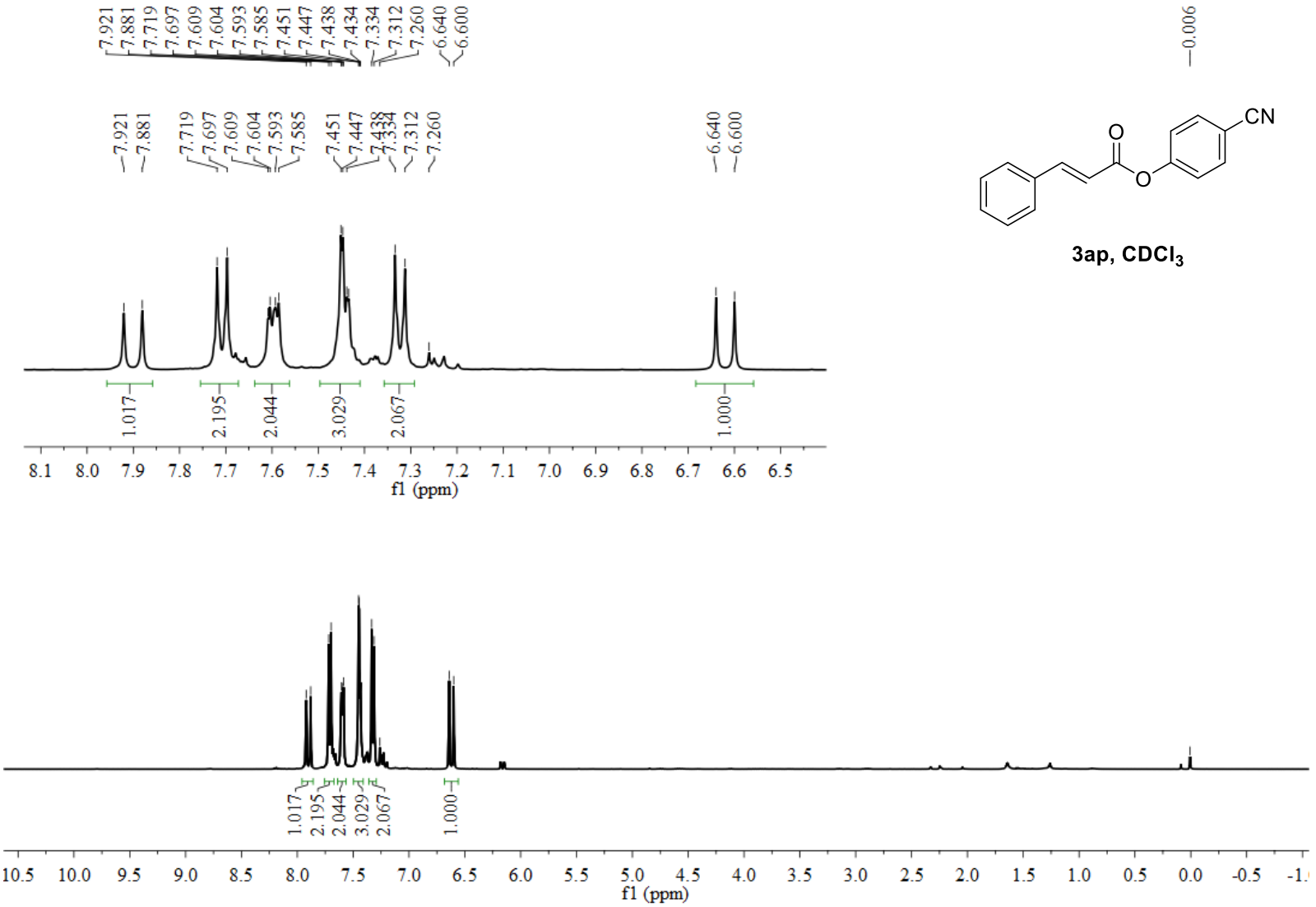

7.774
7.768
7.763
7.751
7.746
7.740
7.713
7.707
7.705
7.698
7.695
7.689
7.388
7.382
7.376
7.365
7.360
7.353
7.260
7.153
7.147
7.141
7.132
7.126
7.120
7.111
7.105
7.099
-0.006
F
O
O
CN
F
1.978
1.979
2.000
0.988
f1 (ppm)

3ao, $CDCl_3$

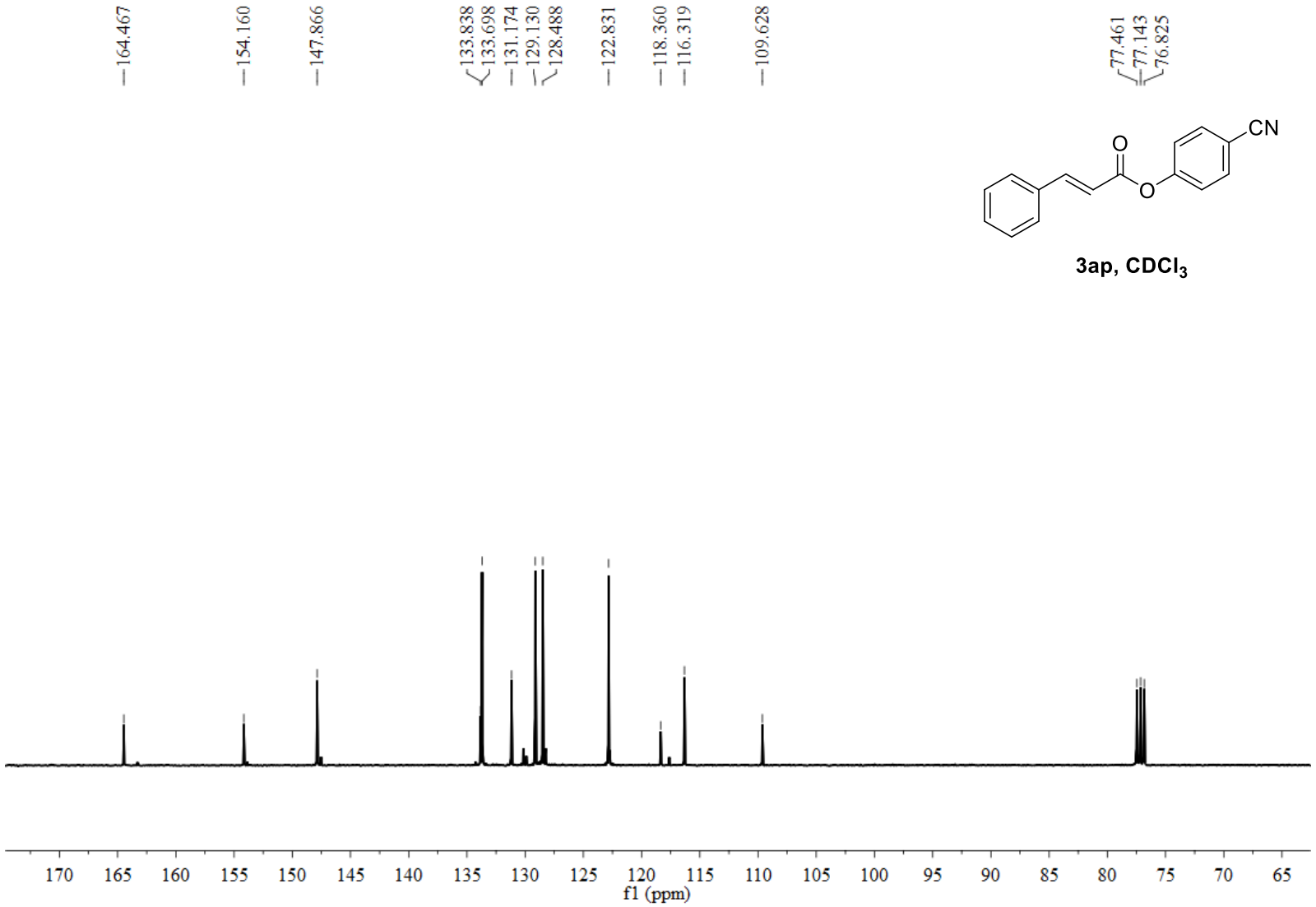

164.239
164.120
162.249
162.213
162.177
161.742
161.624
153.698
133.879
131.903
131.811
131.718
122.717
118.074
113.511
113.435
113.318
113.242
110.383
109.930
109.680
109.429
77.381
77.063
76.745
F
O
O
CN
F
3ao, CDCl3
f1 (ppm)
f1 (ppm)

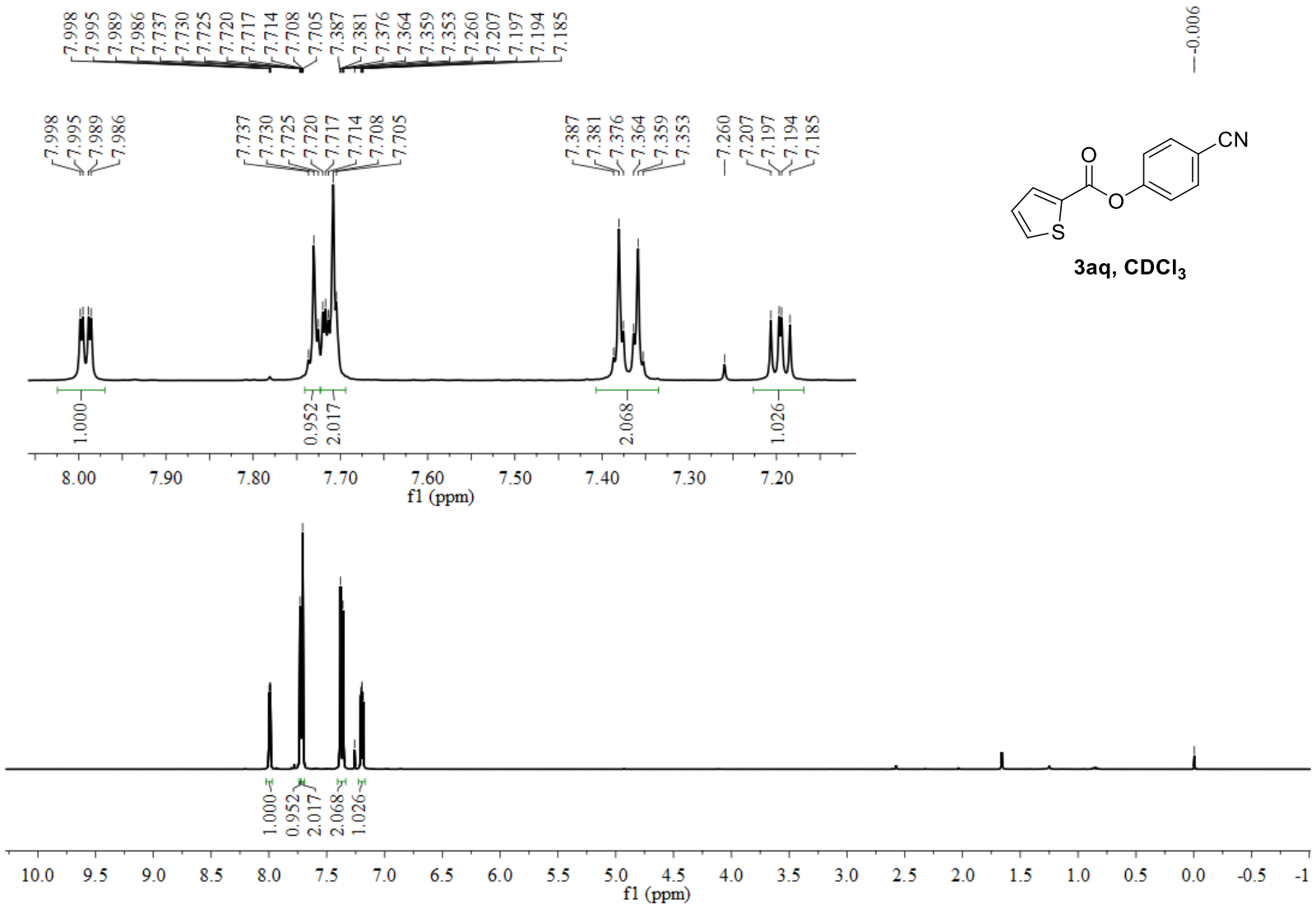

-107.409
F
O
O
CN
F
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

3ao, $CDCl_3$

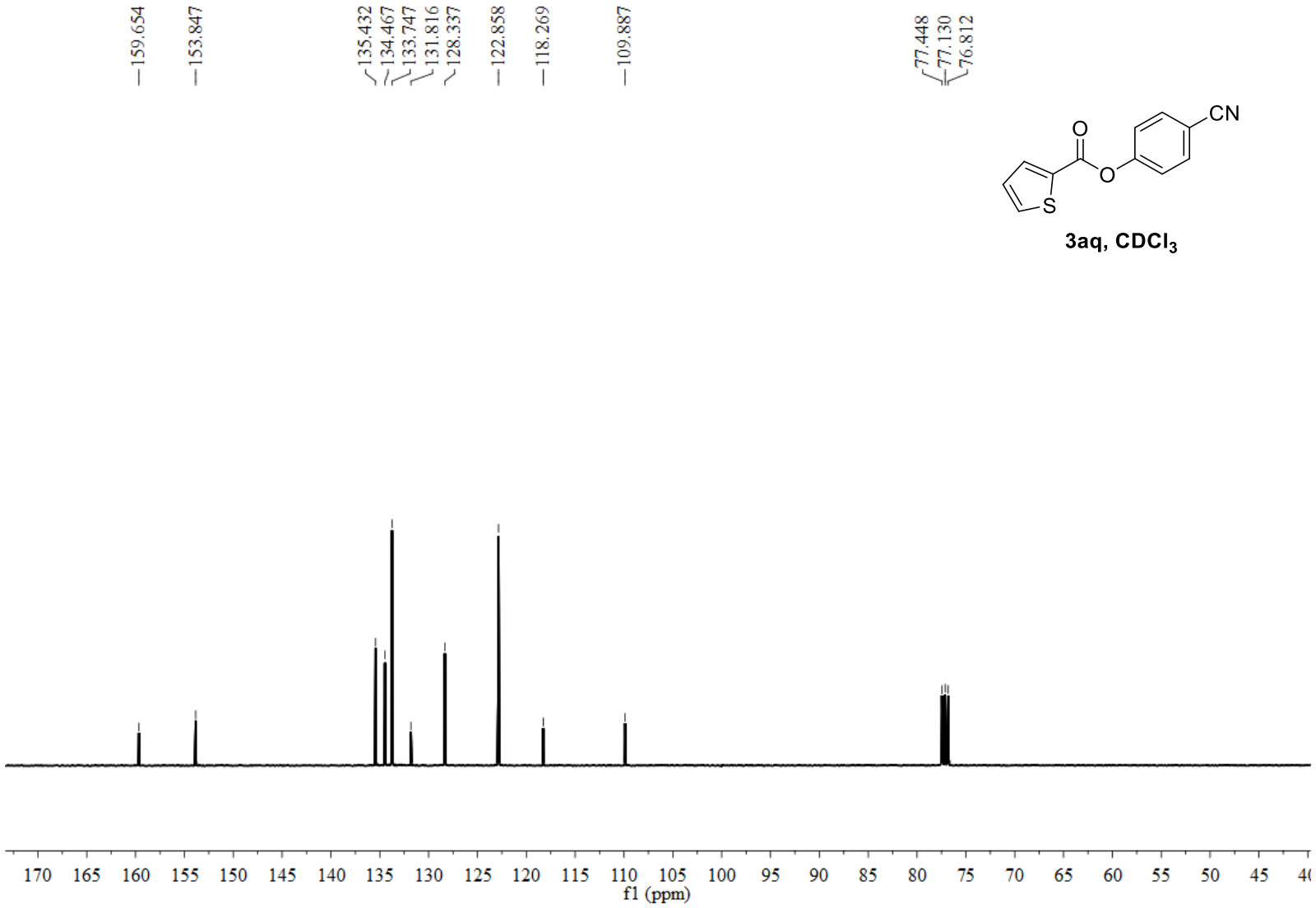

7.921
7.881
7.719
7.697
7.609
7.604
7.593
7.585
7.451
7.447
7.438
7.434
7.334
7.312
7.260
6.640
6.600
0.006
CN
O
O
1.017
2.195
2.044
3.029
2.067
1.000
f1 (ppm)

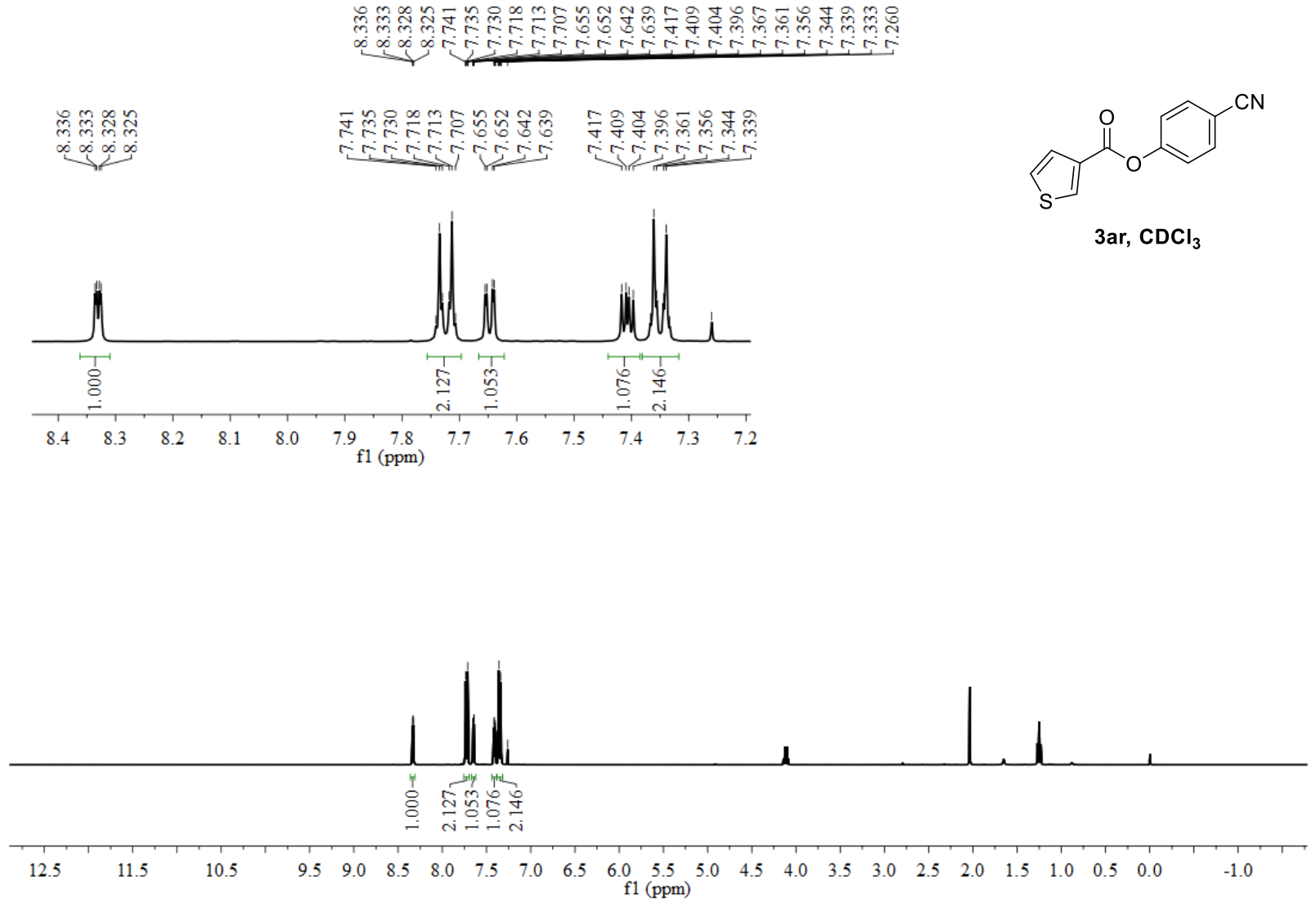
3ap, $CDCl_3$

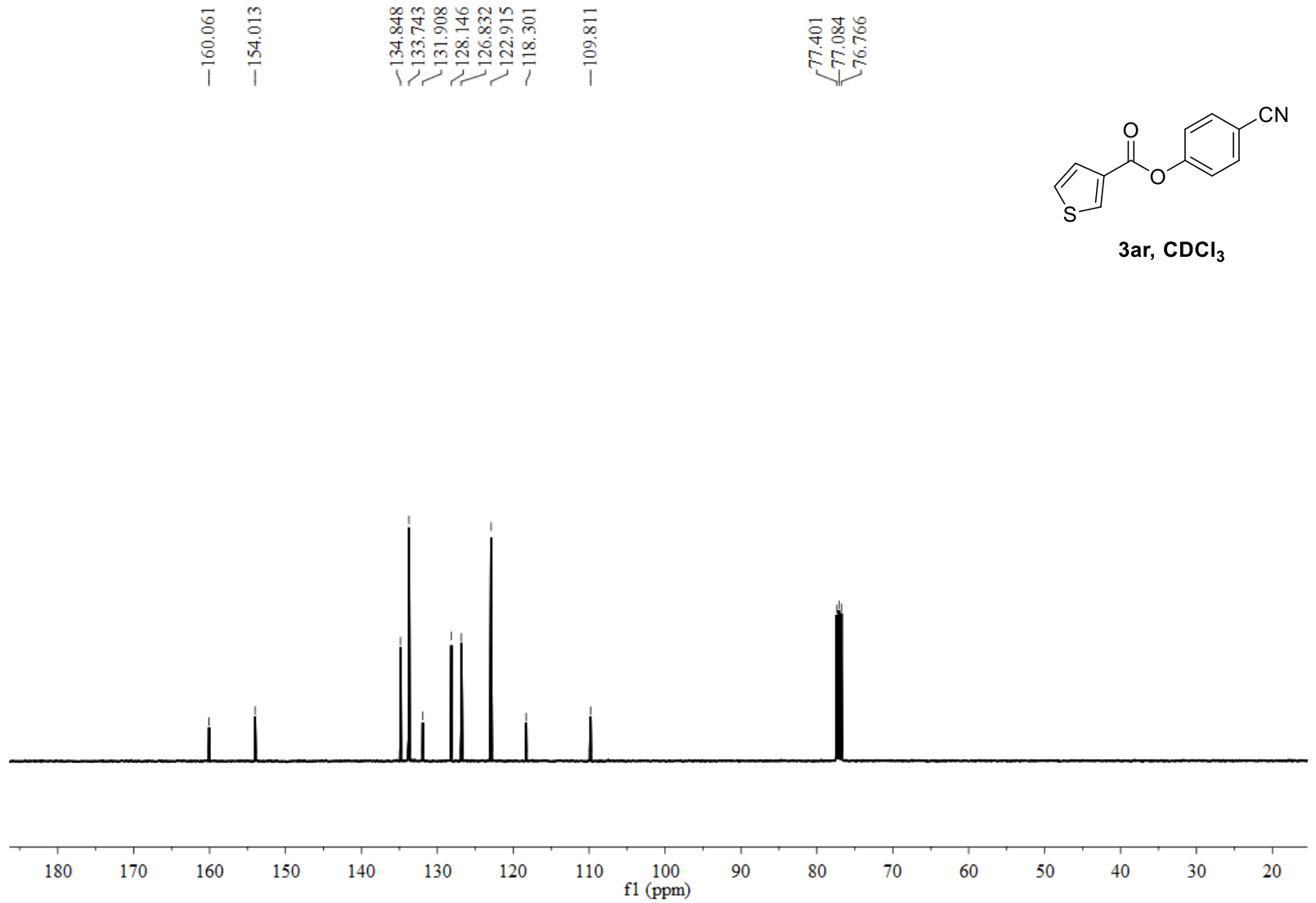

164.467
154.160
147.866
133.838
133.698
131.174
129.130
128.488
122.831
118.360
116.319
109.628
77.461
77.143
76.825
O
O
CN
3ap, CDCl3
170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65
f1 (ppm)


7.998
7.995
7.989
7.986
7.737
7.730
7.725
7.720
7.717
7.714
7.708
7.705
7.387
7.381
7.376
7.364
7.359
7.353
7.260
7.207
7.197
7.194
7.185
-0.006
1.000
0.952
2.017
2.068
1.026
8.00
7.90
7.80
7.70
7.60
7.50
7.40
7.30
7.20
f1 (ppm)
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)
O
O
S
CN

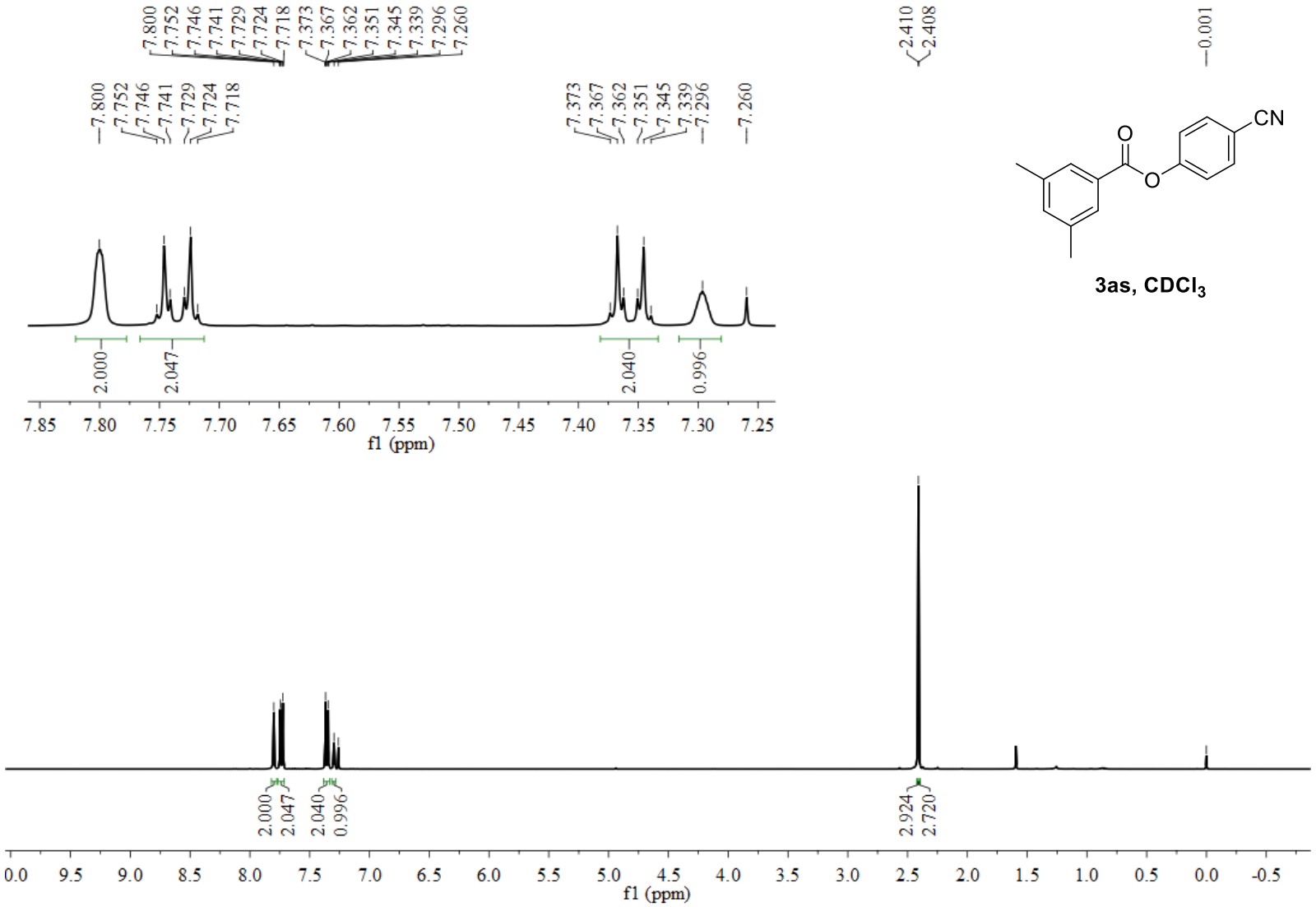
3aq, $CDCl_3$


159.654
153.847
135.432
134.467
133.747
131.816
128.337
122.858
118.269
109.887
77.448
77.130
76.812
O
O
S
CN
3aq, CDCl3
170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45
f1 (ppm)

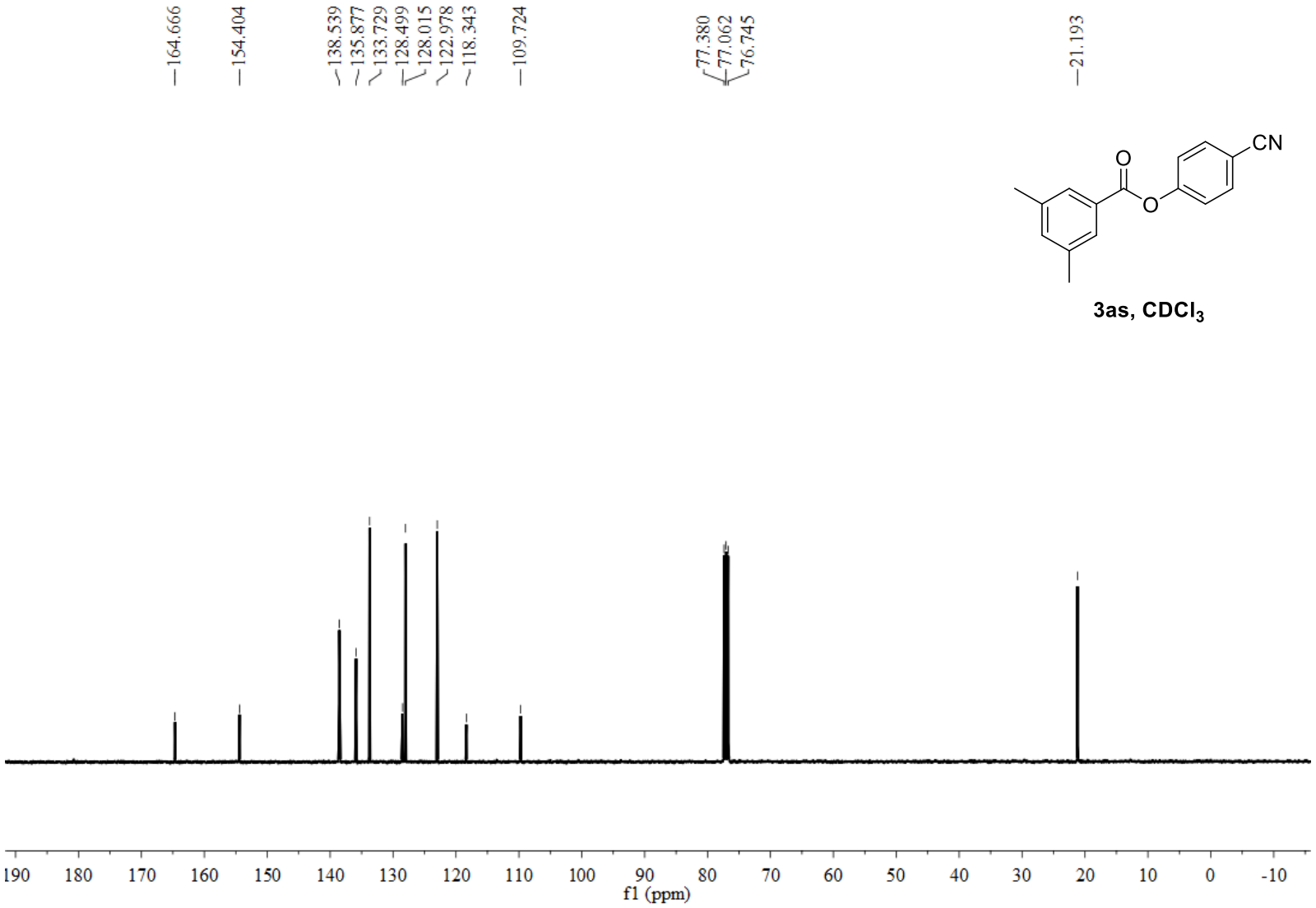

8.336
8.333
8.328
8.325
7.741
7.735
7.730
7.718
7.713
7.707
7.655
7.652
7.642
7.639
7.417
7.409
7.404
7.396
7.367
7.361
7.356
7.344
7.339
7.333
7.260
1.000
2.127
1.053
1.076
2.146
f1 (ppm)
O
O
S
CN
3ar, CDCl3


160.061
154.013
134.848
133.743
131.908
128.146
126.832
122.915
118.301
109.811
77.401
77.084
76.766
O
O
S
CN
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

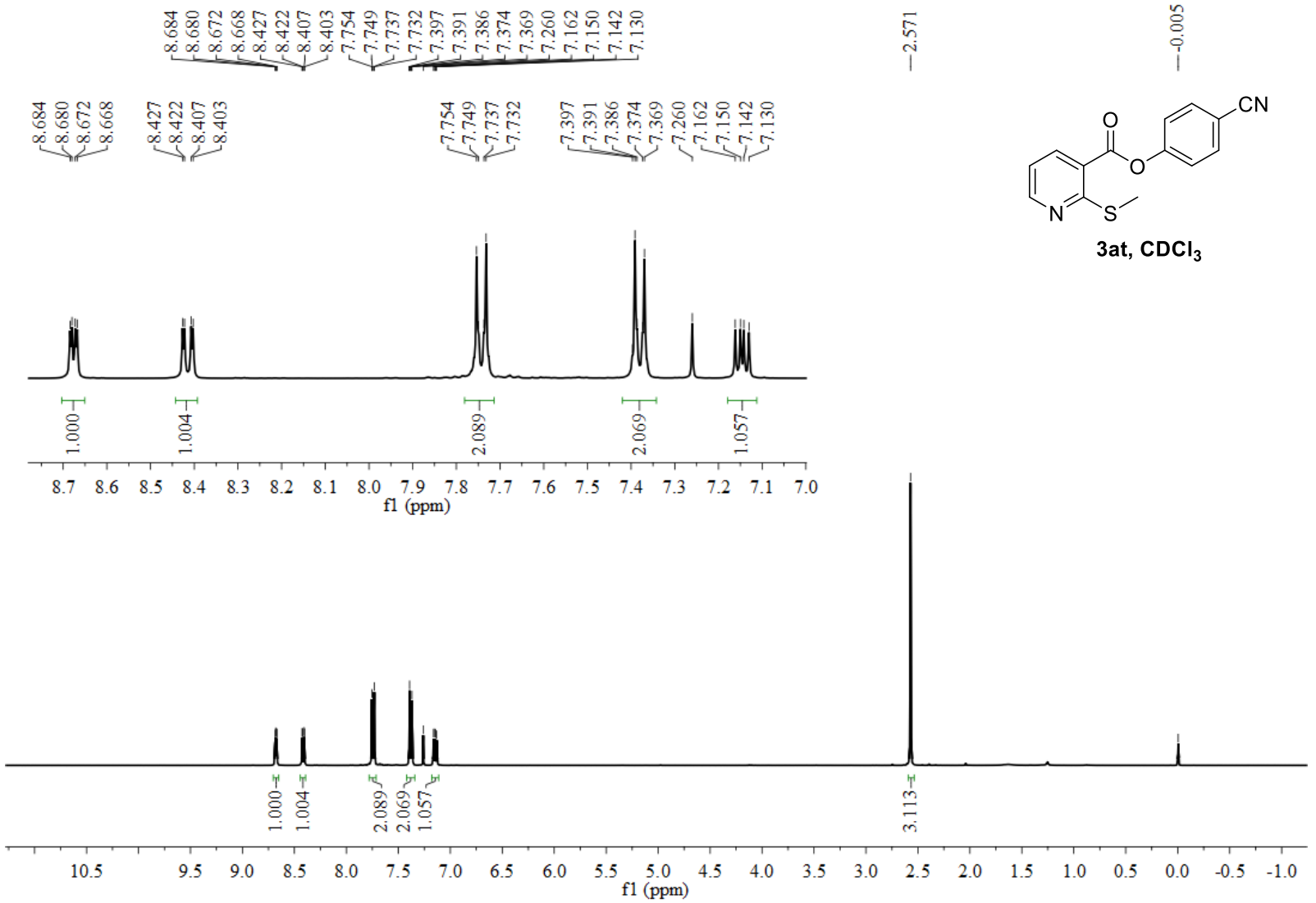
3ar, $CDCl_3$


7.800
7.752
7.746
7.741
7.729
7.724
7.718
7.373
7.367
7.362
7.351
7.345
7.339
7.296
7.260
2.410
2.408
0.001
O
O
CN
2.000
2.047
2.040
0.996
2.924
2.720
f1 (ppm)
f1 (ppm)

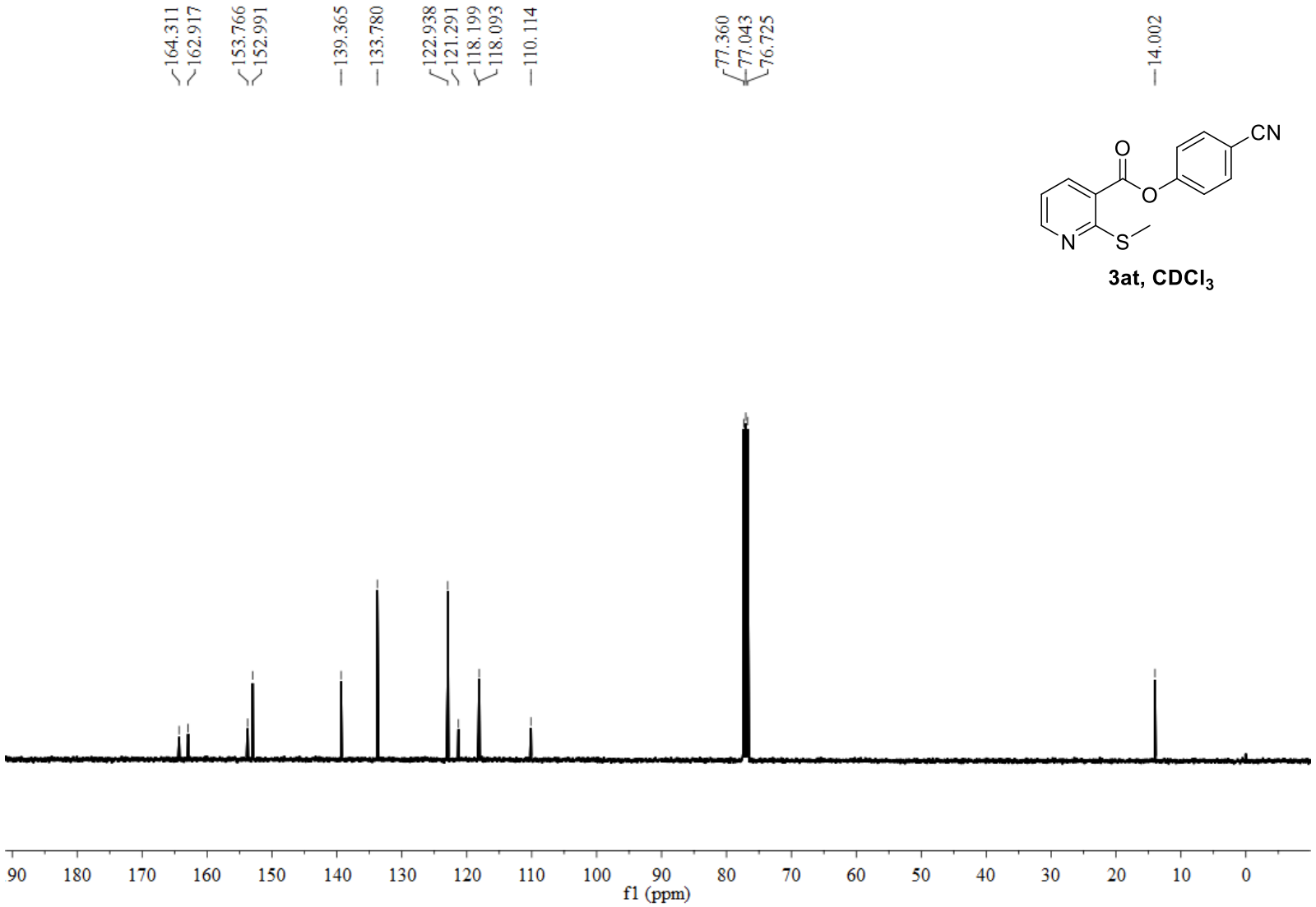
3as, $CDCl_3$


164.666
154.404
138.539
135.877
133.729
128.499
128.015
122.978
118.343
109.724
77.380
77.062
76.745
21.193
O
O
CN
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

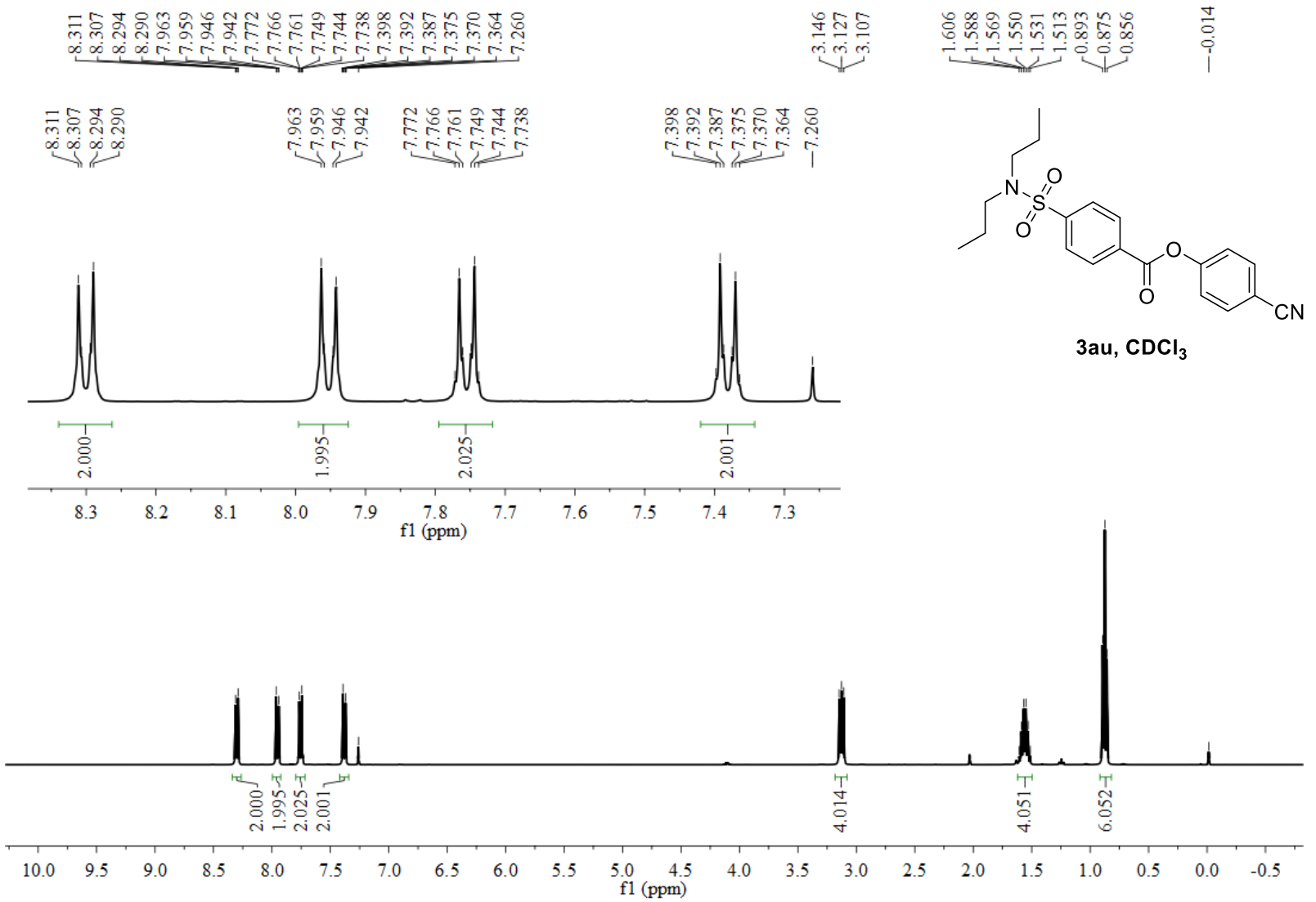
3as, $CDCl_3$


8.684
8.680
8.672
8.668
8.427
8.422
8.407
8.403
7.754
7.749
7.737
7.732
7.397
7.391
7.386
7.374
7.369
7.260
7.162
7.150
7.142
7.130
2.571
0.005
1.000
1.004
2.089
2.069
1.057
3.113
f1 (ppm)
O
O
N
S
CN

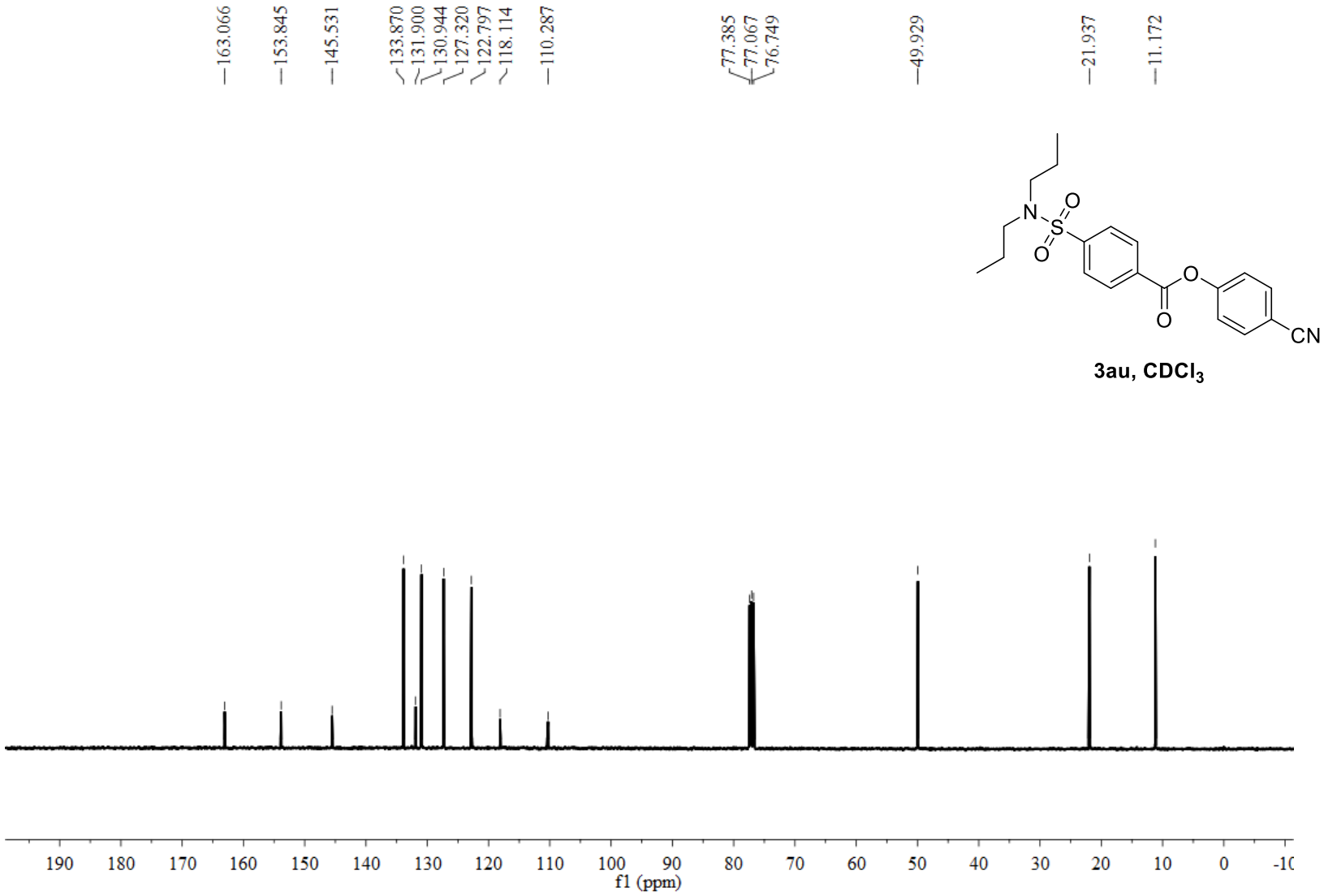
3at, $CDCl_3$


164.311
162.917
153.766
152.991
139.365
133.780
122.938
121.291
118.199
118.093
110.114
77.360
77.043
76.725
14.002
O
O
CN
N
S
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

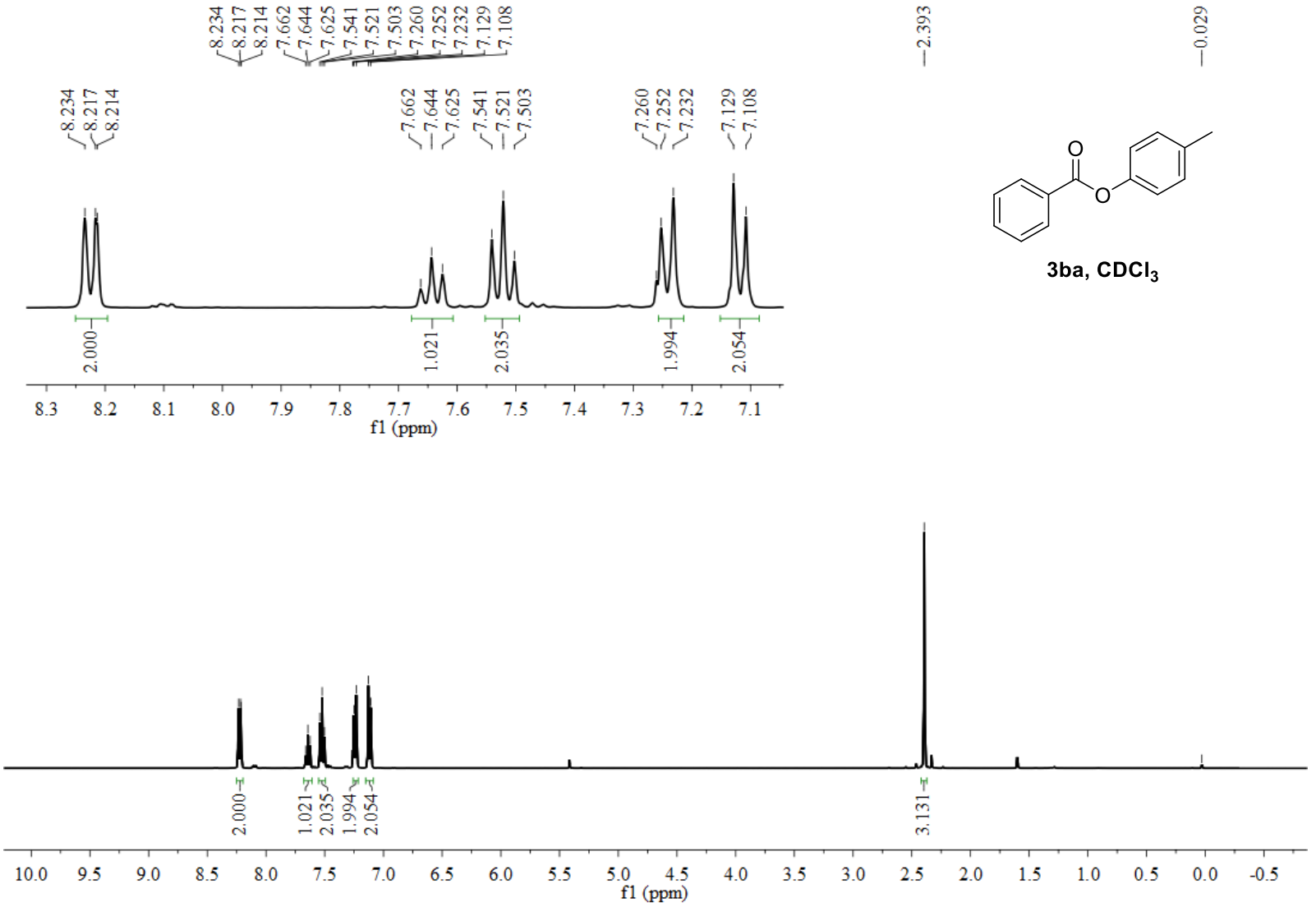
3at, $CDCl_3$

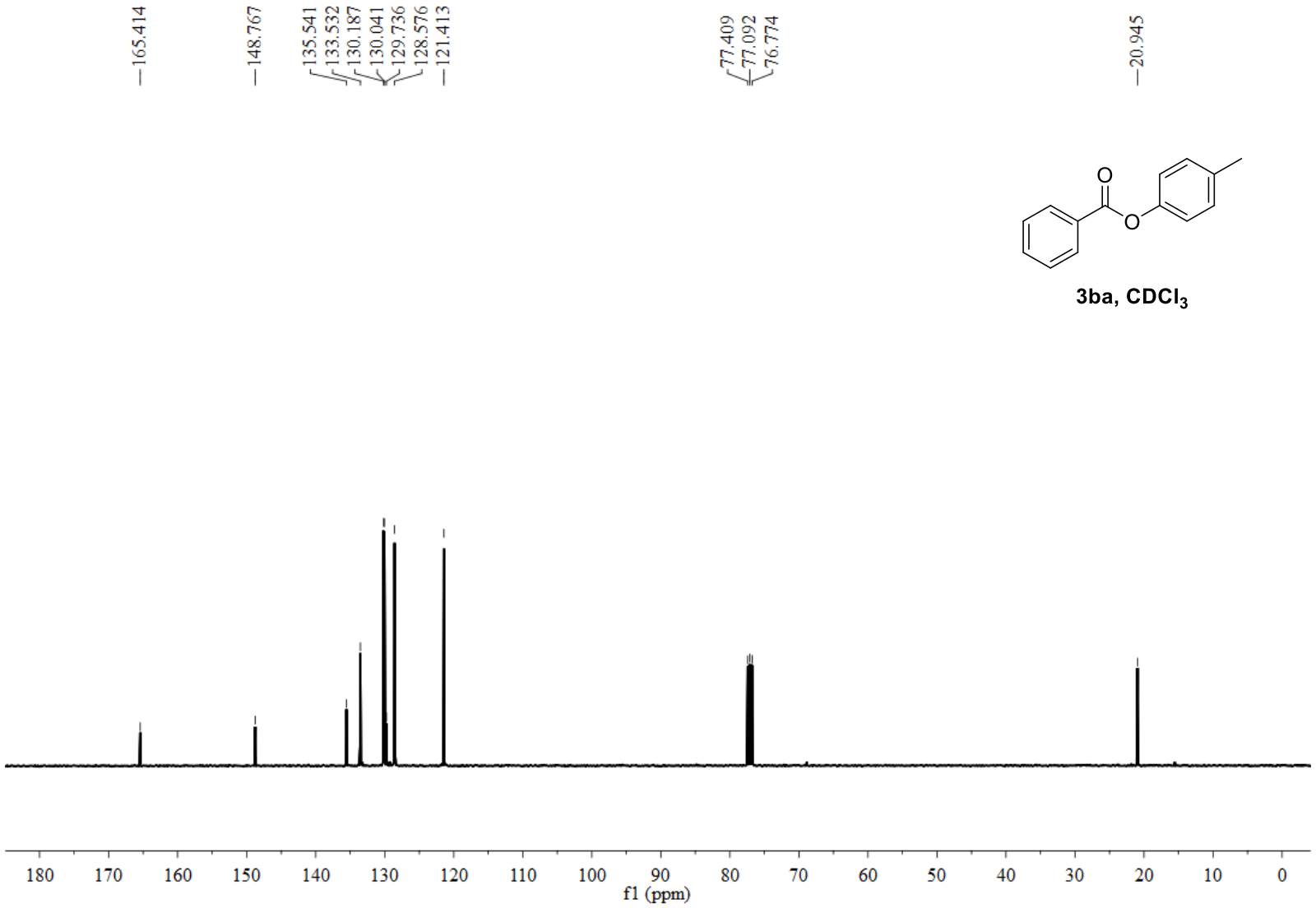

8.311
8.307
8.294
8.290
7.963
7.959
7.946
7.942
7.772
7.766
7.761
7.749
7.744
7.738
7.398
7.392
7.387
7.375
7.370
7.364
7.260
3.146
3.127
3.107
1.606
1.588
1.569
1.550
1.531
1.513
0.893
0.875
0.856
-0.014
2.000
1.995
2.025
2.001
f1 (ppm)
4.014
4.051
6.052
f1 (ppm)
N
S
O
O
O
O
CN

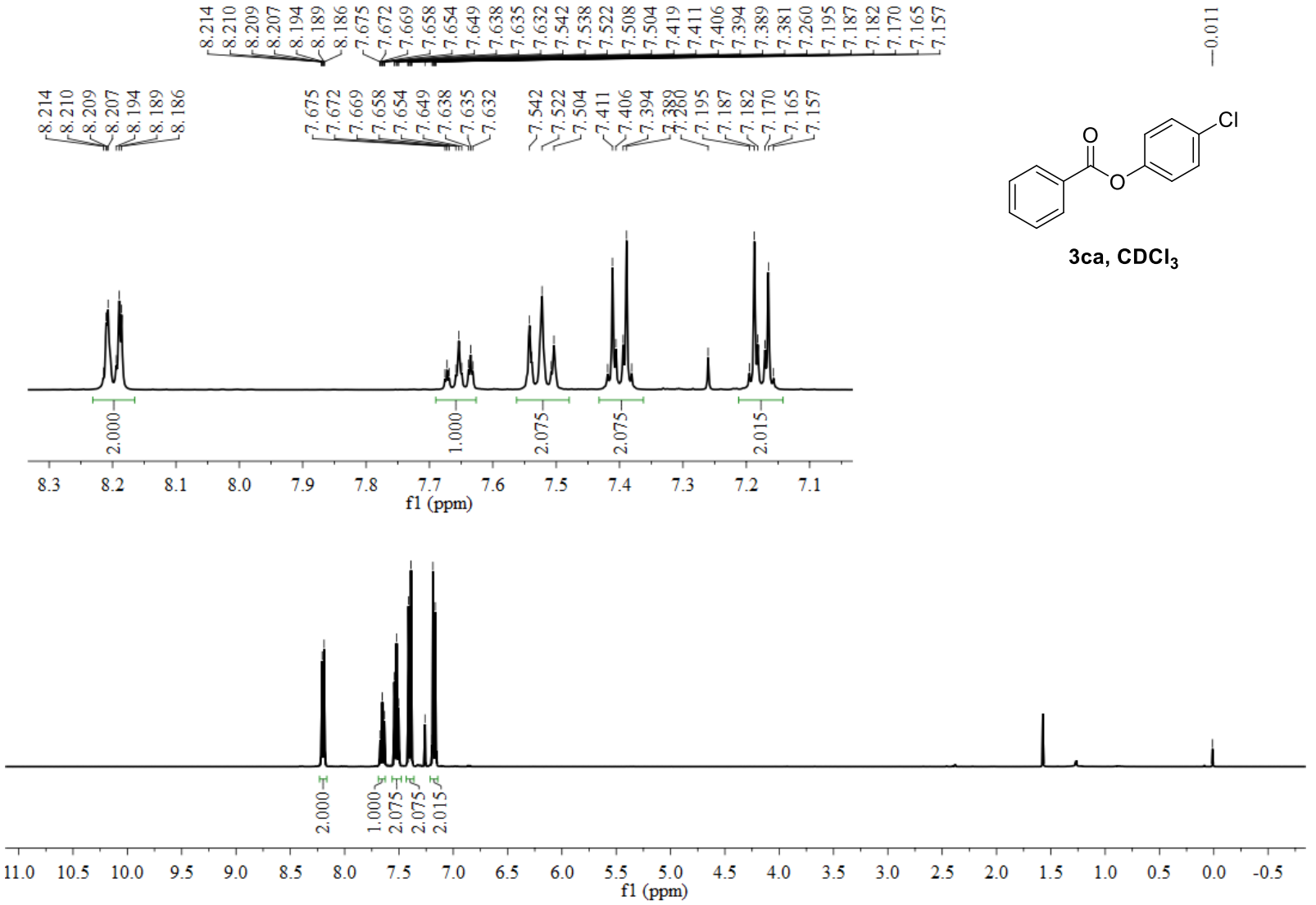
3au, $CDCl_3$

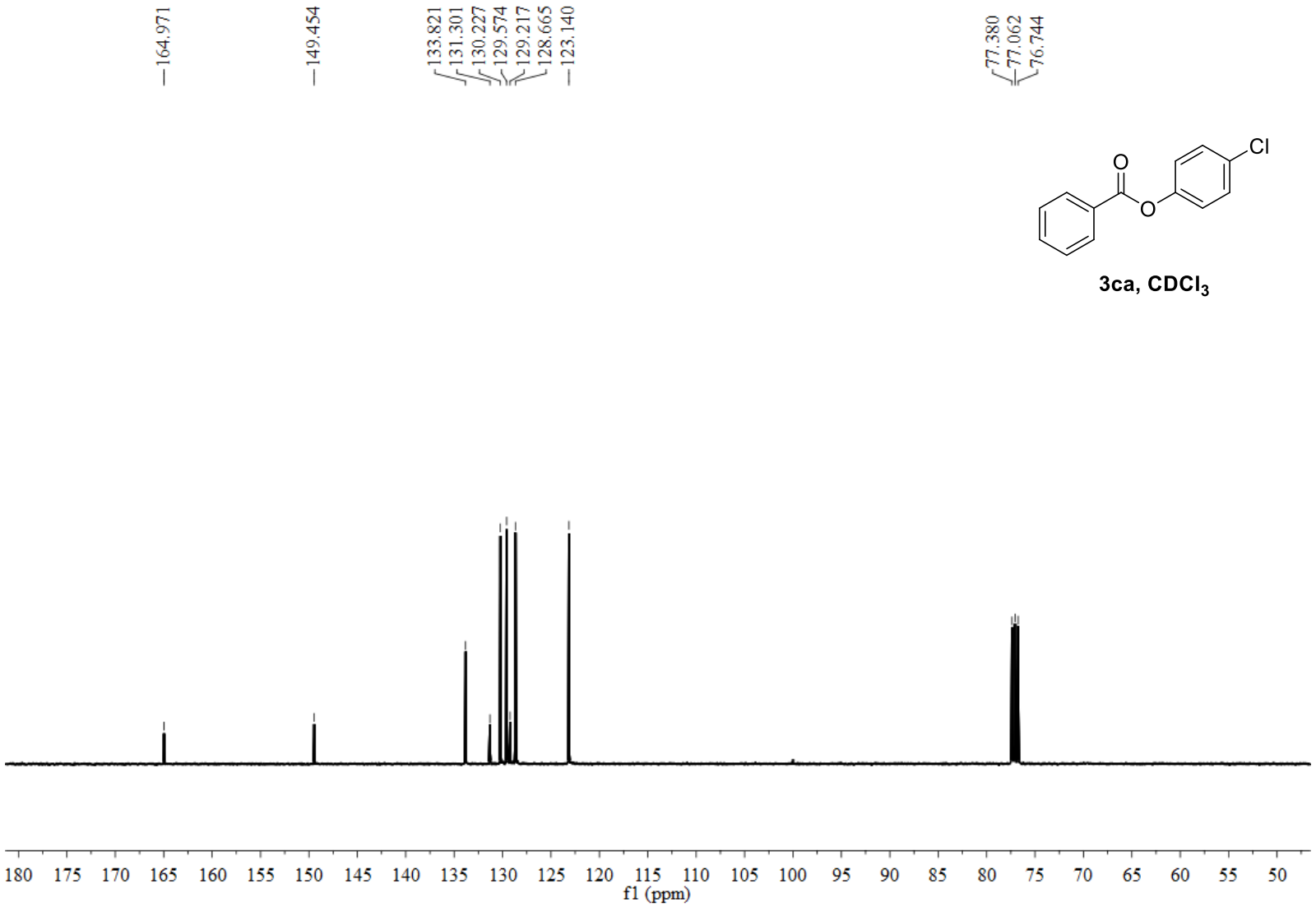

163.066
153.845
145.531
133.870
131.900
130.944
127.320
122.797
118.114
110.287
77.385
77.067
76.749
49.929
21.937
11.172
N
S
O
O
O
O
CN
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

3au, $CDCl_3$

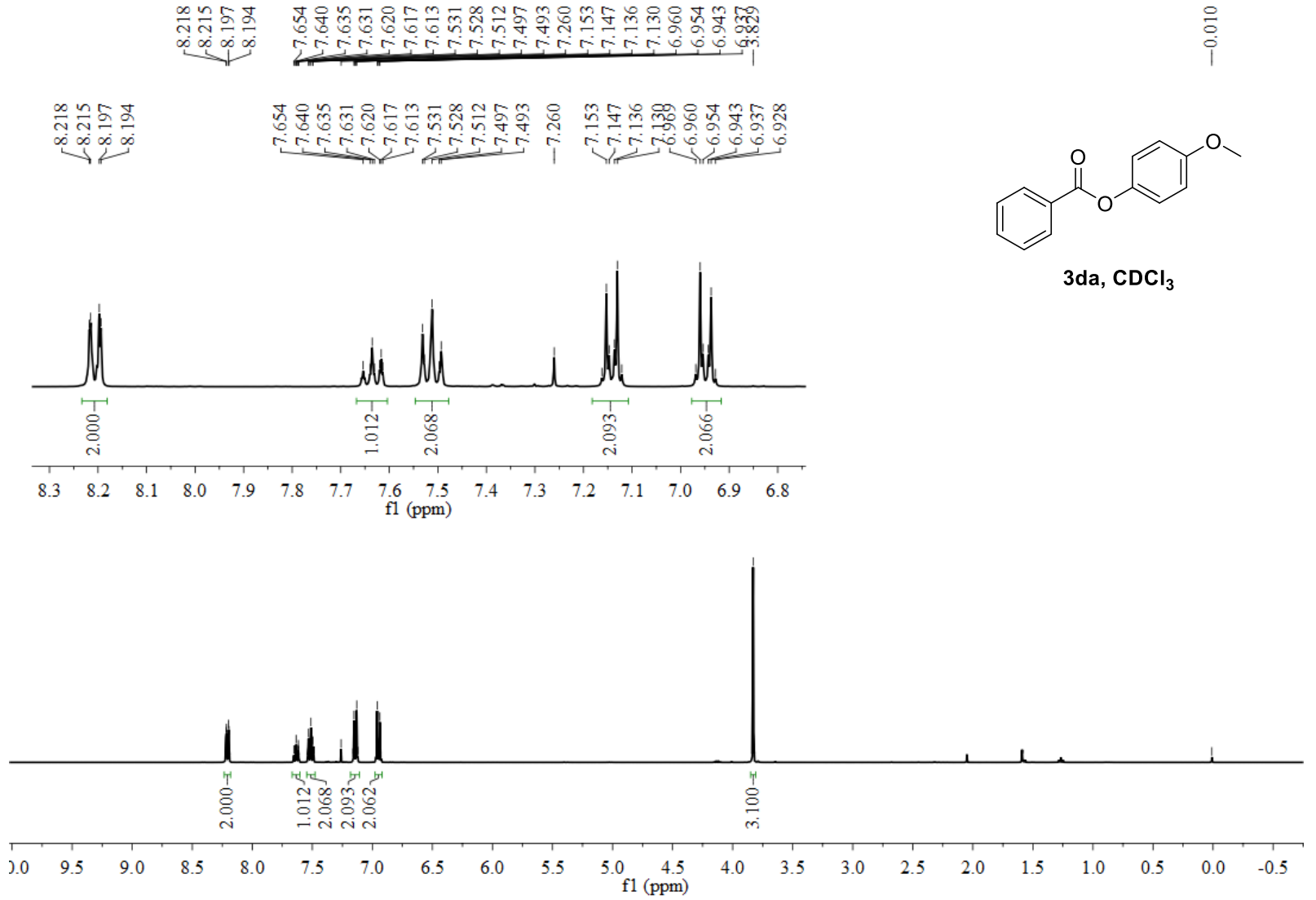

8.234
8.217
8.214
7.662
7.644
7.625
7.541
7.521
7.503
7.260
7.252
7.232
7.129
7.108
2.393
0.029
2.000
1.021
2.035
1.994
2.054
3.131
f1 (ppm)
3ba, CDCl3


165.414
148.767
135.541
133.532
130.187
130.041
129.736
128.576
121.413
77.409
77.092
76.774
20.945
O
O
3ba, CDCl3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

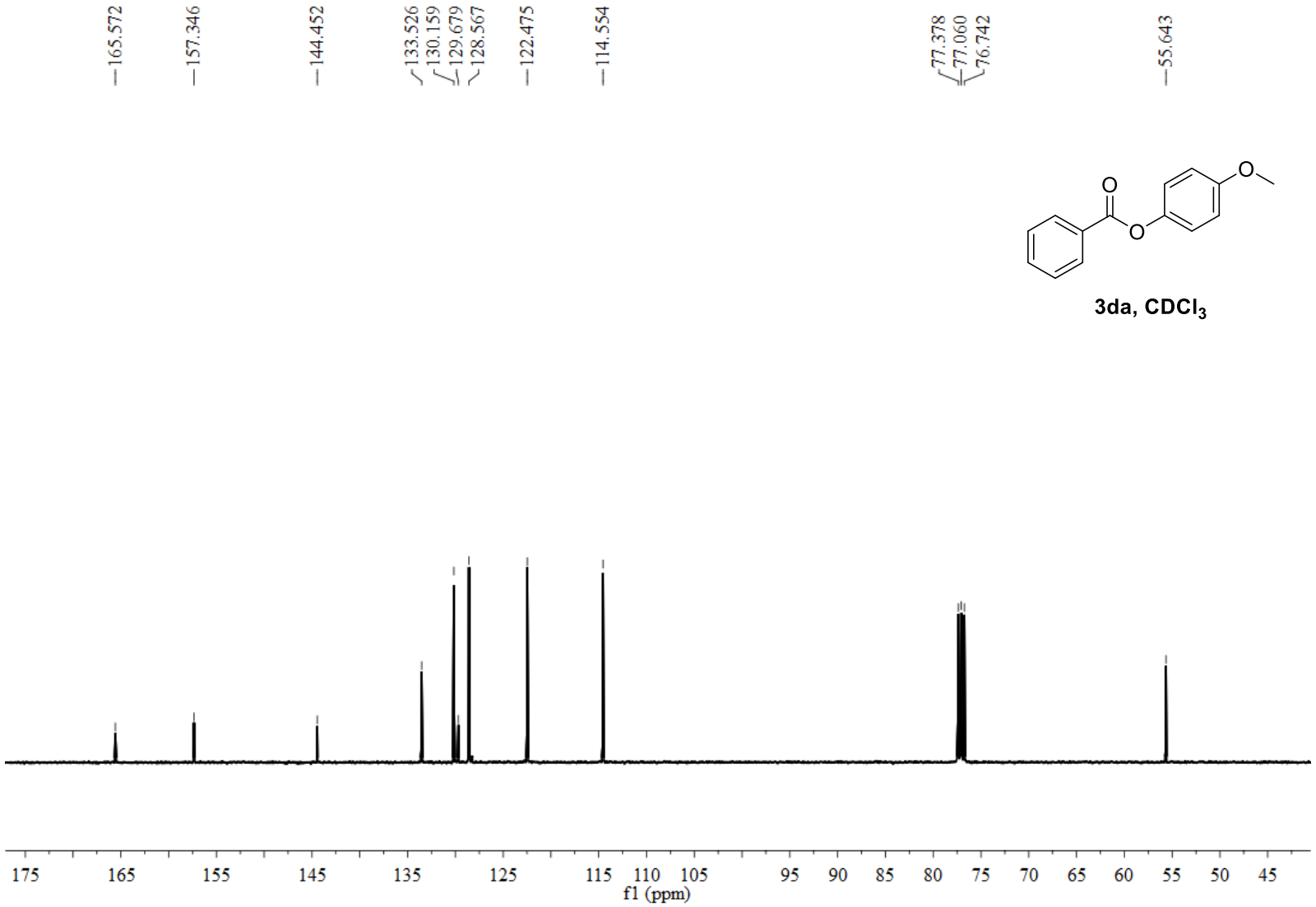

8.214
8.210
8.209
8.207
8.194
8.189
8.186
7.675
7.672
7.669
7.658
7.654
7.649
7.638
7.635
7.632
7.542
7.538
7.522
7.508
7.504
7.419
7.411
7.406
7.394
7.389
7.381
7.260
7.195
7.187
7.182
7.170
7.165
7.157
0.011
Cl
O
O
3ca, CDCl3
2.000
1.000
2.075
2.075
2.015
f1 (ppm)
f1 (ppm)

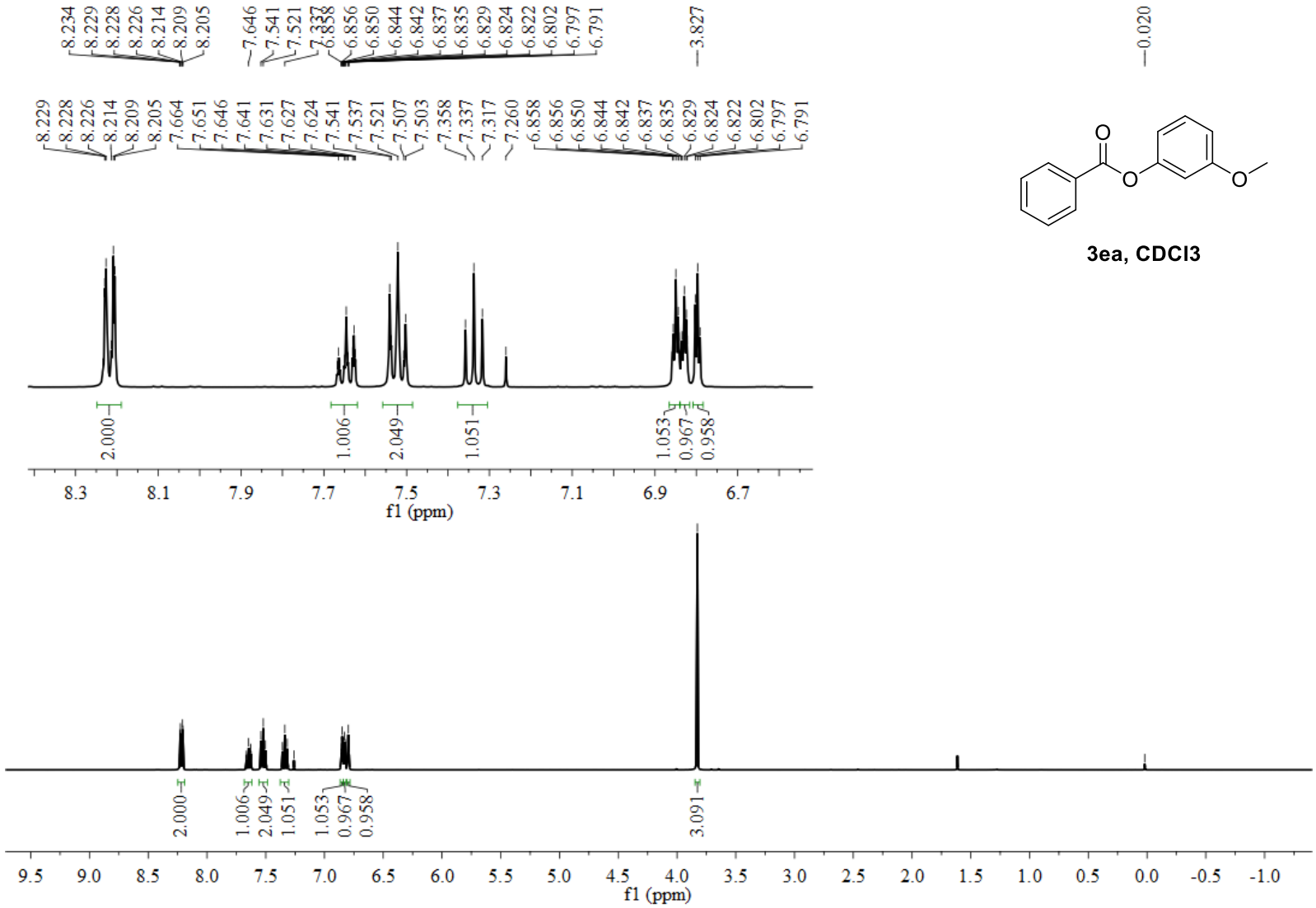

164.971
149.454
133.821
131.301
130.227
129.574
129.217
128.665
123.140
77.380
77.062
76.744
O
O
Cl
180 175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50
f1 (ppm)

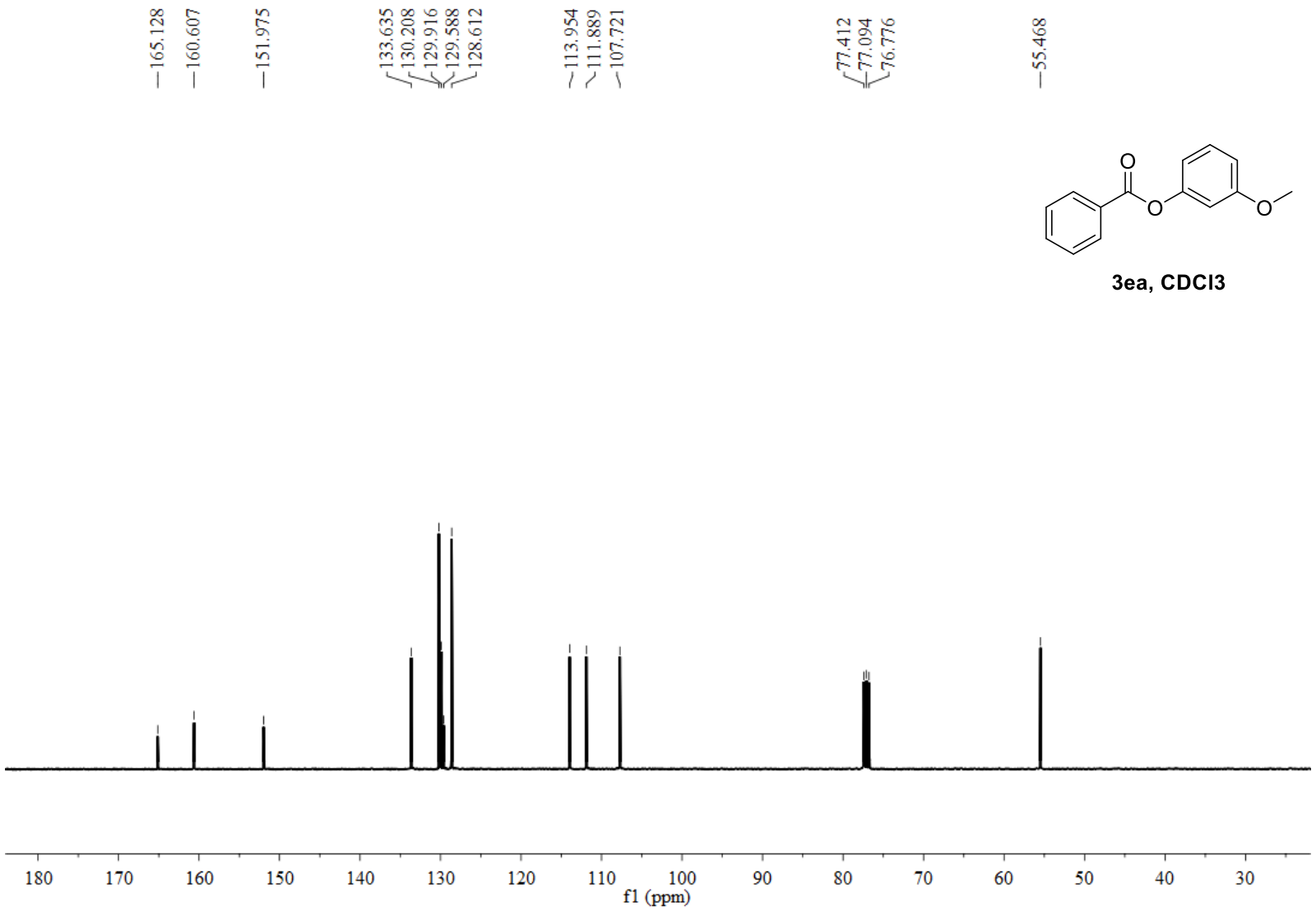
3ca, $CDCl_3$

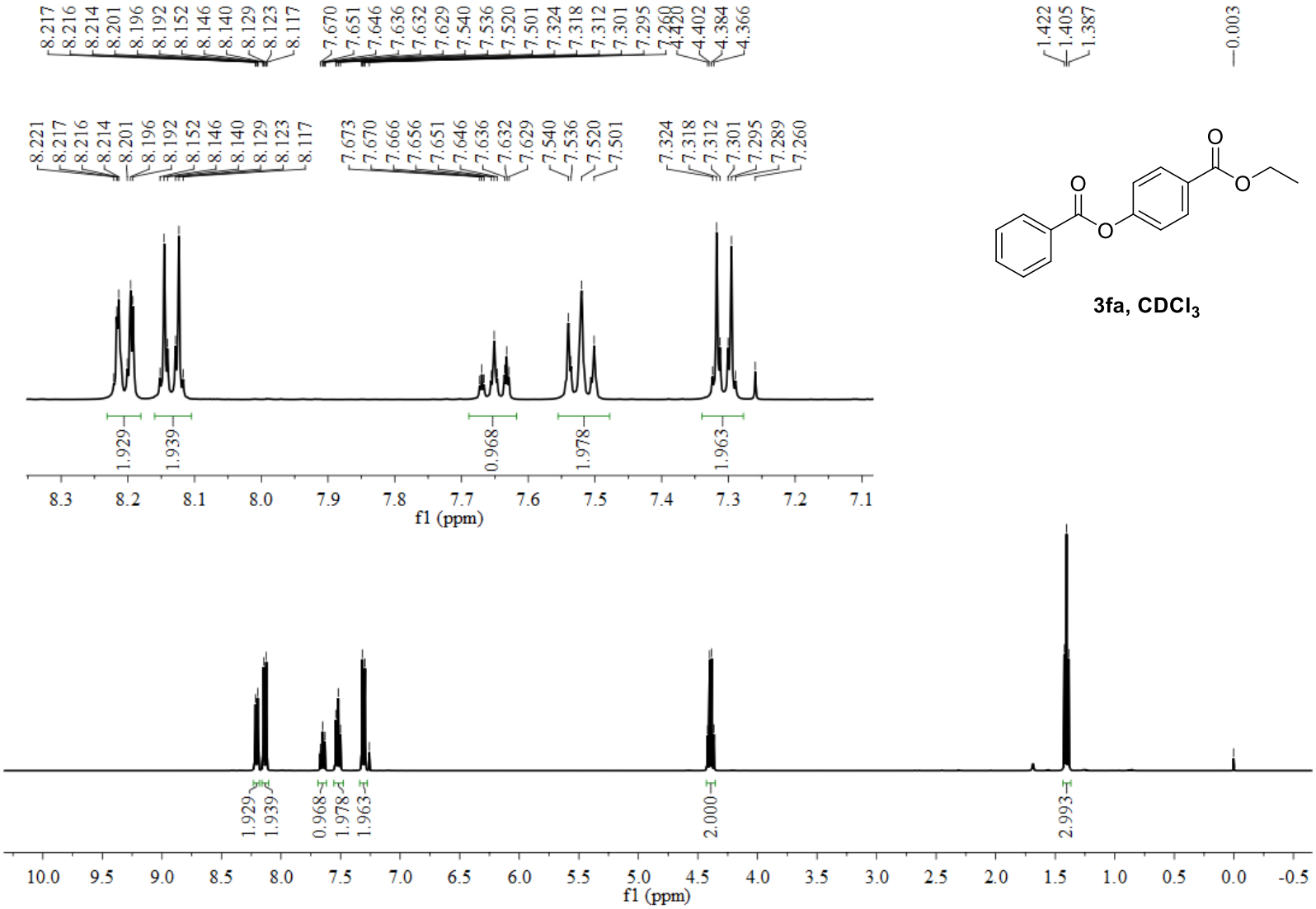

8.218
8.215
8.197
8.194
7.654
7.640
7.635
7.631
7.620
7.617
7.613
7.531
7.528
7.512
7.497
7.493
7.260
7.153
7.147
7.136
7.130
6.960
6.954
6.943
6.937
3.825
0.010
2.000
1.012
2.068
2.093
2.066
f1 (ppm)
2.000
1.012
2.068
2.093
2.062
3.100
f1 (ppm)

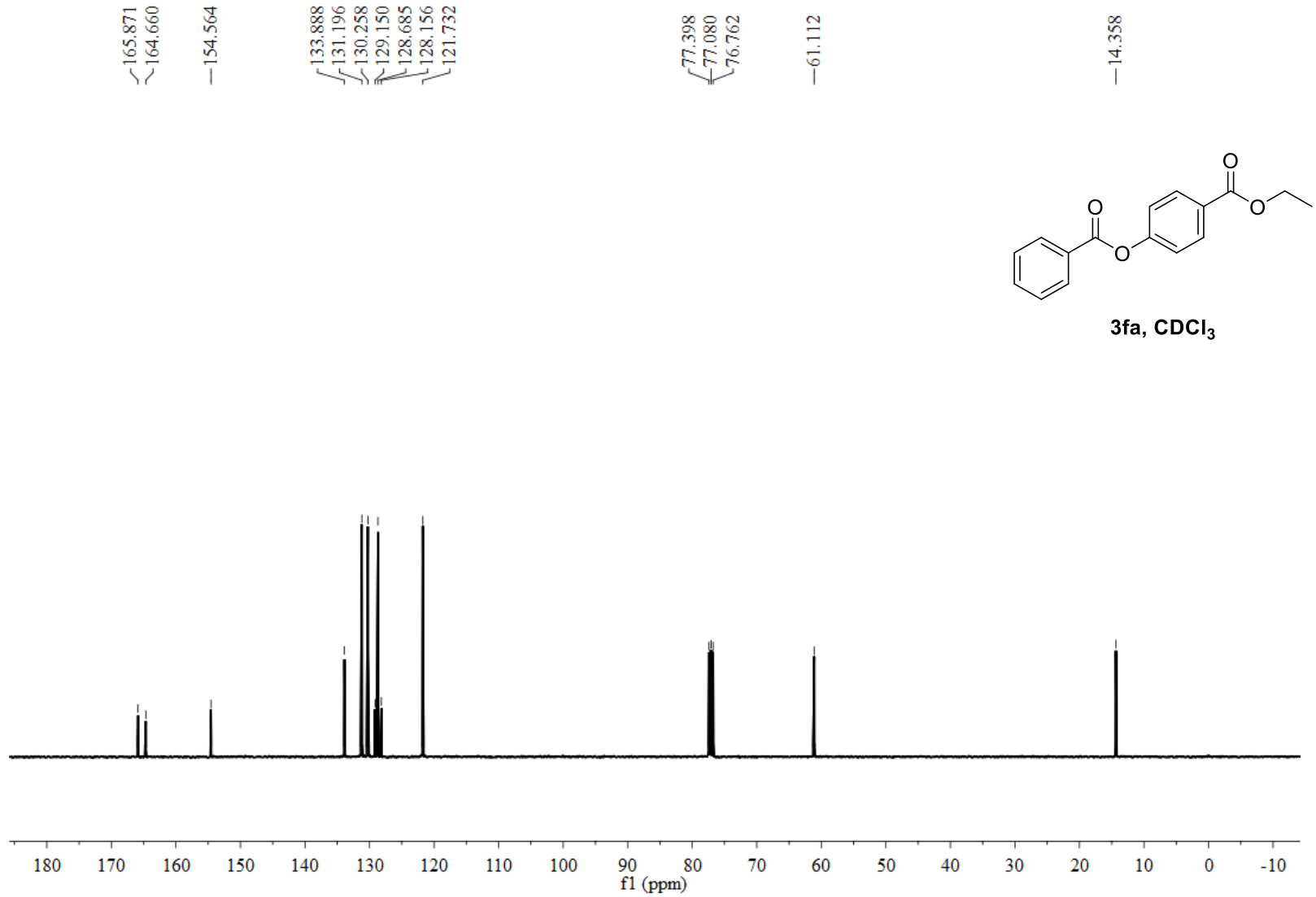
3da, $CDCl_3$

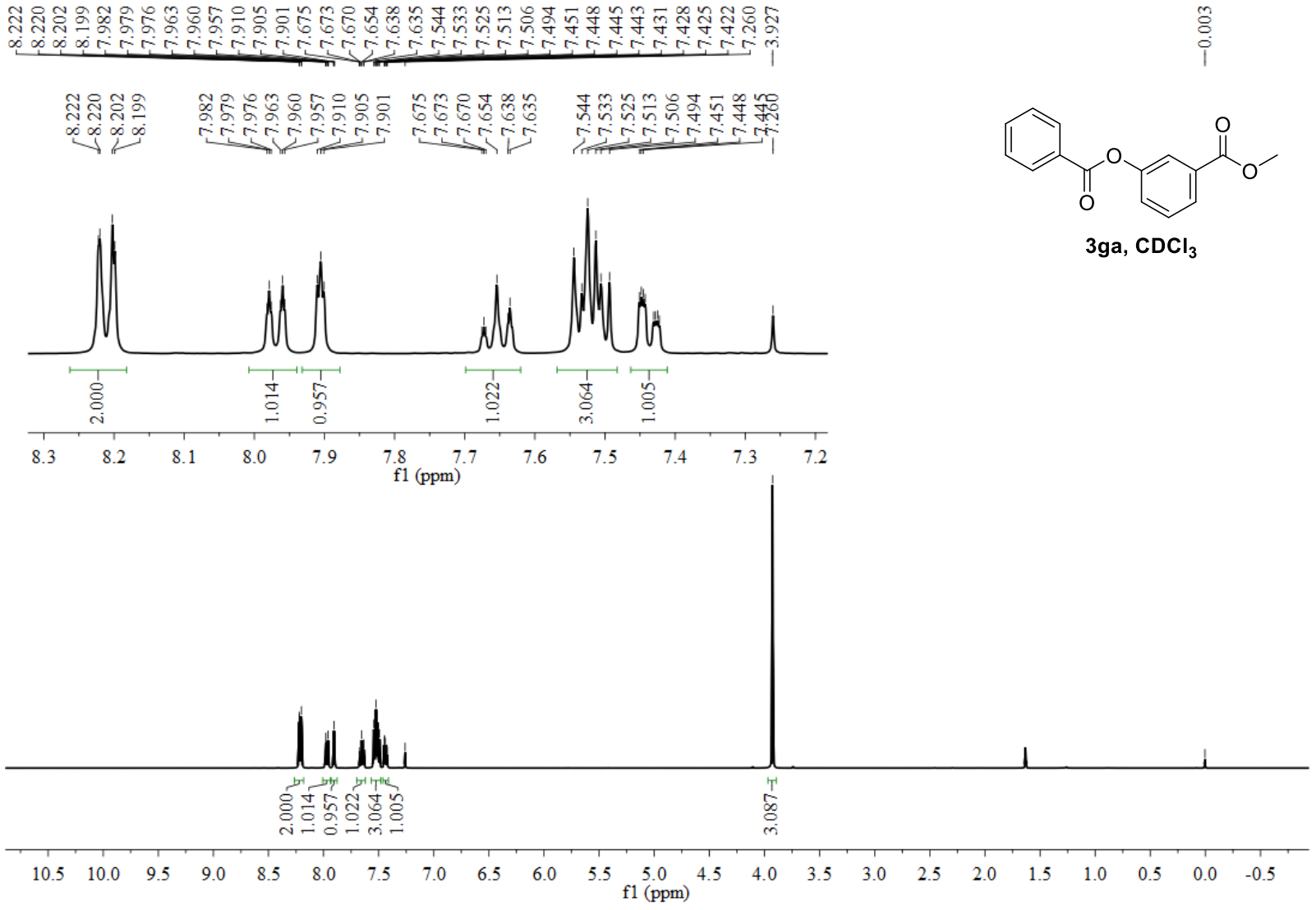

165.572
157.346
144.452
133.526
130.159
129.679
128.567
122.475
114.554
77.378
77.060
76.742
55.643
O
O
O
3da, CDCl3
175
165
155
145
135
125
115
110
105
95
90
85
80
75
70
65
60
55
50
45
f1 (ppm)


8.234
8.229
8.228
8.226
8.214
8.209
8.205
7.646
7.541
7.521
7.337
6.858
6.856
6.850
6.844
6.842
6.837
6.835
6.829
6.824
6.822
6.802
6.797
6.791
3.827
0.020
8.229
8.228
8.226
8.214
8.209
8.205
7.664
7.651
7.646
7.641
7.631
7.627
7.624
7.541
7.537
7.521
7.507
7.503
7.358
7.337
7.317
7.260
6.858
6.856
6.850
6.844
6.842
6.837
6.835
6.829
6.824
6.822
6.802
6.797
6.791
2.000
1.006
2.049
1.051
1.053
0.967
0.958
8.3
8.1
7.9
7.7
7.5
7.3
7.1
6.9
6.7
f1 (ppm)
3ea, CDCl3
2.000
1.006
2.049
1.051
1.053
0.967
0.958
3.091
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)

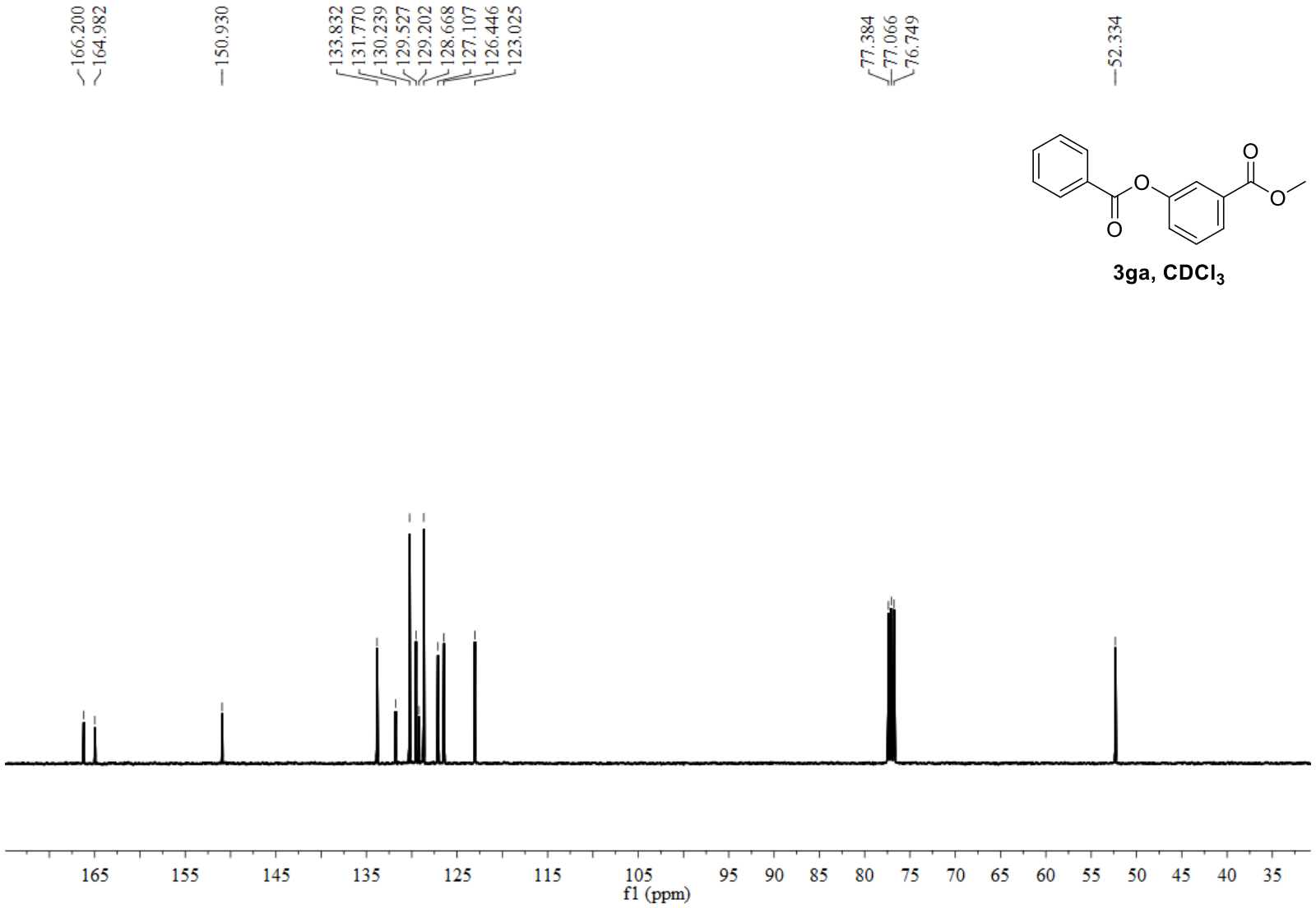

165.128
160.607
151.975
133.635
130.208
129.916
129.588
128.612
113.954
111.889
107.721
77.412
77.094
76.776
55.468
O
O
O
3ea, CDCl3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
f1 (ppm)

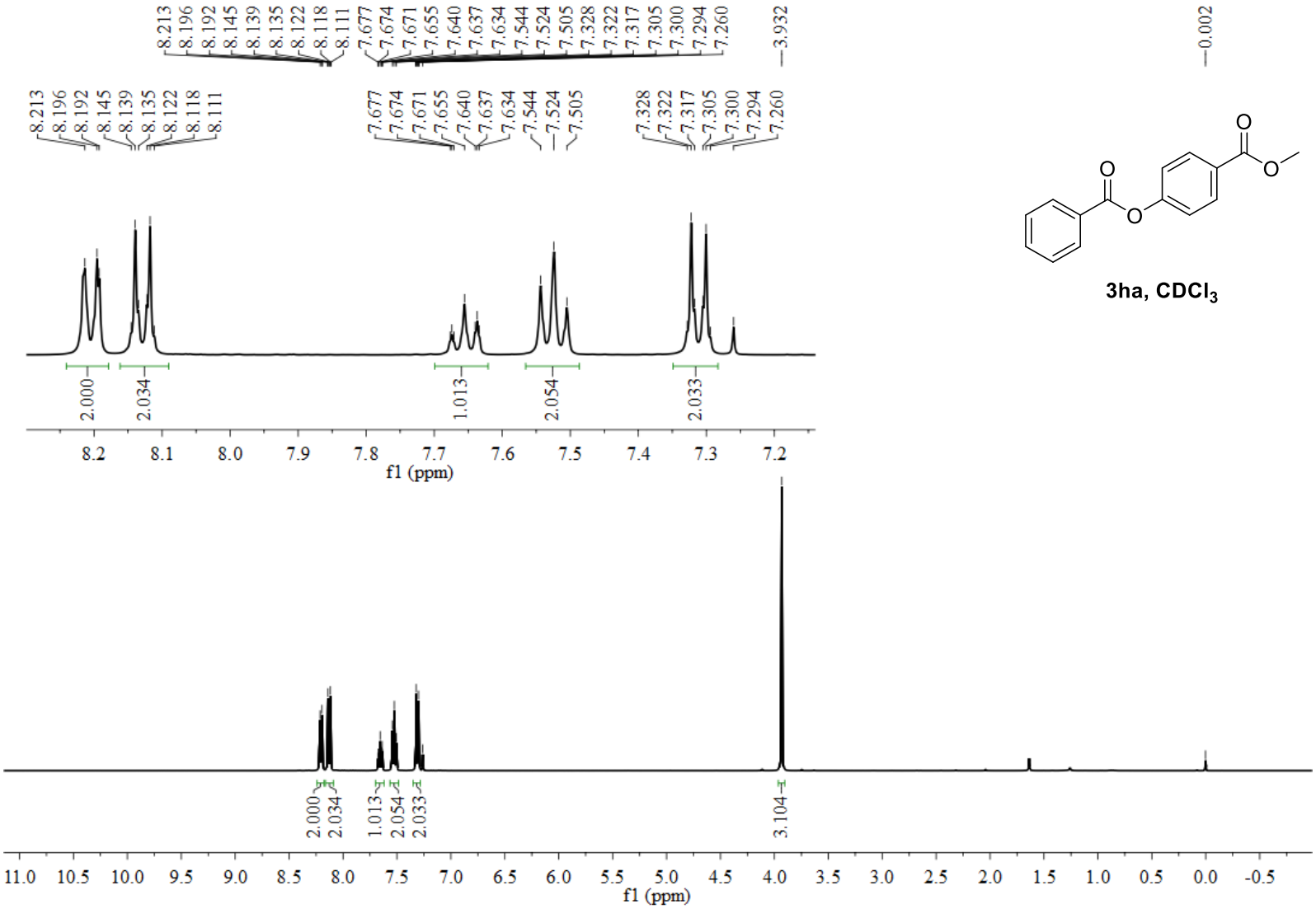

8.217
8.216
8.214
8.201
8.196
8.192
8.152
8.146
8.140
8.129
8.123
8.117
7.670
7.651
7.646
7.636
7.632
7.629
7.540
7.536
7.520
7.501
7.324
7.318
7.312
7.301
7.295
7.260
4.420
4.402
4.384
4.366
1.422
1.405
1.387
0.003
1.929
1.939
0.968
1.978
1.963
f1 (ppm)
2.000
2.993
3fa, CDCl3

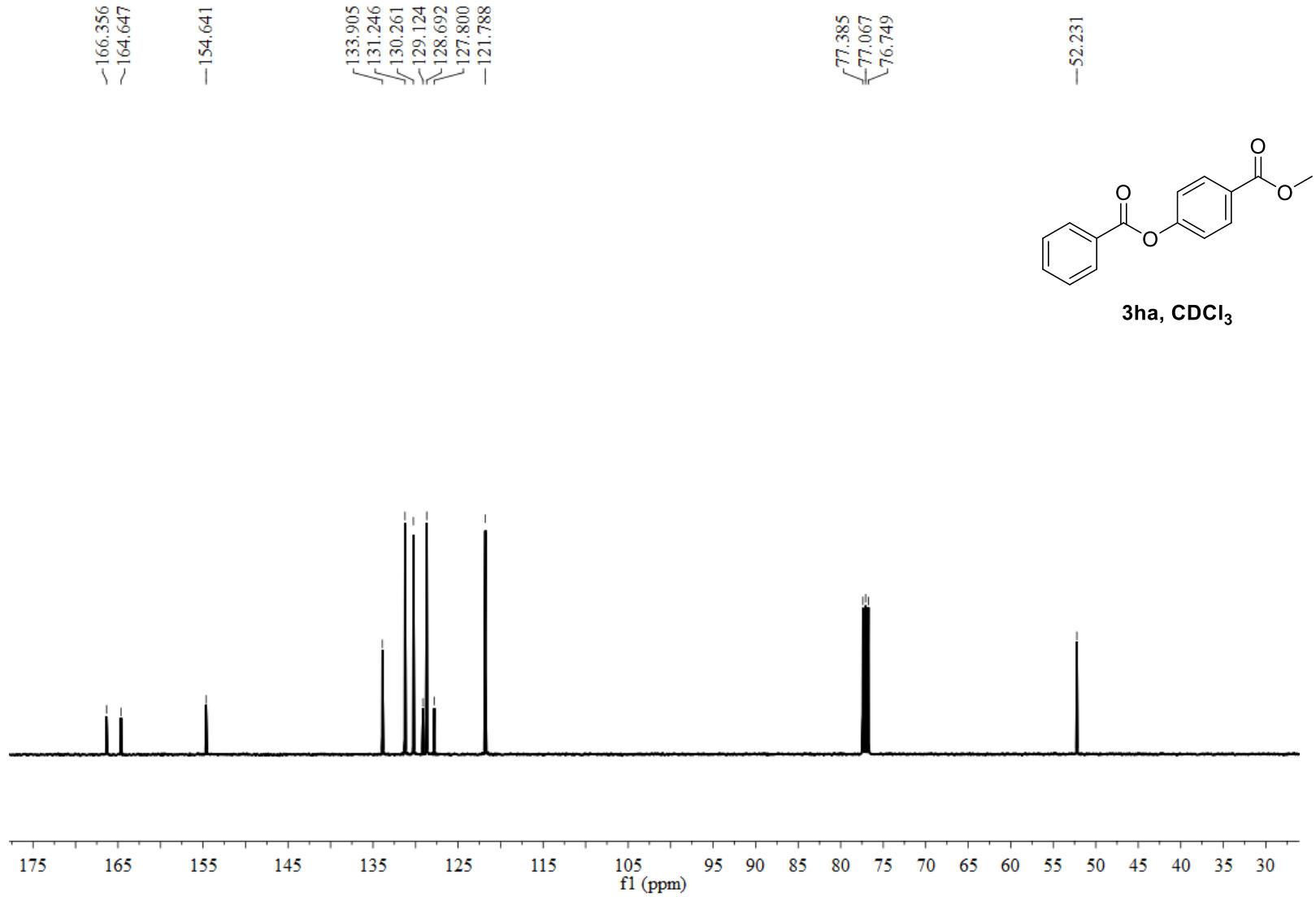

165.871
164.660
154.564
133.888
131.196
130.258
129.150
128.685
128.156
121.732
77.398
77.080
76.762
61.112
14.358
O
O
O
O
3fa, CDCl3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

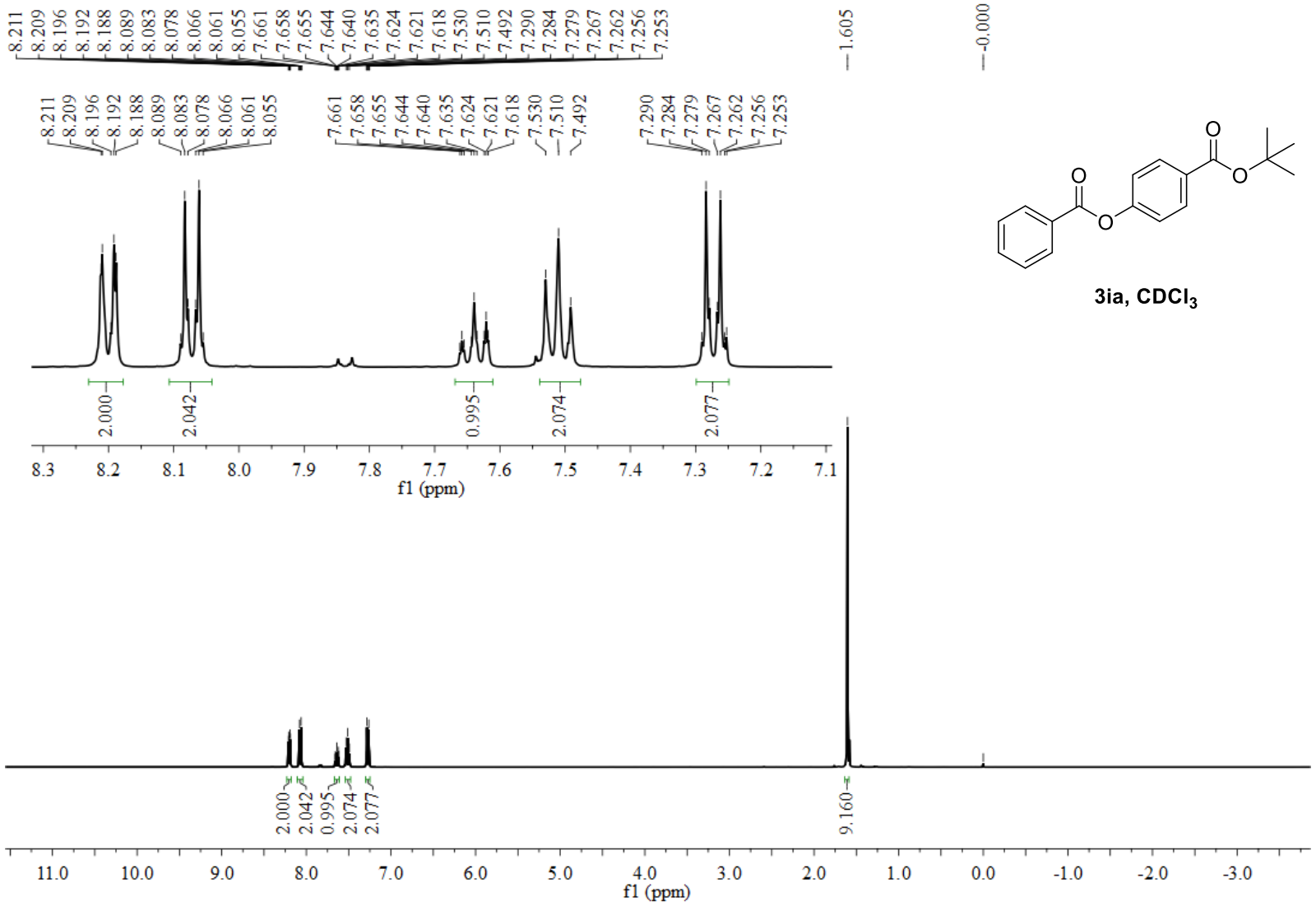

8.222
8.220
8.202
8.199
7.982
7.979
7.976
7.963
7.960
7.957
7.910
7.905
7.901
7.675
7.673
7.670
7.654
7.638
7.635
7.544
7.533
7.525
7.513
7.506
7.494
7.451
7.448
7.445
7.443
7.431
7.428
7.425
7.422
7.260
3.927
0.003
2.000
1.014
0.957
1.022
3.064
1.005
3.087
f1 (ppm)

3ga, $CDCl_3$

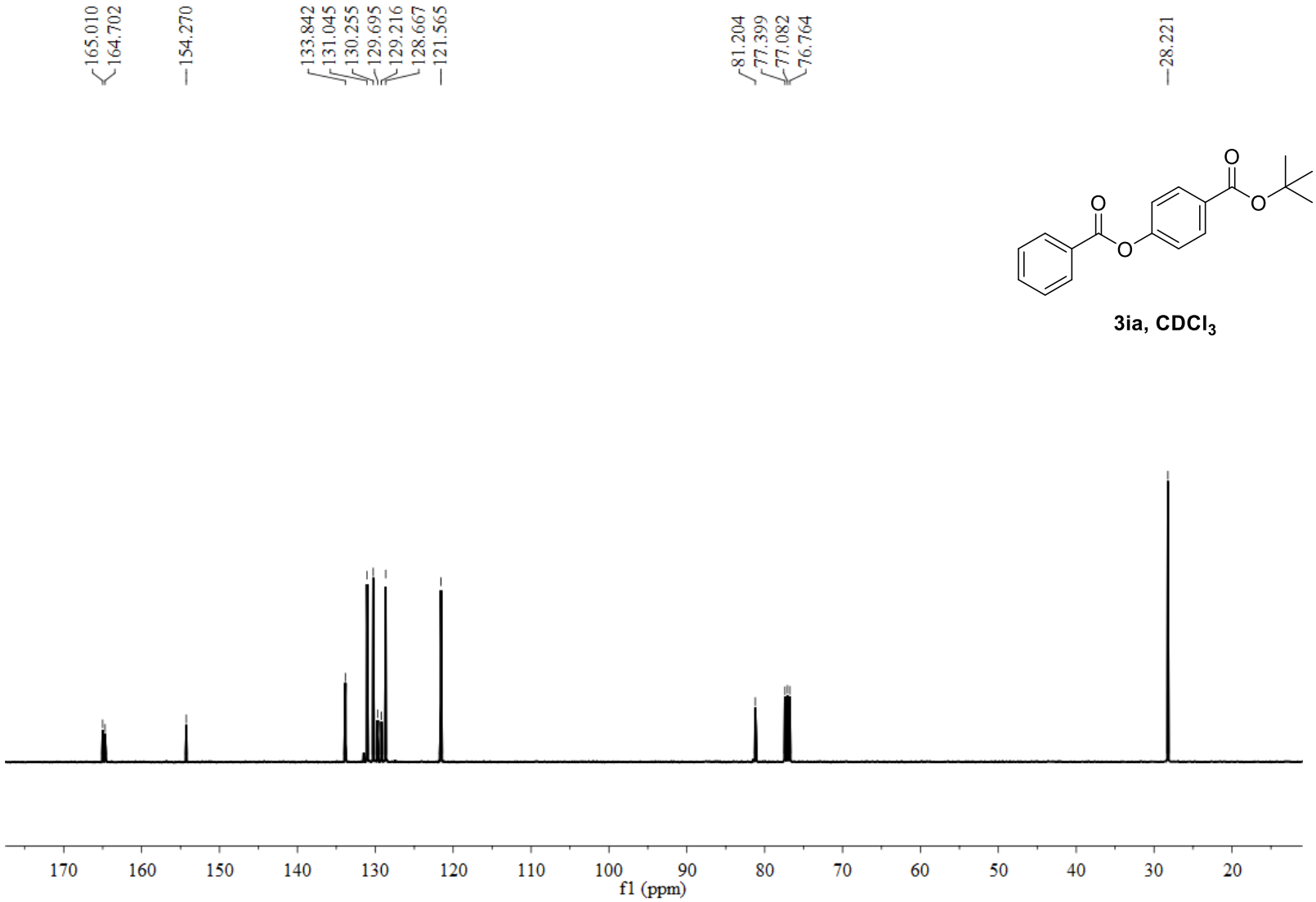

166.200
164.982
150.930
133.832
131.770
130.239
129.527
129.202
128.668
127.107
126.446
123.025
77.384
77.066
76.749
52.334
O
O
O
O
3ga, CDCl3
165
155
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
f1 (ppm)

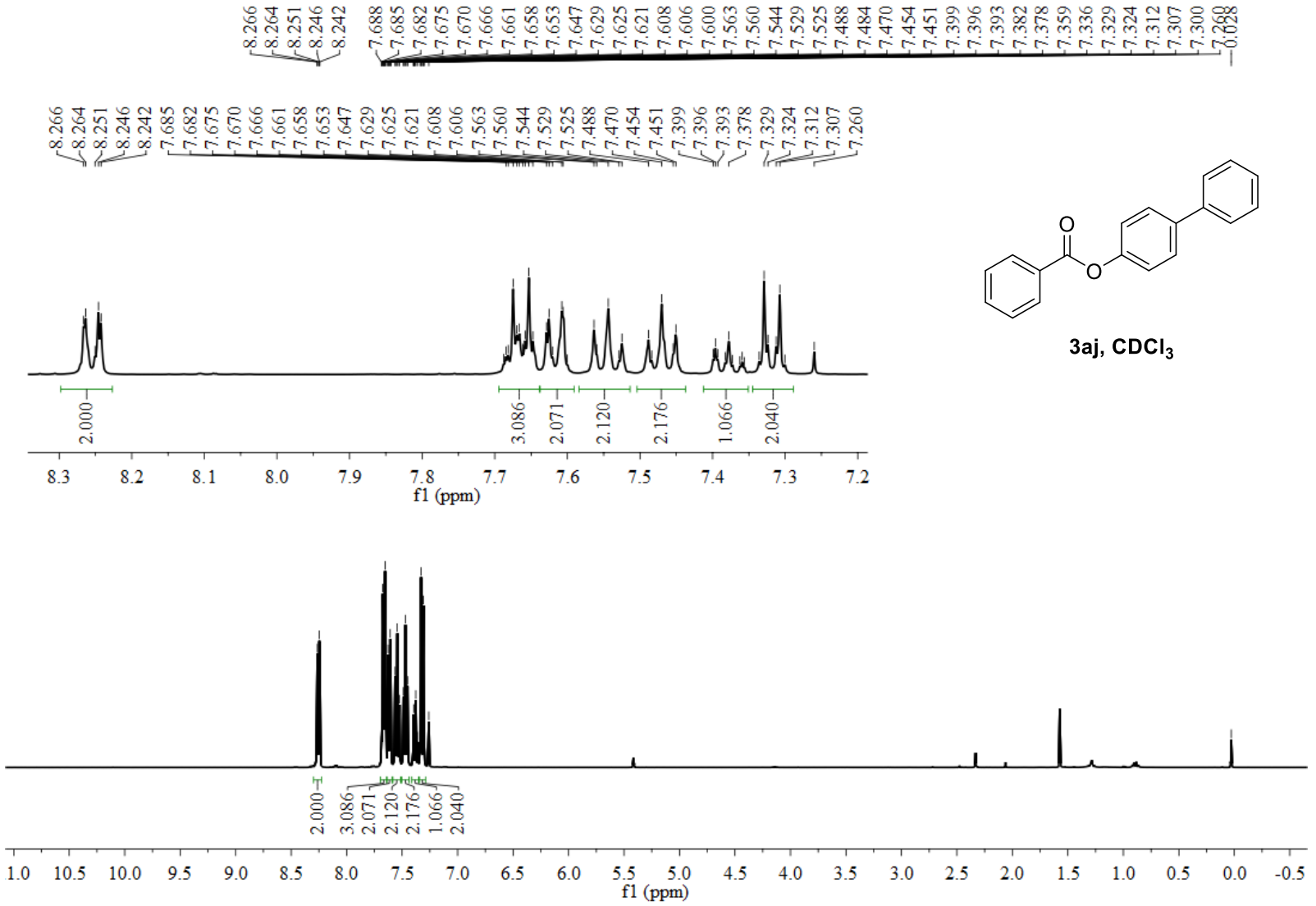

8.213
8.196
8.192
8.145
8.139
8.135
8.122
8.118
8.111
7.677
7.674
7.671
7.655
7.640
7.637
7.634
7.544
7.524
7.505
7.328
7.322
7.317
7.305
7.300
7.294
7.260
3.932
0.002
2.000
2.034
1.013
2.054
2.033
3.104
f1 (ppm)
3ha, CDCl3

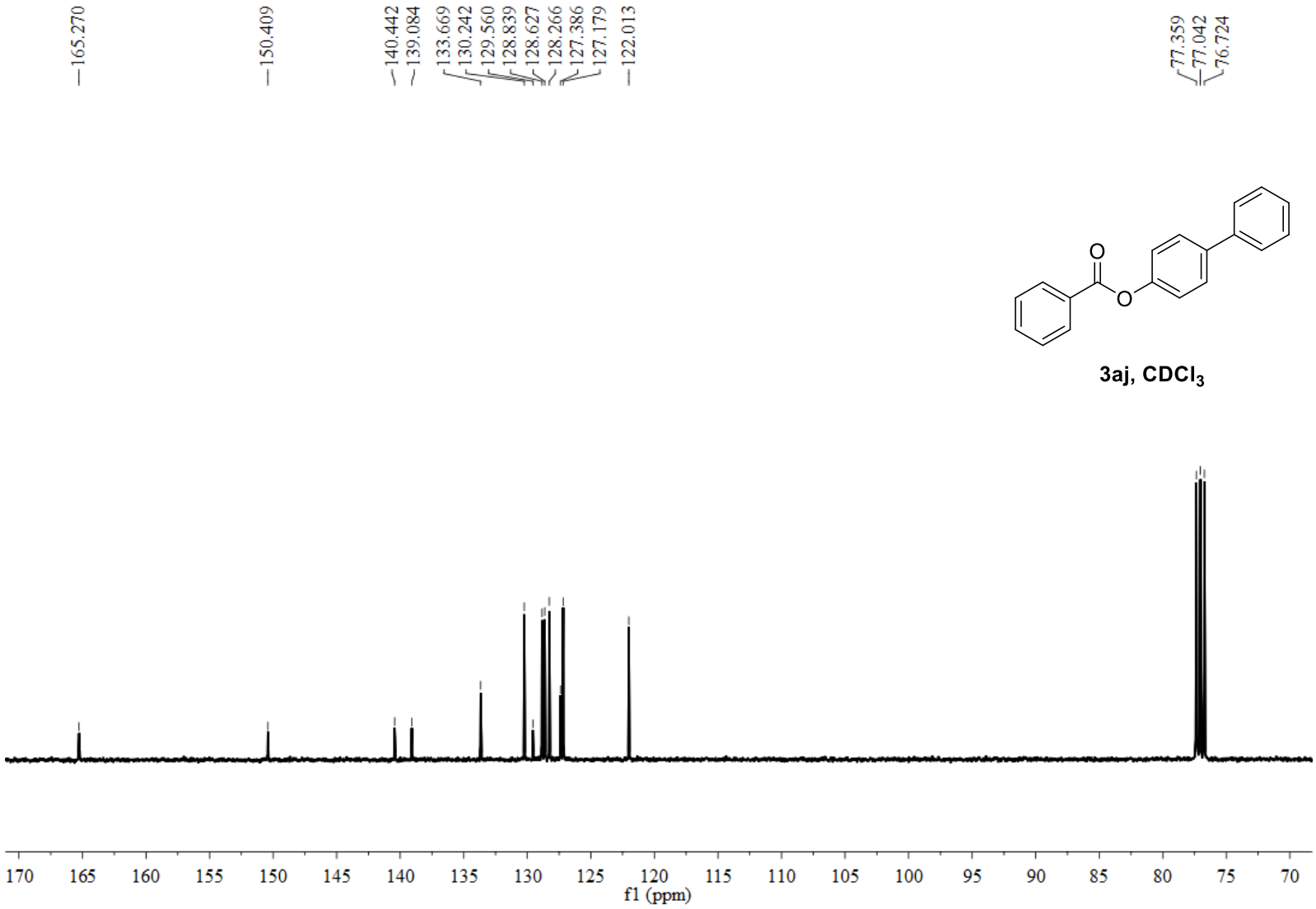

166.356
164.647
154.641
133.905
131.246
130.261
129.124
128.692
127.800
121.788
77.385
77.067
76.749
52.231
O
O
O
O
3ha, CDCl3
175
165
155
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
f1 (ppm)

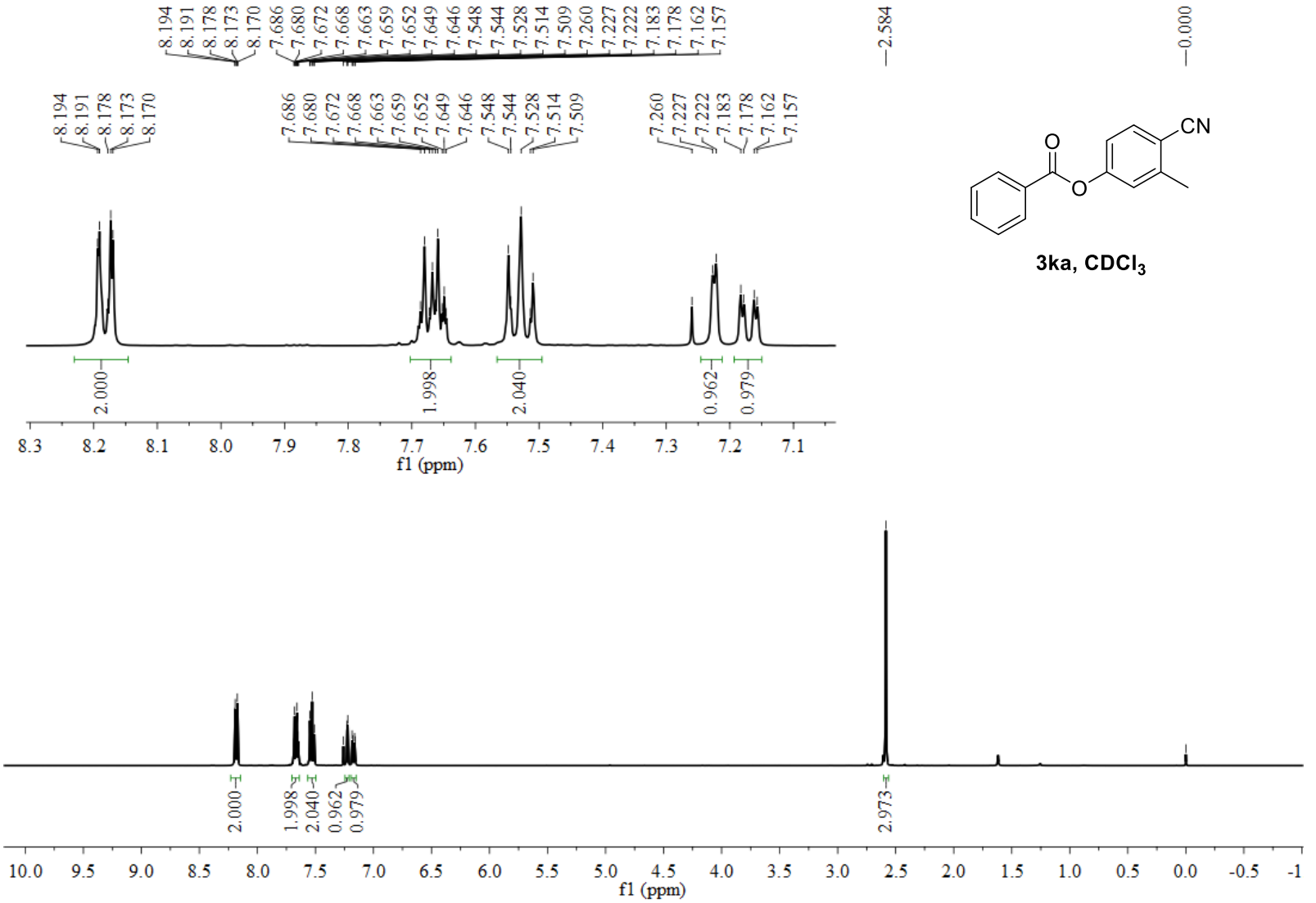

8.211
8.209
8.196
8.192
8.188
8.089
8.083
8.078
8.066
8.061
8.055
7.661
7.658
7.655
7.644
7.640
7.635
7.624
7.621
7.618
7.530
7.510
7.492
7.290
7.284
7.279
7.267
7.262
7.256
7.253
1.605
0.000
2.000
2.042
0.995
2.074
2.077
9.160
f1 (ppm)
f1 (ppm)

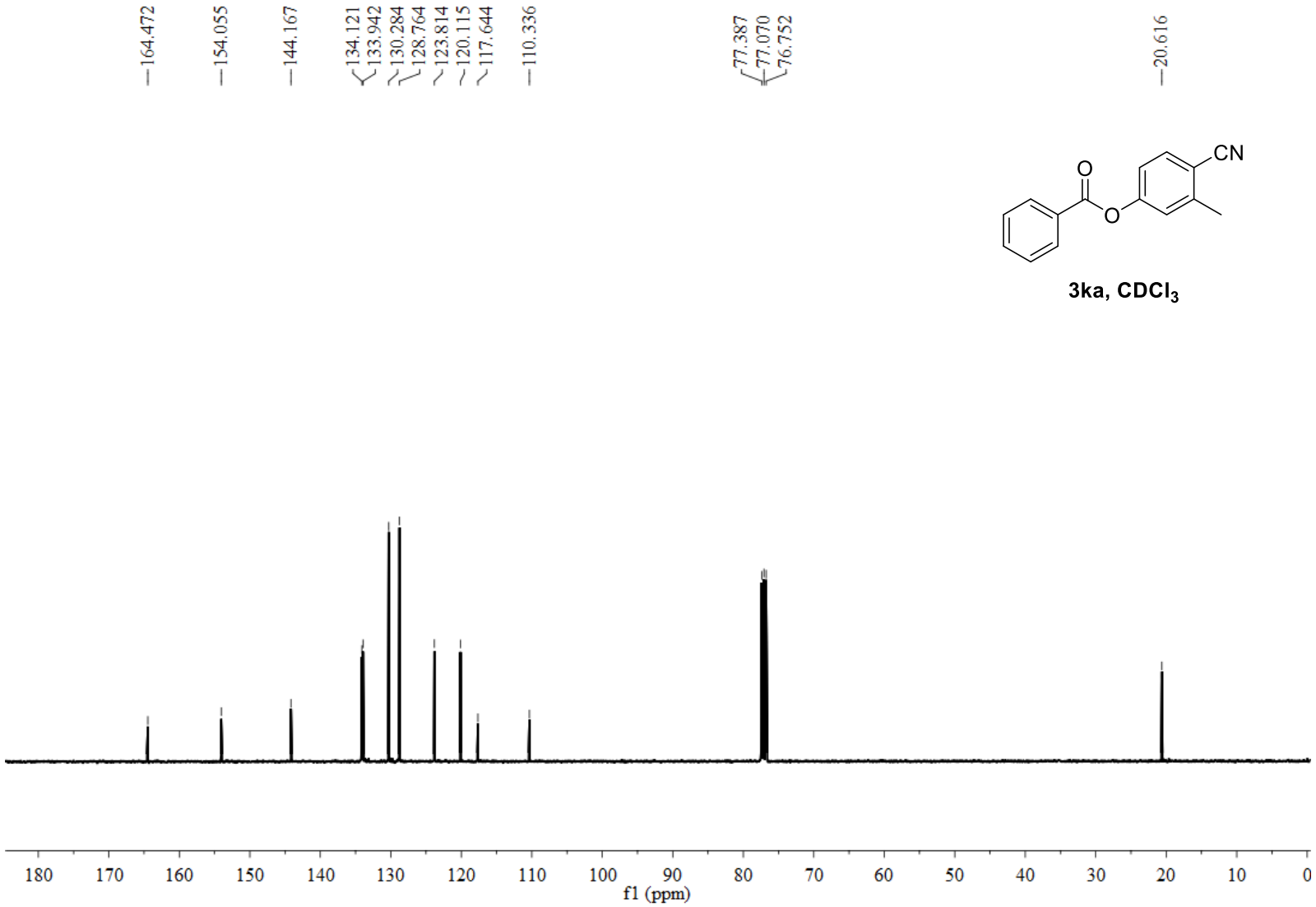
3ia, $CDCl_3$

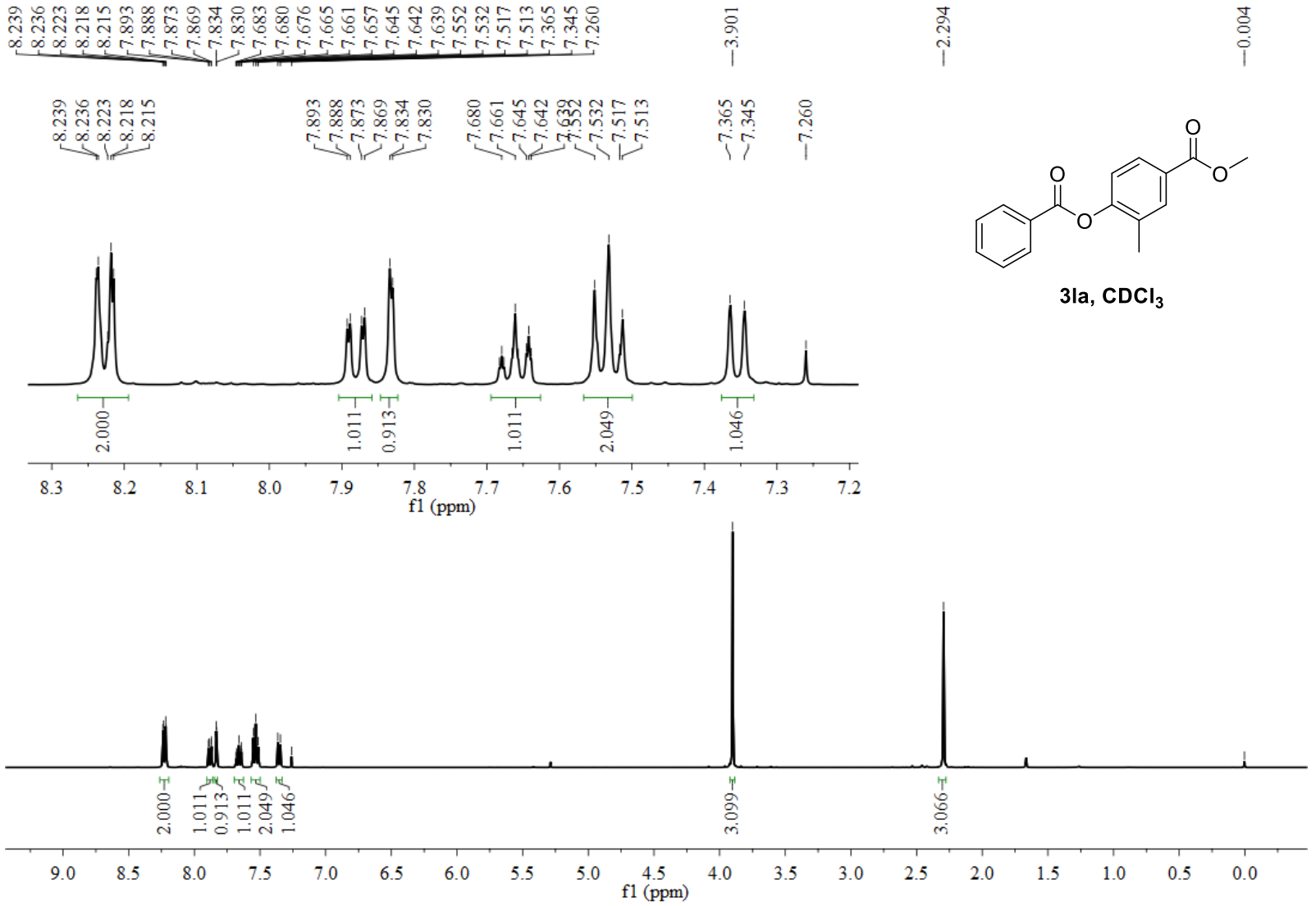

165.010
164.702
154.270
133.842
131.045
130.255
129.695
129.216
128.667
121.565
81.204
77.399
77.082
76.764
28.221
O
O
O
O
3ia, CDCl3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

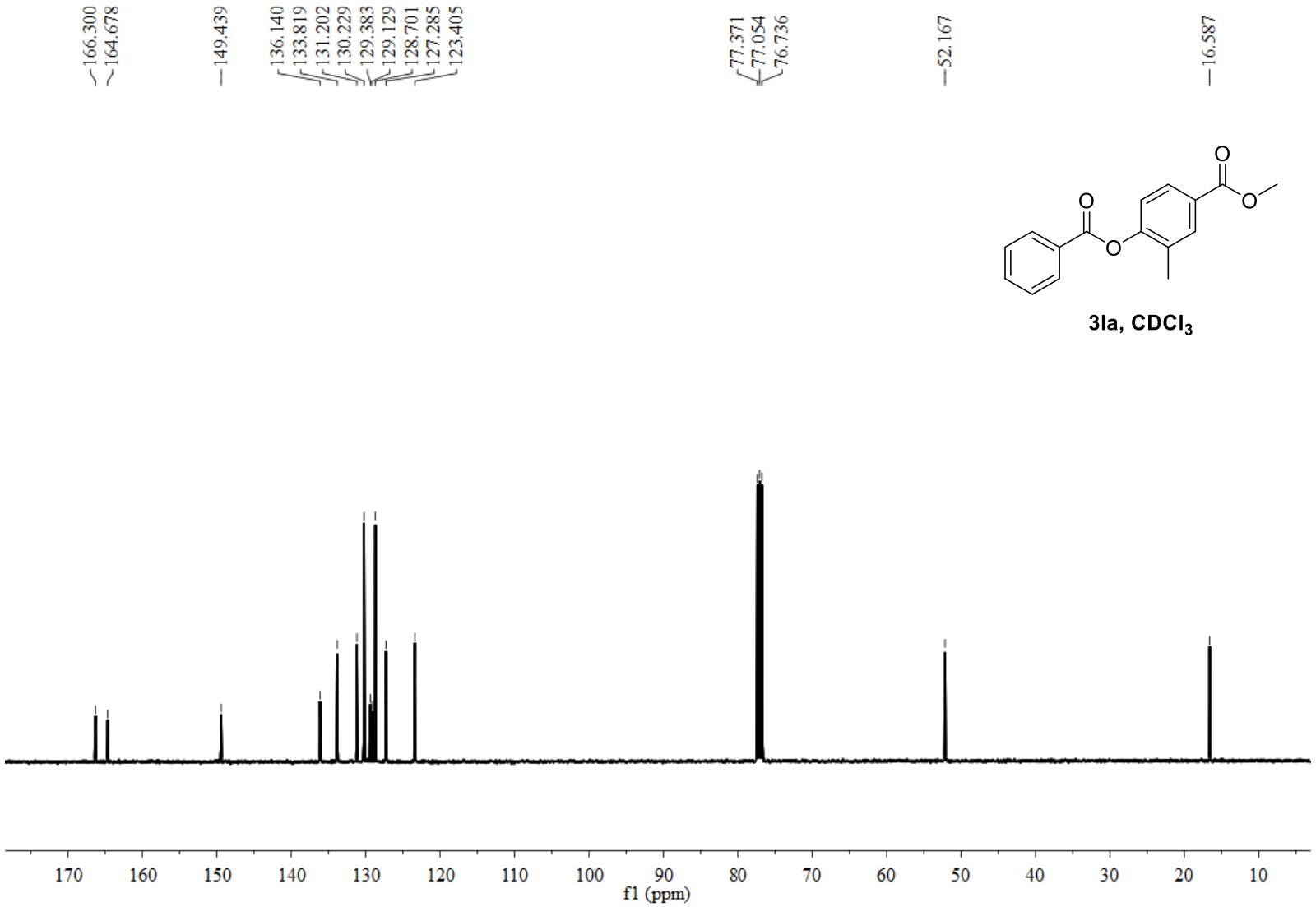

8.266
8.264
8.251
8.246
8.242
7.688
7.685
7.682
7.675
7.670
7.666
7.661
7.658
7.653
7.647
7.629
7.625
7.621
7.608
7.606
7.600
7.563
7.560
7.544
7.529
7.525
7.488
7.484
7.470
7.454
7.451
7.399
7.396
7.393
7.382
7.378
7.359
7.336
7.329
7.324
7.312
7.307
7.300
7.260
0.028
2.000
3.086
2.071
2.120
2.176
1.066
2.040
f1 (ppm)
O
O
3aj, CDCl3
f1 (ppm)

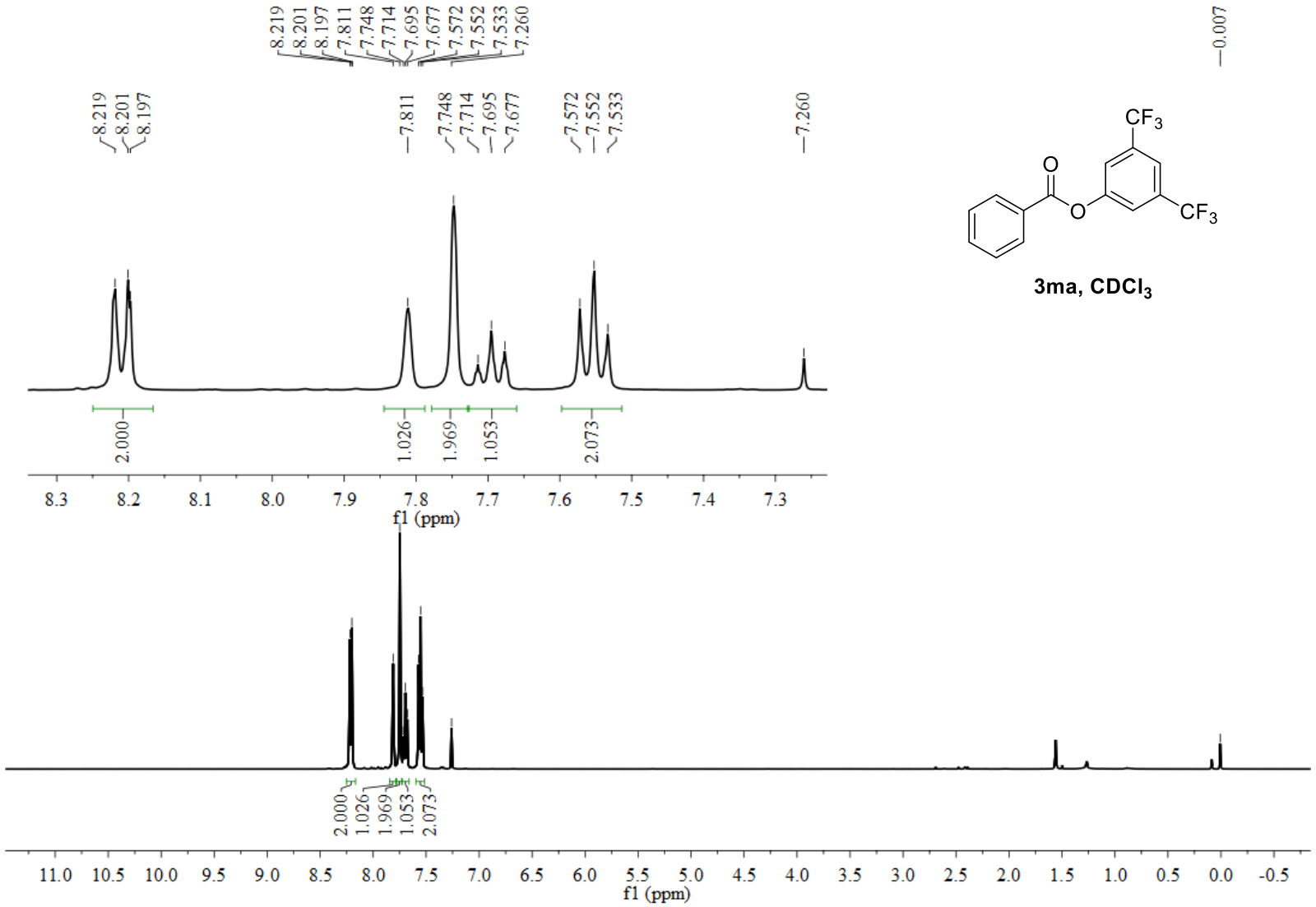

165.270
150.409
140.442
139.084
133.669
130.242
129.560
128.839
128.627
128.266
127.386
127.179
122.013
77.359
77.042
76.724
O
O
3aj, CDCl3
170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70
f1 (ppm)

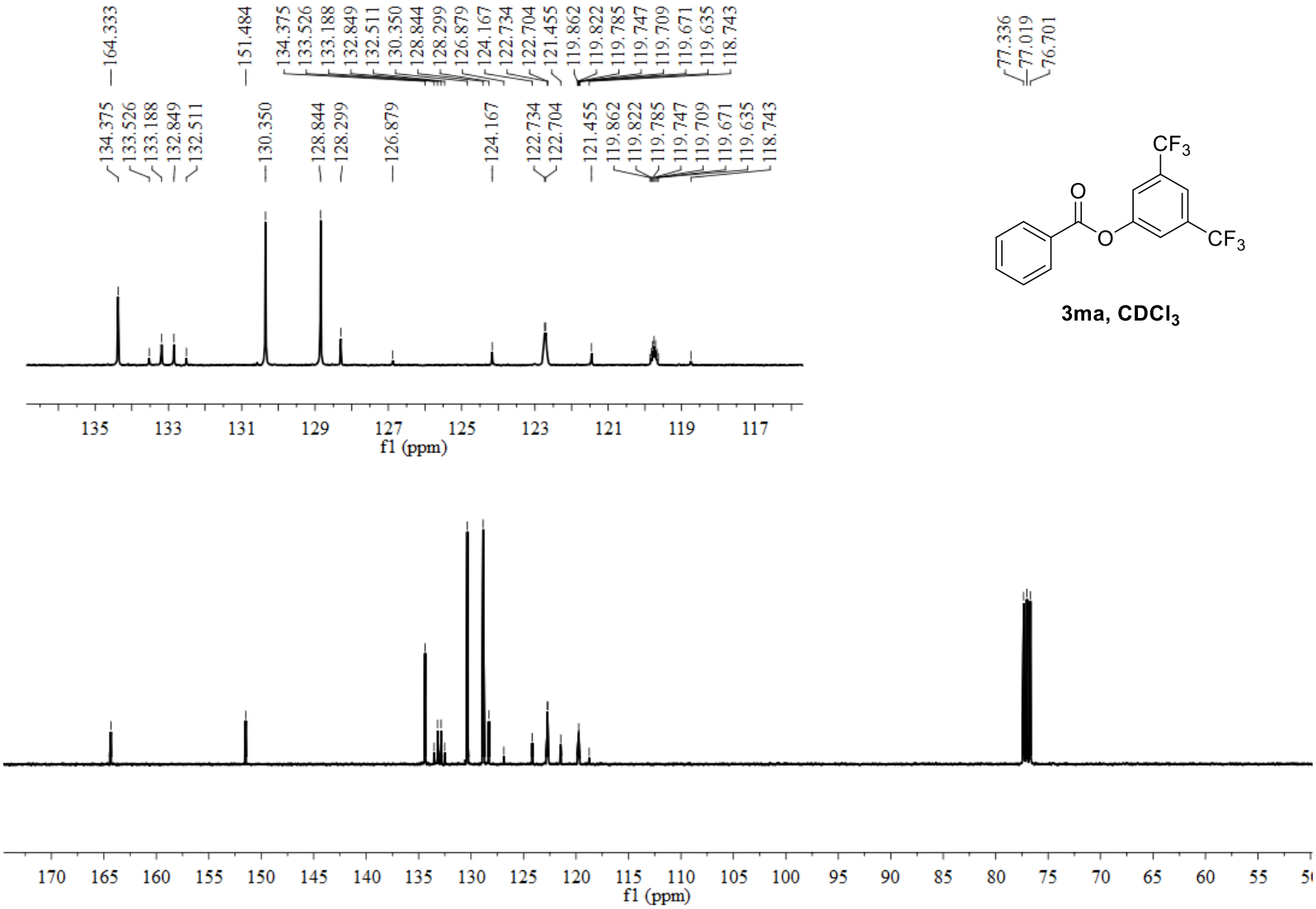

8.194
8.191
8.178
8.173
8.170
7.686
7.680
7.672
7.668
7.663
7.659
7.652
7.649
7.646
7.548
7.544
7.528
7.514
7.509
7.260
7.227
7.222
7.183
7.178
7.162
7.157
2.584
0.000
CN
O
O
3ka, CDCl3
2.000
1.998
2.040
0.962
0.979
2.973
f1 (ppm)

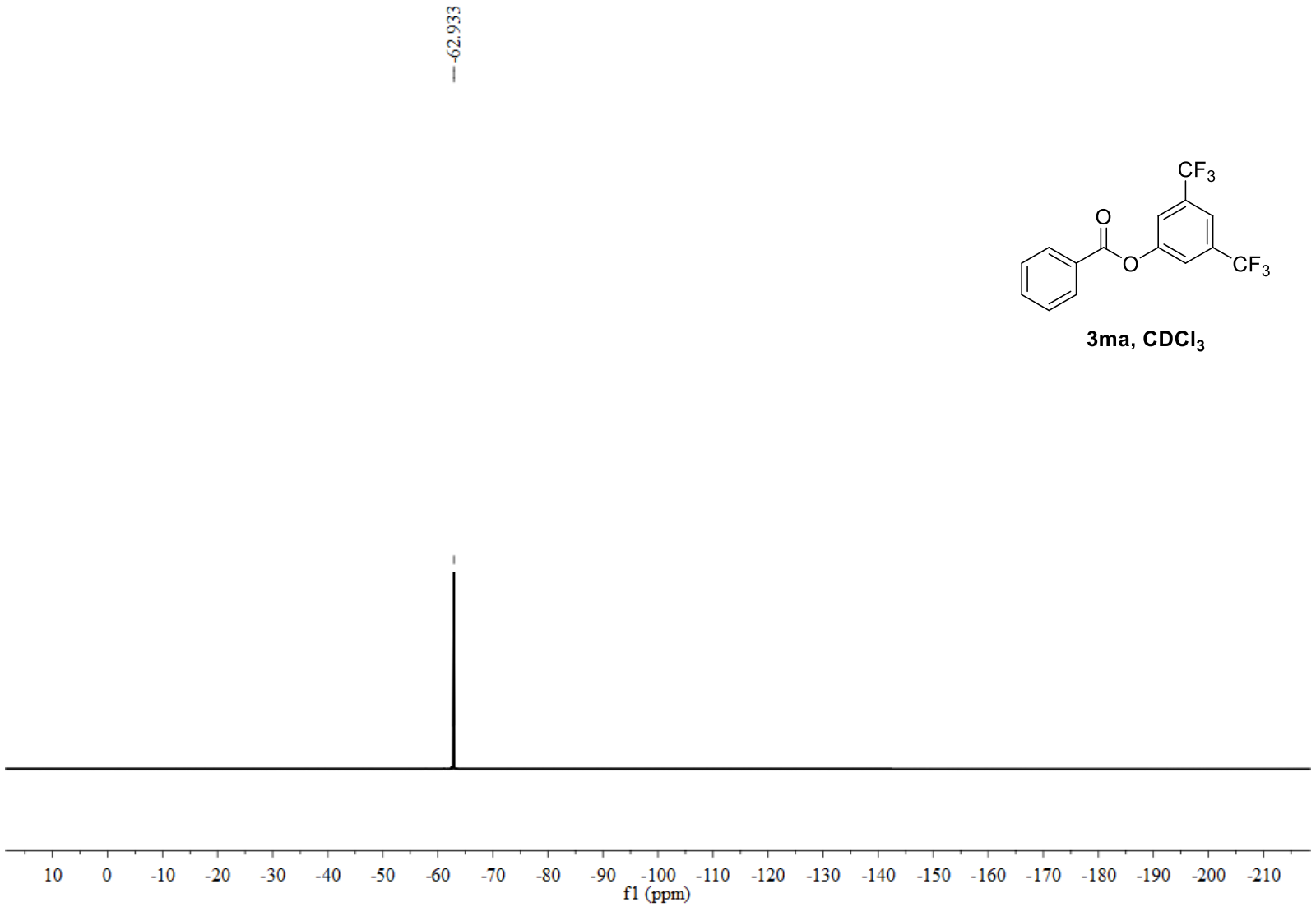

164.472
154.055
144.167
134.121
133.942
130.284
128.764
123.814
120.115
117.644
110.336
77.387
77.070
76.752
20.616
CN
O
O
3ka, CDCl3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.239
8.236
8.223
8.218
8.215
7.893
7.888
7.873
7.869
7.834
7.830
7.683
7.680
7.676
7.665
7.661
7.657
7.645
7.642
7.639
7.552
7.532
7.517
7.513
7.365
7.345
7.260
3.901
2.294
0.004
2.000
1.011
0.913
1.011
2.049
1.046
f1 (ppm)
3.099
3.066
O
O
O
O
3la, CDCl3

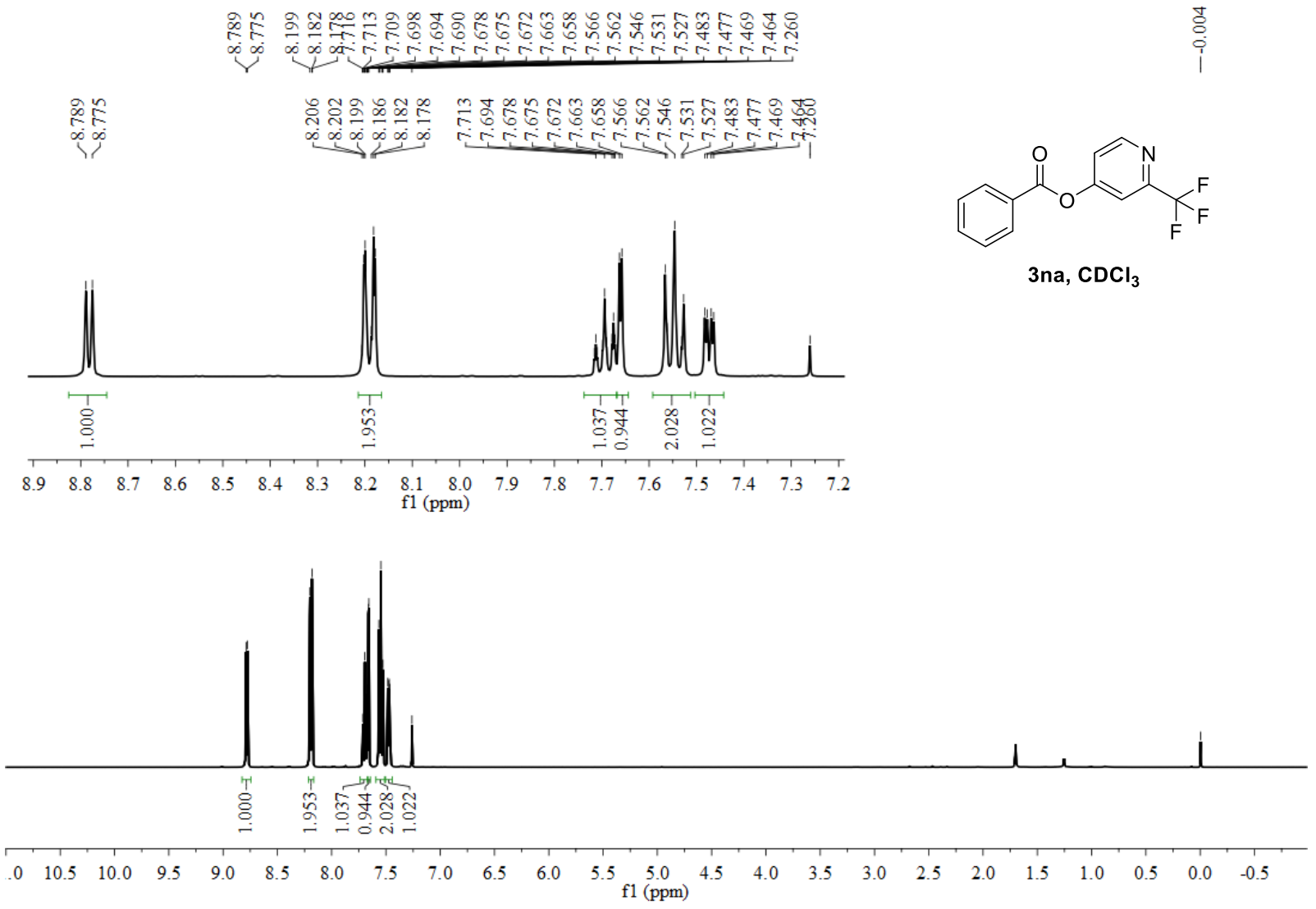

166.300
164.678
149.439
136.140
133.819
131.202
130.229
129.383
129.129
128.701
127.285
123.405
77.371
77.054
76.736
52.167
16.587
O
O
O
O
3la, CDCl3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

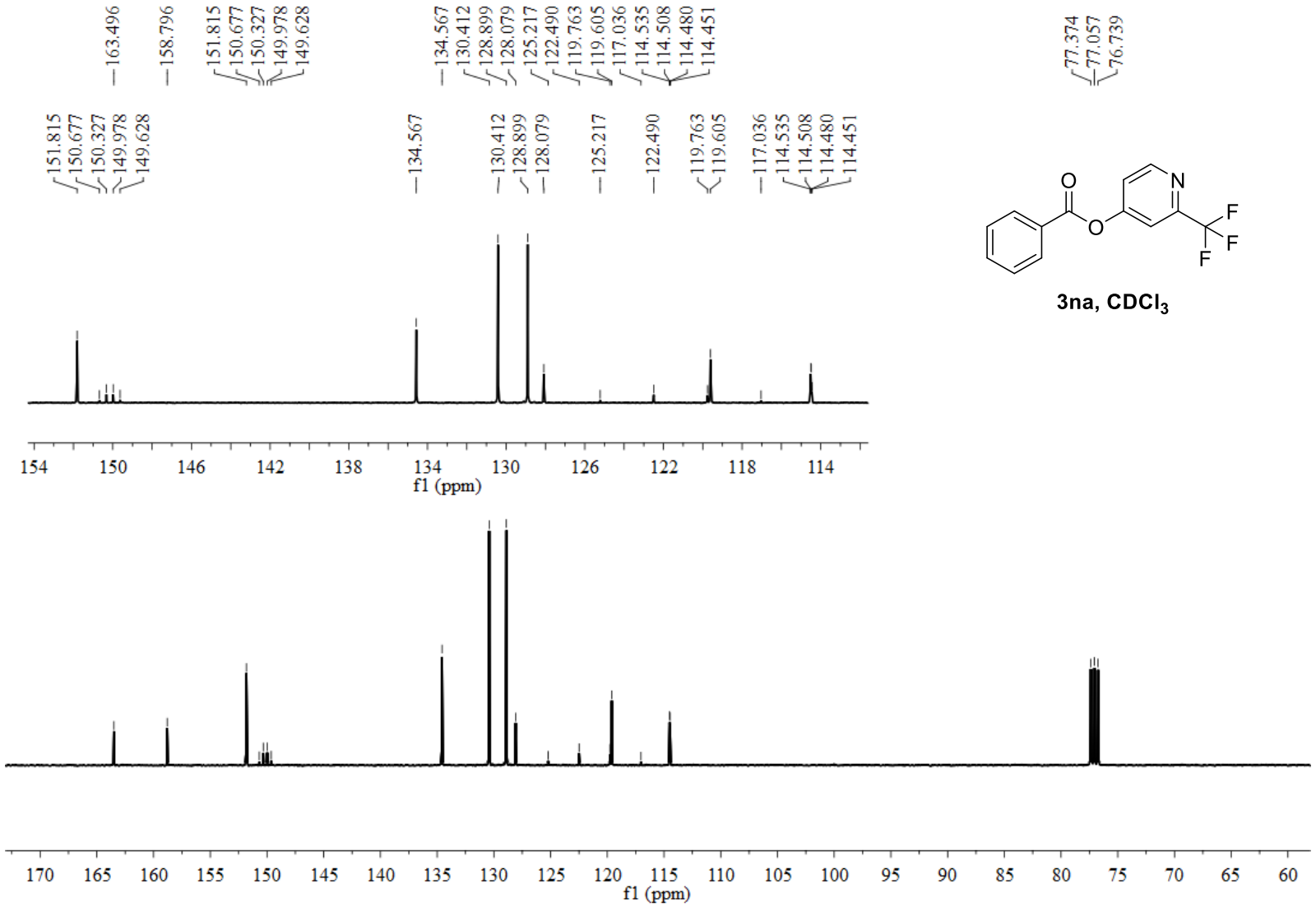

8.219
8.201
8.197
7.811
7.748
7.714
7.695
7.677
7.572
7.552
7.533
7.260
0.007
2.000
1.026
1.969
1.053
2.073
f1 (ppm)
CF3
CF3
O
O
3ma, CDCl3

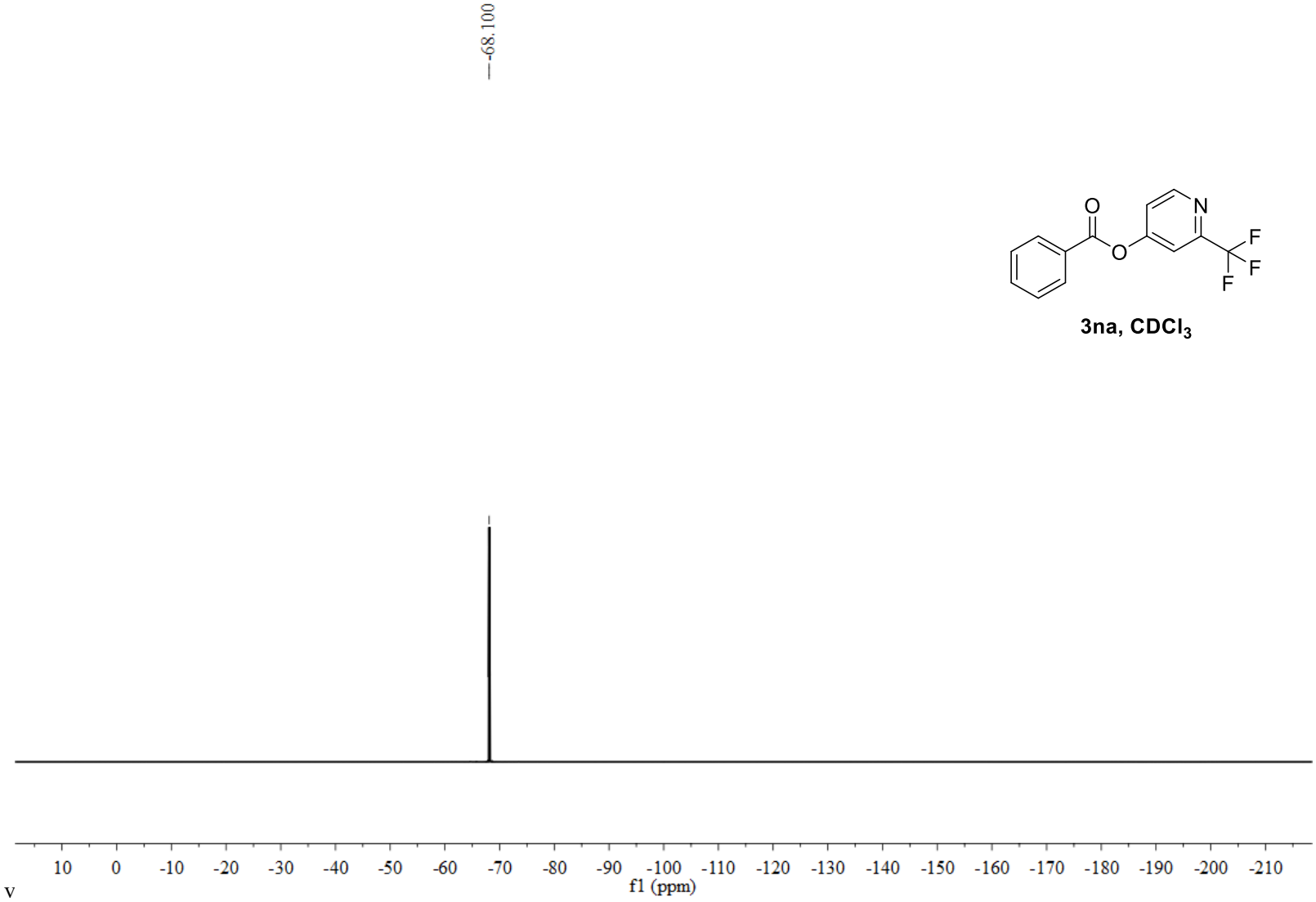

164.333
151.484
134.375
133.526
133.188
132.849
132.511
130.350
128.844
128.299
126.879
124.167
122.734
122.704
121.455
119.862
119.822
119.785
119.747
119.709
119.671
119.635
118.743
77.336
77.019
76.701
CF3
CF3
O
O
3ma, CDCl3
f1 (ppm)
f1 (ppm)


-62.933
CF3
O
O
CF3
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)

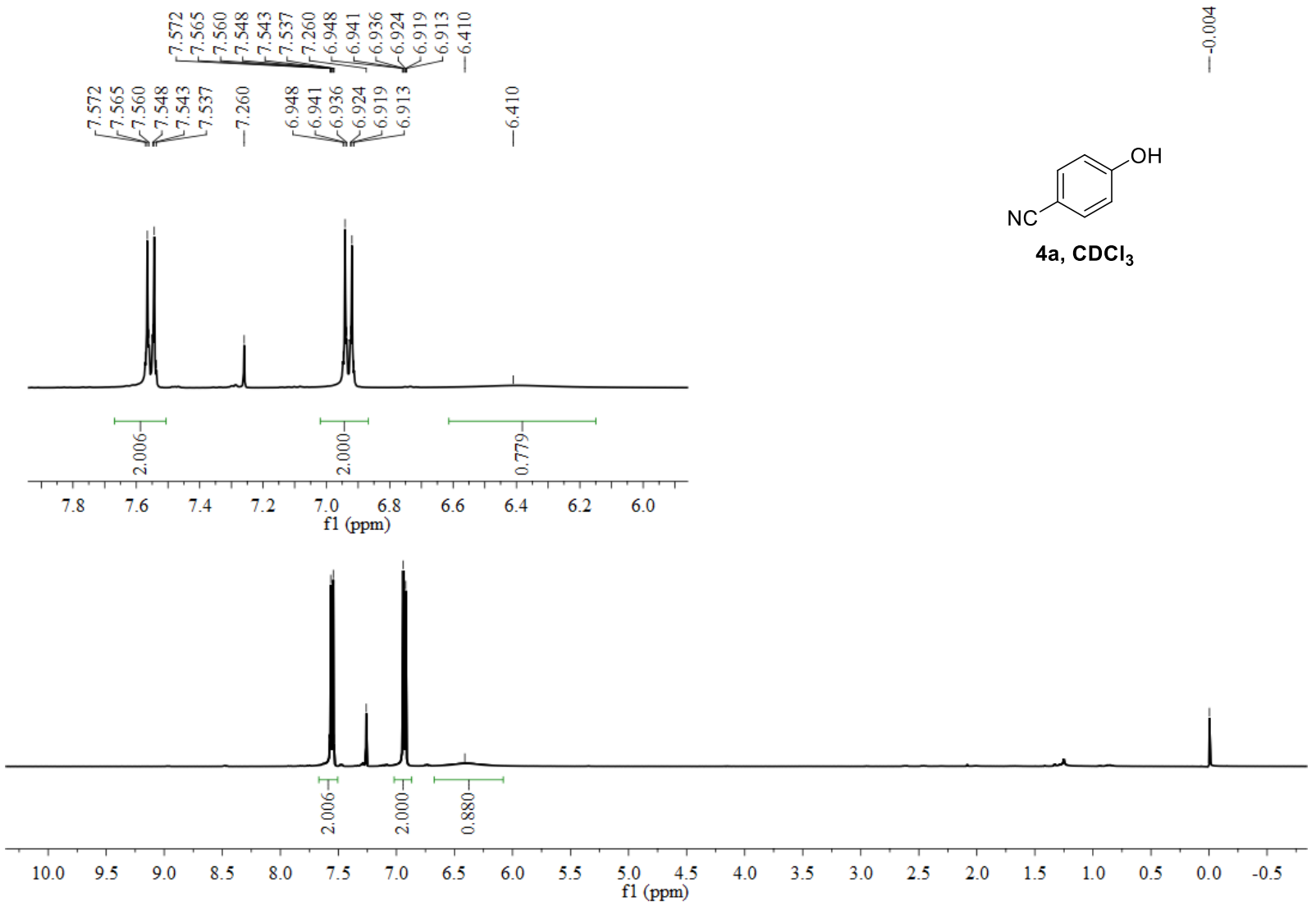
3ma, $CDCl_3$

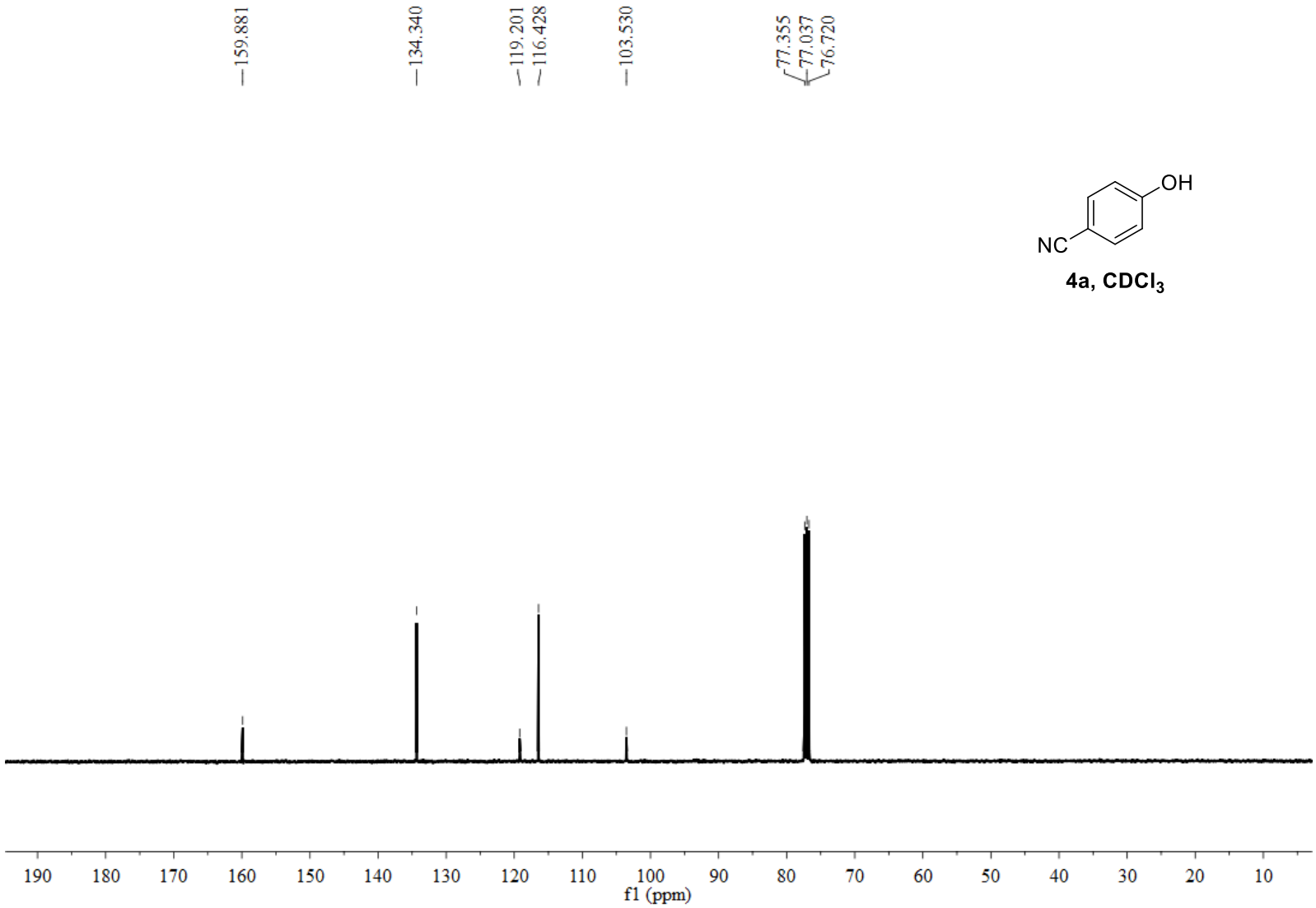

8.789
8.775
8.199
8.182
8.178
7.713
7.709
7.698
7.694
7.690
7.678
7.675
7.672
7.663
7.658
7.566
7.562
7.546
7.531
7.527
7.483
7.477
7.469
7.464
7.260
-0.004
8.206
8.202
8.199
8.186
8.182
8.178
7.713
7.694
7.678
7.675
7.672
7.663
7.658
7.566
7.562
7.546
7.531
7.527
7.483
7.477
7.469
7.464
7.260
1.000
1.953
1.037
0.944
2.028
1.022
f1 (ppm)
O
N
O
F
F
F
3na, CDCl3
1.000
1.953
1.037
0.944
2.028
1.022
f1 (ppm)

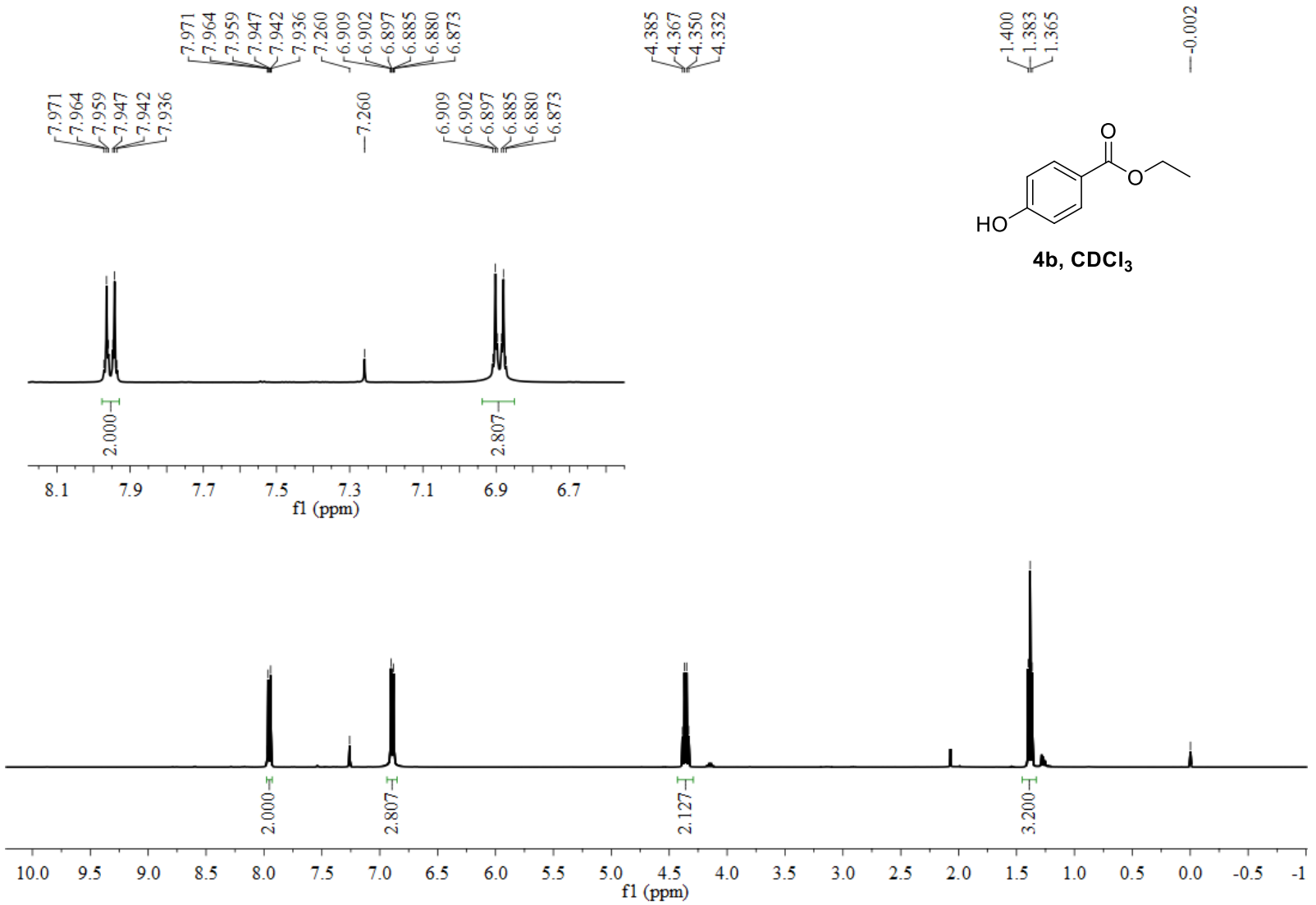

163.496
158.796
151.815
150.677
150.327
149.978
149.628
134.567
130.412
128.899
128.079
125.217
122.490
119.763
119.605
117.036
114.535
114.508
114.480
114.451
77.374
77.057
76.739
O
O
N
F
F
F
3na, CDCl3
f1 (ppm)
f1 (ppm)


-68.100
O
N
O
F
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)

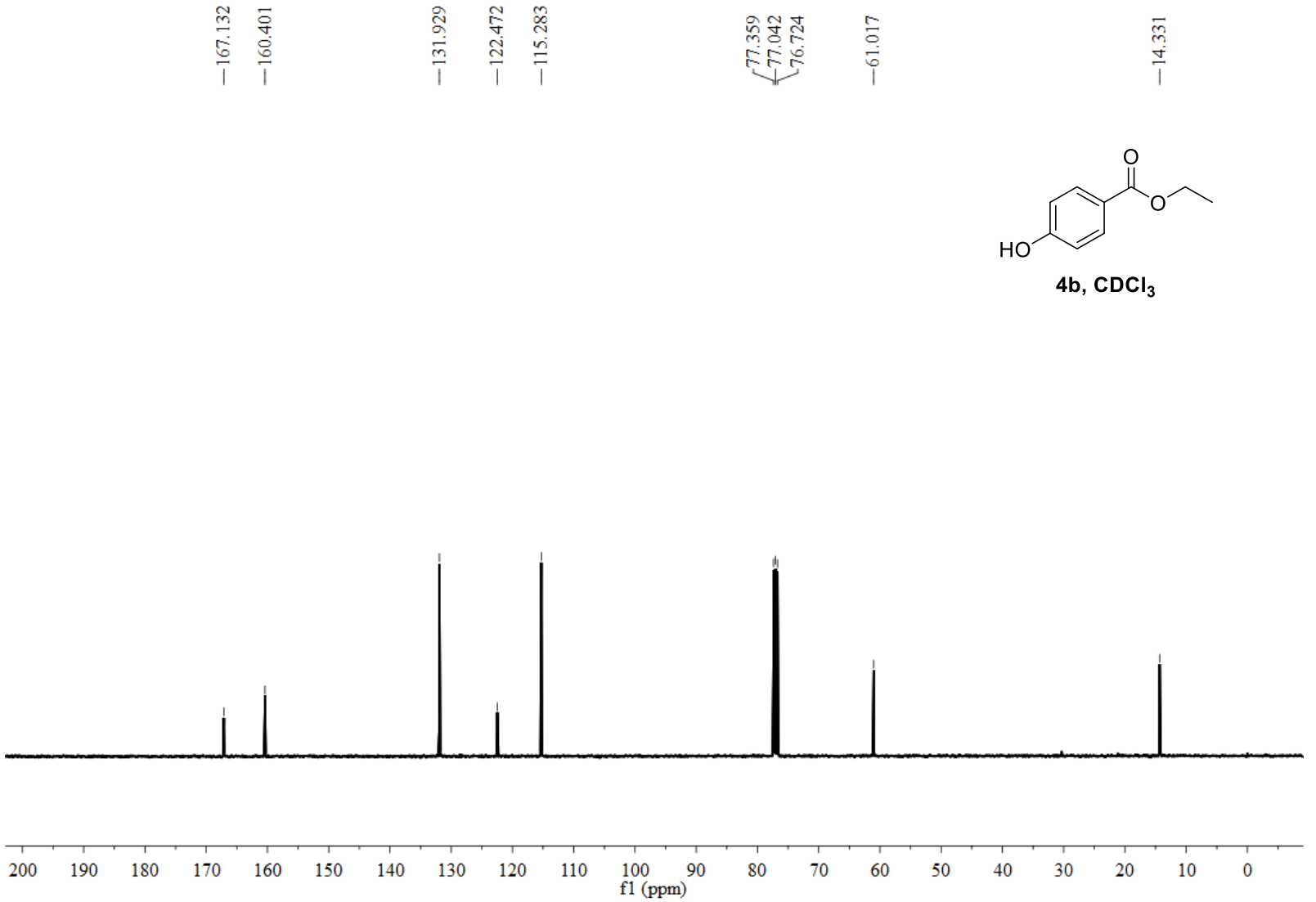
3na, $CDCl_3$

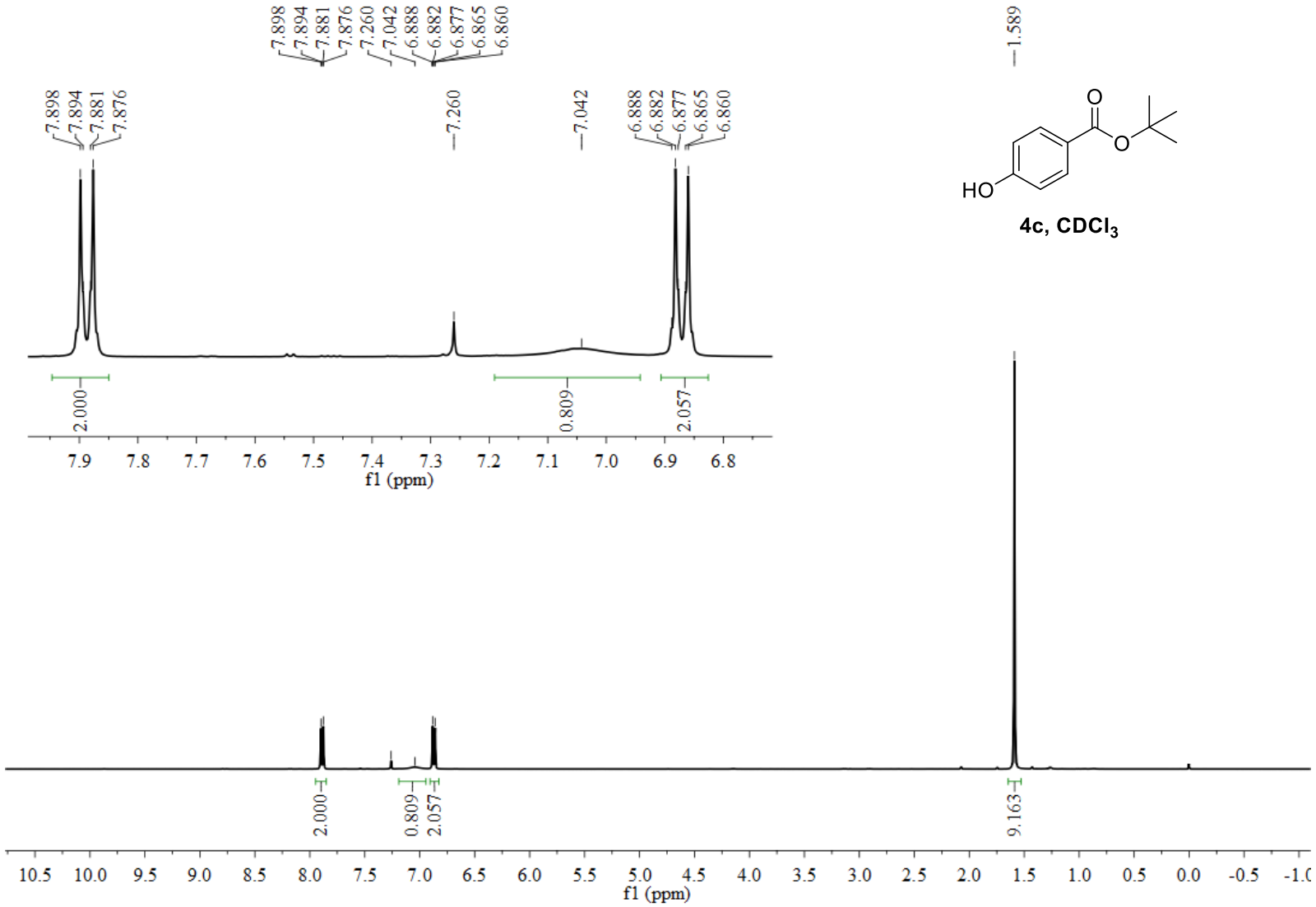

7.572
7.565
7.560
7.548
7.543
7.537
7.260
6.948
6.941
6.936
6.924
6.919
6.913
6.410
-0.004
OH
NC
4a, CDCl3
2.006
2.000
0.779
f1 (ppm)
2.006
2.000
0.880
f1 (ppm)

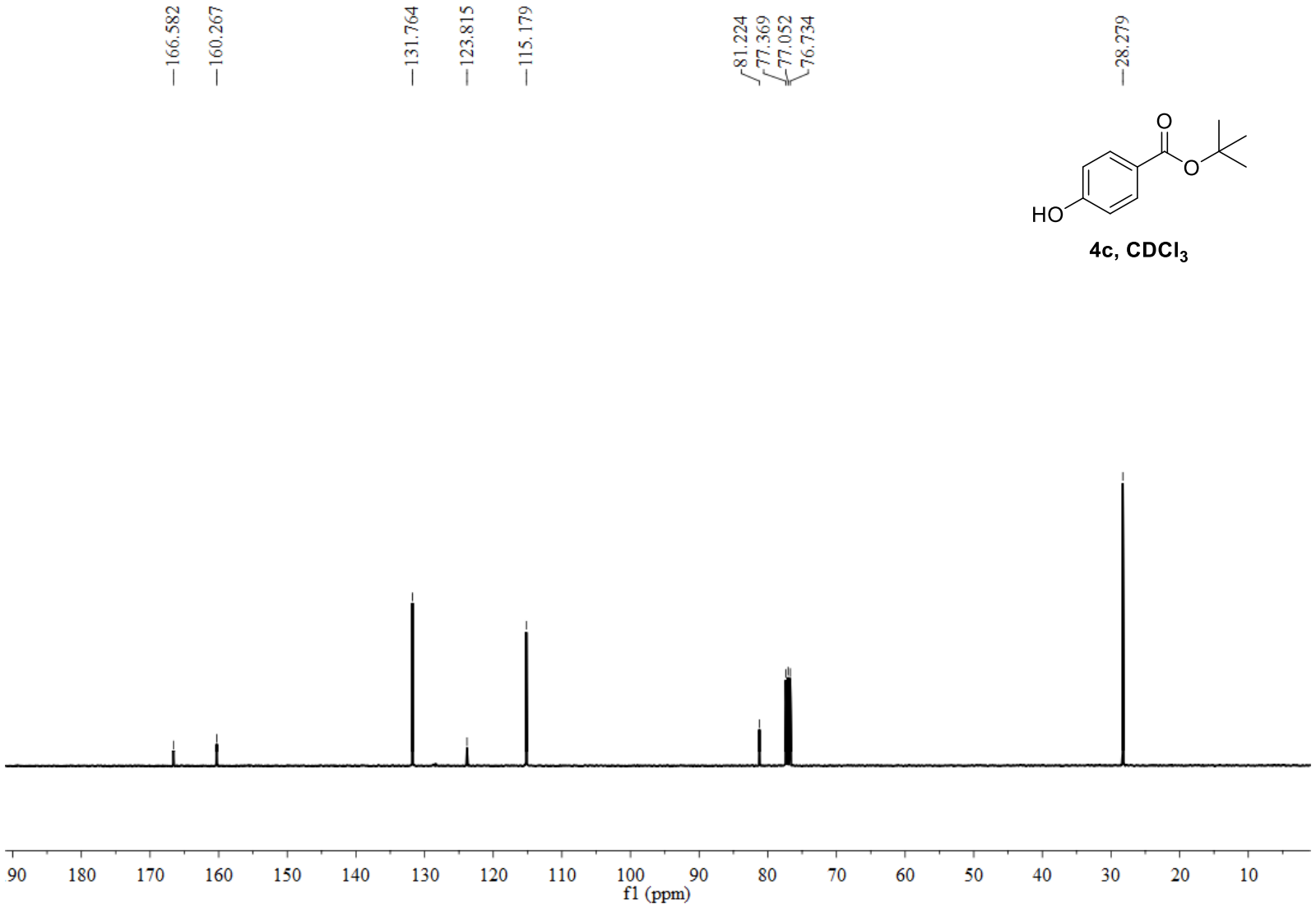

159.881
134.340
119.201
116.428
103.530
77.355
77.037
76.720
OH
NC
4a, CDCl3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

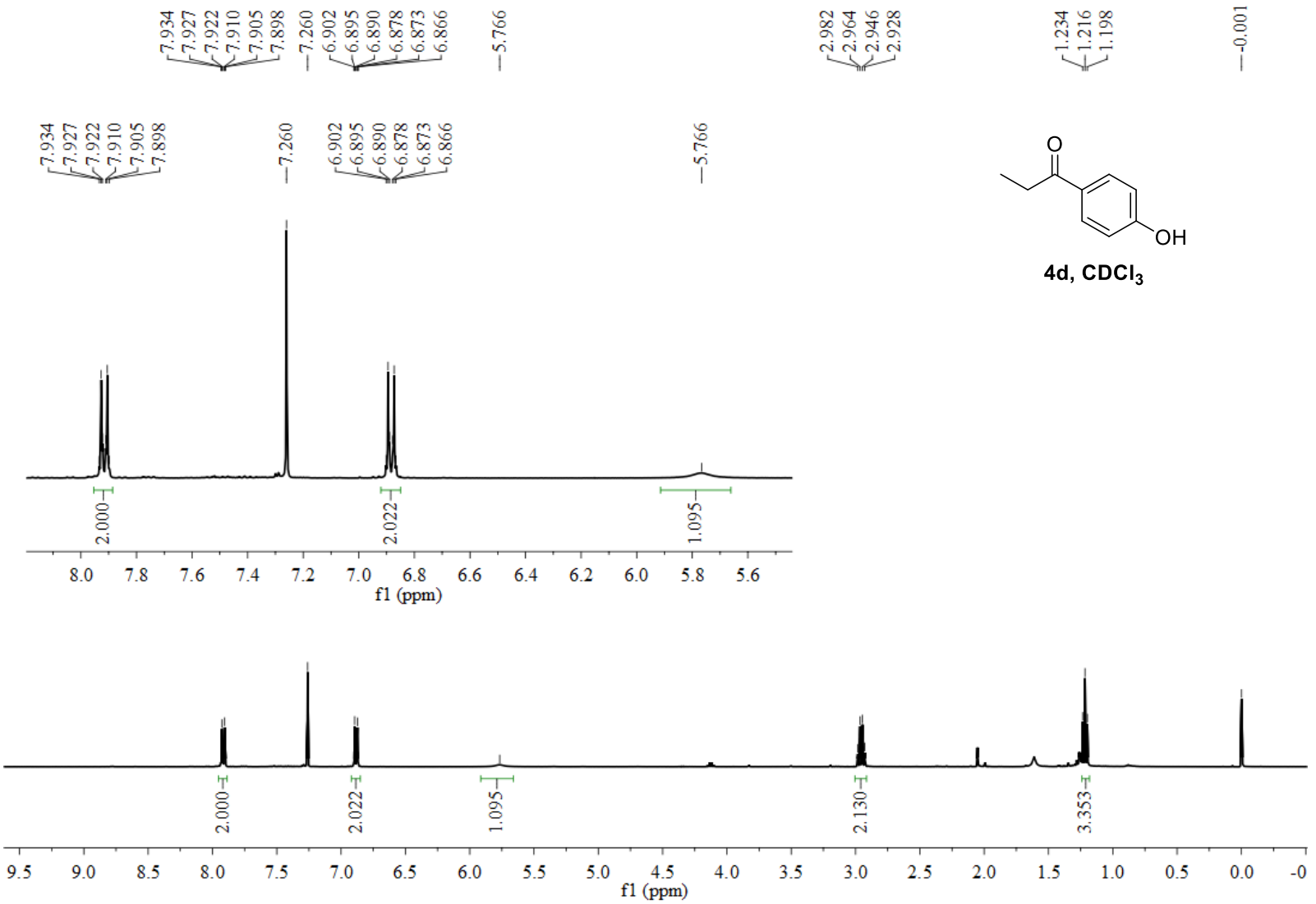

7.971
7.964
7.959
7.947
7.942
7.936
7.260
6.909
6.902
6.897
6.885
6.880
6.873
4.385
4.367
4.350
4.332
1.400
1.383
1.365
-0.002
HO
O
O
2.000
2.807
8.1
7.9
7.7
7.5
7.3
7.1
6.9
6.7
f1 (ppm)
2.000
2.807
2.127
3.200
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

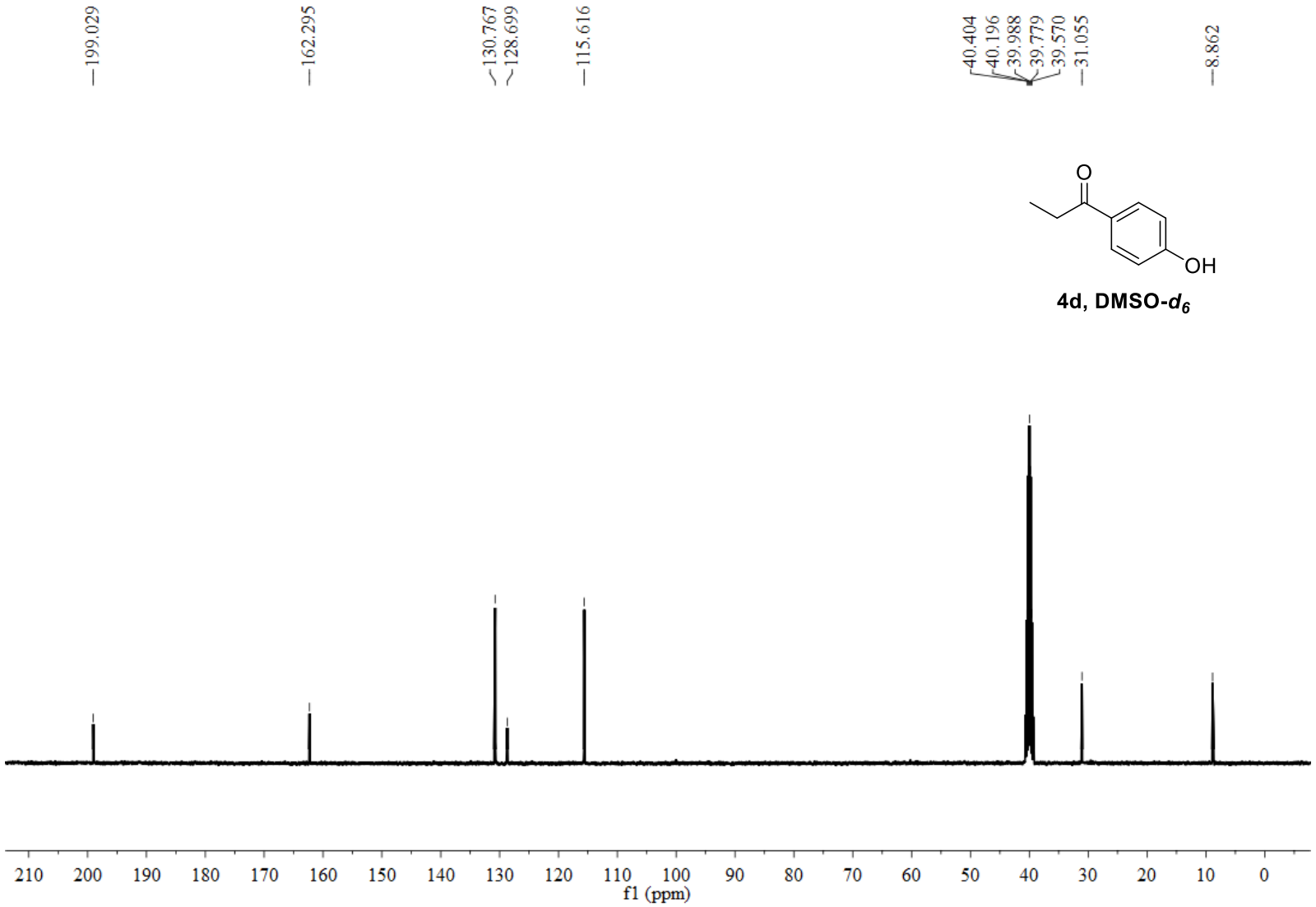
4b, $CDCl_3$

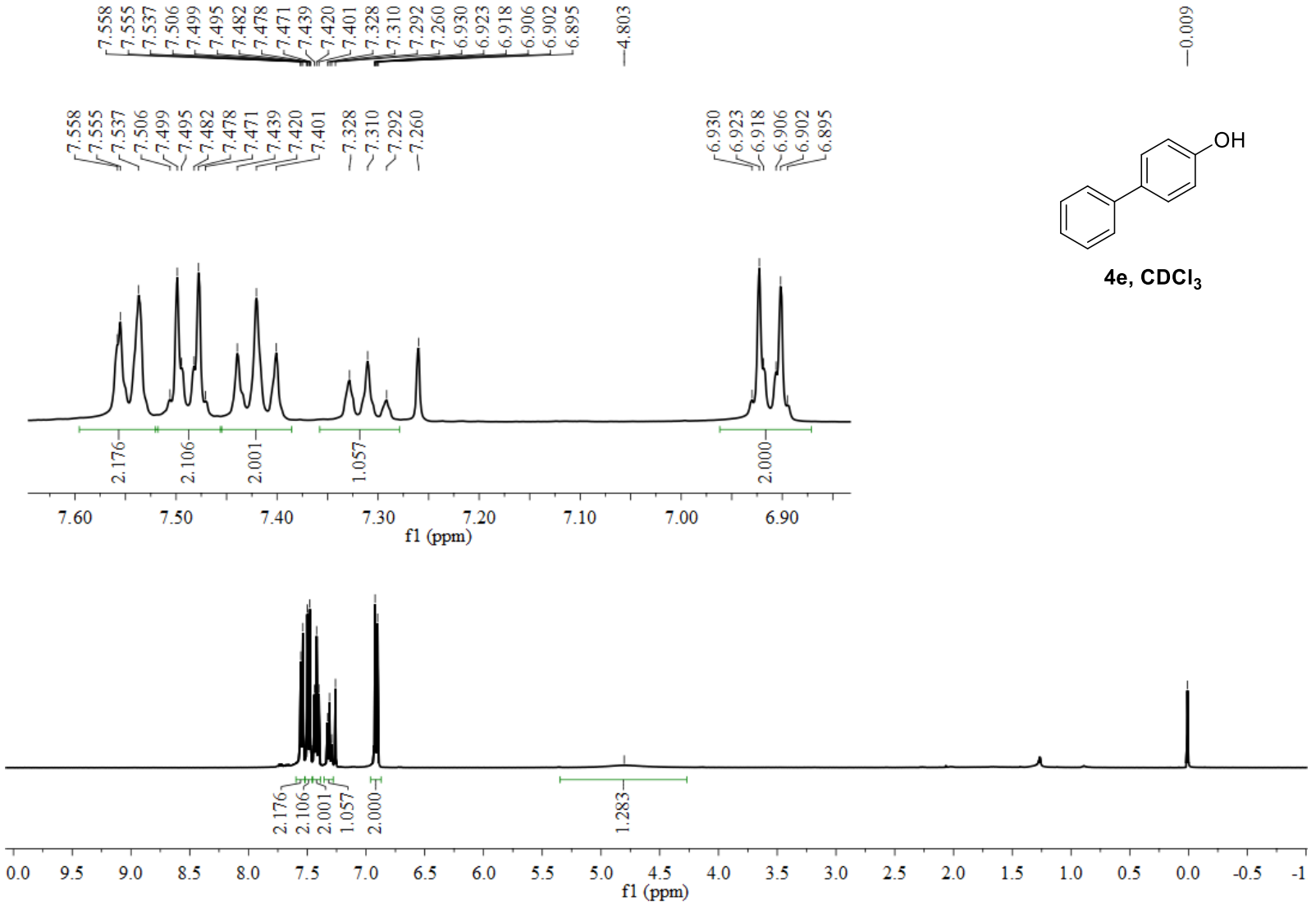

167.132
160.401
131.929
122.472
115.283
77.359
77.042
76.724
61.017
14.331
O
O
HO
4b, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.898
7.894
7.881
7.876
7.260
7.042
6.888
6.882
6.877
6.865
6.860
1.589
HO
O
O
4c, CDCl3
2.000
0.809
2.057
9.163
f1 (ppm)

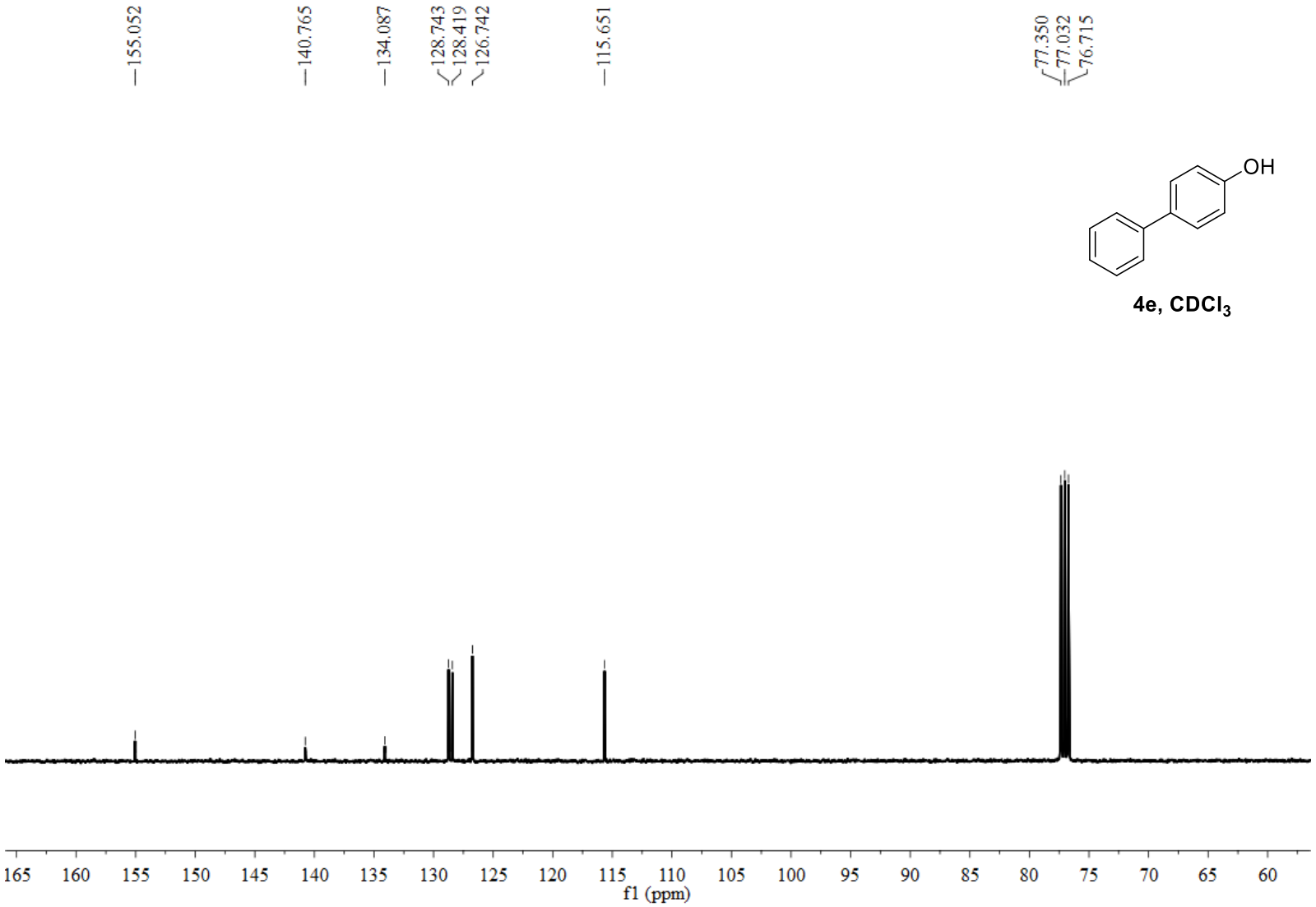

166.582
160.267
131.764
123.815
115.179
81.224
77.369
77.052
76.734
28.279
O
O
HO
4c, CDCl3
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

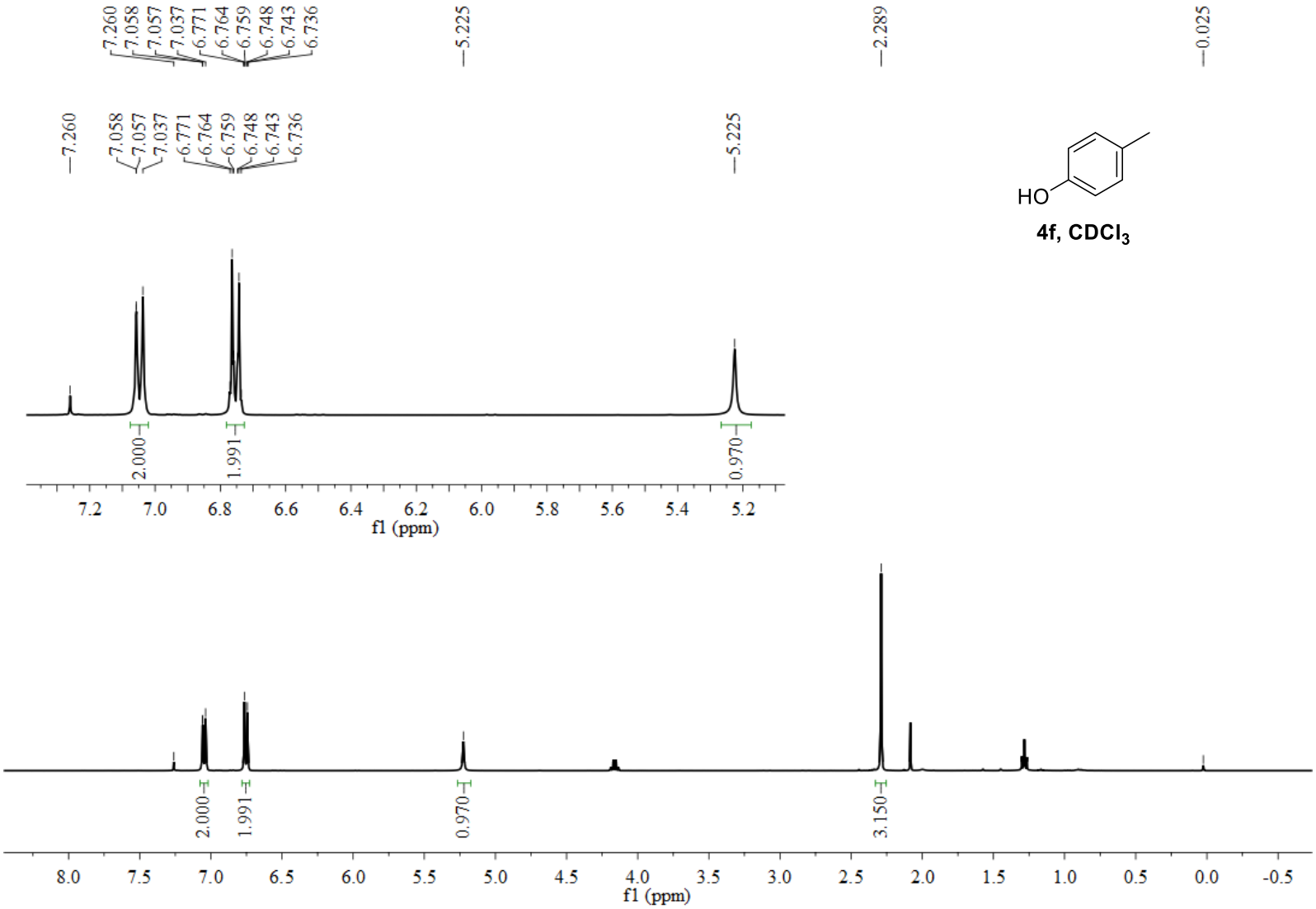

7.934
7.927
7.922
7.910
7.905
7.898
7.260
6.902
6.895
6.890
6.878
6.873
6.866
5.766
2.982
2.964
2.946
2.928
1.234
1.216
1.198
0.001
O
OH
4d, CDCl3
2.000
2.022
1.095
2.130
3.353
f1 (ppm)

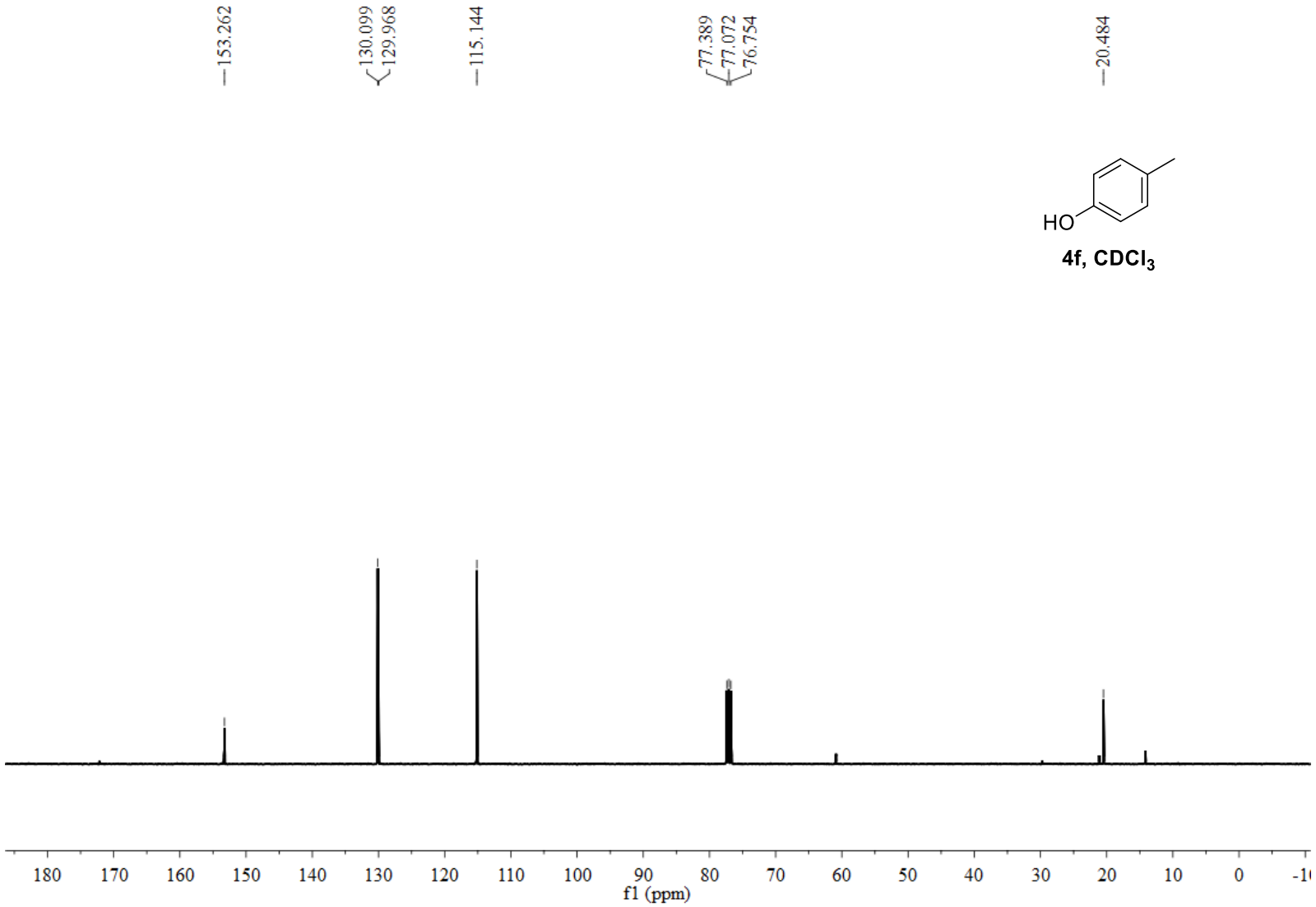

199.029
162.295
130.767
128.699
115.616
40.404
40.196
39.988
39.779
39.570
31.055
8.862
O
OH
4d, DMSO-d_6
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

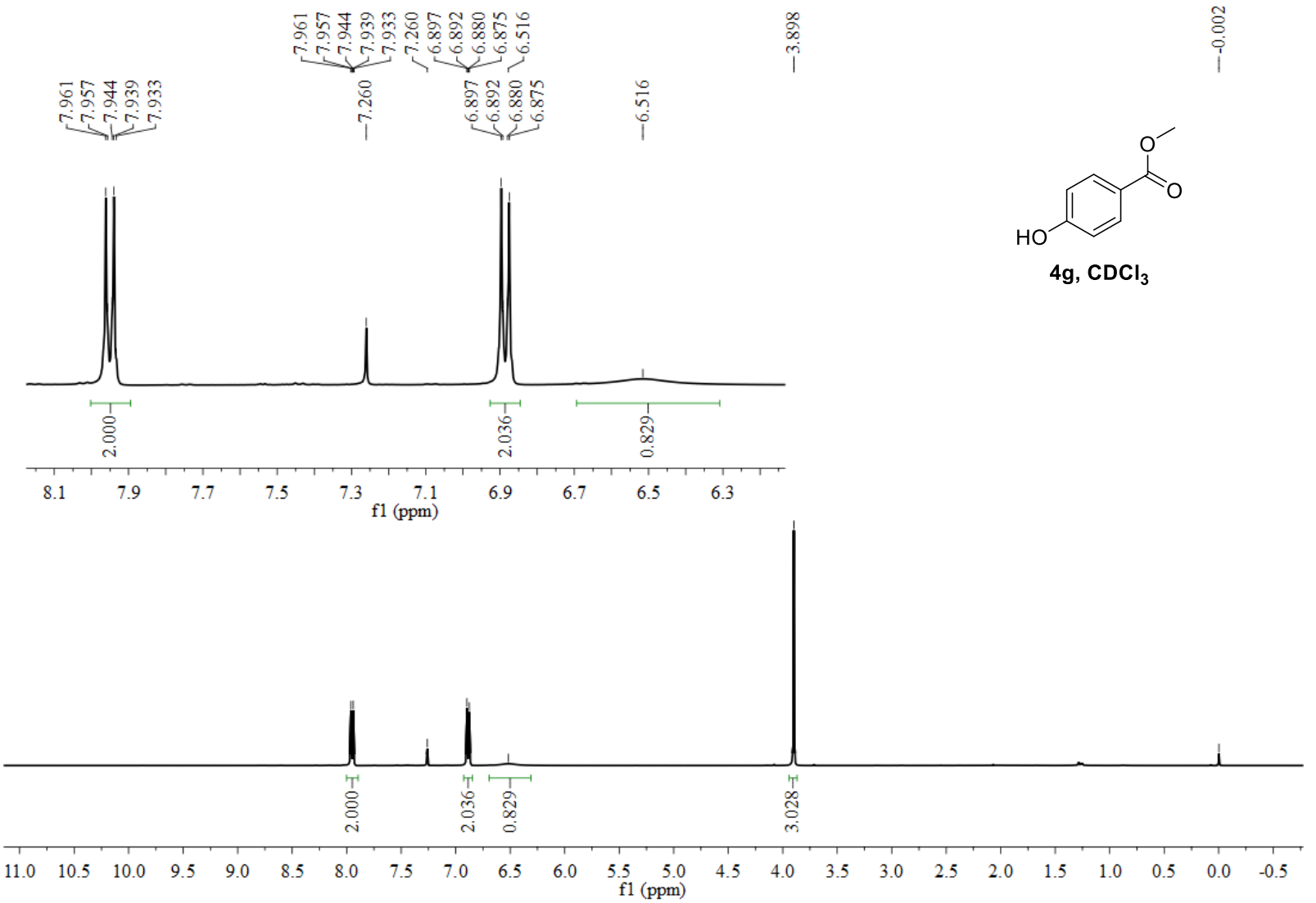

7.558
7.555
7.537
7.506
7.499
7.495
7.482
7.478
7.471
7.439
7.420
7.401
7.328
7.310
7.292
7.260
6.930
6.923
6.918
6.906
6.902
6.895
4.803
0.009
OH
2.176
2.106
2.001
1.057
2.000
1.283
f1 (ppm)

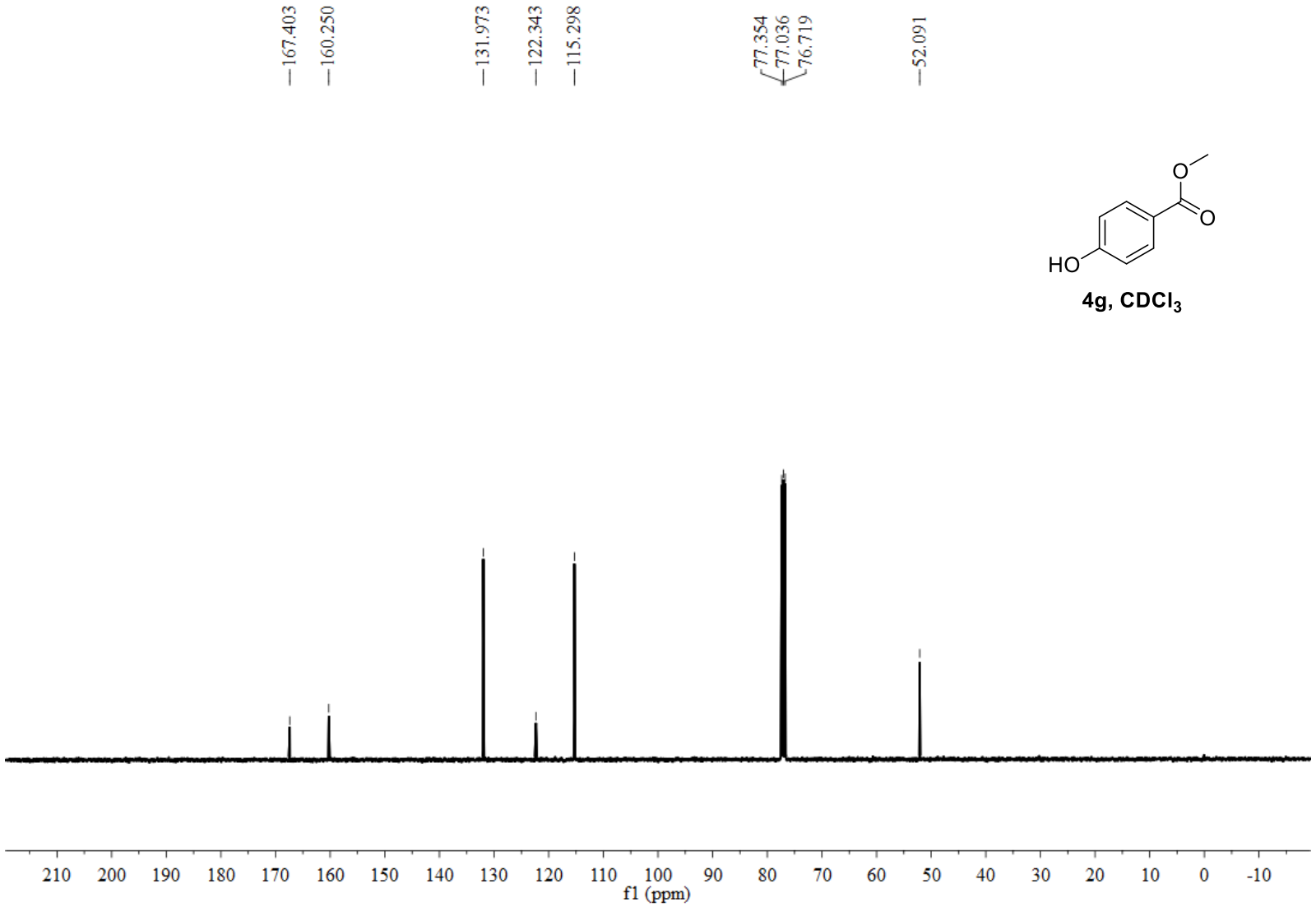
4e, $CDCl_3$


155.052
140.765
134.087
128.743
128.419
126.742
115.651
77.350
77.032
76.715
OH
4e, CDCl3
165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60
f1 (ppm)

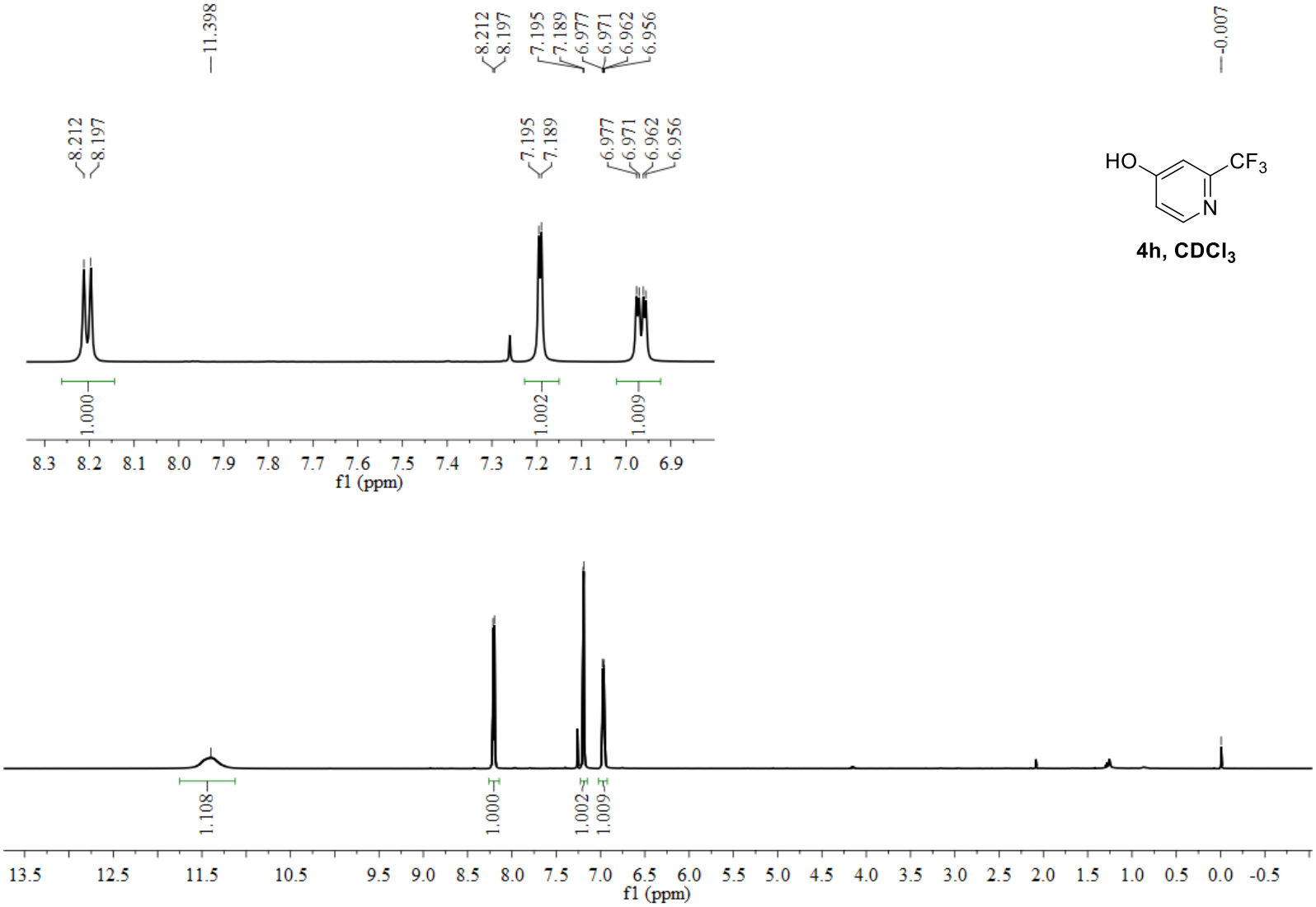

7.260
7.058
7.057
7.037
6.771
6.764
6.759
6.748
6.743
6.736
5.225
2.289
0.025
HO
4f, CDCl3
2.000
1.991
0.970
3.150
f1 (ppm)

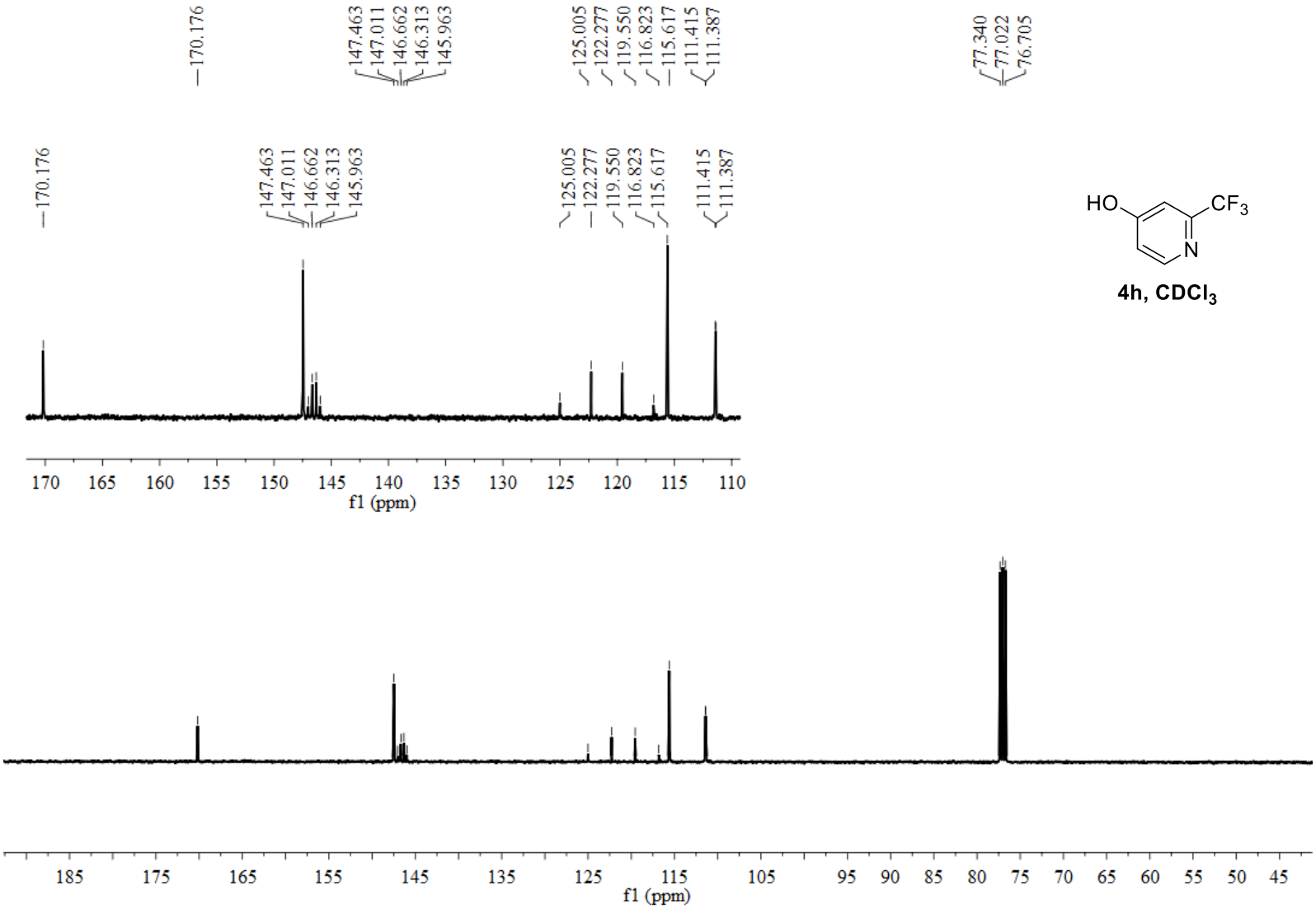

153.262
130.099
129.968
115.144
77.389
77.072
76.754
20.484
HO
4f, CDCl3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

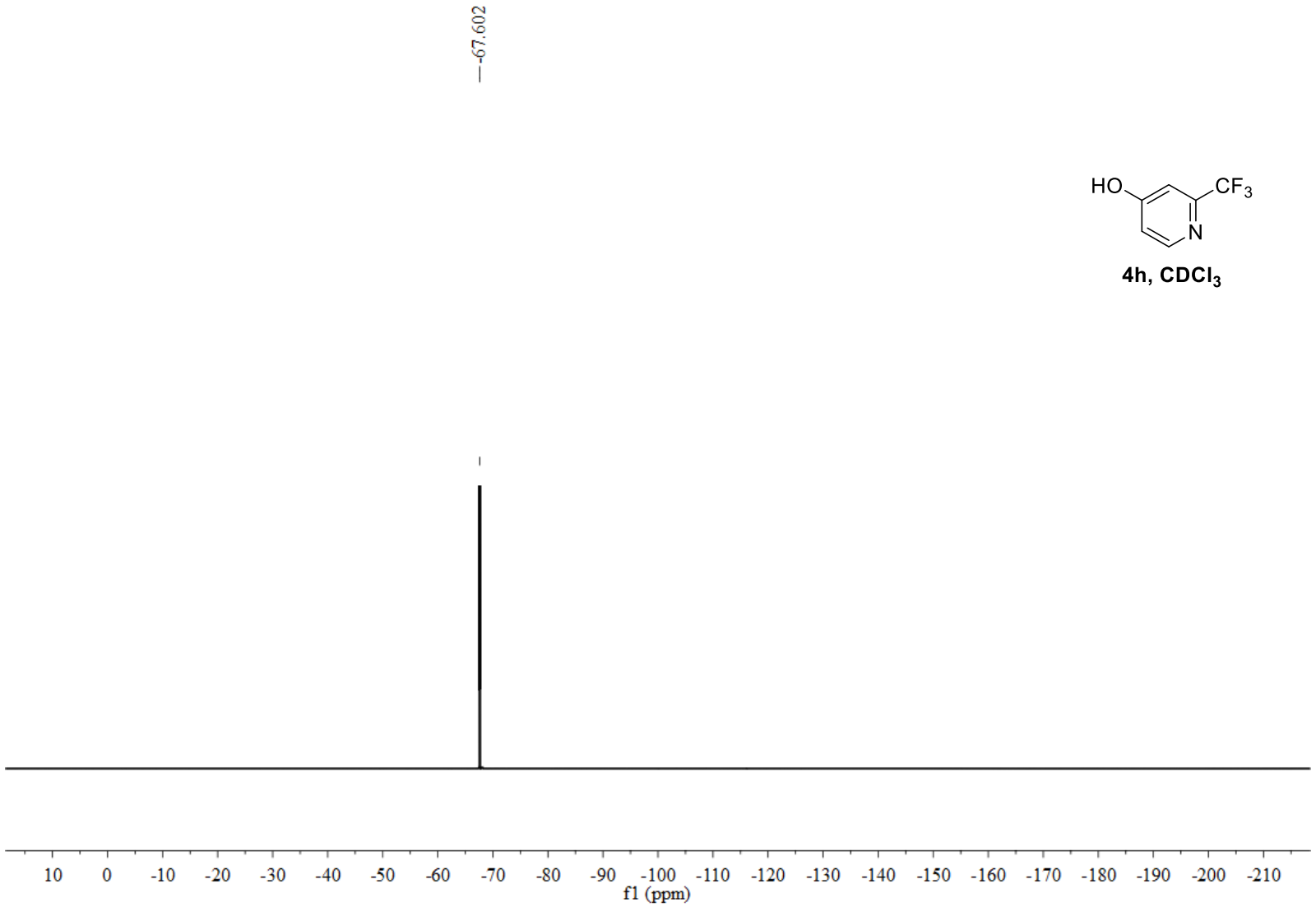

7.961
7.957
7.944
7.939
7.933
7.260
6.897
6.892
6.880
6.875
6.516
3.898
-0.002
HO
O
O
4g, CDCl3
2.000
2.036
0.829
3.028
f1 (ppm)

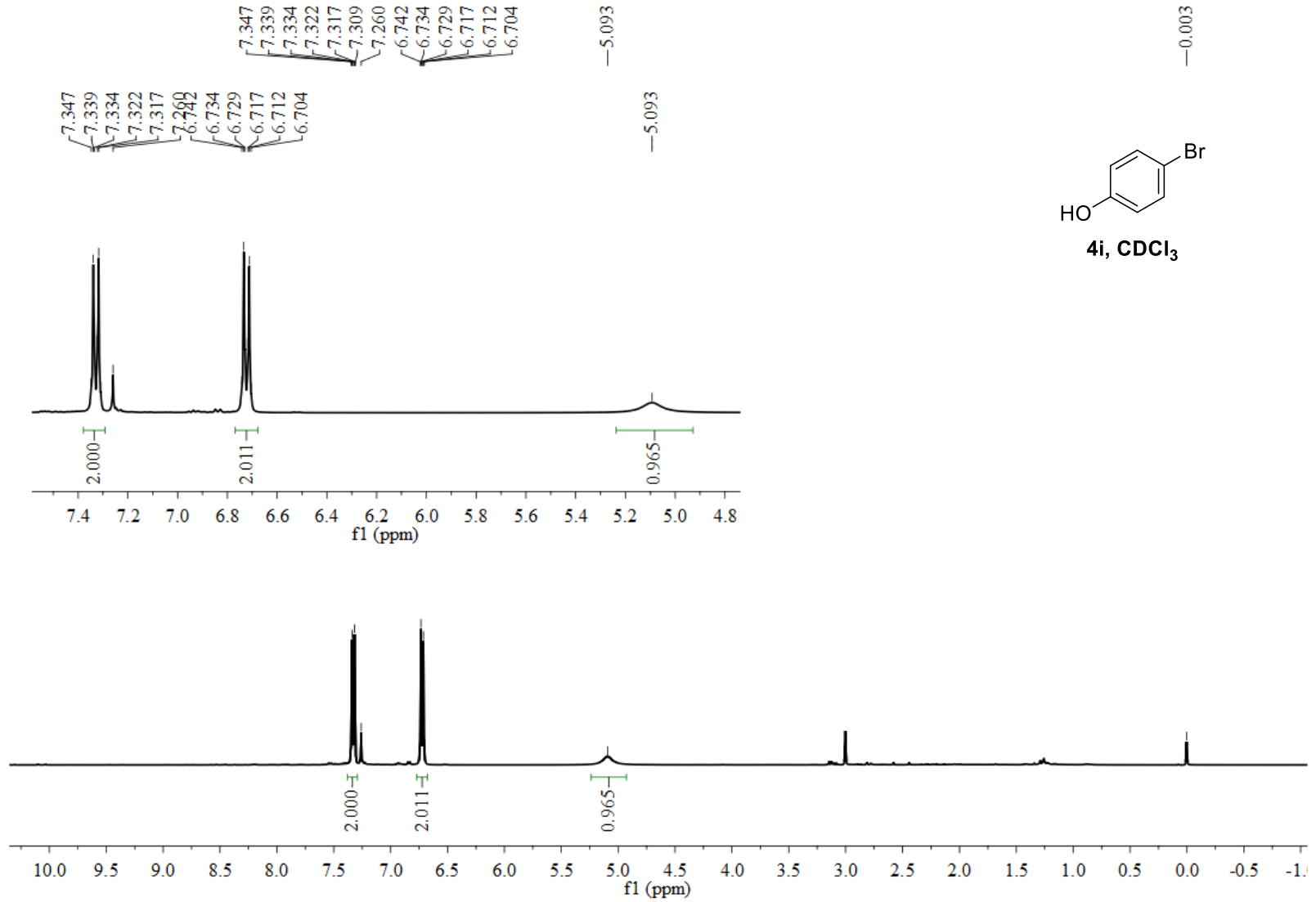

167.403
160.250
131.973
122.343
115.298
77.354
77.036
76.719
52.091
O
O
HO
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

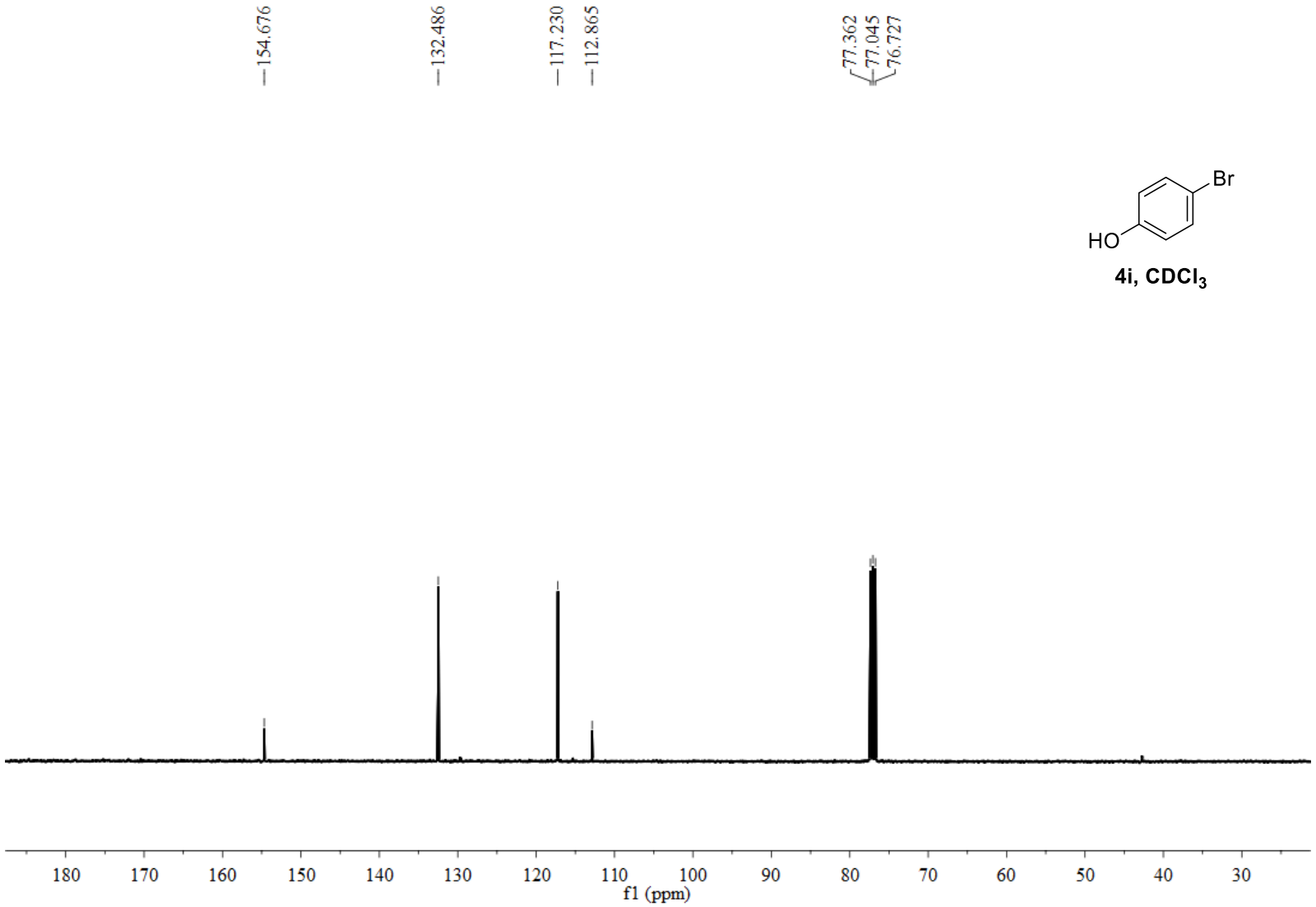
4g, $CDCl_3$


11.398
8.212
8.197
7.195
7.189
6.977
6.971
6.962
6.956
-0.007
HO
CF3
N
4h, CDCl3
1.000
1.002
1.009
1.108
f1 (ppm)

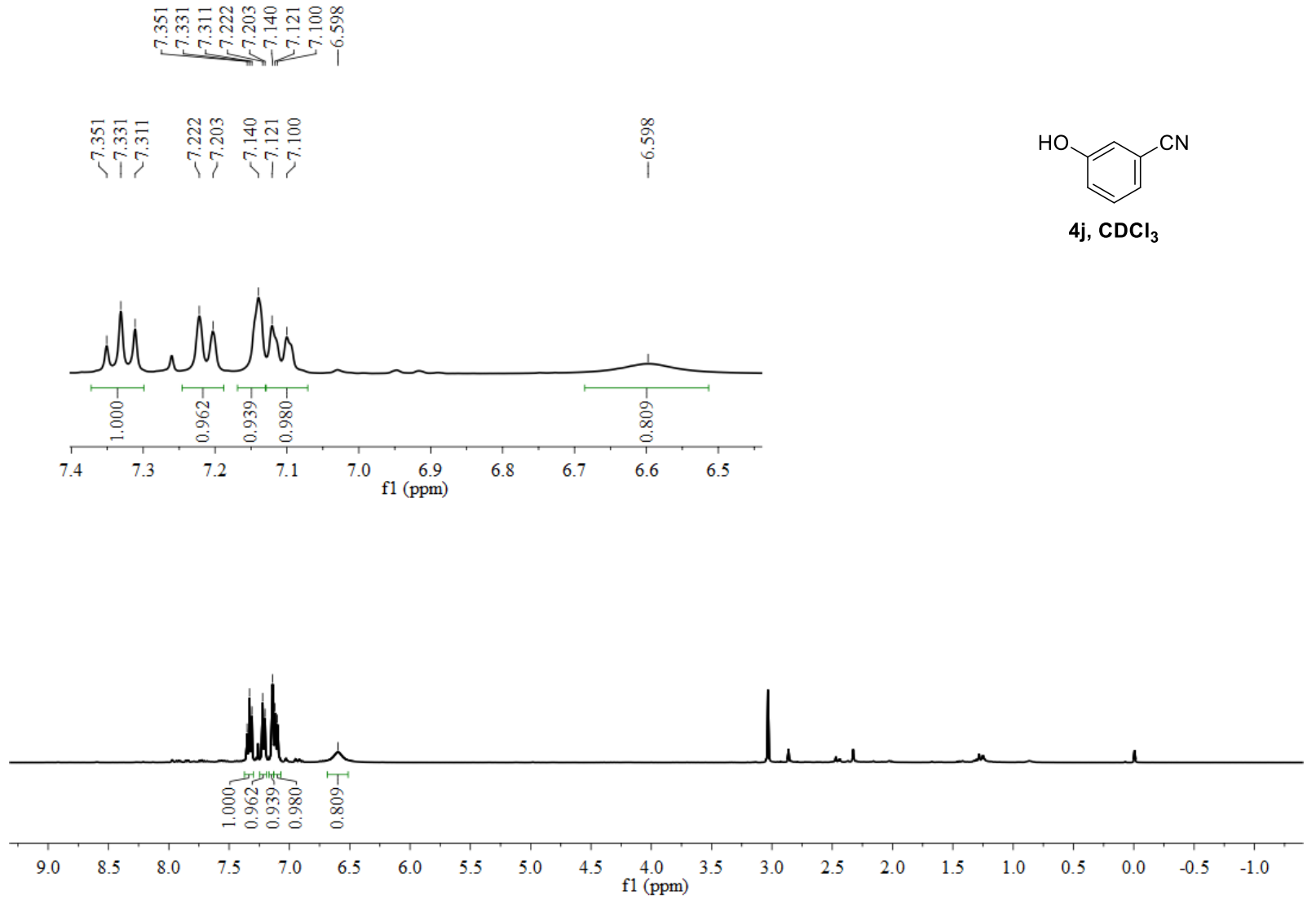

170.176
147.463
147.011
146.662
146.313
145.963
125.005
122.277
119.550
116.823
115.617
111.415
111.387
77.340
77.022
76.705
HO
CF3
N
4h, CDCl3
f1 (ppm)
f1 (ppm)

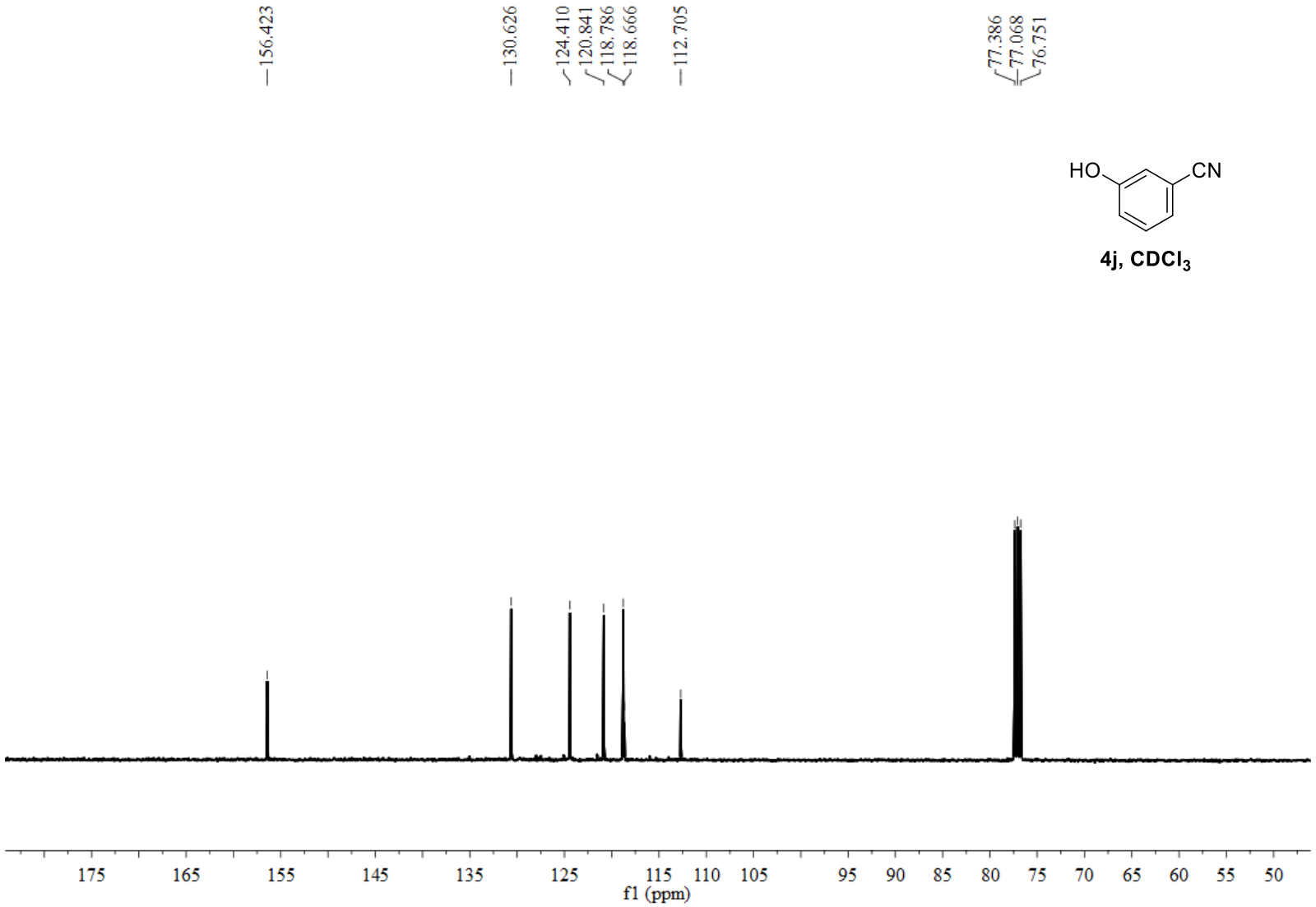

-67.602
HO
CF3
N
4h, CDCl3
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

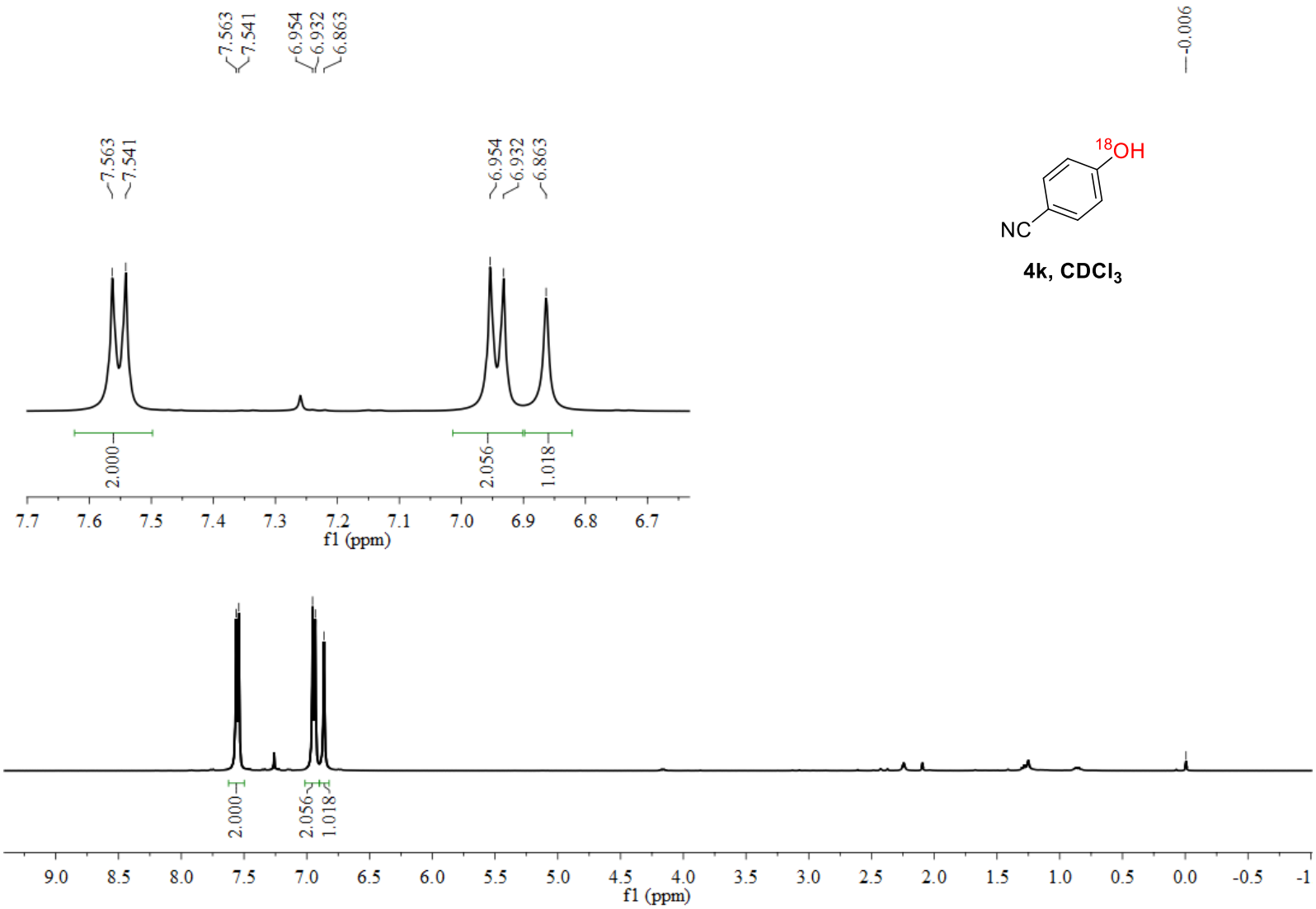

7.347
7.339
7.334
7.322
7.317
7.309
7.260
6.742
6.734
6.729
6.717
6.712
6.704
5.093
0.003
Br
HO
4i, CDCl3
2.000
2.011
0.965
f1 (ppm)

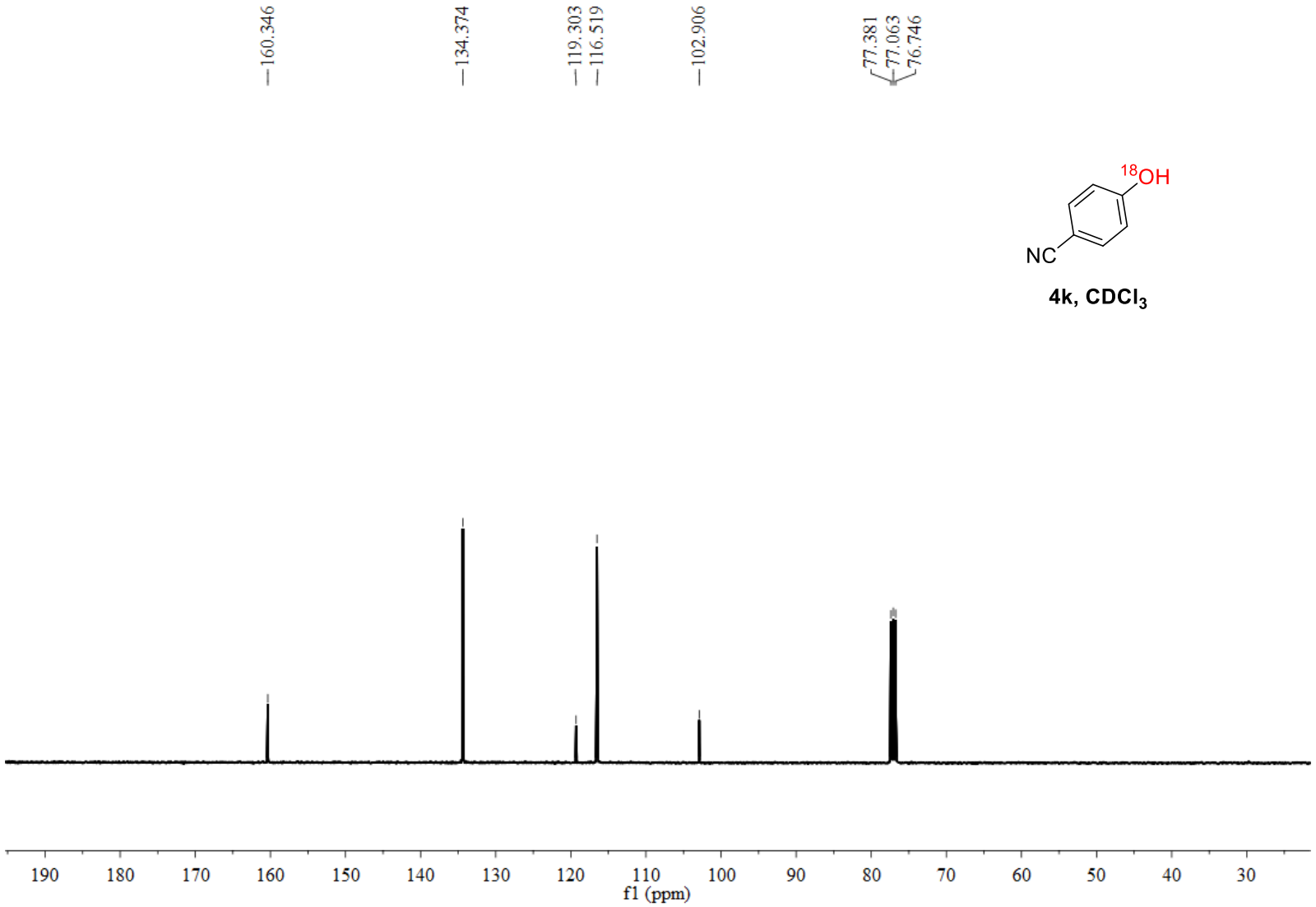

154.676
132.486
117.230
112.865
77.362
77.045
76.727
Br
HO
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
f1 (ppm)

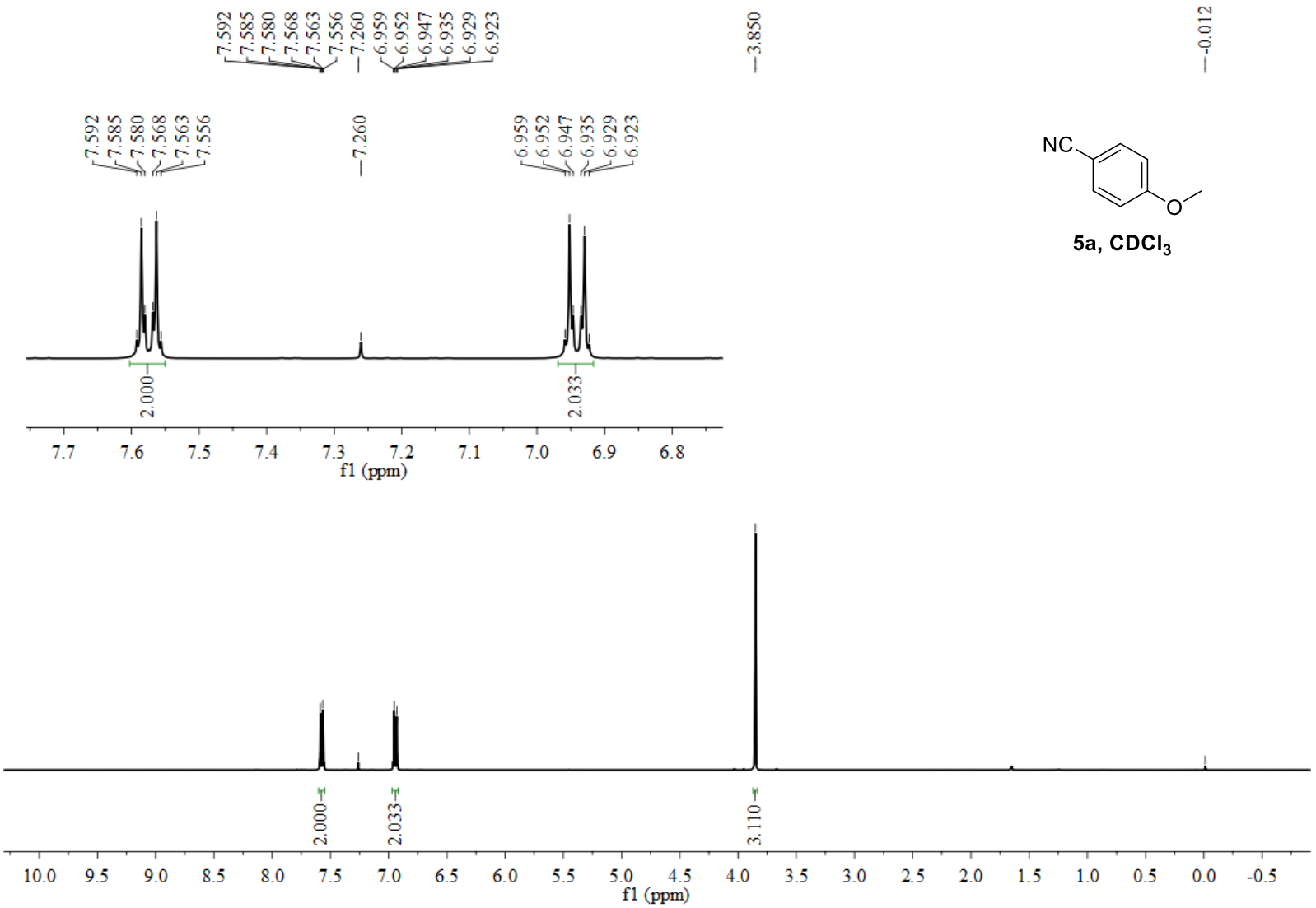
4i, $CDCl_3$


7.351
7.331
7.311
7.222
7.203
7.140
7.121
7.100
6.598
1.000
0.962
0.939
0.980
0.809
f1 (ppm)
HO
CN
4j, CDCl3

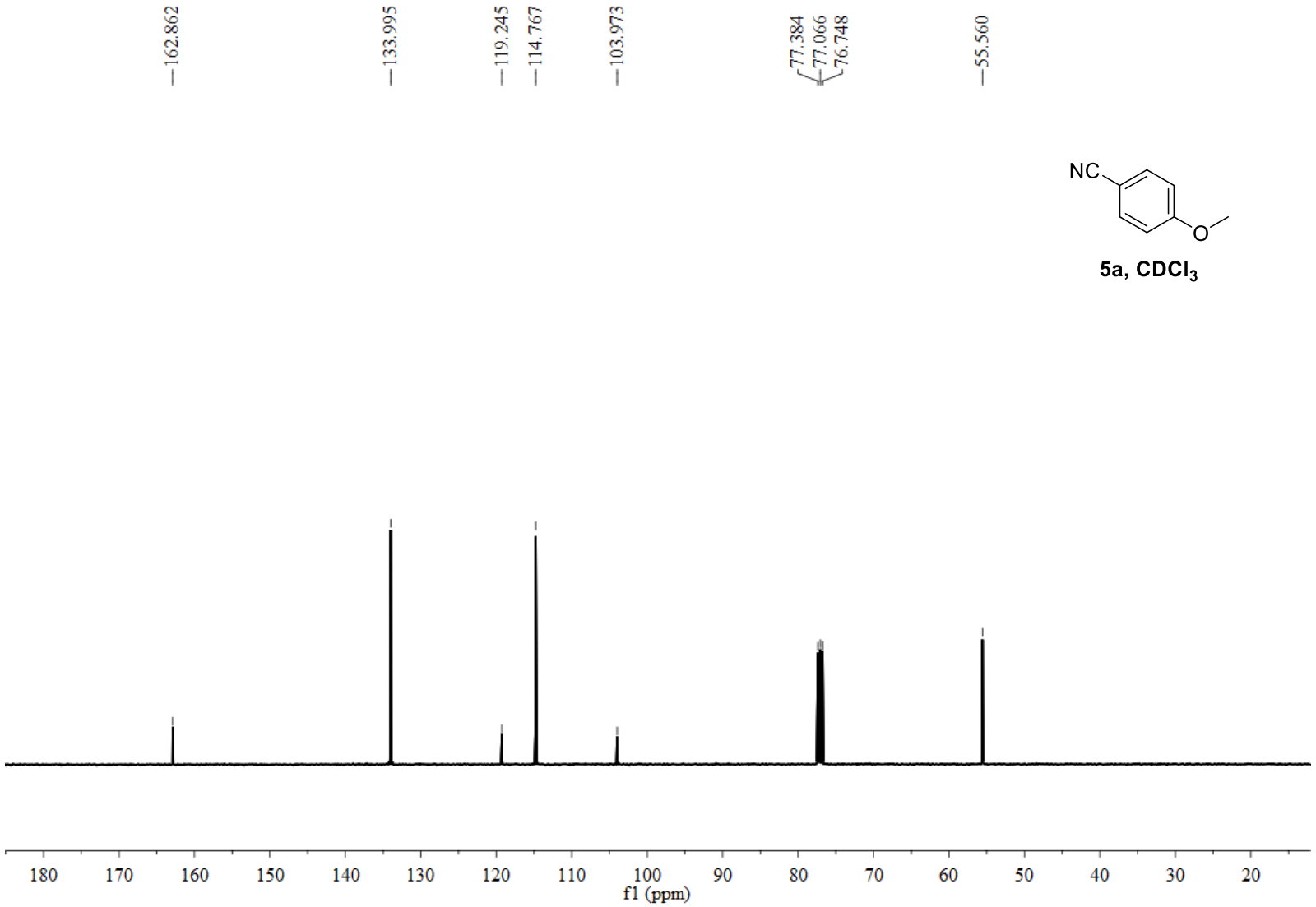

156.423
130.626
124.410
120.841
118.786
118.666
112.705
77.386
77.068
76.751
HO
CN
4j, CDCl3
175
165
155
145
135
125
115
110
105
95
90
85
80
75
70
65
60
55
50
f1 (ppm)


7.563
7.541
6.954
6.932
6.863
-0.006
18OH
NC
4k, CDCl3
2.000
2.056
1.018
f1 (ppm)

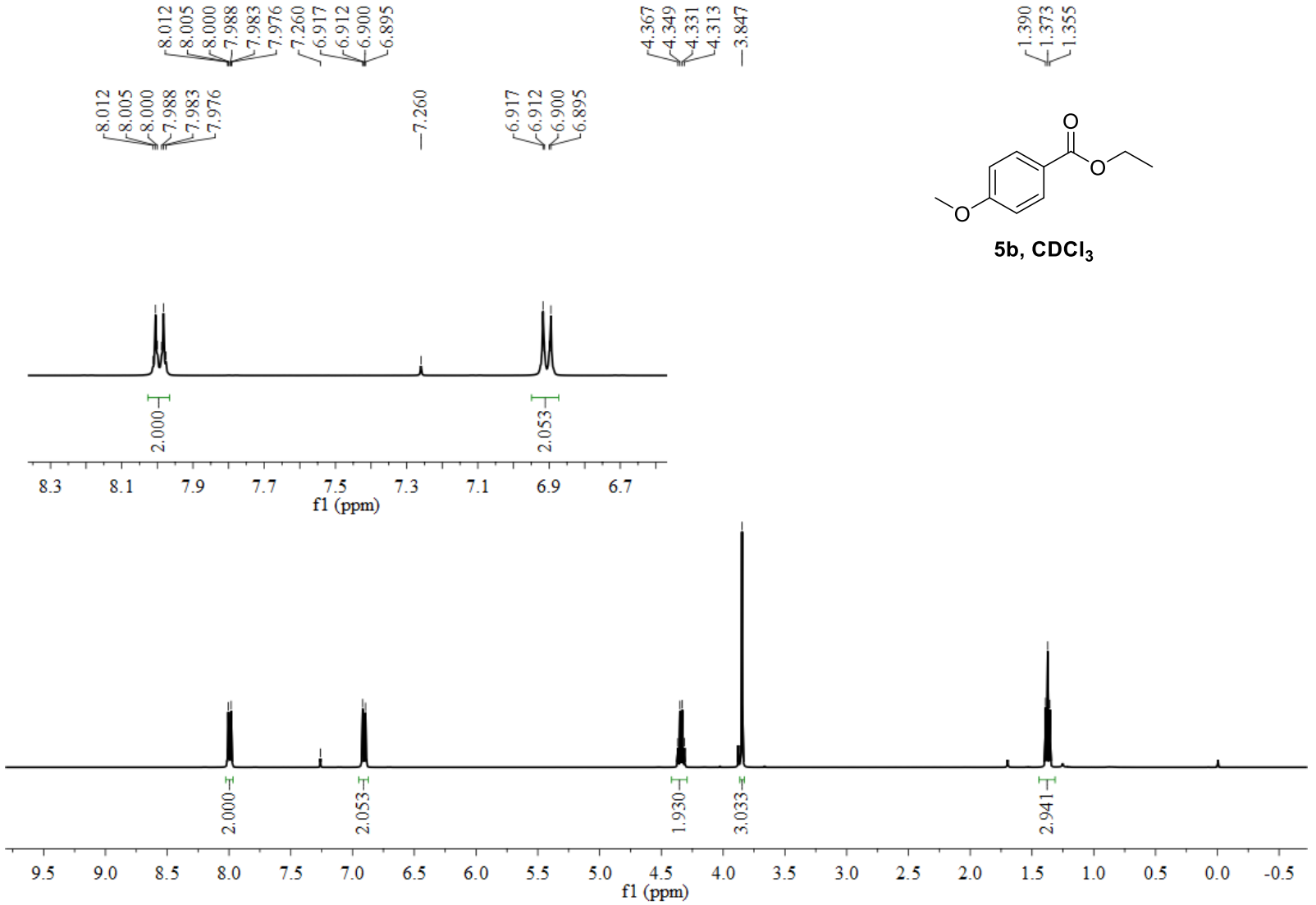

160.346
134.374
119.303
116.519
102.906
77.381
77.063
76.746
18OH
NC
4k, CDCl3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
f1 (ppm)

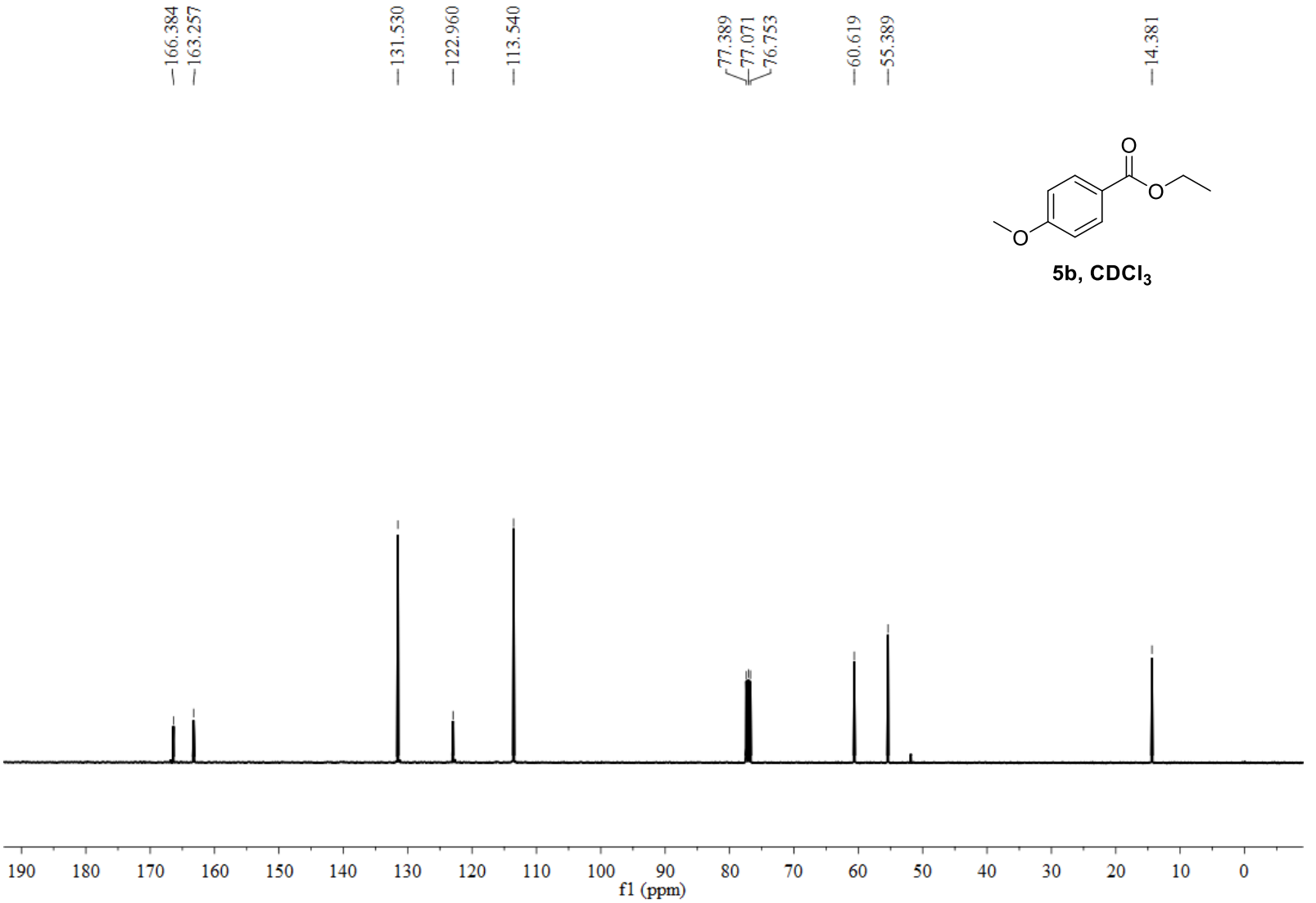

7.592
7.585
7.580
7.568
7.563
7.556
7.260
6.959
6.952
6.947
6.935
6.929
6.923
3.850
-0.012
NC
O
2.000
2.033
3.110
f1 (ppm)

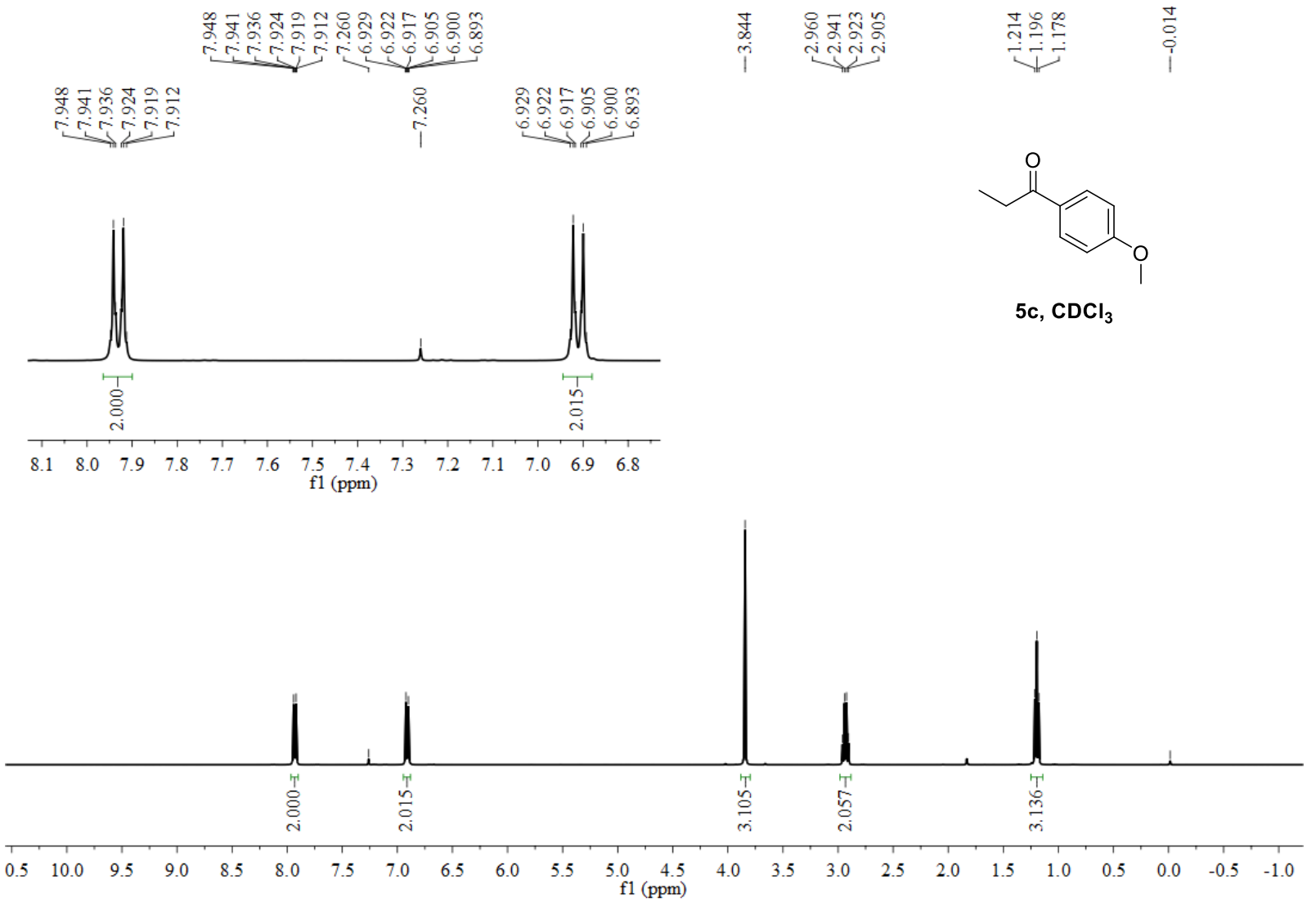
5a, $CDCl_3$

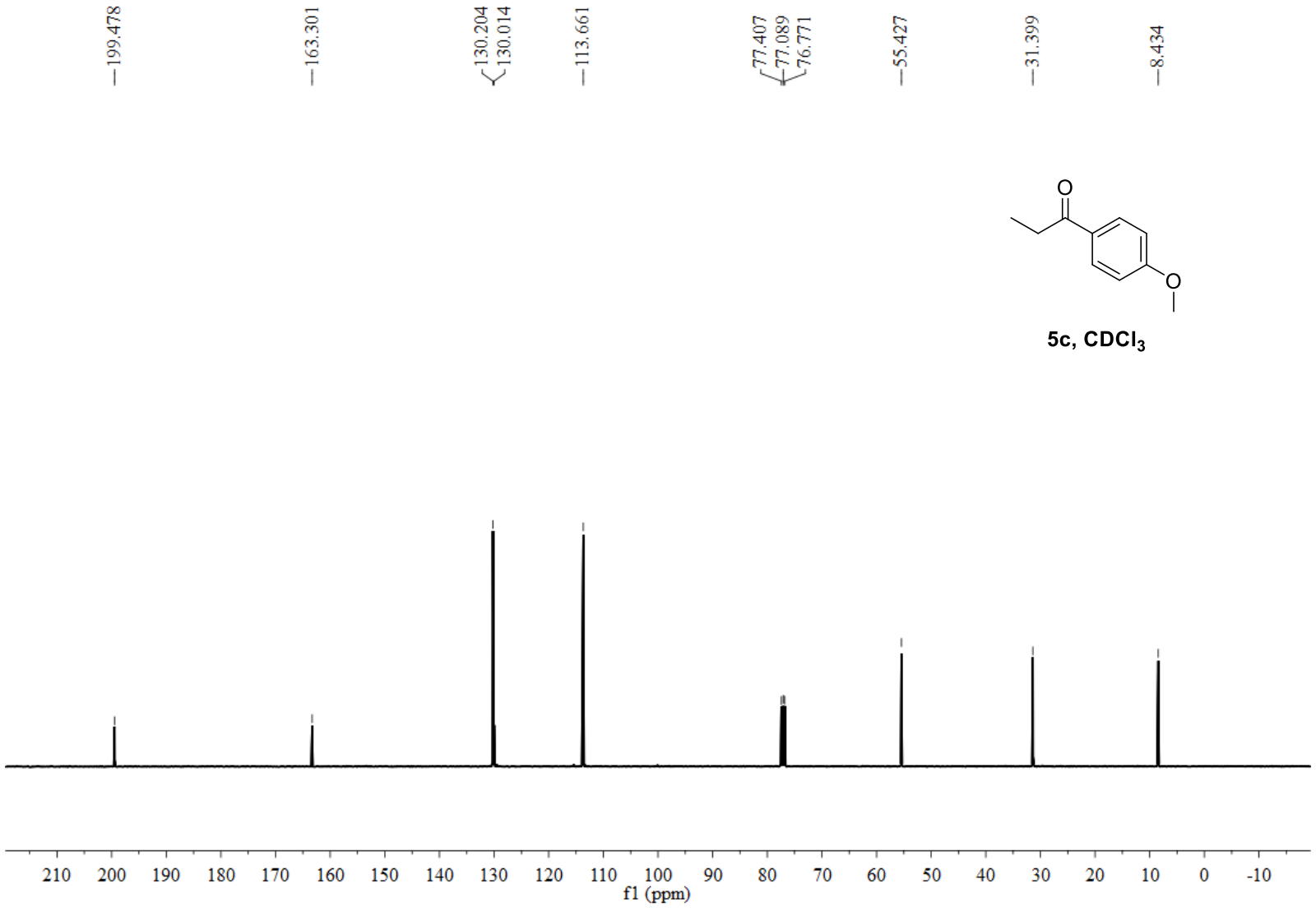

162.862
133.995
119.245
114.767
103.973
77.384
77.066
76.748
55.560
NC
O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

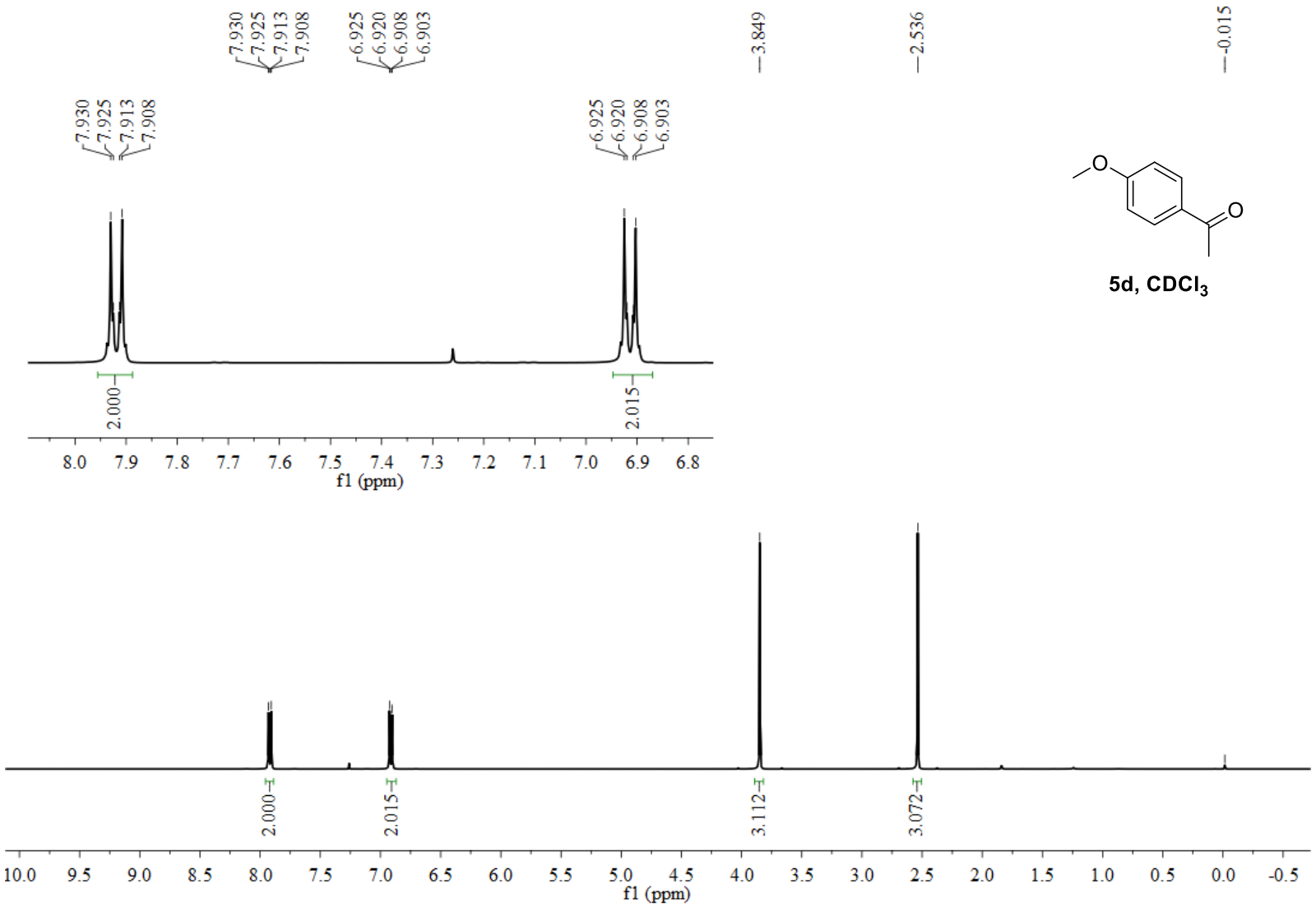
5a, $CDCl_3$


8.012
8.005
8.000
7.988
7.983
7.976
7.260
6.917
6.912
6.900
6.895
4.367
4.349
4.331
4.313
3.847
1.390
1.373
1.355
O
O
O
5b, CDCl3
2.000
2.053
8.3
8.1
7.9
7.7
7.5
7.3
7.1
6.9
6.7
f1 (ppm)
2.000
2.053
1.930
3.033
2.941
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)

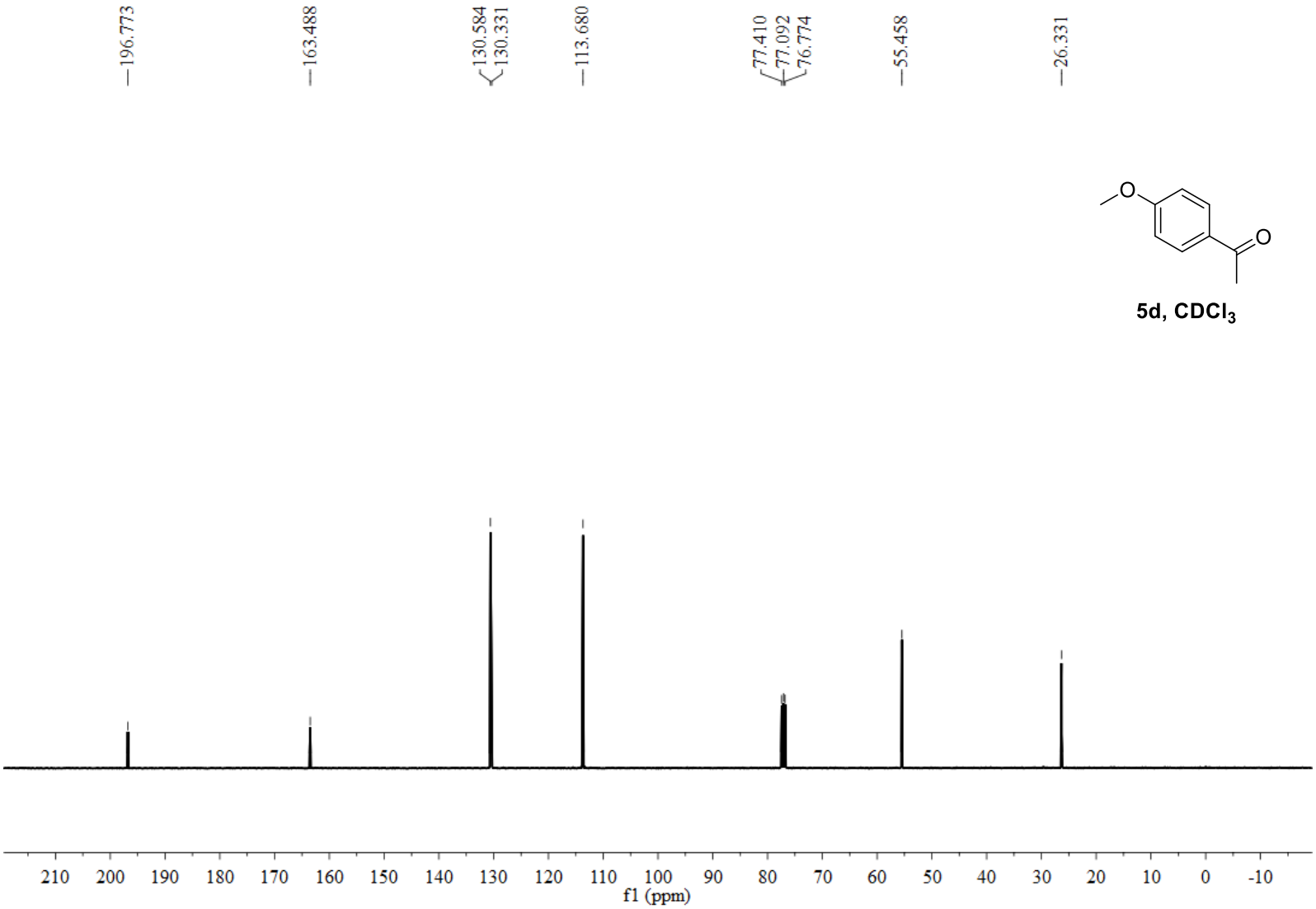

166.384
163.257
131.530
122.960
113.540
77.389
77.071
76.753
60.619
55.389
14.381
O
O
O
5b, CDCl3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

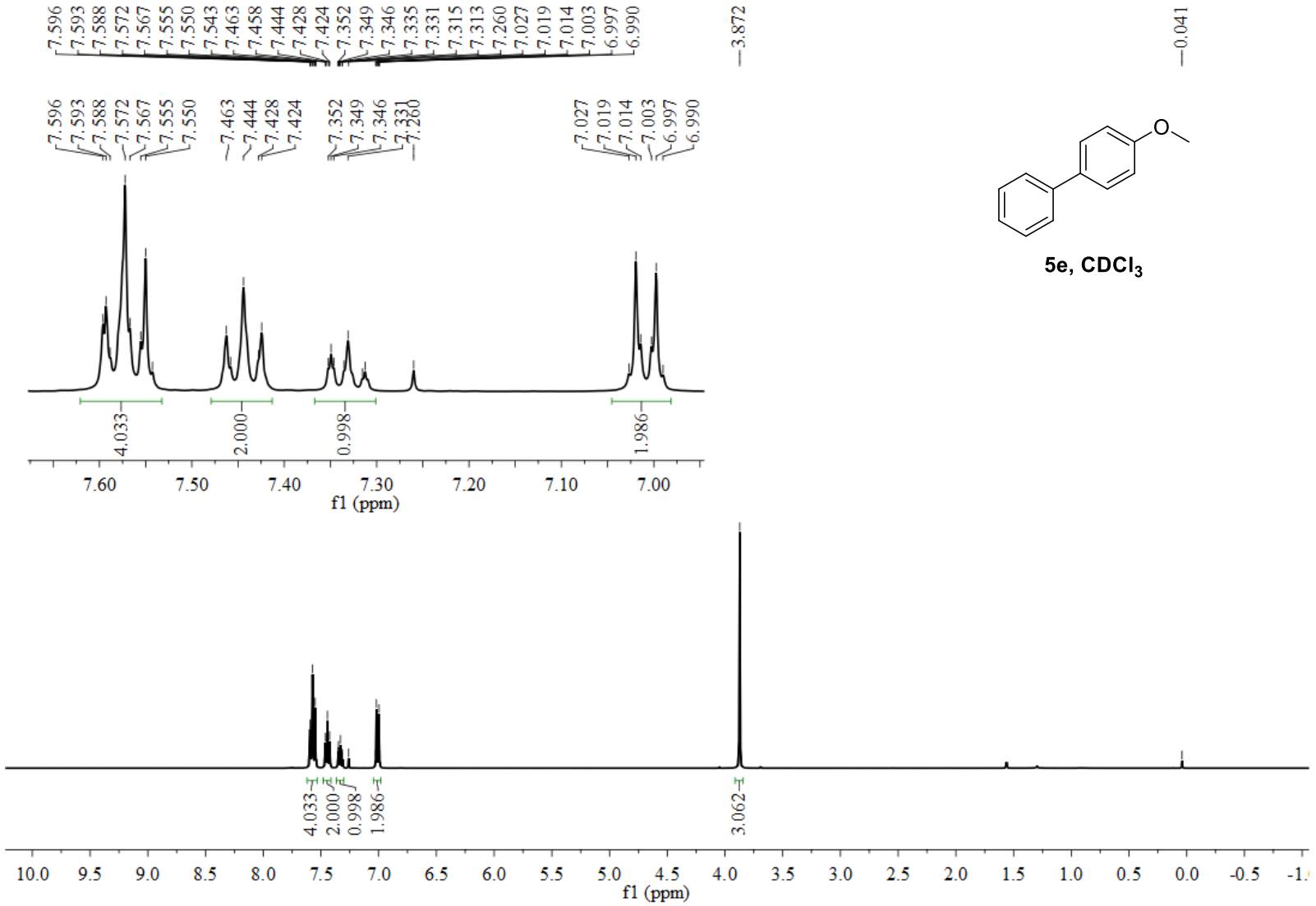

7.948
7.941
7.936
7.924
7.919
7.912
7.260
6.929
6.922
6.917
6.905
6.900
6.893
3.844
2.960
2.941
2.923
2.905
1.214
1.196
1.178
0.014
2.000
2.015
f1 (ppm)
3.105
2.057
3.136
O
O
5c, CDCl3

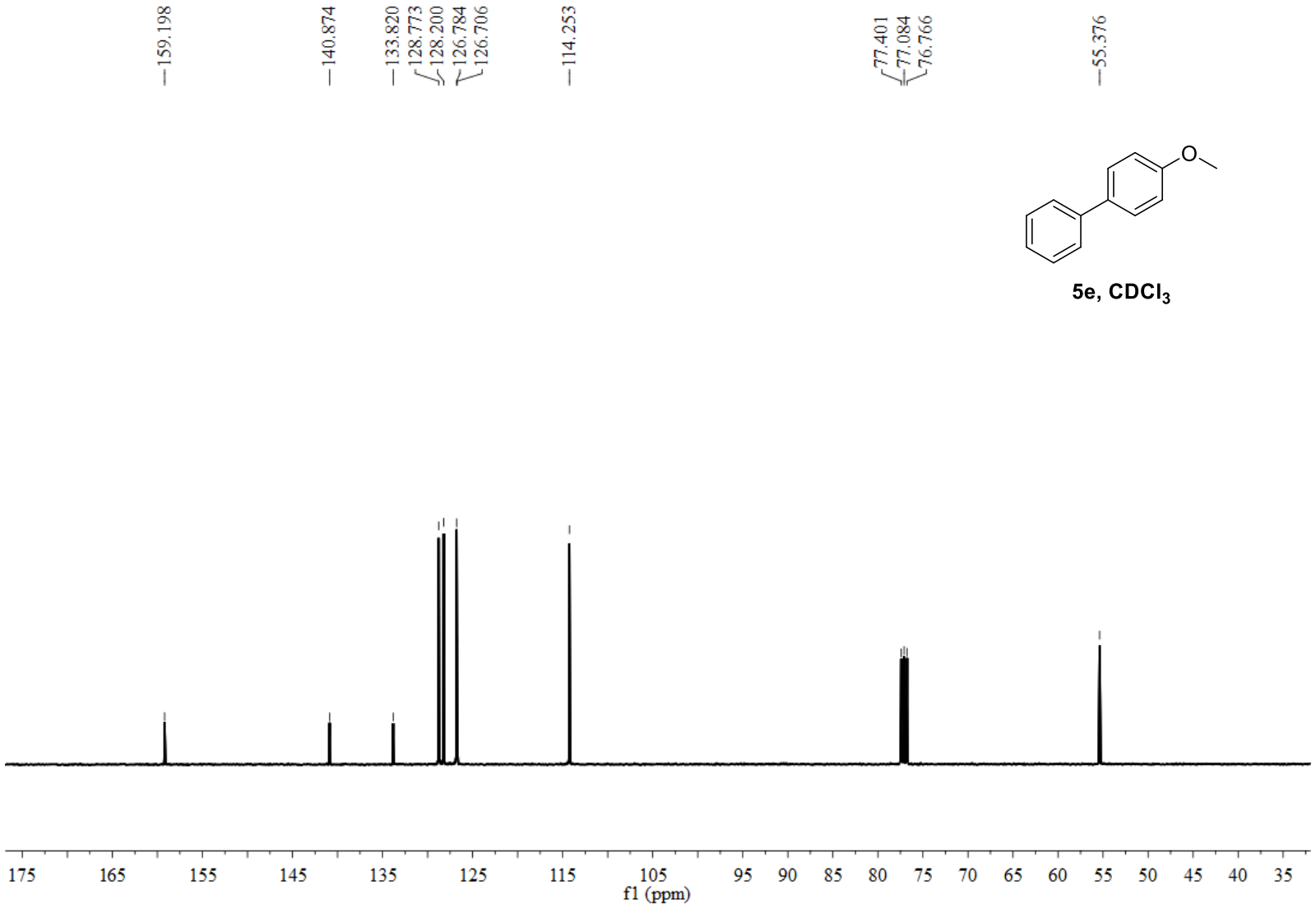

199.478
163.301
130.204
130.014
113.661
77.407
77.089
76.771
55.427
31.399
8.434
O
O
5c, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

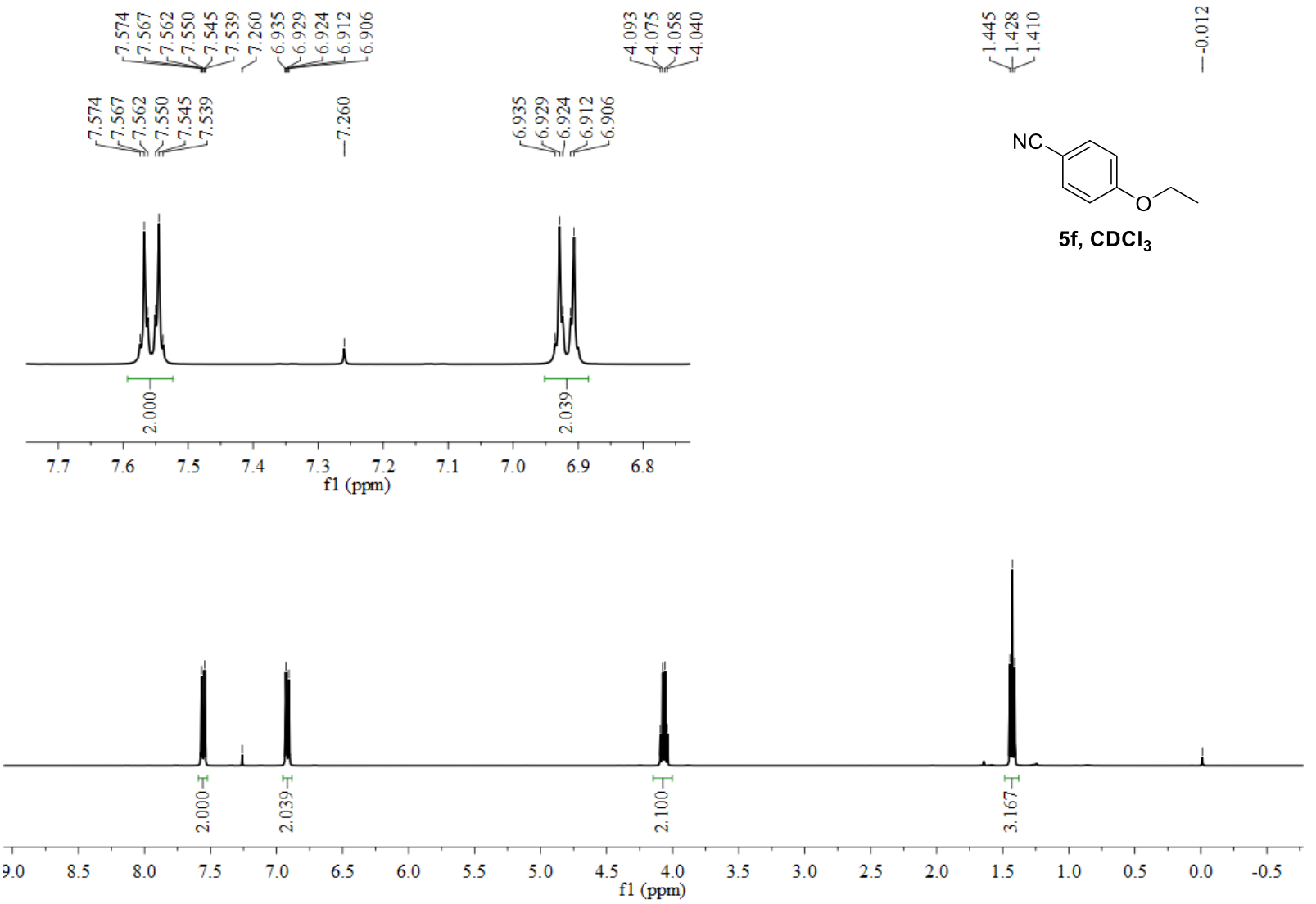

7.930
7.925
7.913
7.908
6.925
6.920
6.908
6.903
3.849
2.536
-0.015
2.000
2.015
f1 (ppm)
3.112
3.072

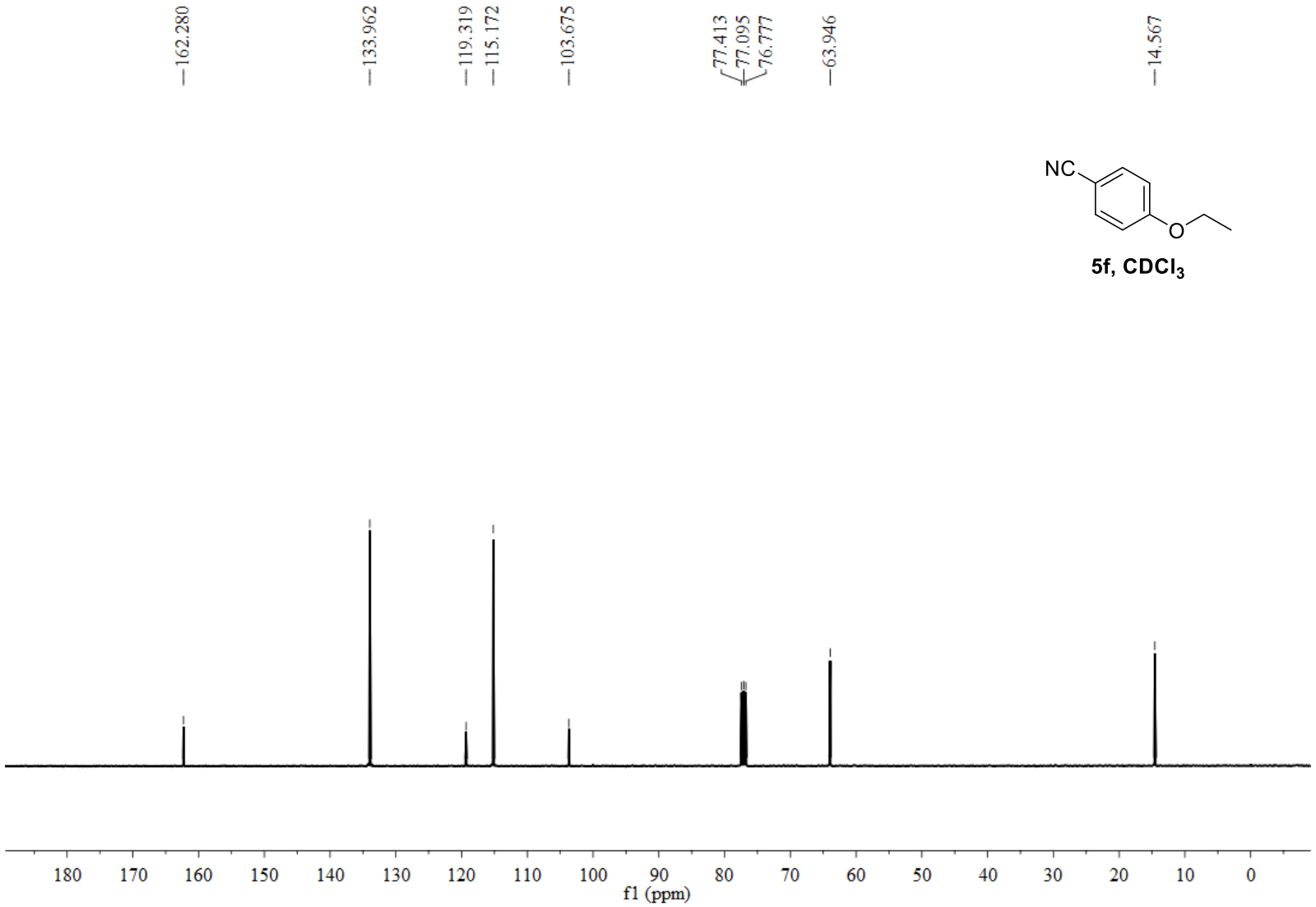
5d, $CDCl_3$

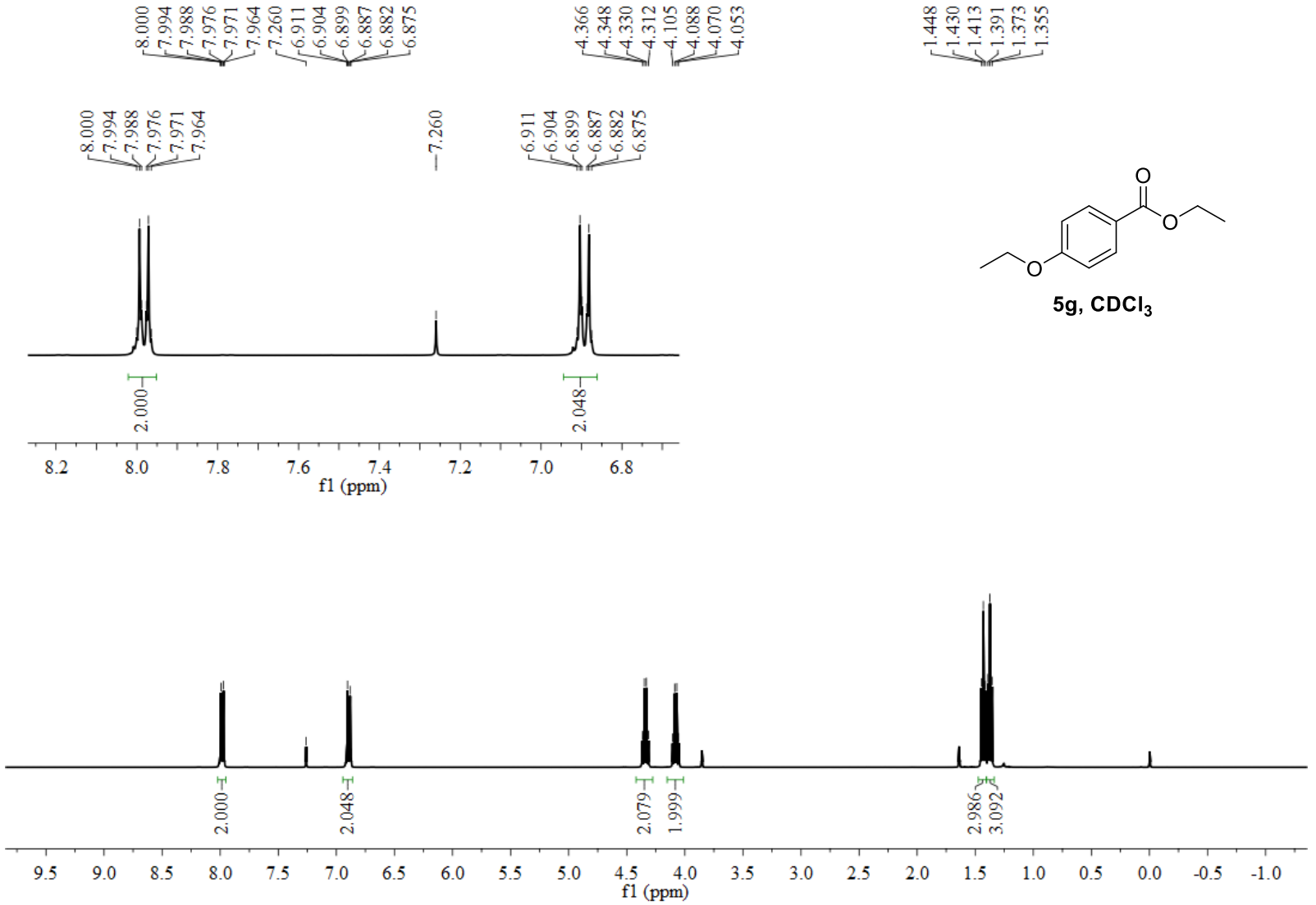

196.773
163.488
130.584
130.331
113.680
77.410
77.092
76.774
55.458
26.331
O
O
5d, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.596
7.593
7.588
7.572
7.567
7.555
7.550
7.543
7.463
7.458
7.444
7.428
7.424
7.352
7.349
7.346
7.335
7.331
7.315
7.313
7.260
7.027
7.019
7.014
7.003
6.997
6.990
3.872
0.041
4.033
2.000
0.998
1.986
3.062
f1 (ppm)
O
5e, CDCl3

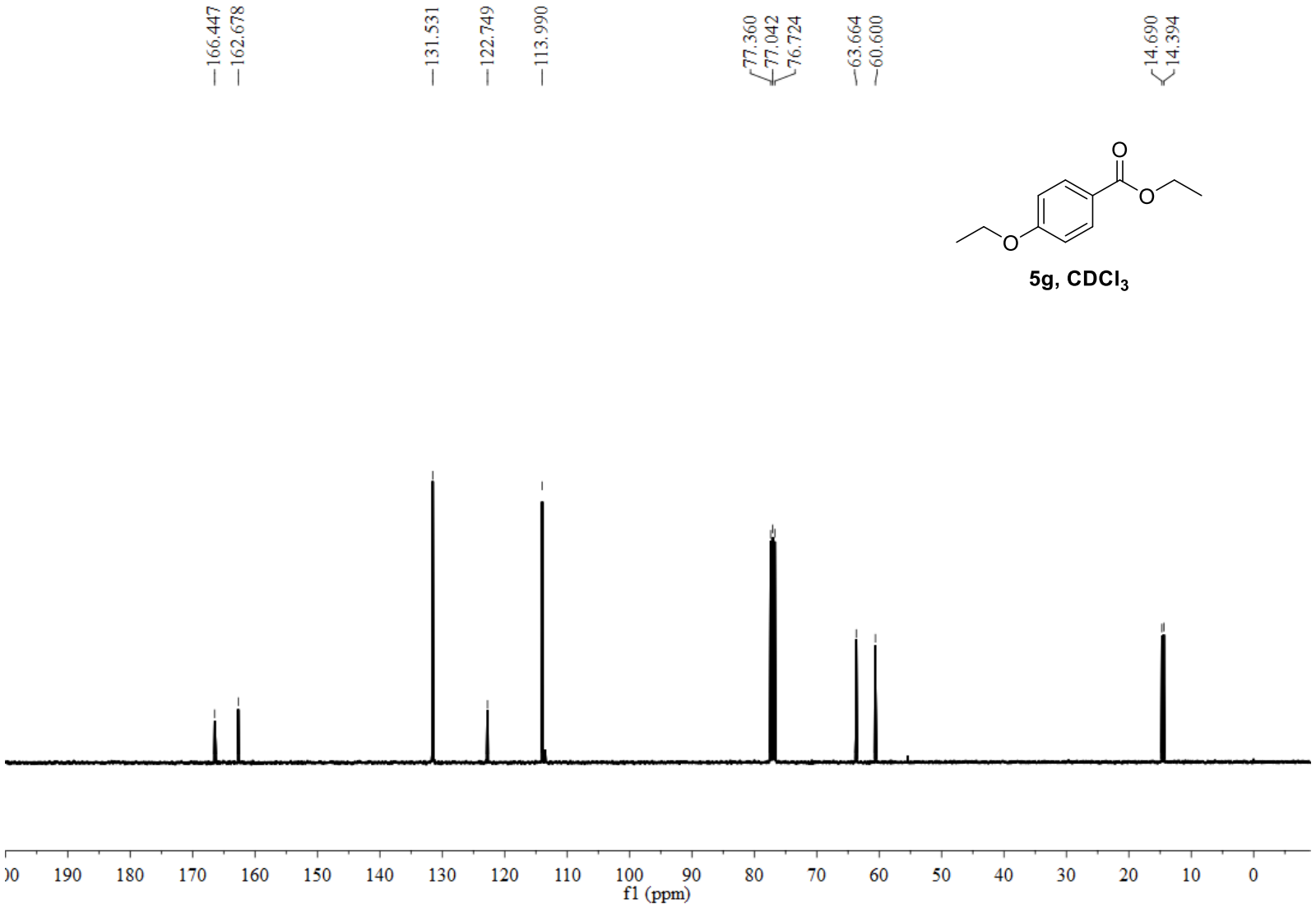

159.198
140.874
133.820
128.773
128.200
126.784
126.706
114.253
77.401
77.084
76.766
55.376
O
5e, CDCl3
175
165
155
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
f1 (ppm)

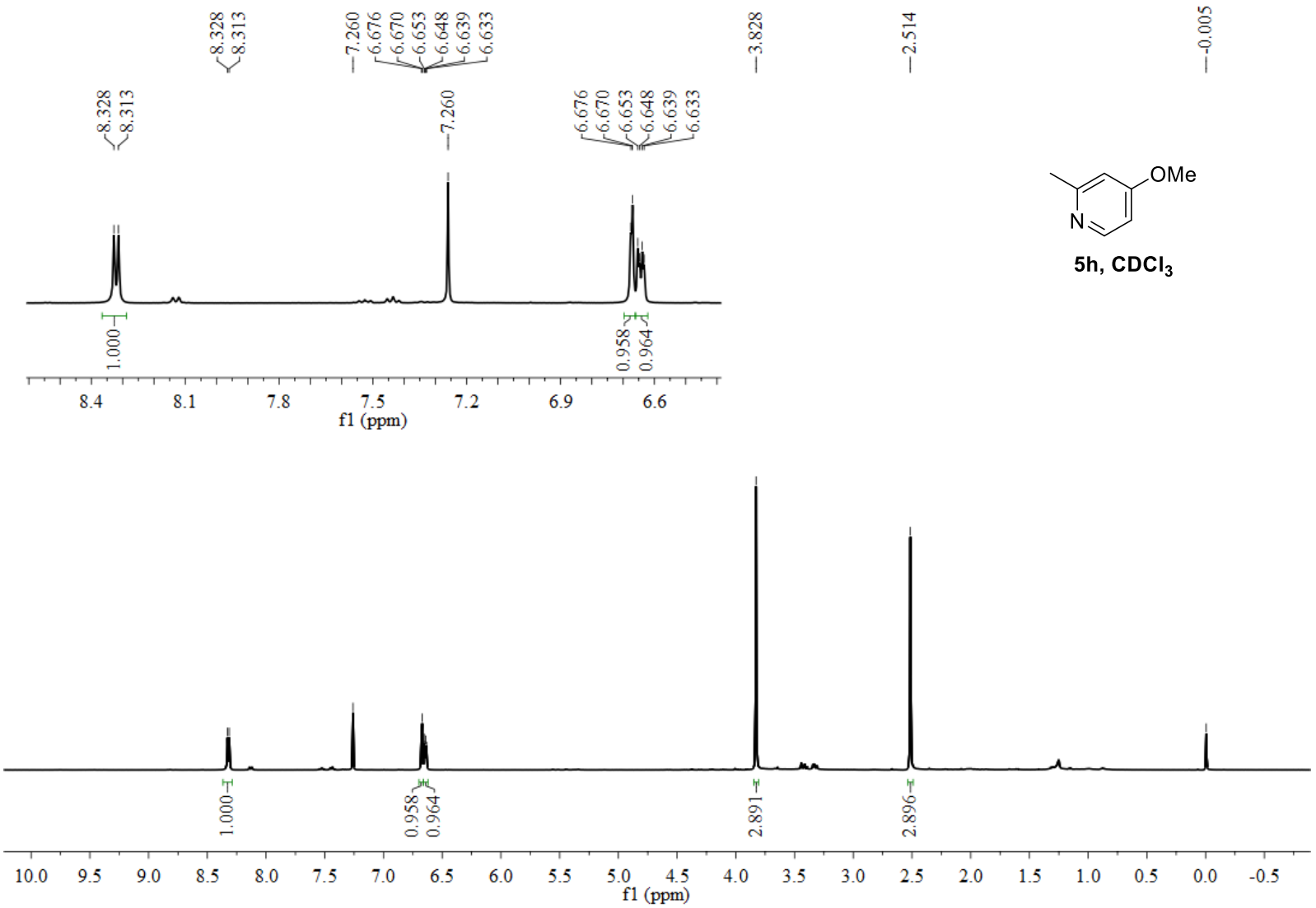

7.574
7.567
7.562
7.550
7.545
7.539
7.260
6.935
6.929
6.924
6.912
6.906
4.093
4.075
4.058
4.040
1.445
1.428
1.410
-0.012
NC
O
5f, CDCl3
2.000
2.039
f1 (ppm)
2.000
2.039
2.100
3.167
f1 (ppm)

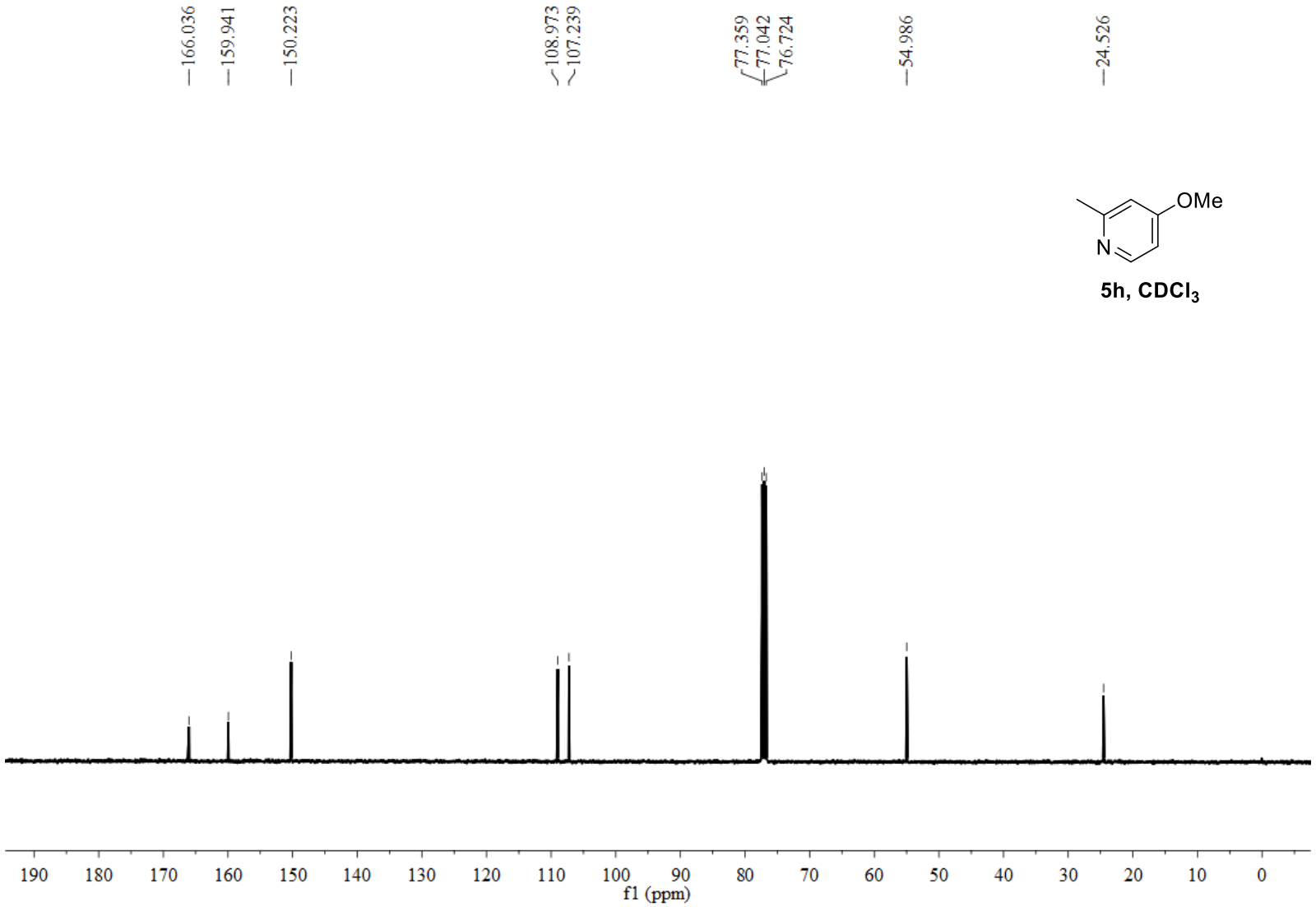

162.280
133.962
119.319
115.172
103.675
77.413
77.095
76.777
63.946
14.567
NC
O
5f, CDCl3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.000
7.994
7.988
7.976
7.971
7.964
7.260
6.911
6.904
6.899
6.887
6.882
6.875
4.366
4.348
4.330
4.312
4.105
4.088
4.070
4.053
1.448
1.430
1.413
1.391
1.373
1.355
2.000
2.048
f1 (ppm)
2.000
2.048
2.079
1.999
2.986
3.092
f1 (ppm)

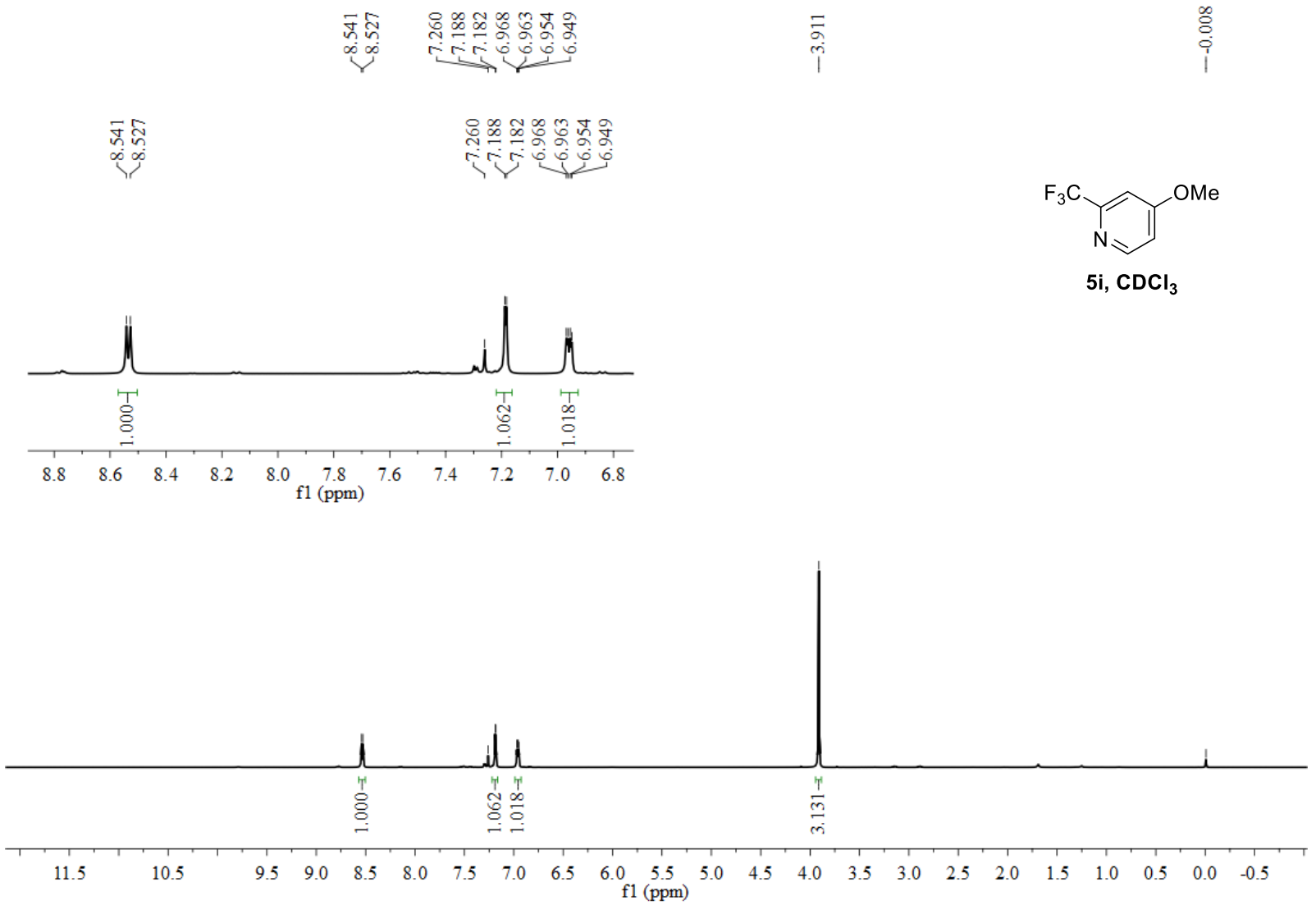
5g, $CDCl_3$

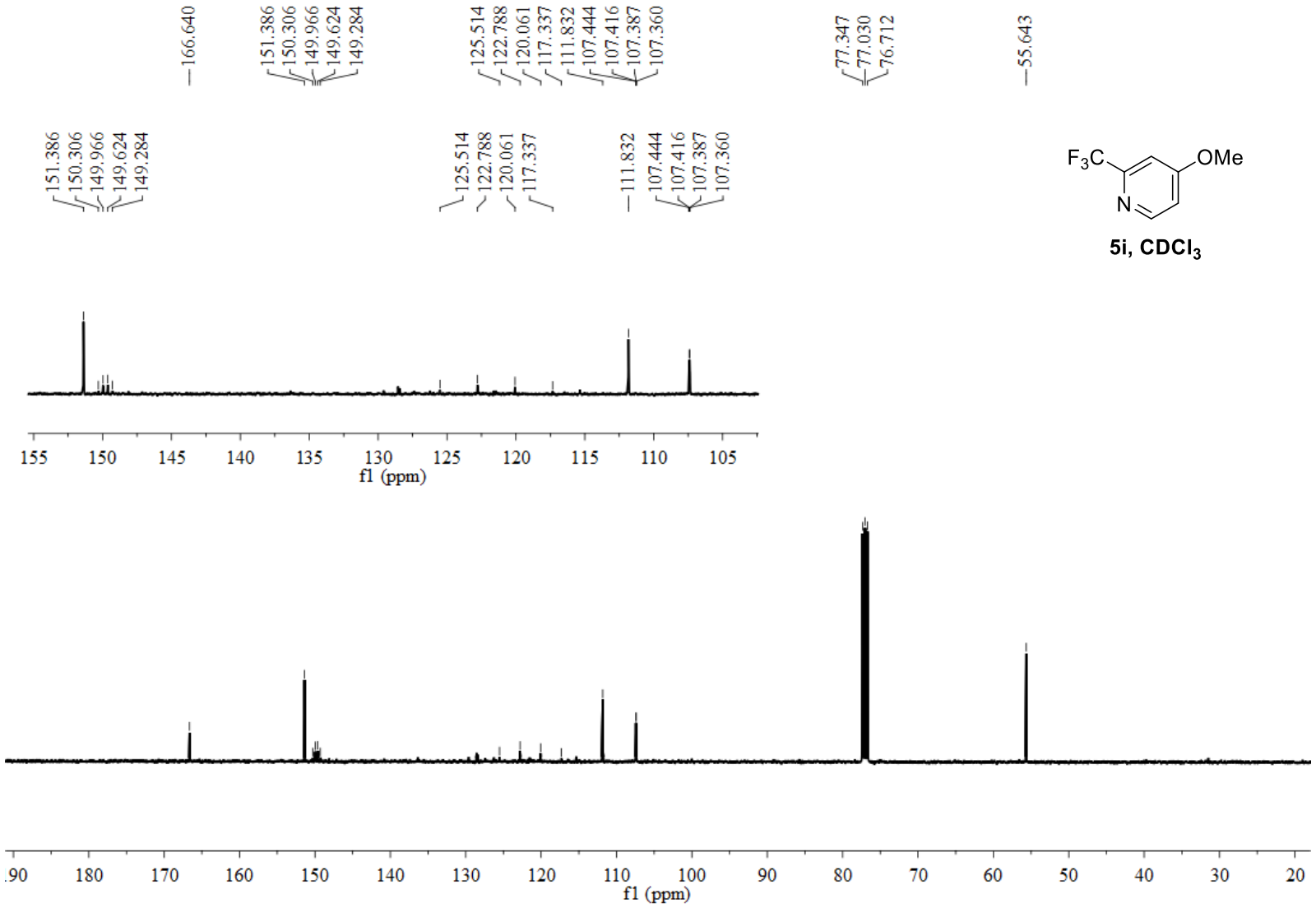

166.447
162.678
131.531
122.749
113.990
77.360
77.042
76.724
63.664
60.600
14.690
14.394
O
O
O
5g, CDCl3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

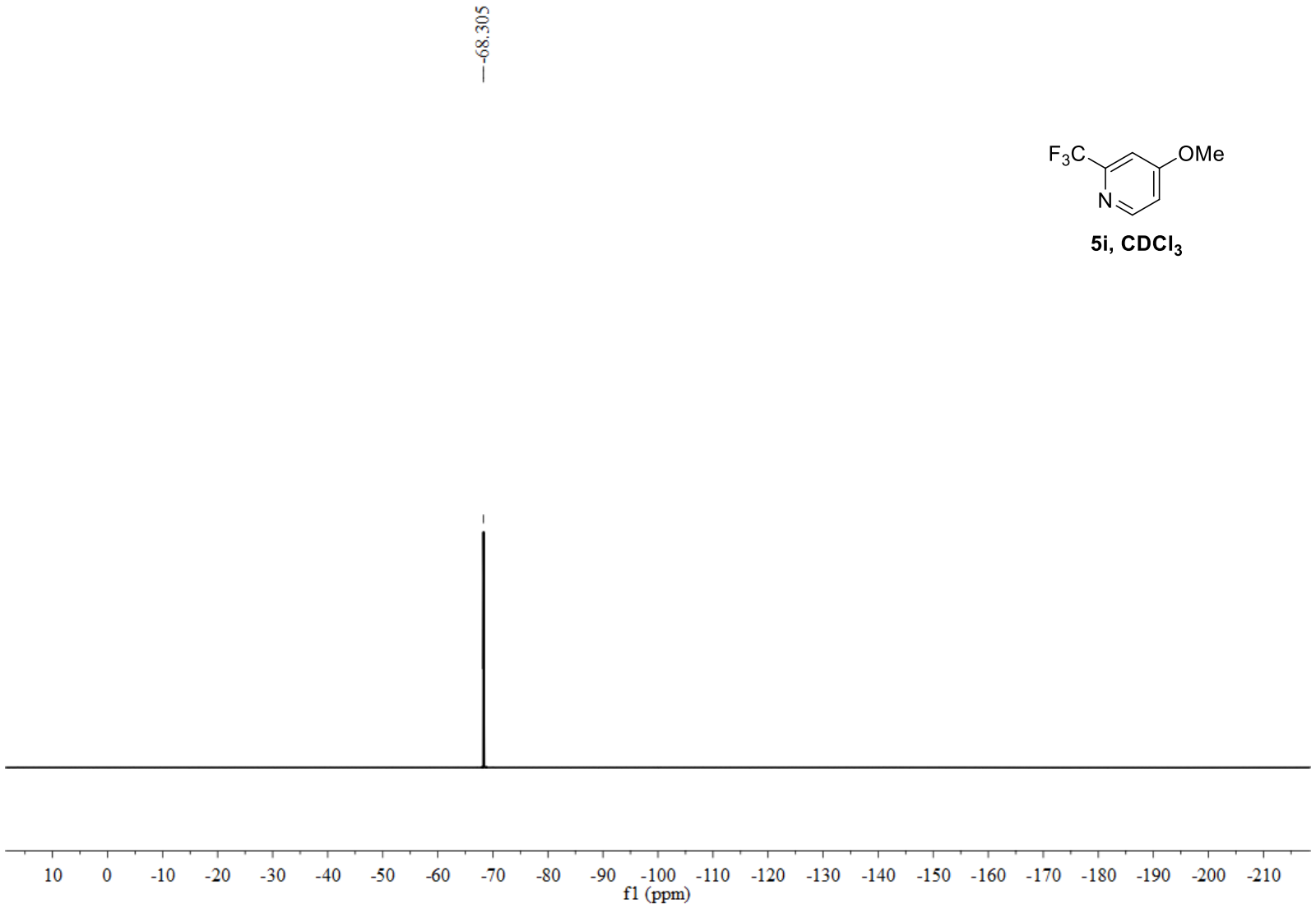

8.328
8.313
7.260
6.676
6.670
6.653
6.648
6.639
6.633
3.828
2.514
-0.005
OMe
N
5h, CDCl3
1.000
0.958
0.964
2.891
2.896
f1 (ppm)


166.036
159.941
150.223
108.973
107.239
77.359
77.042
76.724
54.986
24.526
OMe
N
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

5h, $CDCl_3$


8.541
8.527
7.260
7.188
7.182
6.968
6.963
6.954
6.949
3.911
-0.008
F3C
OMe
N
5i, CDCl3
1.000
1.062
1.018
3.131
f1 (ppm)


166.640
151.386
150.306
149.966
149.624
149.284
125.514
122.788
120.061
117.337
111.832
107.444
107.416
107.387
107.360
77.347
77.030
76.712
55.643
F3C
OMe
N
5i, CDCl3
f1 (ppm)
f1 (ppm)


-68.305
F3C
OMe
N
5i, CDCl3
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)