Supporting Information

Thiourea as a Pre-catalyst for the Electron Donor−Acceptor Complex Photoactivation Platform of Oxime Esters

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1. General Information

All reactions involving air- or moisture-sensitive reagents or intermediates were carried out in oven-dried glassware under nitrogen (N_2) atmosphere using standard *Schlenk* techniques. All reactions under irradiation were conducted in front of a 20 W LEDs bulb. All commercially available reagents were purchased and used directly without further purification. Thin layer chromatography (TLC) was performed on silica gel plates and visualized by fluorescence quenching under UV light or staining with the standard solution of Phosphomolybdic acid. Flash chromatography was carried out using silica gel (200-300 mesh) under a light positive pressure, eluting with the specified solvent system. Organic solutions were concentrated under reduced pressure on a rotatory evaporator. Isolated yields refer to materials of >95% purity as determined by ^{1}H NMR.

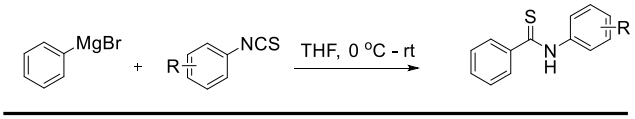
^{1}H NMR spectra were recorded on Bruker Bruker 400 MHz and 600 MHz spectrometers. Chemical shifts are reported in parts per-million (ppm) and the spectra are calibrated to the resonance resulting from incomplete deuteration of the solvent ($CDCl_3$: 7.26ppm, singlet; DMSO-d_6: 2.50ppm, pentet; Acetone-d_6: 2.05ppm, pentet). ^{13}C NMR spectra were recorded on the same spectrometer with complete proton decoupling. Chemical shifts are reported in ppm with the solvent resonance as the internal standard ($^{13}CDCl_3$: 77.16ppm, triplet; DMSO-d_6: 39.52ppm, septet; Acetone-d_6: 29.84ppm, septet). Data are reported as follows: chemical shift δ/ppm, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, m = multiplet or combinations thereof; ^{13}C signals are singlets unless otherwise stated), coupling constants *J* in Hz, and integration (^{1}H only). ^{19}F NMR spectra were recorded on the same Spectrometers.

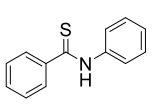
High Resolution Mass Spectrometry (HRMS) were all recorded on an ABI/Sciex QStar Mass Spectrometer using a positive electrospray ionization (ESI+). Measured values are reported to 4 decimal places of the calculated value. The calculated values are based on the most abundant isotope.

2. Synthesis and Characterization of Catalysts and Substrates

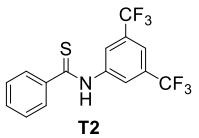
2.1 General Procedure for the Synthesis of Thioureas (Thioamides)

2.1.1 General Procedure for the synthesis of thioamides T1 and T2[1]



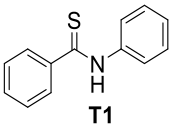


T1



T2

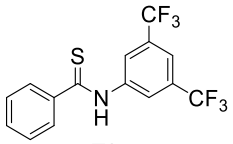
A solution of Phenyl isothiocyanate (1.0 equiv.) in dry THF (0.8 M) under nitrogen was cooled to 0 ºC and stirred. Phenylmagnesium bromide (1.0 equiv., 1.0 M in THF) was added dropwise. The mixture was allowed to warm to room temperature, then monitored by TLC. Upon completion, the mixture was diluted with H_2O and EtOAc. The layers were separated and the aqueous layer was extracted with EtOAc (×2). The combined organic layers were dried over Na_2SO_4, filtered and evaporated. Purification by column chromatography on silica gel gave the corresponding thioamide.



T1

***N*-phenylbenzothioamide** (**T1**): 74% yield as a yellow solid.

^{1}H NMR (600 MHz, DMSO-d_6): δ 11.78 (s, 1H), 7.86 (d, *J* = 7.2 Hz, 4H), 7.54 (t, *J* = 7.2 Hz, 1H), 7.47 (m, 4H), 7.29 (t, *J* = 7.2 Hz, 1H); Data in accordance with literature.[1]

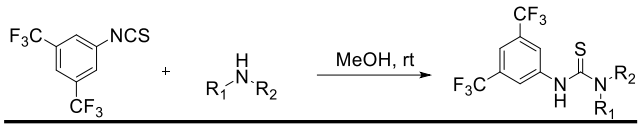


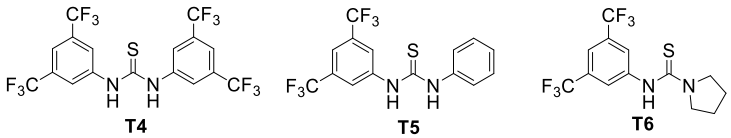
T2

***N*-(3,5-bis(trifluoromethyl)phenyl)benzothioamide** (**T2**): 68% yield as a yellow solid.

^{1}H NMR (600 MHz, DMSO-d_6): δ 12.18 (s, 1H), 8.71 (s, 2H), 8.0 (s, 1H), 7.89 (d, *J* = 7.8 Hz, 2H), 7.58 (t, *J* = 7.2 Hz, 1H), 7.50 (t, *J* = 7.2 Hz, 2H); Data in accordance with literature.[1]

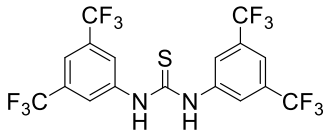
2.1.2 General Procedure for the synthesis of thioureas T4 to T6[2]





T4 **T5** **T6**

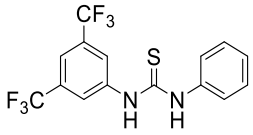
To a solution of 3,5-Bis(trifluoromethyl)phenyl isothiocyanate (1.0 equiv.) in MeOH (0.5 M) was added Amine (1.0 equiv.) dropwise at room temperature. The mixture was allowed to stir for 30 min and monitored by TLC. Upon completion, the solvent was evaporated and the residue was recrystallized from hexane to give the corresponding thiourea.



T4

1,3-Bis(3,5-bis(trifluoromethyl)phenyl)thiourea (**T4**): 75% yield as a white solid.

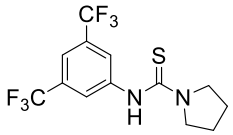
^{1}H NMR (600 MHz, DMSO-d_6): δ 10.68 (s, 2H), 8.24 (s, 4H), 7.85 (s, 2H); Data in accordance with literature.[2]



T5

1-(3,5-Bis(trifluoromethyl)phenyl)-3-phenylthiourea (**T5**): 82% yield as a white solid.

^{1}H NMR (600 MHz, DMSO-d_6): δ 10.33 (s, 1H), 10.25 (s, 1H), 8.28 (s, 2H), 7.78 (s, 1H), 7.47 (d, *J* = 8.4 Hz, 2H), 7.39 (t, *J* = 5.4 Hz, 2H), 7.20 (t, *J* = 7.2 Hz, 1H); Data in accordance with literature.[2a]



T6

***N*-(3,5-Bis(trifluoromethyl)phenyl)pyrrolidine-1-carbothioamide** (**T6**): 79% yield as a white solid.

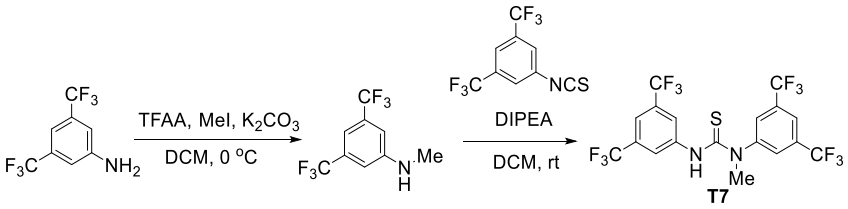
^{1}H NMR (600 MHz, DMSO-d_6): δ 9.34 (s, 1H), 8.24 (s, 2H), 7.75 (s, 1H), 3.68 (br, 4H), 2.02 (br, 2H), 1.89 (br, 2H);

^{13}C NMR (151 MHz, DMSO-d_6): δ 176.68, 142.68, 129.59 (q, *J* = 32.9 Hz), 124.39 (d, *J* = 3.4 Hz), 123.38 (q, *J* = 273.0 Hz), 116.50 (p, *J* = 3.4 Hz), 52.34, 48.67, 25.75, 24.12;

^{19}F NMR (565 MHz, DMSO-d_6): δ -61.50;

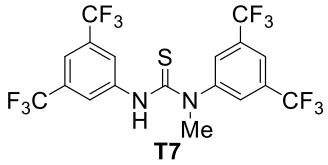
HRMS (ESI) m/z: calculated for $C_{13}H_{14}F_6N_2S$ $[M+H]^+$: 343.0704, found: 343.0698.

2.1.3 Procedure for the synthesis of thiourea T7[3]



A solution of 3,5-Bis(trifluoromethyl)aniline (1.0 equiv.) in dry DCM (0.5 M) under nitrogen was cooled to 0 ºC and stirred. Trifluoroacetic anhydride (3.0 equiv.) was added dropwise. The mixture was allowed to warm to room temperature and stirred for 20 min. The solvent was evaporated and redissolved in Acetone (0.5 M). K_2CO_3 (2.0 equiv.) and MeI (3.0 equiv.) were add stepwise. The mixture was then warmed to 60 ºC and refluxed for 2 h. Upon completion, the mixture was filtrated and the filtrate was evaporated. Then, MeOH : H_2O (5:1, 0.2M) and K_2CO_3 (1.0 equiv.) were added and the mixture was stirred for another 1 h. After evaporation of MeOH, the mixture was diluted with H_2O and DCM. The layers were separated and the aqueous layer was extracted with DCM (×2). The combined organic layers were dried over Na_2SO_4, filtered and evaporated to give the corresponding 3,5-Bis(trifluoromethyl)-N-methylaniline.

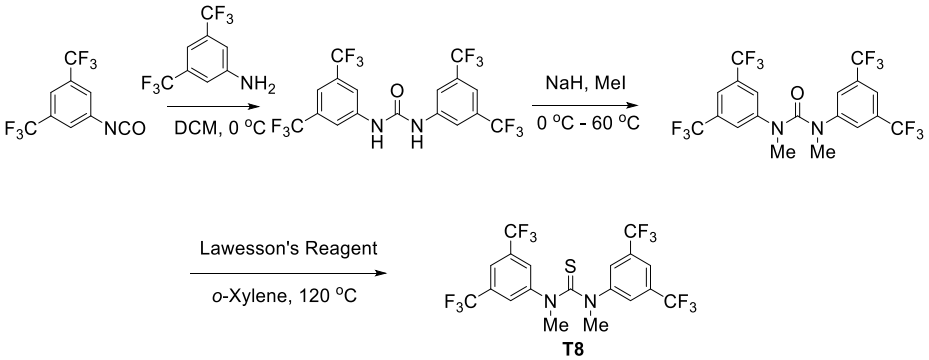
To a solution of 3,5-Bis(trifluoromethyl)-N-methylaniline (1.0 equiv.) and *N*,*N*-Diisopropylethylamine (1.0 equiv.) in DCM (0.5 M) was added Phenyl isothiocyanate (1.0 equiv.) dropwise at room temperature. The mixture was then stirred overnight. Upon completion, the mixture was diluted with DCM and washed with 1M HCl, H_2O and brine. The organic layer was dried over Na_2SO_4, filtered and evaporated. Purification by column chromatography on silica gel gave the corresponding thiourea.



1,3-Bis(3,5-bis(trifluoromethyl)phenyl)-1-methylthiourea (**T7**): 40% yield over 2 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.90 (s, 1H), 7.80 (s, 2H), 7.75 (s, 2H), 7.67 (s, 1H), 7.05 (br, 1H, NH), 3.77 (s, 3H); Data in accordance with literature.[3]

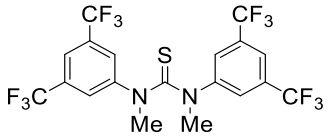
2.1.4 Procedure for the synthesis of thiourea T8[4]



To a solution of *N*,*N*-Diisopropylethylamine (1.0 equiv.) in Toluene (0.5 M) was added 3,5-Bis(trifluoromethyl)phenyl isocyanate (1.0 equiv.) dropwise at room temperature. Large amounts of white solids appeared after stirred for 1 h. Hexane was added and the mixture was stirred vigorously. Then the solid was filtered and washed with Hexane to give 1,3-Bis(3,5-bis(trifluoromethyl)phenyl)urea.

A solution of 1,3-Bis(3,5-bis(trifluoromethyl)phenyl)urea (1.0 equiv.) in dry THF (0.2 M) under nitrogen was cooled to 0 °C and stirred. NaH (3.0 equiv.) was added portionwise during 30 min. After addition of MeI (3.0 equiv.) dropwise, the mixture was then warmed to 60 ºC and refluxed overnight. The reaction was quenched with ice water and diluted with EtOAc. The layers were separated and the aqueous layer was extracted with EtOAc (×2). The combined organic layers were dried over Na_2SO_4, filtered and evaporated. Purification by column chromatography on silica gel gave 1,3-Bis(3,5-bis(trifluoromethyl)phenyl)-1,3-dimethylurea.

To a sealed tube was added 1,3-Bis(3,5-bis(trifluoromethyl)phenyl)-1,3-dimethylurea (1.0 equiv.), Lawesson's reagent (2.0 equiv.) and *o*-Xylene (0.2 M). The mixture was then warmed to 120 ºC and reacted for 10 h. After cooling, direct purification by column chromatography on silica gel gave 1,3-Bis(3,5-bis(trifluoromethyl)phenyl)-1,3-dimethylthiourea.



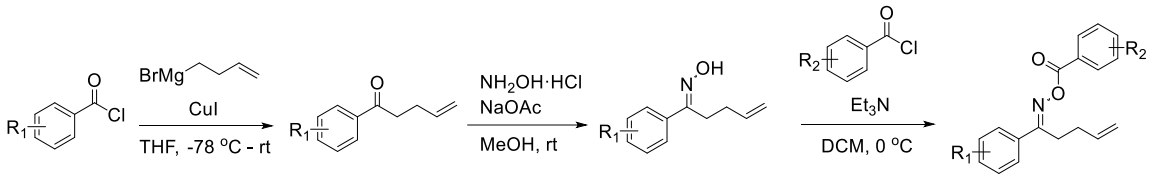
T8

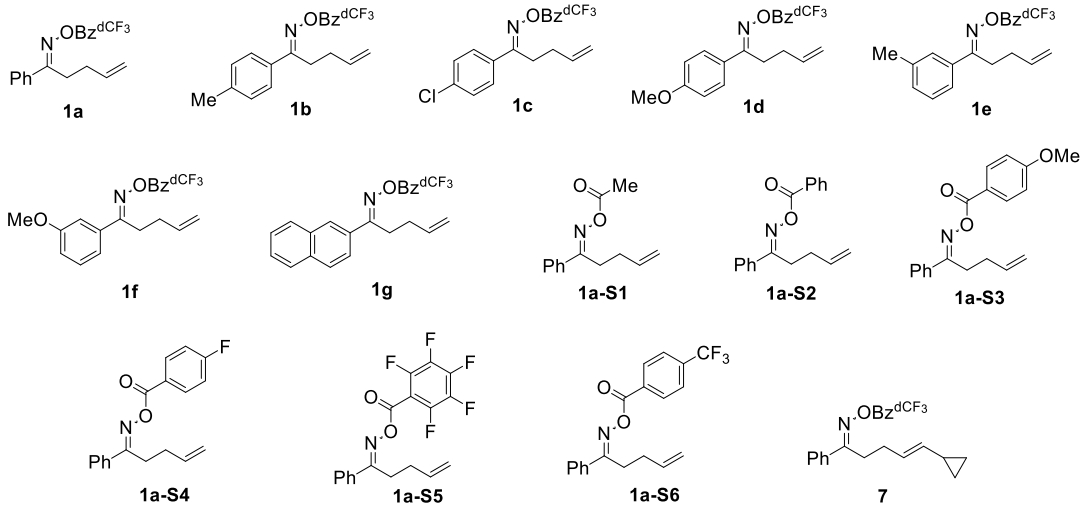
1,3-Bis(3,5-bis(trifluoromethyl)phenyl)-1,3-dimethylthiourea (**T8**): 39% yield over 3 steps as a pale yellow solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.47 (s, 2H), 7.06 (s, 4H), 3.62 (s, 6H); Data in accordance with literature.[4]

2.2 General Procedure for the Synthesis of Oxime Esters

2.2.1 General Procedure for the Synthesis of Oxime Esters 1 and 5[5]

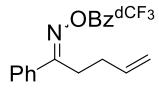




An oven-dried flask was charged with CuI (0.10 equiv.) and then evacuated and refilled with nitrogen (x3). The acid chloride (1.0 equiv.) and dry THF (0.1 M) were added and the mixture was cooled to -78 ºC and stirred. A solution of but-3-en-1-ylmagnesium bromide (1.1equiv., 0.5M in THF) was added dropwise for over 20 min. After stirred at -78 ºC for 2 h, the mixture was allowed to warm to room temperature overnight. Saturated NH_4Cl aqueous solution was added and the mixture was diluted with EtOAc. The layers were separated and the aqueous layer was extracted with EtOAc (×2). The combined organic layers were dried over Na_2SO_4, filtered and evaporated. Purification by column chromatography on silica gel gave the corresponding ketone.

To a solution of the ketone (1.0 equiv) in MeOH (1.0 M) was added sodium acetate (2.0 equiv) and hydroxylamine hydrochloride (1.5 equiv.). The mixture was stirred at room temperature and monitored by TLC. Upon completion, the excess MeOH was removed under reduced pressure and the resulting mixture was diluted with H_2O and EtOAc. The layers were separated and the aqueous layer was extracted with EtOAc (×2). The combined organic layers were dried over Na_2SO_4, filtered and evaporated. The corresponding oxime was used directly in the next step without further purification.

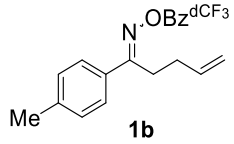
To a solution of the corresponding oxime (1.0 equiv.) in DCM (0.5 M) at 0 ºC was added Et_3N (1.5 equiv.) and acyl chloride (1.1 equiv). The reaction mixture was stirred until the oxime was consumed (determined by TLC, 10 min in most cases). Then saturated $NaHCO_3$ aqueous solution was added and the mixture was extracted with DCM. The combined organic layers were washed with water and brine, and dried over Na_2SO_4. The resulting solution was concentrated under vacuum and the residue was purified by column chromatography on silica gel to afford the corresponding oxime ester. Unless otherwise specified, the major isomer of oxime esters was used for reaction and characterization.



1a

1-Phenylpent-4-en-1-one *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (1a): 73% yield over 3 steps as a white solid.

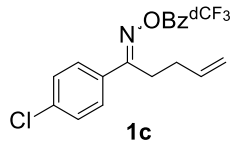
^{1}H NMR (600 MHz, $CDCl_3$): δ 8.56 (s, 2H), 8.13 (s, 1H), 7.80 (d, *J* = 7.2 Hz, 2H), 7.51-7.45 (m, 3H), 5.90-5.84 (m, 1H), 5.15-5.07 (m, 2H), 3.08 (t, *J* = 7.8 Hz, 2H), 2.46-2.41 (m, 2H); Data in accordance with literature.[5b]



1b

1-(*p*-Tolyl)pent-4-en-1-one *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (1b): 78% yield over 3 steps as a white solid.

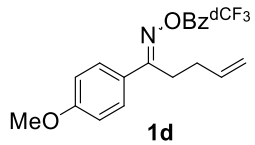
^{1}H NMR (600 MHz, $CDCl_3$): δ 8.55 (s, 2H), 8.12 (s, 1H), 7.70 (d, *J* = 8.4 Hz, 2H), 7.27 (d, *J* = 8.0 Hz, 2H), 5.92-5.82 (m, 1H), 5.15-5.06 (m, 2H), 3.06 (t, *J* = 7.6 Hz, 2H), 2.45-2.39 (m, 5H); Data in accordance with literature.[5b]



1c

1-(4-Chlorophenyl)pent-4-en-1-one *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (1c): 79% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.55 (s, 2H), 8.14 (s, 1H), 7.78-7.74 (m, 2H), 7.45-7.42 (m, 2H), 5.91-5.81 (m, 1H), 5.16-5.07 (m, 2H), 3.07 (t, *J* = 7.6 Hz, 2H), 2.45-2.42 (m, 2H); Data in accordance with literature.[5b]



1d

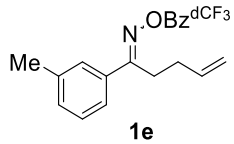
1-(4-Methoxyphenyl)pent-4-en-1-one *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (1d): 78% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.54 (s, 2H), 8.12 (s, 1H), 7.79-7.77 (m, 2H), 6.97-6.95 (m, 2H), 5.91-5.84 (m, 1H), 5.14-5.06 (m, 2H), 3.86 (s, 3H), 3.04 (t, *J* = 7.8 Hz, 2H), 2.42 (q, *J* = 7.2 Hz, 2H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 167.43, 162.19, 161.40, 136.31, 132.62 (q, *J* = 34.1 Hz), 131.75, 129.79 (q, *J* = 3.8 Hz), 129.19, 126.78 (p, *J* = 3.6 Hz), 125.45, 122.94 (q, *J* = 273.0 Hz), 116.36, 114.37, 55.52, 31.22, 28.31;

^{19}F NMR (565 MHz, $CDCl_3$): δ -63.01;

HRMS (ESI) m/z: calculated for $C_{13}H_9F_6NO_3Na$ $[M+Na]^+$: 468.1010, found: 468.1002.



1e

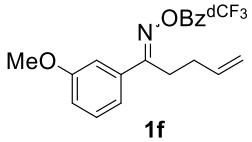
1-(*m*-tolyl)pent-4-en-1-one *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (1e): 70% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.56 (s, 2H), 8.13 (s, 1H), 7.64 (s, 1H), 7.56 (d, *J* = 7.2 Hz, 1H), 7.35 (t, *J* = 7.2 Hz, 1H), 7.31 (d, *J* = 7.2 Hz, 1H), 5.91-5.84 (m, 1H), 5.15-5.07 (m, 2H), 3.07 (t, *J* = 7.8 Hz, 2H), 2.45-2.41 (m, 5H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 168.35, 161.33, 138.80, 136.25, 133.26, 132.63 (q, *J* = 34.1 Hz), 132.06, 131.66, 129.80 (q, *J* = 3.8 Hz), 128.84, 128.13, 126.83 (p, *J* = 3.6 Hz), 124.72, 122.93 (q, *J* = 273.0 Hz), 116.38, 31.06, 28.67, 21.50;

^{19}F NMR (565 MHz, $CDCl_3$): δ -63.02;

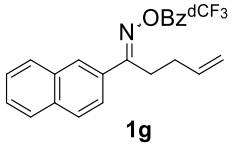
HRMS (ESI) m/z: calculated for $C_{21}H_{17}F_6NO_2Na$ $[M+Na]^+$: 452.1056, found: 452.1051.



1f

1-(3-Methoxyphenyl)pent-4-en-1-one *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (1f): 65% yield over 3 steps as a white solid.

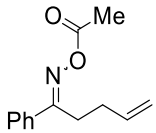
^{1}H NMR (600 MHz, $CDCl_3$): δ 8.55 (s, 2H), 8.13 (s, 1H), 7.39-7.34 (m, 3H), 7.05 (d, *J* = 7.8 Hz, 1H), 5.89-5.85 (m, 1H), 5.14-5.07 (m, 2H), 3.87 (s, 3H), 3.06 (t, *J* = 7.8 Hz, 2H), 2.45-2.41 (m, 2H); Data in accordance with literature.[5b]



1g

1-(Naphthalen-2-yl)pent-4-en-1-one *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (1e): 77% yield over 3 steps as a white solid.

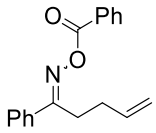
^{1}H NMR (600 MHz, $CDCl_3$): δ 8.58 (s, 2H), 8.23 (s, 1H), 8.14 (s, 1H), 7.97 (d, *J* = 8.4 Hz, 2H), 7.95-7.88 (m, 3H), 7.59-7.54 (m, 2H), 5.94-5.89 (m, 1H), 5.17-5.09 (m, 2H), 3.20 (t, *J* = 7.8 Hz, 2H), 2.52-2.48 (m, 2H); Data in accordance with literature.[5b]



1a-S1

1-Phenylpent-4-en-1-one *O*-acetyl oxime (1a-S1): 70% yield over 3 steps as a yellow oil.

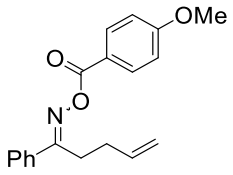
^{1}H NMR (600 MHz, $CDCl_3$): δ 7.71-7.70 (m, 2H), 7.46-7.40 (m, 3H), 5.84-5.80 (m, 1H), 5.07-5.01 (m, 2H), 2.95 (t, *J* = 7.8 Hz, 2H), 2.34-2.30 (m, 2H), 2.27 (s, 3H); Data in accordance with literature.[5b]



1a-S2

1-Phenylpent-4-en-1-one *O*-benzoyl oxime (1a-S2): 71% yield over 3 steps as a white solid.

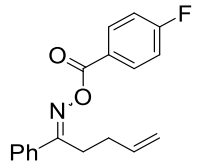
^{1}H NMR (600 MHz, $CDCl_3$): δ 8.12 (d, *J* = 7.2 Hz, 2H), 7.79 (d, *J* = 7.2 Hz, 2H), 7.62 (t, *J* = 7.2 Hz, 1H), 7.51 (t, *J* = 7.8 Hz, 2H), 7.48-7.43 (m, 3H), 5.91-5.85 (m, 1H), 5.12-5.04 (m, 2H), 3.08 (t, *J* = 7.8 Hz, 2H), 2.45-2.41 (m, 2H); Data in accordance with literature.[5b]



1a-S3

1-Phenylpent-4-en-1-one *O*-(4-methoxybenzoyl) oxime (1a-S3): 72% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.08 (d, *J* = 8.4 Hz, 2H), 7.79 (d, *J* = 7.2 Hz, 2H), 7.48-7.42 (m, 3H), 6.98 (d, *J* = 9.0 Hz, 2H), 5.90-5.85 (m, 1H), 5.12-5.04 (m, 2H), 3.89 (s, 3H), 3.06 (t, *J* = 7.8 Hz, 2H), 2.41-2.44 (m, 2H); Data in accordance with literature.[5b]



1a-S4

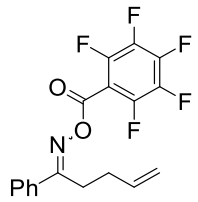
1-Phenylpent-4-en-1-one *O*-(4-fluorobenzoyl) oxime (1a-S4): 67% yield over 3 steps as a yellow oil.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.10-8.08 (m, 4H), 7.75 (d, *J* = 8.4 Hz, 2H), 7.41-7.35 (m, 3H), 7.11 (td, *J* = 8.4, 1.8 Hz, 2H), 5.86-5.79 (m, 1H), 5.06-4.98 (m, 2H), 3.01 (t, *J* = 7.8 Hz, 2H), 2.36 (q, *J* = 7.2 Hz, 2H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 166.63, 165.75 (d, *J* = 254.6 Hz), 162.58, 136.28, 133.58, 132.0 (d, *J* = 9.5 Hz), 130.55, 128.53, 127.23, 125.21 (d, *J* = 3.2 Hz), 115.83, 115.69 (d, *J* = 21.9 Hz), 30.65, 27.84;

^{19}F NMR (565 MHz, $CDCl_3$): δ -104.52;

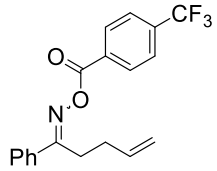
HRMS (ESI) m/z: calculated for $C_{18}H_{16}FNO_2Na$ $[M+Na]^+$: 320.1057, found: 320.1052.



1a-S5

1-Phenylpent-4-en-1-one *O*-perfluorobenzoyl oxime (1a-S5): 76% yield over 3 steps as a white solid.

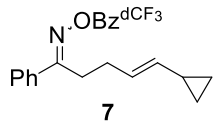
^{1}H NMR (600 MHz, $CDCl_3$): δ 7.75-7.74 (m, 2H), 7.51-7.49 (m, 1H), 7.48-7.43 (m, 2H), 5.82-5.78 (m, 1H), 5.06-5.01 (m, 2H), 3.00 (t, *J* = 7.8 Hz, 2H), 2.36-2.32 (m, 2H); Data in accordance with literature.[5b]



1a-S6

1-Phenylpent-4-en-1-one *O*-(4-(trifluoromethyl)benzoyl) oxime (1a-S6): 80% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.23 (d, *J* = 7.8 Hz, 2H), 7.82-7.77 (m, 4H), 7.50-7.44 (m, 3H), 5.89-5.85 (m, 1H), 5.12-5.05 (m, 2H), 3.08 (t, *J* = 7.2 Hz, 2H), 2.44-2.41 (m, 2H); Data in accordance with literature.[5b]

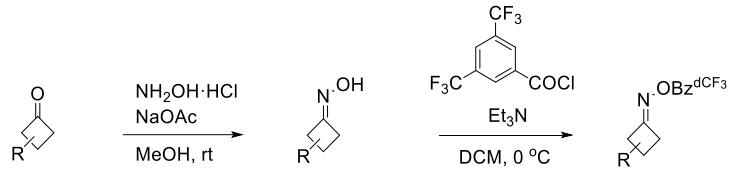


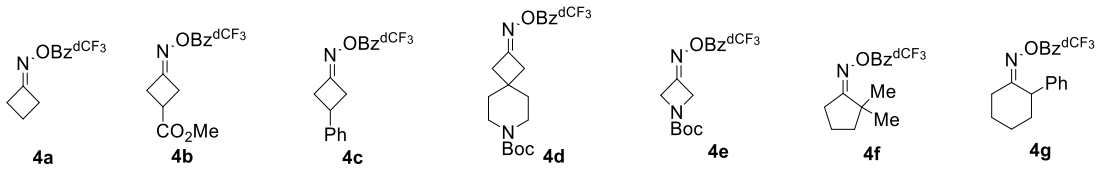
7

(4E)-5-Cyclopropyl-1-phenylpent-4-en-1-one *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (7): 68% yield over 3 steps as a pale yellow solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.56 (s, 2H), 8.13 (s, 1H), 7.82-7.78 (m, 2H), 7.51-7.45 (m, 3H), 5.53-5.49 (m, 0.3H, minor), 5.35-5.31 (m, 0.7H, major), 5.07-5.04 (m, 0.3H, minor), 4.82-4.97 (m, 0.7H, major), 3.09 (t, J = 7.2 Hz, 1.4H, major), 3.03 (t, J = 7.8 Hz, 0.6H, minor), 2.56-2.52 (m, 1.4H, major), 2.37-2.33 (m, 0.6H, minor), 1.37-1.33 (m, 0.7H, major), 1.30-1.28 (m, 0.3H, minor), 0.65-0.61 (m, 2H), 0.28-0.26 (m, 2H).; Data in accordance with literature.[5b]

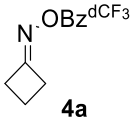
2.2.2 General Procedure for the Synthesis of Oxime Esters 4[6]





To a solution of cyclobutanone (1.0 equiv) in MeOH (1.0 M) was added sodium acetate (2.0 equiv) and hydroxylamine hydrochloride (1.5 equiv.). The mixture was stirred at room temperature and monitored by TLC. Upon completion, the excess MeOH was removed under reduced pressure and the resulting mixture was diluted with H_2O and EtOAc. The layers were separated and the aqueous layer was extracted with EtOAc (×2). The combined organic layers were dried over Na_2SO_4, filtered and evaporated. The corresponding oxime was used directly in the next step without further purification.

To a solution of the corresponding oxime (1.0 equiv.) in DCM (0.5 M) at 0 ºC was added Et_3N (1.5 equiv.) and 3,5-Bis(trifluoromethyl)benzoyl chloride (1.1 equiv). The reaction mixture was stirred until the oxime was consumed (determined by TLC, 10 min in most cases). Then saturated $NaHCO_3$ aqueous solution was added and the mixture was extracted with DCM. The combined organic layers were washed with water and brine, and dried over Na_2SO_4. The resulting solution was concentrated under vacuum and the residue was purified by column chromatography on silica gel to afford the corresponding oxime ester. Unless otherwise specified, the major isomer of oxime esters was used for reaction and characterization.



4a

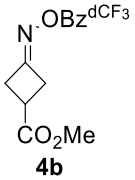
Cyclobutanone *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (4a): 44% yield over 2 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.44 (s, 2H), 8.06 (s, 1H), 3.18-3.13 (m, 4H), 2.17-2.11 (m, 2H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 170.88, 161.55, 132.44 (q, *J* = 34.1 Hz), 131.51, 129.75 (d, *J* = 3.0 Hz), 126.68 (p, *J* = 3.5Hz), 121.88 (q, *J* = 273.0 Hz), 31.95, 14.30;

^{19}F NMR (565 MHz, $CDCl_3$): δ -63.11;

HRMS (ESI) m/z: calculated for $C_{13}H_9F_6NO_2Na$ $[M+Na]^+$: 348.0430, found: 348.0430.



4b

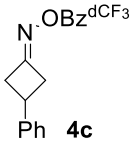
Methyl 3-(((3,5-bis(trifluoromethyl)benzoyl)oxy)imino)cyclobutane-1-carboxylate (4b): 76% yield over 2 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.43 (s, 2H), 8.07 (s, 1H), 3.75 (s, 3H), 3.45-3.39 (m, 4H), 3.32-3.27 (m, 1H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 173.52, 166.04, 161.27, 132.50 (q, *J* = 34.1 Hz), 131.17, 129.78 (d, *J* = 3.5 Hz), 126.85 (p, *J* = 3.5 Hz), 122.83 (q, *J* = 273.0 Hz), 52.55, 35.80, 35.76, 30.87;

^{19}F NMR (565 MHz, $CDCl_3$): δ -63.09;

HRMS (ESI) m/z: calculated for $C_{15}H_{11}F_6NO_4Na$ $[M+Na]^+$: 406.0484, found: 406.0479.



4c

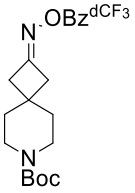
3-Phenylcyclobutan-1-one O-(3,5-bis(trifluoromethyl)benzoyl) oxime (4c): 75% yield over 2 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.47 (s, 2H), 8.07 (s, 1H), 7.35 (d, *J* = 7.2 Hz, 2H), 7.29-7.24 (m, 3H), 3.75-3.70 (m, 1H), 3.68-3.62 (m, 1H), 3.61-3.56 (m, 1H), 3.30-3.23 (m, 2H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 167.68, 161.48, 142.72, 132.45 (q, *J* = 34.1 Hz), 131.39, 129.76 (d, *J* = 3.3 Hz), 128.88, 127.13, 126.73 (p, *J* = 3.6 Hz), 126.37, 122.86 (q, *J* = 273.0 Hz), 39.57, 39.51, 32.51;

^{19}F NMR (565 MHz, $CDCl_3$): δ -63.03;

HRMS (ESI) m/z: calculated for $C_{19}H_{13}F_6NO_2Na$ $[M+Na]^+$: 424.0743, found: 424.0739.



4d

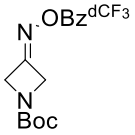
***tert*-Butyl 2-(((3,5-bis(trifluoromethyl)benzoyl)oxy)imino)-7-azaspiro[3.5]nonane-7-carboxylate (4d)**: 76% yield over 2 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.41 (s, 2H), 8.03 (s, 1H), 3.40-3.33 (m, 4H), 2.89-2.85 (m, 4H), 1.68-1.61 (m, 4H), 1.41 (s, 9H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 166.71, 161.36, 154.79, 132.39 (q, *J* = 34.1 Hz), 131.29, 129.69 (d, *J* = 3.3 Hz), 126.67 (p, *J* = 3.8 Hz), 123.79 (q, *J* = 273.0 Hz), 79.74, 41.93, 41.87, 36.29, 33.45, 28.39;

^{19}F NMR (565 MHz, $CDCl_3$): δ -63.07;

HRMS (ESI) m/z: calculated for $C_{22}H_{24}F_6N_2O_4Na$ $[M+Na]^+$: 517.1532, found: 517.1529.



4e

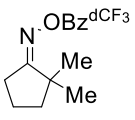
***tert*-Butyl 3-(((3,5-bis(trifluoromethyl)benzoyl)oxy)imino)azetidine-1-carboxylate (4e)**: 70% yield over 2 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.41 (s, 2H), 8.10 (s, 1H), 4.84-4.80 (m, 4H), 1.47 (s, 9H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 160.91, 160.40, 155.98, 132.70 (q, *J* = 34.1 Hz), 130.55, 129.84 (q, *J* = 3.9 Hz), 127.20 (p, *J* = 3.8 Hz), 122.77 (q, *J* = 273.1 Hz), 81.49, 58.31, 28.31;

^{19}F NMR (565 MHz, $CDCl_3$): δ -63.08;

HRMS (ESI) m/z: calculated for $C_{17}H_{16}F_6N_2O_4Na$ $[M+Na]^+$: 449.0906, found: 449.0904.



4f

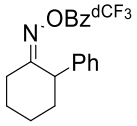
2,2-Dimethylcyclopentan-1-one *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (4f): 68% yield over 2 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.46 (s, 2H), 8.07 (s, 1H), 2.79 (t, *J* = 7.2 Hz, 2H), 1.87 (p, *J* = 7.2 Hz, 2H), 1.74 (t, *J* = 7.2 Hz, 2H), 1.32 (s, 6H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 182.14, 161.46, 132.45 (q, *J* = 34.1 Hz), 132.00, 129.68 (d, *J* = 3.6 Hz), 126.58 (p, *J* = 3.5 Hz), 122.95 (q, *J* = 273.1 Hz), 43.79, 41.13, 29.22, 26.36, 20.82;

^{19}F NMR (565 MHz, $CDCl_3$): δ -63.03;

HRMS (ESI) m/z: calculated for $C_{16}H_{15}F_6NO_2Na$ $[M+Na]^+$: 390.0899, found: 390.0898.



4g

2-Phenylcyclohexan-1-one *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (4g): 73% yield over 2 steps as a white solid.

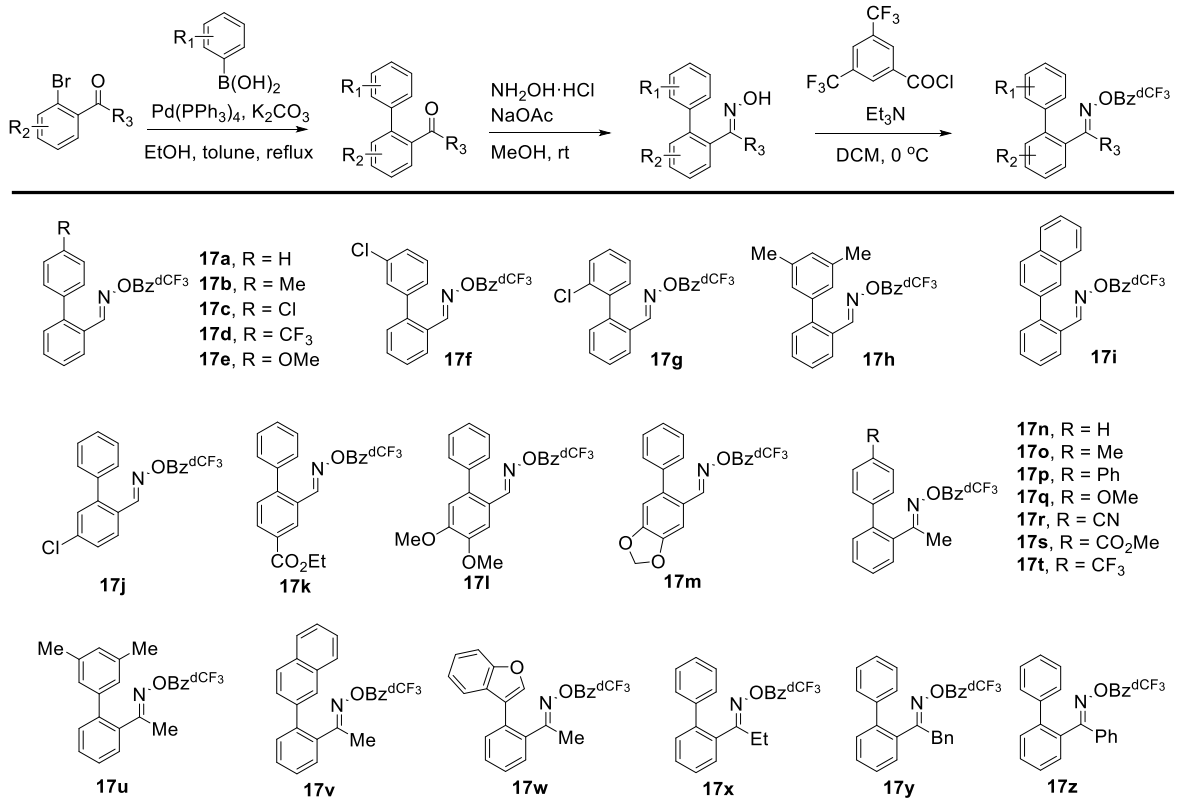
^{1}H NMR (600 MHz, $CDCl_3$): δ 8.51 (s, 2H), 8.10 (s, 1H), 7.40-7.35 (m, 4H), 7.27 (dq, *J* = 8.4, 3.2, 2.7 Hz, 1H), 4.03 (t, *J* = 5.1 Hz, 1H), 2.97-2.86 (m, 1H), 2.53 (dddq, *J* = 13.0, 5.5, 3.8, 1.7 Hz, 1H), 2.37 (ddd, *J* = 14.2, 10.5, 5.1 Hz, 1H), 2.15-2.06 (m, 1H), 1.93-1.86 (m, 1H), 1.83 (ddt, *J* = 14.6, 7.3, 3.9 Hz, 1H), 1.74 (dtd, *J* = 16.6, 9.9, 9.2, 4.2 Hz, 2H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 173.00, 161.86, 138.72, 132.49 (q, *J* = 34.1 Hz), 131.86, 129.78 (d, *J* = 3.6 Hz), 128.81, 127.81, 127.01, 126.68 (p, *J* = 3.6 Hz), 122.94 (q, *J* = 273.0 Hz), 45.67, 31.20, 26.53, 25.72, 22.27;

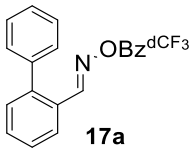
^{19}F NMR (565 MHz, $CDCl_3$): δ -63.03;

HRMS (ESI) m/z: calculated for $C_{21}H_{17}F_6NO_2Na$ $[M+Na]^+$: 452.1056, found: 452.1054.

2.2.3 General Procedure for the Synthesis of Oxime Esters 17a-17z[7]



An oven-dried flask was charged with aryl boronic acid (1.2 equiv.), $Pd(PPh_3)_4$ (0.05 equiv.) and K_2CO_3 (3.0 equiv.) and then evacuated and refilled with nitrogen (x3). Tolune and EtOH (0.4 M, 4:1) were added and the mixture was stirred at room temperature. Brominated aldehyde or ketone (1.0 equiv.) was added dropwise and then the mixture was allowed to reflux overnight. The mixture was filtered and evaporated. Purification by column chromatography on silica gel gave the corresponding aldehyde or ketone. The corresponding oxime ester was obtained following the previous General Procedures. Unless otherwise specified, the major isomer of oxime esters was used for reaction and characterization.



17a

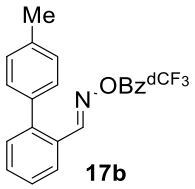
[1,1'-Biphenyl]-2-carbaldehyde O-(3,5-bis(trifluoromethyl)benzoyl) oxime (17a) : 58% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.57 (s, 1H), 8.52 (s, 2H), 8.24 (d, *J* = 7.8 Hz, 2H), 8.10 (s, 1H), 7.58 (t, *J* = 7.2 Hz, 1H), 7.52-7.44 (m, 5H), 7.37 (d, *J* = 6.6 Hz, 2H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 161.67, 157.34, 143.89, 139.01, 132.51 (q, *J* = 34.1 Hz), 131.14, 129.96, 128.81, 128.24, 128.07, 127.81, 127.38, 126.88 (p, *J* = 3.5 Hz), 122.93 (q, *J* = 273.0 Hz);

^{19}F NMR (565 MHz, $CDCl_3$): δ -63.03;

HRMS (ESI) m/z: calculated for $C_{22}H_{13}F_6NO_2Na$ $[M+Na]^+$: 460.0743, found: 460.0736.



17b

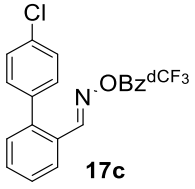
4'-Methyl-[1,1'-biphenyl]-2-carbaldehyde *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (17b): 73% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.59 (s, 1H), 8.53 (s, 2H), 8.22 (d, *J* = 7.8 Hz, 2H), 8.11 (s, 1H), 7.57 (t, *J* = 7.2 Hz, 1H), 7.46 (t, *J* = 7.2 Hz, 1H), 7.43 (d, *J* = 7.8 Hz, 1H), 7.32 (d, *J* = 7.8 Hz, 2H), 7.27 (d, *J* = 7.8 Hz, 2H), 2.45 (s, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 161.70, 157.50, 143.91, 138.16, 136.07, 132.51 (q, *J* = 34.1 Hz), 131.92, 131.19, 130.65, 129.00 (d, *J* = 3.2 Hz), 129.86, 129.53, 127.84, 127.81, 127.36, 126.86 (p, *J* = 3.5 Hz), 122.93 (q, *J* = 273.0 Hz);

^{19}F NMR (565 MHz, $CDCl_3$): δ -62.90;

HRMS (ESI) m/z: calculated for $C_{23}H_{15}F_6NO_2Na$ $[M+Na]^+$: 474.0899, found: 474.0896.



17c

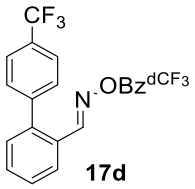
4'-Chloro-[1,1'-biphenyl]-2-carbaldehyde *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (17c): 82% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.52 (s, 3H), 8.22 (d, *J* = 7.8 Hz, 2H), 8.11 (s, 1H), 7.58 (d, *J* = 7.2 Hz, 1H), 7.50-7.47 (m, 3H), 7.40 (d, *J* = 7.8 Hz, 1H), 7.30 (d, *J* = 8.4 Hz, 2H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 161.64, 156.95, 142.52, 137.41, 134.60, 132.55 (q, *J* = 34.1 Hz), 132.06, 131.18, 131.03, 130.51, 129.99 (q, *J* = 3.6 Hz), 129.07, 128.42, 128.00, 127.45, 126.95 (p, *J* = 3.5 Hz), 122.92 (q, *J* = 273.0 Hz);

^{19}F NMR (565 MHz, $CDCl_3$): δ -62.90;

HRMS (ESI) m/z: calculated for $C_{22}H_{12}ClF_6NO_2Na$ $[M+Na]^+$: 494.0353, found: 494.0354.



17d

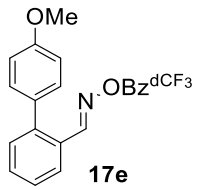
4'-(Trifluoromethyl)-[1,1'-biphenyl]-2-carbaldehyde *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (17d): 75% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.52 (s, 2H), 8.51 (s, 1H), 8.25 (d, *J* = 7.8 Hz, 2H), 7.77 (d, *J* = 7.8 Hz, 2H), 7.62 (t, *J* = 7.2 Hz, 1H), 7.53 (t, *J* = 7.2 Hz, 1H), 7.50 (d, *J* = 7.8 Hz, 1H), 7.43 (d, *J* = 7.2 Hz, 1H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 161.63, 156.72, 142.66, 142.21, 132.58 (q, *J* = 34.1 Hz), 132.14, 130.98, 130.55, 130.52 (q, *J* = 32.9 Hz), 130.27, 129.99 (q, *J* = 3.9 Hz), 128.84, 128.11, 127.53, 126.99 (p, *J* = 3.5 Hz), 125.82 (q, *J* = 3.5 Hz), 124.17 (q, *J* = 272.8 Hz), 122.91 (q, *J* = 273.2 Hz);

^{19}F NMR (565 MHz, $CDCl_3$): δ -62.57, -62.95;

HRMS (ESI) m/z: calculated for $C_{23}H_{12}F_9NO_2Na$ $[M+Na]^+$: 528.0617, found: 528.0616.



17e

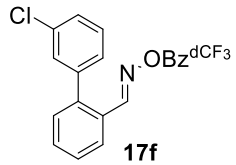
4'-Methoxy-[1,1'-biphenyl]-2-carbaldehyde *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (17e): 83% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.58 (s, 1H), 8.53 (s, 2H), 8.20 (d, *J* = 7.8 Hz, 1H), 8.10 (s, 1H), 7.56 (td, *J* = 7.2, 1.0 Hz, 1H), 7.44 (t, *J* = 7.8 Hz, 1H), 7.42 (d, *J* = 7.8 Hz, 1H), 7.29 (d, *J* = 8.4 Hz, 1H), 7.03 (d, *J* = 8.4 Hz, 1H), 3.88 (s, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 161.70, 159.75, 157.56, 142.58, 132.50 (q, *J* = 34.1 Hz), 131.91, 131.28, 131.18, 131.13, 130.63, 129.97 (q, *J* = 3.6 Hz), 128.86, 127.68, 127.38, 126.86 (p, *J* = 3.5 Hz), 122.93 (q, *J* = 273.5 Hz), 114.25, 55.50;

^{19}F NMR (565 MHz, $CDCl_3$): δ -62.90;

HRMS (ESI) m/z: calculated for $C_{23}H_{15}F_6NO_3Na$ $[M+Na]^+$: 490.0848 , found: 490.0847.



17f

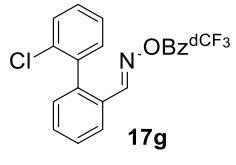
3'-Chloro-[1,1'-biphenyl]-2-carbaldehyde *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (17f): 76% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.52 (s, 3H), 8.23 (d, *J* = 7.8 Hz, 1H), 8.10 (s, 1H), 7.59 (t, *J* = 7.2 Hz, 1H), 7.50 (t, *J* = 7.8 Hz, 1H), 7.44-7.38 (m, 4H), 7.24-7.22 (m, 1H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 161.61, 156.76, 142.32, 140.78, 134.86, 132.53 (q, *J* = 34.1 Hz), 132.04, 131.04, 130.50, 130.0, 129.77, 128.59, 128.45, 128.23, 127.89, 127.46, 126.94 (p, *J* = 3.5 Hz), 122.92 (q, *J* = 273.5 Hz);

^{19}F NMR (565 MHz, $CDCl_3$): δ -62.91;

HRMS (ESI) m/z: calculated for $C_{22}H_{12}ClF_6NO_2Na$ $[M+Na]^+$: 494.0353, found: 494.0352.



17g

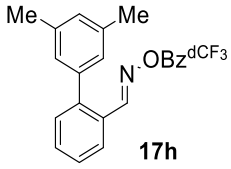
2'-Chloro-[1,1'-biphenyl]-2-carbaldehyde *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (17g): 66% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.50 (s, 2H), 8.30 (s, 1H), 8.28 (d, *J* = 7.8 Hz, 1H), 8.09 (s, 1H), 7.59 (t, *J* = 7.2 Hz, 1H), 7.56-7.51 (m, 2H), 7.44-7.38 (m, 2H), 7.34-7.30 (m, 2H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 161.60, 156.31, 141.02, 137.64, 133.54, 132.47 (q, *J* = 34.1 Hz), 131.93, 131.90, 131.08, 130.86, 130.07, 129.98, 128.74, 128.12, 127.17, 127.12, 126.88 (p, *J* = 3.5 Hz), 122.92 (q, *J* = 273.5 Hz);

^{19}F NMR (565 MHz, $CDCl_3$): δ -62.90;

HRMS (ESI) m/z: calculated for $C_{22}H_{12}ClF_6NO_2Na$ $[M+Na]^+$: 494.0353, found: 494.0355.



17h

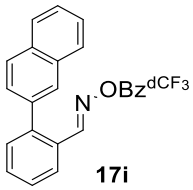
3',5'-Dimethyl-[1,1'-biphenyl]-2-carbaldehyde *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (17h): 74% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.58 (s, 1H), 8.53 (s, 2H), 8.22 (d, *J* = 7.8 Hz, 1H), 8.11 (s, 1H), 7.56 (t, *J* = 7.8 Hz, 1H), 7.46 (t, *J* = 7.8 Hz, 1H), 7.41 (d, *J* = 7.8 Hz, 1H), 7.10 (s, 1H), 6.98 (s, 2H), 2.40 (s, 6H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 161.70, 157.49, 144.24, 138.98, 138.39, 132.51 (q, *J* = 34.1 Hz), 131.82, 131.21, 130.58, 129.98 (q, *J* = 3.6 Hz), 129.84, 127.85, 127.82, 127.61, 127,32, 126.85 (p, *J* = 3.6 Hz), 122.94 (q, *J* = 273.0 Hz), 21.45;

^{19}F NMR (565 MHz, $CDCl_3$): δ -62.92;

HRMS (ESI) m/z: calculated for $C_{24}H_{17}F_6NO_2Na$ $[M+Na]^+$: 488.1056, found: 488.1057.



17i

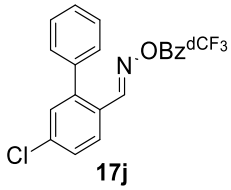
2-(Naphthalen-2-yl)benzaldehyde *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (17i): 80% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.59 (s, 1H), 8.49 (s, 2H), 8.28 (d, *J* = 7.8 Hz, 1H), 8.08 (s, 1H), 7.98 (d, *J* = 8.4 Hz, 1H), 7.95-7.91 (m, 2H), 7.83 (s, 1H), 7.62 (t, *J* = 7.8 Hz, 1H), 7.59-7.56 (m, 2H), 7.54-7.50 (m, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 161.71, 157.35, 143.89, 136.47, 133.25, 132.85, 132.48 (q, *J* = 34.1 Hz), 131.94, 131.07, 130.86, 129.97 (d, *J* = 4.0 Hz), 129.14, 128.56, 128.33, 128.16, 127,95, 127.84, 127.68, 127.02, 126.84, 122.89 (q, *J* = 273.0 Hz);

^{19}F NMR (565 MHz, $CDCl_3$): δ -62.90;

HRMS (ESI) m/z: calculated for $C_{26}H_{15}F_6NO_2Na$ $[M+Na]^+$: 510.0899, found: 510.0894.



17j

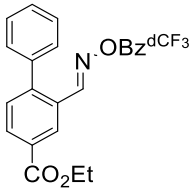
5-Chloro-[1,1'-biphenyl]-2-carbaldehyde *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (17j): 64% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.50 (s, 2H), 8.49 (s, 1H), 8.18 (d, *J* = 7.8 Hz, 1H), 8.10 (s, 1H), 7.53-7.47 (m, 3H), 7.46-7.44 (m, 2H), 7.35 (d, *J* = 7.2 Hz, 2H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 161.55, 156.30, 145.33, 138.0, 137.68, 132.55 (q, *J* = 34.1 Hz), 130.97, 130.62, 129.98 (d, *J* = 4.0 Hz), 129.76, 129.12, 129.0, 128.78, 128.37, 126.96 (p, *J* = 3.6 Hz), 125.93, 122.89 (q, *J* = 273.0 Hz);

^{19}F NMR (565 MHz, $CDCl_3$): δ -62.92;

HRMS (ESI) m/z: calculated for $C_{22}H_{12}ClF_6NO_2Na$ $[M+Na]^+$: 494.0353, found: 494.0349.



17k

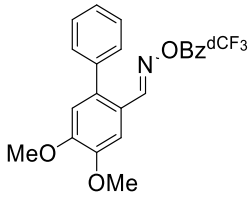
Ethyl 2-((((3,5-bis(trifluoromethyl)benzoyl)oxy)imino)methyl)-[1,1'-biphenyl]-4-carboxylate (17k): 66% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.83 (s, 1H), 8.57 (s, 1H), 8.52 (s, 2H), 8.23 (d, *J* = 7.8 Hz, 1H), 8.10 (s, 1H), 7.54-7.48 (m, 4H), 7.38 (d, *J* = 6.6 Hz, 2H), 4.45 (q, *J* = 7.2 Hz, 2H), 1.44 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 165.75, 161.56, 156.93, 147.62, 138.14, 132.59, 132.55 (q, *J* = 34.1 Hz), 130.99, 130.82, 130.45, 129.98 (d, *J* = 4.0 Hz), 129.76, 129.16, 128.99, 128.85, 127.68, 126.96 (p, *J* = 3.6 Hz), 122.89 (q, *J* = 273.0 Hz), 61.58, 14.49;

^{19}F NMR (565 MHz, $CDCl_3$): δ -62.93;

HRMS (ESI) m/z: calculated for $C_{24}H_{15}F_6NO_4Na$ $[M+Na]^+$: 532.0954, found: 532.0952.



17l

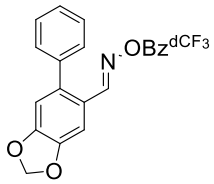
4,5-Dimethoxy-[1,1'-biphenyl]-2-carbaldehyde *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (17l): 83% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.50 (s, 2H), 8.46 (s, 1H), 8.08 (s, 1H), 7.69 (s, 1H), 7.49 (t, *J* = 7.2, 1H), 7.45 (t, *J* = 7.2, 1H), 7.35 (d, *J* = 6.6 Hz, 2H), 6.87 (s, 1H), 4.03 (s, 3H), 3.96 (s, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 161.85, 157.12, 152.18, 148.92, 138.91, 138.68, 132.47 (q, *J* = 34.1 Hz), 131.24, 130.05, 129.91 (d, *J* = 3.2 Hz), 128.75, 128.12, 126.80 (p, *J* = 3.6 Hz), 122.91 (q, *J* = 273.0 Hz), 119.57, 112.83, 108.79, 56.44, 56.19;

^{19}F NMR (565 MHz, $CDCl_3$): δ -62.91;

HRMS (ESI) m/z: calculated for $C_{24}H_{17}F_6NO_4Na$ $[M+Na]^+$: 520.0954, found: 520.0949.



17m

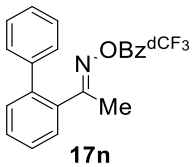
6-Phenylbenzo[*d*][1,3]dioxole-5-carbaldehyde *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (17m): 84% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.49 (s, 2H), 8.41 (s, 1H), 8.08 (s, 1H), 7.69 (s, 1H), 7.49-7.43 (m, 3H), 7.31 (d, *J* = 6.6 Hz, 2H), 6.85 (s, 1H), 6.09 (s, 2H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 161.74, 156.88, 150.99, 147.86, 140.30, 138.82, 132.47 (q, *J* = 34.1 Hz), 131.22, 130.0, 129.94 (d, *J* = 3.2 Hz), 128.78, 128.23, 126.80 (p, *J* = 3.6 Hz), 122.93 (q, *J* = 273.0 Hz), 121.12, 110.37, 106.48, 102.17;

^{19}F NMR (565 MHz, $CDCl_3$): δ -62.91;

HRMS (ESI) m/z: calculated for $C_{23}H_{13}F_6NO_4Na$ $[M+Na]^+$: 504.0641, found: 504.0636.



17n

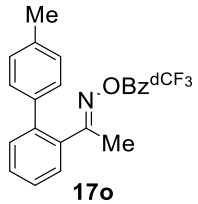
1-([1,1'-Biphenyl]-2-yl)ethan-1-one *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (17n): 61% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.54 (s, 2H), 8.11 (s, 1H), 7.60 (d, *J* = 7.8 Hz, 1H), 7.54 (t, *J* = 7.8 Hz, 1H), 7.47-7.42 (m, 6H), 7.39 (t, *J* = 7.2 Hz, 1H), 1.93 (s, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 169.42, 161.35, 140.88, 140.49, 134.70, 132.54 (q, *J* = 34.1 Hz), 131.68, 130.58, 130.41, 129.86, 129.83, 129.11, 128.86, 127.97, 127.70, 126.80 (p, *J* = 3.6 Hz), 122.92 (q, *J* = 273.0 Hz), 18.54;

^{19}F NMR (565 MHz, $CDCl_3$): δ -62.98;

HRMS (ESI) m/z: calculated for $C_{23}H_{15}F_6NO_2Na$ $[M+Na]^+$: 474.0899, found: 474.0897.



17o

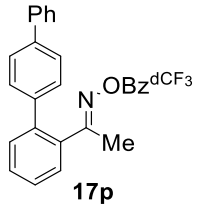
1-(4'-Methyl-[1,1'-biphenyl]-2-yl)ethan-1-one *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (17o): 64% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.54 (s, 2H), 8.12 (s, 1H), 7.59 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.52 (td, *J* = 7.8, 1.2 Hz, 1H), 7.44-7.40 (m, 2H), 7.35 (d, *J* = 7.8 Hz, 2H), 7.24 (d, *J* = 7.8 Hz, 2H), 2.40 (s, 3H), 1.93 (s, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 169.65, 161.38, 140.87, 137.85, 137.56, 134.63, 132.54 (q, *J* = 34.1 Hz), 131.73, 130.56, 130.39, 129.85, 129.59, 128.98, 127.45, 126.79 (p, *J* = 3.6 Hz), 122.93 (q, *J* = 273.0 Hz), 21.32, 18.57;

^{19}F NMR (565 MHz, $CDCl_3$): δ -62.97;

HRMS (ESI) m/z: calculated for $C_{24}H_{17}F_6NO_2Na$ $[M+Na]^+$: 488.1056, found: 488.1053.



17p

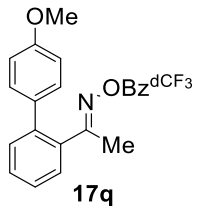
1-([1,1':4',1''-Terphenyl]-2-yl)ethan-1-one *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (17p): 40% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.55 (s, 2H), 8.11 (s, 1H), 7.69 (d, *J* = 7.8 Hz, 2H), 7.65 (d, *J* = 7.8 Hz, 2H), 7.62 (d, *J* = 7.8 Hz, 1H), 7.58-7.55 (m, 3H), 7.50 (d, *J* = 7.8 Hz, 1H), 7.47-7.44(m, 3H), 7.37 (t, *J* = 7.8 Hz, 2H), 1.99 (s, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 169.52, 161.39, 140.77, 140.44, 140.40, 139.39, 134.72, 132.57 (q, *J* = 34.1 Hz), 131.67, 130.57, 130.49, 129.95, 129.87 (d, *J* = 3.6 Hz), 129.54, 129.02, 127.77, 127.75, 127.51, 127.17, 126.83 (p, *J* = 3.6 Hz), 122.92 (q, *J* = 273.0 Hz), 18.75;

^{19}F NMR (565 MHz, $CDCl_3$): δ -62.95;

HRMS (ESI) m/z: calculated for $C_{29}H_{19}F_6NO_2Na$ $[M+Na]^+$: 550.1212, found: 550.1209.



17q

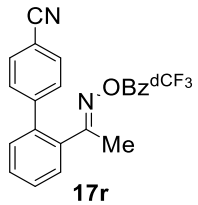
1-(4'-Methoxy-[1,1'-biphenyl]-2-yl)ethan-1-one *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (17q): 68% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.54 (s, 2H), 8.11 (s, 1H), 7.57 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.51 (td, *J* = 7.8, 1.2 Hz, 1H), 7.43-7.37 (m, 4H), 6.98-6.95 (m, 2H), 3.58 (s, 3H), 1.94 (s, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 169.72, 161.40, 159.59, 140.52, 134.59, 132.81, 132.56 (q, *J* = 34.1 Hz), 131.72, 130.49, 130.40, 130.25, 129.85, 127.28, 126.80 (p, *J* = 3.6 Hz), 122.93 (q, *J* = 273.0 Hz), 114.32, 55.42, 18.53;

^{19}F NMR (565 MHz, $CDCl_3$): δ -62.97;

HRMS (ESI) m/z: calculated for $C_{24}H_{17}F_6NO_3Na$ $[M+Na]^+$: 504.1005, found: 504.1006.



17r

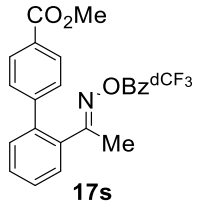
2'-(1-(((3,5-Bis(trifluoromethyl)benzoyl)oxy)imino)ethyl)-[1,1'-biphenyl]-4-carbonitrile (17r): 68% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.52 (s, 2H), 8.12 (s, 1H), 7.73 (d, *J* = 7.8 Hz, 2H), 7.61-7.56 (m, 4H), 7.50 (t, *J* = 7.8 Hz, 1H), 7.42 (d, *J* = 7.8 Hz, 1H), 1.99 (s, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 168.27, 161.21, 145.14, 138.77, 134.69, 132.62, 132.58 (q, *J* = 34.1 Hz), 131.32, 130.64, 130.41, 130.03, 129.83, 128.88, 126.98 (p, *J* = 3.6 Hz), 122.85 (q, *J* = 273.0 Hz), 118.65, 111.87, 18.82;

^{19}F NMR (565 MHz, $CDCl_3$): δ -62.96;

HRMS (ESI) m/z: calculated for $C_{24}H_{14}F_6N_2O_2Na$ $[M+Na]^+$: 499.0852, found: 499.0848.



17s

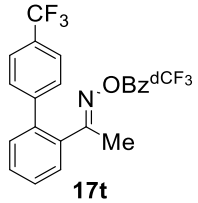
Methyl 2'-(1-(((3,5-bis(trifluoromethyl)benzoyl)oxy)imino)ethyl)-[1,1'-biphenyl]-4-carboxylate (17s): 56% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.54 (s, 2H), 8.11 (s, 1H), 7.58 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.51 (td, *J* = 7.8, 1.2 Hz, 1H), 7.43-7.38 (m, 4H), 6.98-6.95 (m, 2H), 3.85 (s, 3H), 1.94 (s, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 169.71, 161.39, 159.59, 140.52, 134.58, 132.81, 132.55 (q, *J* = 34.1 Hz), 131.72, 130.48, 130.40, 130.24, 129.85, 127.28, 126.79 (p, *J* = 3.6 Hz), 122.93 (q, *J* = 273.0 Hz), 114.31, 55.42, 18.53;

^{19}F NMR (565 MHz, $CDCl_3$): δ -62.97;

HRMS (ESI) m/z: calculated for $C_{25}H_{17}F_6NO_4Na$ $[M+Na]^+$: 532.0954, found: 532.0954.



17t

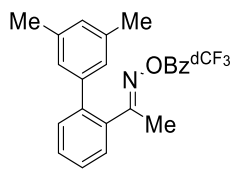
1-(4'-(Trifluoromethyl)-[1,1'-biphenyl]-2-yl)ethan-1-one *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (17t): 60% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.53 (s, 2H), 8.12 (s, 1H), 7.70 (d, *J* = 7.8 Hz, 2H), 7.62-7.60 (m, 3H), 7.57 (td, *J* = 7.8, 1.2 Hz, 1H), 7.49 (td, *J* = 7.8, 1.2 Hz, 1H), 7.44 (dd, *J* = 7.8, 1.2 Hz, 1H), 1.96 (s, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 168.73, 161.32, 144.11, 139.28, 134.80, 132.62 (q, *J* = 34.1 Hz), 131.50, 130.60, 130.57, 130.51, 130.19 (q, *J* = 34.1 Hz), 130.03, 129.87 (d, *J* = 3.6 Hz), 129.48, 128.54, 126.92 (p, *J* = 3.6 Hz), 125.83 (q, *J* = 3.9 Hz), 124.22 (q, *J* = 273.0 Hz), 122.91 (q, *J* = 273.0 Hz), 18.78;

^{19}F NMR (565 MHz, $CDCl_3$): δ -62.53, -63.00;

HRMS (ESI) m/z: calculated for $C_{24}H_{14}F_9NO_2Na$ $[M+Na]^+$: 542.0773, found: 542.0774.



17u

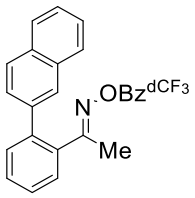
1-(3',5'-Dimethyl-[1,1'-biphenyl]-2-yl)ethan-1-one *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (17u): 65% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.55 (s, 2H), 8.12 (s, 1H), 7.59 (d, *J* = 7.8 Hz, 2H), 7.51 (td, *J* = 7.8, 1.2 Hz, 1H), 7.44-7.40 (m, 2H), 7.09 (s, 2H), 7.03 (s, 1H), 2.35 (s, 6H), 1.93 (s, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 169.79, 161.37, 141.16, 140.40, 138.35, 134.58, 132.56 (q, *J* = 34.1 Hz), 131.74, 130.50, 130.28, 129.82 (d, *J* = 3.6 Hz), 129.68, 129.54, 127.45, 127.01, 126.77 (p, *J* = 3.6 Hz), 122.93 (q, *J* = 273.0 Hz), 21.38, 18.54;

^{19}F NMR (565 MHz, $CDCl_3$): δ -62.99;

HRMS (ESI) m/z: calculated for $C_{25}H_{19}F_6NO_2Na$ $[M+Na]^+$: 502.1212, found: 502.1205.



17v

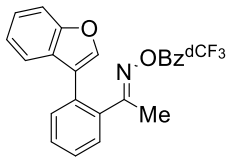
1-(2-(Naphthalen-2-yl)phenyl)ethan-1-one *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (17v): 53% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.53 (s, 2H), 8.10 (s, 1H), 7.96 (s, 1H), 7.93-7.89 (m, 3H), 7.65 (d, *J* = 7.2 Hz, 1H), 7.62-7.52 (m, 5H), 7.48 (t, *J* = 7.2 Hz, 1H), 1.91 (s, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 169.60, 161.41, 140.78, 137.89, 134.96, 133.46, 132.78, 132.55 (q, *J* = 34.1 Hz), 131.64, 130.89, 130.46, 129.92, 129.85 (d, *J* = 3.6 Hz), 128.60, 128.39, 128.29, 127.86, 127.79, 127.02, 126.80 (p, *J* = 3.6 Hz), 126.74, 126.63, 125.62, 122.91 (q, *J* = 273.0 Hz), 18.71;

^{19}F NMR (565 MHz, $CDCl_3$): δ -62.96;

HRMS (ESI) m/z: calculated for $C_{27}H_{17}F_6NO_2Na$ $[M+Na]^+$: 524.1056, found: 524.1064.



17w

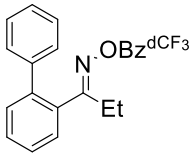
(2-(Benzofuran-3-yl)phenyl)(phenyl)methanone *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (17w): 60% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.53 (s, 2H), 8.12 (s, 1H), 7.79 (s, 1H), 7.67 (d, *J* = 7.8 Hz, 2H), 7.64-7.62 (m, 2H), 7.59 (td, *J* = 7.8, 1.2 Hz, 1H), 7.56 (d, *J* = 8.4 Hz, 1H), 7.49 (td, *J* = 7.8, 1.2 Hz, 1H), 7.37 (td, *J* = 7.8, 1.2 Hz, 1H), 7.30 (t, *J* = 7.8 Hz, 1H), 2.09 (s, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 169.14, 161.40, 155.40, 143.55, 135.44, 132.59 (q, *J* = 34.1 Hz), 131.54, 130.68, 130.41, 130.26, 129.87 (d, *J* = 3.6 Hz), 129.82, 128.15, 127.00, 126.88 (p, *J* = 3.6 Hz), 125.14, 123.43, 122.92 (q, *J* = 273.0 Hz), 120.47, 120.22, 111.92, 18.49;

^{19}F NMR (565 MHz, $CDCl_3$): δ -62.97;

HRMS (ESI) m/z: calculated for $C_{25}H_{15}F_6NO_3Na$ $[M+Na]^+$: 514.0848, found: 514.0848.



17x

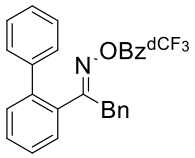
1-([1,1'-Biphenyl]-2-yl)propan-1-one *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (17x): 51% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.53 (s, 2H), 8.12 (s, 1H), 7.55-7.52 (m, 4H), 7.46-7.41 (m, 4H), 7.37 (t, *J* = 7.8 Hz, 1H), 2.29 (q, *J* = 7.8 Hz, 2H), 0.90 (t, *J* = 7.8 Hz, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 174.44, 161.48, 140.63, 140.40, 133.27, 132.56 (q, *J* = 34.1 Hz), 131.74, 130.50, 130.44, 130.32, 129.82 (q, *J* = 3.6 Hz), 129.19, 128.81, 127.90, 127.59, 126.79 (p, *J* = 3.6 Hz), 122.93 (q, *J* = 273.0 Hz), 25.13, 10.45;

^{19}F NMR (565 MHz, $CDCl_3$): δ -63.01;

HRMS (ESI) m/z: calculated for $C_{25}H_{19}F_6NO_2Na$ $[M+Na]^+$: 488.1056, found: 488.1050.



17y

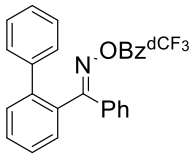
1-([1,1'-Biphenyl]-2-yl)-2-phenylethan-1-one *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (17y): 63% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.29 (s, 2H), 7.96 (s, 1H), 7.43-7.38 (m, 4H), 7.34 (t, *J* = 7.8 Hz, 3H), 7.28 (t, *J* = 7.8 Hz, 1H), 7.06 (t, *J* = 7.8 Hz, 2H), 7.01 (t, *J* = 7.8 Hz, 1H), 7.81 (d, *J* = 7.8 Hz, 2H), 3.47 (s, 2H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 170.72, 161.43, 140.75, 140.43, 135.06, 133.83, 132.47 (q, *J* = 34.1 Hz), 131.47, 130.91, 130.55, 130.48, 129.90 (q, *J* = 3.6 Hz), 129.22, 128.98, 128.83, 128.31, 128.06, 127.69, 127.00, 126.75 (p, *J* = 3.6 Hz), 122.88 (q, *J* = 273.0 Hz), 37.97;

^{19}F NMR (565 MHz, $CDCl_3$): δ -62.89;

HRMS (ESI) m/z: calculated for $C_{29}H_{19}F_6NO_2Na$ $[M+Na]^+$: 550.1212, found: 550.1205.



17z

[1,1'-Biphenyl]-2-yl(phenyl)methanone *O*-(3,5-bis(trifluoromethyl)benzoyl) oxime (17z): 43% yield over 3 steps as a white solid.

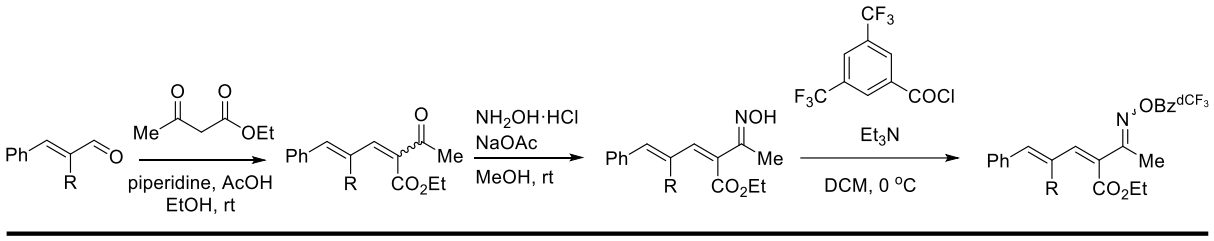
^{1}H NMR (600 MHz, $CDCl_3$): δ 8.12 (s, 2H), 8.04 (s, 1H), 7.70 (dd, *J* = 8.4, 1.2 Hz, 2H), 7.64 (td, *J* = 7.8, 1.2 Hz, 1H), 7.60 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.53 (td, *J* = 7.8, 1.2 Hz, 1H), 7.47-7.43 (m, 1H), 7.36 (ddd, *J* = 7.8, 4.6, 3.2 Hz, 3H), 7.22-7.14 (m, 5H);

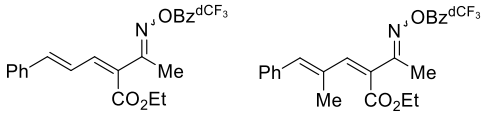
^{13}C NMR (151 MHz, $CDCl_3$): δ 167.26, 160.64, 141.08, 139.78, 133.98, 132.30 (q, *J* = 34.1 Hz), 131.53, 131.48, 131.29, 130.17, 129.79 (q, *J* = 3.6 Hz), 128.85, 128.65, 128.52, 128.17, 127.93, 127.34, 126.61 (p, *J* = 3.6 Hz), 122.87 (q, *J* = 273.0 Hz);

^{19}F NMR (565 MHz, $CDCl_3$): δ -63.05;

HRMS (ESI) m/z: calculated for $C_{28}H_{17}F_6NO_2Na$ $[M+Na]^+$: 536.1056, found: 536.1055.

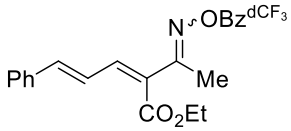
2.2.4 General Procedure for the Synthesis of Oxime Esters 17A-17B[7]





17A 17B

To a solution of cinnamaldehyde (1.0 equiv) in EtOH (0.5 M) was added Ethyl acetoacetate (1.1 equiv), Piperidine (0.5 equiv.) and AcOH (0.5 equiv.). The mixture was stirred at room temperature and monitored by TLC. Upon completion, the excess EtOH was removed under reduced pressure and the resulting mixture was diluted with H_2O and EtOAc. The layers were separated and the aqueous layer was extracted with EtOAc (×2). The combined organic layers were dried over Na_2SO_4, filtered and evaporated. Purification by column chromatography on silica gel gave the corresponding ketone. The corresponding oxime ester was obtained following the previous General Procedures. Unless otherwise specified, the major isomer of oxime esters was used for reaction and characterization.



17A

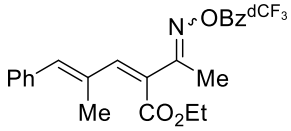
Ehyl (2*Z*,4*E*)-2-(1-(((3,5-bis(trifluoromethyl)benzoyl)oxy)imino)ethyl)-5-phenylpenta-2,4-dienoate (17A): 34% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.53 (s, 2H), 8.12 (s, 1H), 7.80 (dd, *J* = 15.6, 11.5 Hz, 1H), 7.53 (dt, *J* = 6.4, 1.4 Hz, 2H), 7.41-7.32 (m, 3H), 7.17 (dd, *J* = 11.5, 0.9 Hz, 1H), 7.03 (d, *J* = 15.5 Hz, 1H), 4.37 (q, *J* = 7.1 Hz, 2H), 2.35 (s, 3H), 1.40 (t, *J* = 7.1 Hz, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 165.83, 165.00, 161.09, 144.56, 144.20, 136.02, 132.50 (q, *J* = 34.1 Hz), 131.52, 129.74 (q, *J* = 3.6 Hz), 129.70, 128.92, 127.81, 126.79 (p, *J* = 3.6 Hz), 126.36, 124.23, 123.77 (q, *J* = 273.1 Hz), 61.33, 16.44, 14.28;

^{19}F NMR (565 MHz, $CDCl_3$): δ -62.96;

HRMS (ESI) m/z: calculated for $C_{24}H_{19}F_6NO_4Na$ $[M+Na]^+$: 522.1110, found: 522.1108.



17B

Ethyl (2*Z*,4*E*)-2-(1-(((3,5-bis(trifluoromethyl)benzoyl)oxy)imino)ethyl)-4-methyl-5-phenylpenta-2,4-dienoate (17B): 36% yield over 3 steps as a white solid.

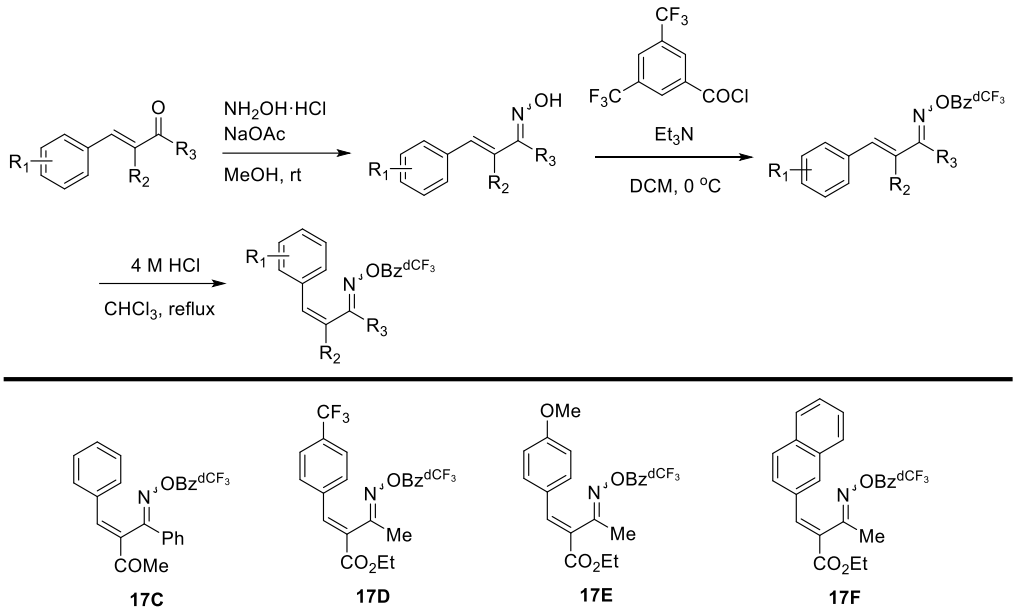
^{1}H NMR (600 MHz, Acetone-d_6): δ 8.62 (s, 2H), 8.40 (s, 1H), 7.41 (m, 4H), 7.32 (m, 1H), 7.10 (s, 1H), 7.02 (s, 1H), 4.34 (q, *J* = 7.2 Hz, 2H), 2.44 (s, 3H), 2.09 (s, 3H), 1.37 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (151 MHz, Acetone-d_6): δ 167.78, 165.01, 161.16, 141.89, 139.87, 137.54, 134.62, 132.81, 132.80 (q, *J* = 34.0 Hz), 130.68 (q, *J* = 3.6 Hz), 130.60, 130.39, 129.28, 128.73, 127.74 (p, *J* = 3.5 Hz), 124.54 (q, *J* = 272.0 Hz), 61.94, 15.54, 14.37, 12.78;

^{19}F NMR (565 MHz, Acetone-d_6): δ -63.46;

HRMS (ESI) m/z: calculated for $C_{25}H_{21}F_6NO_4Na$ $[M+Na]^+$: 536.1267, found: 536.1264.

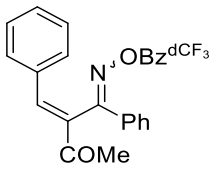
2.2.5 General Procedure for the Synthesis of Oxime Esters 17C-17F[7]



To a solution of alkenyl ketone (1.0 equiv) in MeOH (1.0 M) was added sodium acetate (2.0 equiv) and hydroxylamine hydrochloride (1.5 equiv.). The mixture was stirred at room temperature and monitored by TLC. Upon completion, the excess MeOH was removed under reduced pressure and the resulting mixture was diluted with H_2O and EtOAc. The layers were separated and the aqueous layer was extracted with EtOAc (×2). The combined organic layers were dried over Na_2SO_4, filtered and evaporated. The corresponding oxime was used directly in the next step without further purification.

To a solution of the corresponding oxime (1.0 equiv.) in DCM (0.5 M) at 0 ºC was added Et_3N (1.5 equiv.) and 3,5-Bis(trifluoromethyl)benzoyl chloride (1.1 equiv). The reaction mixture was stirred until the oxime was consumed (determined by TLC, 10 min in most cases). Then saturated $NaHCO_3$ aqueous solution was added and the mixture was extracted with DCM. The combined organic layers were washed with water and brine, and dried over Na_2SO_4. The resulting solution was concentrated under vacuum and the residue was purified by column chromatography on silica gel to afford the corresponding *Z*-configuration oxime ester.

The *Z*-configuration oxime ester was then dissolved in $CHCl_3$ (1.0 M). 4.0 M HCl (1.0 mL) was added to the mixture and stirred under reflux overnight. Then saturated $NaHCO_3$ aqueous solution was added and the mixture was extracted with DCM. The combined organic layers were washed with water and brine, and dried over Na_2SO_4. The resulting solution was concentrated under vacuum and the residue was purified by column chromatography on silica gel to afford the corresponding oxime ester.



17C

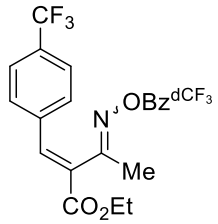
(3*E*)-3-((((3,5-Bis(trifluoromethyl)benzoyl)oxy)imino)(phenyl)methyl)-4-phenylbut-3-en-2-one (17C): 38% yield over 4 steps as a white solid.

^{1}H NMR (600 MHz, Acetone-d_6): δ 8.56 (s, 2H), 8.38 (s, 1H), 7.99 (d, *J* = 7.3 Hz, 2H), 7.65 (s, 1H), 7.59 (t, *J* = 7.4 Hz, 1H), 7.48 (t, *J* = 7.7 Hz, 2H), 7.42 (dd, *J* = 6.8, 3.0 Hz, 2H), 7.30 – 7.25 (m, 3H), 2.62 (s, 3H);

^{13}C NMR (151 MHz, Acetone-d_6): δ 196.70, 166.77, 160.99, 137.70, 137.66, 135.16, 134.46, 132.75 (q, *J* = 34.1 Hz), 132.68, 130.64(q, *J* = 3.8 Hz), 130.47, 130.26, 129.94, 129.69, 129.50, 127.71 (p, *J* = 3.6 Hz), 122.87 (q, *J* = 272.0 Hz), 12.80;

^{19}F NMR (565 MHz, Acetone-d_6): δ -58.25;

HRMS (ESI) m/z: calculated for $C_{26}H_{17}F_6NO_3Na$ $[M+Na]^+$: 528.1005, found: 528.1002.



17D

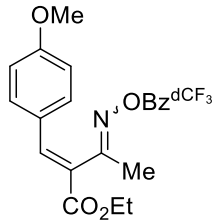
Ethyl 3-(((3,5-bis(trifluoromethyl)benzoyl)oxy)imino)-2-((*E*)-4-(trifluoromethyl)benzylidene)butanoate (17D): 24% yield over 3 steps as a white solid.

^{1}H NMR (600 MHz, Acetone-d_6): δ 8.64 (s, 2H), 8.41 (s, 1H), 7.99 (s, 1H), 7.91 (d, *J* = 8.0 Hz, 2H), 7.74 (d, *J* = 8.1 Hz, 2H), 4.35 (q, *J* = 7.2 Hz, 2H), 2.47 (s, 3H), 1.35 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (151 MHz, Acetone-d_6): δ 165.37, 165.15, 161.40, 141.97, 138.20, 132.83 (q, *J* = 34.1 Hz), 132.74, 131.78 (q, *J* = 32.0 Hz), 131.71, 130.76 (q, *J* = 4.0 Hz), 130.60, 127.82 (p, *J* = 3.6 Hz), 126.45 (q, *J* = 3.5 Hz), 125.00 (q, *J* = 272.0 Hz), 124.03 (q, *J* = 272.2 Hz), 62.48, 17.95, 14.44;

^{19}F NMR (565 MHz, Acetone-d_6): δ -63.46, -63.47;

HRMS (ESI) m/z: calculated for $C_{23}H_{16}F_9NO_4Na$ $[M+Na]^+$: 564.0828, found: 564.0828.



17E

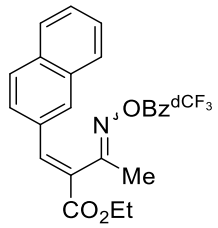
Ethyl 3-(((3,5-bis(trifluoromethyl)benzoyl)oxy)imino)-2-((*E*)-4-methoxybenzylidene)butanoate (17E): 33% yield over 4 steps as a white solid.

^{1}H NMR (600 MHz, Acetone-d_6): δ 8.66 (s, 2H), 8.42 (s, 1H), 7.83 (s, 1H), 7.67 (d, *J* = 8.6 Hz, 2H), 6.96 (d, *J* = 8.6 Hz, 2H), 4.29 (q, *J* = 7.3 Hz, 2H), 3.83 (s, 3H), 2.45 (s, 3H), 1.32 (t, *J* = 7.0 Hz, 3H);

^{13}C NMR (151 MHz, Acetone-d_6): δ 166.01, 165.90, 162.65, 161.47, 143.21, 133.44, 132.92, 132.83 (q, *J* = 34.1 Hz), 130.75 (q, *J* = 3.6 Hz), 127.75 (p, *J* = 3.6 Hz), 126.60, 125.19, 124.05 (q, *J* = 272.1 Hz), 115.23, 61.91, 55.81, 17.90, 14.53;

^{19}F NMR (565 MHz, Acetone-d_6): δ -63.43;

HRMS (ESI) m/z: calculated for $C_{23}H_{19}F_6NO_5Na$ $[M+Na]^+$: 526.1060, found: 526.1057.



17F

Ethyl (2*E*)-3-(((3,5-bis(trifluoromethyl)benzoyl)oxy)imino)-2-(naphthalen-2-ylmethylene)butanoate (17F): 38% yield over 4 steps as a white solid.

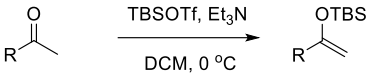
^{1}H NMR (600 MHz, Acetone-d_6): δ 8.67 (s, 2H), 8.42 (s, 1H), 8.32 (s, 1H), 8.08 (s, 1H), 7.98 (d, *J* = 7.9 Hz, 1H), 7.90 (d, *J* = 8.4 Hz, 2H), 7.75 (d, *J* = 8.7 Hz, 1H), 7.59-7.52 (m, 2H), 4.35 (q, *J* = 7.1 Hz, 2H), 2.50 (s, 3H), 1.36 (t, *J* = 7.1 Hz, 3H);

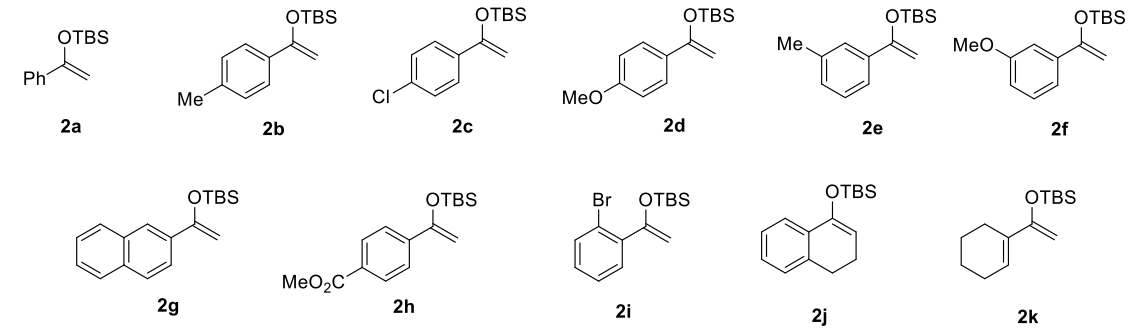
^{13}C NMR (151 MHz, Acetone-d_6): δ 165.87, 165.82, 161.56, 143.69, 134.94, 134.14, 132.86, 132.82 (q, *J* = 34.1 Hz), 132.71, 131.80, 130.77 (q, *J* = 3.6 Hz), 129.77, 129.28, 128.61, 128.51, 128.11, 127.78 (p, *J* = 3.6 Hz), 127.65, 127.15, 124.05 (q, *J* = 272.0 Hz), 62.21, 18.11, 14.52;

^{19}F NMR (565 MHz, Acetone-d_6): δ -63.42;

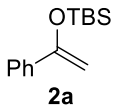
HRMS (ESI) m/z: calculated for $C_{26}H_{19}F_6NO_4Na$ $[M+Na]^+$: 546.1110, found: 546.1108.

2.3 General Procedure for the Synthesis of Silyl Enol Ethers[8]





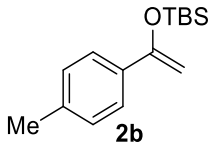
To a solution of the ketone (1.0 equiv.) in DCM (0.5 M) at 0 ºC was added Et_3N (1.5 equiv.) and Trimethylsilyl trifluoromethanesulfonate (1.1 equiv). The reaction mixture was stirred until the ketone was consumed (determined by TLC, 30 min in most cases) at the same temperature. Then saturated NH_4Cl aqueous solution was added and the mixture was extracted with DCM. The combined organic layers were washed with water and brine, and dried over Na_2SO_4. The resulting solution was concentrated under vacuum and the residue was purified by column chromatography on silica gel (1~2% Et_3N in PE) to afford the corresponding silyl enol ethers.



2a

***tert*-Butyldimethyl((1-phenylvinyl)oxy)silane (2a)**: 95% yield as a colorless oil.

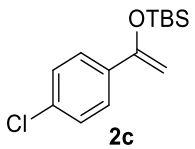
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.64-7.60 (m, 2H), 7.36-7.29 (m, 3H), 4.90 (d, *J* = 1.6 Hz, 1H), 4.43 (d, *J* = 1.6 Hz, 1H), 1.02 (s, 9H), 0.23 (s, 6H); Data in accordance with literature.[8a]



2b

***tert*-Butyldimethyl((1-(*p*-tolyl)vinyl)oxy)silane (2b)**: 92% yield as a colorless oil.

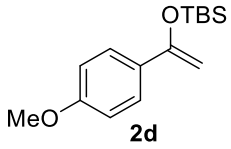
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.52 (d, *J* = 8.0 Hz, 2H), 7.15 (d, *J* = 8.0 Hz, 2H), 4.86 (d, *J* = 1.6 Hz, 1H), 4.39 (d, *J* = 1.6 Hz, 1H), 2.37 (s, 3H), 1.02 (s, 9H), 0.23 (s, 6H); Data in accordance with literature.[8a]



2c

***tert*-Butyl((1-(4-chlorophenyl)vinyl)oxy)dimethylsilane (2c)**: 90% yield as a colorless oil.

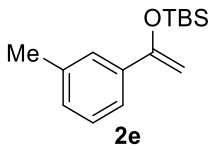
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.55-7.52 (m, 2H), 7.31-7.27 (m, 2H), 4.86 (d, *J* = 1.9 Hz, 1H), 4.43 (d, *J* = 1.9 Hz, 1H), 1.00 (s, 9H), 0.21 (s, 6H); Data in accordance with literature.[8a]



2d

***tert*-Butyl((1-(4-methoxyphenyl)vinyl)oxy)dimethylsilane (2d)**: 92% yield as a colorless oil.

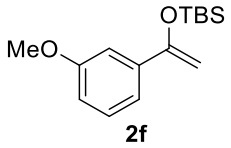
^{1}H NMR (600 MHz, $CDCl_3$): δ 7.55 (d, *J* = 8.4 Hz, 2H), 6.86 (d, *J* = 8.4 Hz, 2H), 4.78 (d, *J* = 1.6 Hz, 1H), 4.33 (d, *J* = 1.6 Hz, 1H), 3.82 (s, 3H), 1.01 (s, 9H), 0.21 (s, 6H); Data in accordance with literature.[8a]



2e

***tert*-Butyldimethyl((1-(*m*-tolyl)vinyl)oxy)silane (2e)**: 90% yield as a colorless oil.

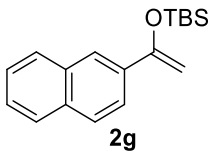
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.25-7.14 (m, 3H), 6.85-6.82 (m, 1H), 4.89 (d, *J* = 1.7 Hz, 1H), 4.42 (d, *J* = 1.7 Hz, 1H), 3.81 (s, 3H), 1.01 (s, 9H), 0.21 (s, 6H); Data in accordance with literature.[8a]



2f

***tert*-Butyl((1-(3-methoxyphenyl)vinyl)oxy)dimethylsilane (2f)**: 95% yield as a colorless oil.

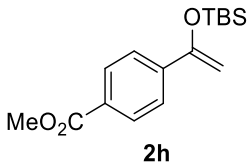
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58-7.54 (m, 2H), 6.88-6.84 (m, 2H), 4.78 (d, *J* = 1.6 Hz, 1H), 4.34 (d, *J* = 1.6 Hz, 1H), 3.82 (s, 3H), 1.02 (s, 9H), 0.22 (s, 6H); Data in accordance with literature.[8a]



2g

***tert*-Butyldimethyl((1-(naphthalen-2-yl)vinyl)oxy)silane (2g)**: 90% yield as a white solid.

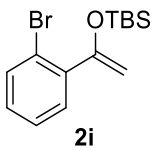
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.08 (s, 1H), 7.85-7.76 (m, 3H), 7.71 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.49-7.44 (m, 2H), 5.04 (d, *J* = 1.7 Hz, 1H), 4.54 (d, *J* = 1.7 Hz, 1H), 1.05 (s, 9H), 0.24 (s, 3H); Data in accordance with literature.[8a]



2h

Methyl 4-(1-((*tert*-butyldimethylsilyl)oxy)vinyl)benzoate (2h): 88% yield as a colorless oil.

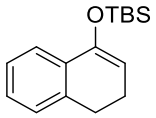
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01-7.98 (m, 2H), 7.68-7.65 (m, 2H), 4.99 (d, *J* = 1.9 Hz, 1H), 4.53 (d, *J* = 1.9 Hz, 1H), 3.91 (s, 3H), 1.00 (s, 9H), 0.21 (s, 6H); Data in accordance with literature.[8a]



2i

((1-(2-Bromophenyl)vinyl)oxy)(*tert*-butyl)dimethylsilane (2i): 85% yield as a colorless oil.

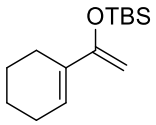
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58 (dd, *J* = 7.6, 1.8 Hz, 1H), 7.29-7.24 (m, 1H), 6.91-6.95 (m, 2H), 5.04 (d, *J* = 1.6 Hz, 1H), 4.52 (d, *J* = 1.6 Hz, 1H), 1.02 (s, 9H), 0.22 (s, 3H); Data in accordance with literature.[8a]



2j

***tert*-Butyl((3,4-dihydronaphthalen-1-yl)oxy)dimethylsilane (2j)**: 82% yield as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.48 (d, *J* = 7.2 Hz, 1H), 7.23-7.11 (m, 3H), 5.18 (t, *J* = 4.6 Hz, 1H), 2.77 (t, *J* = 8.0 Hz, 2H), 2.35-2.29 (m, 2H), 1.03 (s, 9H), 0.22 (s, 6H); Data in accordance with literature.[8a]



2k

***tert*-Butyl((1-(cyclohex-1-en-1-yl)vinyl)oxy)dimethylsilane (2k)**: 85% yield as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$): δ 6.25 (t, *J* = 3.6 Hz, 1H), 4.34 (d, *J* = 1.2 Hz, 1H), 4.18 (d, *J* = 1.2 Hz, 1H), 2.15-2.13 (m, 4H), 1.69-1.65 (m, 2H), 1.59-1.55 (m, 2H), 0.97 (s, 9H), 0.18 (s, 6H); Data in accordance with literature.[8a]

3. Reaction Investigation and Condition Optimization

3.1 Oxime Esters Substituent Screening

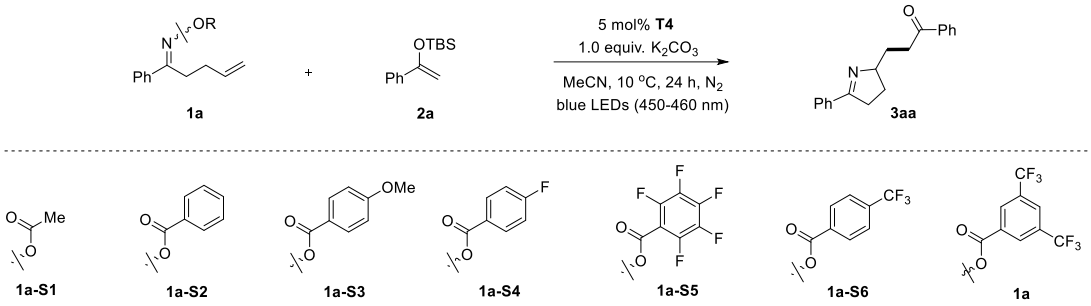


Table S1. Screening of Oxime Ester Substituent [a].

Entry	Oxime ester	Yield of 3aa (%)[b]
1	**1a-S1**	NR
2	**1a-S2**	NR
3	**1a-S3**	NR
4	**1a-S4**	26
5	**1a-S5**	34
6	**1a-S6**	55
7	**1a**	83

[a] Reaction conditions: **1a** (0.20 mmol), **2a** (0.60 mmol), **T4** (0.01 mmol), K_2CO_3 (0.20 mmol), MeCN (1.0 mL), under the irradiation of 20 W blue LEDs for 24 h at 10 ºC in a sealed tube under N_2 atmosphere. [b] Yield determined by ^1H NMR analysis of the crude mixture using trimethoxybenzene as the internal standard.

3.2 Irradiation Wavelength Screening

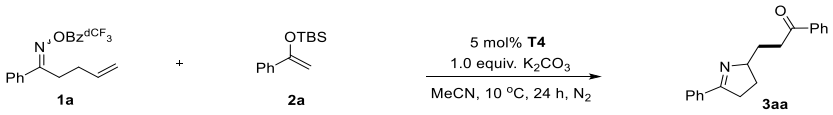


Table S2. Screening of Irradiation Wavelength [a].

Entry	Irradiation Wavelength	Yield of 3aa (%)[b]
1	white LEDs (400-830 nm)	20
2	green LEDs (520-530 nm)	0
3	blue LEDs (450-460 nm)	83
4	blue LEDs (420-430 nm)	75
5	purple LEDs (390-400 nm)	70
6	UV (360-370 nm)	57

[a] Reaction conditions: **1a** (0.20 mmol), **2a** (0.60 mmol), **T4** (0.01 mmol), K_2CO_3 (0.20 mmol), MeCN (1.0 mL), under the irradiation of 20 W LEDs for 24 h at 10 ºC in a sealed tube under N_2 atmosphere. [b] Yield determined by ^1H NMR analysis of the crude mixture using trimethoxybenzene as the internal standard.

3.3 Condition Optimization for the Synthesis of Pyrroline 3

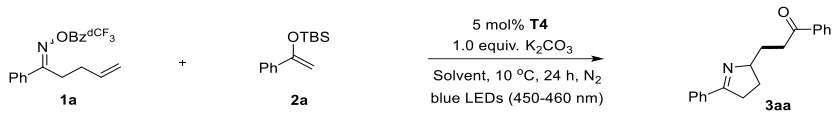


Table S3. Condition Optimization for the Synthesis of **3aa** [a].

Entry	Base	Solvent	Temperature	Time (h)	Yield of **3aa** (%)[b]
1	Na_2CO_3	MeCN	10 ºC	24	49
2	$KHCO_3$	MeCN	10 ºC	24	20
3	K_2CO_3	MeCN	10 ºC	24	83 (77[c])
4	K_3PO_4	MeCN	10 ºC	24	74
5	Cs_2CO_3	MeCN	10 ºC	24	67
6	KOtBu	MeCN	10 ºC	24	trace
7	Et_3N	MeCN	10 ºC	24	5
8	DMAP	MeCN	10 ºC	24	36
9	K_2CO_3	DCM	10 ºC	24	NR
10	K_2CO_3	Dioxane	10 ºC	24	NR
11	K_2CO_3	Acetone	10 ºC	24	7
12	K_2CO_3	DMSO	10 ºC	24	NR
13	K_2CO_3	DMF	10 ºC	24	34
14	K_2CO_3	DMAc	10 ºC	24	22
15	K_2CO_3	MeCN	rt	12	54
16	K_2CO_3	MeCN	0 ºC	24	56
17	none	MeCN	10 ºC	24	trace
18[d]	K_2CO_3	MeCN	10 ºC	24	0
19[e]	K_2CO_3	MeCN	10 ºC	24	0
20[f]	K_2CO_3	MeCN	10 ºC	24	0
21	K_2CO_3	MeCN	10 ºC	12	78
22[g]	K_2CO_3	MeCN	10 ºC	12	52

[a] Reaction conditions: **1a** (0.20 mmol), **2a** (0.60 mmol), **T4** (0.01 mmol), base (0.20 mmol), solvent (1.0 mL), under the irradiation of 20 W blue LEDs in a sealed tube under N_2 atmosphere. [b] Yield determined by ^{1}H NMR analysis of the crude mixture using trimethoxybenzene as the internal standard. [c] Isolated yield. [d] Reaction performed in the absence of **T4**. [e] Reaction performed without irradiation. [f] Reaction performed under Air. [g] Reaction performed using 0.5 equiv. of K_2CO_3.

3.4 Condition Optimization for the Synthesis of Ketonitrile 5

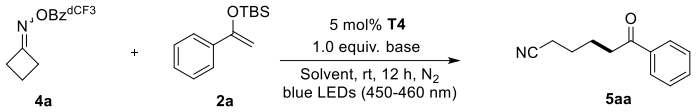


Table S4. Condition Optimization for the Synthesis of **5aa**[a]

entry	Base	Solvent	Yield of **10aa** (%)[b]
1	K_2CO_3	MeCN	52
2	Na_2CO_3	MeCN	56
3	K_3PO_3	MeCN	34
4	Na_2CO_3	DMF	80 (75[c])
5	Na_2CO_3	DMAc	65
6	K_2CO_3	DMF	60
7	none	DMF	0
8[d]	Na_2CO_3	DMF	0
9[e]	Na_2CO_3	DMF	0

[a] Reaction conditions: **4a** (0.20 mmol), **2a** (0.60 mmol), **T4** (0.01 mmol), base (0.20 mmol), solvent (2.0 mL), under the irradiation of 20 W blue LEDs in a sealed tube for 24 h at room temperature under N_2 atmosphere. [b] Yield determined by ^{1}H NMR analysis of the crude mixture using trimethoxybenzene as the internal standard. [c] Isolated yield. [d] Reaction performed in the absence of **T4**. [e] Reaction performed without irradiation.

3.5 Condition Optimization for the Synthesis of Phenanthridine 18

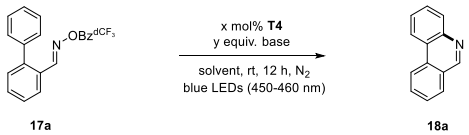


Table S5. Condition Optimization for the Synthesis of **18a**[a]

Entry	x	y	Base	Solvent	Yield of **18a** (%)[b]
1	10	1.0	K_2CO_3	MeCN	65
2	10	1.0	K_2CO_3	DMF	72
3	10	1.0	K_2CO_3	DMAc	72
4	10	1.0	K_2CO_3	DMSO	56
5	10	1.0	Na_2CO_3	DMF	80
6	10	1.0	$NaHCO_3$	DMF	76
7	10	1.0	DMAP	DMF	67
8	5	1.0	Na_2CO_3	DMF	83
9	2	0.5	Na_2CO_3	DMF	85 (82[c])
10	2	0.4	Na_2CO_3	DMF	70
11	1	0.5	Na_2CO_3	DMF	72
12	2	0	none	DMF	0
13[d]	0	0.5	Na_2CO_3	DMF	0
14[e]	2	0.5	Na_2CO_3	DMF	0

[a] Reaction conditions: **17a** (0.20 mmol), **T4** (x mol%), base (y equiv.), solvent (2.0 mL), under the irradiation of 20 W blue LEDs in a sealed tube for 12 h at room temperature under N_2 atmosphere. [b] Yield determined by ^{1}H NMR analysis of the crude mixture using trimethoxybenzene as the internal standard. [c] Isolated yield. [d] Reaction performed in the absence of **T4**. [e] Reaction performed without irradiation.

4. Mechanisms Study Experiments

4.1 On-Off-On Experiment

A series of identical reactions between oxime ester **1a** and silyl enol ether **2a** were conducted under the standard conditions on a 0.2 mmol scale, using MeCN as the solvent, and employing 5 mol% of thiourea **T4** with 1.0 equiv. of K_2CO_3, under blue LED irradiation. The mixture was subjected to sequential periods of stirring under 20 w blue LED irradiation followed by stirring in the absence of light. At each time point (2h, 3h, 5h, 6h, 8h, 9h, 12h), one of the reactions was terminated and concentrated under reduced pressure. The crude material diluted with a $CDCl_3$ solution and the yields of **3aa** were measured by ^1H NMR analysis.

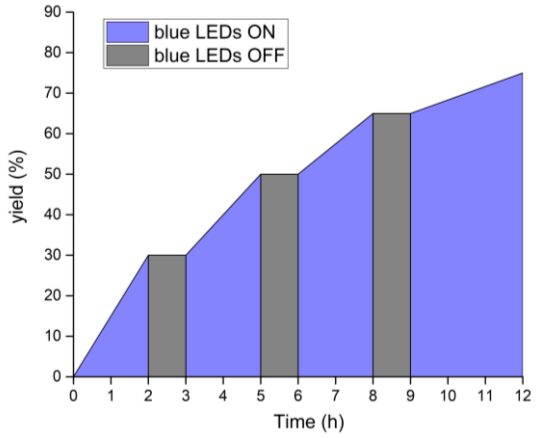
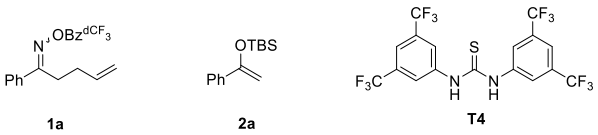


Figure S1: On-Off-On experiment over the time

4.2 UV-Vis Absorption Spectroscopic Measurements



1a **2a** **T4**

0.1M stock solutions of different startingmaterials were prepared using MeCN as solvent for measurements.The solution of **1a**+K_2CO_3 or **1a**+**T4**+K_2CO_3 was stirred under N_2 for 1 h in dark using MeCN as solvent and the supernatant was seperated for measurement.

4.2.1 UV/vis absorption spectra of the combination between 1a, 2a, T4 and K_2CO_3

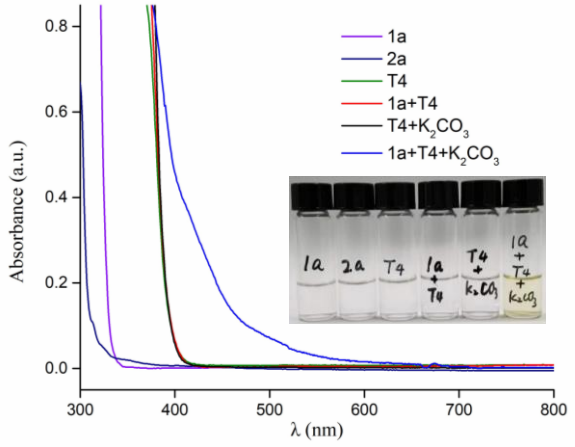


Figure S2: UV/vis absorption spectra of the combination between **1a**, **2a**, **T4** and K_2CO_3.

4.2.2 UV/vis absorption spectra of the combination between 1a, T4 and DMAP

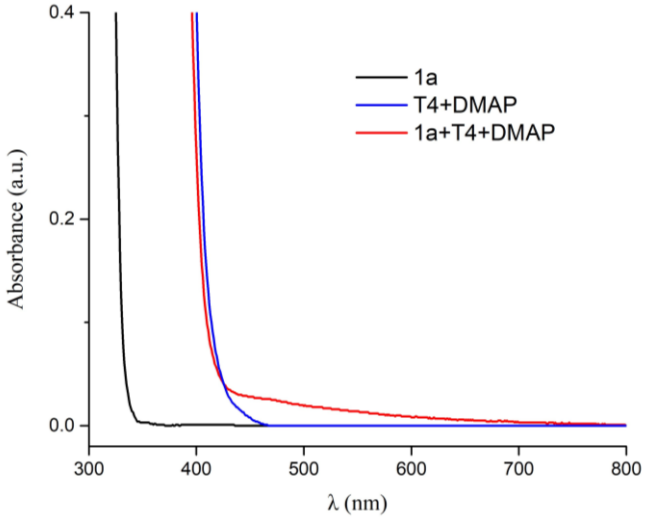


Figure S3: UV/vis absorption spectra of the combination between **1a**, **T4** and DMAP.

4.3 Job's Plot Experiment

Eleven measurements with **T4**+DMAP molar fraction of 0, 10%, 20%, 30%, 40%, 50%, 60%, 70%, 80%, 90%, 100% of the combination of **1a** and **T4**+DMAP were recorded. The absorbance obtained at 460 nm was selected and plotted.

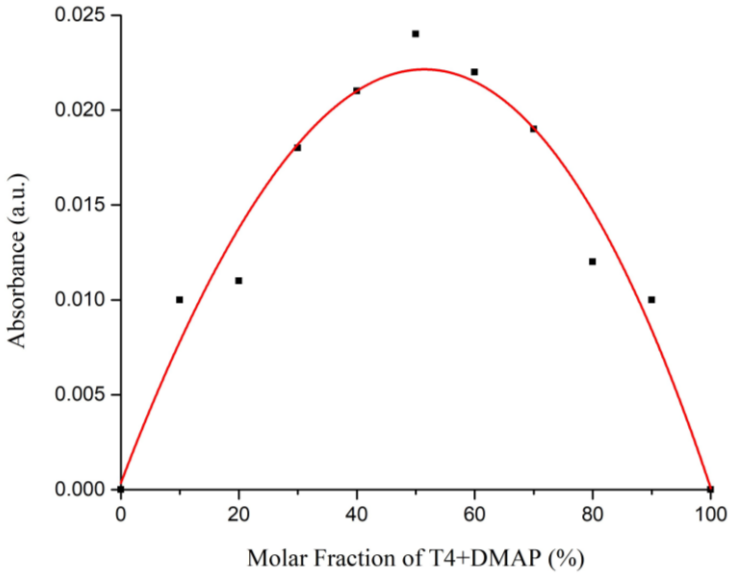


Figure S4: Job's plot of the EDA complexes with UV-Vis absorption spectrometry.

4.4 NMR Titration Experiment

Solutions containing equal molar concentrations of the donor (**T4**+DMAP, 0.1 M in DMSO-d_6) and the acceptor (**1a**, 0.1 M in DMSO-d_6) were prepared and mixed to cover acceptor/donor ratio from 0%, 10%, 20% to 100% donor.

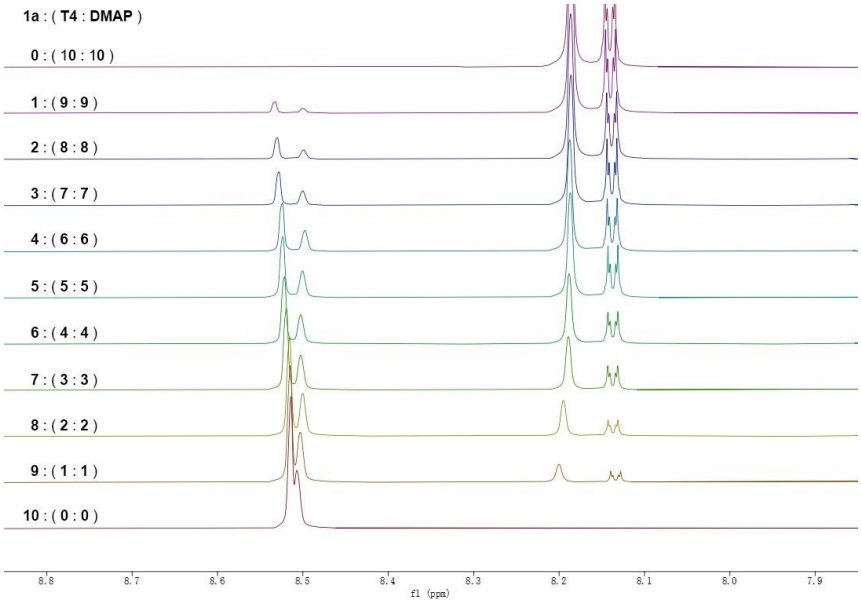
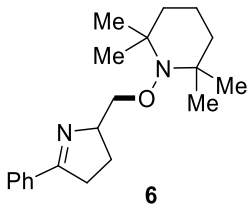


Figure S5: ^{1}H NMR titration of the combination between **1a**, **T4** and DMAP.

4.5 Radical Trap Experiment

An oven-dried Schlenk tube equipped with a stirring bar was charged with **1a** (0.2 mmol, 83.07 mg, 1.0 equiv.), **T4** (0.01 mmol, 5.0 mg, 5 mol%), K_2CO_3 (0.2 mmol, 27.60 mg, 1.0 equiv.) and **Tempo** (0.4 mmol, 62.50 mg, 2.0 equiv.). After refilling with N_2 repeated three times, MeCN (1.0 mL) and **2a** (0.6 mmol, 140.65 mg, 3.0 equiv.) was added through syringe. The mixture was stirred at 10 ºC in a freezer for 24 h in front of a 20 W blue LEDs bulb. Saturated $NaHCO_3$ aqueous solution and EtOAc were added and the mixture was stirred for 10 min. The layers were separated and the aqueous layer was extracted with EtOAc. The combined organic layers were then washed with brine, dried over Na_2SO_4 and concentrated in vacuo. The residue was purified by column chromatography on silica gel to afford the corresponding product.

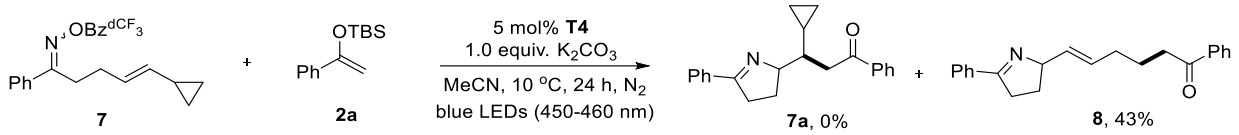


6

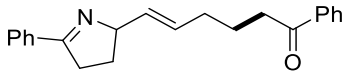
2,2,6,6-Tetramethyl-1-((5-phenyl-3,4-dihydro-2*H*-pyrrol-2-yl)methoxy)piperidine (6): 52.8 mg, 84% yield as a pale yellow solid. **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.87-7.85 (m, 2H), 7.43-7.39 (m, 3H), 4.47-4.43 (m, 1H), 4.07 (dd, *J* = 8.4, 3.6 Hz, 1H), 3.97 (dd, *J* = 8.4, 3.6 Hz, 1H), 3.07-2.94 (m, 2H), 2.19-2.13 (m, 1H), 2.07-2.02 (m, 1H), 1.52-1.27 (m, 6H), 1.23 (s, 3H), 1.17 (s, 3H), 1.12 (s, 3H), 0.96 (s, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 173.21, 134.52, 130.05, 128.13, 127.49, 78.90, 72.12, 59.65, 39.40, 35.17, 33.00, 32.79, 25.68, 20.02, 19.77, 16.86; Data in accordance with literature.[5b]

4.6 Radical Clock Experiment



An oven-dried Schlenk tube equipped with a stirring bar was charged with **5** (0.2 mmol, 91.03 mg, 1.0 equiv.), **T4** (0.01 mmol, 5.0 mg, 5 mol%) and K_2CO_3 (0.2 mmol, 27.60 mg, 1.0 equiv.). After refilling with N_2 repeated three times, MeCN (1.0 mL) and **2a** (0.6 mmol, 140.65 mg, 3.0 equiv.) was added through syringe. The mixture was stirred at 10 ºC in a freezer for 24 h in front of a 20 W blue LEDs bulb. Saturated $NaHCO_3$ aqueous solution and EtOAc were added and the mixture was stirred for 10 min. The layers were separated and the aqueous layer was extracted with EtOAc. The combined organic layers were then washed with brine, dried over Na_2SO_4 and concentrated in vacuo. The residue was purified by column chromatography on silica gel to afford the corresponding product.



8

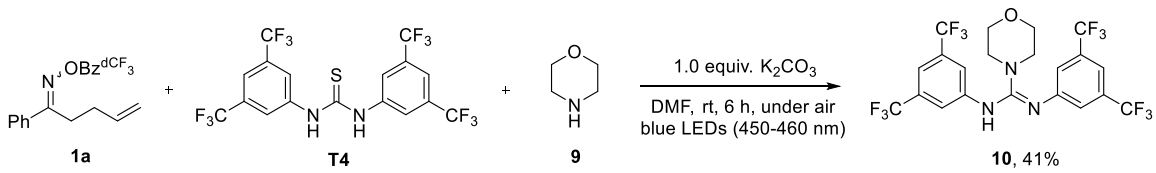
(E)-1-Phenyl-6-(5-phenyl-3,4-dihydro-2*H*-pyrrol-2-yl)hex-5-en-1-one (8): 27.0 mg, 43% yield as a pale yellow solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.95 (d, *J* = 7.2 Hz, 2H), 7.86 (d, *J* = 6.7 Hz, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.47-7.37 (m, 5H), 5.71 (dt, *J* = 15.4, 6.6 Hz, 1H), 5.60 (dd, *J* = 15.4, 7.1 Hz, 1H), 4.69 (q, *J* = 7.4 Hz, 1H), 3.08-2.96 (m, 3H), 2.90 (dddd, *J* = 16.9, 9.5, 7.4, 1.9 Hz, 1H), 2.26 (dddd, *J* = 12.9, 9.6, 7.9, 4.9 Hz, 1H), 2.17 (q, *J* = 7.4 Hz, 2H), 1.87 (p, *J* = 7.4 Hz, 3H), 1.73 (ddt, *J* = 12.7, 9.8, 7.2 Hz, 1H);

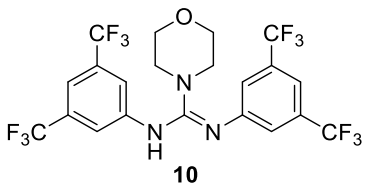
^{13}C NMR (151 MHz, $CDCl_3$): δ 200.53, 173.19, 137.23, 134.60, 133.04, 133.02, 130.64, 130.42, 128.69, 128.54, 128.21, 127.94, 74.48, 37.99, 35.21, 32.01, 29.85, 23.83;

HRMS (ESI) m/z: calculated for $C_{22}H_{24}NO$ $[M+H]^+$: 318.1852, found: 318.1850.

4.7 Radical Conversion Experiment



A glass tube equipped with a stirring bar was charged with **1a** (0.2 mmol, 83.07 mg, 1.0 equiv.), **T4** (0.2 mmol, 100.06 mg, 1.0 equiv) and K_2CO_3 (0.2 mmol, 27.60 mg, 1.0 equiv.). DMF (2.0 mL) and **7** (0.4 mmol, 34.82 mg, 2.0 equiv.) was added through syringe. The mixture was stirred at room temperature for 6 h in front of a 20 W blue LEDs bulb. Saturated $NaHCO_3$ aqueous solution and EtOAc were added and the mixture was stirred for 10 min. The layers were separated and the aqueous layer was extracted with EtOAc. The combined organic layers were then washed with brine, dried over Na_2SO_4 and concentrated in vacuo. The residue was purified by column chromatography on silica gel to afford the corresponding product.



10

***N*,*N*'-Bis(3,5-bis(trifluoromethyl)phenyl)morpholine-4-carboximidamide (10)**: 45.3 mg, 41% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.37 (s, 2H), 7.23 (s, 4H), 3.76 (t, *J* = 4.8 Hz, 4H), 3.46 (t, *J* = 4.8 Hz, 4H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 149.72, 132.76 (q, *J* = 33.2 Hz), 123.14 (q, *J* = 273.0 Hz), 115.90 (p, *J* = 3.9 Hz), 66.41, 47.42; *(2 aromatic carbon signals are not observed due to signal weakness.)*

^{19}F NMR (565 MHz, $CDCl_3$): δ -63.34;

HRMS (ESI) m/z: calculated for $C_{21}H_{16}F_{12}N_3O$ $[M+H]^+$: 554.1096, found: 554.1085.

5. Computational Study Experiments

5.1 Computational Methods

All the density functional theory (DFT) calculations were carried out with the Gaussian16[9] series of programs. DFT method B3LYP[10] with a 6-31G(d) basis set was used for geometry optimizations. Frequency analysis was performed at the same level to provide correction to thermodynamic functions and confirm the nature of optimized structures (minima and transition states featured zero or one imaginary frequency, respectively). The M06[11] functional in combination with the 6-311+G(d,p) basis set was used to calculate the single point energies to give more accurate energy information. The solvent effects (acetonitrile, MeCN) were evaluated implicitly by a self-consistent reaction field (SCRF) approach for all the intermediates and transitions states, using the integral equation formalism polarizable continuum model (IEF-PCM) [12]. The discussed energies were obtained at M06/6-311+G(d,p)/IEF-PCM(MeCN)//B3LYP/6-31G(d)/IEF-PCM(MeCN) level. Linear response time dependent DFT (TD-DFT) were calculation at B3LYP/6-31G(d)/IEF-PCM(MeCN) level.

5.2 Absolute SPE, GFEC, GFE, and IF of the Optimized Structures

Table S6. The Single-Point Energies (SPE) Calculated at M06/6-311+G(d,p)/IEF-PCM(MeCN) Level, Gibbs Free Energy Corrections (GFEC) Calculated at B3LYP/6-31G(d)/IEF-PCM(MeCN) Level, Gibbs Free Energies (GFE = SPE + GFEC) of the Stationary Points Involved in the Reaction Models, and Imaginary Frequencies (IF) Calculated at B3LYP/6-31G(d)/IEF-PCM(MeCN) Level for the Transition States.

	SPE (a.u.)	GFEC (a.u.)	GFE (a.u.)	IF(*i*)
T4	-2358.137739	0.173813	-2357.963926	-
K_2CO_3	-1463.777307	-0.018844	-1463.796151	-
int1	-3821.955174	0.176994	-3821.77818	-
ts1	-3821.953497	0.171671	-3821.781826	1097.02
int2	-3821.961021	0.177700	-3821.783321	-
1a	-1574.945228	0.254984	-1574.690244	-
int3	-5396.923029	0.457468	-5396.465561	
S1	-5396.83467	0.458989	-5396.375681	
int4	-2357.484438	0.15783	-2357.326608	-
int5	-1575.050345	0.250650	-1574.799695	-
$K_2CO_3 \cdot H^+$	-1464.262022	-0.007846	-1464.269868	-
ts2	-1575.028896	0.247002	-1574.781894	833.86
-OBz^{dCF3}	-1094.279873	0.065748	-1094.214125	-
int6	-480.811784	0.160308	-480.651476	-
ts3	-480.794543	0.161849	-480.632694	474.49
int7	-480.824761	0.162664	-480.662097	-
ts3′	-480.787929	0.163153	-480.624776	480.28
int7′	-480.826936	0.164378	-480.662558	-
2a	-911.199867	0.275543	-910.924324	-
ts4	-1392.027831	0.460307	-1391.567524	305.41
int8	-1392.089404	0.467511	-1391.621893	-
int9	-2357.676251	0.159276	-2357.516975	-
int10	-1391.942534	0.472057	-1391.470477	
$K_2CO_3 \cdot TBS^+$	-1990.76519	0.165075	-1990.600115	-
3aa	-865.018622	0.286232	-864.732390	-

5.3 The Energies and Cartesian Coordinates of the Optimized Structures

T4

Zero-point correction= 0.241219 (Hartree/Particle)
Thermal correction to Energy= 0.269685
Thermal correction to Enthalpy= 0.270629
Thermal correction to Gibbs Free Energy= 0.173813
Sum of electronic and zero-point Energies= -2358.225595
Sum of electronic and thermal Energies= -2358.197129
Sum of electronic and thermal Enthalpies= -2358.196185
Sum of electronic and thermal Free Energies= -2358.293001

Cartesian coordinates

C	3.40309900	-0.81927700	-1.21032000
C	2.48242500	0.02212400	-0.57779100
C	2.92699700	0.94800900	0.37272700
C	4.28153900	1.00267600	0.69710600
C	5.20771300	0.16359100	0.07565400
C	4.75754800	-0.74034100	-0.88488300
H	3.06293300	-1.53402300	-1.95243400
H	2.22388200	1.61809500	0.84779300
H	6.25876400	0.21755600	0.33197900
C	4.76245500	2.04175800	1.67591400
F	3.82612700	2.33257600	2.60482900
F	5.07310200	3.20546200	1.05550000
F	5.87378400	1.63984900	2.33060300
C	5.72935800	-1.69407400	-1.52812600
F	6.97465600	-1.17546900	-1.59463000
F	5.82392100	-2.85380300	-0.83505000
F	5.35672600	-2.02020800	-2.78541500
N	1.13051200	-0.04709200	-0.98621500
C	-0.00159300	-0.00712600	-0.21383300
S	-0.00550400	-0.04934400	1.47049000
N	-1.13024600	0.07126800	-0.98867100
C	-2.48361900	-0.01507900	-0.58935600
C	-2.93376300	-0.98453500	0.31411900
C	-3.40136700	0.85214200	-1.19043400
C	-4.29067100	-1.05589000	0.62555200
H	-2.23527600	-1.68276700	0.75394100
C	-4.75826700	0.75526200	-0.88061400
H	-3.05760700	1.59741700	-1.90014300
C	-5.21396800	-0.19184100	0.03469800
H	-6.26851600	-0.26749400	0.27009200
C	-4.76085900	-2.06482500	1.64051800
C	-5.72867100	1.72753100	-1.49782700
F	-6.97042900	1.20569000	-1.59650900
F	-5.83615500	2.86006300	-0.76291800
F	-5.34533400	2.10259500	-2.73821400
F	-6.03285900	-2.45691300	1.40904300
F	-3.98913200	-3.17385600	1.64620600
F	-4.72918800	-1.55962700	2.89671500
H	-0.99524600	0.37911900	-1.94611800
H	1.00017300	-0.30548600	-1.95881300

K_2CO_3

Zero-point correction= 0.015868 (Hartree/Particle)
Thermal correction to Energy= 0.023089
Thermal correction to Enthalpy= 0.024033
Thermal correction to Gibbs Free Energy= -0.018844
Sum of electronic and zero-point Energies= -1463.757268
Sum of electronic and thermal Energies= -1463.750047
Sum of electronic and thermal Enthalpies= -1463.749103
Sum of electronic and thermal Free Energies= -1463.791980

Cartesian coordinates

C	-0.00000500	0.84478900	-0.00006400
O	-1.12685100	1.47797500	0.04257100
O	1.12684100	1.47796900	-0.04251700
O	-0.00001300	-0.47506200	-0.00024200
K	-2.59548300	-0.65568200	-0.00772800
K	2.59549400	-0.65567600	0.00782700

int1

Zero-point correction= 0.257892 (Hartree/Particle)
Thermal correction to Energy= 0.294826
Thermal correction to Enthalpy= 0.295770
Thermal correction to Gibbs Free Energy= 0.176994
Sum of electronic and zero-point Energies= -3822.037976
Sum of electronic and thermal Energies= -3822.001041
Sum of electronic and thermal Enthalpies= -3822.000097
Sum of electronic and thermal Free Energies= -3822.118874

Cartesian coordinates

C	3.34504500	0.41270700	0.26509200
C	2.49849700	-0.68235300	-0.00217000
C	3.08613700	-1.90437700	-0.37007300
C	4.47710200	-2.01233900	-0.43944000
C	5.31594100	-0.93485300	-0.15864800
C	4.72653900	0.28189900	0.18997700
H	2.89008500	1.36484800	0.51734100
H	2.46374300	-2.75664600	-0.59779800
H	6.39241500	-1.03730700	-0.21365900
C	5.08105600	-3.35146700	-0.76754900
F	4.31051800	-4.06319700	-1.62100300
F	5.23877200	-4.11672600	0.34114400
F	6.30371500	-3.23342700	-1.33341000
C	5.57913800	1.49757100	0.42972500
F	6.84710300	1.17708200	0.76549600
F	5.65174400	2.28861400	-0.66969000
F	5.08424900	2.27497300	1.42525100
N	1.13094100	-0.40600300	0.07994700
C	0.02535800	-1.21299900	0.05724300
S	0.05220000	-2.90874300	0.22141700
N	-1.09729200	-0.44885000	-0.09487400
C	-2.46439700	-0.72634100	0.01761000
C	-3.06148700	-1.97602800	0.25169800
C	-3.30325500	0.39822100	-0.12551400
C	-4.45353700	-2.07499200	0.33091500
H	-2.44449700	-2.85563600	0.35875600
C	-4.68448500	0.27399900	-0.05344800
H	-2.83952900	1.36514200	-0.29021800
C	-5.28375000	-0.96642400	0.17692800
H	-6.36066400	-1.06353500	0.23447200
C	-5.06159700	-3.41433100	0.65141600
C	-5.52905400	1.49506100	-0.29398100
F	-6.76419300	1.37952300	0.23818900
F	-4.96666400	2.61239600	0.23021700
F	-5.69341500	1.74009600	-1.61918200
F	-6.32731100	-3.52336000	0.18788300
F	-4.35107400	-4.43657400	0.12356200
F	-5.11749600	-3.63255000	1.98898300
H	-0.91823300	0.56040500	-0.37122100
H	0.93505800	0.61760700	0.28949600
C	-0.02953400	2.82057400	-0.08431700
O	-0.79334300	2.13197700	-0.88733500
O	0.75648800	2.19039000	0.74374300
O	-0.05461800	4.10636000	-0.10721300
K	-2.12738900	4.27229200	-1.76323500
K	1.91774900	4.42014700	1.64067400

ts1

Zero-point correction= 0.253112 (Hartree/Particle)
Thermal correction to Energy= 0.289963
Thermal correction to Enthalpy= 0.290907
Thermal correction to Gibbs Free Energy= 0.171671
Sum of electronic and zero-point Energies= -3822.038872
Sum of electronic and thermal Energies= -3822.002021
Sum of electronic and thermal Enthalpies= -3822.001077
Sum of electronic and thermal Free Energies= -3822.120313

Cartesian coordinates

C	-3.44021000	0.50048300	-0.21553100
C	-2.54697700	-0.58349100	-0.09051100
C	-3.08393300	-1.86837500	0.09714100

C	-4.46916100	-2.04544900	0.12815400
C	-5.35318700	-0.97575600	-0.00794200
C	-4.81503500	0.30263900	-0.17224000
H	-3.03332200	1.49773300	-0.33776800
H	-2.42365800	-2.71471900	0.21673200
H	-6.42454300	-1.13103900	0.01810400
C	-5.01232900	-3.44284600	0.25818200
F	-4.23743200	-4.21907700	1.05003500
F	-5.08387800	-4.06837100	-0.94339400
F	-6.26057100	-3.45972900	0.77843700
C	-5.72498500	1.49820600	-0.23467700
F	-6.93099500	1.19531100	-0.76334200
F	-5.95922500	2.01862700	0.99641000
F	-5.19995200	2.50194700	-0.97962000
N	-1.19378300	-0.25028800	-0.09266000
C	-0.04910400	-0.99422100	-0.29428200
S	-0.07067400	-2.60490700	-0.89371500
N	1.04496800	-0.25314700	-0.03858300
C	2.38445200	-0.63681000	-0.14723000
C	2.90602800	-1.90223400	0.17881300
C	3.29153800	0.37926900	-0.50257900
C	4.28306400	-2.12710600	0.13168000
H	2.23620900	-2.69554300	0.47813200
C	4.66439500	0.14568000	-0.51993800
H	2.89991800	1.35941400	-0.74744600
C	5.17952900	-1.11387500	-0.21280900
H	6.24634700	-1.29854300	-0.23293300
C	4.80362900	-3.50897100	0.41992200
C	5.58954700	1.29797800	-0.79101800
F	6.80709100	0.89817800	-1.21358600
F	5.09373800	2.14536900	-1.72247300
F	5.79311200	2.04616400	0.33024400
F	6.08197300	-3.49164800	0.86186500
F	4.06429000	-4.14685100	1.35612900
F	4.78621800	-4.29418100	-0.68606000
H	0.95098700	0.91881500	0.40940200
H	-1.03163300	0.78237100	-0.06833200
C	0.14430400	2.92858900	0.45467500
O	1.05490500	2.06442400	0.89766900
O	-0.86500400	2.48464600	-0.20581200
O	0.31892200	4.16626500	0.70532400
K	2.88669400	3.93878900	1.47325200
K	-2.06654200	4.87739500	-0.32356100

int2

Zero-point correction= 0.257309 (Hartree/Particle)
Thermal correction to Energy= 0.293830
Thermal correction to Enthalpy= 0.294774
Thermal correction to Gibbs Free Energy= 0.177700
Sum of electronic and zero-point Energies= -3822.040859
Sum of electronic and thermal Energies= -3822.004338
Sum of electronic and thermal Enthalpies= -3822.003393
Sum of electronic and thermal Free Energies= -3822.120468

Cartesian coordinates

C	-3.39265700	0.43370200	-0.16101600
C	-2.51839100	-0.66674600	-0.05276400
C	-3.07864900	-1.95566000	-0.00407900
C	-4.46396900	-2.11478500	-0.07974500
C	-5.32965800	-1.02505200	-0.18336900
C	-4.76997500	0.25340000	-0.21565700
H	-2.96940400	1.43076300	-0.20196400
H	-2.43176100	-2.81541000	0.09309800
H	-6.40187100	-1.16668300	-0.23372600
C	-5.02918200	-3.50904900	-0.09817300
F	-4.29811700	-4.36721600	0.64933000
F	-5.06143500	-4.02259100	-1.35370500
F	-6.29815300	-3.55201600	0.36912700
C	-5.64970100	1.47167700	-0.24772400
F	-6.87813000	1.21044000	-0.74286400
F	-5.83011900	1.99601800	0.99243200
F	-5.11371900	2.46482000	-1.00132700

N	-1.16751100	-0.35407400	0.06806900
C	0.00736000	-1.04584300	-0.21061900
S	-0.00578700	-2.65344800	-0.85957400
N	1.06479600	-0.27592100	0.01288300
C	2.39034300	-0.67431000	-0.08585500
C	2.92319300	-1.86633200	0.45030400
C	3.29736500	0.24860500	-0.64160100
C	4.29742600	-2.10100400	0.42886400
H	2.25576000	-2.59019200	0.89852900
C	4.67085600	0.00870000	-0.64117600
H	2.90487300	1.16899600	-1.06002400
C	5.19166400	-1.17043900	-0.11057400
H	6.25814400	-1.35663500	-0.10672800
C	4.82623500	-3.40557700	0.95755400
C	5.57721400	1.08529200	-1.16515000
F	6.85387200	0.67352800	-1.30851100
F	5.16735500	1.55811000	-2.36617900
F	5.60613100	2.16436500	-0.32997500
F	6.09217700	-3.29288700	1.42382500
F	4.07042400	-3.89374800	1.96793100
F	4.85359400	-4.36561400	-0.00156200
H	1.06771000	1.40867400	0.45570500
H	-1.00531000	0.64287000	0.26993600
C	0.10533800	3.11646500	0.62870500
O	1.26385500	2.38427800	0.63381400
O	-0.99264200	2.49295600	0.54126300
O	0.25682500	4.36430600	0.71748500
K	3.00304500	4.42246300	0.47748100
K	-2.47118400	4.76455200	0.67183400

1a

Zero-point correction=	0.317016 (Hartree/Particle)
Thermal correction to Energy=	0.343224
Thermal correction to Enthalpy=	0.344168
Thermal correction to Gibbs Free Energy=	0.254984
Sum of electronic and zero-point Energies=	-1575.059369
Sum of electronic and thermal Energies=	-1575.033161
Sum of electronic and thermal Enthalpies=	-1575.032216
Sum of electronic and thermal Free Energies=	-1575.121401

Cartesian coordinates

C	1.43052500	0.48799700	-0.14156500
C	1.25289800	-0.89585400	-0.06486000
C	2.36963800	-1.73758000	0.00747100
C	3.65089000	-1.19399200	0.00679000
C	3.83383000	0.19041100	-0.06111200
C	2.71989400	1.02371100	-0.13439000
H	0.57184000	1.14428800	-0.21029300
H	2.21868800	-2.80933900	0.06002800
H	4.83201200	0.61151800	-0.06415100
C	4.85213700	-2.09466100	0.13425000
F	4.60671900	-3.33296600	-0.34302600
F	5.23191600	-2.23704200	1.42586200
F	5.91810700	-1.60290300	-0.53459000
C	2.87397000	2.52125000	-0.18711200
F	4.16099500	2.90368500	-0.29821500
F	2.19757500	3.05259100	-1.23001200
F	2.37602300	3.10540900	0.93174500
C	-0.09747000	-1.53770400	-0.04379800
O	-0.28322400	-2.73025800	0.04600200
O	-1.07562100	-0.59541500	-0.13476200
N	-2.39425400	-1.13060900	-0.01064000
C	-3.27269100	-0.21182500	-0.23878100
C	-4.68661000	-0.66167900	-0.13139400
C	-5.72241700	0.26589500	0.06985800
C	-5.01287200	-2.02878200	-0.21767900
C	-7.04555800	-0.16122700	0.19145200
H	-5.50483300	1.32586200	0.14666900
C	-6.33390000	-2.45062700	-0.10228900
H	-4.22214200	-2.75146000	-0.38596800
C	-7.35638300	-1.51859900	0.10435000
H	-7.83164900	0.57067600	0.35303100

H	-6.56855500	-3.50846300	-0.18006400
H	-8.38739300	-1.84952700	0.19152500
C	-2.93886100	1.22389200	-0.58039800
C	-2.59132500	2.08140800	0.66679000
H	-3.77748300	1.67484100	-1.11745200
H	-2.08291100	1.22807400	-1.26057600
C	-2.26859400	3.50104800	0.28496300
H	-1.74627400	1.62979300	1.19673900
H	-3.44652700	2.06860100	1.35650200
C	-1.09023600	4.09868500	0.47359200
H	-3.07665600	4.05795800	-0.19251100
H	-0.25008100	3.58934400	0.94103200
H	-0.92070100	5.12791300	0.16734100

int3

Zero-point correction= 0.575558 (Hartree/Particle)
Thermal correction to Energy= 0.640970
Thermal correction to Enthalpy= 0.641914
Thermal correction to Gibbs Free Energy= 0.457468
Sum of electronic and zero-point Energies= -5397.114929
Sum of electronic and thermal Energies= -5397.049517
Sum of electronic and thermal Enthalpies= -5397.048573
Sum of electronic and thermal Free Energies= -5397.233020

Cartesian coordinates

C	1.90765200	2.29499100	1.50407200
C	1.94210200	0.95886500	1.91223600
C	3.16119700	0.26989600	1.94836200
C	4.33445100	0.91840600	1.57239300
C	4.30836000	2.25731700	1.17224200
C	3.09186900	2.93832700	1.13938600
H	0.96826500	2.83170900	1.48065500
H	3.17561500	-0.76321800	2.27266700
H	5.22654600	2.76478500	0.89751800
C	5.65027400	0.18417900	1.54654600
F	5.59825100	-0.98925600	2.20519800
F	6.63978400	0.92203900	2.09882700
F	6.03416500	-0.08585600	0.27427900
C	3.04372700	4.35948500	0.64757800
F	4.20286200	5.01187000	0.85468600
F	2.80339000	4.41126200	-0.69615200
F	2.05886500	5.07017800	1.23562500
C	0.71675100	0.21986100	2.34882500
O	0.72713300	-0.90233700	2.80260400
O	-0.39638500	0.98012400	2.16563000
N	-1.56853600	0.41430100	2.76470300
C	-2.62616600	1.03371800	2.35977800
C	-3.87829000	0.61377500	3.04846300
C	-5.12318500	0.65112700	2.39743400
C	-3.82610900	0.16289200	4.38117600
C	-6.27986200	0.23850600	3.06018100
H	-5.20168600	0.97990200	1.36737200
C	-4.98341700	-0.24417100	5.03963300
H	-2.87152800	0.14787800	4.89571300
C	-6.21581000	-0.20853900	4.38088300
H	-7.23273600	0.26586700	2.53934500
H	-4.92505200	-0.58137800	6.07066000
H	-7.11959100	-0.52240000	4.89553800
C	-2.64340500	2.14164700	1.33151000
C	-2.40267100	3.52750900	1.98995100
H	-3.61032300	2.15442900	0.82272900
H	-1.87768200	1.95458600	0.57421400
C	-2.58122100	4.65941000	1.01381000
H	-1.39822800	3.55708400	2.42544200
H	-3.11669300	3.65234600	2.81541600
C	-1.61496800	5.49441400	0.61561400
H	-3.59272000	4.79458000	0.62516700
H	-0.59178100	5.40260000	0.97457600
H	-1.81828200	6.31292400	-0.07167700
C	2.93171000	-1.90917900	-1.84382300
C	1.86430200	-2.20029700	-0.97366200
C	2.15545300	-2.93893300	0.19238000

C	3.45986300	-3.34857700	0.46408700
C	4.51685300	-3.04536900	-0.39962600
C	4.23375000	-2.31902800	-1.55476300
H	2.72633200	-1.34122300	-2.74550500
H	1.35887000	-3.15797400	0.89153000
H	5.52728800	-3.35936300	-0.17294400
C	3.74042400	-4.04724400	1.76446000
F	2.75429900	-4.90624600	2.10755700
F	3.85219700	-3.16553600	2.79750600
F	4.89450400	-4.74983400	1.73613700
C	5.33069000	-1.91507500	-2.49794700
F	6.51613700	-2.48580200	-2.19822800
F	5.04125400	-2.23967800	-3.78157100
F	5.52965500	-0.56779100	-2.48953400
N	0.63216400	-1.62056700	-1.24328900
C	-0.53790200	-2.24150600	-1.15446200
S	-0.79526800	-3.94254900	-0.94497100
N	-1.58288400	-1.33832700	-1.32219100
C	-2.96931000	-1.43252200	-1.36671000
C	-3.75130200	-2.57432400	-1.11226900
C	-3.63992700	-0.23227900	-1.68714300
C	-5.14413900	-2.49356700	-1.17878600
H	-3.26284300	-3.50872500	-0.87535000
C	-5.02696100	-0.17406400	-1.73526400
H	-3.04881900	0.65111300	-1.89901600
C	-5.80690700	-1.30464300	-1.48321600
H	-6.88745500	-1.26185300	-1.53176300
C	-5.94974900	-3.72018700	-0.84419200
C	-5.66926700	1.15595500	-2.00744200
F	-6.95964100	1.04793900	-2.37889000
F	-5.64667900	1.96120400	-0.90388800
F	-5.02406500	1.84763300	-2.97986700
F	-7.17186300	-3.70211300	-1.42463200
F	-5.33615800	-4.85891300	-1.23895300
F	-6.15735300	-3.83716400	0.49145400
H	-1.24733100	-0.37687300	-1.47162700
H	0.92703500	0.00579000	-1.74863600
O	1.27350200	0.89337200	-2.09015100
C	0.25663600	1.80196700	-2.19412500
K	3.27328600	2.51962600	-2.87674300
O	-0.90392100	1.44604900	-1.83057000
O	0.58705900	2.93040000	-2.64744400
K	-1.93468700	3.90972200	-2.42215300

S1

Zero-point correction= 0.572460 (Hartree/Particle)
Thermal correction to Energy= 0.638006
Thermal correction to Enthalpy= 0.638950
Thermal correction to Gibbs Free Energy= 0.458989
Sum of electronic and zero-point Energies= -5397.042530
Sum of electronic and thermal Energies= -5396.976984
Sum of electronic and thermal Enthalpies= -5396.976040
Sum of electronic and thermal Free Energies= -5397.156001

Cartesian coordinates

C	1.48832400	2.23968700	1.62616900
C	1.68427400	0.85120500	1.93434900
C	3.02266500	0.34350500	1.85383500
C	4.06711800	1.16004300	1.48152000
C	3.87461600	2.53312100	1.16146400
C	2.55103900	3.03651100	1.25410900
H	0.49416700	2.65986600	1.69397300
H	3.19209800	-0.69742600	2.09521300
H	4.71278200	3.18290000	0.94215300
C	5.44134300	0.60078000	1.31114300
F	5.57352400	-0.67084700	1.73955000
F	6.38986000	1.33664700	1.93908500
F	5.81172700	0.59653200	-0.01786700
C	2.33786900	4.49010100	0.97509100
F	2.76167100	5.29112400	1.98313600
F	3.00370000	4.90290900	-0.13643000
F	1.02320000	4.80883300	0.77129400

C	0.62808300	-0.04252800	2.29604000
O	0.72234700	-1.23632200	2.59660400
O	-0.62763900	0.61381800	2.23551500
N	-1.67620200	-0.13452200	2.78876200
C	-2.82730800	0.34160700	2.44611400
C	-3.99741700	-0.33014000	3.07529100
C	-5.20377200	-0.50510700	2.37658300
C	-3.90384500	-0.83133500	4.38681300
C	-6.27876300	-1.17105300	2.96677000
H	-5.30277900	-0.14916100	1.35629600
C	-4.98081900	-1.48932500	4.97724800
H	-2.97974000	-0.69105200	4.93767900
C	-6.17375700	-1.66249700	4.26928300
H	-7.19480800	-1.31310200	2.40059400
H	-4.89129600	-1.86222400	5.99401800
H	-7.01398000	-2.17463200	4.73001700
C	-3.01816800	1.51937500	1.51743200
C	-2.99998400	2.86892300	2.27964600
H	-3.96787900	1.43270700	0.98337000
H	-2.21671500	1.51529000	0.77427600
C	-3.17881300	4.04464600	1.35678900
H	-2.06385500	2.96771300	2.84020400
H	-3.81736000	2.86135000	3.01506800
C	-2.37469000	5.11292200	1.30573000
H	-4.04440900	3.99961600	0.69379300
H	-1.49812200	5.20077100	1.94528500
H	-2.57698700	5.94738600	0.63757200
C	3.17527800	-2.08149400	-1.88982200
C	1.86858800	-2.33864100	-1.38709600
C	1.74292500	-2.99917200	-0.12896700
C	2.87807700	-3.37533700	0.56315800
C	4.16156800	-3.11906900	0.05526100
C	4.29623800	-2.46425600	-1.17337300
H	3.27198100	-1.57922000	-2.84446300
H	0.76362300	-3.16859800	0.29587900
H	5.03982900	-3.41103700	0.61789100
C	2.77611800	-4.03143000	1.91700500
F	1.51130000	-4.33494400	2.25254800
F	3.28276300	-3.23464300	2.88691900
F	3.49449800	-5.17924000	1.95091400
C	5.66798700	-2.21041100	-1.74586800
F	6.60327100	-2.10478500	-0.78228900
F	6.05501200	-3.20777100	-2.57170600
F	5.69913200	-1.06816200	-2.47534400
N	0.83970900	-1.85322900	-2.11573500
C	-0.48362000	-2.21529200	-1.96166500
S	-0.91216100	-3.84819000	-2.08075000
N	-1.29642100	-1.14070600	-1.90592900
C	-2.69743900	-1.00605800	-1.89311600
C	-3.61331300	-2.03137400	-1.62542200
C	-3.17226900	0.29502900	-2.13435000
C	-4.98039600	-1.74275500	-1.61608400
H	-3.26956100	-3.03661900	-1.43277000
C	-4.53528400	0.56196400	-2.10539500
H	-2.46142000	1.08503500	-2.34465100
C	-5.45823700	-0.45609600	-1.85624100
H	-6.52258200	-0.25073800	-1.85237200
C	-5.96595700	-2.82836700	-1.26878800
C	-5.02706000	1.97469000	-2.26999200
F	-6.12389100	2.04069900	-3.05282900
F	-5.37553700	2.51544300	-1.07099200
F	-4.09217100	2.78990200	-2.80693900
F	-7.10682100	-2.71486100	-1.98519400
F	-5.46893500	-4.06293200	-1.48977600
F	-6.32197200	-2.77346700	0.03857200
H	-0.79714100	-0.22930000	-1.95507800
H	1.34376200	-0.15698700	-2.90357400
O	1.79999000	0.70866400	-3.01923500
C	0.99614600	1.71441400	-2.52108500
K	4.07558100	1.98600100	-1.97199300
O	-0.16551000	1.40430300	-2.12600200
O	1.52553400	2.84937700	-2.49747500

K	-0.70292100	3.99843800	-1.37667400

int4

Zero-point correction= 0.227521 (Hartree/Particle)
Thermal correction to Energy= 0.255837
Thermal correction to Enthalpy= 0.256782
Thermal correction to Gibbs Free Energy= 0.157830
Sum of electronic and zero-point Energies= -2357.591691
Sum of electronic and thermal Energies= -2357.563375
Sum of electronic and thermal Enthalpies= -2357.562431
Sum of electronic and thermal Free Energies= -2357.661382

Cartesian coordinates

C	3.59728700	-0.84526100	-1.26191300
C	2.43378700	-0.54276200	-0.50296000
C	2.57183200	0.25566000	0.66881600
C	3.82176600	0.71581000	1.04662200
C	4.96516400	0.40225900	0.29669200
C	4.83884000	-0.38067800	-0.85729200
H	3.48495700	-1.44442800	-2.15780700
H	1.69602900	0.50217200	1.25578700
H	5.93759300	0.76764200	0.60600800
C	3.96729000	1.61537200	2.24888800
F	2.91697800	1.51484300	3.08802100
F	4.06420300	2.91418900	1.88288100
F	5.08318600	1.32258200	2.95172900
C	6.07654400	-0.75925300	-1.63142600
F	6.99472100	0.23113700	-1.61476200
F	6.67099700	-1.85530800	-1.10699700
F	5.79807700	-1.03752000	-2.92149900
N	1.25477600	-0.98912400	-0.99230400
C	0.06899000	-1.00916200	-0.31417600
S	-0.07327600	-1.96183700	1.07634000
N	-0.92214200	-0.33801500	-0.95270300
C	-2.29354400	-0.19721300	-0.63980200
C	-3.05607700	-1.22242000	-0.06948100
C	-2.90578800	1.01444500	-0.98539000
C	-4.41432400	-1.01183100	0.17263700
H	-2.60164500	-2.17387200	0.16581000
C	-4.26541800	1.20057800	-0.74767500
H	-2.32080500	1.80653300	-1.44108000
C	-5.03105000	0.19315000	-0.15968900
H	-6.08929300	0.33923500	0.01916600
C	-5.21549200	-2.10113800	0.83793000
C	-4.90112800	2.52678000	-1.07426300
F	-6.20752700	2.39278800	-1.38877800
F	-4.83522700	3.38141700	-0.02609700
F	-4.29171200	3.13550700	-2.11475400
F	-6.52215800	-2.04261700	0.50171100
F	-4.76548200	-3.33139200	0.50754100
F	-5.15230500	-2.01049000	2.18749500
H	-0.59868900	0.21984900	-1.73778500

int5

Zero-point correction= 0.313032 (Hartree/Particle)
Thermal correction to Energy= 0.339527
Thermal correction to Enthalpy= 0.340471
Thermal correction to Gibbs Free Energy= 0.250650
Sum of electronic and zero-point Energies= -1575.149078
Sum of electronic and thermal Energies= -1575.122582
Sum of electronic and thermal Enthalpies= -1575.121638
Sum of electronic and thermal Free Energies= -1575.211460

Cartesian coordinates

C	1.41105200	0.46939300	-0.22739600
C	1.20781600	-0.94551300	-0.11857200
C	2.37803400	-1.76180600	0.01304700
C	3.63701100	-1.20166900	0.05365800
C	3.83370900	0.20133800	-0.03454100
C	2.68536900	1.00799800	-0.18115800
H	0.55707100	1.12443500	-0.34791200
H	2.25013300	-2.83531300	0.08619100

H	4.82561800	0.63318300	-0.00016600
C	4.84993300	-2.06884300	0.17695800
F	4.56122100	-3.38170300	0.33105400
F	5.62648100	-1.71321000	1.23704600
F	5.65935600	-1.97561300	-0.91456900
C	2.82776000	2.49982400	-0.21247700
F	4.06803400	2.90181100	-0.58128100
F	1.95328400	3.09241000	-1.06458700
F	2.59395200	3.06683800	1.00743300
C	-0.07468900	-1.57900200	-0.12215200
O	-0.32547300	-2.78776300	-0.02514500
O	-1.10286200	-0.61181900	-0.25376000
N	-2.38954400	-1.11964200	-0.11703700
C	-3.28553600	-0.19224600	-0.27587700
C	-4.69459200	-0.63177500	-0.13517400
C	-5.73918800	0.29826800	0.02339800
C	-5.02807600	-2.00323500	-0.14349700
C	-7.06209600	-0.12391100	0.16846700
H	-5.52607600	1.36190800	0.04789800
C	-6.34710000	-2.42075600	-0.00095100
H	-4.23521500	-2.73219200	-0.26904400
C	-7.37532700	-1.48359600	0.15567100
H	-7.84794100	0.61640000	0.29314100
H	-6.57751100	-3.48293700	-0.01739700
H	-8.40550400	-1.81140700	0.26406700
C	-2.93987600	1.25199700	-0.56789300
C	-2.54219700	2.05115100	0.70178000
H	-3.77821000	1.74686400	-1.06752700
H	-2.09658800	1.26780000	-1.26500100
C	-2.16140800	3.47024200	0.37701200
H	-1.70959300	1.54306100	1.19917600
H	-3.39017000	2.04619800	1.40147900
C	-0.95546300	4.00815700	0.57381200
H	-2.94796300	4.08187400	-0.06961000
H	-0.13394800	3.44329100	1.00929600
H	-0.74235500	5.04010700	0.30535900

$K_2CO_3 \cdot H^+$

Zero-point correction= 0.027829 (Hartree/Particle)
Thermal correction to Energy= 0.035667
Thermal correction to Enthalpy= 0.036611
Thermal correction to Gibbs Free Energy= -0.007846
Sum of electronic and zero-point Energies= -1464.245528
Sum of electronic and thermal Energies= -1464.237689
Sum of electronic and thermal Enthalpies= -1464.236745
Sum of electronic and thermal Free Energies= -1464.281203

Cartesian coordinates

H	0.89993600	2.45877000	-0.00064100
C	-0.10729700	0.82326100	0.00015400
O	1.11318300	1.51062600	0.00057200
O	-1.15034500	1.51023800	-0.00065100
O	0.02194100	-0.42973600	0.00079500
K	2.69055500	-0.75251300	-0.00026100
K	-2.69762700	-0.72787400	-0.00005500

ts2

Zero-point correction= 0.311001 (Hartree/Particle)
Thermal correction to Energy= 0.337527
Thermal correction to Enthalpy= 0.338471
Thermal correction to Gibbs Free Energy= 0.247002
Sum of electronic and zero-point Energies= -1575.135755
Sum of electronic and thermal Energies= -1575.109230
Sum of electronic and thermal Enthalpies= -1575.108285
Sum of electronic and thermal Free Energies= -1575.199755

Cartesian coordinates

C	1.40316000	0.48363000	0.11475100
C	1.27940800	-0.87097100	-0.27997100
C	2.46329600	-1.65132900	-0.33085500
C	3.69640900	-1.09551500	-0.01339900
C	3.81339600	0.24784400	0.37376600

C	2.63971000	1.02394500	0.43388500
H	0.51292100	1.09752100	0.15943200
H	2.38101500	-2.69181800	-0.62186600
H	4.77808300	0.67643700	0.61805200
C	4.94409000	-1.92019300	-0.14423500
F	4.70481600	-3.24865400	-0.05177100
F	5.86109800	-1.61544600	0.80758500
F	5.56207900	-1.72329300	-1.33929200
C	2.74493200	2.44435500	0.90186000
F	3.79757100	3.08875000	0.33794400
F	1.63917600	3.17703400	0.62252100
F	2.93088300	2.52997500	2.24591900
C	0.00486000	-1.46968200	-0.68231700
O	-0.13318000	-2.69314500	-0.90220200
O	-0.98583600	-0.57235300	-0.81541300
N	-2.34383200	-1.01520500	0.05190700
C	-3.33529900	-0.31329200	-0.36535000
C	-4.67726600	-0.73445400	0.13073800
C	-5.72287700	0.19550300	0.28544700
C	-4.92002300	-2.07519100	0.49103700
C	-6.96316000	-0.20074100	0.78866600
H	-5.56902500	1.23746800	0.02207700
C	-6.16033700	-2.46884000	0.98465400
H	-4.12278800	-2.80101900	0.36769800
C	-7.18998600	-1.53289300	1.13972700
H	-7.75403100	0.53587500	0.90419900
H	-6.32898000	-3.51084600	1.24420000
H	-8.15771600	-1.84115100	1.52575400
C	-3.20906800	0.90588200	-1.26494500
C	-2.70223200	2.15647200	-0.50226700
H	-4.17106500	1.12251900	-1.74065300
H	-2.49262200	0.66357000	-2.05373700
C	-2.47383000	3.33042600	-1.41488600
H	-1.77482800	1.90023000	0.01944000
H	-3.44005300	2.42683000	0.26734500
C	-1.30369500	3.94969200	-1.58763400
H	-3.34556000	3.67679000	-1.97376300
H	-0.40716300	3.64245600	-1.05197200
H	-1.19876200	4.79234800	-2.26682200

$^{-}$OBzd^{CF3}

Zero-point correction= 0.111469 (Hartree/Particle)
Thermal correction to Energy= 0.125814
Thermal correction to Enthalpy= 0.126758
Thermal correction to Gibbs Free Energy= 0.065748
Sum of electronic and zero-point Energies= -1094.315124
Sum of electronic and thermal Energies= -1094.300778
Sum of electronic and thermal Enthalpies= -1094.299834
Sum of electronic and thermal Free Energies= -1094.360845

Cartesian coordinates

C	1.20187600	0.97290900	-0.02215500
C	-0.00003400	1.68525100	-0.01159400
C	-1.20190100	0.97288100	-0.02201800
C	-1.20283500	-0.42407500	-0.04143600
C	0.00002000	-1.13287000	-0.05014100
C	1.20287300	-0.42402000	-0.04153100
H	2.12890300	1.53564300	-0.02303500
H	-2.12900200	1.53549700	-0.02277800
H	0.00005200	-2.21605400	-0.07547600
C	-2.50820500	-1.16746500	-0.00069100
F	-3.47742900	-0.53098100	-0.69823900
F	-2.97431100	-1.30261900	1.26719000
F	-2.40452500	-2.41765900	-0.50843900
C	2.50822200	-1.16743800	-0.00063400
F	2.40475700	-2.41733800	-0.50916900
F	3.47778100	-0.53053900	-0.69735600
F	2.97374500	-1.30336500	1.26736500
C	-0.00001800	3.22772400	0.00326600
O	-1.13288800	3.77563600	0.00971900
O	1.13287500	3.77561900	0.00912300

int6

Zero-point correction= 0.199980 (Hartree/Particle)
Thermal correction to Energy= 0.211384
Thermal correction to Enthalpy= 0.212328
Thermal correction to Gibbs Free Energy= 0.160308
Sum of electronic and zero-point Energies= -480.874636
Sum of electronic and thermal Energies= -480.863232
Sum of electronic and thermal Enthalpies= -480.862288
Sum of electronic and thermal Free Energies= -480.914308

Cartesian coordinates

N	0.14479100	2.49782300	0.36775100
C	0.18889500	1.23790700	0.43275800
C	-1.03379900	0.40778700	0.18100000
C	-1.15955300	-0.88954100	0.70057800
C	-2.09177200	0.94554700	-0.57266800
C	-2.32147100	-1.63009000	0.47532400
H	-0.36038400	-1.32592100	1.29082700
C	-3.24832300	0.20329000	-0.79772600
H	-1.99383200	1.94422600	-0.98694100
C	-3.36720300	-1.08764600	-0.27348600
H	-2.40635500	-2.63200400	0.88631600
H	-4.05577400	0.62952000	-1.38637900
H	-4.26844700	-1.66757200	-0.45117800
C	1.52773500	0.57035600	0.75975300
C	2.09858400	-0.23501300	-0.43043900
H	1.39721500	-0.08242400	1.63165400
H	2.23618400	1.35173100	1.04902400
C	3.39401800	-0.91246500	-0.07202400
H	2.24867600	0.43694400	-1.28364600
H	1.36149800	-0.98823400	-0.73927800
C	4.57012000	-0.67115700	-0.65413400
H	3.33819000	-1.64677700	0.73353900
H	4.67109600	0.05431100	-1.45936900
H	5.47501400	-1.19240700	-0.35243500

ts3

Zero-point correction= 0.199126 (Hartree/Particle)
Thermal correction to Energy= 0.209444
Thermal correction to Enthalpy= 0.210388
Thermal correction to Gibbs Free Energy= 0.161849
Sum of electronic and zero-point Energies= -480.859405
Sum of electronic and thermal Energies= -480.849087
Sum of electronic and thermal Enthalpies= -480.848143
Sum of electronic and thermal Free Energies= -480.896682

Cartesian coordinates

N	1.23782100	-0.99138000	-0.31301200
C	0.55004500	0.05610900	-0.10032800
C	-0.94393300	-0.01868700	-0.03337100
C	-1.73288400	1.13927800	-0.11414000
C	-1.58256300	-1.26438600	0.09918200
C	-3.12618600	1.05337500	-0.06752500
H	-1.26594300	2.11299000	-0.22237700
C	-2.97120300	-1.34786600	0.15102200
H	-0.97473100	-2.16107400	0.16621800
C	-3.74926700	-0.18804900	0.06682300
H	-3.72241000	1.95916700	-0.13502400
H	-3.44923800	-2.31762000	0.25982700
H	-4.83300900	-0.25351500	0.10816200
C	1.25980900	1.39939500	0.03978500
C	2.72310100	1.07631200	0.35706800
H	0.79939900	2.03098700	0.80653800
H	1.16924300	1.94055300	-0.91269400
C	3.13946600	-0.18069500	-0.37279800
H	2.84717000	0.92144600	1.43543500
H	3.37094300	1.91489500	0.07257100
C	4.03102400	-1.07871900	0.18014700
H	3.09376000	-0.13299500	-1.46059400
H	4.25135000	-1.06857900	1.24488900
H	4.46426300	-1.88300100	-0.40706300

int7

Zero-point correction= 0.200144 (Hartree/Particle)
Thermal correction to Energy= 0.210851
Thermal correction to Enthalpy= 0.211795
Thermal correction to Gibbs Free Energy= 0.162664
Sum of electronic and zero-point Energies= -480.884992
Sum of electronic and thermal Energies= -480.874285
Sum of electronic and thermal Enthalpies= -480.873341
Sum of electronic and thermal Free Energies= -480.922472

Cartesian coordinates

N	-1.36773800	-0.82685600	0.27443300
C	-0.59084600	0.18394300	0.11136900
C	0.87967100	0.03529100	0.04113900
C	1.71739900	1.16006800	-0.02909400
C	1.46594000	-1.24382600	0.04790800
C	3.10450800	1.01176500	-0.08953800
H	1.28904600	2.15756000	-0.03164600
C	2.84815300	-1.39091600	-0.01614600
H	0.81845000	-2.11274400	0.10295400
C	3.67372500	-0.26249900	-0.08475100
H	3.73826600	1.89273400	-0.14102900
H	3.28594600	-2.38549400	-0.01269700
H	4.75295200	-0.37845200	-0.13424400
C	-1.29521700	1.53304000	0.03963600
C	-2.75611500	1.10661400	-0.17745900
H	-0.90788300	2.17652700	-0.75675000
H	-1.15645300	2.07373800	0.98644200
C	-2.77257900	-0.36716100	0.35242300
H	-2.99722200	1.11294200	-1.24609400
H	-3.48243700	1.74129900	0.33662900
C	-3.70468600	-1.27651400	-0.37036100
H	-3.04621800	-0.35526400	1.42021000
H	-3.37987700	-1.77767900	-1.27727700
H	-4.76012400	-1.29601400	-0.11829100

ts3′

Zero-point correction= 0.199871 (Hartree/Particle)
Thermal correction to Energy= 0.209919
Thermal correction to Enthalpy= 0.210863
Thermal correction to Gibbs Free Energy= 0.163153
Sum of electronic and zero-point Energies= -480.850653
Sum of electronic and thermal Energies= -480.840605
Sum of electronic and thermal Enthalpies= -480.839661
Sum of electronic and thermal Free Energies= -480.887371

Cartesian coordinates

N	1.17076200	-1.19790700	-0.57711600
C	0.63947300	-0.08429600	-0.26210300
C	-0.85529500	-0.04443900	-0.10050800
C	-1.59653500	1.10650900	-0.41186300
C	-1.54071800	-1.19081000	0.33691400
C	-2.98776200	1.10916600	-0.29105900
H	-1.09411500	2.00096400	-0.76739800
C	-2.92790100	-1.18337000	0.46729400
H	-0.97034900	-2.08102400	0.58249100
C	-3.65748700	-0.03275700	0.15223600
H	-3.54662900	2.00620400	-0.54345500
H	-3.44088700	-2.07453100	0.81888300
H	-4.73917600	-0.02653300	0.25434200
C	1.43413100	1.21864100	-0.06945200
C	2.66586200	1.02758100	0.84142200
H	0.79491900	2.00202900	0.34407800
H	1.75385000	1.56636900	-1.06062300
C	3.41731200	-0.23089200	0.51071100
H	2.33793600	0.97816600	1.88815300
H	3.30050700	1.92539400	0.77305700
C	3.22256300	-0.86102400	-0.69266000
H	3.88975700	-0.77125800	1.32816300
H	3.63882800	-1.84862400	-0.86953900
H	2.99817200	-0.29765900	-1.59394000

int7′

Zero-point correction=	0.201424 (Hartree/Particle)
Thermal correction to Energy=	0.211675
Thermal correction to Enthalpy=	0.212619
Thermal correction to Gibbs Free Energy=	0.164378
Sum of electronic and zero-point Energies=	-480.885497
Sum of electronic and thermal Energies=	-480.875245
Sum of electronic and thermal Enthalpies=	-480.874301
Sum of electronic and thermal Free Energies=	-480.922542

Cartesian coordinates

N	-1.23395000	1.18762900	-0.18119700
C	-0.67140600	0.04019100	-0.06665000
C	0.82538800	0.01234800	-0.02303000
C	1.54460900	1.19546100	0.22500300
C	1.54822200	-1.17186600	-0.24254300
C	2.93627100	1.19332500	0.25820900
H	0.98894400	2.11171000	0.39308900
C	2.94501700	-1.17281900	-0.21902400
H	1.02776300	-2.10159600	-0.44842800
C	3.64445600	0.00741100	0.03480900
H	3.47213700	2.11704900	0.46057400
H	3.48400100	-2.09901100	-0.39926300
H	4.73079700	0.00540800	0.06004300
C	-1.41235200	-1.28858400	0.01262300
C	-2.85744500	-1.11850500	0.51483200
H	-0.86763900	-1.97902500	0.66466400
H	-1.41747500	-1.74597700	-0.98693000
C	-3.49212600	0.06181300	-0.13317500
H	-2.82890600	-0.98802300	1.61337400
H	-3.43160000	-2.03456200	0.33615600
C	-2.68780700	1.31091800	-0.26541600
H	-4.56673800	0.11032300	-0.28623600
H	-2.97970900	2.05126300	0.50438300
H	-2.91088900	1.82088100	-1.21687900

2a

Zero-point correction=	0.325298 (Hartree/Particle)
Thermal correction to Energy=	0.344872
Thermal correction to Enthalpy=	0.345816
Thermal correction to Gibbs Free Energy=	0.275543
Sum of electronic and zero-point Energies=	-911.194188
Sum of electronic and thermal Energies=	-911.174615
Sum of electronic and thermal Enthalpies=	-911.173671
Sum of electronic and thermal Free Energies=	-911.243943

Cartesian coordinates

C	-1.00265500	-1.09587600	-0.14676300
C	-0.96544900	-2.43212500	-0.29497300
H	-1.87977300	-3.00508600	-0.38432000
H	-0.03527400	-2.98435400	-0.35035300
C	-2.26632900	-0.31315600	-0.06147800
C	-2.27675600	1.05197900	-0.39323900
C	-3.47203800	-0.90880300	0.34950200
C	-3.45869300	1.79187900	-0.33841100
H	-1.35294300	1.52821400	-0.70197200
C	-4.65186100	-0.16892500	0.40423000
H	-3.48444400	-1.95190700	0.64994700
C	-4.65218600	1.18541700	0.05790400
H	-3.44524300	2.84514200	-0.60615900
H	-5.57091900	-0.64878200	0.72983400
H	-5.57171500	1.76235000	0.10488800
O	0.10599600	-0.29926200	-0.08456800
Si	1.77358600	-0.64981300	-0.02075200
C	2.30985200	-1.53519300	-1.59925600
H	1.89879200	-2.54827000	-1.66228700
H	1.98947900	-0.98861400	-2.49330100
H	3.40258800	-1.62162800	-1.63503500
C	2.13321000	-1.70932900	1.49845800
H	1.59868300	-2.66450200	1.46031200
H	3.20458900	-1.93287400	1.56629900
H	1.83848800	-1.19940400	2.42251200

C	2.01890900	1.82689400	1.35092200
H	2.47564800	2.82429100	1.42777700
H	0.93331200	1.96136200	1.28950300
H	2.23938400	1.29478700	2.28434800
C	2.27076000	1.91137700	-1.14925800
H	1.19354100	2.04789300	-1.29963600
H	2.72239500	2.91049100	-1.06484300
H	2.67928000	1.44380900	-2.05320800
C	4.10369400	0.93144800	0.26614600
H	4.55516900	0.42265200	-0.59443600
H	4.57416800	1.92228600	0.34162300
H	4.37717900	0.37171100	1.16877100
C	2.57278200	1.08139900	0.11735000

ts4

Zero-point correction= 0.527259 (Hartree/Particle)
Thermal correction to Energy= 0.558125
Thermal correction to Enthalpy= 0.559070
Thermal correction to Gibbs Free Energy= 0.460307
Sum of electronic and zero-point Energies= -1392.072156
Sum of electronic and thermal Energies= -1392.041290
Sum of electronic and thermal Enthalpies= -1392.040346
Sum of electronic and thermal Free Energies= -1392.139108

Cartesian coordinates

N	-2.50265400	-0.92612800	1.25502600
C	-3.48627500	-1.25047100	0.49407200
C	-4.39116300	-0.23807200	-0.09583600
C	-4.16986200	1.13394200	0.12520900
C	-5.49046700	-0.62407500	-0.88000400
C	-5.01996200	2.08792700	-0.42612800
H	-3.32429200	1.43523400	0.73446000
C	-6.34464300	0.33359600	-1.43037800
H	-5.68633600	-1.67621900	-1.06135600
C	-6.11184000	1.69129900	-1.20697300
H	-4.83437900	3.14365300	-0.24743400
H	-7.19104100	0.01664200	-2.03335600
H	-6.77531100	2.43706100	-1.63623500
C	-3.67093800	-2.74925500	0.28616100
C	-2.34863400	-3.30755100	0.84016600
H	-3.84999400	-3.01413600	-0.76079400
H	-4.54326300	-3.09702200	0.85699100
C	-1.82378600	-2.15384100	1.73362200
H	-1.64298900	-3.49338000	0.02304800
H	-2.47245600	-4.24248500	1.39338100
C	-0.33542400	-2.00330800	1.79579700
H	-2.19709900	-2.30733400	2.76690500
H	0.06227500	-1.15005400	2.33752800
H	0.25965100	-2.91172600	1.84383300
C	0.45907600	-1.20493600	-0.39958900
C	1.76171000	-0.81619000	-0.28528500
H	0.21510700	-2.16567000	-0.83193100
C	2.91506600	-1.72031700	-0.46404200
O	2.12407400	0.45401700	0.07764600
C	4.22631400	-1.20607200	-0.49038600
C	2.75282200	-3.11442900	-0.60871700
Si	1.29534700	1.94216200	0.04857000
C	5.32526000	-2.04573400	-0.67038600
H	4.37512800	-0.13942300	-0.37021200
C	3.85187300	-3.94977500	-0.78984500
H	1.76187800	-3.55421800	-0.56428300
C	0.04602600	2.01002400	1.45976600
C	0.43614900	2.16826800	-1.61771900
C	2.69187300	3.22740800	0.29400500
C	5.14695600	-3.42213800	-0.82411800
H	6.32555900	-1.62061700	-0.69031000
H	3.69702500	-5.02029100	-0.89668300
H	-0.70631000	1.21731900	1.37687600
H	0.53730600	1.90437600	2.43422200
H	-0.48070700	2.97246200	1.45690800
H	-0.42596700	1.50262300	-1.73027700
H	0.07152600	3.19775900	-1.71867700

H	1.12042500	1.97427100	-2.45134000
C	3.65019000	3.21556200	-0.91654700
C	3.49358900	2.90617300	1.57379800
C	2.07516600	4.63790400	0.42926600
H	6.00311100	-4.07648300	-0.96306500
H	4.46021100	3.94439800	-0.76757200
H	4.11383600	2.23284100	-1.06121300
H	3.13682900	3.48364400	-1.84779800
H	3.96327100	1.91782000	1.52023400
H	4.29234700	3.64832700	1.71807400
H	2.86144000	2.92915700	2.46995400
H	1.41266100	4.71598300	1.29957100
H	2.87003300	5.38707700	0.55556200
H	1.49806500	4.92418200	-0.45882700
H	-0.35086200	-0.49091900	-0.33796100

int8

Zero-point correction= 0.532772 (Hartree/Particle)
Thermal correction to Energy= 0.563008
Thermal correction to Enthalpy= 0.563952
Thermal correction to Gibbs Free Energy= 0.467511
Sum of electronic and zero-point Energies= -1392.127697
Sum of electronic and thermal Energies= -1392.097462
Sum of electronic and thermal Enthalpies= -1392.096517
Sum of electronic and thermal Free Energies= -1392.192959

Cartesian coordinates

N	-2.44186100	0.72812600	-1.10065500
C	-3.48418000	1.14922800	-0.47725000
C	-4.51108800	0.22568000	0.05371400
C	-4.33899400	-1.16736700	-0.04565900
C	-5.67805600	0.71797100	0.66067500
C	-5.30389100	-2.03878800	0.45046300
H	-3.43951300	-1.55011000	-0.51627700
C	-6.64721700	-0.15701100	1.15522900
H	-5.83654000	1.78847900	0.74581300
C	-6.46312600	-1.53664300	1.05320900
H	-5.15531300	-3.11210200	0.36795300
H	-7.54487100	0.24119400	1.62004800
H	-7.21614900	-2.21804600	1.43953700
C	-3.59616900	2.66535400	-0.37121700
C	-2.18773600	3.11442300	-0.80096700
H	-3.87387100	3.00138700	0.63299700
H	-4.37596900	3.02720600	-1.05577000
C	-1.63484100	1.87720300	-1.55537400
H	-1.57809800	3.33252000	0.08264100
H	-2.19371300	4.01174000	-1.42566700
C	-0.12799500	1.60838300	-1.41050600
H	-1.83327000	1.98931700	-2.63283500
H	0.14603400	0.79502100	-2.09259100
H	0.42140800	2.49774100	-1.74449700
C	0.32349000	1.22777500	0.02006600
C	1.77627500	0.85195300	0.09757300
H	0.12014400	2.05404800	0.70881300
C	2.83860400	1.77468100	0.32151300
O	2.13360700	-0.42906500	-0.20304400
C	4.20049500	1.34674300	0.31495200
C	2.60040900	3.16160300	0.56233600
Si	1.40851200	-1.95520000	0.02953700
C	5.23739200	2.24020600	0.54406900
H	4.41748800	0.30222500	0.12265000
C	3.64904400	4.04253600	0.79046600
H	1.58524100	3.54493500	0.56491400
C	0.06794200	-2.23755400	-1.26625000
C	0.68808000	-2.05385800	1.77203500
C	2.86274100	-3.17708500	-0.20042300
C	4.97860900	3.59709700	0.78663200
H	6.26328200	1.87906700	0.53307000
H	3.43020000	5.09227000	0.97127100
H	-0.73235700	-1.49206200	-1.19532700
H	0.47672800	-2.19498000	-2.28257900
H	-0.38518800	-3.22775800	-1.13273000

H	-0.20382400	-1.42726200	1.88296300
H	0.39394700	-3.08460500	2.00473200
H	1.41710900	-1.73671500	2.52606000
C	3.89771100	-2.99881100	0.93140500
C	3.55439900	-2.93284400	-1.55903500
C	2.32677900	-4.62614400	-0.16316400
H	5.79402100	4.29208100	0.96546200
H	4.74061300	-3.69036900	0.78770100
H	4.30599000	-1.98190000	0.95598000
H	3.46635700	-3.21011200	1.91725400
H	3.96327500	-1.91878700	-1.62903500
H	4.38700200	-3.63869500	-1.69346800
H	2.86630000	-3.07638200	-2.40115500
H	1.61523700	-4.82323600	-0.97381100
H	3.15675700	-5.33832600	-0.27657900
H	1.82768600	-4.85853900	0.78587400
H	-0.29321000	0.39081900	0.36505800

int9

Zero-point correction= 0.227702 (Hartree/Particle)
Thermal correction to Energy= 0.255951
Thermal correction to Enthalpy= 0.256895
Thermal correction to Gibbs Free Energy= 0.159276
Sum of electronic and zero-point Energies= -2357.767578
Sum of electronic and thermal Energies= -2357.739329
Sum of electronic and thermal Enthalpies= -2357.738385
Sum of electronic and thermal Free Energies= -2357.836005

Cartesian coordinates

C	3.36103300	1.33827700	-0.60933900
C	2.44293800	0.51540000	0.07396400
C	2.96535500	-0.57611000	0.80233700
C	4.33627100	-0.82611900	0.82726500
C	5.23670000	-0.01491500	0.13150300
C	4.72957000	1.07069900	-0.58413200
H	2.97861600	2.19395000	-1.15592000
H	2.28648900	-1.21624600	1.35103600
H	6.30003600	-0.21857100	0.15374700
C	4.86350600	-1.94694200	1.67879200
F	3.99432100	-2.98026900	1.76429000
F	5.10703600	-1.54440500	2.95310900
F	6.03029400	-2.44476700	1.20558200
C	5.66152100	1.93051300	-1.39037100
F	6.92321800	1.91982900	-0.90066600
F	5.74588000	1.51637900	-2.68081900
F	5.25983800	3.22268100	-1.43010700
N	1.11338200	0.89166900	0.08676100
C	0.10562200	0.07197300	-0.10729500
S	0.13994200	-1.58853100	-0.62691200
N	-1.10867900	0.73537800	0.14753700
C	-2.45741700	0.42242400	0.03771200
C	-2.98897400	-0.68570900	-0.64702400
C	-3.36203800	1.32624100	0.63609700
C	-4.37062600	-0.87307400	-0.70564900
H	-2.31541700	-1.38207900	-1.12558600
C	-4.73512700	1.12369400	0.55721400
H	-2.97872600	2.19593900	1.16078100
C	-5.26342300	0.01695000	-0.11143900
H	-6.33335200	-0.13556600	-0.17776300
C	-4.90051200	-2.10206300	-1.39405800
C	-5.66491300	2.07634400	1.25772200
F	-6.85246900	2.18514900	0.61935600
F	-5.94193300	1.67056800	2.52209300
F	-5.14597400	3.32116000	1.35627700
F	-6.15980000	-1.92583400	-1.85585300
F	-4.13560200	-2.46918100	-2.44733800
F	-4.94080000	-3.16871000	-0.55645500
H	-0.92263500	1.66086900	0.51920300

int10

Zero-point correction= 0.535937 (Hartree/Particle)
Thermal correction to Energy= 0.565958

Thermal correction to Enthalpy=	0.566902
Thermal correction to Gibbs Free Energy=	0.472057
Sum of electronic and zero-point Energies=	-1391.988069
Sum of electronic and thermal Energies=	-1391.958048
Sum of electronic and thermal Enthalpies=	-1391.957104
Sum of electronic and thermal Free Energies=	-1392.051948

Cartesian coordinates

N	-2.29306000	-0.92180500	1.04537300
C	-3.34524000	-1.30021900	0.40829300
C	-4.38948800	-0.34729900	-0.02453300
C	-4.24719900	1.03051600	0.22424000
C	-5.54435400	-0.79726000	-0.68536500
C	-5.22876800	1.92923400	-0.18194400
H	-3.35992300	1.38094400	0.74062400
C	-6.52975500	0.10500200	-1.08979800
H	-5.68059600	-1.85552700	-0.88413300
C	-6.37462200	1.46951600	-0.84129500
H	-5.10424300	2.99028800	0.01620700
H	-7.41742000	-0.25998300	-1.59866400
H	-7.14083100	2.17220100	-1.15688300
C	-3.44274600	-2.80296100	0.17761300
C	-2.02096900	-3.27088800	0.53817300
H	-3.73764300	-3.05718400	-0.84507300
H	-4.20254800	-3.23054600	0.84591600
C	-1.47348300	-2.09720500	1.38796300
H	-1.42871600	-3.40393400	-0.37420400
H	-2.00240000	-4.21871300	1.08196300
C	0.02825400	-1.79354100	1.25259800
H	-1.64137800	-2.30466700	2.45560000
H	0.29948400	-1.03638200	1.99514000
H	0.60390000	-2.69486500	1.48725100
C	0.40200800	-1.27379000	-0.16592400
C	1.80958200	-0.77347500	-0.20294700
H	0.27121600	-2.06616100	-0.90634900
C	2.95306200	-1.65482400	-0.33516800
O	2.05293200	0.47725000	-0.06872400
C	4.26258300	-1.12268200	-0.26155400
C	2.78416100	-3.04465300	-0.53664300
Si	1.14897000	2.03235700	0.00989200
C	5.36361500	-1.95641100	-0.38346400
H	4.39755200	-0.05965400	-0.10453500
C	3.89297700	-3.87199000	-0.65773200
H	1.79445900	-3.47980200	-0.60423300
C	0.06069800	1.96241500	1.53189700
C	0.19609800	2.14559300	-1.60236500
C	2.58288300	3.27341000	0.13829500
C	5.18063100	-3.33087100	-0.58169000
H	6.36500400	-1.54289600	-0.32452700
H	3.75680000	-4.93681000	-0.81426200
H	-0.73728800	1.21734600	1.43856100
H	0.63906400	1.74504400	2.43616900
H	-0.41381800	2.94198400	1.66991200
H	-0.67530200	1.48356900	-1.62075300
H	-0.17036500	3.17128800	-1.73018200
H	0.82901100	1.90805400	-2.46354500
C	3.48038400	3.19805600	-1.11660800
C	3.43193700	2.99356500	1.39817200
C	1.98042300	4.69568000	0.24263900
H	6.04488300	-3.98111100	-0.67831300
H	4.30030800	3.92391000	-1.03020100
H	3.93092600	2.20713600	-1.24408200
H	2.92697900	3.43635400	-2.03222900
H	3.88361500	1.99515900	1.37920300
H	4.24997900	3.72372000	1.46345200
H	2.84270000	3.07898100	2.31848900
H	1.35199100	4.81576000	1.13292900
H	2.79085400	5.43357300	0.31368100
H	1.37870800	4.95782700	-0.63579800
H	-0.27862000	-0.46276500	-0.43056200

$K_2CO_3 \cdot TBS^+$

Zero-point correction= 0.215054 (Hartree/Particle)
Thermal correction to Energy= 0.234568
Thermal correction to Enthalpy= 0.235513
Thermal correction to Gibbs Free Energy= 0.165075
Sum of electronic and zero-point Energies= -1990.707255
Sum of electronic and thermal Energies= -1990.687740
Sum of electronic and thermal Enthalpies= -1990.686796
Sum of electronic and thermal Free Energies= -1990.757234

Cartesian coordinates

Si	1.16867600	-0.93669200	-0.01356800
C	1.07957200	-1.95486500	-1.59859800
C	1.07102100	-2.02887300	1.52083900
C	2.76895500	0.12321900	0.01724200
H	0.12831000	-2.49286700	-1.64310500
H	1.15397300	-1.32083800	-2.48986900
H	1.89239300	-2.68950200	-1.64297300
H	0.15538300	-2.62652600	1.49963900
H	1.92755700	-2.71152300	1.57520300
H	1.06386500	-1.42969600	2.43884000
C	2.86043300	0.93453400	1.32749300
C	2.80311500	1.09308900	-1.18295400
C	3.99731700	-0.81139800	-0.07035900
H	3.77467000	1.54626600	1.33469500
H	2.00911300	1.61420800	1.45202000
H	2.89666300	0.28315800	2.20875900
H	1.95879400	1.79205600	-1.16914500
H	3.72627000	1.69100300	-1.16546300
H	2.77700700	0.56045500	-2.14120800
H	4.00716300	-1.39263500	-1.00019200
H	4.92497900	-0.22129900	-0.04455400
H	4.03877900	-1.51815100	0.76738200
C	-1.43835800	-0.13967900	0.00212200
O	-1.70814100	-1.36222600	-0.01159300
O	-0.09148900	0.23410500	0.00630000
O	-2.24878200	0.82709100	0.01278500
K	-4.38036200	-0.88686200	0.01277600
K	-0.84392300	3.05221300	-0.00986700

3aa

Zero-point correction= 0.335808 (Hartree/Particle)
Thermal correction to Energy= 0.353685
Thermal correction to Enthalpy= 0.354629
Thermal correction to Gibbs Free Energy= 0.286232
Sum of electronic and zero-point Energies= -865.118851
Sum of electronic and thermal Energies= -865.100975
Sum of electronic and thermal Enthalpies= -865.100031
Sum of electronic and thermal Free Energies= -865.168428

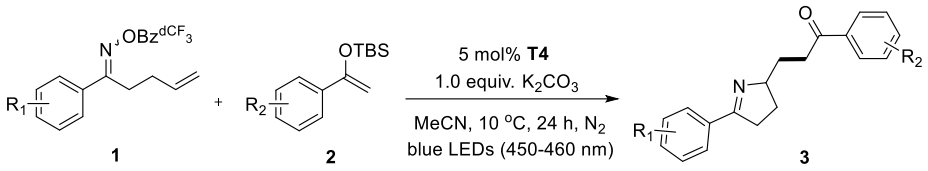
Cartesian coordinates

N	1.61021900	0.14765900	1.08345900
C	2.49615000	0.73414300	0.36030700
C	3.75711600	0.06515500	-0.02878500
C	3.98261000	-1.28066600	0.31438300
C	4.75128500	0.75487900	-0.74132100
C	5.16641000	-1.91609500	-0.04763500
H	3.21442900	-1.81277000	0.86583600
C	5.94034100	0.11748700	-1.10127900
H	4.60206000	1.79501500	-1.01404600
C	6.15098800	-1.21862600	-0.75735900
H	5.32507700	-2.95665300	0.22236300
H	6.70033900	0.66613700	-1.65063400
H	7.07520900	-1.71557900	-1.03925400
C	2.16240900	2.17050400	-0.02313600
C	0.67450500	2.25960300	0.36349500
H	2.35231900	2.38321400	-1.08011800
H	2.78584700	2.86350000	0.55875200
C	0.49140200	1.07191100	1.34405300
H	0.04873100	2.12827000	-0.52599800
H	0.40385300	3.21674800	0.81733800
C	-0.86405700	0.34657900	1.29497400
H	0.61409800	1.42959500	2.37822700

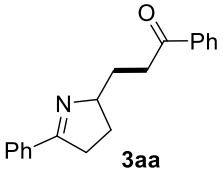
H	-0.88670000	-0.39419700	2.10348100
H	-1.65783400	1.07310500	1.50835700
C	-1.14458500	-0.38247100	-0.03817600
C	-2.42298100	-1.20249700	0.04204900
H	-1.18703700	0.32832300	-0.86939200
C	-3.75020900	-0.55445400	-0.21186900
O	-2.36389500	-2.39037600	0.34807500
C	-4.90718100	-1.34413100	-0.09127100
C	-3.88589000	0.79964400	-0.56015900
C	-6.16676400	-0.79698600	-0.31449600
H	-4.79331700	-2.38887600	0.17838600
C	-5.14935800	1.34934600	-0.78103100
H	-3.01186700	1.43418600	-0.66060900
C	-6.29037600	0.55336100	-0.65993000
H	-7.05308400	-1.41803300	-0.21983400
H	-5.24163500	2.39790900	-1.04891000
H	-7.27320600	0.98248800	-0.83422800
H	-0.32854200	-1.08310000	-0.23540800

6. Synthesis Procedure and Characterization of Products

6.1. Synthesis Procedure and Characterization of Pyrroline 3



An oven-dried Schlenk tube equipped with a stirring bar was charged with **1** (0.2 mmol, 1.0 equiv.), **T4** (0.01 mmol, 5.0 mg, 5 mol%) and K_2CO_3 (0.2 mmol, 27.60 mg, 1.0 equiv.). After refilling with N_2 repeated three times, MeCN (1.0 mL) and **2** (0.6 mmol, 3.0 equiv.) was added through syringe. The mixture was stirred at 10 ºC in a freezer for 24 h in front of a 20 W blue LEDs bulb. Saturated $NaHCO_3$ aqueous solution and EtOAc were added and the mixture was stirred for 10 min. The layers were separated and the aqueous layer was extracted with EtOAc. The combined organic layers were then washed with brine, dried over Na_2SO_4 and concentrated in vacuo. The residue was purified by column chromatography on silica gel to afford the corresponding product.

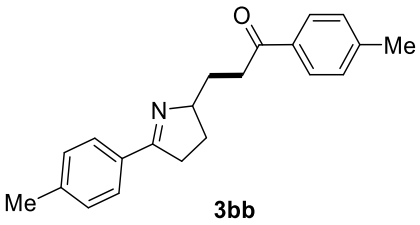


3aa

1-Phenyl-3-(5-phenyl-3,4-dihydro-2*H*-pyrrol-2-yl)propan-1-one (3aa): 42.7 mg, 77% yield as a pale yellow solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.05-7.97 (m, 2H), 7.84 (dd, *J* = 7.9, 1.8 Hz, 2H), 7.58-7.52 (m, 1H), 7.45 (t, *J* = 7.8 Hz, 2H), 7.44-7.36 (m, 3H), 4.27 (dtdd, *J* = 9.8, 7.8, 5.1, 2.0 Hz, 1H), 3.33 (ddd, *J* = 17.1, 9.3, 5.5 Hz, 1H), 3.24 (ddd, *J* = 17.0, 9.3, 5.9 Hz, 1H), 3.04 (dddd, *J* = 16.8, 9.9, 4.6, 2.2 Hz, 1H), 2.91 (dddd, *J* = 17.1, 9.8, 7.8, 1.9 Hz, 1H), 2.27 (dddd, *J* = 12.5, 9.9, 7.7, 4.5 Hz, 1H), 2.14 (ddt, *J* = 13.6, 9.3, 5.8 Hz, 1H), 2.01 (dtd, *J* = 14.0, 8.9, 5.5 Hz, 1H), 1.65 (ddt, *J* = 12.7, 9.9, 7.4 Hz, 1H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 200.48, 172.46, 137.16, 134.74, 132.97, 130.45, 128.62, 128.48, 128.24, 127.75, 72.60, 36.25, 35.13, 31.43, 28.98; Data in accordance with literature.[13]



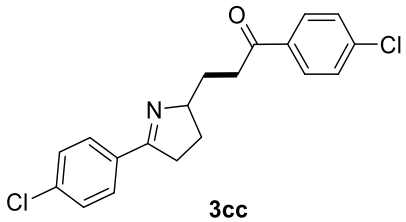
3bb

1-(*p*-Tolyl)-3-(5-(*p*-tolyl)-3,4-dihydro-2*H*-pyrrol-2-yl)propan-1-one (3bb): 46.0 mg, 75% yield as a pale yellow solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.91 (d, *J* = 8.4 Hz, 2H), 7.73 (d, *J* = 8.4 Hz, 2H), 7.25 (d, *J* = 7.8 Hz, 2H), 7.20 (d, *J* = 7.8 Hz, 2H), 4.30-4.21 (m, 1H), 3.29 (ddd, *J* = 16.8, 9.5, 5.5 Hz, 1H), 3.19 (ddd, *J* = 16.8, 9.5, 5.8 Hz, 1H), 3.02 (dddd, *J* = 16.8, 9.9, 4.6, 2.1 Hz, 1H), 2.88 (dddd, *J* = 17.0, 9.7, 7.7, 1.8 Hz, 1H), 2.40 (s, 3H), 2.38 (s, 3H), 2.25 (dddd, *J* = 12.6, 9.9, 7.7, 4.7 Hz, 1H), 2.11 (ddt, *J* = 13.7, 9.5, 5.8 Hz, 1H), 2.00 (dddd, *J* = 13.6, 9.3, 8.1, 5.5 Hz, 1H), 1.64 (ddt, *J* = 12.7, 9.9, 7.4 Hz, 1H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 200.24, 172.40, 143.69, 140.66, 134.70, 132.05, 129.30, 129.20, 128.39, 127.75, 72.53, 36.15, 35.12, 31.54, 28.93, 21.71, 21.53;

HRMS (ESI) m/z: calculated for $C_{21}H_{24}NO$ $[M+H]^+$: 306.1852, found: 306.1850.



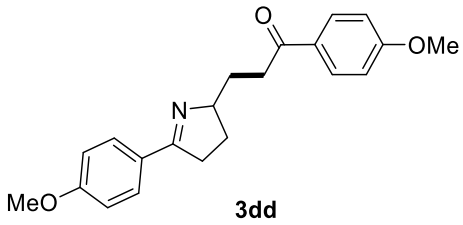
3cc

1-(4-Chlorophenyl)-3-(5-(4-chlorophenyl)-3,4-dihydro-2*H*-pyrrol-2-yl)propan-1-one (3cc): 37.0 mg, 53% yield as a yellow solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.97-7.92 (m, 2H), 7.79-7.72 (m, 2H), 7.45-7.40 (m, 2H), 7.39-7.33 (m, 2H), 4.27-4.21 (m, 1H), 3.30 (ddd, *J* = 17.1, 9.1, 5.5 Hz, 1H), 3.19 (ddd, *J* = 17.1, 9.0, 6.0 Hz, 1H), 3.00 (dddd, *J* = 16.8, 10.0, 4.5, 2.2 Hz, 1H), 2.87 (dddd, *J* = 17.1, 9.9, 7.9, 2.0 Hz, 1H), 2.27 (dddd, *J* = 12.5, 9.9, 7.7, 4.5 Hz, 1H), 2.17-2.08 (m, 1H), 1.95 (dtd, *J* = 14.1, 8.8, 5.5 Hz, 1H), 1.64 (ddt, *J* = 12.8, 10.0, 7.5 Hz, 1H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 199.18, 171.57, 139.47, 136.62, 135.48, 133.12, 129.70, 129.12, 128.98, 128.77, 72.63, 36.25, 35.15, 31.33, 29.11;

HRMS (ESI) m/z: calculated for $C_{19}H_{18}Cl_2NO$ $[M+H]^+$: 346.0760, found: 346.0757.



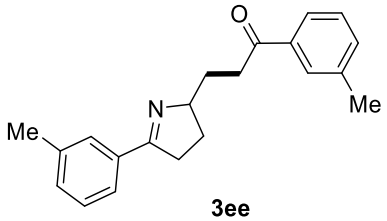
3dd

1-(4-Methoxyphenyl)-3-(5-(4-methoxyphenyl)-3,4-dihydro-2*H*-pyrrol-2-yl)propan-1-one (3dd): 40.5 mg, 60% yield as a yellow solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.99 (d, *J* = 8.8 Hz, 2H), 7.78 (d, *J* = 8.8 Hz, 2H), 6.96-6.86 (m, 4H), 4.27-4.19 (m, 1H), 3.85 (s, 3H), 3.83 (s, 3H), 3.25 (ddd, *J* = 16.5, 9.5, 5.5 Hz, 1H), 3.15 (ddd, *J* = 16.5, 9.5, 5.8 Hz, 1H), 3.00 (dddd, *J* = 16.6, 9.9, 4.6, 2.0 Hz, 1H), 2.86 (dddd, *J* = 17.0, 9.7, 7.7, 1.8 Hz, 1H), 2.24 (dddd, *J* = 12.4, 9.8, 7.7, 4.6 Hz, 1H), 2.09 (ddt, *J* = 13.5, 9.4, 5.8 Hz, 1H), 2.02-1.94 (m, 1H), 1.63 (ddt, *J* = 12.6, 9.9, 7.3 Hz, 1H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 199.21, 171.83, 163.43, 161.47, 130.54, 130.30, 129.39, 127.60, 113.80, 113.75, 72.47, 55.54, 55.42, 35.95, 35.07, 31.74, 29.01;

HRMS (ESI) m/z: calculated for $C_{21}H_{24}NO_3$ $[M+H]^+$: 338.1751, found: 338.1747.



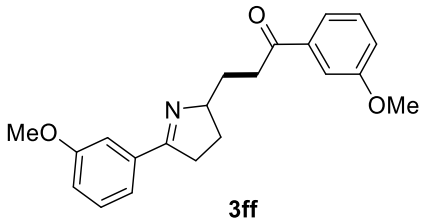
3ee

1-(*m*-Tolyl)-3-(5-(*m*-tolyl)-3,4-dihydro-2*H*-pyrrol-2-yl)propan-1-one (3ee): 43.7 mg, 72% yield as a pale yellow solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.86-7.78 (m, 2H), 7.70 (d, *J* = 2.0 Hz, 1H), 7.59 (dt, *J* = 7.6, 1.5 Hz, 1H), 7.38-7.32 (m, 2H), 7.29 (t, *J* = 7.6 Hz, 1H), 7.23 (d, *J* = 7.6 Hz, 1H), 4.32-4.21 (m, 1H), 3.32 (ddd, *J* = 16.9, 9.4, 5.5 Hz, 1H), 3.21 (ddd, *J* = 17.0, 9.4, 5.8 Hz, 1H), 3.03 (dddd, *J* = 16.8, 10.0, 4.6, 2.2 Hz, 1H), 2.90 (dddd, *J* = 17.2, 9.8, 7.8, 1.9 Hz, 1H), 2.41 (s, 3H), 2.38 (s, 3H), 2.26 (dddd, *J* = 12.5, 9.8, 7.6, 4.6 Hz, 1H), 2.12 (ddt, *J* = 13.8, 9.5, 5.8 Hz, 1H), 2.01 (dddd, *J* = 13.7, 9.4, 8.1, 5.5 Hz, 1H), 1.65 (ddt, *J* = 12.7, 9.9, 7.4 Hz, 1H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 200.71, 172.71, 138.35, 138.14, 137.19, 134.65, 133.72, 131.25, 128.79, 128.49, 128.36, 128.22, 125.46, 125.02, 72.59, 36.33, 35.17, 31.46, 28.94, 21.41, 21.40;

HRMS (ESI) m/z: calculated for $C_{21}H_{24}NO$ $[M+H]^+$: 306.1852, found: 306.1848.



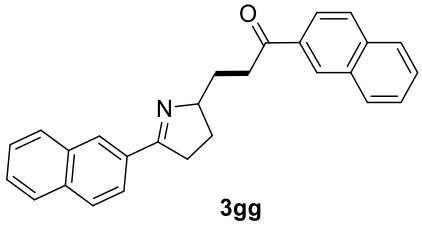
3ff

1-(3-Methoxyphenyl)-3-(5-(3-methoxyphenyl)-3,4-dihydro-2*H*-pyrrol-2-yl)propan-1-one (3ff): 47.8 mg, 71% yield as a yellow solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.60 (dt, *J* = 7.7, 1.2 Hz, 1H), 7.53 (dd, *J* = 2.6, 1.5 Hz, 1H), 7.43 (dd, *J* = 2.5, 1.5 Hz, 1H), 7.38-7.33 (m, 2H), 7.30 (t, *J* = 7.9 Hz, 1H), 7.09 (ddd, *J* = 8.3, 2.7, 0.9 Hz, 1H), 6.97 (ddd, *J* = 8.2, 2.7, 1.0 Hz, 1H), 4.31-4.22 (m, 1H), 3.84 (s, 3H), 3.83 (s, 3H), 3.31 (ddd, *J* = 17.0, 9.3, 5.5 Hz, 1H), 3.21 (ddd, *J* = 16.9, 9.3, 6.0 Hz, 1H), 3.02 (dddd, *J* = 16.8, 9.9, 4.6, 2.2 Hz, 1H), 2.89 (dddd, *J* = 17.1, 9.8, 7.8, 1.9 Hz, 1H), 2.26 (dddd, *J* = 12.5, 9.8, 7.7, 4.6 Hz, 1H), 2.12 (ddt, *J* = 13.6, 9.3, 5.8 Hz, 1H), 2.05-1.95 (m, 1H), 1.64 (ddt, *J* = 12.8, 10.0, 7.4 Hz, 1H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 200.31, 172.46, 159.91, 159.73, 138.56, 136.13, 129.63, 129.47, 120.94, 120.53, 119.50, 116.82, 112.45, 112.26, 72.60, 55.52, 55.45, 36.39, 35.28, 31.48, 28.99;

HRMS (ESI) m/z: calculated for $C_{21}H_{24}NO_3$ $[M+H]^+$: 338.1751, found: 338.1748.



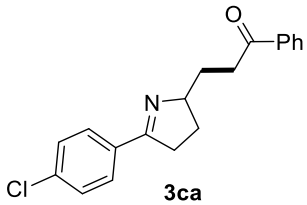
3gg

1-(Naphthalen-2-yl)-3-(5-(naphthalen-2-yl)-3,4-dihydro-2*H*-pyrrol-2-yl)propan-1-one (3gg): 48.1 mg, 64% yield as a yellow solid.

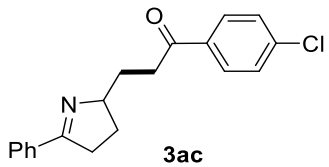
^{1}H NMR (600 MHz, $CDCl_3$): δ 8.58 (d, *J* = 1.7 Hz, 1H), 8.17 (d, *J* = 1.7 Hz, 1H), 8.11 (ddd, *J* = 12.4, 8.6, 1.8 Hz, 2H), 7.97 (d, *J* = 8.1 Hz, 1H), 7.92-7.81 (m, 5H), 7.59 (ddd, *J* = 8.2, 6.7, 1.3 Hz, 1H), 7.57-7.46 (m, 3H), 4.42-4.33 (m, 1H), 3.53 (ddd, *J* = 16.9, 9.4, 5.5 Hz, 1H), 3.40 (ddd, *J* = 16.8, 9.3, 5.9 Hz, 1H), 3.19 (dddd, *J* = 16.7, 10.0, 4.6, 2.1 Hz, 1H), 3.04 (dddd, *J* = 16.9, 9.8, 7.8, 1.8 Hz, 1H), 2.35 (dddd, *J* = 12.4, 9.8, 7.6, 4.5 Hz, 1H), 2.25 (ddt, *J* = 13.6, 9.3, 5.8 Hz, 1H), 2.12 (dtd, *J* = 14.0, 9.0, 5.4 Hz, 1H), 1.74 (ddt, *J* = 12.7, 9.9, 7.4 Hz, 1H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 200.50, 172.63, 135.65, 134.50, 133.10, 132.69, 132.24, 129.99, 129.70, 128.82, 128.47, 128.43, 128.35, 128.22, 127.86, 127.16, 126.78, 126.49, 124.72, 124.12, 72.81, 36.44, 35.19, 31.70, 29.12;

HRMS (ESI) m/z: calculated for $C_{27}H_{24}NO$ $[M+H]^+$: 378.1852, found: 378.1845.



3ca



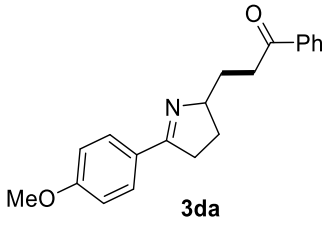
3ac

3-(5-(4-Chlorophenyl)-3,4-dihydro-2*H*-pyrrol-2-yl)-1-phenylpropan-1-one (3ca) and **1-(4-Chlorophenyl)-3-(5-phenyl-3,4-dihydro-2*H*-pyrrol-2-yl)propan-1-one (3ac)**: 47.6 mg (**3ca**:**3ac** = 1:1), 76% yield as a yellow solid.

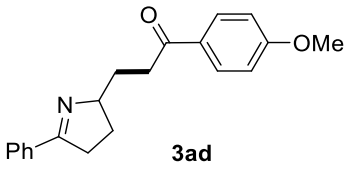
^{1}H NMR (600 MHz, $CDCl_3$): δ 8.04-7.99 (m, **3ca** 1H), 7.98-7.92 (m, **3ac** 1H), 7.86-7.81 (m, **3ac** 1H), 7.79-7.73 (m, **3ca** 1H), 7.57-7.52 (m, **3ca** 1H), 7.46 (t, *J* = 7.8 Hz, **3ac** 1H), 7.44-7.38 (m, 3H, **3ca** 1H, **3ac** 2H), 7.38-7.34 (m, **3ca** 1H), 4.26 (pd, *J* = 8.1, 2.2 Hz, 1H), 3.32 (dtd, *J* = 17.1, 9.2, 5.5 Hz, 1H), 3.22 (dddd, *J* = 17.3, 11.6, 9.1, 6.0 Hz, 1H), 3.09-2.96 (m, 1H), 2.90 (ddddd, *J* = 24.9, 17.0, 9.9, 7.8, 1.9 Hz, 1H), 2.28 (ddddd, *J* = 12.5, 10.1, 7.3, 4.6, 2.6 Hz, 1H), 2.20-2.07 (m, 1H), 1.98 (ddtd, *J* = 16.0, 14.1, 8.9, 5.5 Hz, 1H), 1.65 (dddd, *J* = 19.5, 10.2, 7.4, 4.4 Hz, 1H) *(the unlabled hydrogen signals belong to both **3ca** and **3ac**)*;

^{13}C NMR (151 MHz, $CDCl_3$): δ 200.43 (**3ca**), 199.30, 172.75, 171.45 (**3ca**), 139.42, 137.16 (**3ca**), 136.54 (**3ca**), 135.49, 134.61, 133.20 (**3ca**), 133.06 (**3ca**), 130.61, 129.73, 129.12 (**3ca**), 128.95, 128.74 (**3ca**), 128.67 (**3ca**), 128.55, 128.26 (**3ca**), 127.81, 72.73 (**3ca**),

72.47, 36.27 (**3ca**), 36.24, 35.19 (**3ca**), 35.14, 31.39 (**3ca**), 31.37, 29.09 (**3ca**), 29.00 *(the unlabled carbon signals belong to **3ac**)*; Data in accordance with literature.[13]



3da



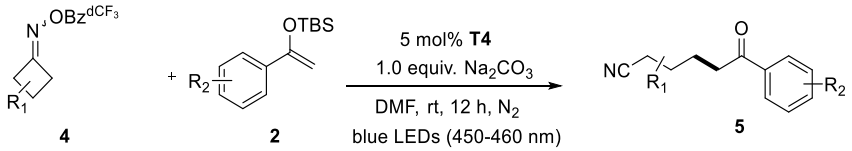
3ad

3-(5-(4-Methoxyphenyl)-3,4-dihydro-2*H*-pyrrol-2-yl)-1-phenylpropan-1-one (3da) and **1-(4-Methoxyphenyl)-3-(5-phenyl-3,4-dihydro-2*H*-pyrrol-2-yl)propan-1-one (3ad)**: 39.7 mg (**3da**:**3ad** = 2:1), 65% yield as a yellow solid.

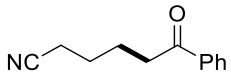
^{1}H NMR (600 MHz, $CDCl_3$): δ 8.03-7.96 (m, **3ca** $\frac{4}{3}$H, **3ad** $\frac{2}{3}$H), 7.86-7.81 (m, **3da** $\frac{4}{3}$H,), 7.80-7.75 (m, **3ad** $\frac{2}{3}$H), 7.53 (tt, *J* = 7.2, 1.8 Hz, **3ad** $\frac{1}{3}$H), 7.44 (t, *J* = 7.8 Hz, **3da** $\frac{2}{3}$H), 7.42-7.36 (m, **3da** $\frac{4}{3}$H, **3ac** $\frac{2}{3}$H), 6.95-6.87 (m, **3da** $\frac{4}{3}$H, **3ac** $\frac{2}{3}$H), 4.32-4.18 (m, 1H), 3.35-3.12 (m, 2H), 3.01 (tddd, *J* = 16.3, 9.9, 4.7, 2.1 Hz, 1H), 2.94-2.83 (m, 1H), 2.26 (dddd, *J* = 12.6, 9.7, 7.8, 4.6 Hz, 1H), 2.11 (ddtd, *J* = 13.6, 9.5, 5.8, 1.9 Hz, 1H), 2.04-1.95 (m, 1H), 1.64 (dtt, *J* = 12.7, 9.8, 7.4 Hz, 1H) *(the unlabled hydrogen signals belong to both **3da** and **3ad**)*;

^{13}C NMR (151 MHz, $CDCl_3$): δ 200.54 (**3da**), 199.11, 172.52 (**3da**), 171.90, 163.42 (**3da**), 161.48, 137.14, 134.72 (**3da**), 132.96, 130.50 (**3da**), 130.45 (**3da**), 130.25 (**3da**), 129.39, 128.61 (**3da**), 128.47, 128.24, 127.75 (**3da**), 127.48, 113.79 (**3da**), 113.73, 72.63 (**3da**), 72.32, 55.50 (**3da**), 55.39, 36.24 (**3da**), 35.87, 35.13 (**3da**), 35.05, 31.61 (**3da**), 31.46, 28.97 (**3da**), 28.93 *(the unlabled carbon signals belong to **3ad**)*; Data in accordance with literature.[13]

6.2. Synthesis Procedure and Characterization of Ketonitrile 5



An oven-dried Schlenk tube equipped with a stirring bar was charged with **9** (0.2 mmol, 1.0 equiv.), **T4** (0.01 mmol, 5.0 mg, 5 mol%) and Na_2CO_3 (0.2 mmol, 21.20 mg, 1.0 equiv.). After refilling with N_2 repeated three times, DMF (2.0 mL) and **2** (0.6 mmol, 3.0 equiv.) was added through syringe. The mixture was stirred at room temperature for 12 h in front of a 20 W blue LEDs bulb. Saturated $NaHCO_3$ aqueous solution and EtOAc were added and the mixture was stirred for 10 min. The layers were separated and the aqueous layer was extracted with EtOAc. The combined organic layers were then washed with brine, dried over Na_2SO_4 and concentrated in vacuo. The residue was purified by column chromatography on silica gel to afford the corresponding product.

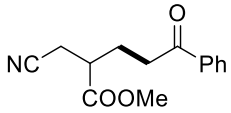


5aa

6-Oxo-6-phenylhexanenitrile (5aa): 28.1 mg, 75% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.95-7.93 (m, 2H), 7.58-7.55 (m, 1H), 7.47-7.45 (m, 2H), 3.03 (t, *J* = 7.0 Hz, 2H), 2.40 (t, *J* = 7.1 Hz, 2H), 1.92-1.87 (m, 2H), 1.78-1.73 (m, 2H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 199.21, 136.80, 133.32, 128.77, 128.07, 119.62, 37.45, 25.11, 23.19, 17.28; Data in accordance with literature.[14]

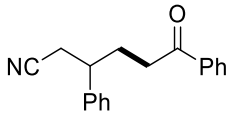


5ba

Methyl 2-(cyanomethyl)-5-oxo-5-phenylpentanoate (5ba): 35.9 mg, 73% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.95-7.93 (m, 2H), 7.60-7.54 (m, 1H), 7.50-7.43 (m, 2H), 3.73 (s, 3H), 3.15-3.06 (m, 2H), 2.90 (dtd, *J* = 8.4, 6.8, 5.5 Hz, 1H), 2.72 (dd, *J* = 16.9, 7.0 Hz, 1H), 2.64 (dd, *J* = 16.9, 6.7 Hz, 1H), 2.24-2.10 (m, 2H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 198.41, 172.84, 136.59, 133.50, 128.83, 128.09, 117.67, 52.58, 40.80, 35.31, 25.65, 19.95; Data in accordance with literature.[14]

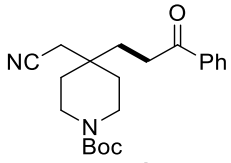


5ca

6-Oxo-3,6-diphenylhexanenitrile (5ca): 36.1 mg, 68% yield as a pale yellow solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.84-7.82 (m, 2H), 7.53 (td, *J* = 7.3, 1.4 Hz, 1H), 7.41 (t, *J* = 7.8 Hz, 2H), 7.36 (dd, *J* = 8.2, 6.9 Hz, 2H), 7.31-7.27 (m, 1H), 7.25-7.22 (m, 2H), 3.09 (dtd, *J* = 11.4, 6.9, 4.6 Hz, 1H), 2.90 (ddd, *J* = 17.6, 8.4, 6.9 Hz, 1H), 2.82 (ddd, *J* = 17.6, 8.4, 5.3 Hz, 1H), 2.68 (d, *J* = 7.0 Hz, 2H), 2.33 (dddd, *J* = 13.5, 8.5, 6.9, 4.6 Hz, 1H), 2.16 (dddd, *J* = 13.8, 10.8, 8.4, 5.3 Hz, 1H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 199.21, 140.88, 136.76, 133.30, 129.24, 128.72, 128.05, 127.89, 127.42, 118.45, 41.68, 35.98, 29.25, 25.58; Data in accordance with literature.[15]

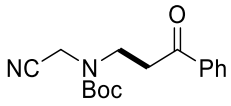


5da

***tert*-Butyl 4-(cyanomethyl)-4-(3-oxo-3-phenylpropyl)piperidine-1-carboxylate (5da)**: 46.5 mg, 65% yield as a pale yellow solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.96-7.94 (m, 2H), 7.59-7.56 (m, 1H), 7.47 (t, *J* = 7.8 Hz, 2H), 3.50-3.45 (m, 2H), 3.39 (ddd, *J* = 14.0, 9.1, 5.2 Hz, 2H), 3.02-2.94 (m, 2H), 2.43 (s, 2H), 2.03-1.95 (m, 2H), 1.57 (dt, *J* = 7.1, 4.0 Hz, 4H), 1.45 (s, 9H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 198.99, 154.83, 136.67, 133.50, 128.88, 128.17, 117.51, 80.01, 34.11, 32.31, 31.17, 28.52, 26.27 *(the carbonyl carbon signal is overlapped)*; Data in accordance with literature.[14]

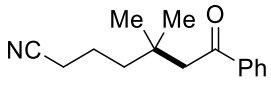


5ea

***tert*-Butyl (cyanomethyl)(3-oxo-3-phenylpropyl)carbamate (5ea)**: 36.7 mg, 64% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.95 (d, *J* = 7.8 Hz, 2H), 7.58 (t, *J* = 7.5 Hz, 1H), 7.47 (t, *J* = 7.8 Hz, 2H), 4.32 (d, *J* = 19.9 Hz, 2H), 3.72 (s, 2H), 3.35 (t, *J* = 16.1 Hz, 2H), 1.47 (d, *J* = 6.8 Hz, 10H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 198.95, 154.22, 136.52, 133.69, 128.88, 128.21, 116.64, 82.12, 43.86, 37.96, 28.35; Data in accordance with literature.[14]



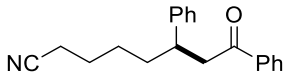
5fa

5,5-Dimethyl-7-oxo-7-phenylheptanenitrile (5fa): 31.1 mg, 68% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.93-7.91 (m, 2H), 7.56-7.54 (m, 1H), 7.45 (t, *J* = 7.8 Hz, 2H), 2.87 (s, 2H), 2.32 (t, *J* = 7.2 Hz, 2H), 1.72-1.64 (m, 2H), 1.59-1.52 (m, 2H), 1.05 (s, 6H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 200.13, 138.50, 133.07, 128.71, 128.21, 119.87, 47.78, 41.11, 33.86, 27.78, 20.83, 17.88;

HRMS (ESI) m/z: calculated for $C_{15}H_{20}NO$ $[M+H]^+$: 230.1539, found: 230.1535.



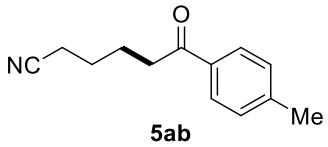
5ga

8-Oxo-6,8-diphenyloctanenitrile (5ga): 20.4 mg, 35% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.91-7.89 (m, 2H), 7.56-7.53 (m, 1H), 7.44 (t, *J* = 7.8 Hz, 2H), 7.30 (t, *J* = 7.6 Hz, 2H), 7.23-7.19 (m, 3H), 3.33 (ddt, *J* = 10.1, 7.4, 5.3 Hz, 1H), 3.30-3.21 (m, 2H), 2.27 (td, *J* = 7.2, 2.2 Hz, 2H), 1.79 (dddd, *J* = 13.4, 10.4, 6.1, 4.5 Hz, 1H), 1.70-1.60 (m, 3H), 1.36 (dddd, *J* = 13.4, 9.6, 6.8, 3.7 Hz, 1H), 1.29 (dtd, *J* = 12.2, 4.8, 2.2 Hz, 1H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 198.99, 144.32, 137.21, 133.22, 128.78, 128.73, 128.17, 127.63, 126.73, 119.80, 45.99, 40.90, 35.25, 26.68, 25.34, 17.08;

HRMS (ESI) m/z: calculated for $C_{15}H_{20}NO$ $[M+H]^+$: 230.1539, found: 230.1535.

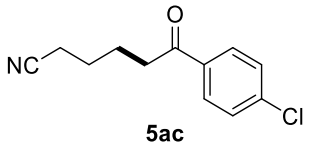


5ab

6-Oxo-6-(*p*-tolyl)hexanenitrile (5ab): 30.5 mg, 74% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): 7.84 (d, *J* = 8.3 Hz, 2H), 7.26 (d, *J* = 8.3 Hz, 2H), 3.00 (t, *J* = 7.0 Hz, 2H), 2.41 (s, 3H), 2.39 (d, *J* = 7.1 Hz, 2H), 1.91-1.86 (m, 2H), 1.78-1.73 (m, 2H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 198.87, 144.14, 134.36, 129.46, 128.22, 119.64, 37.33, 25.15, 23.30, 21.73, 17.29; Data in accordance with literature.[14]

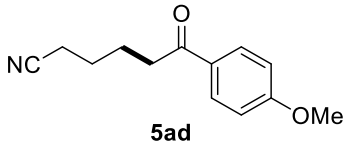


5ac

6-(4-Chlorophenyl)-6-oxohexanenitrile (5ac): 36.4 mg, 82% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.8-7.86 (m, 2H), 7.43-7.41 (m, 2H), 3.00 (t, *J* = 7.0 Hz, 2H), 2.39 (t, *J* = 7.1 Hz, 2H), 1.91-1.86 (m, 2H), 1.77-1.72 (m, 2H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 197.90, 139.73, 135.09, 129.49, 129.07, 119.56, 37.43, 25.03, 23.06, 17.27; Data in accordance with literature.[14]

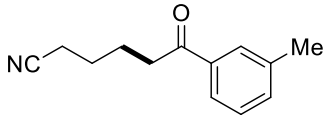


5ad

6-(4-Methoxyphenyl)-6-oxohexanenitrile (5ad): 34.3 mg, 82% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.93-7.91 (m, 2H), 6.94-6.92 (m, 2H), 3.86 (s, 3H), 2.97 (t, *J* = 7.0 Hz, 2H), 2.38 (t, *J* = 7.1 Hz, 2H), 1.90-1.85 (m, 2H), 1.77-1.72 (m, 2H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 197.77, 163.66, 130.35, 129.89, 119.65, 113.88, 55.57, 37.07, 25.14, 23.38, 17.25; Data in accordance with literature.[14]

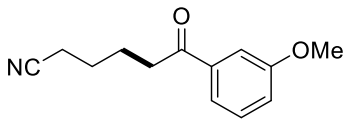


5ae

6-Oxo-6-(*m*-tolyl)hexanenitrile (5ae): 29.7 mg, 74% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.75-7.73 (m, 2H), 7.39-7.33 (m, 2H), 3.02 (t, *J* = 7.0 Hz, 2H), 2.41 (s, 3H), 2.39 (d, *J* = 7.1 Hz, 2H), 1.92-1.87 (m, 2H), 1.78-1.73 (m, 2H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 199.44, 138.60, 136.87, 134.09, 128.66, 128.61, 125.32, 119.63, 37.51, 25.13, 23.25, 21.46, 17.29; Data in accordance with literature.[14]

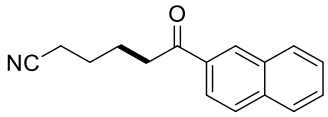


5af

6-(3-Methoxyphenyl)-6-oxohexanenitrile (5af): 34.7 mg, 80% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.52 (dt, *J* = 7.6, 1.2 Hz, 1H), 7.46 (dd, *J* = 2.7, 1.6 Hz, 1H), 7.37 (t, *J* = 7.9 Hz, 1H), 7.11 (ddd, *J* = 8.2, 2.7, 0.9 Hz, 1H), 3.85 (s, 3H), 3.01 (t, *J* = 7.0 Hz, 2H), 2.40 (t, *J* = 7.1 Hz, 2H), 1.94-1.85 (m, 2H), 1.79-1.71 (m, 2H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 199.03, 160.00, 138.18, 129.77, 120.69, 119.69, 119.61, 112.42, 55.55, 37.58, 25.10, 23.25, 17.28; Data in accordance with literature.[16]

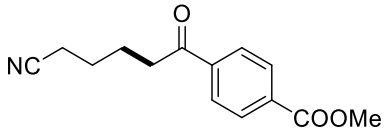


5ag

6-(Naphthalen-2-yl)-6-oxohexanenitrile (5ag): 36.7 mg, 64% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.46 (s, 1H), 8.02 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.97 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.91-7.87 (m, 2H), 7.61 (ddd, *J* = 8.2, 6.8, 1.3 Hz, 1H), 7.56 (ddd, *J* = 8.2, 6.8, 1.3 Hz, 1H), 3.17 (t, *J* = 7.0 Hz, 2H), 2.43 (t, *J* = 7.2 Hz, 2H), 1.99-1.94 (m, 2H), 1.83-1.78 (m, 2H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 199.15, 135.76, 134.16, 132.63, 129.79, 129.68, 128.68, 127.92, 126.99, 123.84, 119.65, 37.54, 25.18, 23.37, 17.33 *(one carbon signal is overlapped)*; Data in accordance with literature.[14]

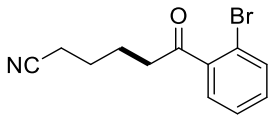


5ah

Methyl 4-(5-cyanopentanoyl)benzoate (5ah): 35.3 mg, 72% yield as a pale yellow solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.12-8.11 (m, 2H), 8.00-7.98 (m, 2H), 3.94 (s, 3H), 3.06 (t, *J* = 7.2 Hz, 2H), 2.41 (t, *J* = 7.2 Hz, 2H), 1.94-1.89 (m, 2H), 1.79-1.74 (m, 2H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 198.66, 166.29, 139.97, 134.13, 130.03, 128.01, 119.55, 52.60, 37.87, 25.06, 23.03, 17.33; Data in accordance with literature.[16]

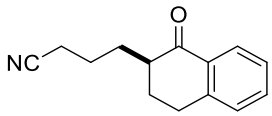


5ai

6-(2-Bromophenyl)-6-oxohexanenitrile (5ai): 27.7 mg, 52% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.60-7.59 (m, 1H), 7.38-7.34 (m, 2H), 7.31-7.28 (m, 1H), 2.97 (t, *J* = 7.2 Hz, 2H), 2.39 (t, *J* = 7.2 Hz, 2H), 1.90-1.85 (m, 2H), 1.79-1.74 (m, 2H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 203.36, 141.63, 133.81, 131.77, 128.34, 127.64, 119.52, 118.62, 41.63, 24.91, 23.08, 17.25; Data in accordance with literature.[14]



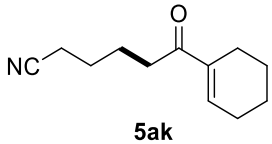
5aj

4-(1-oxo-1,2,3,4-tetrahydronaphthalen-2-yl)butanenitrile (5aj): 31.1 mg, 68% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.01 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.47 (td, *J* = 7.5, 1.5 Hz, 1H), 7.33-7.28 (m, 1H), 7.24 (d, *J* = 7.6 Hz, 1H), 3.05-3.00 (m, 2H), 2.52 (dtd, *J* = 10.5, 6.2, 4.4 Hz, 1H), 2.45-2.37 (m, 2H), 2.23 (dq, *J* = 13.5, 4.6 Hz, 1H), 2.04 (tdd, *J* = 11.2, 8.4, 5.5 Hz, 1H), 1.93 (dddd, *J* = 13.2, 11.6, 9.3, 6.0 Hz, 1H), 1.81 (ddtd, *J* = 12.4, 10.4, 7.1, 5.1 Hz, 2H), 1.74-1.65 (m, 1H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 199.59, 143.91, 133.53, 132.44, 128.88, 127.57, 126.84, 119.72, 46.99, 29.19, 28.89, 28.72, 23.31, 17.56;

HRMS (ESI) m/z: calculated for $C_{14}H_{16}NO$ $[M+H]^+$: 214.1226, found: 214.1224.



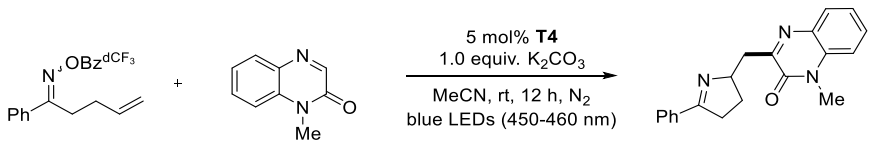
5ak

6-(Cyclohex-1-en-1-yl)-6-oxohexanenitrile (5ak): 22.9 mg, 60% yield as a white solid.

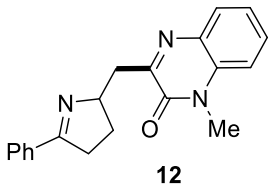
^{1}H NMR (600 MHz, $CDCl_3$): δ 6.87 (tt, *J* = 3.7, 1.6 Hz, 1H), 2.66 (t, *J* = 7.0 Hz, 2H), 2.34 (t, *J* = 7.1 Hz, 2H), 2.26-2.14 (m, 4H), 1.73 (dtd, *J* = 9.2, 7.6, 7.0, 5.6 Hz, 2H), 1.69-1.63 (m, 2H), 1.63-1.53 (m, 4H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 200.28, 140.16, 139.17, 119.65, 35.78, 26.11, 25.13, 23.58, 23.14, 21.96, 21.56, 17.17; Data in accordance with literature.[6b]

6.3. Synthesis Procedure and Characterization of Product 12, 14 and 16



An oven-dried Schlenk tube equipped with a stirring bar was charged with **1a** (0.2 mmol, 83.07 mg, 1.0 equiv.), **11** (0.3 mmol, 48.05 mg, 1.5 equiv.), **T4** (0.01 mmol, 5.0 mg, 5 mol%) and K_2CO_3 (0.2 mmol, 27.60 mg, 1.0 equiv.). After refilling with N_2 repeated three times, MeCN (2.0 mL) was added through syringe. The mixture was stirred at room temperature for 12 h in front of a 20 W blue LEDs bulb. Saturated $NaHCO_3$ aqueous solution and EtOAc were added and the mixture was stirred for 10 min. The layers were separated and the aqueous layer was extracted with EtOAc. The combined organic layers were then washed with brine, dried over Na_2SO_4 and concentrated in vacuo. The residue was purified by column chromatography on silica gel to afford the corresponding product.



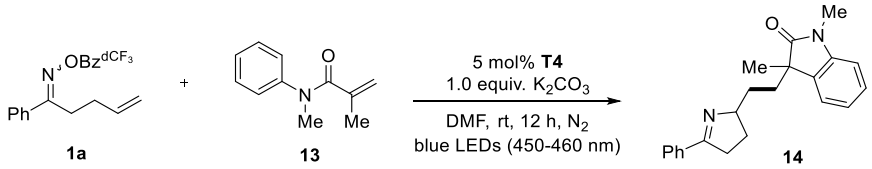
12

1-Methyl-3-((5-phenyl-3,4-dihydro-2*H*-pyrrol-2-yl)methyl)quinoxalin-2(1*H*)-one (12): 58.3 mg, 92% yield as a white solid.

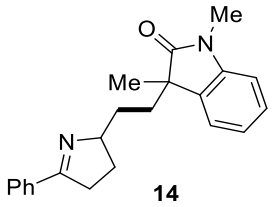
^{1}H NMR (600 MHz, $CDCl_3$): δ 7.86-7.82 (m, 3H), 7.52 (t, *J* = 7.8 Hz, 1H), 7.41-7.36 (m, 3H), 7.33 (t, *J* = 7.8 Hz, 1H), 7.29 (d, *J* = 7.8 Hz, 1H), 4.97-4.92 (m, 1H), 3.70 (s, 3H), 3.52 (dd, *J* = 15.0, 6.0 Hz, 1H), 3.10 (dd, *J* = 11.4, 8.4 Hz, 1H), 3.09-3.04 (m, 1H), 2.96-2.91 (m, 1H), 2.32 (dddd, *J* = 12.7, 9.6, 7.7, 4.9 Hz, 1H), 1.78 (ddt, *J* = 13.3, 9.7, 7.0 Hz, 1H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 172.74, 159.11, 155.16, 134.82, 133.31, 132.93, 130.39, 129.96, 129.78, 128.42, 127.88, 123.58, 113.66, 70.95, 41.13, 35.14, 29.17, 29.00;

HRMS (ESI) m/z: calculated for $C_{20}H_{20}N_3O$ $[M+H]^+$: 318.1601, found: 318.1600.



An oven-dried Schlenk tube equipped with a stirring bar was charged with **1a** (0.2 mmol, 83.07 mg, 1.0 equiv.), **13** (0.4 mmol, 70.10 mg, 2.0 equiv.), **T4** (0.01 mmol, 5.0 mg, 5 mol%) and K_2CO_3 (0.2 mmol, 27.60 mg, 1.0 equiv.). After refilling with N_2 repeated three times, DMF (2.0 mL) was added through syringe. The mixture was stirred at room temperature for 12 h in front of a 20 W blue LEDs bulb. Saturated $NaHCO_3$ aqueous solution and EtOAc were added and the mixture was stirred for 10 min. The layers were separated and the aqueous layer was extracted with EtOAc. The combined organic layers were then washed with brine, dried over Na_2SO_4 and concentrated in vacuo. The residue was purified by column chromatography on silica gel to afford the corresponding product.



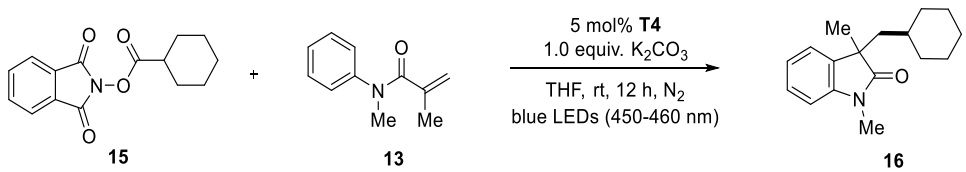
14

1,3-Dimethyl-3-(2-(5-phenyl-3,4-dihydro-2*H*-pyrrol-2-yl)ethyl)indolin-2-one (14): 43.9 mg (d.r. = 1:1), 66% yield as a white solid.

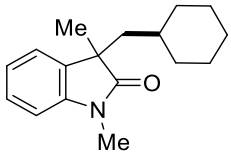
^{1}H NMR (600 MHz, $CDCl_3$): δ 7.78-7.74 (m, 4H), 7.37 (dddd, *J* = 11.2, 8.8, 6.7, 3.9 Hz, 6H), 7.24 (ddd, *J* = 7.6, 6.1, 1.3 Hz, 2H), 7.20 (ddd, *J* = 7.0, 5.6, 1.4 Hz, 2H), 7.05 (tdd, *J* = 7.5, 4.9, 1.0 Hz, 2H), 6.82 (t, *J* = 7.2 Hz, 2H), 4.10-3.94 (m, 2H), 3.21 (s, 3H), 3.19 (s, 3H), 2.95 (dddd, *J* = 16.9, 10.2, 4.8, 2.2 Hz, 2H), 2.87-2.75 (m, 2H), 2.19-1.98 (m, 7H), 1.84 (td, *J* = 13.1, 4.1 Hz, 1H), 1.60 (ddd, *J* = 13.3, 11.1, 6.4 Hz, 1H), 1.54-1.45 (m, 2H), 1.39 (s, 3H), 1.38 (s, 3H), 1.14-1.05 (m, 2H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 180.83, 180.76, 172.24, 143.47, 143.42, 134.66, 134.15, 134.02, 130.43, 128.46, 127.80, 127.77, 127.72, 122.73, 122.71, 122.67, 122.60, 108.08, 108.06, 73.33, 73.02, 48.49, 48.31, 35.96, 35.32, 35.12, 35.00, 31.79, 31.35, 28.54, 28.38, 26.27, 26.23, 24.11, 23.83;

HRMS (ESI) m/z: calculated for $C_{22}H_{25}N_2O$ $[M+H]^+$: 333.1961, found: 333.1958.



An oven-dried Schlenk tube equipped with a stirring bar was charged with **15** (0.4 mmol, 109.32 mg, 2.0 equiv.), **13** (0.2 mmol, 35.05 mg, 1.0 equiv.), **T4** (0.01 mmol, 5.0 mg, 5 mol%) and K_2CO_3 (0.2 mmol, 27.60 mg, 1.0 equiv.). After refilling with N_2 repeated three times, THF (2.0 mL) was added through syringe. The mixture was stirred at room temperature for 12 h in front of a 20 W blue LEDs bulb. Saturated $NaHCO_3$ aqueous solution and EtOAc were added and the mixture was stirred for 10 min. The layers were separated and the aqueous layer was extracted with EtOAc. The combined organic layers were then washed with brine, dried over Na_2SO_4 and concentrated in vacuo. The residue was purified by column chromatography on silica gel to afford the corresponding product.



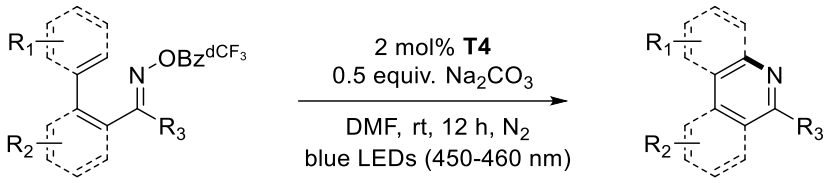
16

3-(Cyclohexylmethyl)-1,3-dimethylindolin-2-one (16): 18.5 mg, 36% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.05-7.99 (m, 2H), 7.87-7.81 (m, 2H), 7.57-7.52 (m, 1H), 7.45 (dd, *J* = 8.4, 7.1 Hz, 2H), 7.42-7.37 (m, 3H), 4.27 (dqd, *J* = 9.9, 7.9, 2.0 Hz, 1H), 3.33 (ddd, *J* = 17.0, 9.3, 5.5 Hz, 1H), 3.23 (ddd, *J* = 16.9, 9.2, 5.9 Hz, 1H), 3.04 (dddd, *J* = 16.8, 10.0, 4.6, 2.1 Hz, 1H), 2.90 (dddd, *J* = 17.0, 9.7, 7.8, 1.9 Hz, 1H), 2.27 (dddd, *J* = 12.5, 9.8, 7.7, 4.6 Hz, 1H), 2.14 (ddt, *J* = 13.7, 9.4, 5.8 Hz, 1H), 2.01 (dddd, *J* = 13.8, 9.4, 8.3, 5.5 Hz, 1H), 1.65 (dddd, *J* = 12.8, 10.0, 7.8, 6.8 Hz, 1H);

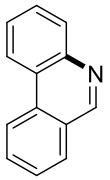
^{13}C NMR (151 MHz, $CDCl_3$): δ 200.47, 172.47, 137.14, 134.73, 132.97, 130.44, 128.61, 128.47, 128.23, 127.74, 72.59, 36.24, 35.12, 31.41, 28.97;Data in accordance with literature.[17]

6.4. Synthesis Procedure and Characterization of Phenanthridine, Quinoline and Pyridine 18



17 **18**

An oven-dried Schlenk tube equipped with a stirring bar was charged with **17** (0.2 mmol, 1.0 equiv.), **T4** (0.004 mmol, 2.0 mg, 2 mol%) and Na_2CO_3 (0.1 mmol, 10.60 mg, 0.5 equiv.). After refilling with N_2 repeated three times, DMF (2.0 mL) was added through syringe. The mixture was stirred at room temperature for 12 h in front of a 20 W blue LEDs bulb. Saturated $NaHCO_3$ aqueous solution and EtOAc were added and the mixture was stirred for 10 min. The layers were separated and the aqueous layer was extracted with EtOAc. The combined organic layers were then washed with brine, dried over Na_2SO_4 and concentrated in vacuo. The residue was purified by column chromatography on silica gel to afford the corresponding product.

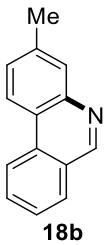


18a

Phenanthridine (18a): 30.4 mg, 85% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 9.28 (s, 1H), 8.59 (d, *J* = 8.4 Hz, 1H), 8.56 (dd, *J* = 8.4, 1.2 Hz, 1H), 8.20 (dd, *J* = 8.4, 1.2 Hz, 1H), 8.03 (dd, J = 7.8, 1.2 Hz, 1H), 7.86-7.83 (m, 1H), 7.76-7.73 (m, 1H), 7.71-7.66 (m, 2H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 153.68, 144.56, 132.67, 131.13, 130.23, 128.87, 128.81, 127.60, 127.20, 126.49, 124.22, 122.33, 121.98; Data in accordance with literature.[7]

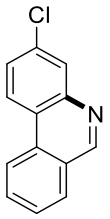


18b

3-Methylphenanthridine (18b): 34.2 mg, 88% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 9.25 (s, 1H), 8.53 (d, *J* = 8.4 Hz, 1H), 8.43 (d, *J* = 8.4 Hz, 1H), 8.02-7.96 (m, 2H), 7.81 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 7.67-7.62 (m, 1H), 7.49 (dd, *J* = 8.4, 1.8 Hz, 1H), 2.59 (s, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 153.65, 144.72, 138.95, 132.72, 131.00, 129.76, 128.90, 128.82, 127.08, 126.21, 122.08, 121.85, 121.76, 21.66; Data in accordance with literature.[7]

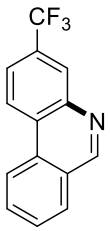


18c

3-Chlorophenanthridine (18c): 37.1 mg, 87% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 9.24 (s, 1H), 8.48 (d, *J* = 8.4 Hz, 1H), 8.42 (d, *J* = 8.4 Hz, 1H), 8.14 (d, *J* = 2.4 Hz, 1H), 8.01 (d, *J* = 7.8 Hz, 1H), 7.84 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 7.70 (t, *J* = 7.8 Hz, 1H), 7.59 (dd, *J* = 8.4, 2.4 Hz, 1H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 154.77, 145.21, 134.39, 132.18, 131.52, 129.43, 129.00, 127.89, 127.71, 126.35, 123.65, 122.68, 121.86; Data in accordance with literature.[7]



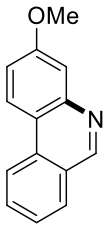
18d

3-(Trifluoromethyl)phenanthridine (18d): 42.0 mg, 85% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 9.32 (s, 1H), 8.63 (d, *J* = 8.8 Hz, 1H), 8.61 (d, *J* = 8.4 Hz, 1H), 8.47 (s, 1H), 8.10 (d, *J* = 8.0 Hz, 1H), 7.96-7.91 (m, 1H), 7.87 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.83-7.77 (m, 1H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 155.01, 143.89, 131.82, 131.70, 130.60 (q, *J* = 33.2 Hz), 129.08, 128.82, 127.78 (q, *J* = 4.6 Hz), 127.01, 126.54, 124.20 (q, *J* = 271.8 Hz), 123.39, 123.06 (q, *J* = 3.0 Hz), 122.33;

^{19}F NMR (565 MHz, $CDCl_3$): δ -62.22; Data in accordance with literature.[7]

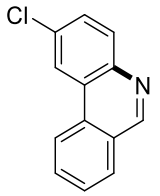


18e

3-Methoxyphenanthridine (18e): 37.8 mg, 90% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 9.23 (s, 1H), 8.47 (d, *J* = 8.4 Hz, 1H), 8.42 (d, *J* = 8.8 Hz, 1H), 8.01 (d, *J* = 8.0 Hz, 1H), 7.86-7.78 (m, 1H), 7.67-7.58 (m, 2H), 7.32 (dd, *J* = 8.8, 2.8 Hz, 1H), 3.98 (s, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 160.18, 154.06, 146.20, 132.86, 131.15, 128.88, 126.48, 125.66, 123.48, 121.45, 118.23, 118.17, 110.08, 55.64; Data in accordance with literature.[7]

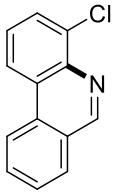


18f1

2-Chlorophenanthridine (18f1): 9.7 mg (of all 38.9 mg, 91% yield) as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 9.27 (s, 1H), 8.55-8.51 (m, 2H), 8.12 (d, *J* = 8.4 Hz, 1H), 8.06 (d, *J* = 7.8 Hz, 1H), 7.92-7.85 (m, 1H), 7.78-7.73 (m, 1H), 7.69 (dd, *J* = 8.4, 2.4 Hz, 1H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 153.90, 143.02, 133.20, 131.75, 131.73, 131.48, 129.38, 129.00, 128.35, 126.65, 125.37, 122.08, 122.05; Data in accordance with literature.[18]

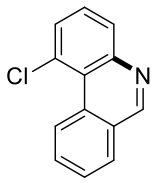


18f2

4-Chlorophenanthridine (18f2): 29.2 mg (of all 38.9 mg, 91% yield) as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 9.37 (s, 1H), 8.56 (d, *J* = 8.4 Hz, 1H), 8.47 (d, *J* = 8.4 Hz, 1H), 8.07 (d, *J* = 7.8 Hz, 1H), 7.90-7.81 (m, 2H), 7.73 (t, *J* = 7.8 Hz, 1H), 7.57 (t, *J* = 7.8 Hz, 1H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 154.22, 140.85, 134.45, 132.40, 131.62, 129.23, 129.10, 128.27, 127.11, 126.48, 125.97, 122.26, 121.29; Data in accordance with literature.[19]



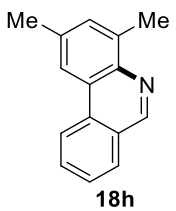
18g

1-Chlorophenanthridine (18g): 23.9 mg, 56% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 9.86 (d, J = 8.6 Hz, 1H), 9.25 (s, 1H), 8.14 (dd, J = 8.1, 1.5 Hz, 1H), 8.06 (dd, J = 7.8, 1.6 Hz, 1H), 7.88 (ddd, J = 8.7, 7.0, 1.6 Hz, 1H), 7.79-7.72 (m, 2H), 7.62 (t, J = 7.9 Hz, 1H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 154.70, 146.87, 131.98, 131.18, 130.90, 130.86, 130.11, 129.13, 128.10, 127.99, 127.51, 126.49, 122.09;

HRMS (ESI) m/z: calculated for $C_{13}H_9ClN$ $[M+H]^+$: 214.0418, found: 214.0416.

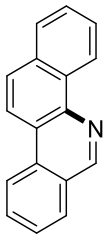


18h

2,4-Dimethylphenanthridine (18h): 35.2 mg, 85% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 9.24 (s, 1H), 8.57 (d, *J* = 8.4 Hz, 1H), 8.20 (s, 1H), 8.02 (d, *J* = 7.8 Hz, 1H), 7.83-7.78 (m, 1H), 7.66 (t, *J* = 7.8 Hz, 1H), 7.44 (s, 1H), 2.85 (s, 3H), 2.58 (s, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 151.38, 141.68, 137.44, 136.53, 132.71, 131.40, 130.65, 128.72, 127.21, 126.35, 123.96, 122.16, 119.80, 22.01, 18.70; Data in accordance with literature.[19]

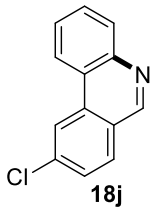


18i

Benzo[*c*]phenanthridine (18i): 35.2 mg, 85% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 9.47 (s, 1H), 9.42 (d, *J* = 8.4 Hz, 1H), 8.63 (d, *J* = 8.4 Hz, 1H), 8.51 (d, *J* = 8.4 Hz, 1H), 8.11 (d, *J* = 7.8 Hz, 1H), 8.01 (d, *J* = 9.0 Hz, 1H), 7.98 (d, *J* = 7.8 Hz, 1H), 7.86 (t, *J* = 7.8 Hz, 2H), 7.70 (t, *J* = 7.8 Hz, 2H), 7.70 (t, *J* = 7.8 Hz, 2H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 152.07, 141.59, 133.38, 132.92, 132.17, 130.89, 128.78, 127.94, 127.79, 127.48, 127.22, 127.11, 126.99, 124.87, 122.29, 121.16, 120.00; Data in accordance with literature.[7]

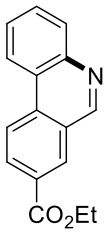


18j

9-Chlorophenanthridine (18j): 34.6 mg, 81% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 9.21 (s, 1H), 8.51 (s, 1H), 8.44 (d, *J* = 8.4 Hz, 1H), 8.17 (d, *J* = 8.4 Hz, 1H), 7.94 (d, *J* = 8.4 Hz, 1H), 7.79-7.73 (m, 1H), 7.70-7.65 (m, 1H), 7.65-7.60 (m, 1H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 152.79, 144.74, 137.57, 133.80, 130.32, 129.49, 128.31, 127.51, 124.66, 123.09, 122.33, 121.81 *(one carbon signal is overlapped)*; Data in accordance with literature.[18]



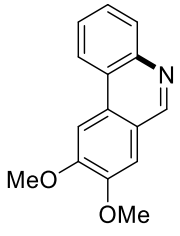
18k

Ethyl phenanthridine-8-carboxylate (18k): 46.7 mg, 93% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 9.32 (s, 1H), 8.71 (s, 1H), 8.58 (d, *J* = 8.4 Hz, 1H), 8.54 (d, *J* = 8.4 Hz, 1H), 8.42 (d, *J* = 8.4 Hz, 1H), 8.19 (d, *J* = 8.4 Hz, 1H), 7.78 (t, *J* = 7.8 Hz, 1H), 7.68 (t, *J* = 7.8 Hz, 1H), 4.47 (q, *J* = 7.2 Hz, 2H), 1.47 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 165.92, 153.81, 145.21, 135.47, 131.04, 130.92, 130.31, 129.91, 129.45, 127.60, 125.80, 123.57, 122.86, 122.25, 61.58, 14.48;

HRMS (ESI) m/z: calculated for $C_{16}H_{14}NO_2$ $[M+H]^+$: 252.1019, found: 252.1017.

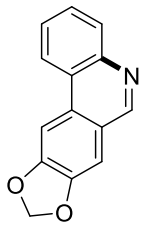


18l

8,9-Dimethoxyphenanthridine (18l): 41.2 mg, 86% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 9.12 (s, 1H), 8.40 (d, *J* = 8.4 Hz, 1H), 8.14 (d, *J* = 8.4 Hz, 1H), 7.82 (s, 1H), 7.67 (t, *J* = 7.8 Hz, 1H), 7.61 (t, *J* = 7.8 Hz, 1H), 7.31 (s, 1H), 4.11 (s, 3H), 4.04 (s, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 152.98, 151.83, 150.03, 144.06, 130.22, 128.24, 127.88, 126.68, 123.91, 121.88, 121.81, 107.84, 101.86, 56.25, 56.19; Data in accordance with literature.[7]

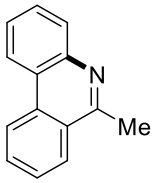


18m

[1,3]Dioxolo[4,5-*j*]phenanthridine (18m): 40.6 mg, 91% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 9.05 (s, 1H), 8.32 (d, *J* = 8.4 Hz, 1H), 8.13 (d, *J* = 8.4 Hz, 1H), 7.84 (s, 1H), 7.67 (t, *J* = 7.8 Hz, 1H), 7.60 (t, *J* = 7.8 Hz, 1H), 7.27 (s, 1H), 6.12 (s, 2H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 151.89, 151.52, 148.26, 144.22, 130.28, 130.15, 128.07, 126.75, 124.36, 123.15, 122.08, 105.53, 102.01, 99.98; Data in accordance with literature.[7]

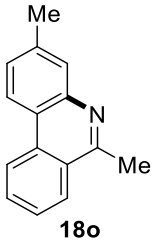


18n

6-Methylphenanthridine (18n): 37.5 mg, 97% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.58 (d, *J* = 7.8 Hz, 1H), 8.50 (d, *J* = 8.4 Hz, 1H), 8.18 (d, *J* = 7.8 Hz, 1H), 8.10 (d, *J* = 8.4 Hz, 1H), 7.82-7.29 (m, 1H), 7.71-7.65 (m, 2H), 7.61-7.59 (m, 1H), 3.03 (s, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 158.96, 143.77, 132.64, 130.57, 129.42, 128.73, 127.39, 126.62, 126.42, 125.98, 123.87, 122.39, 122.04, 23.45; Data in accordance with literature.[7]

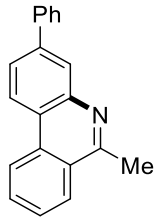


18o

3,6-Dimethylphenanthridine (18o): 39.4 mg, 95% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.53 (d, *J* = 8.4 Hz, 1H), 8.36 (d, *J* = 8.4 Hz, 1H), 8.15 (d, *J* = 8.4 Hz, 1H), 7.89 (s, 1H), 7.80-7.74 (m, 1H), 7.64-7.57 (m, 1H), 7.41 (dd, *J* = 8.4, 1.8 Hz, 1H), 3.01 (s, 3H), 2.57 (s, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 158.89, 143.89, 138.79, 132.69, 130.45, 129.05, 128.08, 126.86, 126.57, 125.67, 122.18, 121.81, 121.49, 23.42, 21.64; Data in accordance with literature.[20]

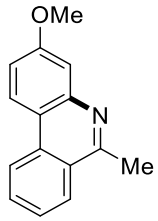


18p

6-Methyl-3-phenylphenanthridine (18p): 52.8 mg, 98% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.56 (d, *J* = 8.4 Hz, 1H), 8.52 (d, *J* = 8.4 Hz, 1H), 8.36 (d, *J* = 1.8 Hz, 1H), 8.18 (d, *J* = 7.8 Hz, 1H), 7.85 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.82-7.77 (m, 3H), 7.68-7.63 (m, 1H), 7.51 (t, *J* = 7.8 Hz, 2H), 7.43-7.38 (m, 1H), 3.04 (s, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 159.41, 144.12, 141.30, 140.42, 132.45, 130.63, 129.05, 127.74, 127.39, 127.34, 127.30, 126.65, 125.95, 125.47, 122.91, 122.58, 122.40, 23.50; Data in accordance with literature.[7]

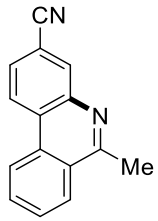


18q

3-Methoxy-6-methylphenanthridine (18q): 44.2 mg, 99% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.46 (d, *J* = 8.4 Hz, 1H), 8.36 (d, *J* = 9.0 Hz, 1H), 8.14 (d, *J* = 8.4 Hz, 1H), 7.78-7.73 (m, 1H), 7.58 (t, *J* = 7.8 Hz, 1H), 7.50 (s, 1H), 7.22 (d, *J* = 9.0 Hz, 1H), 3.96 (s, 3H), 3.00 (s, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 160.18, 159.47, 145.34, 132.85, 130.61, 126.63, 126.26, 125.05, 123.25, 121.88, 117.84, 117.38, 109.36, 55.62, 23.41; Data in accordance with literature.[7]

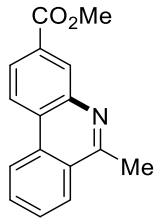


18r

6-Methylphenanthridine-3-carbonitrile (18r): 43.0 mg, 98% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.52 (d, *J* = 8.4 Hz, 1H), 8.48 (d, *J* = 8.4 Hz, 1H), 8.30 (d, *J* = 1.8 Hz, 1H), 8.20 (d, *J* = 7.8 Hz, 1H), 7.91-7.85 (m, 1H), 7.80-7.74 (m, 1H), 7.70 (dd, *J* = 8.4, 1.8 Hz, 1H), 3.00 (s, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 161.21, 142.96, 134.34, 131.34, 131.32, 129.20, 127.87, 127.07, 126.85, 126.64, 123.29, 122.84, 118.86, 111.78, 23.45; Data in accordance with literature.[7]

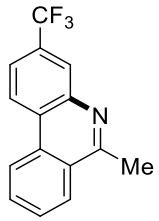


18s

Methyl 6-methylphenanthridine-3-carboxylate (18s): 46.9 mg, 93% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.44 (d, *J* = 8.4 Hz, 1H), 8.35 (d, *J* = 9.0 Hz, 1H), 8.12 (d, *J* = 8.4 Hz, 1H), 7.77-7.72 (m, 1H), 7.59-7.54 (m, 1H), 7.49 (d, *J* = 2.8 Hz, 1H), 7.21 (dd, *J* = 9.0, 2.8 Hz, 1H), 3.95 (s, 3H), 2.99 (s, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 160.16, 159.46, 145.28, 132.84, 130.61, 126.62, 126.25, 125.02, 123.24, 121.87, 117.83, 117.36, 109.31, 55.61, 23.35; Data in accordance with literature.[20]



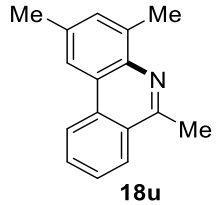
18t

6-Methyl-3-(trifluoromethyl)phenanthridine (18t): 51.2 mg, 98% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.52 (t, *J* = 9.0 Hz, 2H), 8.34 (s, 1H), 8.17 (d, *J* = 8.4 Hz, 1H), 7.86-7.81 (m, 1H), 7.77-7.69 (m, 2H), 3.00 (s, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 160.58, 143.06, 131.69, 131.07, 130.42 (q, *J* = 33.4 Hz), 128.57, 126.98 (q, *J* = 4.5 Hz), 126.76, 126.49, 126.14, 124.29 (q, *J* = 271.8 Hz), 123.01, 122.70, 122.21 (q, *J* = 3.0 Hz), 23.46;

^{19}F NMR (565 MHz, $CDCl_3$): δ -62.23; Data in accordance with literature.[20]

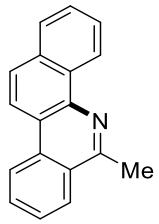


18u

2,4,6-Trimethylphenanthridine (18u): 38.5 mg, 87% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.59 (d, *J* = 8.4 Hz, 1H), 8.17 (d, *J* = 7.8 Hz, 1H), 8.16 (s, 1H), 7.77 (t, *J* = 7.8 Hz, 1H), 7.64 (t, *J* = 7.8 Hz, 1H), 7.41 (s, 1H), 3.04 (s, 3H), 2.86 (s, 3H), 2.57 (s, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 156.37, 140.91, 136.92, 135.43, 132.74, 131.18, 129.95, 126.91, 126.45, 125.83, 123.51, 122.59, 119.50, 23.74, 21.98, 18.32; Data in accordance with literature.[19]

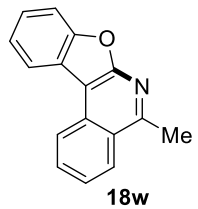


18v

6-Methylbenzo[*c*]phenanthridine (18v): 47.9 mg, 98% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 9.49 (d, *J* = 8.4 Hz, 1H), 8.63 (d, *J* = 8.4 Hz, 1H), 8.47 (d, *J* = 9.0 Hz, 1H), 8.25 (d, *J* = 7.8 Hz, 1H), 7.97 (d, *J* = 7.8 Hz, 1H), 7.94 (d, *J* = 9.0 Hz, 1H), 7.82 (t, *J* = 7.8 Hz, 1H), 7.77 (t, *J* = 7.8 Hz, 1H), 7.72-7.64 (m, 2H), 3.17 (s, 3H);

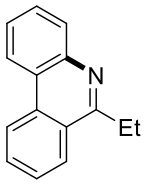
^{13}C NMR (151 MHz, $CDCl_3$): δ 157.72, 140.55, 133.40, 132.91, 131.95, 130.25, 127.67, 127.25, 126.96, 126.92, 126.81, 126.56, 126.22, 124.93, 122.74, 120.40, 119.93, 23.71; Data in accordance with literature.[7]



18w

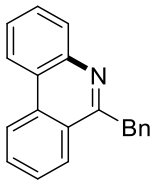
6-Methylbenzo[*c*]phenanthridine (18w): 38.3 mg, 82% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.46 (d, *J* = 8.4 Hz, 1H), 8.25 (d, *J* = 8.4 Hz, 1H), 8.22 (d, *J* = 7.8 Hz, 1H), 7.83 (td, *J* = 7.8, 1.2 Hz, 1H), 7.70 (d, *J* = 7.8 Hz, 1H), 7.58 (td, *J* = 7.8, 1.2 Hz, 1H), 7.49 (td, *J* = 7.8, 1.2 Hz, 1H), 7.44 (td, *J* = 7.8, 1.2 Hz, 1H), 3.08 (s, 3H);
^{13}C NMR (151 MHz, $CDCl_3$): δ 159.14, 158.17, 153.71, 133.02, 131.09, 127.33, 126.33, 125.30, 125.17, 124.02, 123.61, 123.50, 121.89, 112.31, 106.67, 22.96;
HRMS (ESI) m/z: calculated for $C_{16}H_{12}NO$ $[M+H]^+$: 234.0913, found: 234.0914.



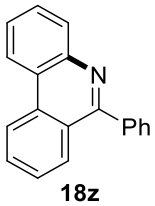
18x

6-Ethylphenanthridine (18x): 55.1 mg, 95% yield as a white solid.
^{1}H NMR (600 MHz, $CDCl_3$): δ 8.61 (d, *J* = 8.4 Hz, 1H), 8.52 (d, *J* = 8.4 Hz, 1H), 8.24 (d, *J* = 8.4 Hz, 1H), 8.14 (d, *J* = 8.4 Hz, 1H), 7.80 (t, *J* = 7.8 Hz, 1H), 7.71 (t, *J* = 7.8 Hz, 1H), 7.67 (t, *J* = 7.8 Hz, 1H), 7.60 (t, *J* = 7.8 Hz, 1H), 3.40 (q, *J* = 7.8 Hz, 2H), 1.52 (t, *J* = 7.8 Hz, 3H);
^{13}C NMR (151 MHz, $CDCl_3$): δ 163.30, 143.89, 133.02, 130.35, 129.67, 128.66, 127.32, 126.37, 126.30, 125.12, 123.77, 122.58, 122.01, 29.47, 13.65; Data in accordance with literature.[7]



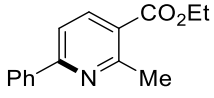
18y

6-Benzylphenanthridine (18y): 51.2 mg, 95% yield as a white solid.
^{1}H NMR (600 MHz, $CDCl_3$): δ 8.57 (d, *J* = 8.4 Hz, 1H), 8.52 (d, *J* = 8.4 Hz, 1H), 8.20 (d, *J* = 7.8 Hz, 1H), 8.16 (d, *J* = 8.4 Hz, 1H), 7.74-7.71 (m, 2H), 7.63 (t, *J* = 7.8 Hz, 1H), 7.54 (t, *J* = 7.8 Hz, 1H), 7.30 (d, *J* = 7.8 Hz, 2H), 7.22 (t, *J* = 7.8 Hz, 2H), 7.14 (t, *J* = 7.8 Hz, 1H), 4.74 (s, 2H);
^{13}C NMR (151 MHz, $CDCl_3$): δ 160.27, 143.79, 139.20, 133.36, 130.48, 129.89, 128.80, 128.65, 127.44, 127.16, 126.80, 126.44, 125.46, 124.04, 122.51, 122.09, 43.12 *(one carbon signal is overlapped)*; Data in accordance with literature.[7]



18z

6-Phenylphenanthridine (18z): 50.2 mg, 98% yield as a white solid.
^{1}H NMR (600 MHz, $CDCl_3$): δ 8.71 (d, *J* = 8.4 Hz, 1H), 8.63 (d, *J* = 8.4 Hz, 1H), 8.26 (d, *J* = 7.8 Hz, 1H), 8.11 (d, *J* = 8.4 Hz, 1H), 7.89-7.83 (m, 1H), 7.80-7.73 (m, 3H), 7.70 (td, *J* = 7.8, 1.2 Hz, 1H), 7.62 (t, *J* = 7.8 Hz, 1H), 7.59-7.51 (m, 3H);
^{13}C NMR (151 MHz, $CDCl_3$): δ 161.42, 143.93, 139.92, 133.60, 130.71, 130.50, 129.88, 129.07, 129.00, 128.86, 128.57, 127.27, 127.08, 125.40, 123.90, 122.35, 122.09; Data in accordance with literature.[7]

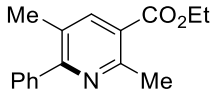


18A

Ethyl 2-methyl-6-phenylnicotinate (18A): 26.5 mg, 55% yield as a yellow oil.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.27 (d, *J* = 8.1 Hz, 1H), 8.06 (d, *J* = 7.6 Hz, 2H), 7.63 (d, *J* = 8.2 Hz, 1H), 7.49 (t, *J* = 7.5 Hz, 2H), 7.47-7.42 (m, 1H), 4.40 (q, *J* = 7.1 Hz, 2H), 2.92 (s, 3H), 1.42 (t, *J* = 7.1 Hz, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 166.84, 160.10, 159.23, 139.45, 138.69, 129.80, 128.96, 127.46, 123.83, 117.51, 61.28, 25.40, 14.45; Data in accordance with literature.[7]

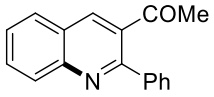


18B

Ethyl 2,5-dimethyl-6-phenylnicotinate (18B): 39.3 mg, 77% yield as a yellow oil.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.09 (s, 1H), 7.57-7.50 (m, 2H), 7.45 (t, *J* = 7.8 Hz, 2H), 7.42-7.36 (m, 1H), 4.40 (q, *J* = 7.1 Hz, 2H), 2.84 (s, 3H), 2.35 (s, 3H), 1.42 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 166.95, 160.72, 156.83, 140.95, 140.07, 129.04, 128.49, 128.37, 128.01, 123.92, 61.25, 24.62, 19.54, 14.44; Data in accordance with literature.[7]

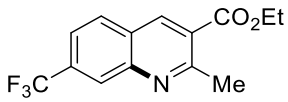


18C

1-(2-Phenylquinolin-3-yl)ethan-1-one (18C): 24.1 mg, 56% yield as a pale yellow solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.13 (s, 1H), 8.09 (d, *J* = 8.4 Hz, 1H), 7.85 (d, *J* = 7.7 Hz, 2H), 7.79 (dd, *J* = 11.8, 8.0 Hz, 2H), 7.64 (t, *J* = 7.5 Hz, 1H), 7.55 (t, *J* = 7.5 Hz, 1H), 7.50 (t, *J* = 7.6 Hz, 2H), 2.75 (s, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 196.94, 156.84, 148.20, 137.44, 136.95, 133.87, 132.40, 131.24, 130.33, 128.90, 128.82, 128.80, 128.25, 126.84, 125.45, 24.37; Data in accordance with literature.[7]



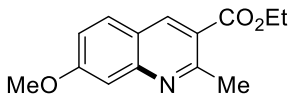
18D

Ethyl 2-methyl-7-(trifluoromethyl)quinoline-3-carboxylate (18D): 39.6 mg, 70% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.75 (s, 1H), 8.34 (s, 1H), 7.98 (d, *J* = 8.5 Hz, 1H), 7.70 (d, *J* = 8.4 Hz, 1H), 4.46 (q, *J* = 7.1 Hz, 2H), 3.00 (s, 3H), 1.46 (t, *J* = 7.1 Hz, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 166.21, 160.14, 147.74, 139.48, 133.18 (q, *J* = 33.4 Hz), 129.71, 127.36, 126.62 (q, *J* = 4.5 Hz), 126.00, 123.89 (q, *J* = 271.8 Hz), 122.31 (q, *J* = 3.0 Hz), 61.87, 25.80, 14.41;

^{19}F NMR (565 MHz, $CDCl_3$): δ -62.95; Data in accordance with literature.[7]

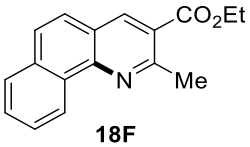


18E

Ethyl 7-methoxy-2-methylquinoline-3-carboxylate (18E): 35.8 mg, 73% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.65 (s, 1H), 7.72 (d, *J* = 8.9 Hz, 1H), 7.37-7.32 (m, 1H), 7.16 (dd, *J* = 8.9, 2.4 Hz, 1H), 4.41 (q, *J* = 7.2 Hz, 2H), 3.95 (s, 3H), 2.96 (s, 3H), 1.43 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 166.87, 157.96, 147.46, 139.12, 134.69, 130.89, 129.05, 127.93, 127.70, 127.24, 125.27, 125.19, 123.98, 123.81, 61.41, 26.02, 14.48; Data in accordance with literature.[7]



18F

Ethyl 2-methylbenzo[*h*]quinoline-3-carboxylate (18F): 47.7 mg, 90% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 9.34 (d, *J* = 7.8 Hz, 1H), 8.70 (s, 1H), 7.89 (d, *J* = 7.5 Hz, 1H), 7.81-7.64 (m, 4H), 4.46 (q, *J* = 7.2 Hz, 2H), 3.10 (s, 3H), 1.47 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (151 MHz, $CDCl_3$): δ 166.75, 162.79, 159.30, 150.79, 139.69, 129.70, 121.65, 121.04, 119.99, 106.72, 61.28, 55.77, 25.87, 14.47; Data in accordance with literature.[7]

References

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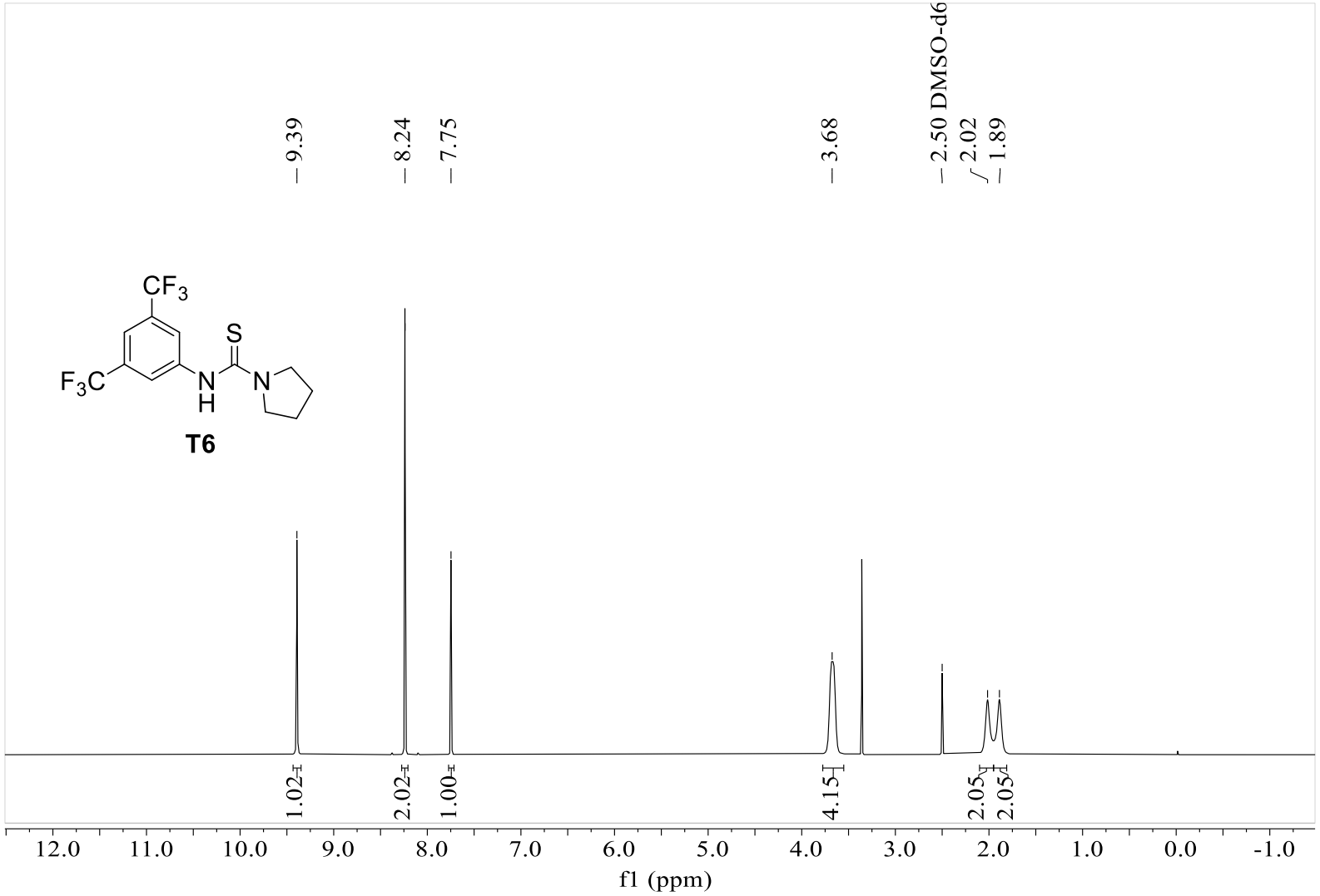
NMR Spectra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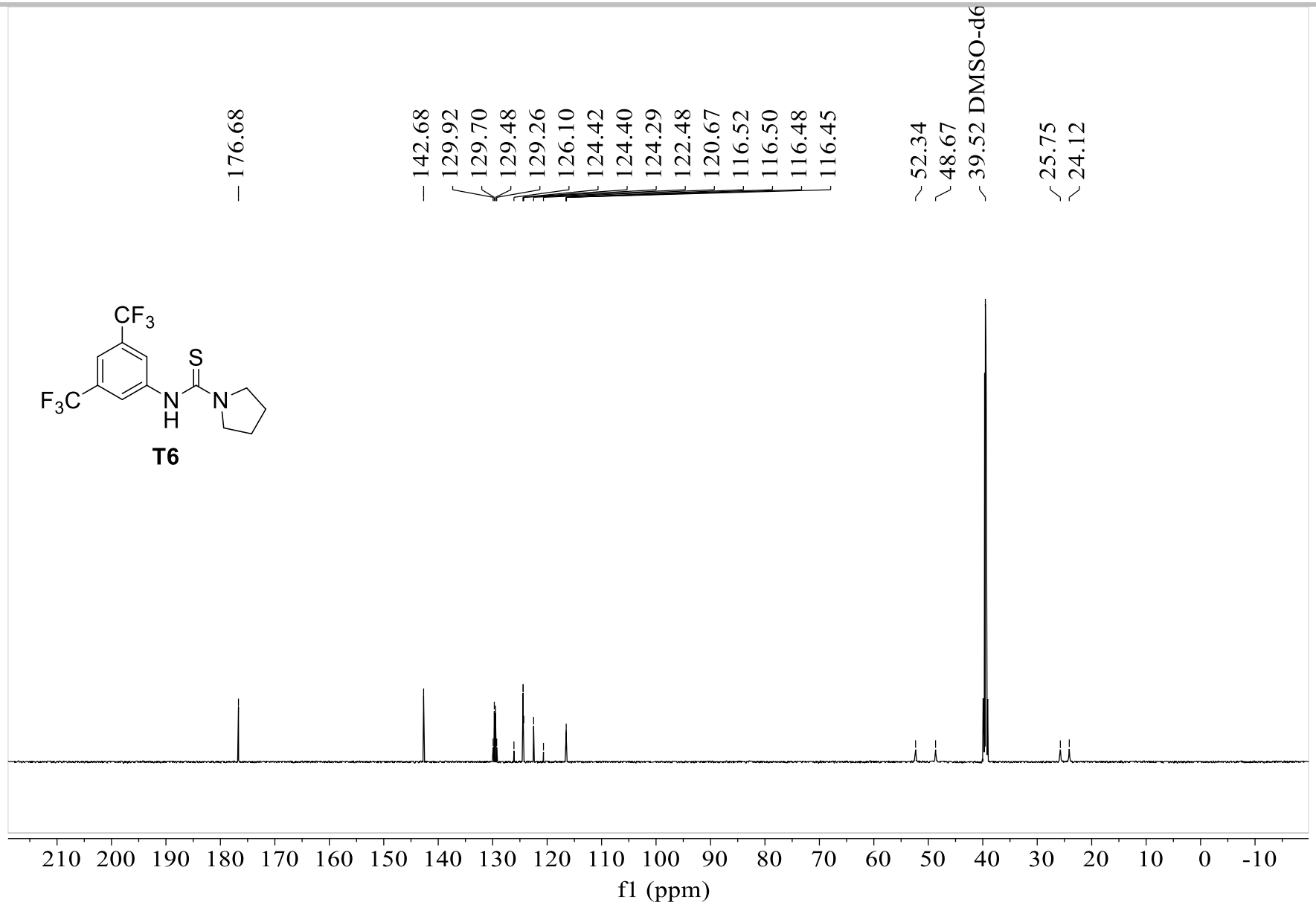
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48.67
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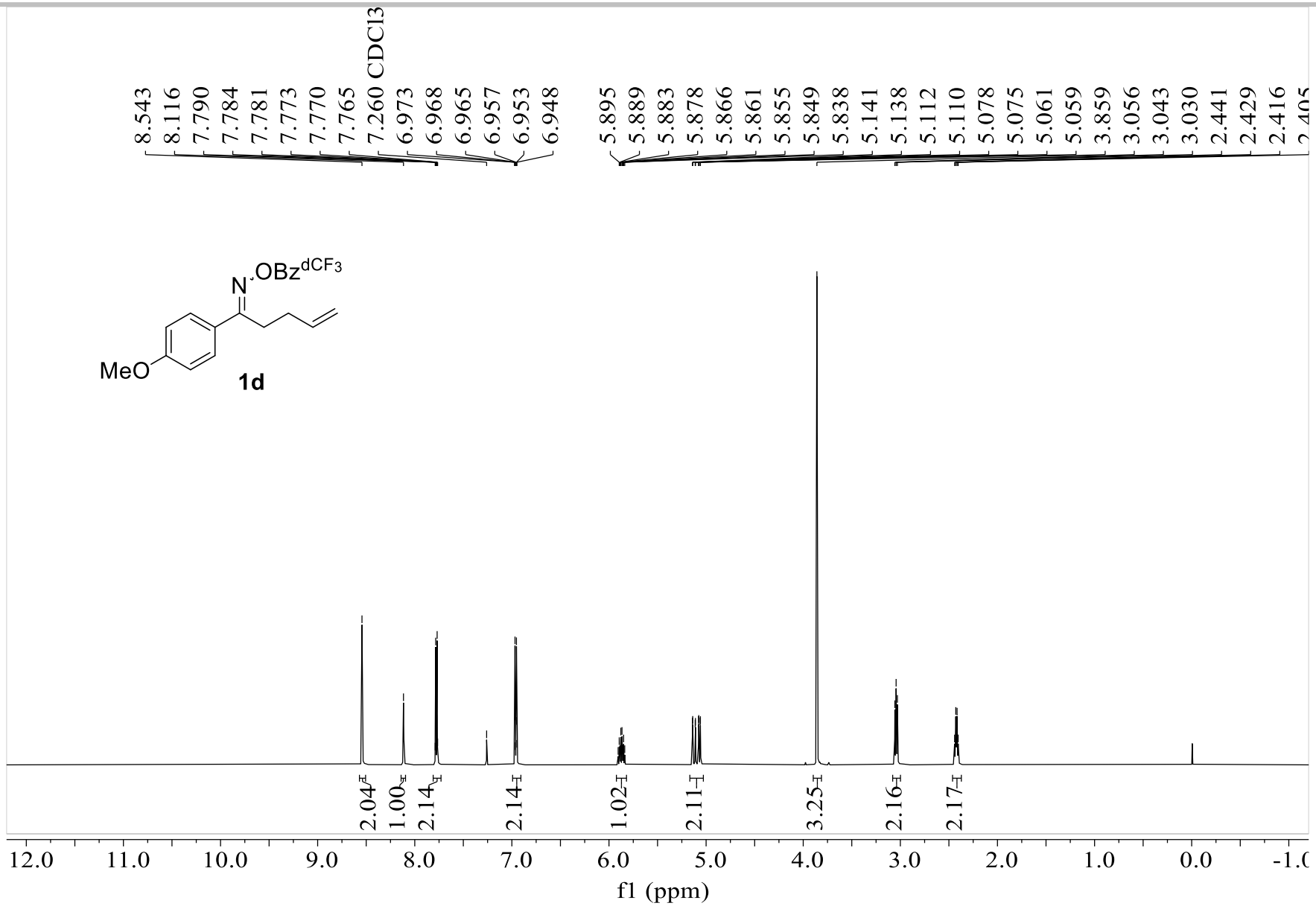
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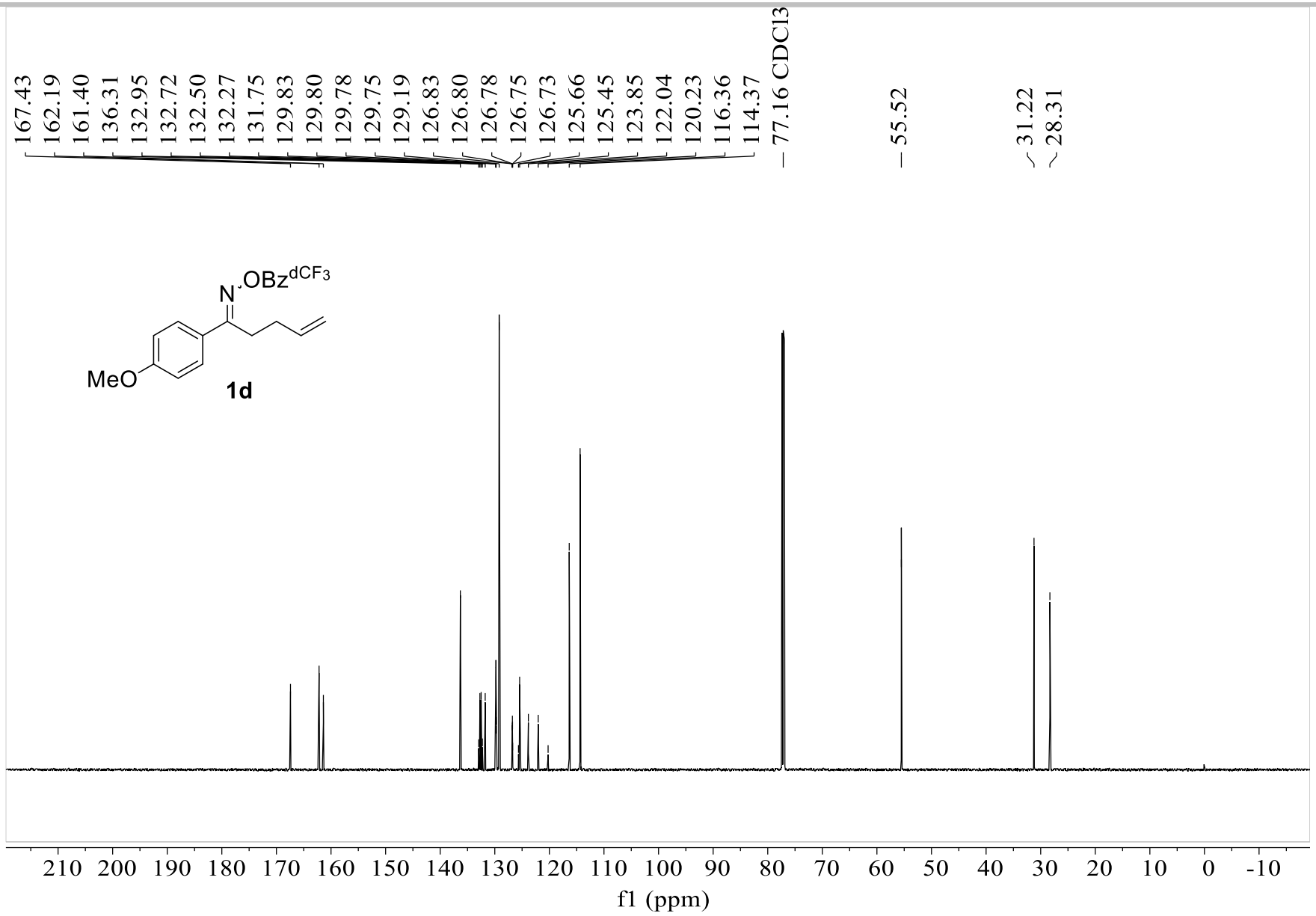
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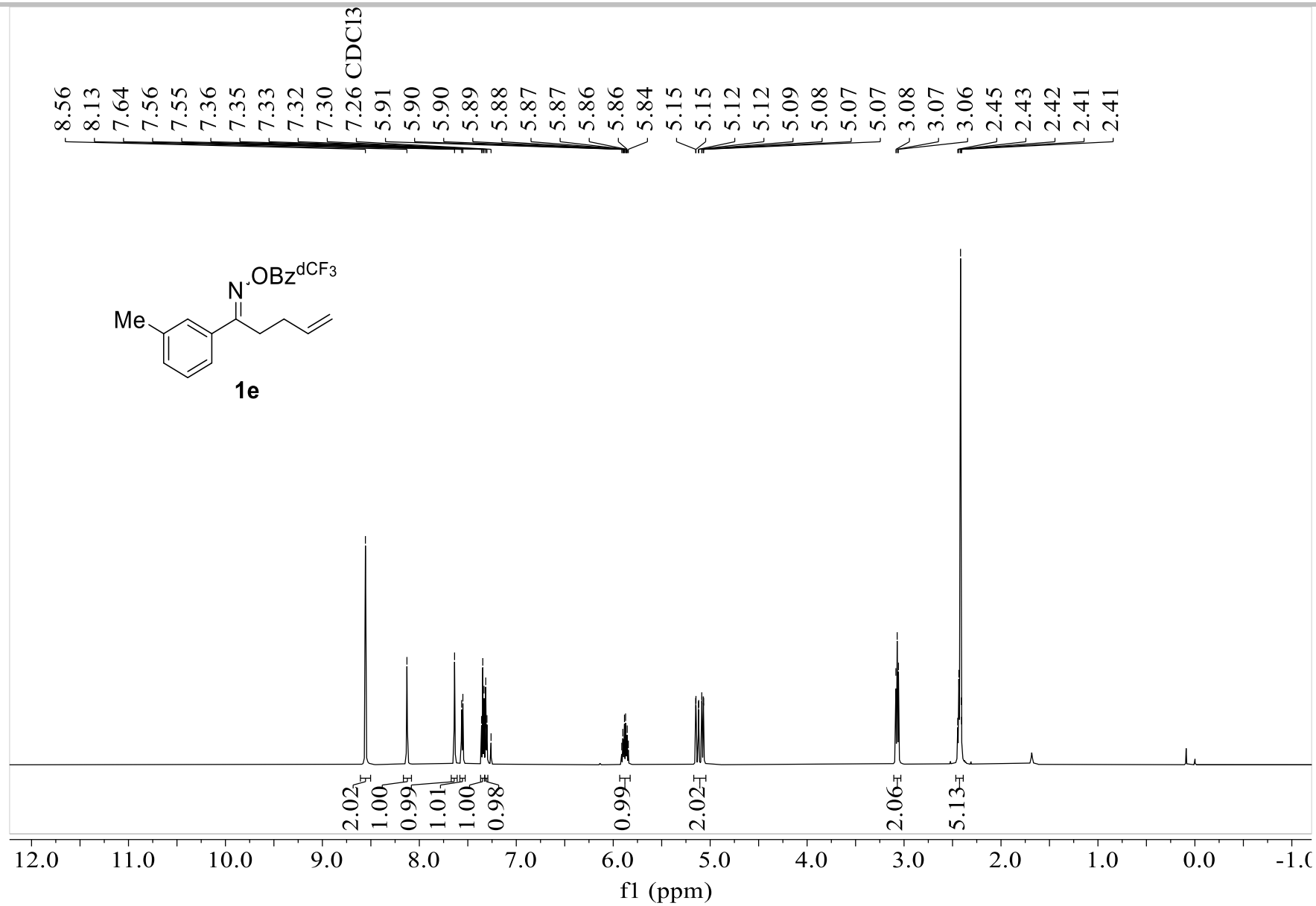
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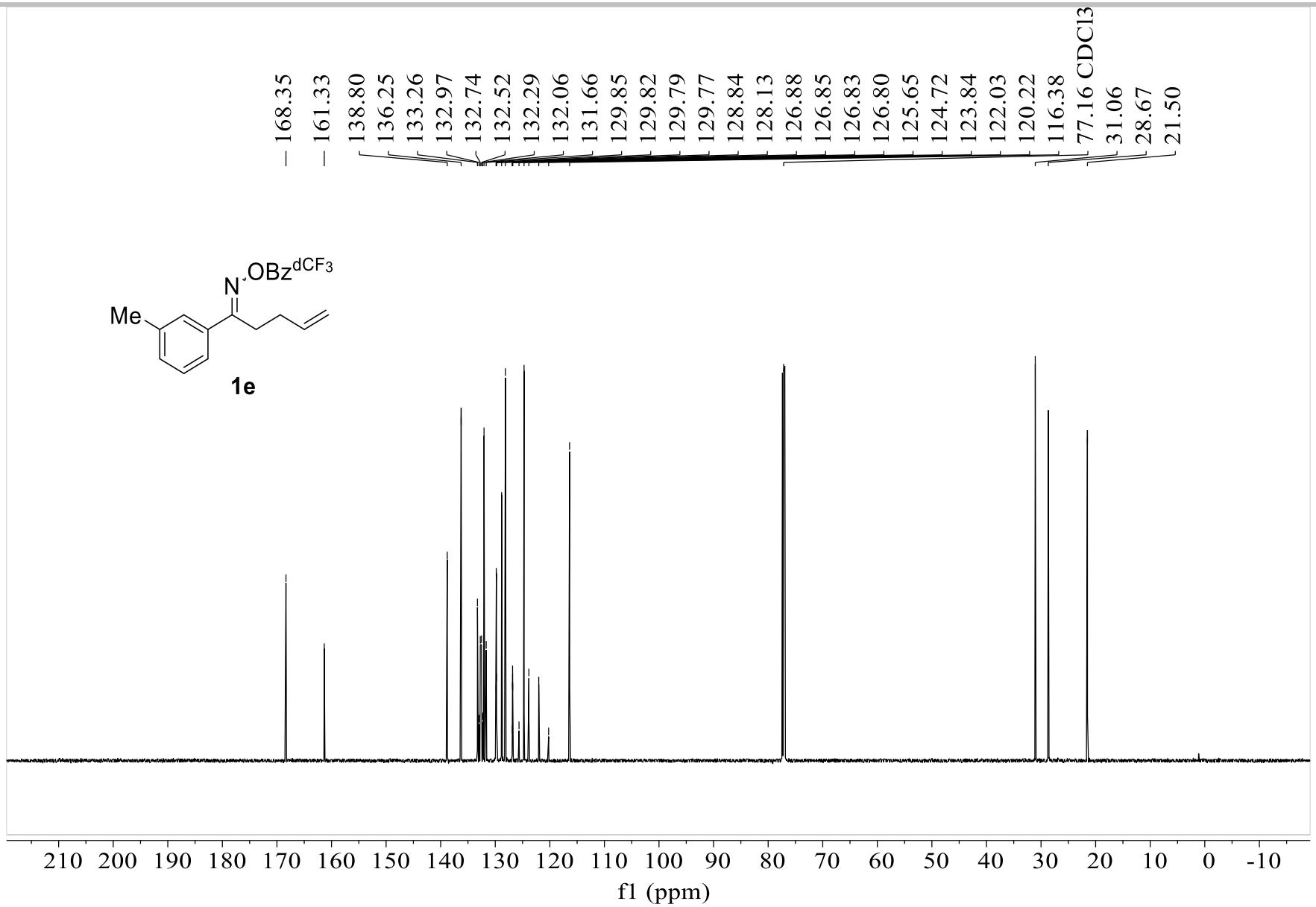
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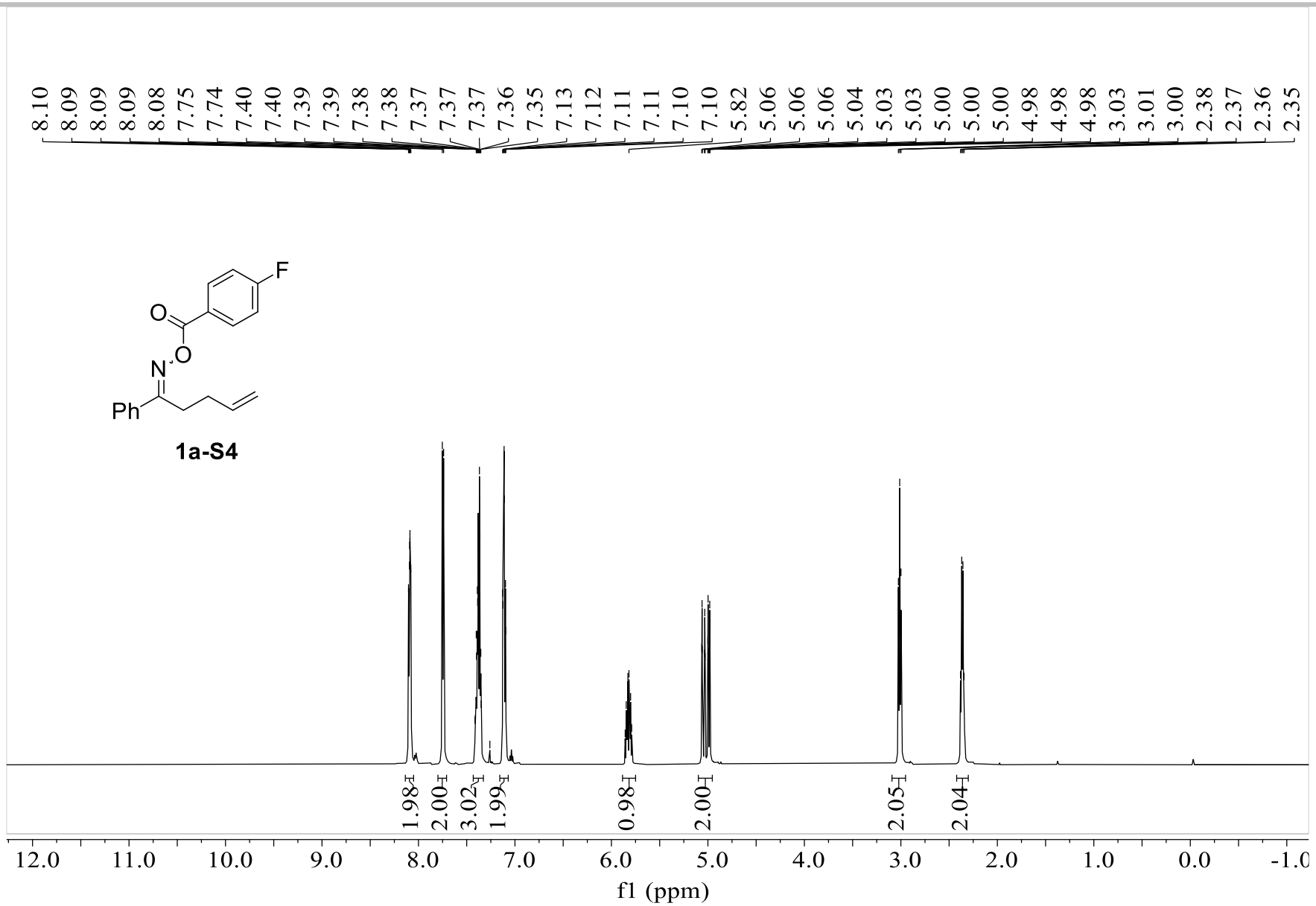
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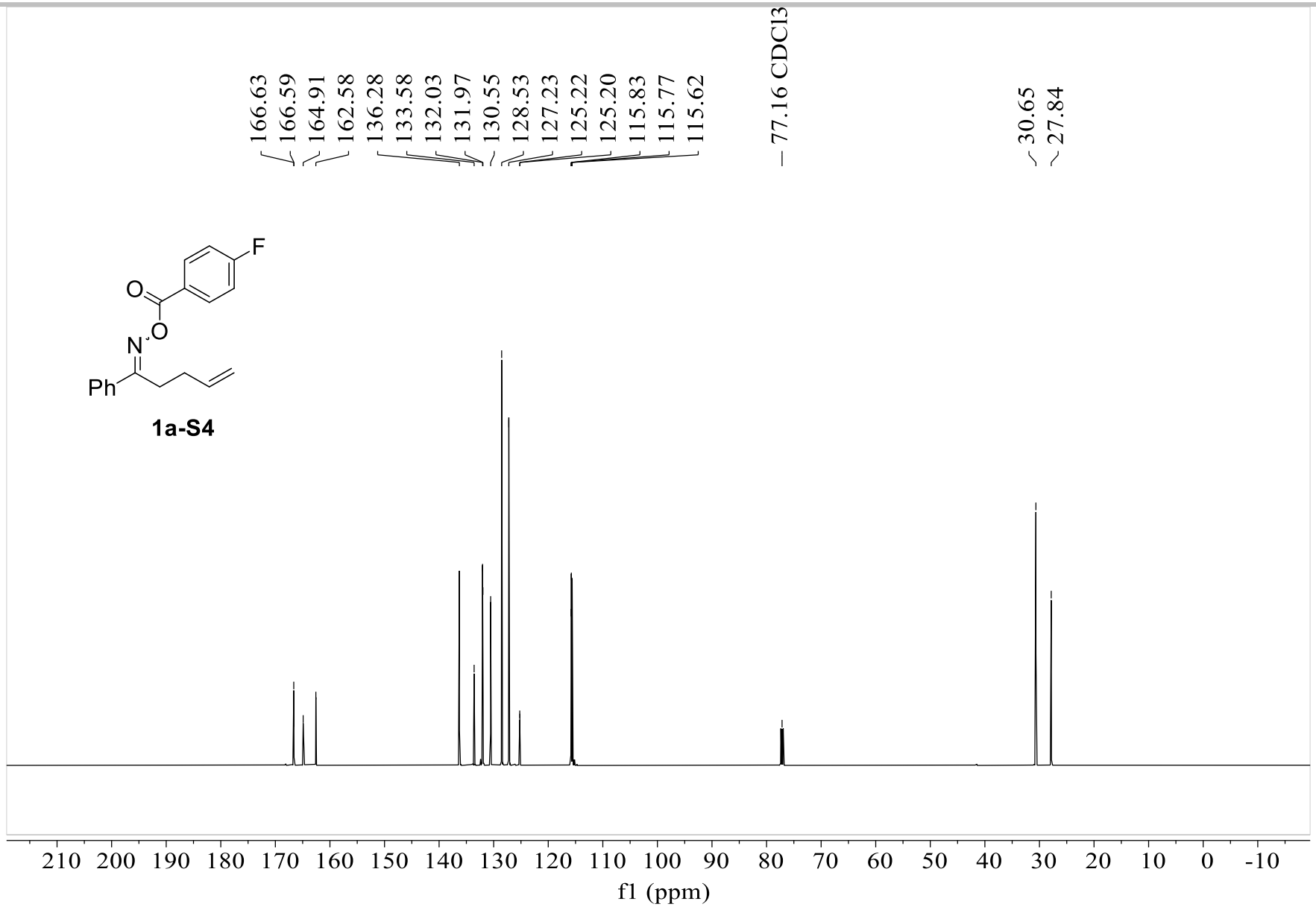
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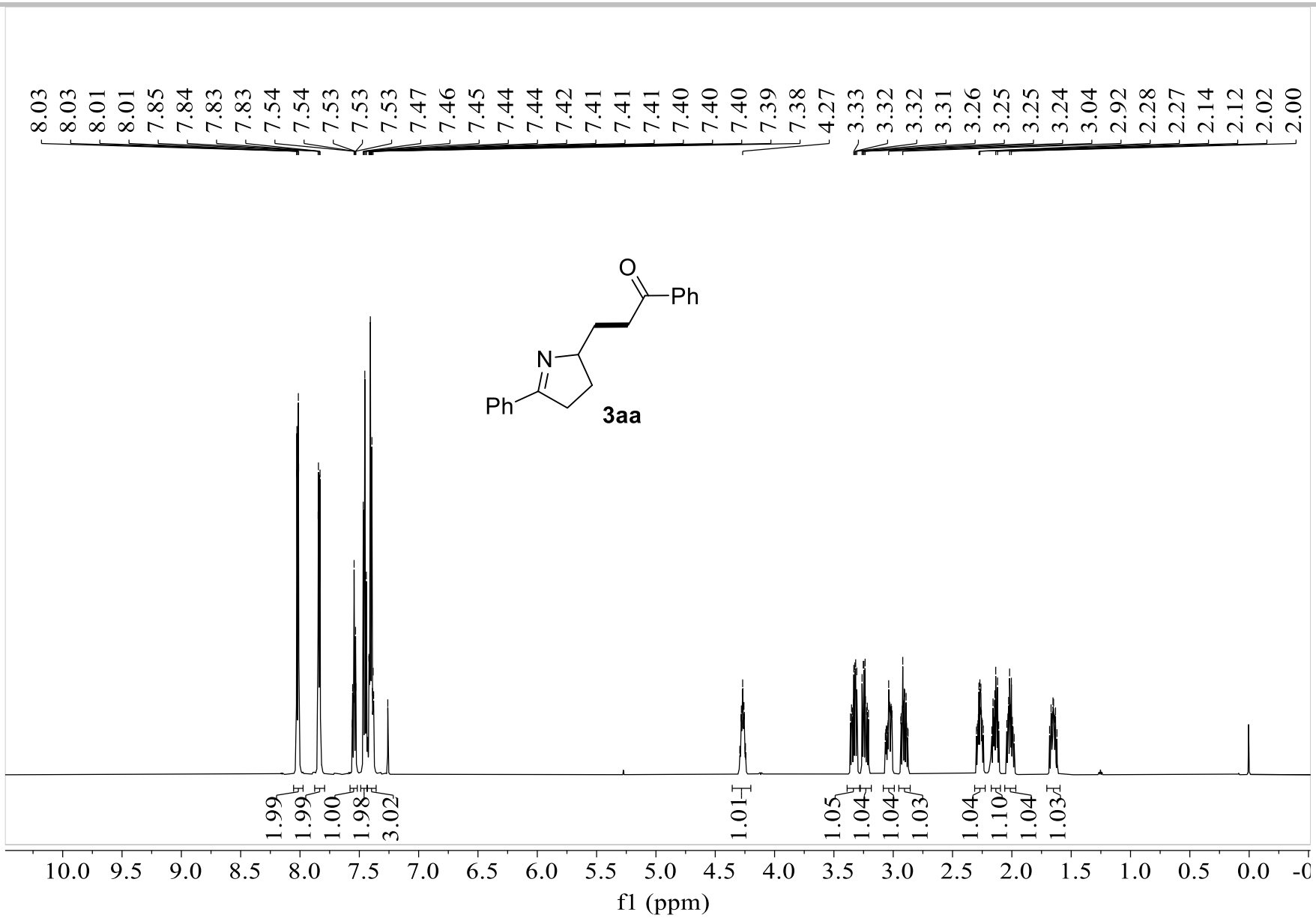
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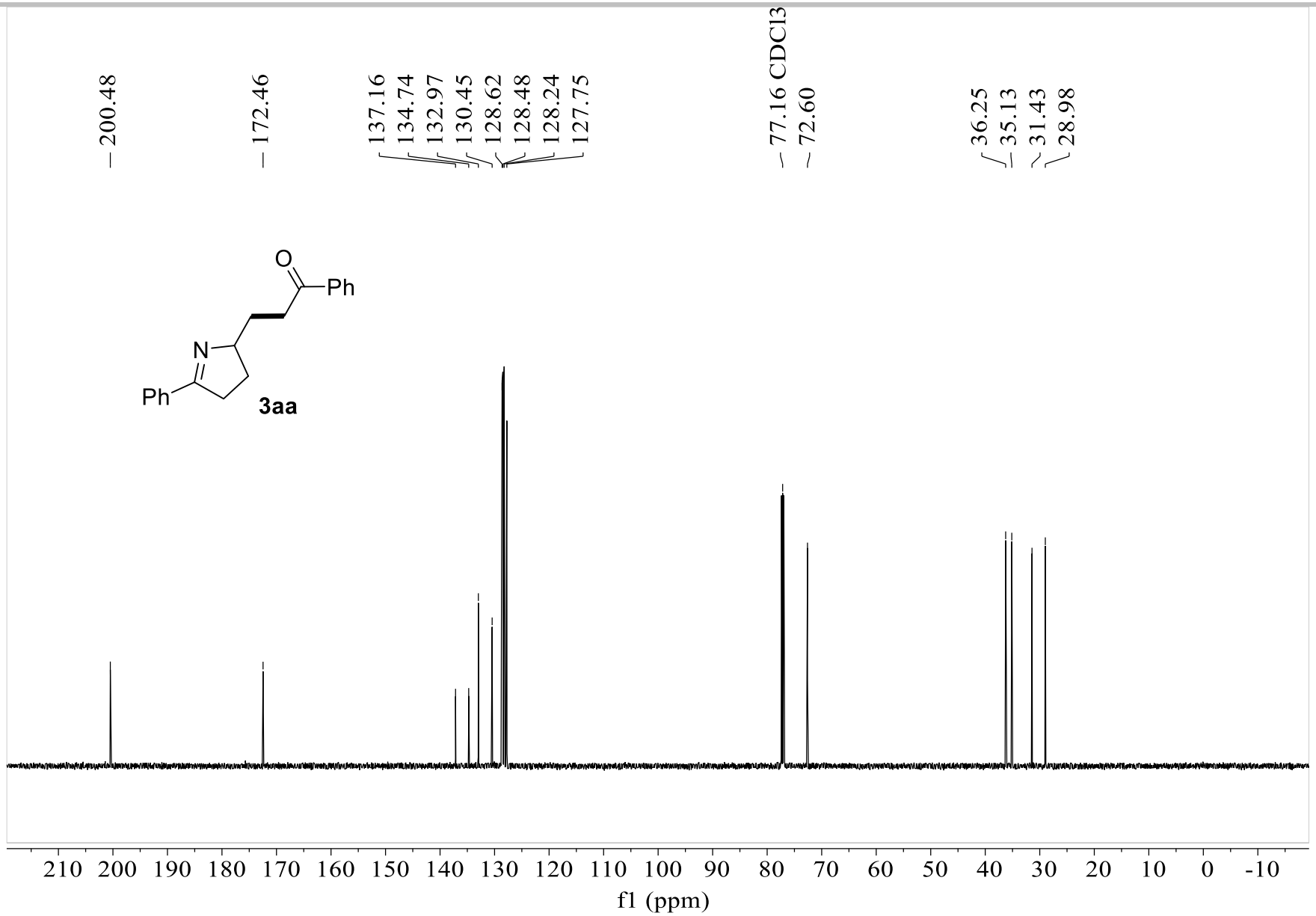
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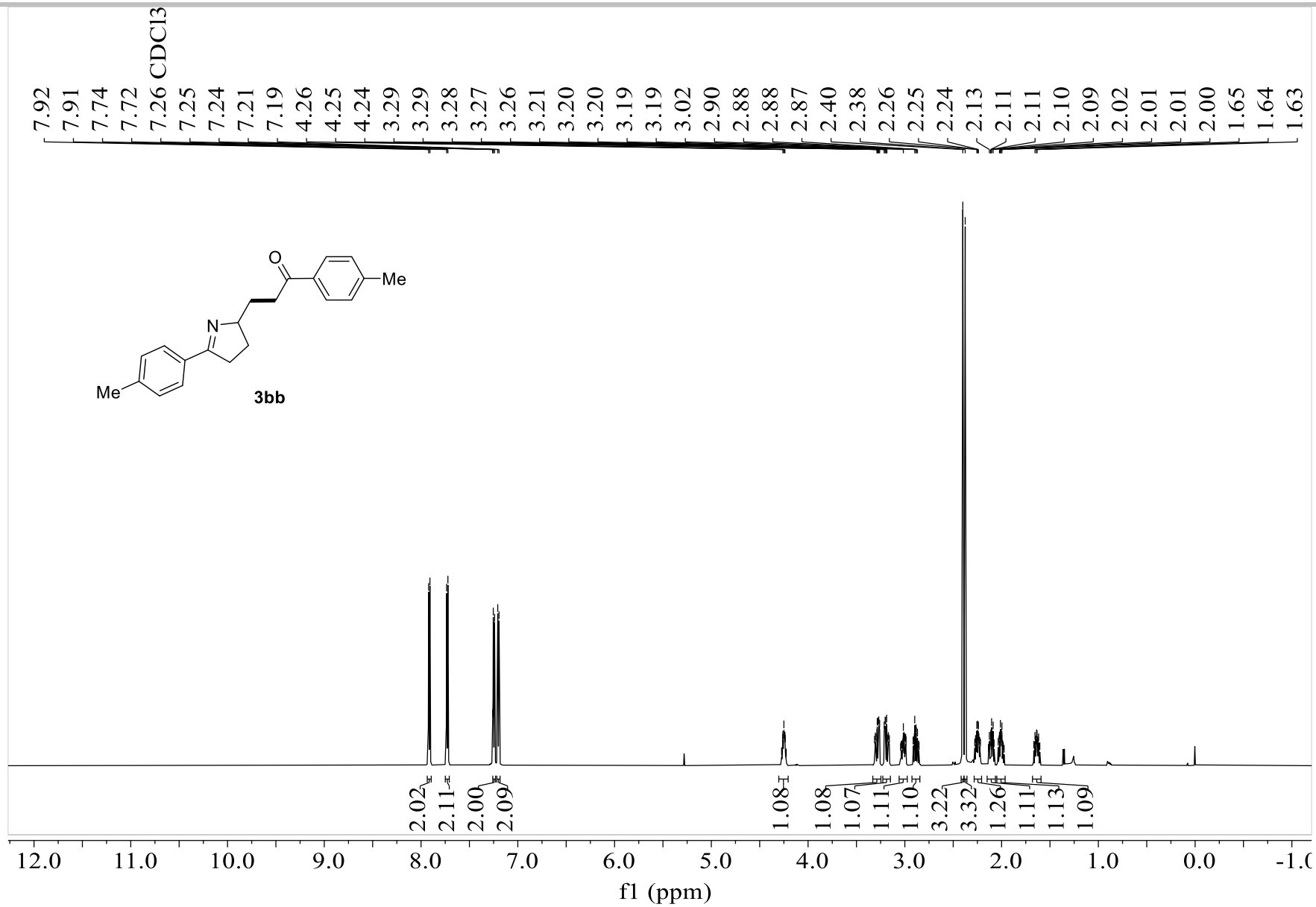
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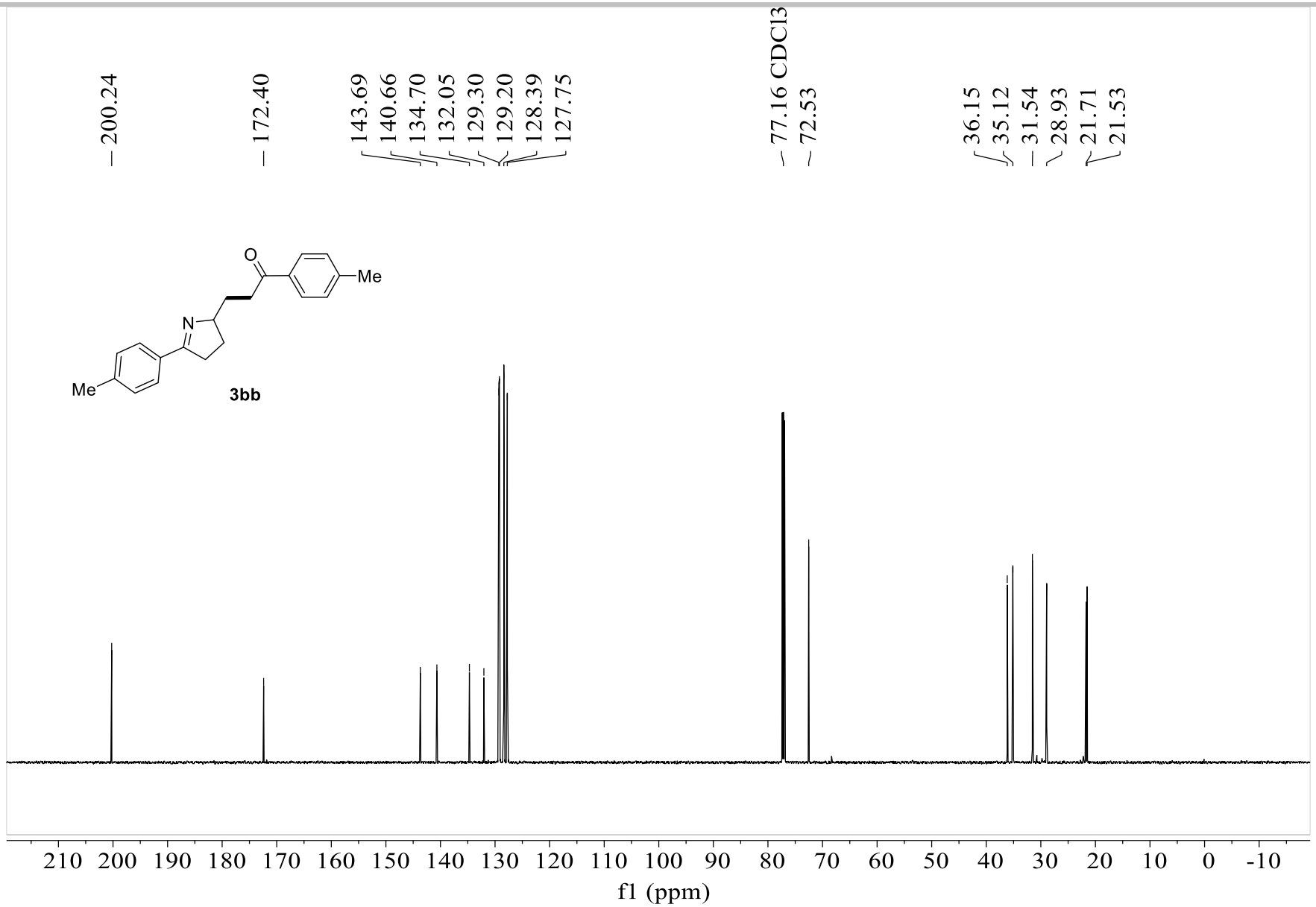
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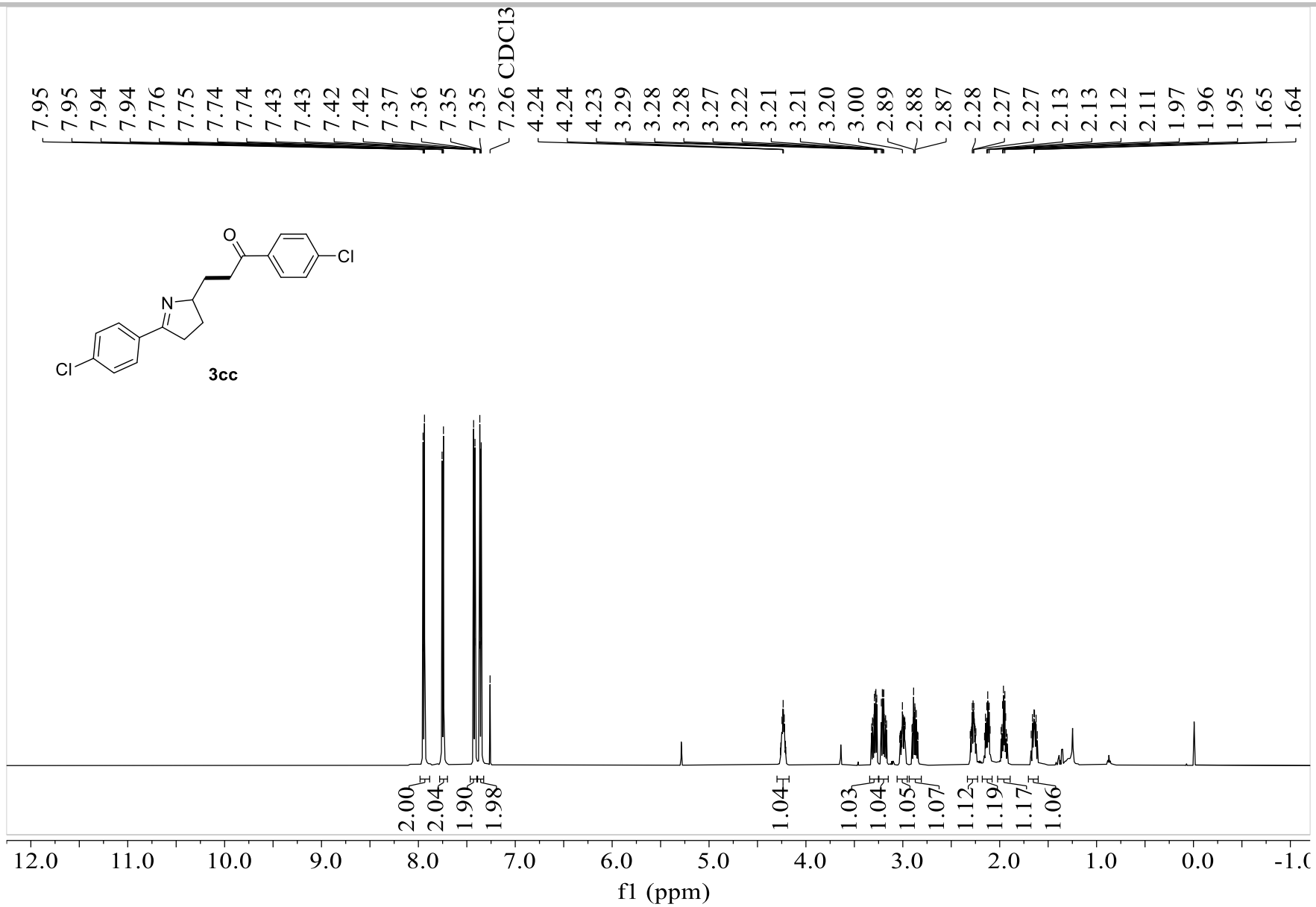
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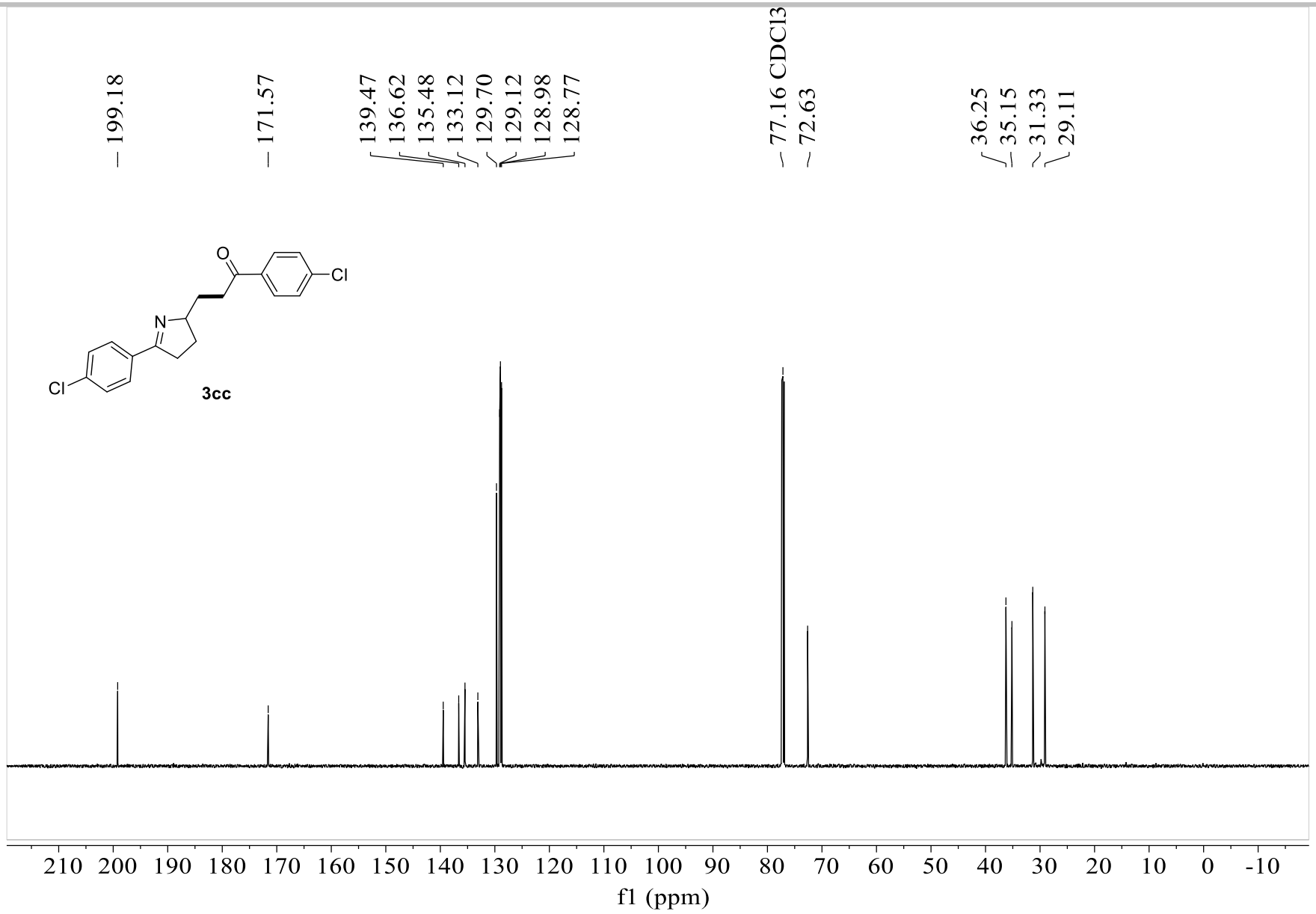
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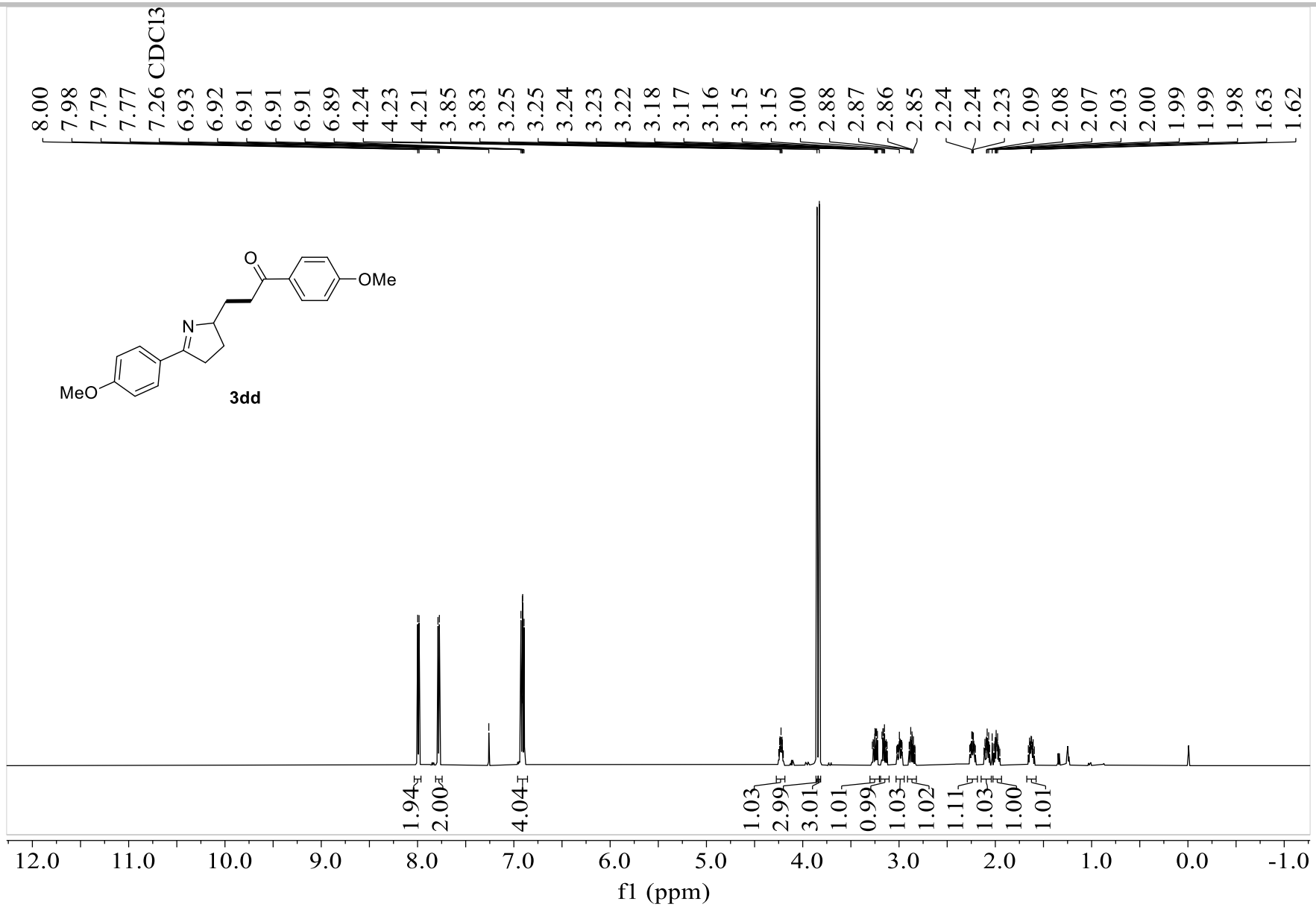
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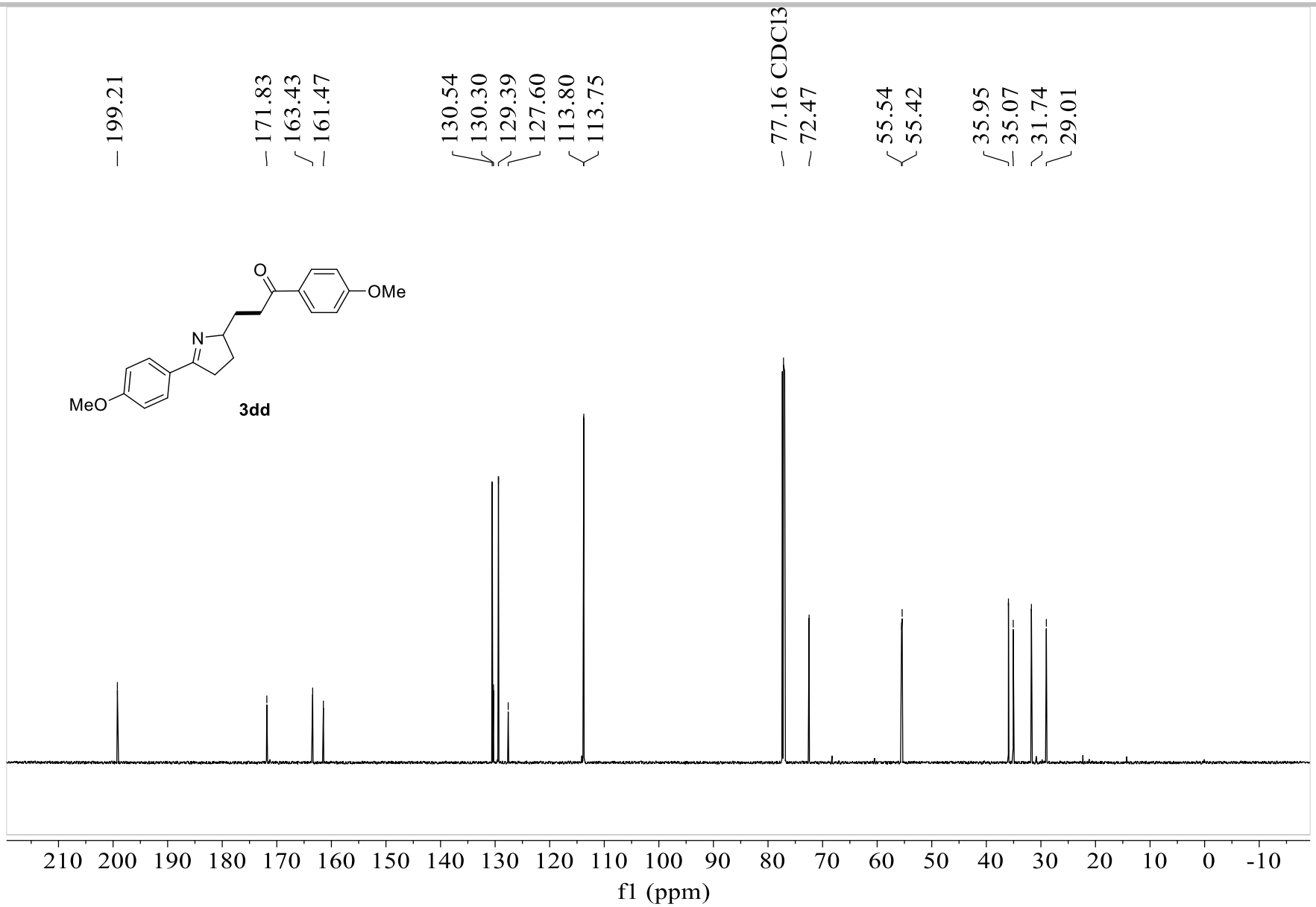
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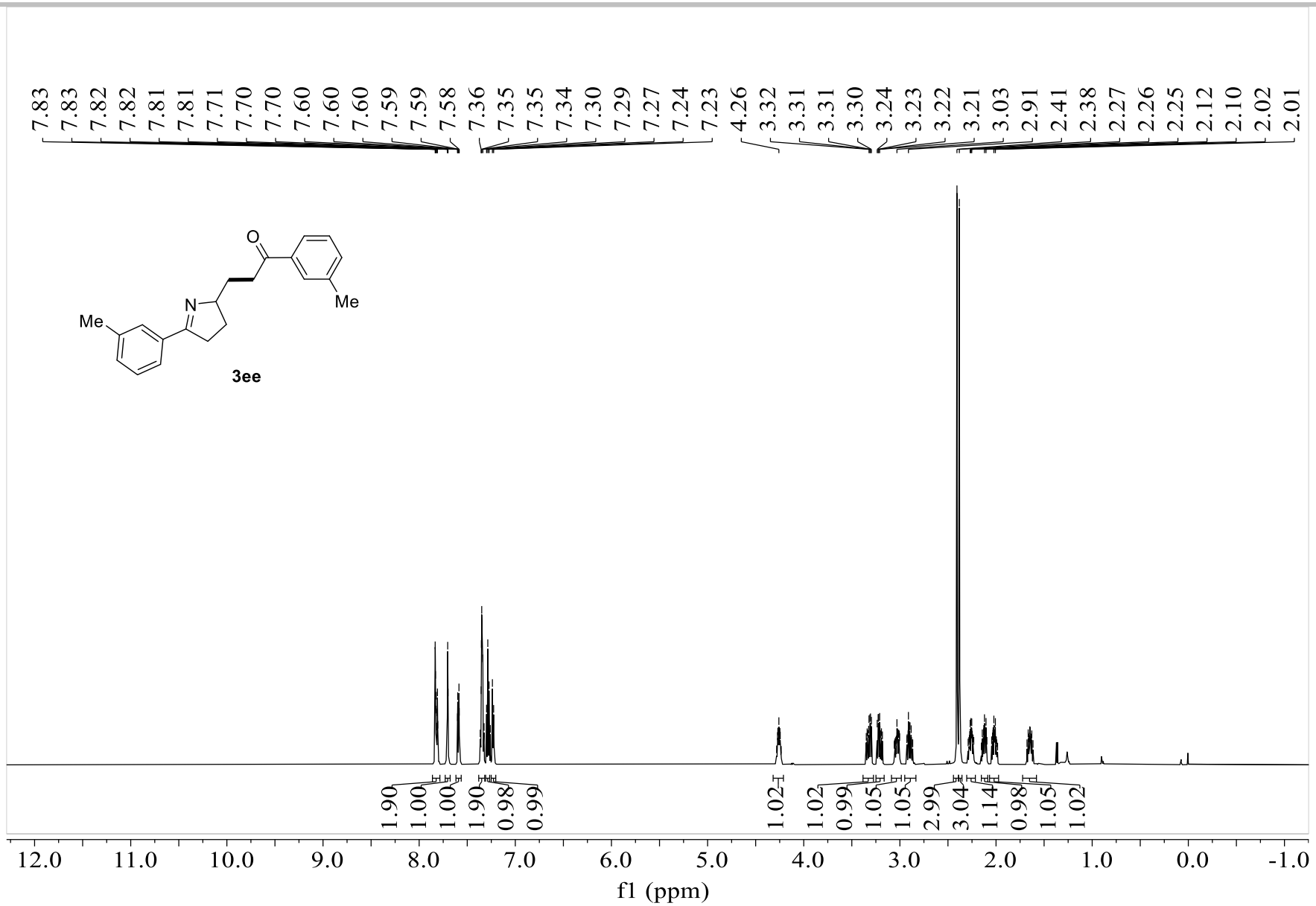
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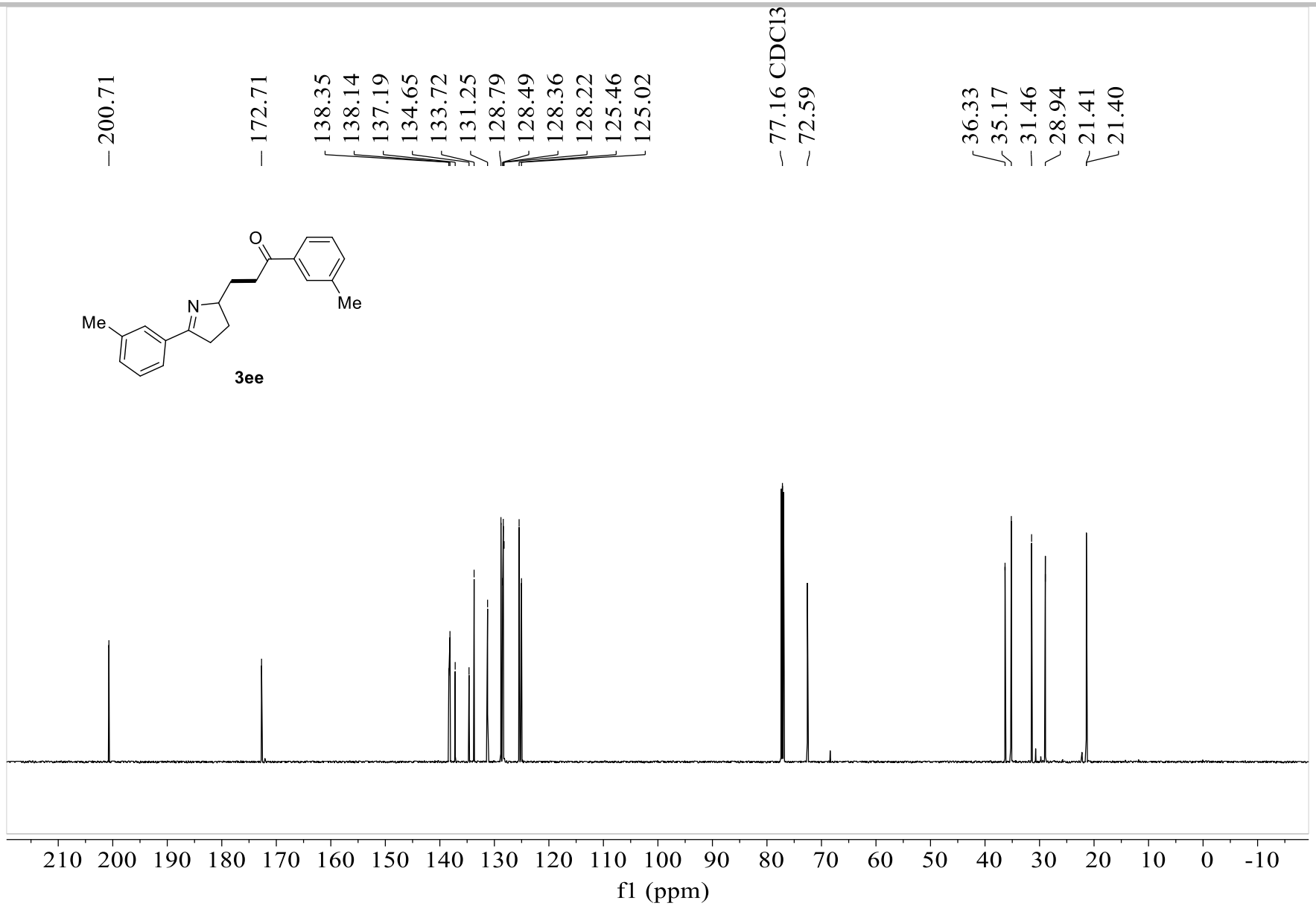
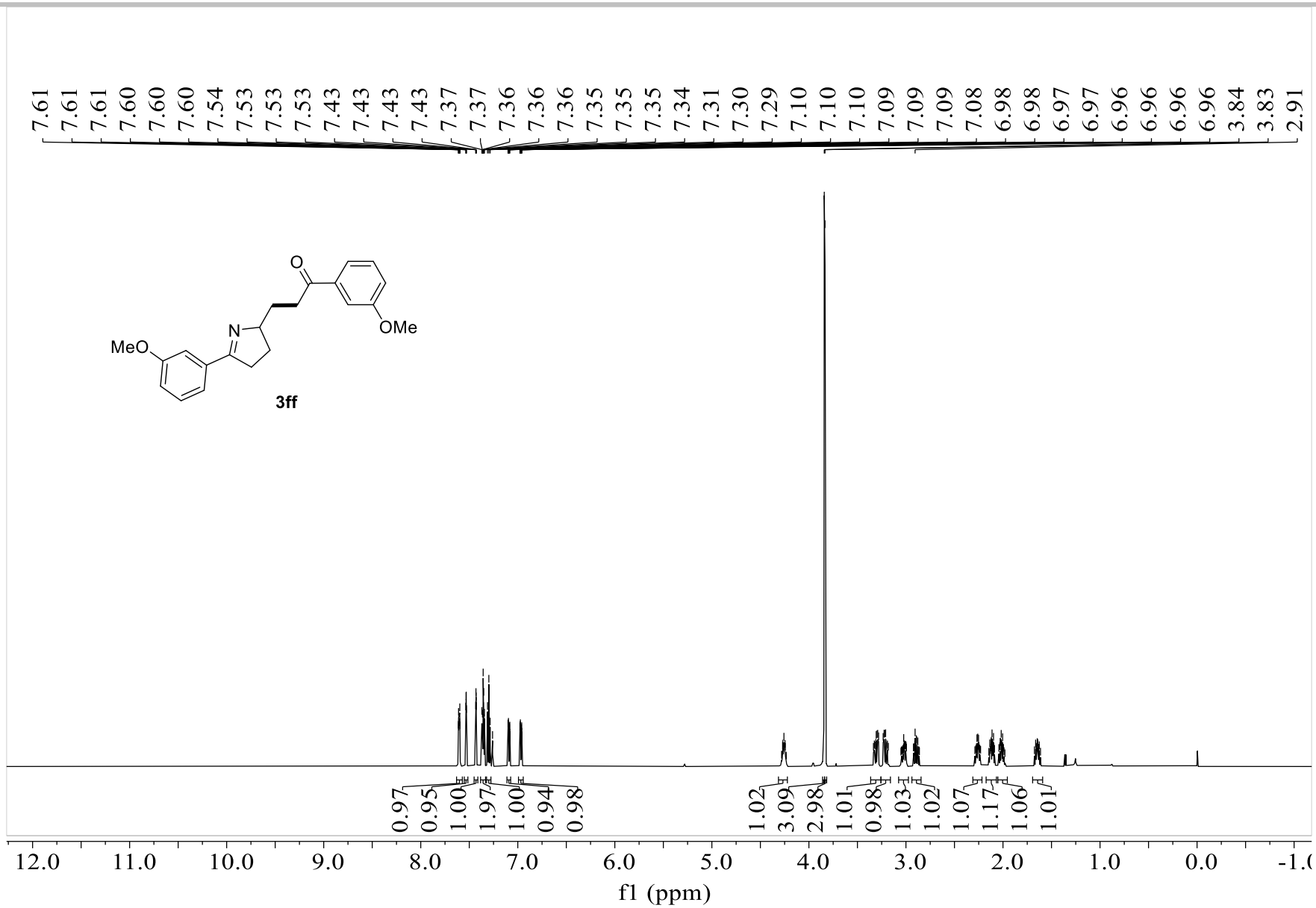
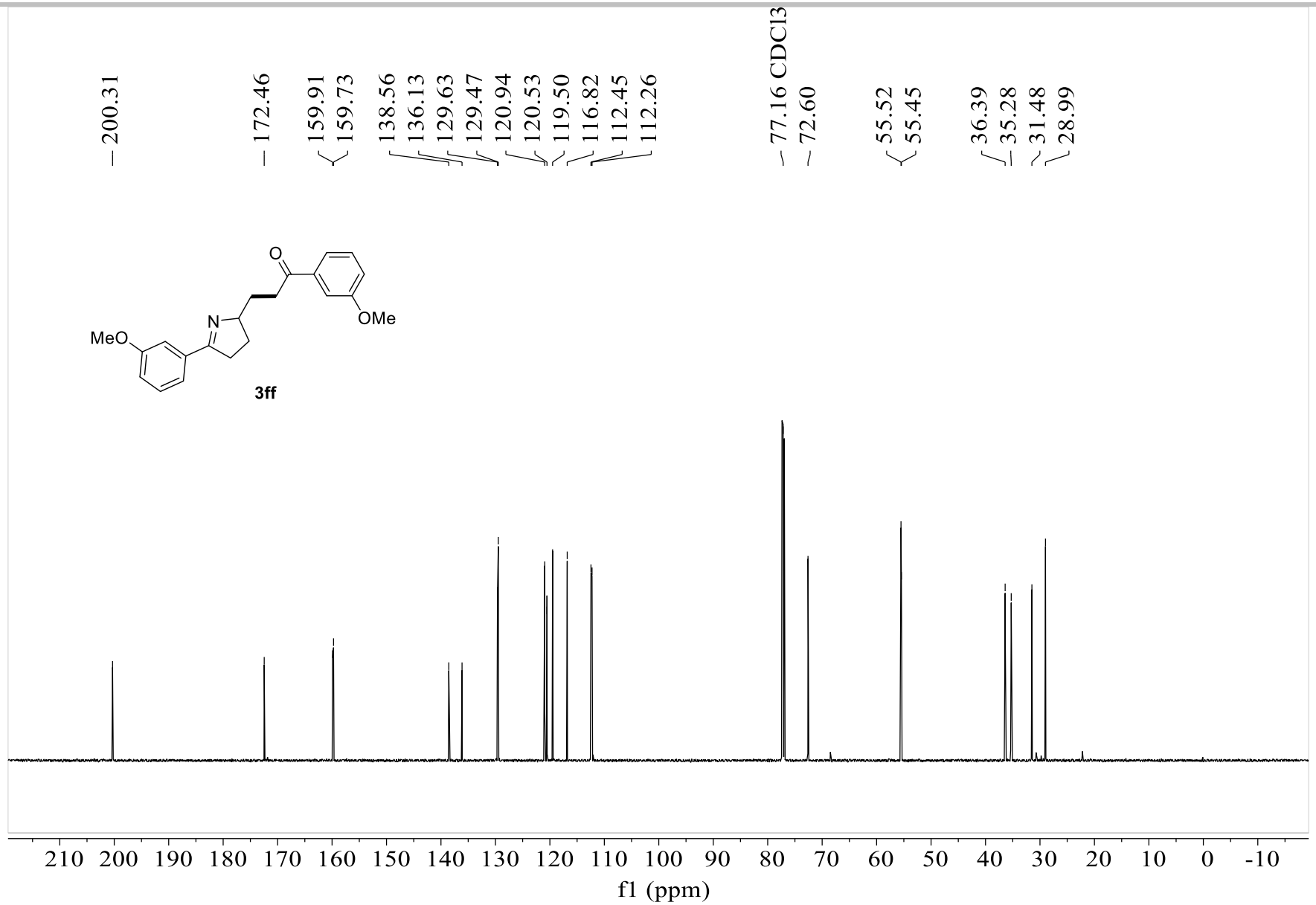
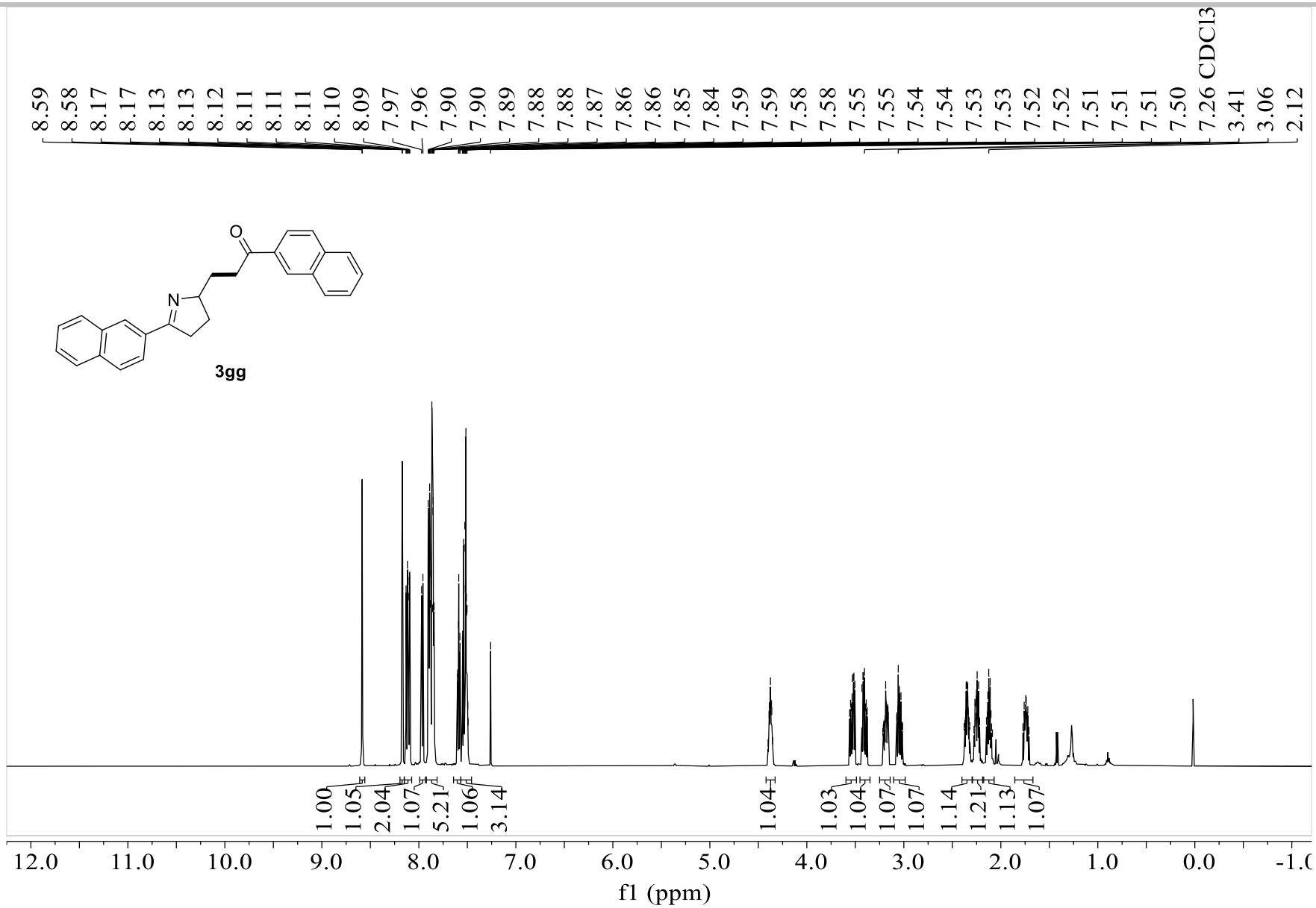
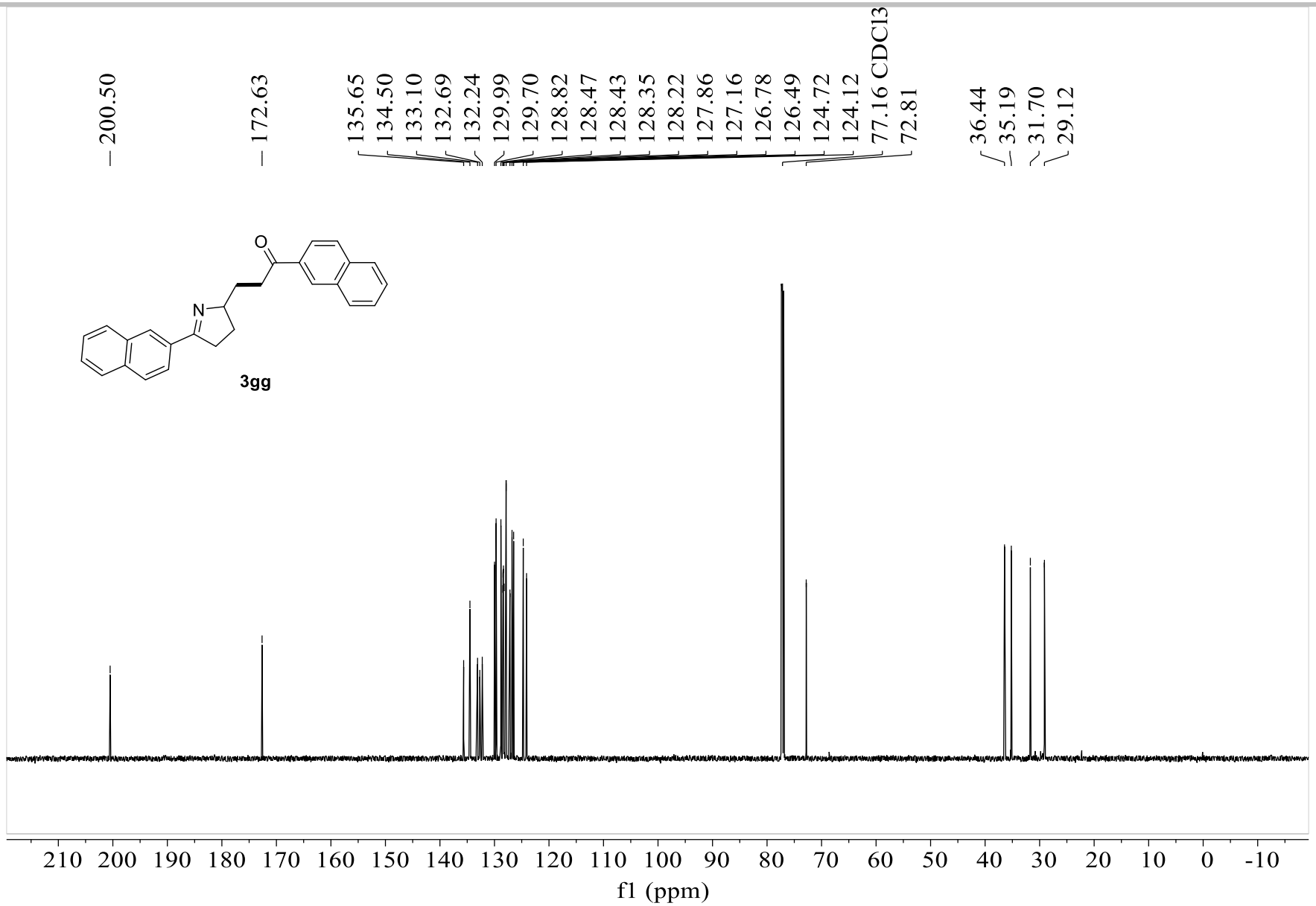
3.04
1.14
0.98
1.05
1.02
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)

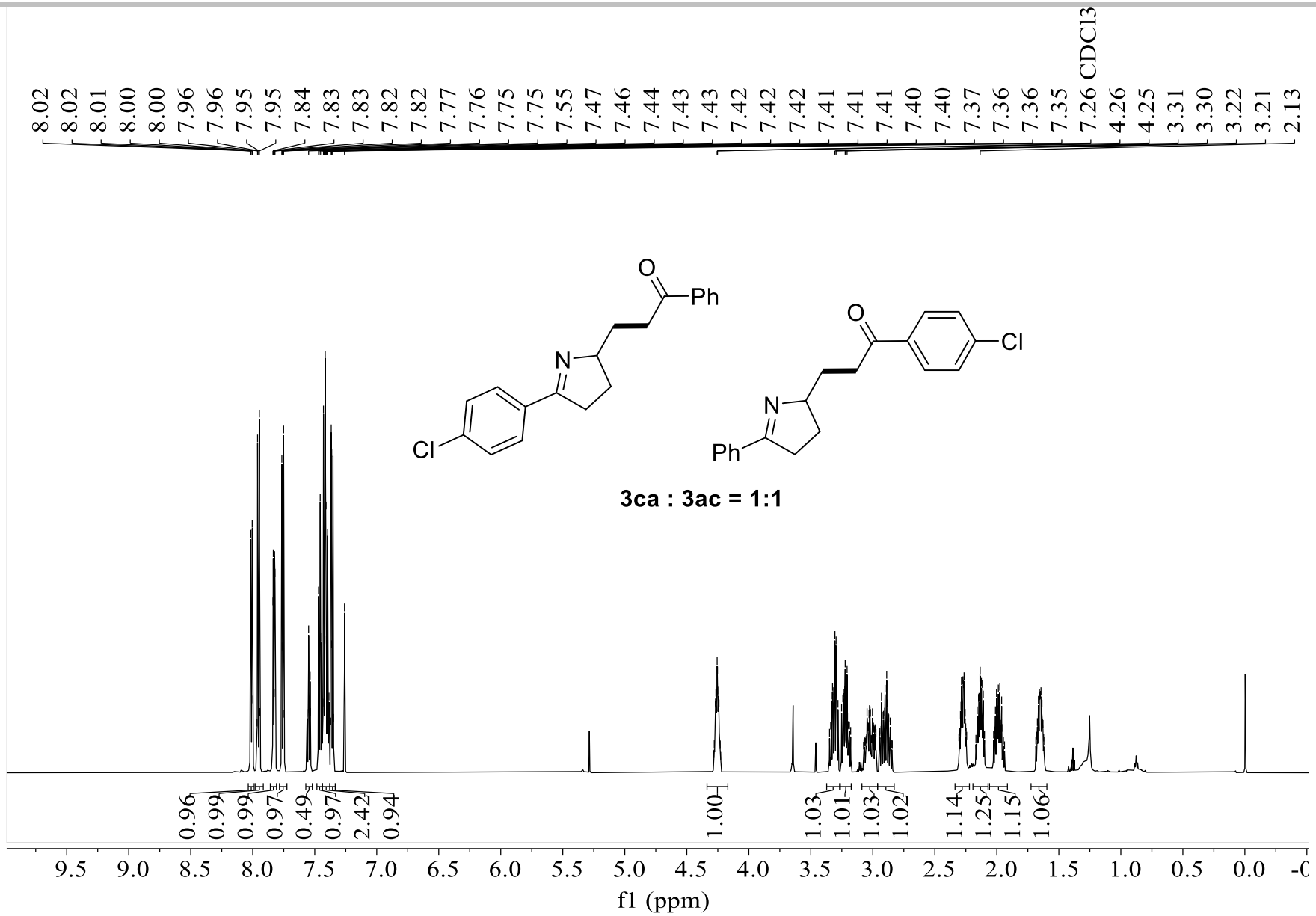

200.71
172.71
138.35
138.14
137.19
134.65
133.72
131.25
128.79
128.49
128.36
128.22
125.46
125.02
77.16 CDCl3
72.59
36.33
35.17
31.46
28.94
21.41
21.40
O
N
Me
Me
3ee
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

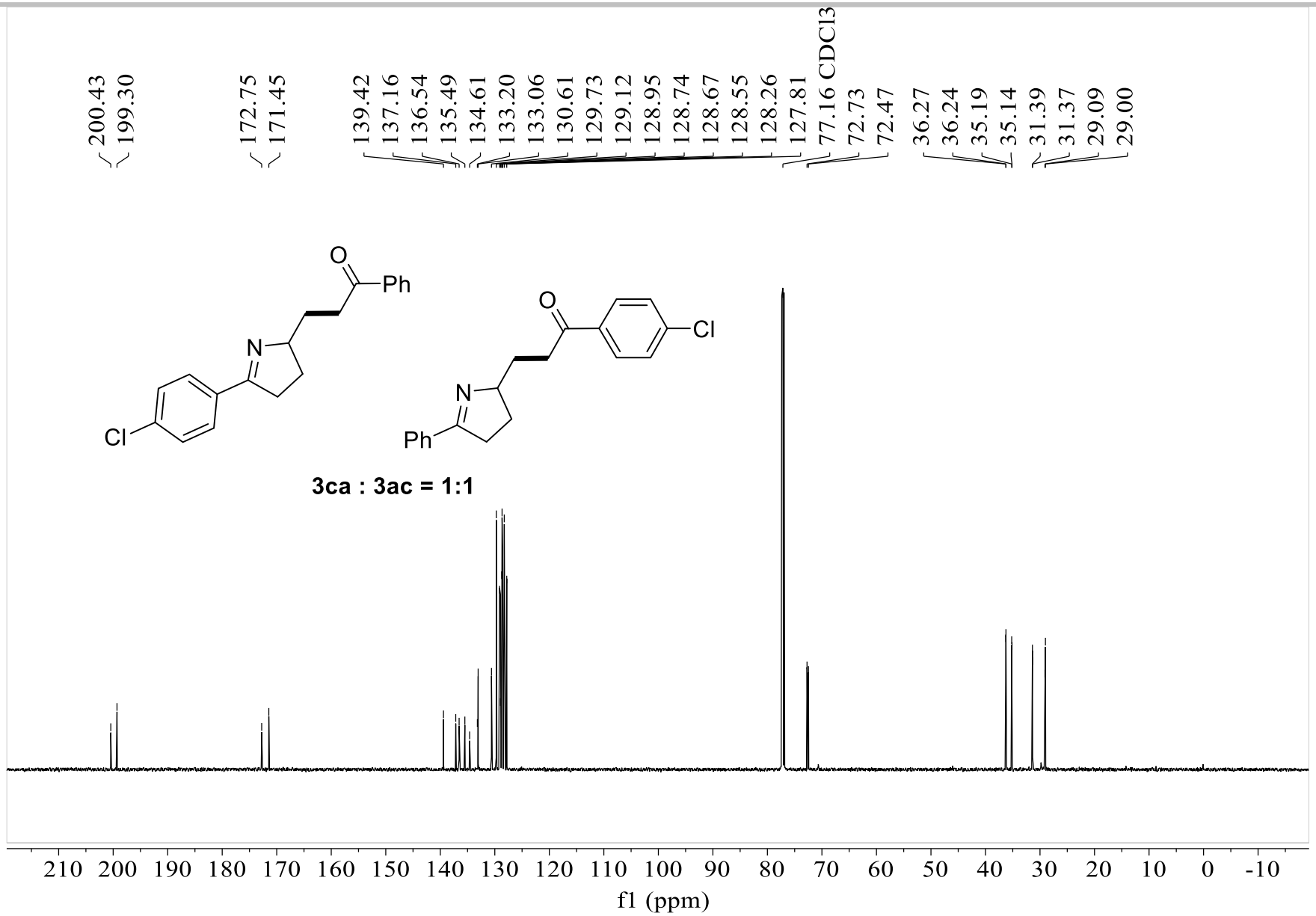

7.61 7.61 7.61 7.60 7.60 7.60 7.54 7.53 7.53 7.53 7.43 7.43 7.43 7.43 7.37 7.37 7.36 7.36 7.36 7.35 7.35 7.35 7.34 7.31 7.30 7.29 7.10 7.10 7.10 7.09 7.09 7.09 7.08 6.98 6.98 6.97 6.97 6.96 6.96 6.96 6.96 3.84 3.83 2.91
O
N
MeO
OMe
3ff
0.97 0.95 1.00 1.97 1.00 0.94 0.98
1.02 3.09 2.98 1.01 0.98 1.03 1.02 1.07 1.17 1.06 1.01
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)

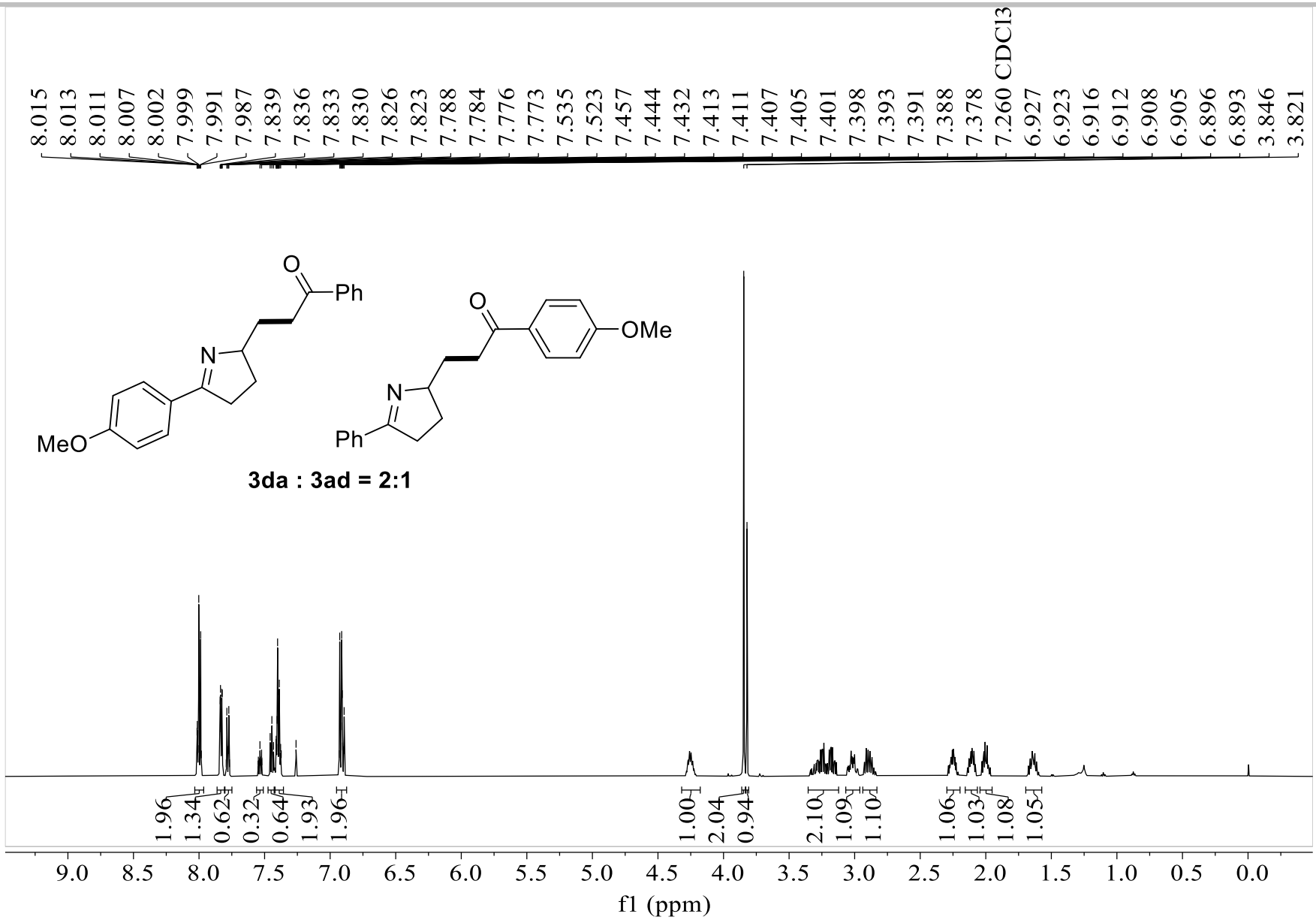

200.31
172.46
159.91
159.73
138.56
136.13
129.63
129.47
120.94
120.53
119.50
116.82
112.45
112.26
77.16 CDCl3
72.60
55.52
55.45
36.39
35.28
31.48
28.99
O
N
MeO
OMe
3ff
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

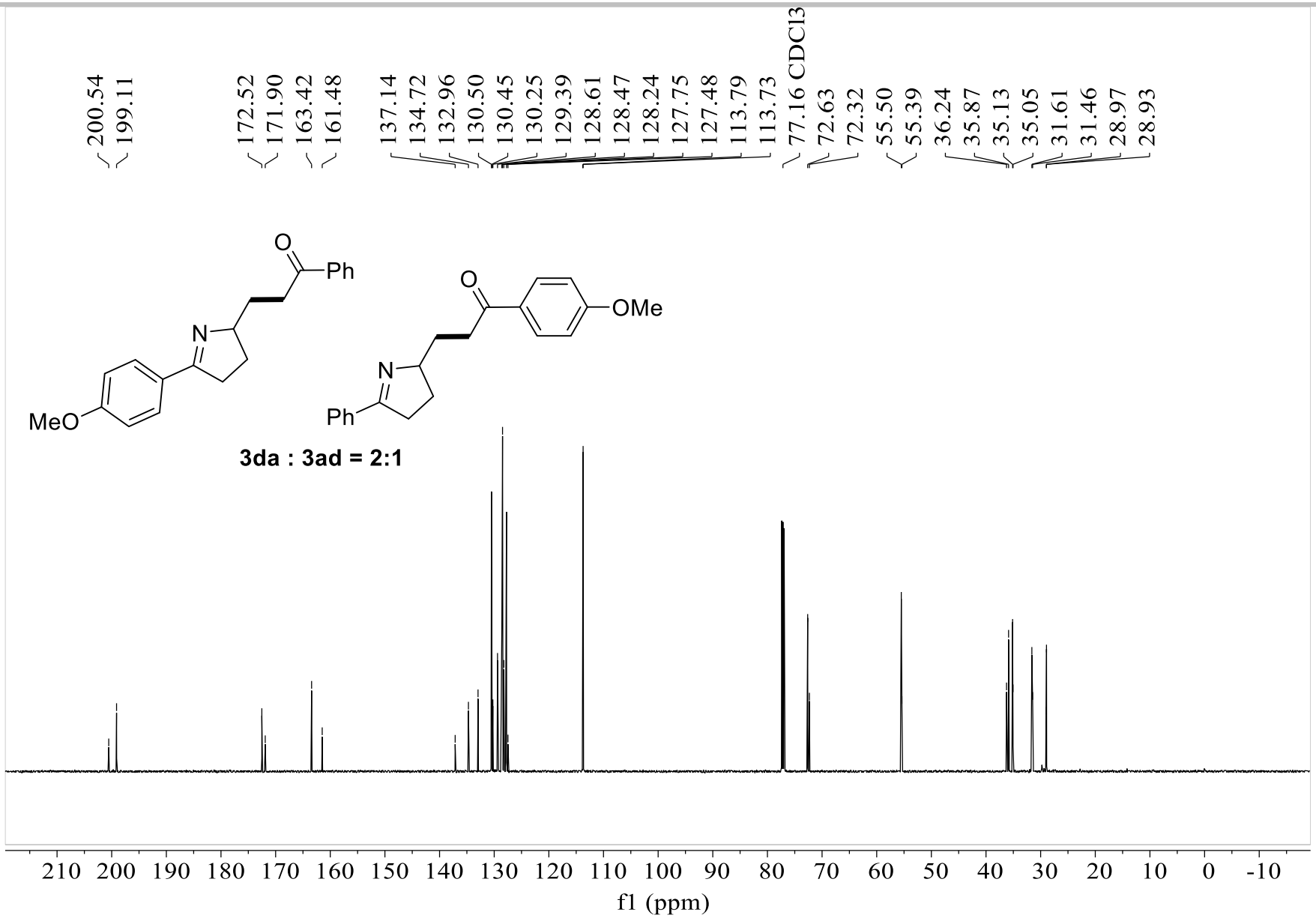

8.59
8.58
8.17
8.17
8.13
8.13
8.12
8.11
8.11
8.11
8.10
8.09
7.97
7.96
7.90
7.90
7.89
7.88
7.88
7.87
7.86
7.86
7.85
7.84
7.59
7.59
7.58
7.58
7.55
7.55
7.54
7.54
7.53
7.53
7.52
7.52
7.51
7.51
7.51
7.50
7.26 CDCl3
3.41
3.06
2.12
O
N
3gg
1.00
1.05
2.04
1.07
5.21
1.06
3.14
1.04
1.03
1.04
1.07
1.07
1.14
1.21
1.13
1.07
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

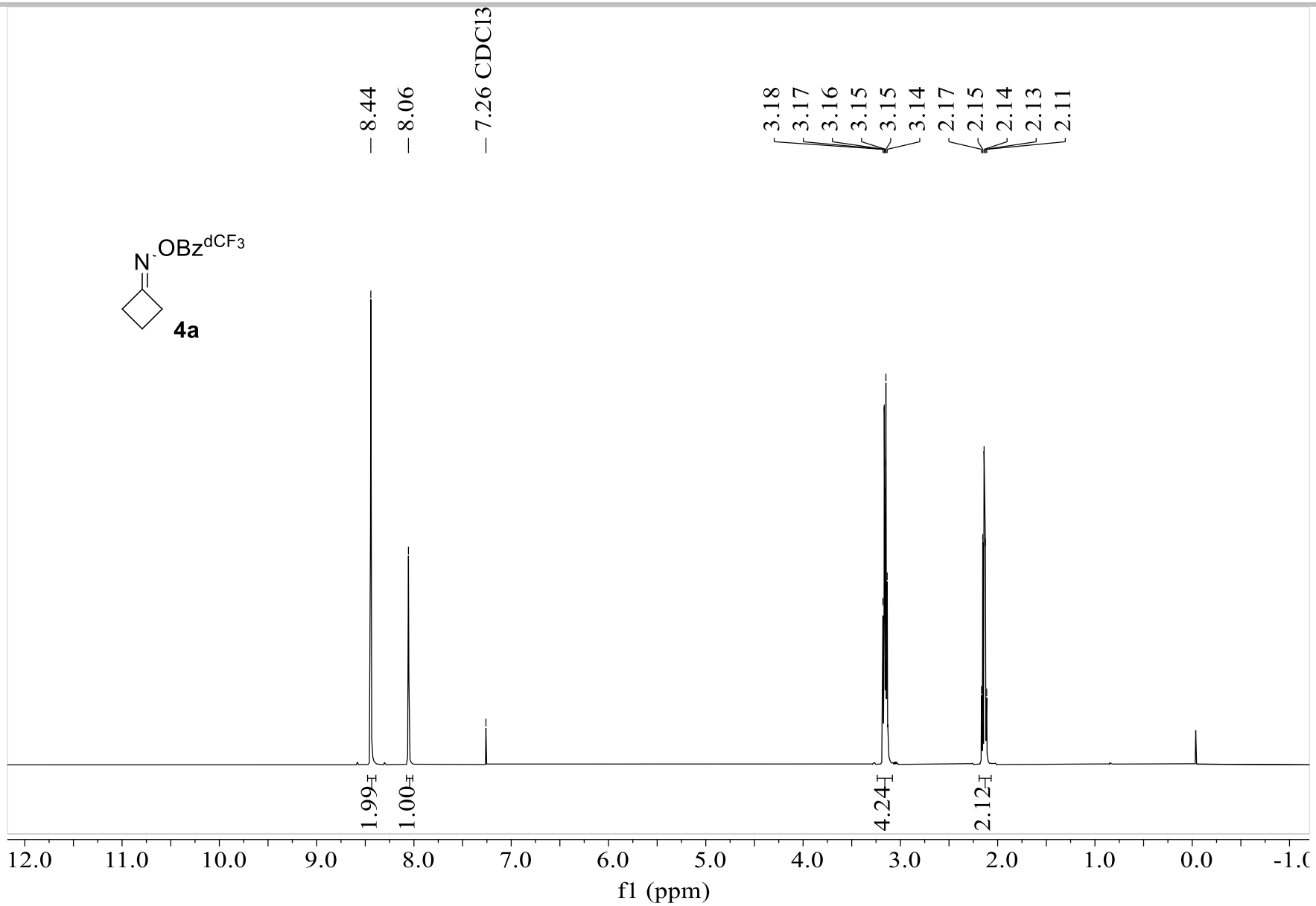

200.50
172.63
135.65
134.50
133.10
132.69
132.24
129.99
129.70
128.82
128.47
128.43
128.35
128.22
127.86
127.16
126.78
126.49
124.72
124.12
77.16 CDCl3
72.81
36.44
35.19
31.70
29.12
O
N
3gg
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

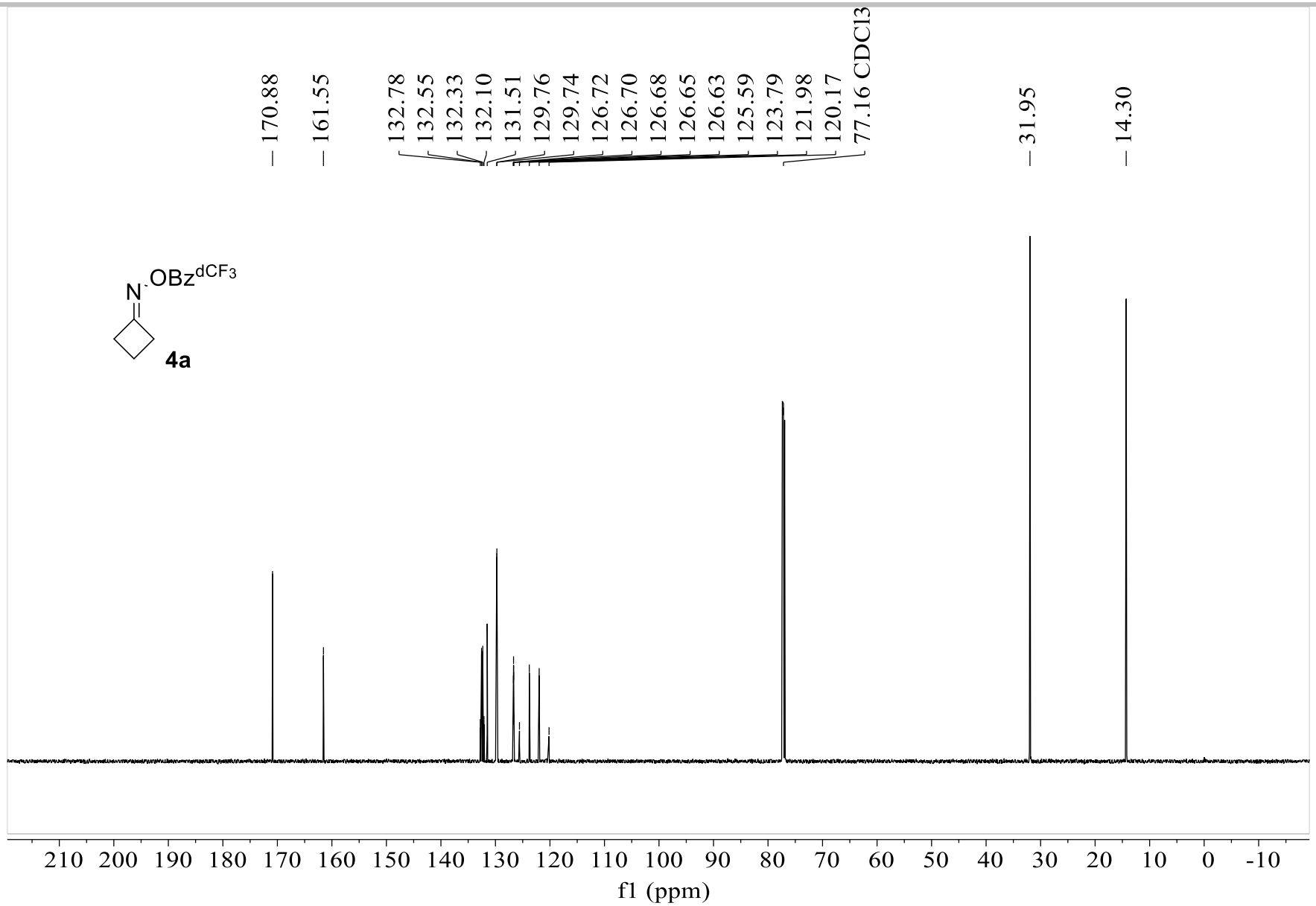

8.02 8.02 8.01 8.00 8.00 7.96 7.96 7.95 7.95 7.84 7.83 7.83 7.82 7.82 7.77 7.76 7.75 7.75 7.55 7.47 7.46 7.44 7.43 7.43 7.42 7.42 7.42 7.41 7.41 7.41 7.40 7.40 7.37 7.36 7.36 7.35 7.26 CDCl3 4.26 4.25 3.31 3.30 3.22 3.21 2.13
O
Ph
N
Cl
O
Cl
N
Ph
3ca : 3ac = 1:1
0.96 0.99 0.99 0.97 0.49 0.97 2.42 0.94 1.00 1.03 1.01 1.03 1.02 1.14 1.25 1.15 1.06
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

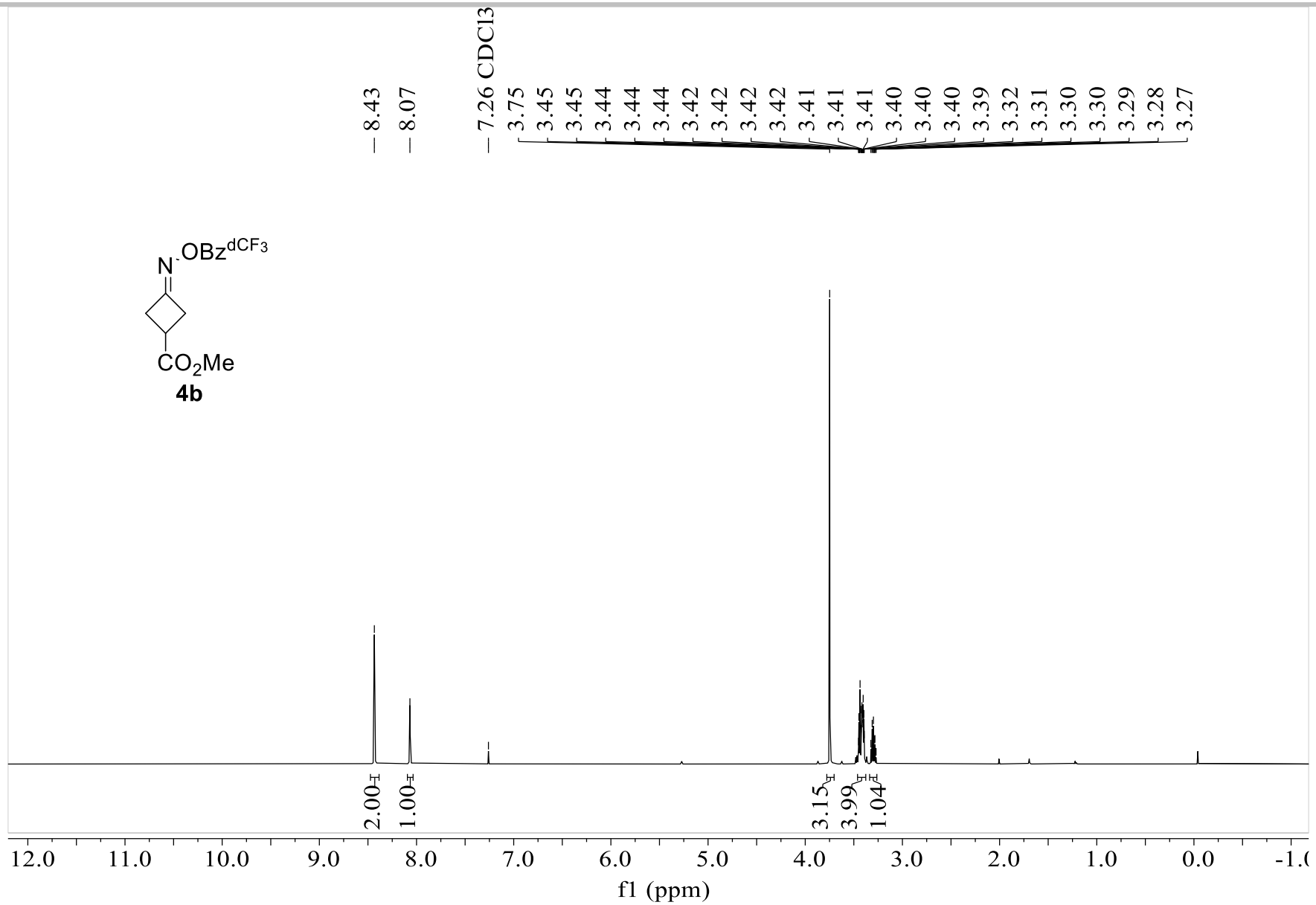

200.43
199.30
172.75
171.45
139.42
137.16
136.54
135.49
134.61
133.20
133.06
130.61
129.73
129.12
128.95
128.74
128.67
128.55
128.26
127.81
77.16 CDCl3
72.73
72.47
36.27
36.24
35.19
35.14
31.39
31.37
29.09
29.00
O
Ph
N
Cl
O
Cl
N
Ph
3ca : 3ac = 1:1
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

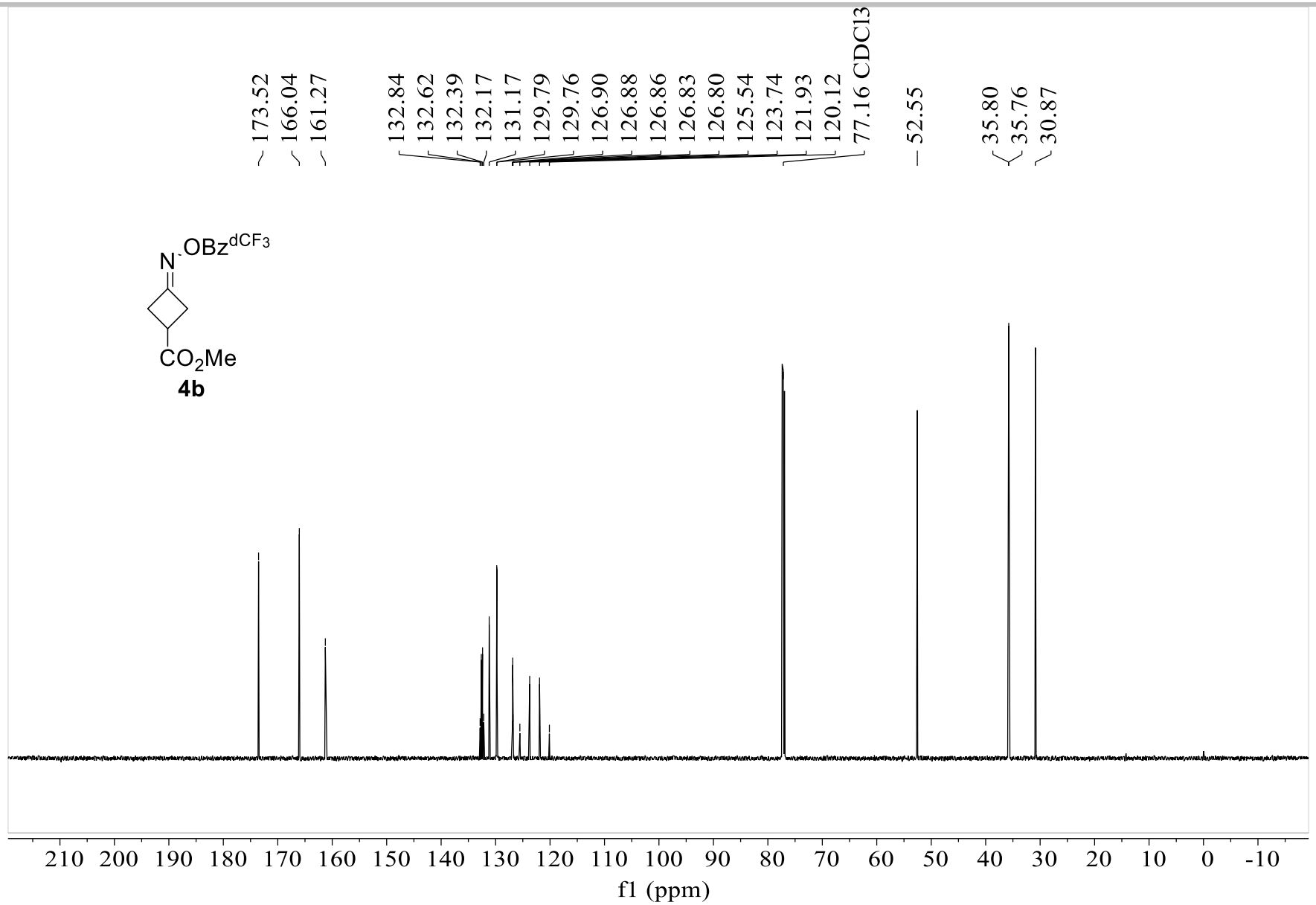

8.015
8.013
8.011
8.007
8.002
7.999
7.991
7.987
7.839
7.836
7.833
7.830
7.826
7.823
7.788
7.784
7.776
7.773
7.535
7.523
7.457
7.444
7.432
7.413
7.411
7.407
7.405
7.401
7.398
7.393
7.391
7.388
7.378
7.260 CDCl3
6.927
6.923
6.916
6.912
6.908
6.905
6.896
6.893
3.846
3.821
O
Ph
N
MeO
O
OMe
N
Ph
3da : 3ad = 2:1
1.96
1.34
0.62
0.32
0.64
1.93
1.96
1.00
2.04
0.94
2.10
1.09
1.10
1.06
1.03
1.08
1.05
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

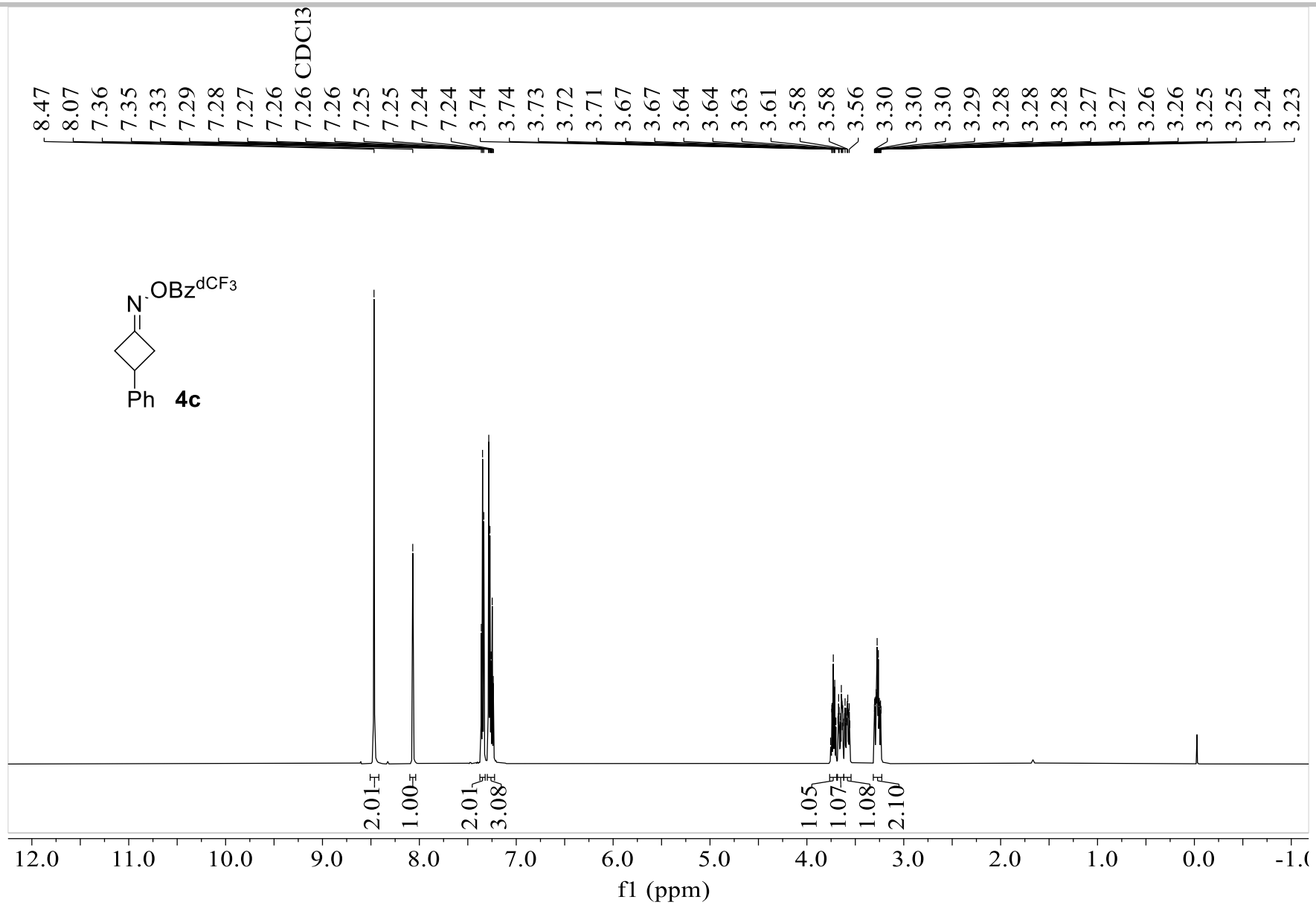

200.54
199.11
172.52
171.90
163.42
161.48
137.14
134.72
132.96
130.50
130.45
130.25
129.39
128.61
128.47
128.24
127.75
127.48
113.79
113.73
77.16 CDCl3
72.63
72.32
55.50
55.39
36.24
35.87
35.13
35.05
31.61
31.46
28.97
28.93
O
Ph
N
MeO
O
OMe
N
Ph
3da : 3ad = 2:1
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

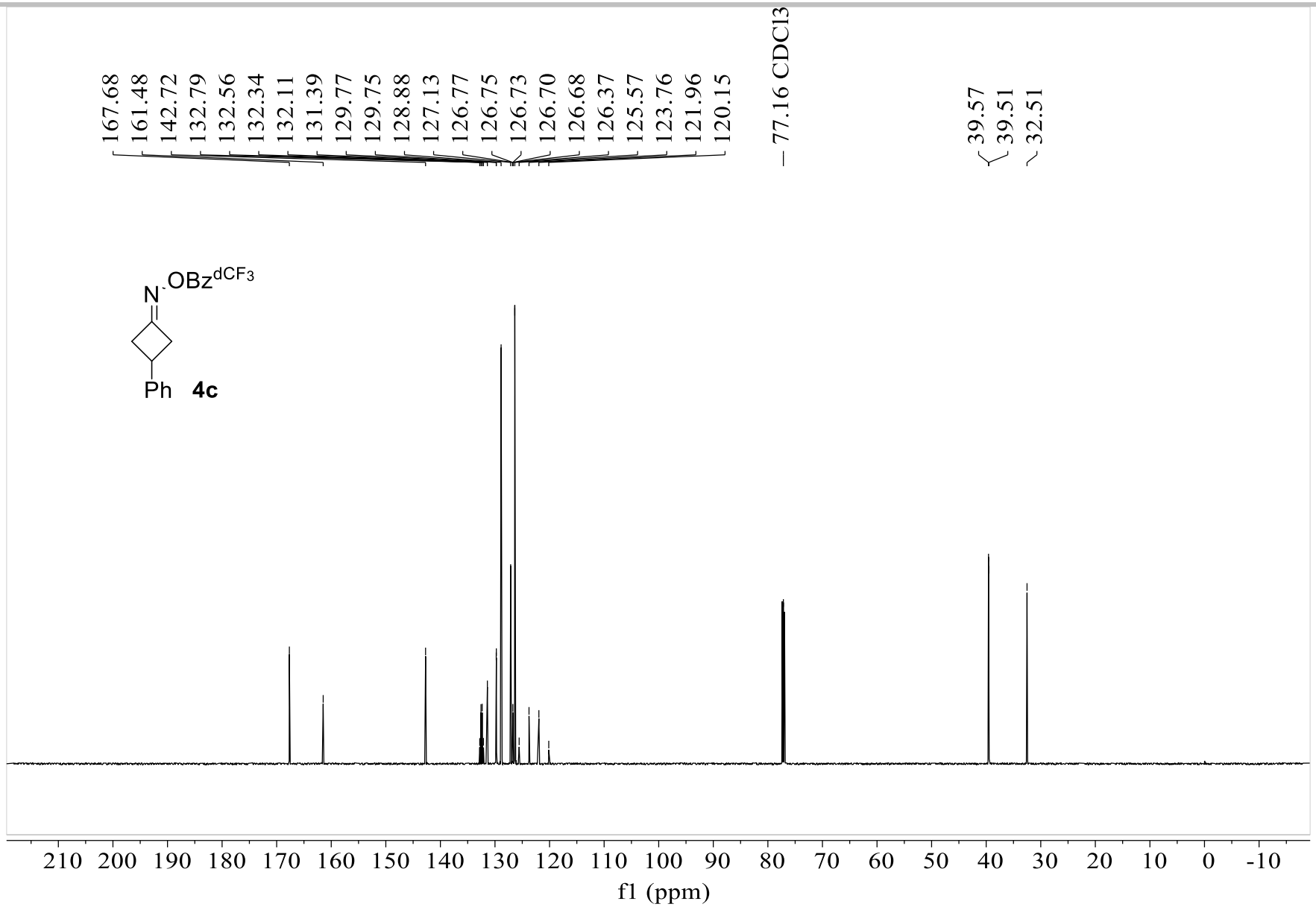

8.44
8.06
7.26 CDCl3
3.18
3.17
3.16
3.15
3.15
3.14
2.17
2.15
2.14
2.13
2.11
N
OBz^dCF3
4a
1.99
1.00
4.24
2.12
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

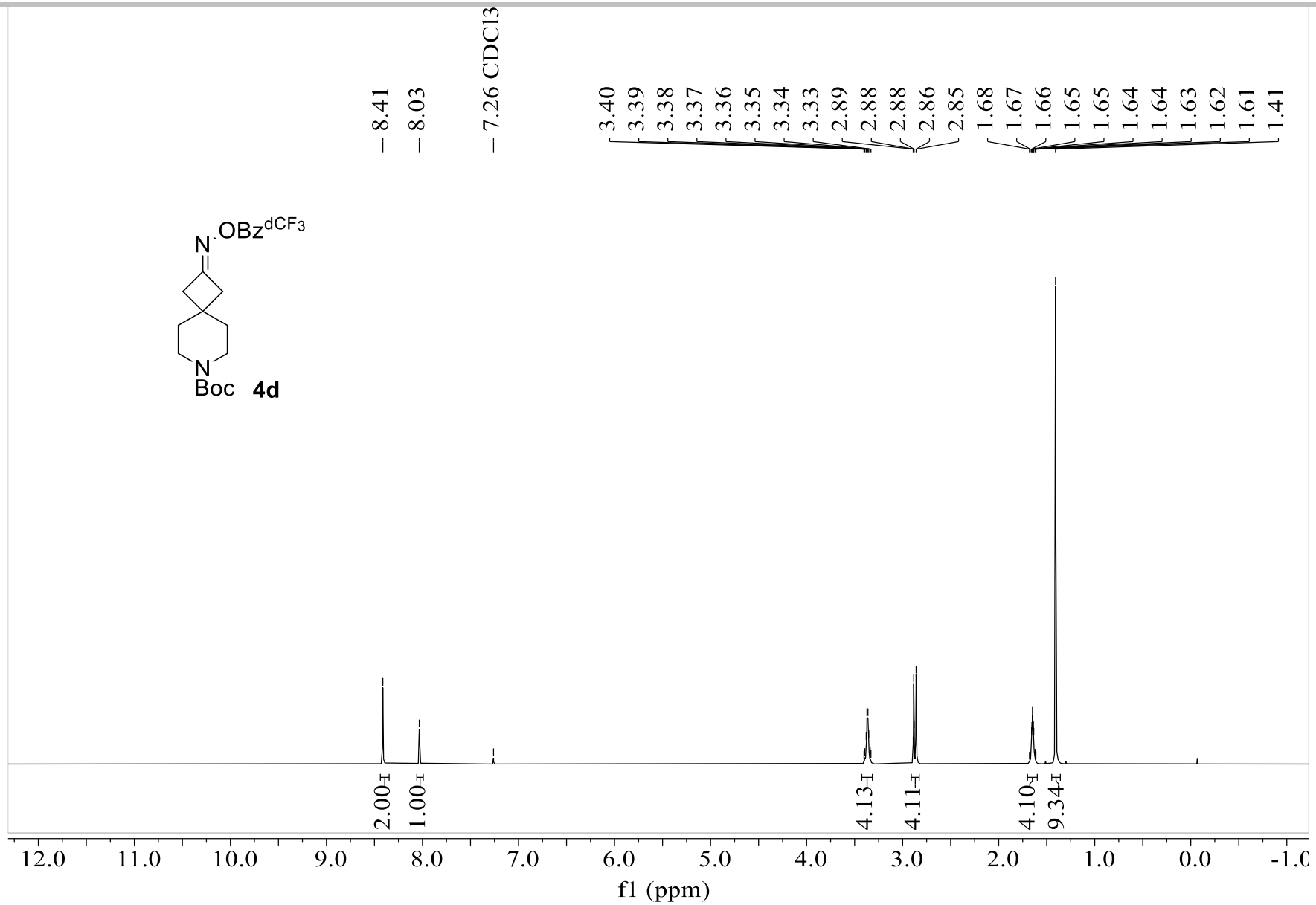

170.88
161.55
132.78
132.55
132.33
132.10
131.51
129.76
129.74
126.72
126.70
126.68
126.65
126.63
125.59
123.79
121.98
120.17
77.16 CDCl3
31.95
14.30
N
OBz^dCF3
4a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

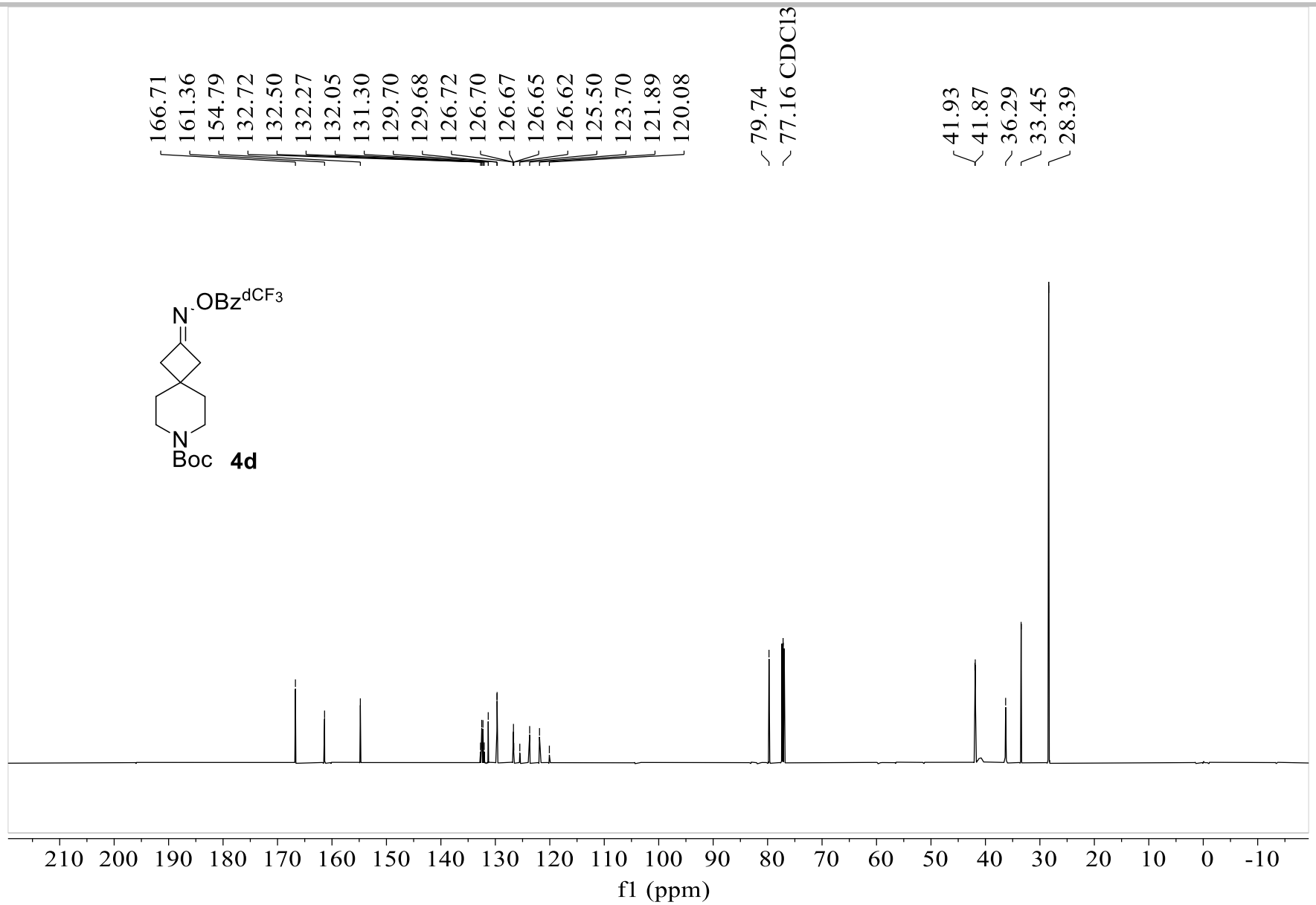

8.43
8.07
7.26 CDCl3
3.75
3.45
3.45
3.44
3.44
3.44
3.42
3.42
3.42
3.42
3.41
3.41
3.41
3.40
3.40
3.40
3.39
3.32
3.31
3.30
3.30
3.29
3.28
3.27
N
OBz^dCF3
CO2Me
4b
2.00
1.00
3.15
3.99
1.04
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

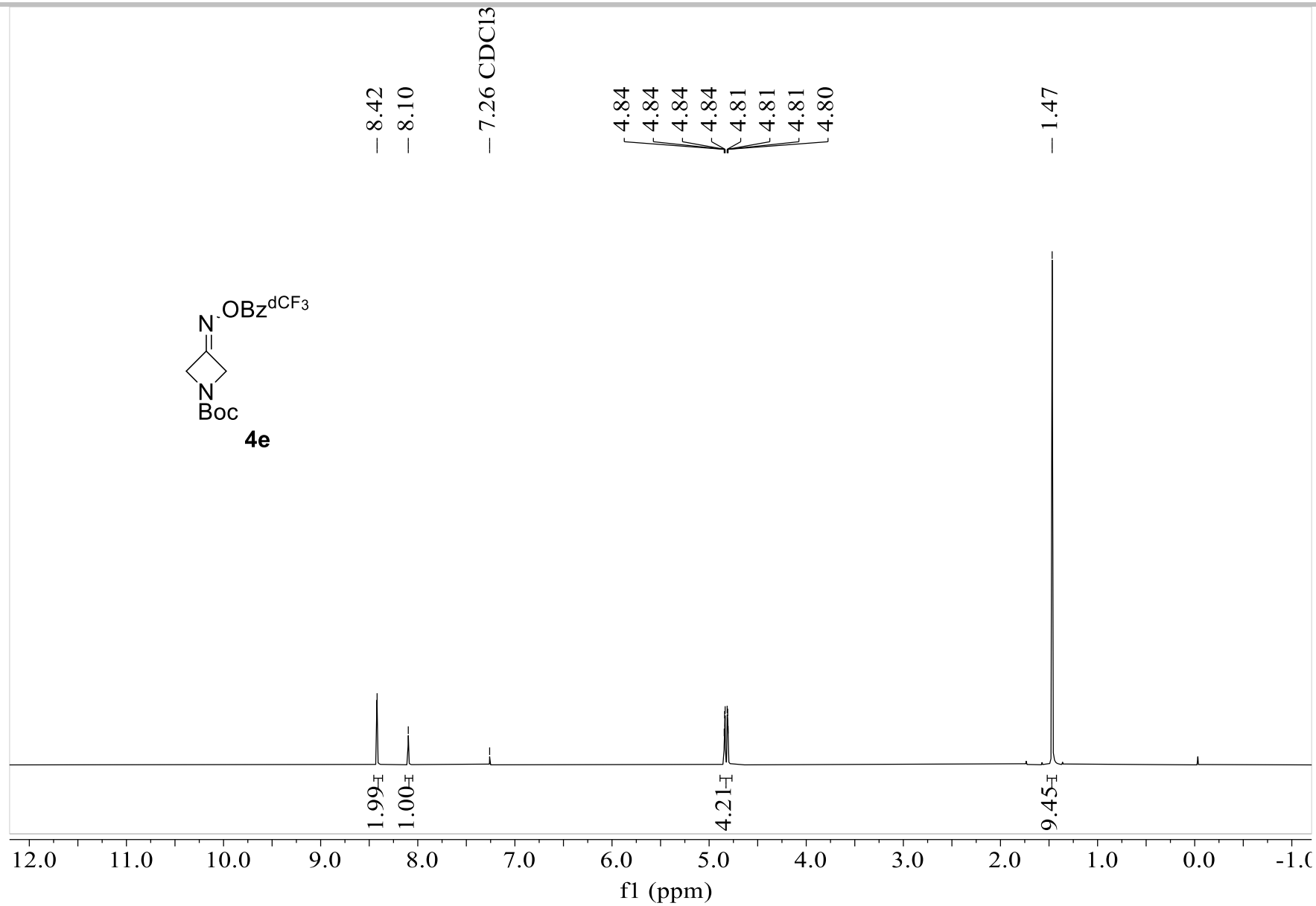

173.52
166.04
161.27
132.84
132.62
132.39
132.17
131.17
129.79
129.76
126.90
126.88
126.86
126.83
126.80
125.54
123.74
121.93
120.12
77.16 CDCl3
52.55
35.80
35.76
30.87
N
OBz^dCF3
CO2Me
4b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

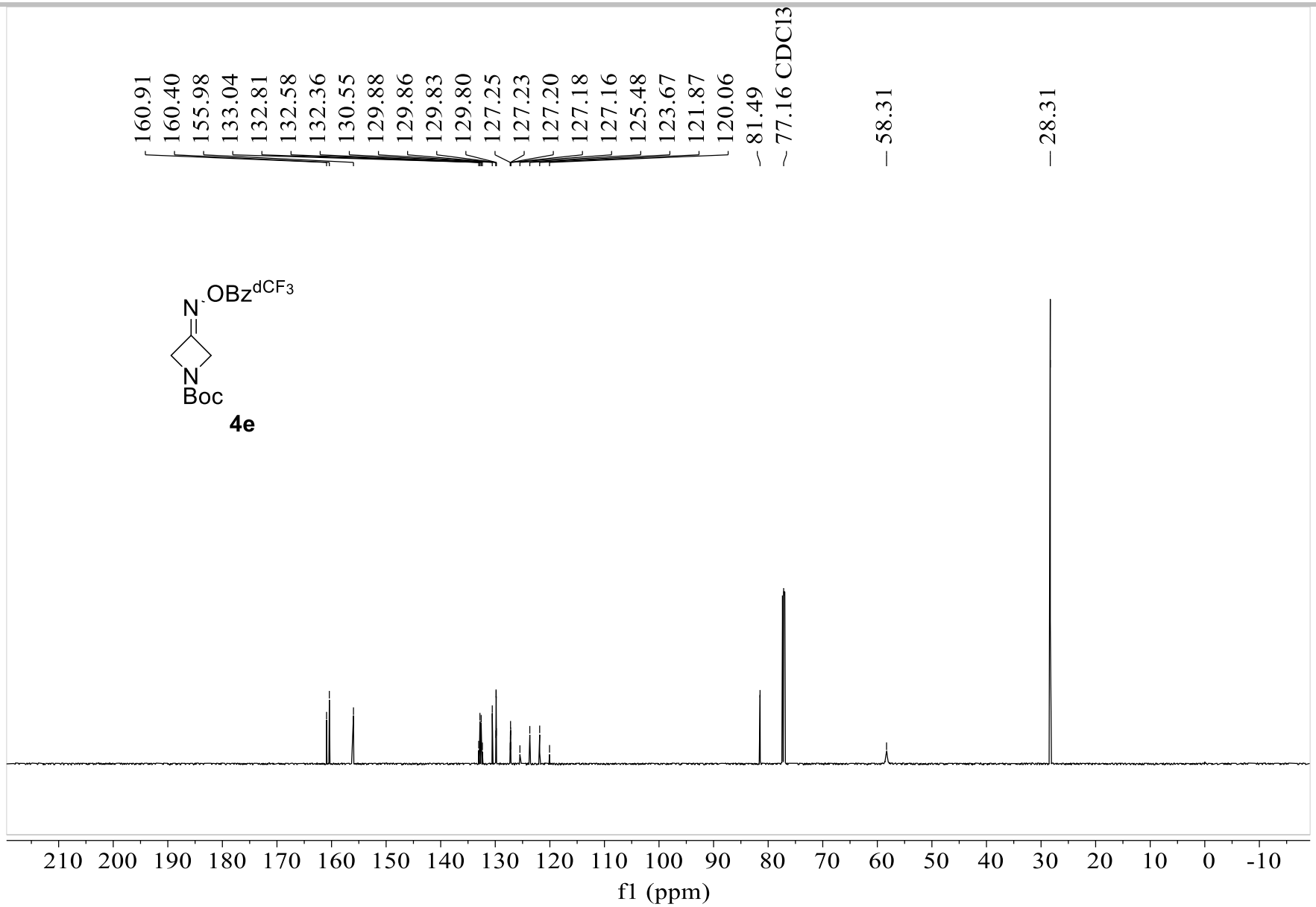

8.47
8.07
7.36
7.35
7.33
7.29
7.28
7.27
7.26
7.26 CDCl3
7.26
7.25
7.25
7.24
7.24
3.74
3.74
3.73
3.72
3.71
3.67
3.67
3.64
3.64
3.63
3.61
3.58
3.58
3.56
3.30
3.30
3.30
3.29
3.28
3.28
3.28
3.27
3.27
3.26
3.26
3.25
3.25
3.24
3.23
N
OBz^dCF3
Ph
4c
2.01
1.00
2.01
3.08
1.05
1.07
1.08
2.10
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

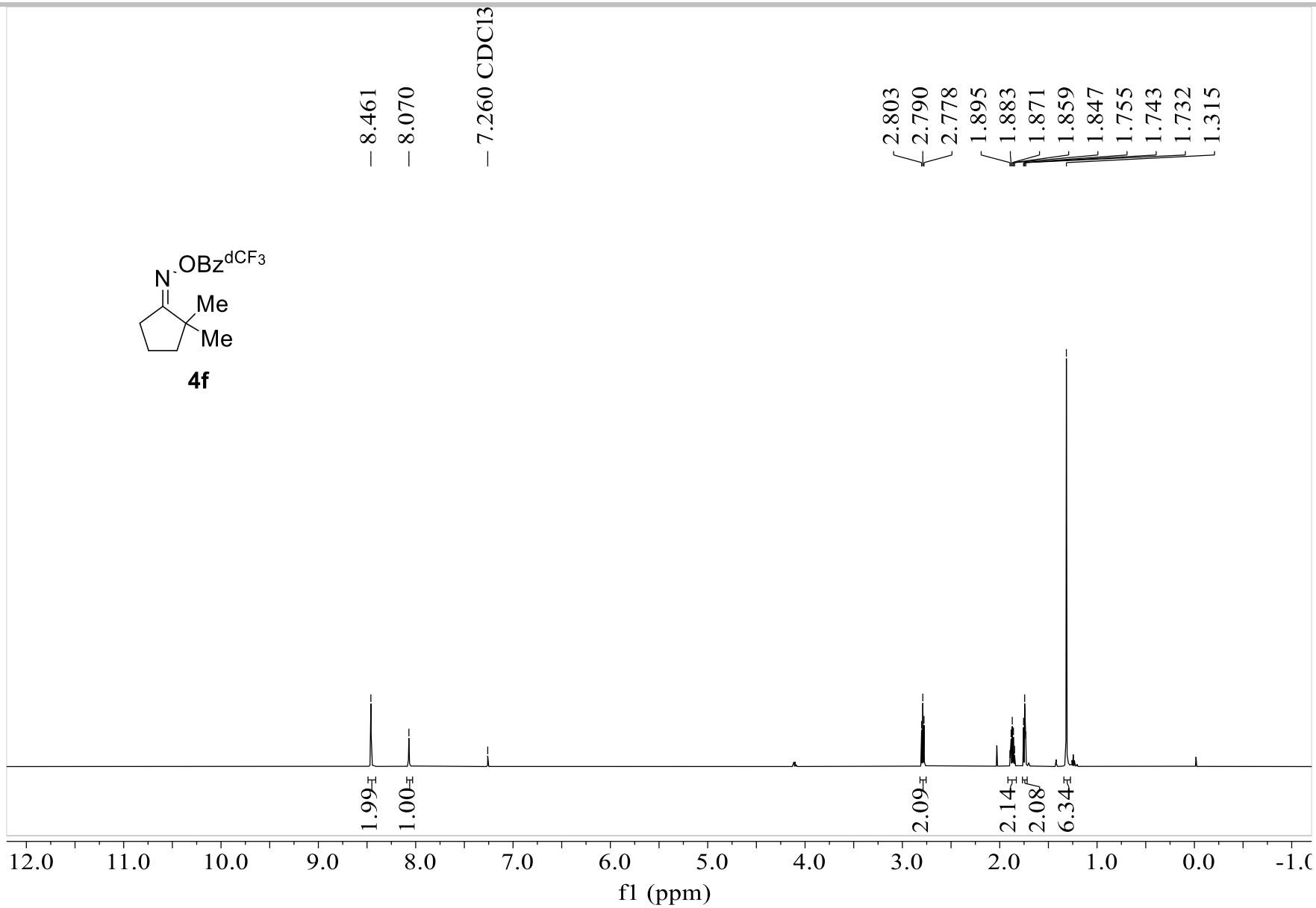

167.68
161.48
142.72
132.79
132.56
132.34
132.11
131.39
129.77
129.75
128.88
127.13
126.77
126.75
126.73
126.70
126.68
126.37
125.57
123.76
121.96
120.15
77.16 CDCl3
39.57
39.51
32.51
N
OBz^dCF3
Ph
4c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

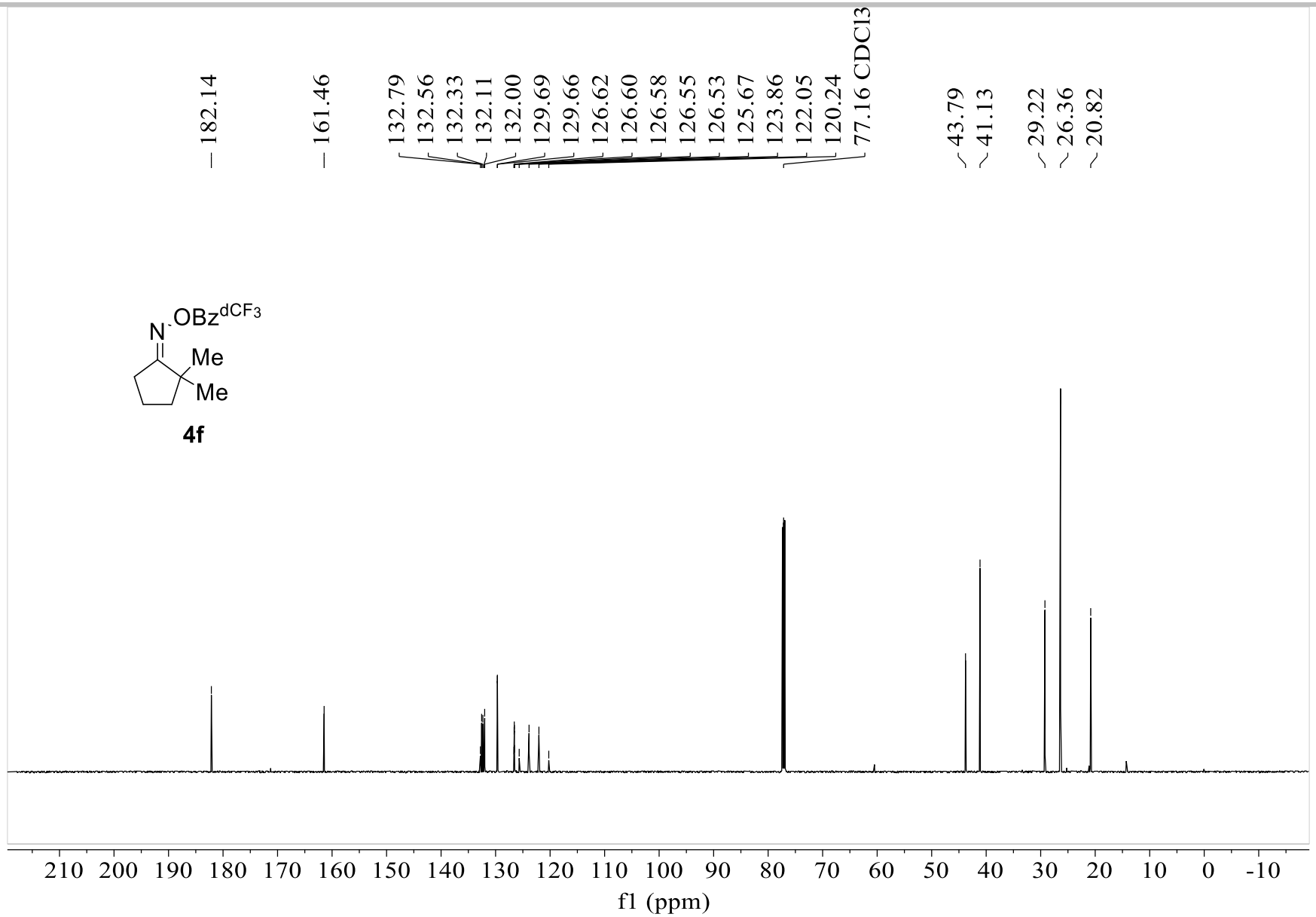

8.41
8.03
7.26 CDCl3
3.40
3.39
3.38
3.37
3.36
3.35
3.34
3.33
2.89
2.88
2.88
2.86
2.85
1.68
1.67
1.66
1.65
1.65
1.64
1.64
1.63
1.62
1.61
1.41
N
OBz^dCF3
N
Boc
4d
2.00
1.00
4.13
4.11
4.10
9.34
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)

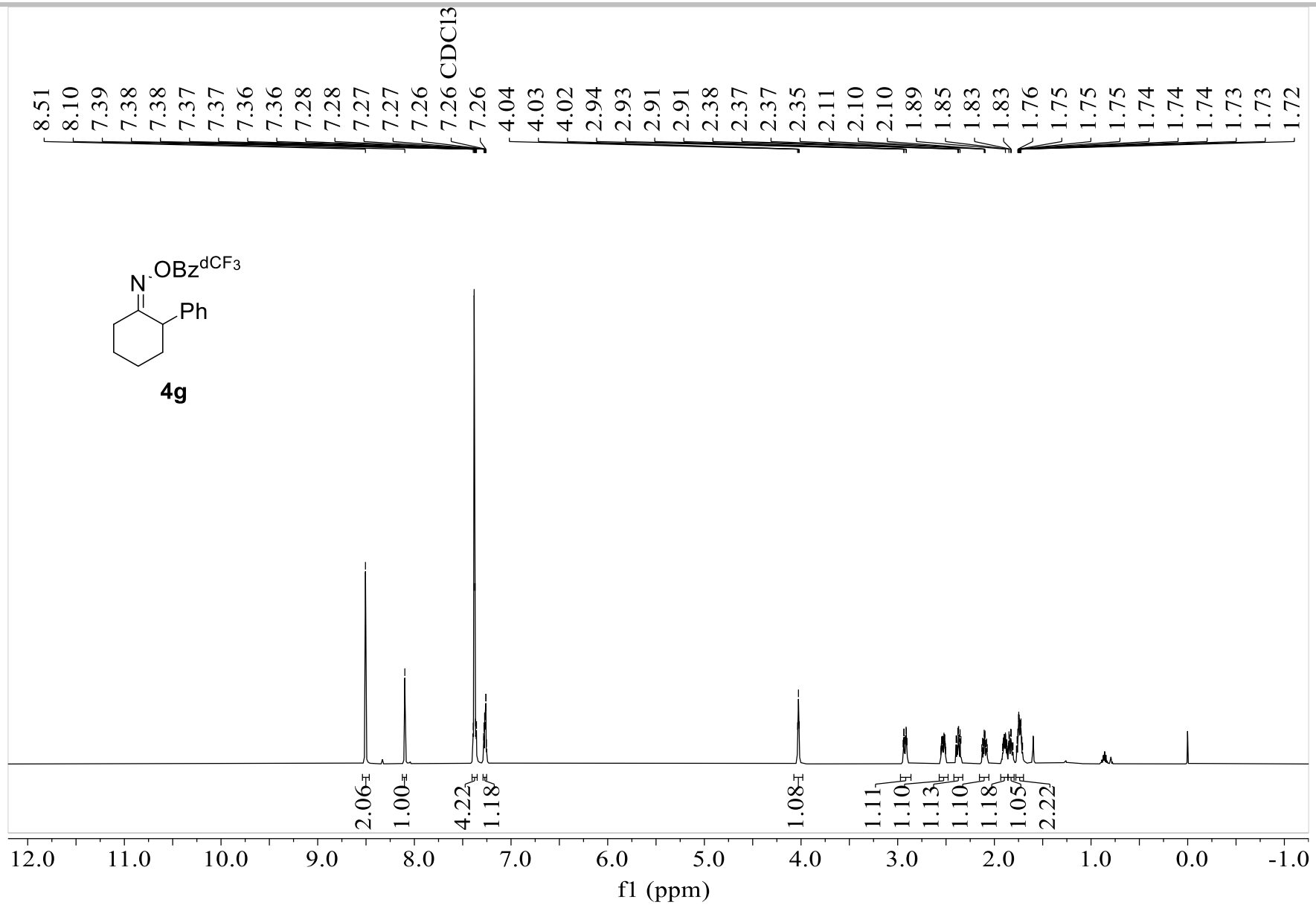

166.71
161.36
154.79
132.72
132.50
132.27
132.05
131.30
129.70
129.68
126.72
126.70
126.67
126.65
126.62
125.50
123.70
121.89
120.08
79.74
77.16 CDCl3
41.93
41.87
36.29
33.45
28.39
N
OBz^dCF3
N
Boc
4d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

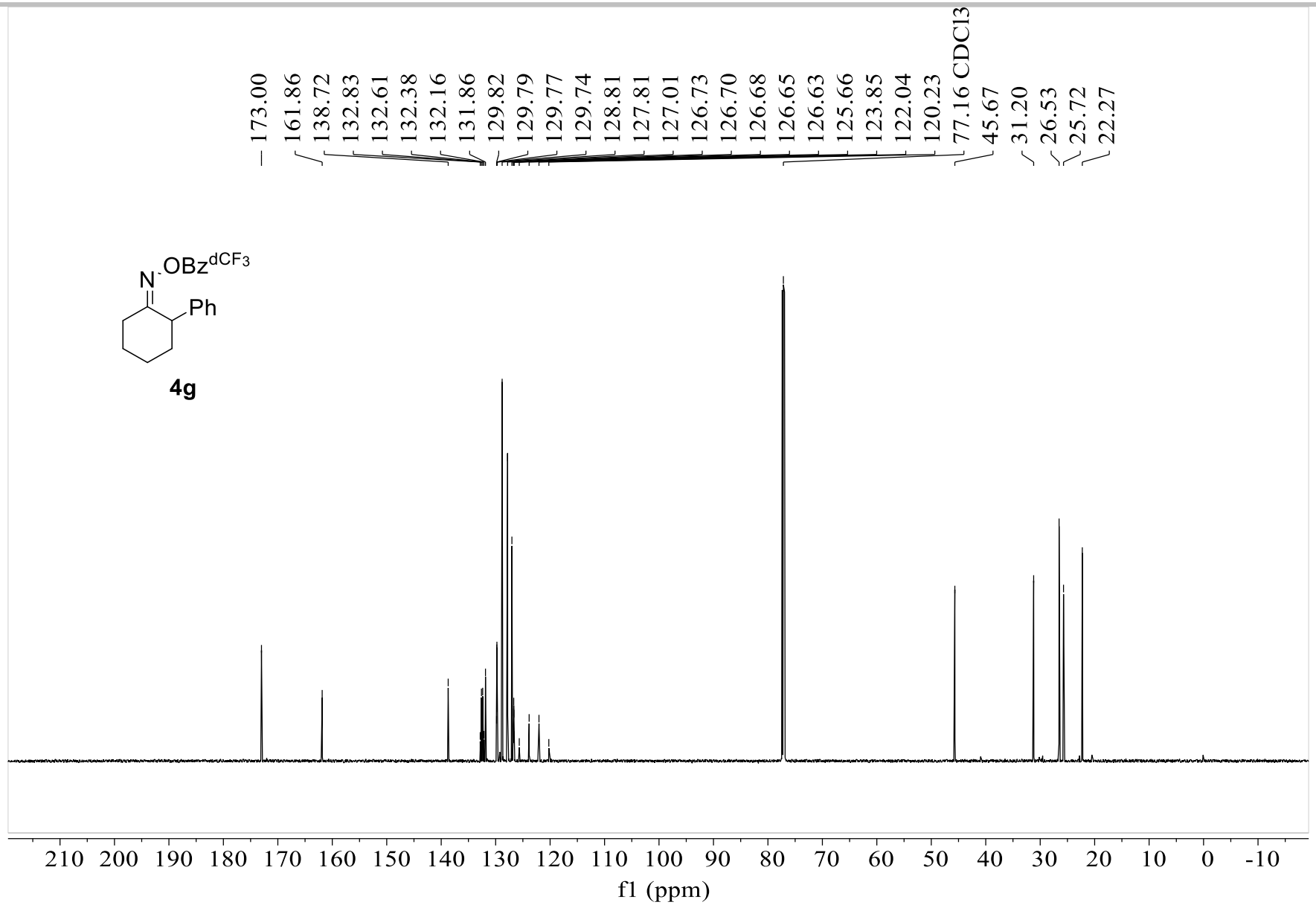

8.42
8.10
7.26 CDCl3
4.84
4.84
4.84
4.84
4.81
4.81
4.81
4.80
1.47
OBz^dCF3
N
N
Boc
4e
1.99
1.00
4.21
9.45
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


160.91
160.40
155.98
133.04
132.81
132.58
132.36
130.55
129.88
129.86
129.83
129.80
127.25
127.23
127.20
127.18
127.16
125.48
123.67
121.87
120.06
81.49
77.16 CDCl3
58.31
28.31
OBz^dCF3
N
N
Boc
4e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.461
8.070
7.260 CDCl3
2.803
2.790
2.778
1.895
1.883
1.871
1.859
1.847
1.755
1.743
1.732
1.315
N
OBz^dCF3
Me
Me
4f
1.99
1.00
2.09
2.14
2.08
6.34
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


182.14
161.46
132.79
132.56
132.33
132.11
132.00
129.69
129.66
126.62
126.60
126.58
126.55
126.53
125.67
123.86
122.05
120.24
77.16 CDCl3
43.79
41.13
29.22
26.36
20.82
N
OBz^dCF3
Me
Me
4f
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.51
8.10
7.39
7.38
7.38
7.37
7.37
7.36
7.36
7.28
7.28
7.27
7.27
7.26
7.26 CDCl3
7.26
4.04
4.03
4.02
2.94
2.93
2.91
2.91
2.38
2.37
2.37
2.35
2.11
2.10
2.10
1.89
1.85
1.83
1.83
1.76
1.75
1.75
1.75
1.74
1.74
1.74
1.73
1.73
1.72
N
OBz^dCF3
Ph
4g
2.06
1.00
4.22
1.18
1.08
1.11
1.10
1.13
1.10
1.18
1.05
2.22
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)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129.77
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128.81
127.81
127.01
126.73
126.70
126.68
126.65
126.63
125.66
123.85
122.04
120.23
77.16 CDCl3
45.67
31.20
26.53
25.72
22.27
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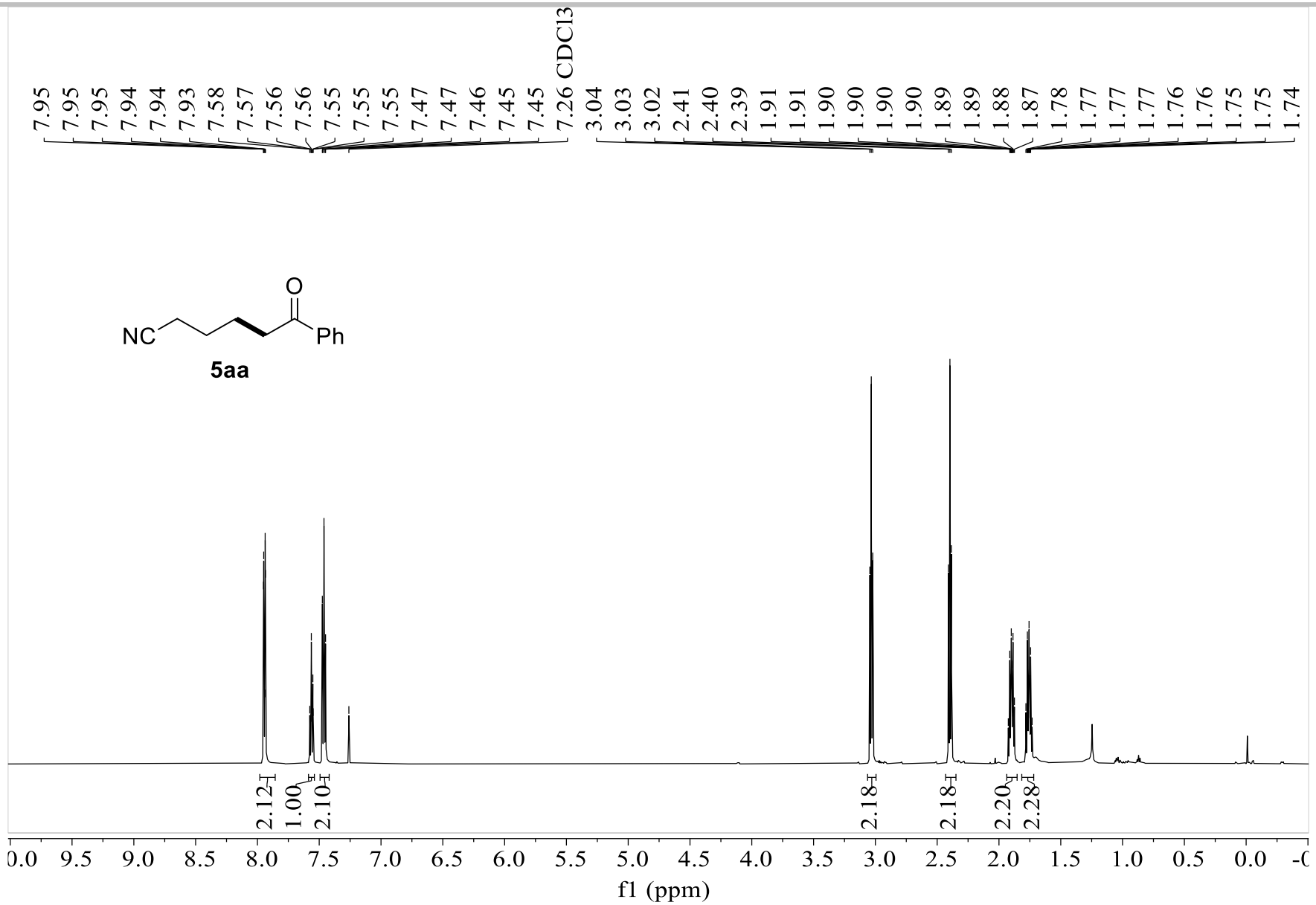
OBz^dCF3
Ph
4g
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.55
7.47
7.47
7.46
7.45
7.45
7.26 CDCl3
3.04
3.03
3.02
2.41
2.40
2.39
1.91
1.91
1.90
1.90
1.90
1.90
1.89
1.89
1.88
1.87
1.78
1.77
1.77
1.77
1.76
1.76
1.75
1.75
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Ph
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2.18
2.18
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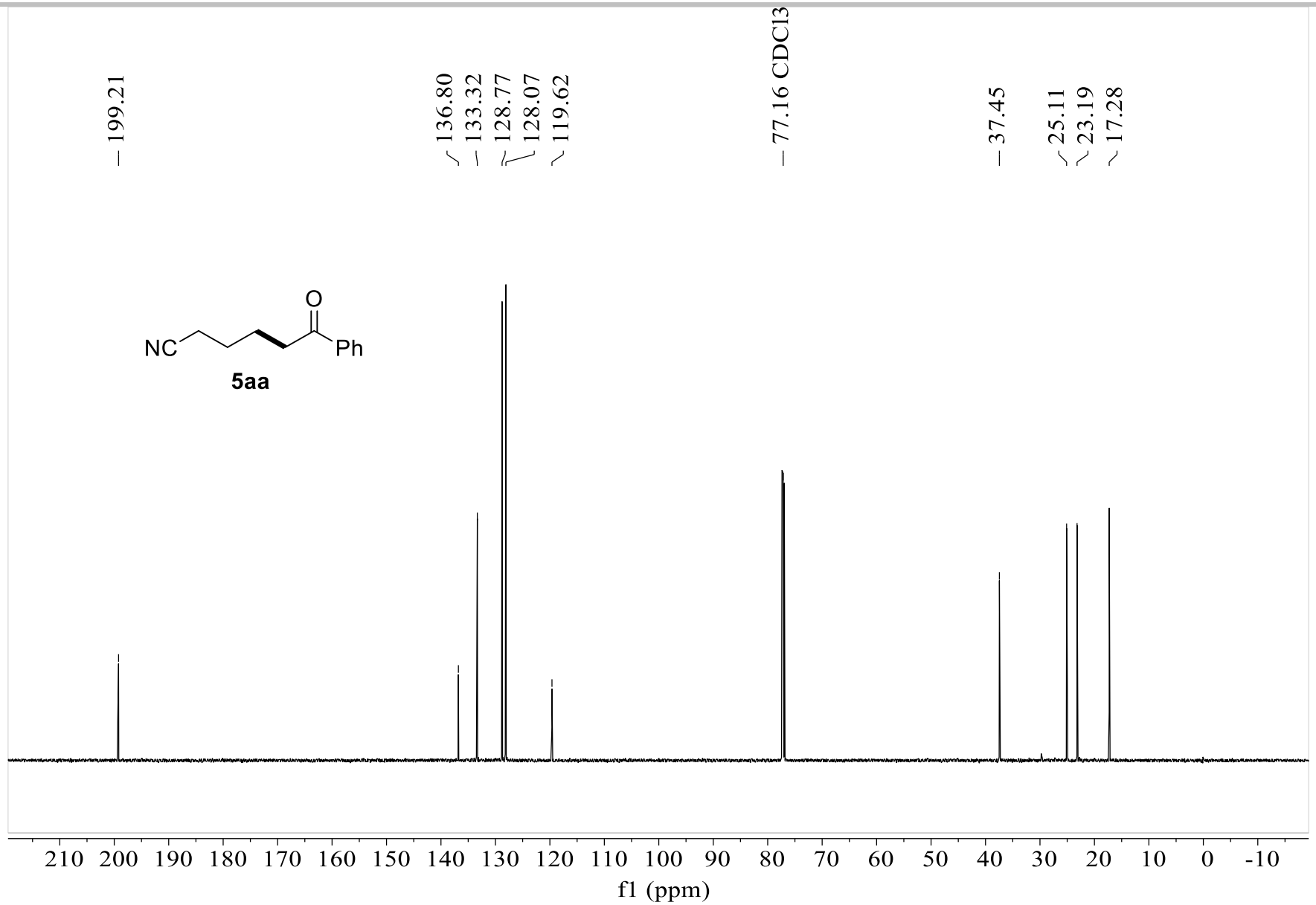
2.28
f1 (ppm)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37.45
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NC
Ph
5aa
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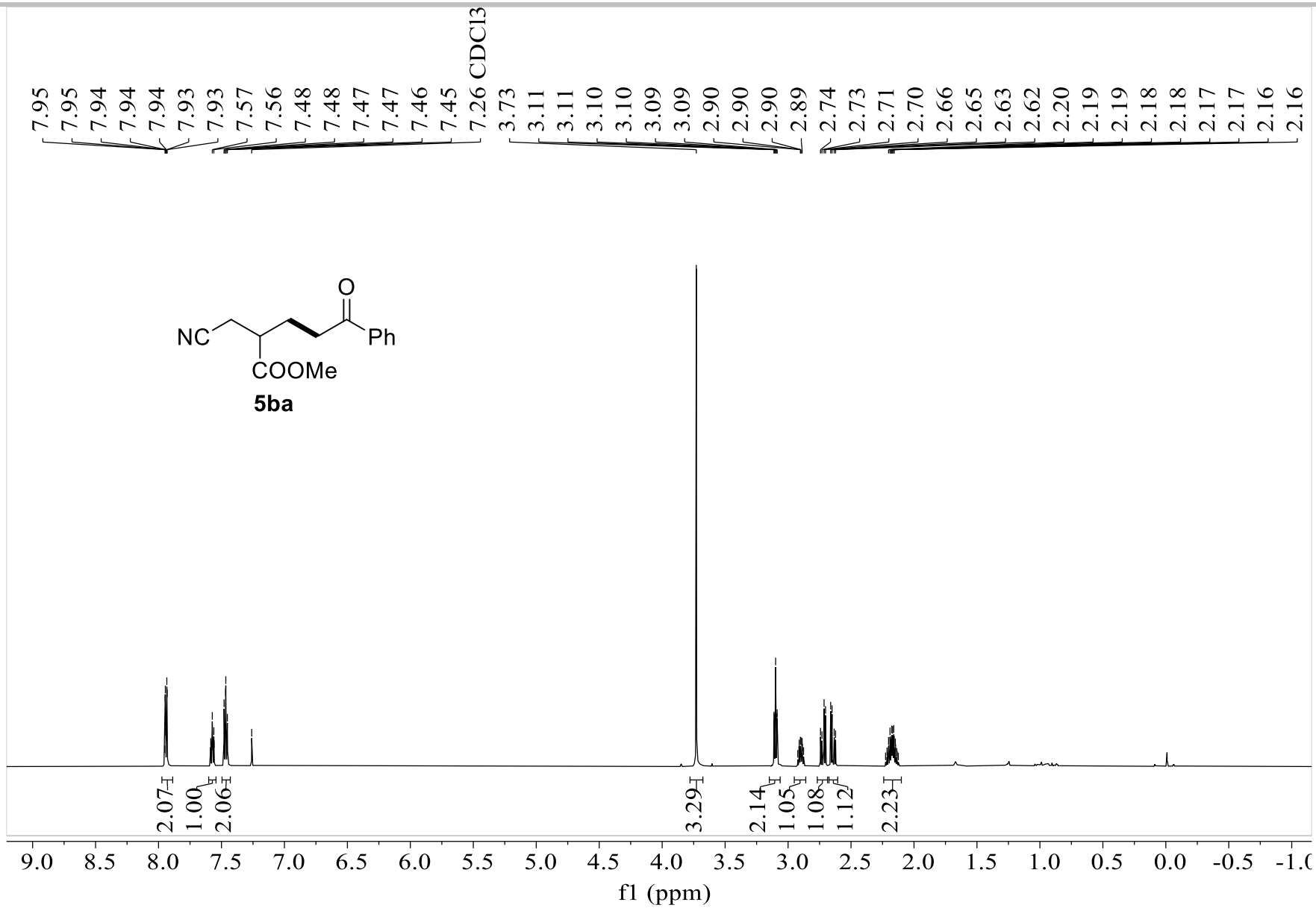
f1 (ppm)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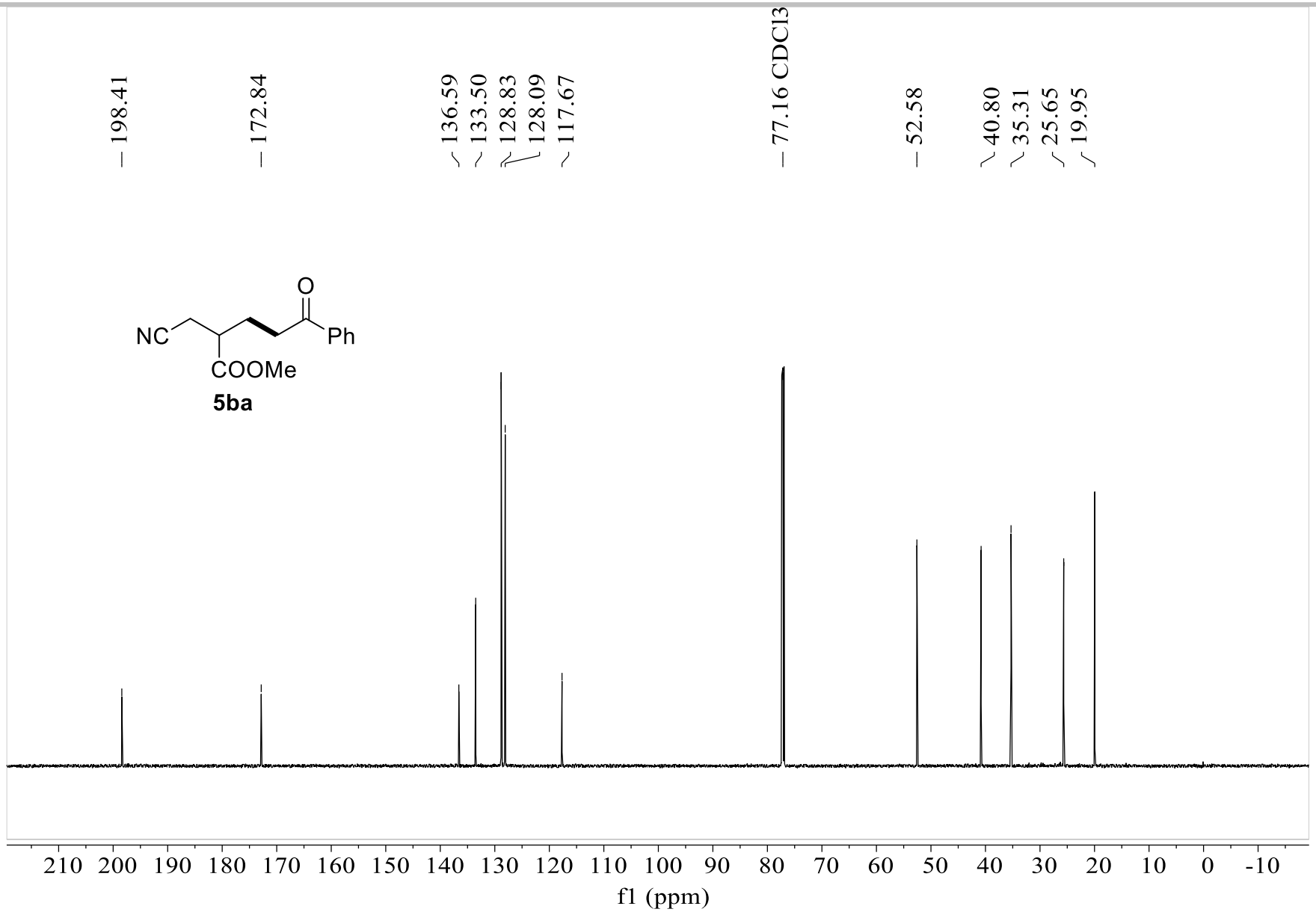
7.48
7.47
7.47
7.46
7.45
7.26 CDCl3
3.73
3.11
3.11
3.10
3.10
3.09
3.09
2.90
2.90
2.90
2.89
2.74
2.73
2.71
2.70
2.66
2.65
2.63
2.62
2.20
2.19
2.19
2.18
2.18
2.17
2.17
2.16
2.16
O
NC
Ph
COOMe
5ba
2.07
1.00
2.06
3.29
2.14
1.05
1.08
1.12
2.23
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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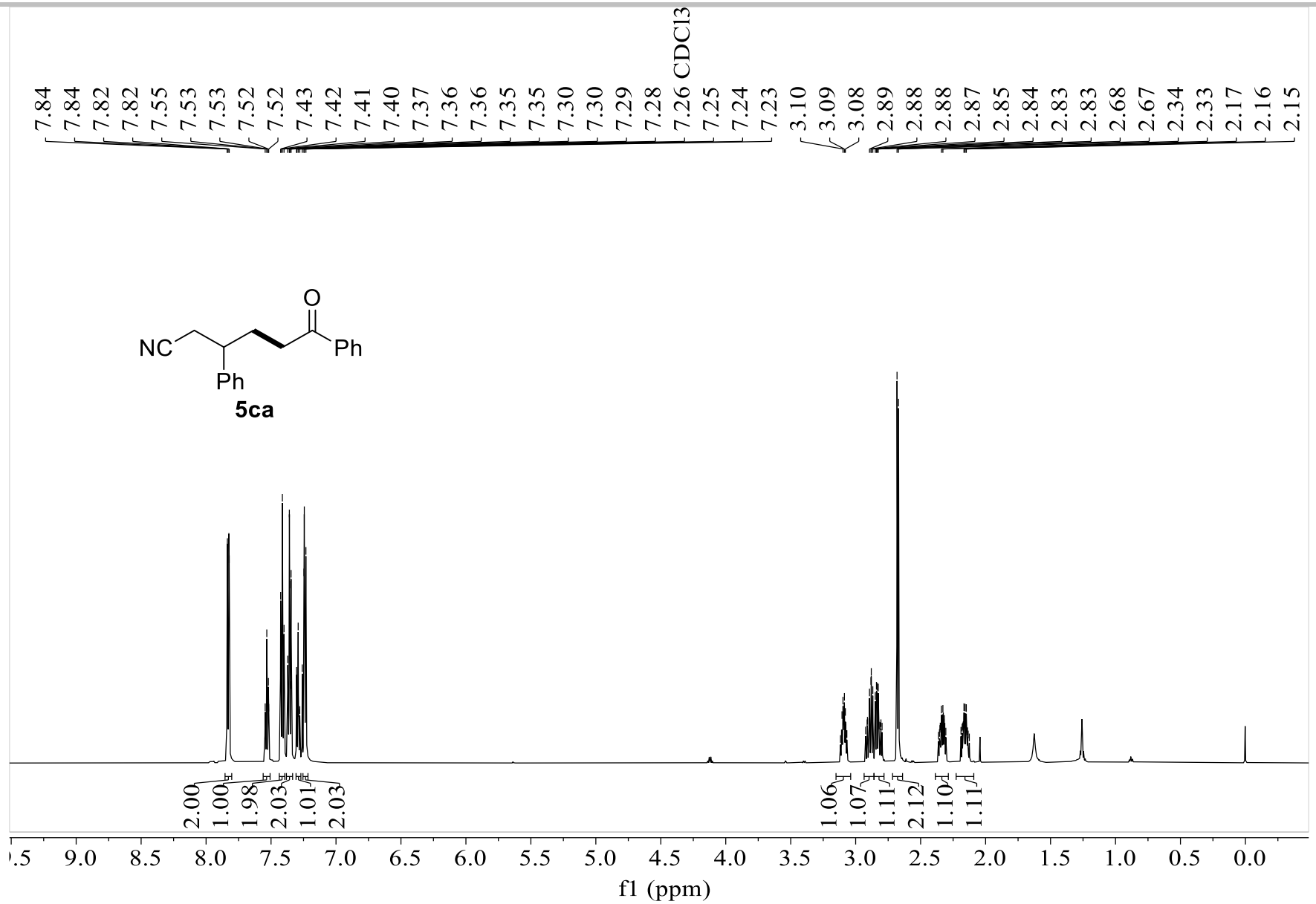
NC
Ph
COOMe
5ba
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.82
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7.53
7.52
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7.43
7.42
7.41
7.40
7.37
7.36
7.36
7.35
7.35
7.30
7.30
7.29
7.28
7.26 CDCl3
7.25
7.24
7.23
3.10
3.09
3.08
2.89
2.88
2.88
2.87
2.85
2.84
2.83
2.83
2.68
2.67
2.34
2.33
2.17
2.16
2.15
O
NC
Ph
Ph
5ca
2.00
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1.98
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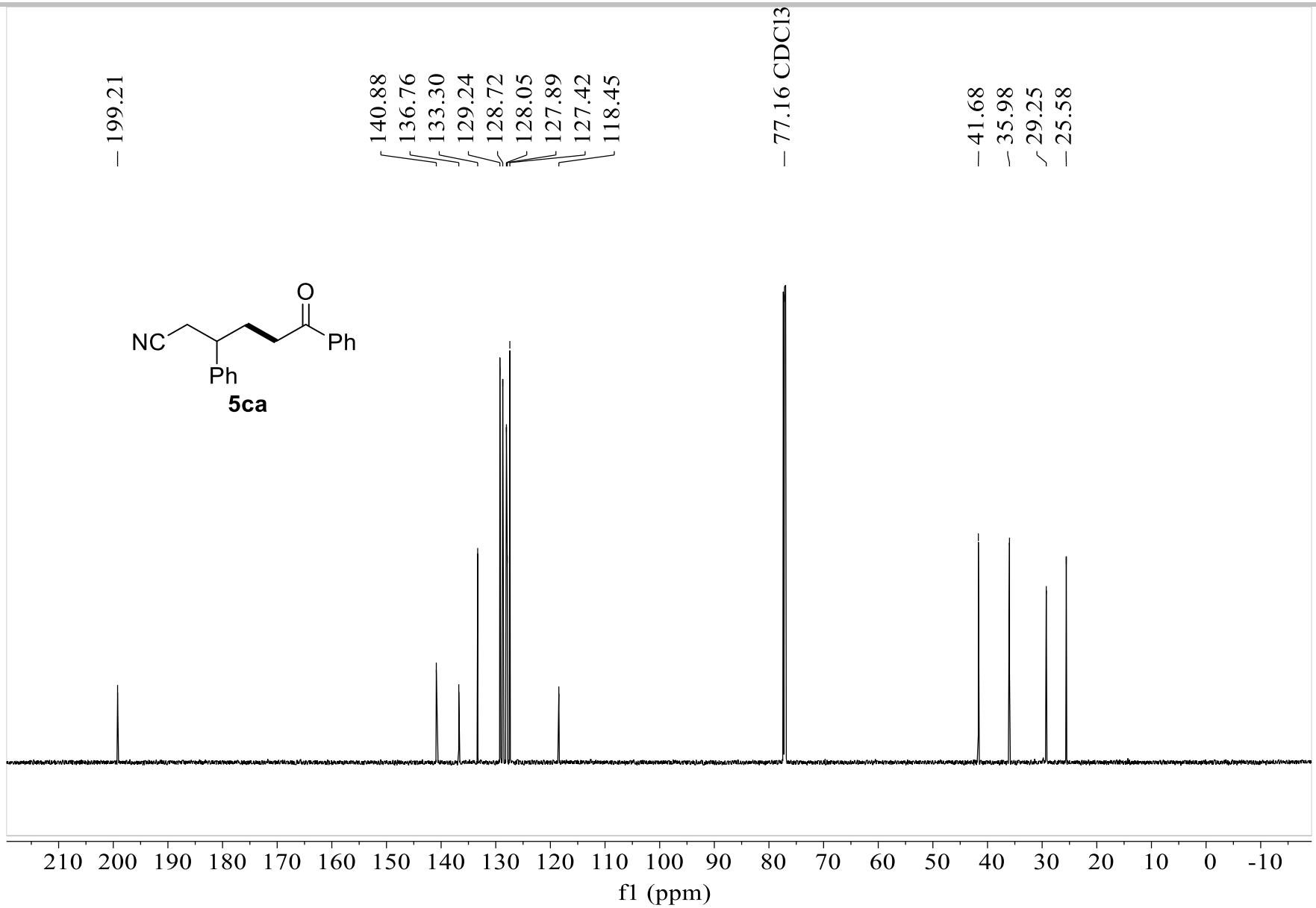
1.01
2.03
1.06
1.07
1.11
2.12
1.10
1.11
f1 (ppm)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140.88
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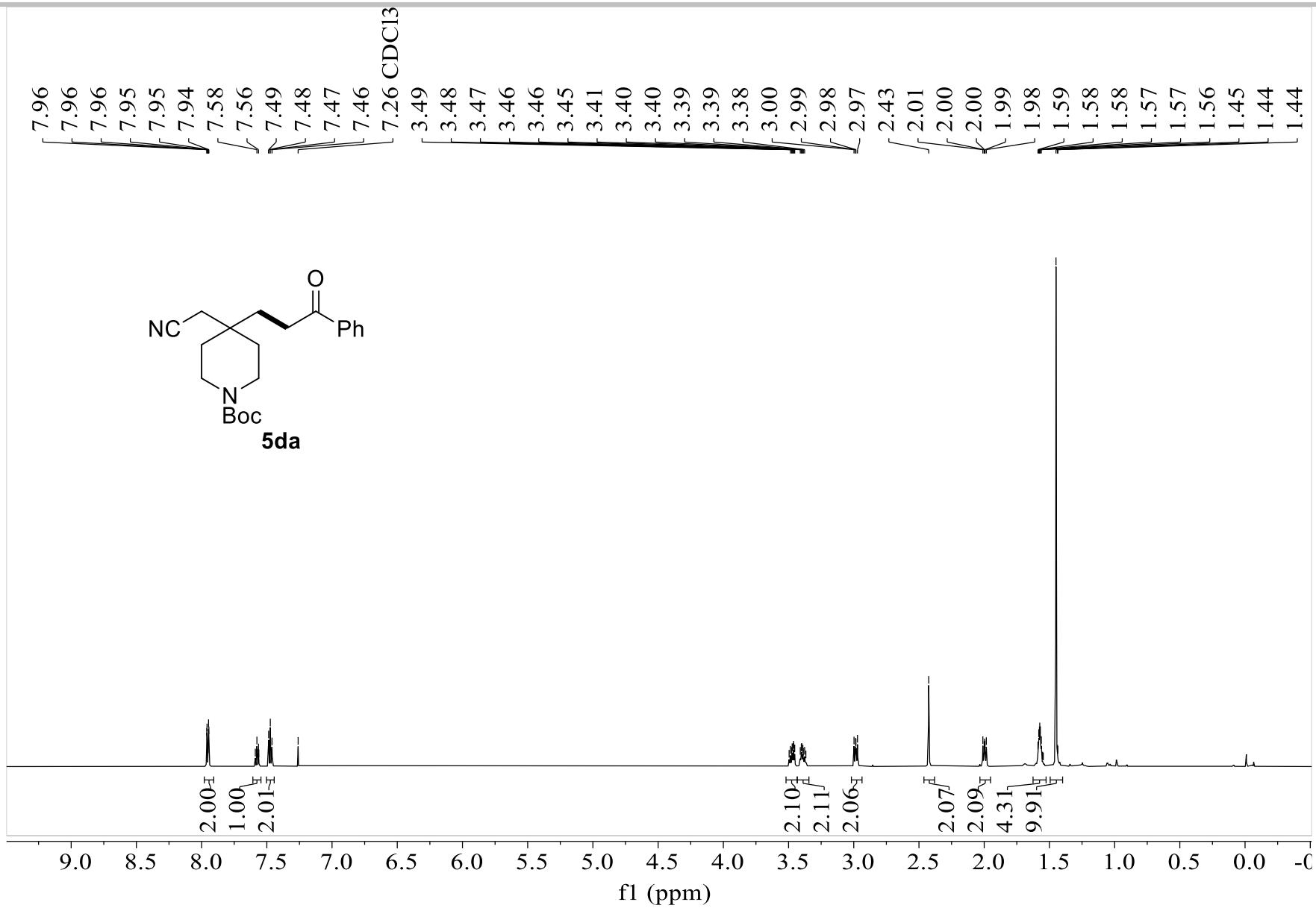
128.72
128.05
127.89
127.42
118.45
77.16 CDCl3
41.68
35.98
29.25
25.58
O
NC
Ph
Ph
5ca
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.94
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7.56
7.49
7.48
7.47
7.46
7.26 CDCl3
3.49
3.48
3.47
3.46
3.46
3.45
3.41
3.40
3.40
3.39
3.39
3.38
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2.98
2.97
2.43
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2.00
1.99
1.98
1.59
1.58
1.58
1.57
1.57
1.56
1.45
1.44
1.44
O
NC
Ph
N
Boc
5da
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1.00
2.01
2.10
2.11
2.06
2.07
2.09
4.31
9.91
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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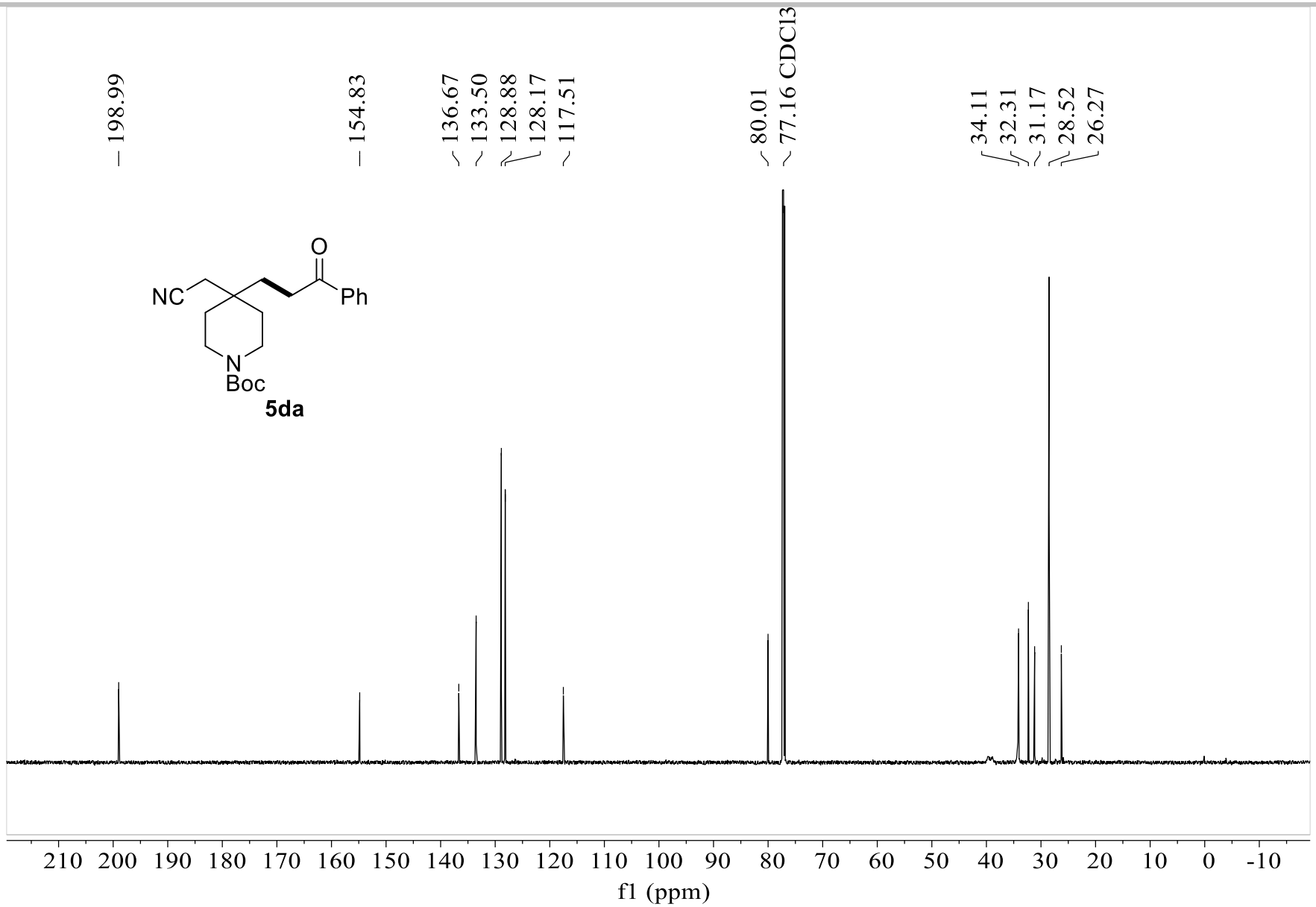
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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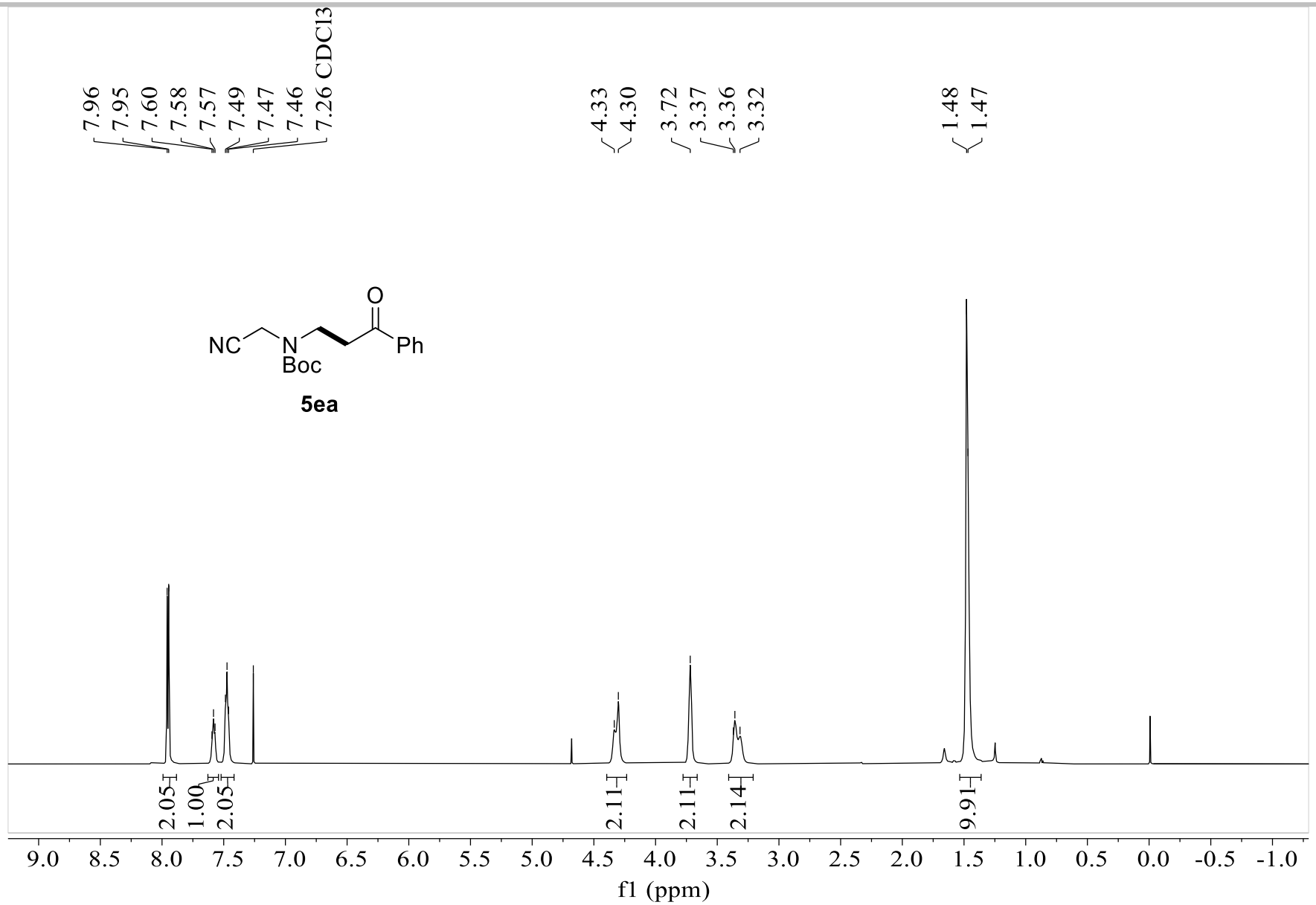
128.88
128.17
117.51
80.01
77.16 CDCl3
34.11
32.31
31.17
28.52
26.27
NC
O
Ph
N
Boc
5da
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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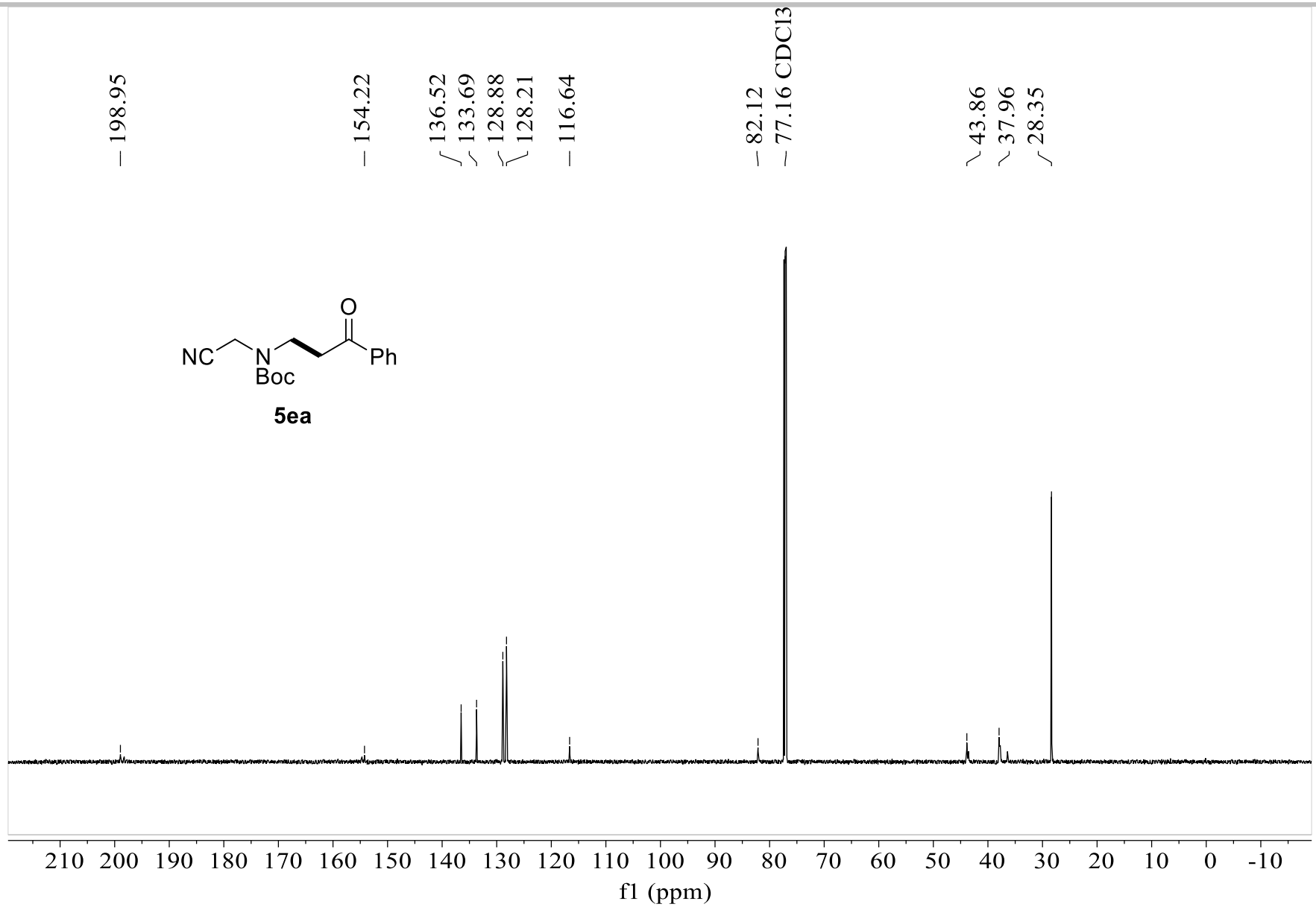
7.95
7.60
7.58
7.57
7.49
7.47
7.46
7.26 CDCl3
4.33
4.30
3.72
3.37
3.36
3.32
1.48
1.47
NC
N
Boc
O
Ph
5ea
2.05
1.00
2.05
2.11
2.11
2.14
9.91
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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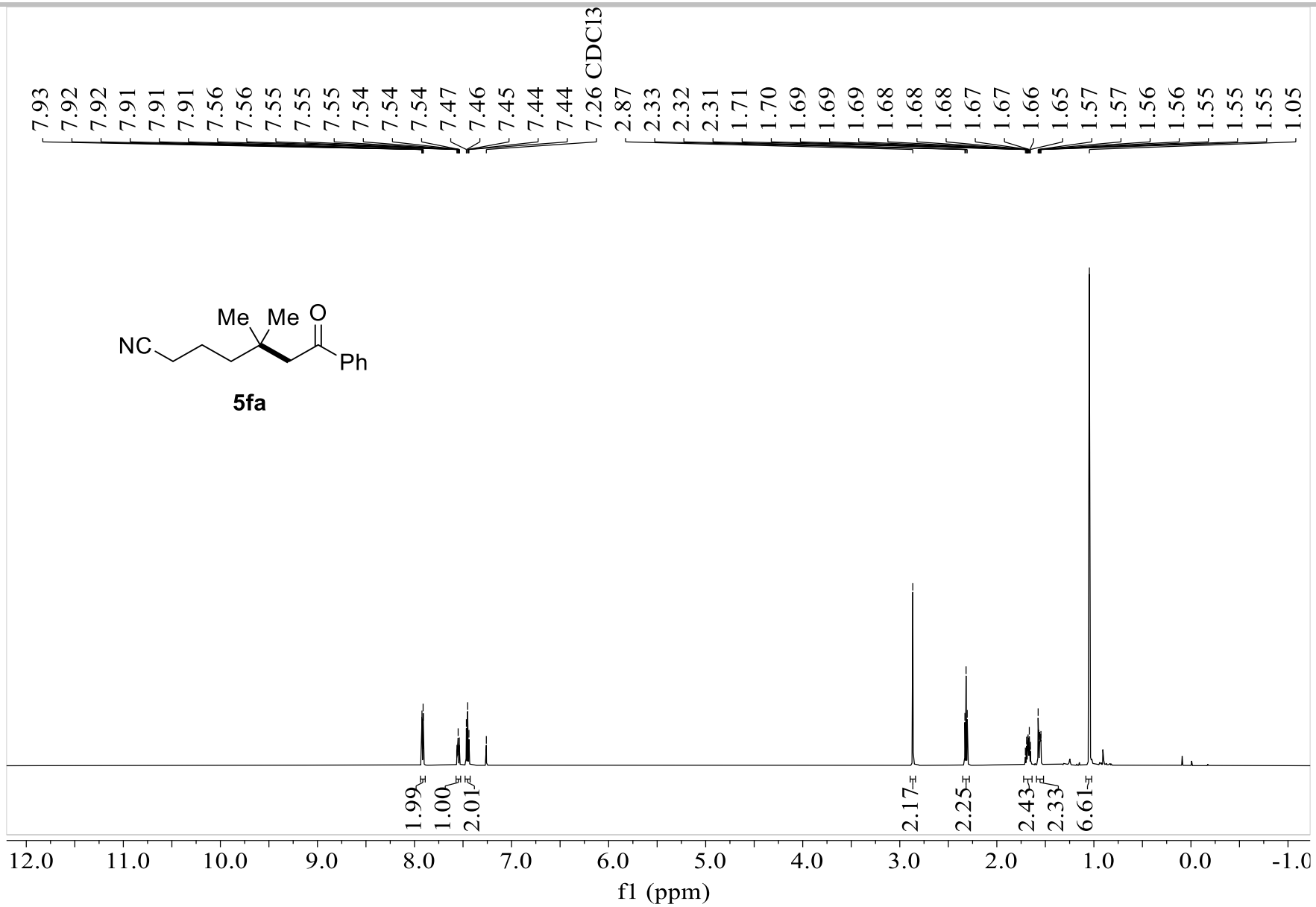
128.21
116.64
82.12
77.16 CDCl3
43.86
37.96
28.35
NC
N
Boc
O
Ph
5ea
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.91
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7.56
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7.55
7.55
7.54
7.54
7.54
7.47
7.46
7.45
7.44
7.44
7.26 CDCl3
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2.33
2.32
2.31
1.71
1.70
1.69
1.69
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1.67
1.67
1.66
1.65
1.57
1.57
1.56
1.56
1.55
1.55
1.55
1.05
Me
Me
O
NC
Ph
5fa
1.99
1.00
2.01
2.17
2.25
2.43
2.33
6.61
12.0
11.0
10.0
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8.0
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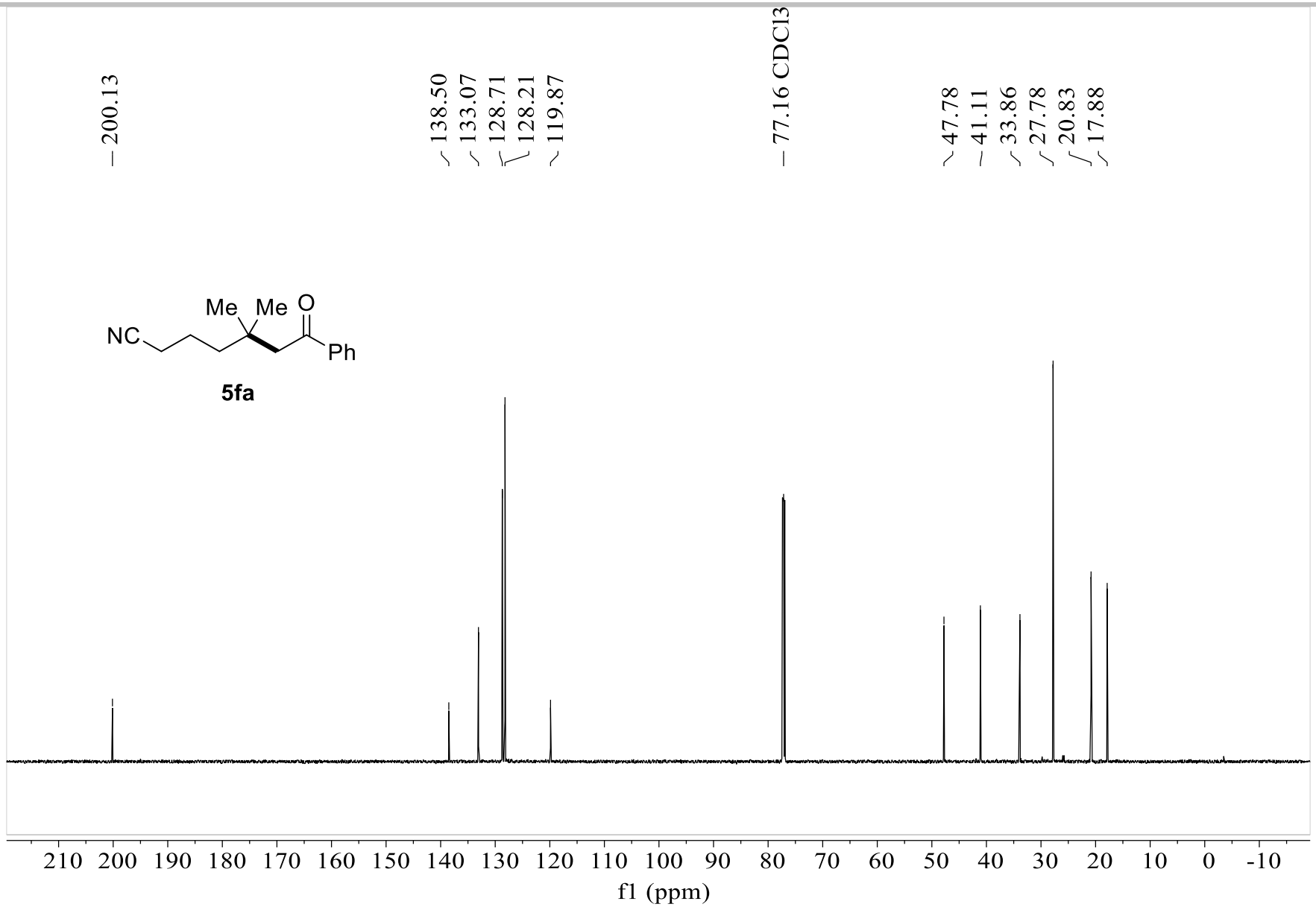
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)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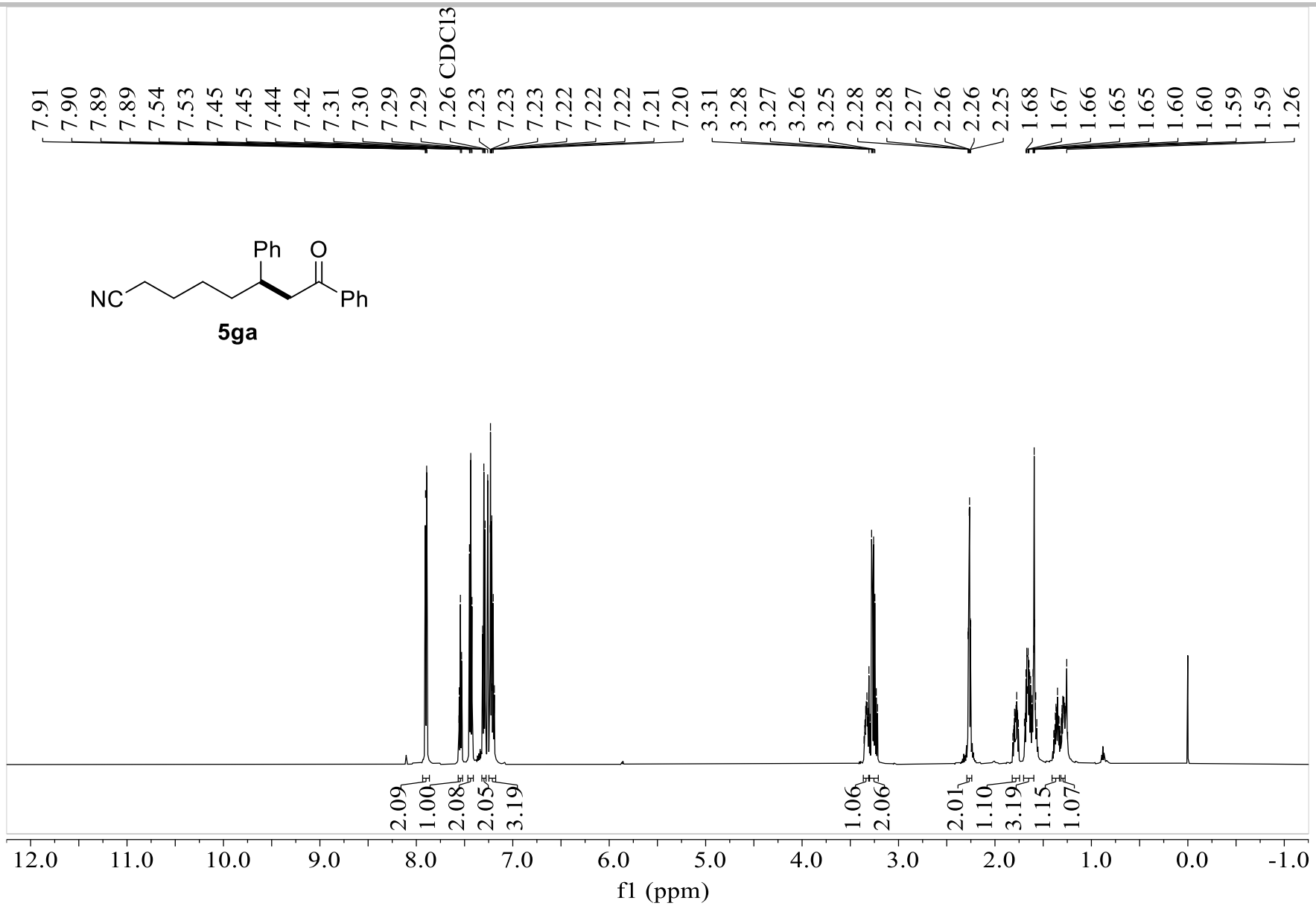
47.78
41.11
33.86
27.78
20.83
17.88
Me
Me
O
NC
Ph
5fa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.45
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7.42
7.31
7.30
7.29
7.29
7.26 CDCl3
7.23
7.23
7.23
7.22
7.22
7.22
7.21
7.20
3.31
3.28
3.27
3.26
3.25
2.28
2.28
2.27
2.26
2.26
2.25
1.68
1.67
1.66
1.65
1.65
1.60
1.60
1.59
1.59
1.26
Ph
O
NC
Ph
5ga
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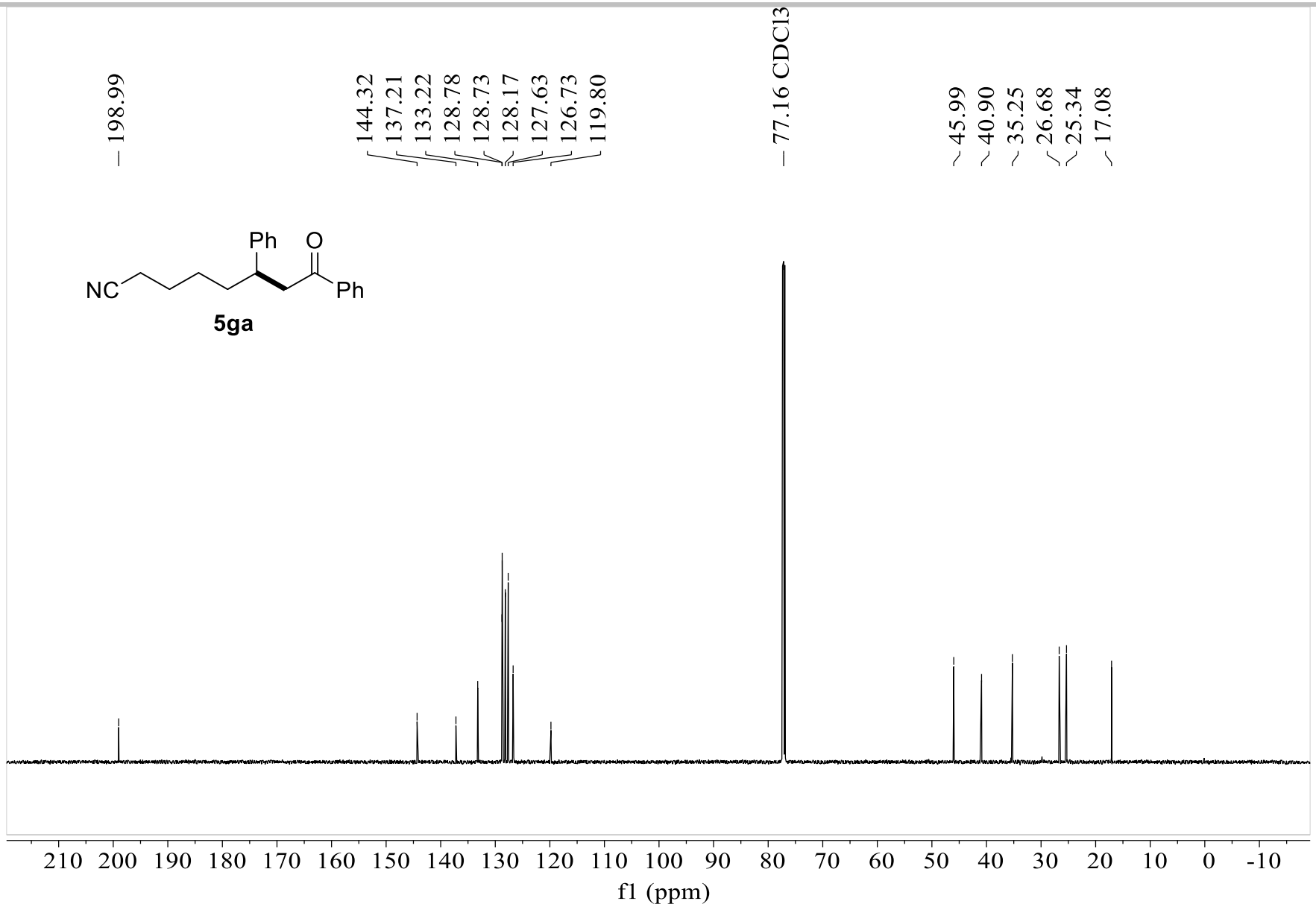
1.00
2.08
2.05
3.19
1.06
2.06
2.01
1.10
3.19
1.15
1.07
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)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128.17
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119.80
77.16 CDCl3
45.99
40.90
35.25
26.68
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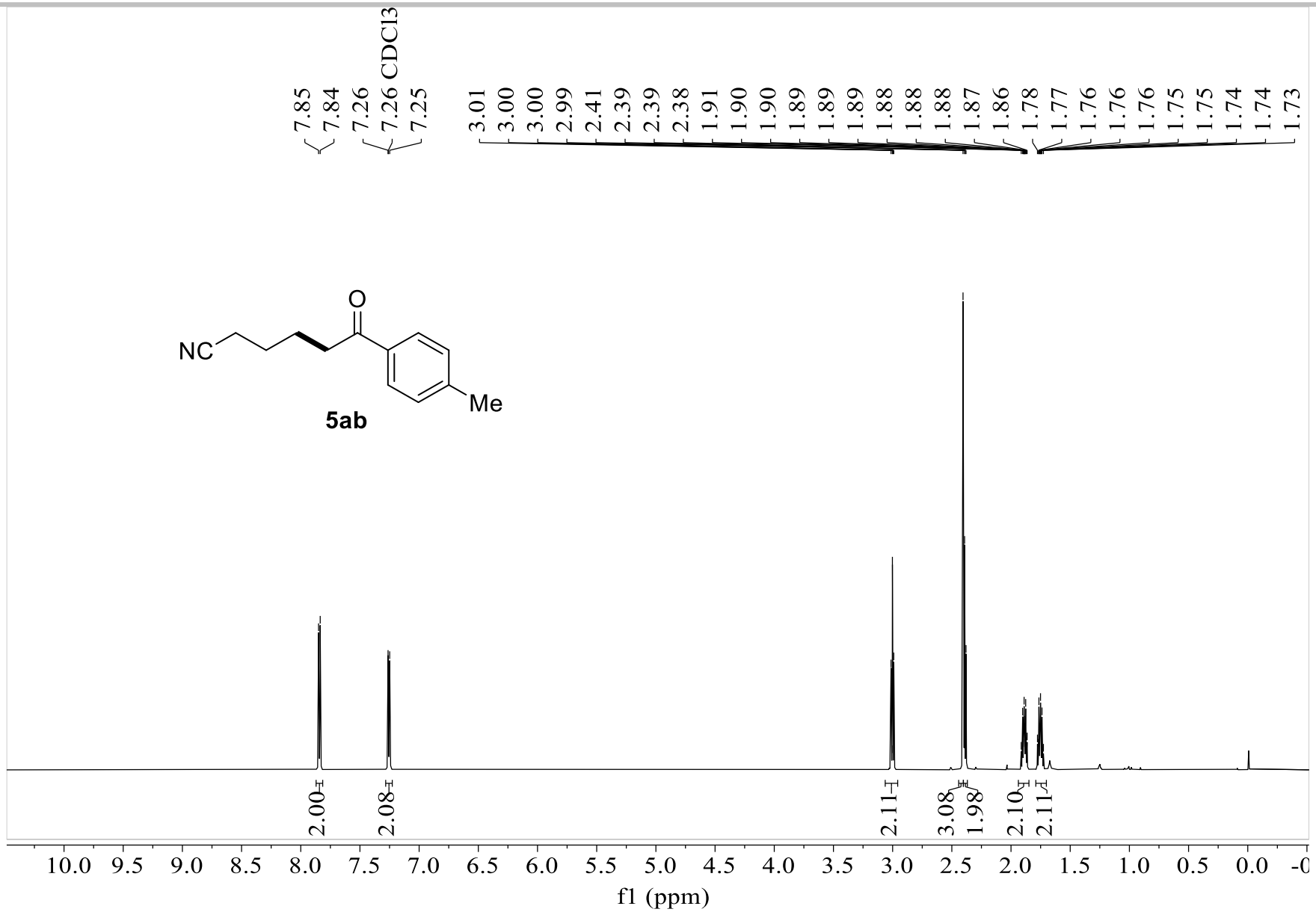
Ph
O
NC
Ph
5ga
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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3.00
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2.39
2.38
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1.90
1.89
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1.89
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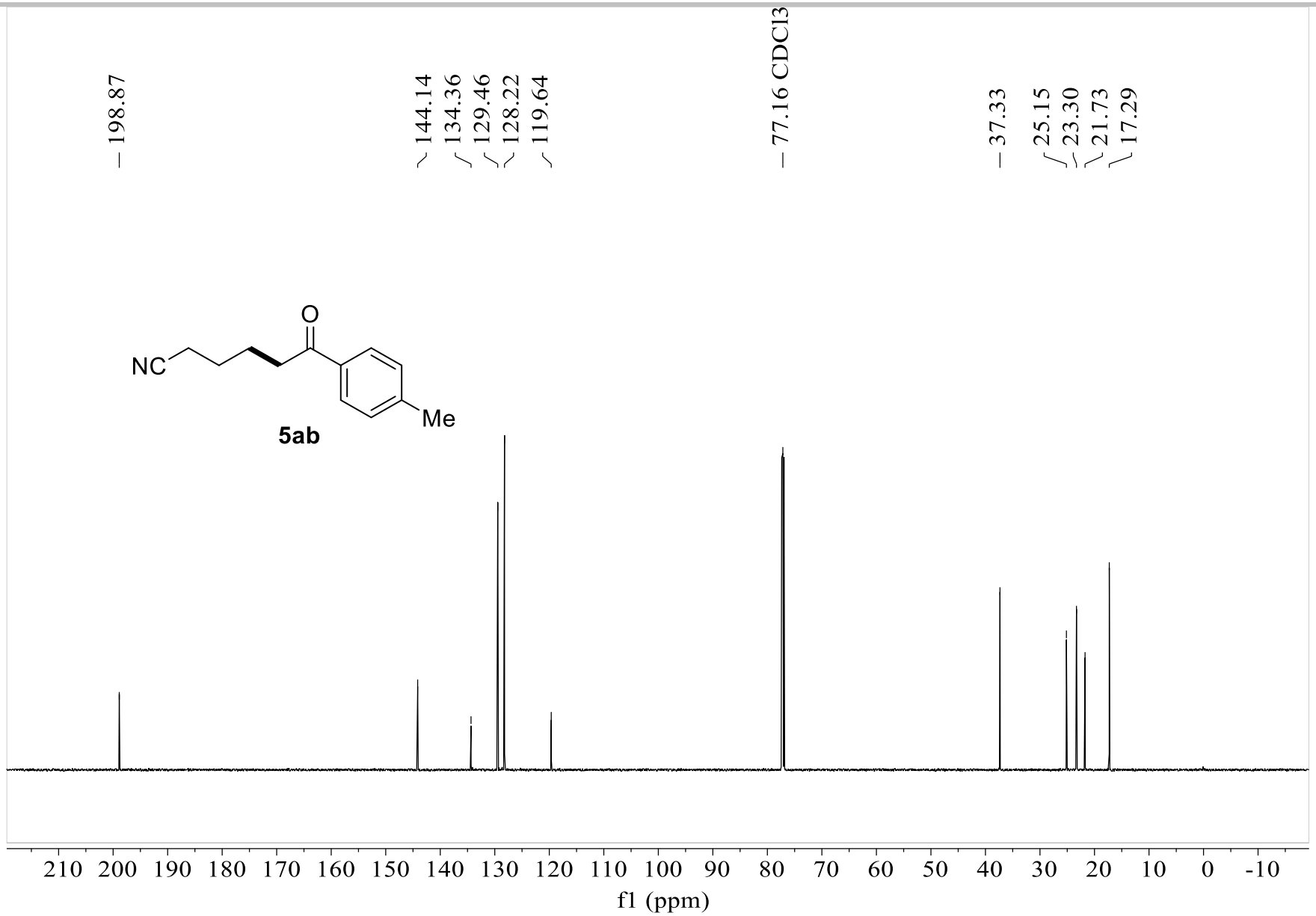
1.88
1.87
1.86
1.78
1.77
1.76
1.76
1.76
1.75
1.75
1.74
1.74
1.73
O
NC
Me
5ab
2.00
2.08
2.11
3.08
1.98
2.10
2.11
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)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37.33
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23.30
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NC
Me
5ab
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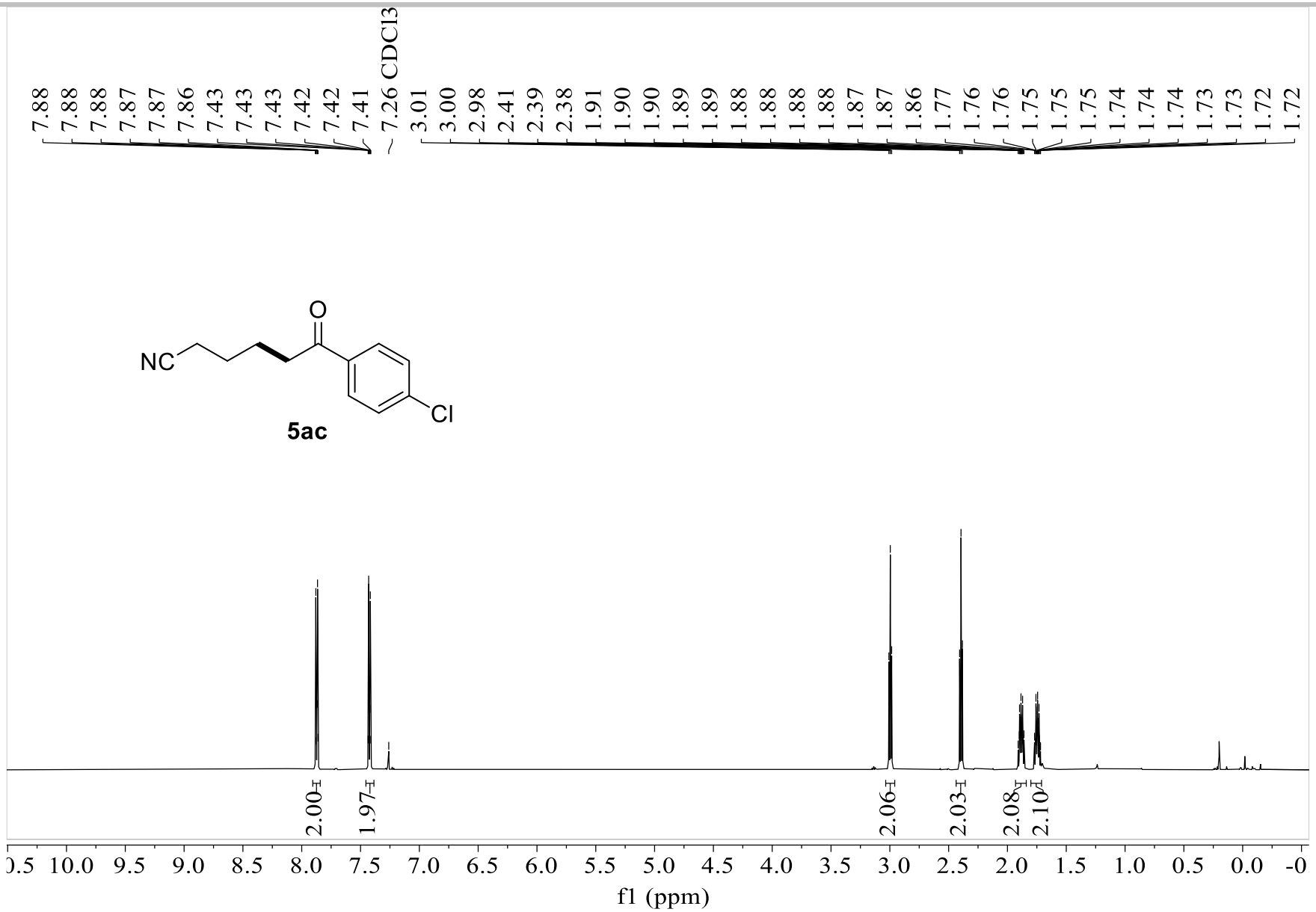
f1 (ppm)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7.86
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7.43
7.43
7.42
7.42
7.41
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3.01
3.00
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2.41
2.39
2.38
1.91
1.90
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1.73
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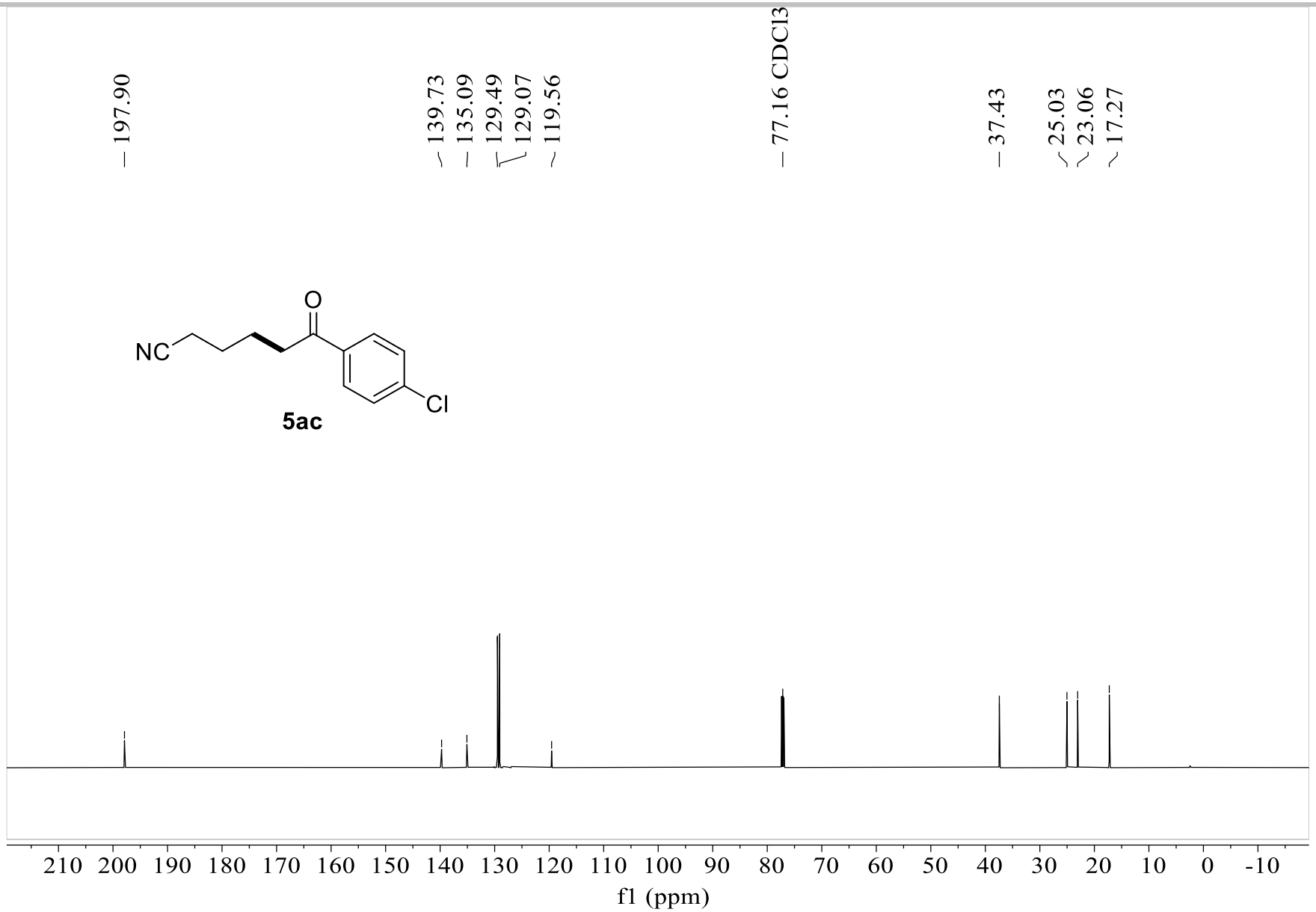
2.08
2.10
f1 (ppm)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37.43
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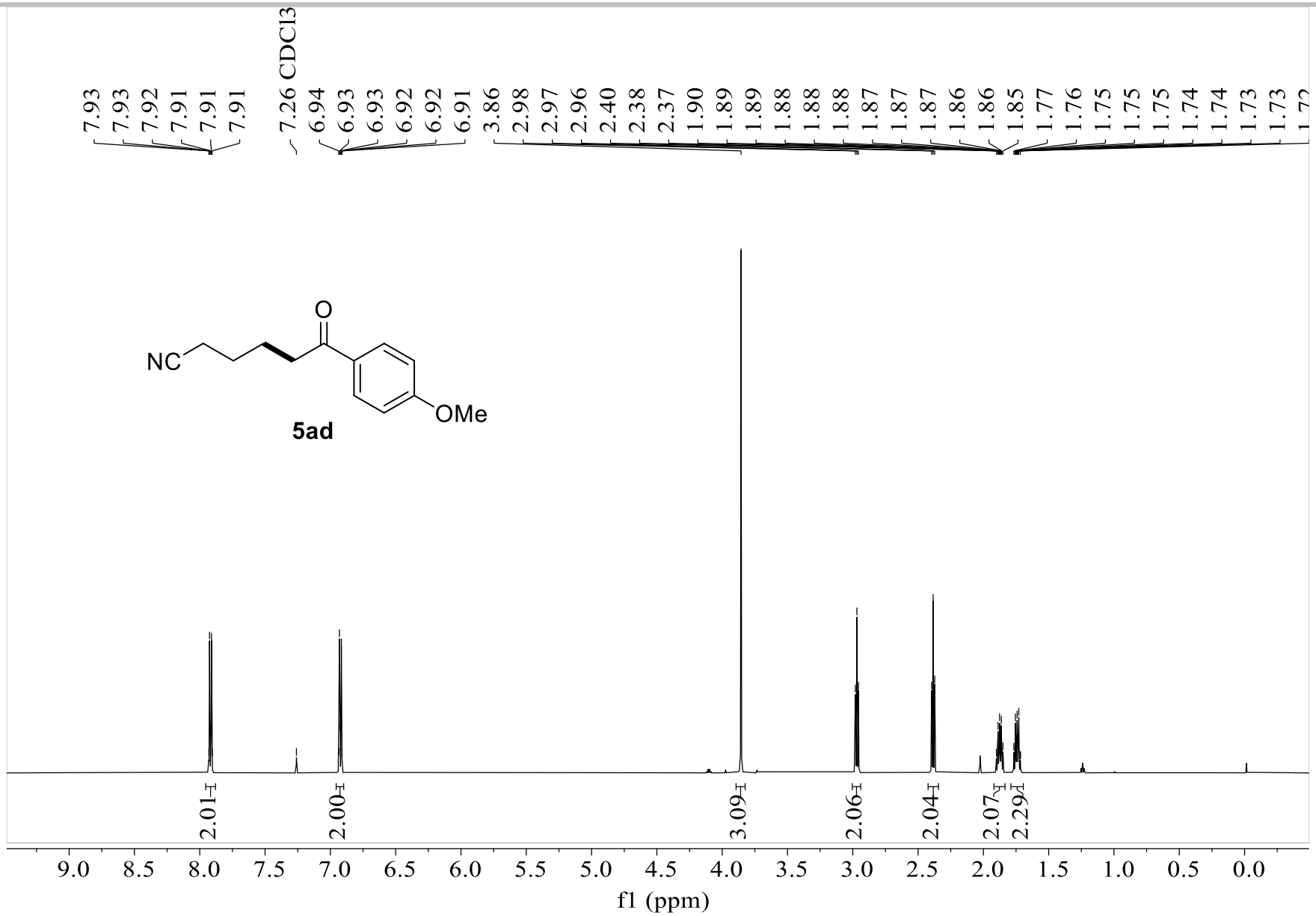
f1 (ppm)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1.86
1.85
1.77
1.76
1.75
1.75
1.75
1.74
1.74
1.73
1.73
O
NC
OMe
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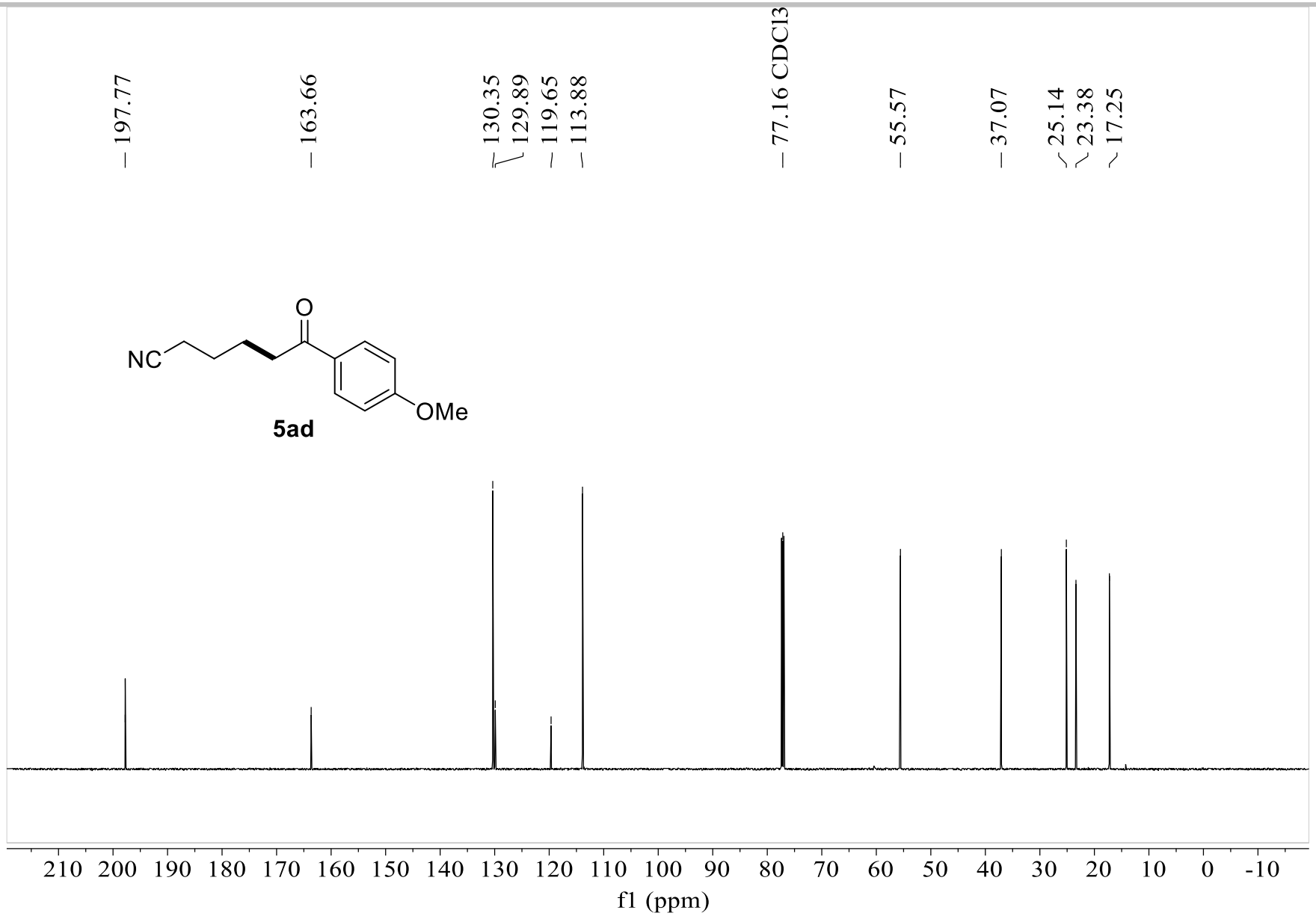
2.01
2.00
3.09
2.06
2.04
2.07
2.29
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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113.88
77.16 CDCl3
55.57
37.07
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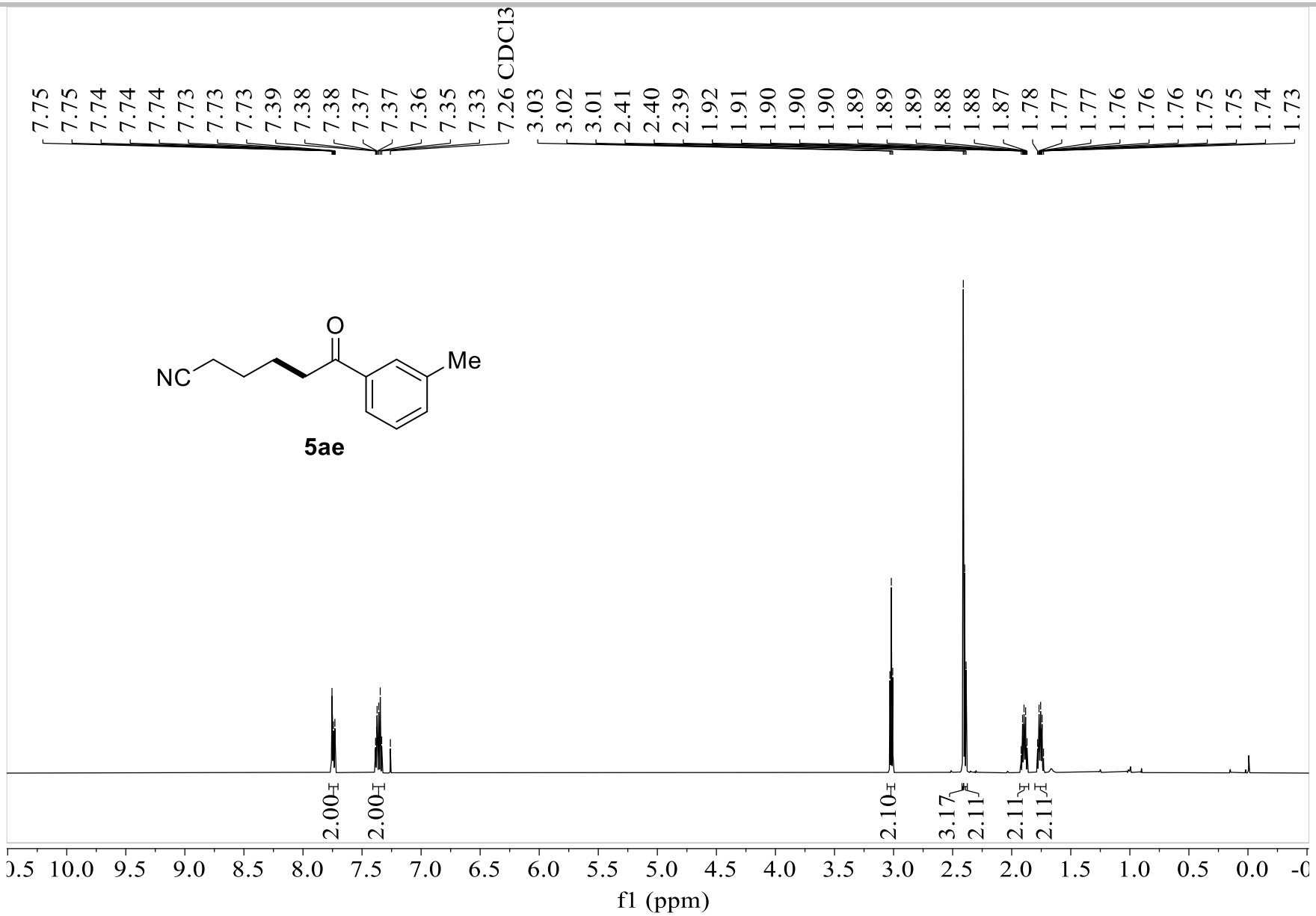
O
NC
OMe
5ad
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.36
7.35
7.33
7.26 CDCl3
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3.02
3.01
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1.78
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1.77
1.76
1.76
1.76
1.75
1.75
1.74
1.73
O
NC
Me
5ae
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2.00
2.10
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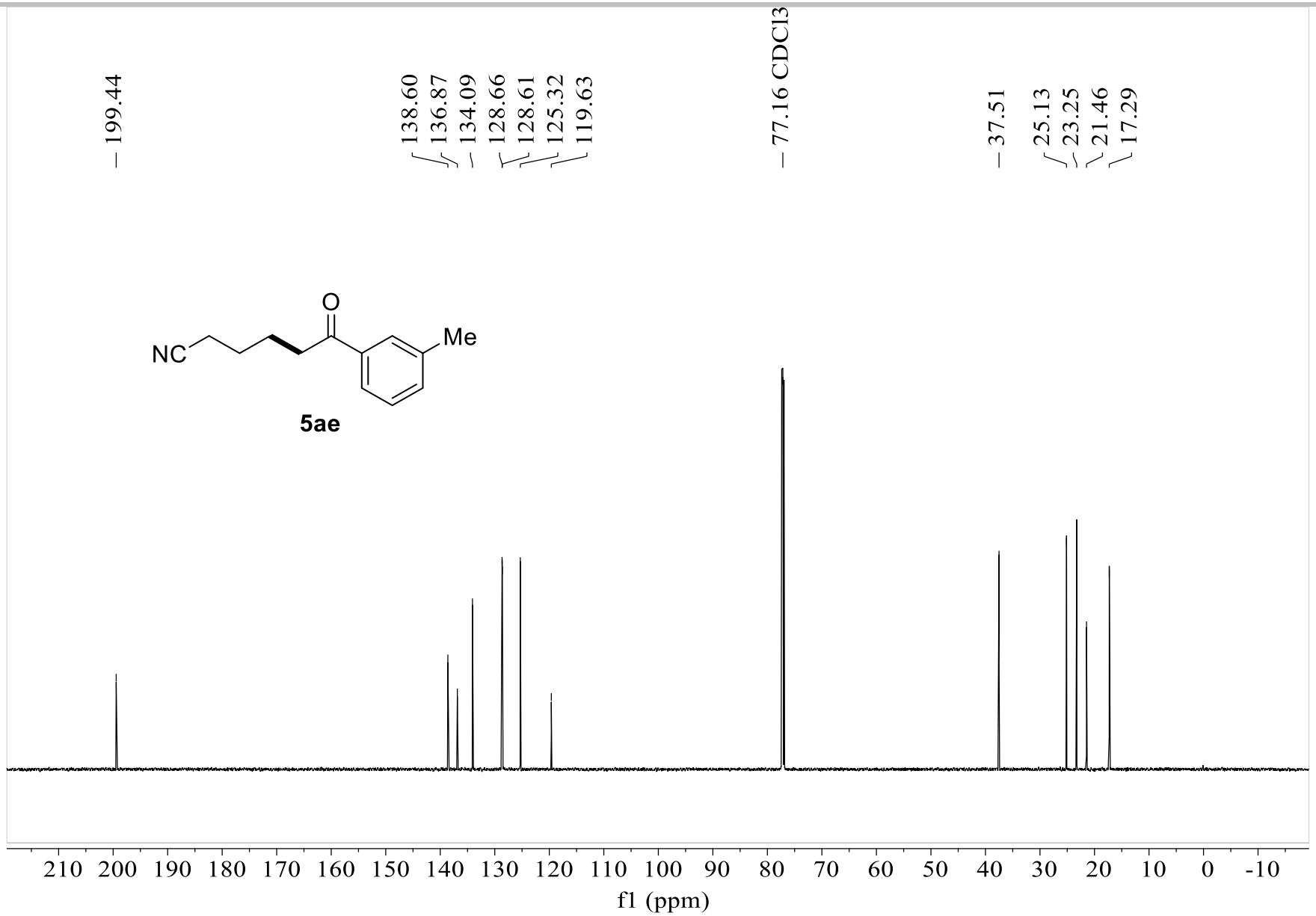
2.11
2.11
2.11
f1 (ppm)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119.63
77.16 CDCl3
37.51
25.13
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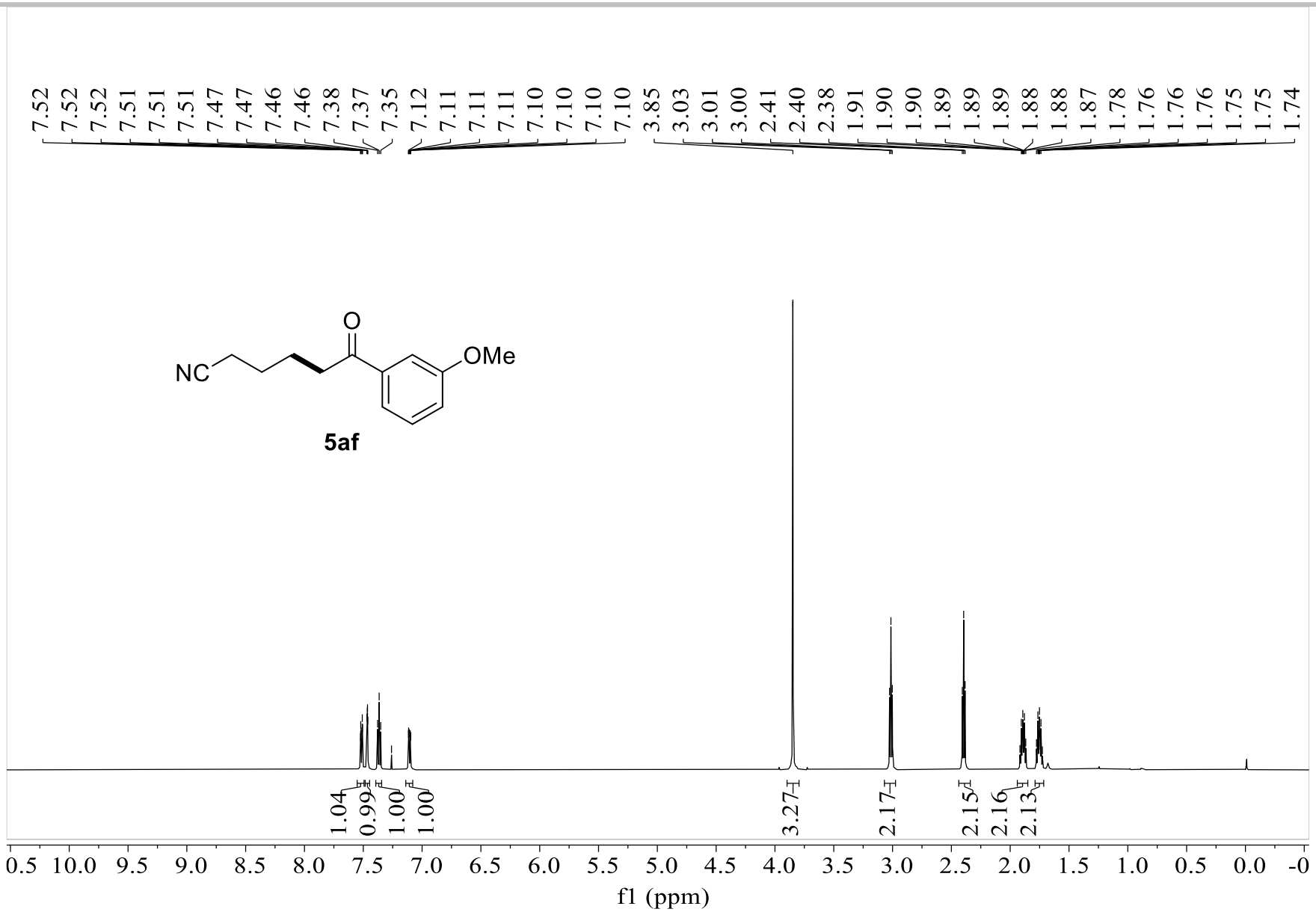
21.46
17.29
O
NC
Me
5ae
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.11
7.10
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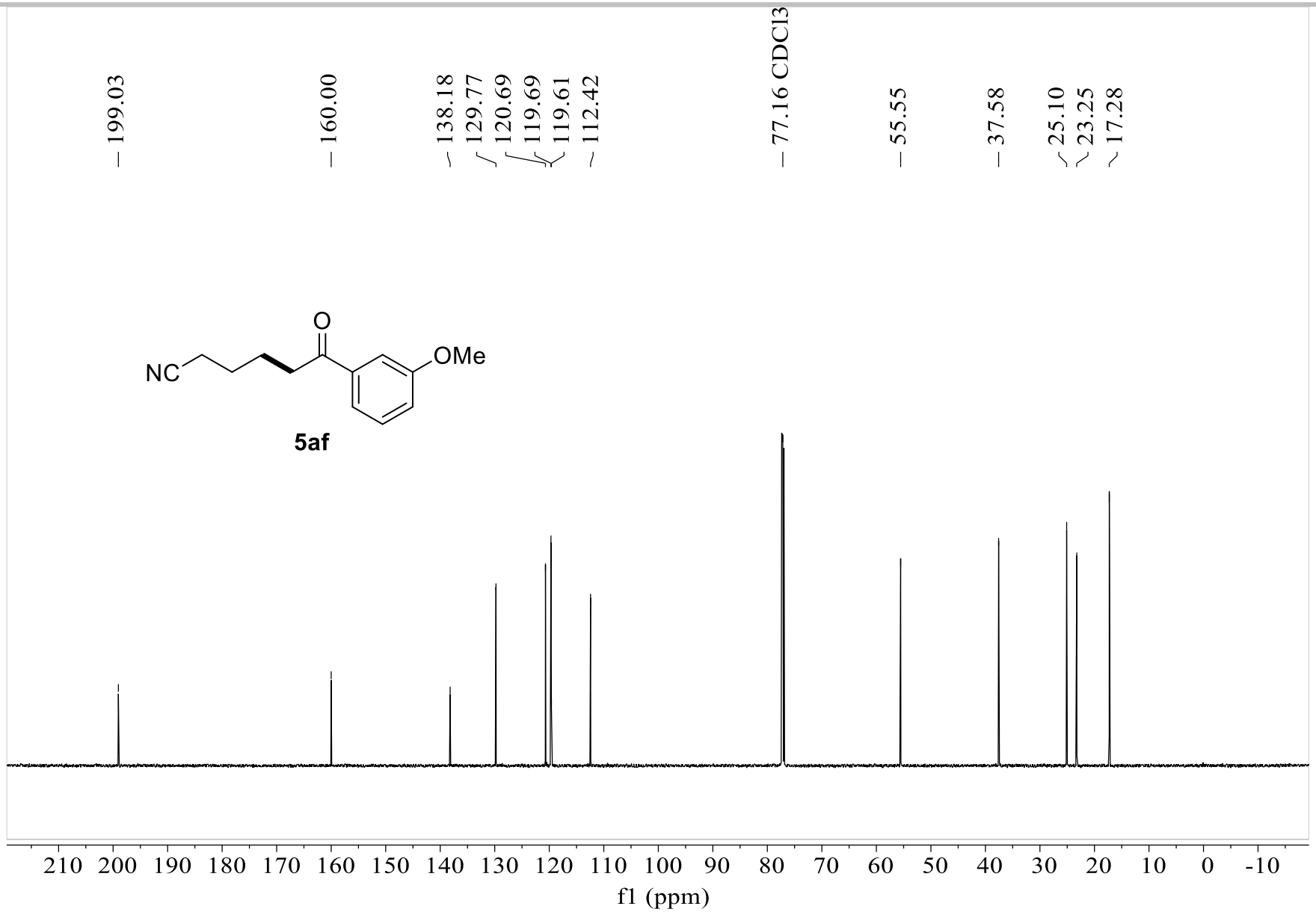
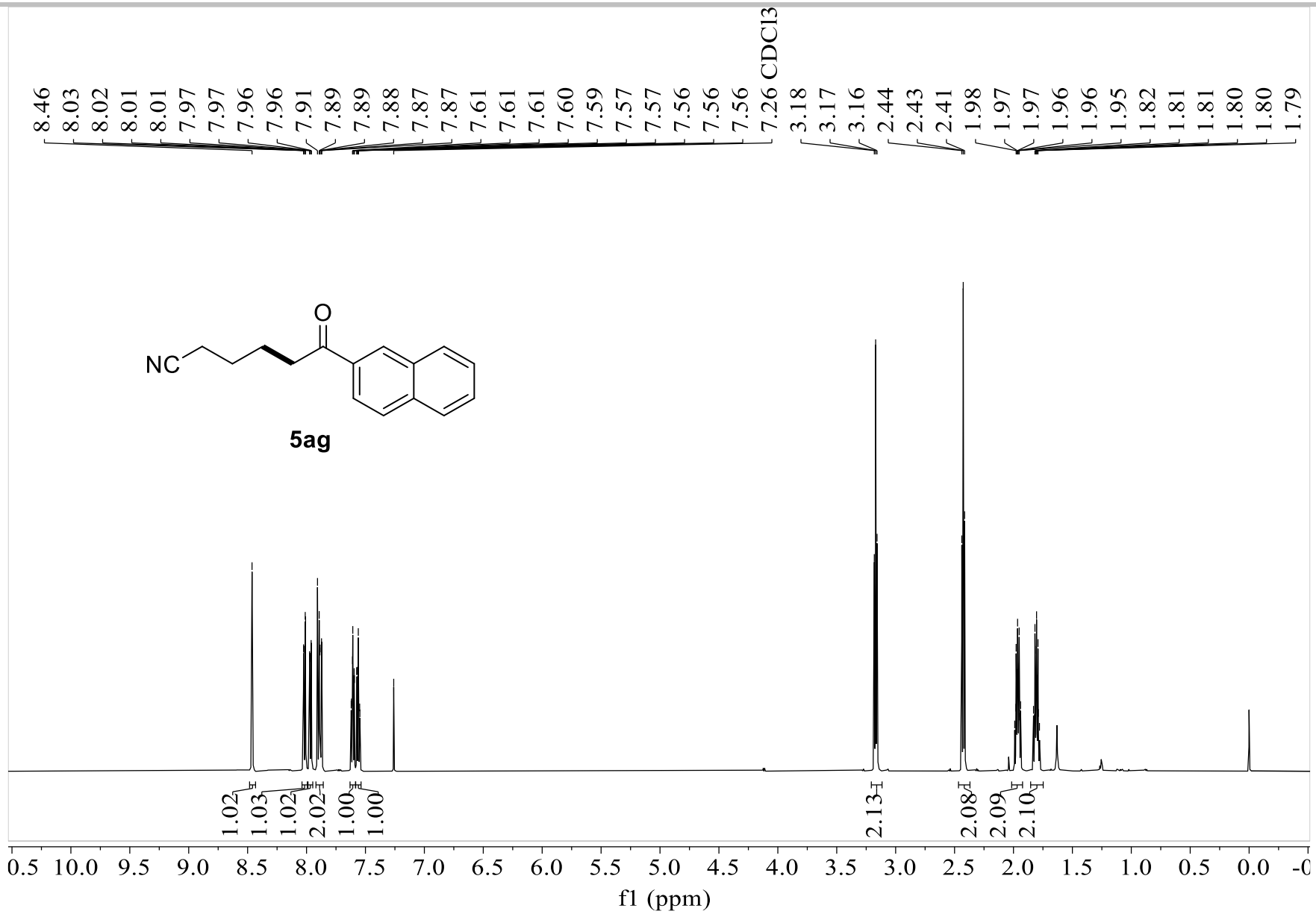
7.10
3.85
3.03
3.01
3.00
2.41
2.40
2.38
1.91
1.90
1.90
1.89
1.89
1.89
1.88
1.88
1.87
1.78
1.76
1.76
1.76
1.75
1.75
1.74
O
NC
OMe
5af
1.04
0.99
1.00
1.00
3.27
2.17
2.15
2.16
2.13
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)


199.03
160.00
138.18
129.77
120.69
119.69
119.61
112.42
77.16 CDCl3
55.55
37.58
25.10
23.25
17.28
O
NC
OMe
5af
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)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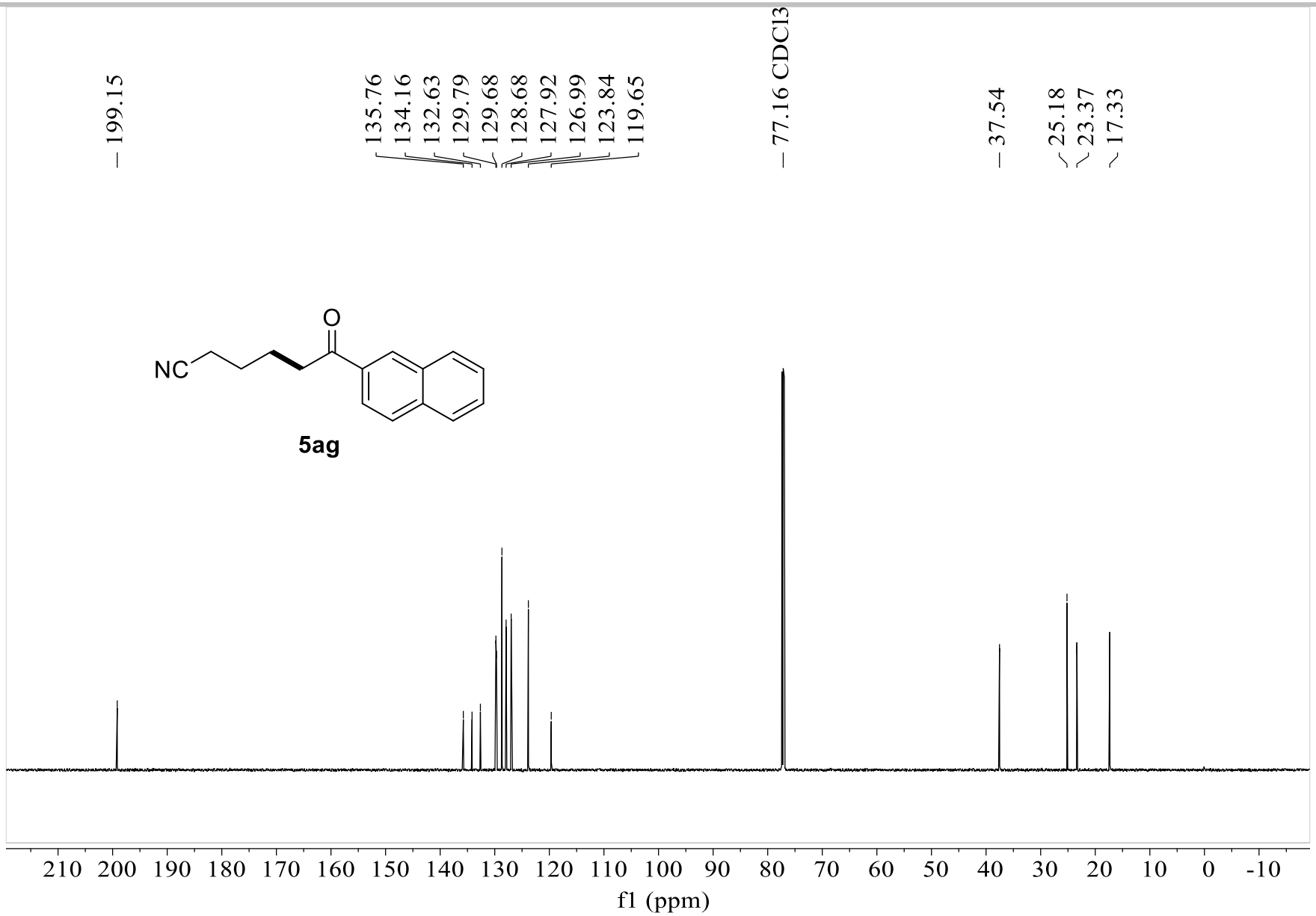
8.03
8.02
8.01
8.01
7.97
7.97
7.96
7.96
7.91
7.89
7.89
7.88
7.87
7.87
7.61
7.61
7.61
7.60
7.59
7.57
7.57
7.56
7.56
7.56
7.26 CDCl3
3.18
3.17
3.16
2.44
2.43
2.41
1.98
1.97
1.97
1.96
1.96
1.95
1.82
1.81
1.81
1.80
1.80
1.79
O
NC
5ag
1.02
1.03
1.02
2.02
1.00
1.00
2.13
2.08
2.09
2.10
f1 (ppm)


199.15
135.76
134.16
132.63
129.79
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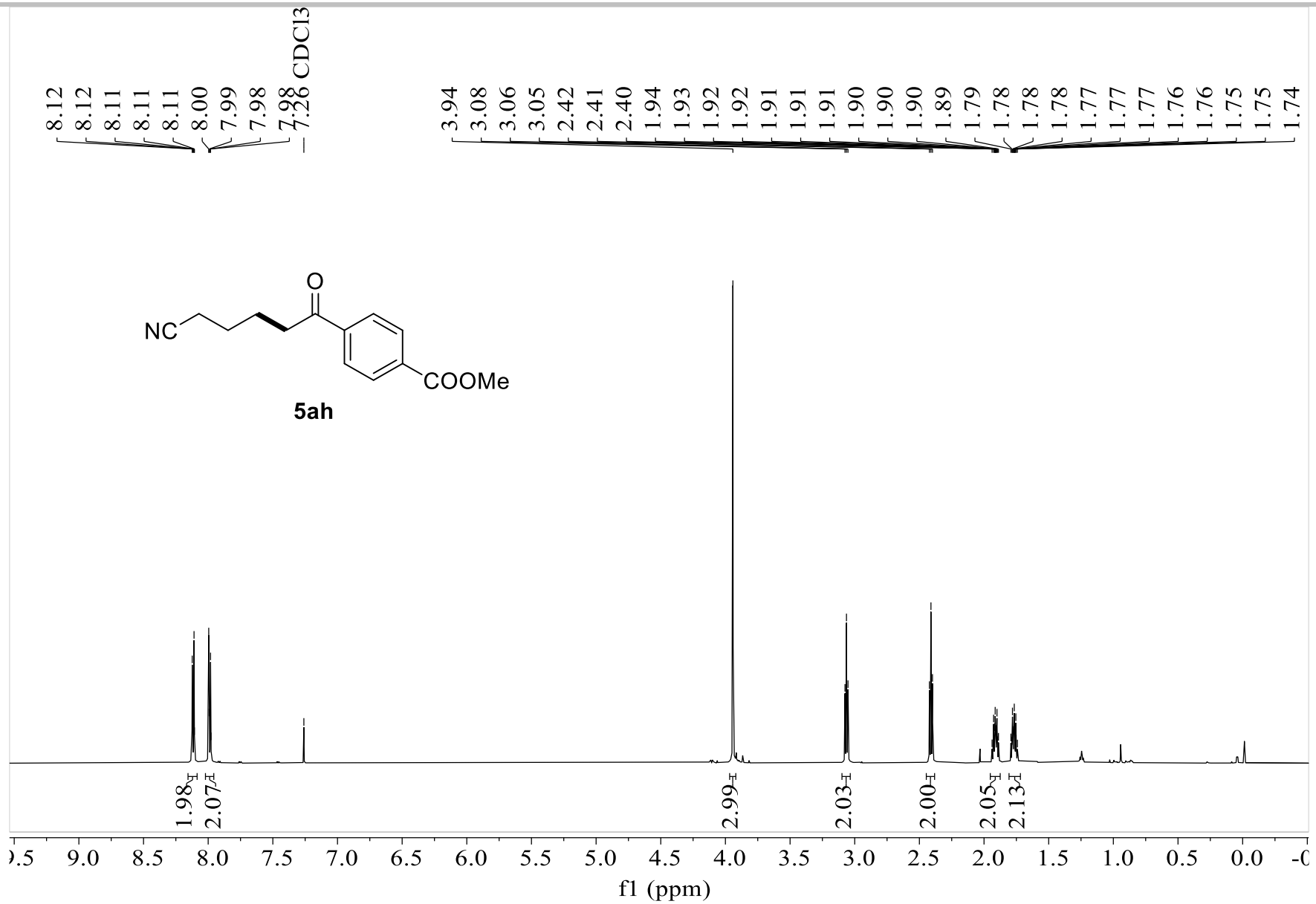
128.68
127.92
126.99
123.84
119.65
77.16 CDCl3
37.54
25.18
23.37
17.33
O
NC
5ag
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.12
8.12
8.11
8.11
8.11
8.00
7.99
7.98
7.98
7.26 CDCl3
3.94
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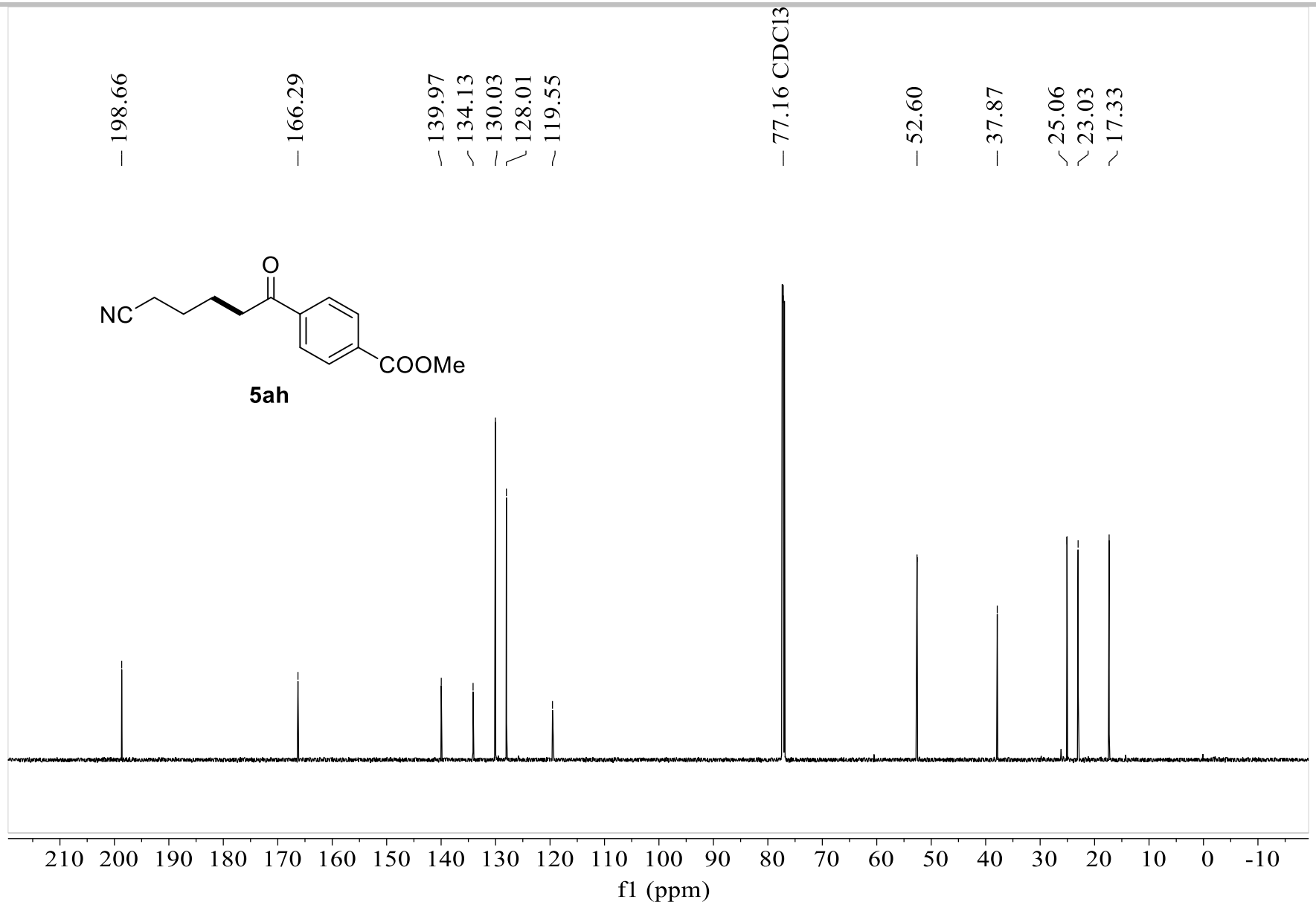
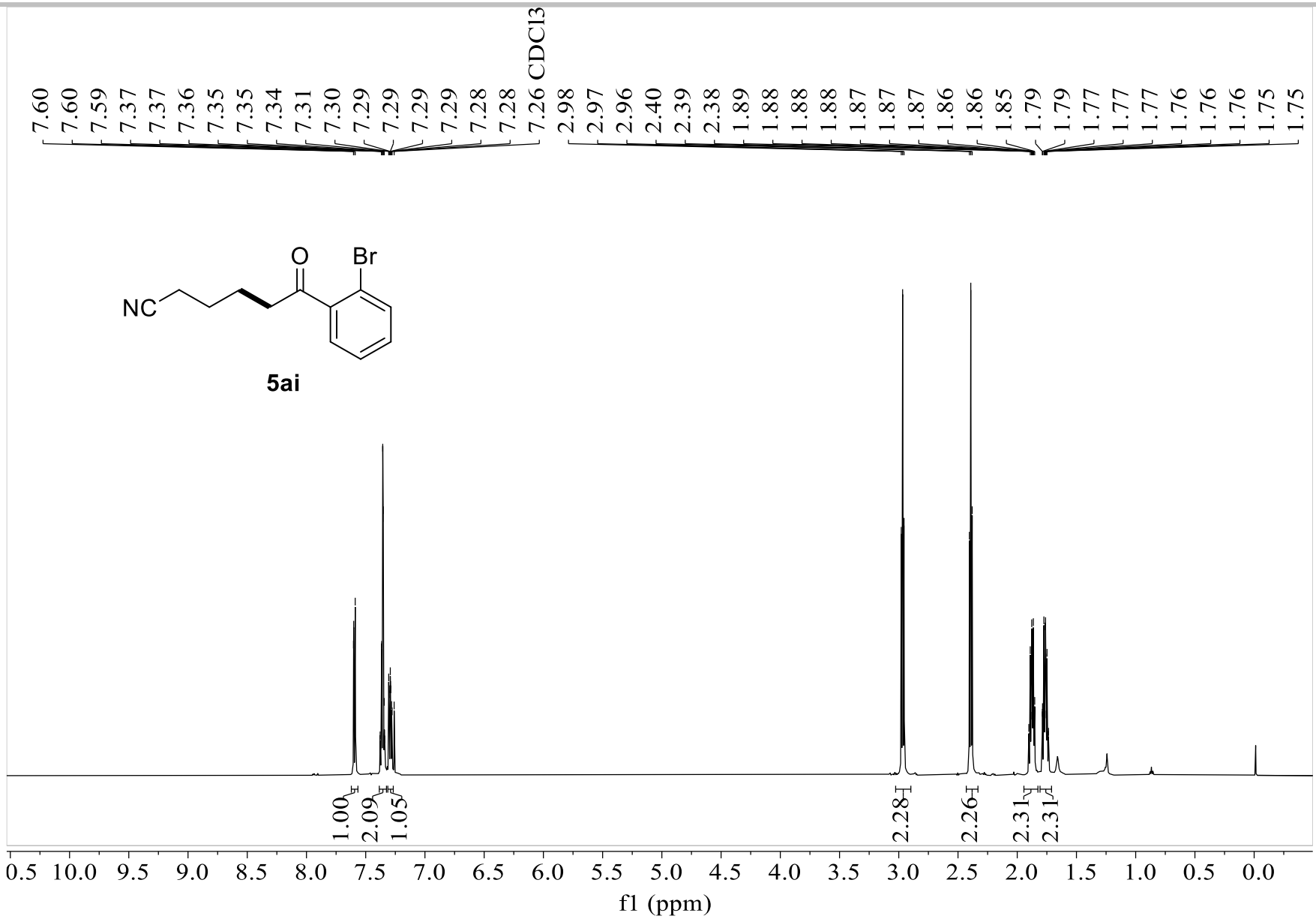
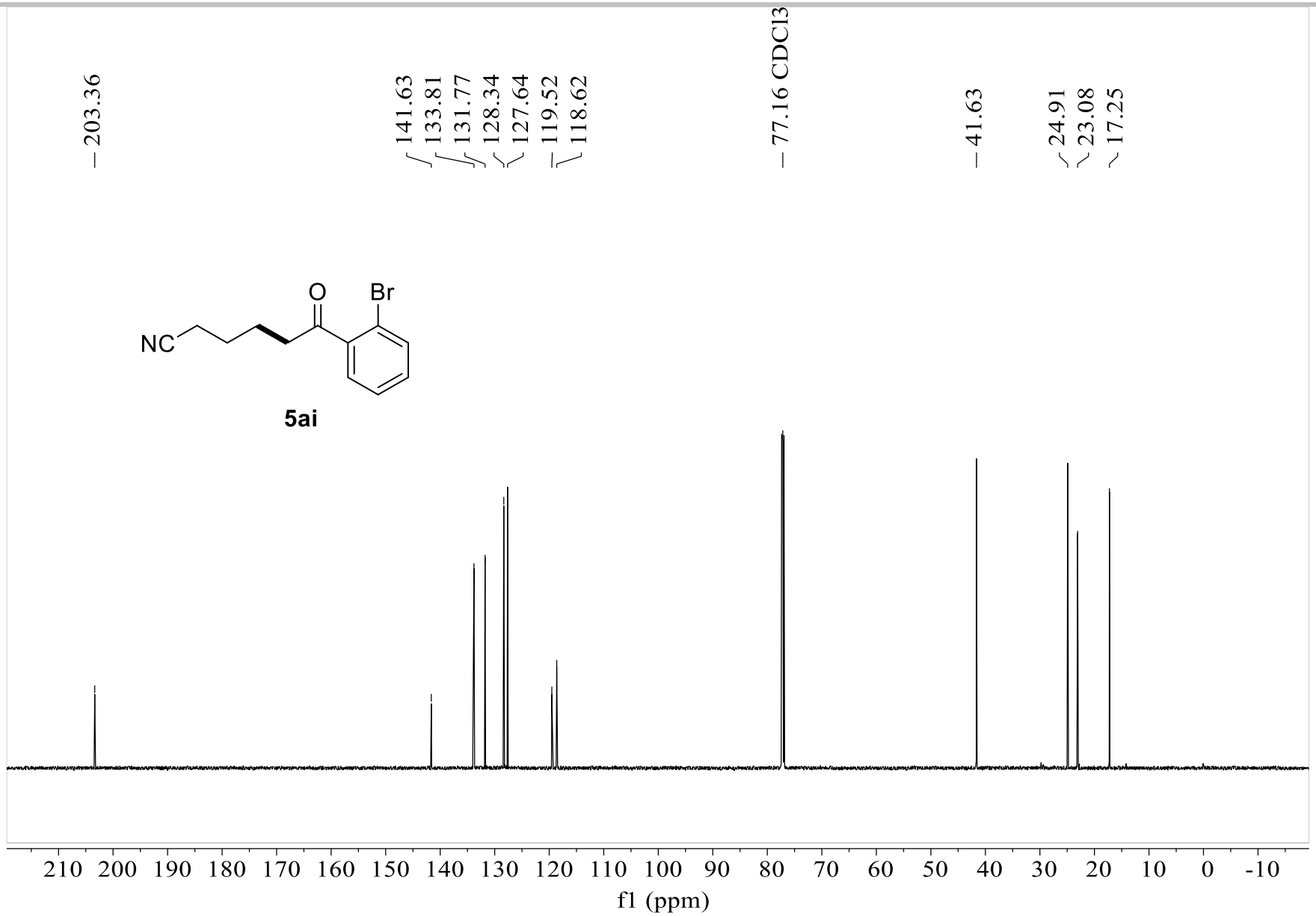
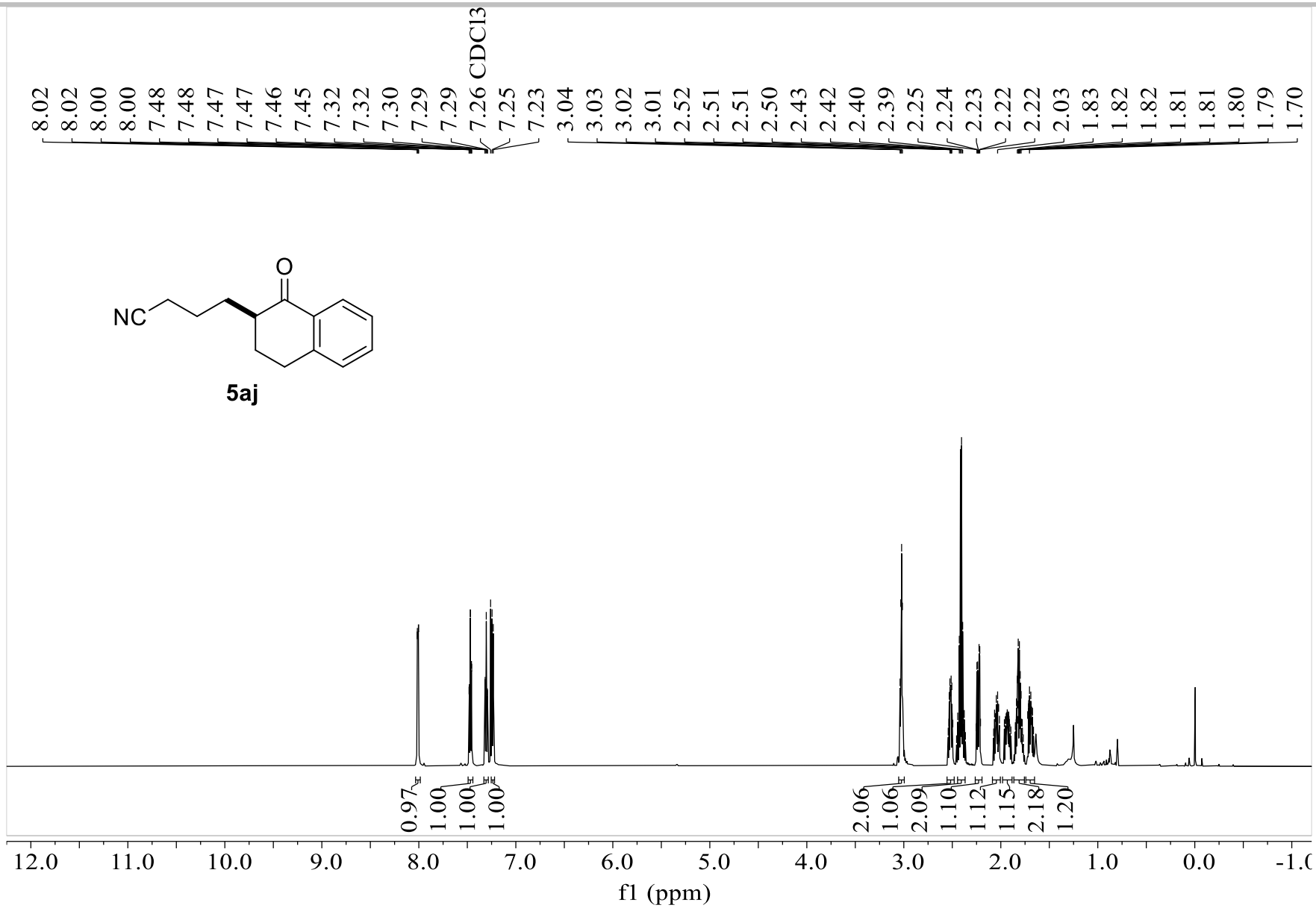
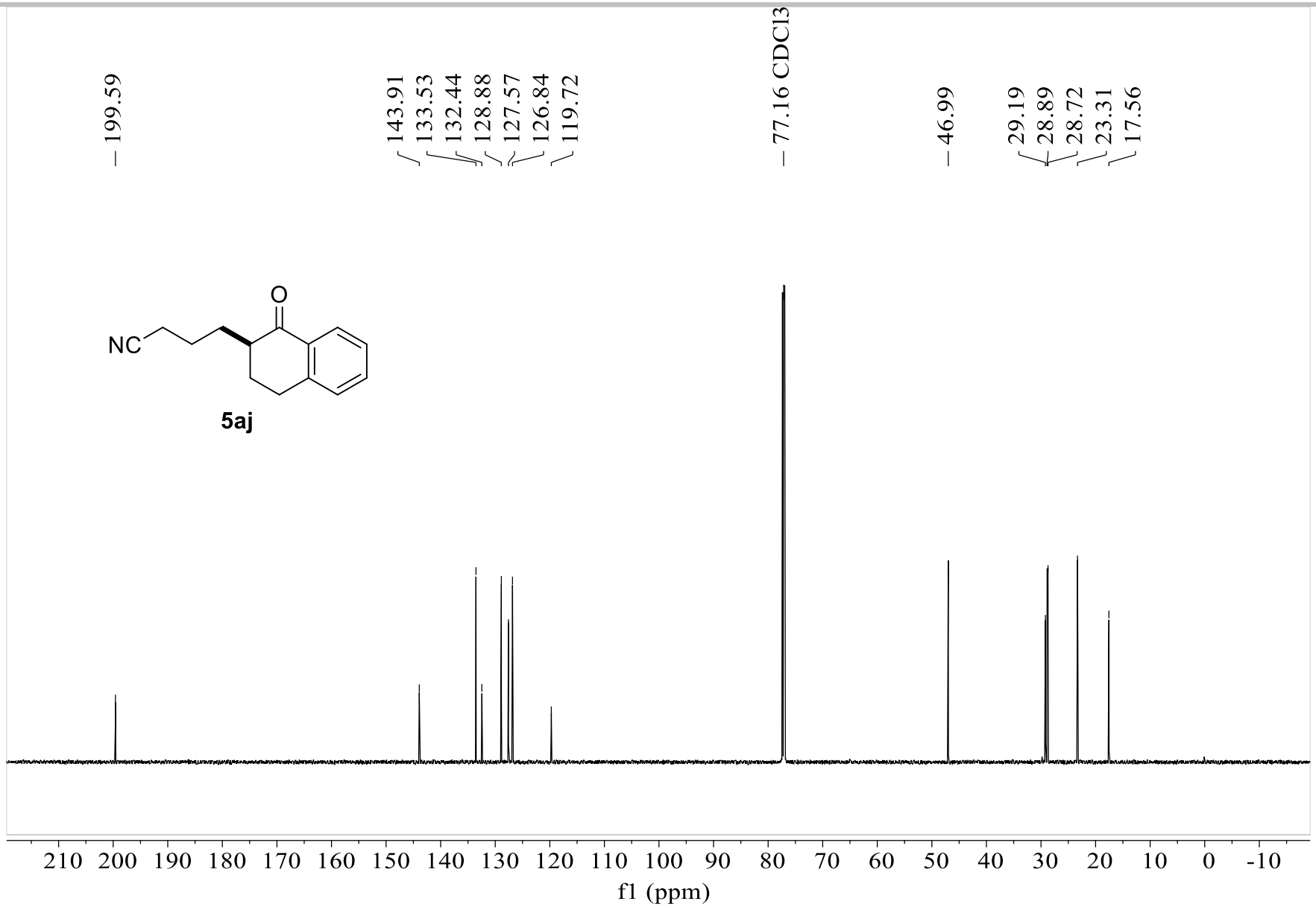
3.06
3.05
2.42
2.41
2.40
1.94
1.93
1.92
1.92
1.91
1.91
1.91
1.90
1.90
1.90
1.89
1.79
1.78
1.78
1.78
1.77
1.77
1.77
1.76
1.76
1.75
1.75
1.74
O
NC
COOMe
5ah
1.98
2.07
2.99
2.03
2.00
2.05
2.13
f1 (ppm)

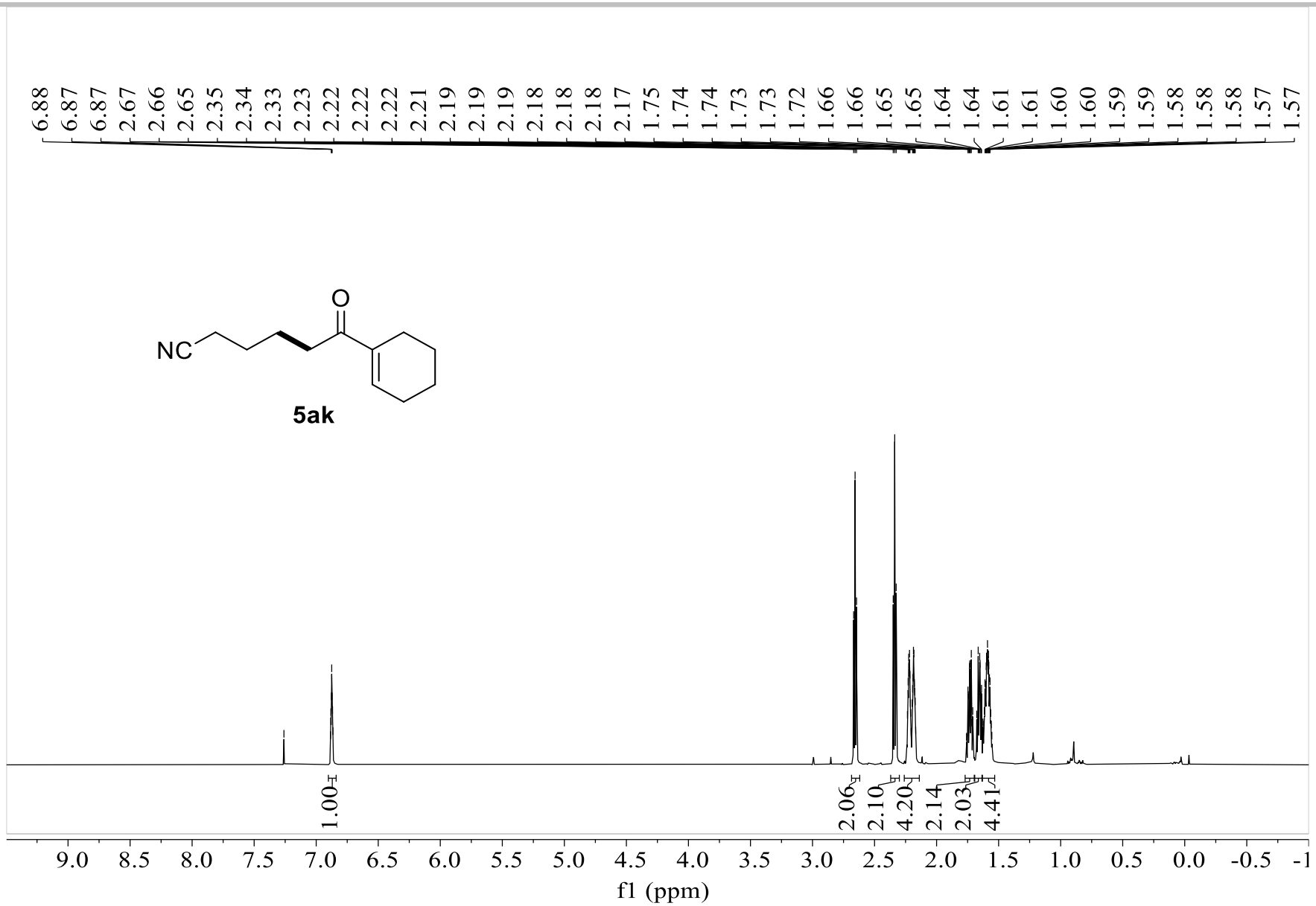

198.66
166.29
139.97
134.13
130.03
128.01
119.55
77.16 CDCl3
52.60
37.87
25.06
23.03
17.33
NC
O
COOMe
5ah
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.60
7.60
7.59
7.37
7.37
7.36
7.35
7.35
7.34
7.31
7.30
7.29
7.29
7.29
7.29
7.28
7.28
7.26 CDCl3
2.98
2.97
2.96
2.40
2.39
2.38
1.89
1.88
1.88
1.88
1.87
1.87
1.87
1.86
1.86
1.85
1.79
1.79
1.77
1.77
1.77
1.76
1.76
1.76
1.75
1.75
O
Br
NC
5ai
1.00
2.09
1.05
2.28
2.26
2.31
2.31
0.5 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
f1 (ppm)


203.36
141.63
133.81
131.77
128.34
127.64
119.52
118.62
77.16 CDCl3
41.63
24.91
23.08
17.25
O
Br
NC
5ai
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.02
8.02
8.00
8.00
7.48
7.48
7.47
7.47
7.46
7.45
7.32
7.32
7.30
7.29
7.29
7.26 CDCl3
7.25
7.23
3.04
3.03
3.02
3.01
2.52
2.51
2.51
2.50
2.43
2.42
2.40
2.39
2.25
2.24
2.23
2.22
2.22
2.03
1.83
1.82
1.82
1.81
1.81
1.80
1.79
1.70
O
NC
5aj
0.97
1.00
1.00
1.00
2.06
1.06
2.09
1.10
1.12
1.15
2.18
1.20
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


199.59
143.91
133.53
132.44
128.88
127.57
126.84
119.72
77.16 CDCl3
46.99
29.19
28.89
28.72
23.31
17.56
O
NC
5aj
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


6.88
6.87
6.87
2.67
2.66
2.65
2.35
2.34
2.33
2.23
2.22
2.22
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2.21
2.19
2.19
2.19
2.18
2.18
2.18
2.17
1.75
1.74
1.74
1.73
1.73
1.72
1.66
1.66
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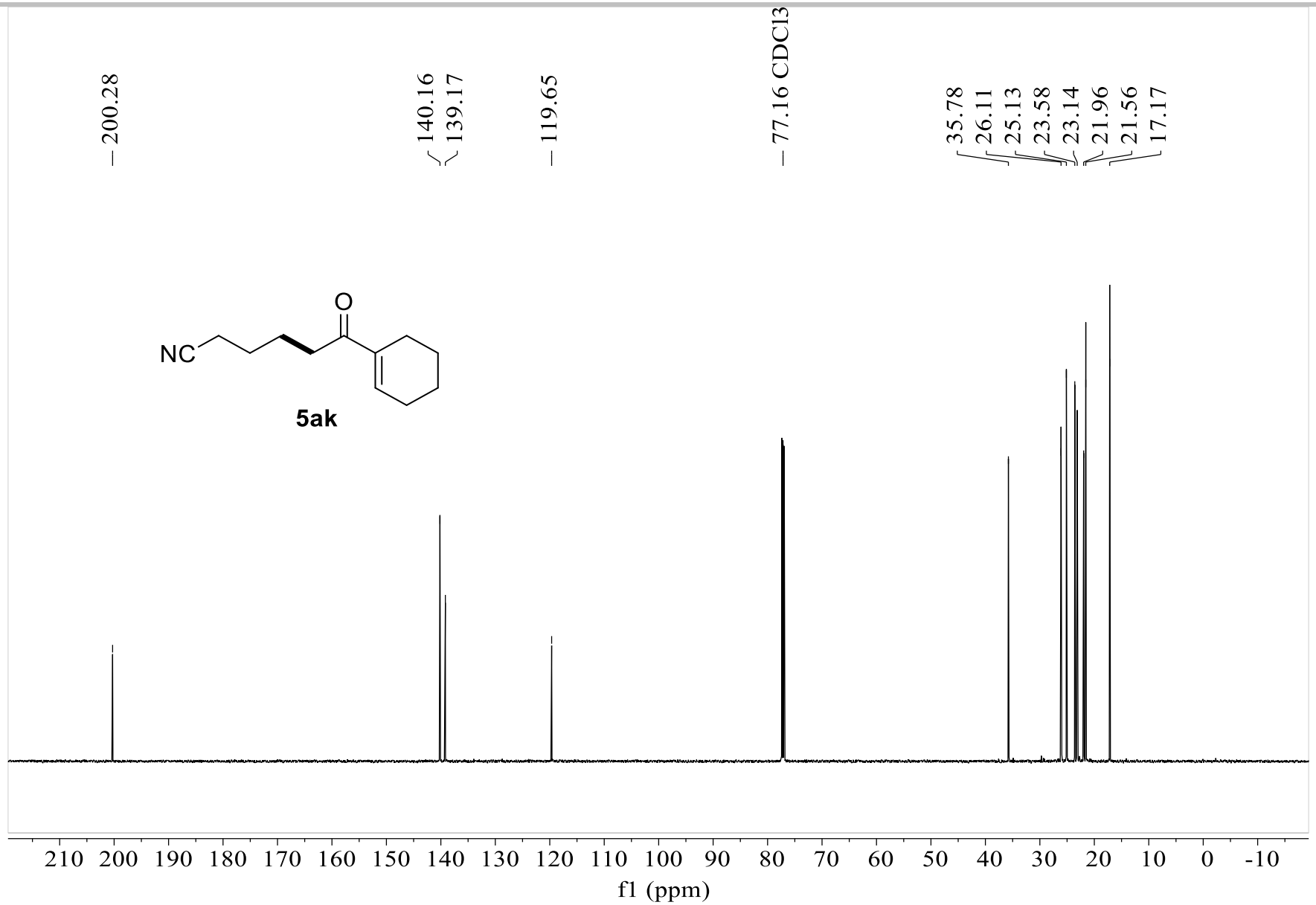
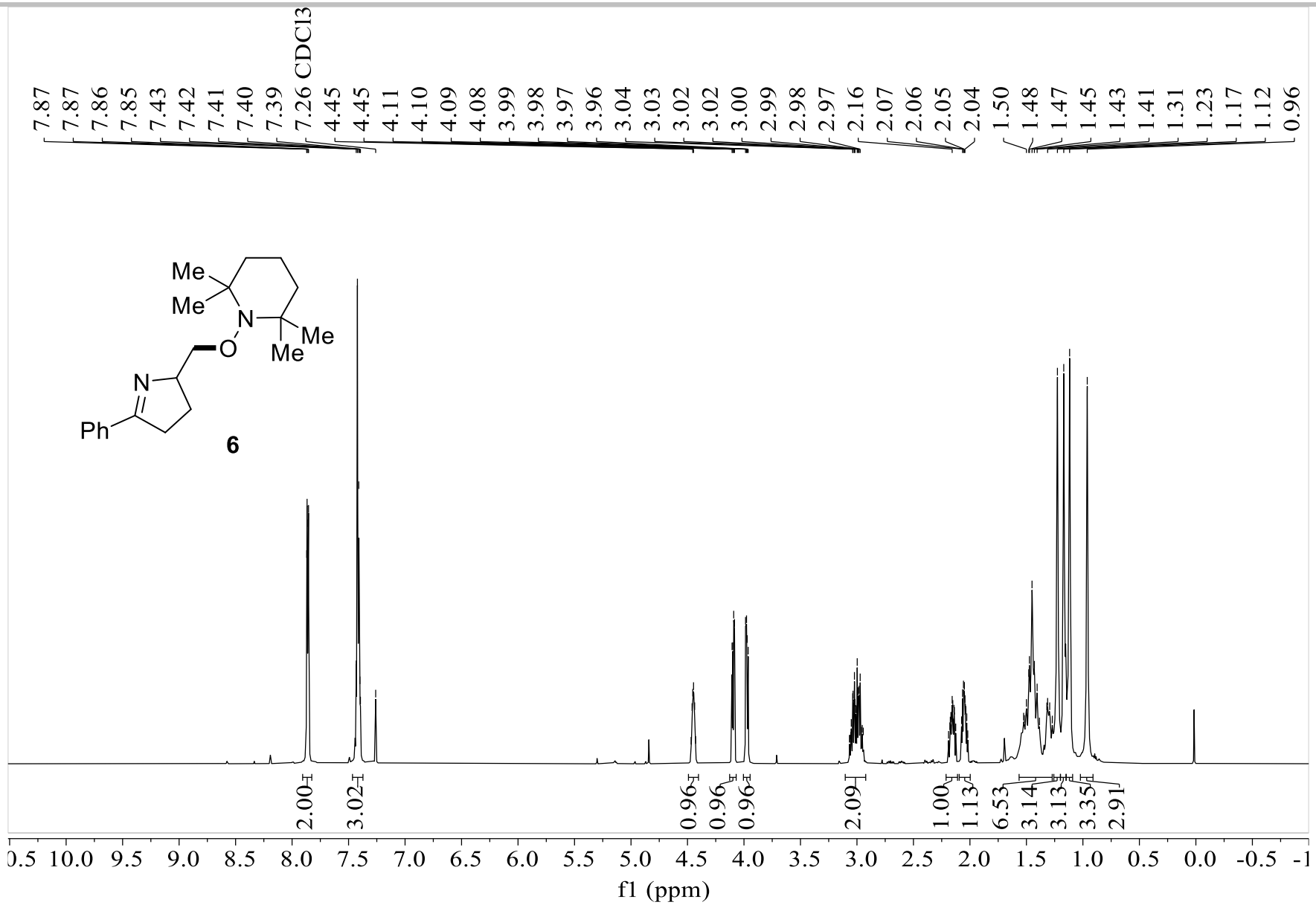
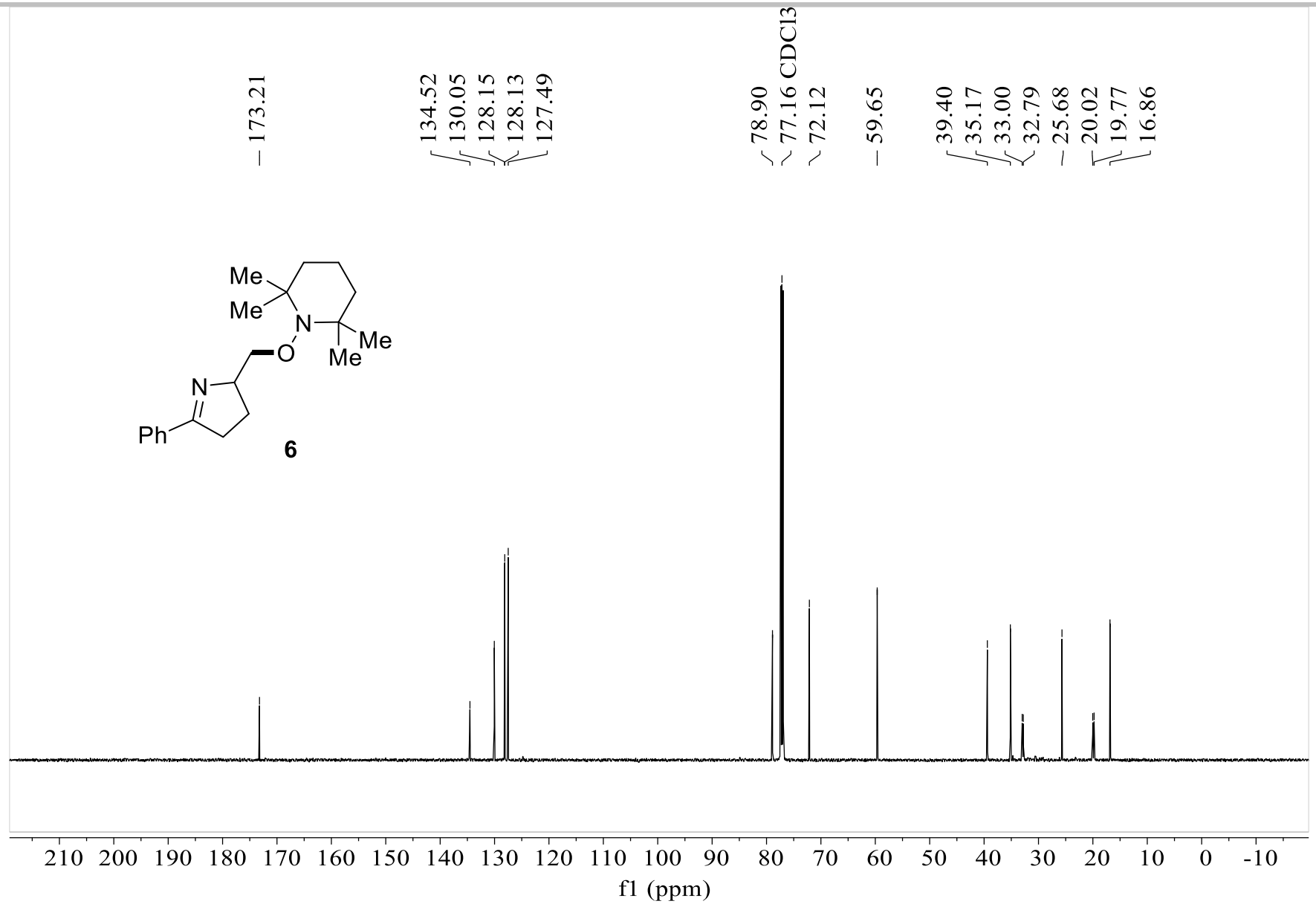
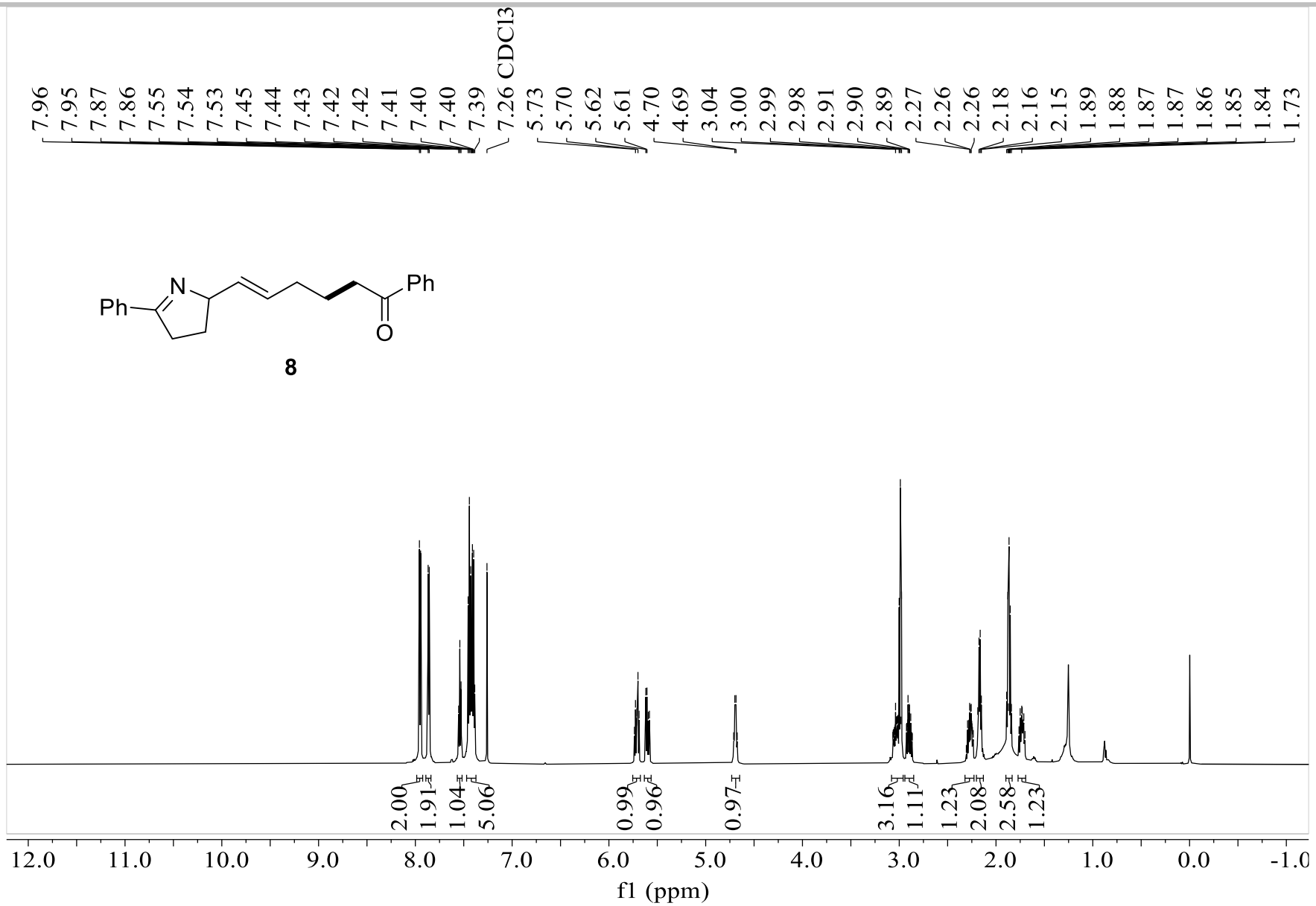
1.65
1.64
1.64
1.61
1.61
1.60
1.60
1.59
1.59
1.58
1.58
1.58
1.57
1.57
O
NC
5ak
1.00
2.06
2.10
4.20
2.14
2.03
4.41
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

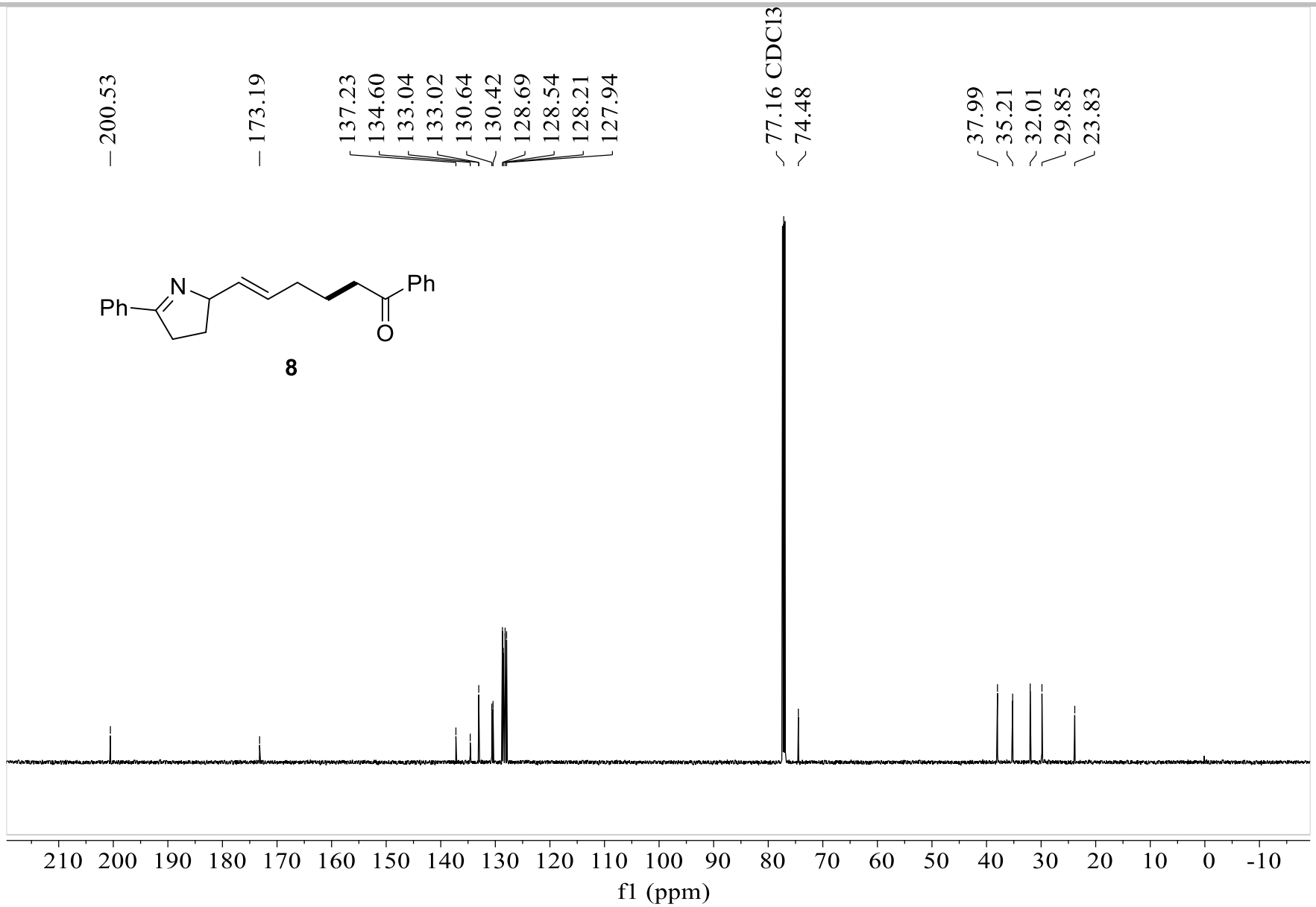

200.28
140.16
139.17
119.65
77.16 CDCl3
35.78
26.11
25.13
23.58
23.14
21.96
21.56
17.17
O
NC
5ak
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

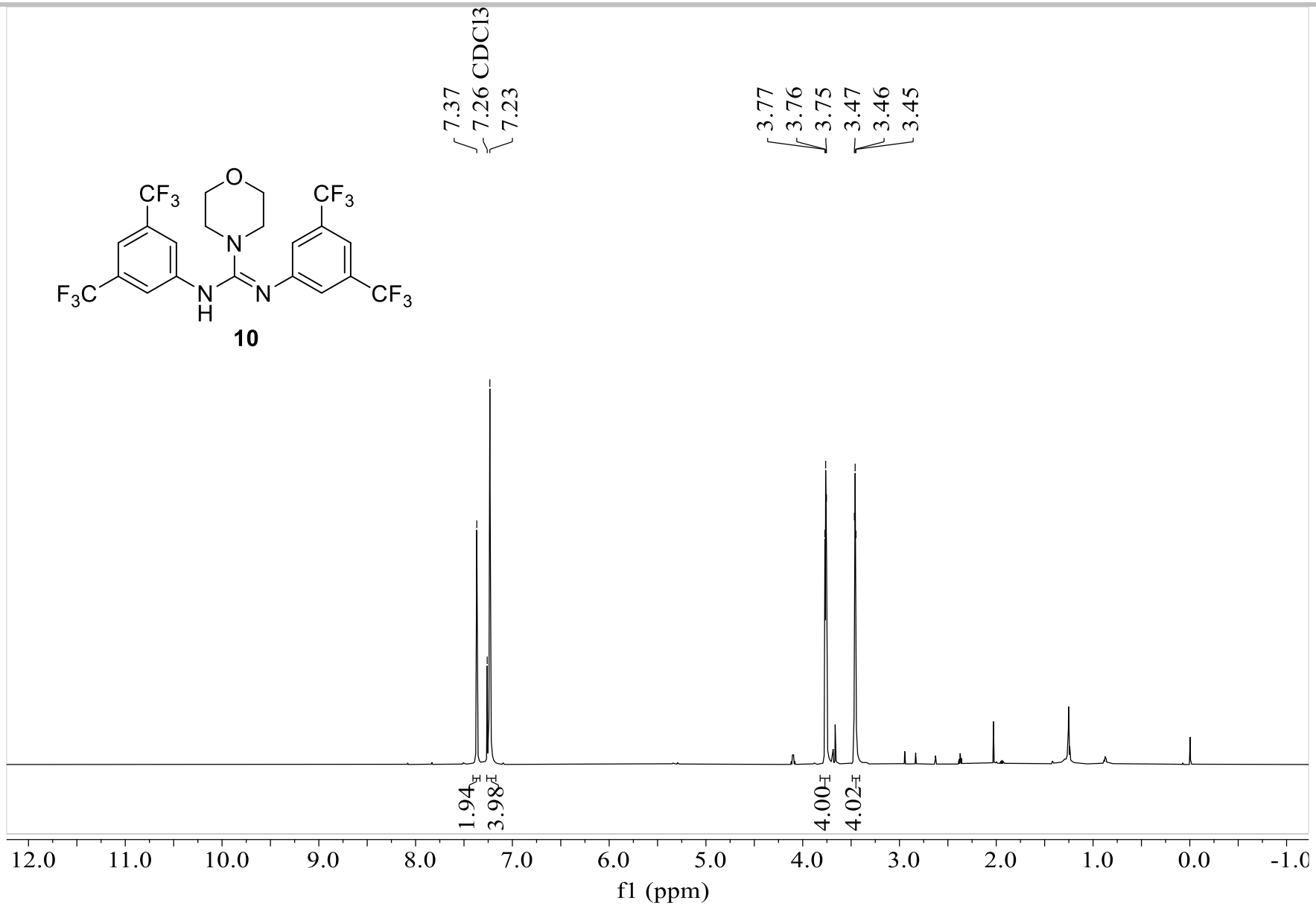

7.87
7.87
7.86
7.85
7.43
7.42
7.41
7.40
7.39
7.26 CDCl3
4.45
4.45
4.11
4.10
4.09
4.08
3.99
3.98
3.97
3.96
3.04
3.03
3.02
3.02
3.00
2.99
2.98
2.97
2.16
2.07
2.06
2.05
2.04
1.50
1.48
1.47
1.45
1.43
1.41
1.31
1.23
1.17
1.12
0.96
Me
Me
N
Me
Me
O
N
Ph
6
2.00
3.02
0.96
0.96
0.96
2.09
1.00
1.13
6.53
3.14
3.13
3.35
2.91
f1 (ppm)

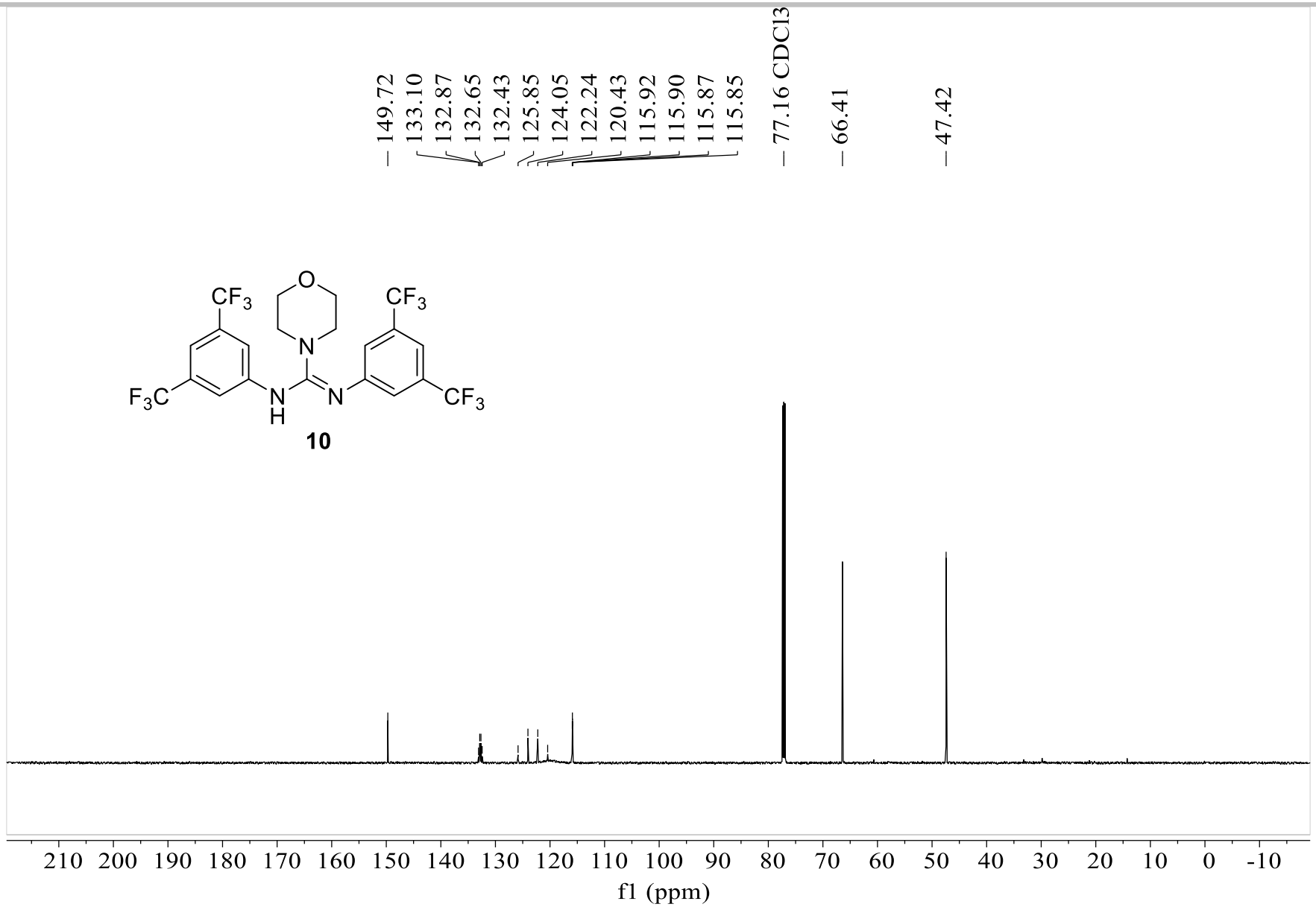

173.21
134.52
130.05
128.15
128.13
127.49
78.90
77.16 CDCl3
72.12
59.65
39.40
35.17
33.00
32.79
25.68
20.02
19.77
16.86
Me
Me
N
O
Me
Me
N
Ph
6
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

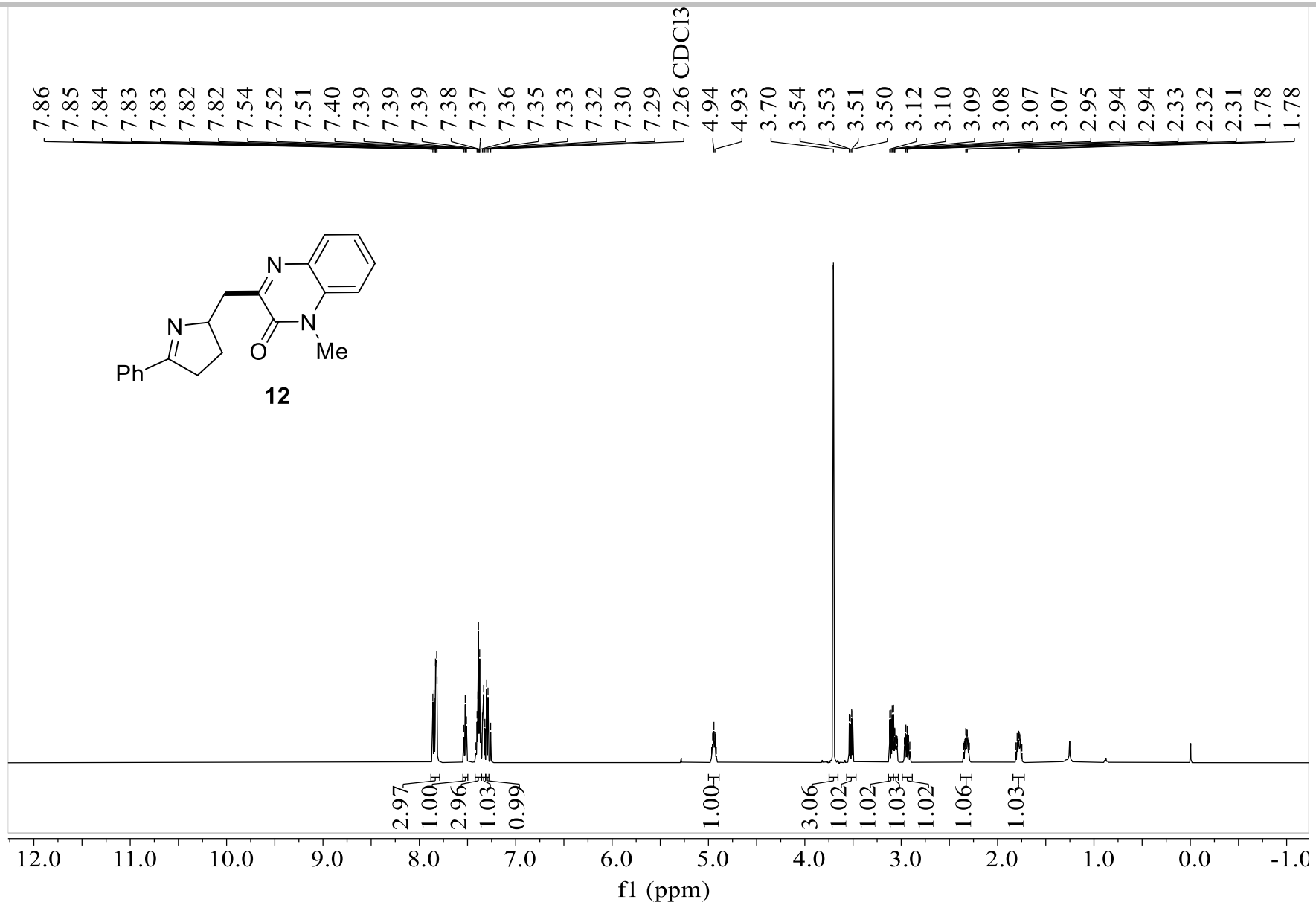

7.96
7.95
7.87
7.86
7.55
7.54
7.53
7.45
7.44
7.43
7.42
7.42
7.41
7.40
7.40
7.39
7.26 CDCl3
5.73
5.70
5.62
5.61
4.70
4.69
3.04
3.00
2.99
2.98
2.91
2.90
2.89
2.27
2.26
2.26
2.18
2.16
2.15
1.89
1.88
1.87
1.87
1.86
1.85
1.84
1.73
N
Ph
Ph
O
2.00
1.91
1.04
5.06
0.99
0.96
0.97
3.16
1.11
1.23
2.08
2.58
1.23
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)

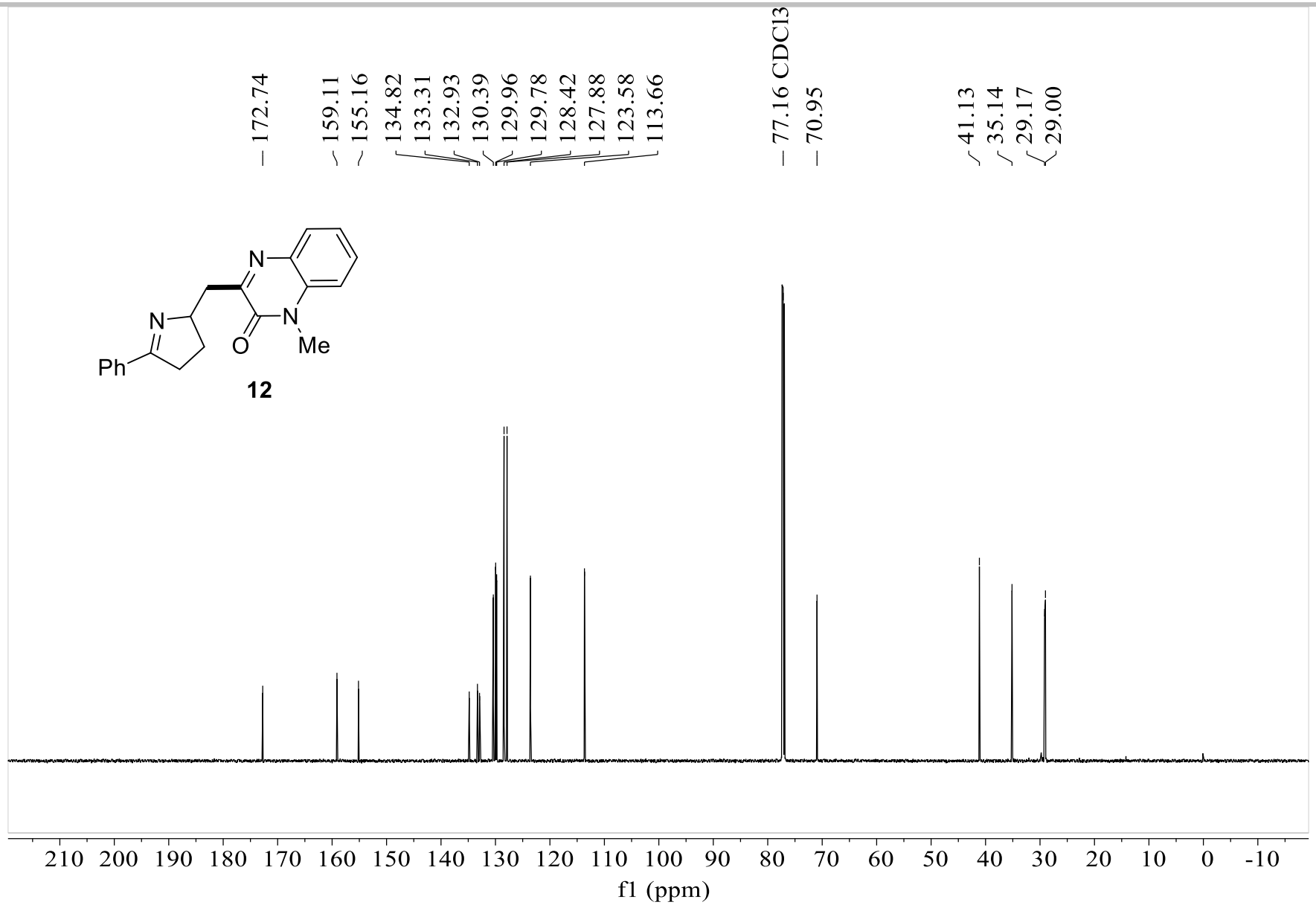
8

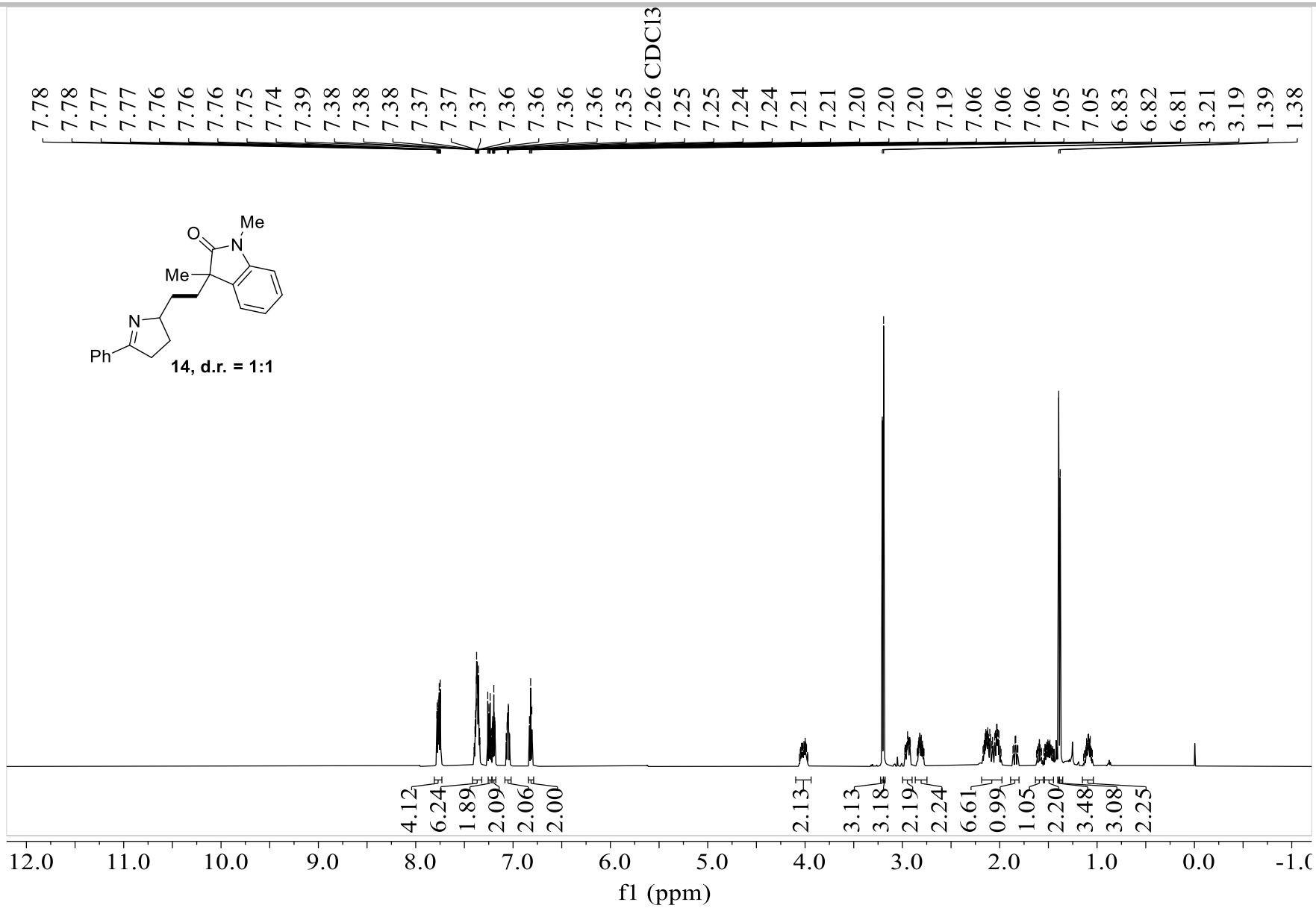

200.53
173.19
137.23
134.60
133.04
133.02
130.64
130.42
128.69
128.54
128.21
127.94
77.16 CDCl3
74.48
37.99
35.21
32.01
29.85
23.83
N
Ph
Ph
O
8
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

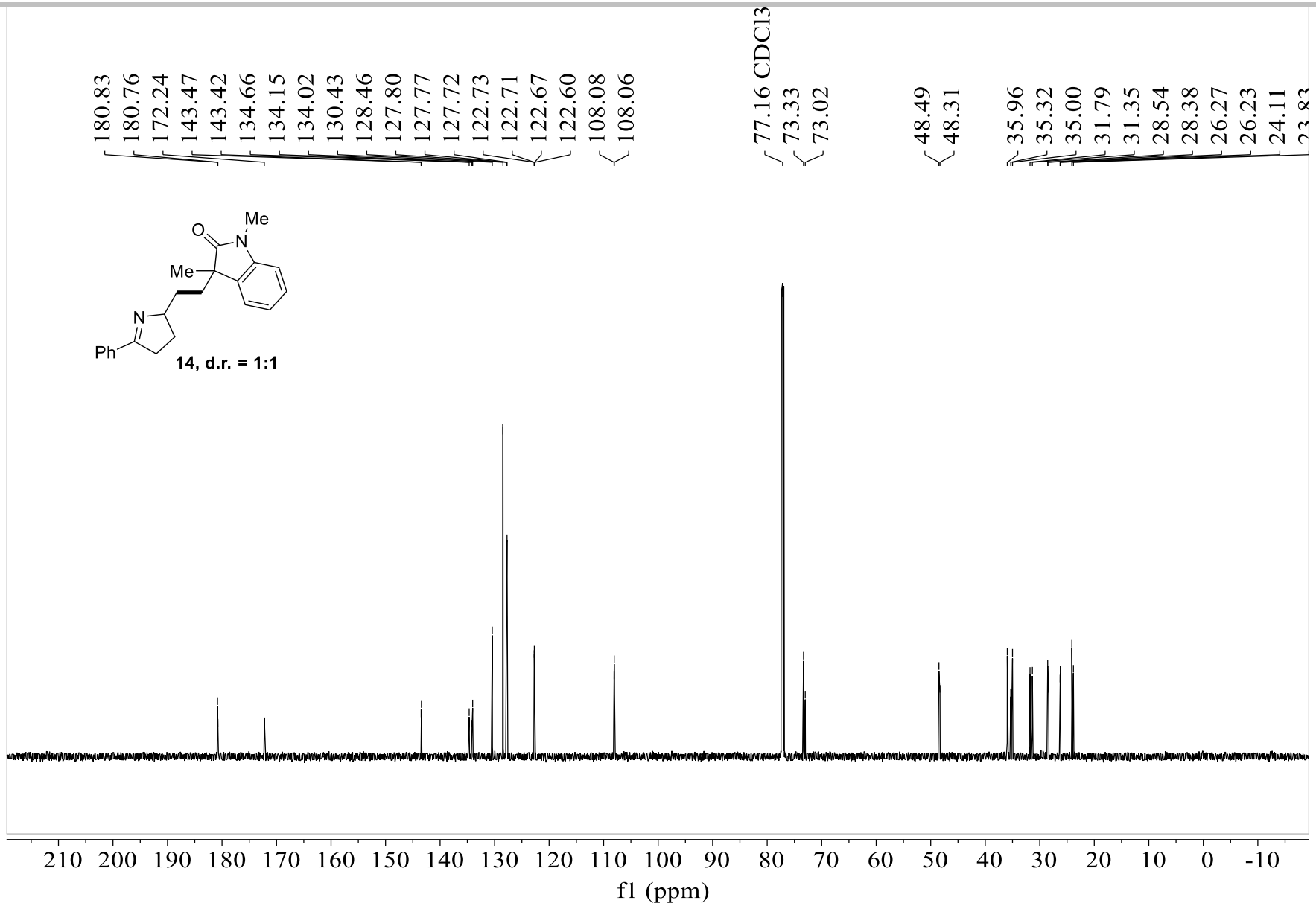

7.37
7.26 CDCl3
7.23
3.77
3.76
3.75
3.47
3.46
3.45
CF3
CF3
F3C
CF3
O
N
N
H
N
10
1.94
3.98
4.00
4.02
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)

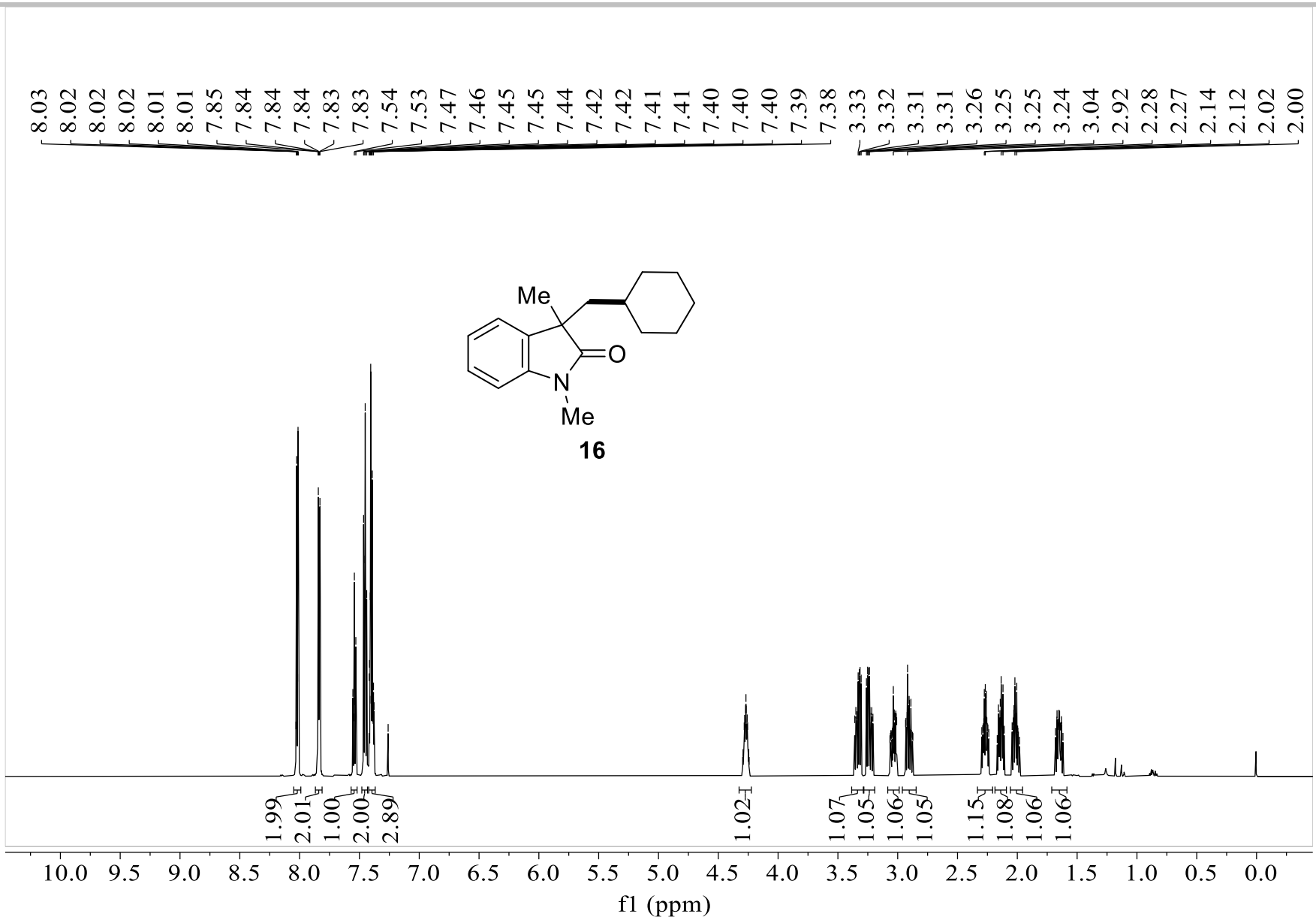

149.72
133.10
132.87
132.65
132.43
125.85
124.05
122.24
120.43
115.92
115.90
115.87
115.85
77.16 CDCl3
66.41
47.42
CF3
CF3
F3C
CF3
O
N
N
H
N
10
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

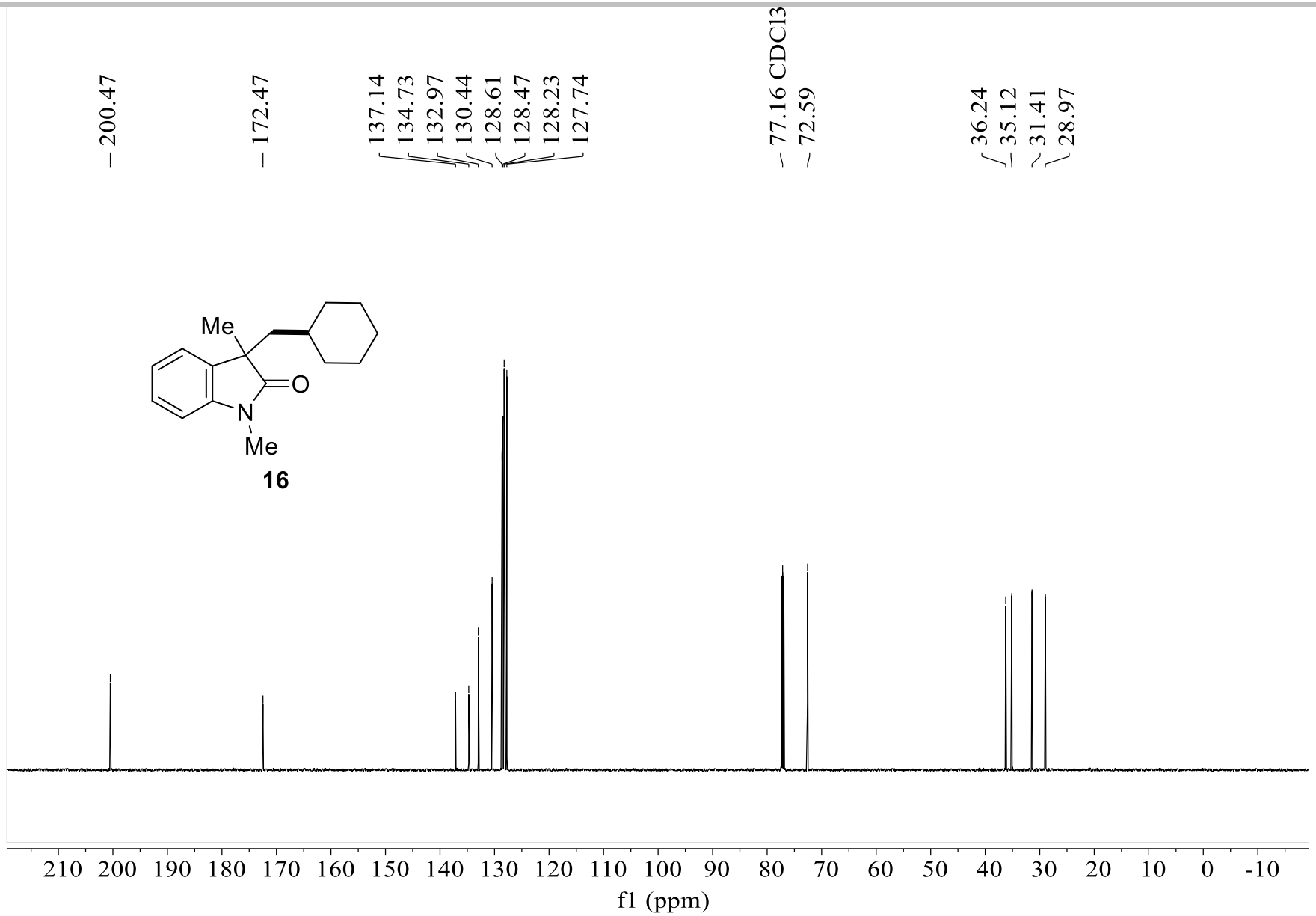

7.86
7.85
7.84
7.83
7.83
7.82
7.82
7.54
7.52
7.51
7.40
7.39
7.39
7.39
7.38
7.37
7.36
7.35
7.33
7.32
7.30
7.29
7.26 CDCl3
4.94
4.93
3.70
3.54
3.53
3.51
3.50
3.12
3.10
3.09
3.08
3.07
3.07
2.95
2.94
2.94
2.33
2.32
2.31
1.78
1.78
N
N
O
N
Me
Ph
12
2.97
1.00
2.96
1.03
0.99
1.00
3.06
1.02
1.02
1.03
1.02
1.06
1.03
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)


172.74
159.11
155.16
134.82
133.31
132.93
130.39
129.96
129.78
128.42
127.88
123.58
113.66
77.16 CDCl3
70.95
41.13
35.14
29.17
29.00
N
N
O
N
Me
Ph
12
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)


7.78 7.78 7.77 7.77 7.76 7.76 7.76 7.75 7.74 7.39 7.38 7.38 7.38 7.37 7.37 7.37 7.36 7.36 7.36 7.36 7.35 7.26 CDCl3 7.25 7.25 7.24 7.24 7.21 7.21 7.20 7.20 7.20 7.19 7.06 7.06 7.06 7.05 7.05 6.83 6.82 6.81 3.21 3.19 1.39 1.38
O
N
Me
Me
N
Ph
14, d.r. = 1:1
4.12 6.24 1.89 2.09 2.06 2.00 2.13 3.13 3.18 2.19 2.24 6.61 0.99 1.05 2.20 3.48 3.08 2.25
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.0
f1 (ppm)


180.83
180.76
172.24
143.47
143.42
134.66
134.15
134.02
130.43
128.46
127.80
127.77
127.72
122.73
122.71
122.67
122.60
108.08
108.06
77.16 CDCl3
73.33
73.02
48.49
48.31
35.96
35.32
35.00
31.79
31.35
28.54
28.38
26.27
26.23
24.11
O
N
Me
Me
N
Ph
14, d.r. = 1:1
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.03 8.02 8.02 8.02 8.01 8.01 7.85 7.84 7.84 7.84 7.83 7.83 7.54 7.53 7.47 7.46 7.45 7.45 7.44 7.42 7.42 7.41 7.41 7.40 7.40 7.40 7.39 7.38
3.33 3.32 3.31 3.31 3.26 3.25 3.25 3.24 3.04 2.92 2.28 2.27 2.14 2.12 2.02 2.00
Me
O
N
Me
16
1.99 2.01 1.00 2.00 2.89 1.02 1.07 1.05 1.06 1.05 1.15 1.08 1.06 1.06
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
f1 (ppm)


200.47
172.47
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130.44
128.61
128.47
128.23
127.74
77.16 CDCl3
72.59
36.24
35.12
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Me
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N
Me
16
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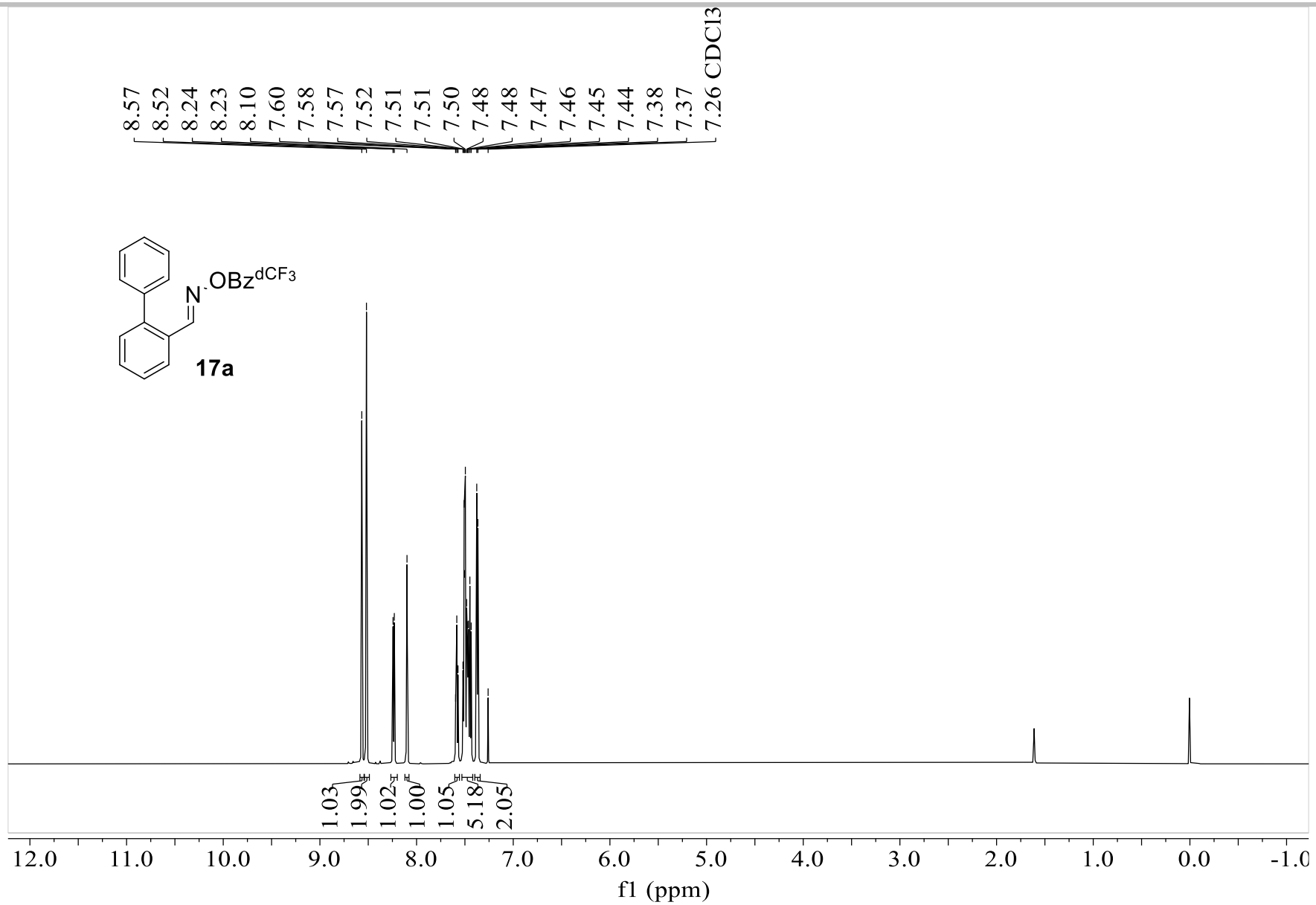
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7.45
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7.38
7.37
7.26 CDCl3
N
OBz^dCF3
17a
1.03
1.99
1.02
1.00
1.05
5.18
2.05
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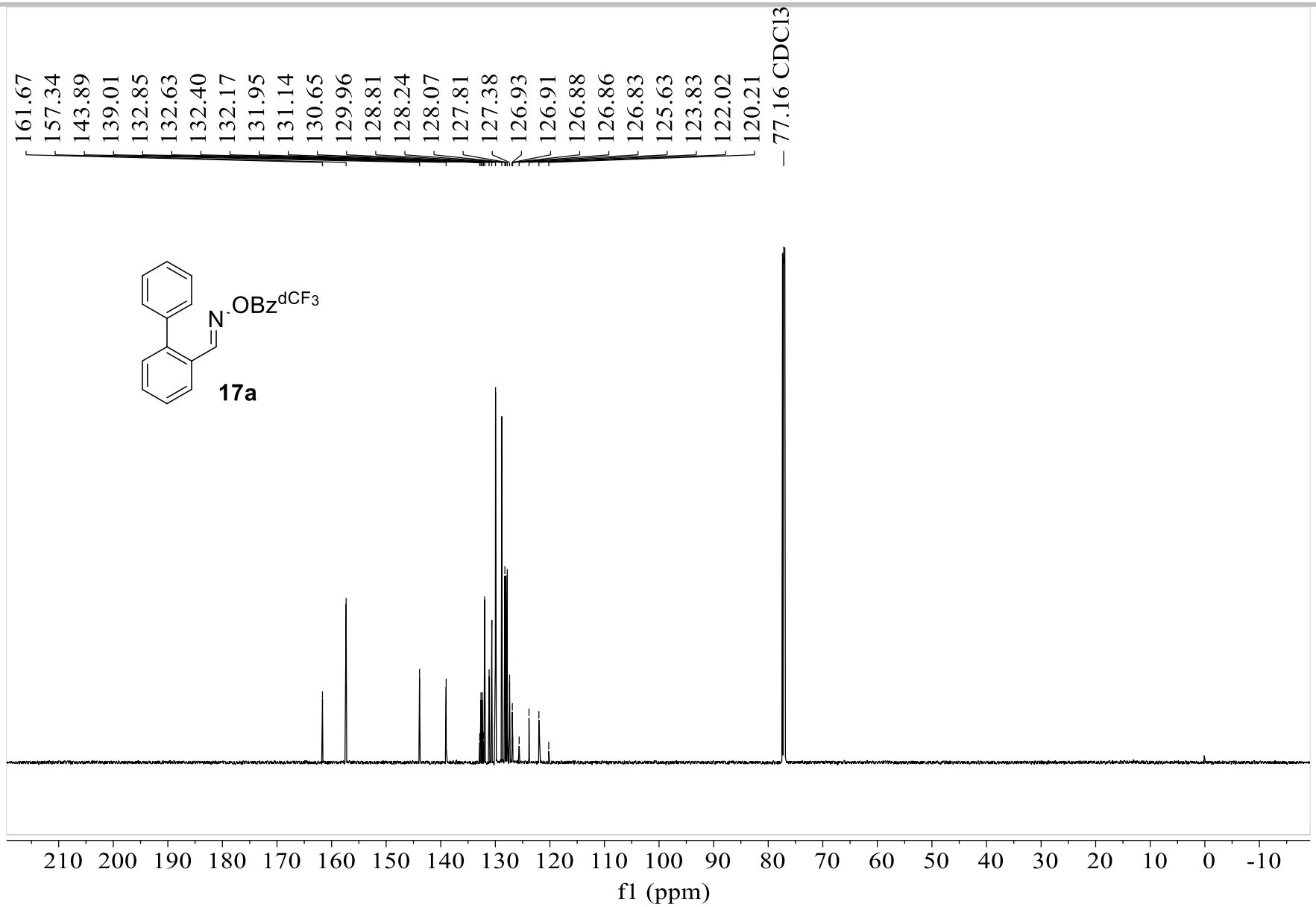
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128.07
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126.91
126.88
126.86
126.83
125.63
123.83
122.02
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77.16 CDCl3
N
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17a
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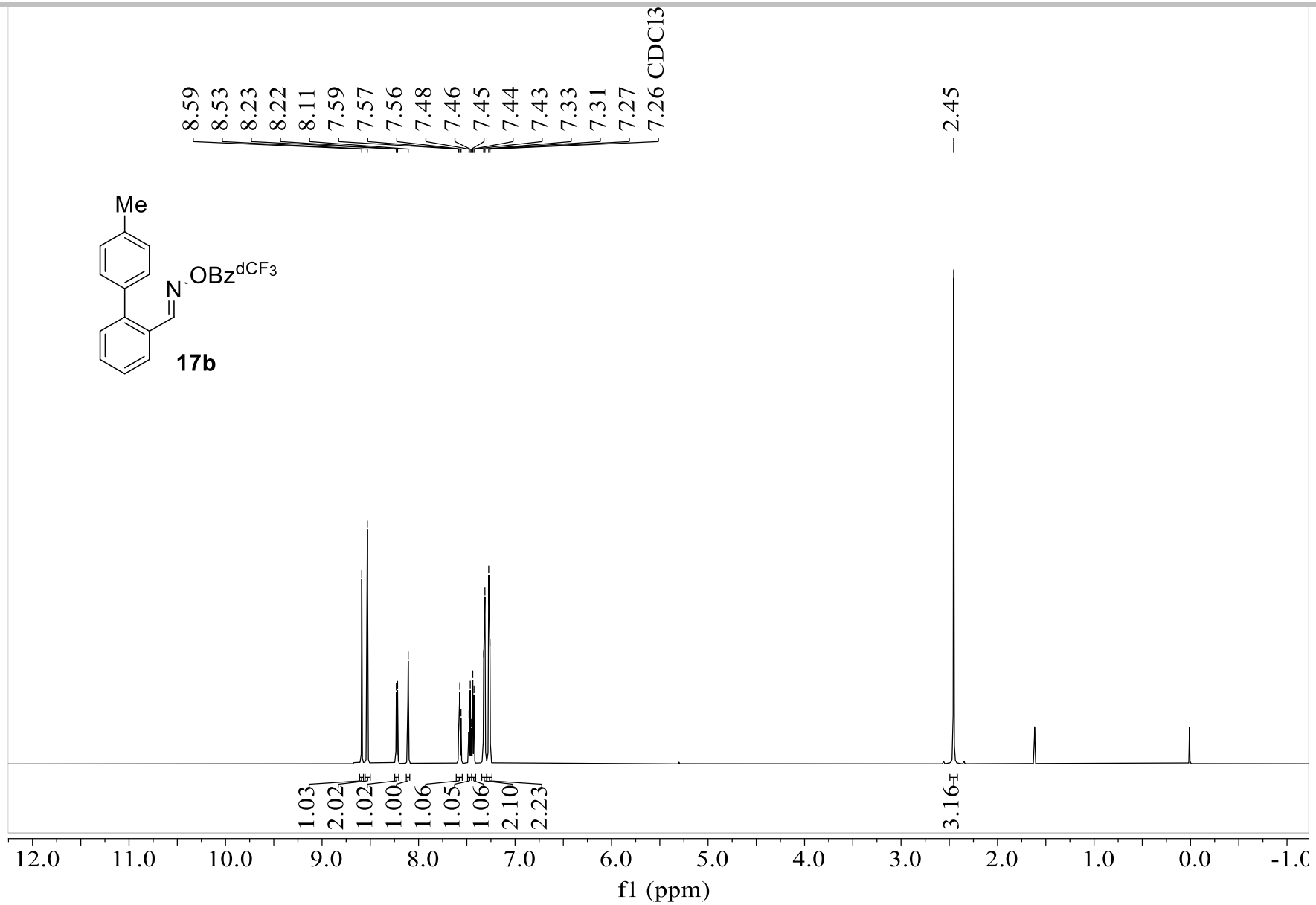
f1 (ppm)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7.43
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7.31
7.27
7.26 CDCl3
2.45
Me
N
OBz^dCF3
17b
1.03
2.02
1.02
1.00
1.06
1.05
1.06
2.10
2.23
3.16
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11.0
10.0
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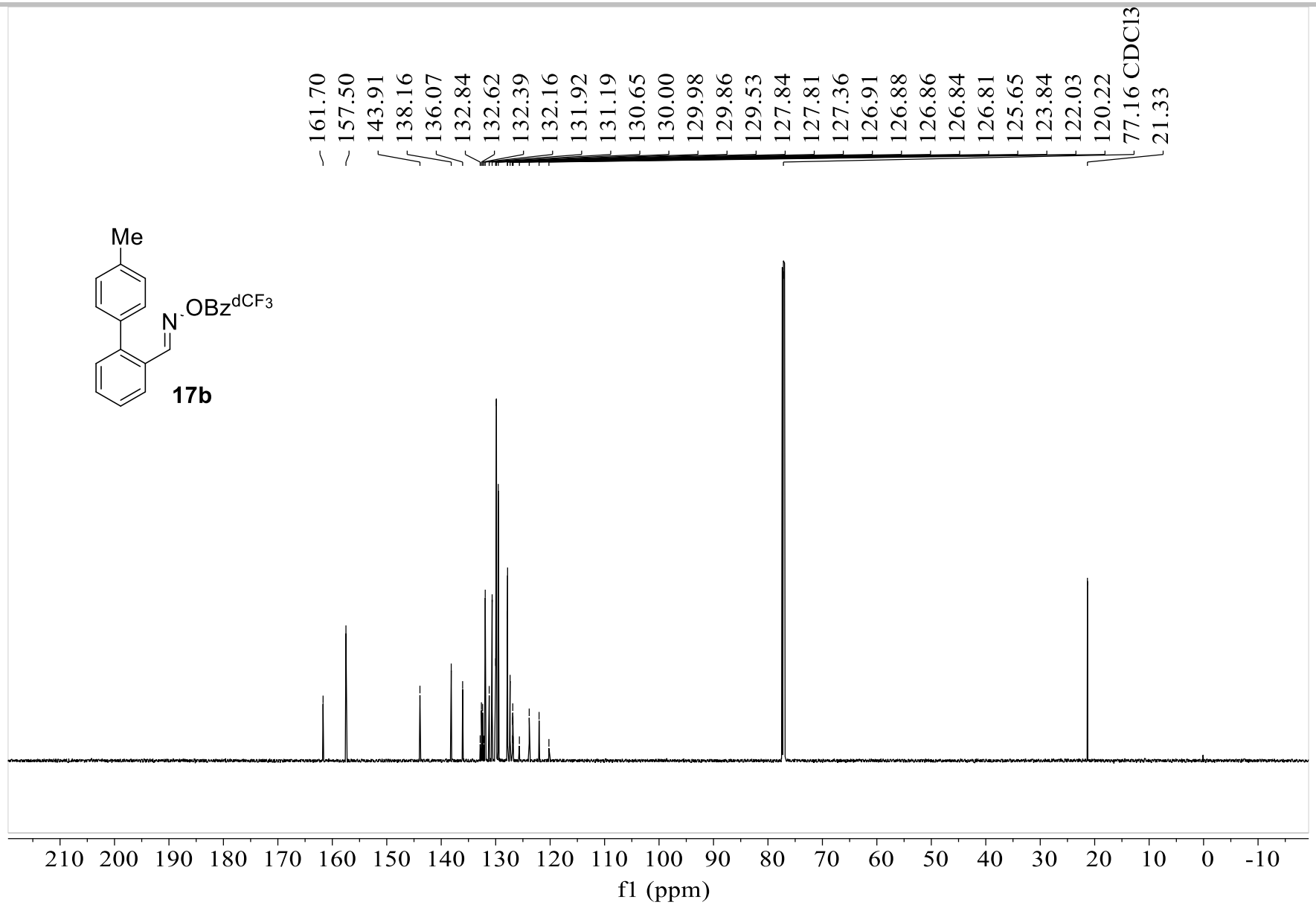
f1 (ppm)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123.84
122.03
120.22
77.16 CDCl3
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17b
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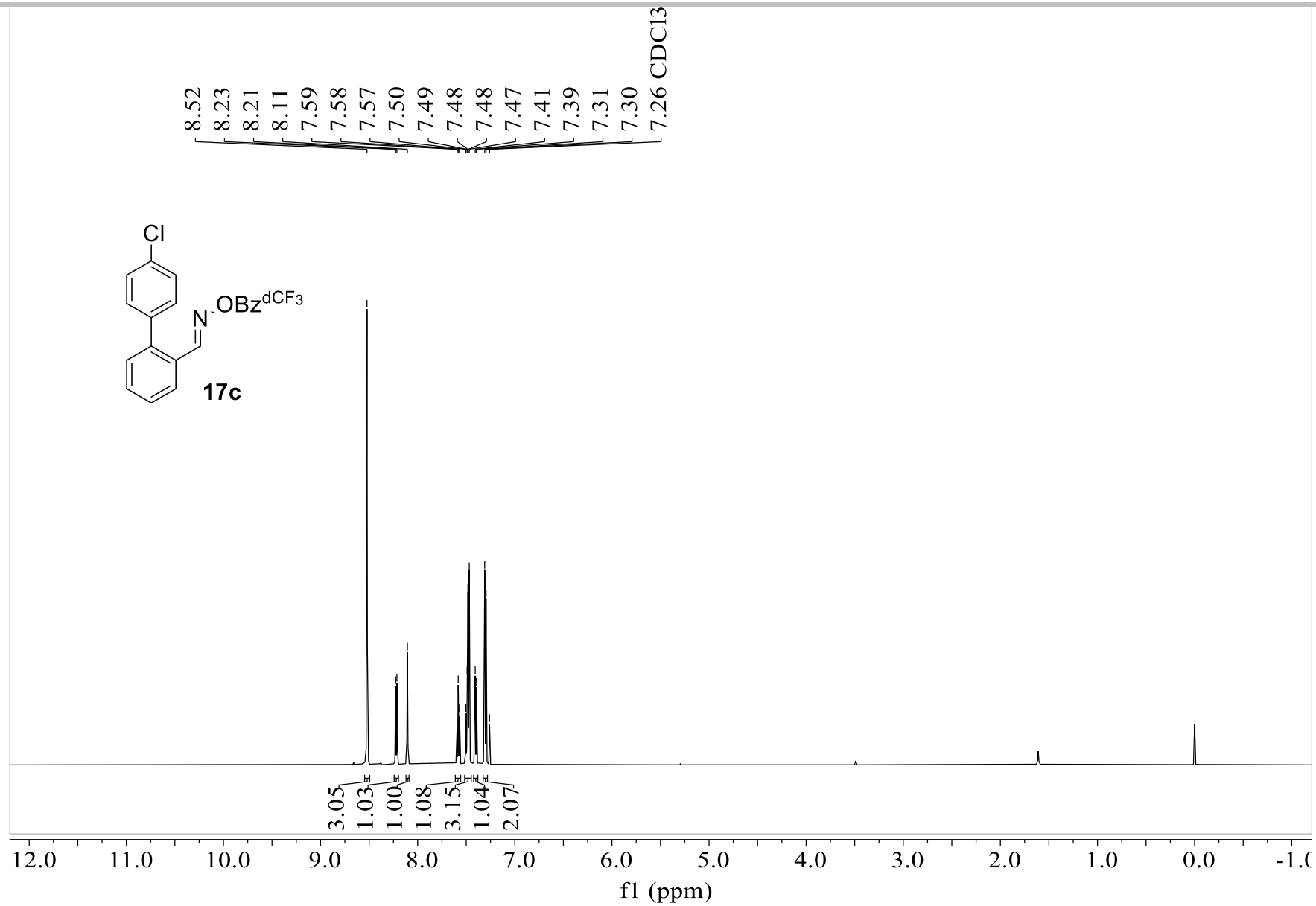
f1 (ppm)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7.41
7.39
7.31
7.30
7.26 CDCl3
Cl
N
OBz^dCF3
17c
3.05
1.03
1.00
1.08
3.15
1.04
2.07
12.0
11.0
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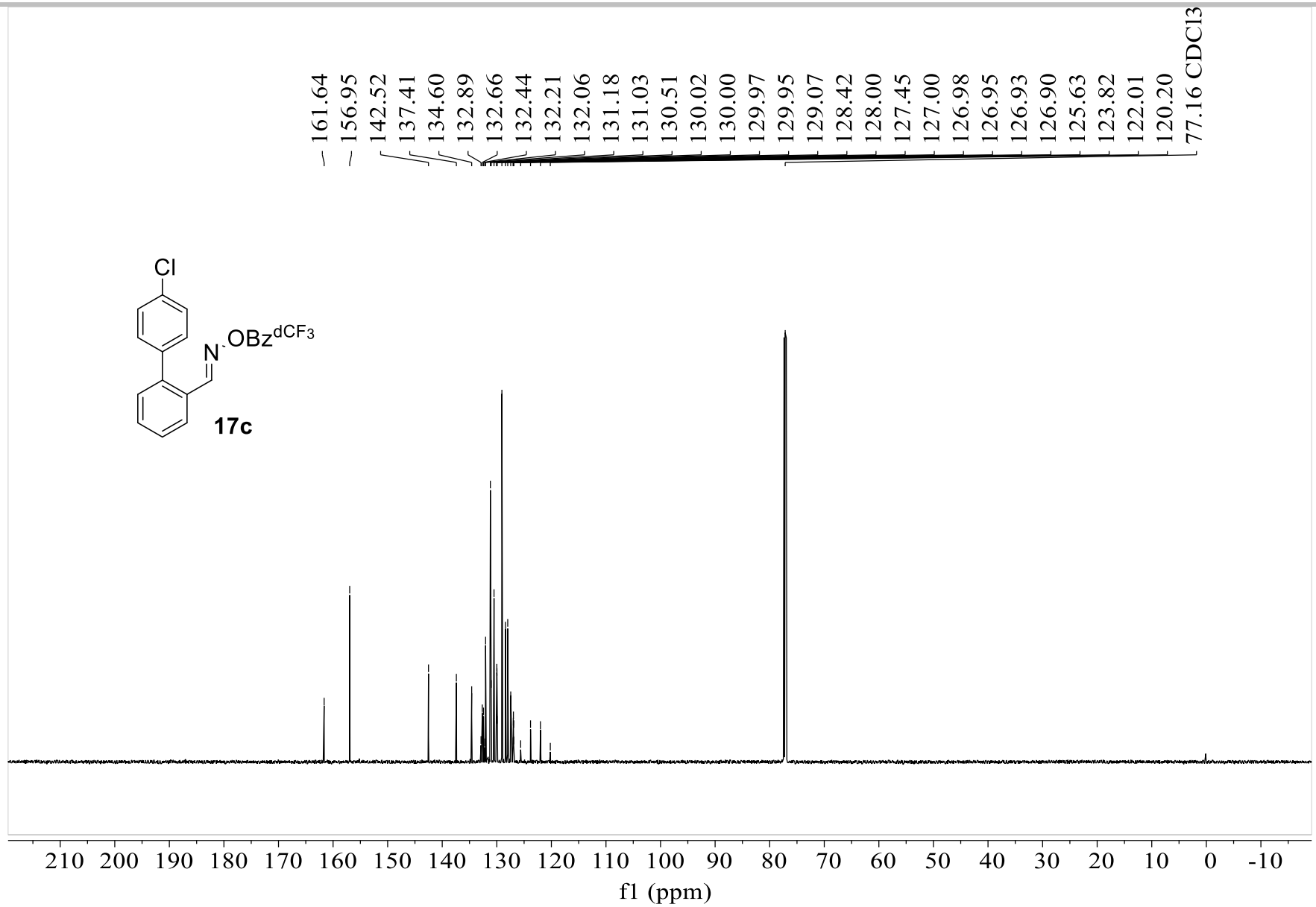
f1 (ppm)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127.00
126.98
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126.90
125.63
123.82
122.01
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N
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17c
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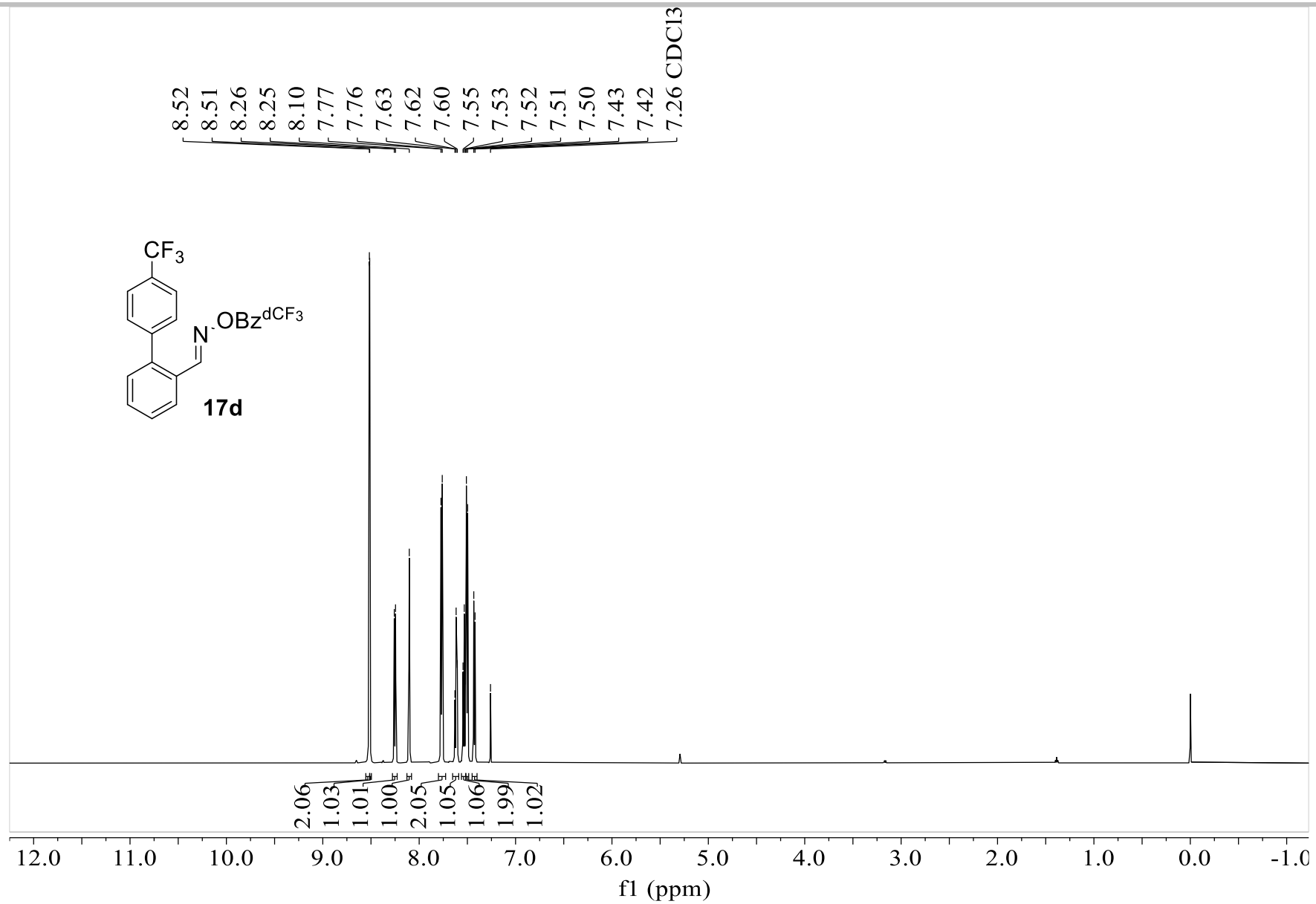
f1 (ppm)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7.55
7.53
7.52
7.51
7.50
7.43
7.42
7.26 CDCl3
CF3
N
OBzdCF3
17d
2.06
1.03
1.01
1.00
2.05
1.05
1.06
1.99
1.02
12.0
11.0
10.0
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1.0
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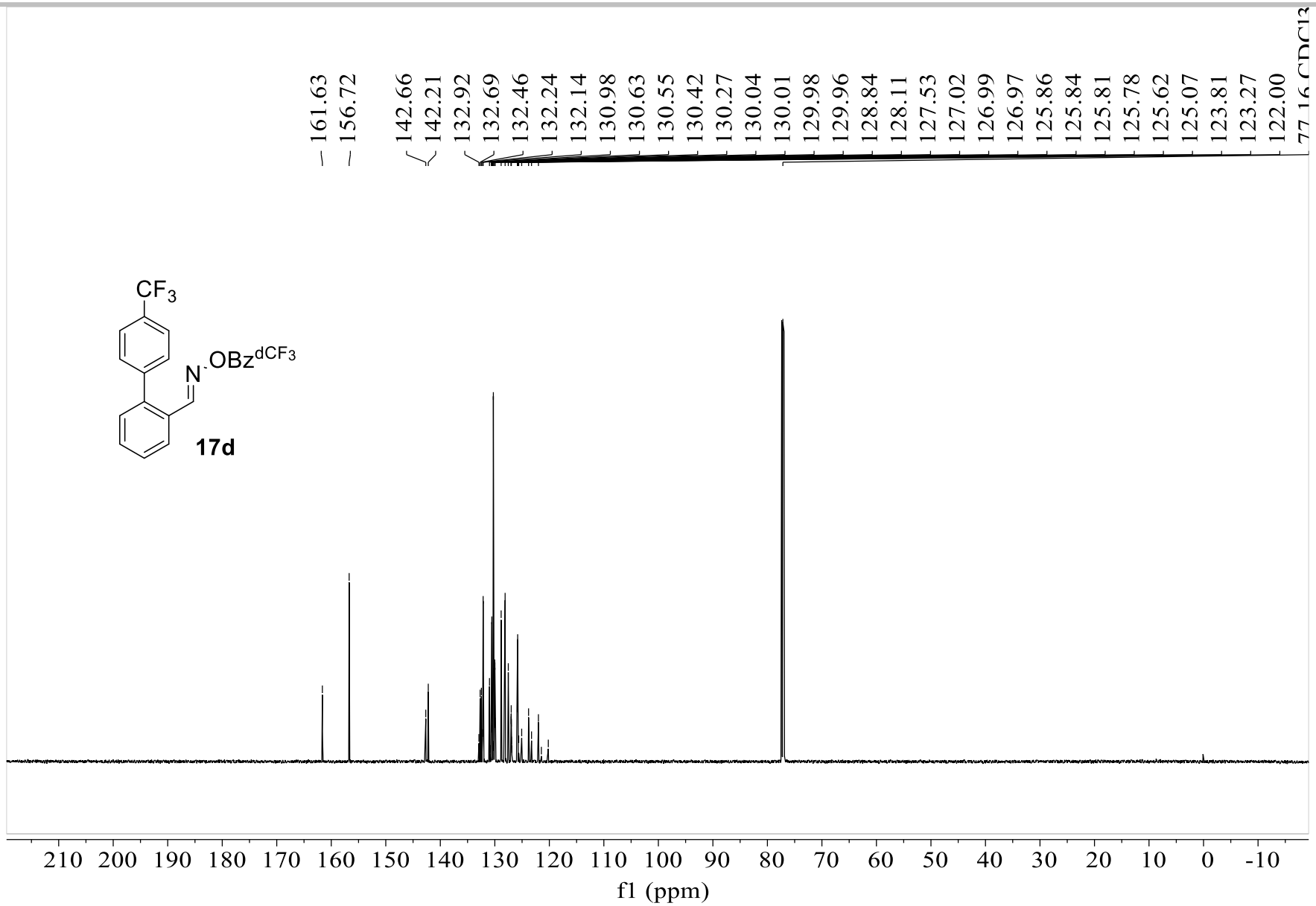
f1 (ppm)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130.42
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130.01
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128.11
127.53
127.02
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126.97
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125.81
125.78
125.62
125.07
123.81
123.27
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CF3
N
OBzdCF3
17d
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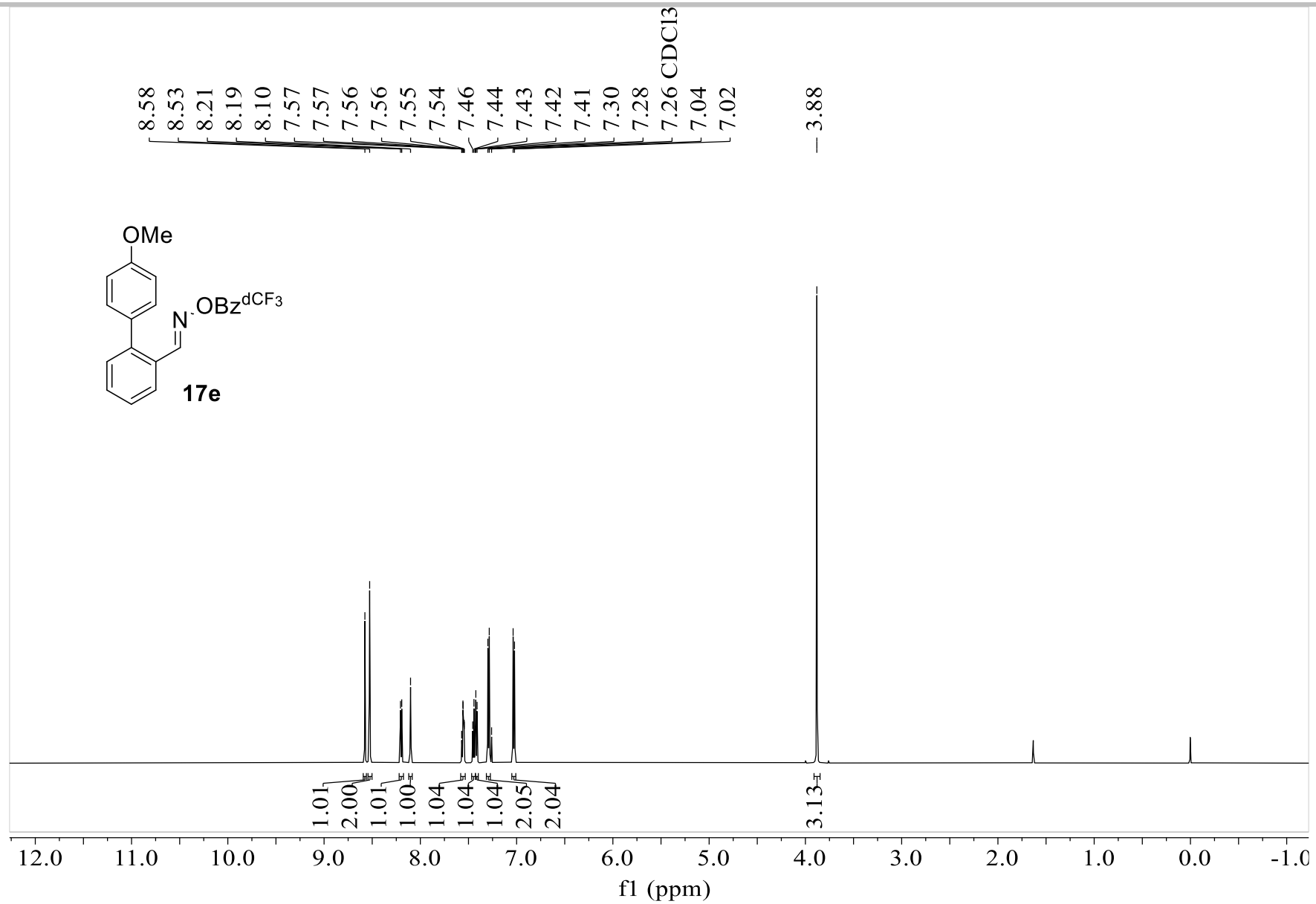
f1 (ppm)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7.44
7.43
7.42
7.41
7.30
7.28
7.26 CDCl3
7.04
7.02
3.88
OMe
N
OBz^dCF3
17e
1.01
2.00
1.01
1.00
1.04
1.04
1.04
2.05
2.04
3.13
12.0
11.0
10.0
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6.0
5.0
4.0
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1.0
0.0
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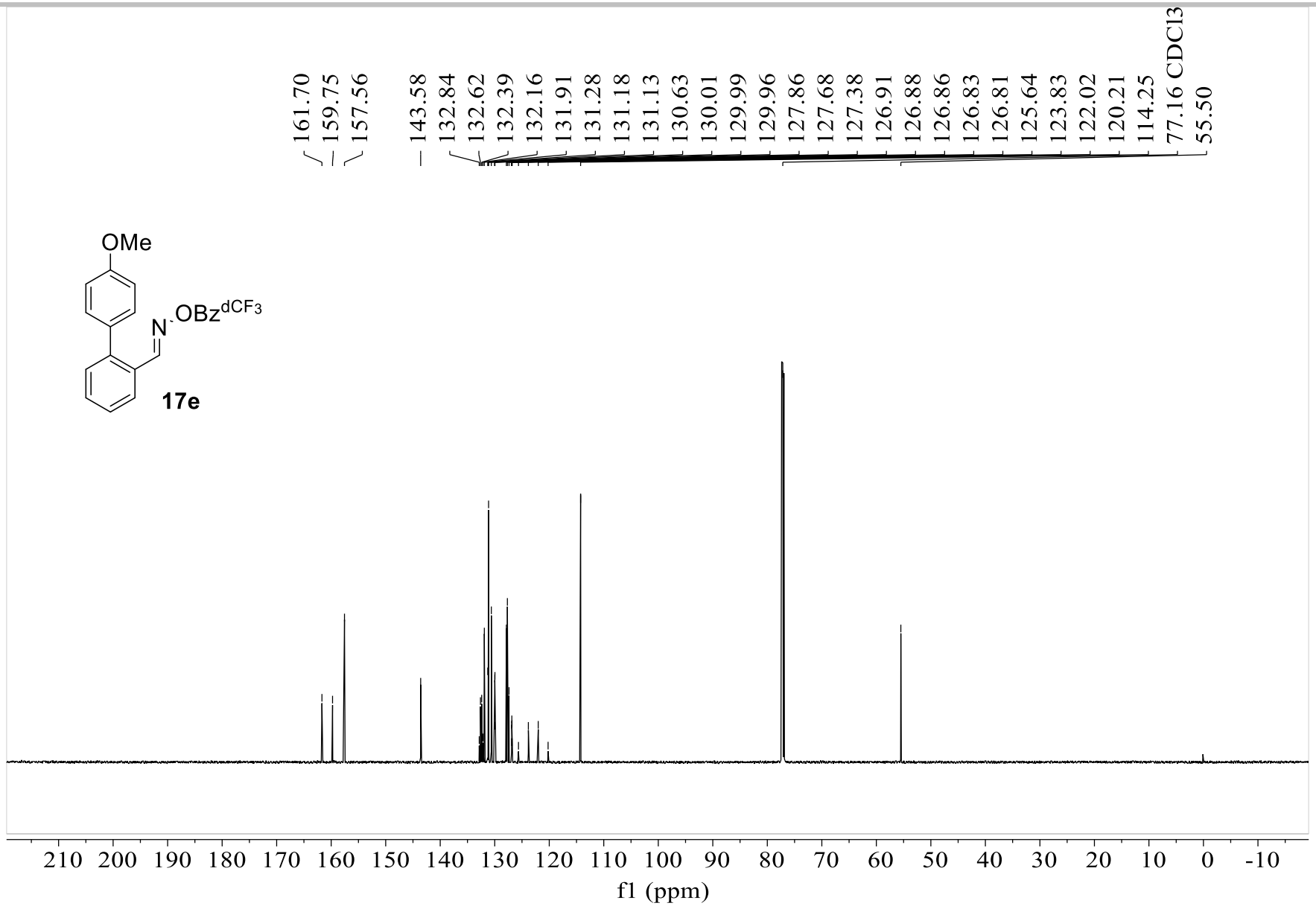
f1 (ppm)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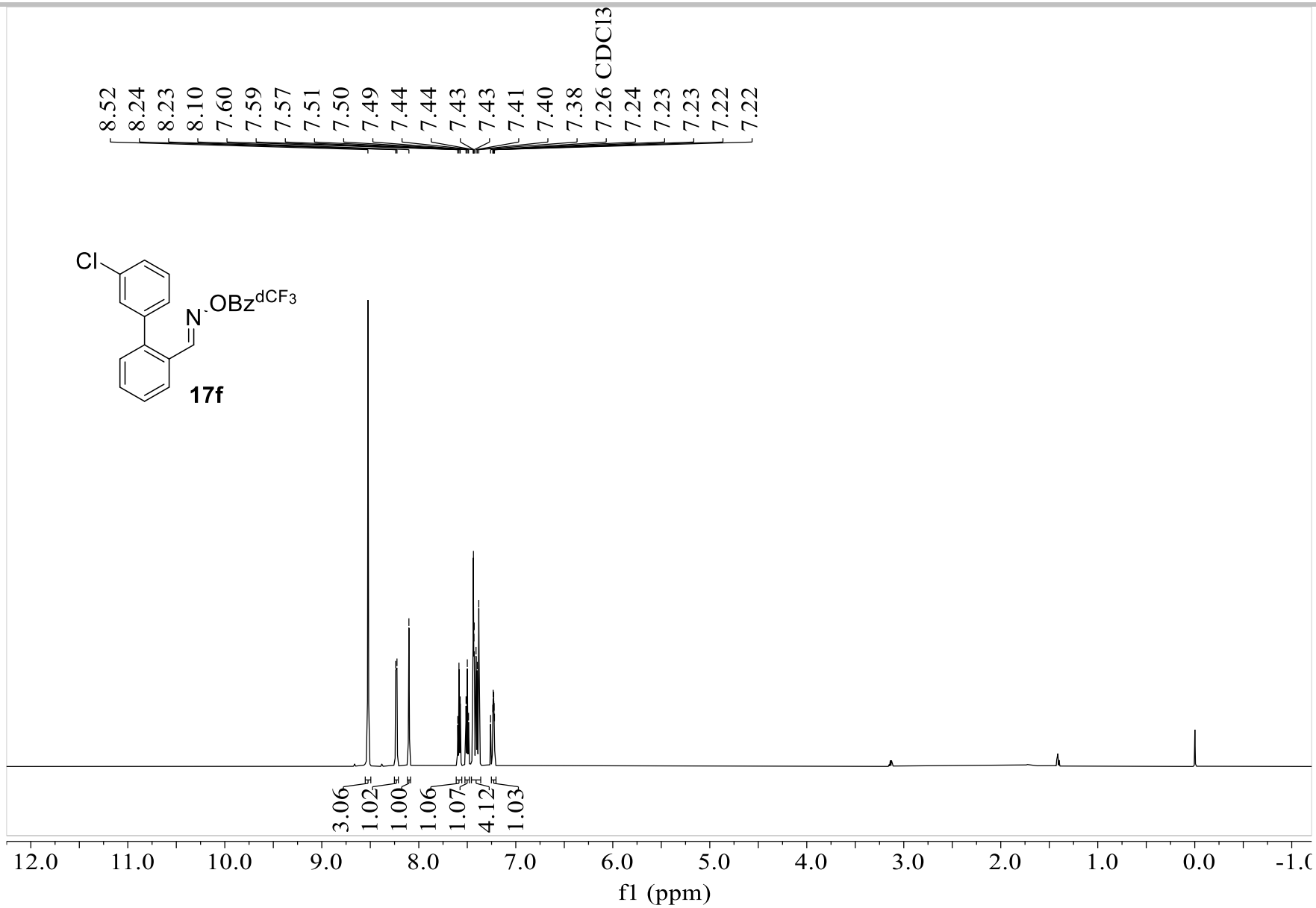
126.81
125.64
123.83
122.02
120.21
114.25
77.16 CDCl3
55.50
OMe
N
OBz^dCF3
17e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.43
7.43
7.41
7.40
7.38
7.26 CDCl3
7.24
7.23
7.23
7.22
7.22
Cl
N
OBz^dCF3
17f
3.06
1.02
1.00
1.06
1.07
4.12
1.03
12.0
11.0
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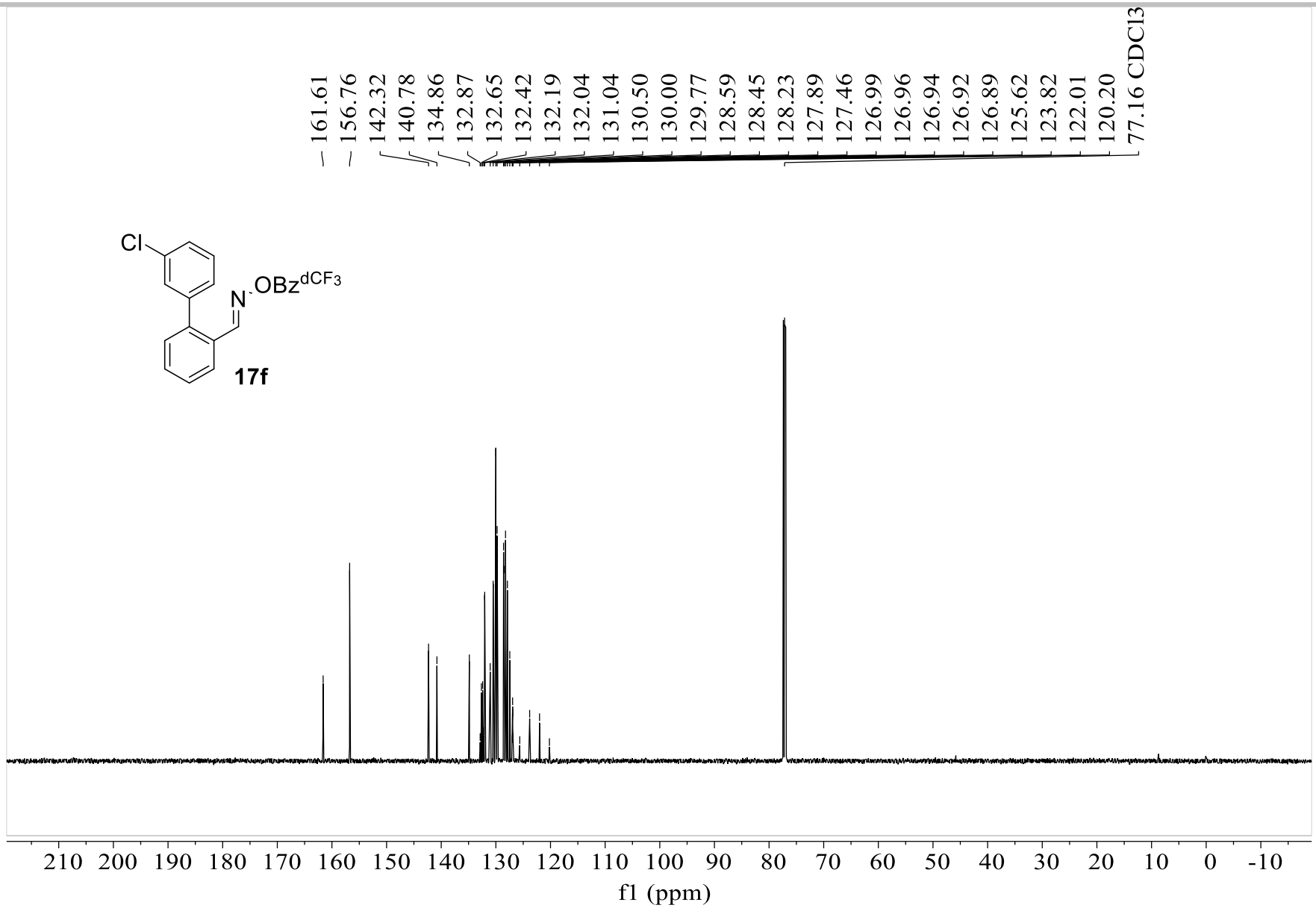
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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129.77
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128.45
128.23
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127.46
126.99
126.96
126.94
126.92
126.89
125.62
123.82
122.01
120.20
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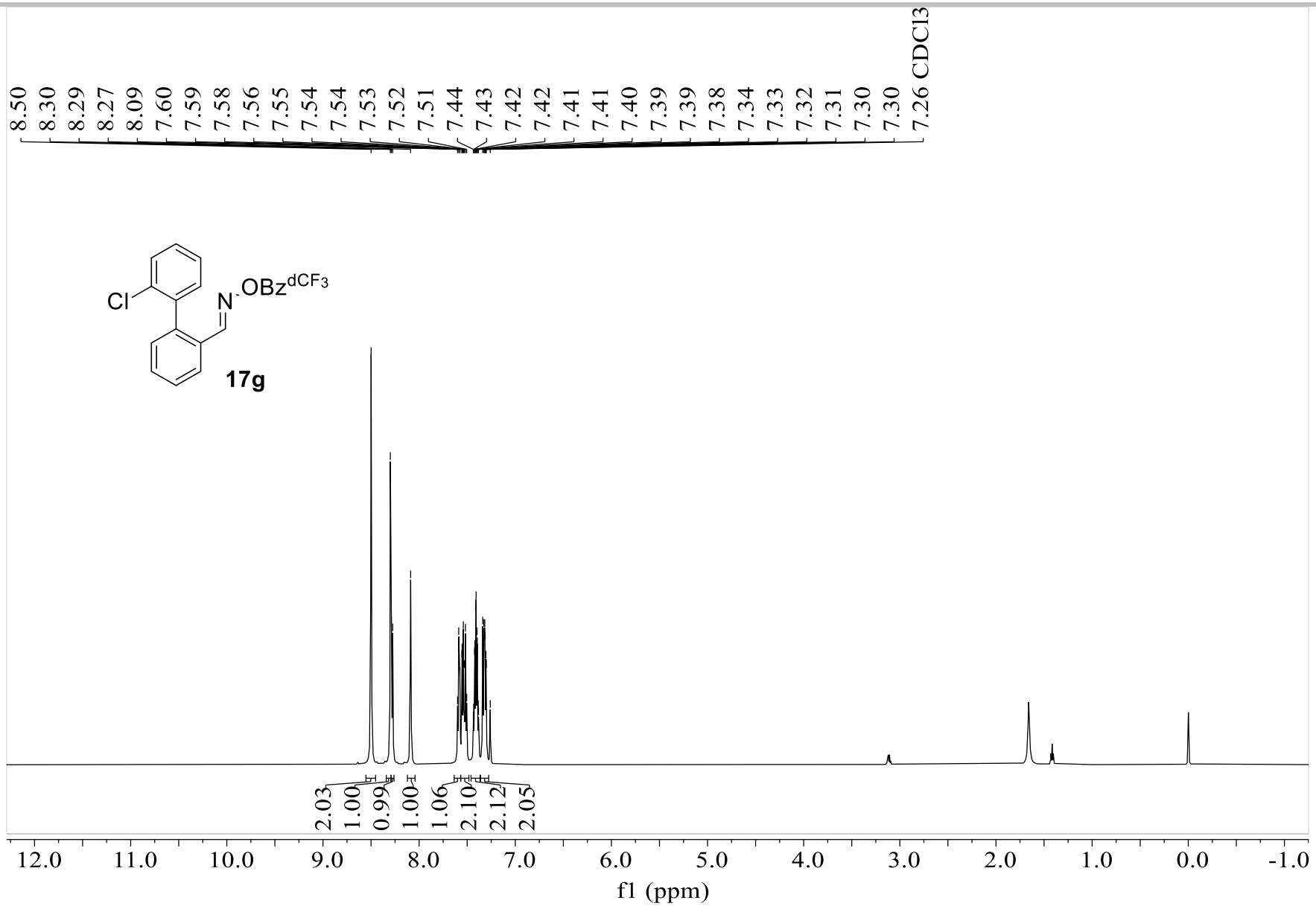
Cl
N
OBz^dCF3
17f
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.51
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7.42
7.42
7.41
7.41
7.40
7.39
7.39
7.38
7.34
7.33
7.32
7.31
7.30
7.30
7.26 CDCl3
Cl
N
OBz^dCF3
17g
2.03
1.00
0.99
1.00
1.06
2.10
2.12
2.05
12.0
11.0
10.0
9.0
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5.0
4.0
3.0
2.0
1.0
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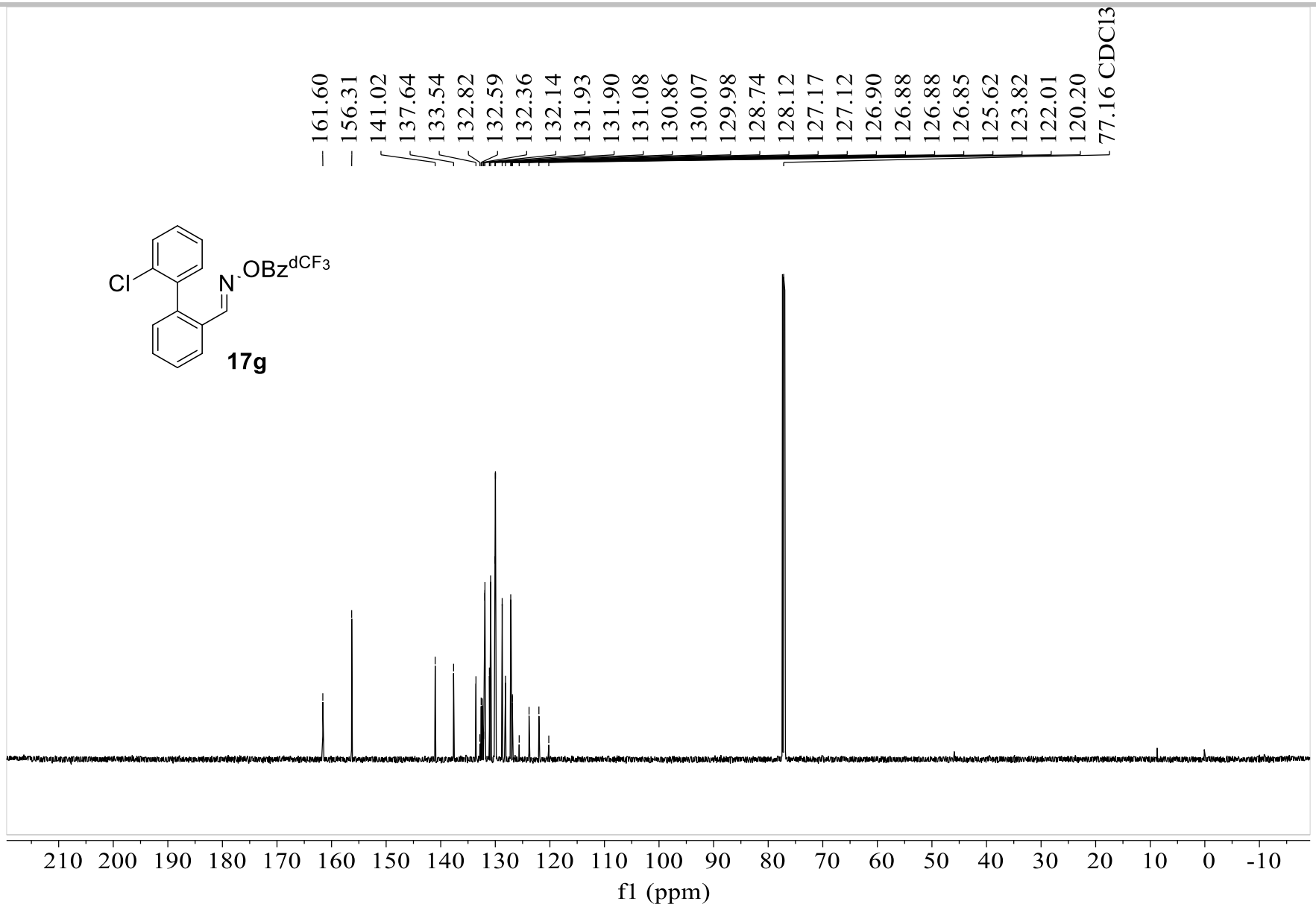
-1.0
f1 (ppm)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127.12
126.90
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126.88
126.85
125.62
123.82
122.01
120.20
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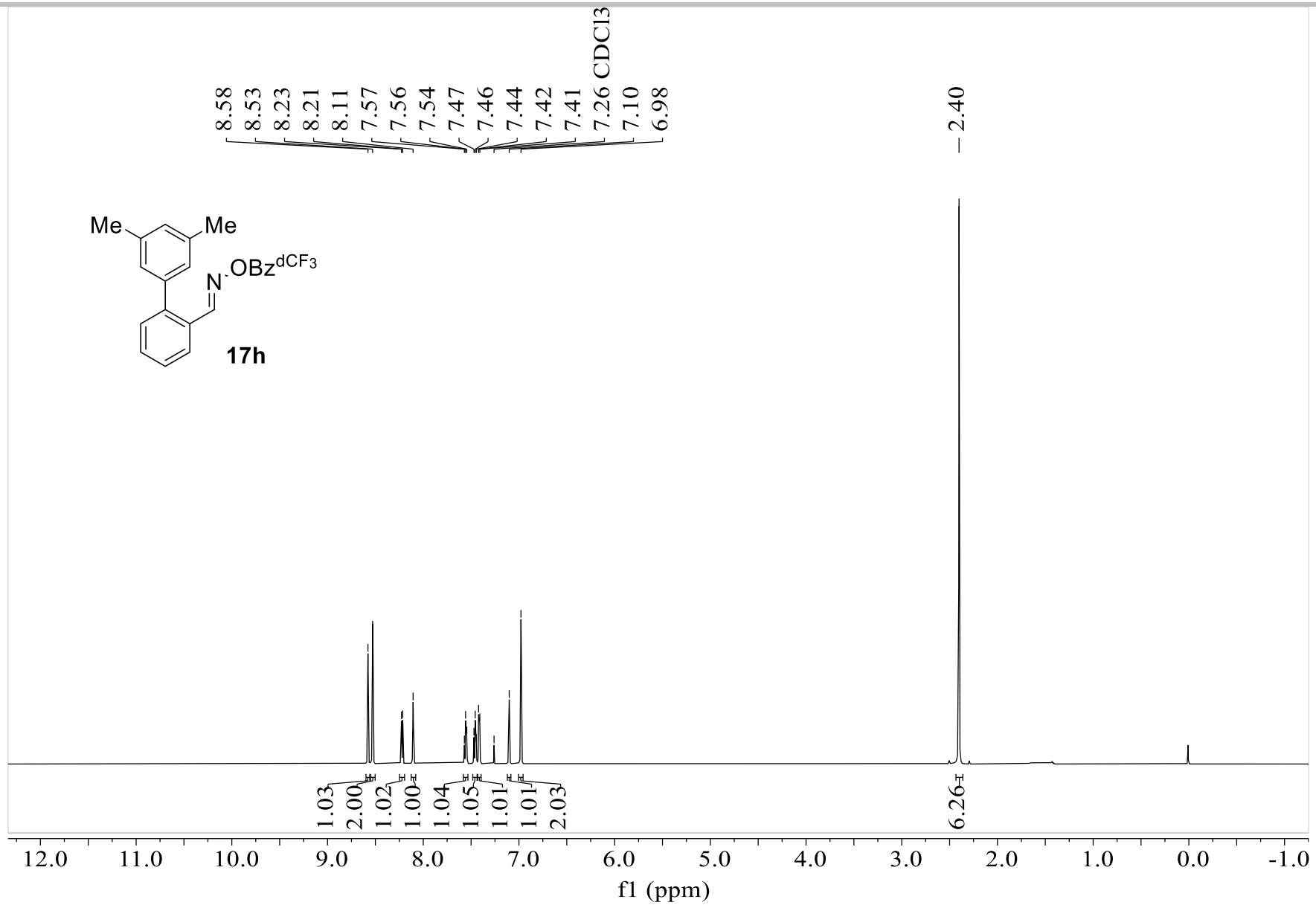
Cl
N
OBz^{dCF_3}
17g
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.41
7.26 CDCl3
7.10
6.98
2.40
Me
Me
N
OBz^dCF3
17h
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2.00
1.02
1.00
1.04
1.05
1.01
1.01
2.03
6.26
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10.0
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4.0
3.0
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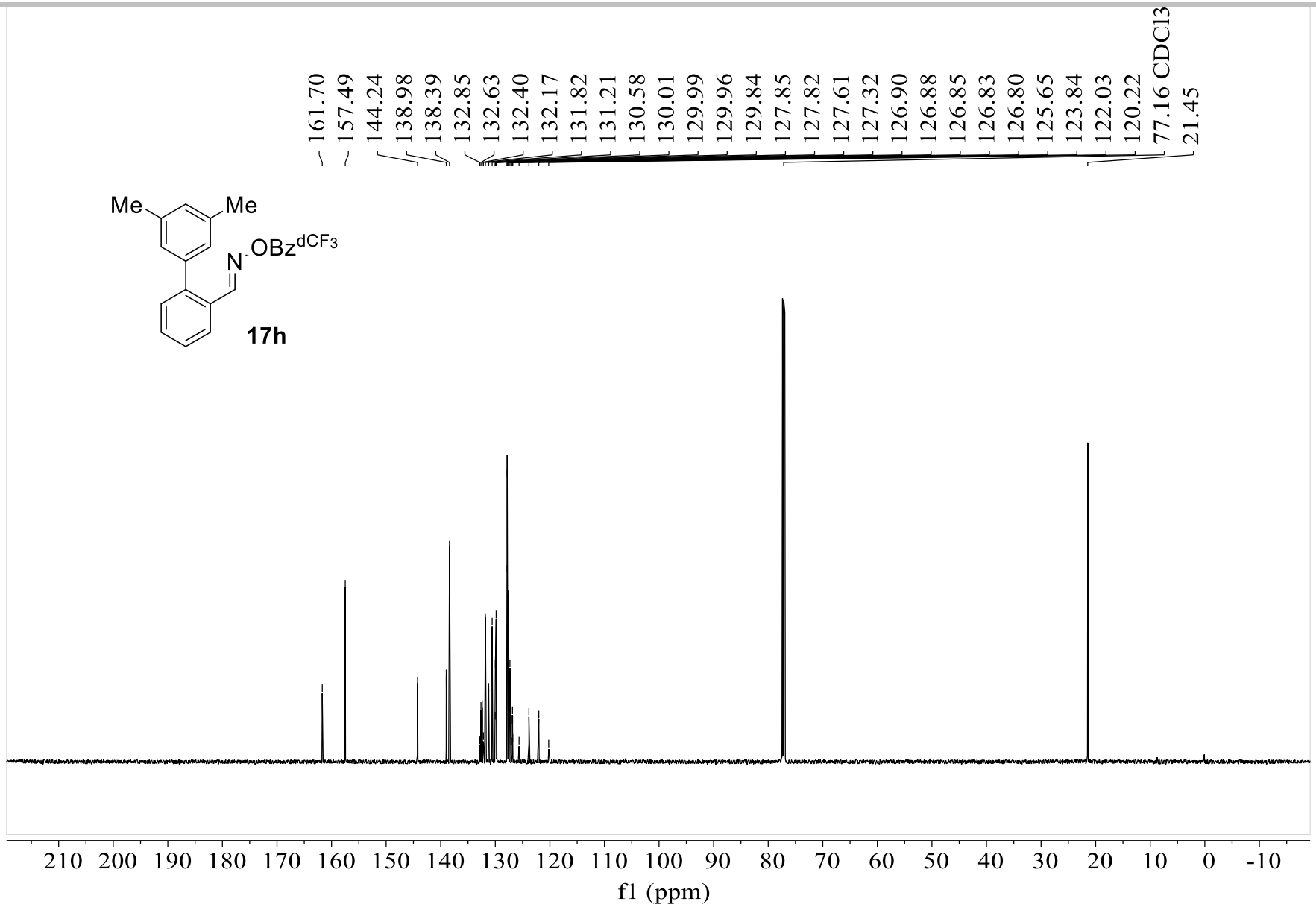
-1.0
f1 (ppm)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126.90
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126.85
126.83
126.80
125.65
123.84
122.03
120.22
77.16 CDCl3
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Me
Me
N
OBz^{dCF_3}
17h
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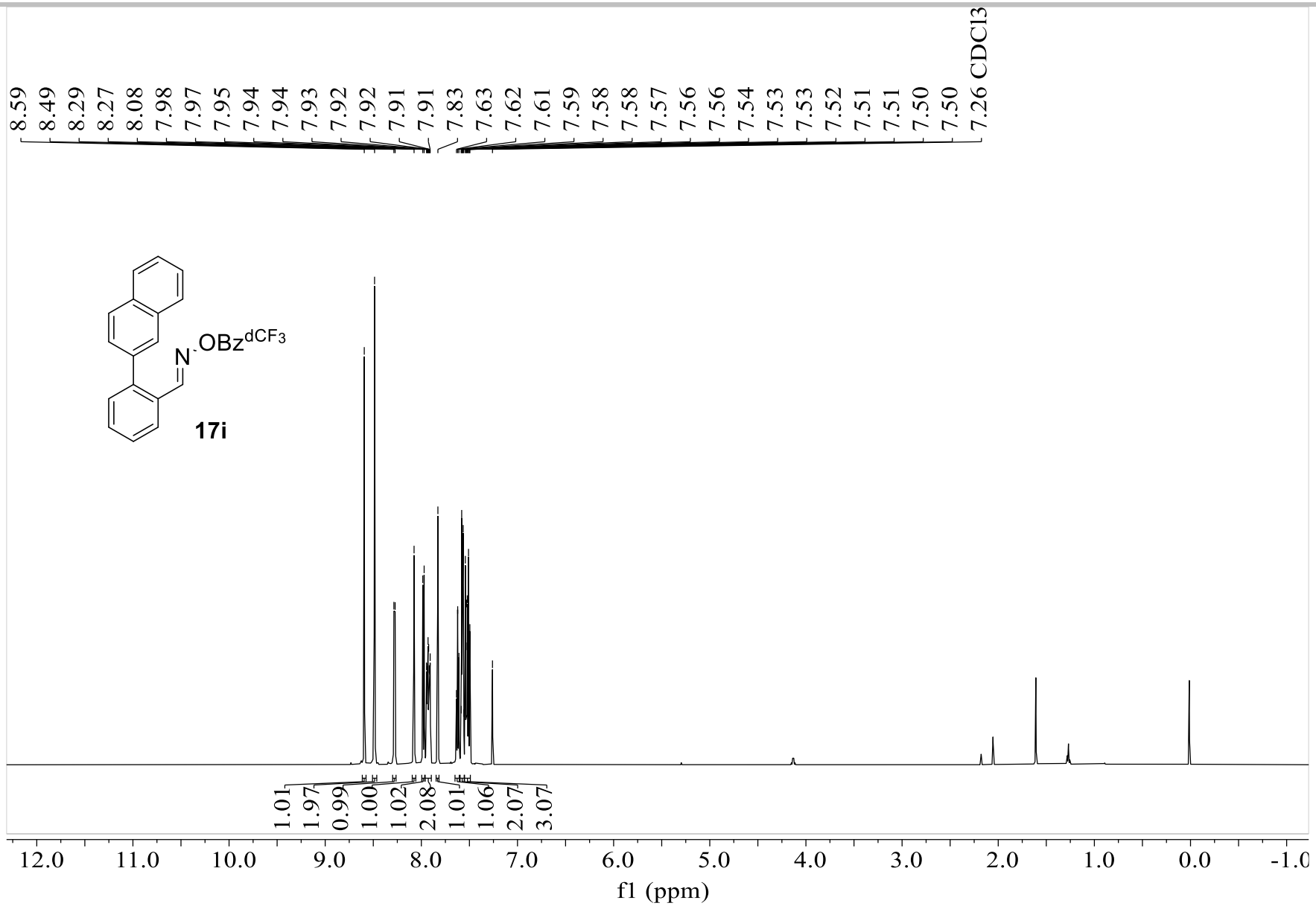
f1 (ppm)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7.61
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7.58
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7.57
7.56
7.56
7.54
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7.50
7.50
7.26 CDCl3
N
OBz^{dCF_3}
17i
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0.99
1.00
1.02
2.08
1.01
1.06
2.07
3.07
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11.0
10.0
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5.0
4.0
3.0
2.0
1.0
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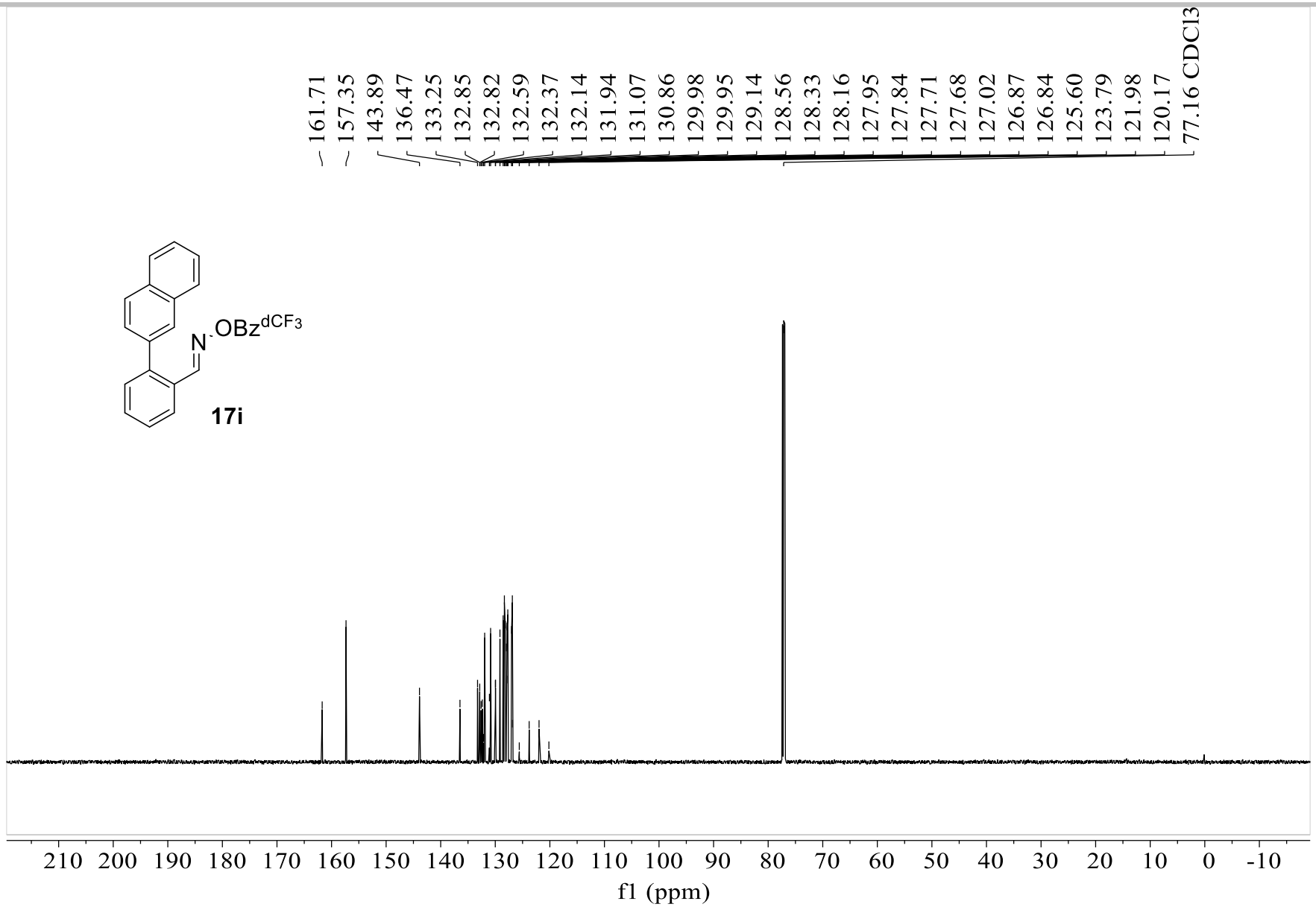
f1 (ppm)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N
OBz^dCF3
17i
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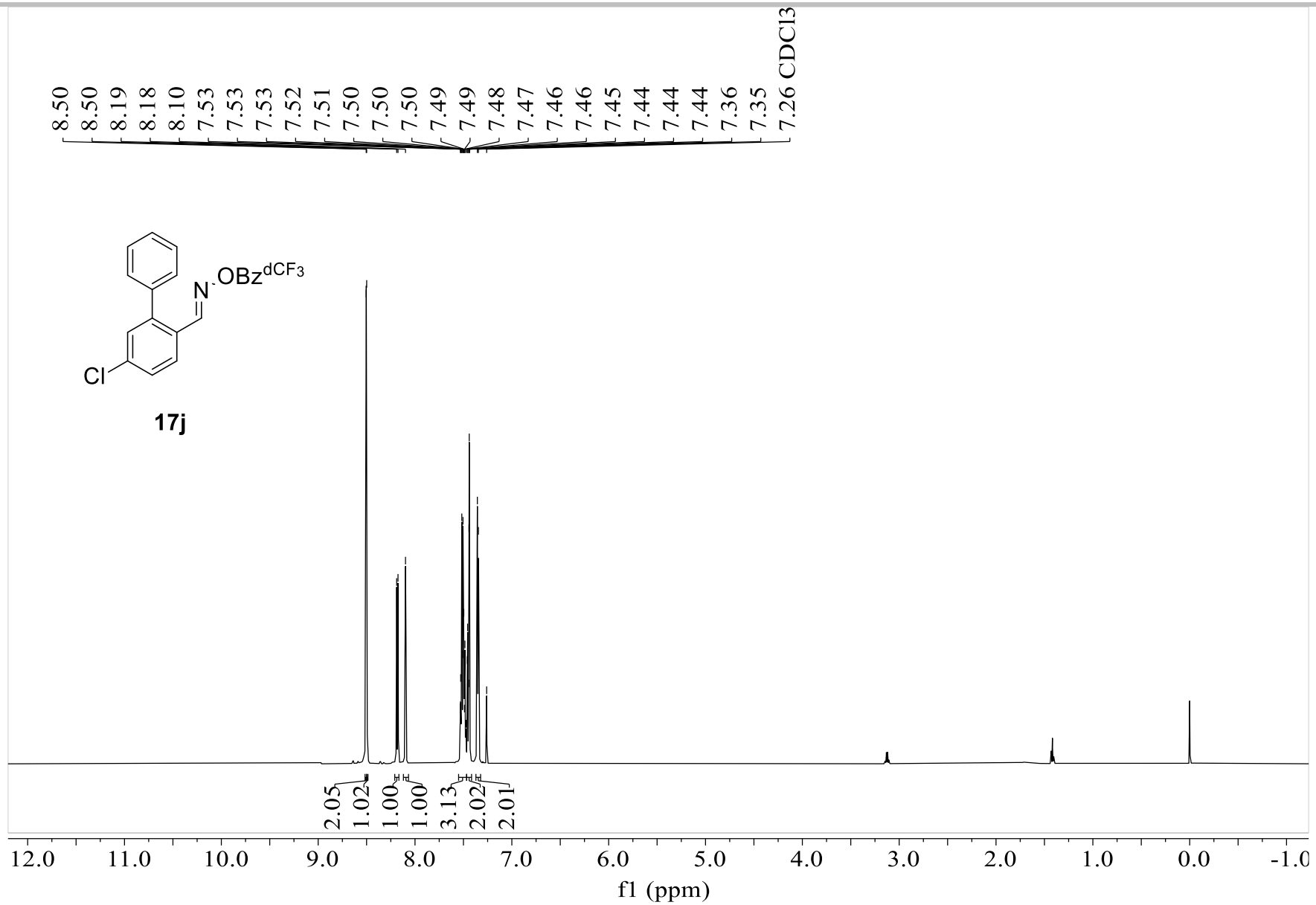
f1 (ppm)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7.46
7.45
7.44
7.44
7.44
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7.35
7.26 CDCl3
N
OBz^dCF3
Cl
17j
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1.00
1.00
3.13
2.02
2.01
12.0
11.0
10.0
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5.0
4.0
3.0
2.0
1.0
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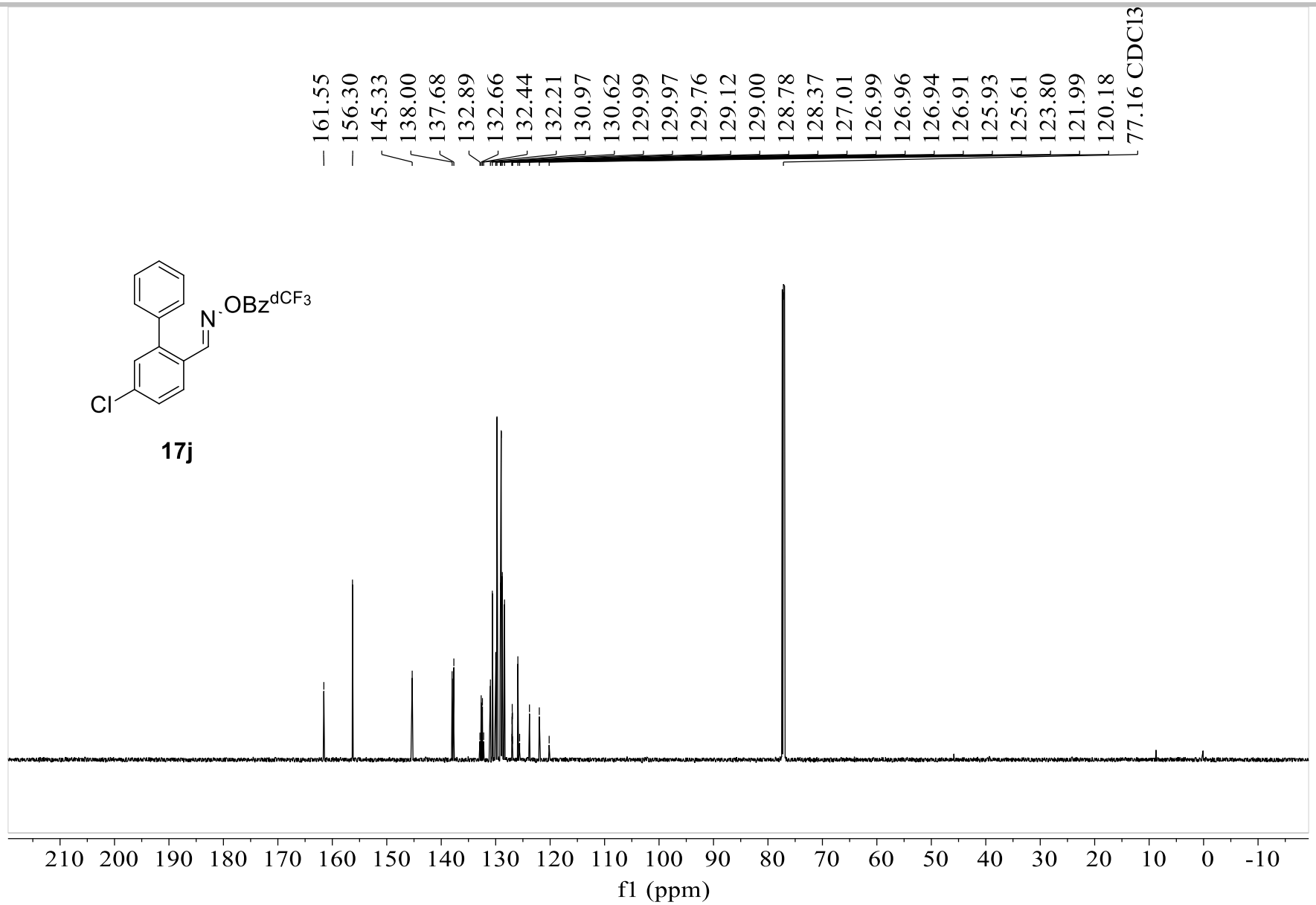
-1.0
f1 (ppm)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126.94
126.91
125.93
125.61
123.80
121.99
120.18
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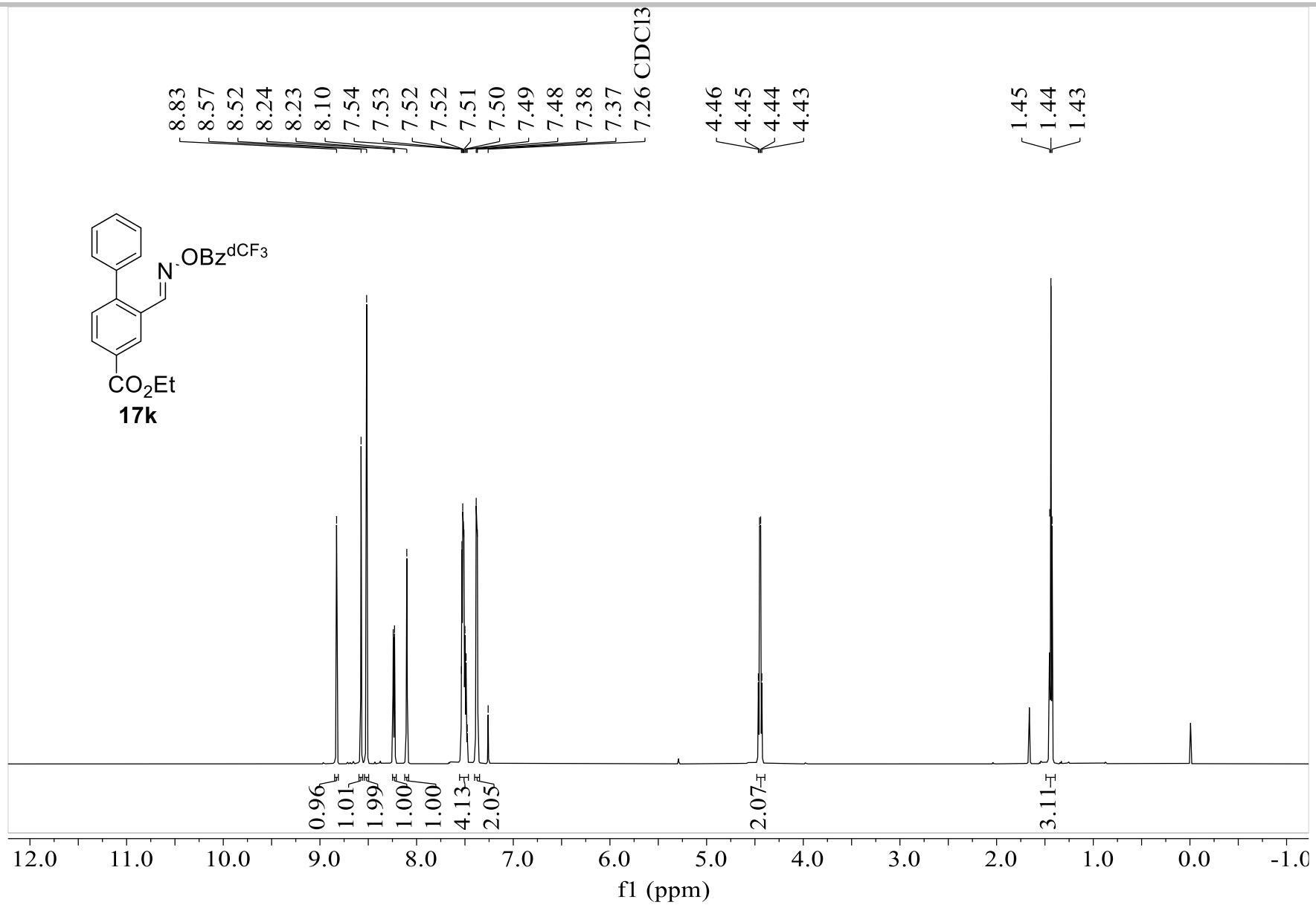
OBz^dCF3
Cl
17j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.48
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7.37
7.26 CDCl3
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4.45
4.44
4.43
1.45
1.44
1.43
N
OBz^dCF3
CO2Et
17k
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1.99
1.00
1.00
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2.07
3.11
12.0
11.0
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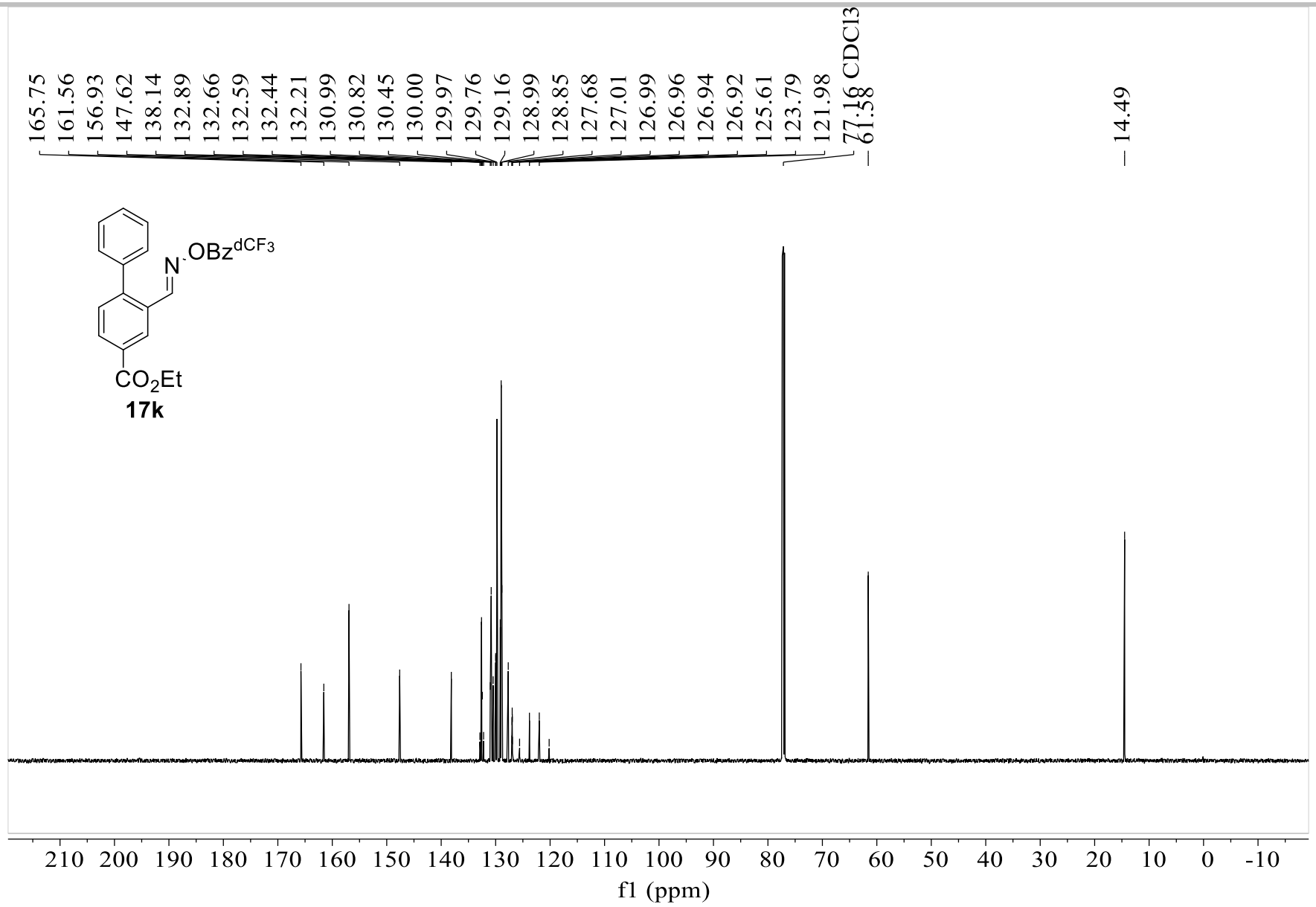
f1 (ppm)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77.16 CDCl3
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CO2Et
17k
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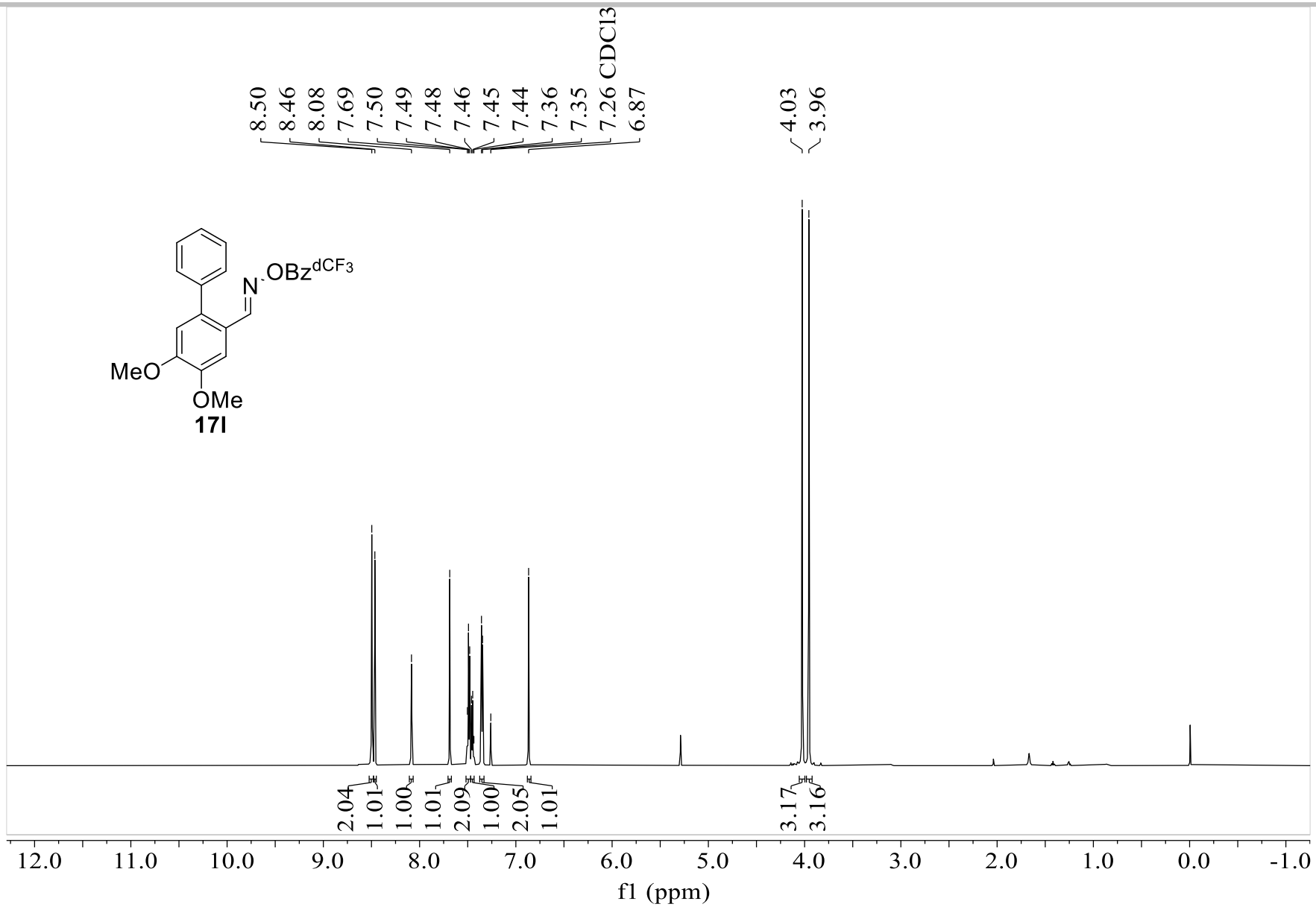
f1 (ppm)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7.44
7.36
7.35
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MeO
OMe
17l
2.04
1.01
1.00
1.01
2.09
1.00
2.05
1.01
3.17
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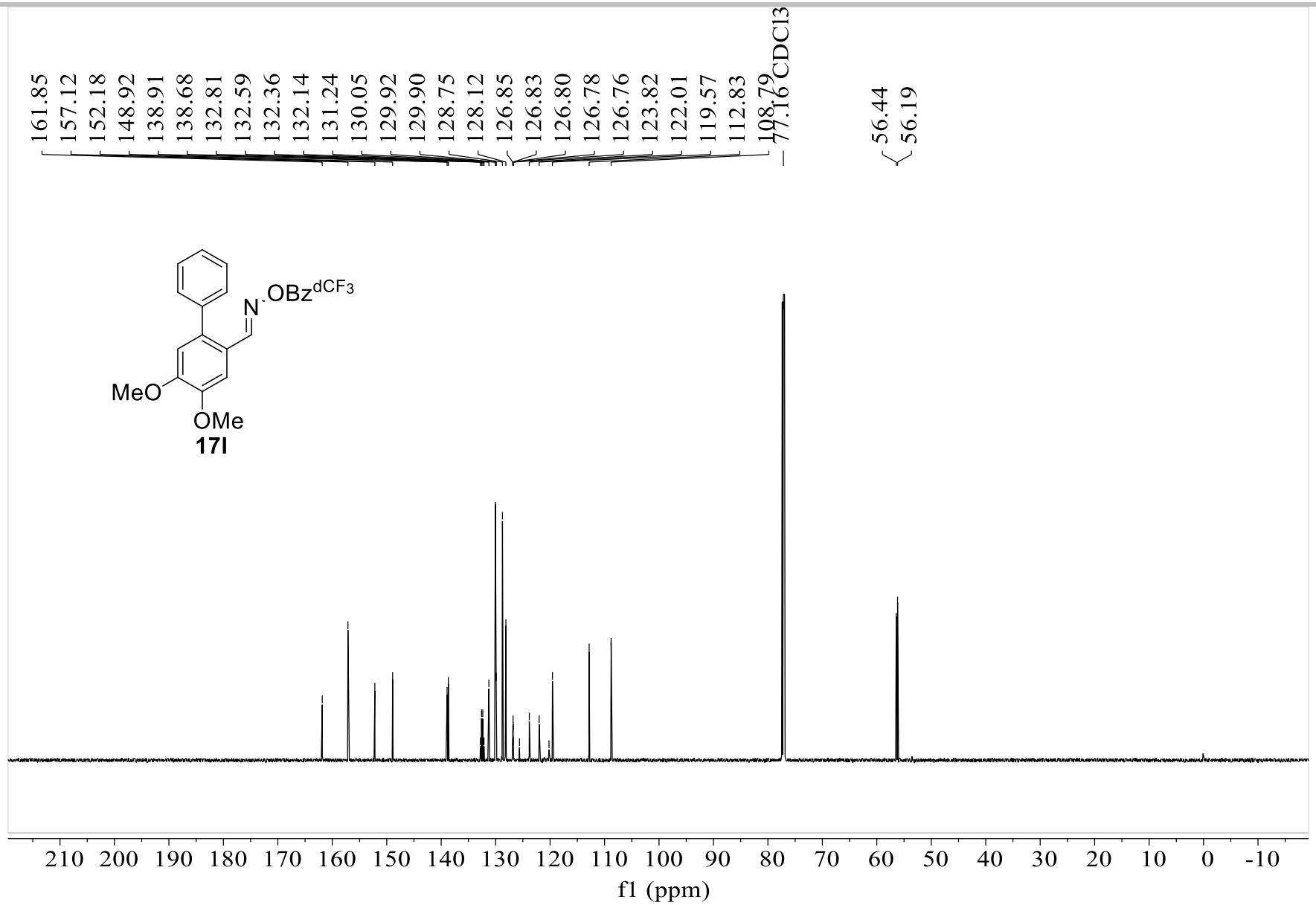
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122.01
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108.79
77.16 CDCl3
56.44
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OMe
17l
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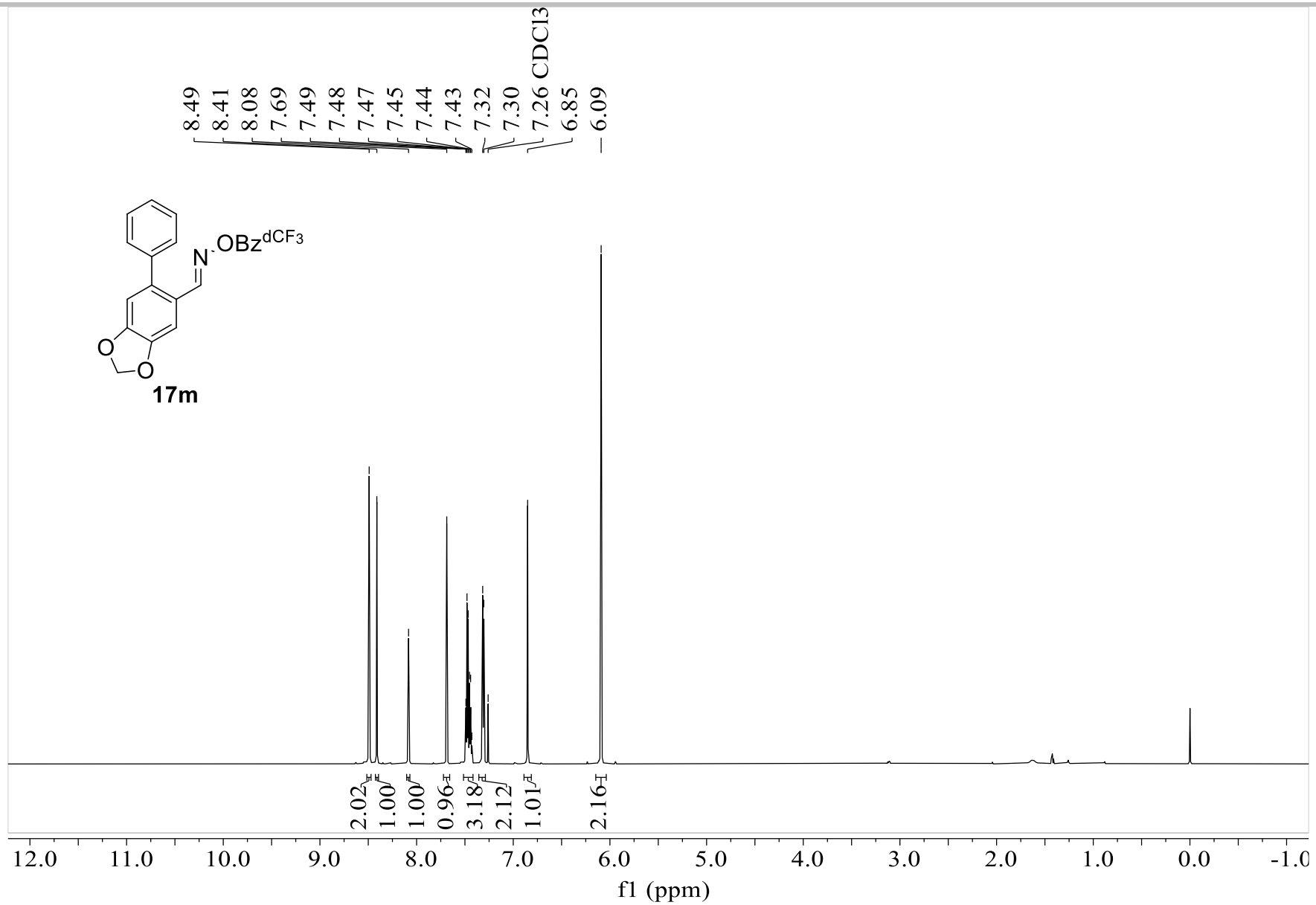
f1 (ppm)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7.30
7.26 CDCl3
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6.09
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OBz^dCF3
O
O
17m
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1.00
1.00
0.96
3.18
2.12
1.01
2.16
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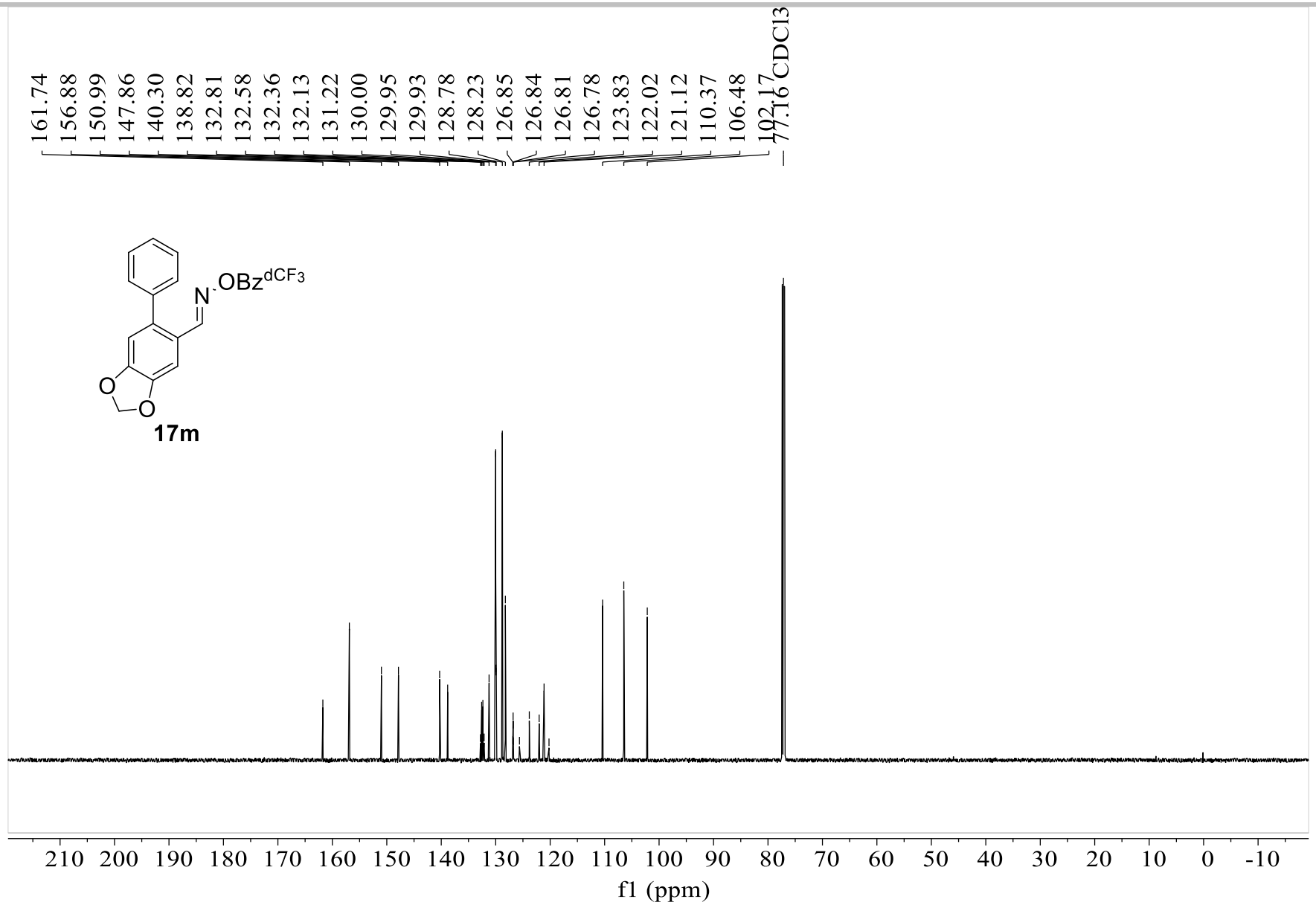
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123.83
122.02
121.12
110.37
106.48
102.17
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O
O
17m
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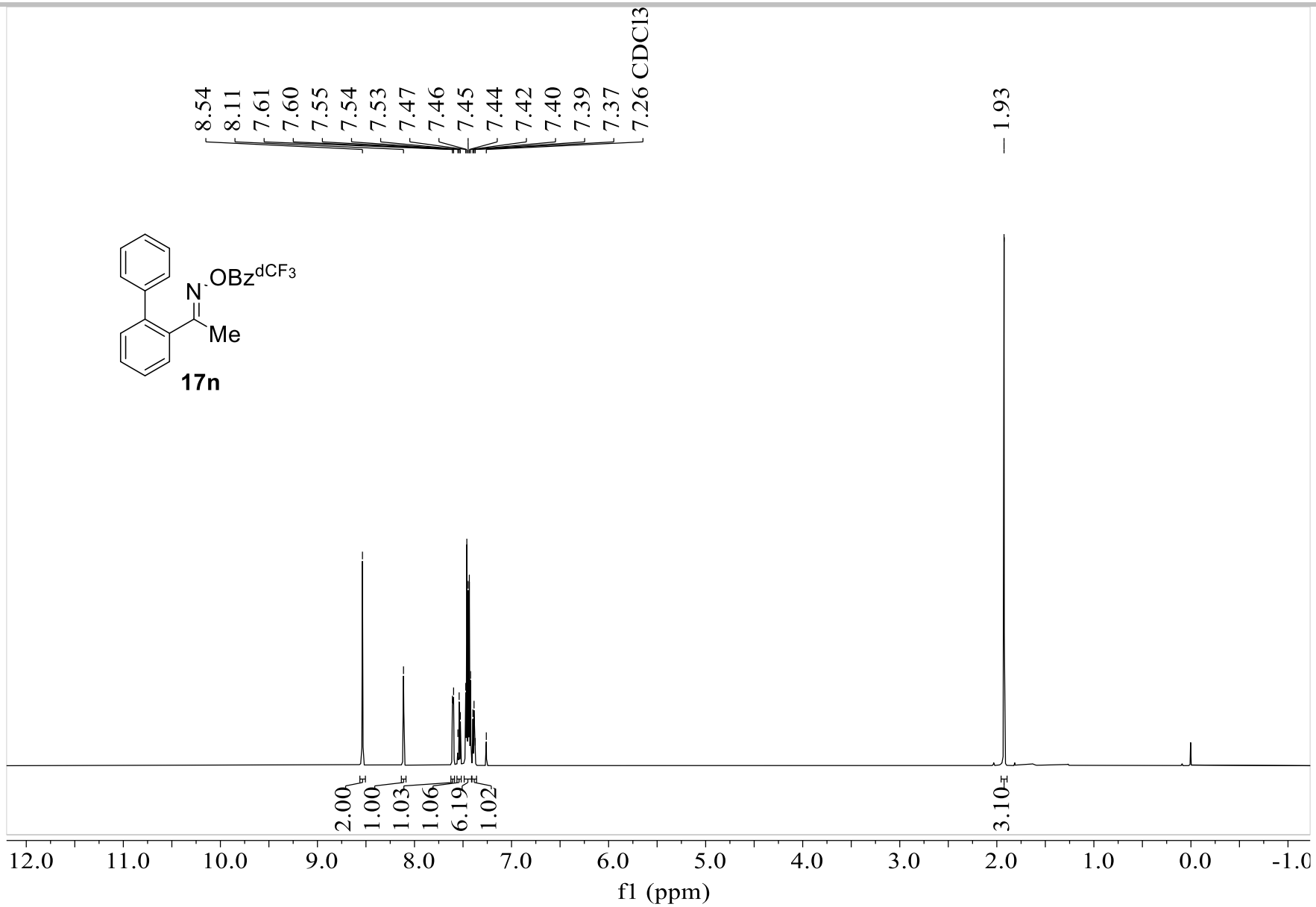
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7.39
7.37
7.26 CDCl3
1.93
N
OBz^dCF3
Me
17n
2.00
1.00
1.03
1.06
6.19
1.02
3.10
12.0
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10.0
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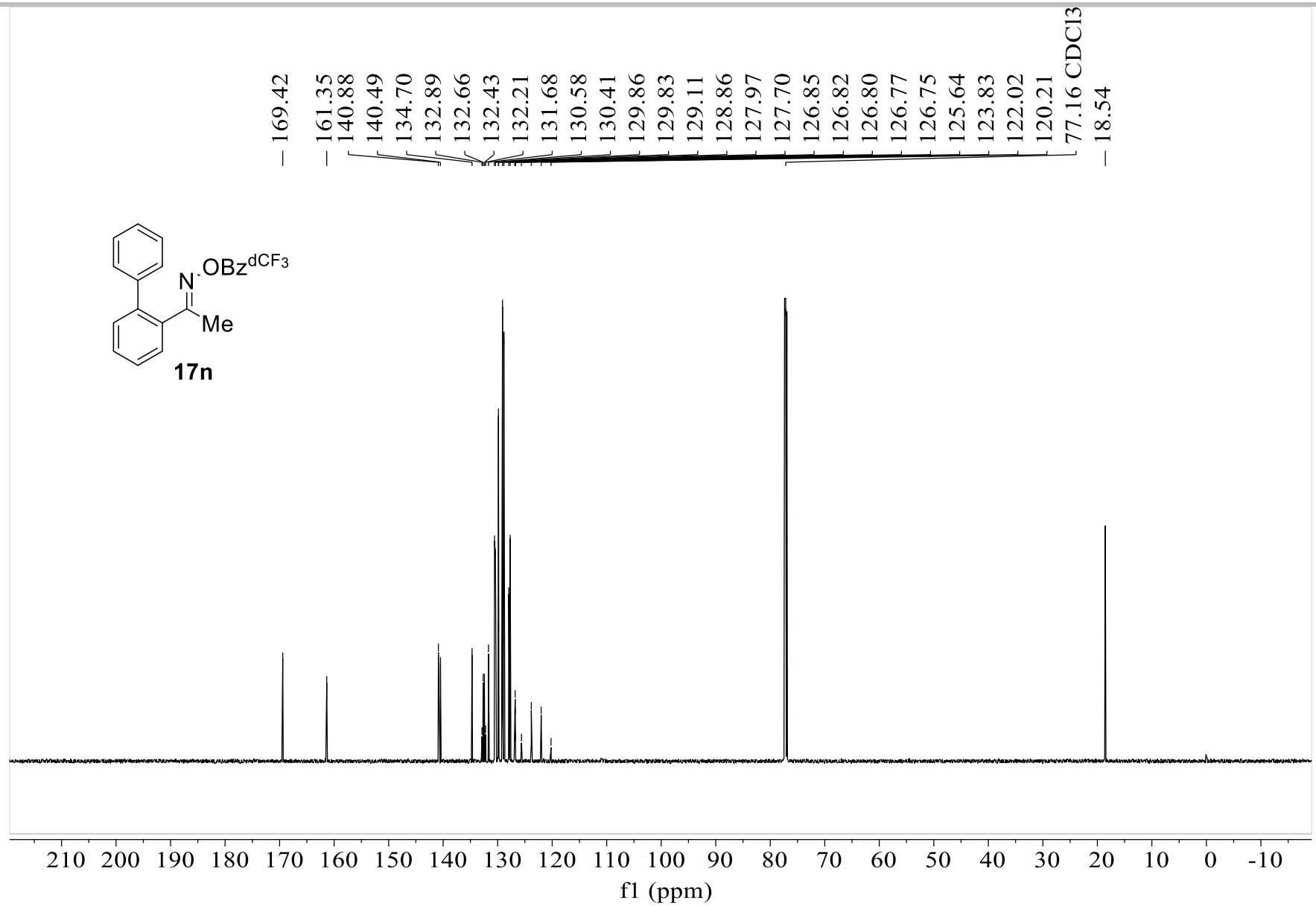
f1 (ppm)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123.83
122.02
120.21
77.16 CDCl3
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Me
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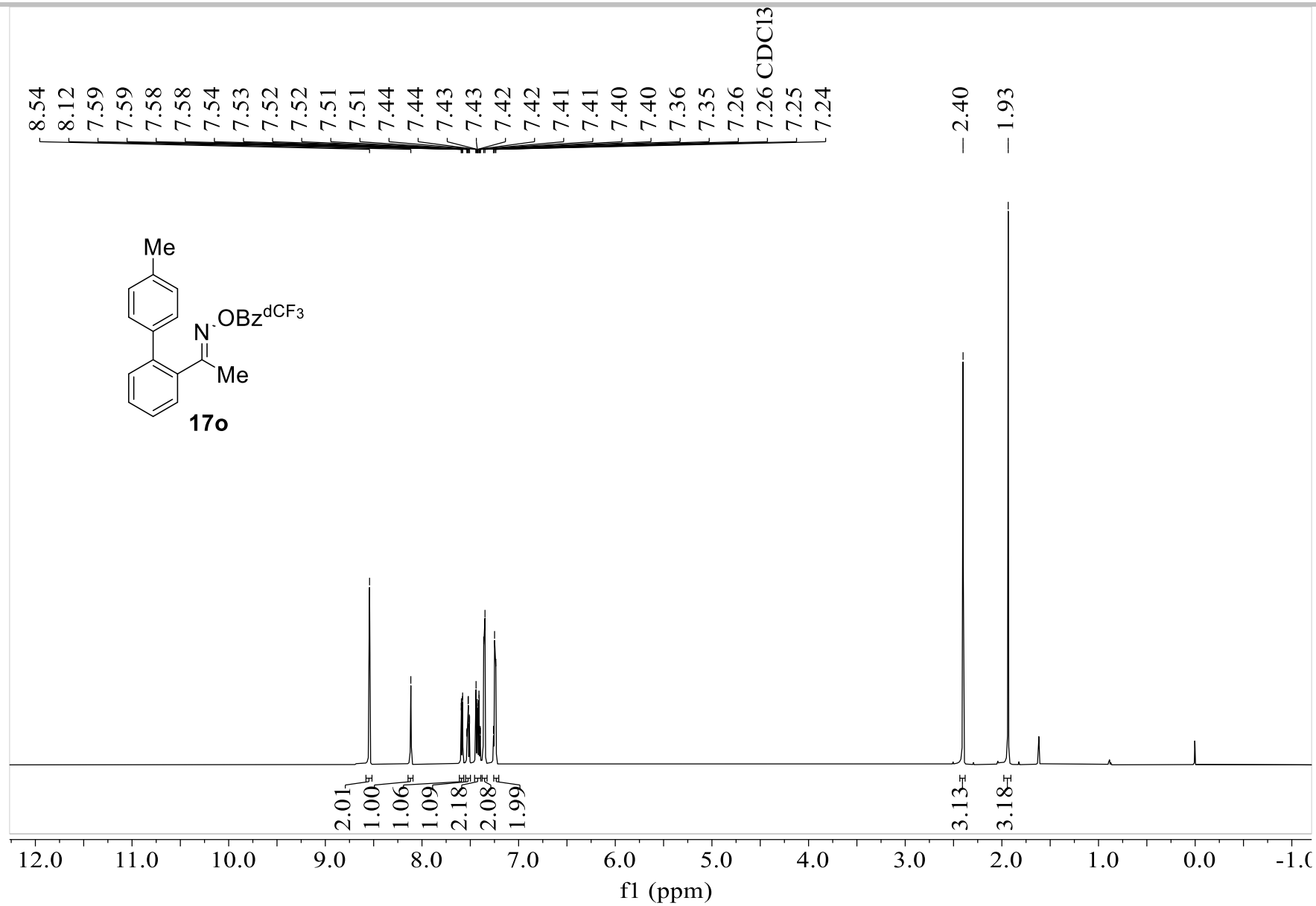
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.41
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7.26
7.26 CDCl3
7.25
7.24
2.40
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Me
N
OBz^dCF3
Me
17o
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1.00
1.06
1.09
2.18
2.08
1.99
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3.18
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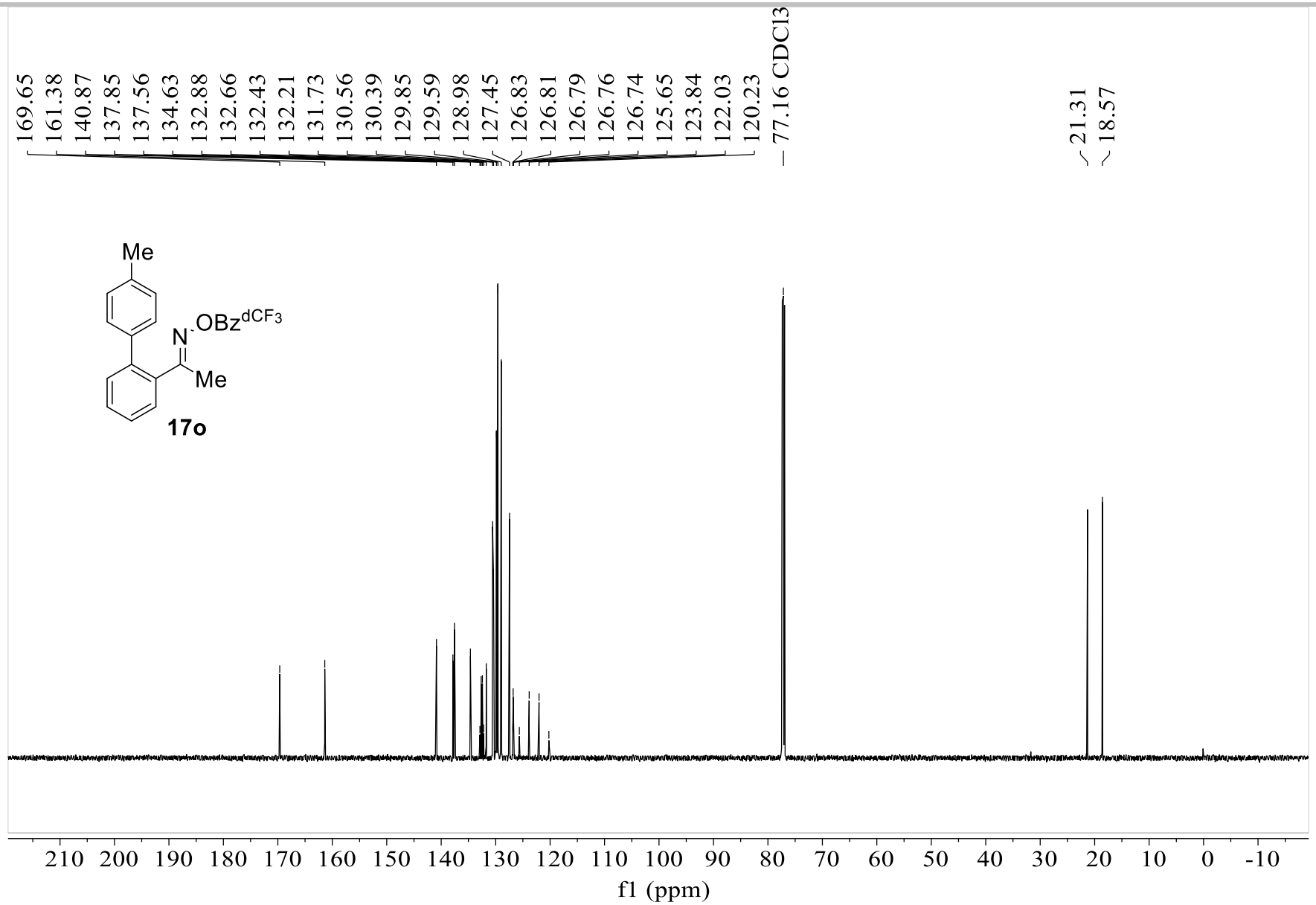
f1 (ppm)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132.21
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129.59
128.98
127.45
126.83
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125.65
123.84
122.03
120.23
77.16 CDCl3
21.31
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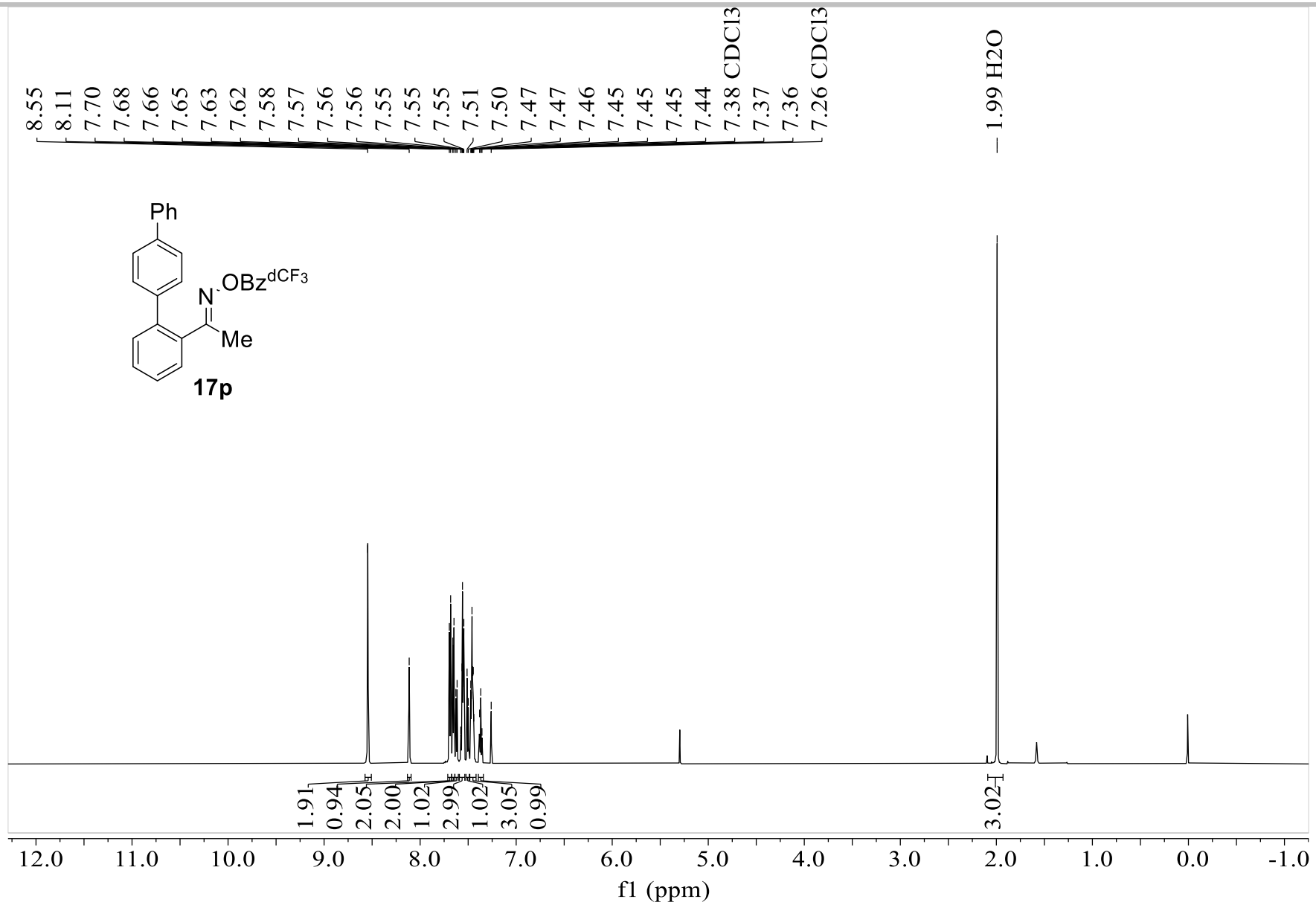
OBz^{dCF_3}
Me
17o
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.55
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7.50
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7.46
7.45
7.45
7.45
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7.38 CDCl3
7.37
7.36
7.26 CDCl3
1.99 H2O
Ph
N
OBz^dCF3
Me
17p
1.91
0.94
2.05
2.00
1.02
2.99
1.02
3.05
0.99
3.02
12.0
11.0
10.0
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5.0
4.0
3.0
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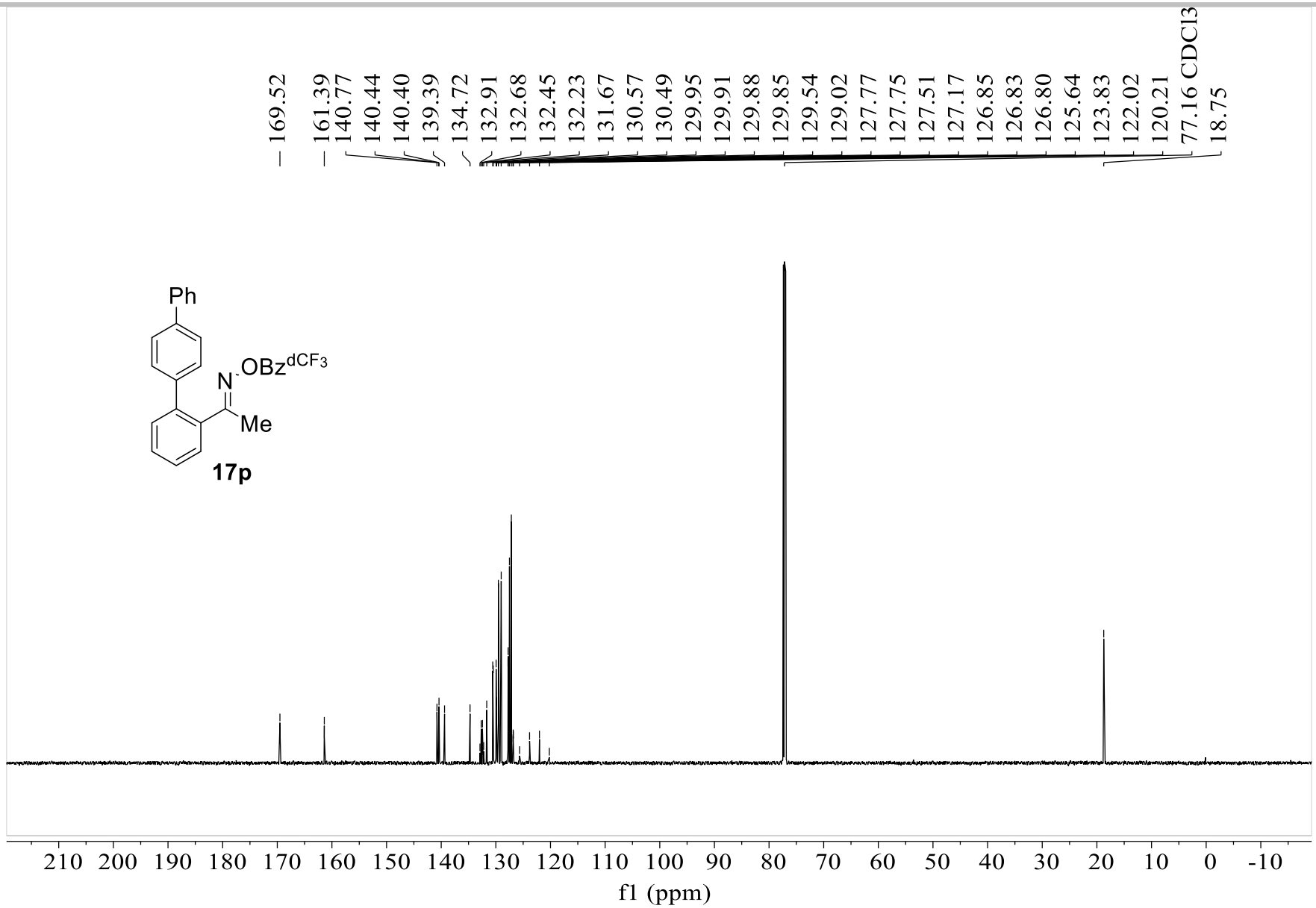
f1 (ppm)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123.83
122.02
120.21
77.16 CDCl3
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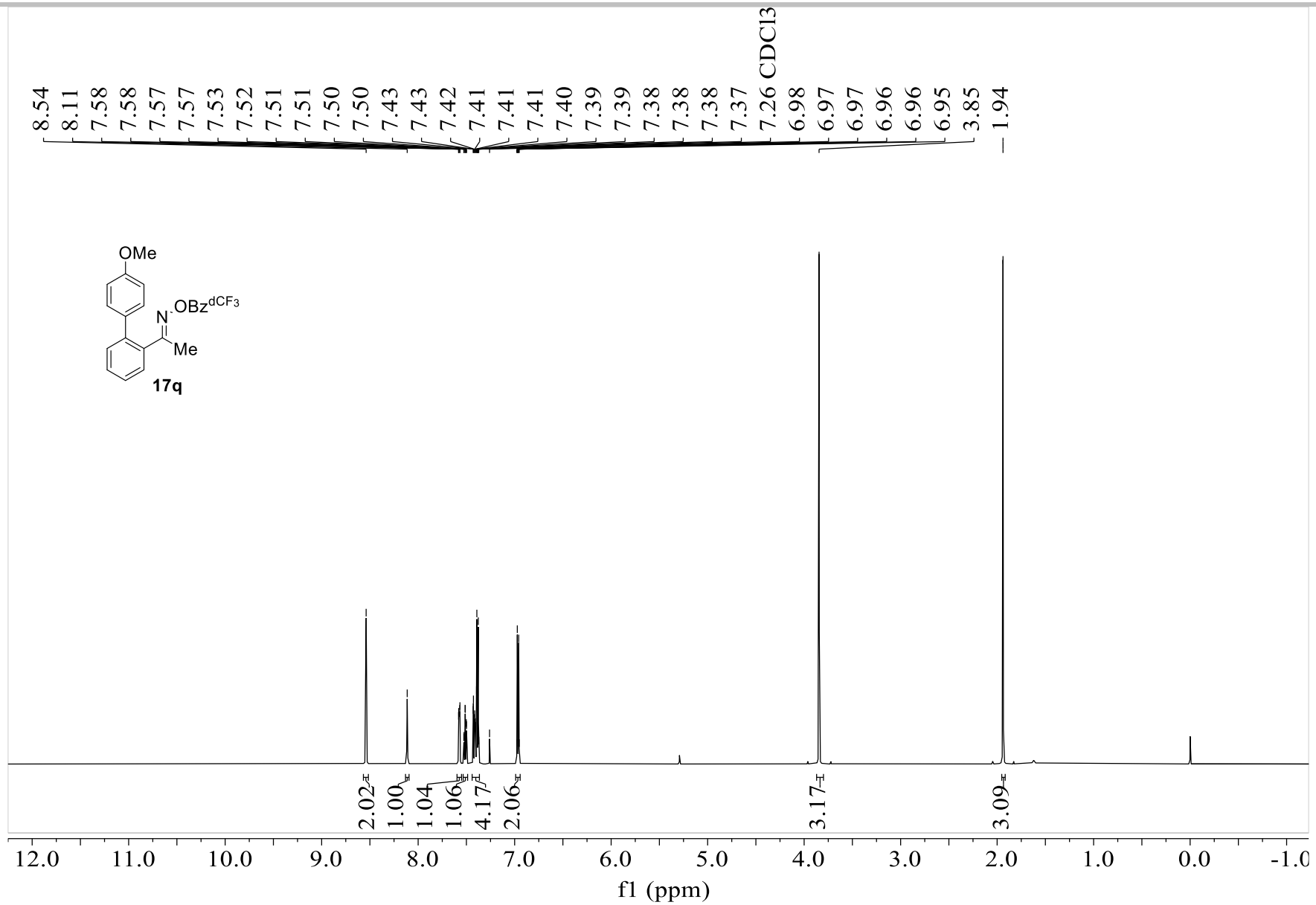
Ph
N
OBz^dCF3
Me
17p
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.41
7.41
7.40
7.39
7.39
7.38
7.38
7.38
7.37
7.26 CDCl3
6.98
6.97
6.97
6.96
6.96
6.95
3.85
1.94
OMe
N
OBz^dCF3
Me
17q
2.02
1.00
1.04
1.06
4.17
2.06
3.17
3.09
12.0
11.0
10.0
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4.0
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1.0
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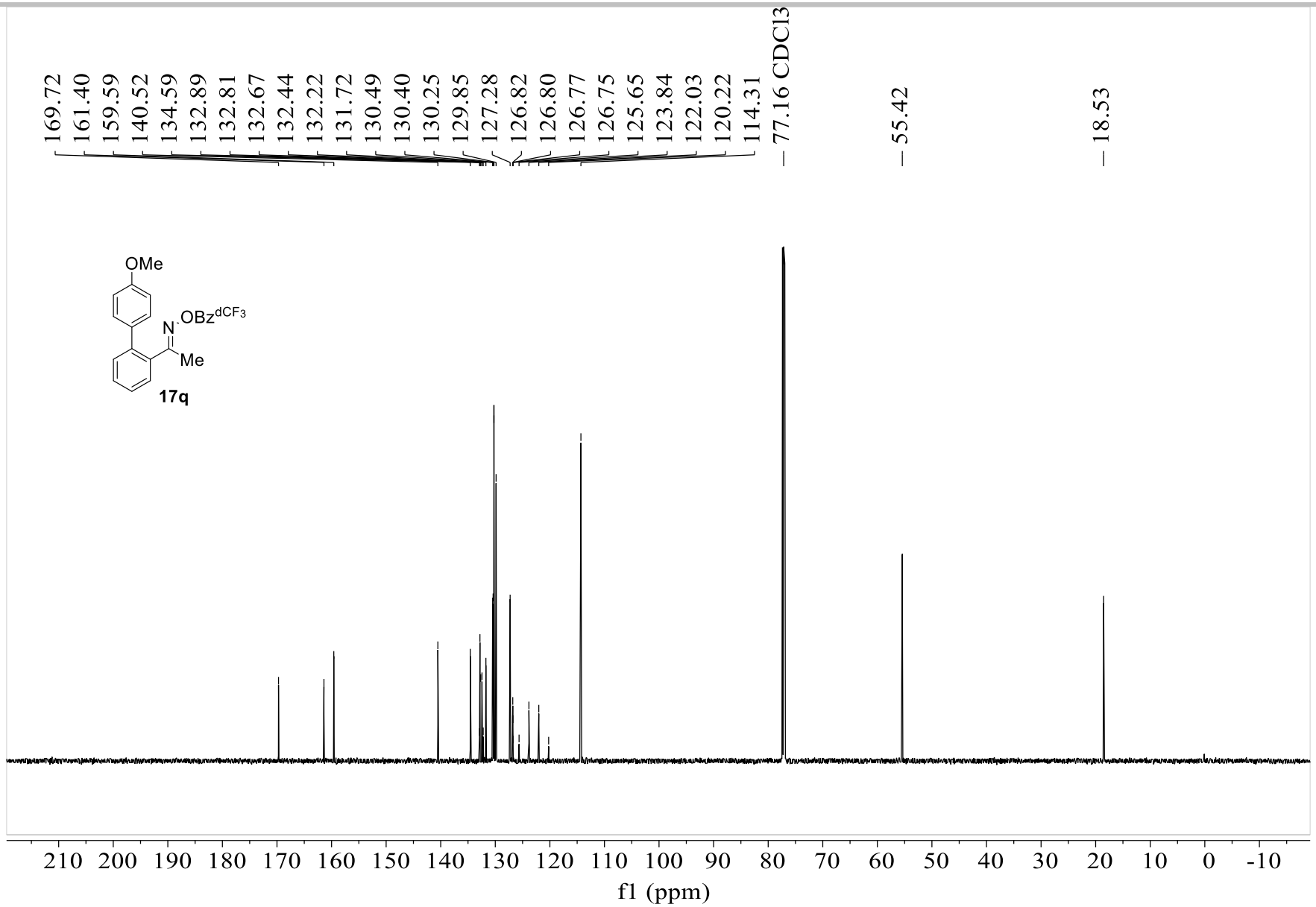
f1 (ppm)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126.80
126.77
126.75
125.65
123.84
122.03
120.22
114.31
77.16 CDCl3
55.42
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OMe
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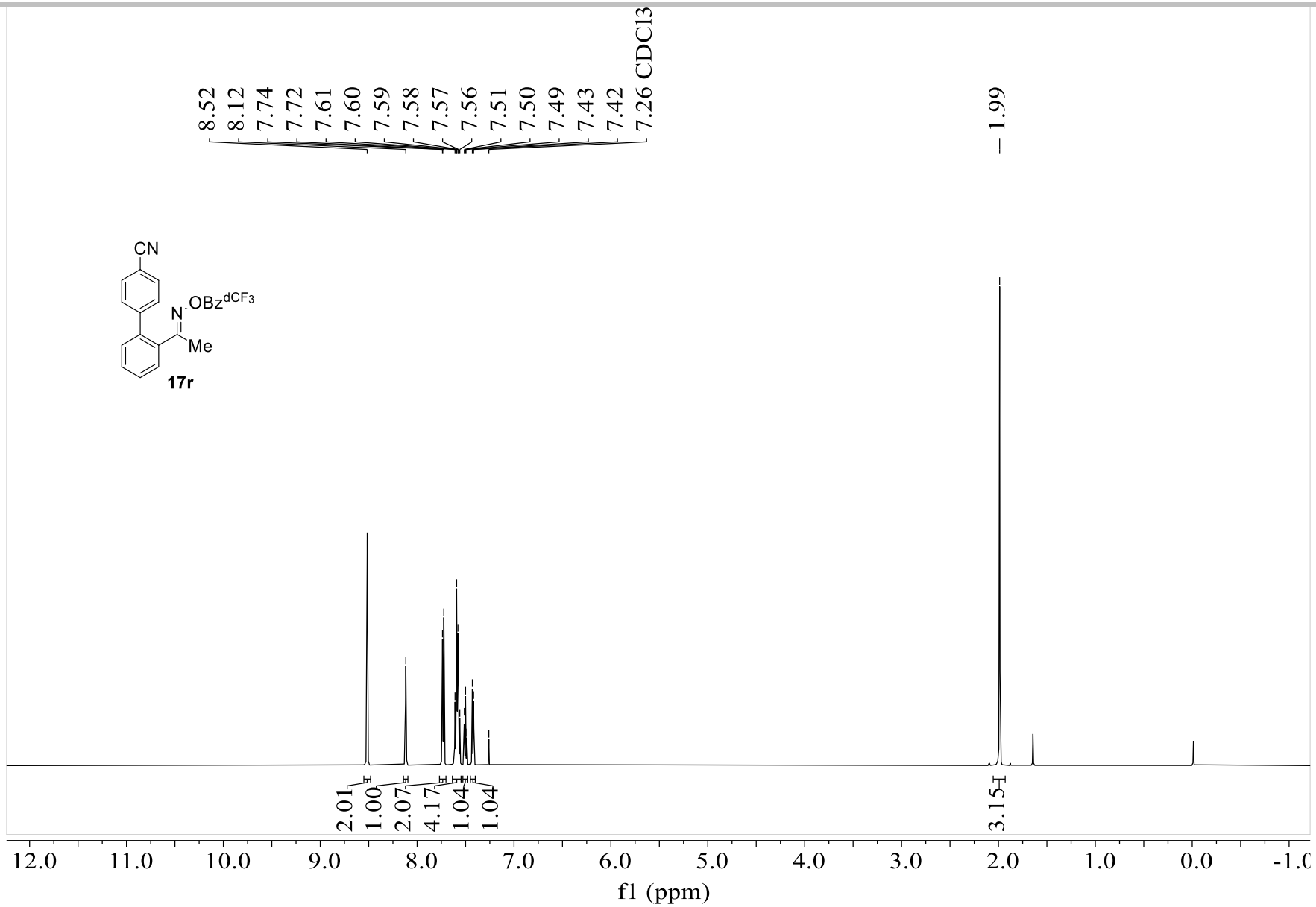
OBz^{dCF_3}
Me
17q
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.50
7.49
7.43
7.42
7.26 CDCl3
1.99
CN
N
OBz^dCF3
Me
17r
2.01
1.00
2.07
4.17
1.04
1.04
3.15
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11.0
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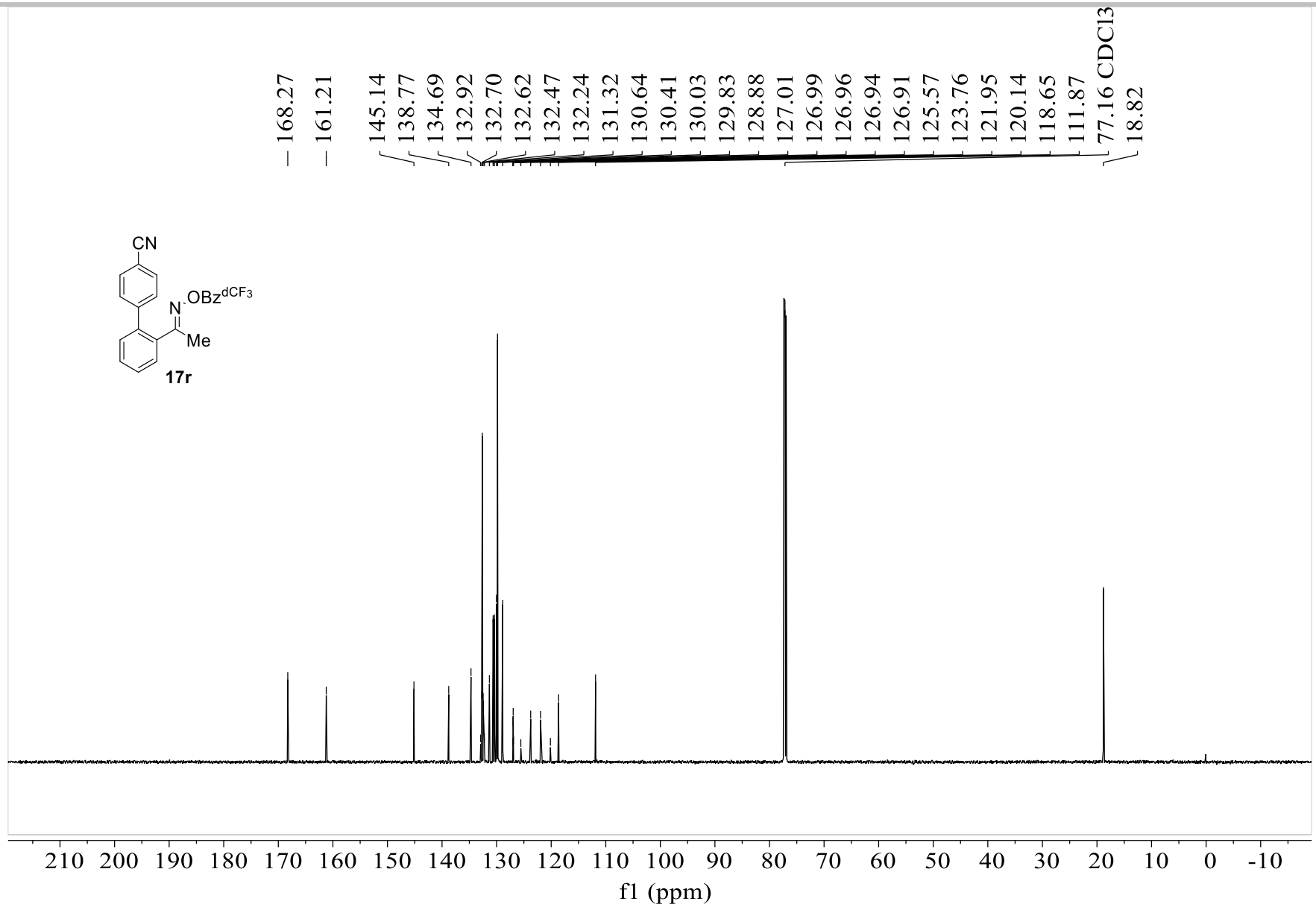
f1 (ppm)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130.41
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129.83
128.88
127.01
126.99
126.96
126.94
126.91
125.57
123.76
121.95
120.14
118.65
111.87
77.16 CDCl3
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OBz^dCF3
Me
17r
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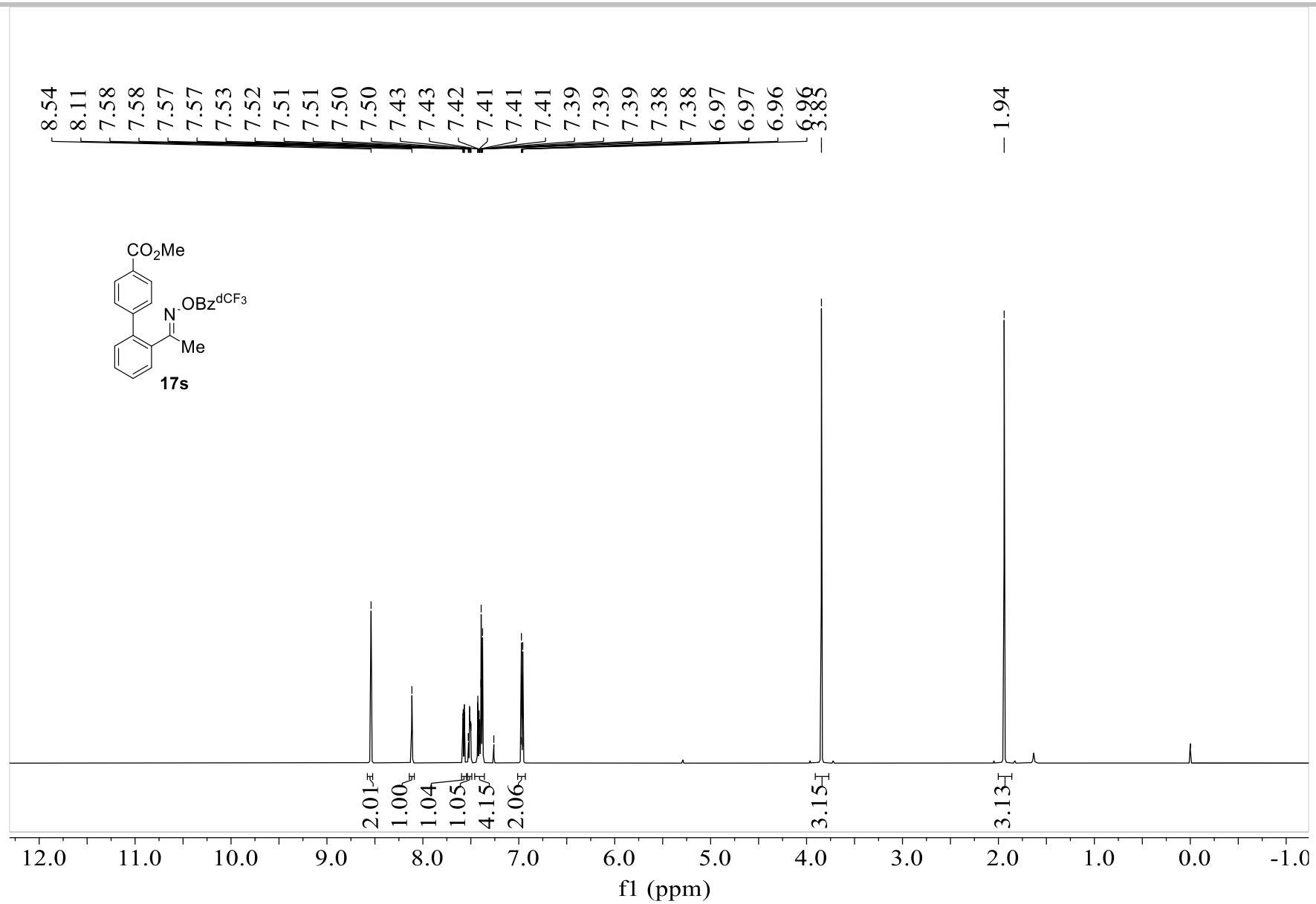
f1 (ppm)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7.41
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7.39
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7.38
6.97
6.97
6.96
6.96
3.85
1.94
CO2Me
N
OBzdCF3
Me
17s
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1.00
1.04
1.05
4.15
2.06
3.15
3.13
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10.0
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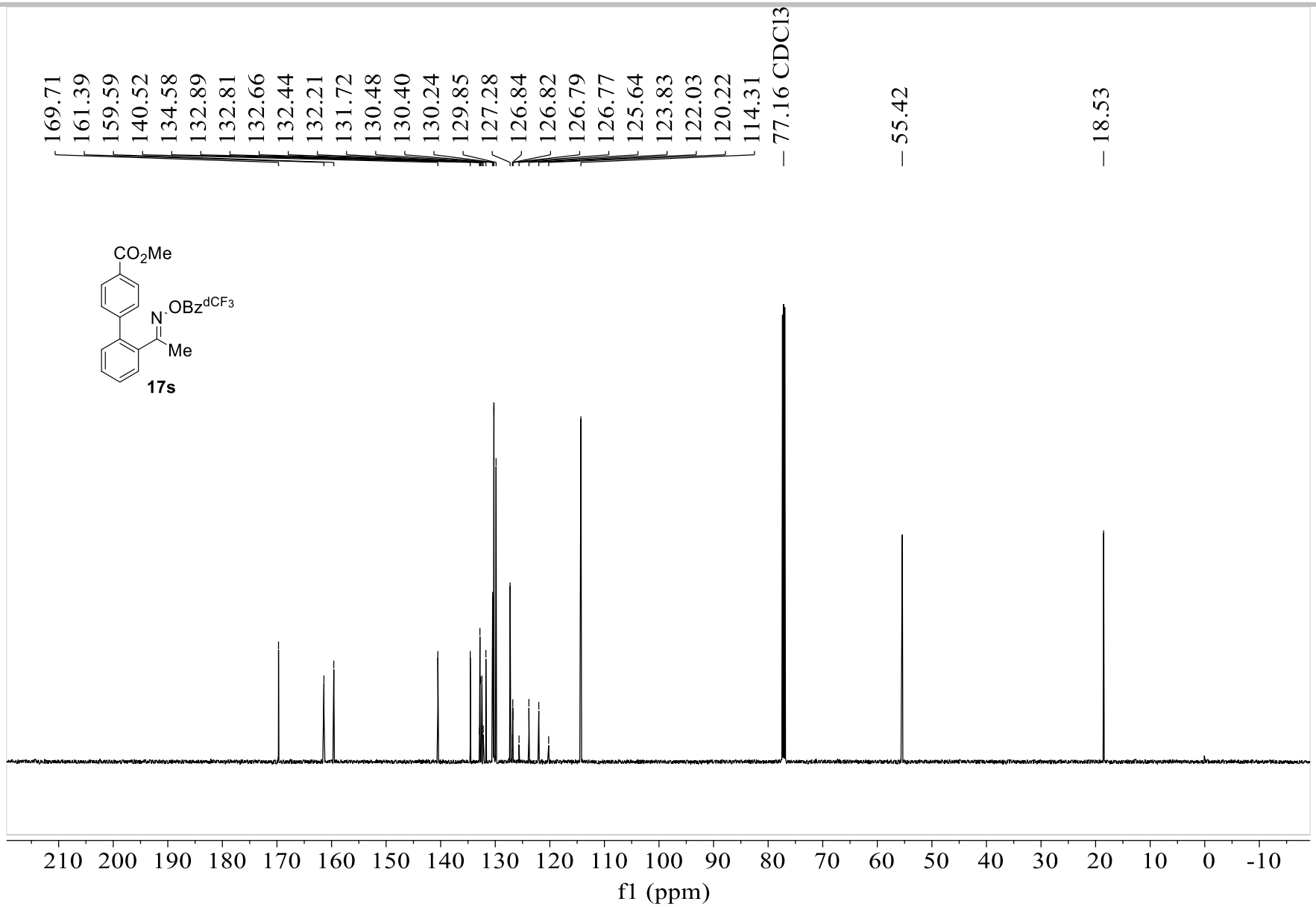
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122.03
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77.16 CDCl3
55.42
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N
OBzdCF3
Me
17s
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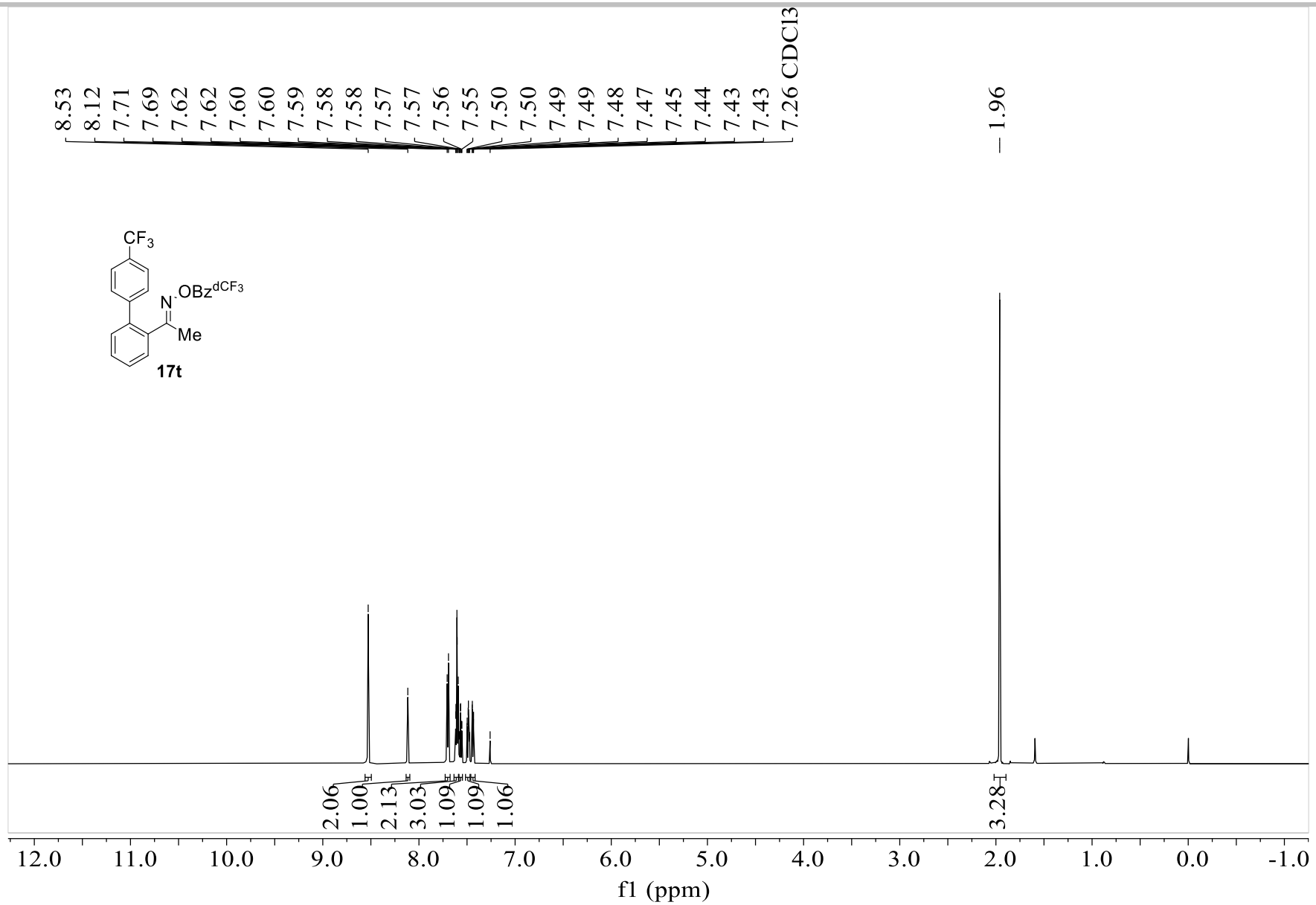
f1 (ppm)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7.56
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7.50
7.50
7.49
7.49
7.48
7.47
7.45
7.44
7.43
7.43
7.26 CDCl3
1.96
CF3
N
OBzdCF3
Me
17t
2.06
1.00
2.13
3.03
1.09
1.09
1.06
3.28
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10.0
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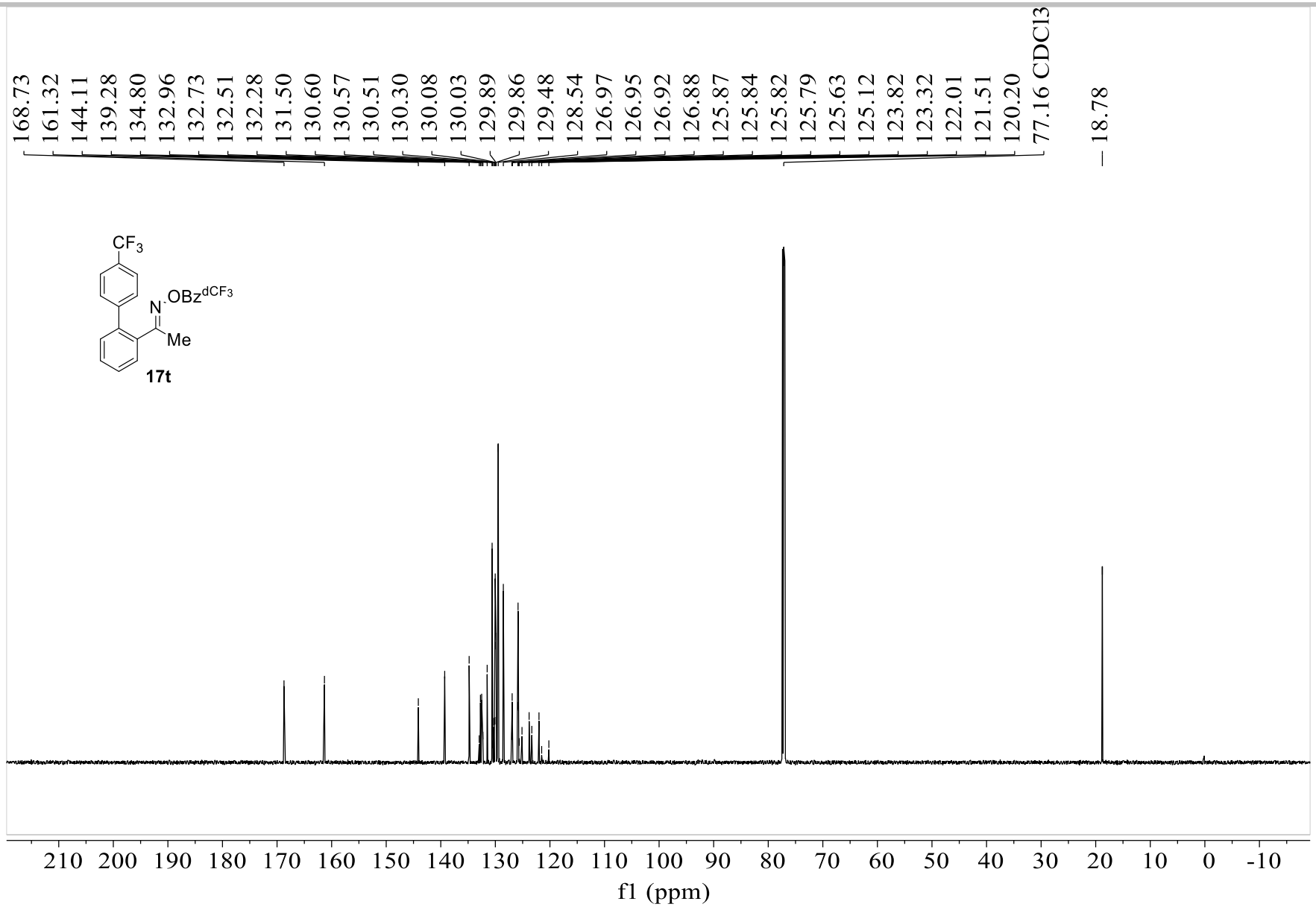
f1 (ppm)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122.01
121.51
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77.16 CDCl3
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OBzdCF3
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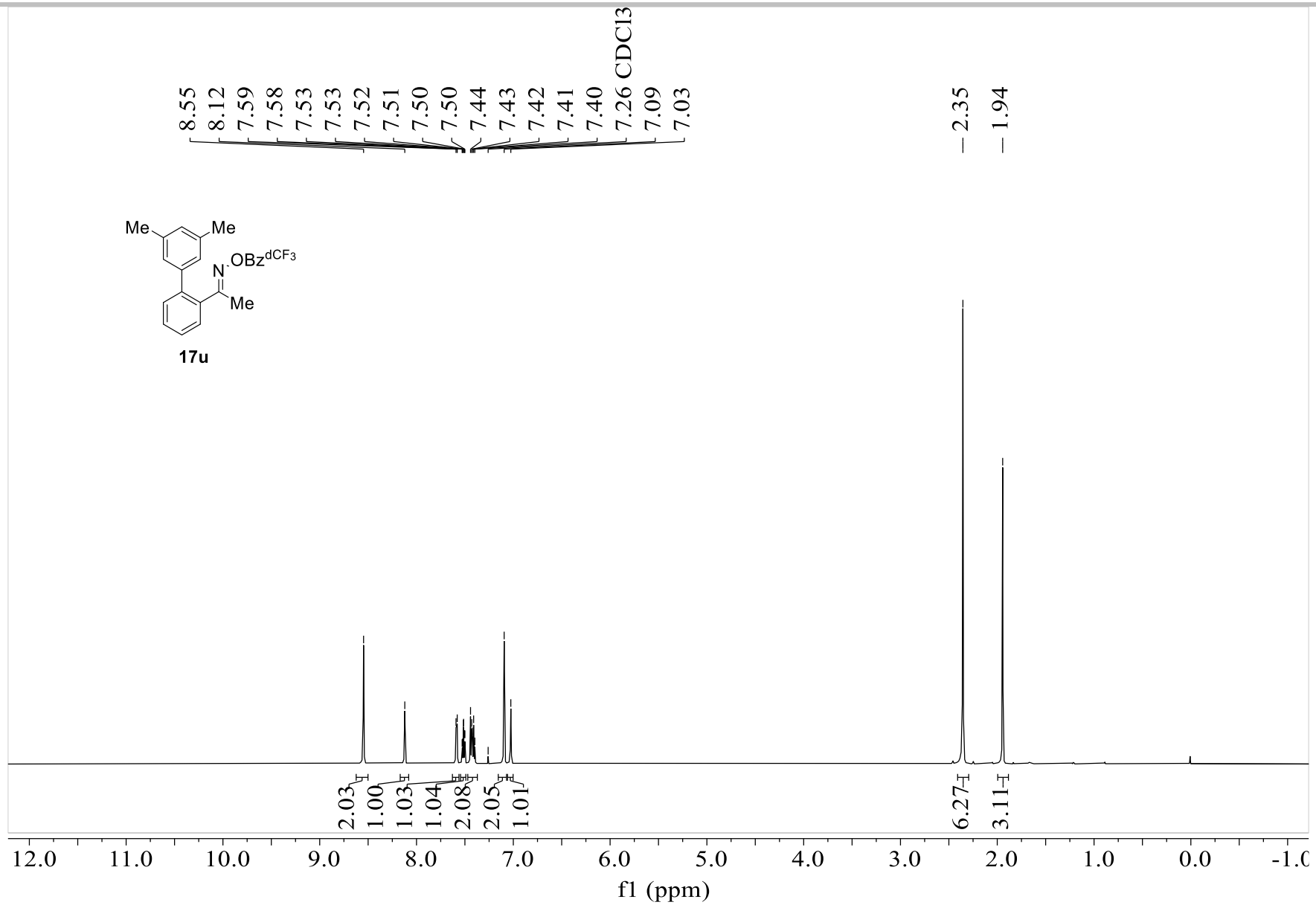
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.40
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2.35
1.94
Me
Me
N
OBz^dCF3
Me
17u
2.03
1.00
1.03
1.04
2.08
2.05
1.01
6.27
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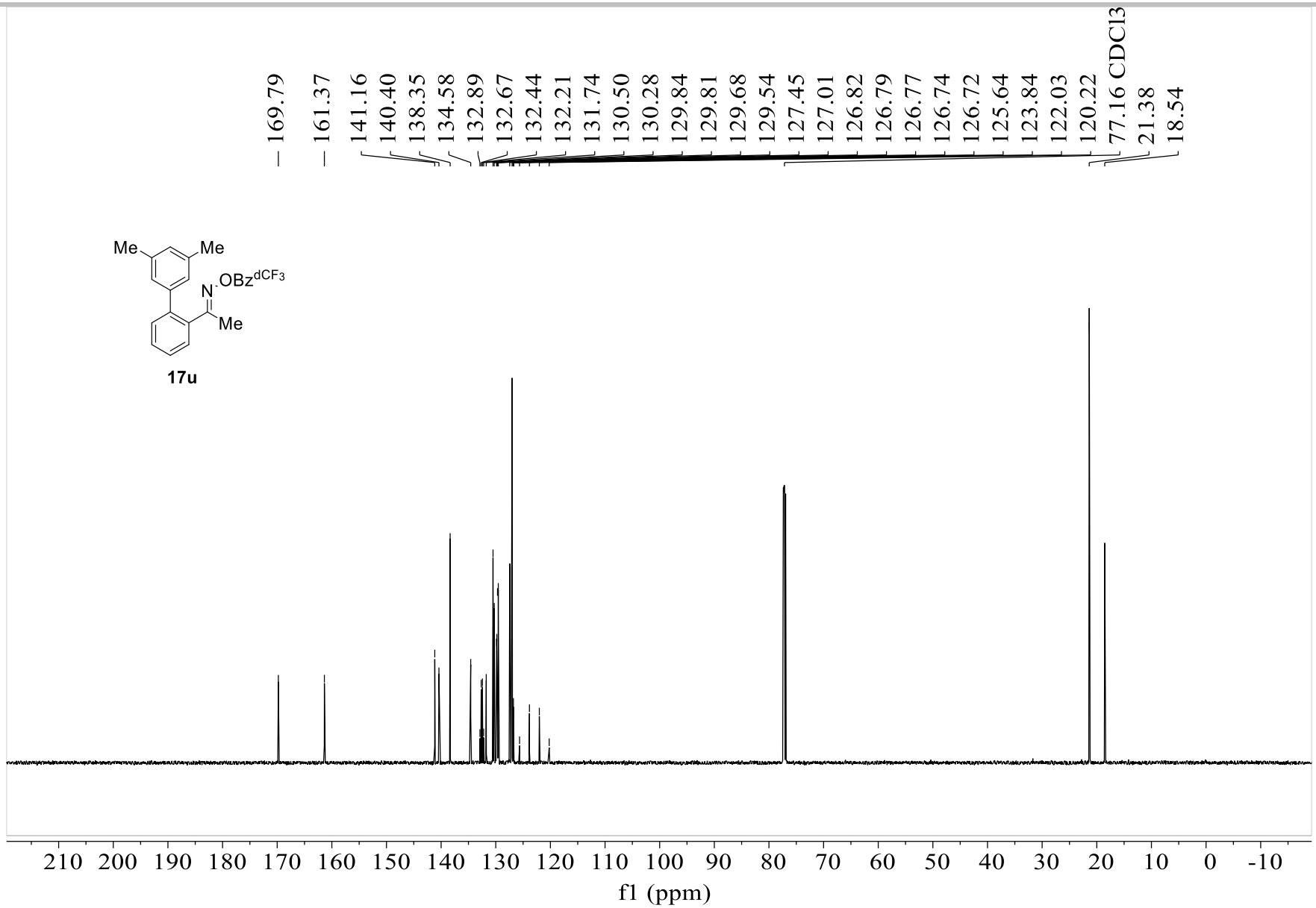
f1 (ppm)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122.03
120.22
77.16 CDCl3
21.38
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OBz^dCF3
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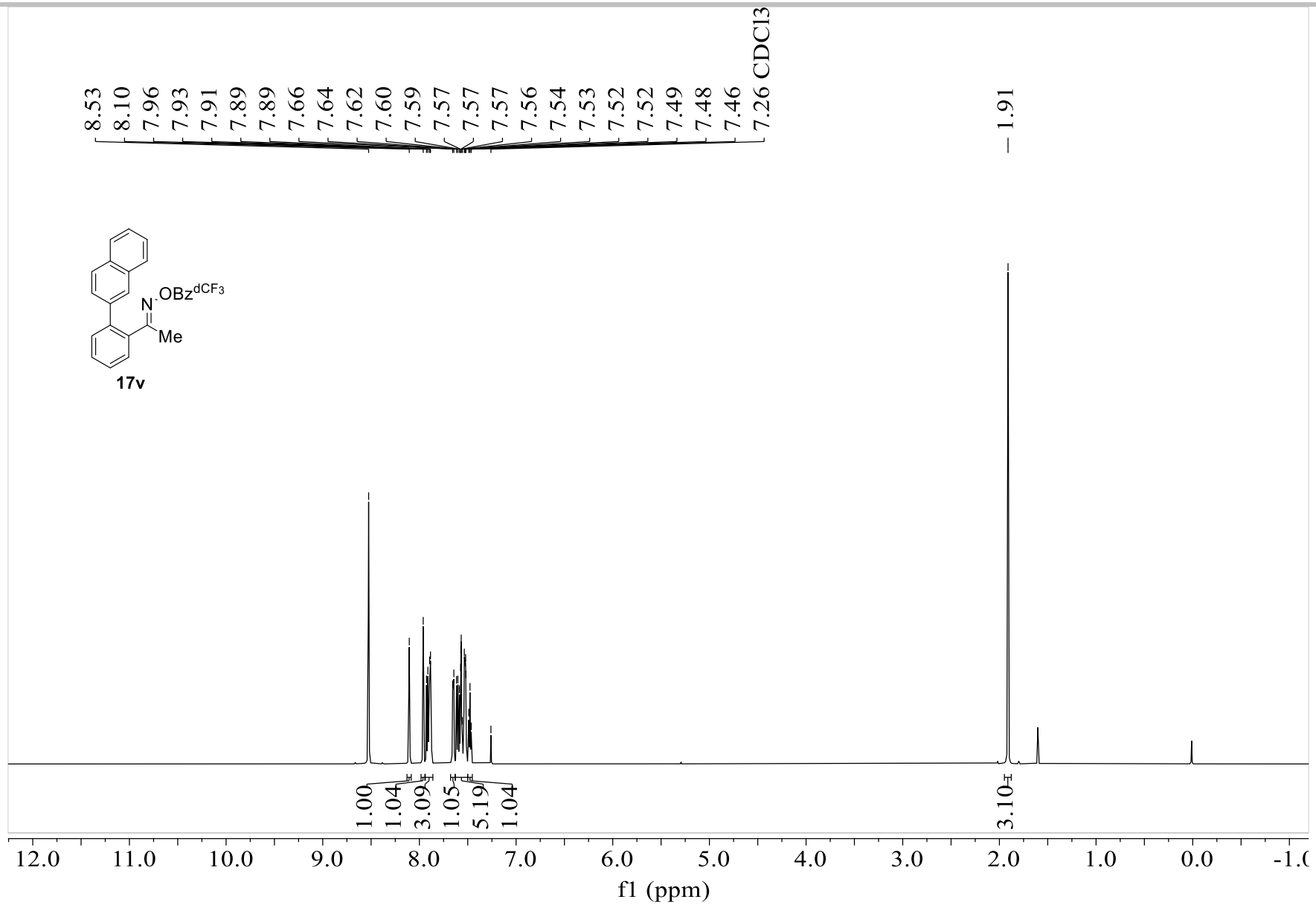
f1 (ppm)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7.46
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OBz^dCF3
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17v
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1.05
5.19
1.04
3.10
12.0
11.0
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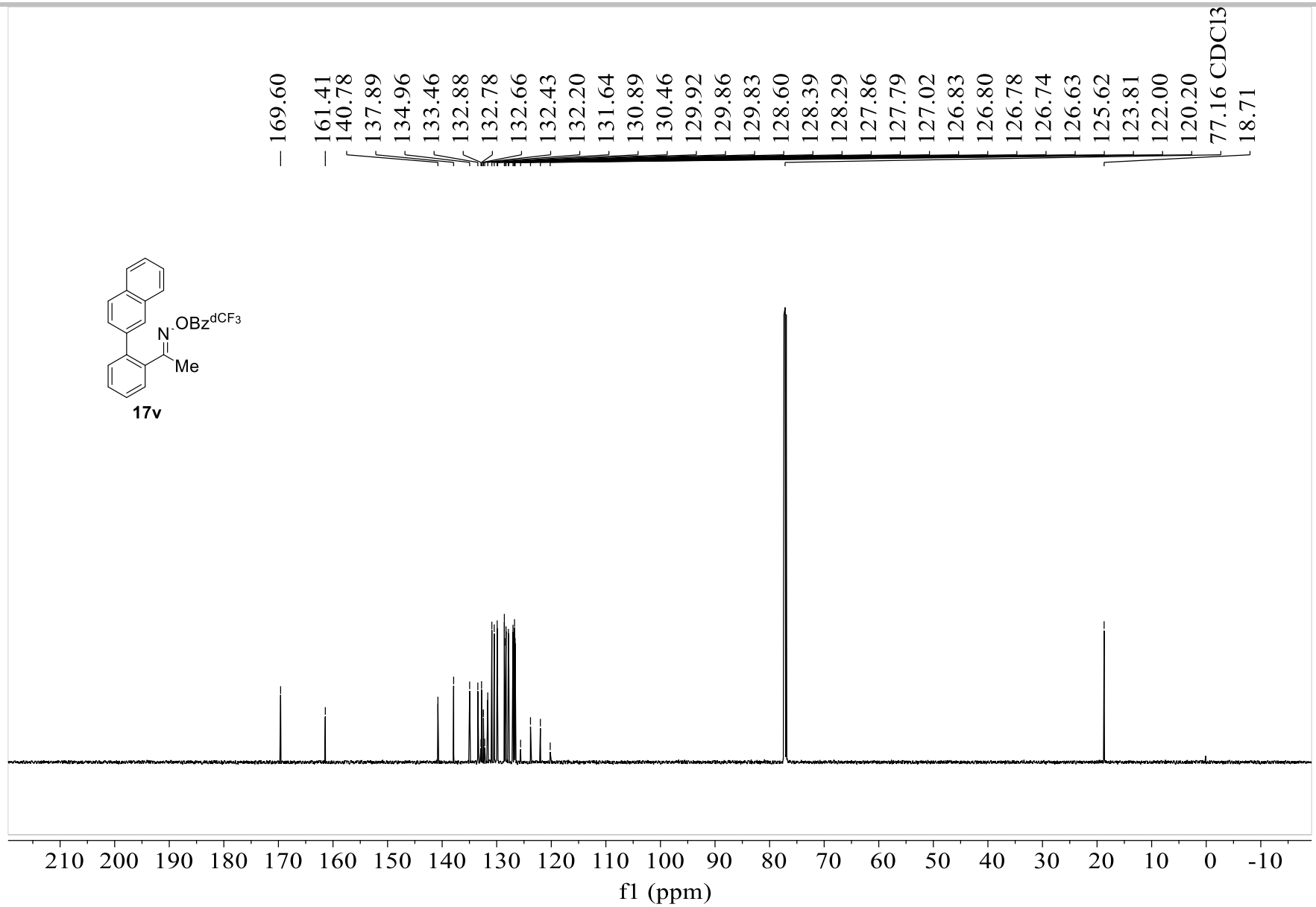
0.0
f1 (ppm)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126.63
125.62
123.81
122.00
120.20
77.16 CDCl3
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Me
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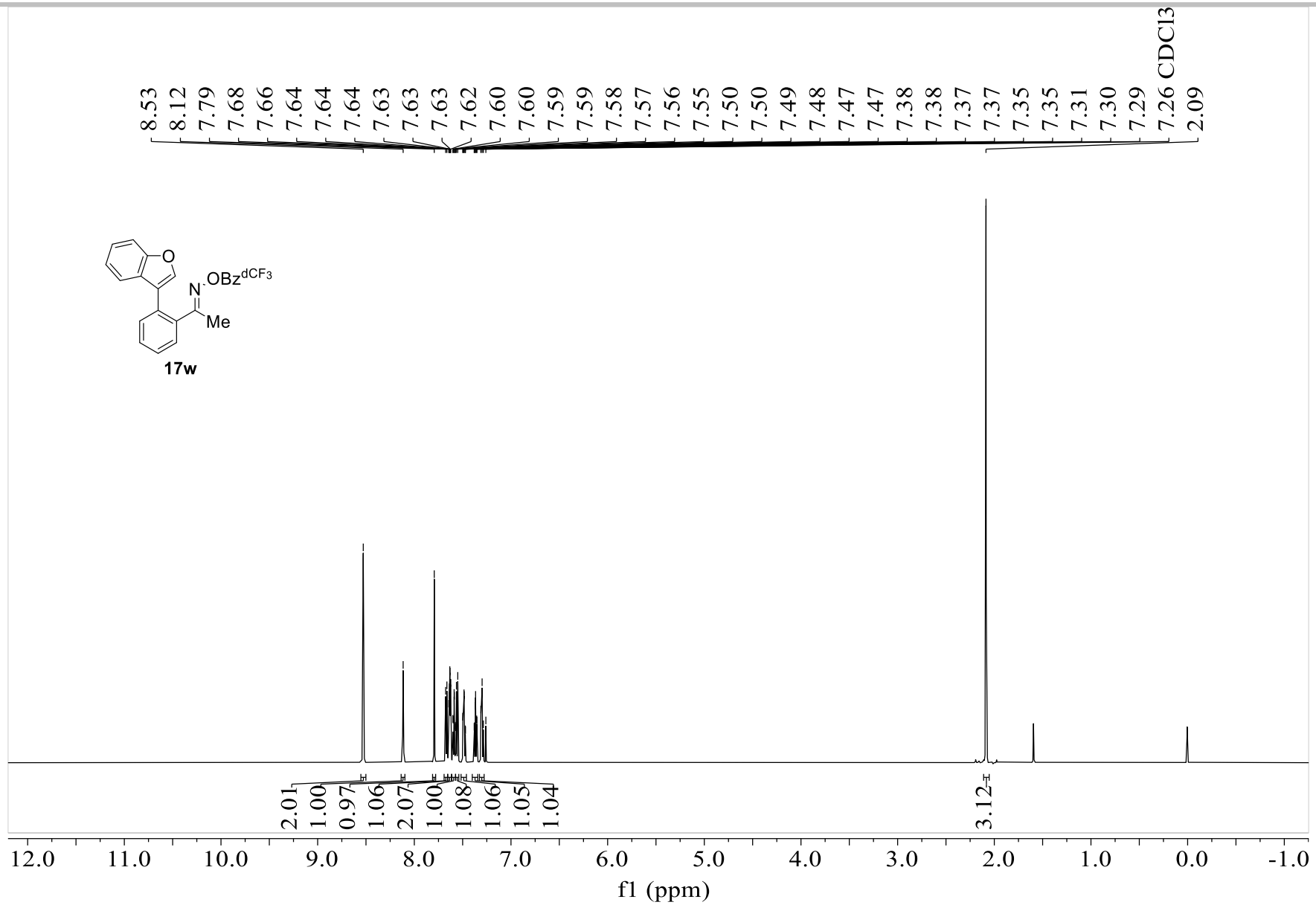
f1 (ppm)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7.29
7.26 CDCl3
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OBz^dCF3
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1.06
2.07
1.00
1.08
1.06
1.05
1.04
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12.0
11.0
10.0
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4.0
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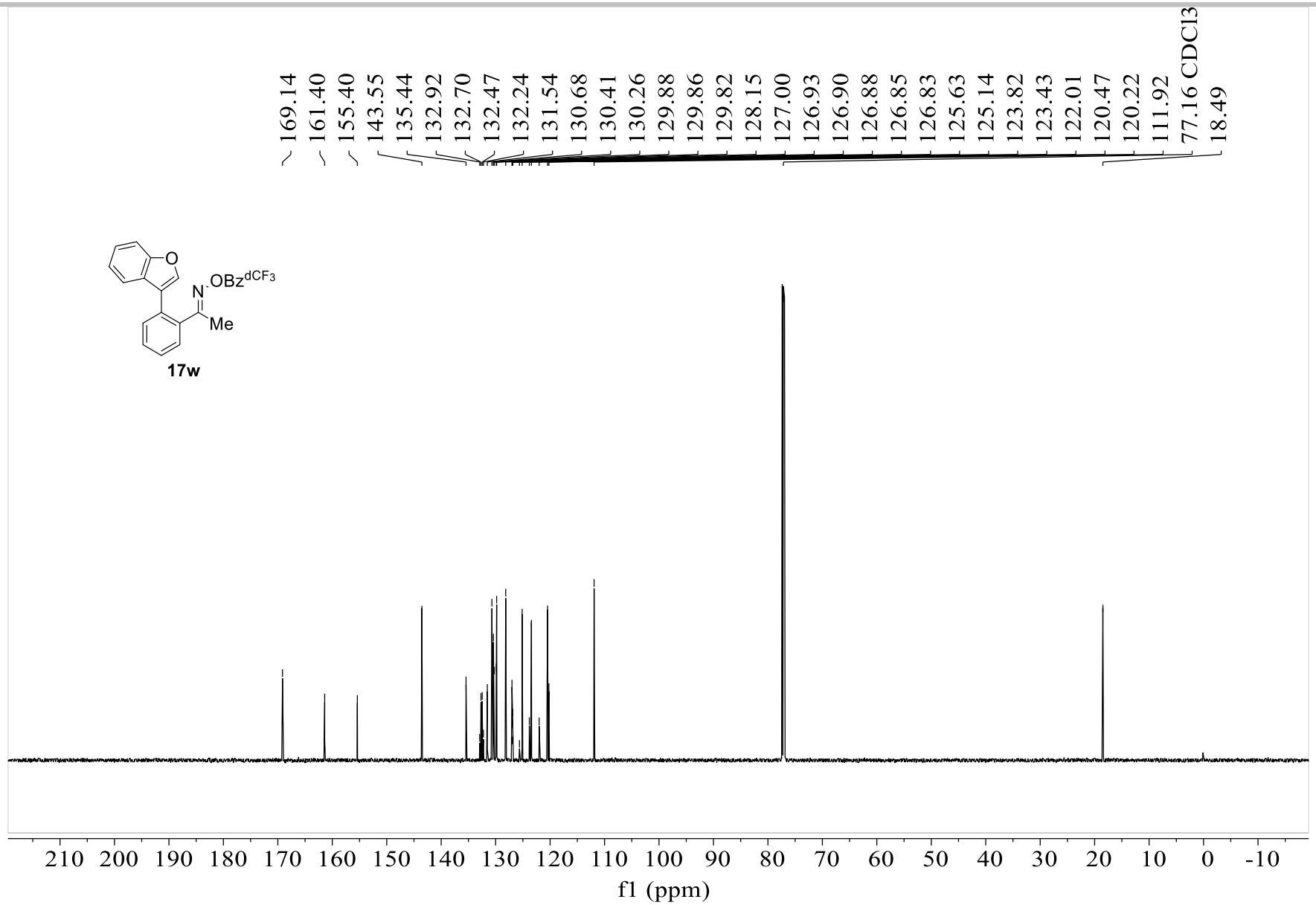
-1.0
f1 (ppm)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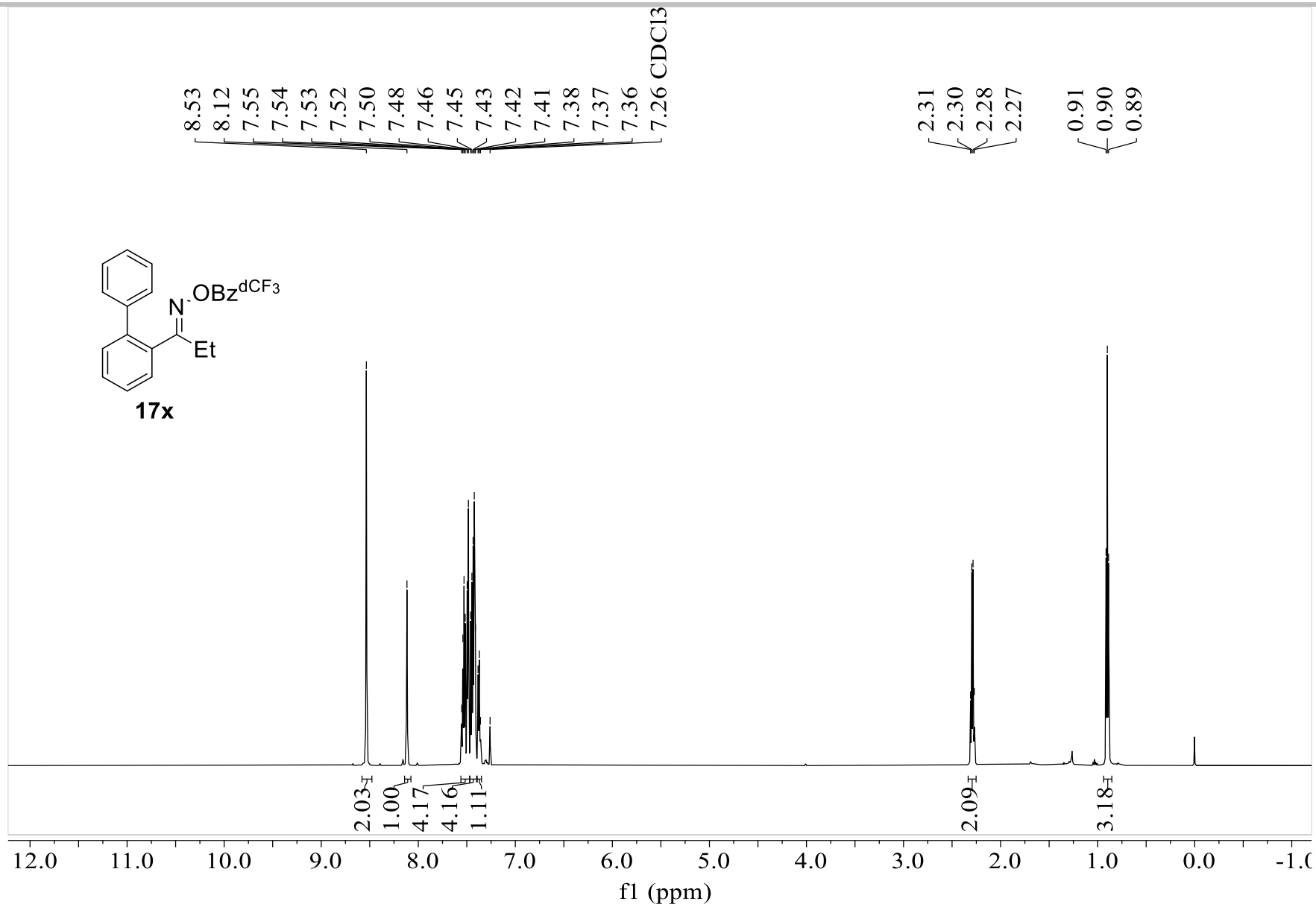
130.26
129.88
129.86
129.82
128.15
127.00
126.93
126.90
126.88
126.85
126.83
125.63
125.14
123.82
123.43
122.01
120.47
120.22
111.92
77.16 CDCl3
18.49
O
N
OBz^dCF3
Me
17w
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.41
7.38
7.37
7.36
7.26 CDCl3
2.31
2.30
2.28
2.27
0.91
0.90
0.89
N
OBz^dCF3
Et
17x
2.03
1.00
4.17
4.16
1.11
2.09
3.18
12.0
11.0
10.0
9.0
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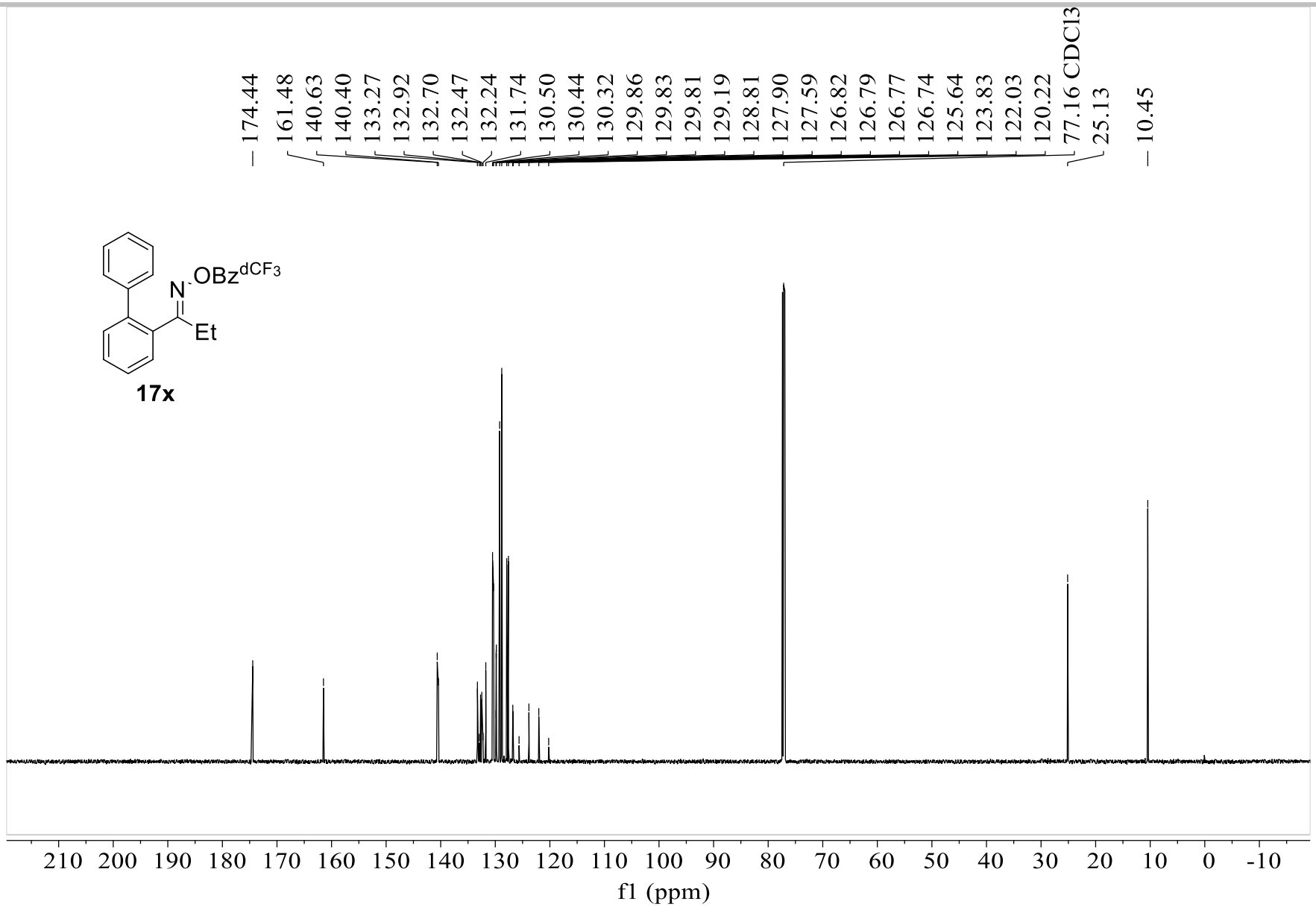
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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129.19
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127.90
127.59
126.82
126.79
126.77
126.74
125.64
123.83
122.03
120.22
77.16 CDCl3
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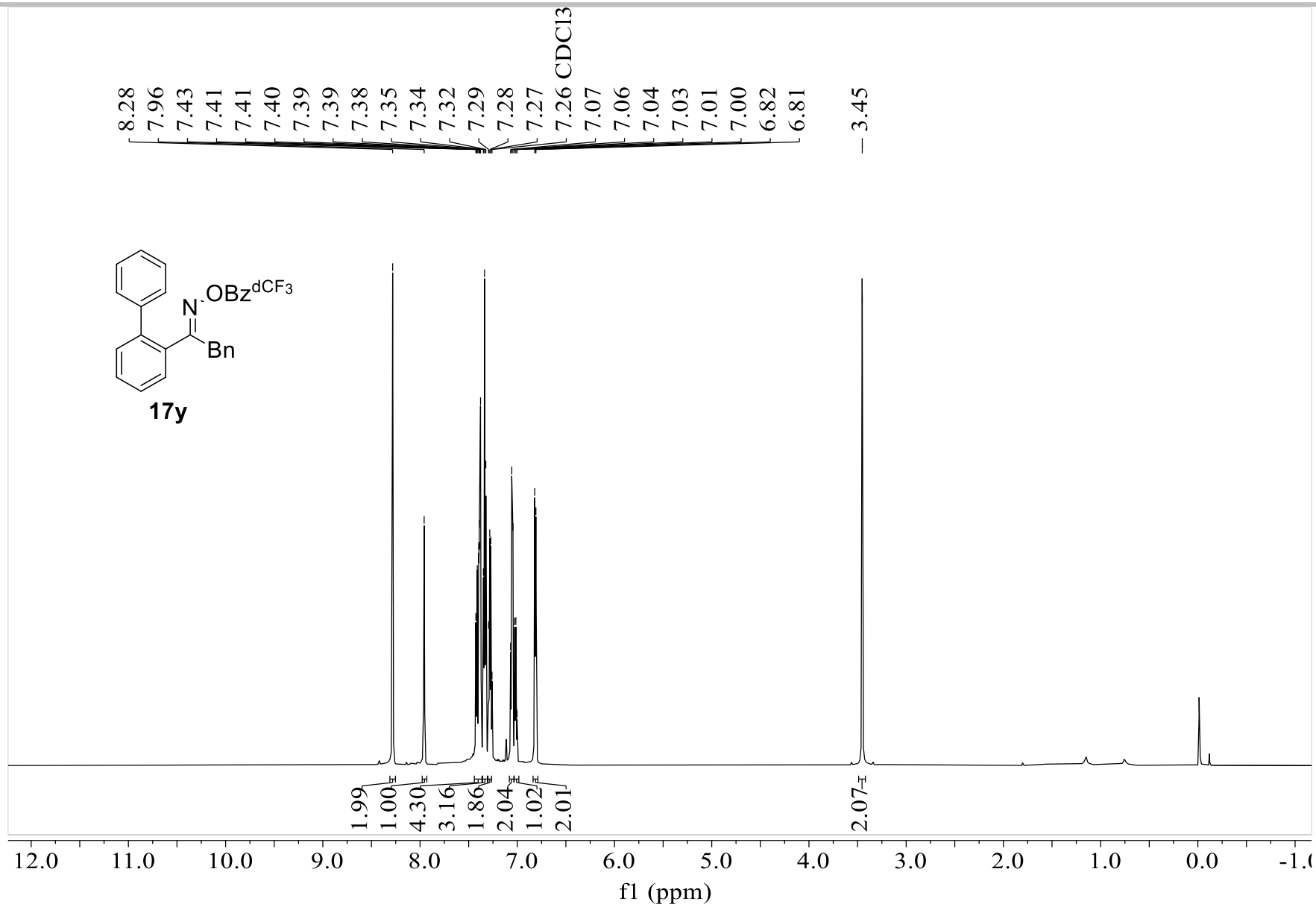
N
OBz^dCF3
Et
17x
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.32
7.29
7.28
7.27
7.26 CDCl3
7.07
7.06
7.04
7.03
7.01
7.00
6.82
6.81
3.45
N
OBz^dCF3
Bn
17y
1.99
1.00
4.30
3.16
1.86
2.04
1.02
2.01
2.07
12.0
11.0
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5.0
4.0
3.0
2.0
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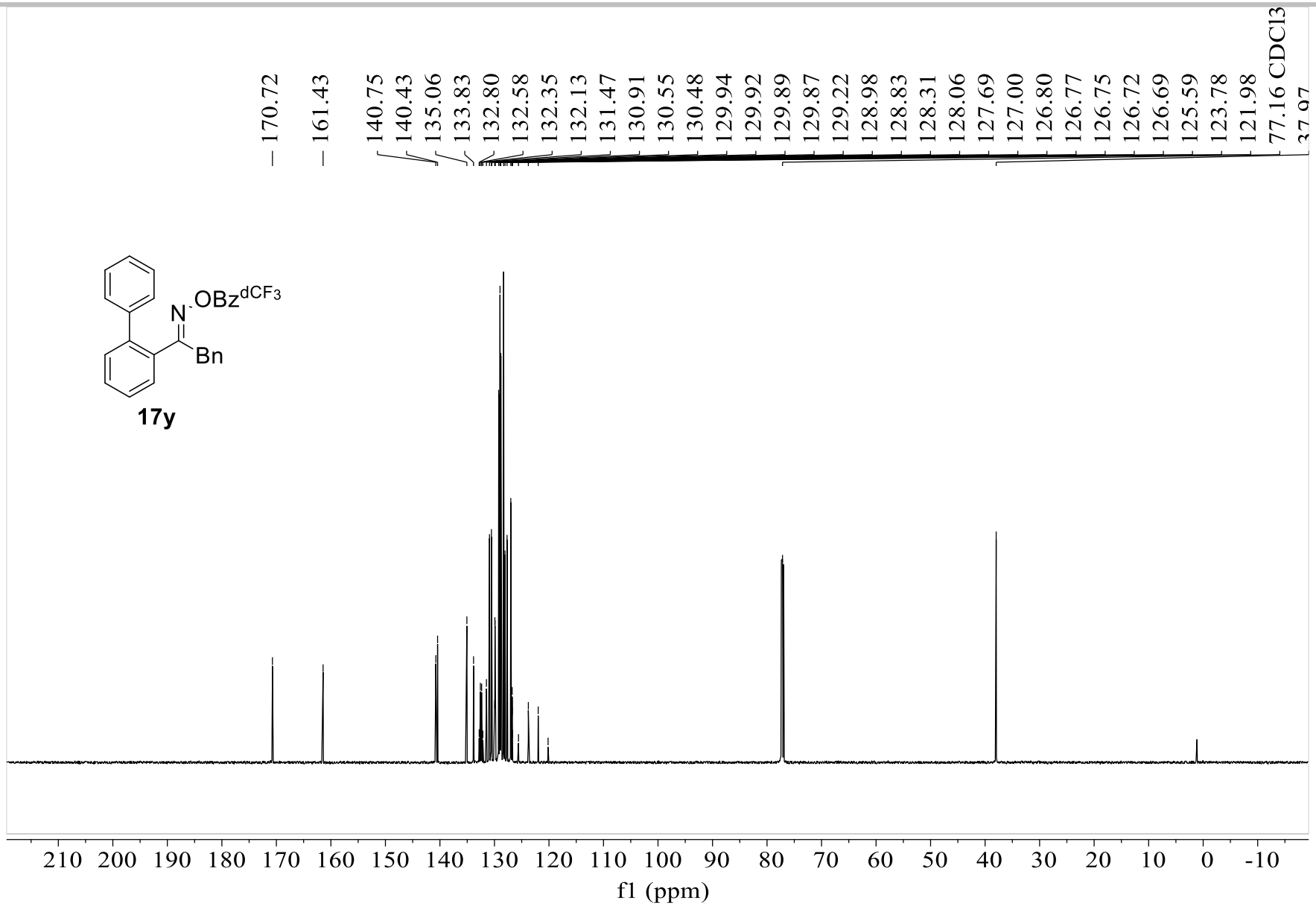
f1 (ppm)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128.31
128.06
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127.00
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126.75
126.72
126.69
125.59
123.78
121.98
77.16 CDCl3
37.97
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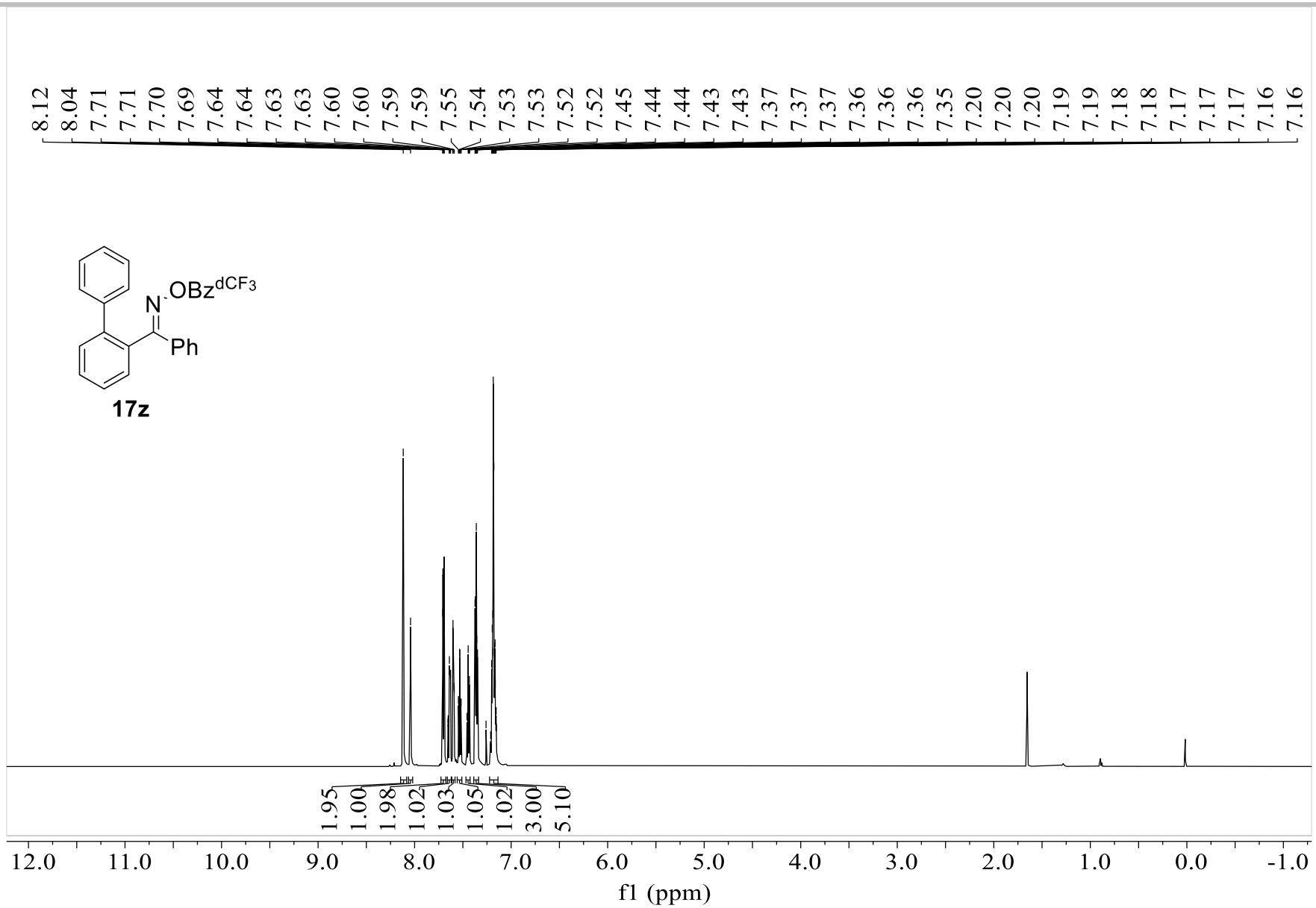
OBz^dCF3
Bn
17y
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.59
7.59
7.55
7.54
7.53
7.53
7.52
7.52
7.45
7.44
7.44
7.43
7.43
7.37
7.37
7.37
7.36
7.36
7.36
7.35
7.20
7.20
7.20
7.19
7.19
7.18
7.18
7.17
7.17
7.17
7.16
7.16
N
OBz^dCF3
Ph
17z
1.95
1.00
1.98
1.02
1.03
1.05
1.02
3.00
5.10
12.0
11.0
10.0
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6.0
5.0
4.0
3.0
2.0
1.0
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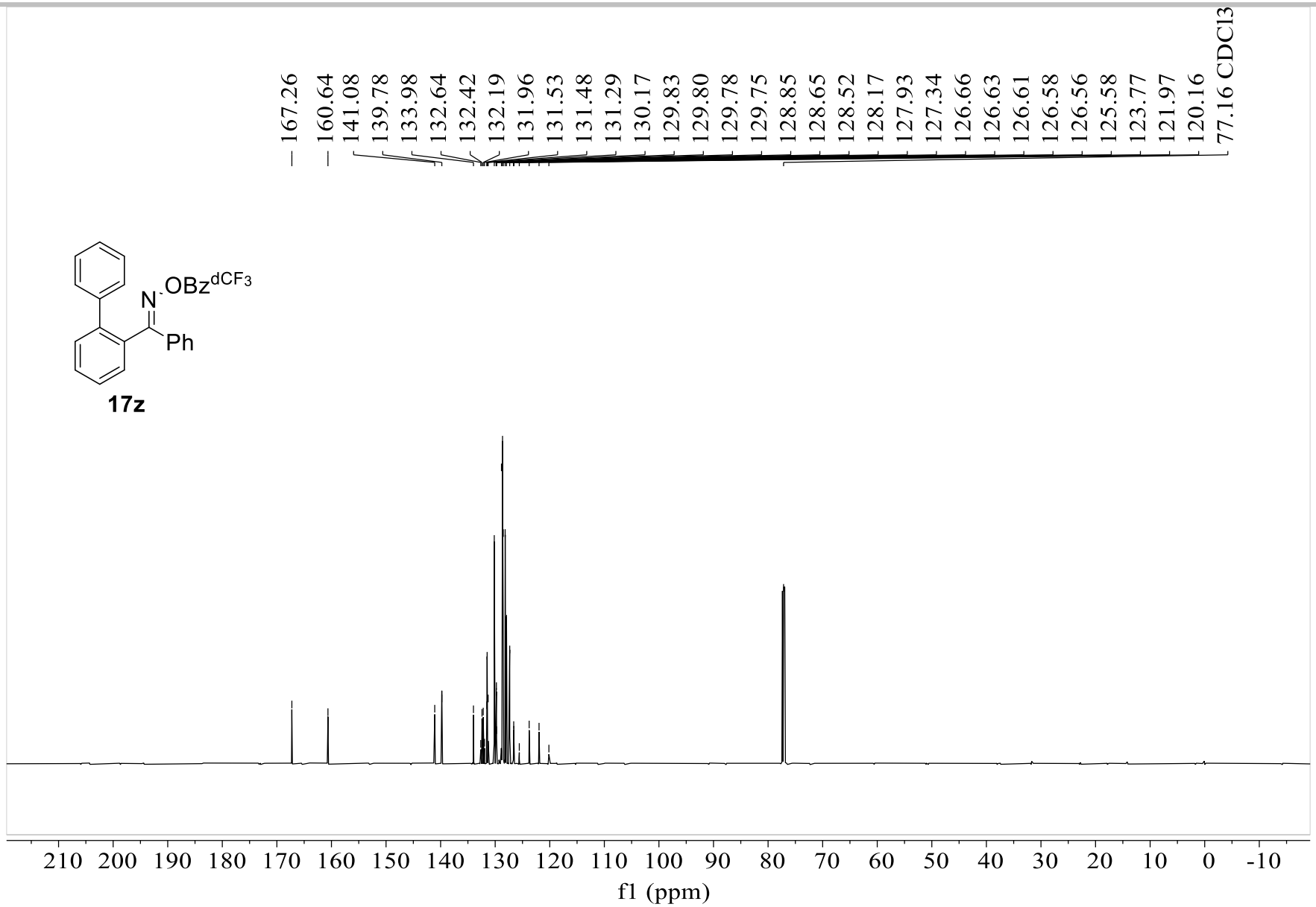
-1.0
f1 (ppm)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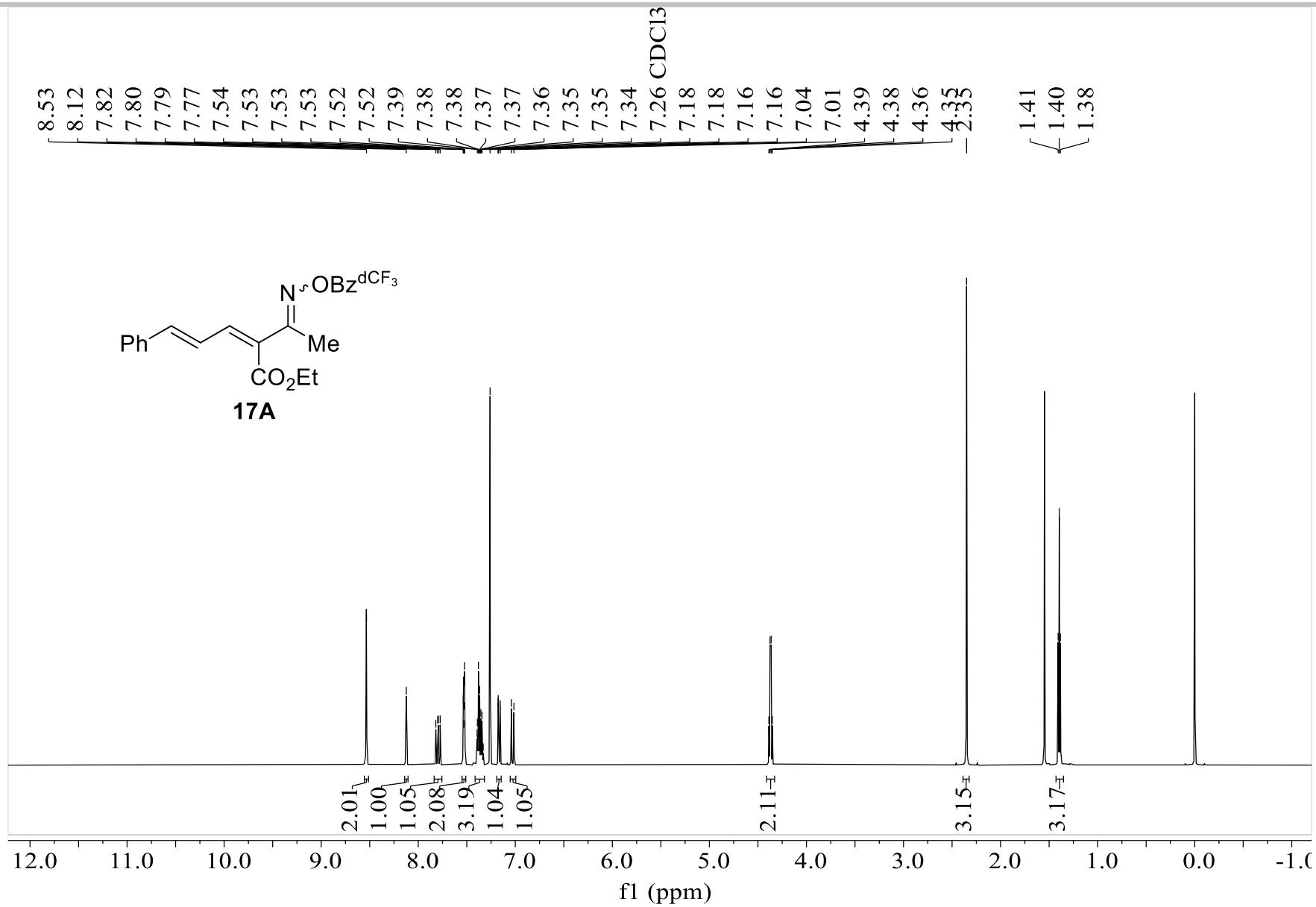
129.83
129.80
129.78
129.75
128.85
128.65
128.52
128.17
127.93
127.34
126.66
126.63
126.61
126.58
126.56
125.58
123.77
121.97
120.16
77.16 CDCl3
N
OBz^dCF3
Ph
17z
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.52
7.52
7.39
7.38
7.38
7.37
7.37
7.36
7.35
7.35
7.34
7.26 CDCl3
7.18
7.18
7.16
7.16
7.04
7.01
4.39
4.38
4.36
4.35
4.33
2.35
1.41
1.40
1.38
N
OBz^dCF3
Ph
Me
CO2Et
17A
2.01
1.00
1.05
2.08
3.19
1.04
1.05
2.11
3.15
3.17
12.0
11.0
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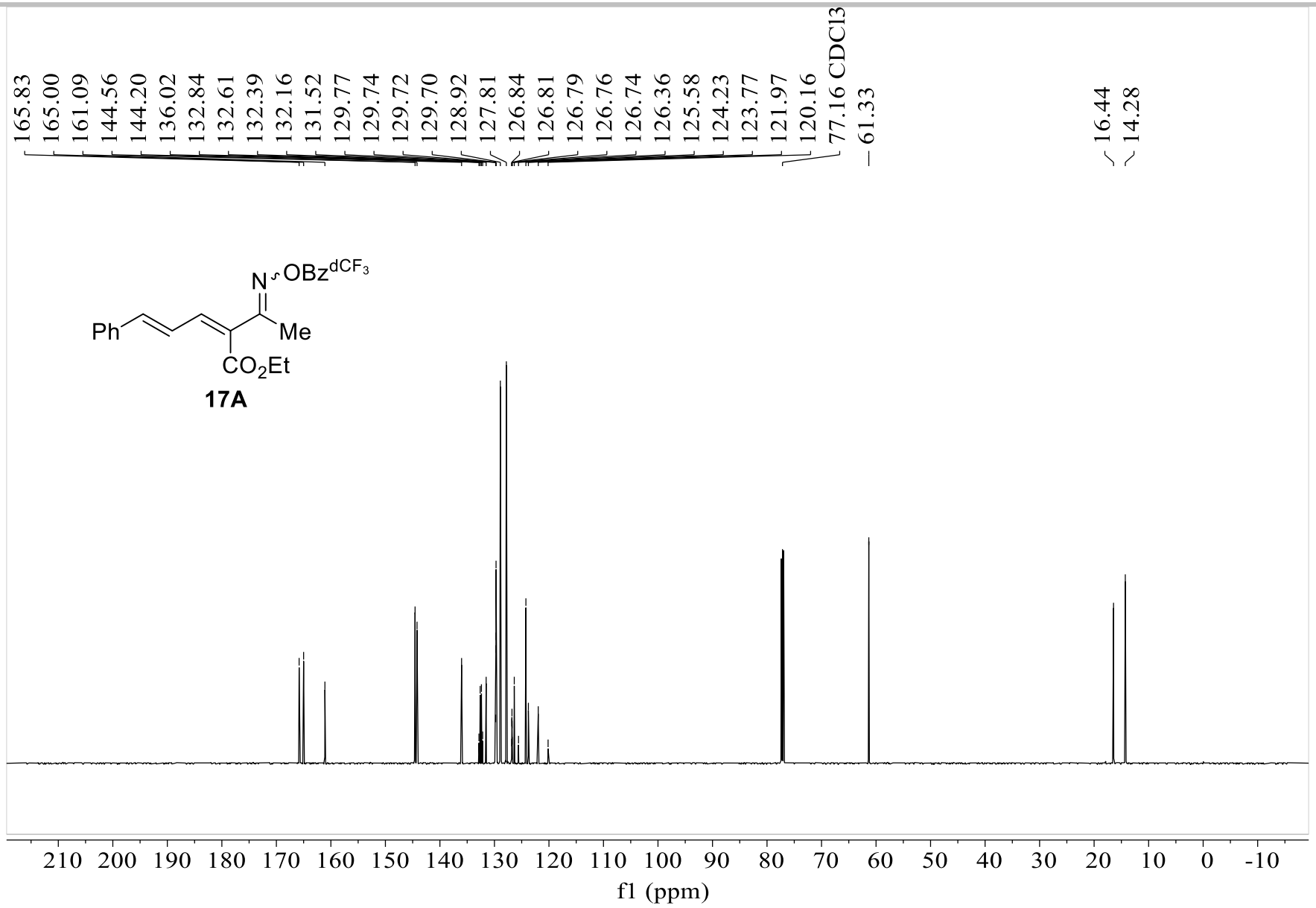
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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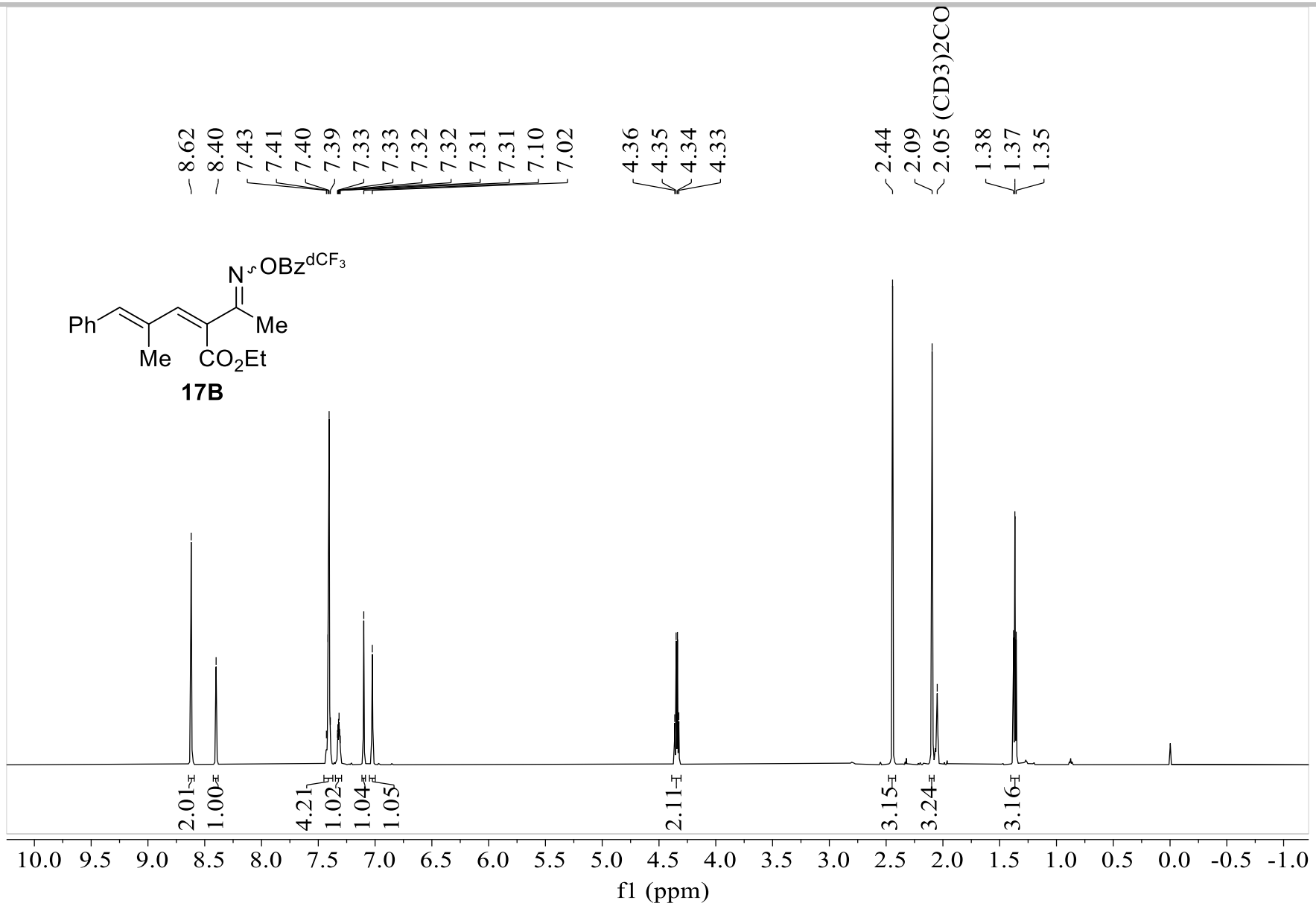
126.84
126.81
126.79
126.76
126.74
126.36
125.58
124.23
123.77
121.97
120.16
77.16 CDCl3
61.33
16.44
14.28
N
OBz^dCF3
Ph
Me
CO2Et
17A
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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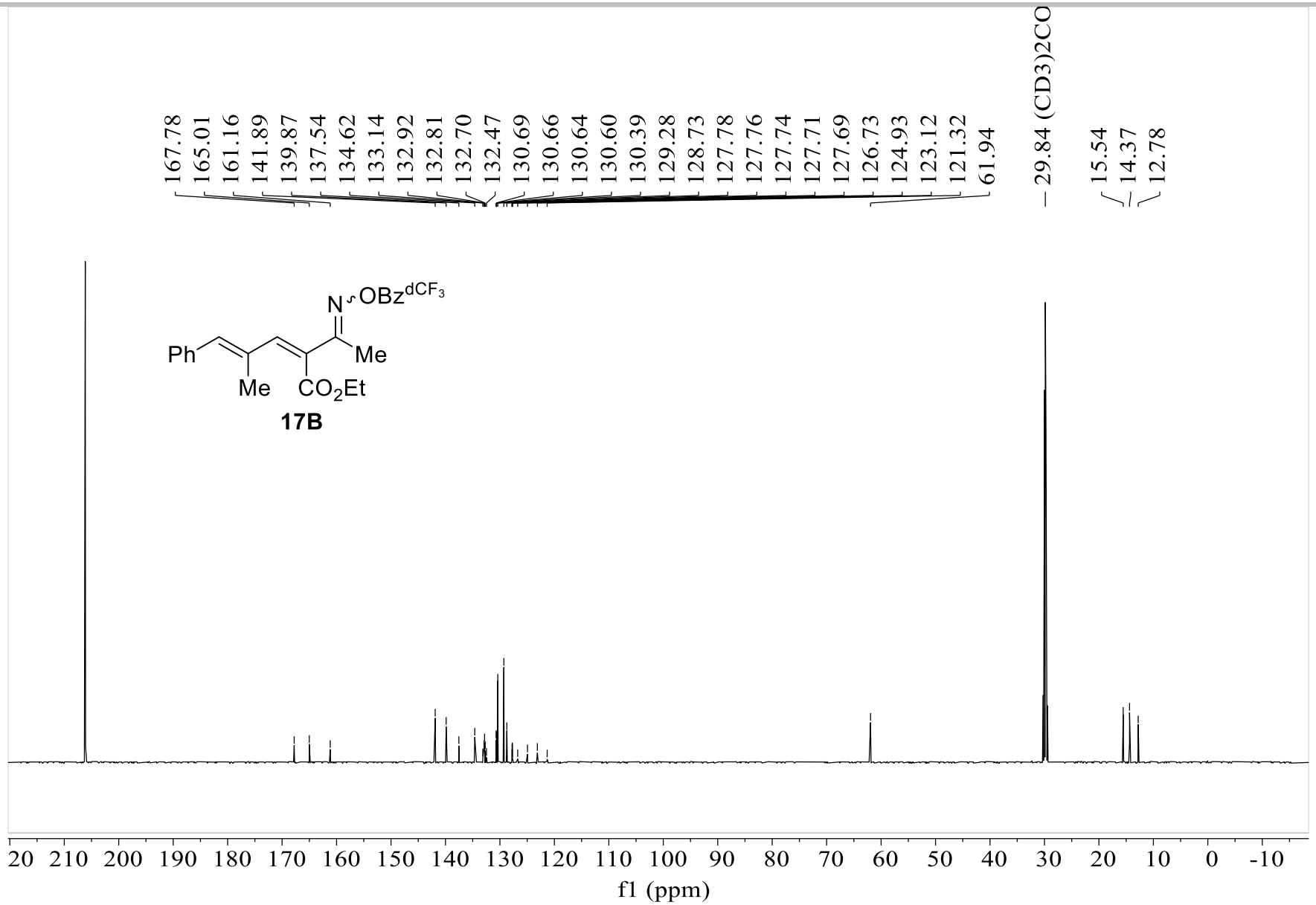
7.33
7.32
7.32
7.31
7.31
7.10
7.02
4.36
4.35
4.34
4.33
2.44
2.09
2.05 (CD3)2CO
1.38
1.37
1.35
N
OBz^dCF3
Ph
Me
Me
CO2Et
17B
2.01
1.00
4.21
1.02
1.04
1.05
2.11
3.15
3.24
3.16
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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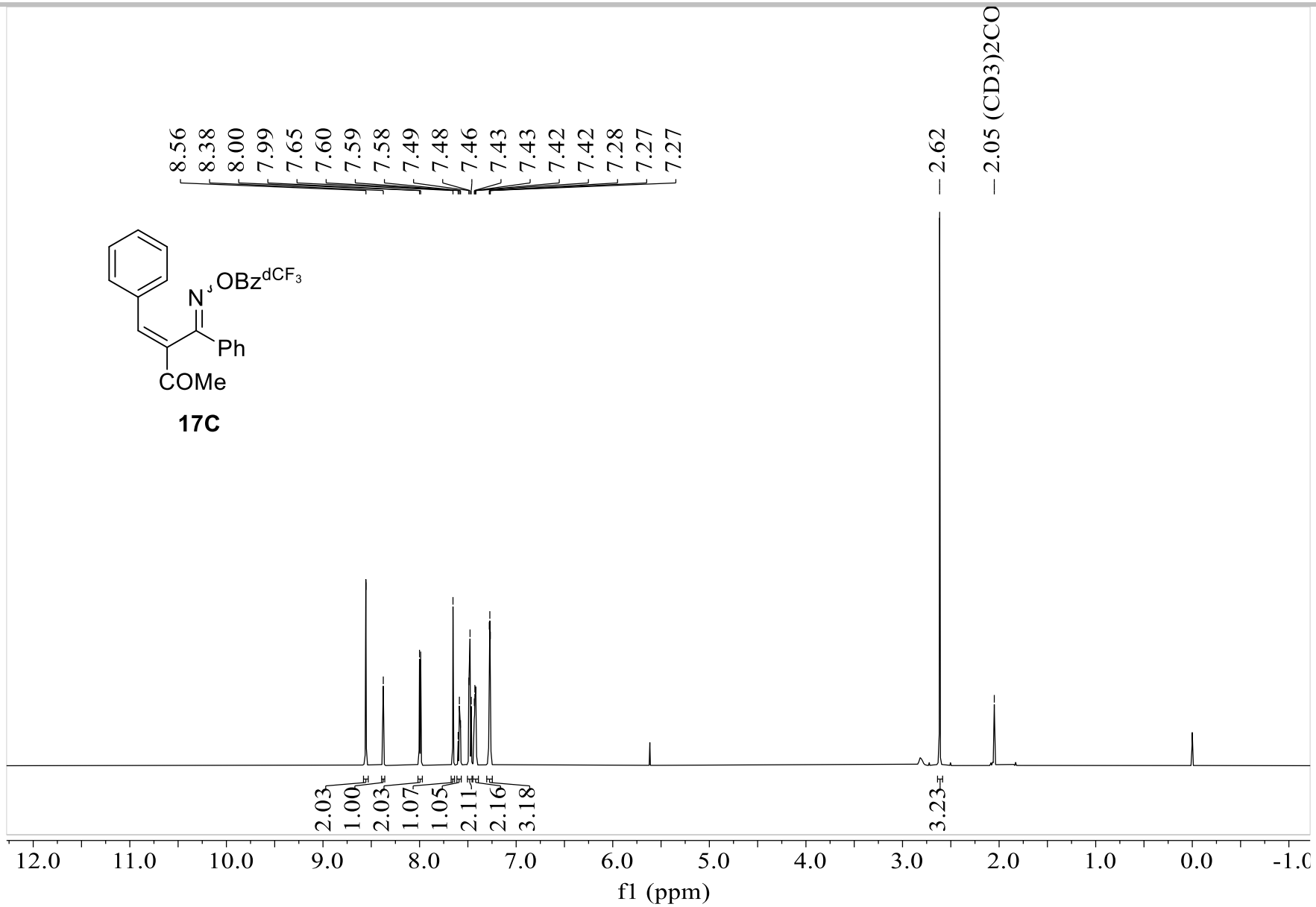
130.66
130.64
130.60
130.39
129.28
128.73
127.78
127.76
127.74
127.71
127.69
126.73
124.93
123.12
121.32
61.94
29.84 (CD3)2CO
15.54
14.37
12.78
N
OBz^dCF3
Ph
Me
Me
CO2Et
17B
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.48
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7.43
7.42
7.42
7.28
7.27
7.27
2.62
2.05 (CD3)2CO
OBz^dCF3
N
Ph
COMe
17C
2.03
1.00
2.03
1.07
1.05
2.11
2.16
3.18
3.23
12.0
11.0
10.0
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6.0
5.0
4.0
3.0
2.0
1.0
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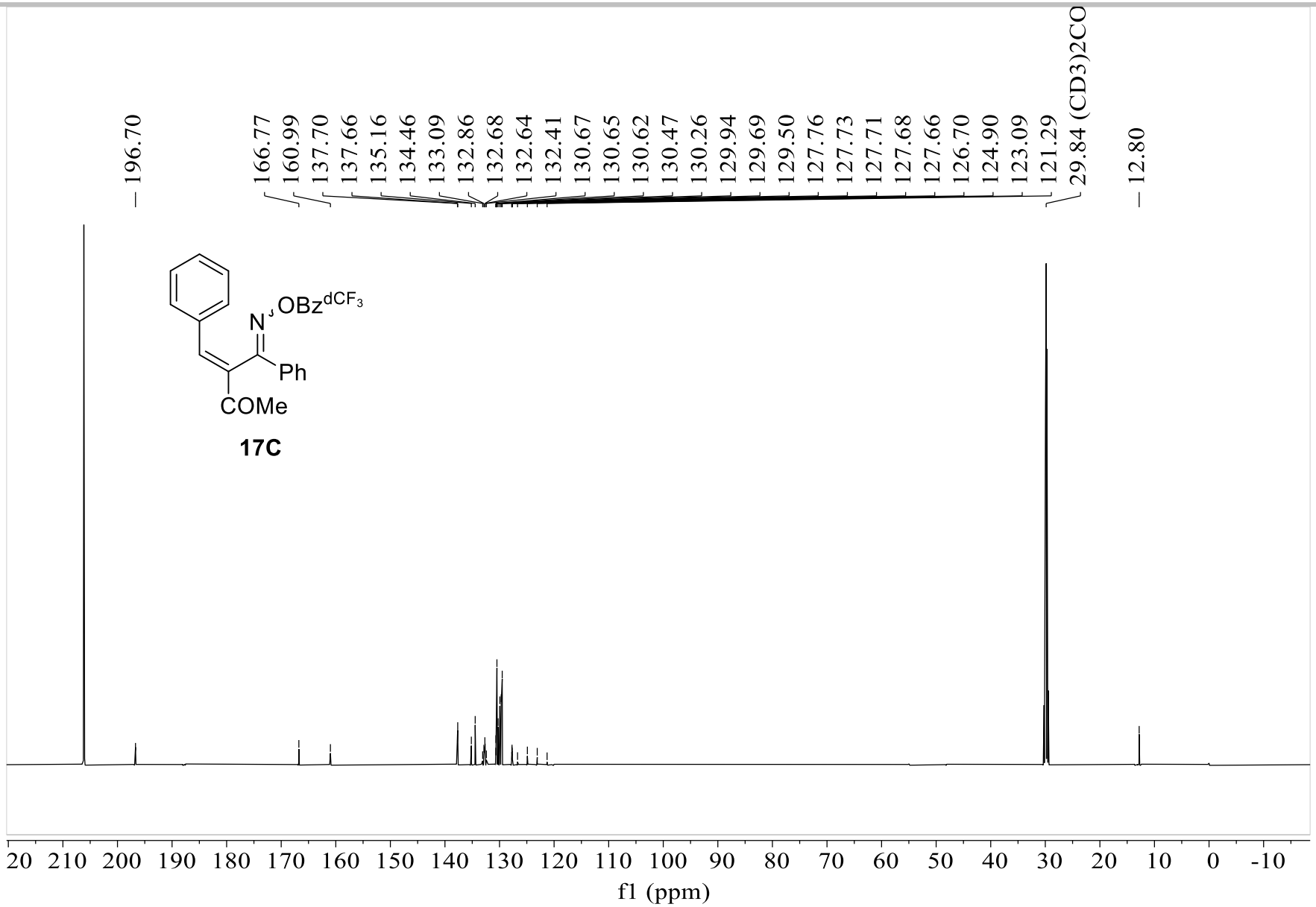
-1.0
f1 (ppm)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130.47
130.26
129.94
129.69
129.50
127.76
127.73
127.71
127.68
127.66
126.70
124.90
123.09
121.29
29.84 (CD3)2CO
12.80
N
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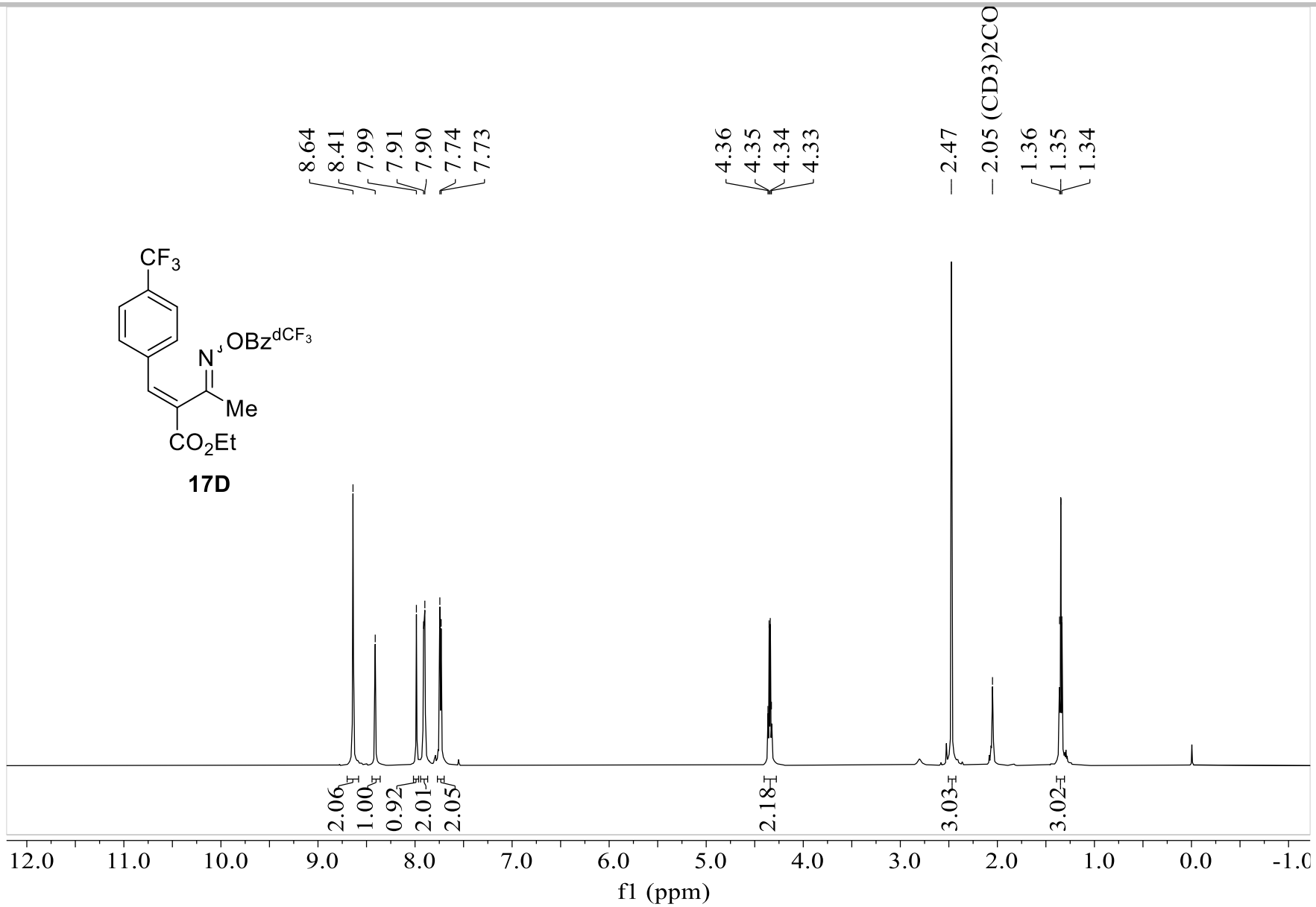
Ph
COMe
17C
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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4.35
4.34
4.33
2.47
2.05 (CD3)2CO
1.36
1.35
1.34
CF3
N
OBzdCF3
Me
CO2Et
17D
2.06
1.00
0.92
2.01
2.05
2.18
3.03
3.02
12.0
11.0
10.0
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8.0
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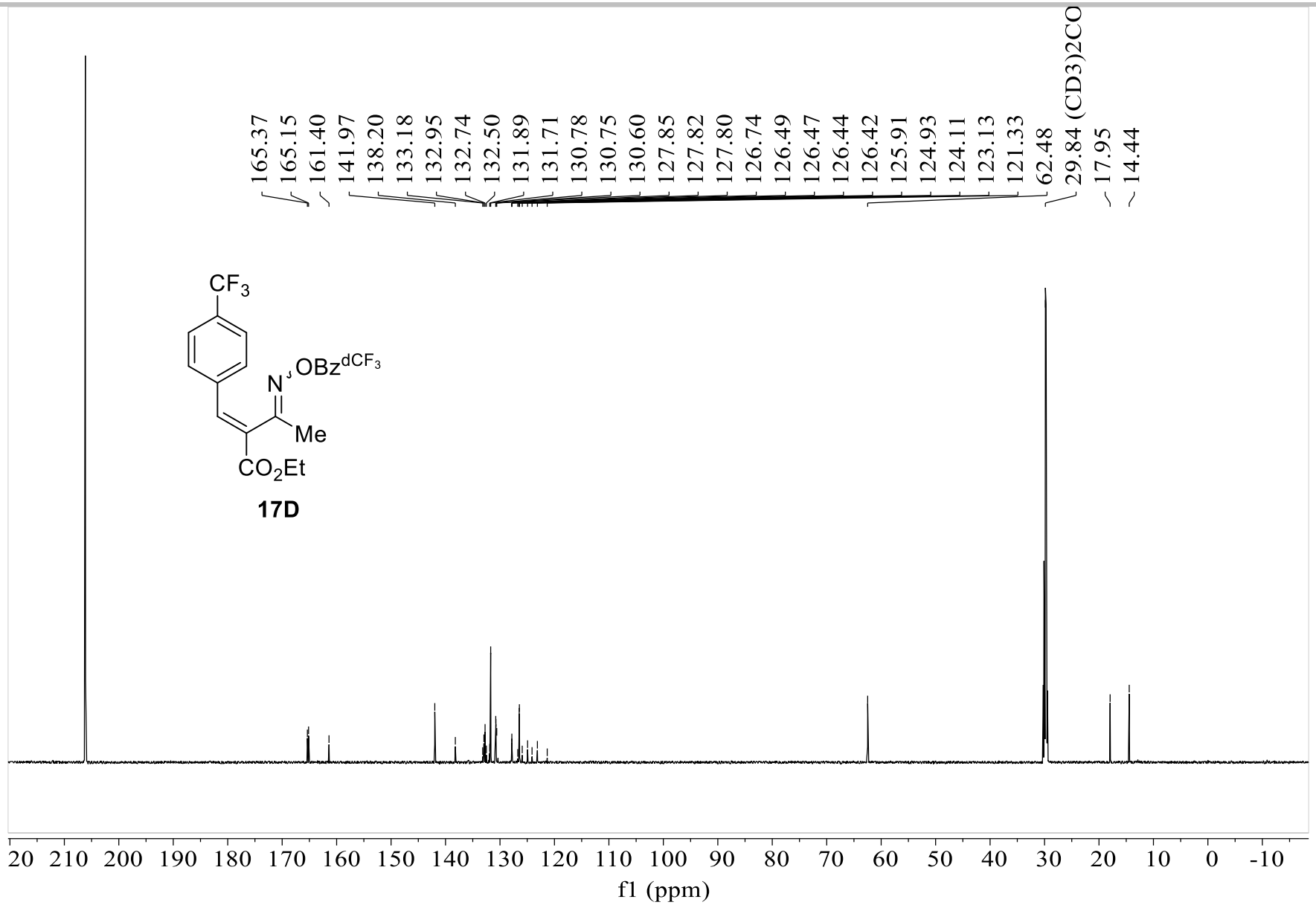
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)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130.60
127.85
127.82
127.80
126.74
126.49
126.47
126.44
126.42
125.91
124.93
124.11
123.13
121.33
62.48
29.84 (CD3)2CO
17.95
14.44
CF3
N
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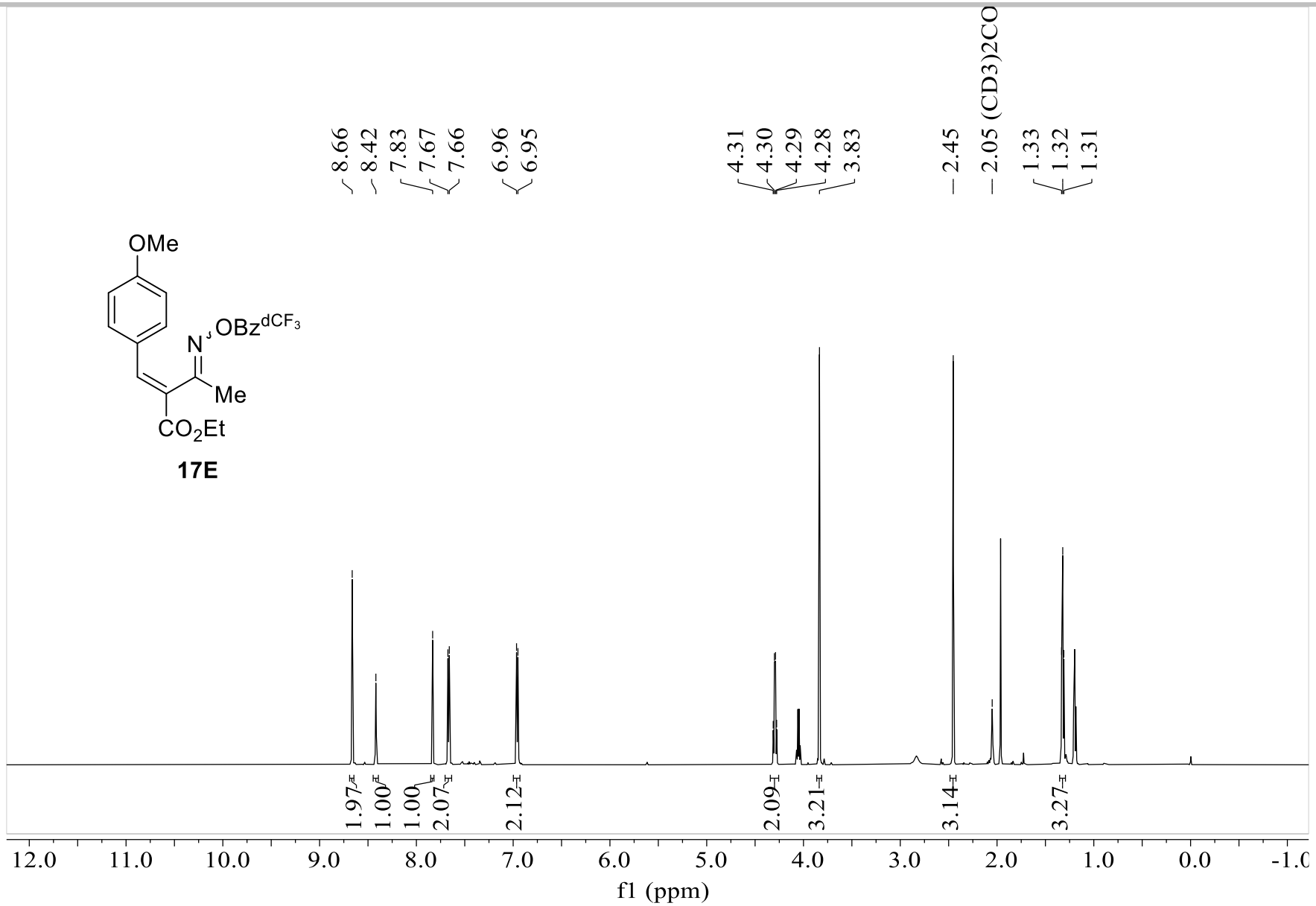
Me
CO2Et
17D
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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6.95
4.31
4.30
4.29
4.28
3.83
2.45
2.05 (CD3)2CO
1.33
1.32
1.31
OMe
N
OBz^dCF3
Me
CO2Et
17E
1.97
1.00
1.00
2.07
2.12
2.09
3.21
3.14
3.27
12.0
11.0
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4.0
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2.0
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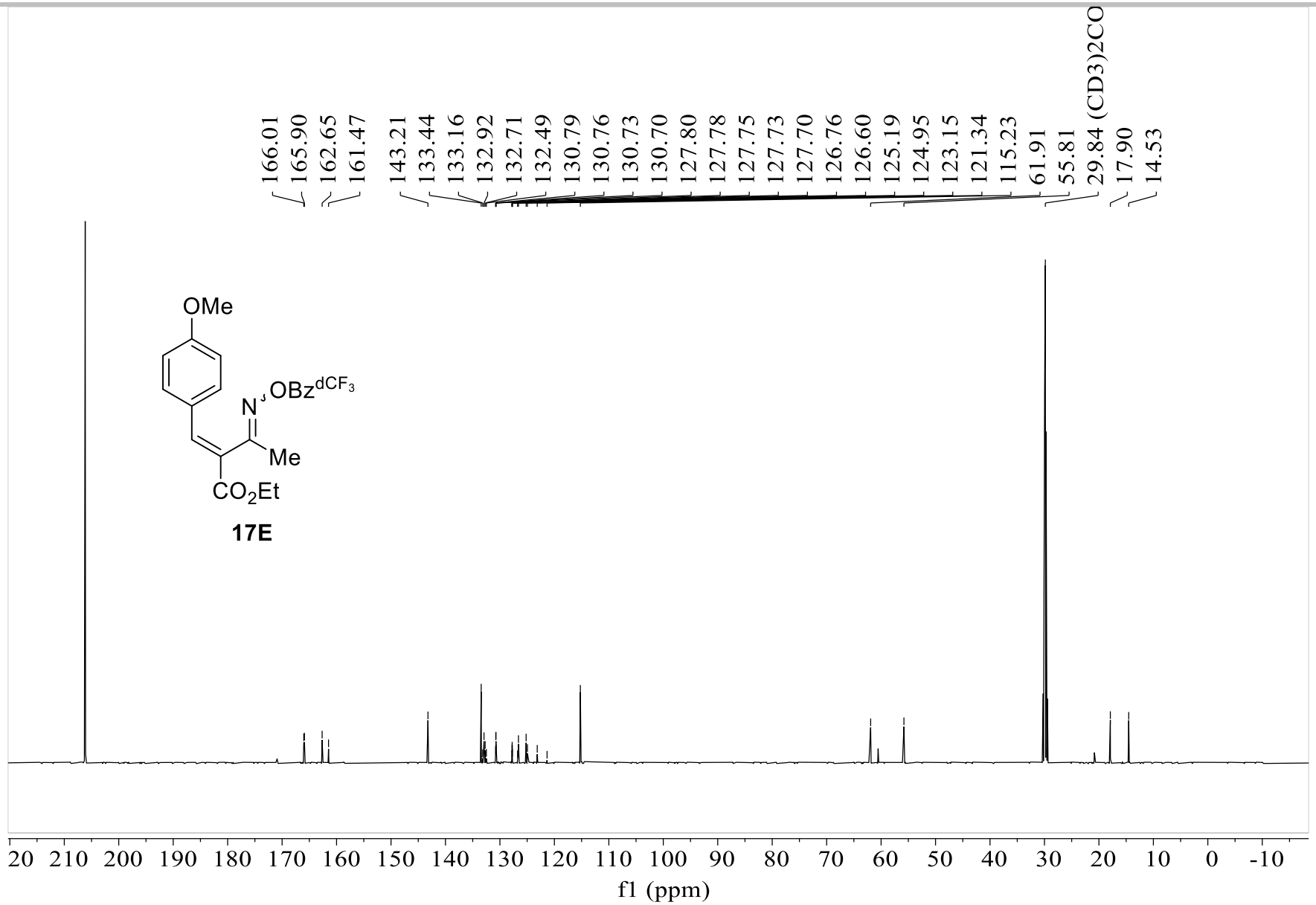
0.0
f1 (ppm)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127.75
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126.76
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125.19
124.95
123.15
121.34
115.23
61.91
55.81
29.84 (CD3)2CO
17.90
14.53
OMe
N
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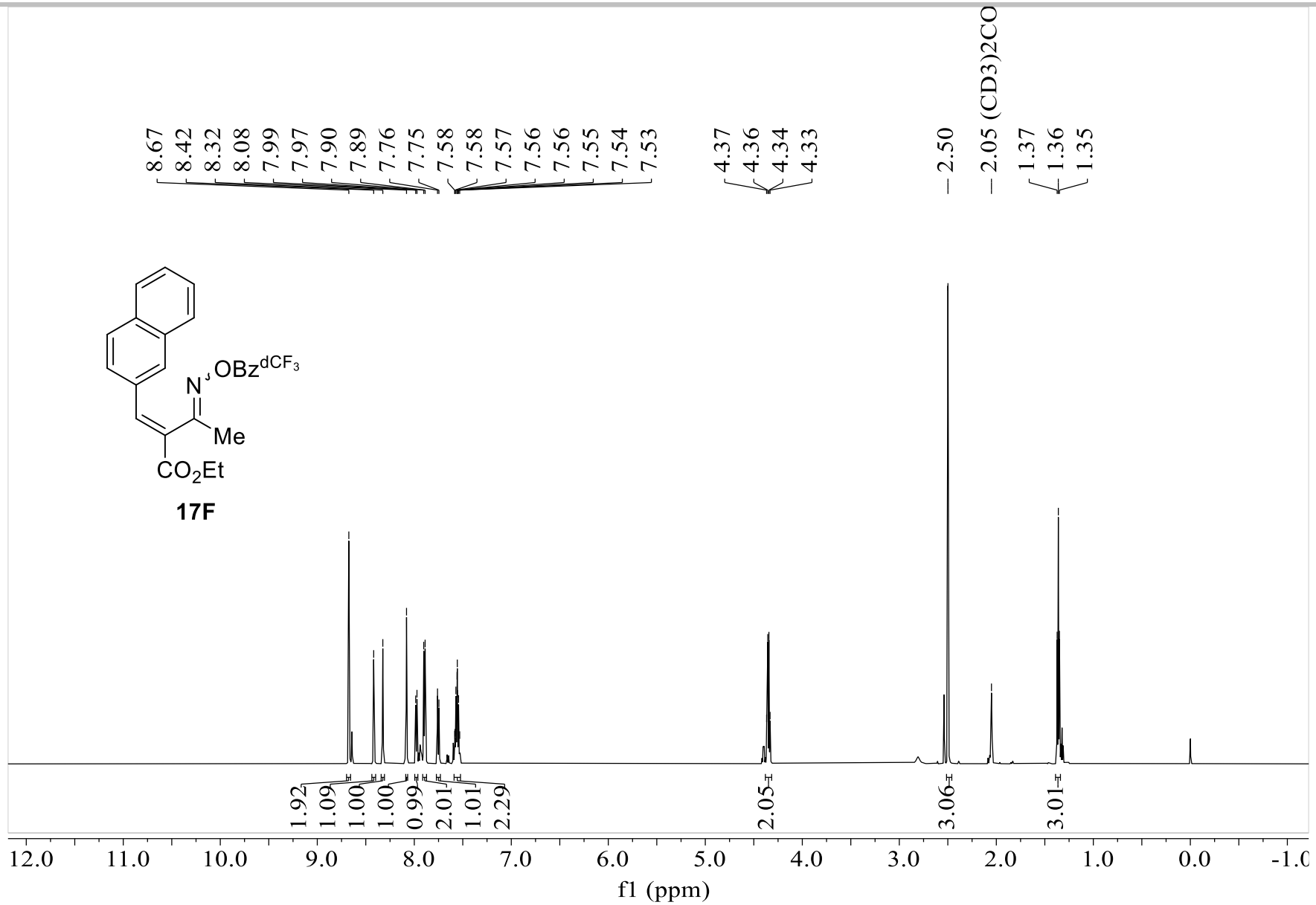
Me
CO2Et
17E
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.57
7.56
7.56
7.55
7.54
7.53
4.37
4.36
4.34
4.33
2.50
2.05 (CD3)2CO
1.37
1.36
1.35
N
OBz^dCF3
Me
CO2Et
17F
1.92
1.09
1.00
1.00
0.99
2.01
1.01
2.29
2.05
3.06
3.01
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11.0
10.0
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6.0
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4.0
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1.0
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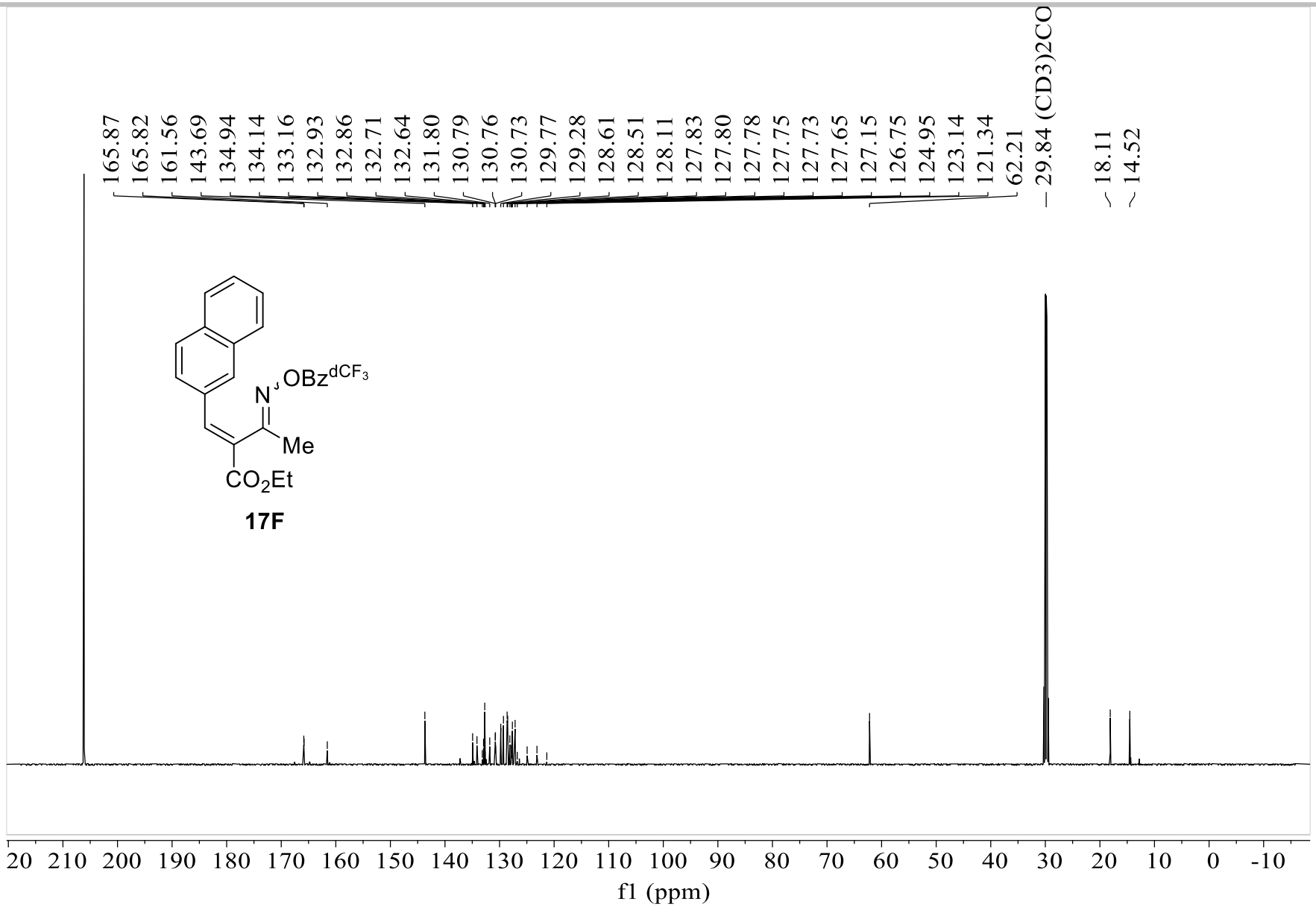
-1.0
f1 (ppm)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127.78
127.75
127.73
127.65
127.15
126.75
124.95
123.14
121.34
62.21
29.84 (CD3)2CO
18.11
14.52
N
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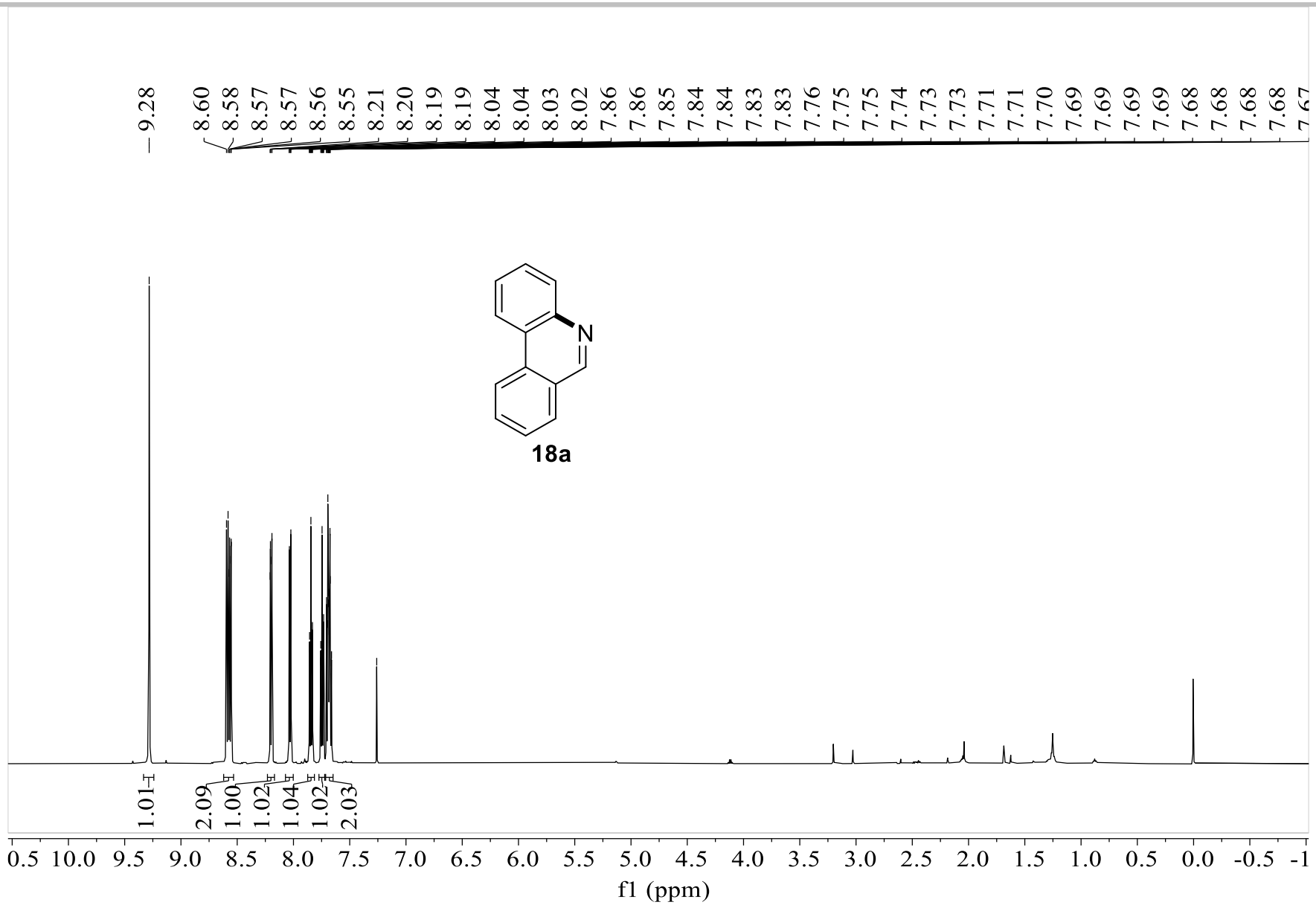
Me
CO2Et
17F
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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8.04
8.03
8.02
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7.86
7.85
7.84
7.84
7.83
7.83
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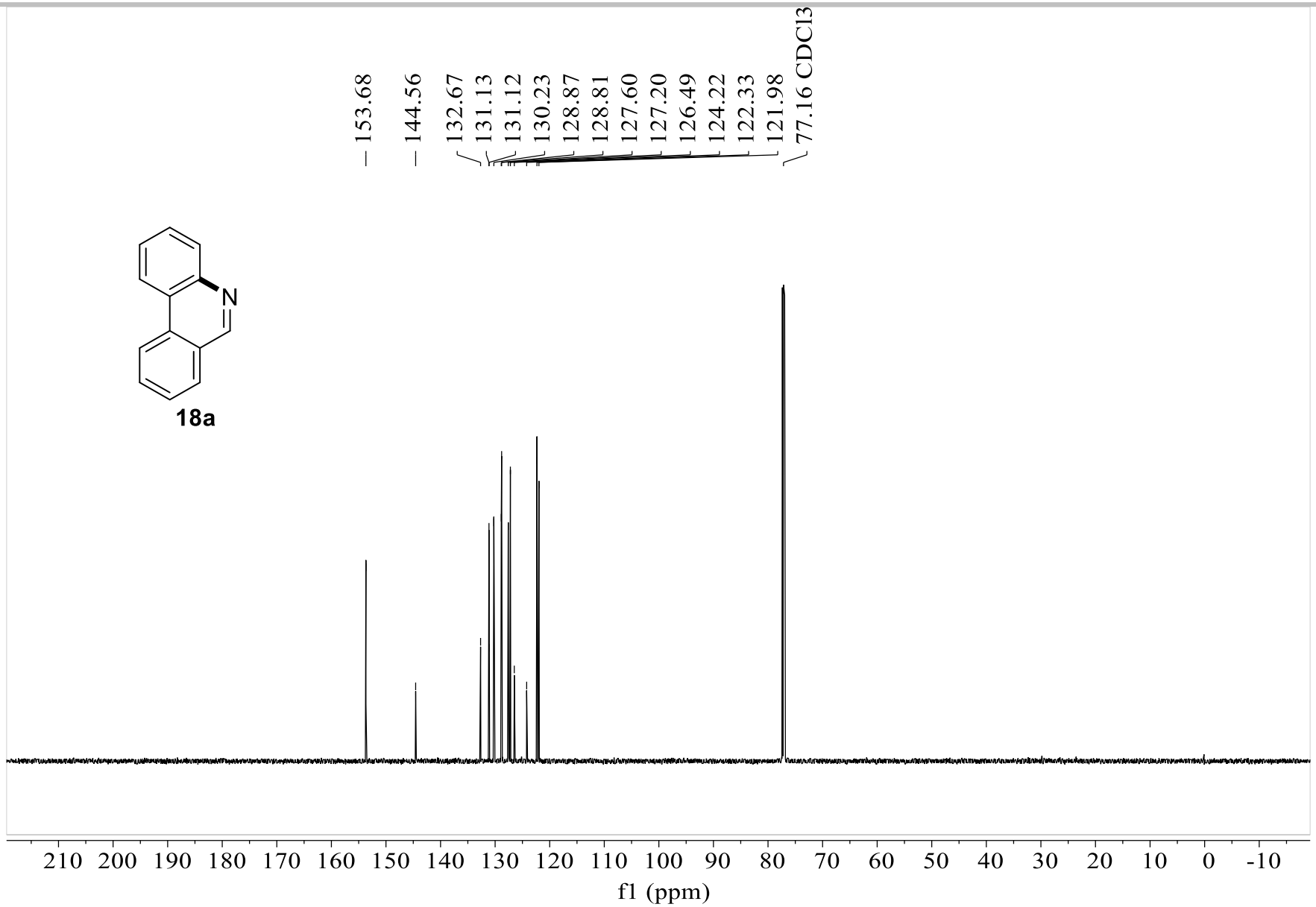
7.68
7.68
7.68
7.67
N
18a
1.01
2.09
1.00
1.02
1.04
1.02
2.03
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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127.20
126.49
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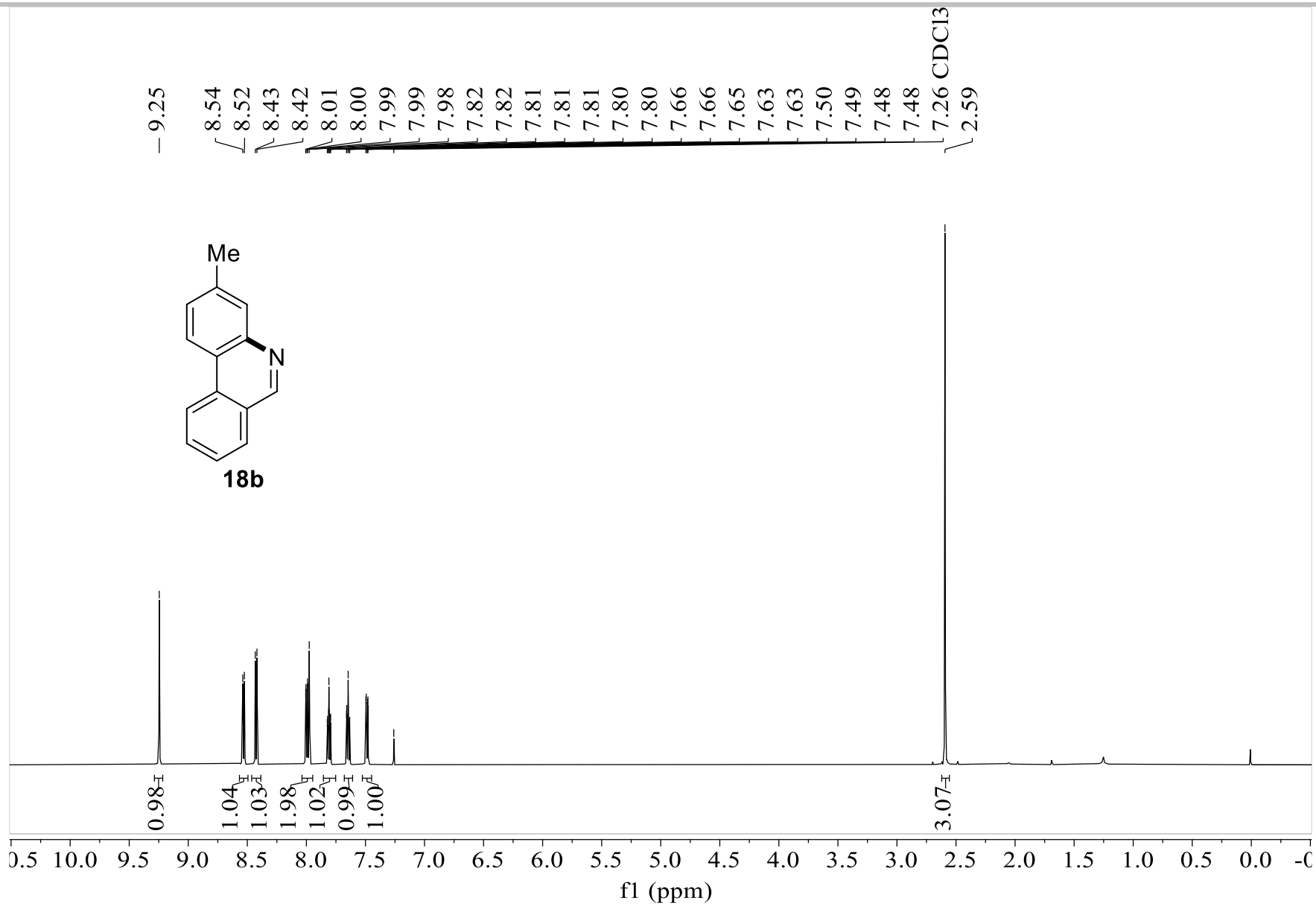
121.98
77.16 CDCl3
N
18a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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8.00
7.99
7.99
7.98
7.82
7.82
7.81
7.81
7.81
7.80
7.80
7.66
7.66
7.65
7.63
7.63
7.50
7.49
7.48
7.48
7.26 CDCl3
2.59
Me
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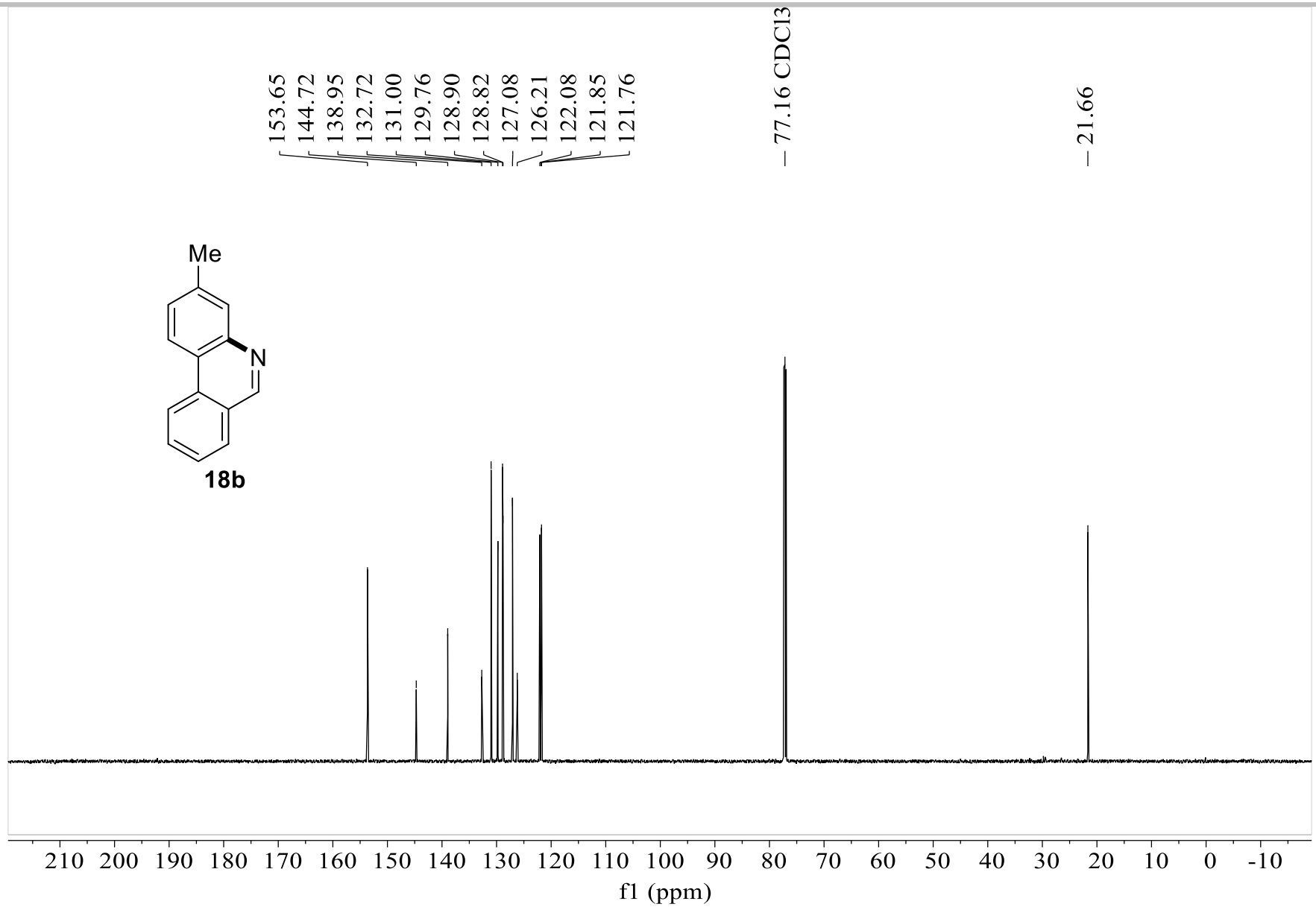
18b
0.98
1.04
1.03
1.98
1.02
0.99
1.00
3.07
f1 (ppm)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138.95
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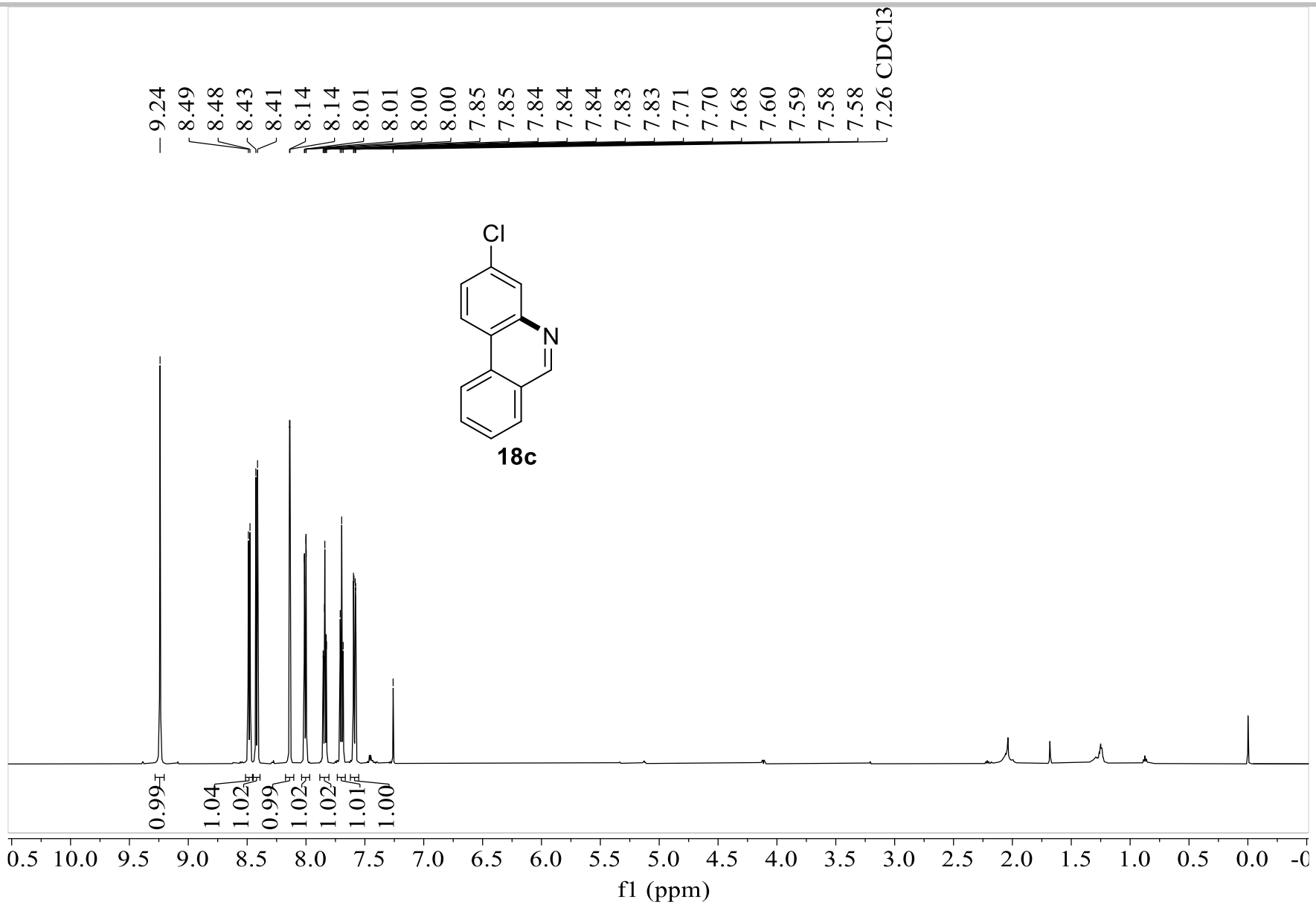
129.76
128.90
128.82
127.08
126.21
122.08
121.85
121.76
77.16 CDCl3
21.66
Me
N
18b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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8.14
8.01
8.01
8.00
8.00
7.85
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7.84
7.84
7.84
7.83
7.83
7.71
7.70
7.68
7.60
7.59
7.58
7.58
7.26 CDCl3
Cl
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18c
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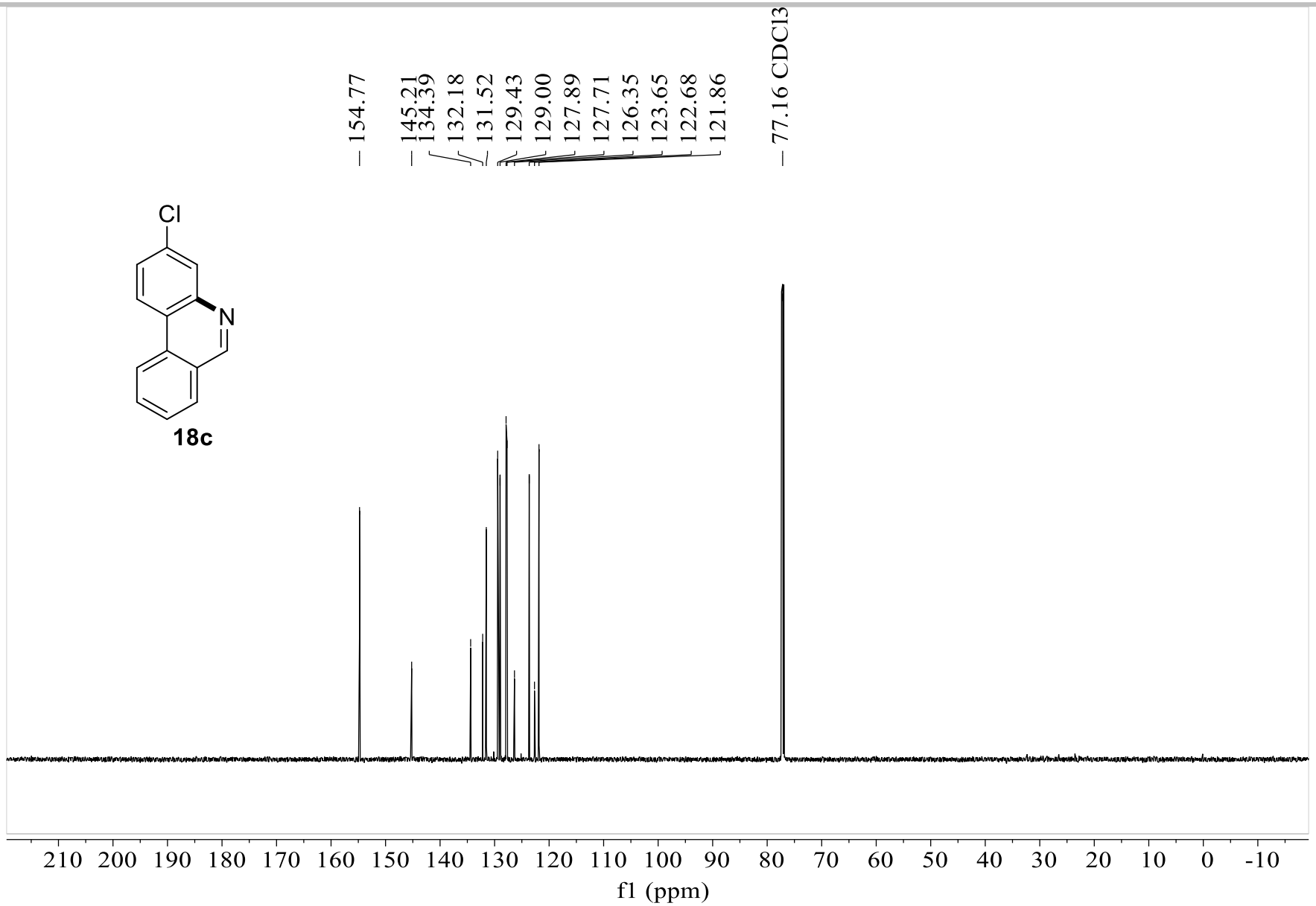
1.02
0.99
1.02
1.02
1.01
1.00
f1 (ppm)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126.35
123.65
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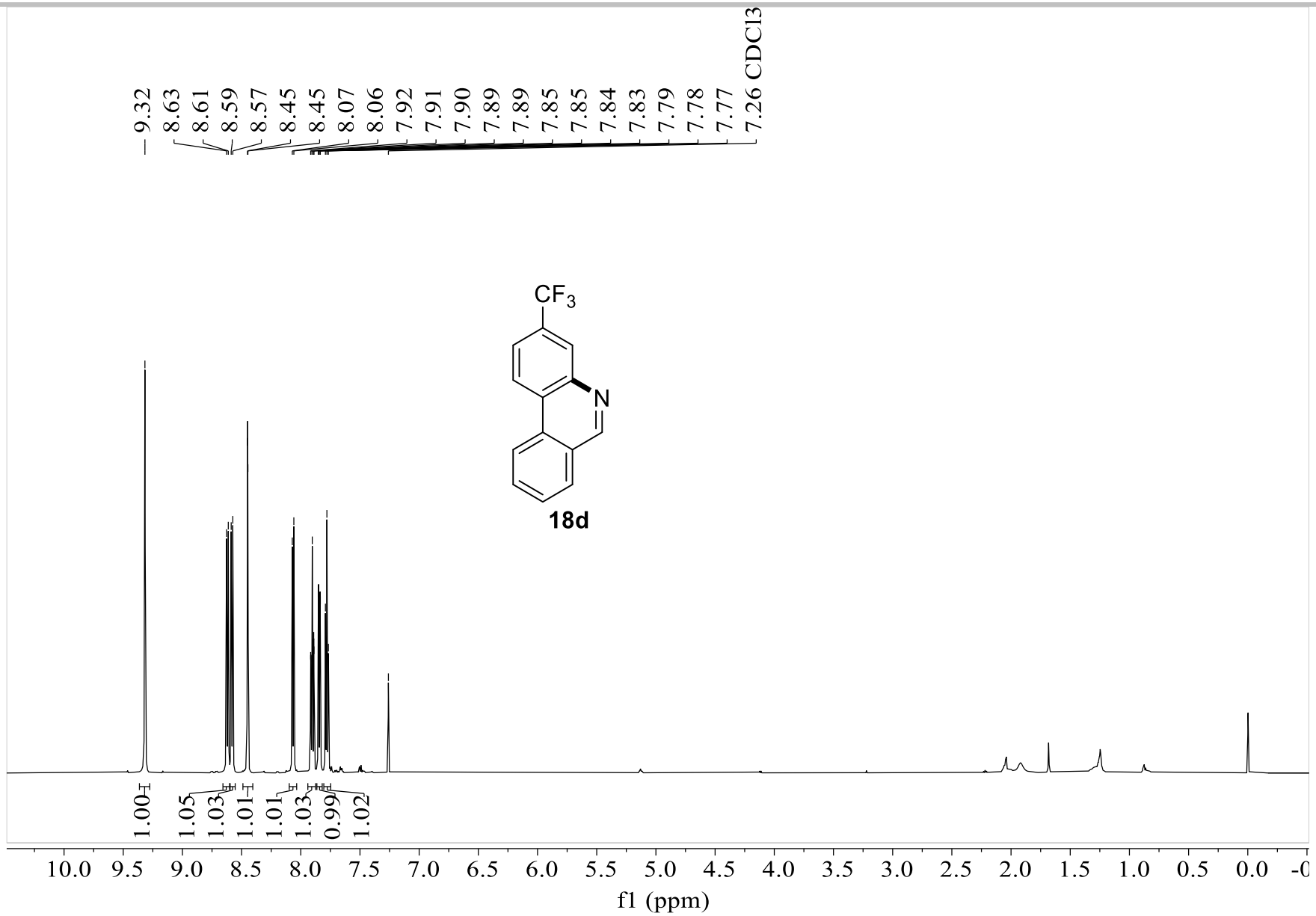
Cl
N
18c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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8.07
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7.91
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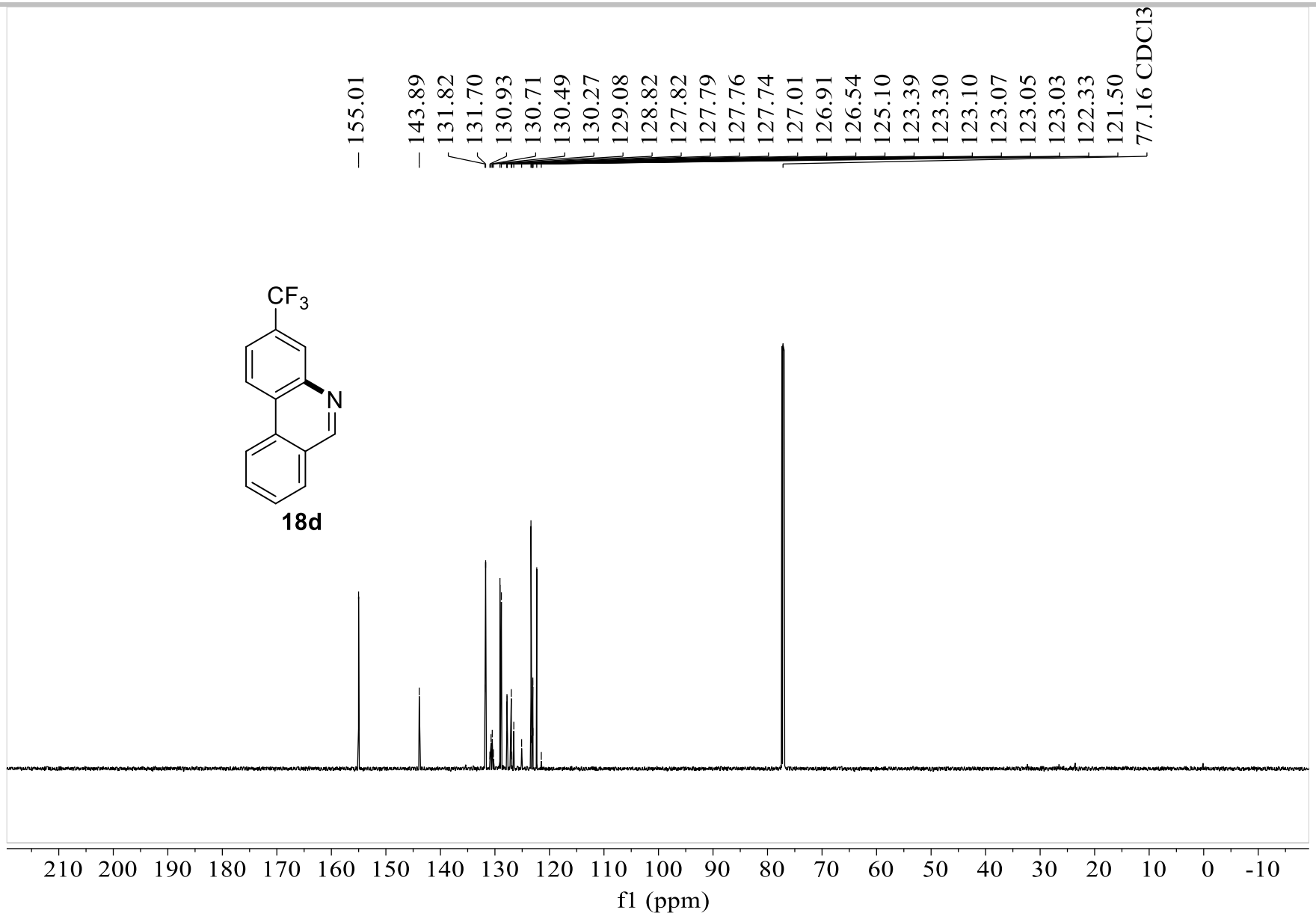
7.89
7.89
7.85
7.85
7.84
7.83
7.79
7.78
7.77
7.26 CDCl3
CF3
N
18d
1.00
1.05
1.03
1.01
1.01
1.03
0.99
1.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)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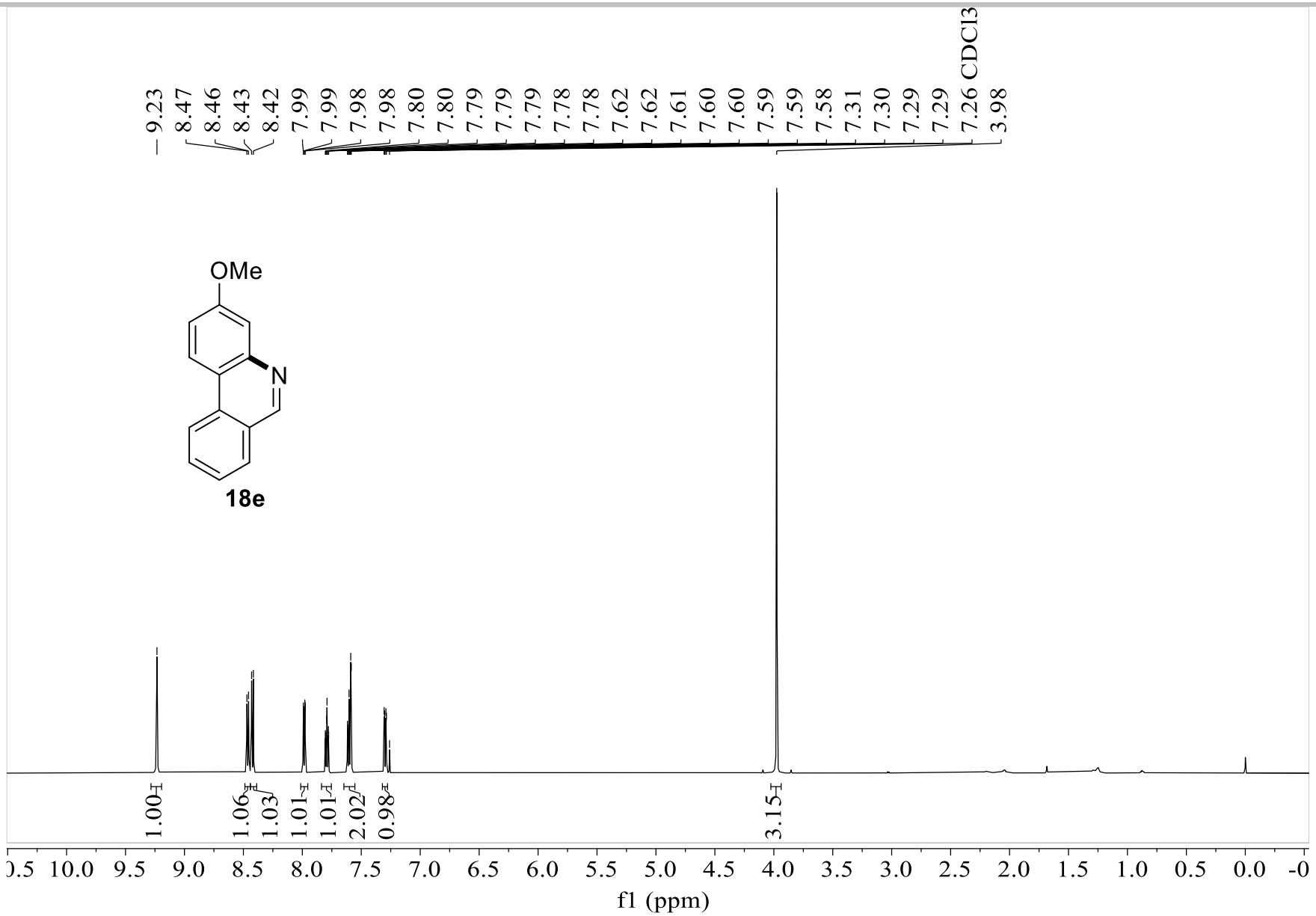
127.74
127.01
126.91
126.54
125.10
123.39
123.30
123.10
123.07
123.05
123.03
122.33
121.50
77.16 CDCl3
CF3
N
18d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.78
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7.61
7.60
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7.59
7.59
7.58
7.31
7.30
7.29
7.29
7.26 CDCl3
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OMe
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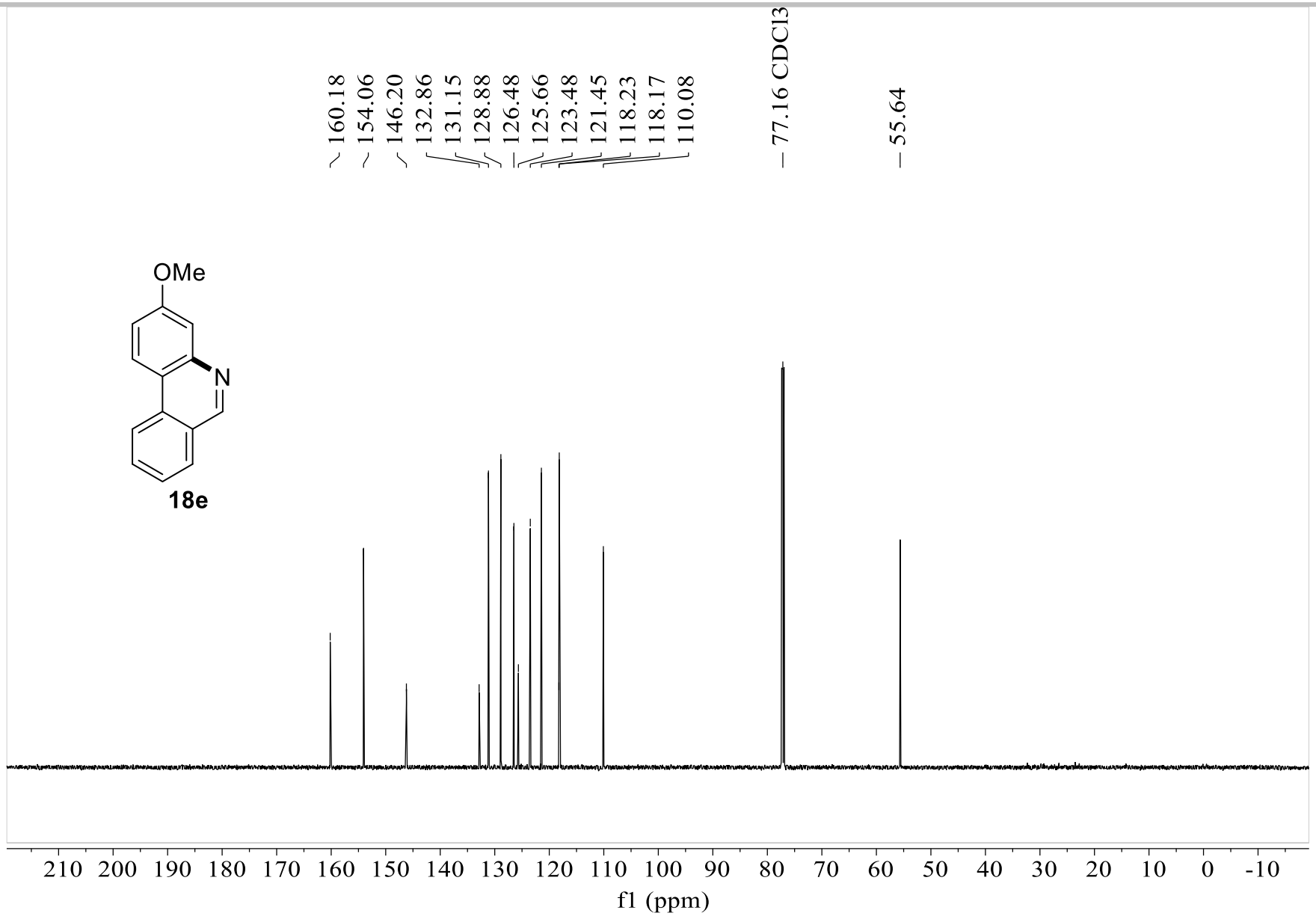
18e
1.00
1.06
1.03
1.01
1.01
2.02
0.98
3.15
f1 (ppm)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126.48
125.66
123.48
121.45
118.23
118.17
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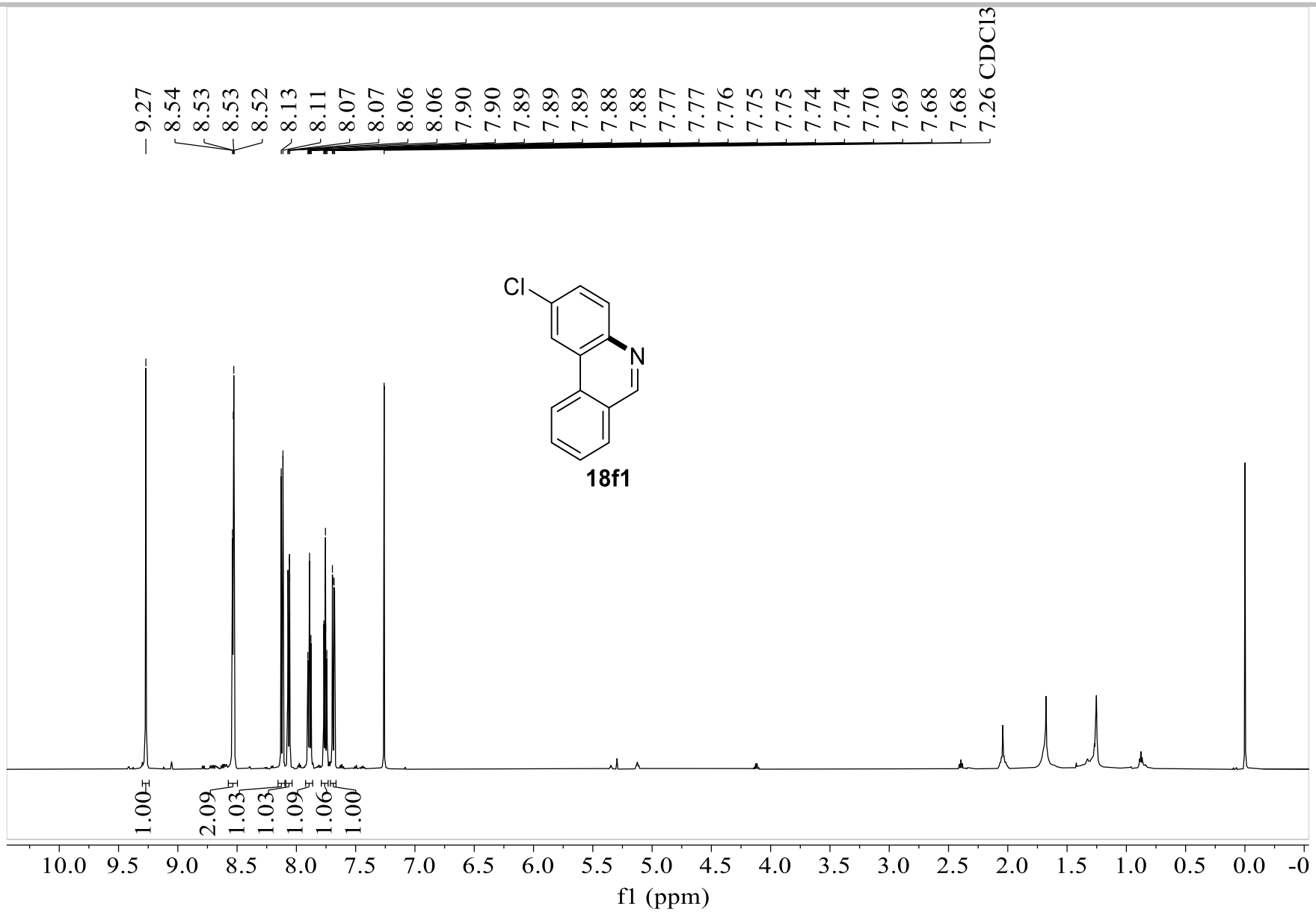
77.16 CDCl3
55.64
OMe
N
18e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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8.13
8.11
8.07
8.07
8.06
8.06
7.90
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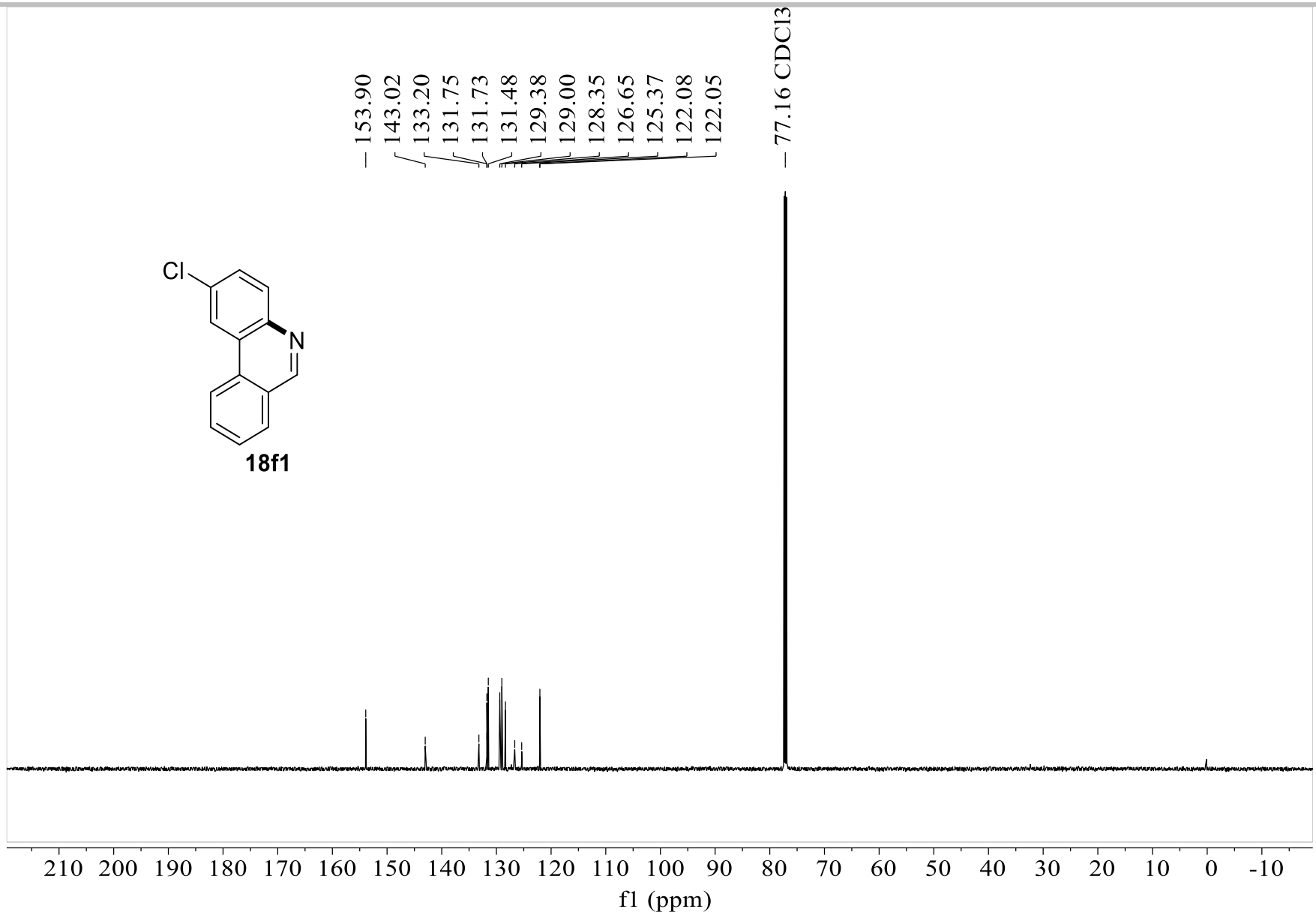
7.89
7.89
7.89
7.88
7.88
7.77
7.77
7.76
7.75
7.75
7.74
7.74
7.70
7.69
7.68
7.68
7.26 CDCl3
Cl
N
18f1
1.00
2.09
1.03
1.03
1.09
1.06
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)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143.02
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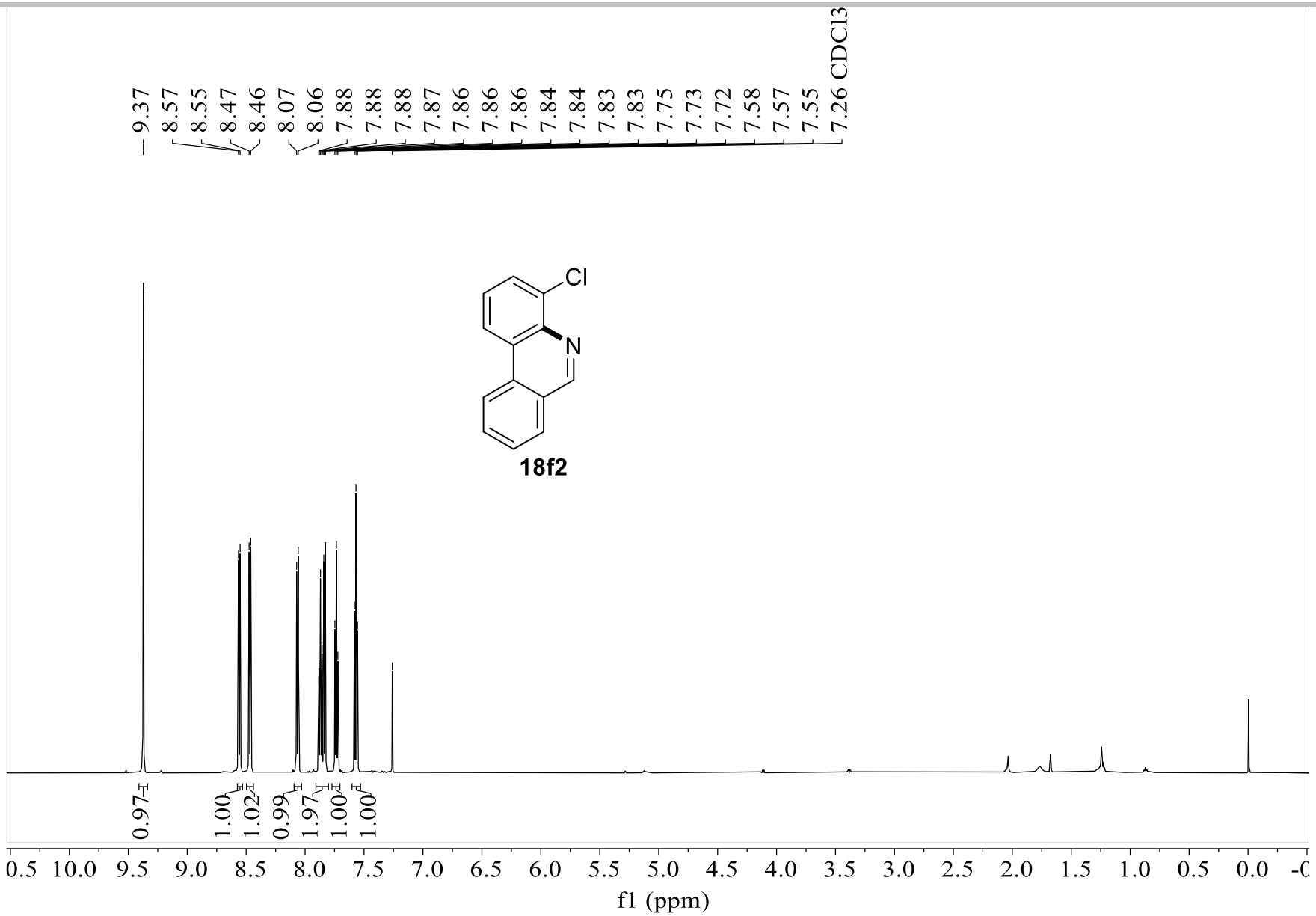
131.48
129.38
129.00
128.35
126.65
125.37
122.08
122.05
77.16 CDCl3
Cl
N
18f1
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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8.07
8.06
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7.88
7.88
7.87
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7.86
7.84
7.84
7.83
7.83
7.75
7.73
7.72
7.58
7.57
7.55
7.26 CDCl3
Cl
N
18f2
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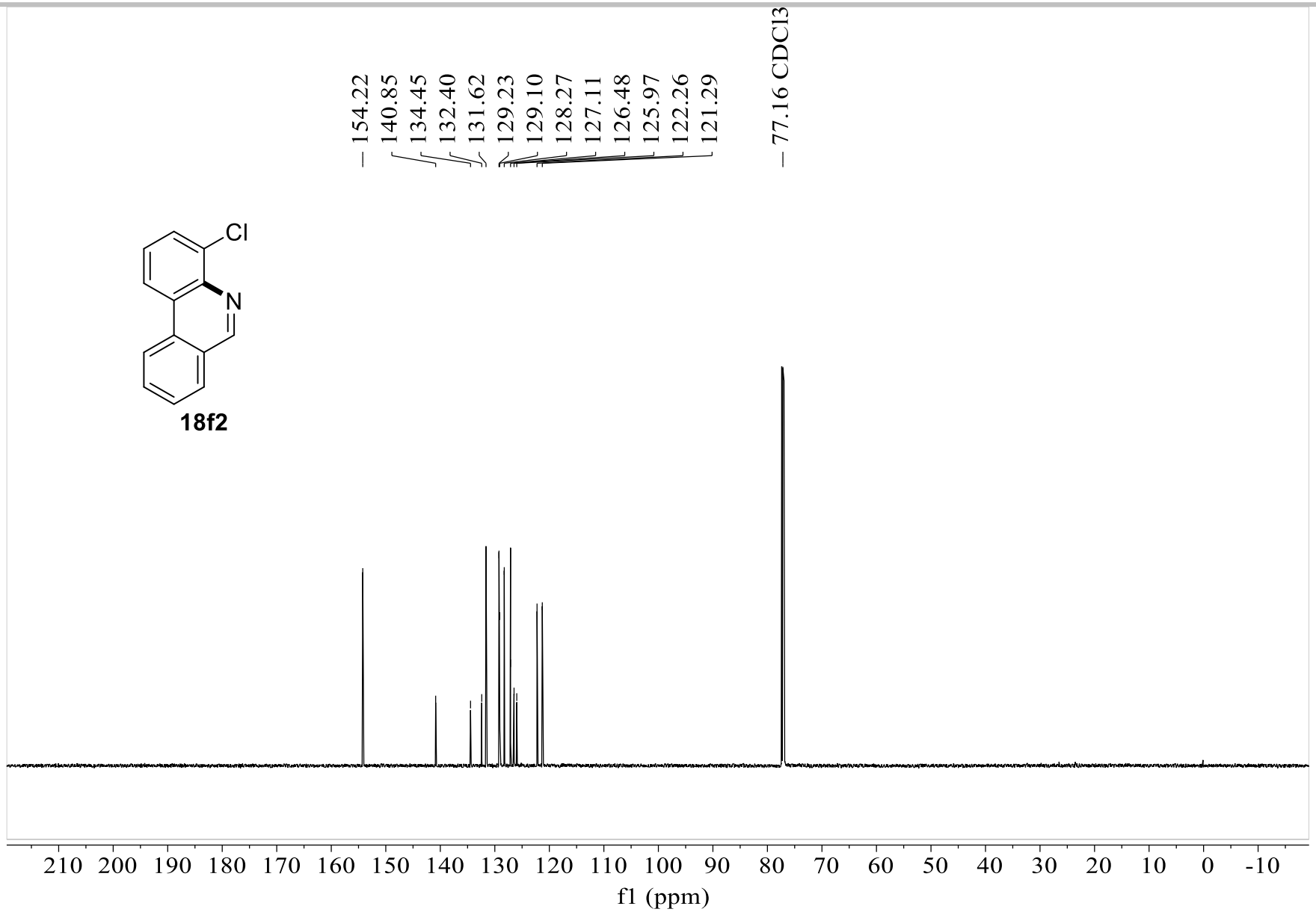
1.00
1.02
0.99
1.97
1.00
1.00
f1 (ppm)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140.85
134.45
132.40
131.62
129.23
129.10
128.27
127.11
126.48
125.97
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121.29
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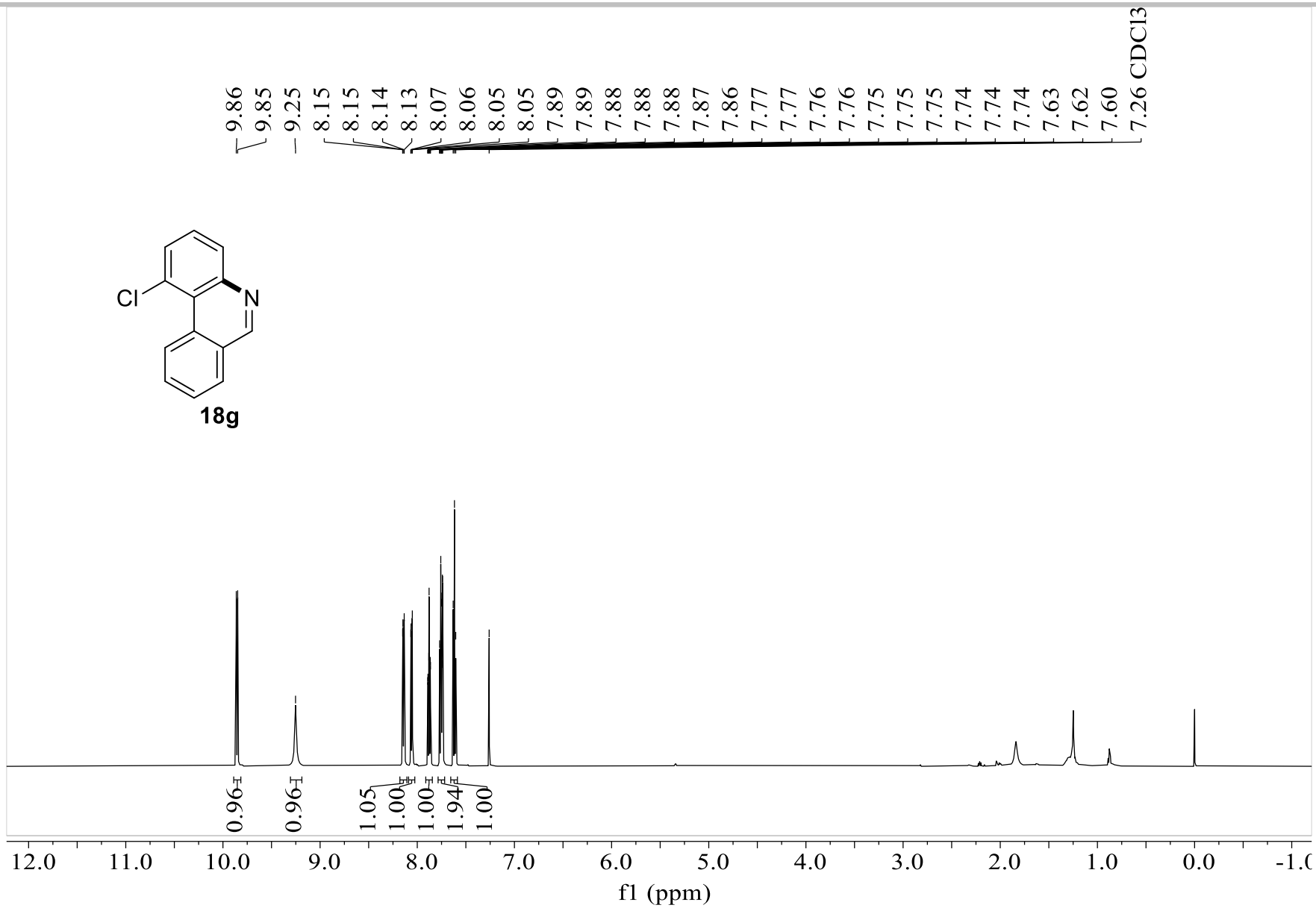
Cl
N
18f2
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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9.85
9.25
8.15
8.15
8.14
8.13
8.07
8.06
8.05
8.05
7.89
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7.88
7.88
7.88
7.87
7.86
7.77
7.77
7.76
7.76
7.75
7.75
7.75
7.74
7.74
7.74
7.63
7.62
7.60
7.26 CDCl3
Cl
N
18g
0.96
0.96
1.05
1.00
1.00
1.94
1.00
12.0
11.0
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7.0
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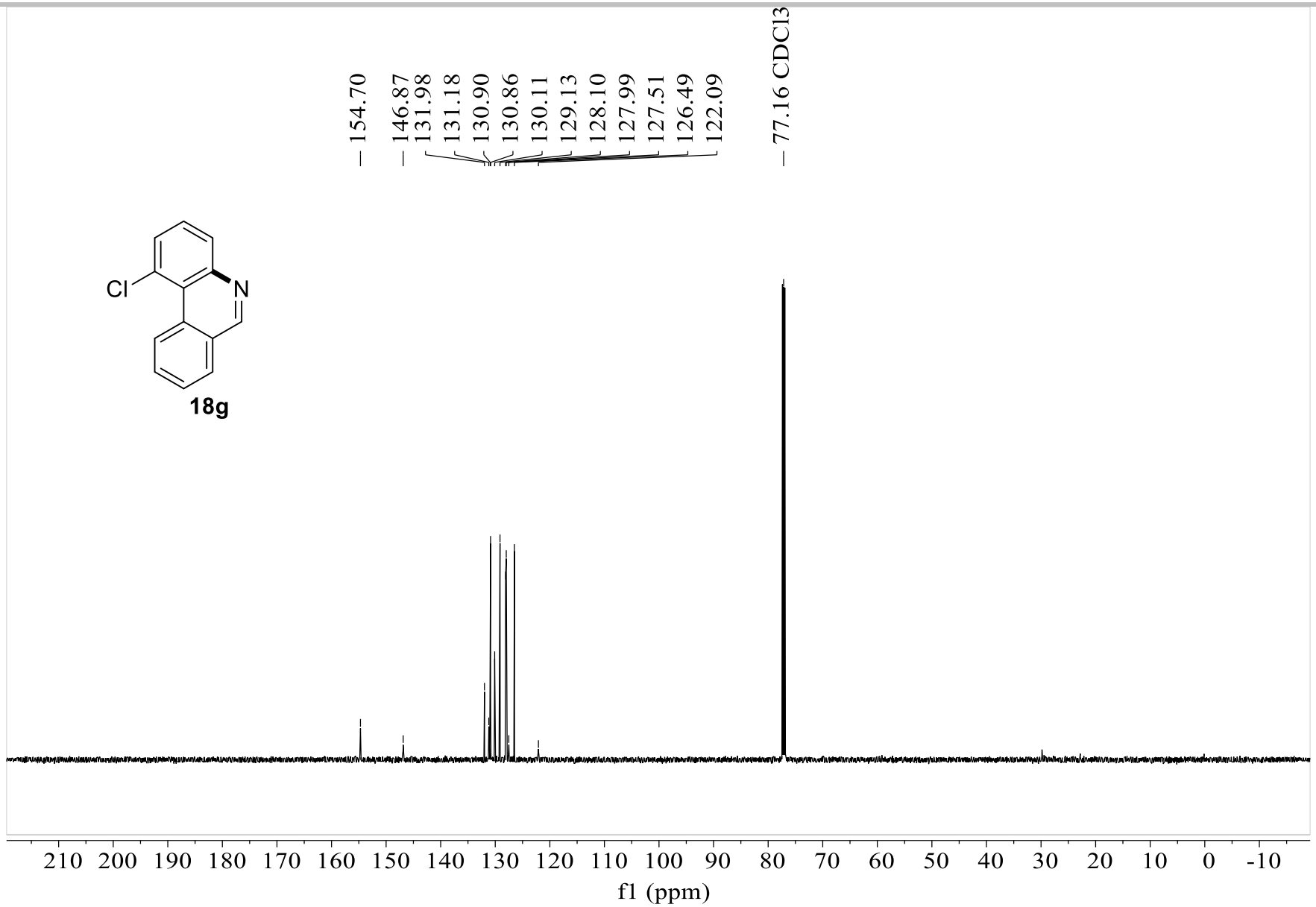
3.0
2.0
1.0
0.0
f1 (ppm)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130.11
129.13
128.10
127.99
127.51
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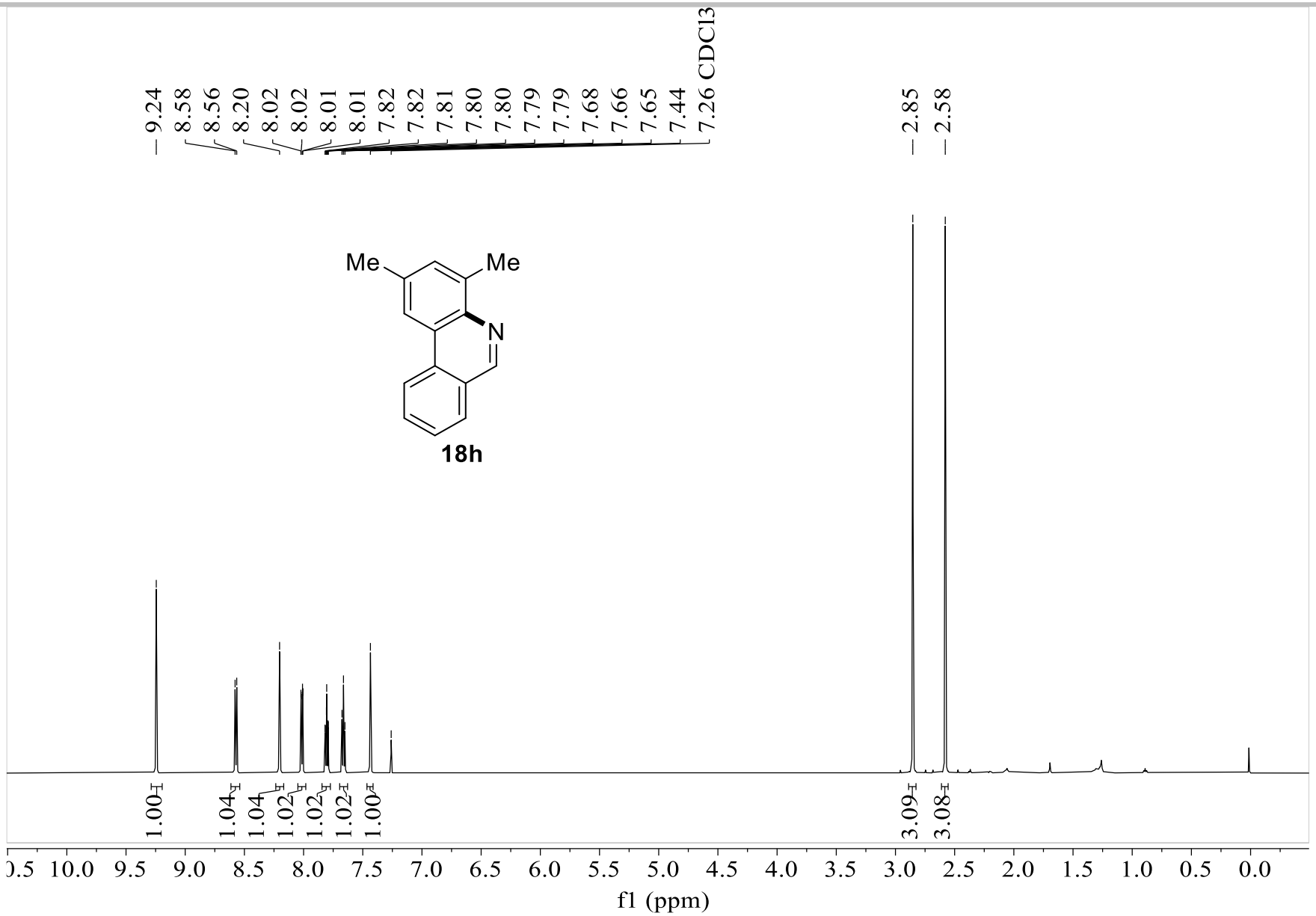
122.09
77.16 CDCl3
Cl
N
18g
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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8.02
8.01
8.01
7.82
7.82
7.81
7.80
7.80
7.79
7.79
7.68
7.66
7.65
7.44
7.26 CDCl3
2.85
2.58
Me
Me
N
18h
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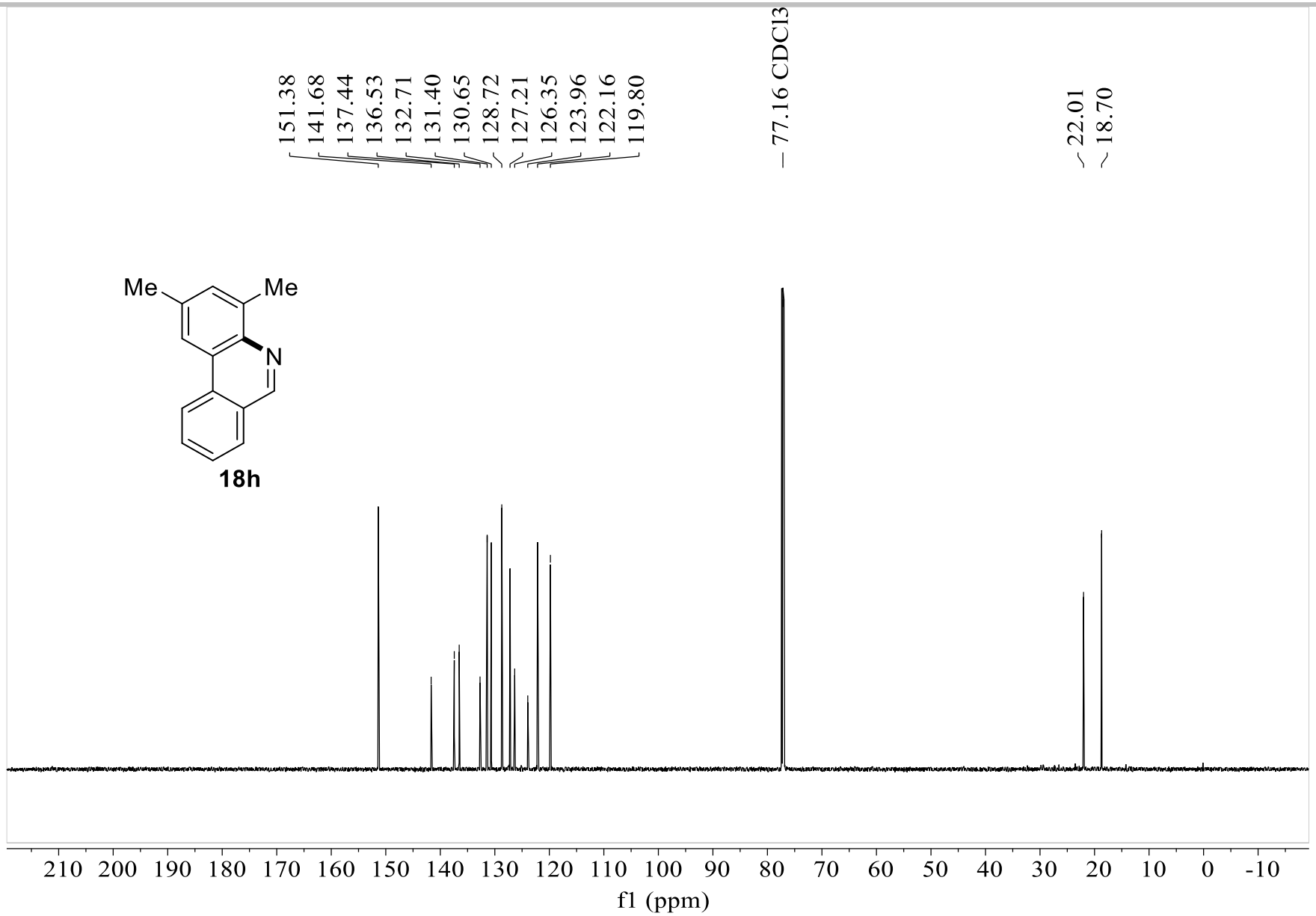
1.04
1.04
1.02
1.02
1.02
1.00
3.09
3.08
f1 (ppm)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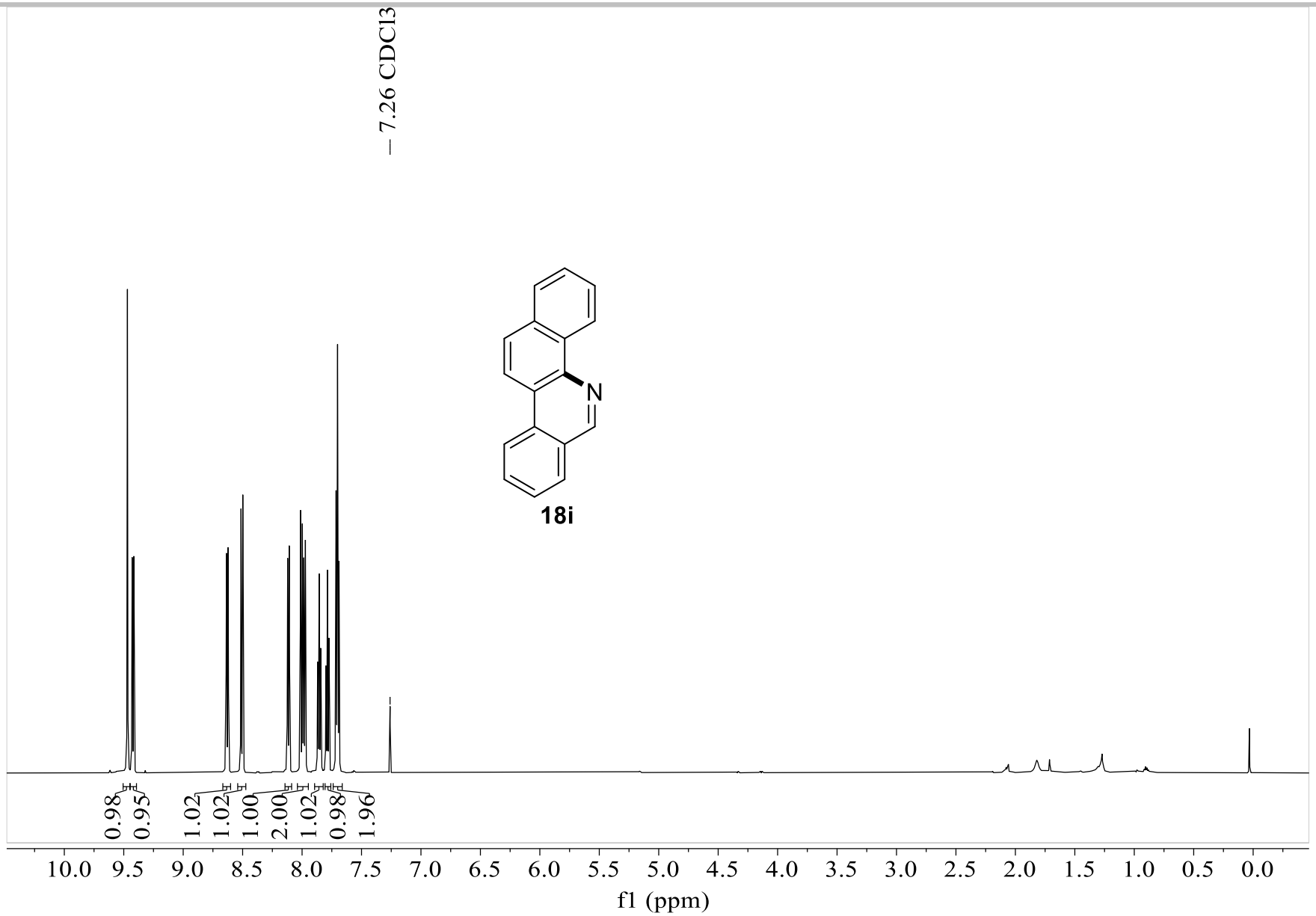
127.21
126.35
123.96
122.16
119.80
77.16 CDCl3
22.01
18.70
Me
Me
N
18h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.26 CDCl3
N
18i
0.98
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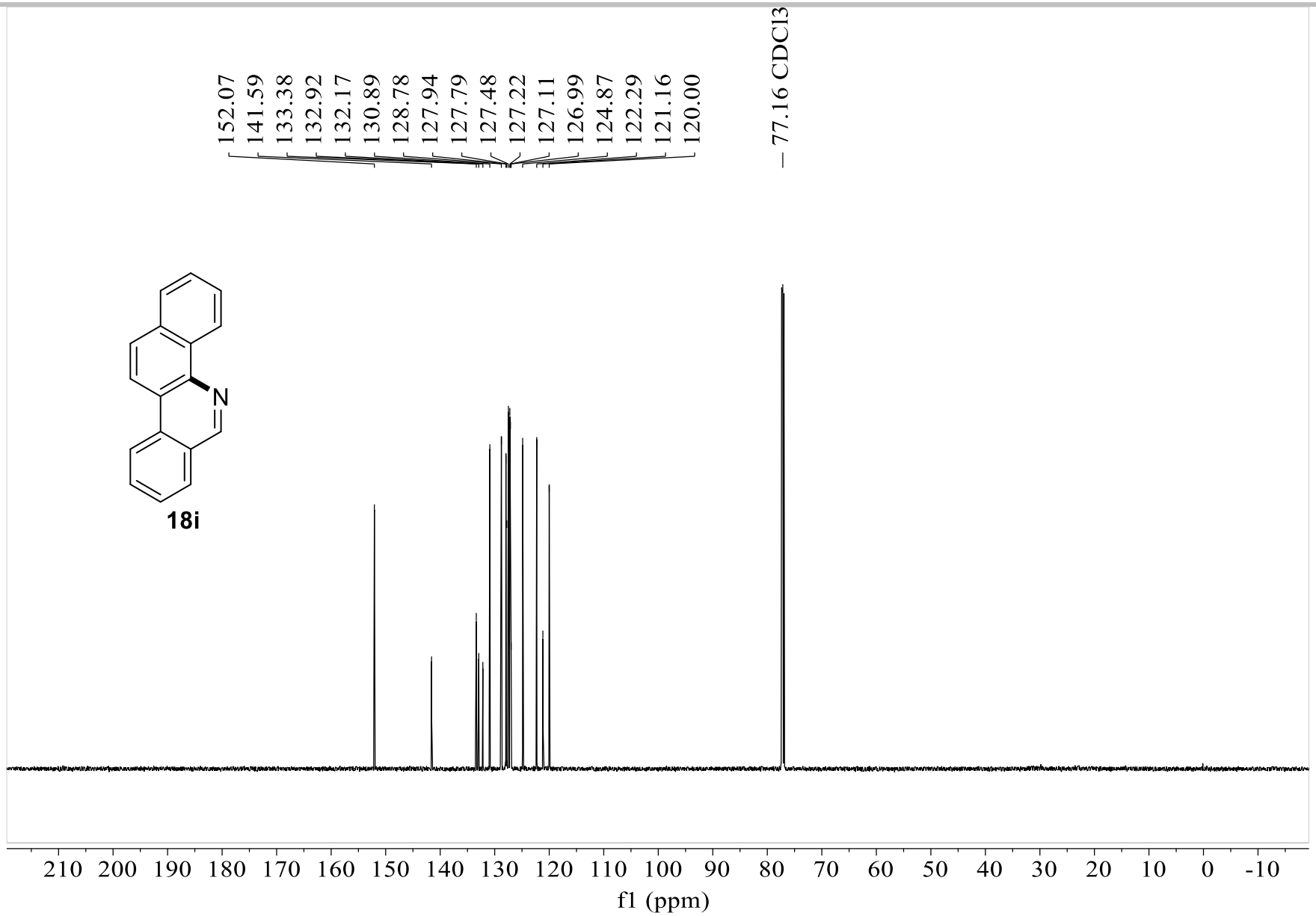
1.02
1.02
1.00
2.00
1.02
0.98
1.96
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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128.78
127.94
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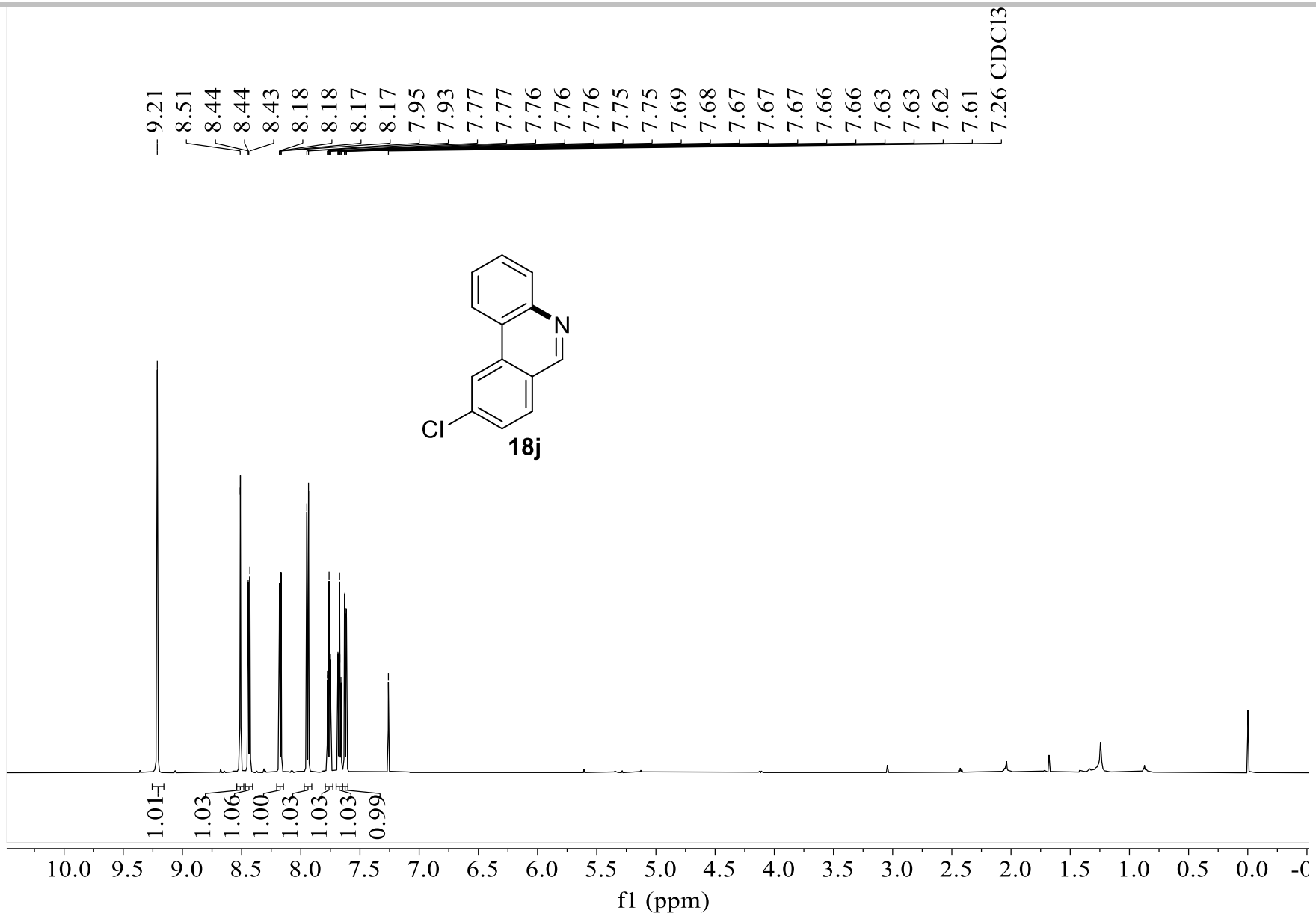
127.48
127.22
127.11
126.99
124.87
122.29
121.16
120.00
77.16 CDCl3
N
18i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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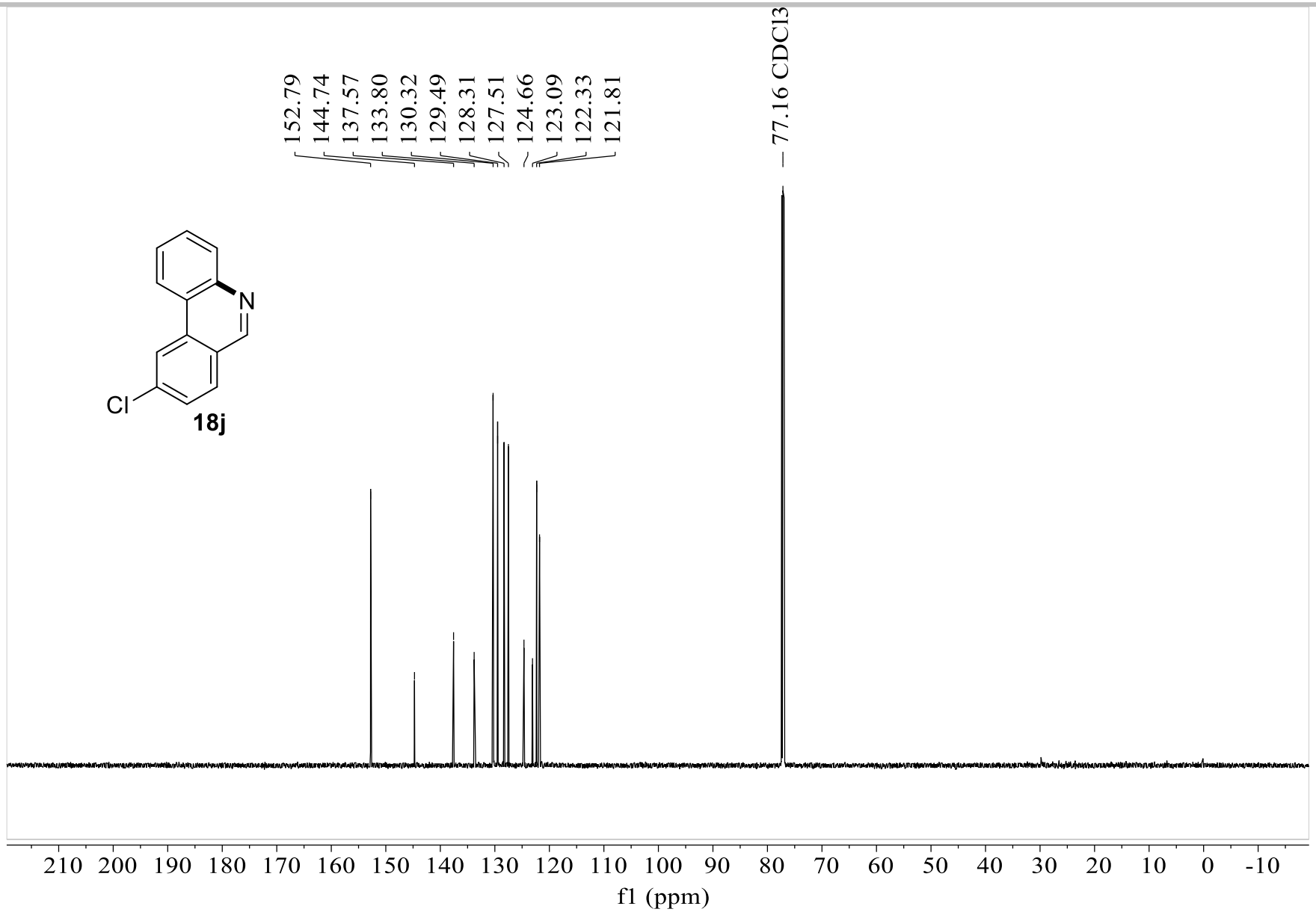
7.76
7.76
7.75
7.75
7.69
7.68
7.67
7.67
7.67
7.66
7.66
7.63
7.63
7.62
7.61
7.26 CDCl3
N
Cl
18j
1.01
1.03
1.06
1.00
1.03
1.03
1.03
0.99
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)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129.49
128.31
127.51
124.66
123.09
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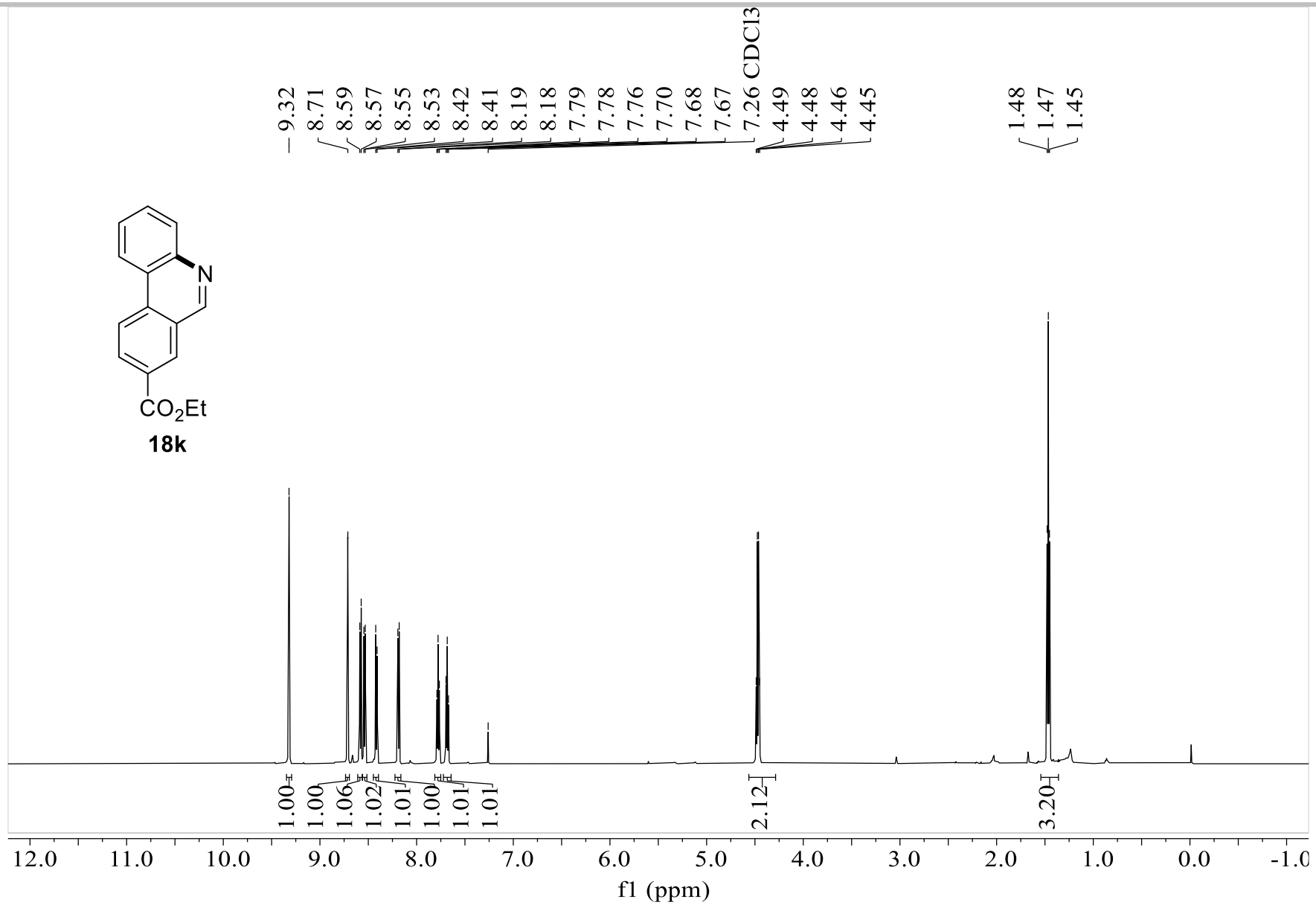
121.81
77.16 CDCl3
N
Cl
18j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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8.41
8.19
8.18
7.79
7.78
7.76
7.70
7.68
7.67
7.26 CDCl3
4.49
4.48
4.46
4.45
1.48
1.47
1.45
N
CO2Et
18k
1.00
1.00
1.06
1.02
1.01
1.00
1.01
1.01
2.12
3.20
12.0
11.0
10.0
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1.0
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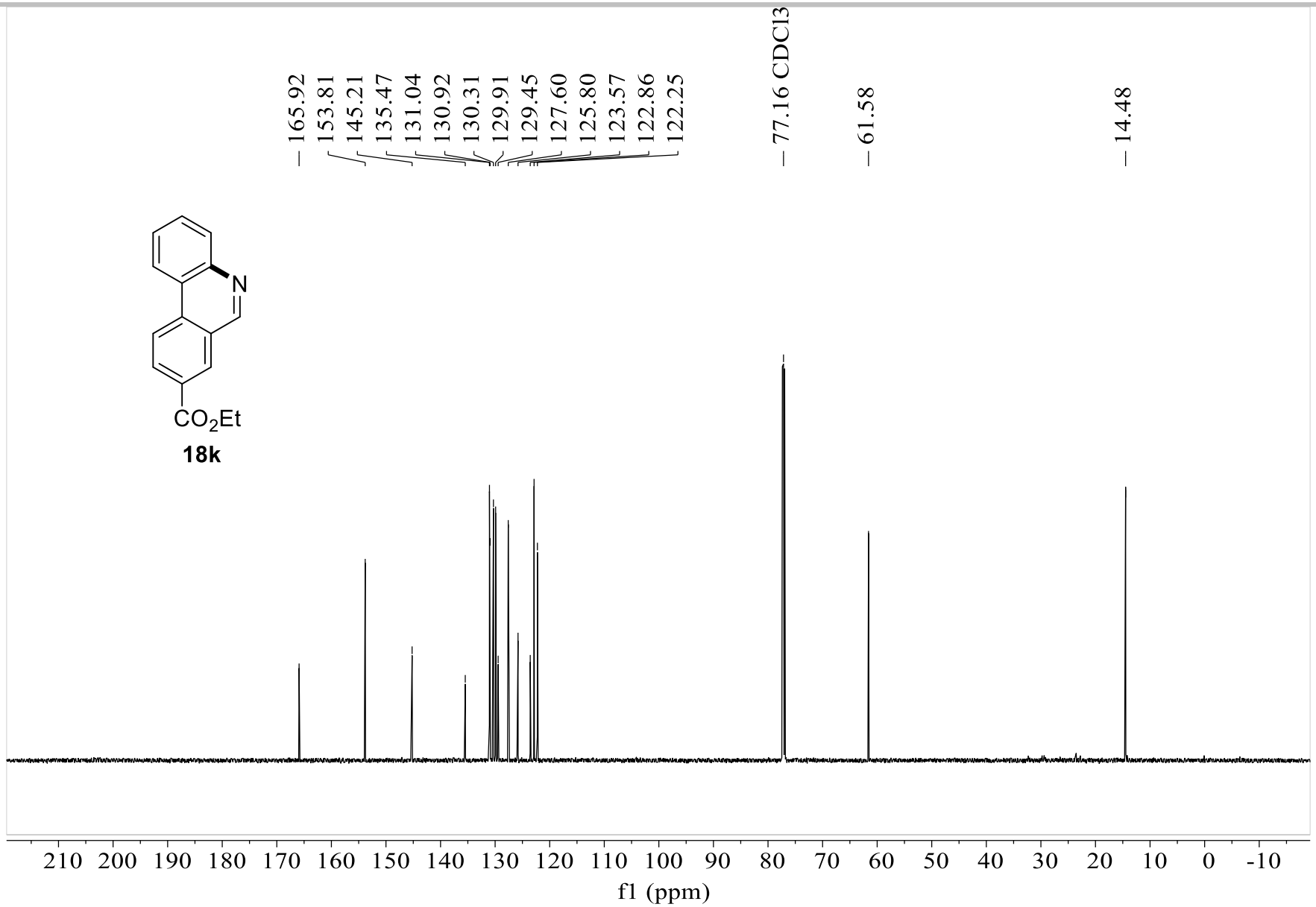
-1.0
f1 (ppm)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127.60
125.80
123.57
122.86
122.25
77.16 CDCl3
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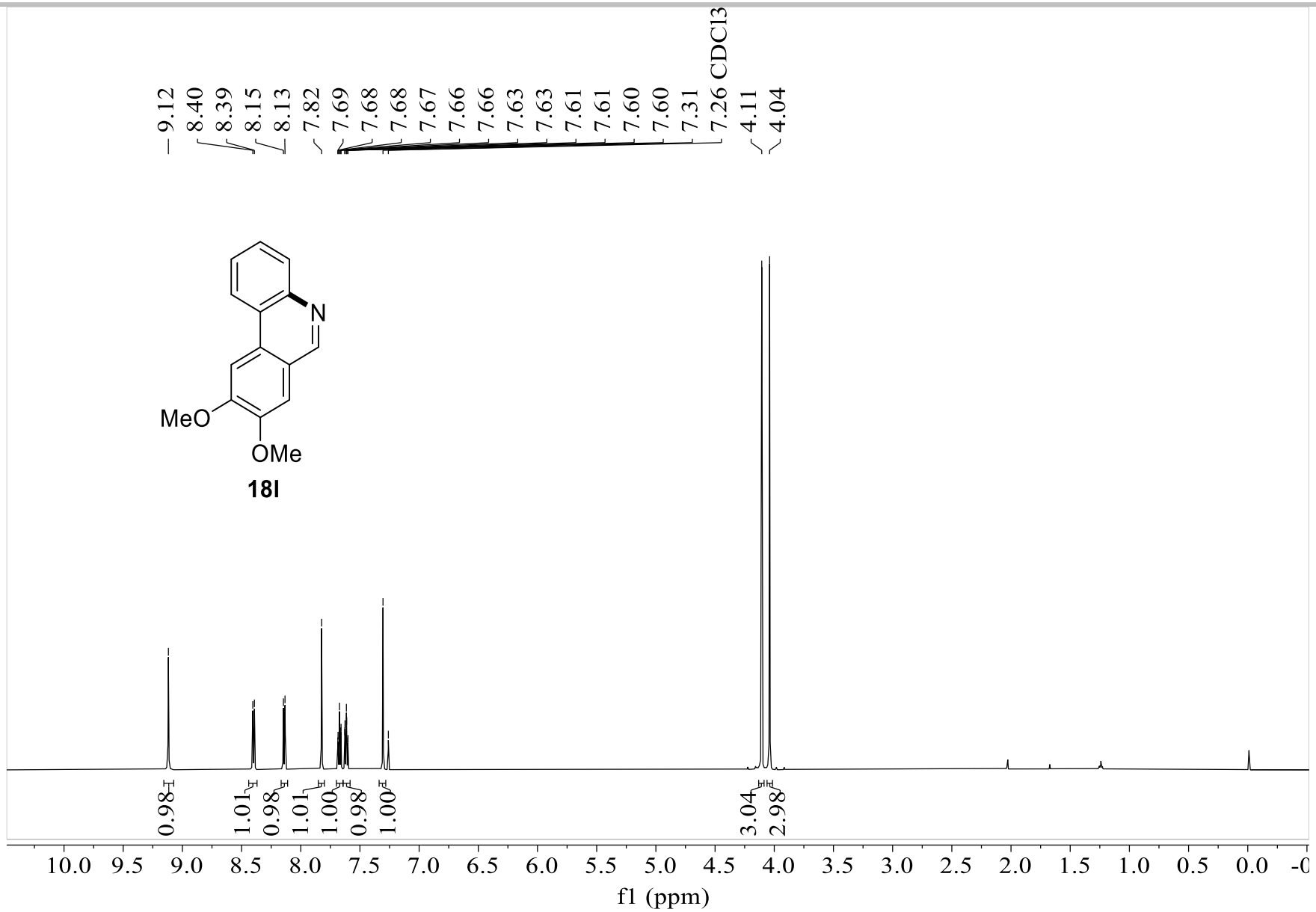
N
CO2Et
18k
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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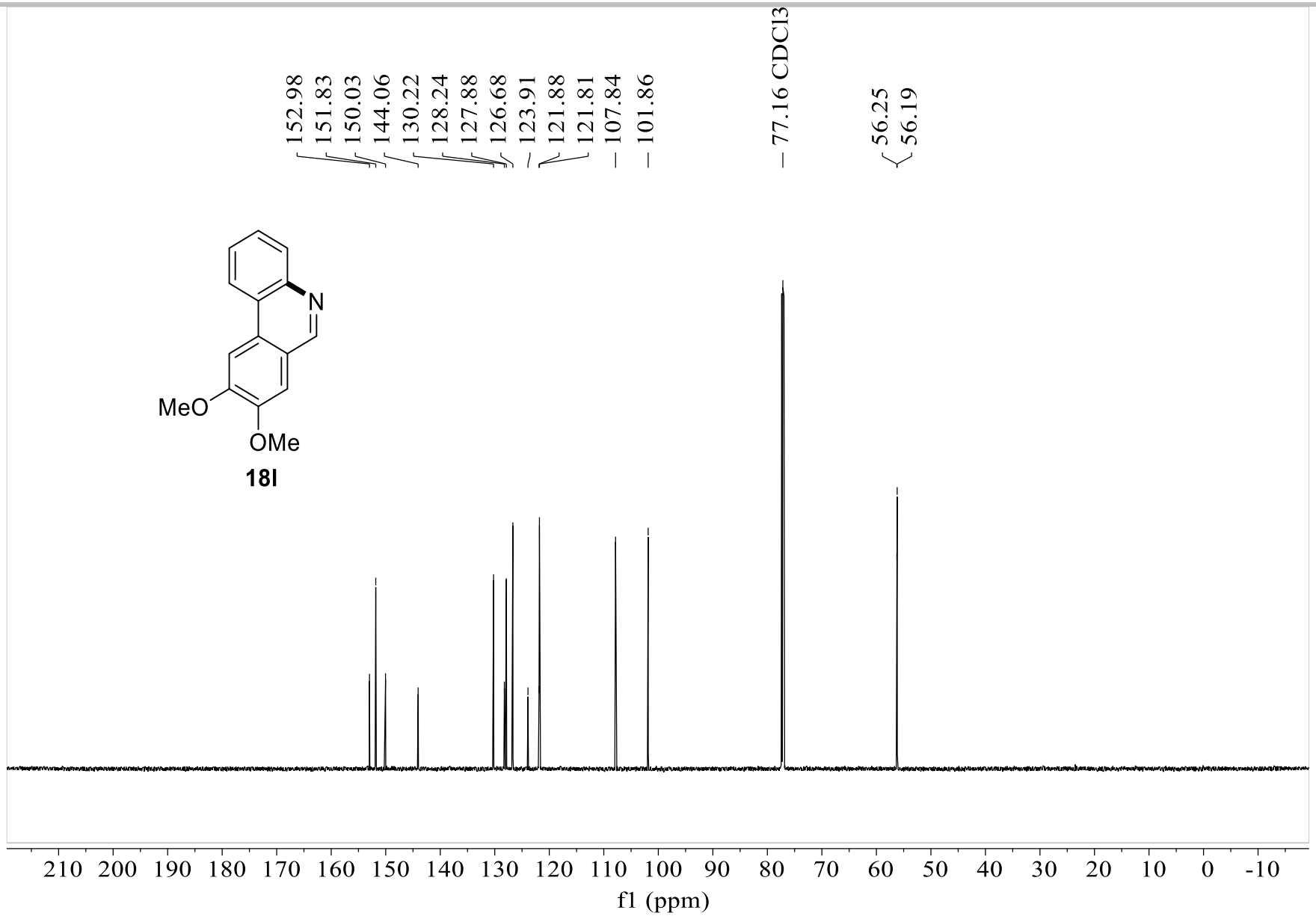
7.66
7.63
7.63
7.61
7.61
7.60
7.60
7.31
7.26 CDCl3
4.11
4.04
N
MeO
OMe
18l
0.98
1.01
0.98
1.01
1.00
0.98
1.00
3.04
2.98
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)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121.81
107.84
101.86
77.16 CDCl3
56.25
56.19
N
MeO
OMe
18l
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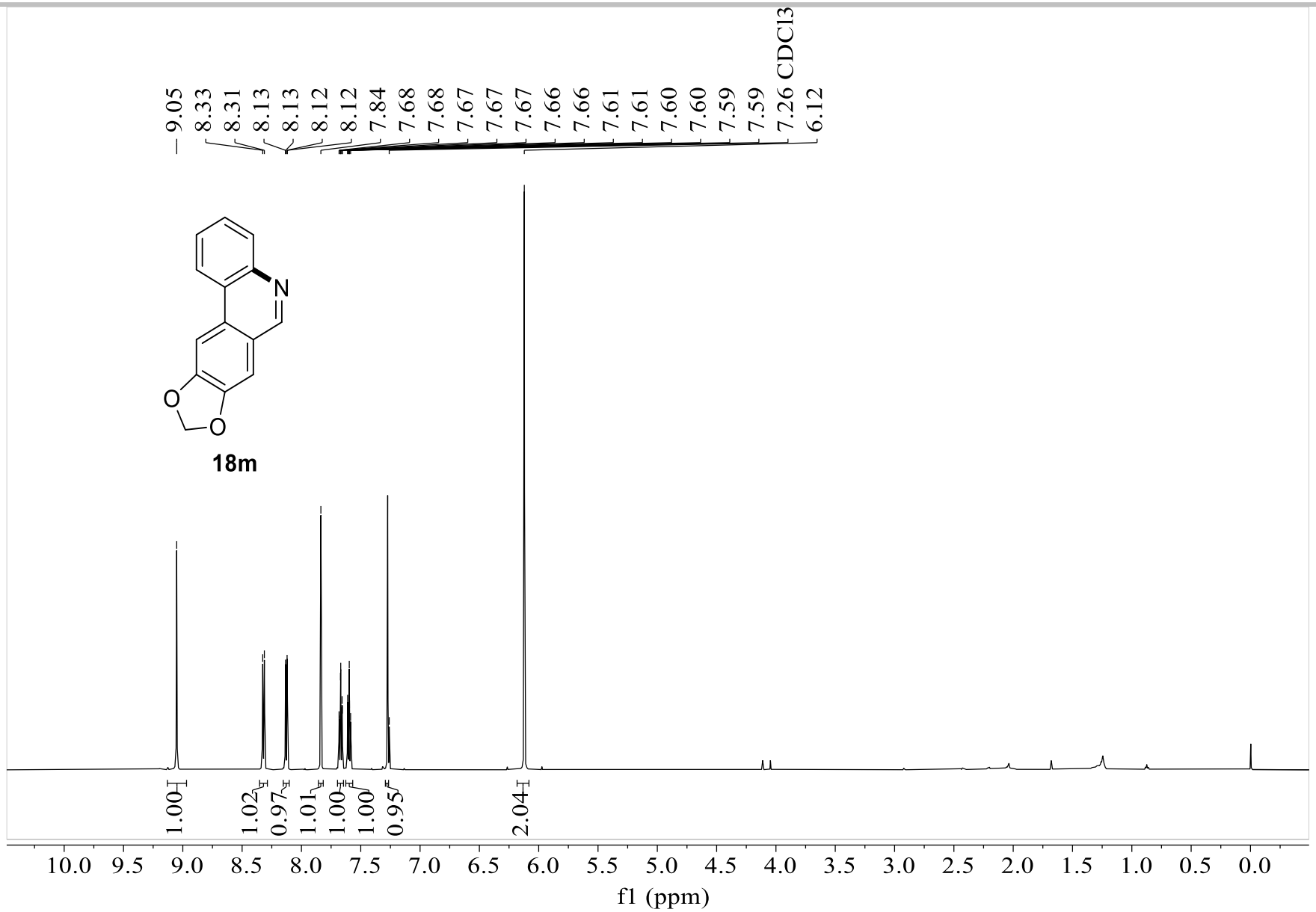
f1 (ppm)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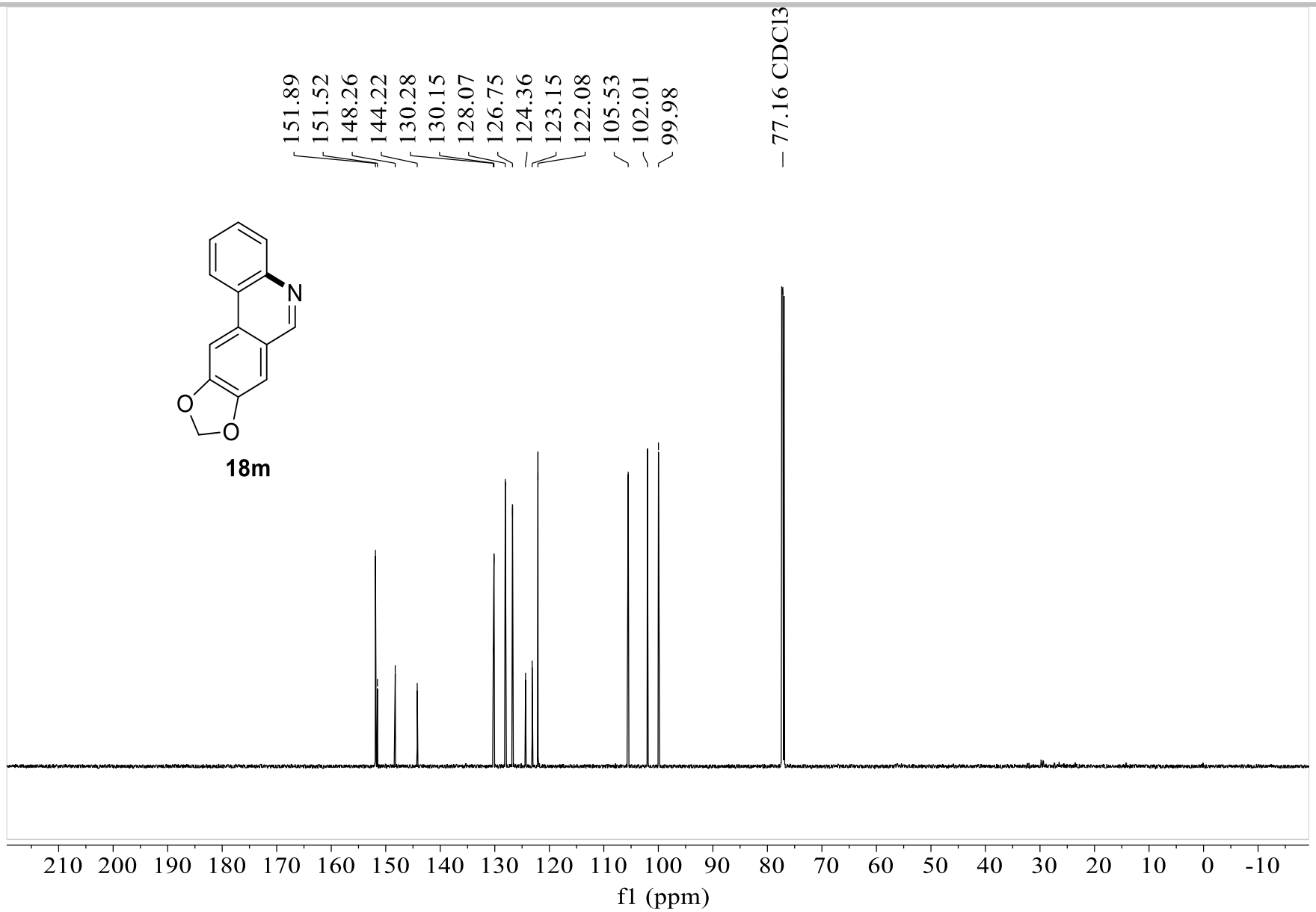
7.66
7.66
7.61
7.61
7.60
7.60
7.59
7.59
7.26 CDCl3
6.12
N
O
O
18m
1.00
1.02
0.97
1.01
1.00
1.00
0.95
2.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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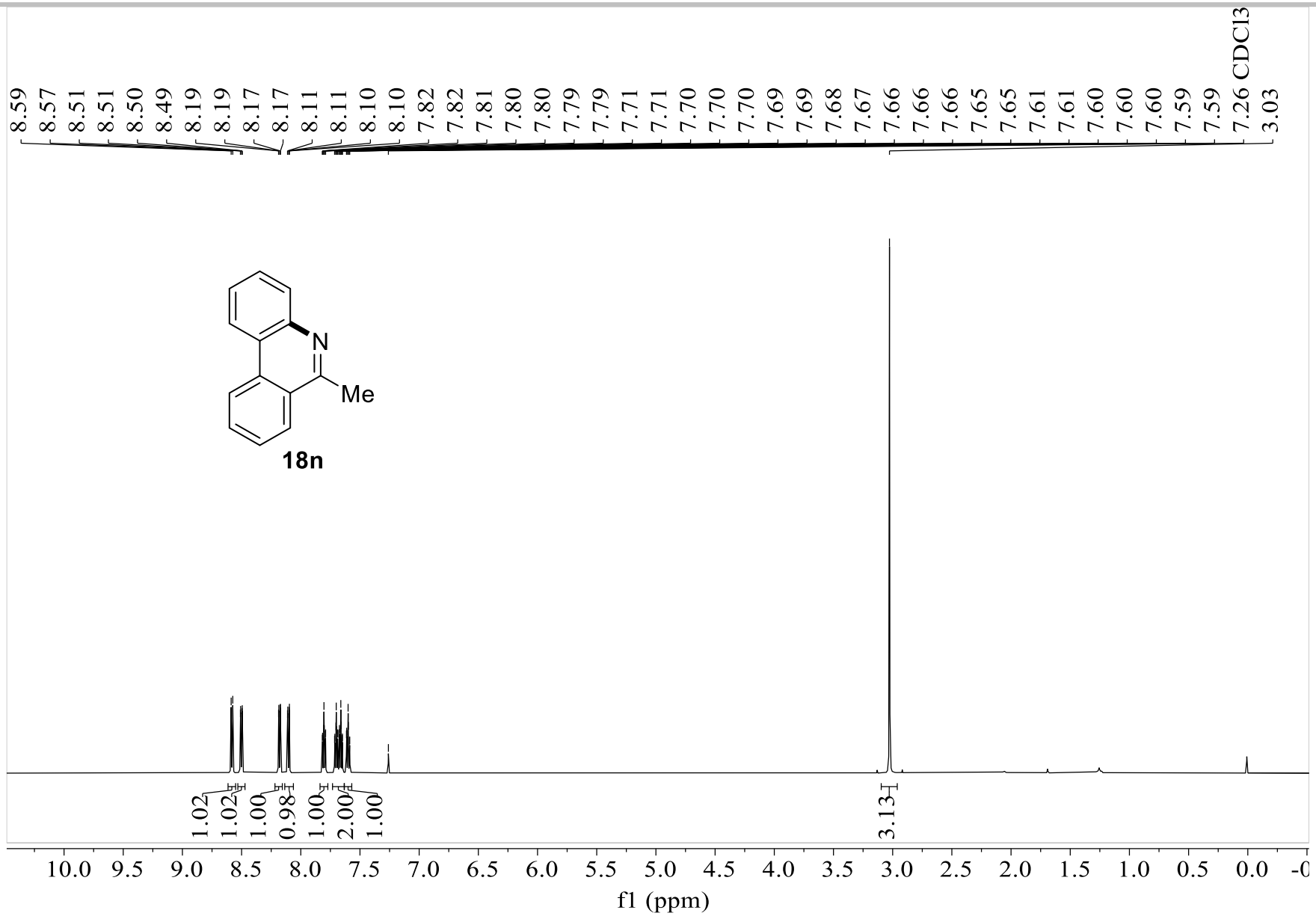
124.36
123.15
122.08
105.53
102.01
99.98
77.16 CDCl3
N
O
O
18m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.60
7.60
7.59
7.59
7.26 CDCl3
3.03
N
Me
18n
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1.02
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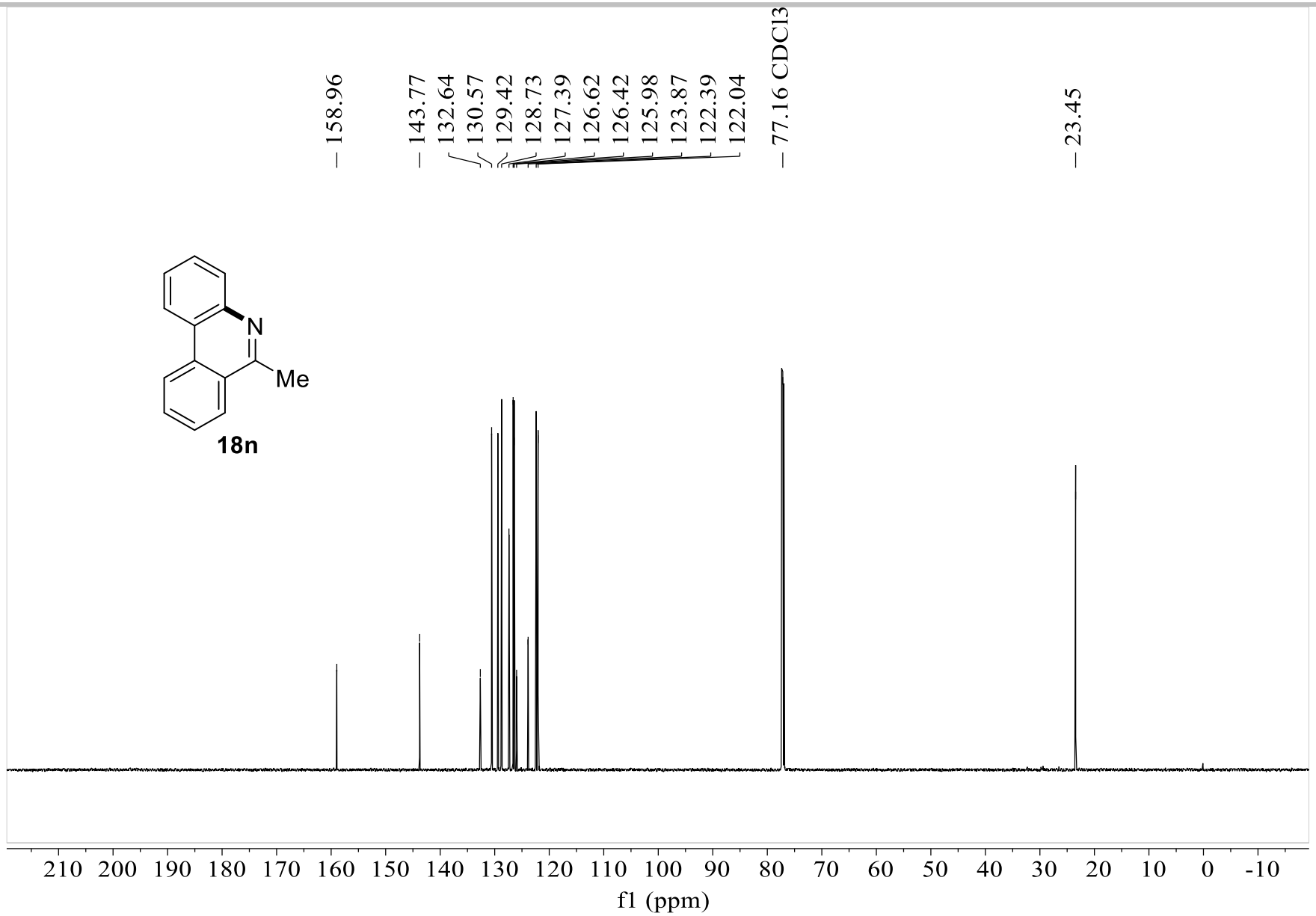
1.00
2.00
1.00
3.13
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)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123.87
122.39
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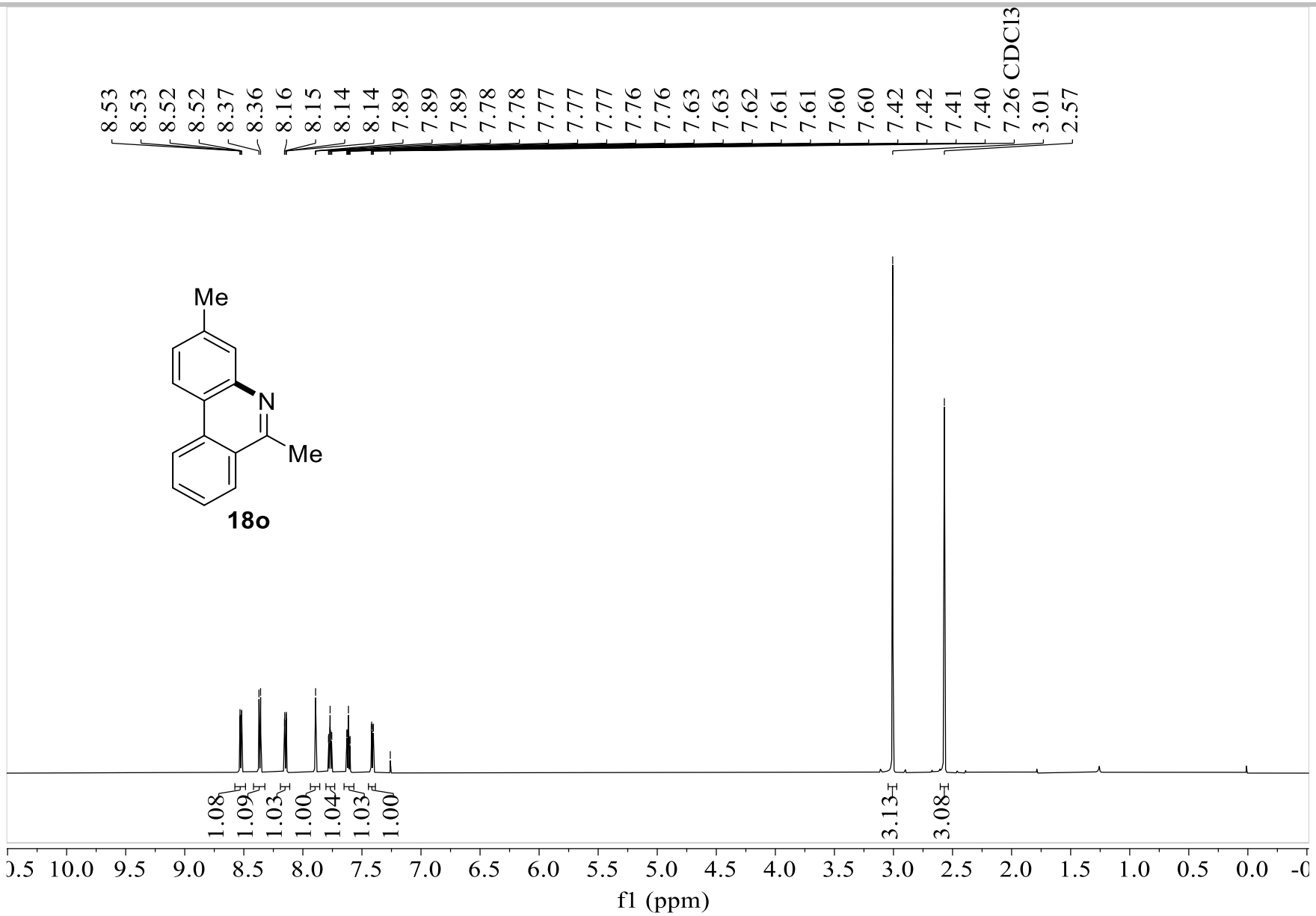
23.45
N
Me
18n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.76
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7.63
7.62
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7.60
7.42
7.42
7.41
7.40
7.26 CDCl3
3.01
2.57
Me
N
Me
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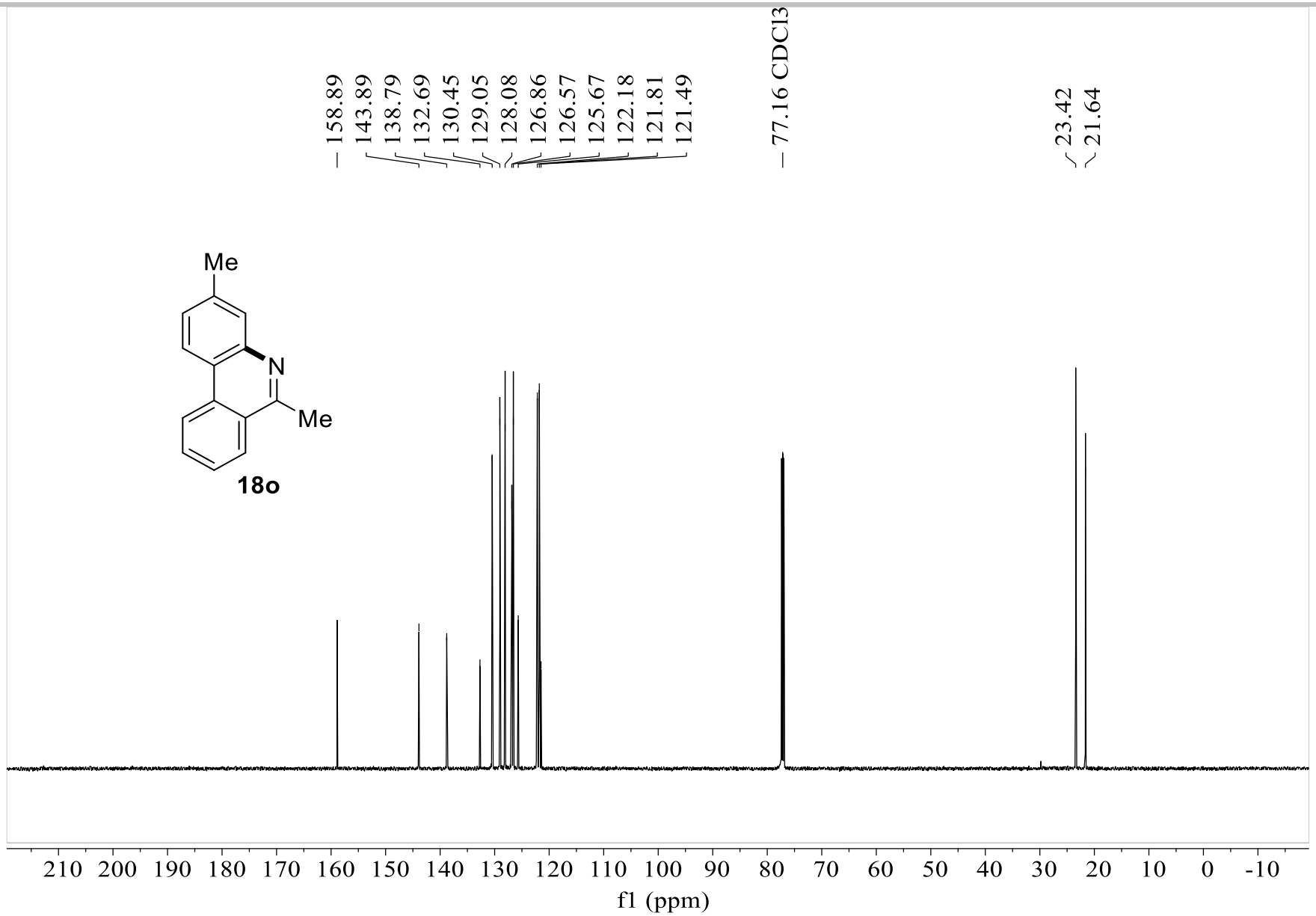
1.09
1.03
1.00
1.04
1.03
1.00
3.13
3.08
f1 (ppm)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121.81
121.49
77.16 CDCl3
23.42
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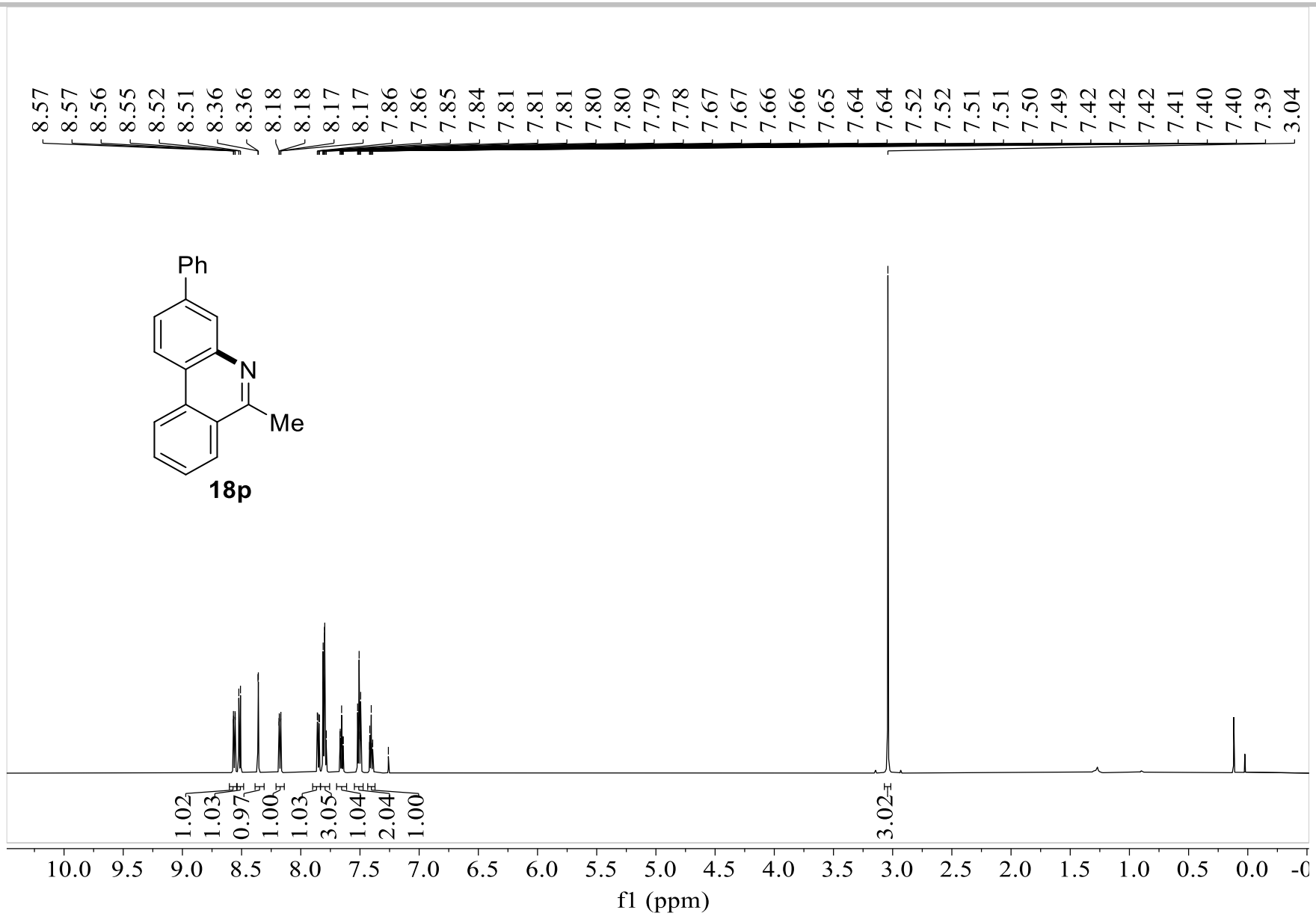
Me
N
Me
18o
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.42
7.41
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7.40
7.39
3.04
Ph
N
Me
18p
1.02
1.03
0.97
1.00
1.03
3.05
1.04
2.04
1.00
3.02
10.0 9.5 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
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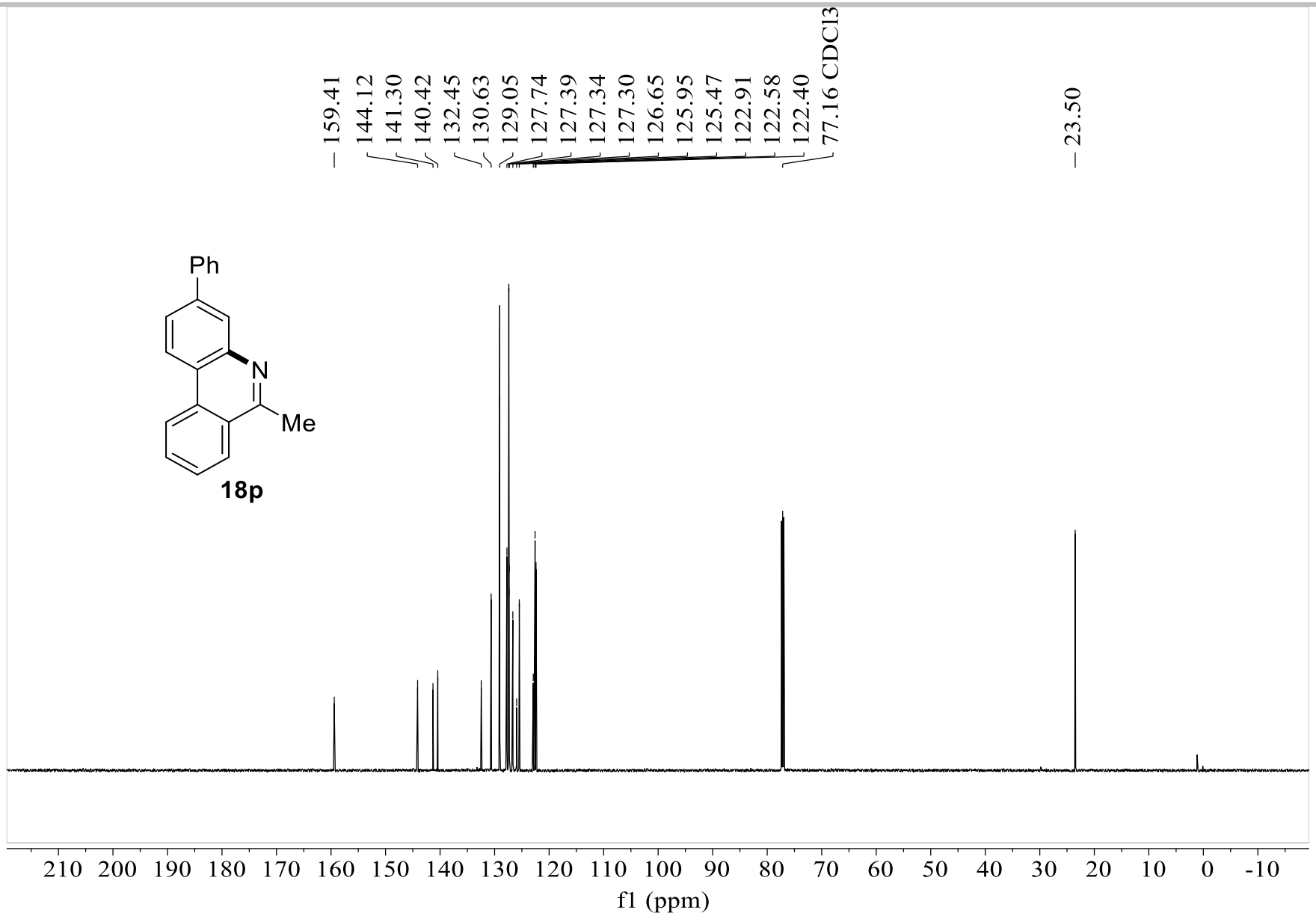
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125.47
122.91
122.58
122.40
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Ph
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Me
18p
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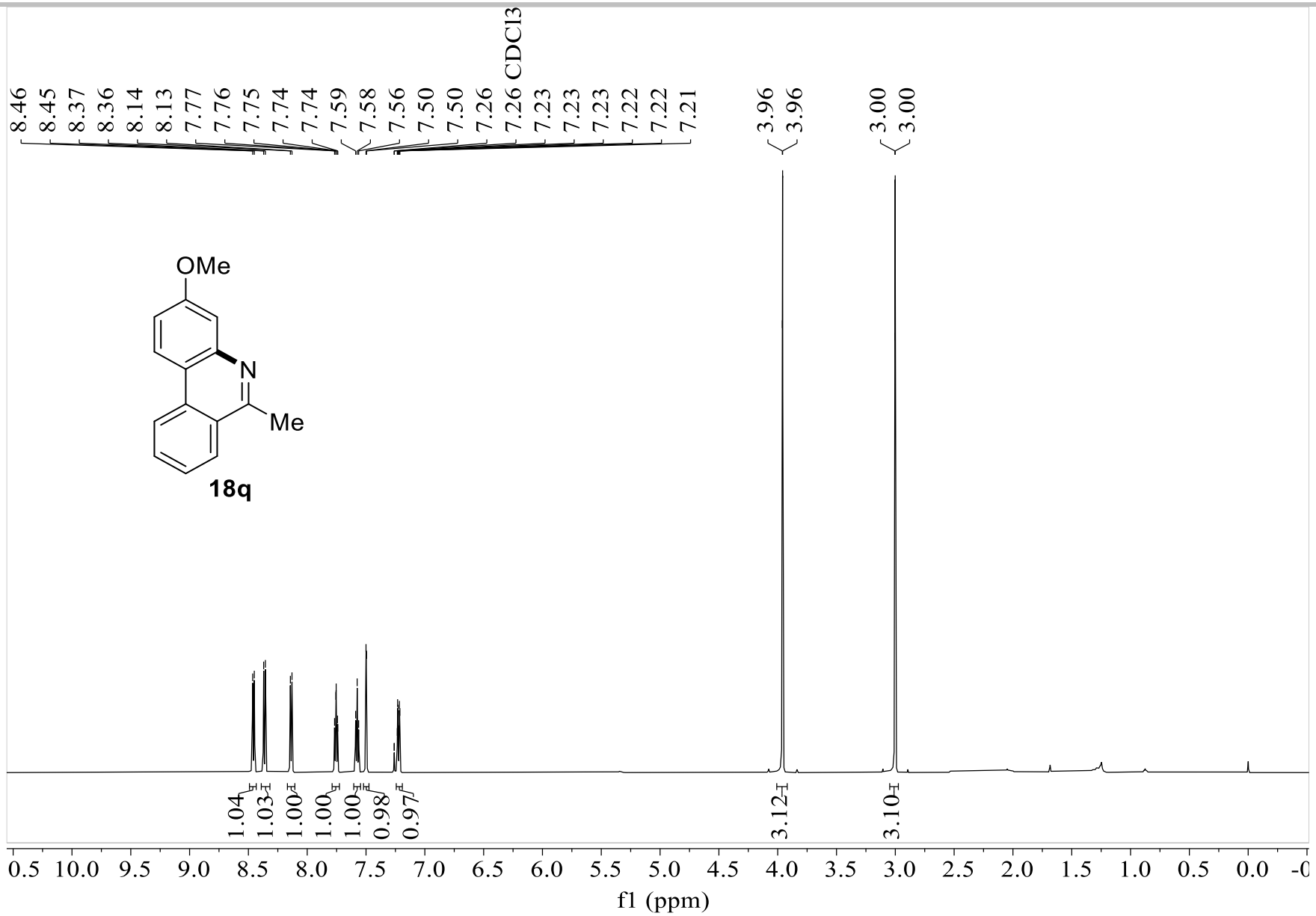
f1 (ppm)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7.58
7.56
7.50
7.50
7.26
7.26 CDCl3
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7.22
7.22
7.21
3.96
3.96
3.00
3.00
OMe
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1.00
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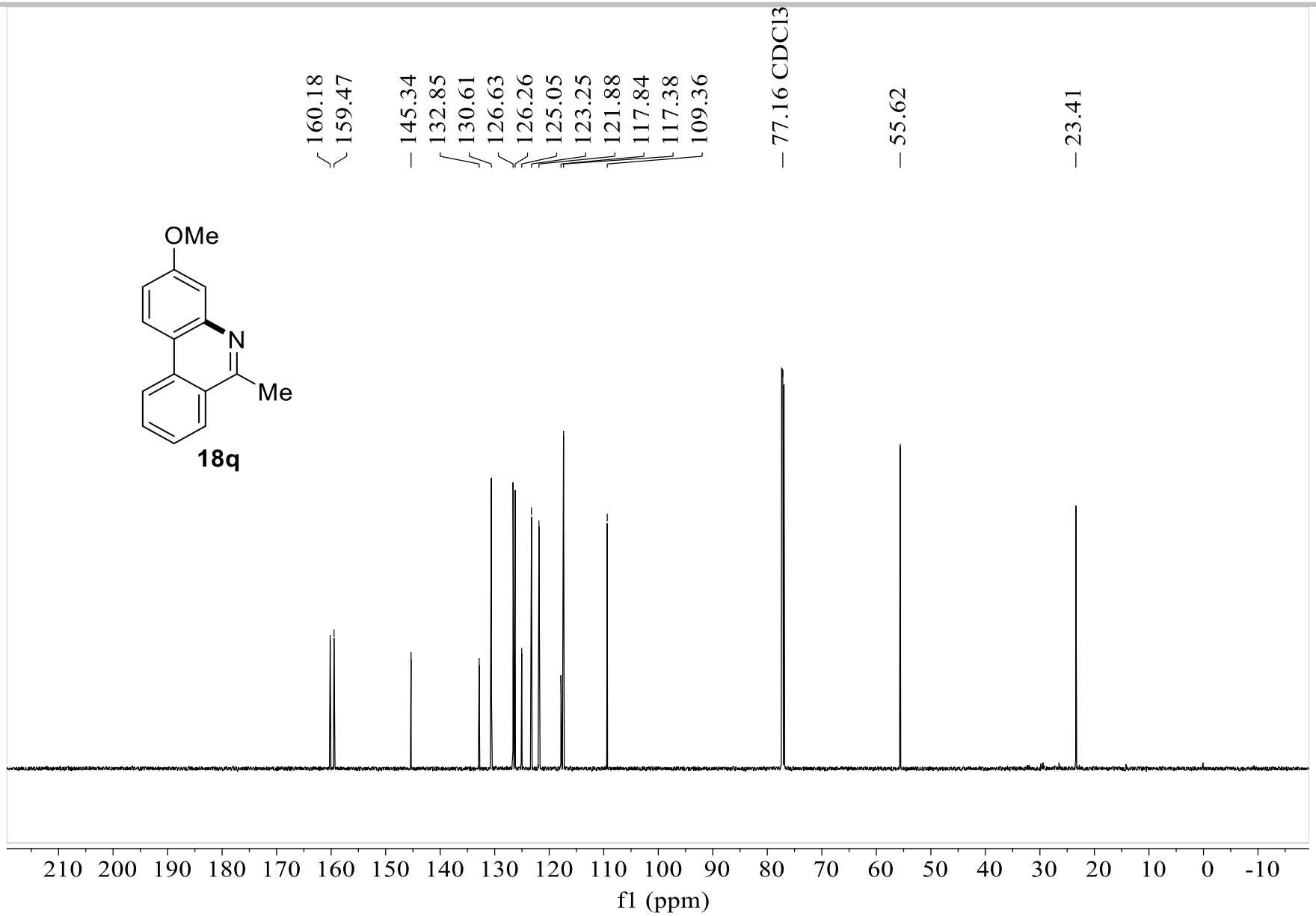
3.10
f1 (ppm)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123.25
121.88
117.84
117.38
109.36
77.16 CDCl3
55.62
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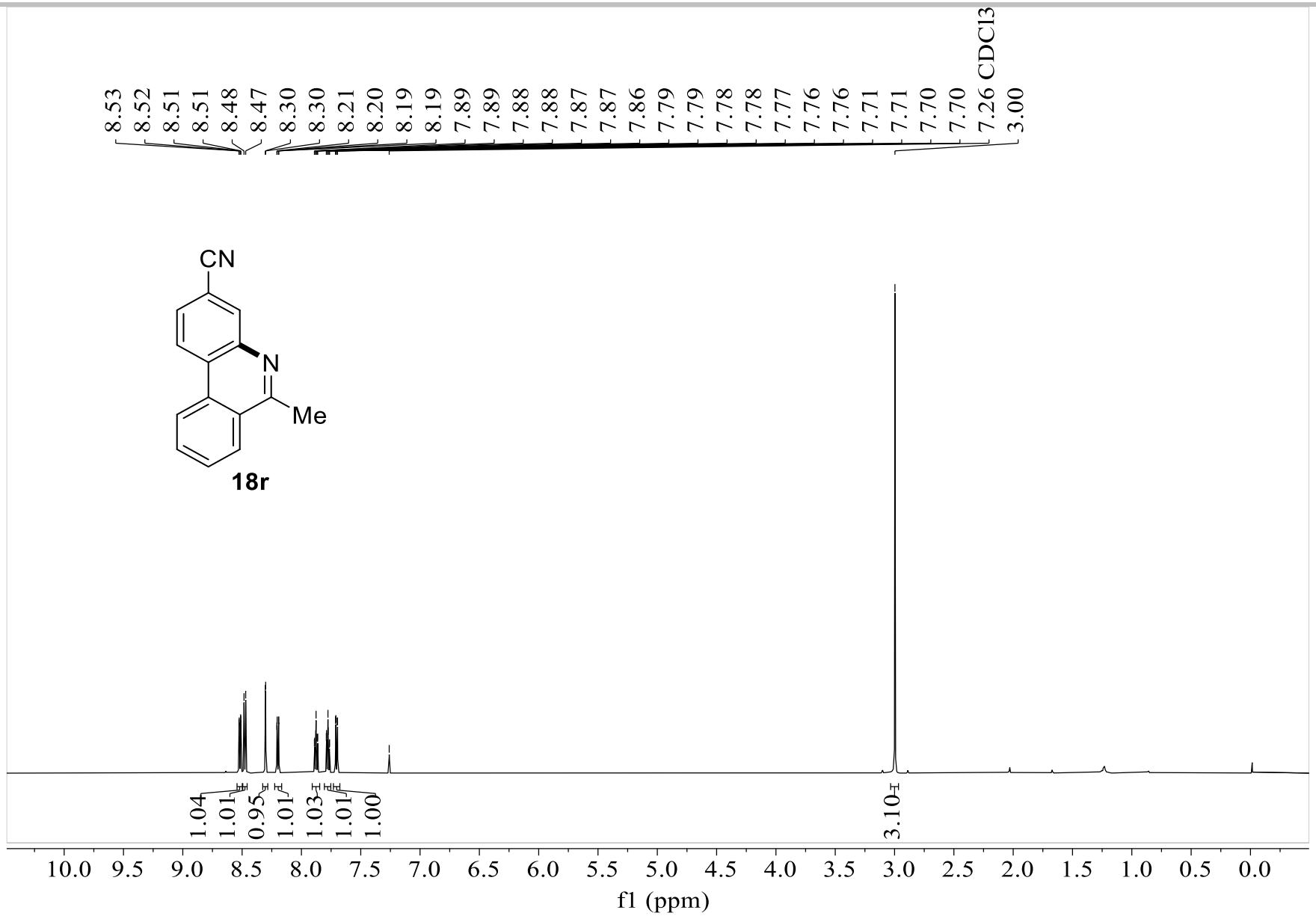
OMe
N
Me
18q
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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8.19
8.19
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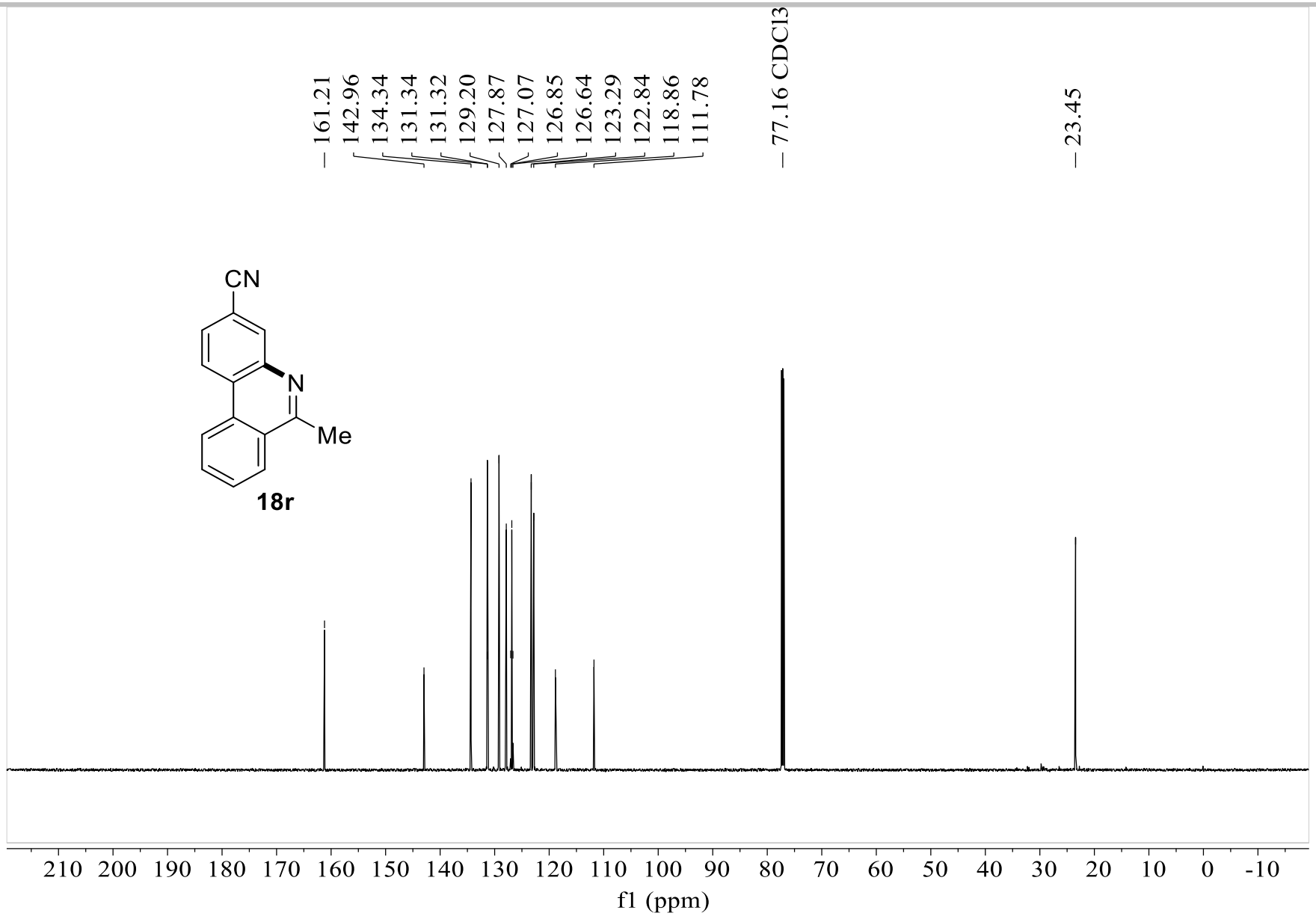
7.78
7.77
7.76
7.76
7.71
7.71
7.70
7.70
7.26 CDCl3
3.00
CN
N
Me
18r
1.04
1.01
0.95
1.01
1.03
1.01
1.00
3.10
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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122.84
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111.78
77.16 CDCl3
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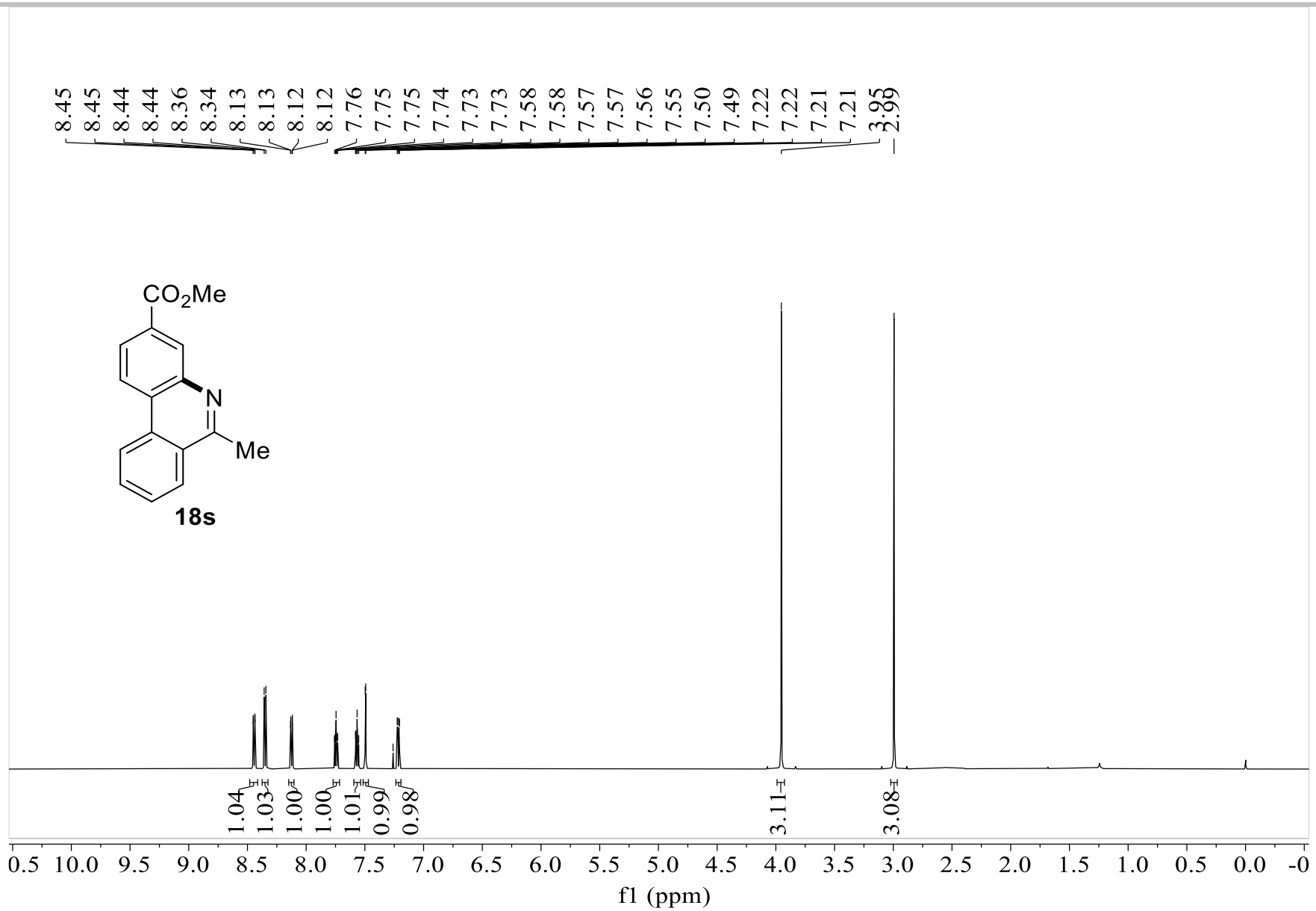
CN
N
Me
18r
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.57
7.56
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7.50
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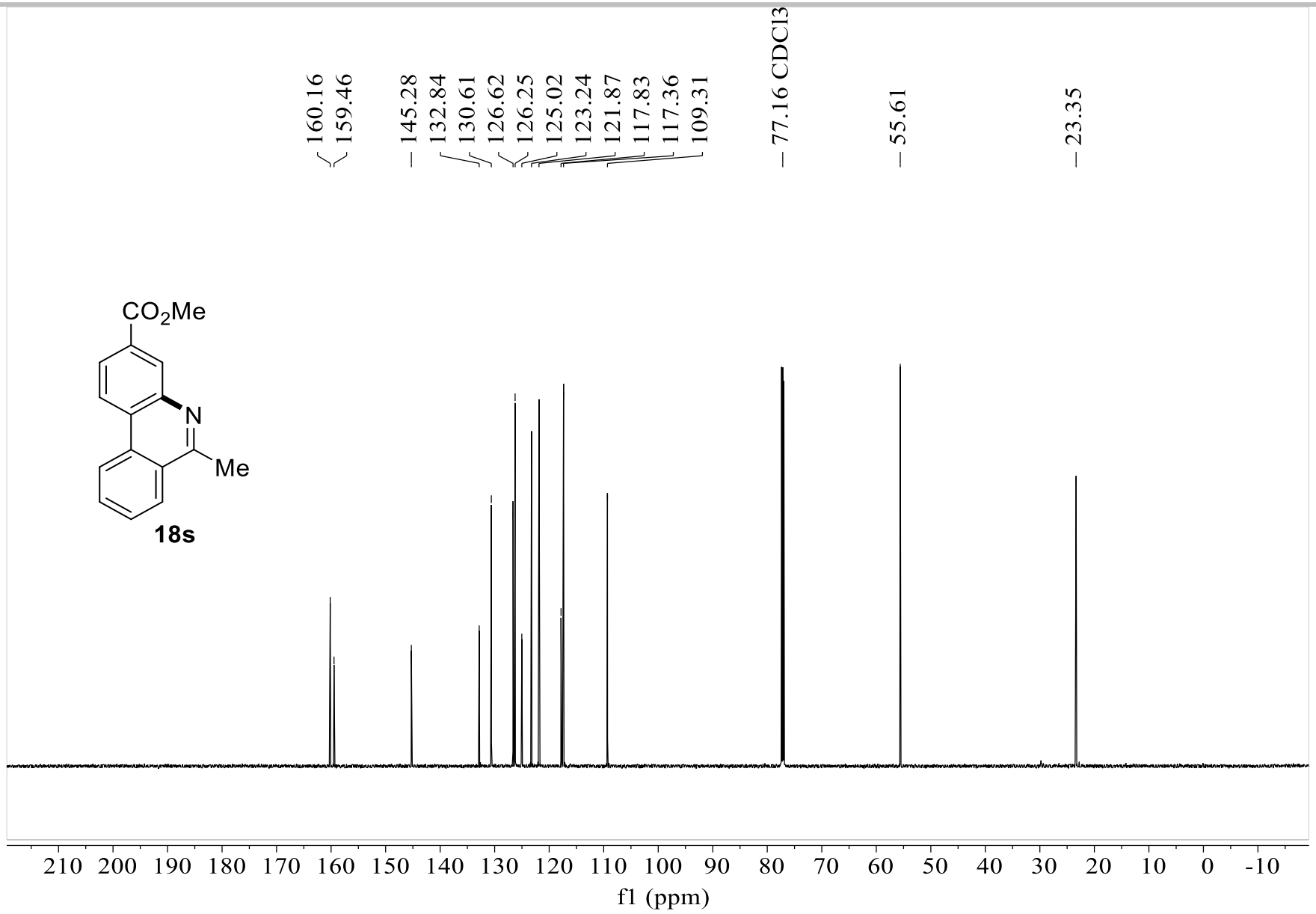
7.22
7.21
7.21
3.95
2.99
CO2Me
N
Me
18s
1.04
1.03
1.00
1.00
1.01
0.99
0.98
3.11
3.08
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)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125.02
123.24
121.87
117.83
117.36
109.31
77.16 CDCl3
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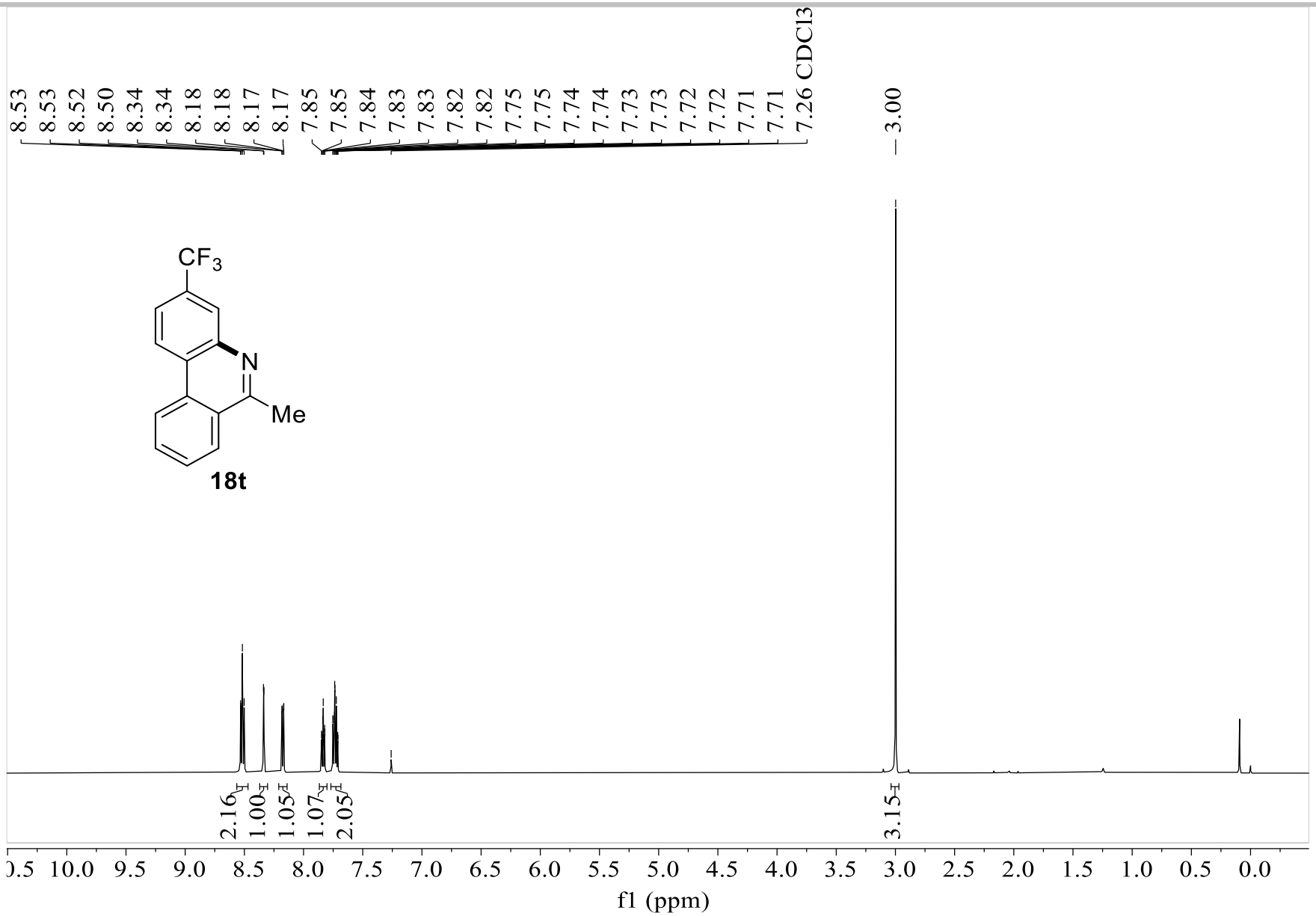
CO2Me
N
Me
18s
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.85
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7.82
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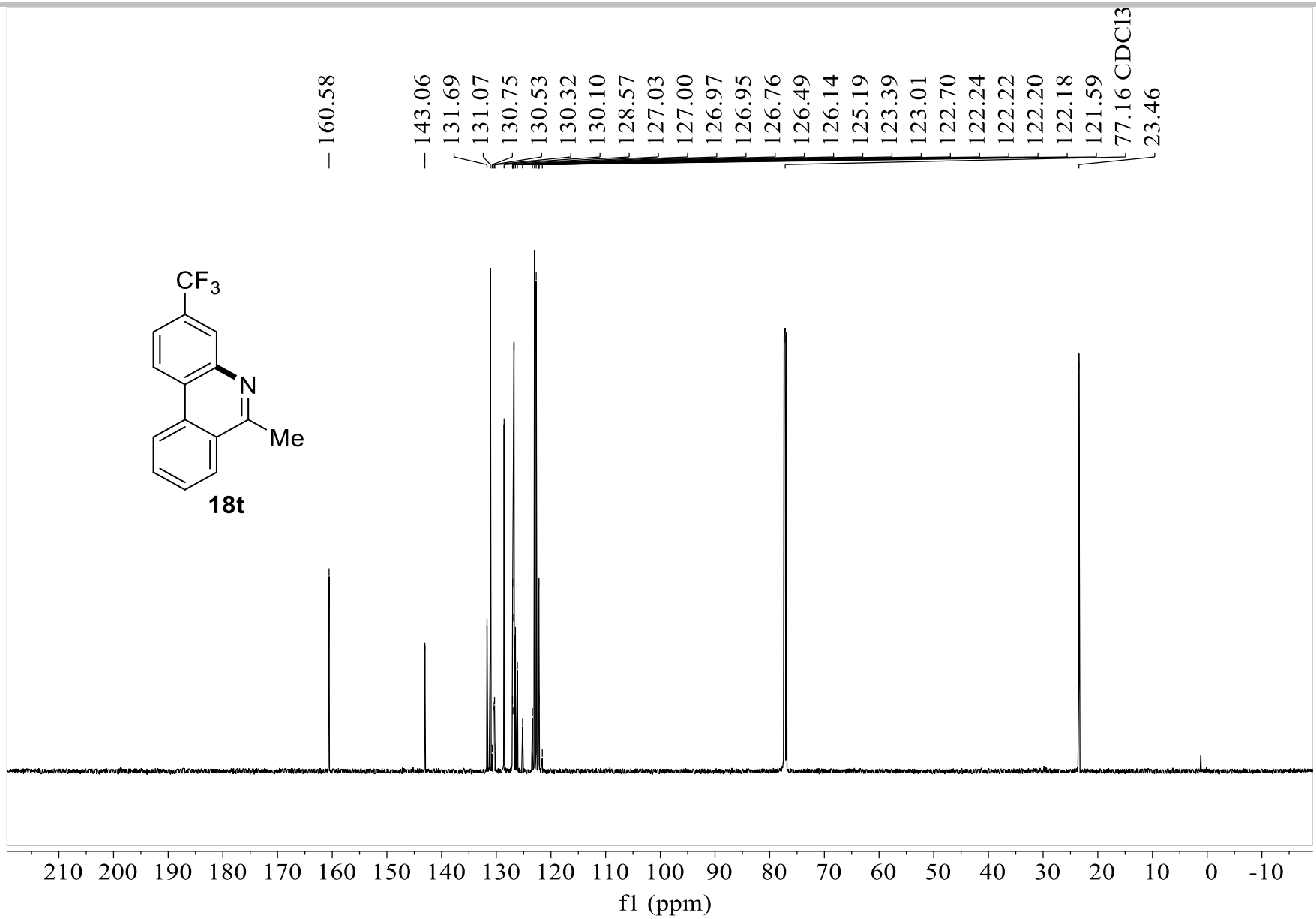
7.75
7.75
7.74
7.74
7.73
7.73
7.72
7.72
7.71
7.71
7.26 CDCl3
3.00
CF3
N
Me
18t
2.16
1.00
1.05
1.07
2.05
3.15
f1 (ppm)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126.95
126.76
126.49
126.14
125.19
123.39
123.01
122.70
122.24
122.22
122.20
122.18
121.59
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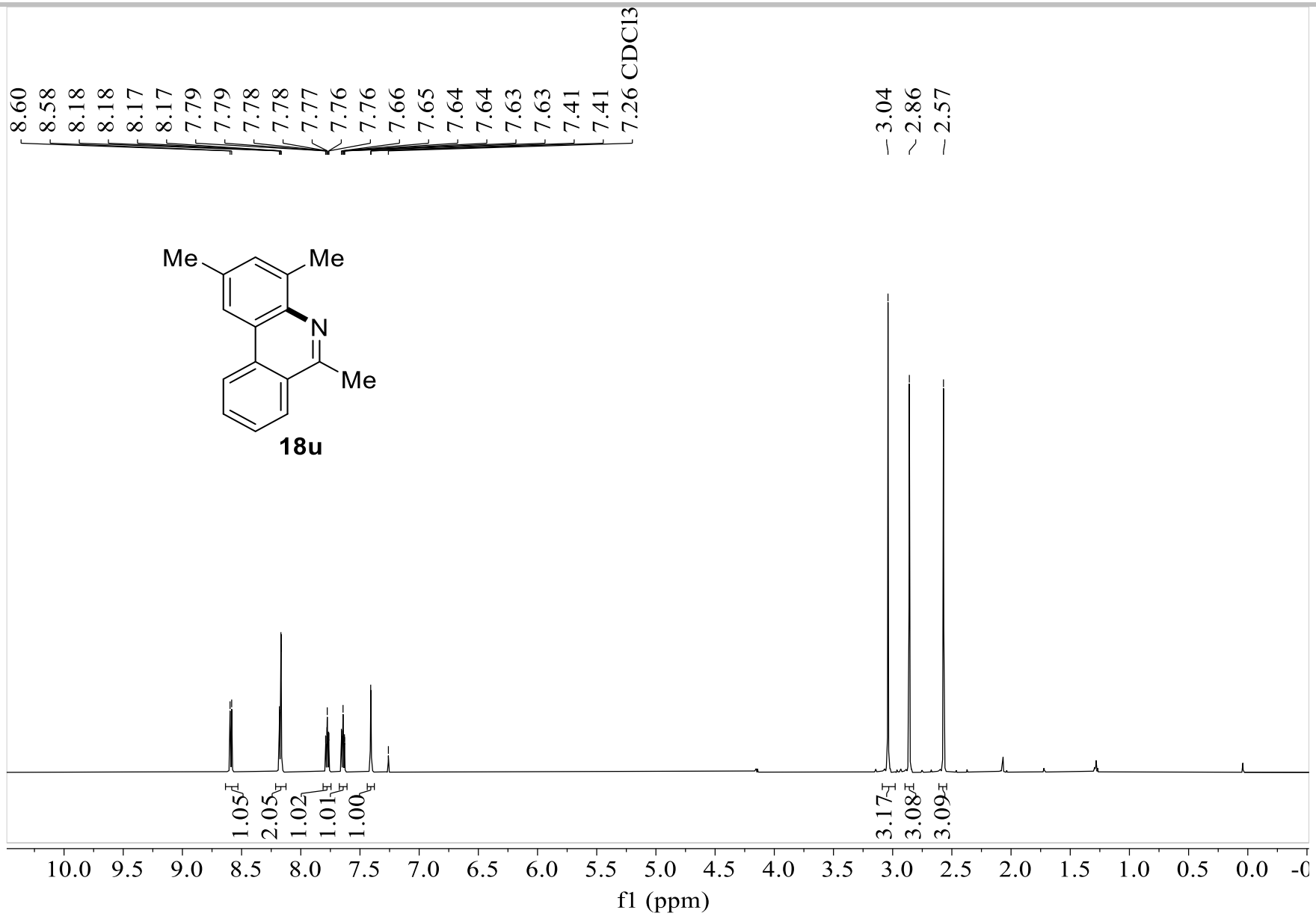
CF3
N
Me
18t
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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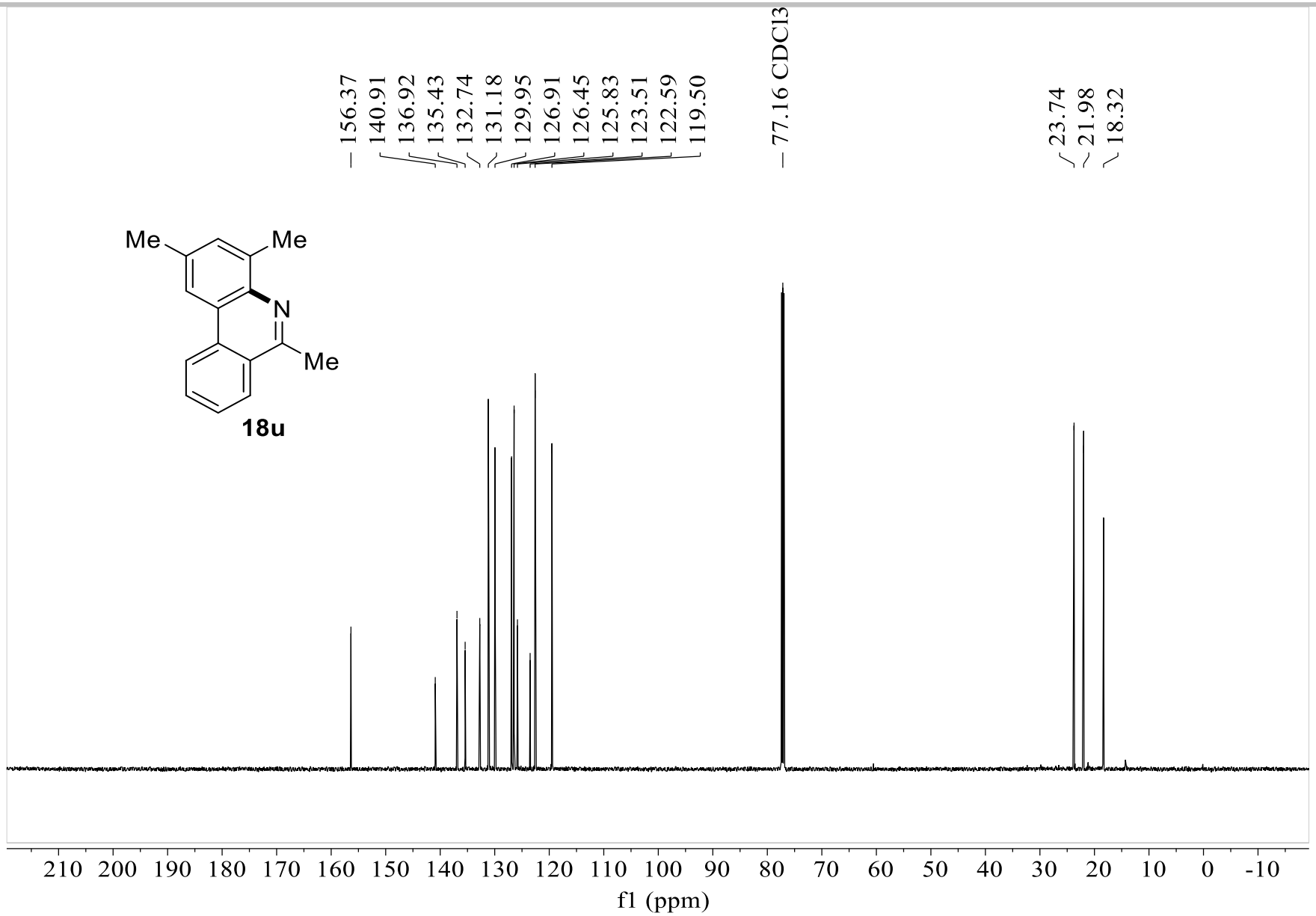
7.65
7.64
7.64
7.63
7.63
7.41
7.41
7.26 CDCl3
3.04
2.86
2.57
Me
Me
N
Me
18u
1.05
2.05
1.02
1.01
1.00
3.17
3.08
3.09
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)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123.51
122.59
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77.16 CDCl3
23.74
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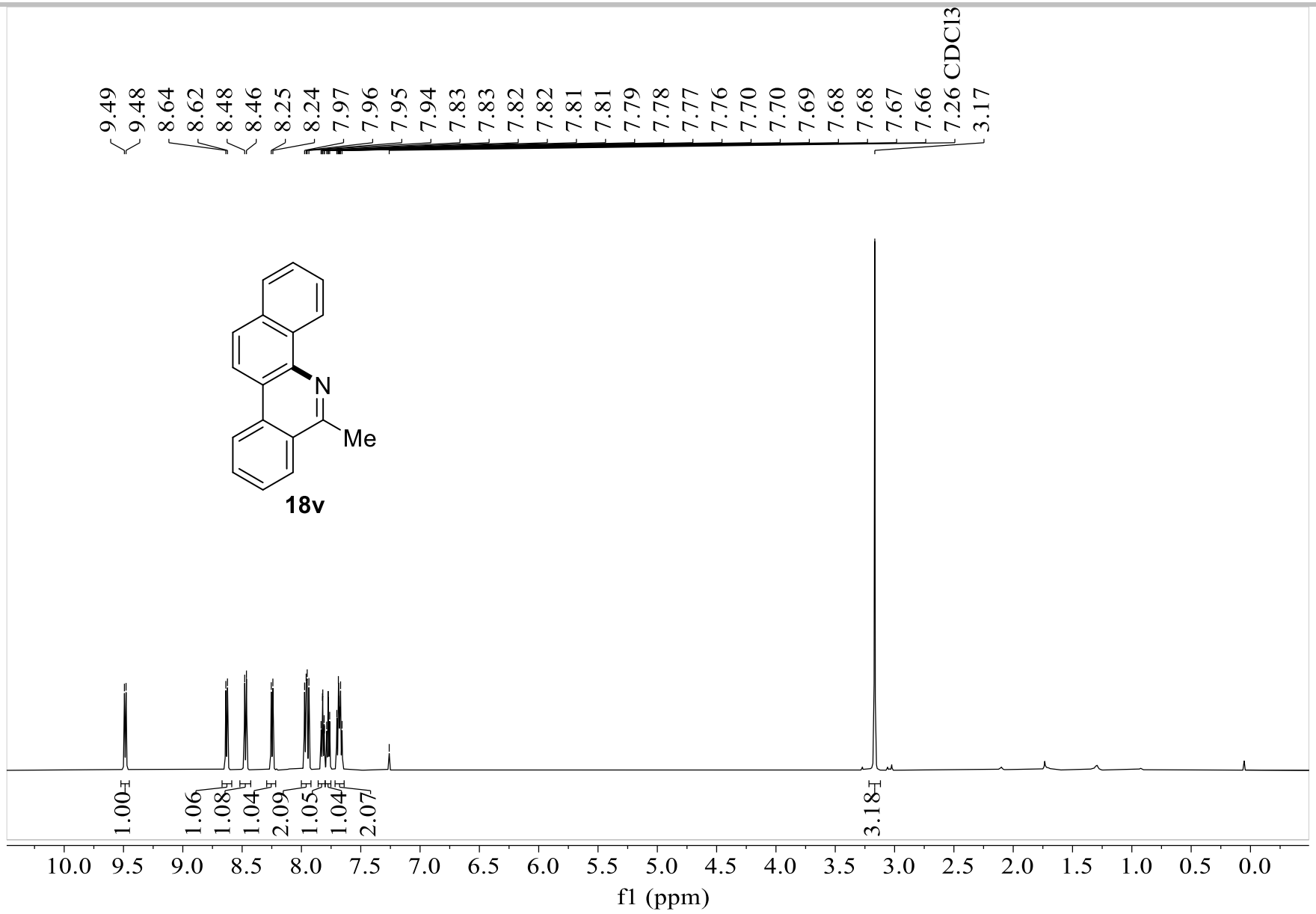
Me
Me
N
Me
18u
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.83
7.82
7.82
7.81
7.81
7.79
7.78
7.77
7.76
7.70
7.70
7.69
7.68
7.68
7.67
7.66
7.26 CDCl3
3.17
N
Me
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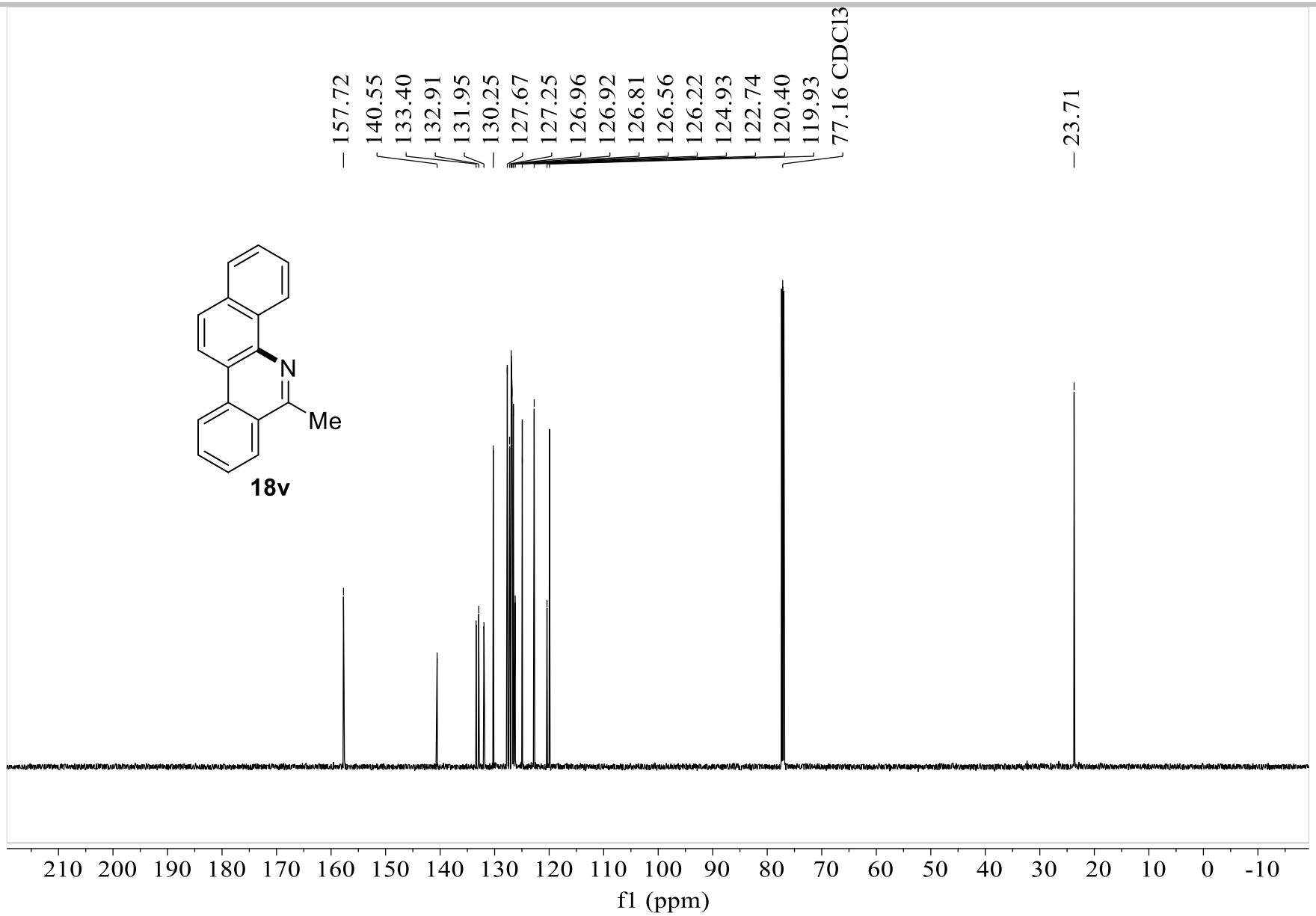
1.08
1.04
2.09
1.05
1.04
2.07
3.18
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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126.22
124.93
122.74
120.40
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Me
18v
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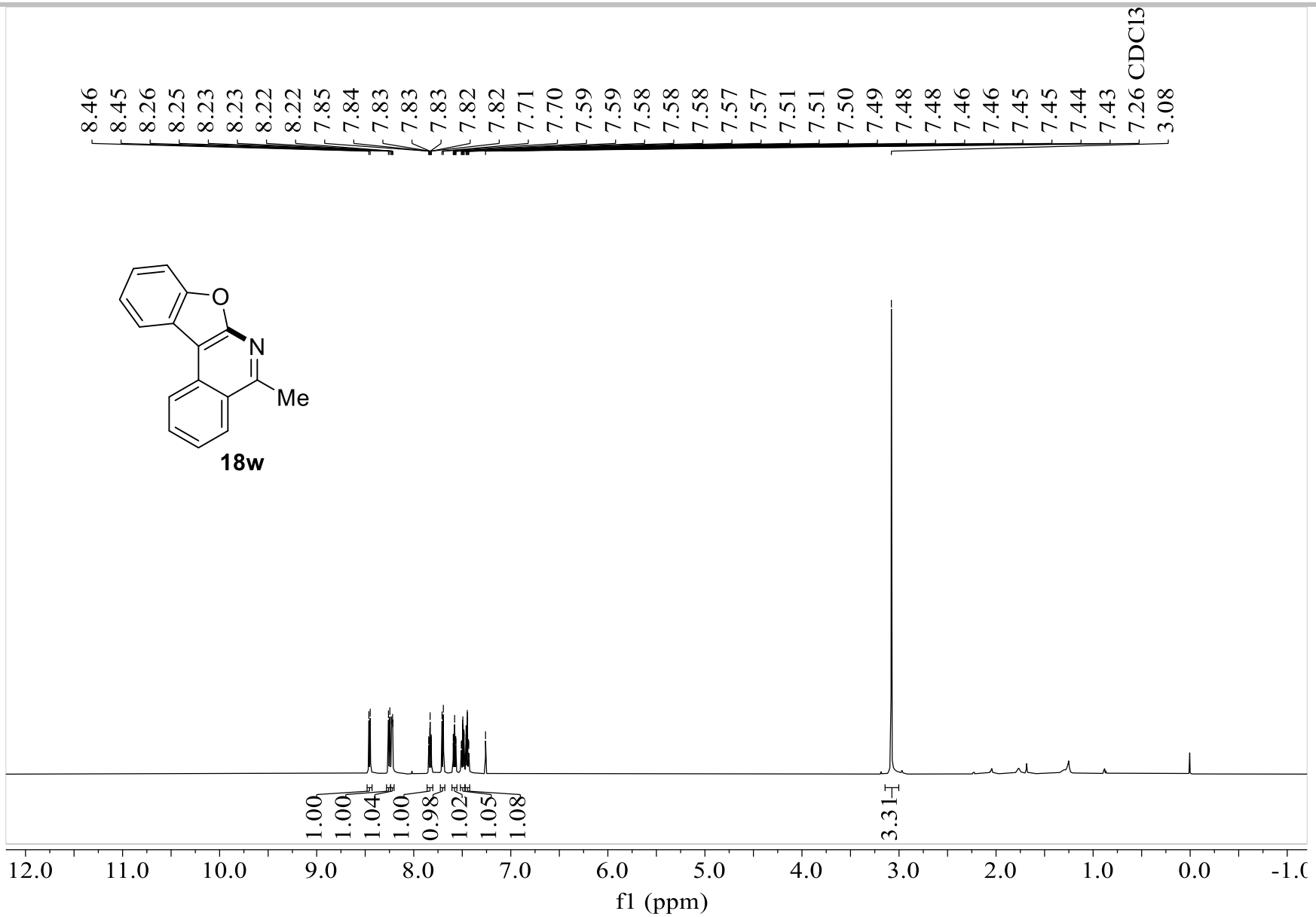
f1 (ppm)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7.45
7.44
7.43
7.26 CDCl3
3.08
O
N
Me
18w
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1.00
1.04
1.00
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1.02
1.05
1.08
3.31
12.0
11.0
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4.0
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2.0
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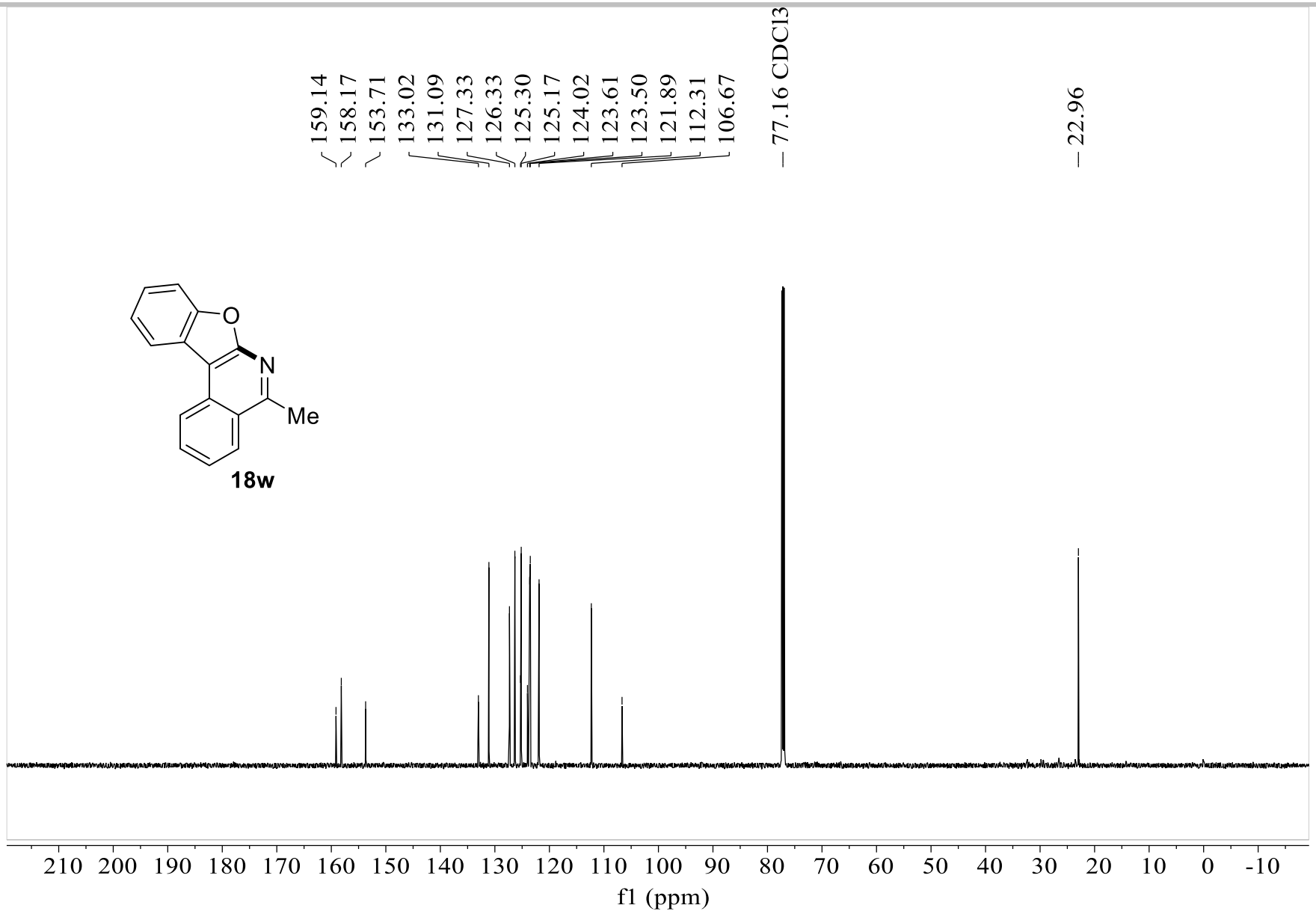
f1 (ppm)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O
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Me
18w
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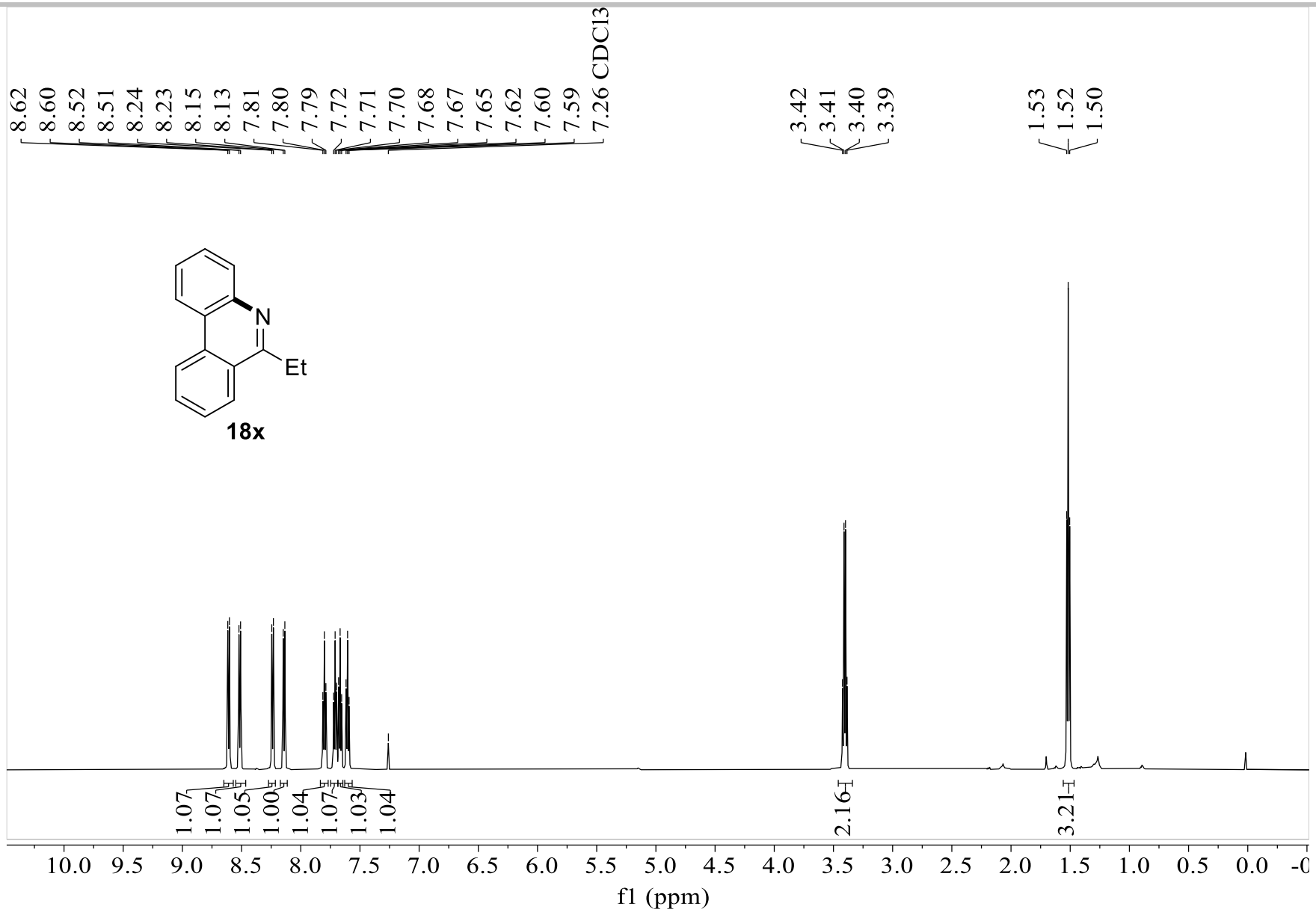
f1 (ppm)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7.67
7.65
7.62
7.60
7.59
7.26 CDCl3
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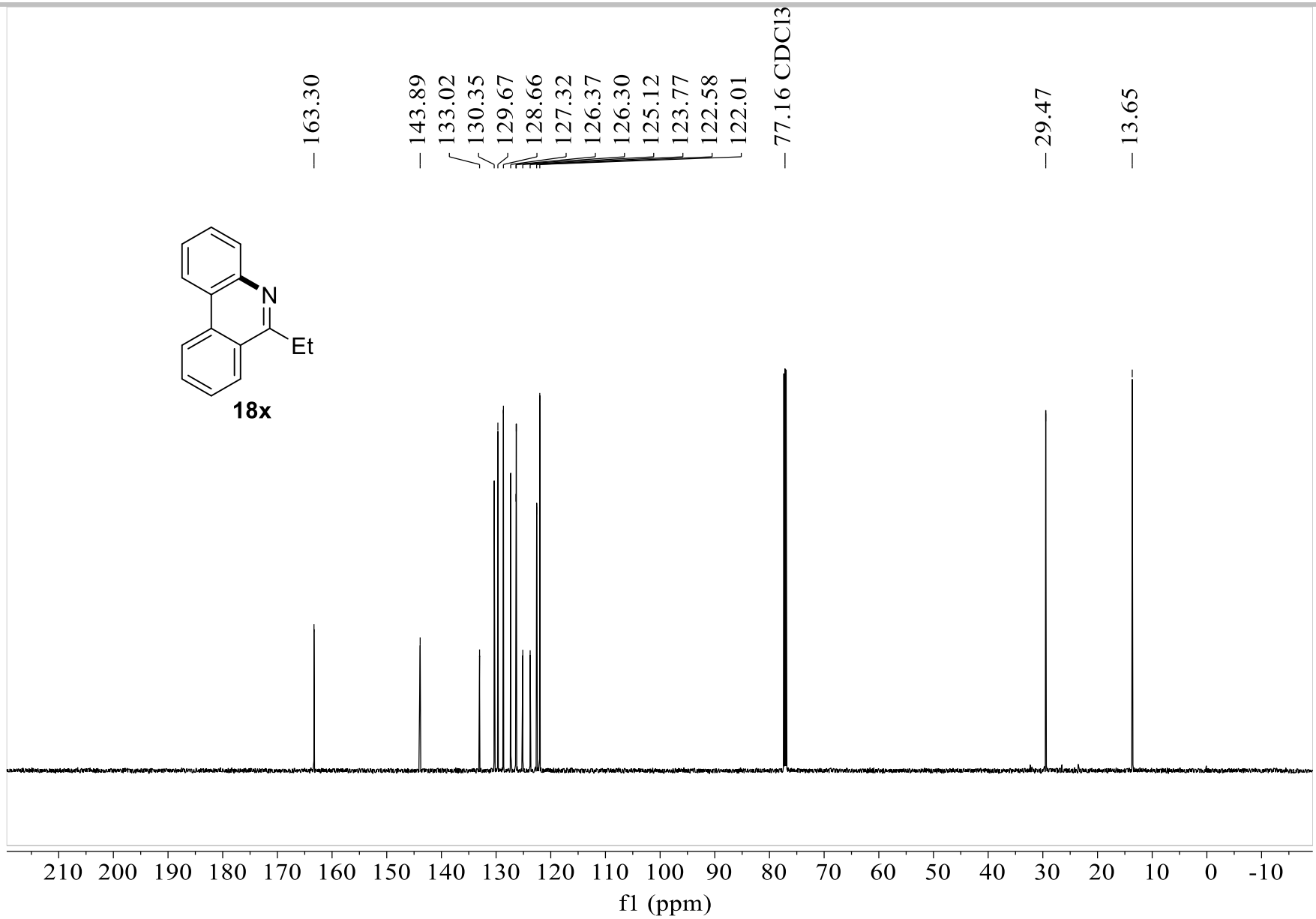
3.41
3.40
3.39
1.53
1.52
1.50
N
Et
18x
1.07
1.07
1.05
1.00
1.04
1.07
1.03
1.04
2.16
3.21
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)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125.12
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122.01
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13.65
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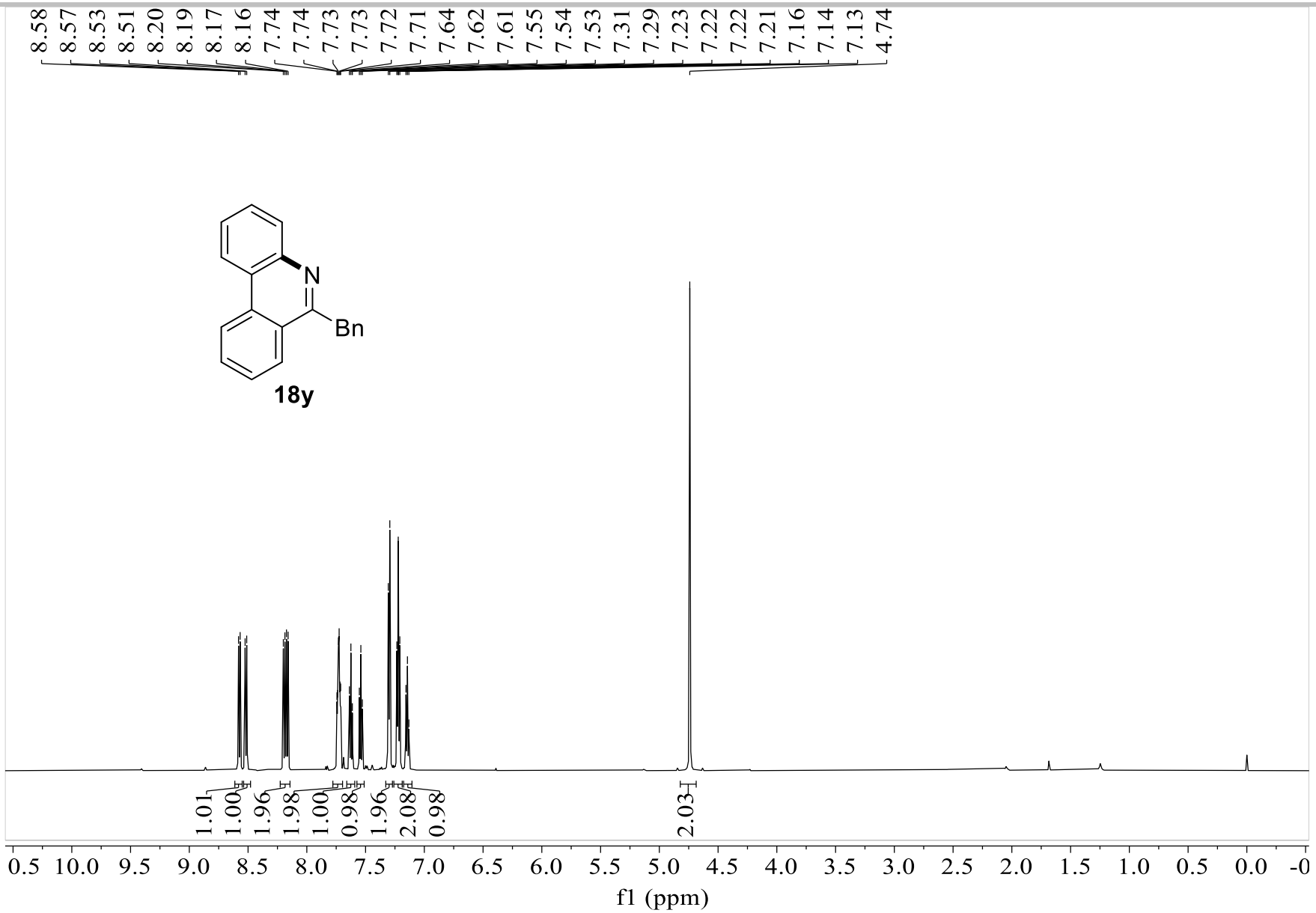
Et
18x
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.22
7.21
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7.14
7.13
4.74
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Bn
18y
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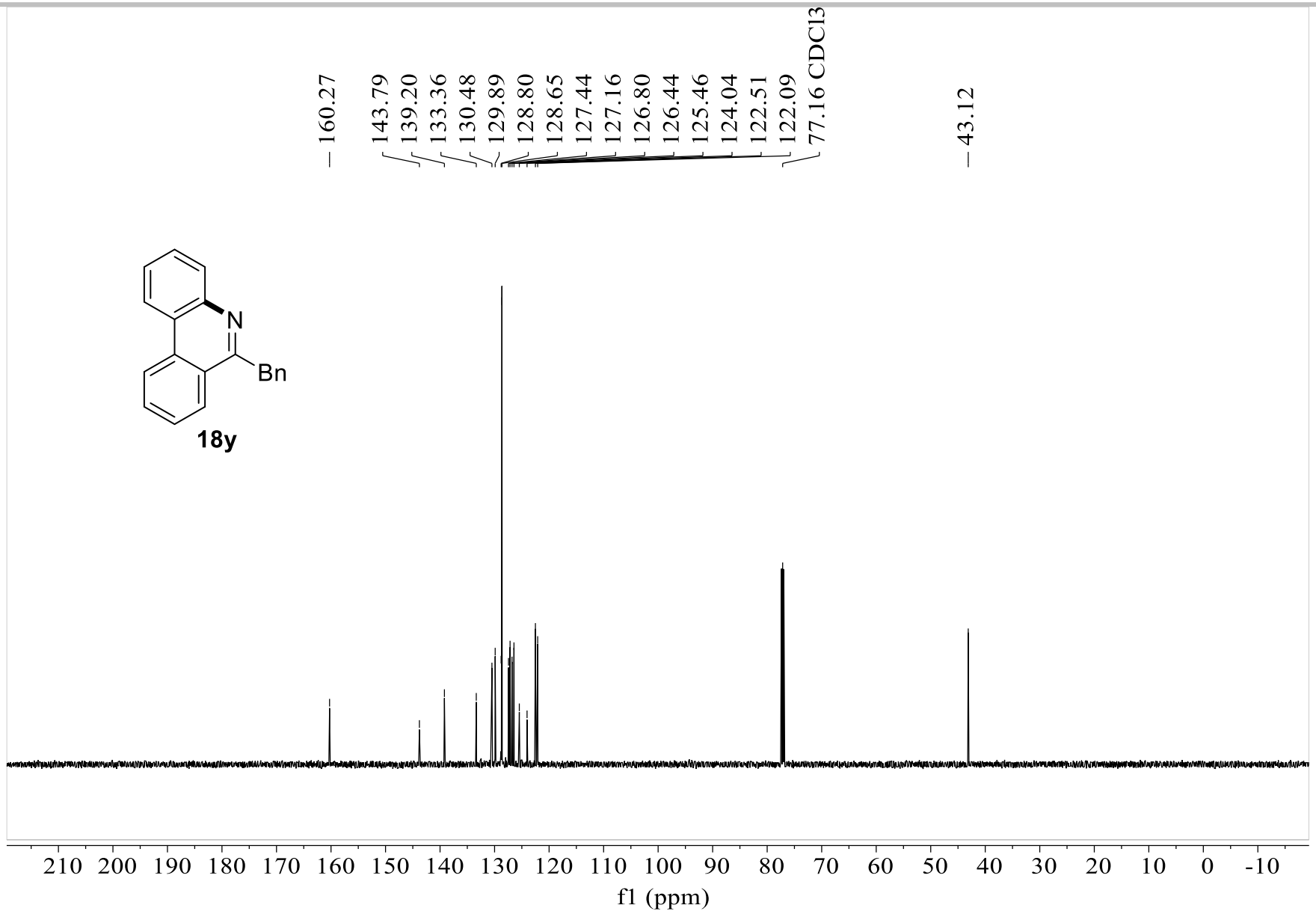
1.00
1.96
1.98
1.00
0.98
1.96
2.08
0.98
2.03
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)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125.46
124.04
122.51
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77.16 CDCl3
43.12
N
Bn
18y
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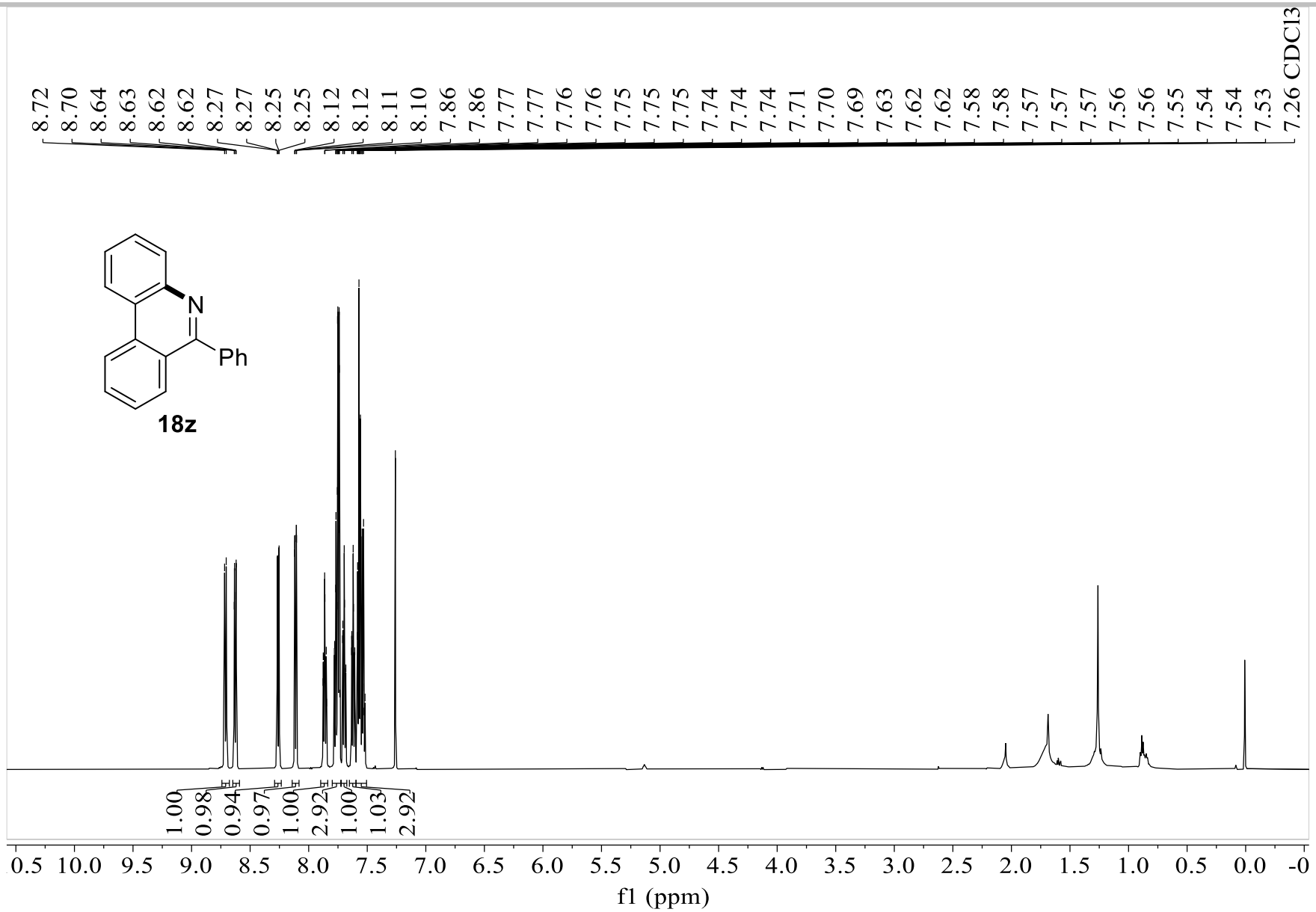
f1 (ppm)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Ph
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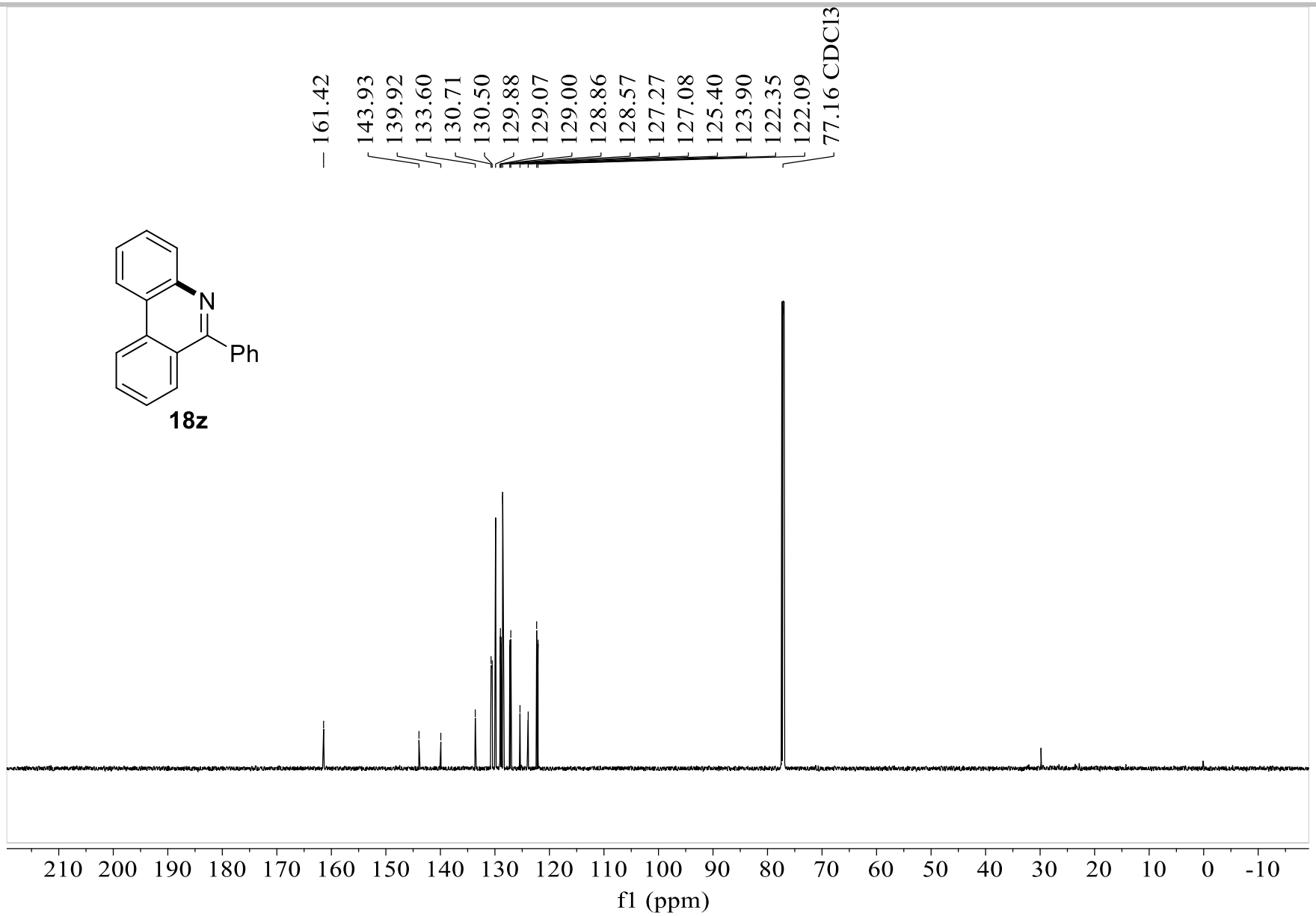
1.00
1.03
2.92
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)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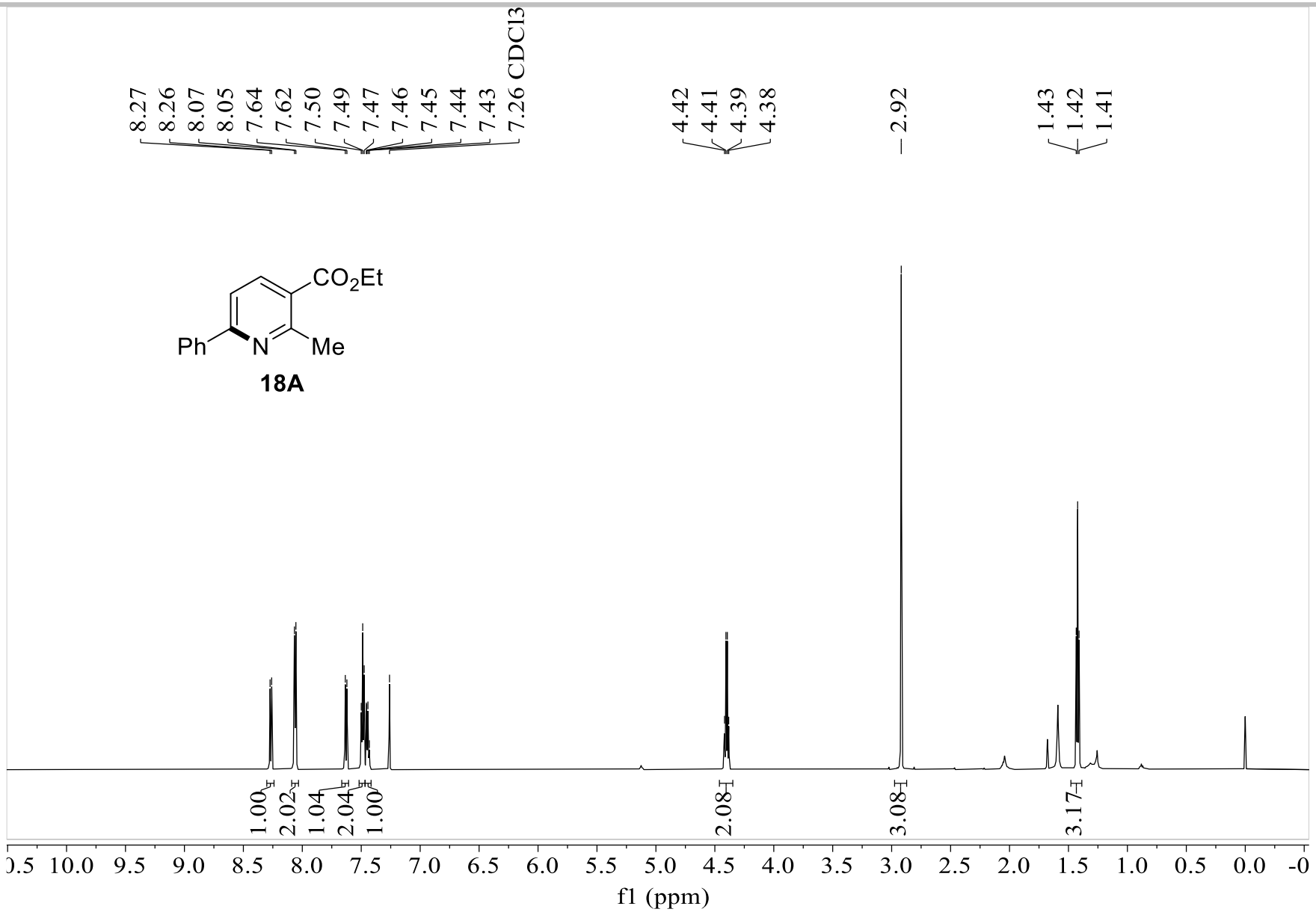
143.93
139.92
133.60
130.71
130.50
129.88
129.07
129.00
128.86
128.57
127.27
127.08
125.40
123.90
122.35
122.09
77.16 CDCl3
N
Ph
18z
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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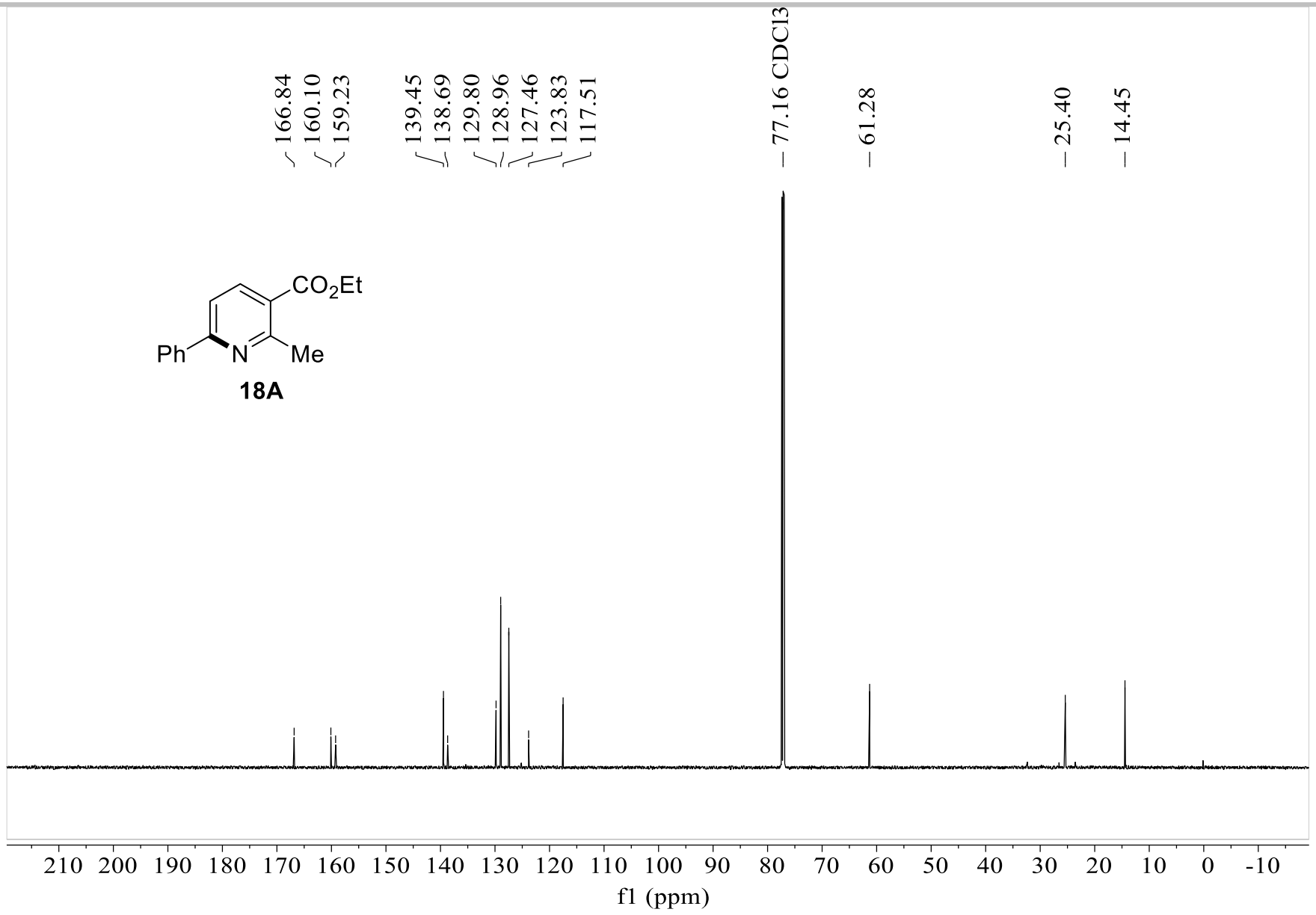
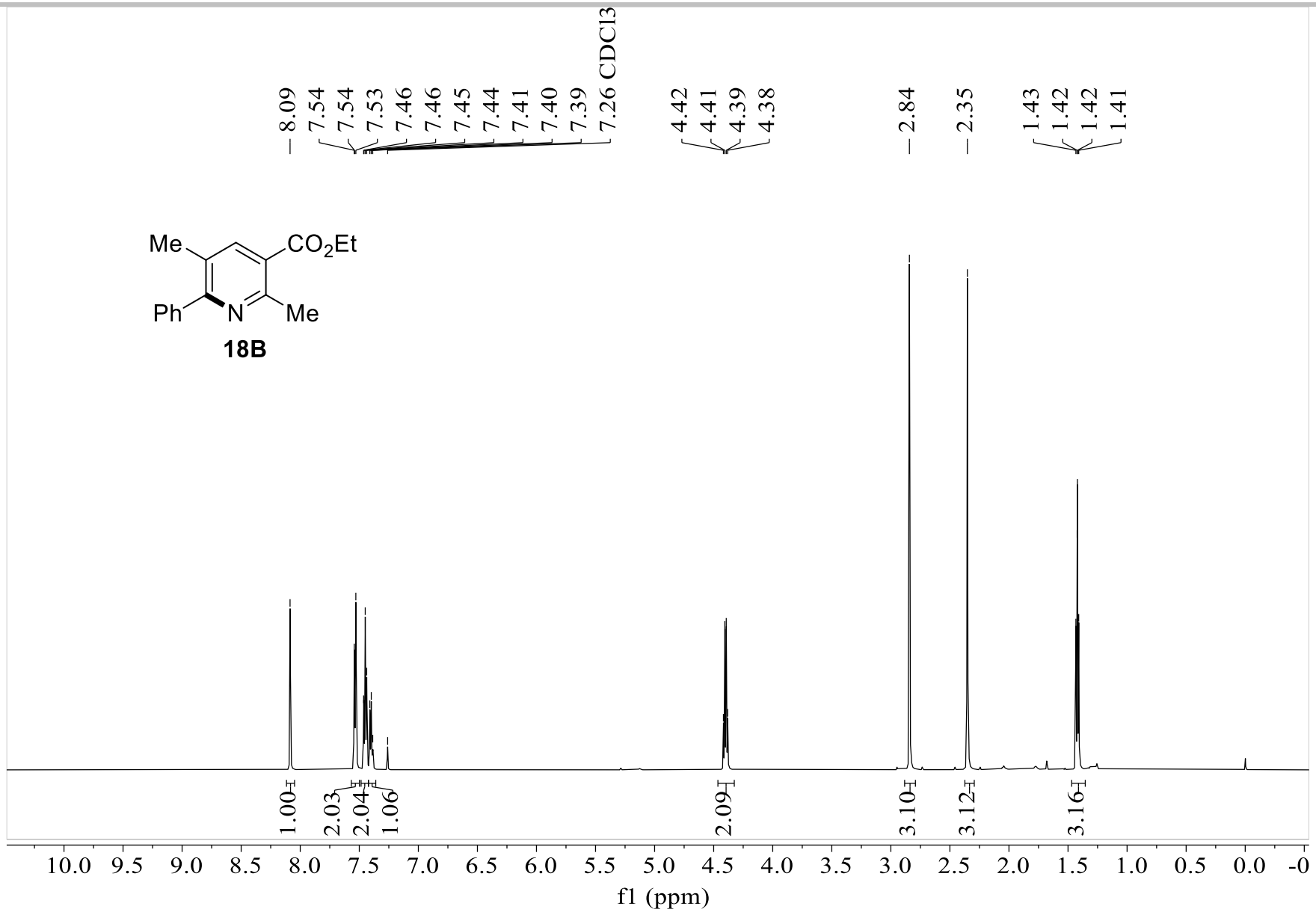
8.26
8.07
8.05
7.64
7.62
7.50
7.49
7.47
7.46
7.45
7.44
7.43
7.26 CDCl3
4.42
4.41
4.39
4.38
2.92
1.43
1.42
1.41
CO2Et
Ph
N
Me
18A
1.00
2.02
1.04
2.04
1.00
2.08
3.08
3.17
f1 (ppm)


166.84
160.10
159.23
139.45
138.69
129.80
128.96
127.46
123.83
117.51
77.16 CDCl3
61.28
25.40
14.45
CO2Et
Ph
N
Me
18A
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)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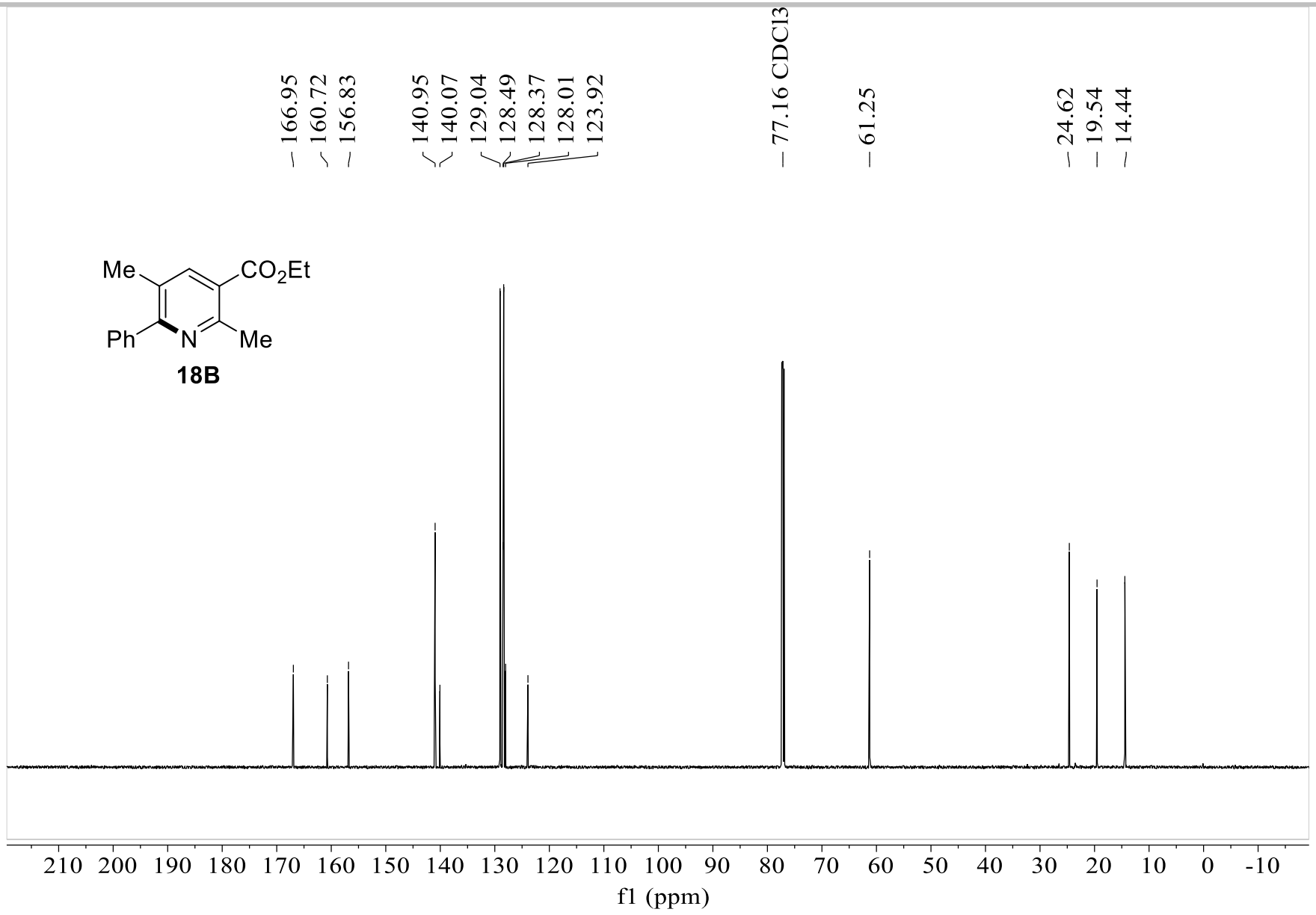
7.54
7.54
7.53
7.46
7.46
7.45
7.44
7.41
7.40
7.39
7.26 CDCl3
4.42
4.41
4.39
4.38
2.84
2.35
1.43
1.42
1.42
1.41
Me
CO2Et
Ph
N
Me
18B
1.00
2.03
2.04
1.06
2.09
3.10
3.12
3.16
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)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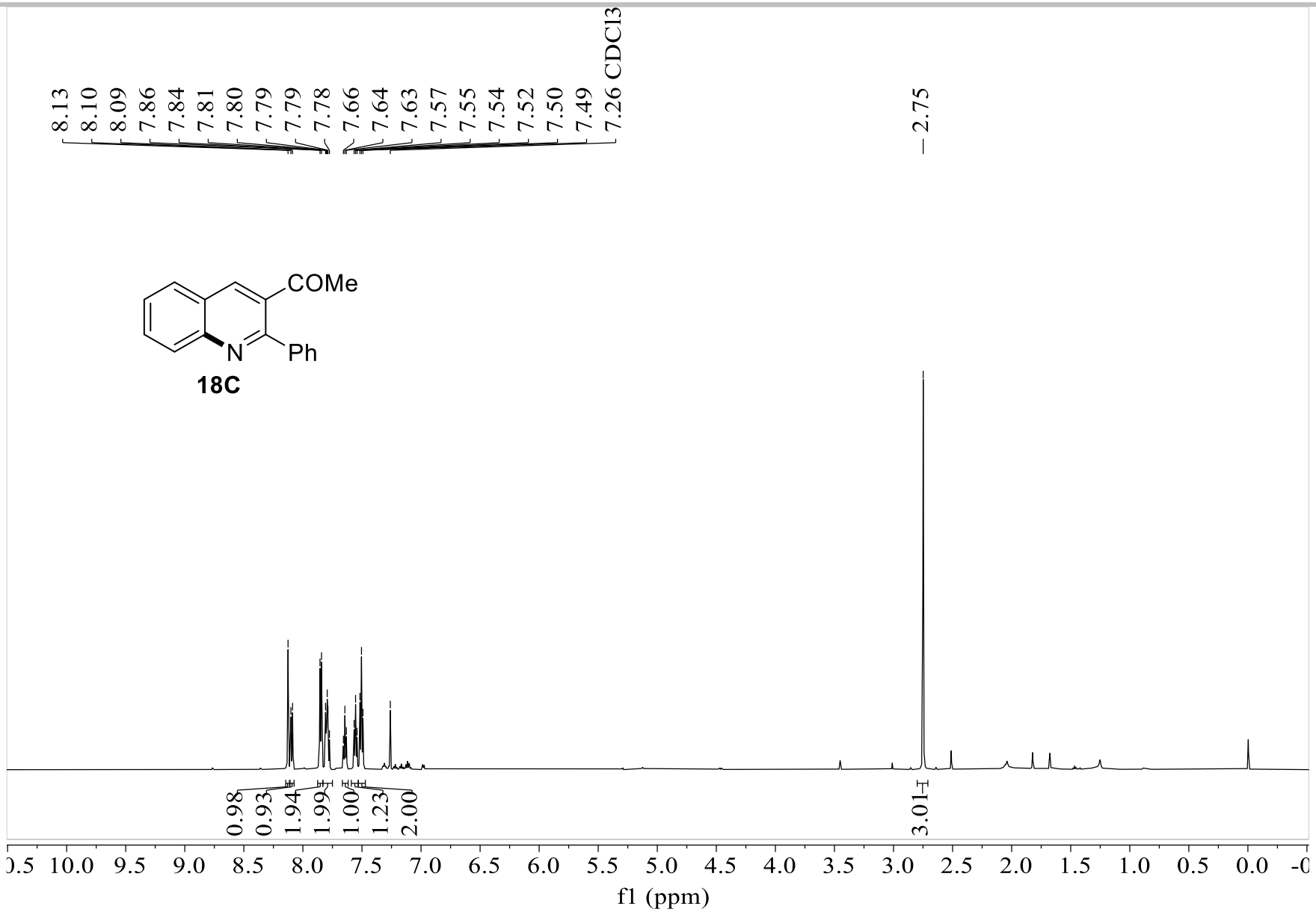
156.83
140.95
140.07
129.04
128.49
128.37
128.01
123.92
77.16 CDCl3
61.25
24.62
19.54
14.44
Me
CO2Et
Ph
N
Me
18B
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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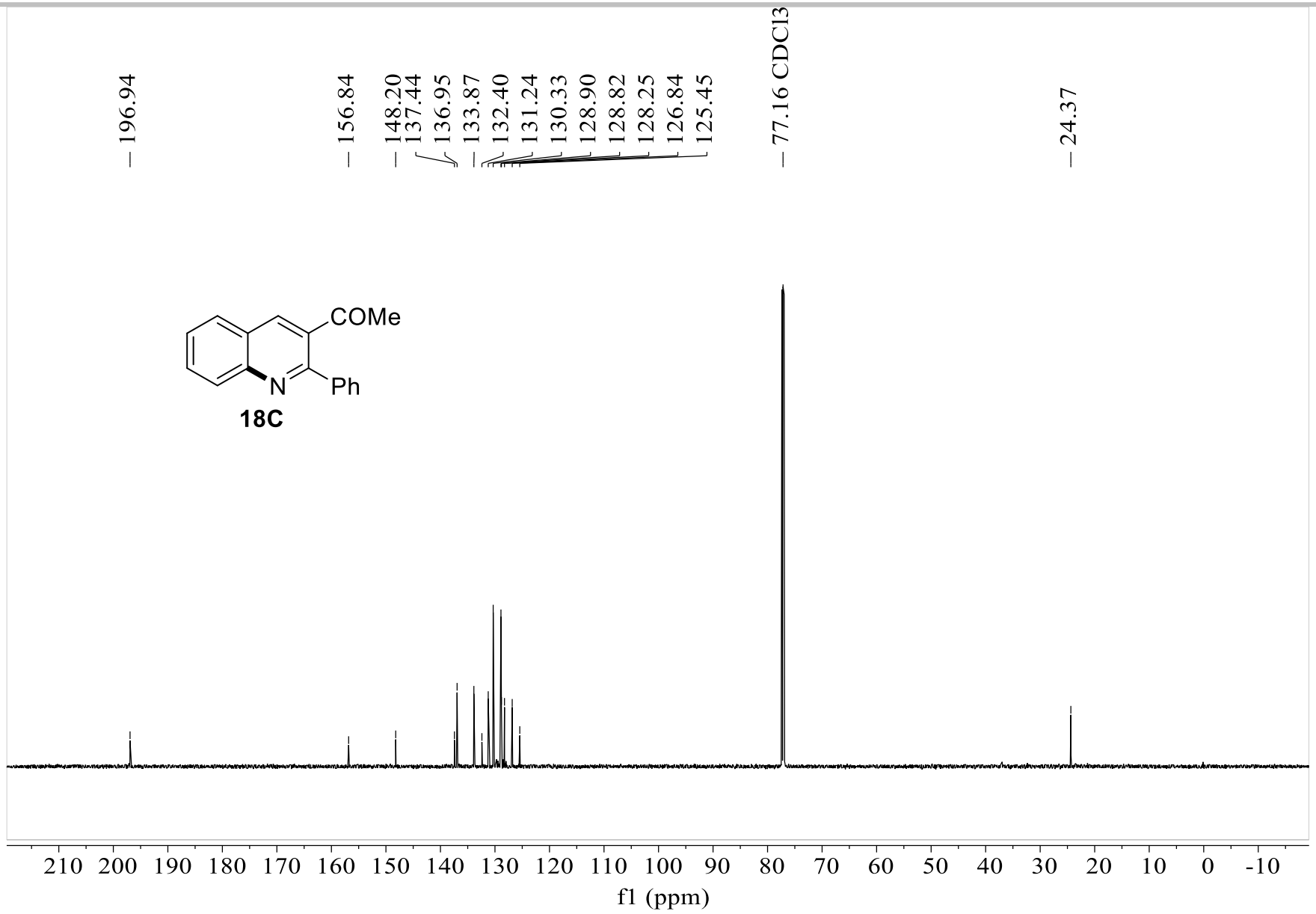
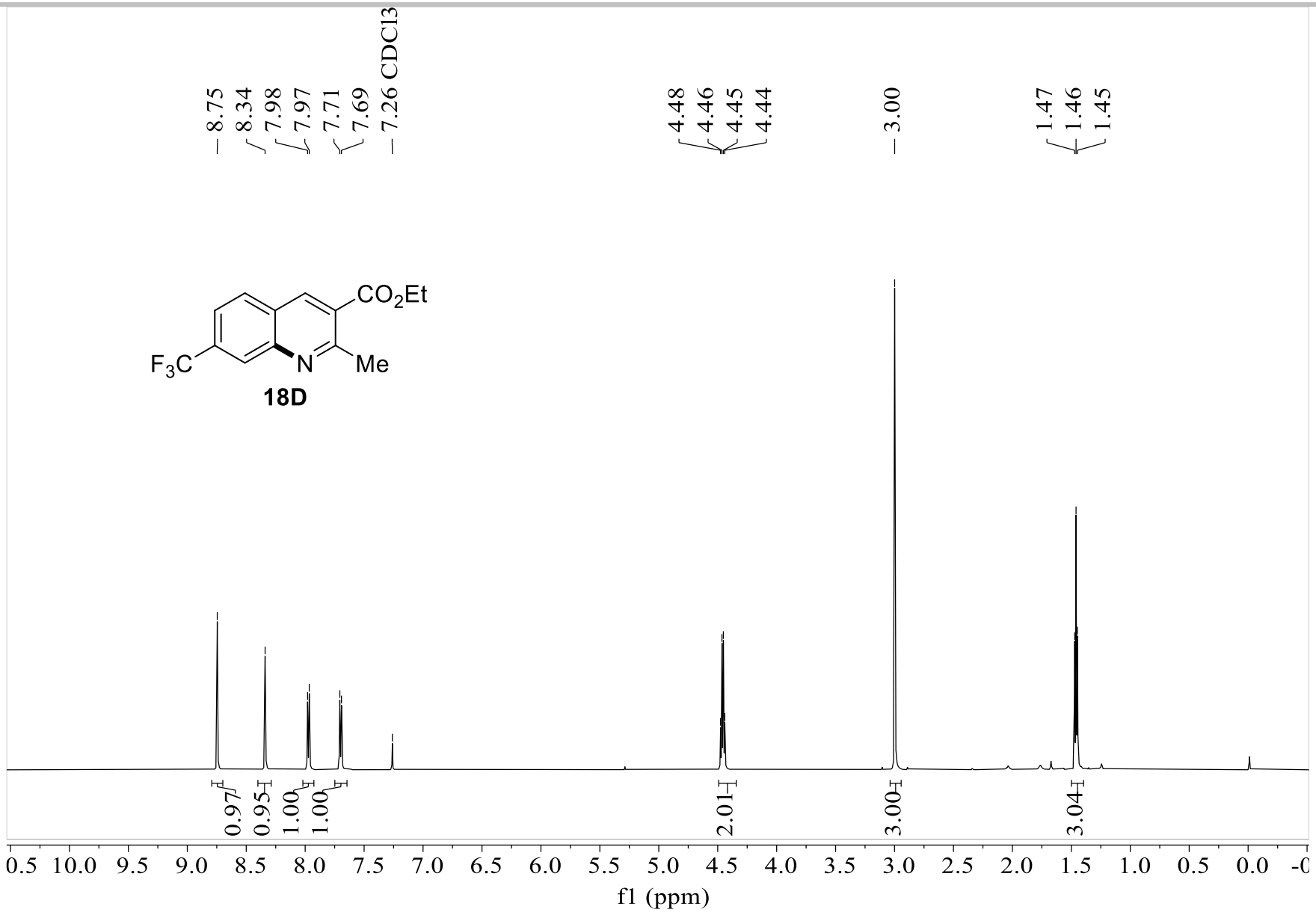
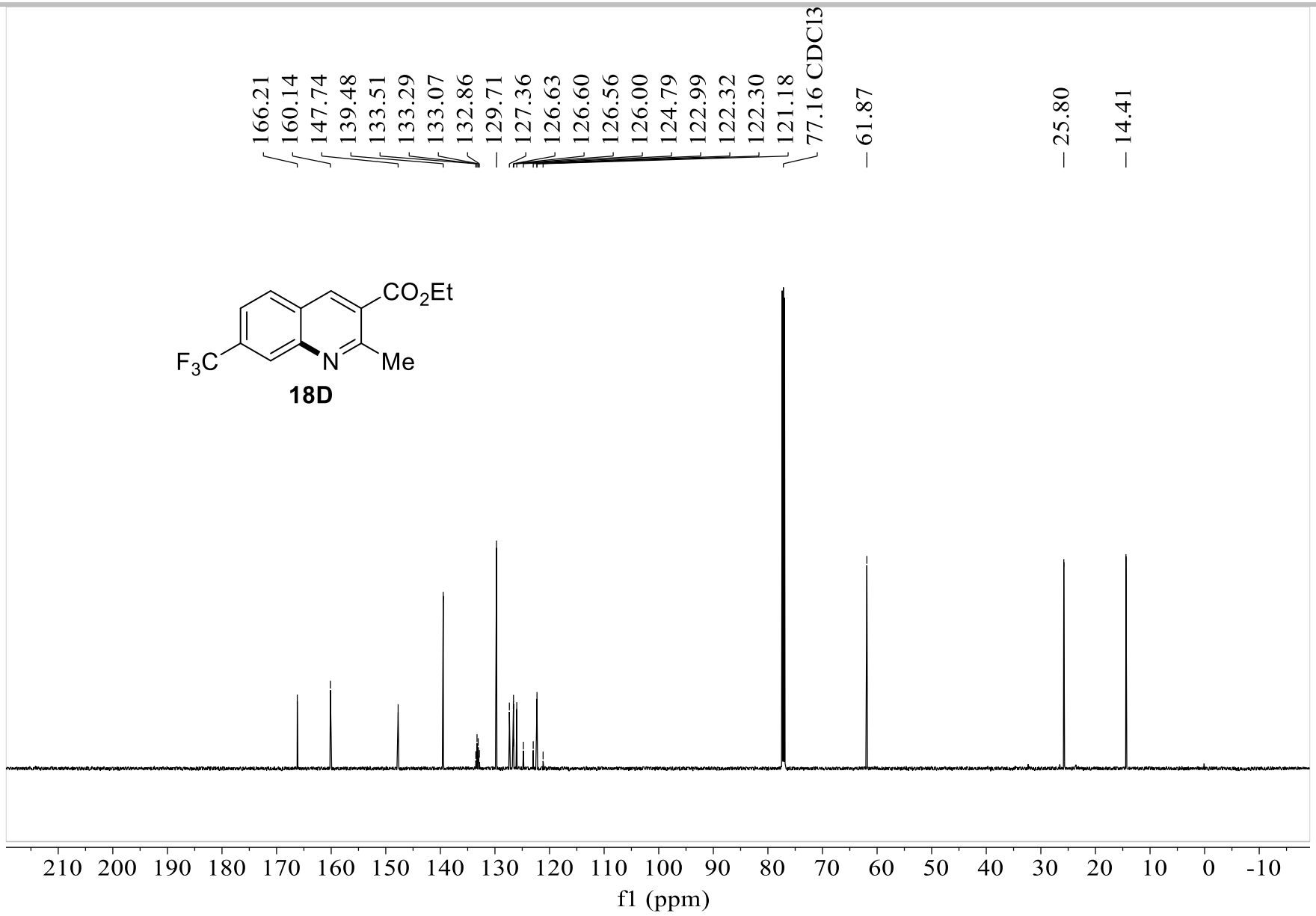
8.10
8.09
7.86
7.84
7.81
7.80
7.79
7.79
7.78
7.66
7.64
7.63
7.57
7.55
7.54
7.52
7.50
7.49
7.26 CDCl3
2.75
COMe
N
Ph
18C
0.98
0.93
1.94
1.99
1.00
1.23
2.00
3.01
f1 (ppm)


196.94
156.84
148.20
137.44
136.95
133.87
132.40
131.24
130.33
128.90
128.82
128.25
126.84
125.45
77.16 CDCl3
24.37
COMe
N
Ph
18C
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.75
8.34
7.98
7.97
7.71
7.69
7.26 CDCl3
4.48
4.46
4.45
4.44
3.00
1.47
1.46
1.45
CO2Et
F3C
N
Me
18D
0.97
0.95
1.00
1.00
2.01
3.00
3.04
f1 (ppm)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147.74
139.48
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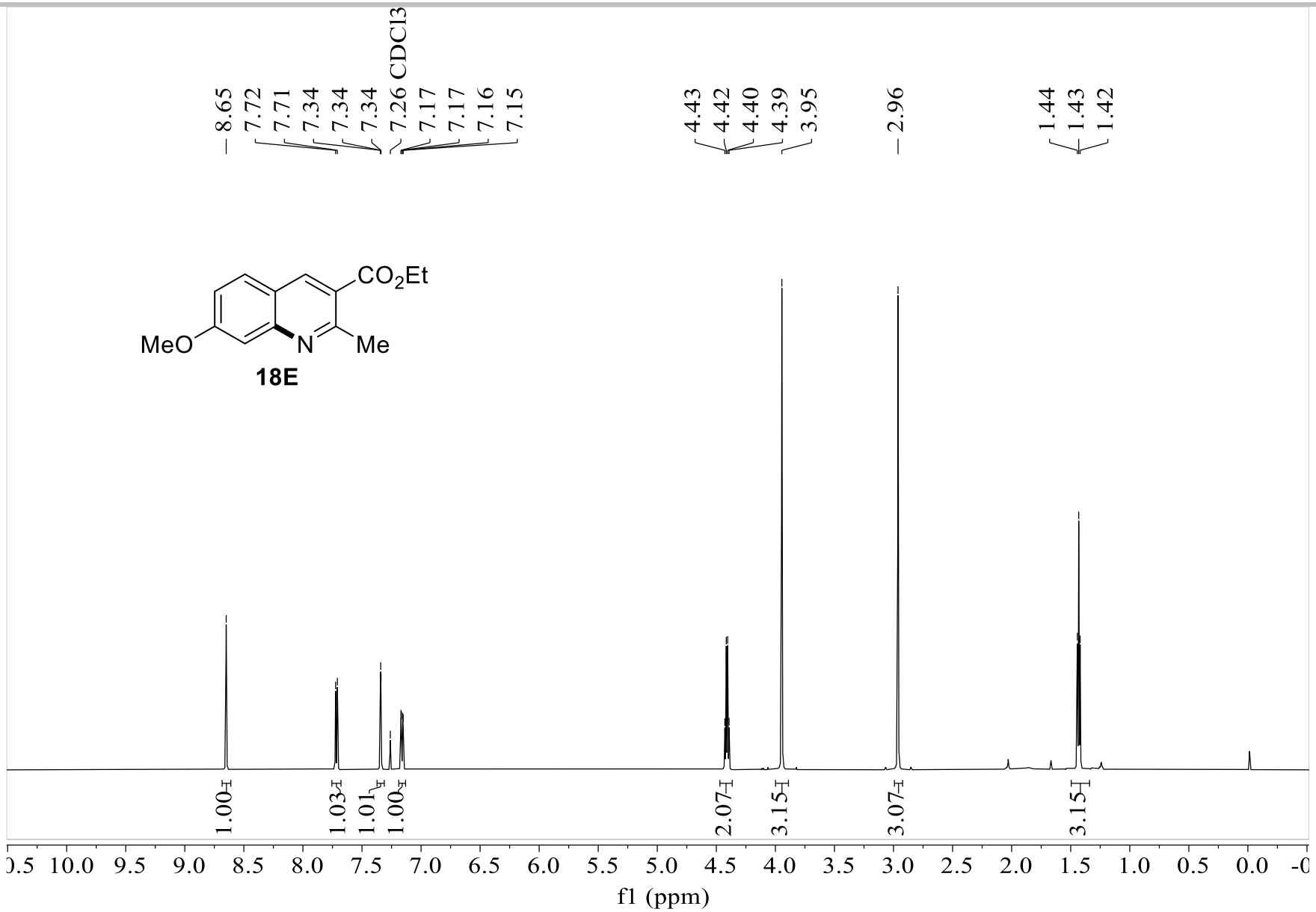
133.29
133.07
132.86
129.71
127.36
126.63
126.60
126.56
126.00
124.79
122.99
122.32
122.30
121.18
77.16 CDCl3
61.87
25.80
14.41
CO2Et
F3C
N
Me
18D
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.72
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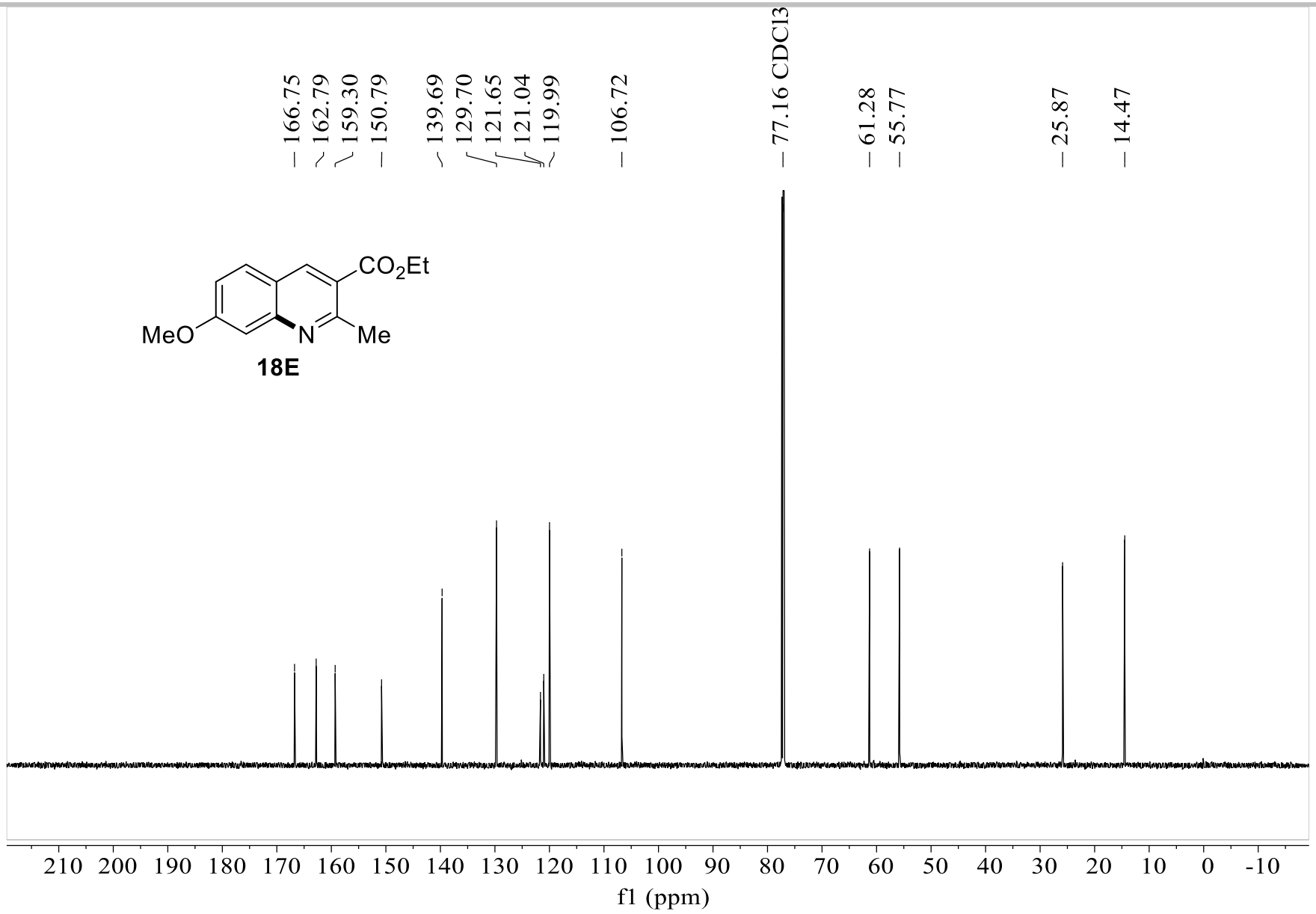
7.34
7.34
7.34
7.26 CDCl3
7.17
7.17
7.16
7.15
4.43
4.42
4.40
4.39
3.95
2.96
1.44
1.43
1.42
CO2Et
MeO
N
Me
18E
1.00
1.03
1.01
1.00
2.07
3.15
3.07
3.15
f1 (ppm)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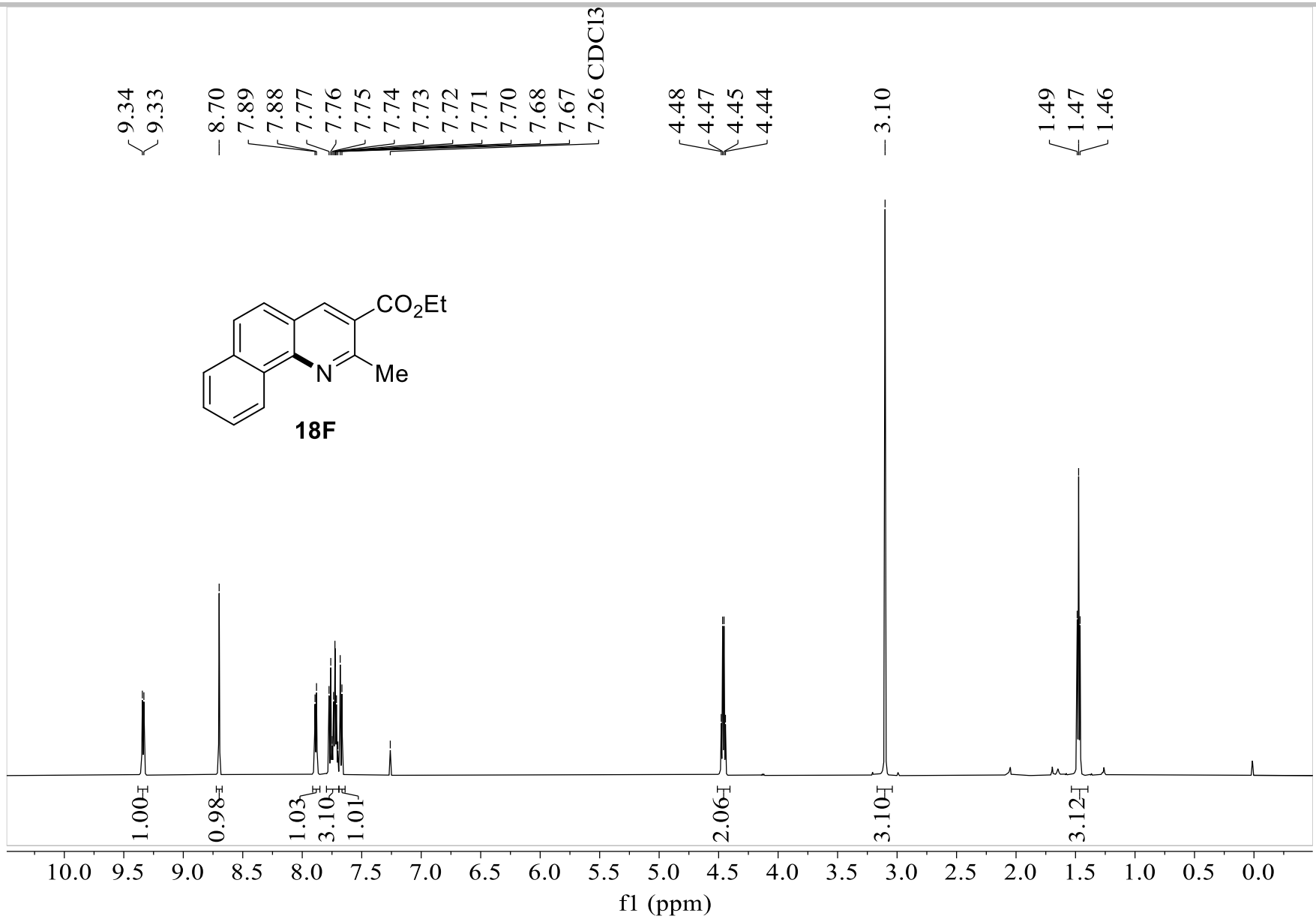
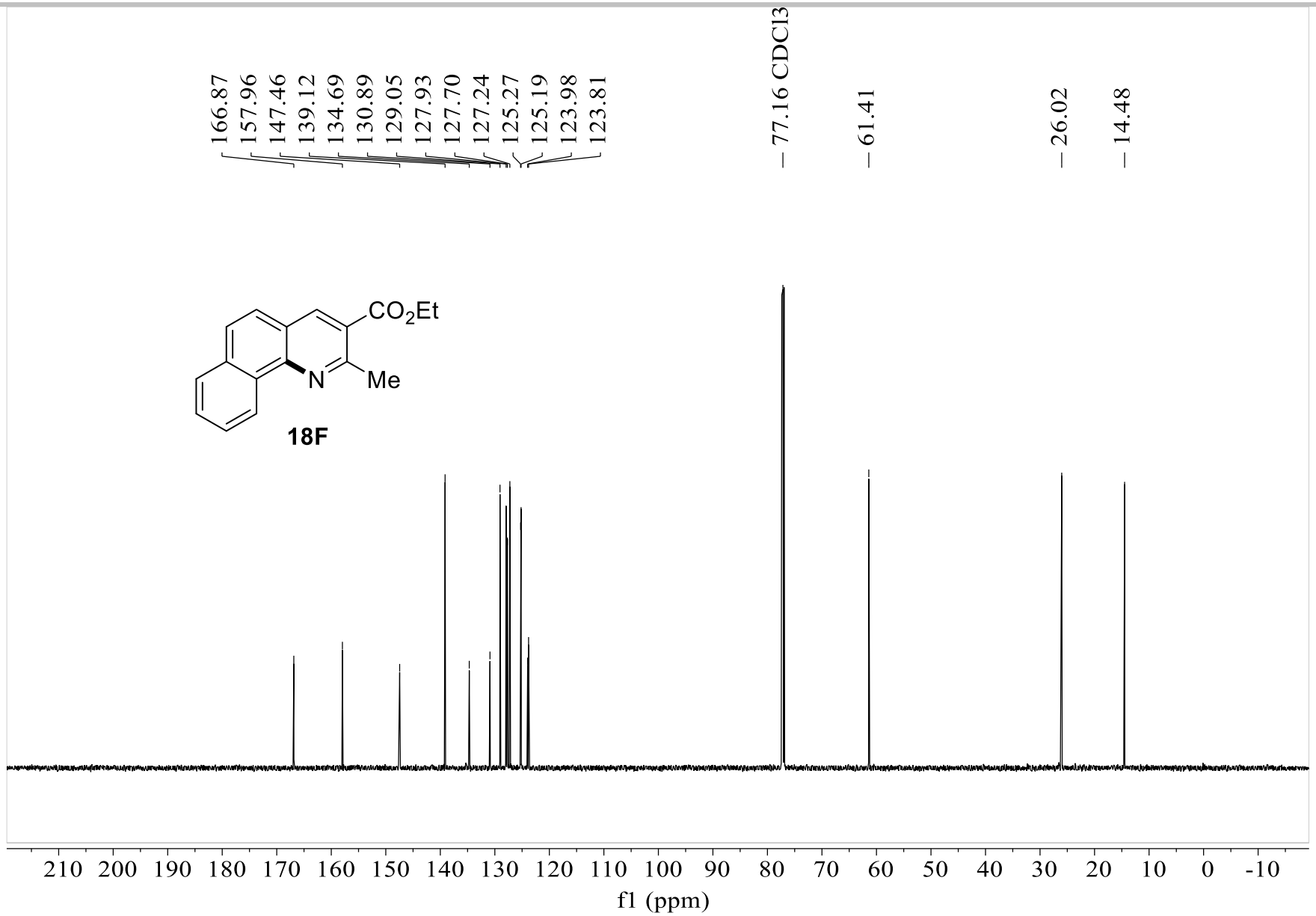
162.79
159.30
150.79
139.69
129.70
121.65
121.04
119.99
106.72
77.16 CDCl3
61.28
55.77
25.87
14.47
CO2Et
MeO
N
Me
18E
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


9.34
9.33
8.70
7.89
7.88
7.77
7.76
7.75
7.74
7.73
7.72
7.71
7.70
7.68
7.67
7.26 CDCl3
4.48
4.47
4.45
4.44
3.10
1.49
1.47
1.46
CO2Et
N
Me
18F
1.00
0.98
1.03
3.10
1.01
2.06
3.10
3.12
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
f1 (ppm)


166.87
157.96
147.46
139.12
134.69
130.89
129.05
127.93
127.70
127.24
125.27
125.19
123.98
123.81
77.16 CDCl3
61.41
26.02
14.48
CO2Et
N
Me
18F
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)