Supporting Information

for

Catalyst-free, visible-light-promoted S–H insertion reaction between thiols and α-diazoesters

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List of Contents

1. General Information

^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra were recorded on an Agilent Technologies DD2 (600 MHz) or a Varian Mercury-400 Plus spectrometer in $CDCl_3$. High-resolution mass spectra (HRMS) were reported from the Thermo Orbitrap Elite or Bruker Daltonics APEXII 47e FT-ICR instrument with an ESI source. UV-Visible absorption spectra were recorded on an Agilent 8453 spectrophotometer. Unless otherwise noted, all reactions were carried out in Pyrex glass tube with magnetic stirring bar. Reactions were monitored by thin layer chromatography (TLC) using pre-coated silica gel plates (GF254). Flash column chromatography was performed on silica gel 60 (particle size 200–400 mesh ASTM, purchased from Liangchen, China) and eluted with petroleum ether/ethylacetate.

All thiols (**1a–1x**) and ethyl diazoacetate (**2a**) used in the substrate expansion study of this work were purchased from Bidepharm.com or Energy Chemical, and were used directly without further purification. Aryldiazoacetates (**2b–2q**) used in this work were prepared according to the corresponding literature procedure.[1] Anhydrous acetylene (MeCN) was distilled from phosphorus pentoxide (P_2O_5) to use.

The 23 W CFL lamps employed in this work were bought from supermarket. The distance from the light source to the irradiation vessel is about 2.5 cm (**Figure S1**). The temperature was controlled by a fan.

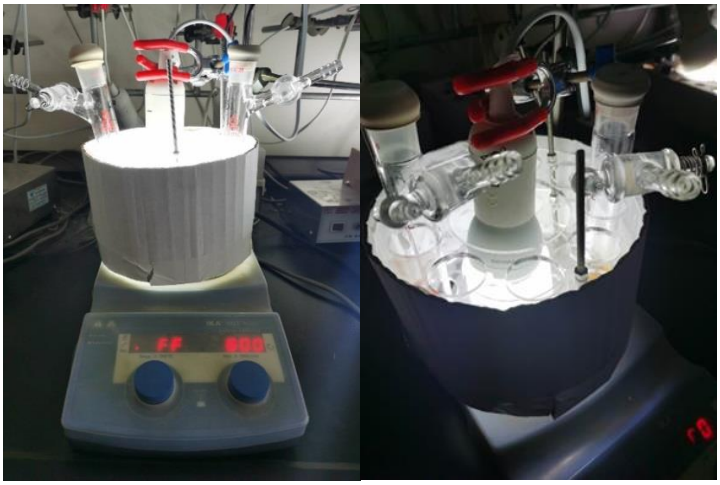
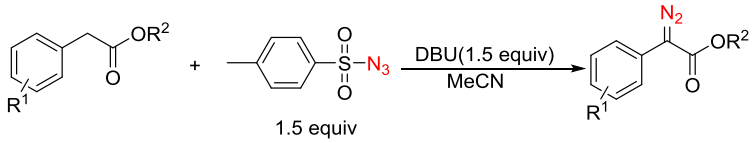


Figure S1. Setup of Photochemical Reaction

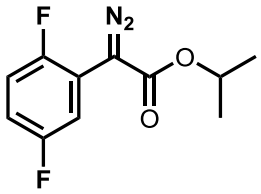
2. General procedure for preparation of α-diazoesters[1]



To a mixture of ester (10 mmol) and tosyl azide (2.96 g, 15 mmol) in anhydrous MeCN (15 mL), 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) (2.24 mL, 2.28 g, 15 mmol) was added. The reaction mixture was stirred at room temperature for overnight. Upon complete consumption of the starting materials, the reaction mixture was quenched with saturated aqueous solution of NH_4Cl (5 mL), extracted with CH_2Cl_2 (3 × 30 mL), washed with brine (3 × 10 mL), dried over $MgSO_4$, and concentrated under reduced pressure. The residue was purified by flash chromatography (hexane : EtOAc = 9:1) to afford the α-diazoester.

Except for α-diazoacetates **2n**, the other aryl diazoacetates **2b–2q** used in this work are all reported products.[1-7] The characterization data of new diazoacetate **2n** are listed as follow:

Isopropyl 2-diazo-2-(2,5-difluorophenyl)acetate (2n)



General procedure above is employed with Isopropyl 2-(2,5-difluorophenyl)acetate (2.14 g, 10 mmol) and tosyl azide (2.96 g, 15 mmol). Purification by flash column chromatography on silica gel (hexane : EtOAc = 9:1) to affords the title product **2n**.

Yellow oil; yield: 1.92 g (80%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.56–7.51 (m, 1H), 7.03–6.97 (m, 1H), 6.89–6.83 (m, 1H), 5.23–5.14 (m, 1H), 1.32 (d, *J* = 6.4 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 164.2, 160.0, 157.6, 155.1, 116.4 (d, *J* = 9.2 Hz), 116.2 (d, *J* = 9.1 Hz), 115.1 (d, *J* = 27.2 Hz), 114.1 (d, *J* = 8.4 Hz), 113.9 (d, *J* = 8.6 Hz), 69.2, 22.0.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -117.94–118.05 (m), -120.99 (s).

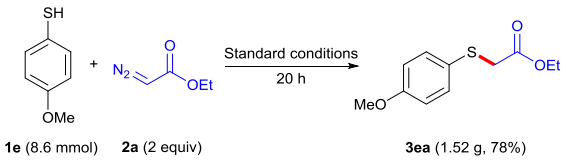
HRMS (ESI): m/z $[M+Na]^+$ calcd for $C_{11}H_{10}F_2N_2NaO_2^+$: 263.0603; found: 263.0598.

3. Experimental Procedures

1) General procedure for synthesis of 3

Thiol **1** (0.3 mmol), α-diazoacetate **2** (0.6 mmol, 2 equiv) and MeCN/H_2O (10:1, 3 mL) were added into a 25 mL Pyrex glass tube. The reaction mixture was continually stirred at room temperature under a 23 W CFL irradiation until thiol **1** was consumed completely (monitored by TLC). The reaction solution was quenched with saturated aq. NaCl (2 mL) and extracted with EtOAc (3 × 5 mL). The combined organic phase was dried over anhydrous Na_2SO_4, filtrated and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (PE : EtOAc = 20:1) to afford the pure product **3**.

2) Procedure for gram-scale synthesis of 3ea

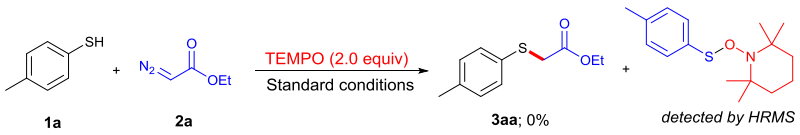


1e (8.6 mmol) **2a** (2 equiv) **3ea** (1.52 g, 78%)

4-Methoxybenzenethiol **1e** (1.21 g, 8.6 mmol), ethyl diazoacetate **2a** (1.96 g, 17.2 mmol, 2 equiv) and MeCN/H_2O (10:1, 15 mL) were added into a 50 mL Pyrex glass tube. The reaction mixture was continually stirred at room temperature under a 23 W CFL irradiation for 20 hours until **1e** was consumed completely (monitored by TLC). The reaction solution was quenched with saturated aq. NaCl (10 mL) and extracted with EtOAc (3 × 15 mL). The combined organic phase was dried over anhydrous Na_2SO_4, filtrated and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (PE : EtOAc = 20:1) to afford the desired product **3ea** (1.52 g, 78% yield).

3) Procedure for control experiments

(1) Radical-trapping experiment with TEMPO



1a **2a** **3aa**; 0% *detected by HRMS*

4-Methylbenzenethiol **1a** (37.3 mg, 0.3 mmol), ethyl diazoacetate **2a** (0.6 mmol, 68.5 mg, 2 equiv), TEMPO (93.8 mg, 0.6 mmol, 2.0 equiv) and MeCN/H_2O (10:1, 3 mL) were added into a 25

mL Pyrex glass tube. The reaction mixture was continually stirred at room temperature under a 23 W CFL irradiation for 18 hours. The reaction solution was concentrated under reduced pressure and the residue was analyzed by TLC and HRMS, respectively. There, **3aa** was not detected with TLC and the TEMPO trapped thiyl radical was detected by HRMS (**Figure S2**, data of $[M+H]^+$ are showed).

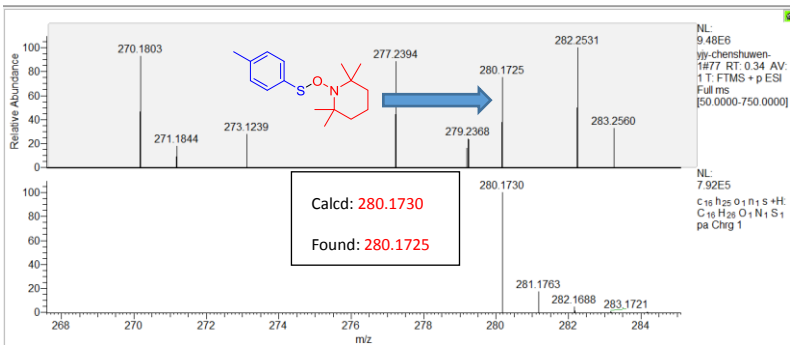
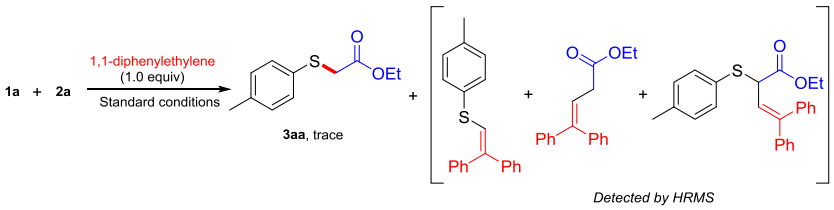


Figure S2

(2) Radical-trapping experiment with 1,1-diphenylethylene



4-Methylbenzenethiol **1a** (37.3 mg, 0.3 mmol), ethyl diazoacetate **2a** (0.6 mmol, 68.5 mg, 2 equiv), 1,1-diphenylethylene (54.1 mg, 0.3 mmol, 1.0 equiv) and MeCN/H_2O (10:1, 3 mL) were added into a 25 mL Pyrex glass tube. The reaction mixture was continually stirred at room temperature under a 23 W CFL irradiation for 18 hours, only a trace amount of **3aa** was detected by TLC and the radical intermediates trapped by 1,1-diphenylethylene were detected by HRMS (**Figure S3-S5**, data of $[M+H]^+$ are showed).

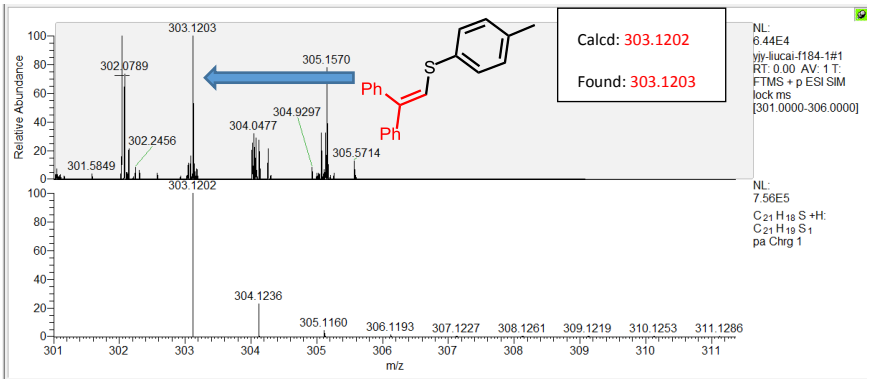


Figure S3

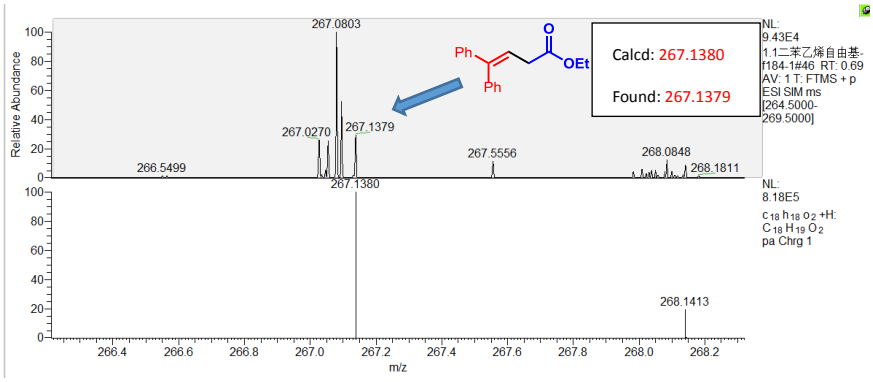


Figure S4

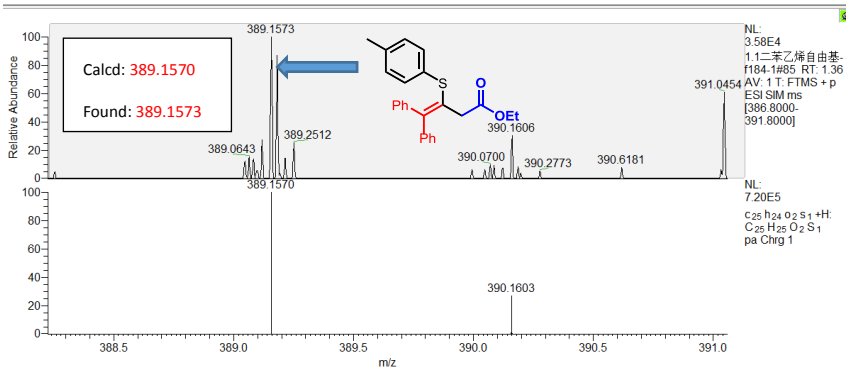
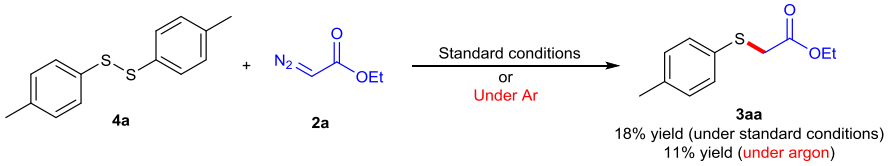


Figure S5

(4) The experiment starting from disulfide 4a

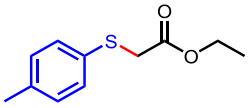


1,2-Di-*p*-tolyldisulfane **4a** (73.9 mg, 0.3 mmol), ethyl diazoacetate **2a** (68.5 mg, 0.6 mmol, 2 equiv) and MeCN:H_2O (10:1, 3 mL) were added into a 25 mL Pyrex glass tube. The reaction

mixture was continually stirred at room temperature under a 23 W CFL irradiation for 18 hours. The reaction solution was quenched with saturated aq. NaCl (2 mL) and extracted with EtOAc (3 × 5 mL). The combined organic phase was dried over anhydrous Na_2SO_4, filtrated and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (PE : EtOAc = 20:1) to afford pure **3aa** in 18% yield. In addition, **3aa** was obtained in 11% yield under argon atmosphere.

4. Characterization Data of Products

1) Ethyl 2-(*p*-tolylthio)acetate (3aa)[8]



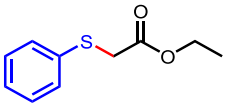
Colorless oil; yield: 56.1 mg (89%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.33 (d, *J* = 8.4 Hz, 2H), 7.11 (d, *J* = 8.4 Hz, 2H), 4.15 (q, *J* = 7.2 Hz, 2H), 3.57 (s, 2H), 2.32 (s, 3H), 1.22 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 169.6, 135.0, 133.3, 130.0, 129.0, 126.9, 61.5, 36.7, 14.0.

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{11}H_{15}O_2S^+$: 211.0787; found: 211.0790.

2) Ethyl 2-(phenylthio)acetate (3ba)[9]

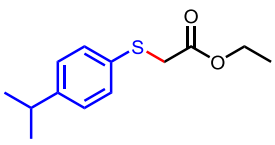


Colorless oil; yield: 49.5 mg (84%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.41–7.40 (m, 2H), 7.30–7.28 (m, 2H), 7.23–7.20 (m, 1H), 4.15 (q, *J* = 7.2 Hz, 2H), 3.63 (s, 2H), 1.21 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 169.7, 137.2, 131.1, 130.9, 129.7, 61.3, 37.3, 21.0, 14.0.

3) Ethyl 2-((4-isopropylphenyl)thio)acetate (3ca)[9]

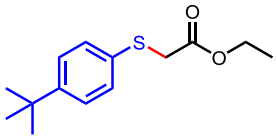


Colorless oil; yield: 57.9 mg (81%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.35 (d, *J* = 8.4 Hz, 2H), 7.16 (d, *J* = 8.4 Hz, 2H), 4.15 (q, *J* = 7.2 Hz, 2H), 3.58 (s, 2H), 2.89–2.85 (m, 1H), 1.23 (s, 3H), 1.22 (s, 3H), 1.21 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 169.8, 148.2, 131.5, 130.9, 127.2, 61.4, 37.3, 33.7, 23.8, 14.0.

4) Ethyl 2-((4-(*tert*-butyl)phenyl)thio)acetate (3da)[9]

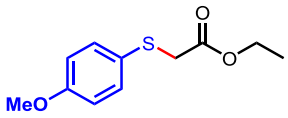


Colorless oil; yield: 56.8 mg (75%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.35 (dd, *J* = 7.8, 1.8 Hz, 2H), 7.32 (dd, *J* = 7.8, 1.8 Hz, 2H), 4.15 (q, *J* = 7.2 Hz, 2H), 3.59 (s, 2H), 1.29 (s, 9H), 1.21 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 169.8, 150.4, 131.3, 130.4, 126.0, 61.4, 37.1, 34.5, 31.2, 14.0.

5) Ethyl 2-((4-methoxyphenyl)thio)acetate (3ea)[8]



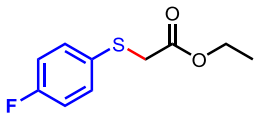
Colorless oil; yield: 64.5 mg (95%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.40 (dd, *J* = 6.6, 2.4 Hz, 2H), 6.83 (dd, *J* = 6.6, 2.4 Hz, 2H), 4.12 (q, *J* = 7.2 Hz, 2H), 3.77 (s, 3H), 3.49 (s, 2H), 1.20 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 169.8, 159.6, 134.1, 124.9, 114.6, 61.3, 55.2, 38.6, 14.0.

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{11}H_{15}O_3S^+$: 227.0736; found: 227.0739.

6) Ethyl 2-((4-fluorophenyl)thio)acetate (3fa)[9]



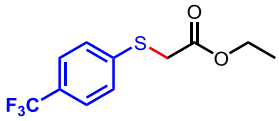
Colorless oil; yield: 54.6 mg (85%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.42 (dd, *J* = 9.0, 5.4 Hz, 2H), 6.99 (t, *J* = 9.0 Hz, 2H), 4.13 (q, *J* = 7.2 Hz, 2H), 3.54(s, 2H), 1.20 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$) :δ = 169.8, 162.4 (d, *J* = 246.15 Hz), 133.4 (d, *J* = 8.1 Hz), 129.7 (d, *J* = 3.3 Hz), 116.1 (d, *J* = 2.75 Hz), 61.5, 37.8, 14.1.

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{10}H_{12}FO_2S^+$: 215.0537; found: 215.0533.

7) Ethyl 2-((4-(trifluoromethyl)phenyl)thio)acetate (3ga)[8]

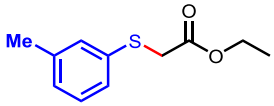


Colorless oil; yield: 47.6 mg (60%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.42 (dd, *J* = 9.0, 5.4 Hz, 2H), 6.99 (t, *J* = 9.0 Hz, 2H), 4.13 (q, *J* = 7.2 Hz, 2H), 3.54 (s, 2H), 1.20 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 169.1, 140.5, 134.9, 128.4 (q, *J* = 32.4 Hz), 128.1, 125.8 (q, *J* = 3.9 Hz), 124.0 (q, *J* = 240.3 Hz), 61.8, 35.4, 14.0.

8) Ethyl 2-(*m*-tolylthio)acetate (3ha)[8]



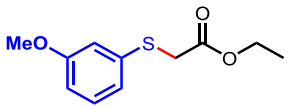
Colorless oil; yield: 55.5 mg (88%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.22 (m, 3H), 7.02 (d, *J* = 7.2 Hz, 1H), 4.16 (q, *J* = 7.2 Hz, 2H), 3.61 (s, 2H), 2.31 (s, 3H), 1.22 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 169.7, 138.7, 134.7, 130.5, 128.8, 127.7, 126.9, 61.4, 36.6, 21.2, 14.0.

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{11}H_{15}O_2S^+$: 211.0787; found: 211.0790.

9) Ethyl 2-((3-methoxyphenyl)thio)acetate (3ia)[8]



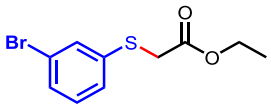
Colorless oil; yield: 56.3 mg (83%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.19 (t, *J* = 8.4 Hz, 1H), 6.97–6.95 (m, 2H), 6.75 (dd, *J* = 8.4, 2.4 Hz, 1H), 4.16 (q, *J* = 7.2 Hz, 2H), 3.78 (s, 3H), 3.63 (s, 2H), 1.22 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 169.6, 159.8, 136.3, 129.8, 121.7, 114.8, 112.7, 61.5, 55.2, 36.5, 14.1.

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{11}H_{15}O_3S^+$: 227.0736; found: 227.0739.

10) Ethyl 2-((3-bromophenyl)thio)acetate (3ja)[10]

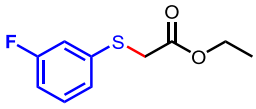


Colorless oil; yield: 63.6 mg (77%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.54 (t, *J* = 1.8 Hz, 1H), 7.34–7.30 (m, 2H), 7.15 (t, *J* = 8.4 Hz, 1H), 4.17 (q, *J* = 7.2 Hz, 2H), 3.63 (s, 2H), 1.23 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 169.2, 137.4, 132.0, 130.3, 129.8, 128.0, 122.8, 61.7, 36.3, 14.1.

11) Ethyl 2-((3-fluorophenyl)thio)acetate (3ka)[9]



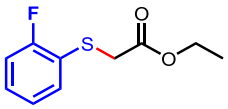
Colorless oil; yield: 48.9 mg (76%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.44 (dd, *J* = 8.8, 5.2 Hz, 2H), 7.00 (t, *J* = 8.8 Hz, 2H), 4.22 (q, *J* = 7.2 Hz, 2H), 3.56 (s, 2H), 1.22 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 169.7, 163.6, 161.1, 133.4 (d, *J* = 8.2 Hz), 129.7, 116.2, 116.0, 61.5, 37.8, 14.0

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{10}H_{12}FO_2S^+$: 215.0537; found: 215.0533.

12) Ethyl 2-((2-fluorophenyl)thio)acetate (3la)



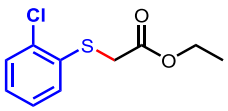
Colorless oil; yield: 59.1 mg (92%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.47–7.44 (m, 1H), 7.28–7.24 (m, 1H), 7.10–7.05 (m, 2H), 4.12 (q, *J* = 7.2 Hz, 2H), 3.60 (s, 2H), 1.18 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 169.3, 161.8 (d, *J* = 245.1 Hz), 133.4 (d, *J* = 1.35 Hz), 129.6 (d, *J* = 7.8 Hz), 124.5 (d, *J* = 3.75 Hz), 121.4 (d, *J* = 17.55 Hz), 115.8 (d, *J* = 22.35 Hz), 61.5, 36.0, 14.0.

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{10}H_{12}FO_2S^+$: 215.0537; found: 215.0533.

13) Ethyl 2-((2-chlorophenyl)thio)acetate (3ma)[9]

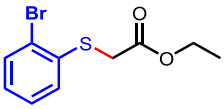


Colorless oil; yield: 56.8 mg (82%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.41–7.36 (m, 2H), 7.23–7.20 (m, 1H), 7.17–7.14 (m, 1H), 4.16 (q, *J* = 7.2 Hz, 2H), 3.67 (s, 2H), 1.22 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 169.1, 134.2, 134.1, 130.0, 129.8, 127.7, 127.2, 61.7, 35.2, 14.0.

14) Ethyl 2-((2-bromophenyl)thio)acetate (3na)[10]

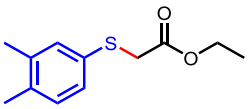


Colorless oil; yield: 59.4 mg (72%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.55 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.38 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.27 (dd, *J* = 7.2, 1.2 Hz, 1H), 7.08–7.05 (m, 1H), 4.17 (q, *J* = 7.2 Hz, 2H), 3.67 (s, 2H), 1.23 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$) δ = 169.1, 134.3, 133.1, 129.5, 127.9, 127.7, 124.2, 61.7, 35.6, 14.1.

15) Ethyl 2-((3,4-dimethylphenyl)thio)acetate (3oa)



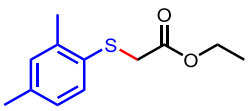
Colorless oil; yield: 57.9 mg (86%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.21 (br, 1H), 7.17–7.16 (m, 1H), 7.06 (d, *J* = 7.8 Hz, 1H), 4.15 (q, *J* = 7.2 Hz, 2H), 3.57 (s, 2H), 2.23 (s, 3H), 2.22 (s, 3H), 1.22 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 169.9, 137.4, 136.0, 132.1, 131.3, 130.3, 128.3, 61.4, 37.4, 19.7, 19.4, 14.1.

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{12}H_{16}NaO_2S^+$: 247.0763; found: 247.0761.

16) Ethyl 2-((2,4-dimethylphenyl)thio)acetate (3pa)[9]



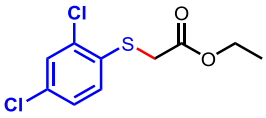
Colorless oil; yield: 61.9 mg (92%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.29 (d, *J* = 8.4 Hz, 1H), 7.01 (s, 1H), 6.96 (d, *J* = 7.8 Hz, 1H), 4.13 (q, *J* = 7.2 Hz, 2H), 3.54 (s, 2H), 2.40 (s, 3H), 2.28 (s, 3H), 1.21 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 169.7, 139.0, 137.3, 131.2, 131.1, 130.2, 127.3, 61.4, 36.6, 20.9, 20.3, 14.0.

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{12}H_{16}NaO_2S^+$: 247.0763; found: 247.0761.

17) Ethyl 2-((2,4-dichlorophenyl)thio)acetate (3qa)



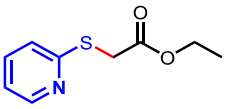
Colorless oil; yield: 70.0 mg (88%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.40 (d, *J* = 8.4 Hz, 1H), 7.35 (d, *J* = 8.4 Hz, 1H), 7.20 (dd, *J* = 8.4, 2.4 Hz, 1H), 4.16 (q, *J* = 7.2 Hz, 2H), 3.64 (s, 2H), 1.23 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 168.9, 135.2, 133.2, 132.8, 131.1, 129.6, 127.5, 61.8, 35.3, 14.1.

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{10}H_{11}Cl_2O_2S^+$: 264.9851; found: 264.9853.

18) Ethyl 2-(pyridin-2-ylthio)acetate (3ra)[9]



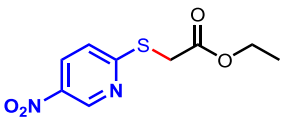
Colorless oil; yield: 48.5 mg (82%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.37 (dd, J = 4.8, 1.2 Hz, 1H), 7.48–7.45 (m, 1H), 7.21 (d, *J* = 8.4 Hz, 1H), 6.98–6.96 (m, 1H), 4.18 (q, *J* = 7.2 Hz, 2H), 3.96 (s, 2H), 1.24 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 169.7, 156.9, 149.3, 136.0, 121.9, 119.7, 61.5, 32.3, 14.1.

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_9H_{12}NO_2S^+$: 198.0583; found: 198.0586.

19) Ethyl 2-((5-nitropyridin-2-yl)thio)acetate (3sa)



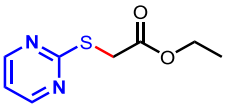
Colorless oil; yield: 63.2 mg (87%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 9.19 (d, *J* = 2.4 Hz, 1H), 8.25 (dd, *J* = 9.0, 3.0 Hz, 1H), 7.36 (d, *J* = 9.0 Hz, 1H), 4.21 (q, *J* = 7.2 Hz, 2H), 4.03 (s, 2H), 1.27 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 168.5, 165.4, 114.9, 130.6, 121.3, 61.9, 32.7, 14.1.

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_9H_{11}N_2O_4S^+$: 243.0434; found: 243.0435.

20) Ethyl 2-(pyrimidin-2-ylthio)acetate (3ta)



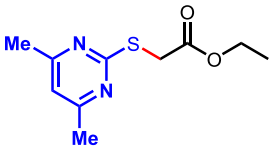
Colorless oil; yield: 53.5 mg (90%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.49 (d, *J* = 4.8 Hz, 2H), 6.96 (t, *J* = 4.8 Hz, 1H), 4.19 (q, *J* = 7.2 Hz, 2H), 3.91 (s, 2H), 1.24 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 170.8, 169.1, 157.2, 116.8, 61.6, 33.4, 14.1.

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_8H_{11}N_2O_2S^+$: 199.0536; found: 199.0537.

21) Ethyl 2-((4,6-dimethylpyrimidin-2-yl)thio)acetate (3ua)[11]

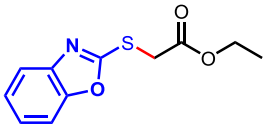


Colorless oil; yield: 63.1 mg (93%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 6.96 (s, 1H), 4.19 (q, *J* = 7.2 Hz, 2H), 3.90 (s, 2H), 2.37 (s, 6H), 1.26 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 169.5, 169.4, 167.0, 115.9, 61.4, 33.5, 23.7, 14.2.

22) Ethyl 2-(benzo[d]oxazol-2-ylthio)acetate (3va)



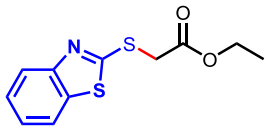
Colorless oil; yield: 34.2 mg (48%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.59–7.58 (m, 1H), 7.44–7.43 (m, 1H), 7.29–7.26 (m, 1H), 7.24–7.23 (m, 1H), 4.25 (q, *J* = 7.2 Hz, 2H), 4.11 (s, 2H), 1.28 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 167.9, 163.3, 152.1, 141.7, 124.4, 124.1, 118.6, 110.0, 62.2, 34.2, 14.1.

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{11}H_{12}NO_3S^+$: 238.0532; found: 238.0535.

23) Ethyl 2-(benzo[*d*]thiazol-2-ylthio)acetate (3wa)



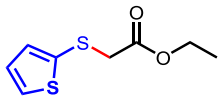
Colorless oil; yield: 47.9 mg (63%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.84 (d, *J* = 7.8 Hz, 1H), 7.74 (d, *J* = 7.8 Hz, 1H), 7.41–7.39 (m, 1H), 7.30–7.28 (m, 1H), 4.24 (q, *J* = 7.2 Hz, 2H), 4.16 (s, 2H), 1.28 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 168.2, 164.7, 152.9, 135.5, 126.0, 124.4, 121.7, 121.0, 62.0, 35.1, 14.1.

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{11}H_{12}NO_2S_2^+$: 254.0304; found: 254.0307.

24) Ethyl 2-(thiophen-2-ylthio)acetate (3xa)[9]



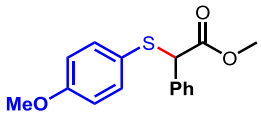
Colorless oil; yield: 48.5 mg (80%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.37 (dd, *J* = 5.4, 1.2 Hz, 1H), 7.20 (dd, *J* = 3.6, 1.2 Hz, 1H), 6.97 (dd, *J* = 5.4, 3.6 Hz, 1H), 4.16 (q, *J* = 7.2 Hz, 2H), 3.49 (s, 2H), 1.24 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 169.3, 135.0, 132.4, 130.5, 127.6, 61.5, 41.0, 14.1.

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_8H_{11}O_2S_2^+$: 203.0195; found: 203.0197.

25) Methyl 2-((4-methoxyphenyl)thio)-2-phenylacetate (3eb)[12]



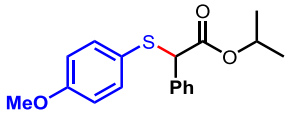
Colorless oil; yield: 61.4 mg (71%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.39–7.38 (m, 2H), 7.32–7.28 (m, 5H), 6.80–6.77 (m, 2H), 4.76 (s, 1H), 3.78 (s, 3H), 3.66 (s, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 171.0, 160.2, 136.2, 135.8, 128.5, 128.1, 123.6, 114.5, 110.0, 57.4, 55.3, 52.5.

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{16}H_{17}O_3S^+$: 289.0893; found: 289.0896.

26) Isopropyl 2-((4-methoxyphenyl)thio)-2-phenylacetate (3ec)



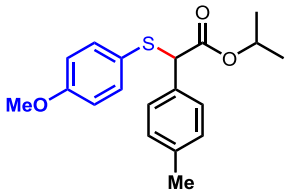
Colorless oil; yield: 74.0 mg (78%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.40 (d, *J* = 7.2 Hz, 2H), 7.33–7.27 (m, 5H), 6.78 (d, *J* = 8.4 Hz, 2H), 4.98–4.94 (m, 1H), 4.72 (s, 1H), 3.78 (s, 3H), 1.14 (t, *J* = 7.2 Hz, 6H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 170.0, 160.1, 136.1, 136.0, 128.6, 128.5, 128.0, 123.9, 114.4, 69.2, 57.5, 55.3, 21.6, 21.5.

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{18}H_{21}O_3S^+$: 317.1206; found: 317.1208.

27) Isopropyl 2-((4-methoxyphenyl)thio)-2-(*p*-tolyl)acetate (3ed)



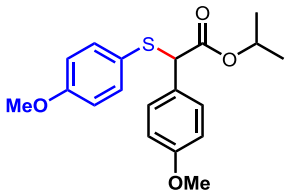
Colorless oil; yield: 75.3 mg (76%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.35 (d, *J* = 8.4 Hz, 2H), 7.31 (d, *J* = 7.8 Hz, 2H), 7.11 (d, *J* = 8.4 Hz, 2H), 6.79 (d, *J* = 8.4 Hz, 2H), 4.98–4.94 (m, 1H), 4.71 (s, 1H), 3.77 (s, 3H), 2.32 (s, 3H), 1.15 (d, *J* = 6.6 Hz, 3H), 1.14 (d, *J* = 6.0 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 170.1, 160.0, 137.8, 135.8, 132.9, 129.1, 128.4, 124.3, 114.4, 69.0, 57.2, 55.2, 21.6, 21.5, 21.1.

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{19}H_{23}O_3S^+$: 331.1362; found: 331.1364.

28) Isopropyl 2-(4-methoxyphenyl)-2-((4-methoxyphenyl)thio)acetate (3ee)



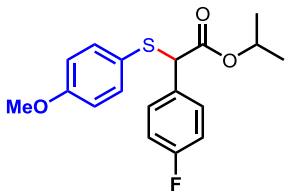
Colorless oil; yield: 85.1 mg (82%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.35–7.26 (m, 4H), 6.85–6.82 (m, 2H), 6.80–6.78 (m, 2H), 4.98–4.92 (m, 1H), 4.70 (s, 1H), 3.78 (d, *J* = 6.6 Hz, 6H), 1.14 (dd, *J* = 12.6, 6.3 Hz, 6H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 170.2, 160.0, 159.4, 136.0, 129.7, 127.9, 124.0, 114.4, 113.9, 69.0, 56.8, 55.3, 55.2, 21.7, 21.6.

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{19}H_{23}O_4S^+$: 347.1312; found: 347.1314.

29) Isopropyl 2-(4-fluorophenyl)-2-((4-methoxyphenyl)thio)acetate (3ef)



Colorless oil; yield: 68.2 mg (68%).

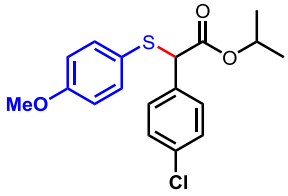
^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.37–7.35 (m, 2H), 7.31–7.29 (m, 2H), 6.97 (t, *J* = 9.0 Hz, 2H), 6.78 (d, *J* = 9.0 Hz, 2H), 4.98–4.94 (m, 1H), 4.69 (s, 1H), 3.77 (s, 3H), 1.15 (d, *J* = 7.2 Hz, 6H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 169.8, 162.5 (d, *J* = 245.7 Hz), 160.3, 136.2, 131.9 (d, *J* = 3.15 Hz), 130.3 (d, *J* = 33.0 Hz), 123.6, 115.3 (d, *J* = 21.45 Hz), 114.5, 69.3, 56.7, 55.3, 21.5.

^{19}F NMR (287 MHz, $CDCl_3$): δ = -114.277—-114.314 (m).

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{18}H_{20}FO_3S^+$: 335.1112; found: 335.1114.

30) Isopropyl 2-(4-chlorophenyl)-2-((4-methoxyphenyl)thio)acetate (3eg)



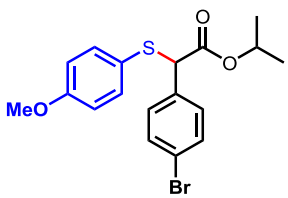
Colorless oil; yield: 73.7 mg (70%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.33–7.29 (m, 4H), 7.25 (d, *J* = 8.4 Hz, 2H), 6.78 (d, *J* = 8.4 Hz, 2H), 5.00–4.93 (m, 1H), 4.67 (s, 1H), 3.77 (s, 3H), 1.15 (d, *J* = 6.0 Hz, 6H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 169.6, 160.3, 136.2, 134.7, 133.9, 129.9, 128.6, 123.4, 114.5, 69.3, 56.8, 55.3, 21.5.

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{18}H_{20}ClO_3S^+$: 351.0816; found: 351.0820.

31) Isopropyl 2-(4-bromophenyl)-2-((4-methoxyphenyl)thio)acetate (3eh)



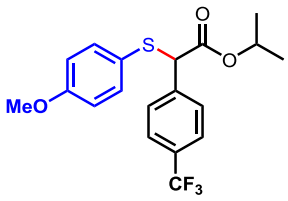
Colorless oil; yield: 77.1 mg (65%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.32–7.29 (m, 4H), 7.26 (d, *J* = 9.0 Hz, 2H), 6.78 (d, *J* = 8.4 Hz, 2H), 4.98–4.94 (m, 1H), 4.67 (s, 1H), 3.77 (s, 3H), 1.15 (d, *J* = 6.0 Hz, 6H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 169.6, 160.3, 136.3, 134.6, 133.9, 129.9, 128.6, 123.4, 114.5, 69.4, 56.7, 55.3, 21.5.

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{18}H_{20}BrO_3S^+$: 395.0311; found: 395.0312.

32) Isopropyl 2-((4-methoxyphenyl)thio)-2-(4-(trifluoromethyl)phenyl)acetate (3ei)



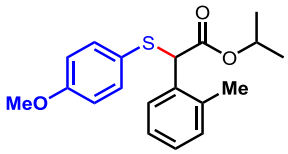
Colorless oil; yield: 69.2 mg (60%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.55 (d, *J* = 7.8 Hz, 2H), 7.49 (d, *J* = 8.4 Hz, 2H), 7.31–7.28 (m, 2H), 6.78 (dd, *J* = 7.2, 2.4 Hz, 2H), 5.00–4.95 (m, 1H), 4.72 (m, 1H), 3.78 (s, 3H), 1.16 (d, *J* = 3.6 Hz, 3H), 1.15 (d, J = 3.0 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 169.4, 160.4, 140.1, 136.4, 130.3, 130.0, 128.9, 125.4 (t, *J* = 3.8 Hz), 124.9, 123.1 (d, *J* = 9.0 Hz), 114.5, 69.6, 57.0, 55.3, 21.5.

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{19}H_{20}F_3O_3S^+$: 385.1080; found: 385.1081.

33) Isopropyl 2-((4-methoxyphenyl)thio)-2-(*o*-tolyl)acetate (3ej)



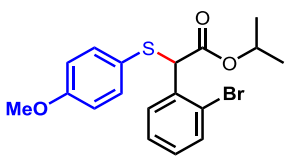
Colorless oil; yield: 71.3 mg (72%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.56–7.52 (m, 1H), 7.38–7.34 (m, 2H), 7.19–7.13 (m, 3H), 6.8–6.77 (m, 2H), 5.03–4.94 (m, 2H), 3.78 (s, 3H), 2.34 (s, 3H), 1.14 (dd, *J* = 6.4, 1.2 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 170.3, 160.0, 136.1, 136.0, 134.2, 130.4, 128.2, 127.8, 126.3, 124.0, 114.3, 69.1, 55.3, 53.8, 21.5, 21.4, 19.5.

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{19}H_{23}O_3S^+$: 331.1362; found: 331.1364.

34) Isopropyl 2-(2-bromophenyl)-2-((4-methoxyphenyl)thio)acetate (3ek)



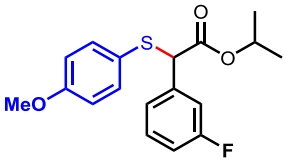
Colorless oil; yield: 85.4 mg (72%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.64 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.53 (dd, *J* =7.8, 1.2 Hz, 1H), 7.39–7.36 (m, 2H), 7.29–7.26 (m, 1H), 7.14–7.11 (m, 1H), 6.80–6.78 (m, 2H), 5.28 (s, 1H), 5.01–4.97 (m, 1H), 3.78 (s, 3H), 1.17 (s, 3H), 1.16 (s, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 169.6, 160.2, 136.3, 135.5, 132.8, 130.2, 129.3, 127.6, 124.5, 123.9, 114.4, 69.4, 55.9, 55.3, 21.6, 21.5.

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{18}H_{20}BrO_3S^+$: 395.0311; found: 395.0312.

35) Isopropyl 2-(3-fluorophenyl)-2-((4-methoxyphenyl)thio)acetate (3el)



Colorless oil; yield: 66.2 mg (66%).

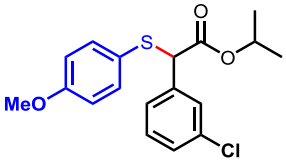
^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.32–7.30 (m, 2H), 7.25–7.22 (m, 1H), 7.17–7.12 (m, 2H), 6.98–6.95 (m, 1H), 6.80–6.77 (m, 2H), 4.99–4.95 (m, 1H), 4.68 (s, 1H), 3.77 (s, 3H), 1.16 (d, *J* = 6.0 Hz, 3H), 1.15 (d, *J* = 6.0 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 169.5, 162.6 (d, *J* = 244.95 Hz), 160.3, 138.4 (d, J = 7.5 Hz), 136.2, 129.8 (d, J = 8.25 Hz), 124.3 (d, J = 2.7 Hz), 123.3, 115.6 (d, J = 22.8 Hz), 115.0 (d, J = 21.0 Hz), 114.5, 69.4, 57.0, 56.9, 55.3, 21.5.

^{19}F NMR (287 MHz, $CDCl_3$): δ = -113.006—-113.070 (m).

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{18}H_{20}FO_3S^+$: 335.1112; found: 335.1113.

36) Isopropyl 2-(3-chlorophenyl)-2-((4-methoxyphenyl)thio)acetate (3em)



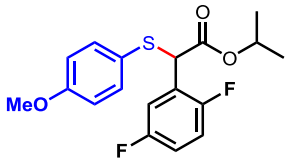
Colorless oil; yield: 82.1 mg (78%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.39 (t, *J* = 1.8 Hz, 1H), 7.34–7.28 (m, 2H), 7.27–7.23 (m, 2H), 7.23–7.19 (m, 1H), 6.83–6.76 (m, 2H), 4.99–4.94 (m, 1H), 4.65 (s, 1H), 3.77 (s, 3H), 1.15 (dd, *J* = 8.7, 6.3 Hz, 6H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 169.5, 160.3, 138.0, 136.3, 134.2, 129.6, 128.7, 128.2, 126.8, 123.2, 114.5, 69.4, 56.9, 55.3, 21.6, 21.5.

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{18}H_{20}ClO_3S^+$: 351.0816; found: 351.0819.

37) Isopropyl 2-(2,5-difluorophenyl)-2-((4-methoxyphenyl)thio)acetate (3en)



Colorless oil; yield: 70.8 mg (67%).

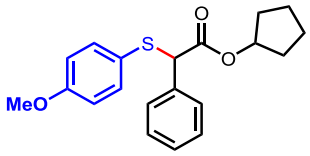
^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.34–7.28 (m, 3H), 6.97–6.91 (m, 2H), 6.79 (d, *J* = 9.0 Hz, 2H), 5.01 (s, 1H), 5.00–4.96 (m, 2H), 3.77 (s, 3H), 1.18 (d, *J* = 2.4 Hz, 3H), 1.17 (d, *J* = 3.0 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 169.0, 160.5, 158.4 (dd, *J* = 241.05, 2.4 Hz), 155.0 (dd, *J* = 242.4, 2.55 Hz), 136.5, 125.2 (q, *J* = 6.6 Hz), 122.7, 116.7 (dd, *J* = 25.5, 3.15 Hz), 116.1 (dd, *J* = 51.45, 8.55 Hz), 116.0 (dd, *J* = 8.55, 2.1 Hz), 114.5, 69.6, 55.3, 48.8, 21.5.

^{19}F NMR (287 MHz, $CDCl_3$): δ = -118.312—-118.393 (m), -123.948—-124.044 (m).

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{18}H_{18}F_2NaO_3S^+$: 375.0837; found: 375.0834.

38) Cyclopentyl 2-((4-methoxyphenyl)thio)-2-phenylacetate (3eo)



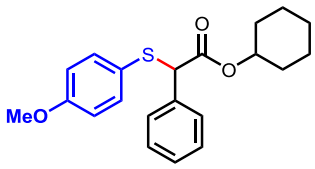
Colorless oil; yield: 67.8 mg (66%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.41–7.39 (m, 2H), 7.33–7.25 (m, 5H), 6.80–6.77 (m, 2H), 5.13–5.10 (m, 1H), 4.71 (s, 1H), 3.78 (s, 3H), 1.77–1.73 (m, 2H), 1.60–1.51 (m, 6H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 170.2, 160.1, 136.0, 135.9, 128.6, 128.5, 128.0, 123.9, 114.4, 76.8, 57.4, 55.3, 32.5, 32.4, 23.6.

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{20}H_{23}O_3S^+$: 343.1362; found: 343.1362.

39) Cyclohexyl 2-((4-methoxyphenyl)thio)-2-phenylacetate (3ep)



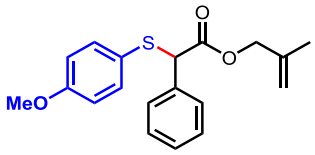
Colorless oil; yield: 86.6 mg (81%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.42–7.39 (m, 2H), 7.35–7.26 (m, 5H), 6.82–6.78 (m, 2H), 4.80–4.69 (m, 2H), 3.78 (s, 3H), 1.74–1.63 (m, 4H), 1.38–1.24 (m, 6H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 170.2, 160.1, 136.0, 135.9, 128.6, 128.5, 128.0, 123.9, 114.4, 76.8, 57.4, 55.3, 32.5, 32.4, 23.6.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{21}H_{24}NaO_3S^+$: 379.1338; found: 379.1343.

40) 2-Methylallyl 2-((4-methoxyphenyl)thio)-2-phenylacetate (3eq)



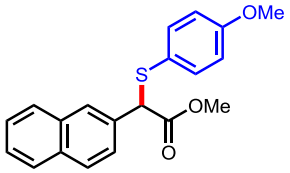
Colorless oil; yield: 62.0 mg (63%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.43–7.40 (m, 2H), 7.34–7.28 (m, 5H), 6.80–6.76 (m, 2H), 4.85 (d, *J* = 1.2 Hz, 2H), 4.79 (s, 1H), 4.48 (s, 2H), 3.78 (s, 3H), 1.63 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 170.2, 160.2, 139.4, 136.1, 135.7, 128.6, 128.2, 114.5, 113.3, 68.7, 57.5, 55.3, 19.3.

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{19}H_{21}O_3S^+$: 329.1206; found: 329.1210.

41) Methyl 2-((4-methoxyphenyl)thio)-2-(naphthalen-2-yl)acetate (3er)



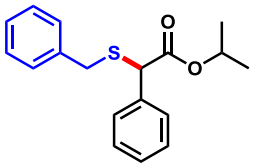
Colorless oil; yield: 73.1 mg (72%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.15 (d, *J* = 8.4 Hz, 1H), 7.88 (d, *J* = 8.0 Hz, 1H), 7.81 (d, *J* = 8.0 Hz, 1H), 7.66 (d, *J* = 7.2 Hz, 1H), 7.58–7.49 (m, 2H), 7.44–7.35 (m, 3H), 6.81–6.77 (m, 2H), 5.54 (s, 1H), 3.78 (s, 3H), 3.67 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 171.4, 160.2, 136.1, 133.9, 131.3, 130.9, 129.0, 128.9, 126.8, 126.6, 125.8, 125.3, 123.1, 114.4, 55.3, 54.1, 52.7.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{20}H_{18}NaO_3S^+$: 361.0869; found: 361.0868.

42) Isopropyl 2-(benzylthio)-2-phenylacetate (3yc)



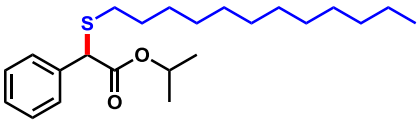
Colorless oil; yield: 65.7 mg (73%).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.41 (d, *J* = 7.2 Hz, 2H), 7.35–7.23 (m, 8H), 5.05–4.99 (m, 1H), 4.39 (s, 1H), 3.78 (d, *J* = 13.2 Hz, 1H), 3.64 (d, *J* = 13.2 Hz, 1H), 1.25 (d, *J* = 6.0 Hz, 3H), 1.19 (d, *J* = 6.0 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 170.1, 137.3, 136.2, 129.1, 128.6, 128.5, 128.0, 127.2, 69.2, 52.1, 36.3, 21.7, 21.6.

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{18}H_{21}O_2S^+$: 301.1257; found: 301.1254.

43) Isopropyl 2-(dodecylthio)-2-phenylacetate (3zc)



Colorless oil; yield: 75.0 mg (66%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.53–7.46 (m, 2H), 7.35–7.26 (m, 3H), 5.09–5.00 (m, 1H), 4.52 (d, *J* = 1.2 Hz, 1H), 2.57–2.45 (m, 2H), 1.59–1.51 (m, 2H), 1.41 (dd, *J* = 6.4, 1.4 Hz, 2H), 1.23 (m, 22H), 0.90–0.86 (m, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 170.5, 136.4, 128.5, 128.4, 127.9, 69.1, 52.4, 31.9, 29.6, 29.5, 29.4, 29.3, 29.1, 29.0, 28.8, 22.7, 21.7, 21.5, 14.1.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{23}H_{38}NaO_2S^+$: 401.2485; found: 401.2485.

5. References

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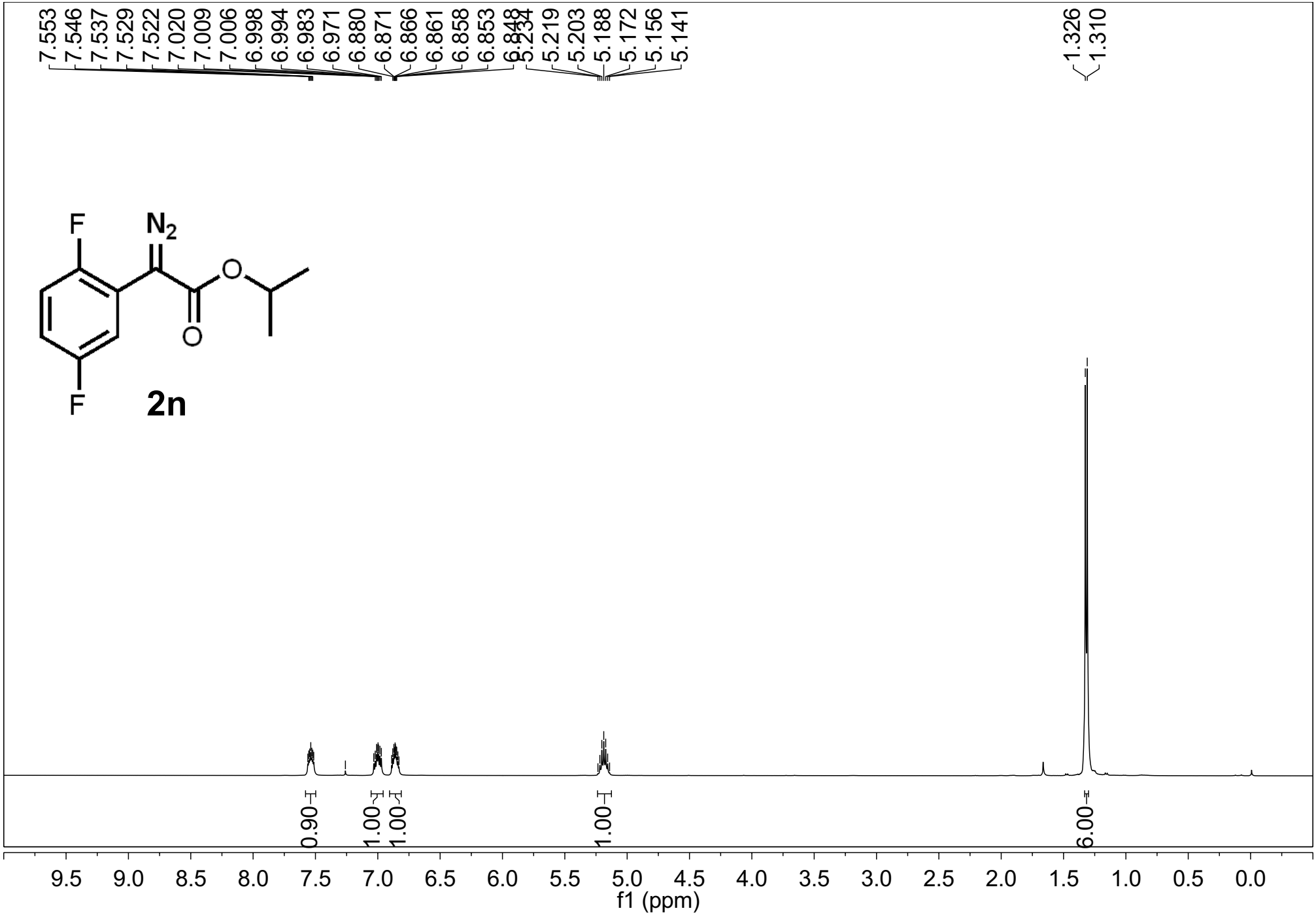
6. Cope of NMR Spectra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7.546
7.537
7.529
7.522
7.020
7.009
7.006
6.998
6.994
6.983
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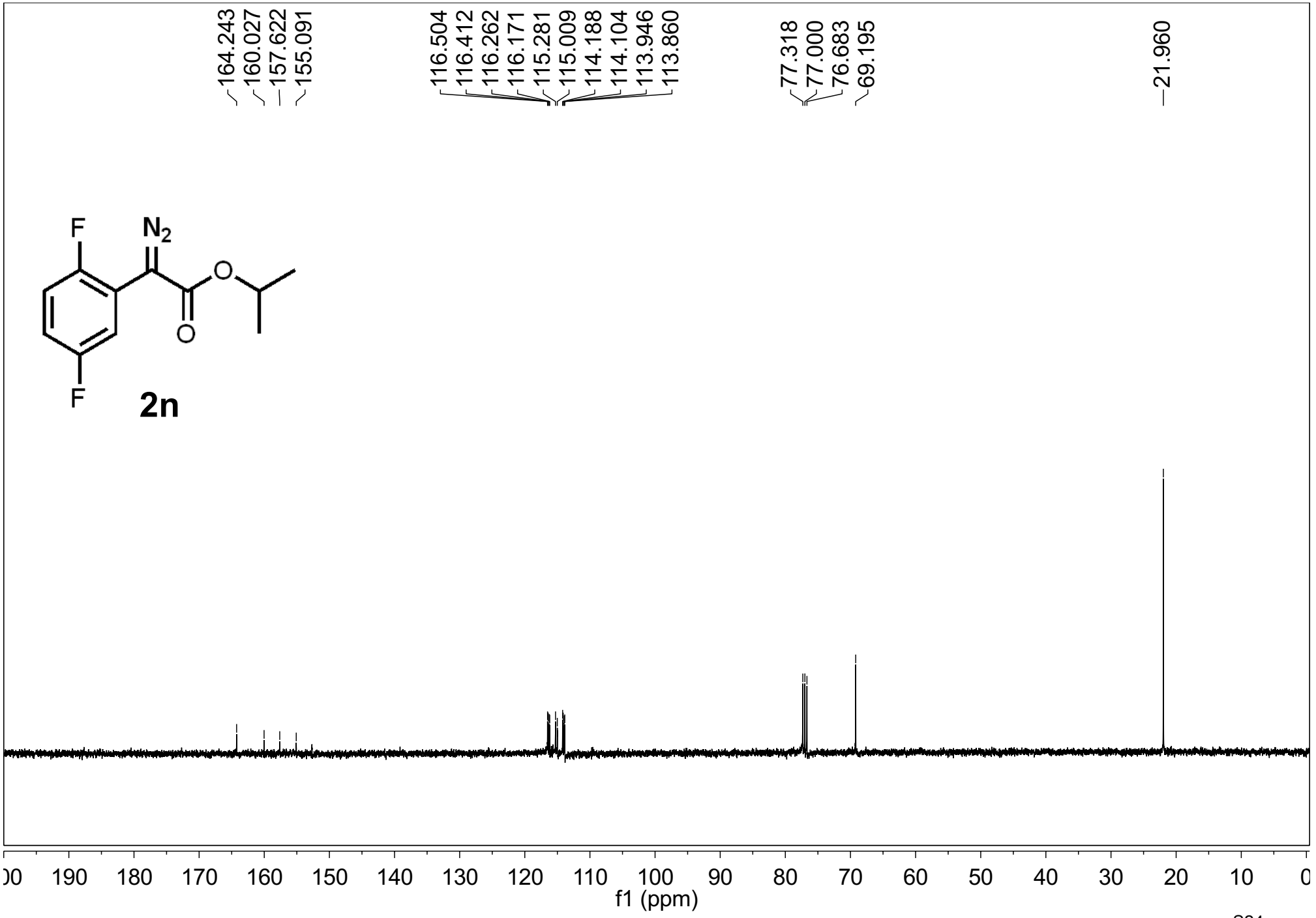
6.880
6.871
6.866
6.861
6.858
6.853
6.848
6.234
5.219
5.203
5.188
5.172
5.156
5.141
1.326
1.310
F
N2
O
O
F
2n
0.90
1.00
1.00
1.00
6.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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160.027
157.622
155.091
116.504
116.412
116.262
116.171
115.281
115.009
114.188
114.104
113.946
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77.000
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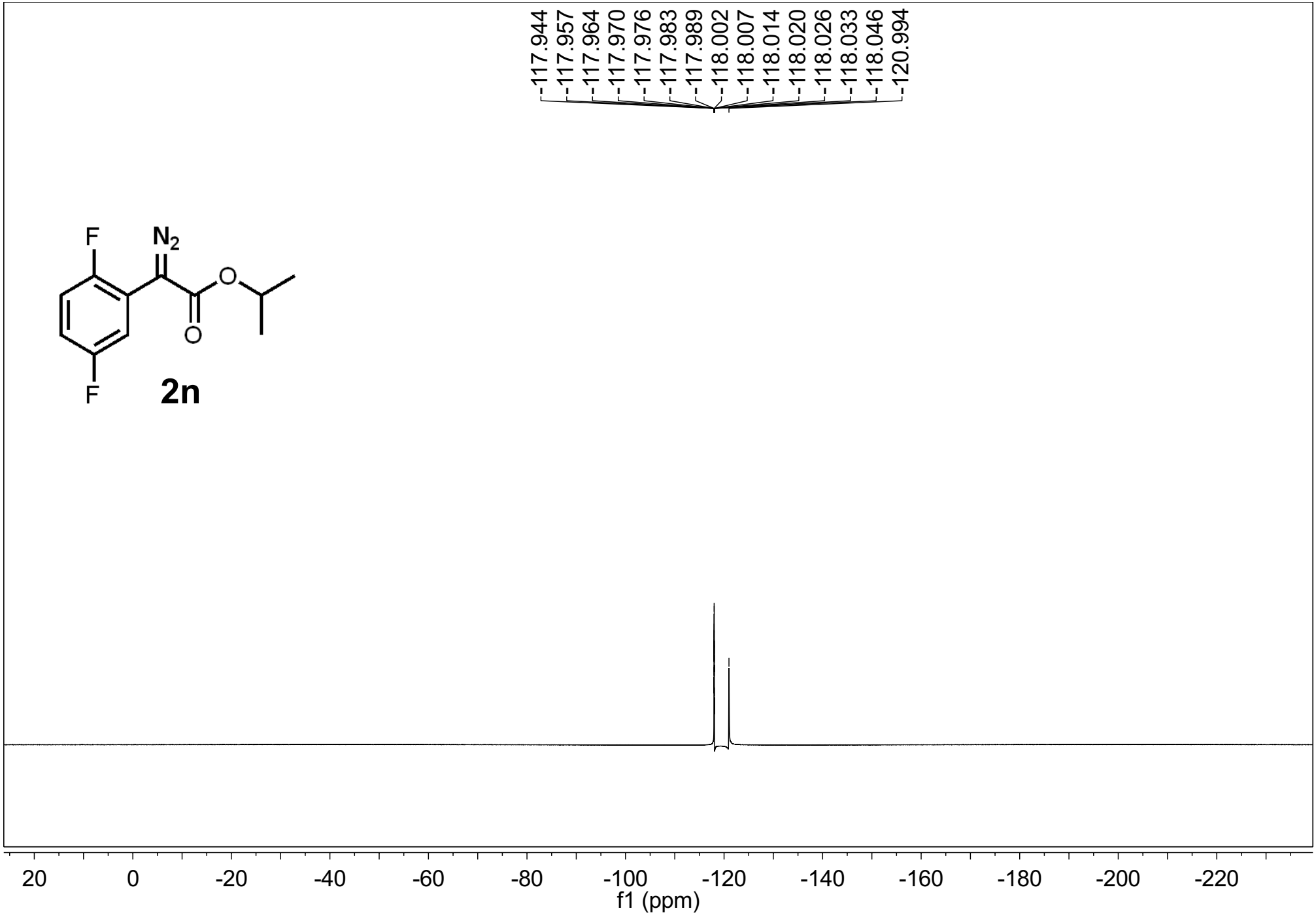
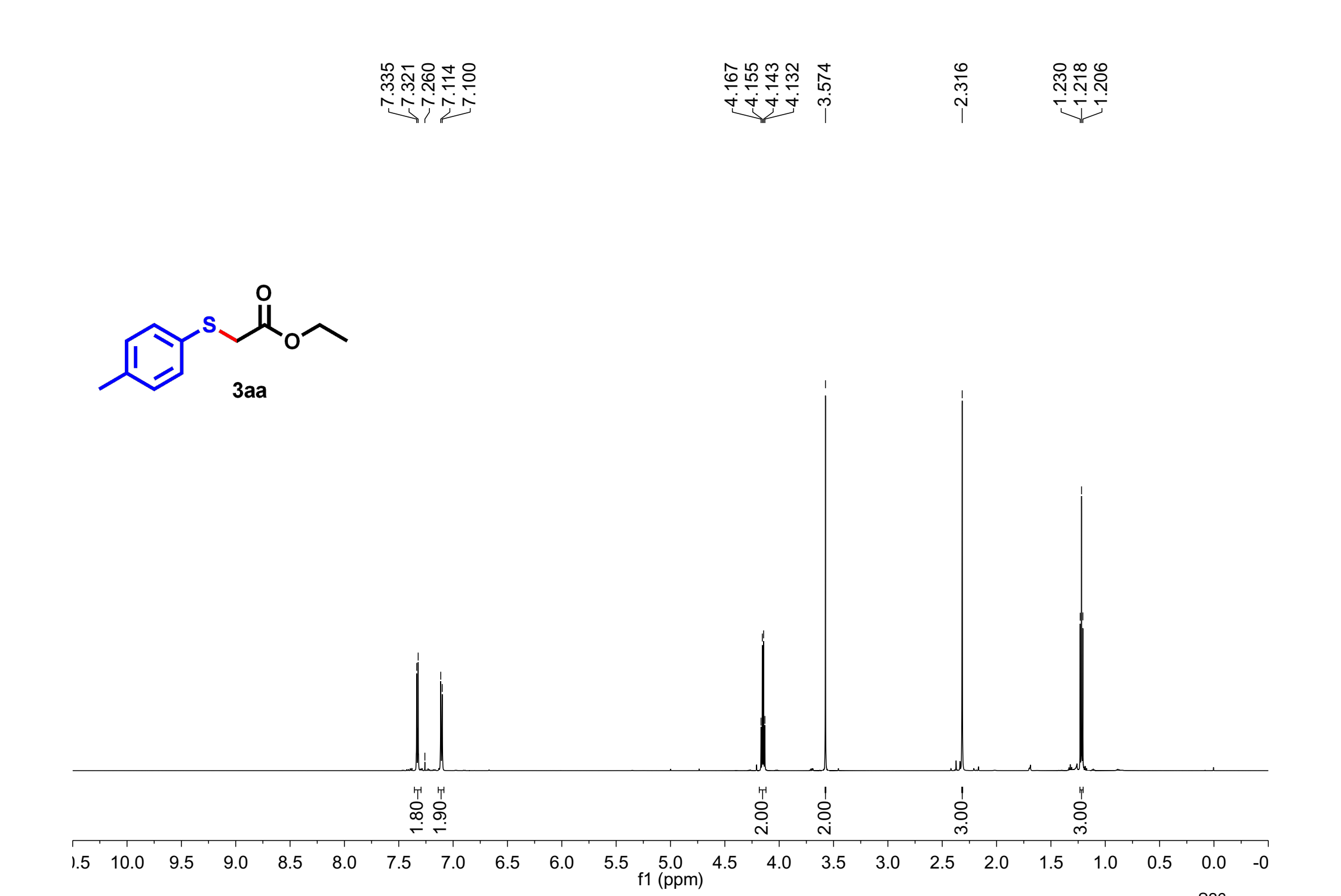
69.195
21.960
F
N2
O
O
F
2n
f1 (ppm)


-117.944
-117.957
-117.964
-117.970
-117.976
-117.983
-117.989
-118.002
-118.007
-118.014
-118.020
-118.026
-118.033
-118.046
-120.994
F
N2
O
O
F
2n
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
f1 (ppm)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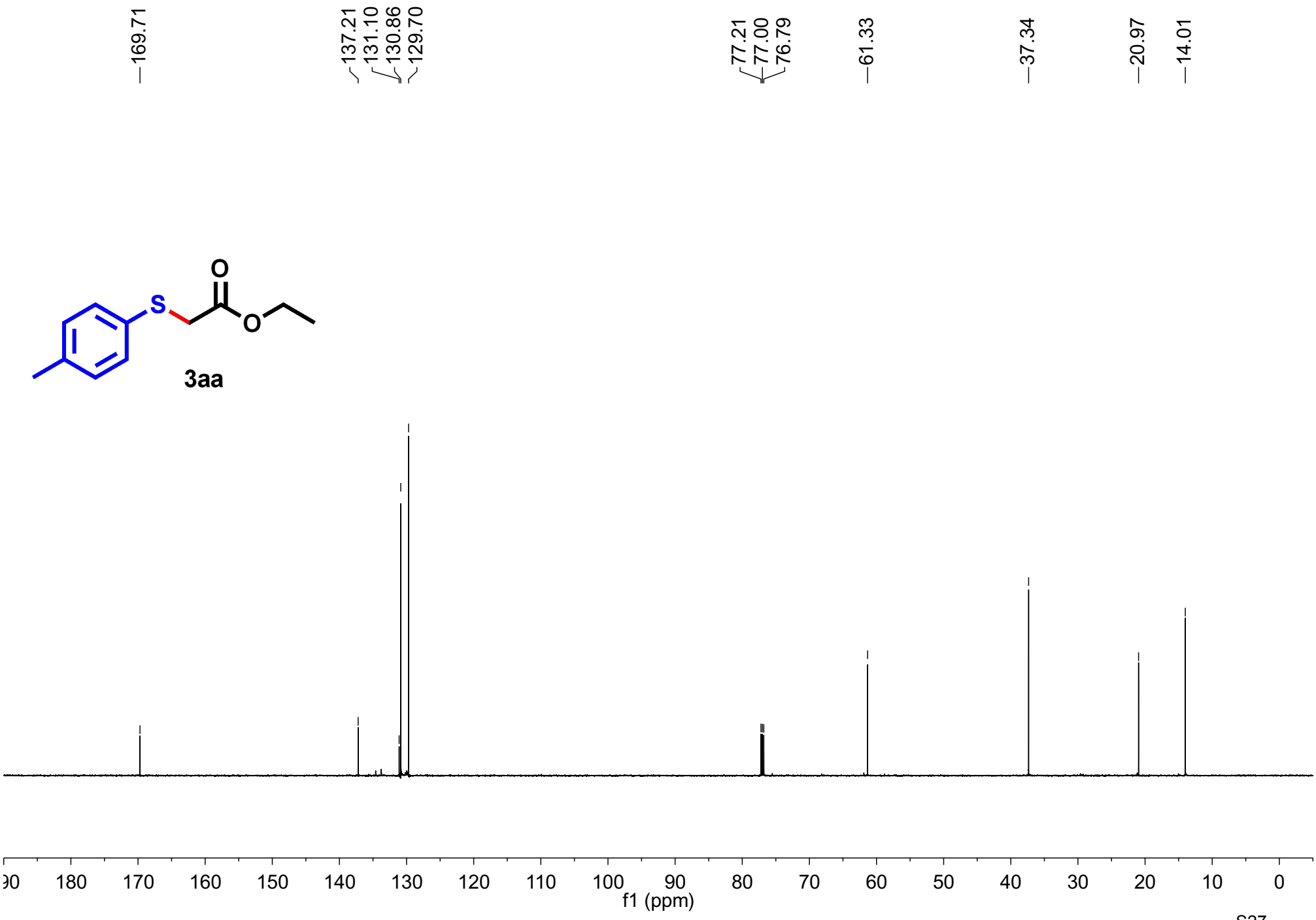
7.321
7.260
7.114
7.100
4.167
4.155
4.143
4.132
3.574
2.316
1.230
1.218
1.206
O
S
O
3aa
1.80
1.90
2.00
2.00
3.00
3.00
f1 (ppm)


169.71
137.21
131.10
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129.70
77.21
77.00
76.79
61.33
37.34
20.97
14.01
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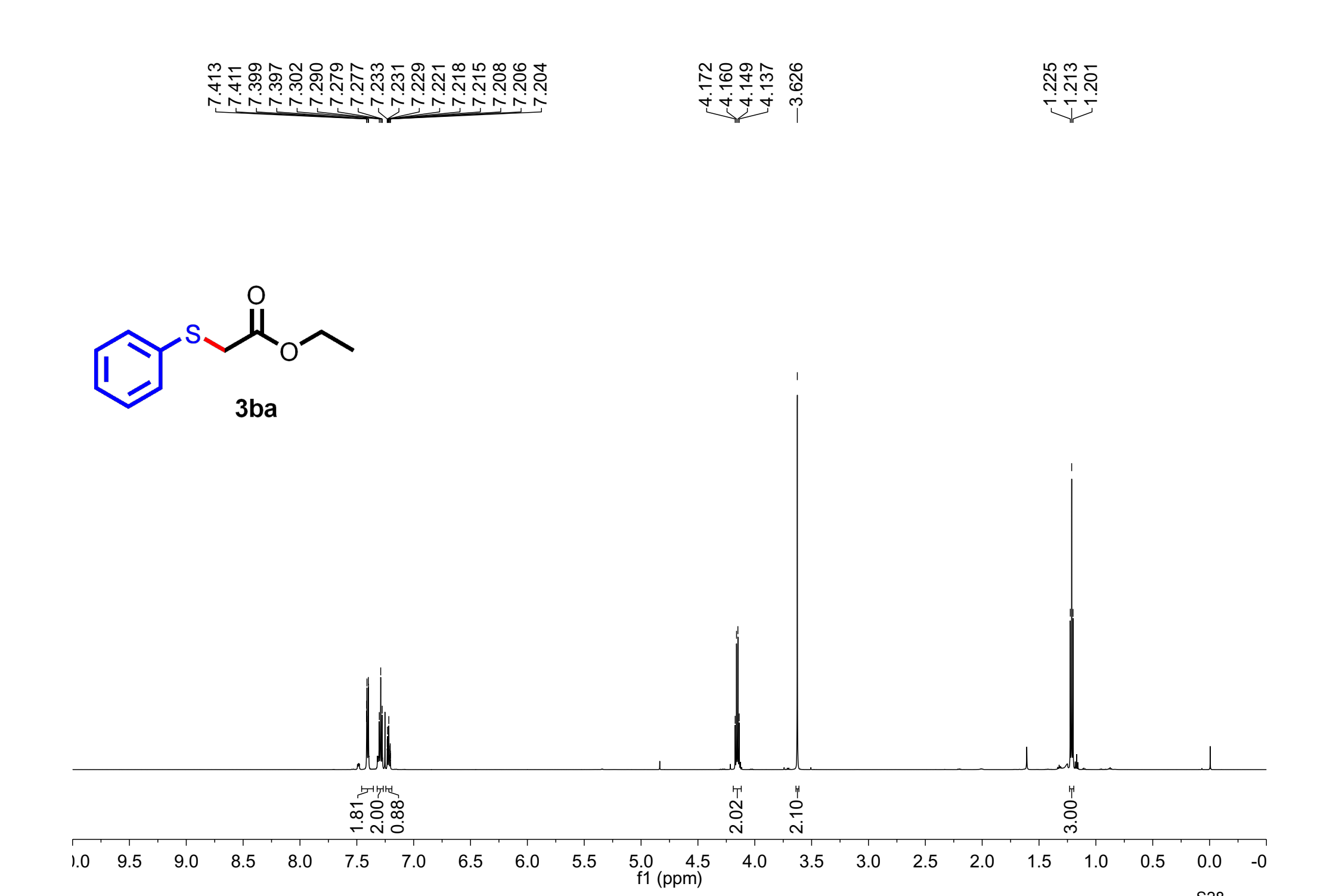
S
O
3aa
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.277
7.233
7.231
7.229
7.221
7.218
7.215
7.208
7.206
7.204
4.172
4.160
4.149
4.137
3.626
1.225
1.213
1.201
O
S
O
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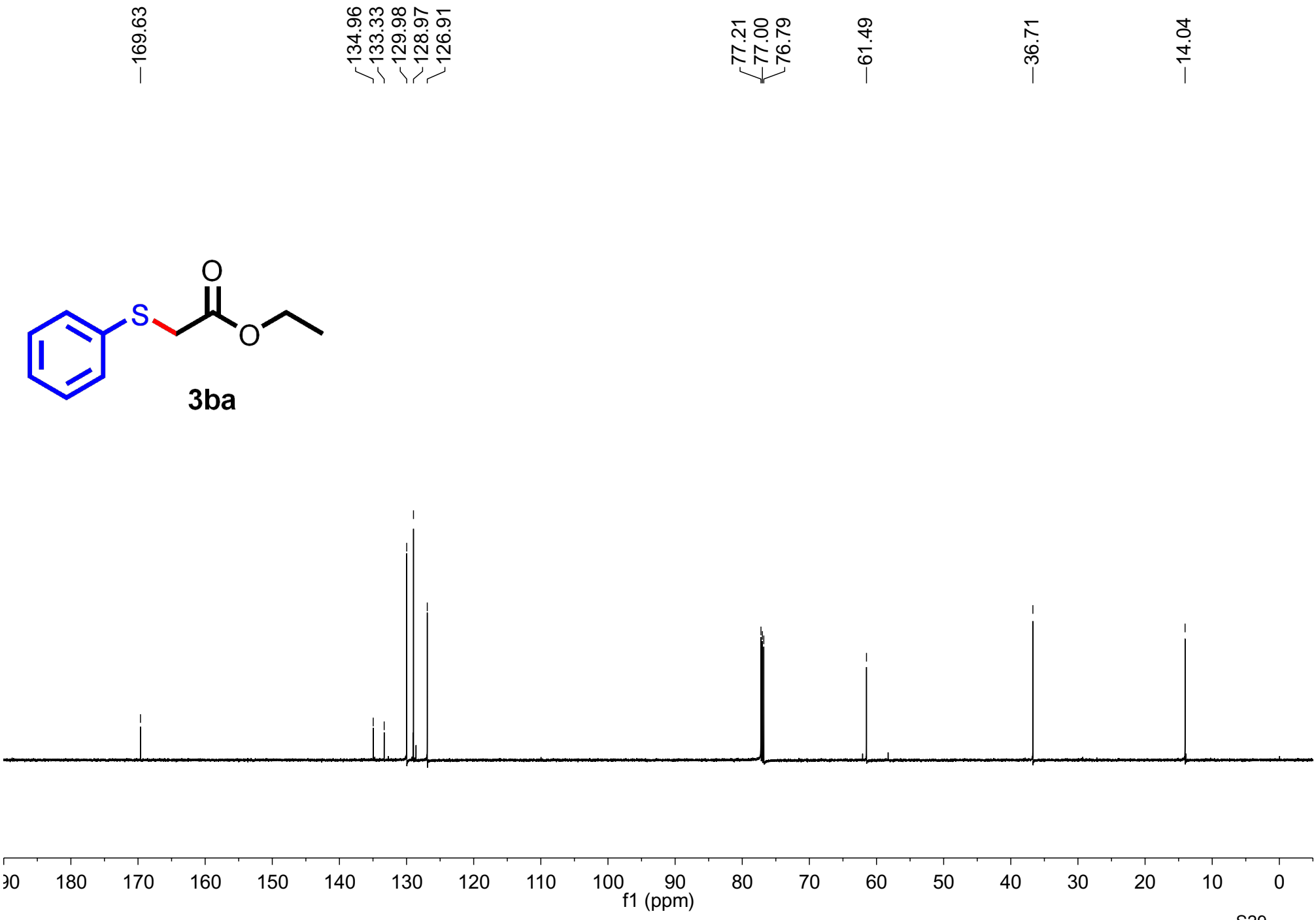
2.00
0.88
2.02
2.10
3.00
f1 (ppm)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129.98
128.97
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61.49
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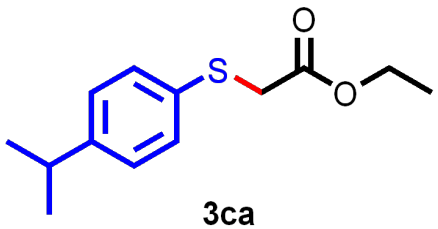
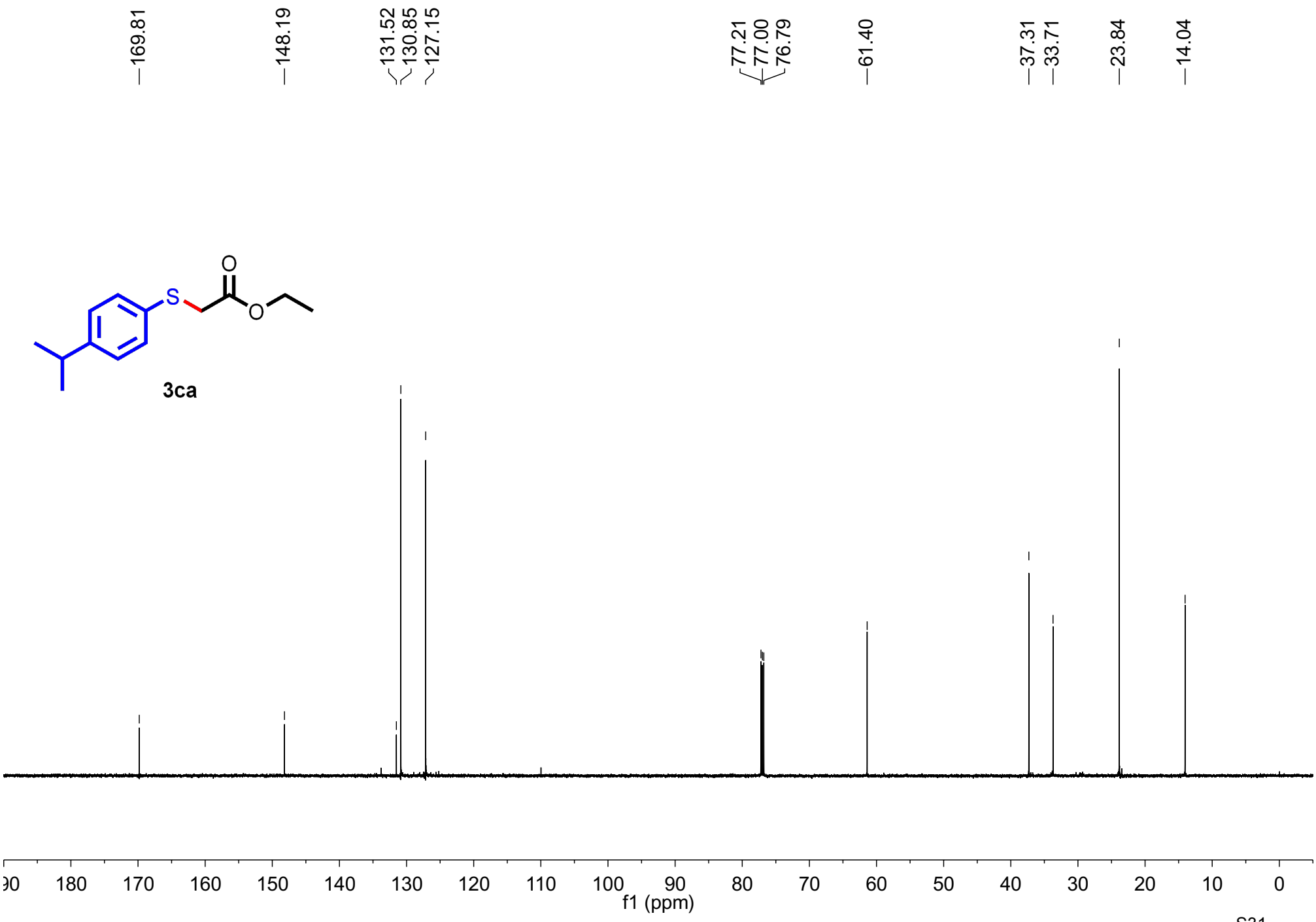
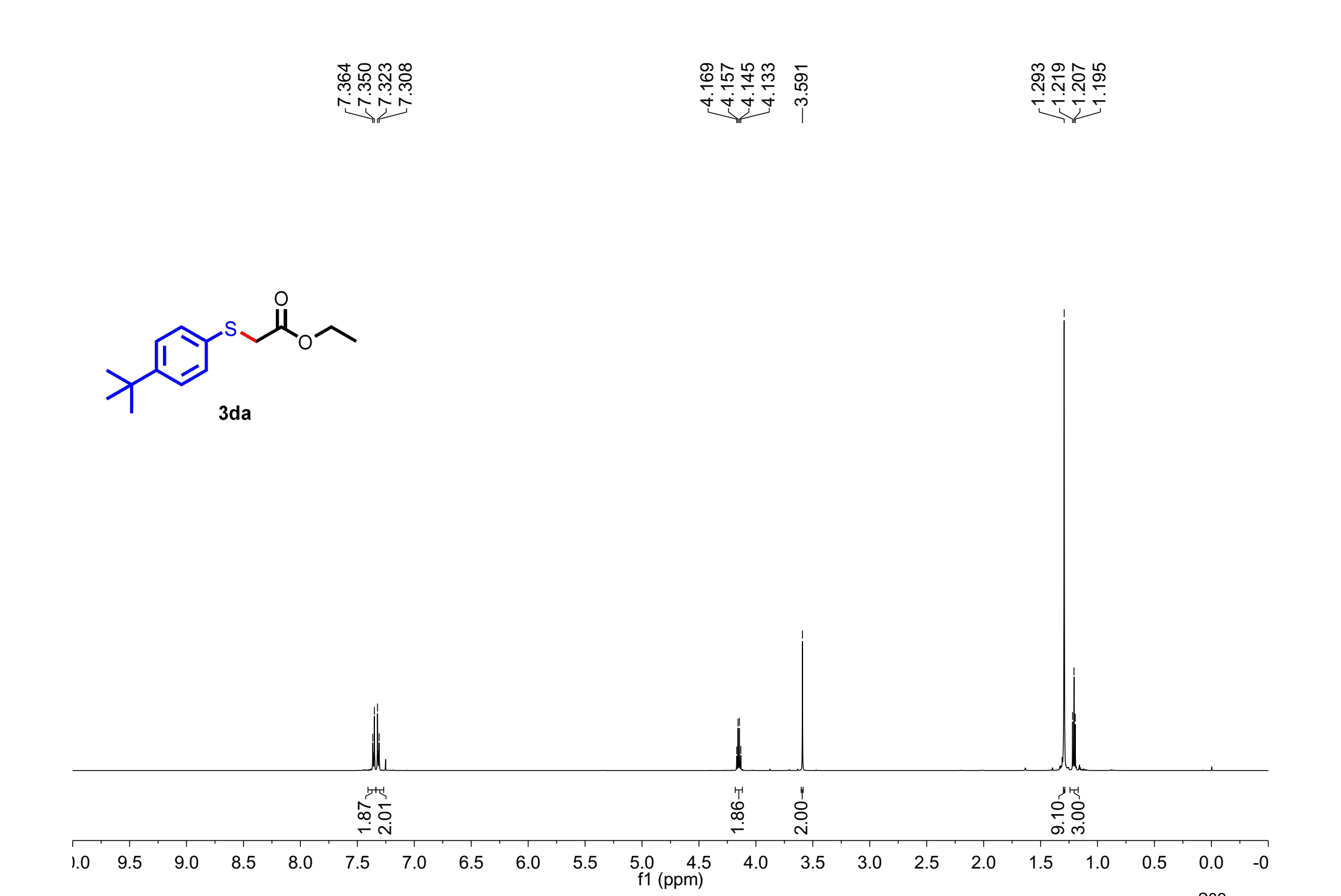
S
O
3ba
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

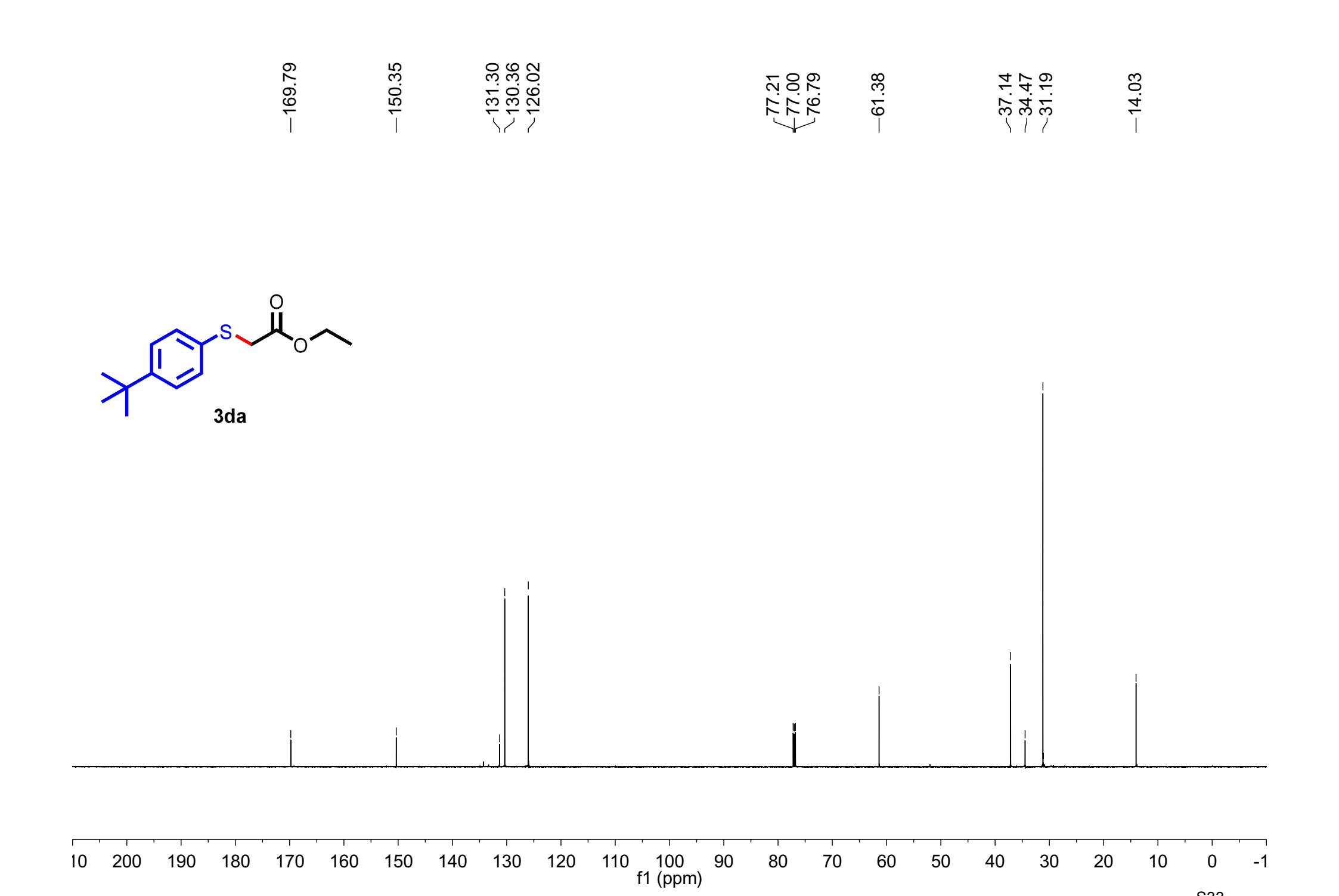

O
S
O

3ca

7.360
7.346
7.164
7.150
4.165
4.153
4.141
4.129
3.583
2.893
2.881
2.870
2.858
2.847
1.226
1.215
1.205
1.194
1.80
2.01
2.00
2.10
1.00
9.05
f1 (ppm)


169.81
148.19
131.52
130.85
127.15
77.21
77.00
76.79
61.40
37.31
33.71
23.84
14.04
O
S
O
3ca
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.364
7.350
7.323
7.308
4.169
4.157
4.145
4.133
3.591
1.293
1.219
1.207
1.195
O
S
O
3da
1.87
2.01
1.86
2.00
9.10
3.00
f1 (ppm)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150.35
131.30
130.36
126.02
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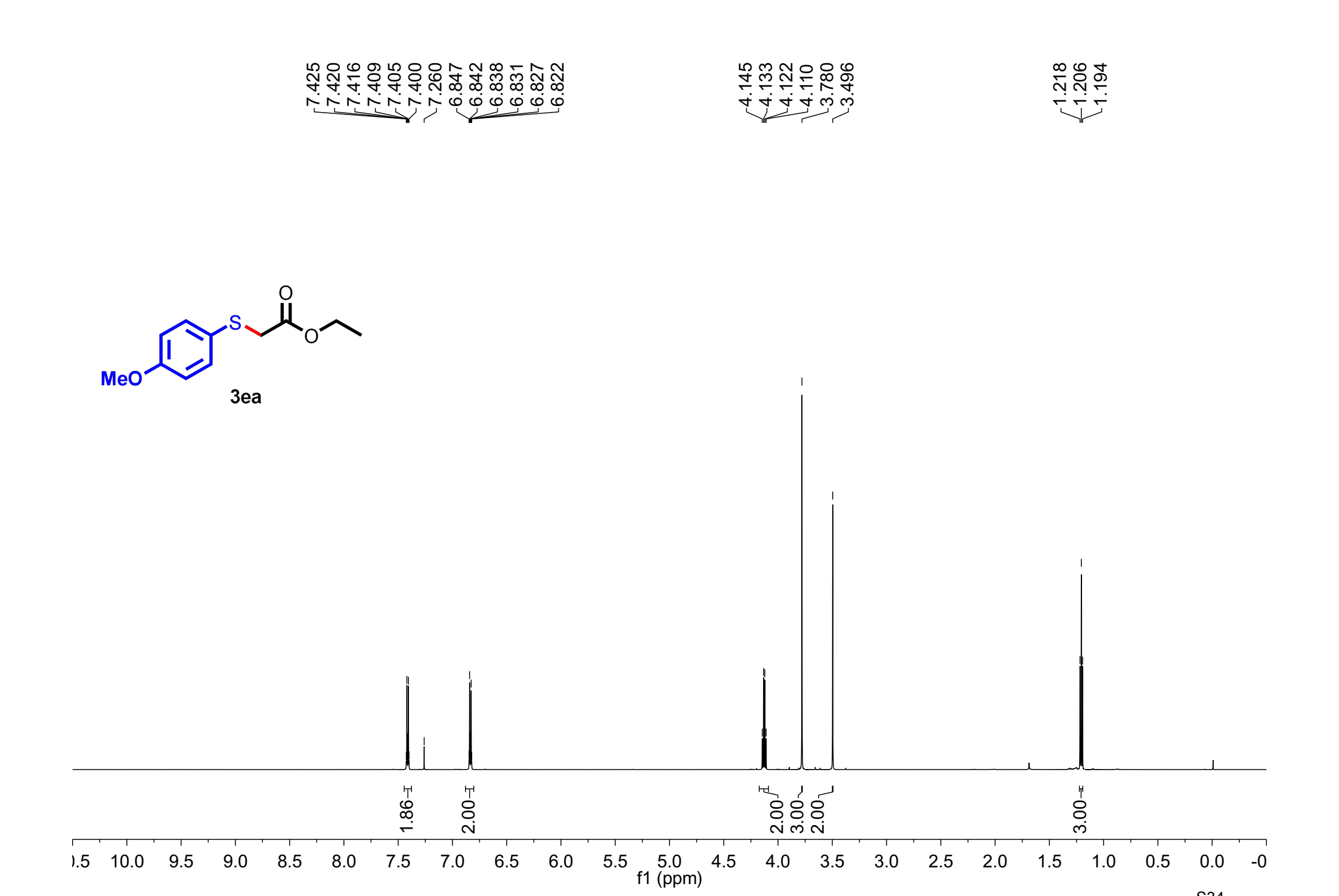
77.00
76.79
61.38
37.14
34.47
31.19
14.03
O
S
O
3da
f1 (ppm)


7.425
7.420
7.416
7.409
7.405
7.400
7.260
6.847
6.842
6.838
6.831
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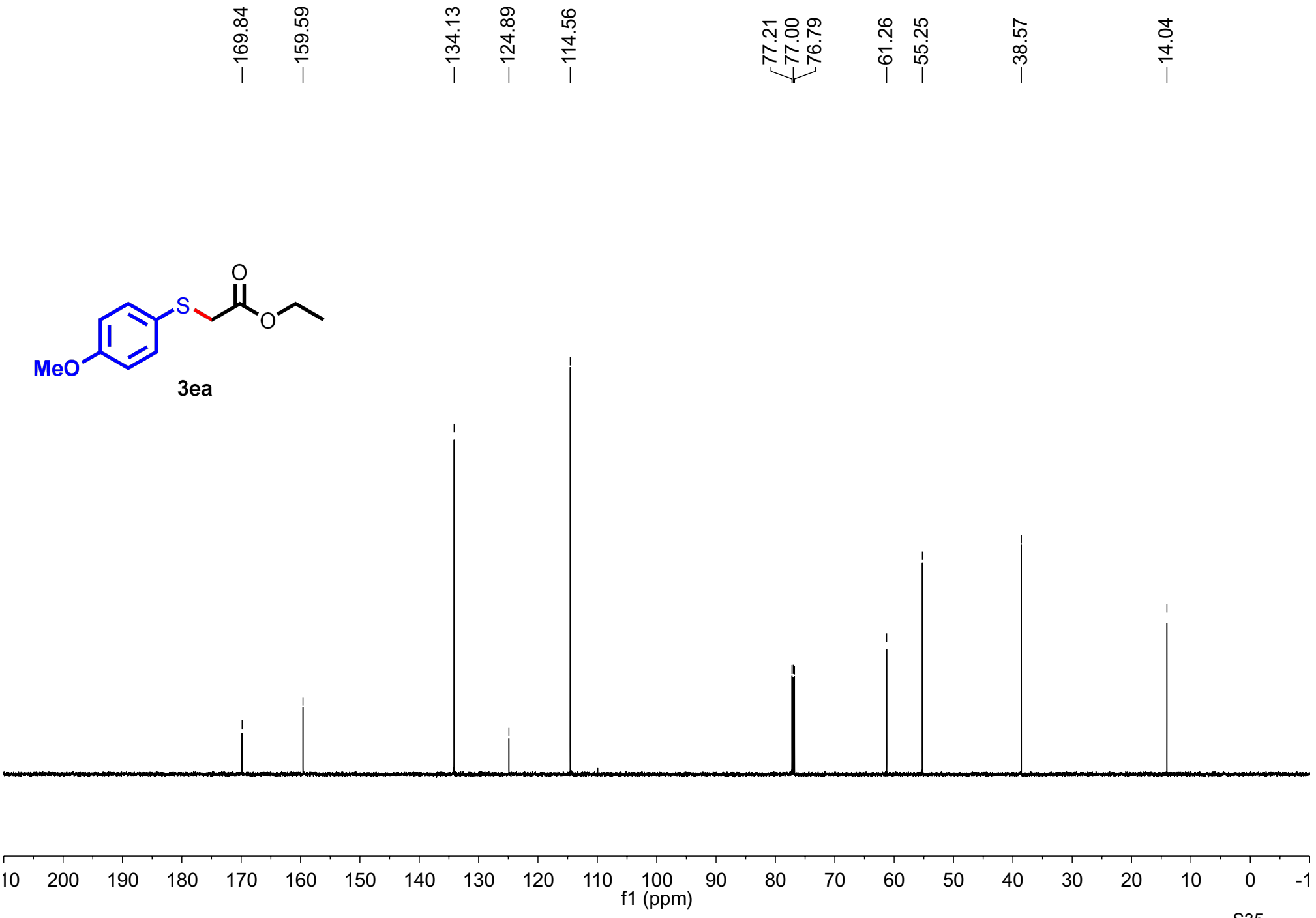
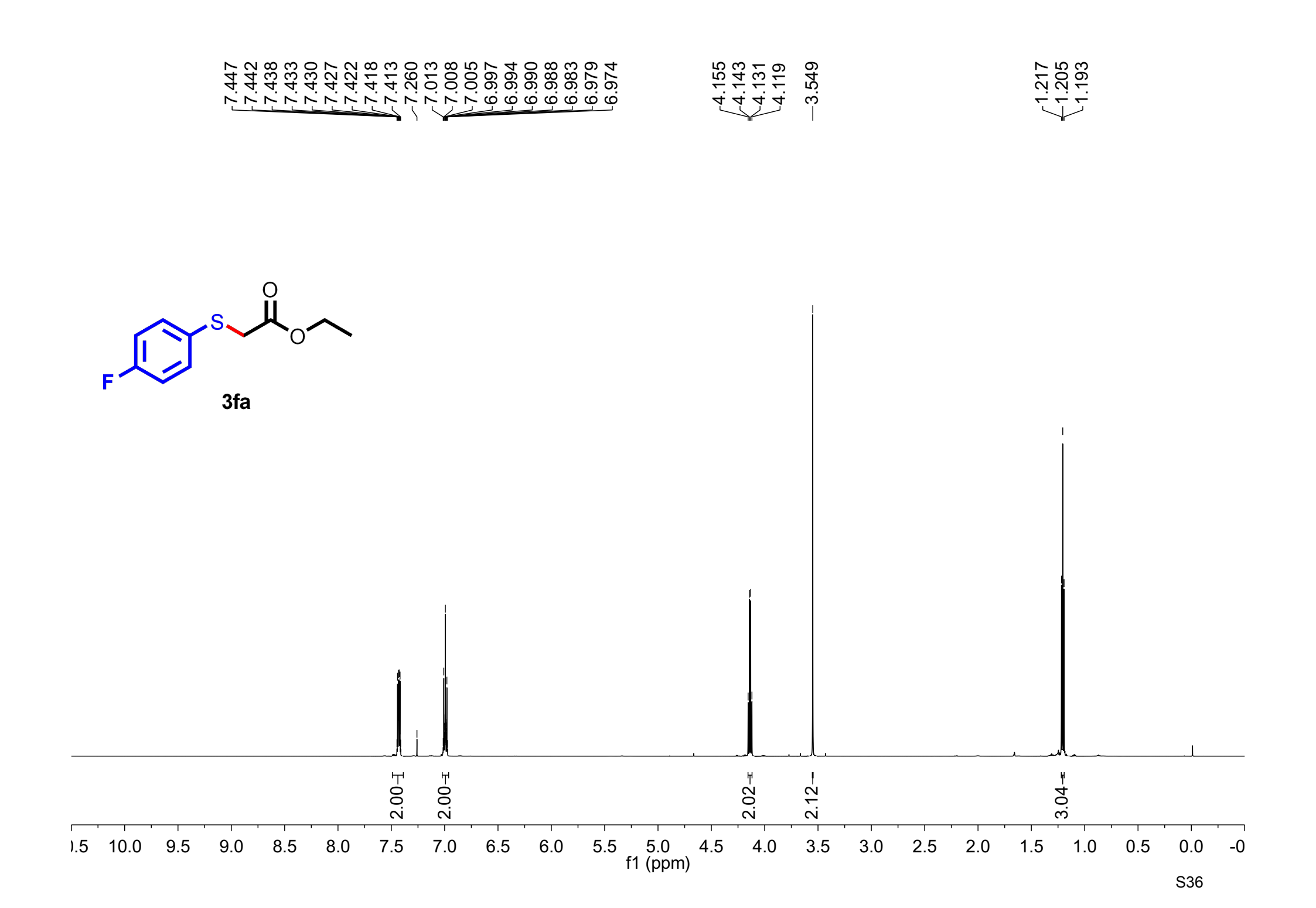
6.822
4.145
4.133
4.122
4.110
3.780
3.496
1.218
1.206
1.194
O
S
O
MeO
3ea
1.86
2.00
2.00
3.00
2.00
3.00
f1 (ppm)


169.84
159.59
134.13
124.89
114.56
77.21
77.00
76.79
61.26
55.25
38.57
14.04
O
S
O
MeO
3ea
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)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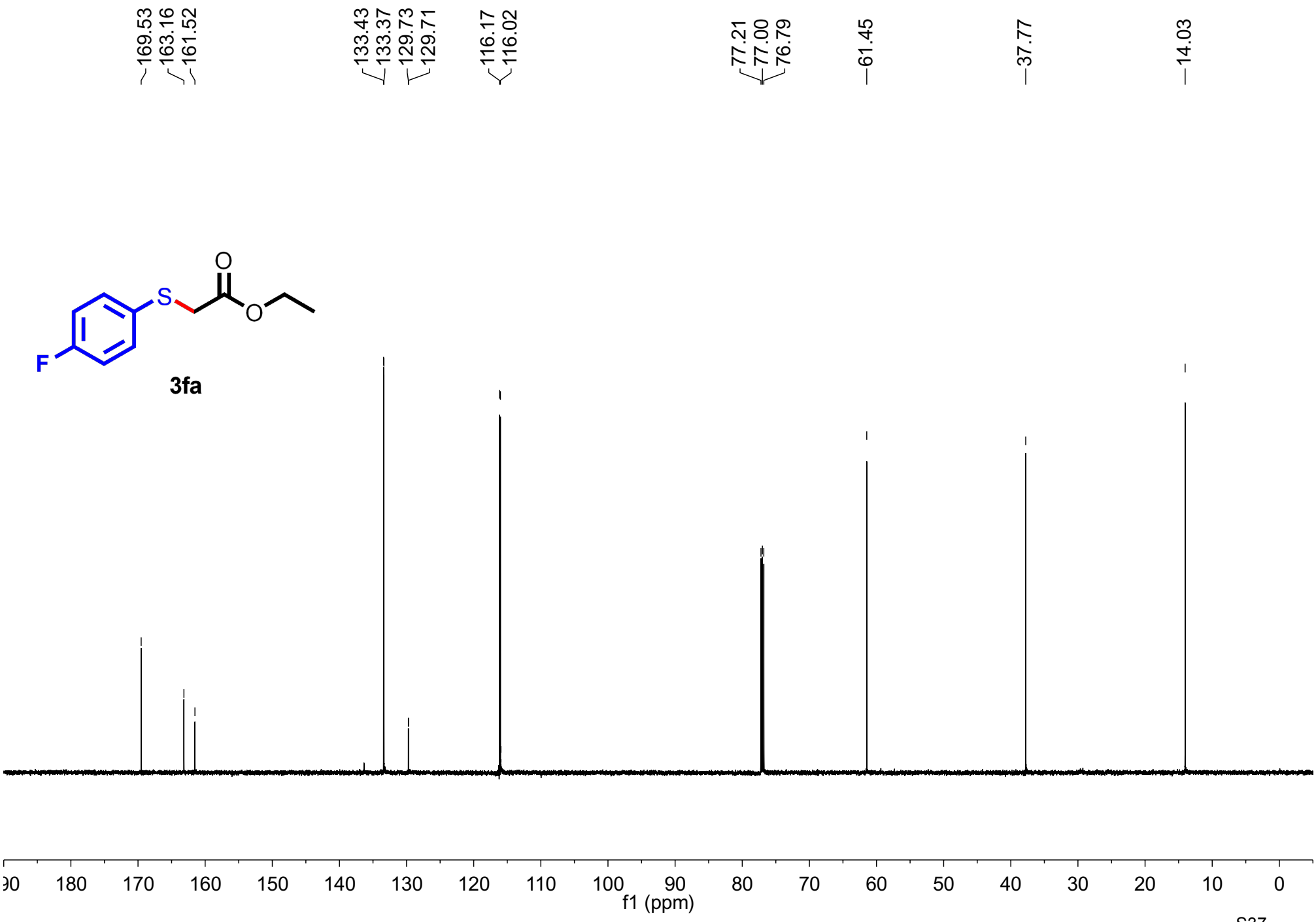
7.442
7.438
7.433
7.430
7.427
7.422
7.418
7.413
7.260
7.013
7.008
7.005
6.997
6.994
6.990
6.988
6.983
6.979
6.974
4.155
4.143
4.131
4.119
3.549
1.217
1.205
1.193
O
S
O
F
3fa
2.00
2.00
2.02
2.12
3.04
f1 (ppm)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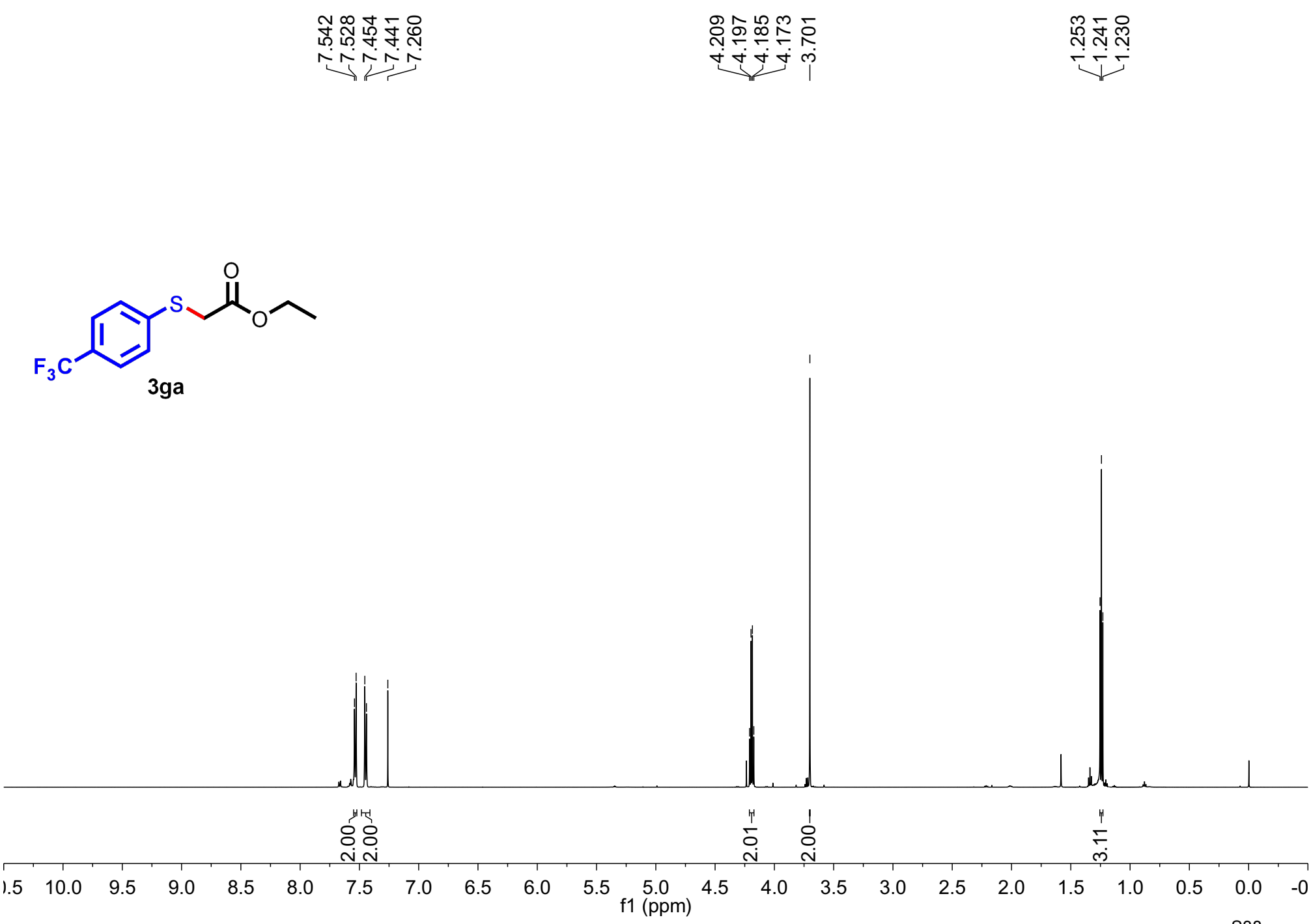
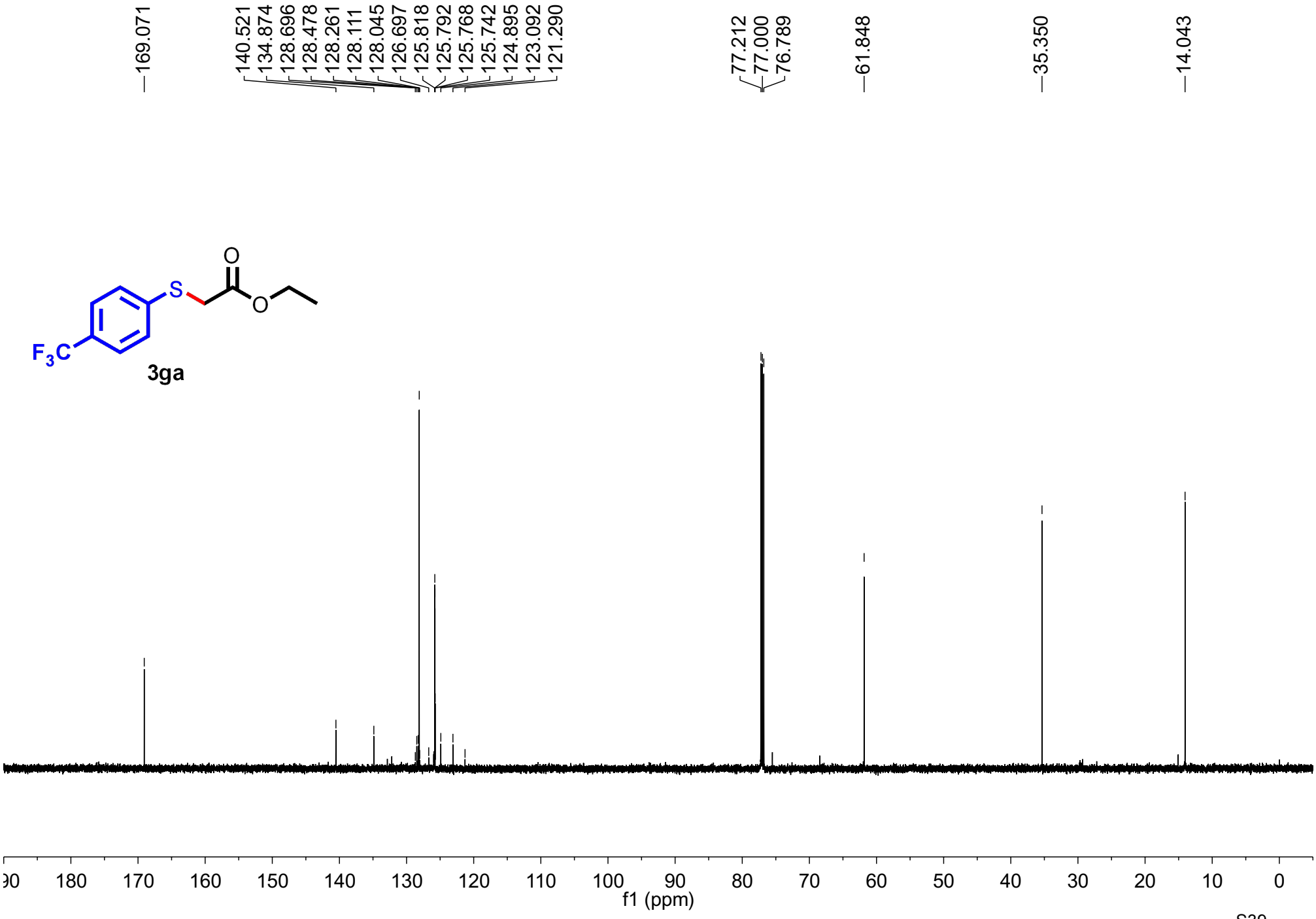
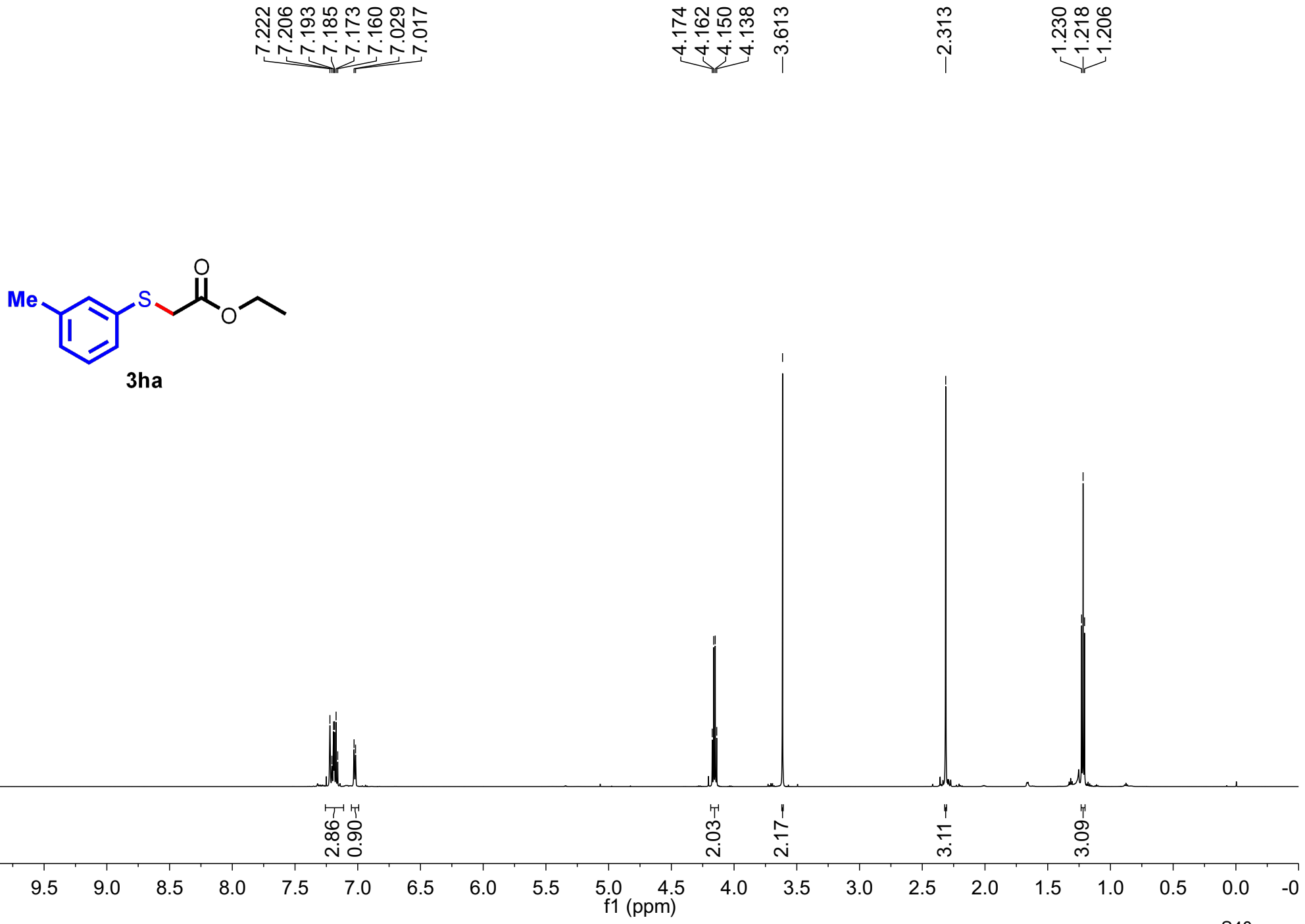
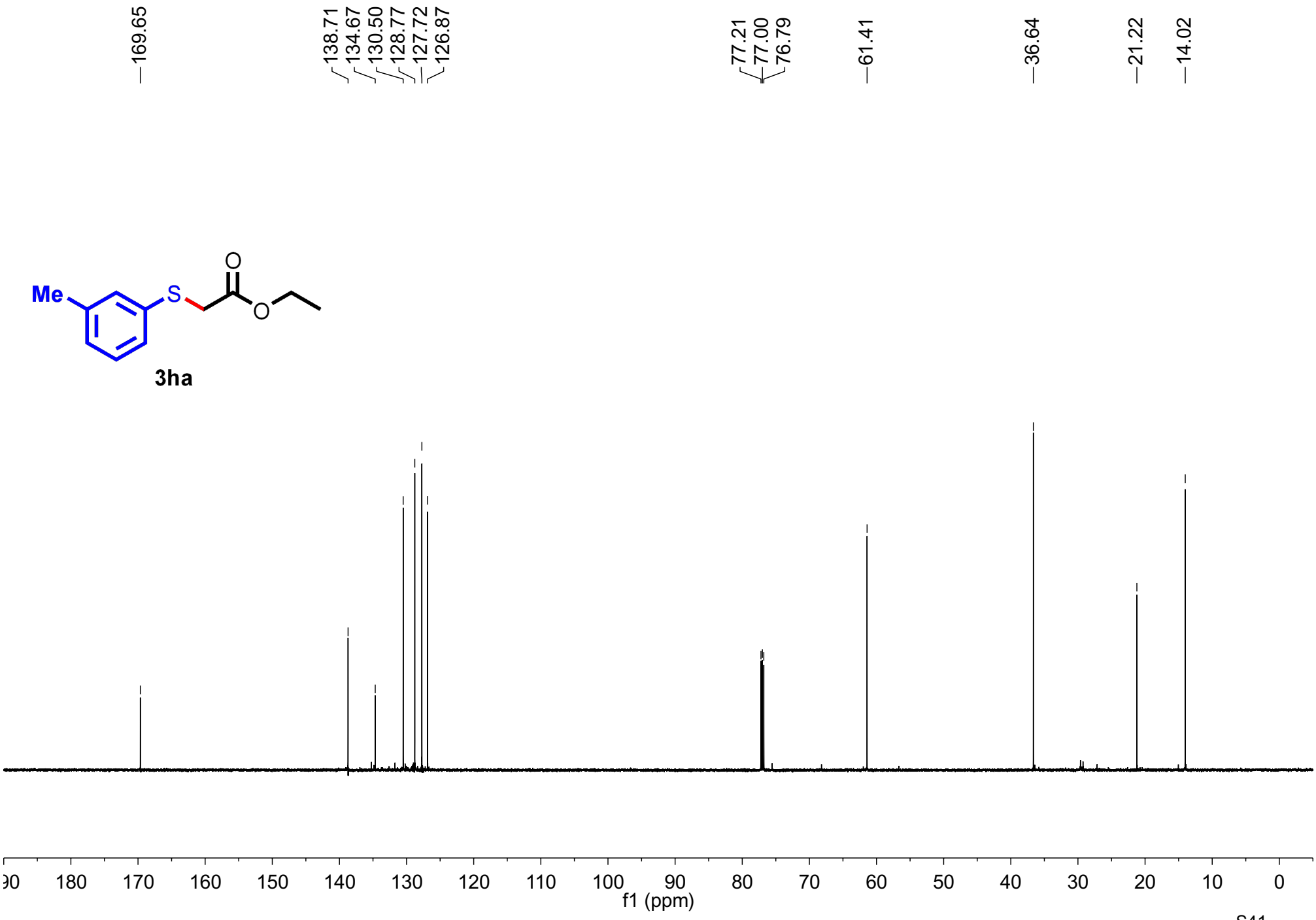
163.16
161.52
133.43
133.37
129.73
129.71
116.17
116.02
77.21
77.00
76.79
61.45
37.77
14.03
O
S
O
F
3fa
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.542
7.528
7.454
7.441
7.260
4.209
4.197
4.185
4.173
3.701
1.253
1.241
1.230
O
S
O
F3C
3ga
2.00
2.00
2.01
2.00
3.11
f1 (ppm)


169.071
140.521
134.874
128.696
128.478
128.261
128.111
128.045
126.697
125.818
125.792
125.768
125.742
124.895
123.092
121.290
77.212
77.000
76.789
61.848
35.350
14.043
O
S
O
F3C
3ga
f1 (ppm)


7.222
7.206
7.193
7.185
7.173
7.160
7.029
7.017
4.174
4.162
4.150
4.138
3.613
2.313
1.230
1.218
1.206
Me
S
O
O
3ha
2.86
0.90
2.03
2.17
3.11
3.09
f1 (ppm)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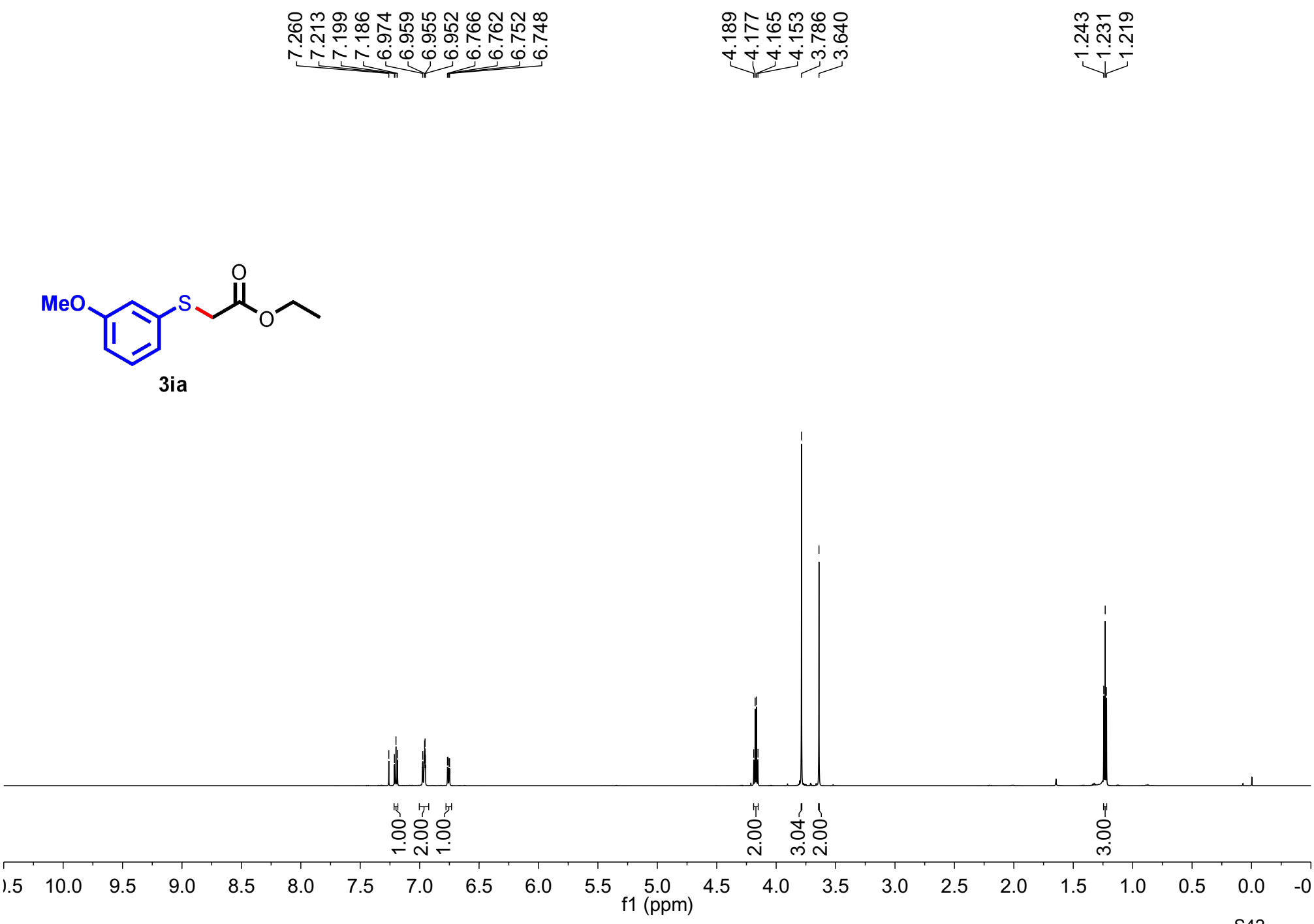
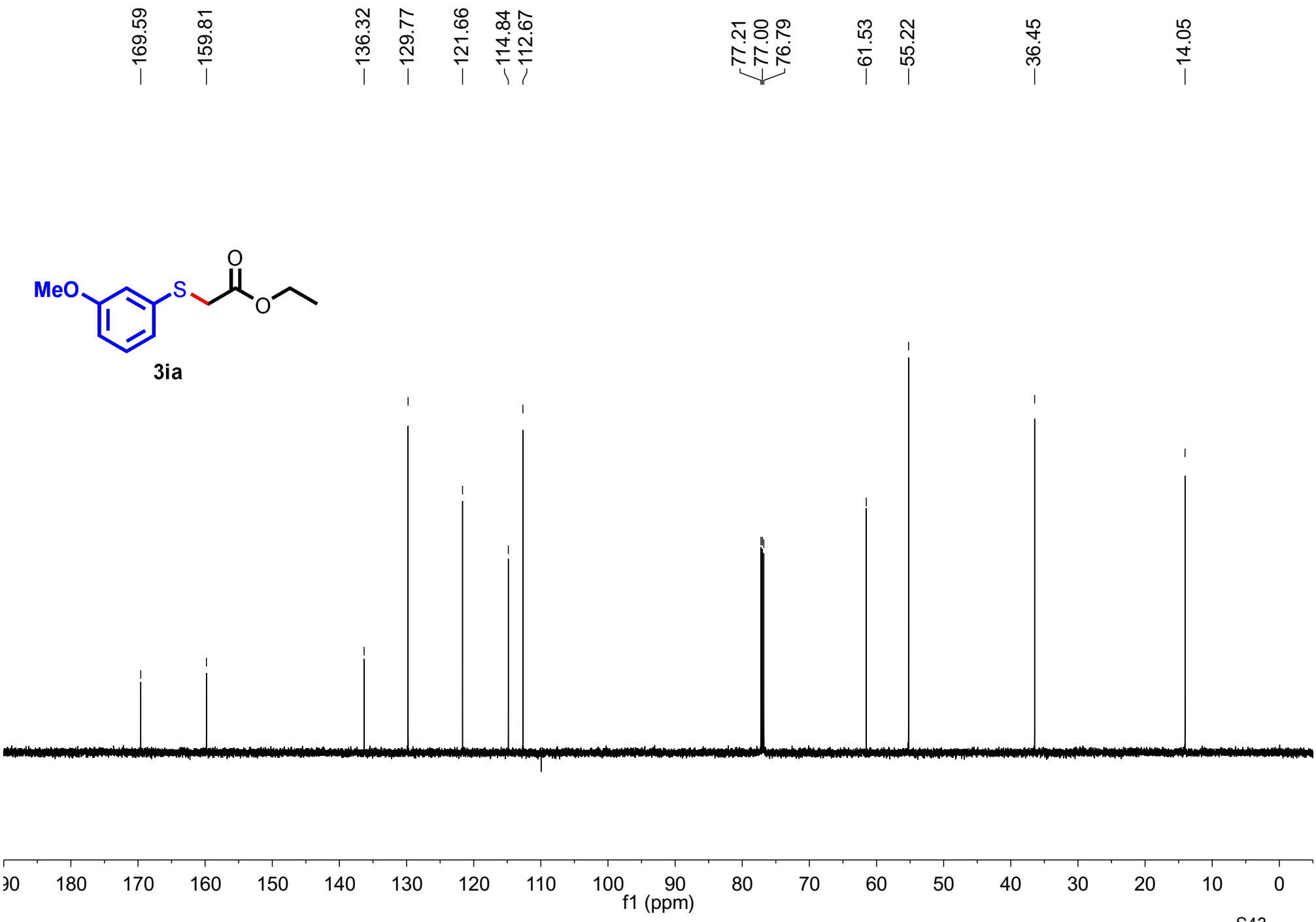
138.71
134.67
130.50
128.77
127.72
126.87
77.21
77.00
76.79
61.41
36.64
21.22
14.02
Me
S
O
O
3ha
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.260
7.213
7.199
7.186
6.974
6.959
6.955
6.952
6.766
6.762
6.752
6.748
4.189
4.177
4.165
4.153
3.786
3.640
1.243
1.231
1.219
MeO
S
O
O
3ia
1.00
2.00
1.00
2.00
3.04
2.00
3.00
f1 (ppm)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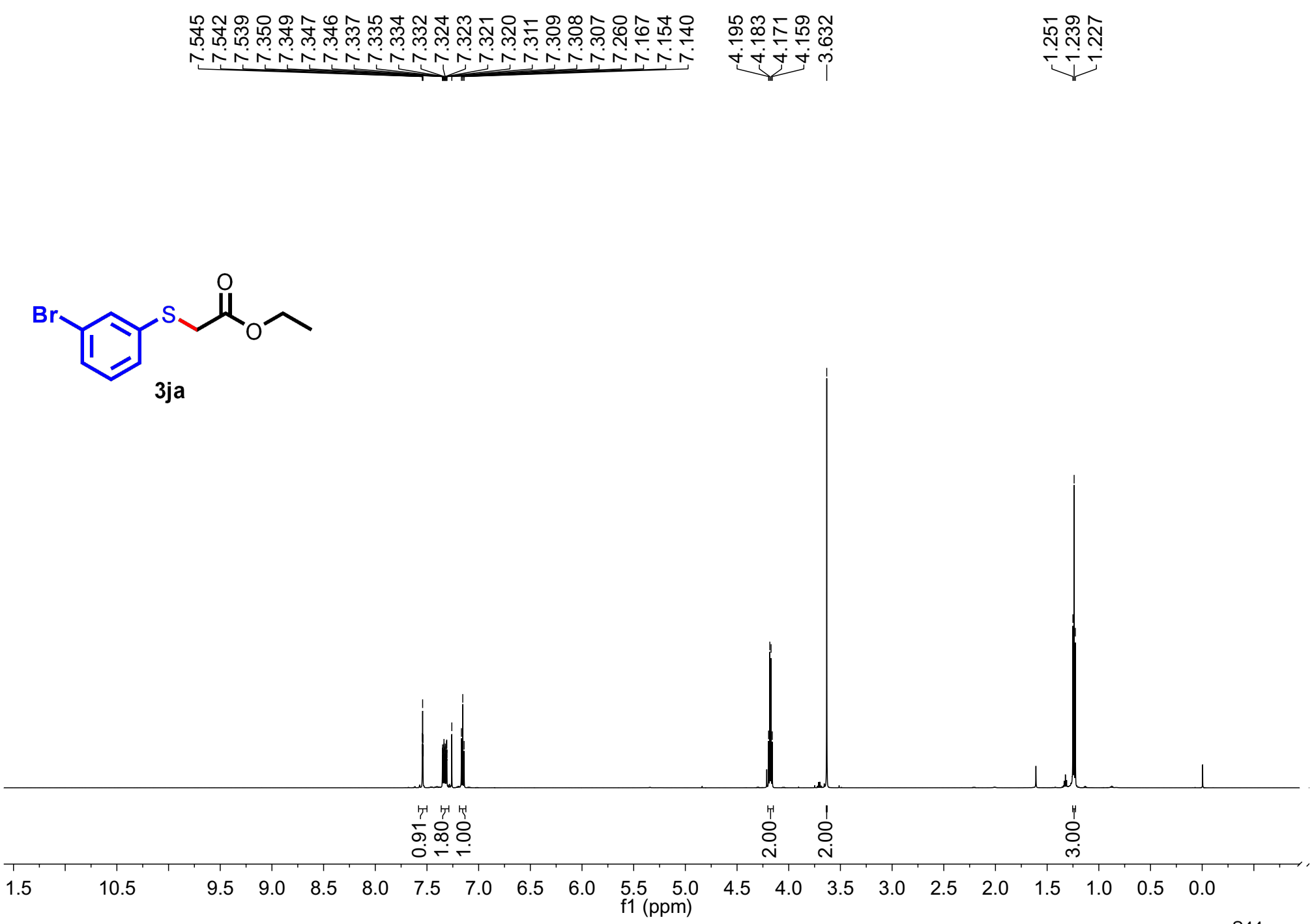
159.81
136.32
129.77
121.66
114.84
112.67
77.21
77.00
76.79
61.53
55.22
36.45
14.05
MeO
S
O
O
3ia
f1 (ppm)


7.545
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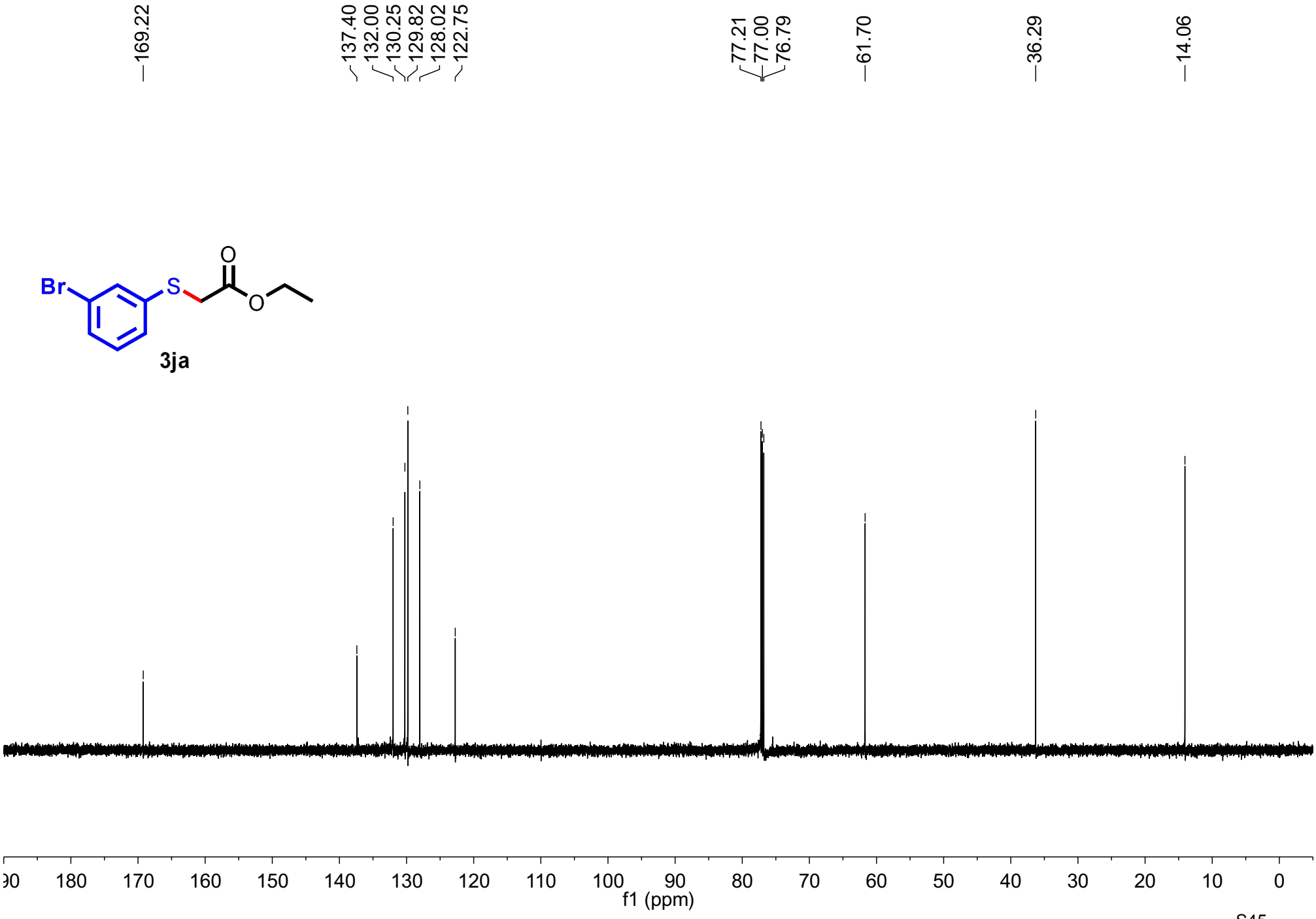
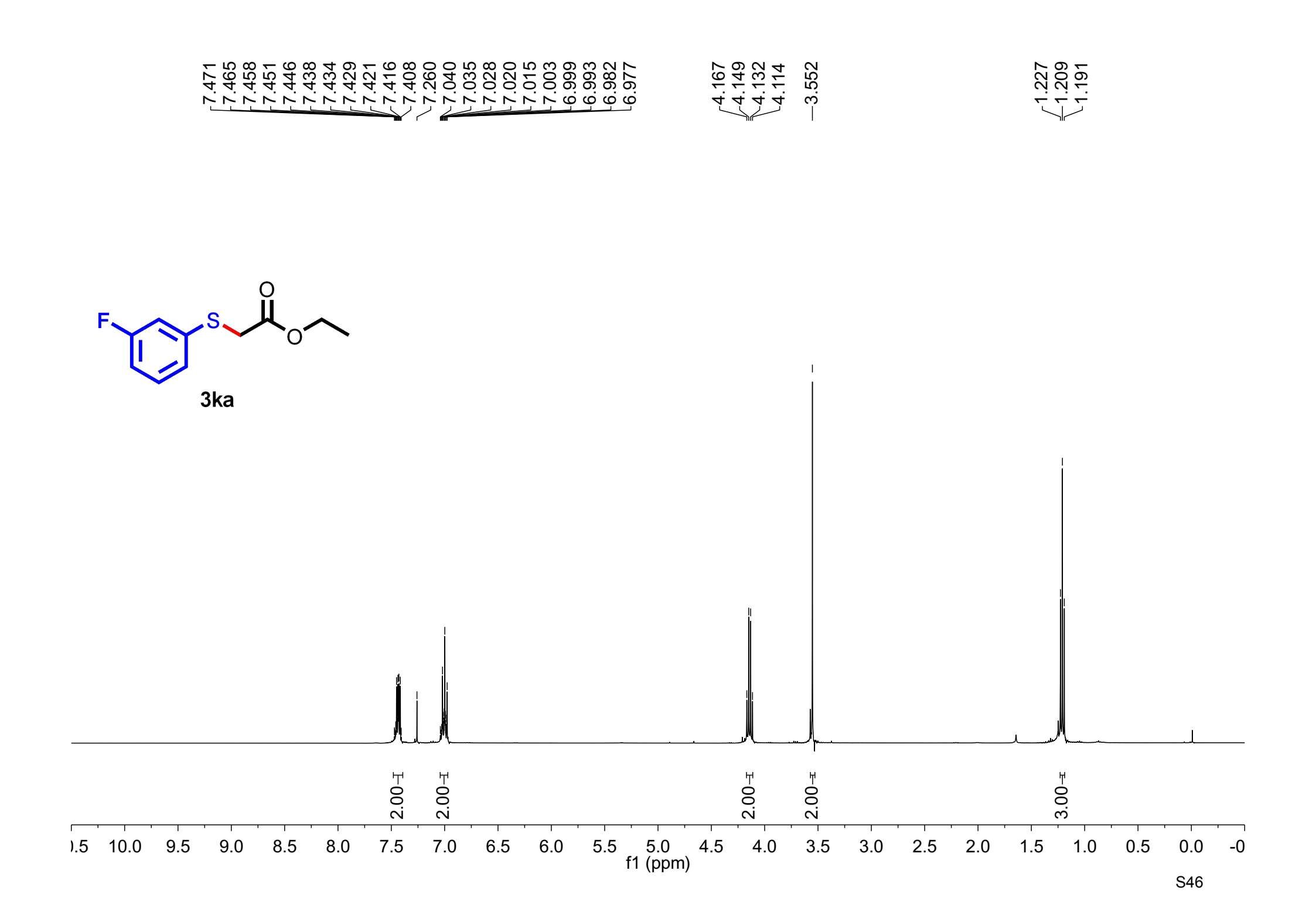
7.539
7.350
7.349
7.347
7.346
7.337
7.335
7.334
7.332
7.324
7.323
7.321
7.320
7.311
7.309
7.308
7.307
7.260
7.167
7.154
7.140
4.195
4.183
4.171
4.159
3.632
1.251
1.239
1.227
Br
S
O
O
3ja
0.91
1.80
1.00
2.00
2.00
3.00
1.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


169.22
137.40
132.00
130.25
129.82
128.02
122.75
77.21
77.00
76.79
61.70
36.29
14.06
Br
S
O
O
3ja
f1 (ppm)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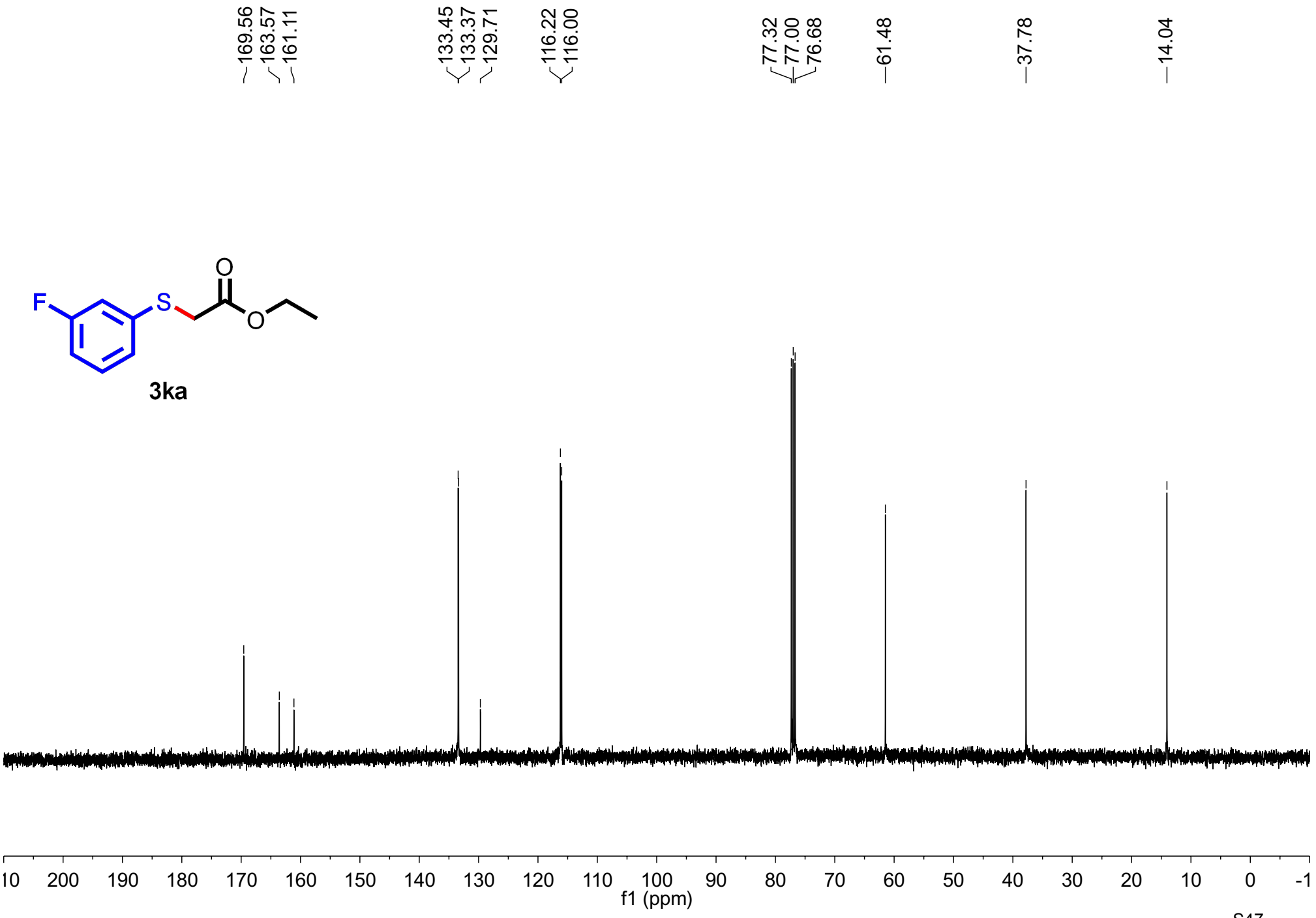
7.458
7.451
7.446
7.438
7.434
7.429
7.421
7.416
7.408
7.260
7.040
7.035
7.028
7.020
7.015
7.003
6.999
6.993
6.982
6.977
4.167
4.149
4.132
4.114
3.552
1.227
1.209
1.191
F
S
O
O
3ka
2.00
2.00
2.00
2.00
3.00
f1 (ppm)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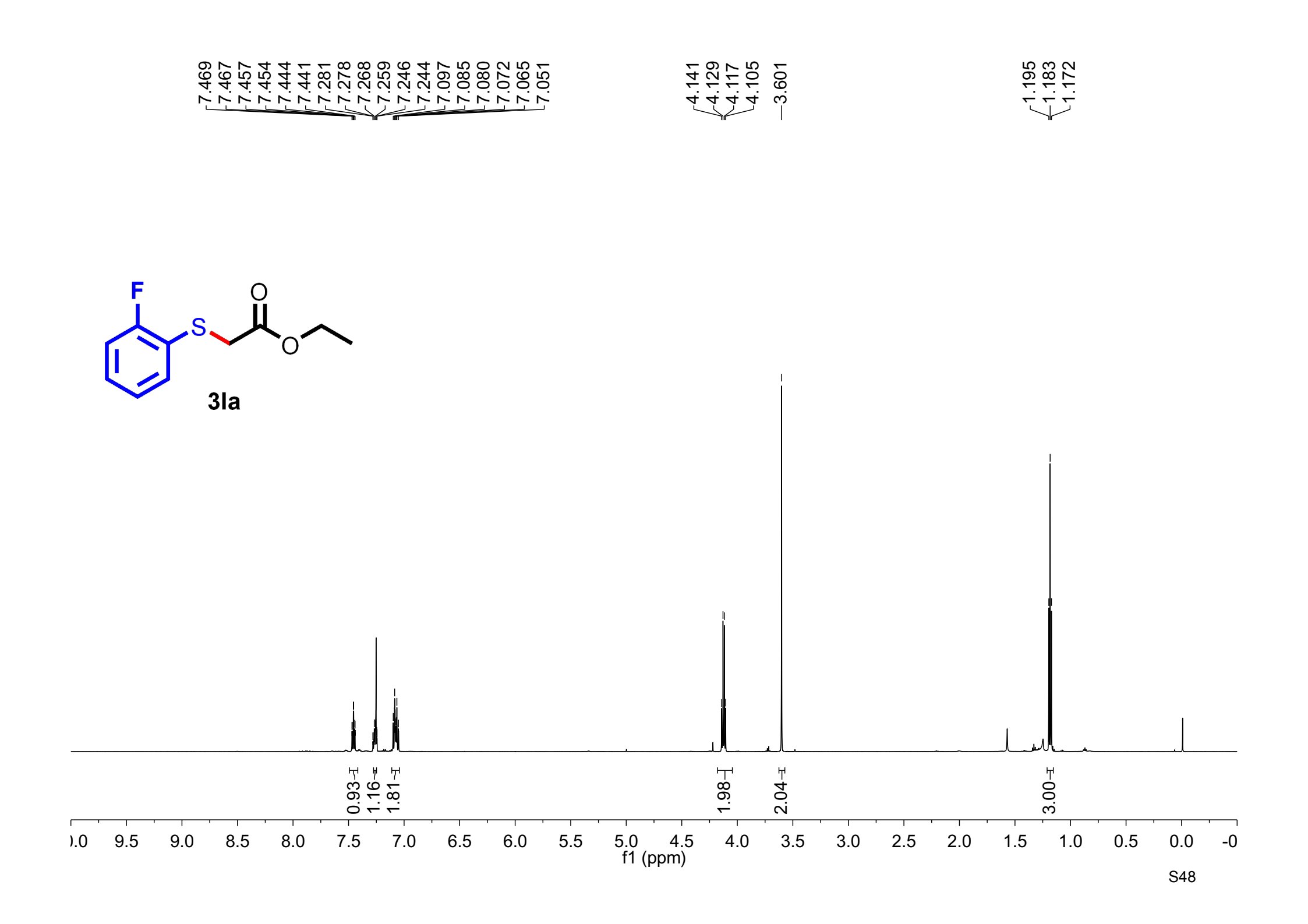
161.11
133.45
133.37
129.71
116.22
116.00
77.32
77.00
76.68
61.48
37.78
14.04
F
S
O
O
3ka
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)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7.454
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7.441
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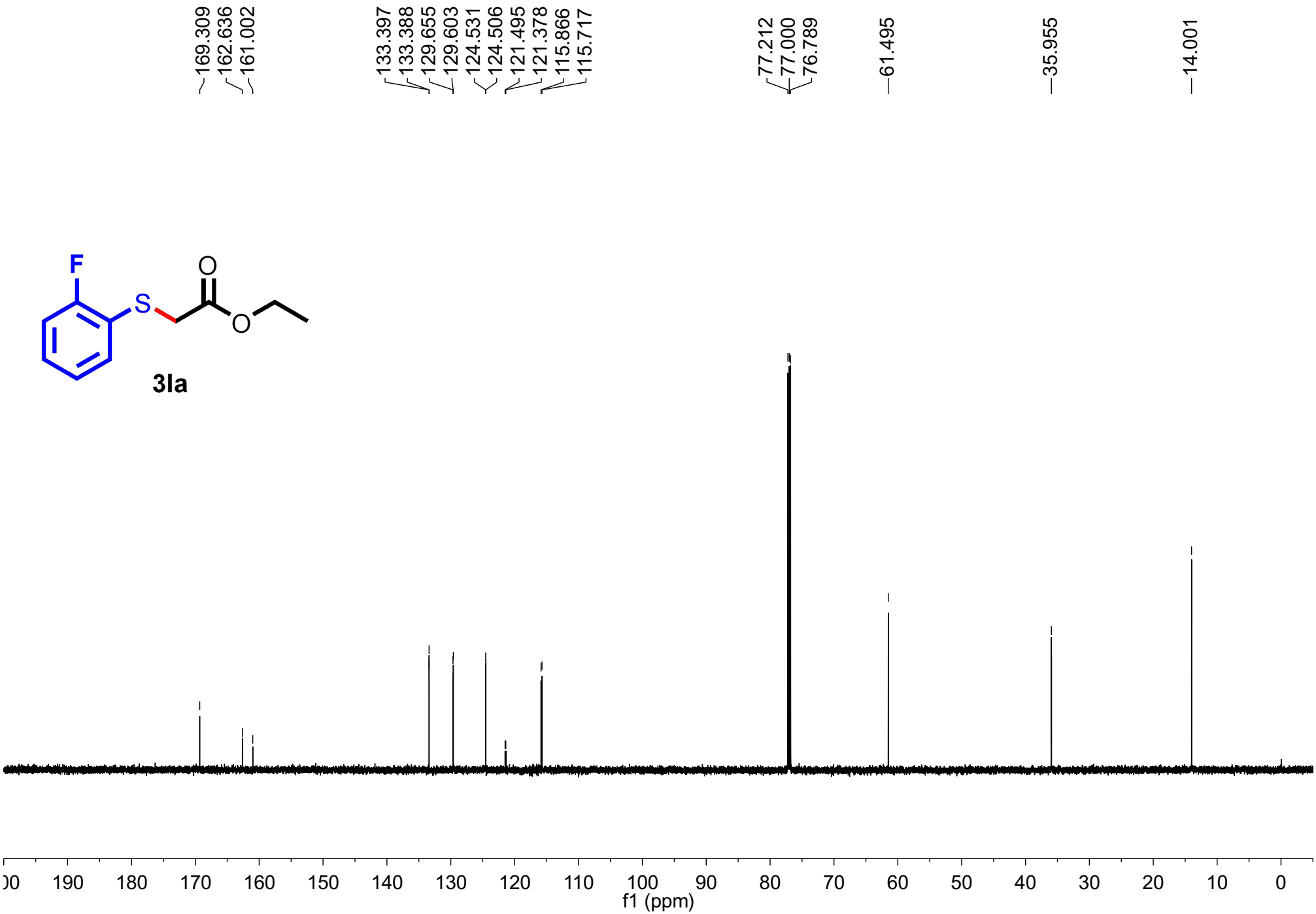
7.278
7.268
7.259
7.246
7.244
7.097
7.085
7.080
7.072
7.065
7.051
4.141
4.129
4.117
4.105
3.601
1.195
1.183
1.172
F
S
O
O
3la
0.93
1.16
1.81
1.98
2.04
3.00
f1 (ppm)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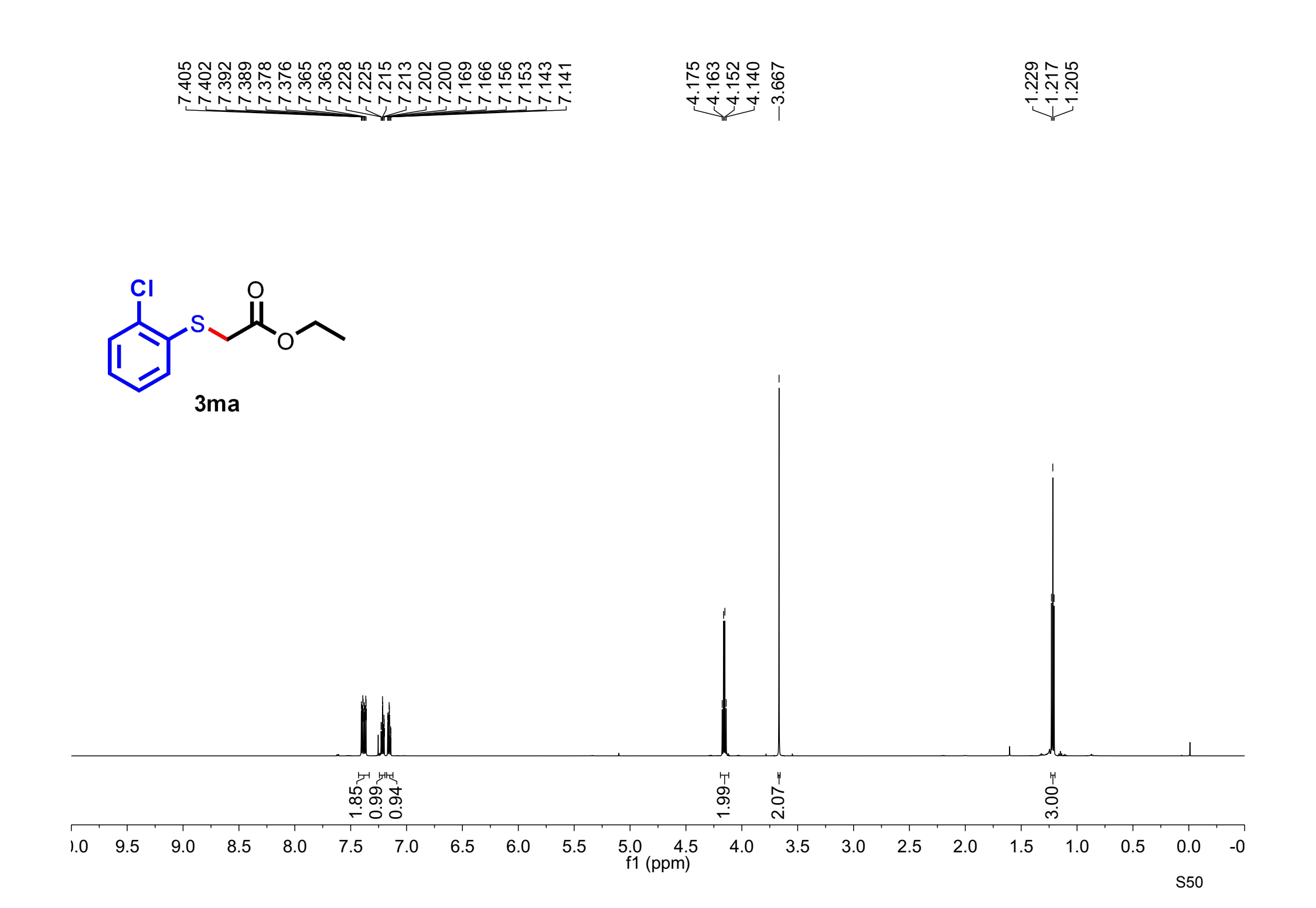
161.002
133.397
133.388
129.655
129.603
124.531
124.506
121.495
121.378
115.866
115.717
77.212
77.000
76.789
61.495
35.955
14.001
F
S
O
O
3la
f1 (ppm)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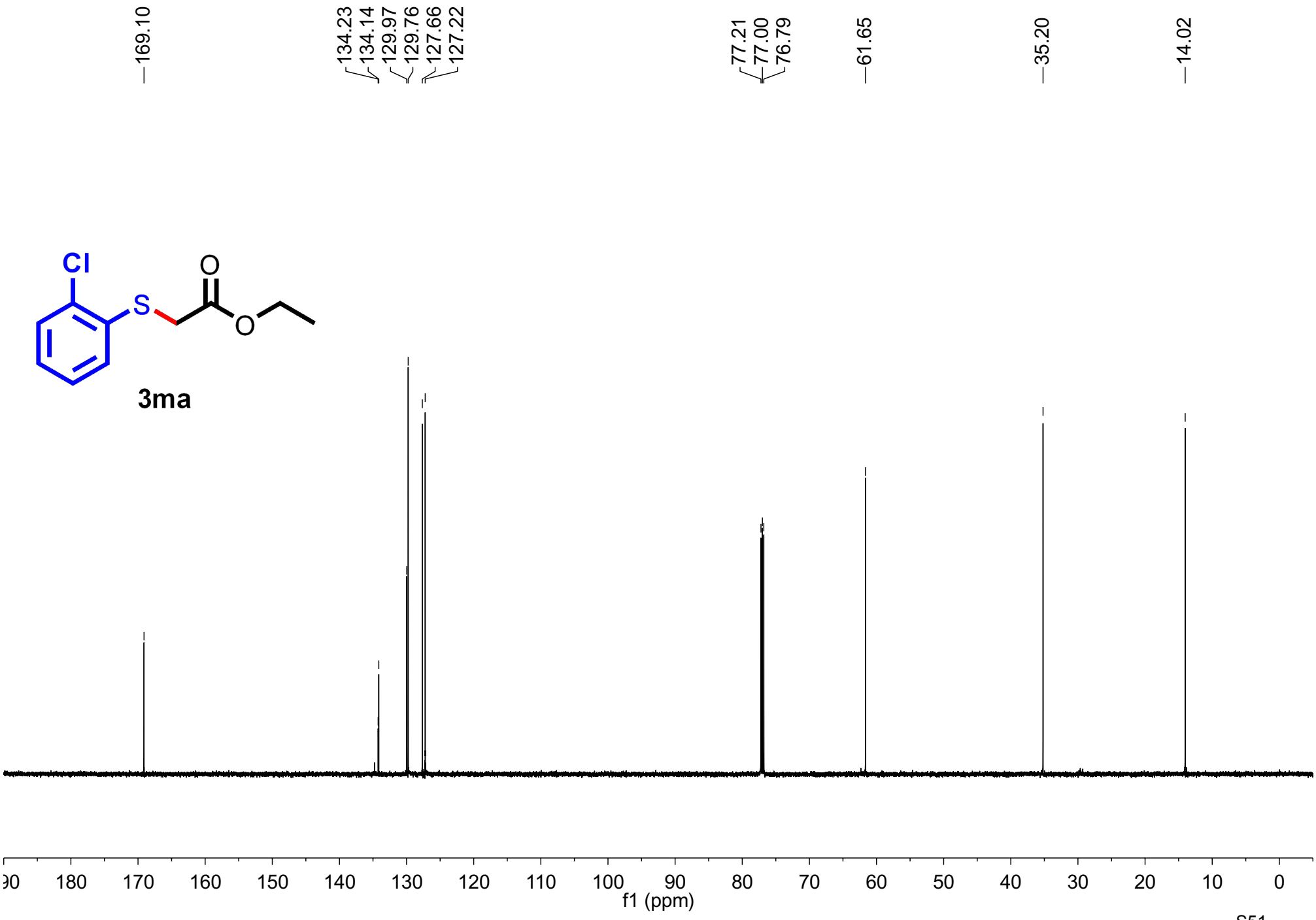
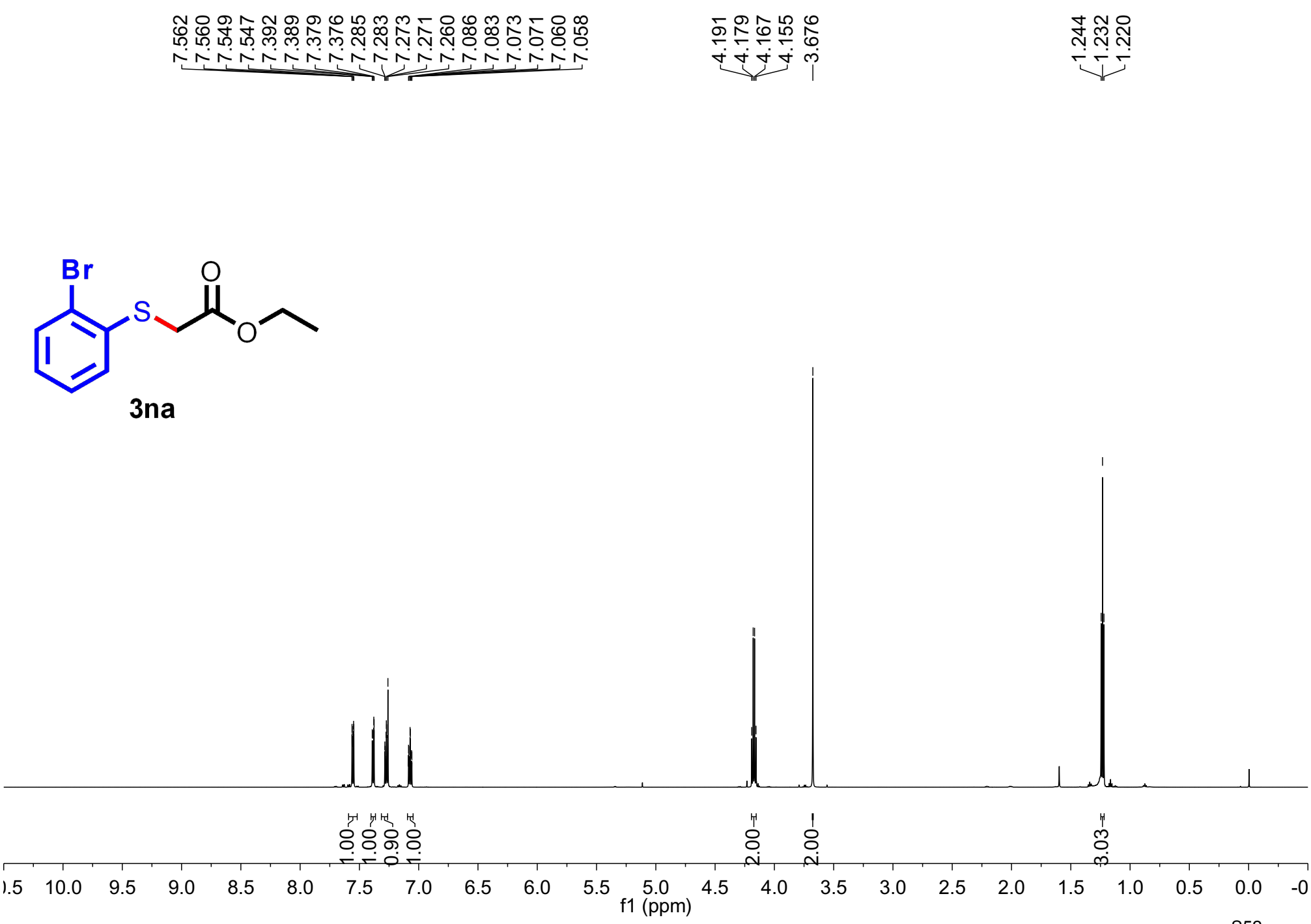
7.392
7.389
7.378
7.376
7.365
7.363
7.228
7.225
7.215
7.213
7.202
7.200
7.169
7.166
7.156
7.153
7.143
7.141
4.175
4.163
4.152
4.140
3.667
1.229
1.217
1.205
Cl
S
O
O
3ma
1.85
0.99
0.94
1.99
2.07
3.00
f1 (ppm)


169.10
134.23
134.14
129.97
129.76
127.66
127.22
77.21
77.00
76.79
61.65
35.20
14.02
Cl
S
O
O
3ma
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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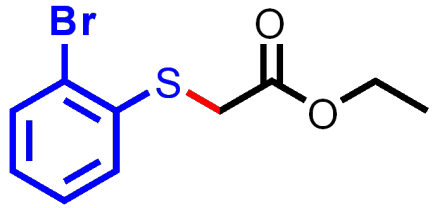
7.547
7.392
7.389
7.379
7.376
7.285
7.283
7.273
7.271
7.260
7.086
7.083
7.073
7.071
7.060
7.058
4.191
4.179
4.167
4.155
3.676
1.244
1.232
1.220
Br
S
O
O
3na
1.00
1.00
0.90
1.00
2.00
2.00
3.03
f1 (ppm)

CARBON_01

169.06
136.28
133.06
129.49
127.88
127.65
124.15
77.21
77.00
76.79
61.69
35.60
14.05



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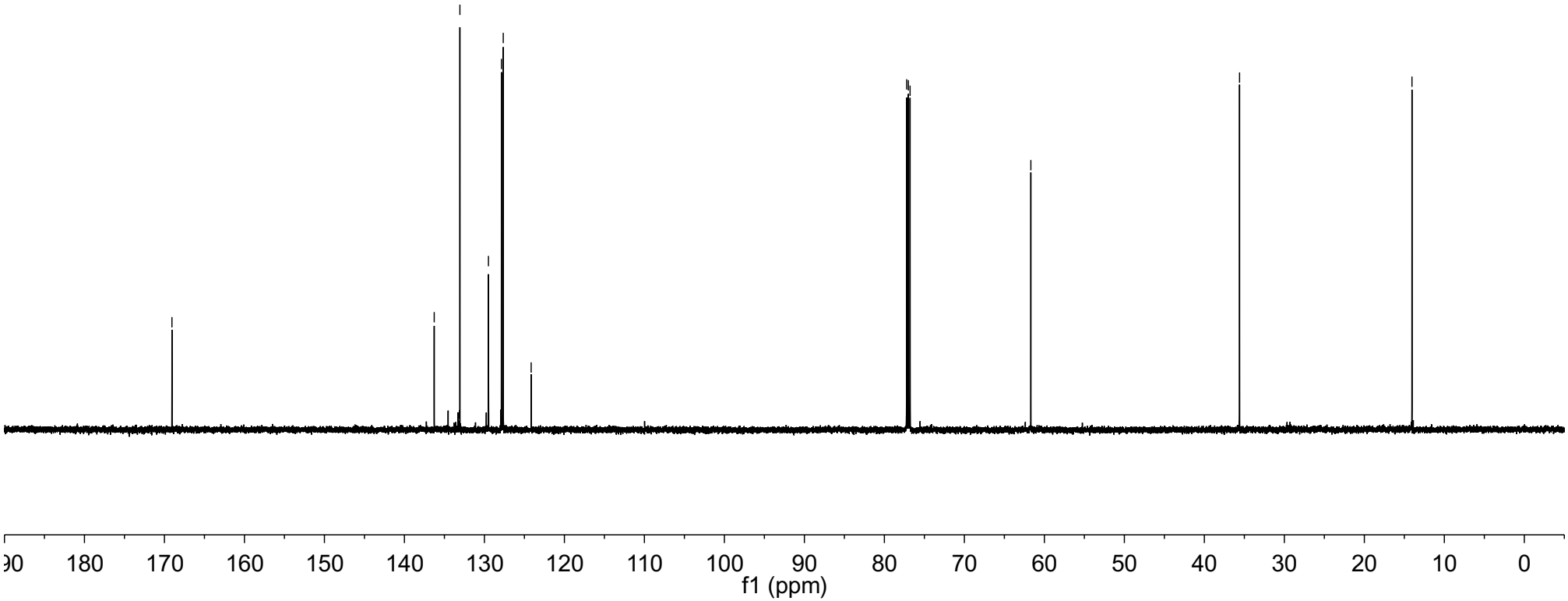

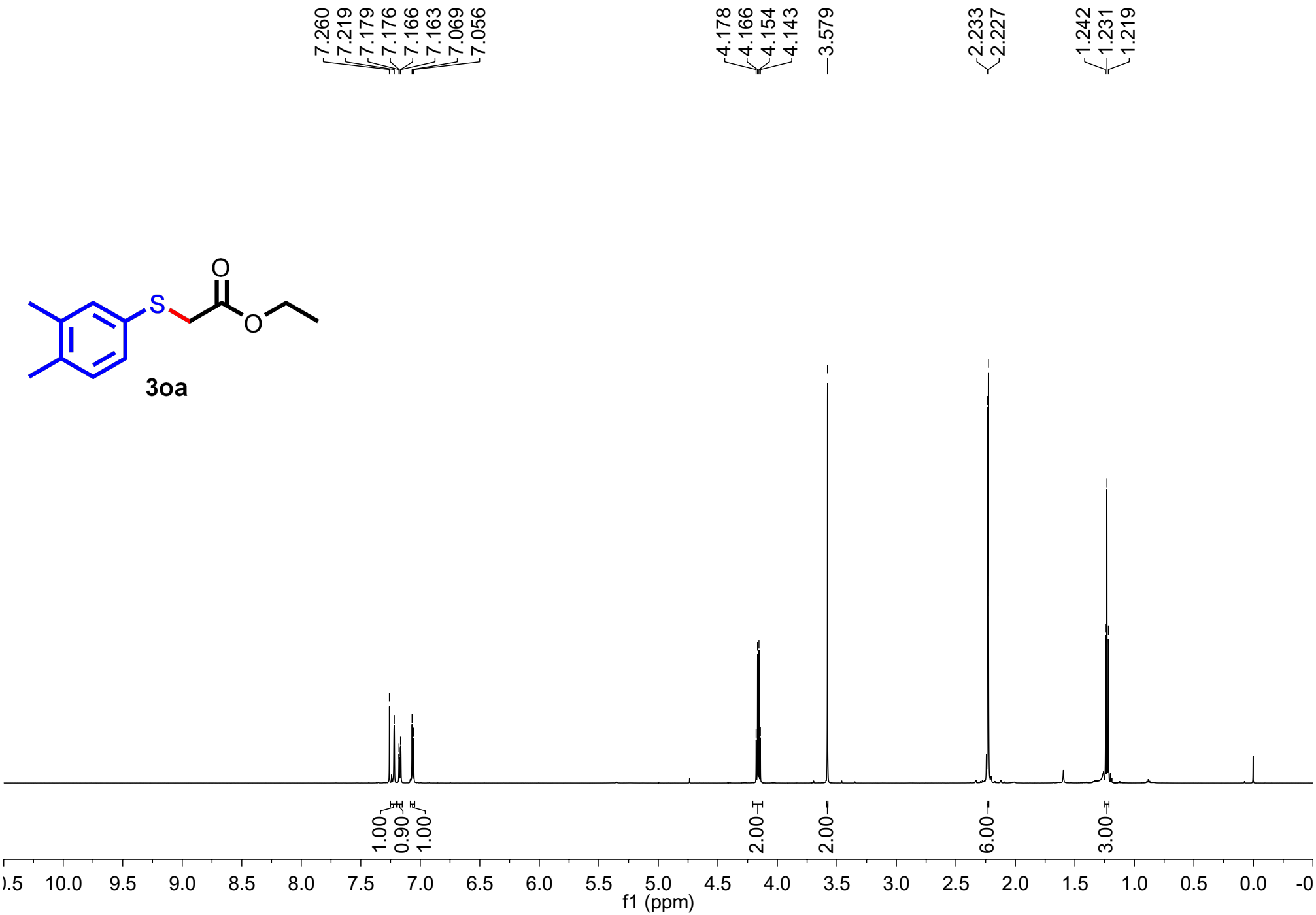
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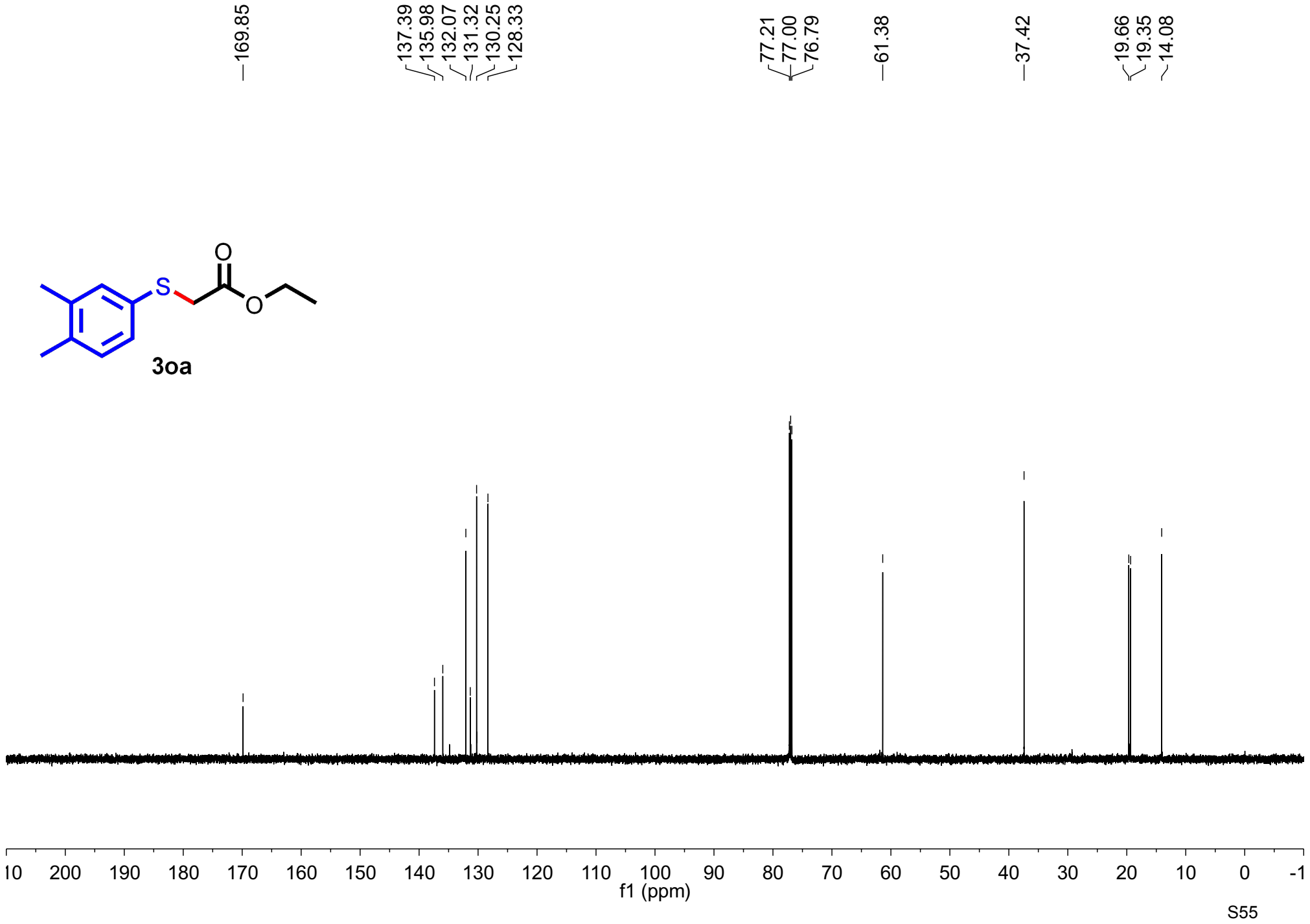
7.219
7.179
7.176
7.166
7.163
7.069
7.056
4.178
4.166
4.154
4.143
3.579
2.233
2.227
1.242
1.231
1.219
O
S
O
3oa
1.00
0.90
1.00
2.00
2.00
6.00
3.00
f1 (ppm)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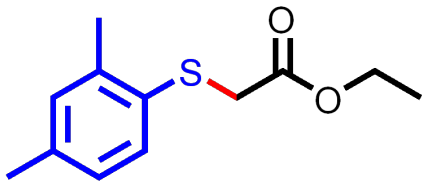
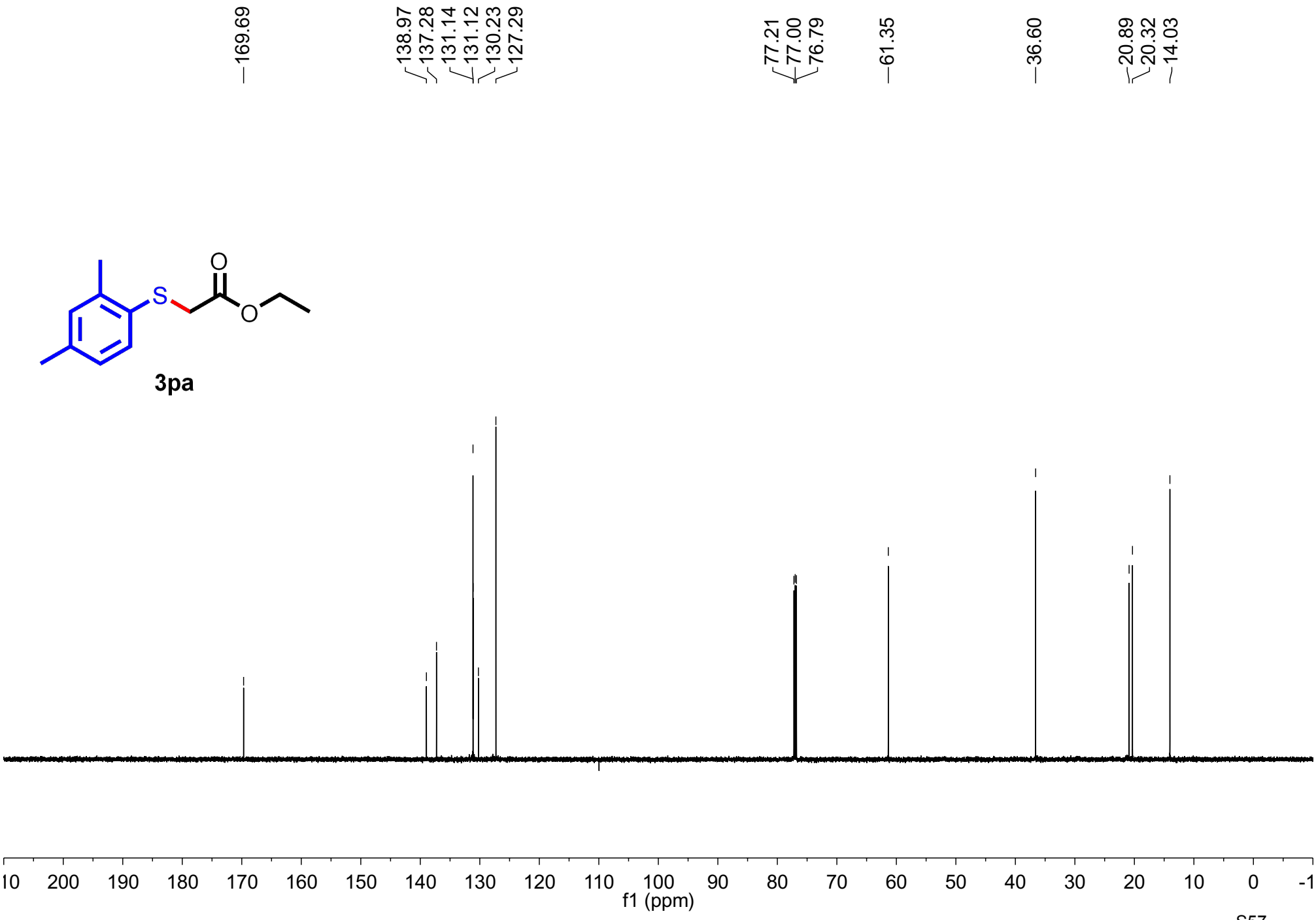
131.32
130.25
128.33
77.21
77.00
76.79
61.38
37.42
19.66
19.35
14.08
O
S
O
3oa
f1 (ppm)


O
S
O

3pa

7.299
7.285
7.260
7.021
6.976
6.963
4.160
4.148
4.136
4.124
3.545
2.406
2.291
1.232
1.220
1.208
1.00
1.00
1.00
2.00
2.05
3.05
3.10
3.05
f1 (ppm)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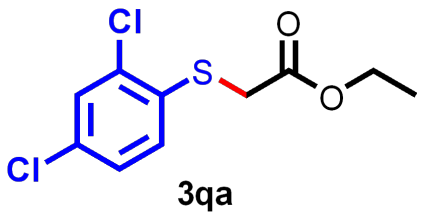
137.28
131.14
131.12
130.23
127.29
77.21
77.00
76.79
61.35
36.60
20.89
20.32
14.03
O
S
O
3pa
f1 (ppm)


Cl
S
O
O
Cl

3qa

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7.400
7.363
7.349
7.260
7.215
7.211
7.201
7.197
4.183
4.171
4.159
4.148
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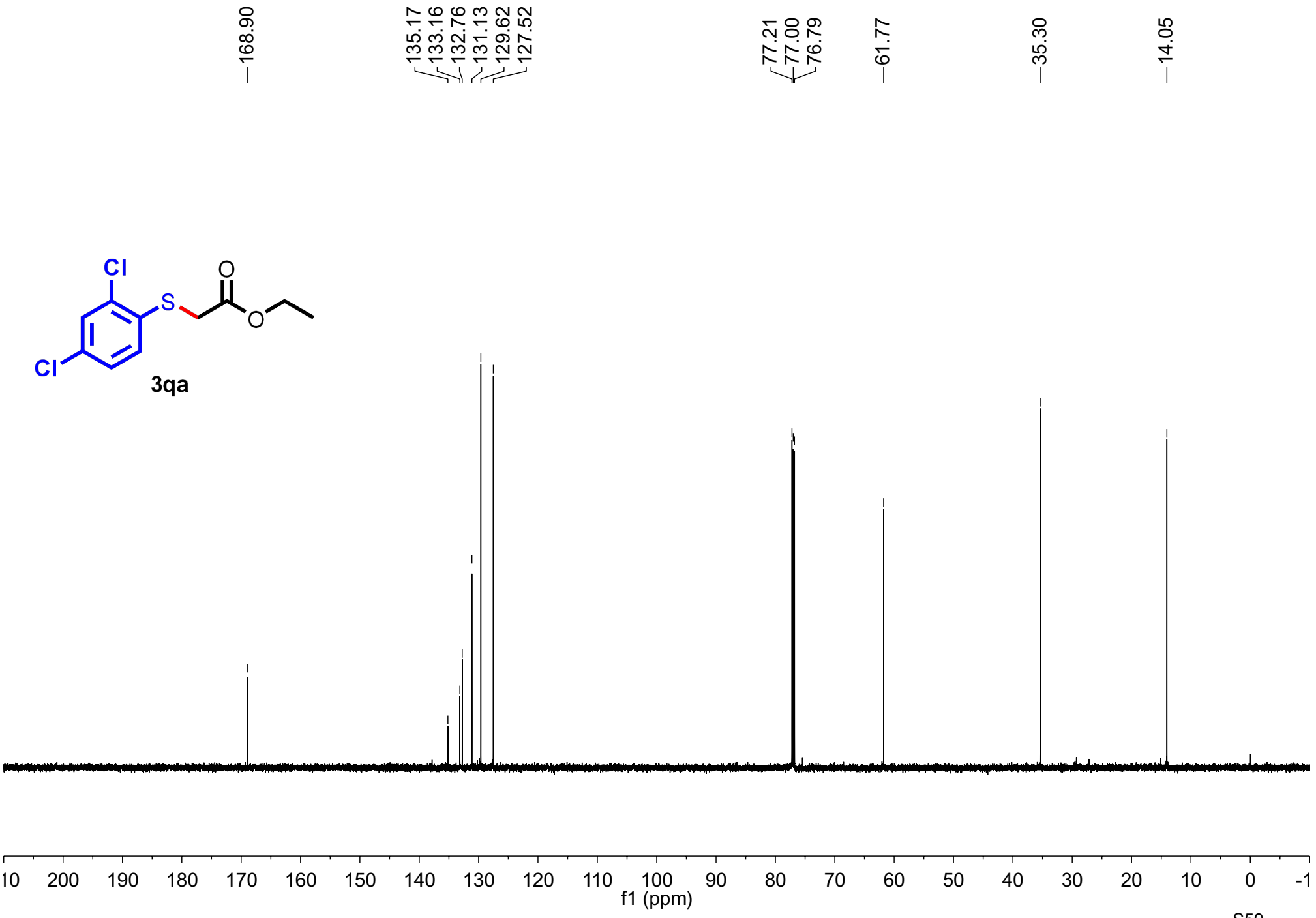
1.232
1.220
0.80
1.00
0.95
2.00
2.00
3.00
f1 (ppm)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132.76
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129.62
127.52
77.21
77.00
76.79
61.77
35.30
14.05
Cl
S
O
O
Cl
3qa
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
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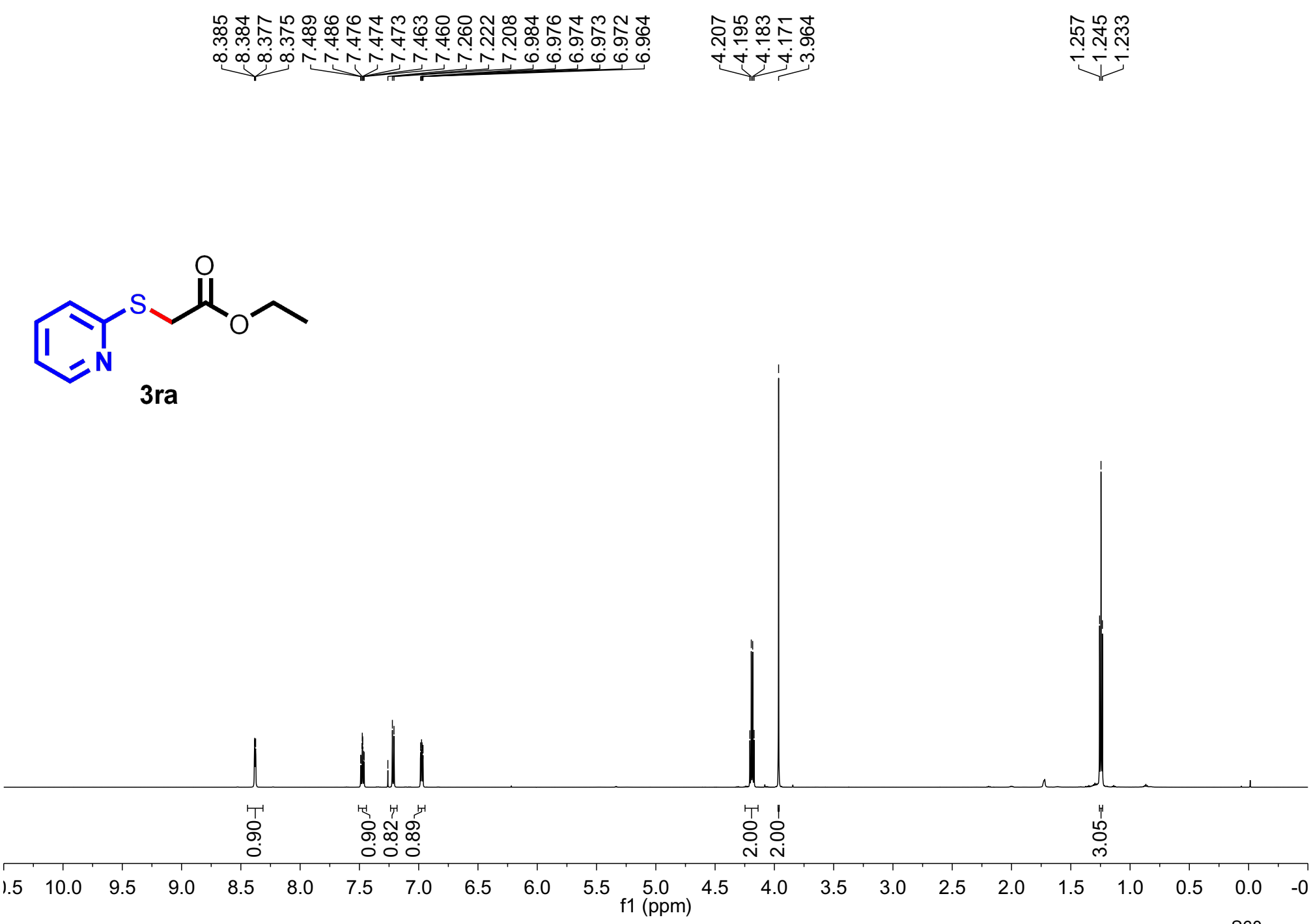
-1
f1 (ppm)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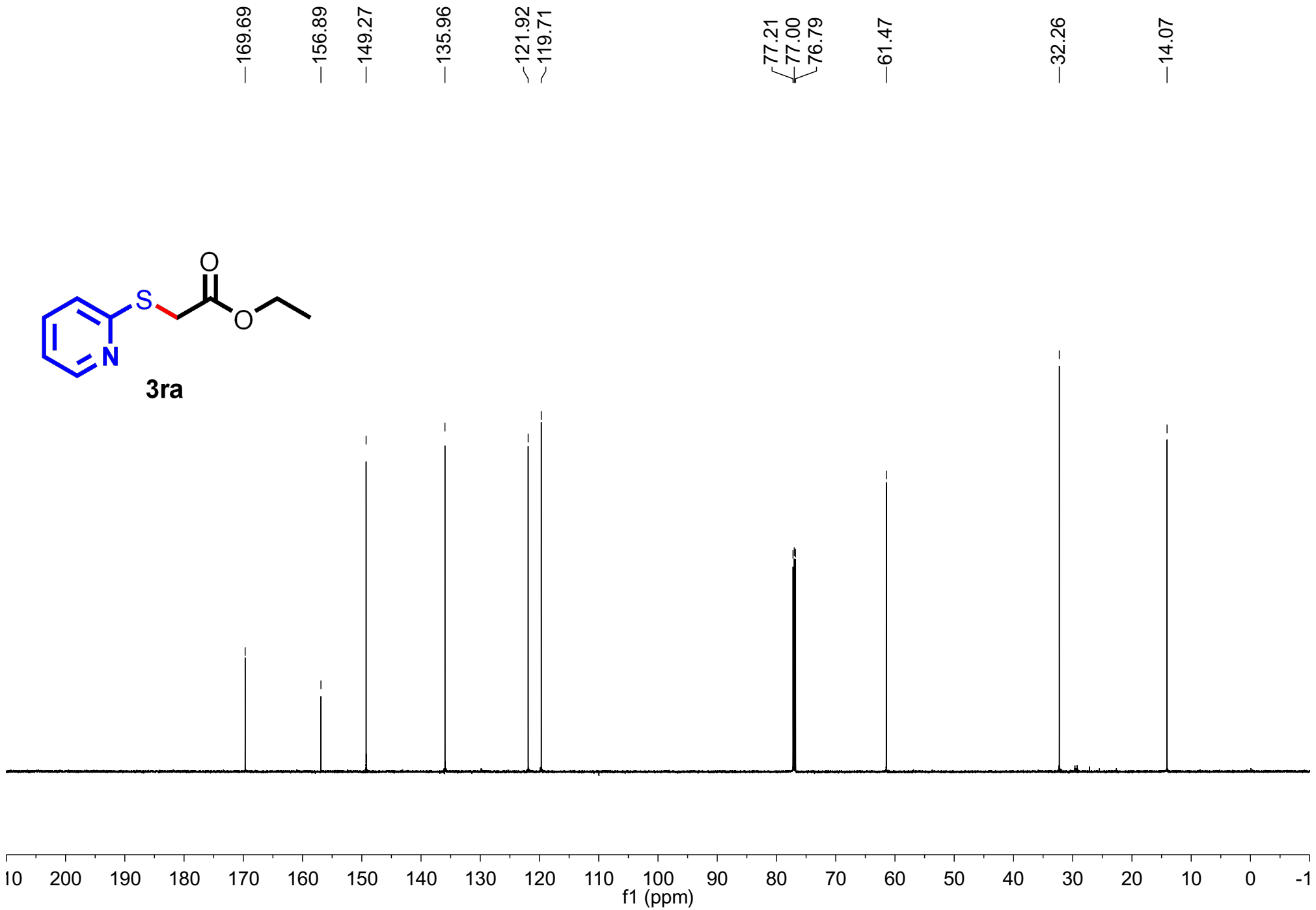
8.375
7.489
7.486
7.476
7.474
7.473
7.463
7.460
7.260
7.222
7.208
6.984
6.976
6.974
6.973
6.972
6.964
4.207
4.195
4.183
4.171
3.964
1.257
1.245
1.233
O
S
O
N
3ra
0.90
0.90
0.82
0.89
2.00
2.00
3.05
f1 (ppm)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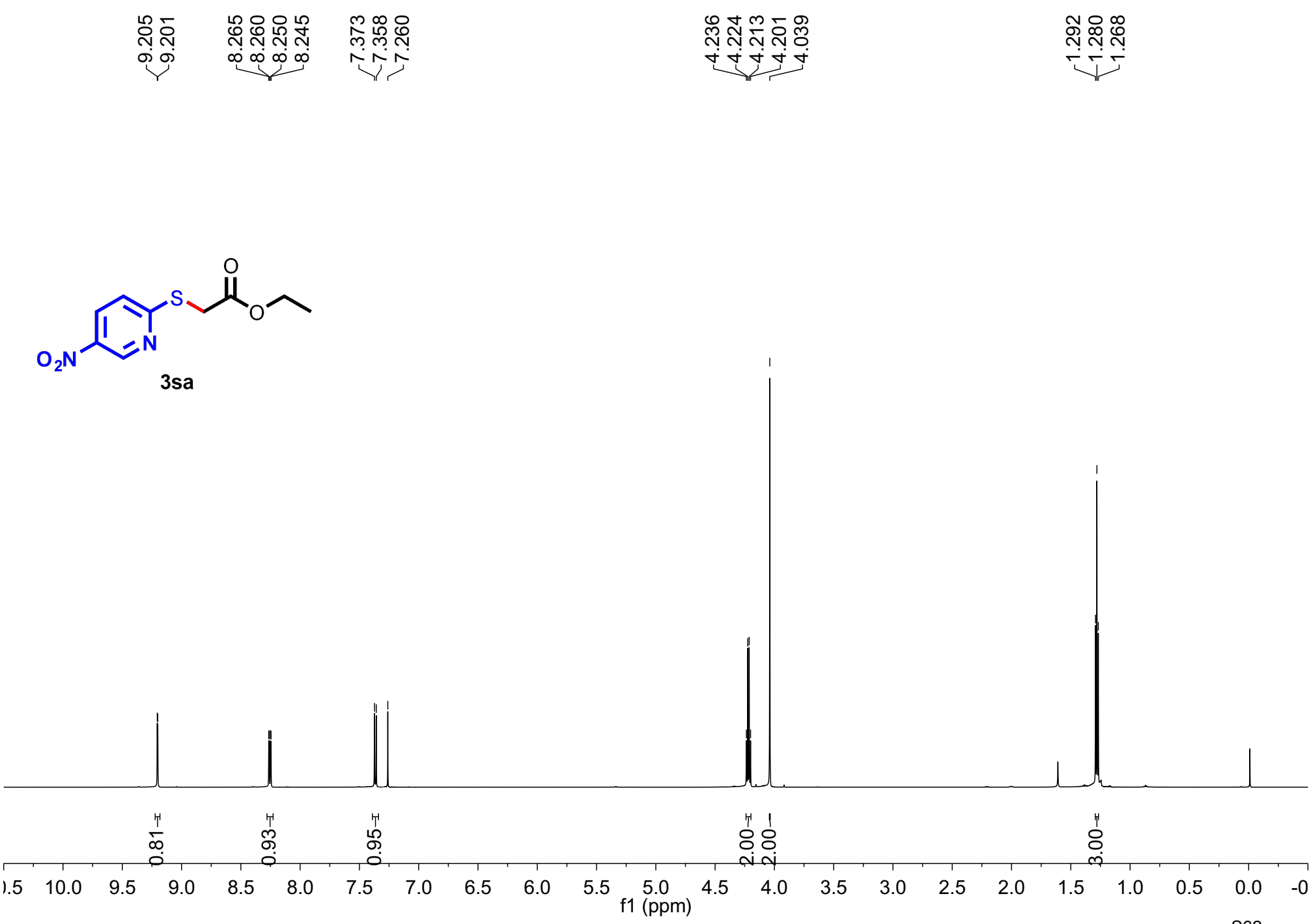
156.89
149.27
135.96
121.92
119.71
77.21
77.00
76.79
61.47
32.26
14.07
O
S
O
N
3ra
f1 (ppm)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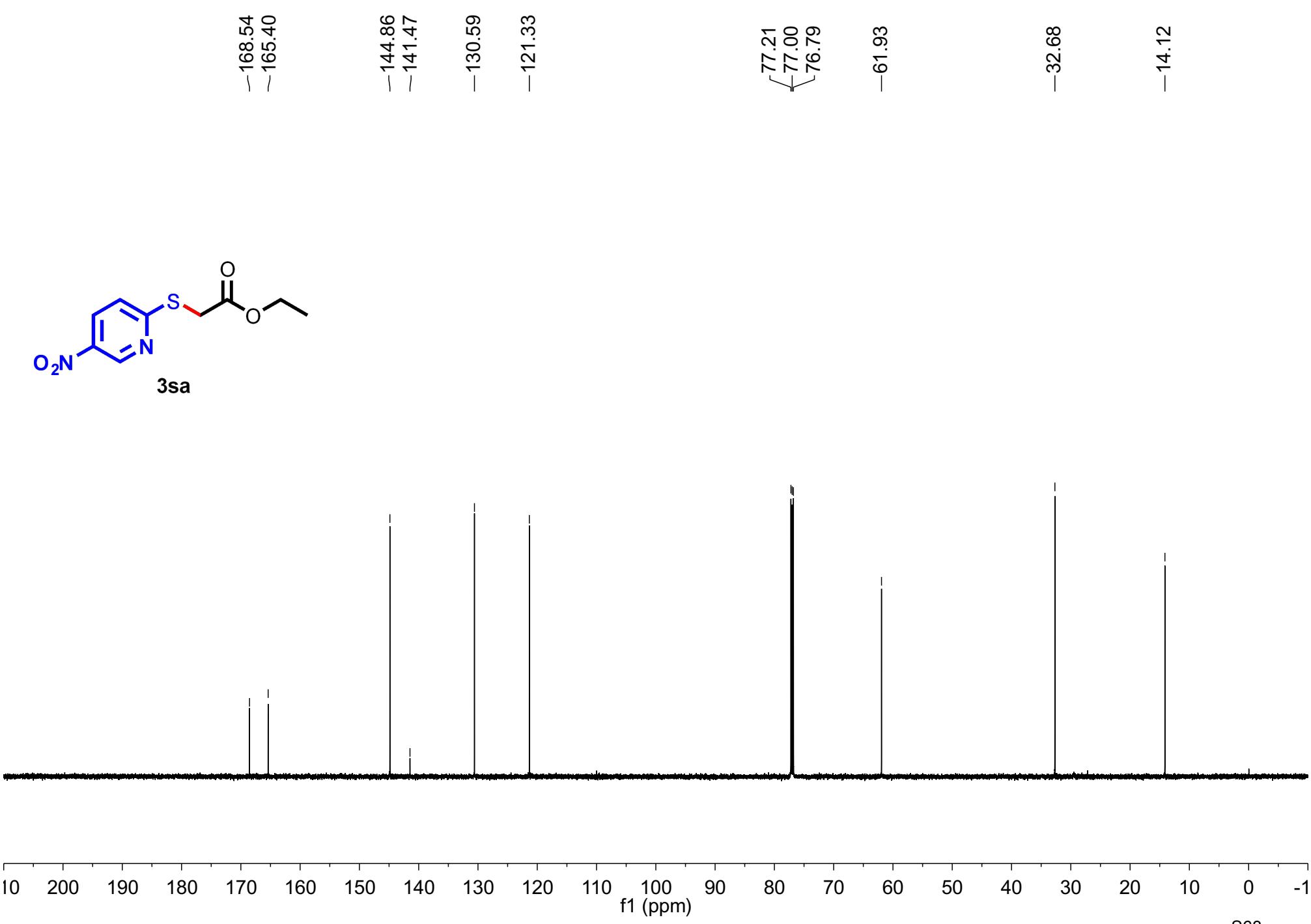
9.201
8.265
8.260
8.250
8.245
7.373
7.358
7.260
4.236
4.224
4.213
4.201
4.039
1.292
1.280
1.268
O
S
O
N
O2N
3sa
0.81
0.93
0.95
2.00
2.00
3.00
f1 (ppm)


168.54
165.40
144.86
141.47
130.59
121.33
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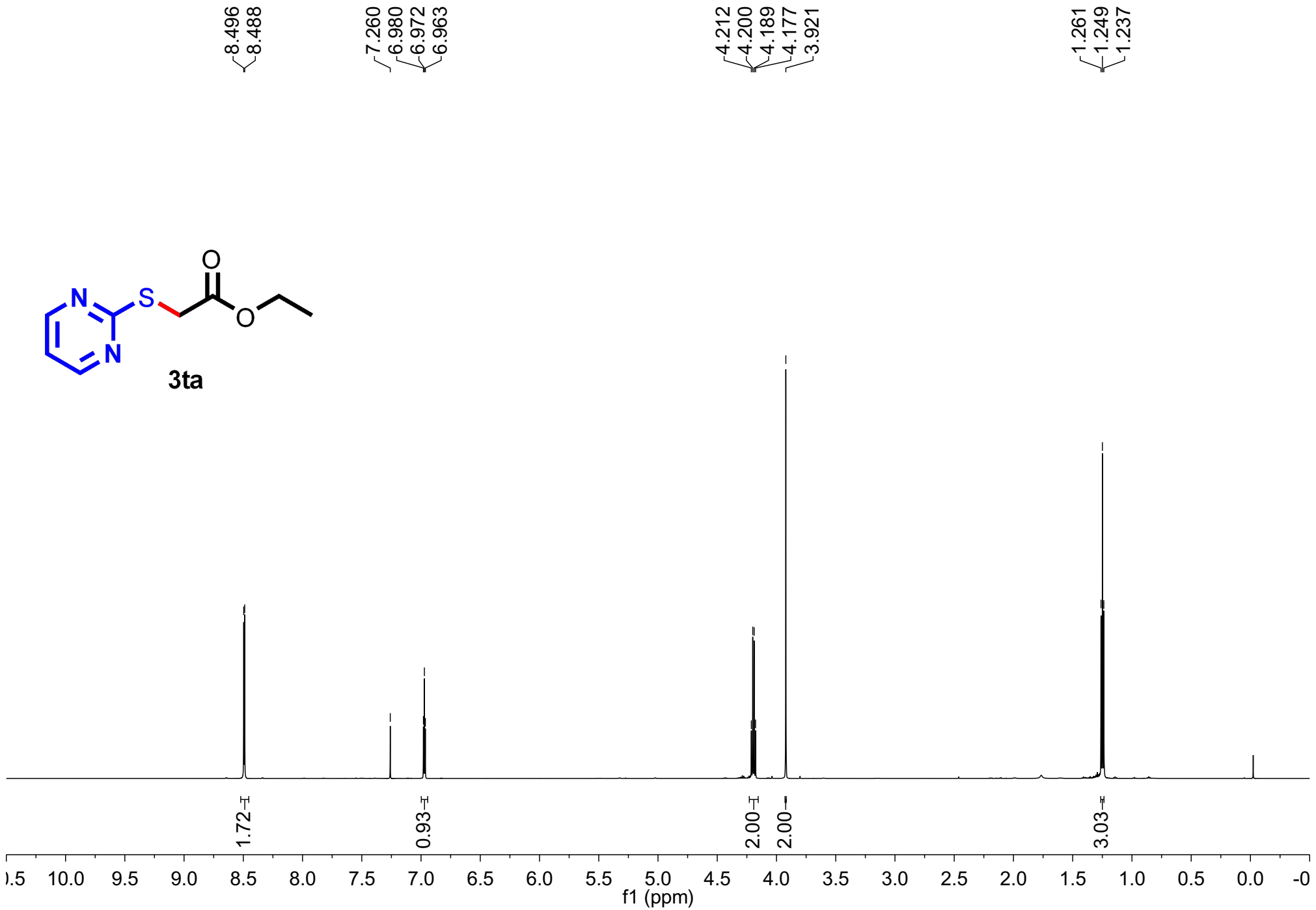
77.00
76.79
61.93
32.68
14.12
O
S
O
N
O2N
3sa
f1 (ppm)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8.488
7.260
6.980
6.972
6.963
4.212
4.200
4.189
4.177
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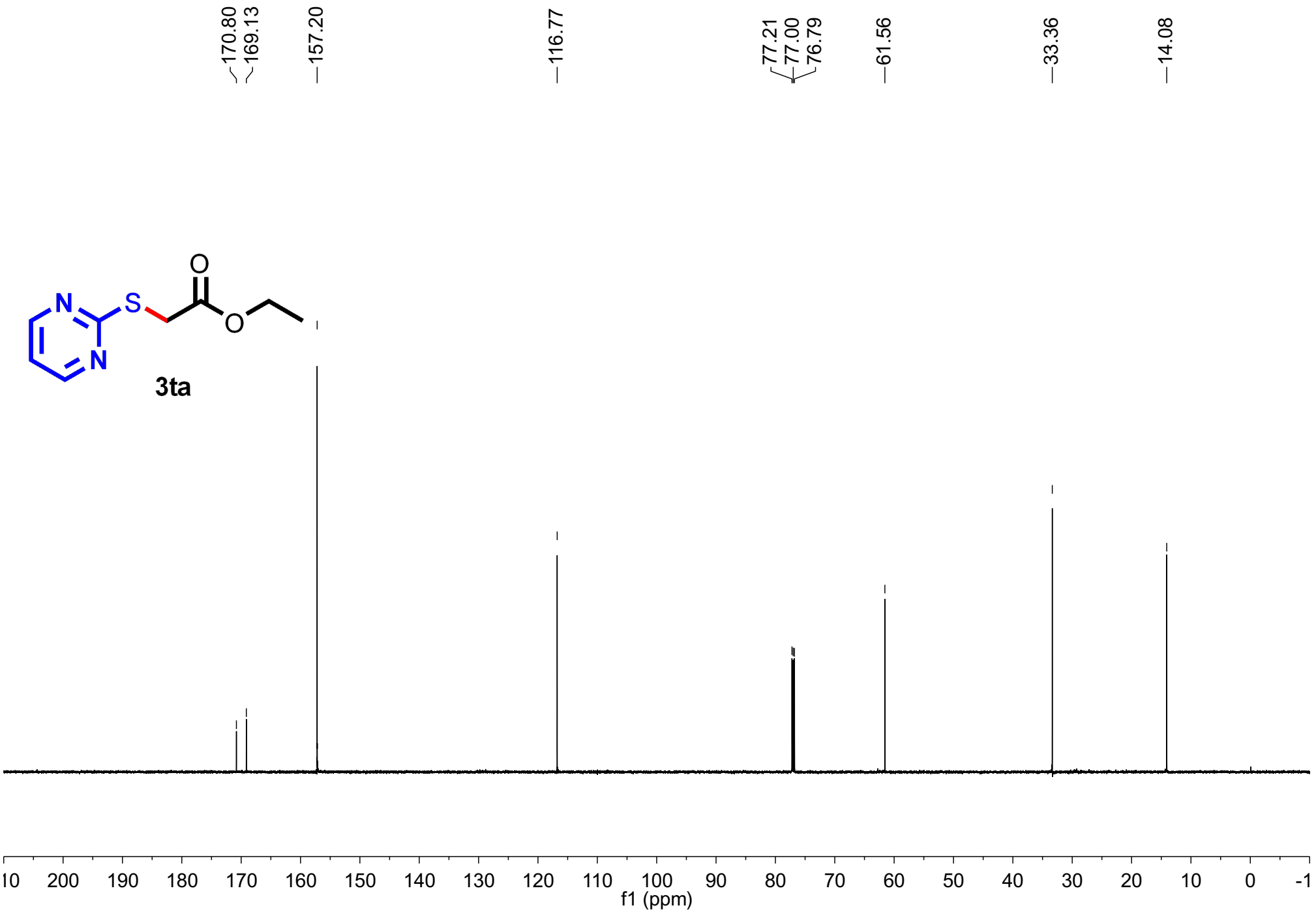
1.261
1.249
1.237
3ta
1.72
0.93
2.00
2.00
3.03
f1 (ppm)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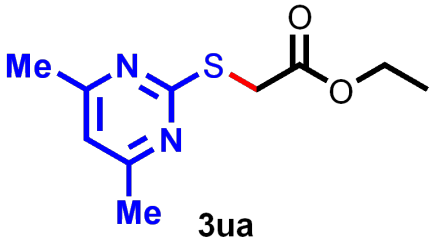
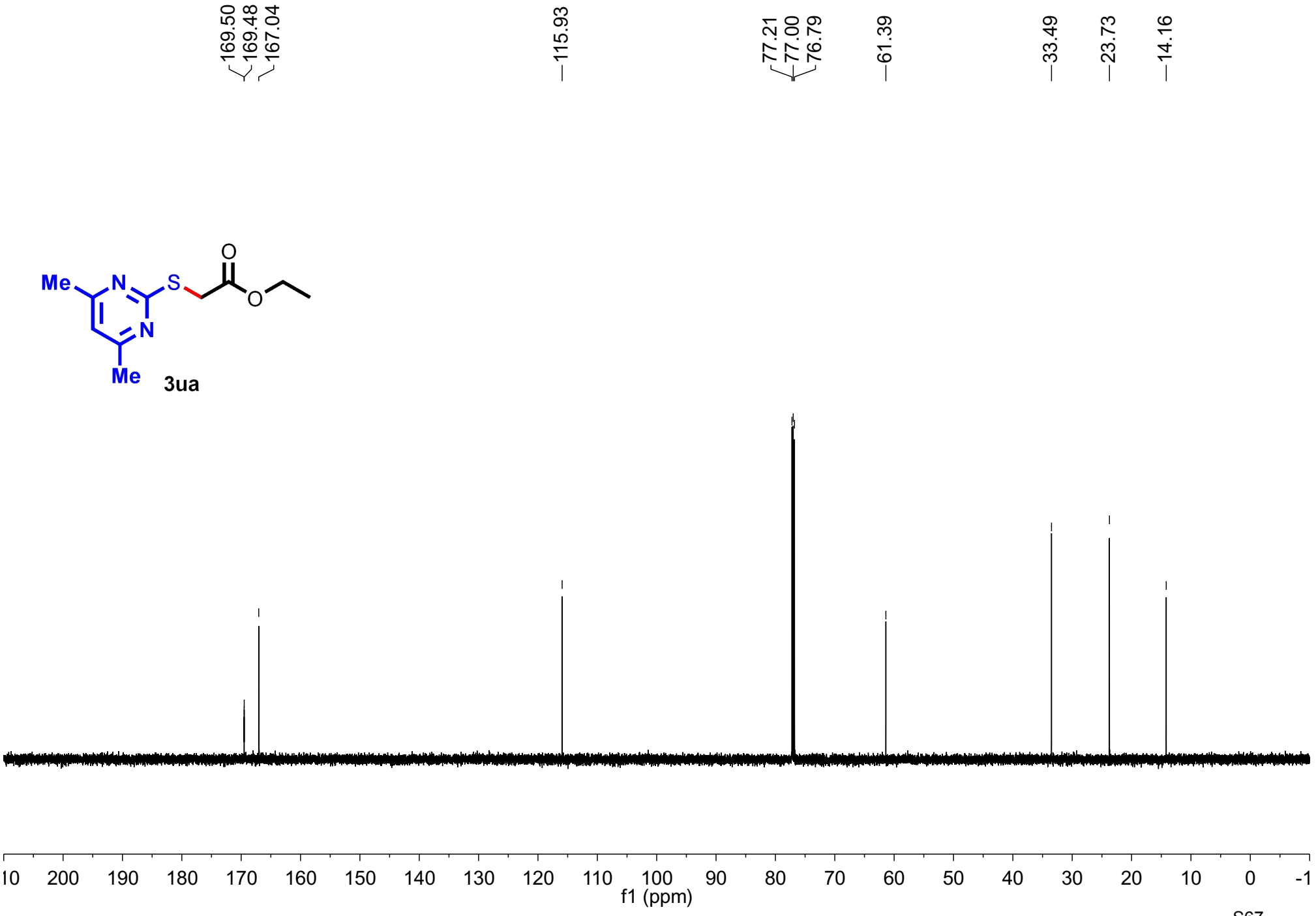
169.13
157.20
116.77
77.21
77.00
76.79
61.56
33.36
14.08
N
S
O
O
N
3ta
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)


Me
N
S
O
O
N
Me

3ua

7.260
6.691
4.221
4.203
4.185
4.167
3.902
2.370
1.277
1.260
1.242
0.87
2.00
2.00
6.00
3.00
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
f1 (ppm)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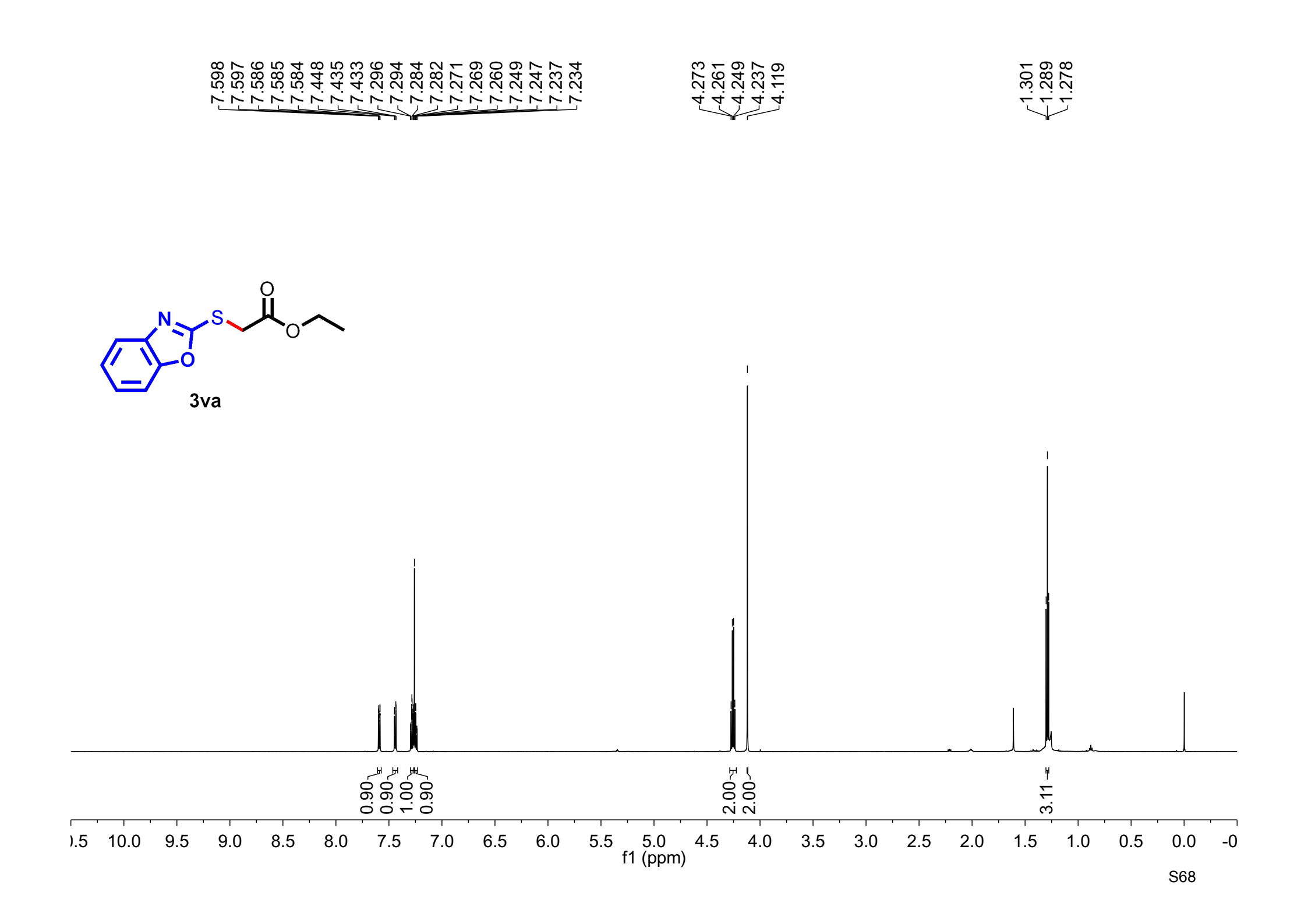
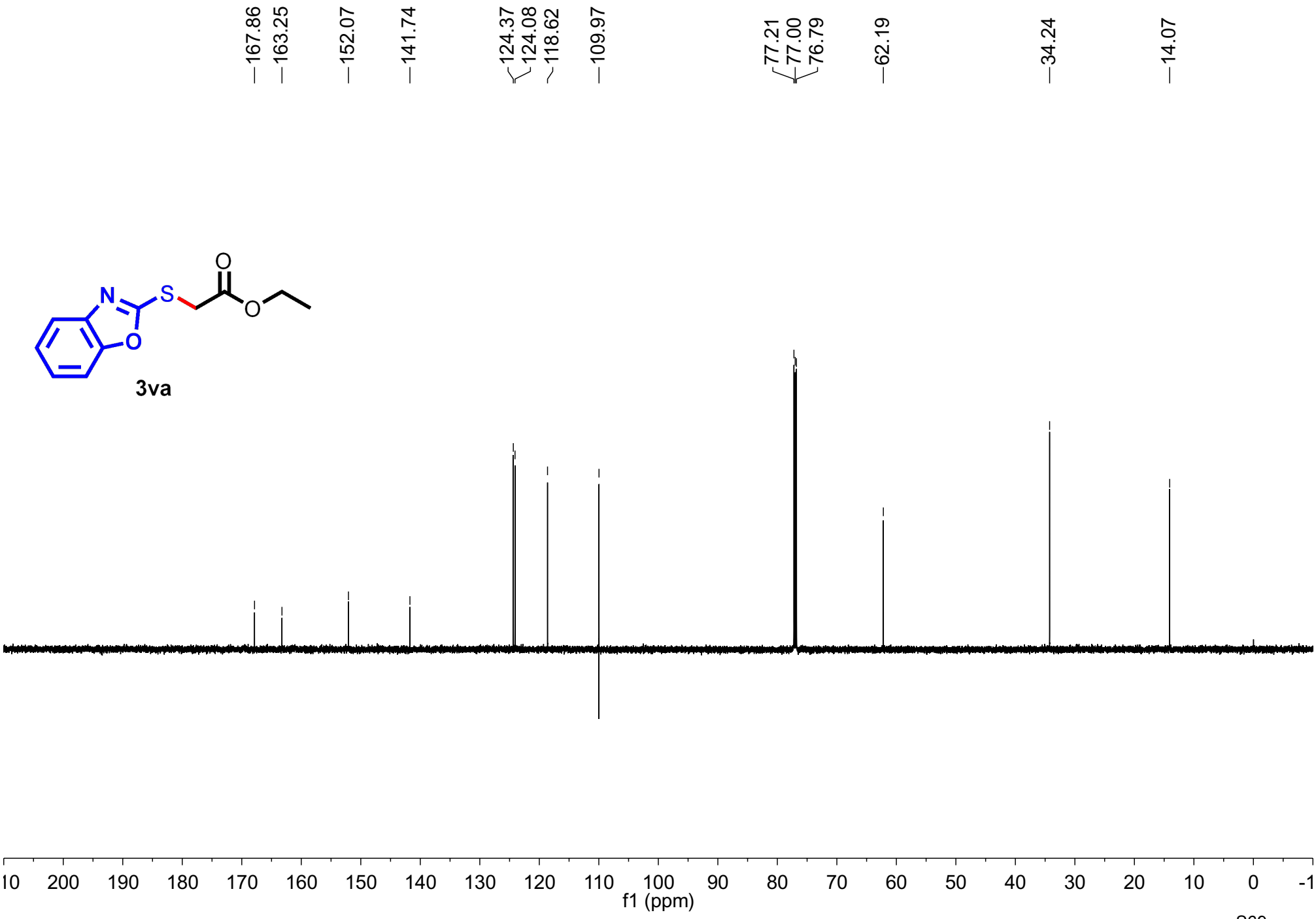
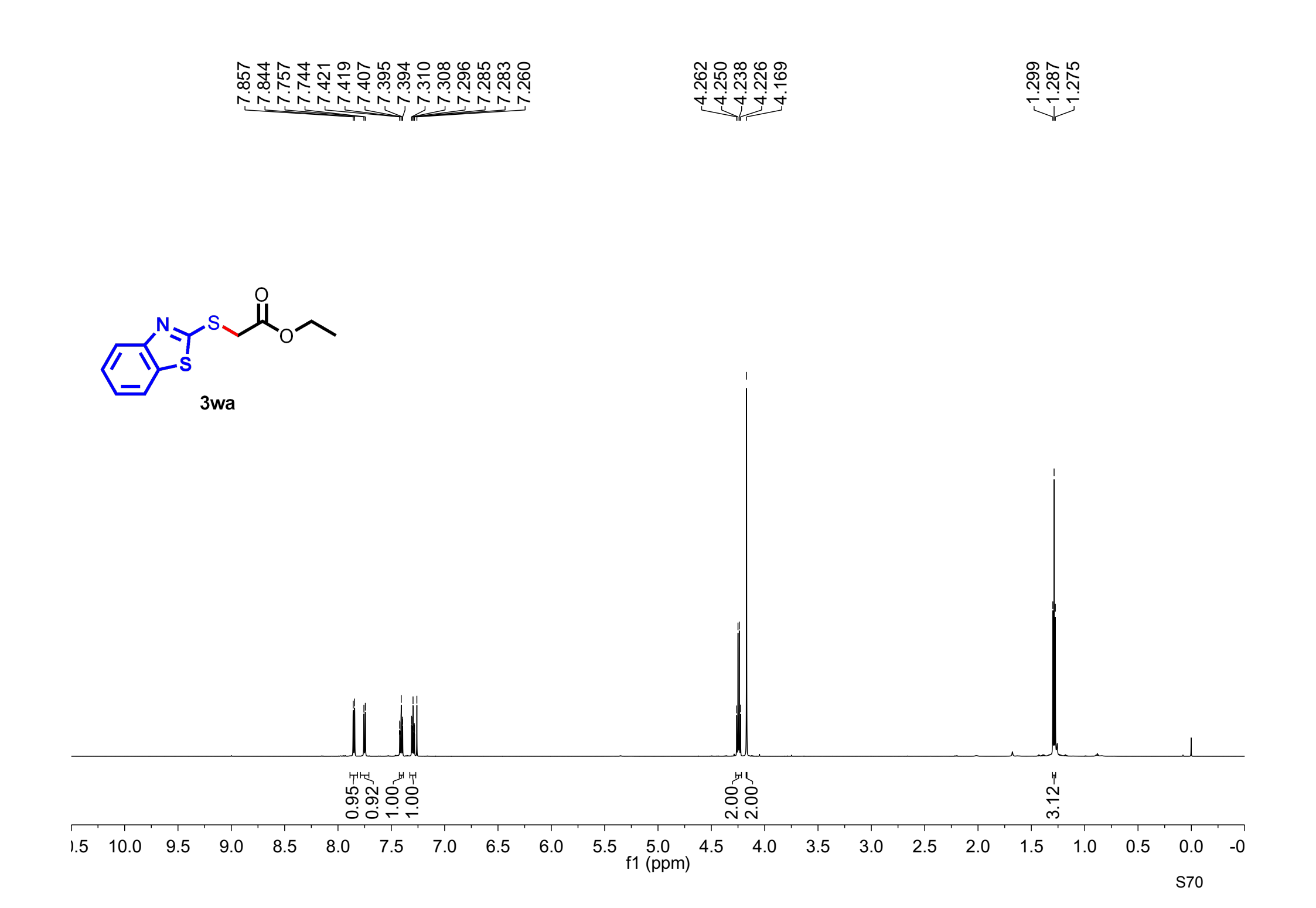
167.04
115.93
77.21
77.00
76.79
61.39
33.49
23.73
14.16
Me
N
S
O
O
N
Me
3ua
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)


7.598
7.597
7.586
7.585
7.584
7.448
7.435
7.433
7.296
7.294
7.284
7.282
7.271
7.269
7.260
7.249
7.247
7.237
7.234
4.273
4.261
4.249
4.237
4.119
1.301
1.289
1.278
O
N
S
O
O
3va
0.90
0.90
1.00
0.90
2.00
2.00
3.11
f1 (ppm)


167.86
163.25
152.07
141.74
124.37
124.08
118.62
109.97
77.21
77.00
76.79
62.19
34.24
14.07
O
N
S
O
O
3va
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)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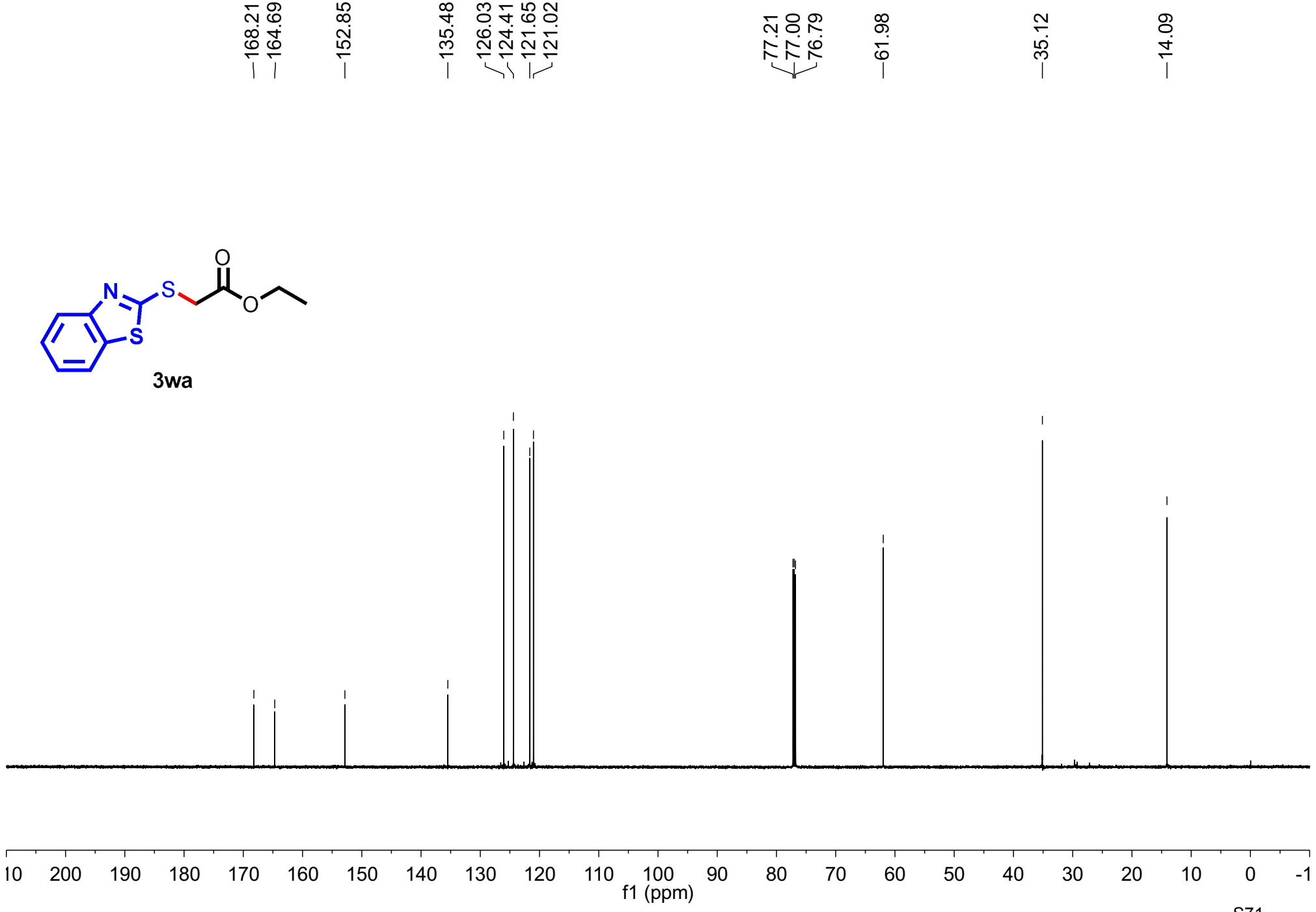
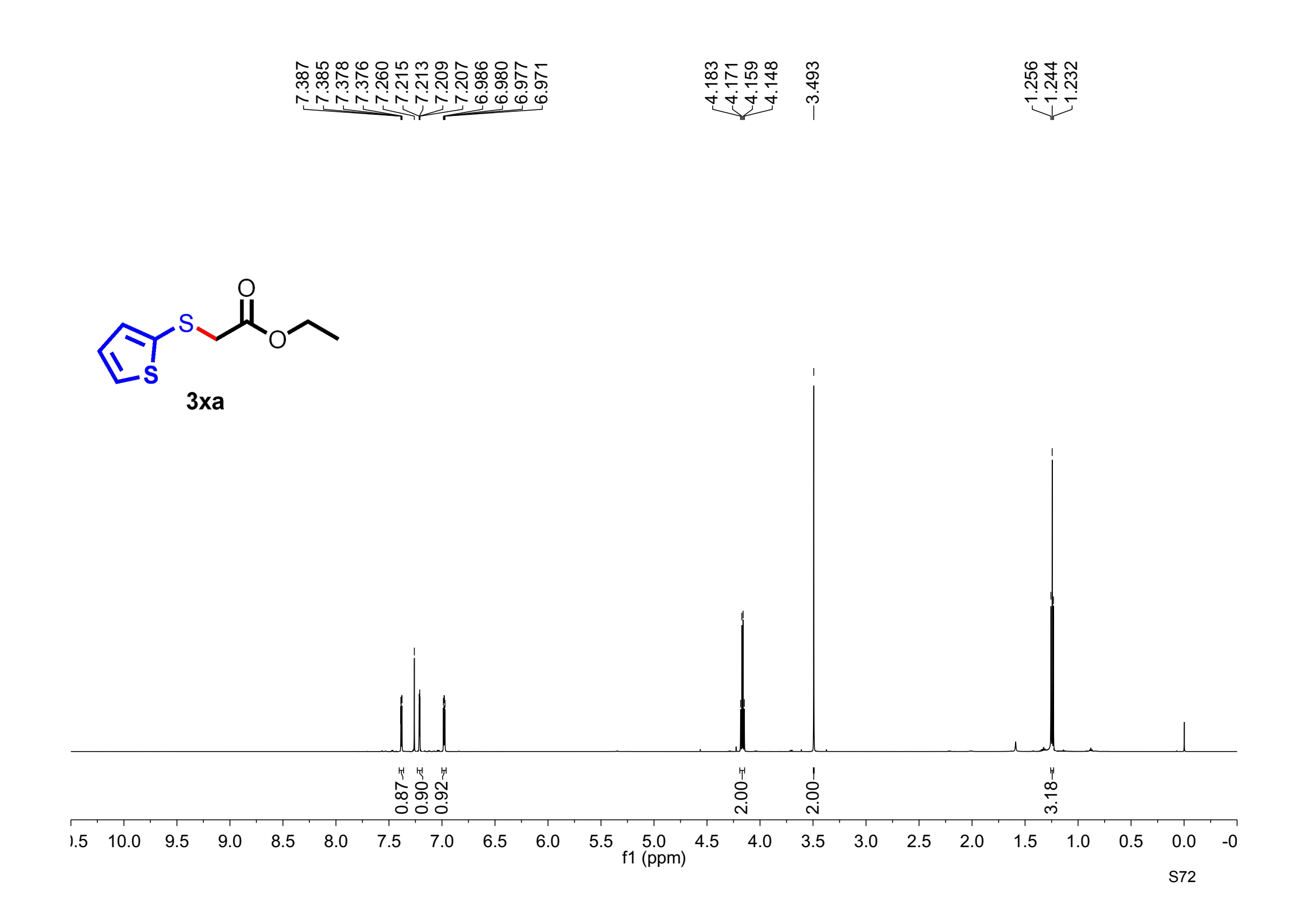
7.757
7.744
7.421
7.419
7.407
7.395
7.394
7.310
7.308
7.296
7.285
7.283
7.260
4.262
4.250
4.238
4.226
4.169
1.299
1.287
1.275
N
S
O
O
S
3wa
0.95
0.92
1.00
1.00
2.00
2.00
3.12
f1 (ppm)


168.21
164.69
152.85
135.48
126.03
124.41
121.65
121.02
77.21
77.00
76.79
61.98
35.12
14.09
N
S
S
O
O
3wa
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)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7.213
7.209
7.207
6.986
6.980
6.977
6.971
4.183
4.171
4.159
4.148
3.493
1.256
1.244
1.232
O
S
O
S
3xa
0.87
0.90
0.92
2.00
2.00
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
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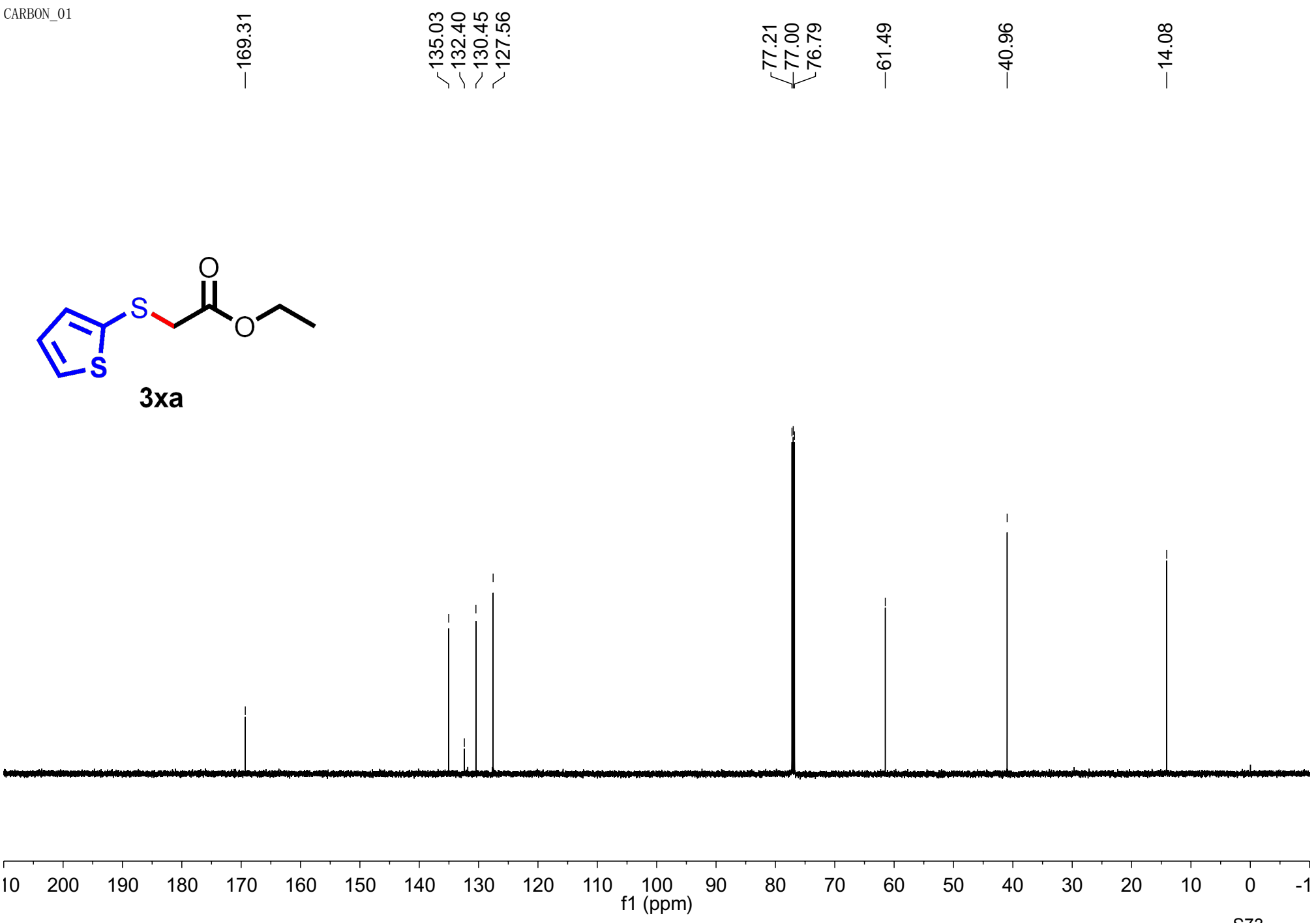
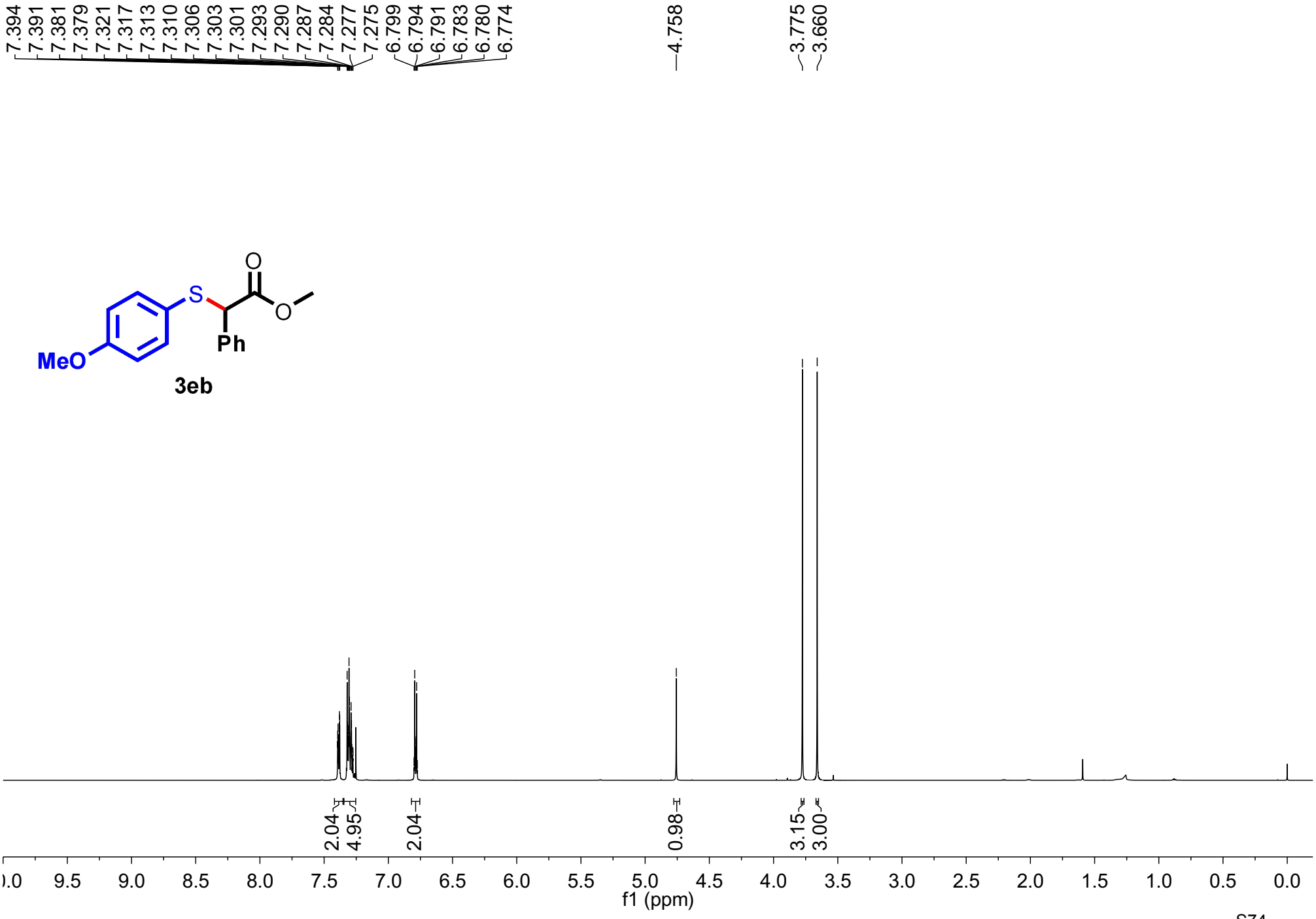
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

CARBON_01


169.31
135.03
132.40
130.45
127.56
77.21
77.00
76.79
61.49
40.96
14.08
O
S
O
S
3xa
f1 (ppm)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7.391
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7.321
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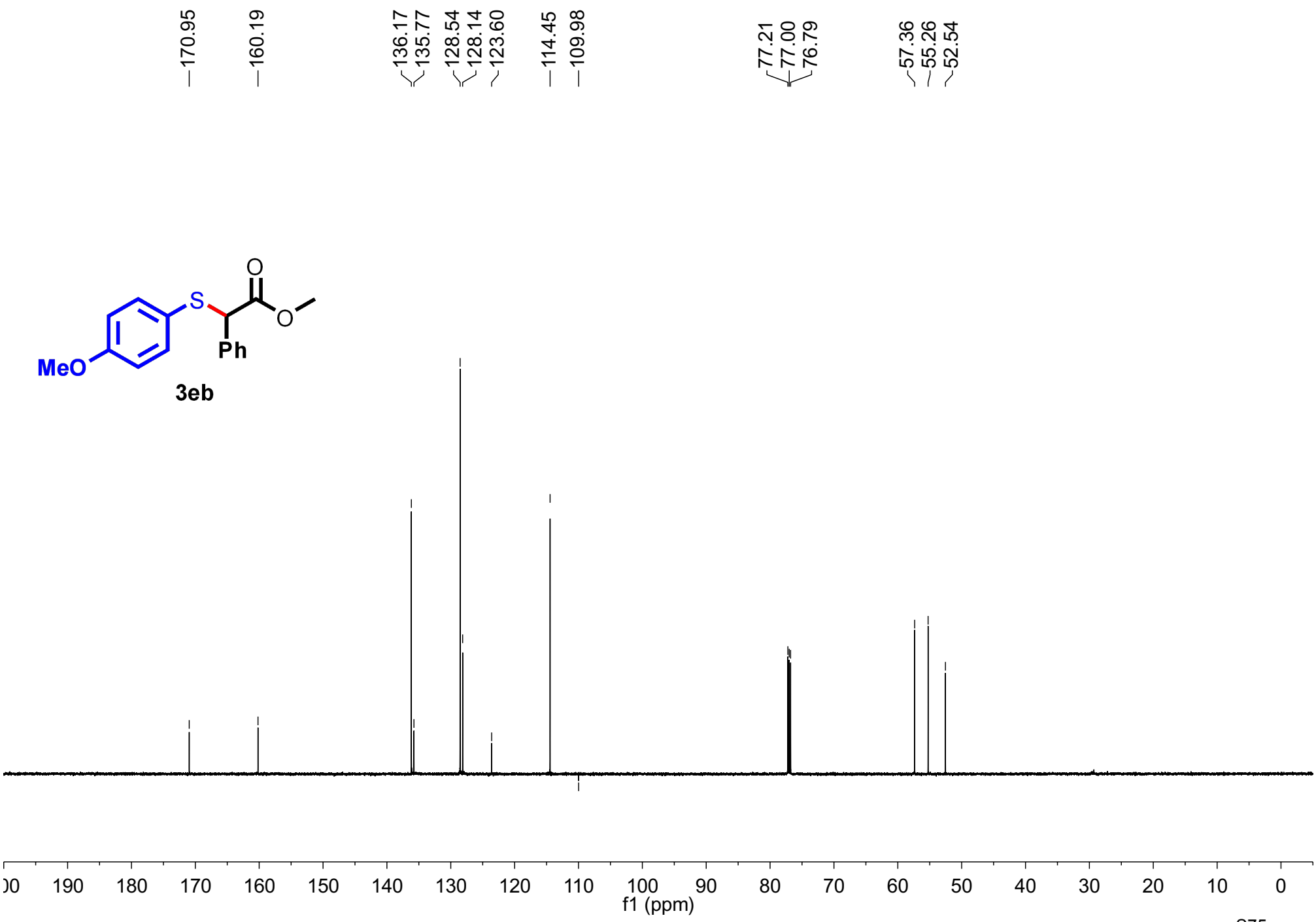
7.310
7.306
7.303
7.301
7.293
7.290
7.287
7.284
7.277
7.275
6.799
6.794
6.791
6.783
6.780
6.774
4.758
3.775
3.660
O
S
O
Ph
MeO
3eb
2.04
4.95
2.04
0.98
3.15
3.00
f1 (ppm)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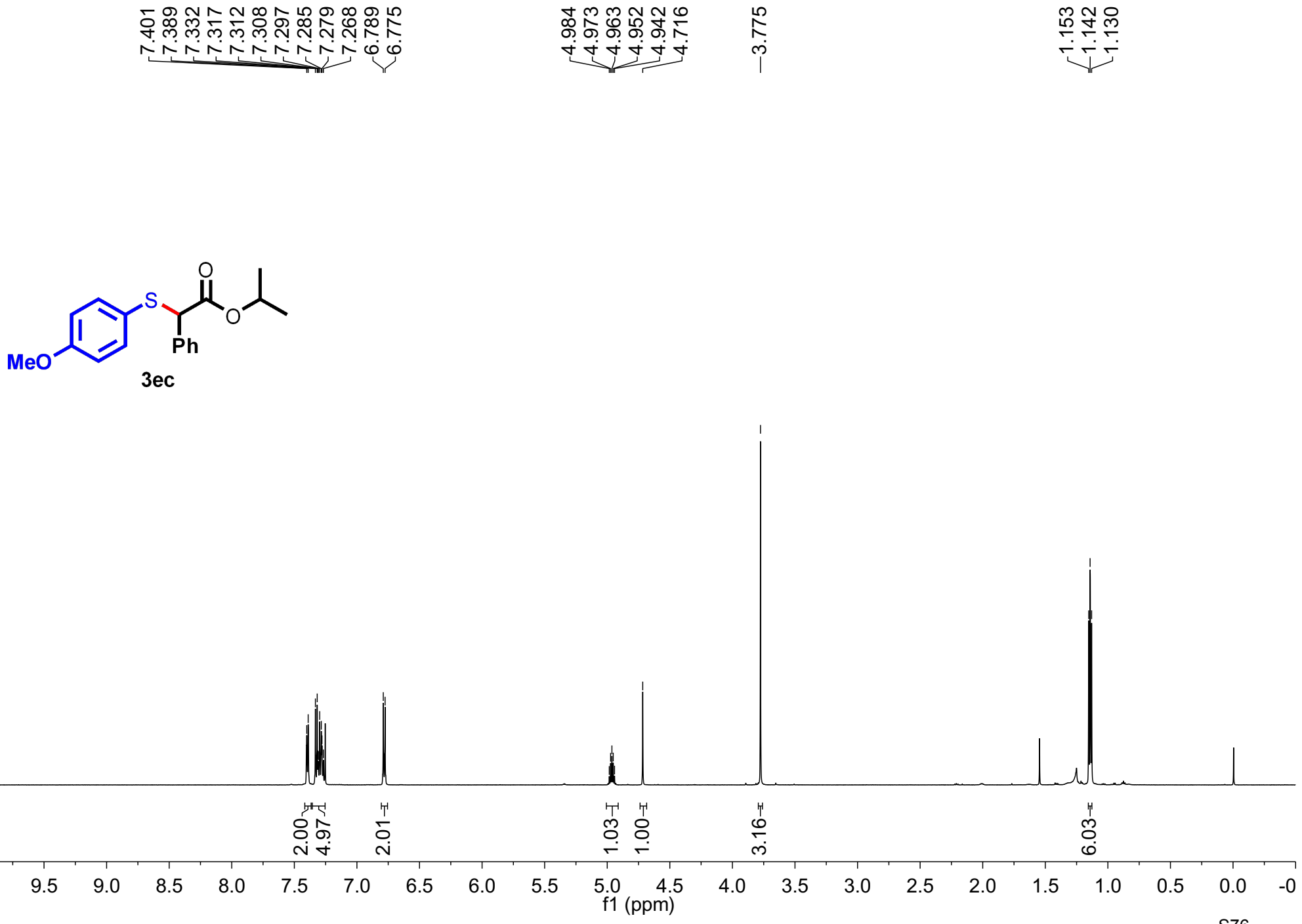
160.19
136.17
135.77
128.54
128.14
123.60
114.45
109.98
77.21
77.00
76.79
57.36
55.26
52.54
O
S
O
Ph
MeO
3eb
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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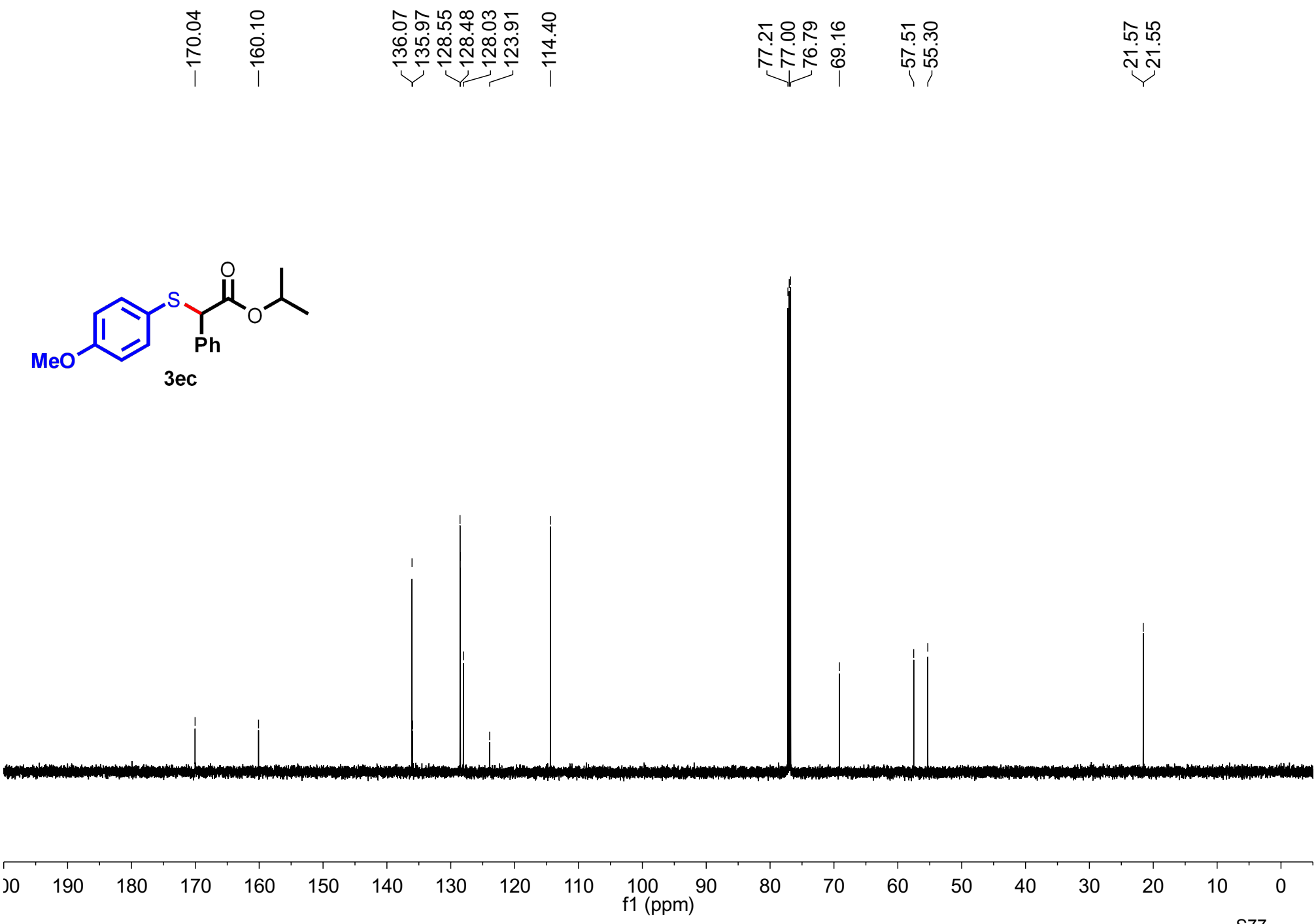
7.308
7.297
7.285
7.279
7.268
6.789
6.775
4.984
4.973
4.963
4.952
4.942
4.716
3.775
1.153
1.142
1.130
MeO
Ph
3ec
2.00
4.97
2.01
1.03
1.00
3.16
6.03
f1 (ppm)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160.10
136.07
135.97
128.55
128.48
128.03
123.91
114.40
77.21
77.00
76.79
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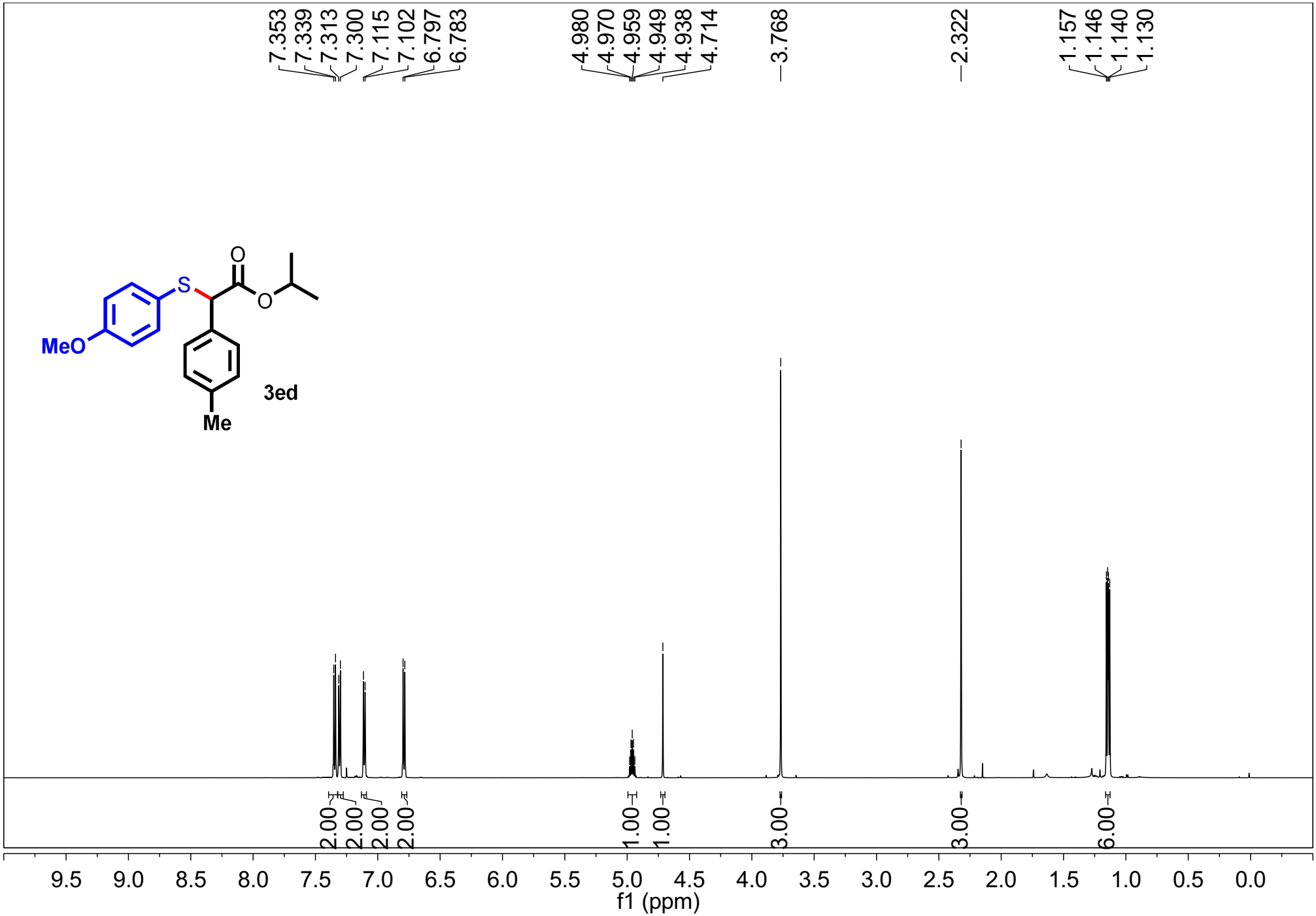
57.51
55.30
21.57
21.55
MeO
S
O
O
Ph
3ec
f1 (ppm)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6.783
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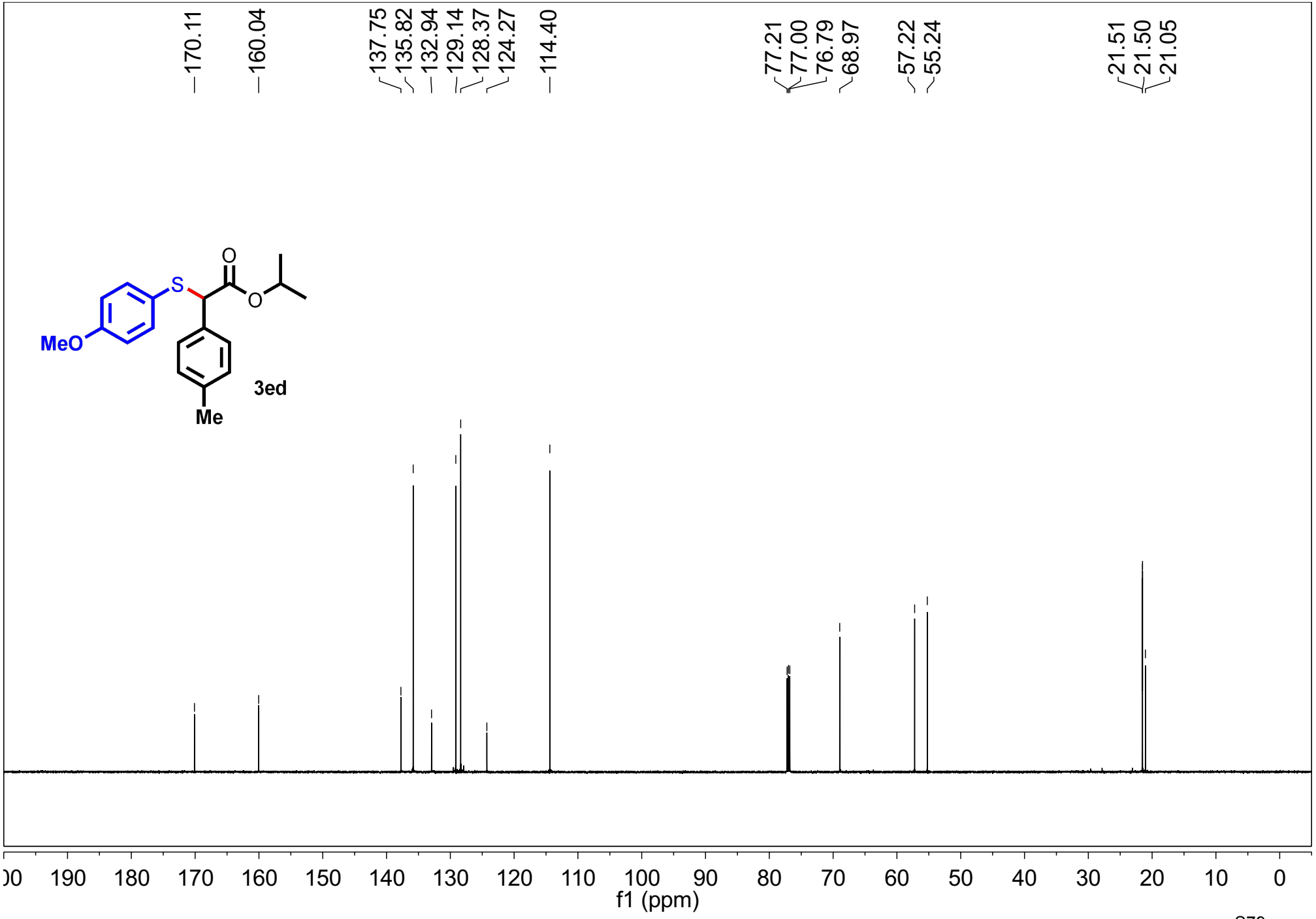
4.970
4.959
4.949
4.938
4.714
3.768
2.322
1.157
1.146
1.140
1.130
MeO
S
O
O
Me
3ed
2.00
2.00
2.00
2.00
1.00
1.00
3.00
3.00
6.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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137.75
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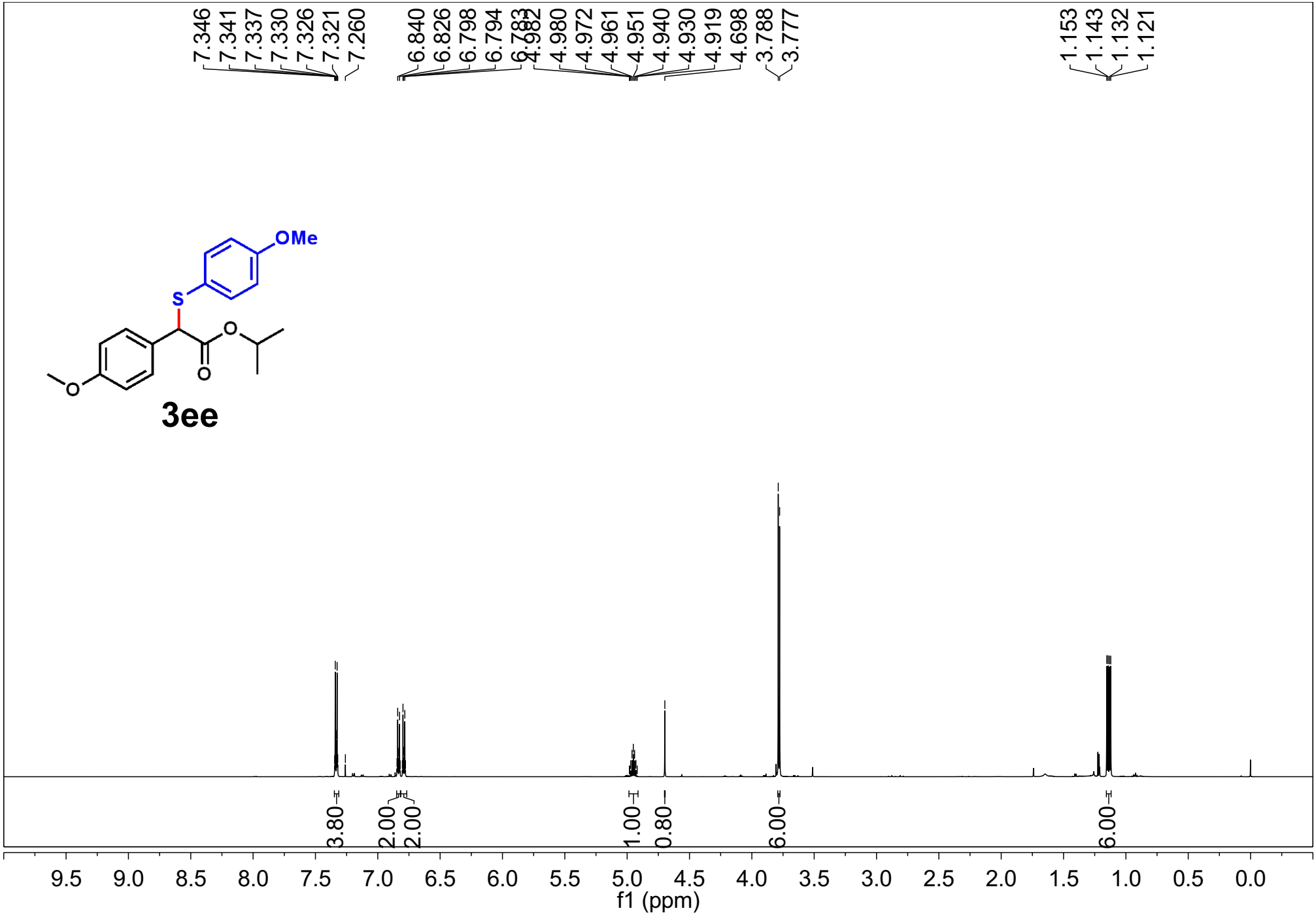
129.14
128.37
124.27
114.40
77.21
77.00
76.79
68.97
57.22
55.24
21.51
21.50
21.05
O
S
O
MeO
Me
3ed
f1 (ppm)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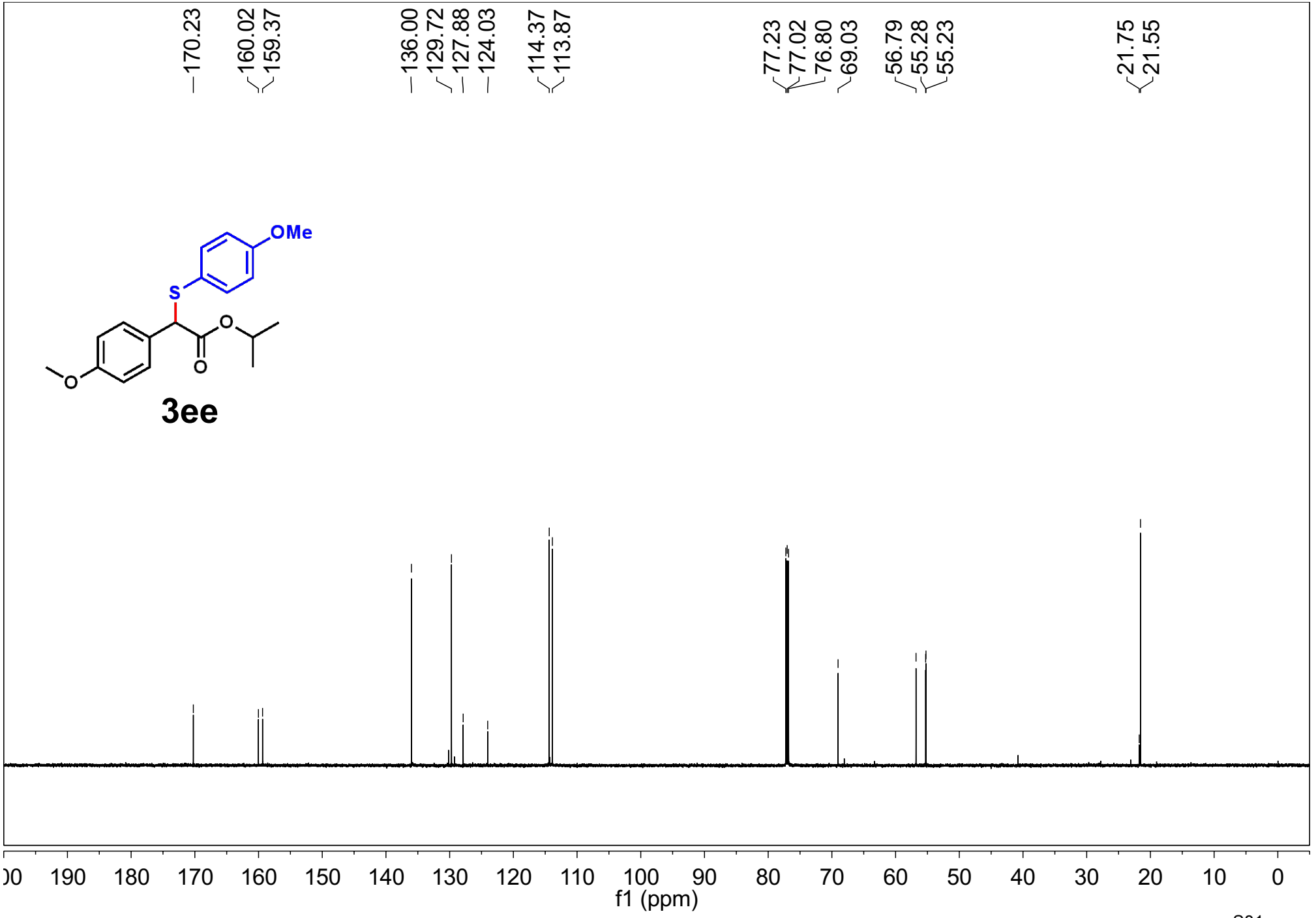
7.321
7.260
6.840
6.826
6.798
6.794
6.783
4.982
4.980
4.972
4.961
4.951
4.940
4.930
4.919
4.698
3.788
3.777
1.153
1.143
1.132
1.121
OMe
S
O
O
O
3ee
3.80
2.00
2.00
1.00
0.80
6.00
6.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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77.23
77.02
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69.03
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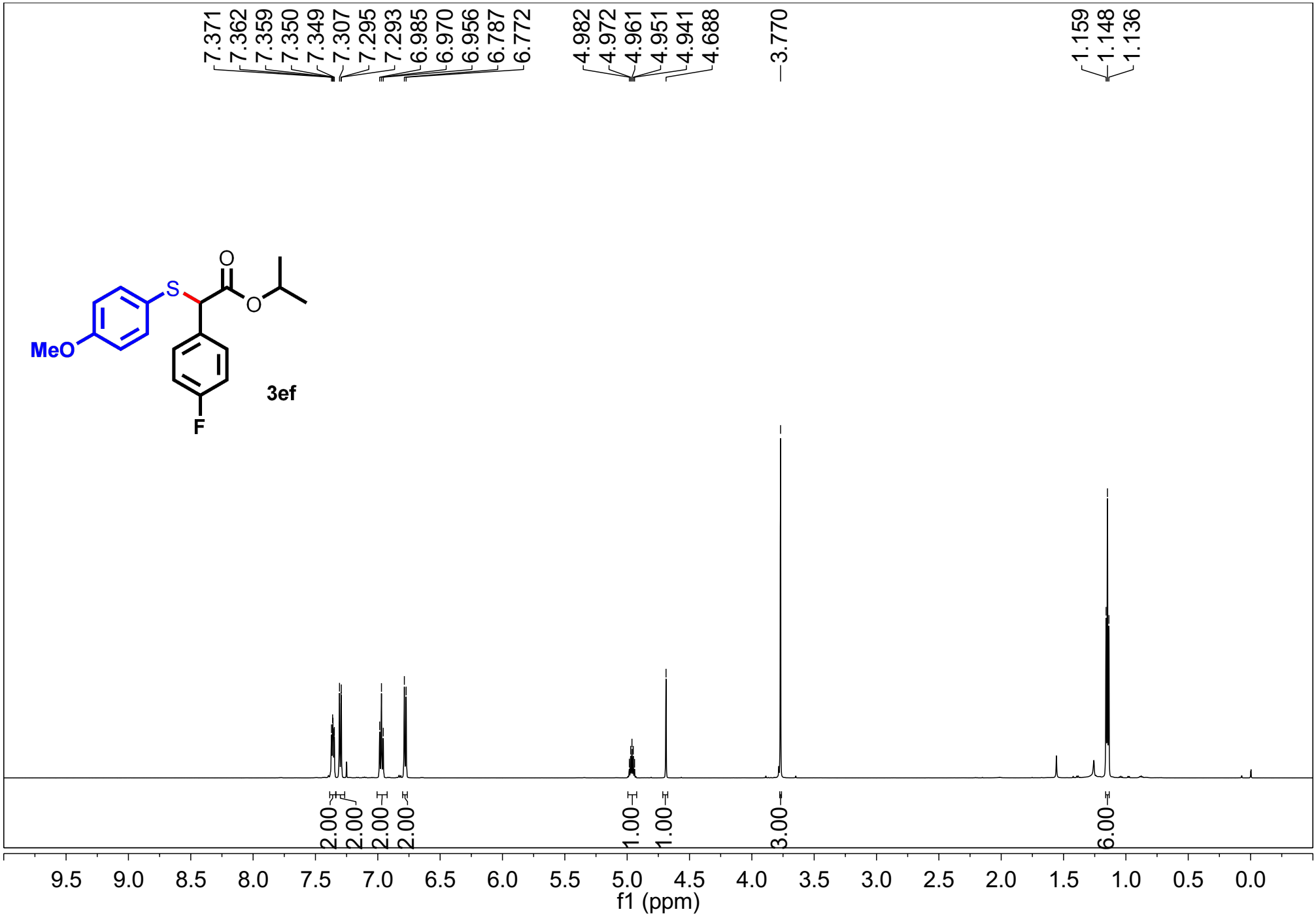
55.28
55.23
21.75
21.55
OMe
S
O
O
O
3ee
f1 (ppm)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7.307
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7.293
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6.970
6.956
6.787
6.772
4.982
4.972
4.961
4.951
4.941
4.688
3.770
1.159
1.148
1.136
MeO
S
O
O
F
3ef
2.00
2.00
2.00
2.00
1.00
1.00
3.00
6.00
9.5
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
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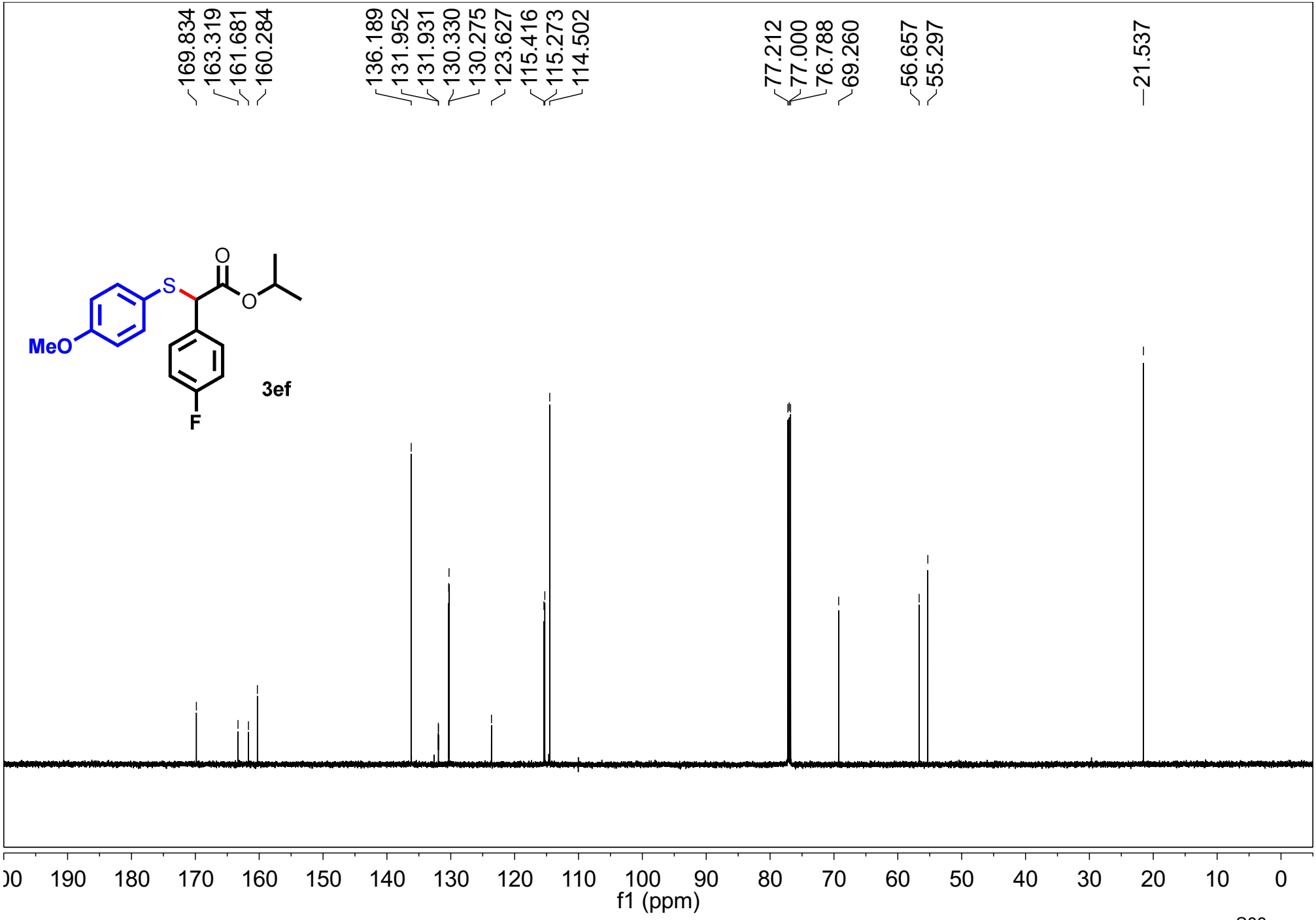
0.0
f1 (ppm)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130.330
130.275
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115.273
114.502
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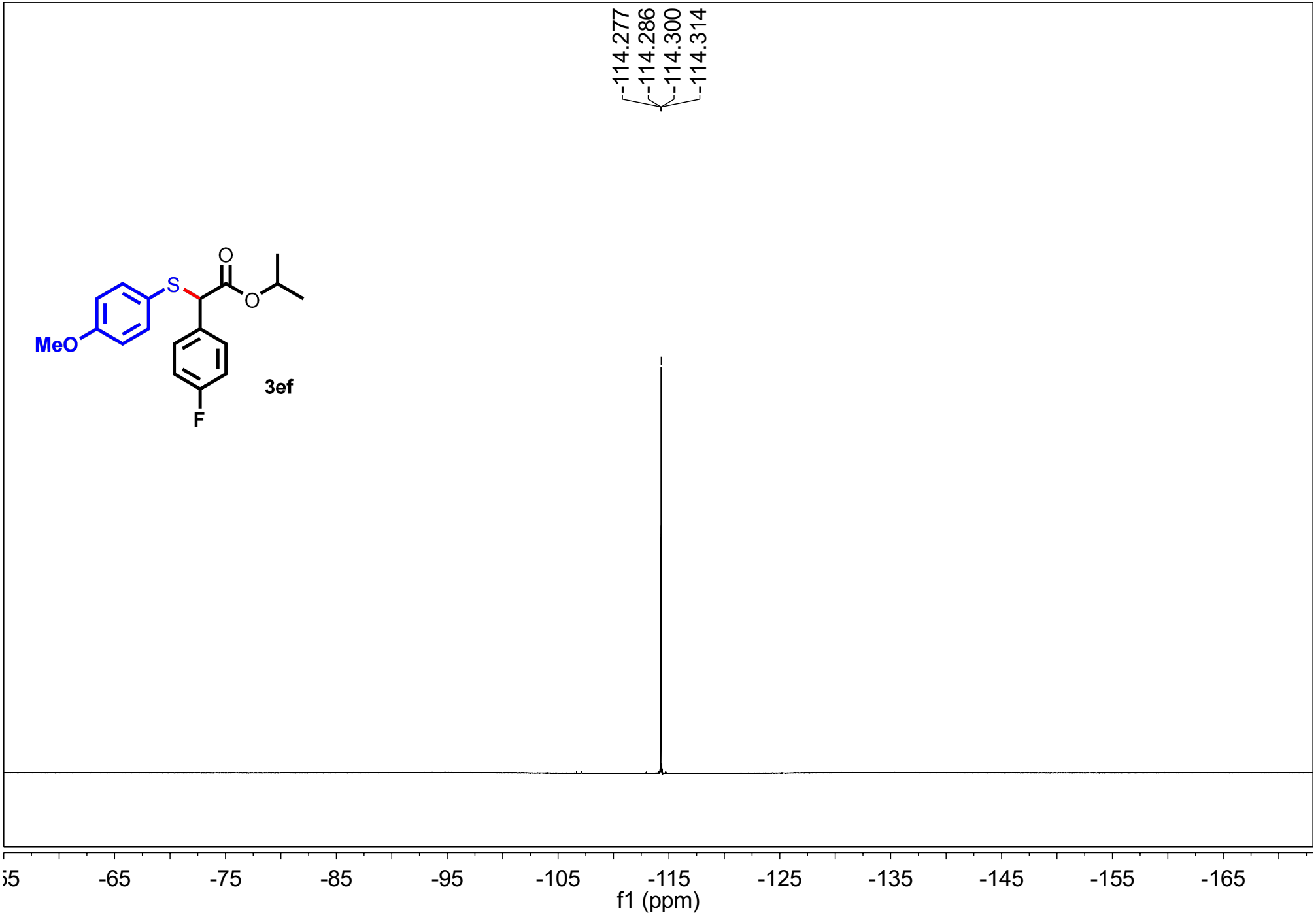
77.000
76.788
69.260
56.657
55.297
21.537
MeO
S
O
O
F
3ef
f1 (ppm)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-114.286
-114.300
-114.314
MeO
S
O
O
F
3ef
-65
-75
-85
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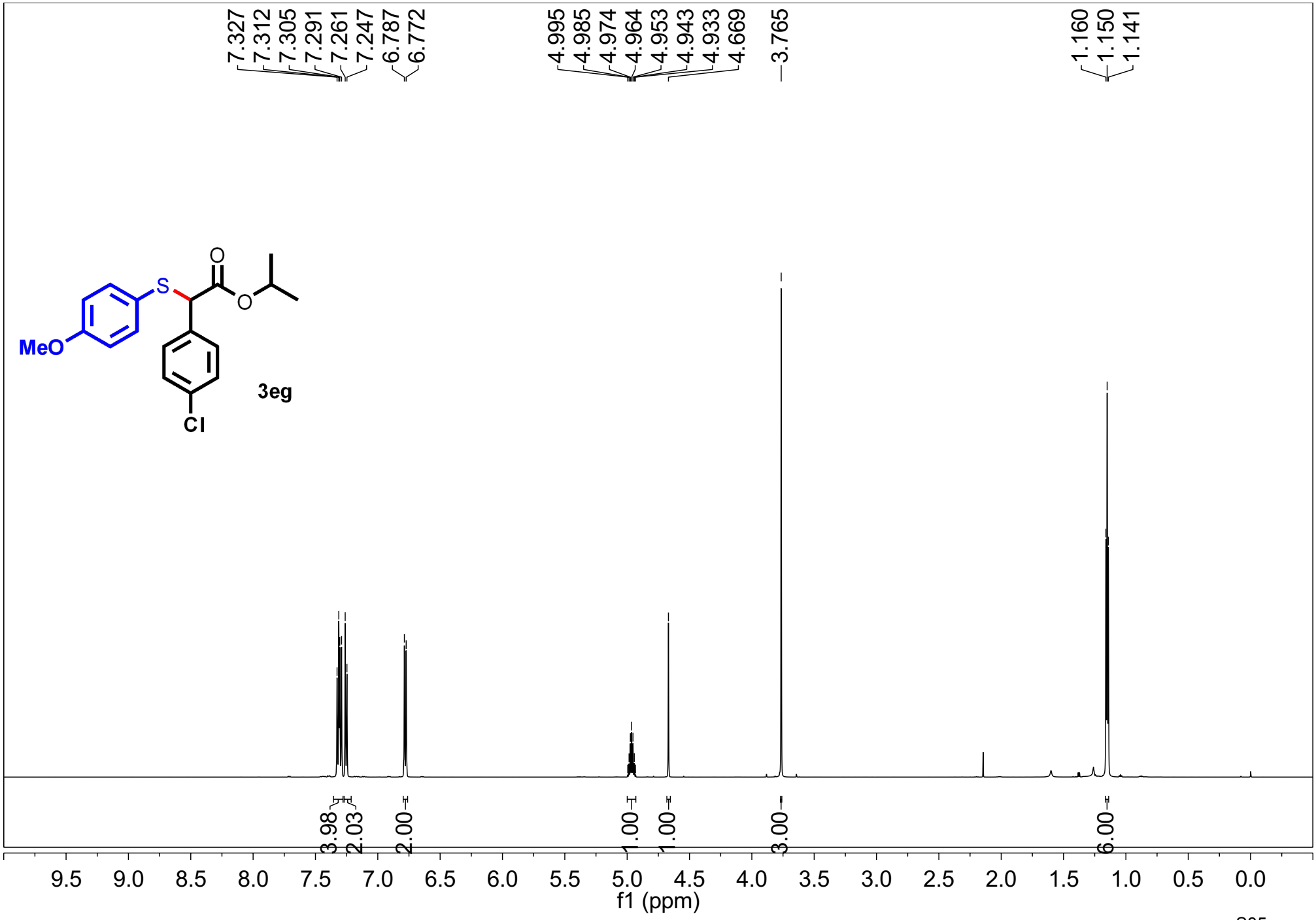
-125
-135
-145
-155
-165
f1 (ppm)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6.772
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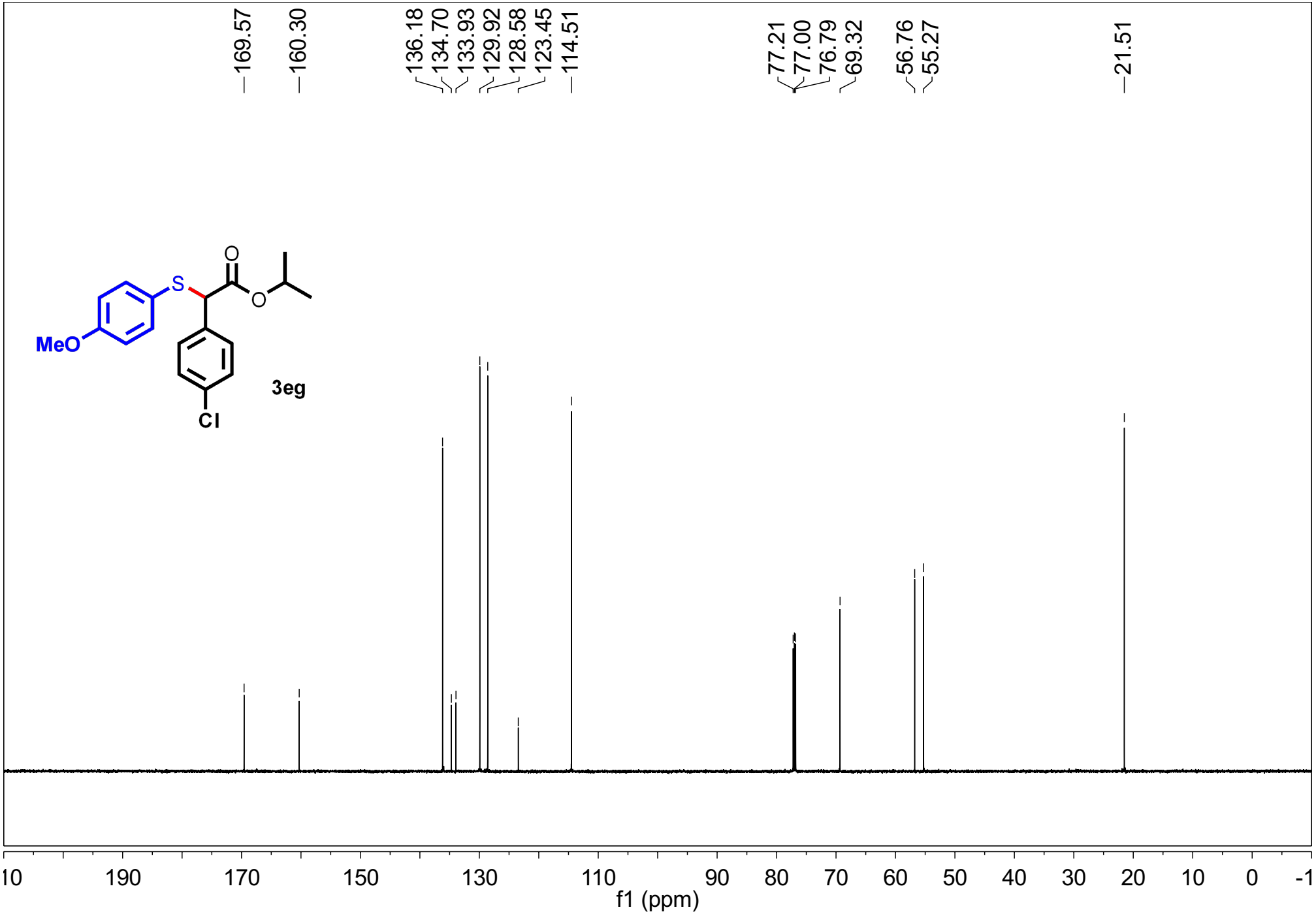
4.985
4.974
4.964
4.953
4.943
4.933
4.669
3.765
1.160
1.150
1.141
MeO
S
O
O
Cl
3eg
3.98
2.03
2.00
1.00
1.00
3.00
6.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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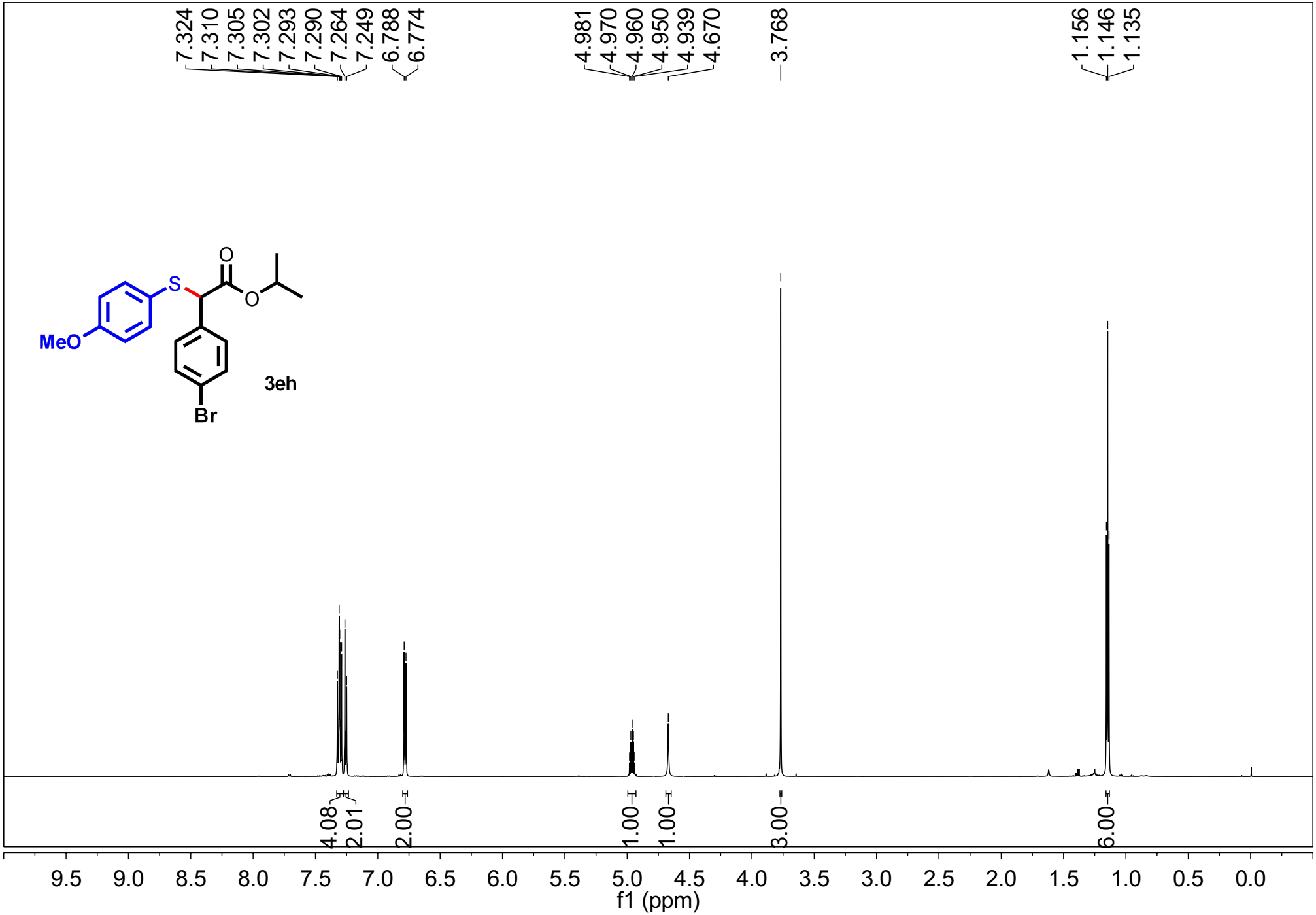
56.76
55.27
21.51
MeO
S
O
O
Cl
3eg
f1 (ppm)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6.774
4.981
4.970
4.960
4.950
4.939
4.670
3.768
1.156
1.146
1.135
MeO
S
O
O
Br
3eh
4.08
2.01
2.00
1.00
1.00
3.00
6.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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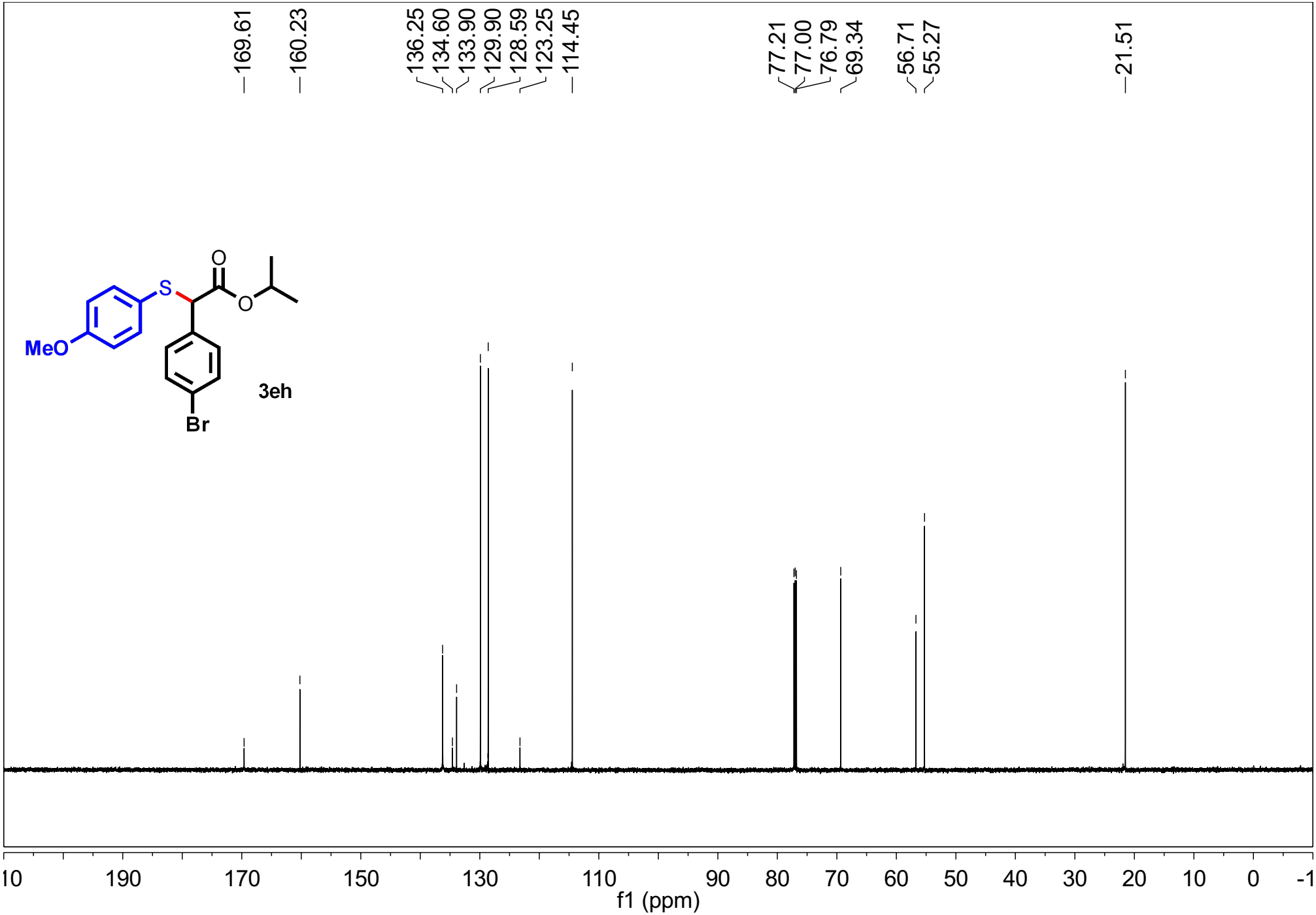
f1 (ppm)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55.27
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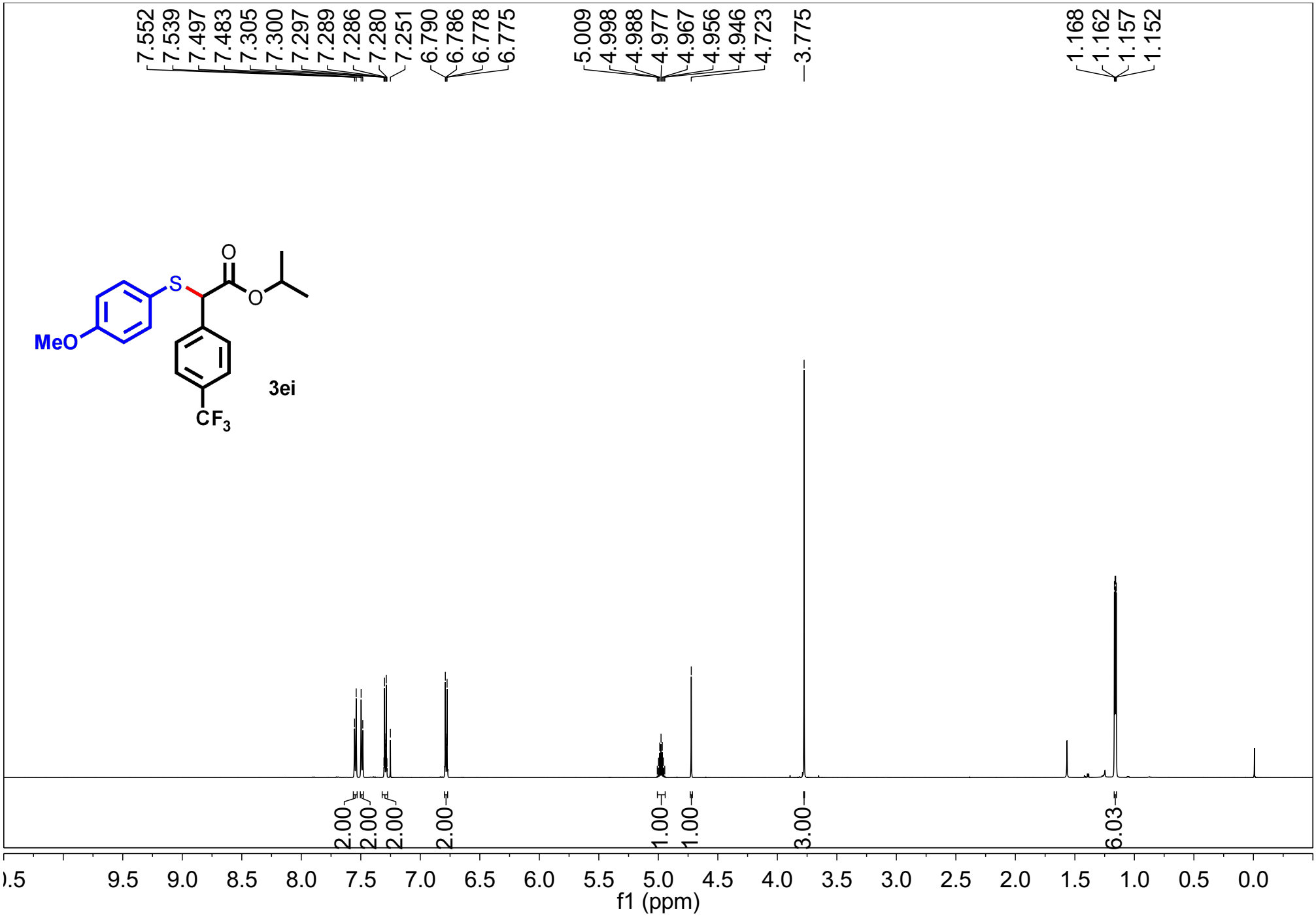
MeO
S
O
O
Br
3eh
f1 (ppm)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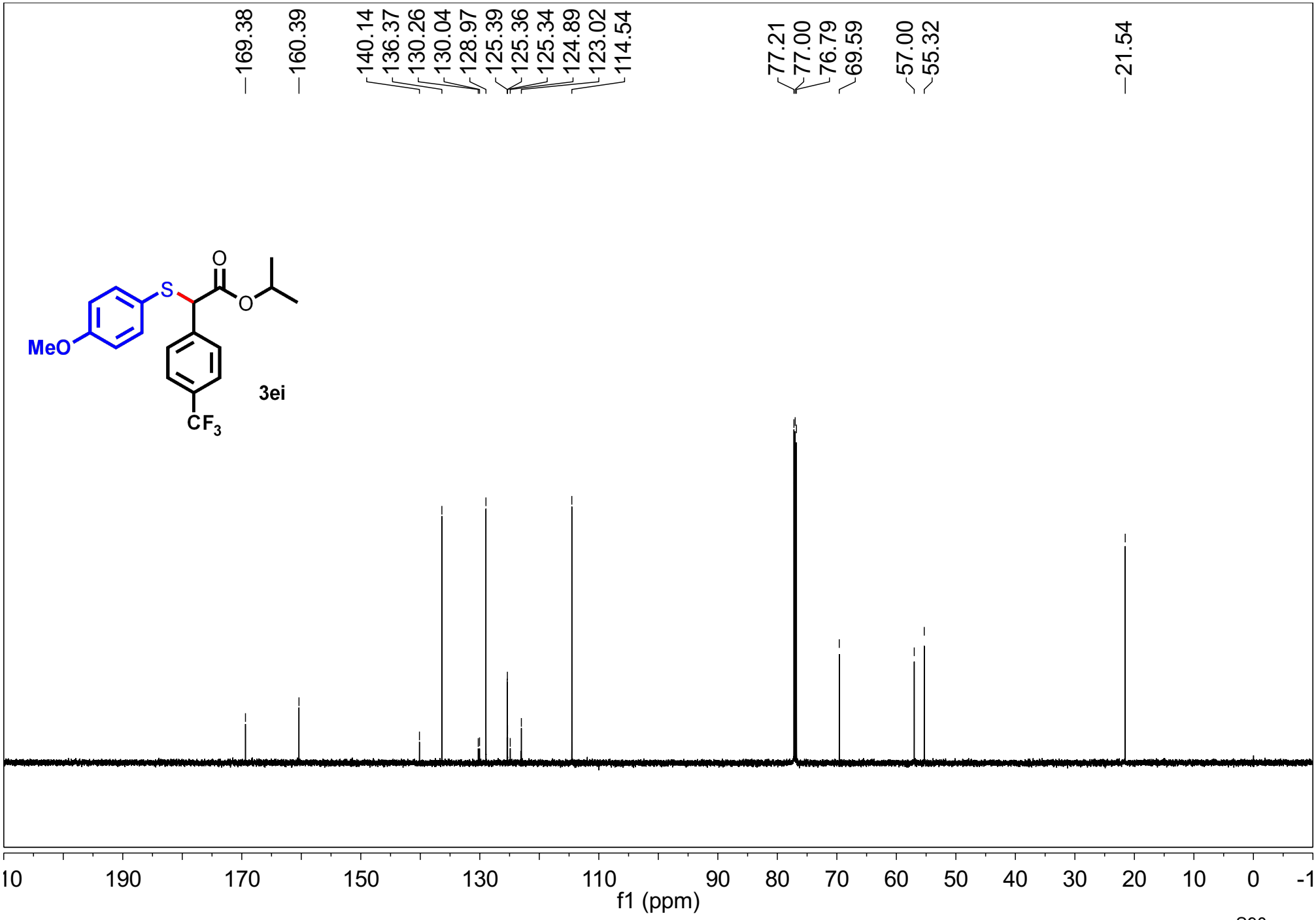
6.786
6.778
6.775
5.009
4.998
4.988
4.977
4.967
4.956
4.946
4.723
3.775
1.168
1.162
1.157
1.152
MeO
O
S
O
CF3
3ei
2.00
2.00
2.00
2.00
1.00
1.00
3.00
6.03
f1 (ppm)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124.89
123.02
114.54
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69.59
57.00
55.32
21.54
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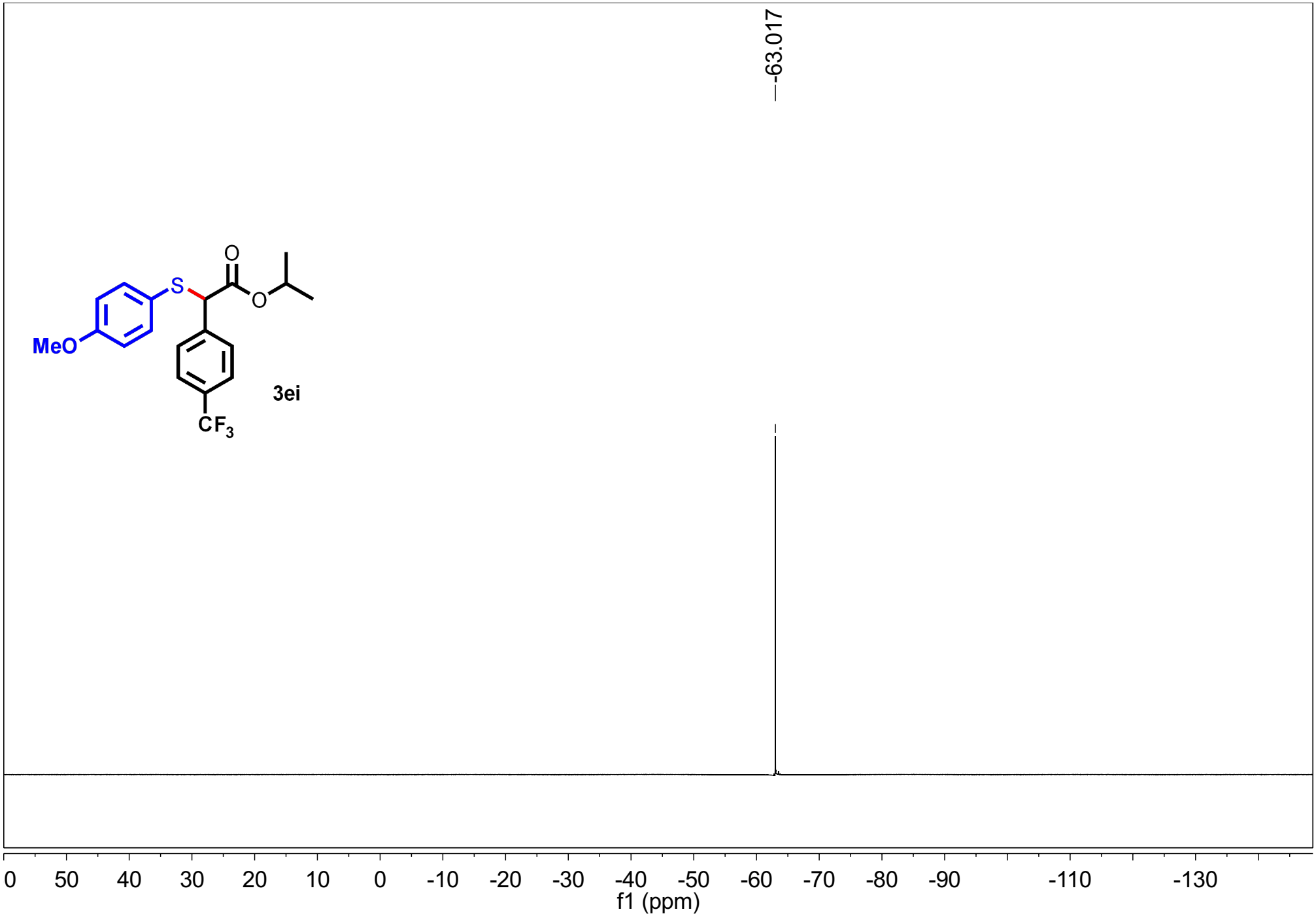
S
O
O
CF3
3ei
f1 (ppm)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50
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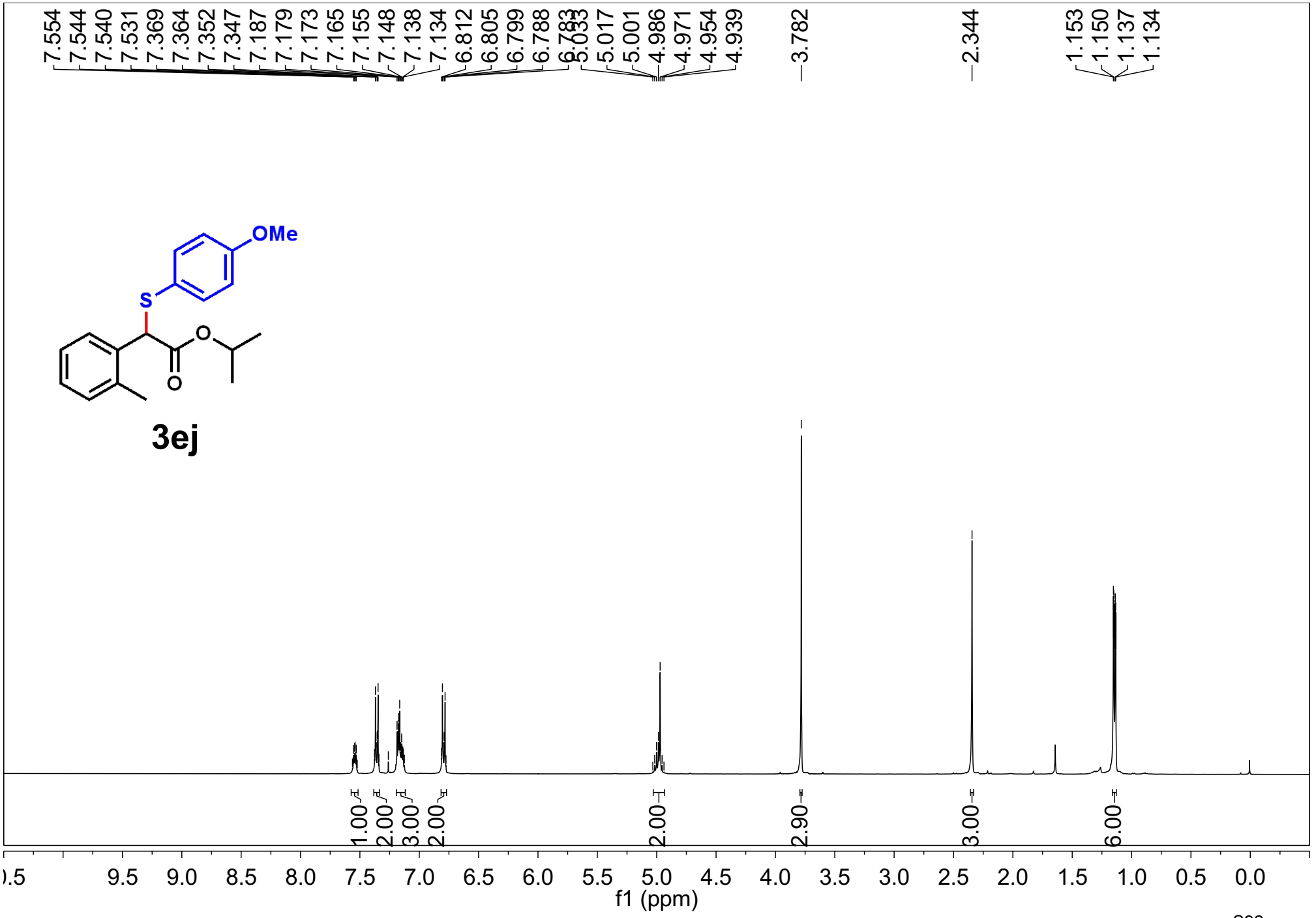
-30
-40
-50
-60
-70
-80
-90
-110
-130
f1 (ppm)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7.155
7.148
7.138
7.134
6.812
6.805
6.799
6.788
6.783
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5.017
5.001
4.986
4.971
4.954
4.939
3.782
2.344
1.153
1.150
1.137
1.134
OMe
S
O
O
3ej
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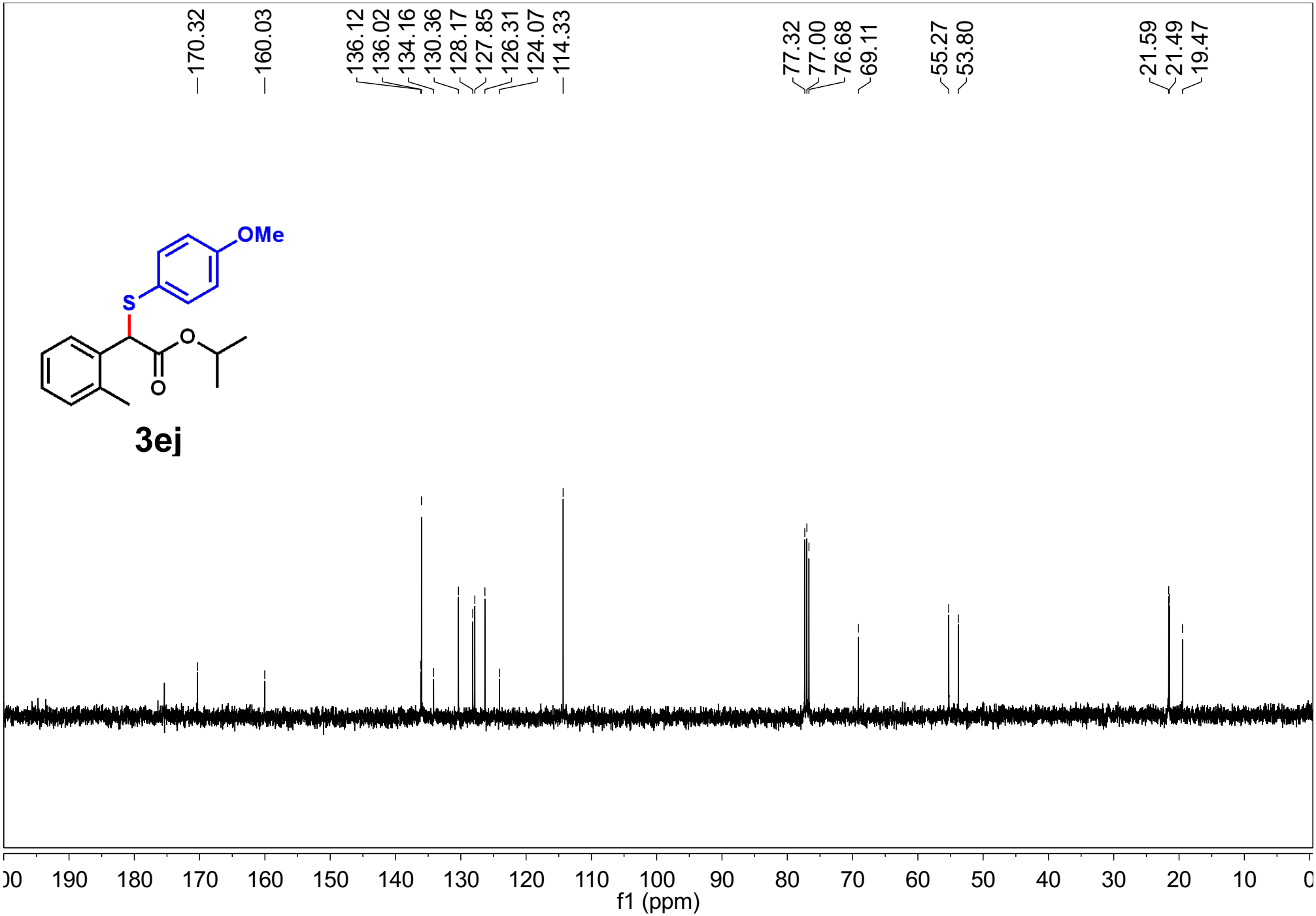
2.00
3.00
2.00
2.00
2.90
3.00
6.00
f1 (ppm)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126.31
124.07
114.33
77.32
77.00
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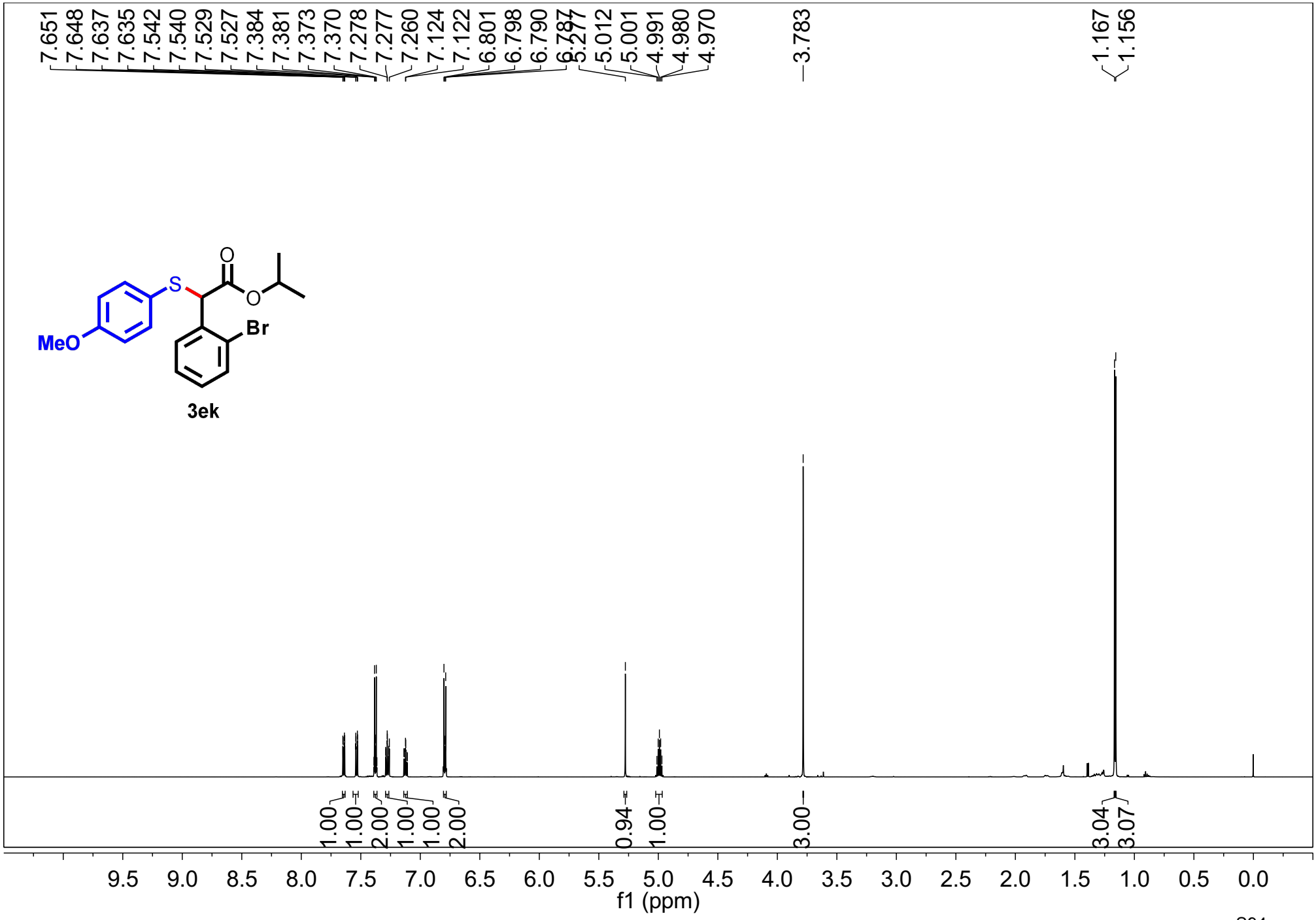
55.27
53.80
21.59
21.49
19.47
OMe
S
O
O
3ej
f1 (ppm)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7.527
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7.370
7.278
7.277
7.260
7.124
7.122
6.801
6.798
6.790
6.787
5.277
5.012
5.001
4.991
4.980
4.970
3.783
1.167
1.156
MeO
S
O
O
Br
3ek
1.00
1.00
2.00
1.00
1.00
2.00
0.94
1.00
3.00
3.04
3.07
9.5
9.0
8.5
8.0
7.5
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6.5
6.0
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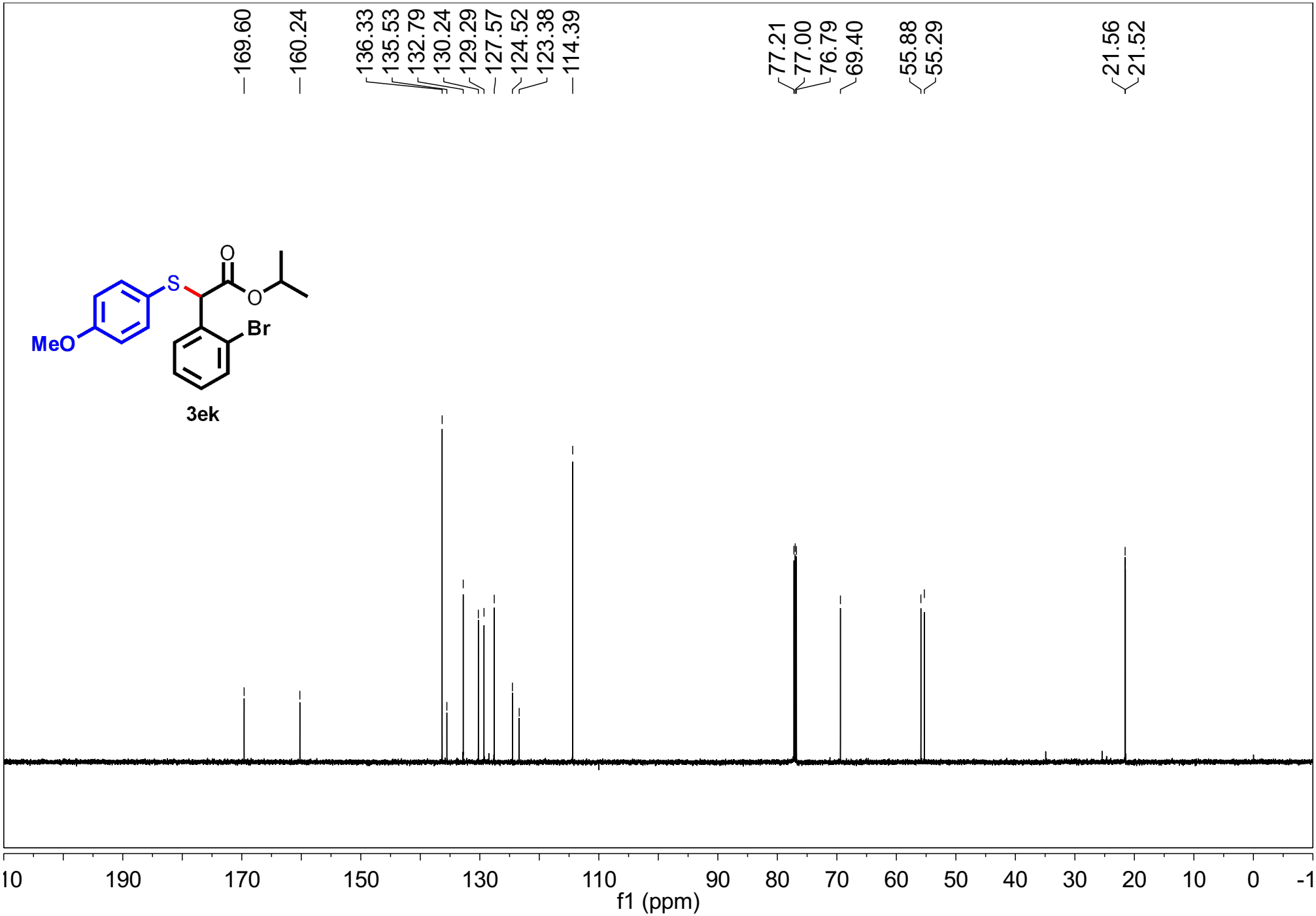
0.0
f1 (ppm)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127.57
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123.38
114.39
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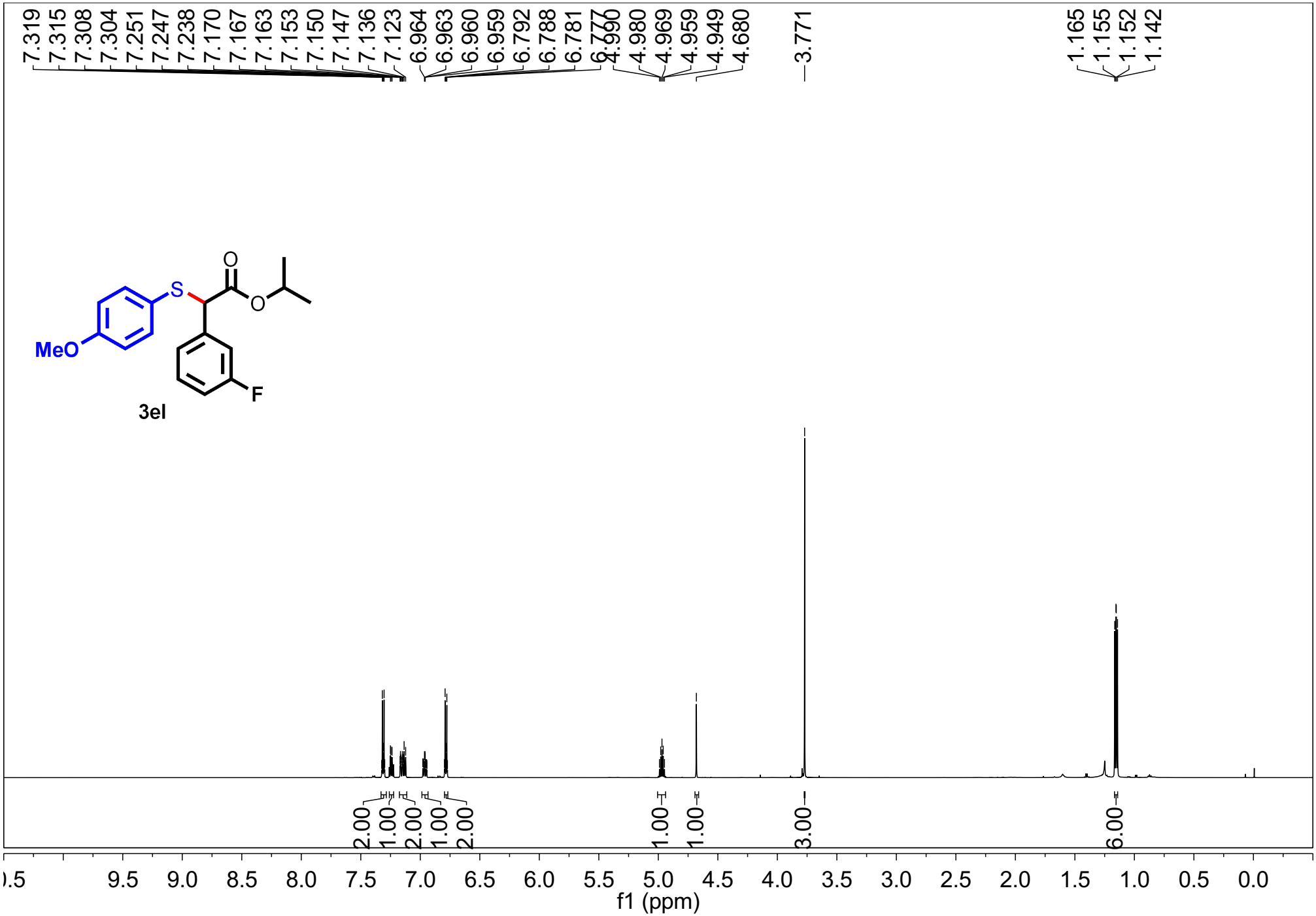
55.88
55.29
21.56
21.52
O
S
O
MeO
Br
3ek
f1 (ppm)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7.304
7.251
7.247
7.238
7.170
7.167
7.163
7.153
7.150
7.147
7.136
7.123
6.964
6.963
6.960
6.959
6.792
6.788
6.781
6.777
4.980
4.969
4.959
4.949
4.680
3.771
1.165
1.155
1.152
1.142
MeO
S
O
O
F
3el
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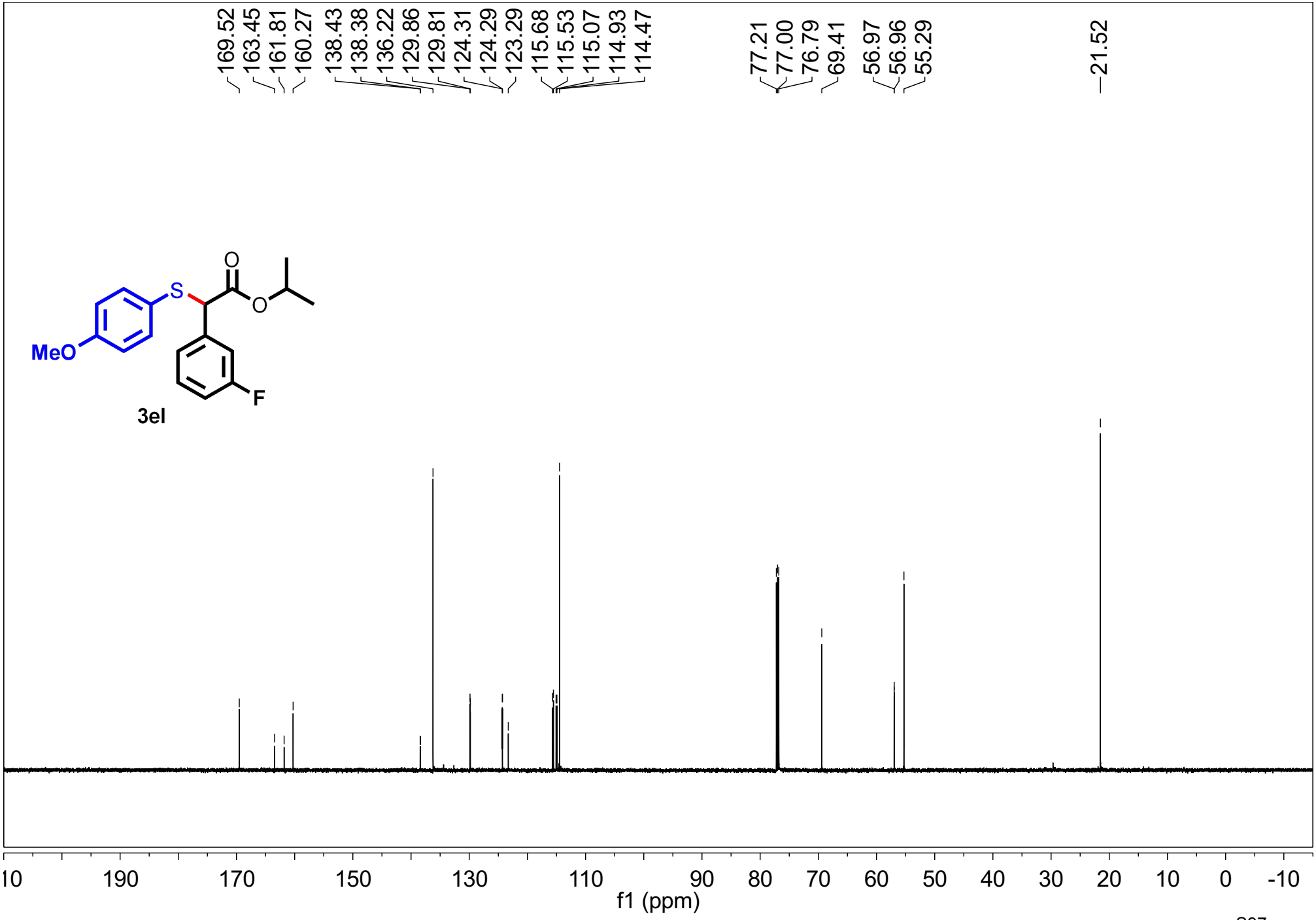
1.00
2.00
1.00
2.00
1.00
1.00
3.00
6.00
f1 (ppm)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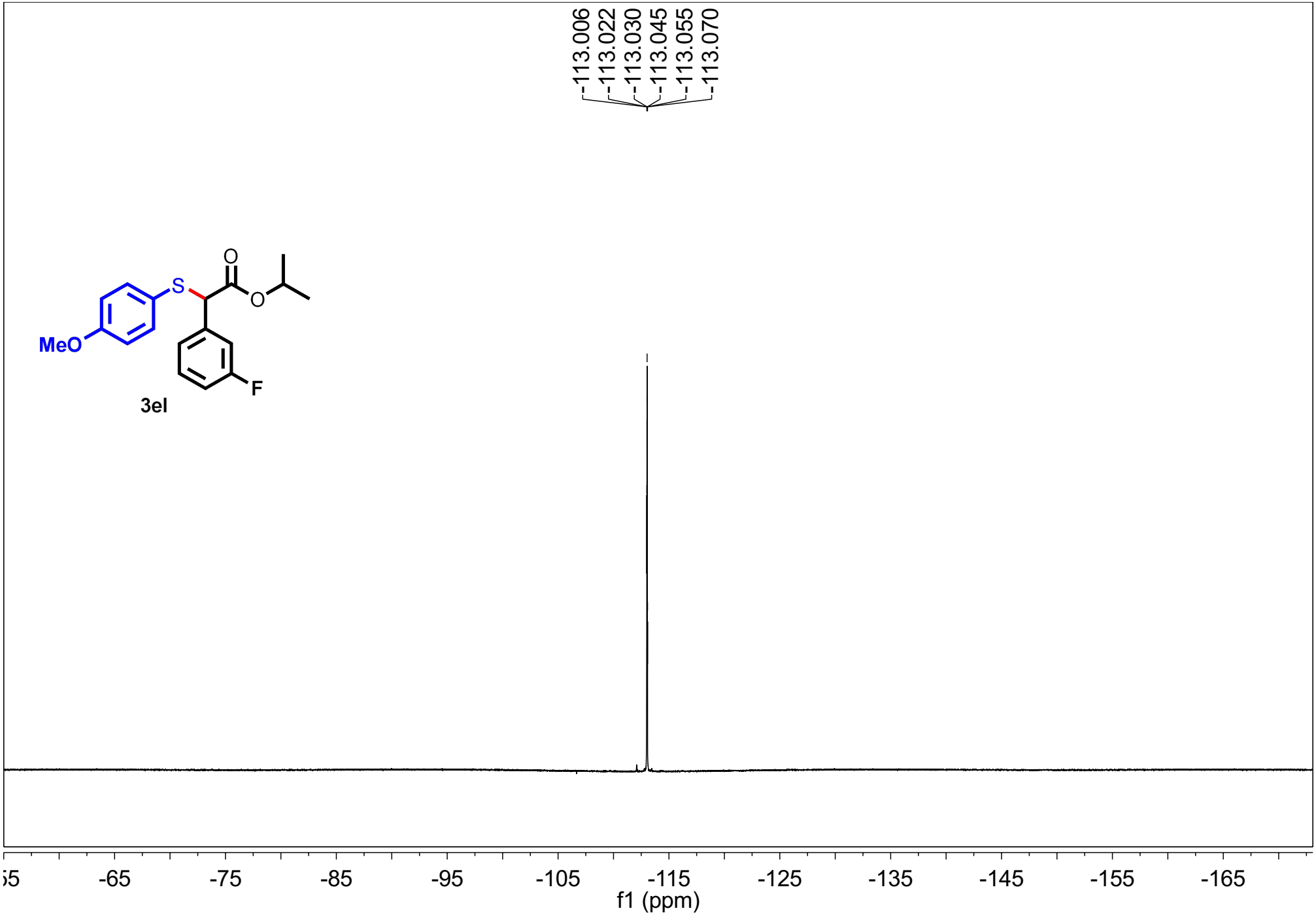
138.43
138.38
136.22
129.86
129.81
124.31
124.29
123.29
115.68
115.53
115.07
114.93
114.47
77.21
77.00
76.79
69.41
56.97
56.96
55.29
21.52
O
S
O
MeO
F
3el
10
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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MeO
S
O
O
F
3el
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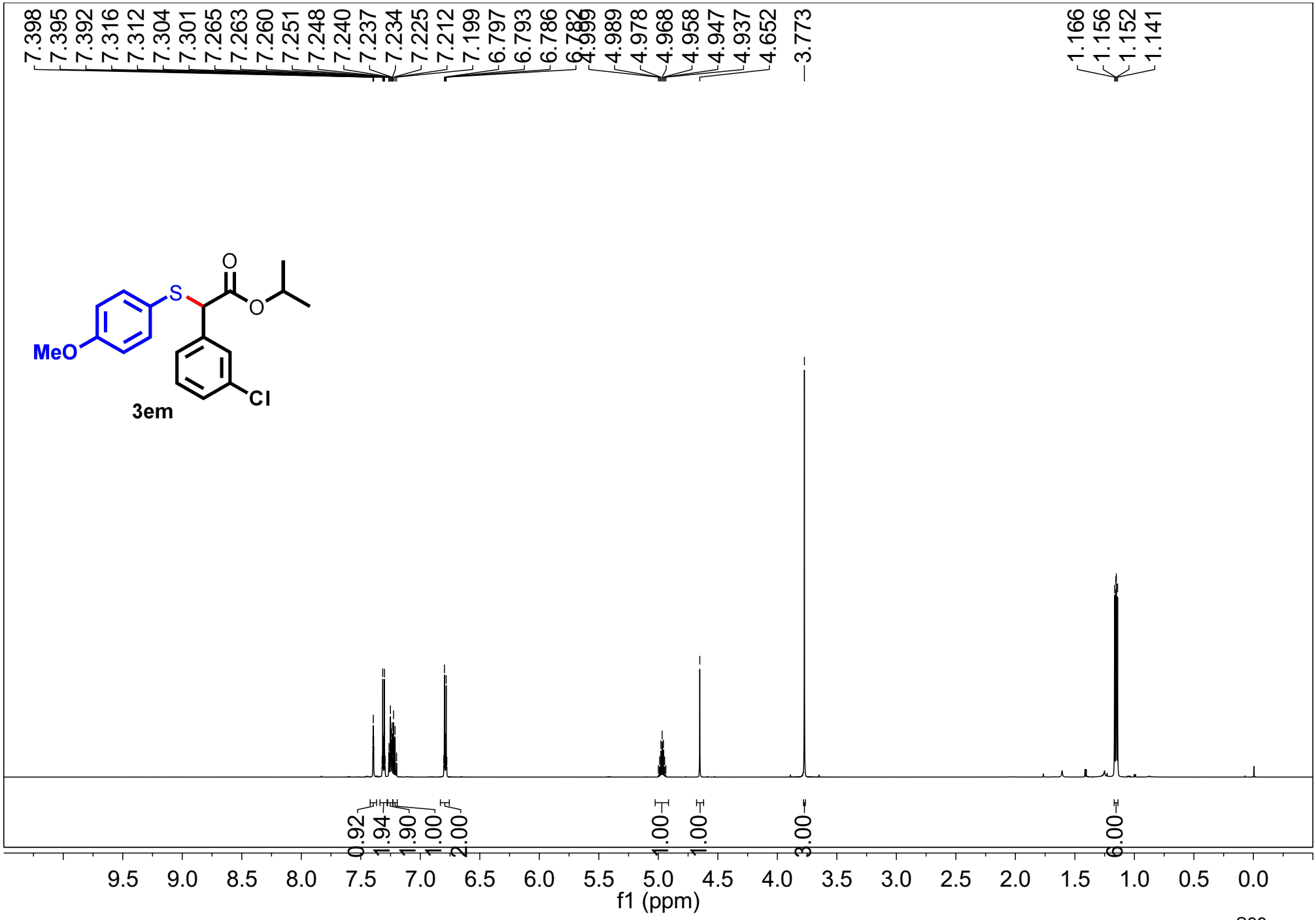
-95
-105
-115
-125
-135
-145
-155
-165
f1 (ppm)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7.260
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7.240
7.237
7.234
7.225
7.212
7.199
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6.793
6.786
4.989
4.978
4.968
4.958
4.947
4.937
4.652
3.773
1.166
1.156
1.152
1.141
MeO
S
O
O
Cl
3em
0.92
1.94
1.90
1.00
2.00
1.00
1.00
3.00
6.00
9.5
9.0
8.5
8.0
7.5
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6.0
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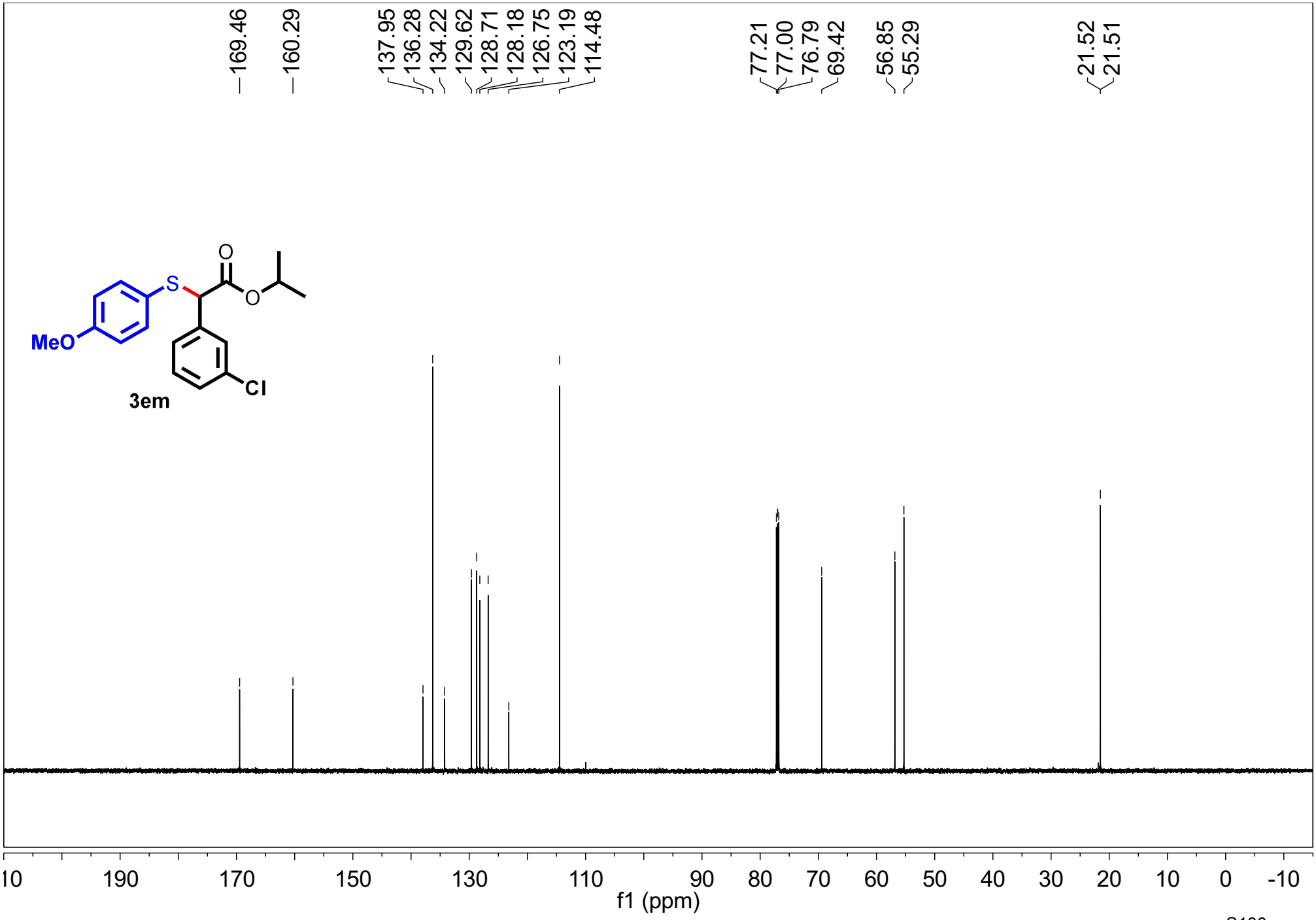
f1 (ppm)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123.19
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77.21
77.00
76.79
69.42
56.85
55.29
21.52
21.51
O
S
O
MeO
Cl
3em
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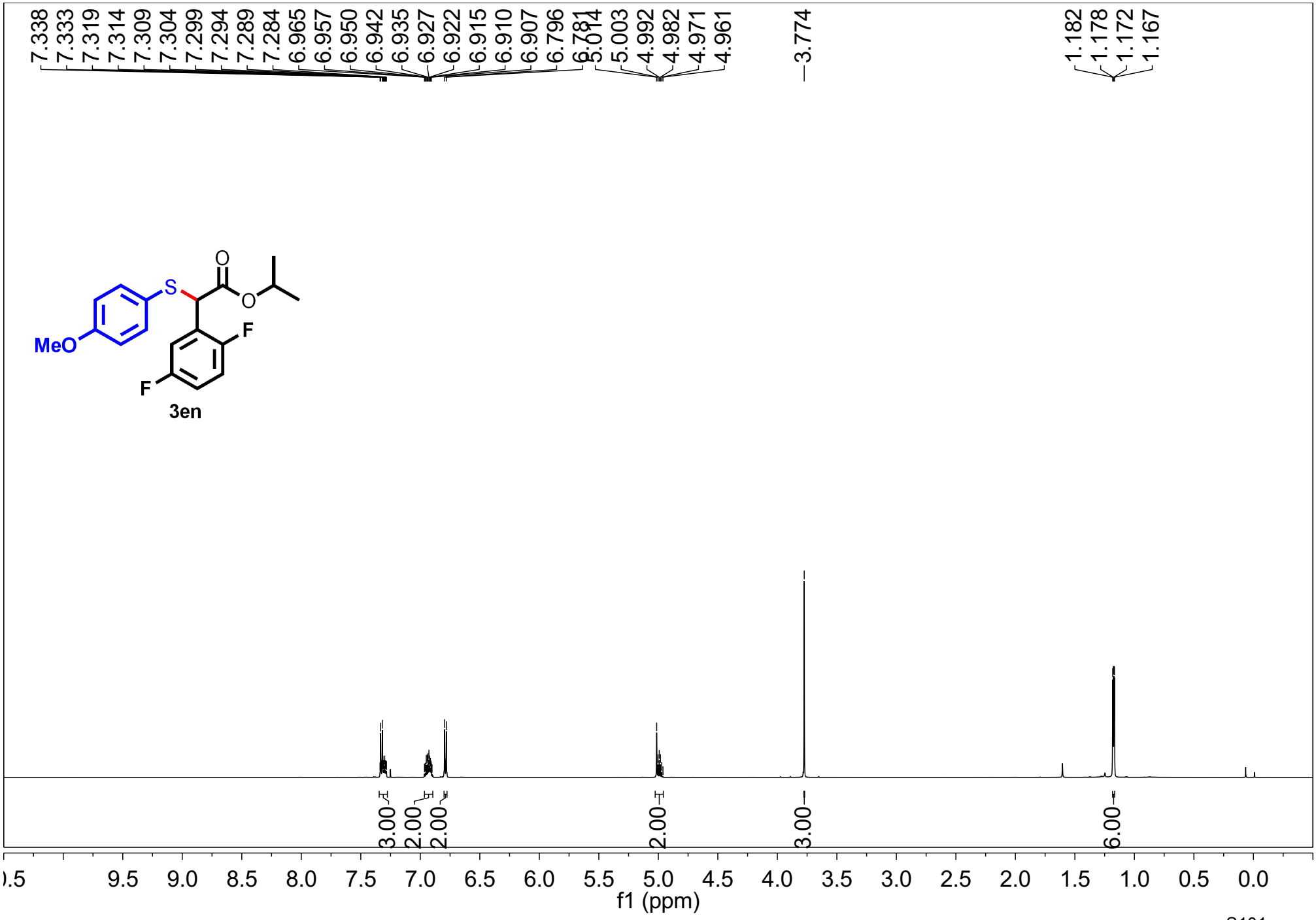
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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6.907
6.796
6.781
5.014
5.003
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4.971
4.961
3.774
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1.178
1.172
1.167
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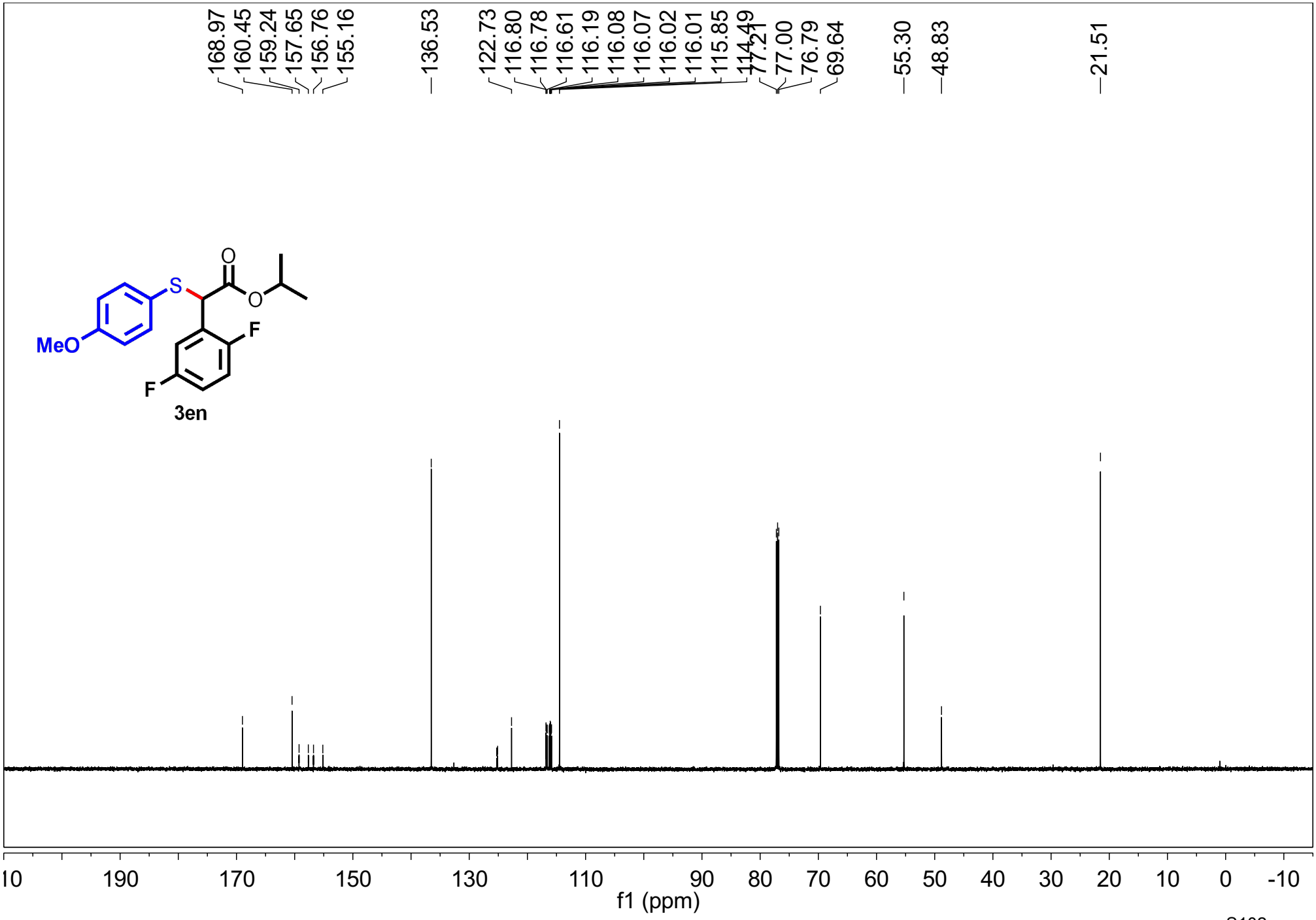
F
F
3en
3.00
2.00
2.00
2.00
3.00
6.00
f1 (ppm)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116.08
116.07
116.02
116.01
115.85
114.49
77.21
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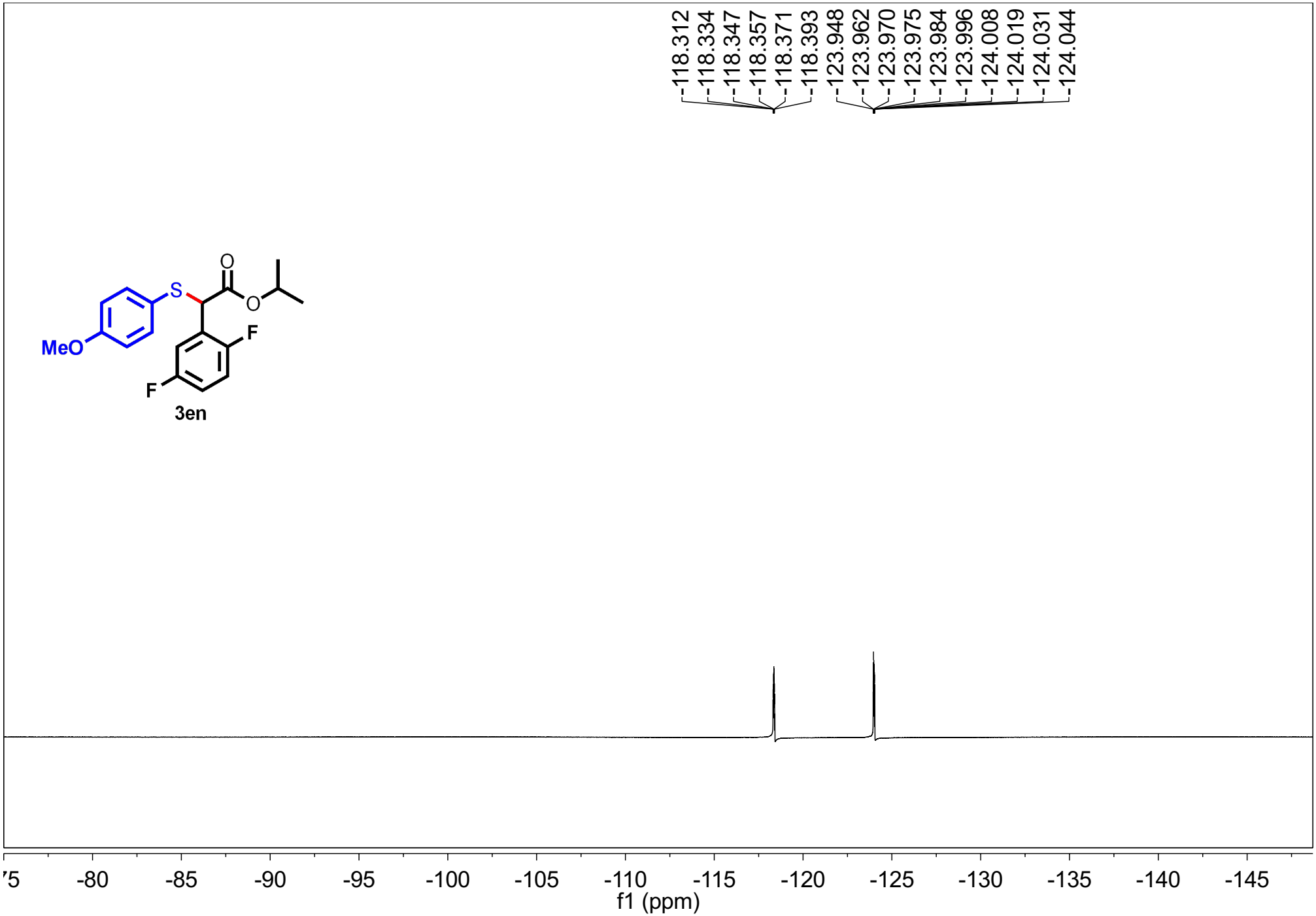
55.30
48.83
21.51
MeO
S
O
O
F
F
3en
f1 (ppm)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123.984
123.996
124.008
124.019
124.031
124.044
MeO
S
O
O
F
F
3en
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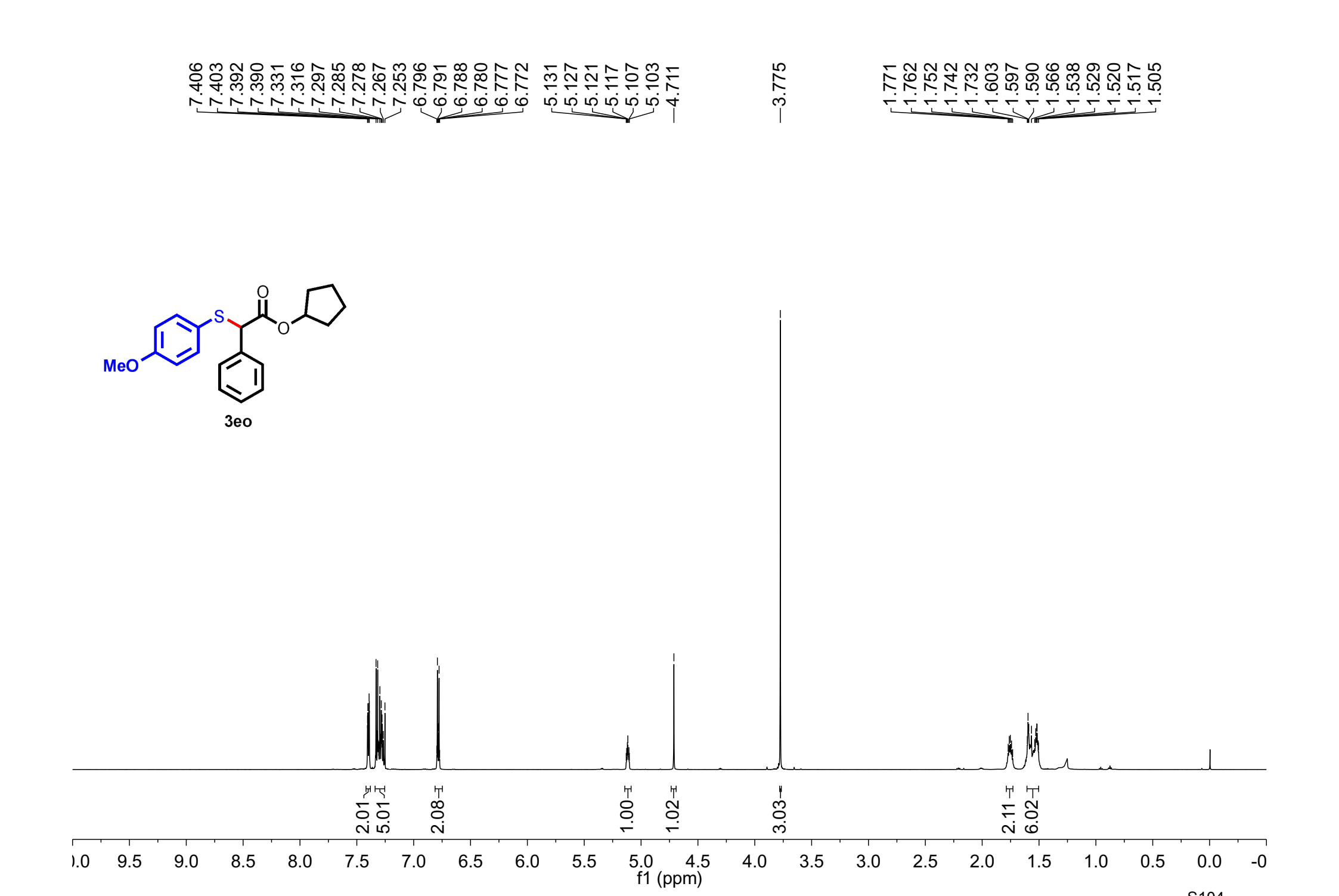
-90
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
-145
f1 (ppm)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6.791
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6.780
6.777
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5.103
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3.775
1.771
1.762
1.752
1.742
1.732
1.603
1.597
1.590
1.566
1.538
1.529
1.520
1.517
1.505
O
S
O
MeO
3eo
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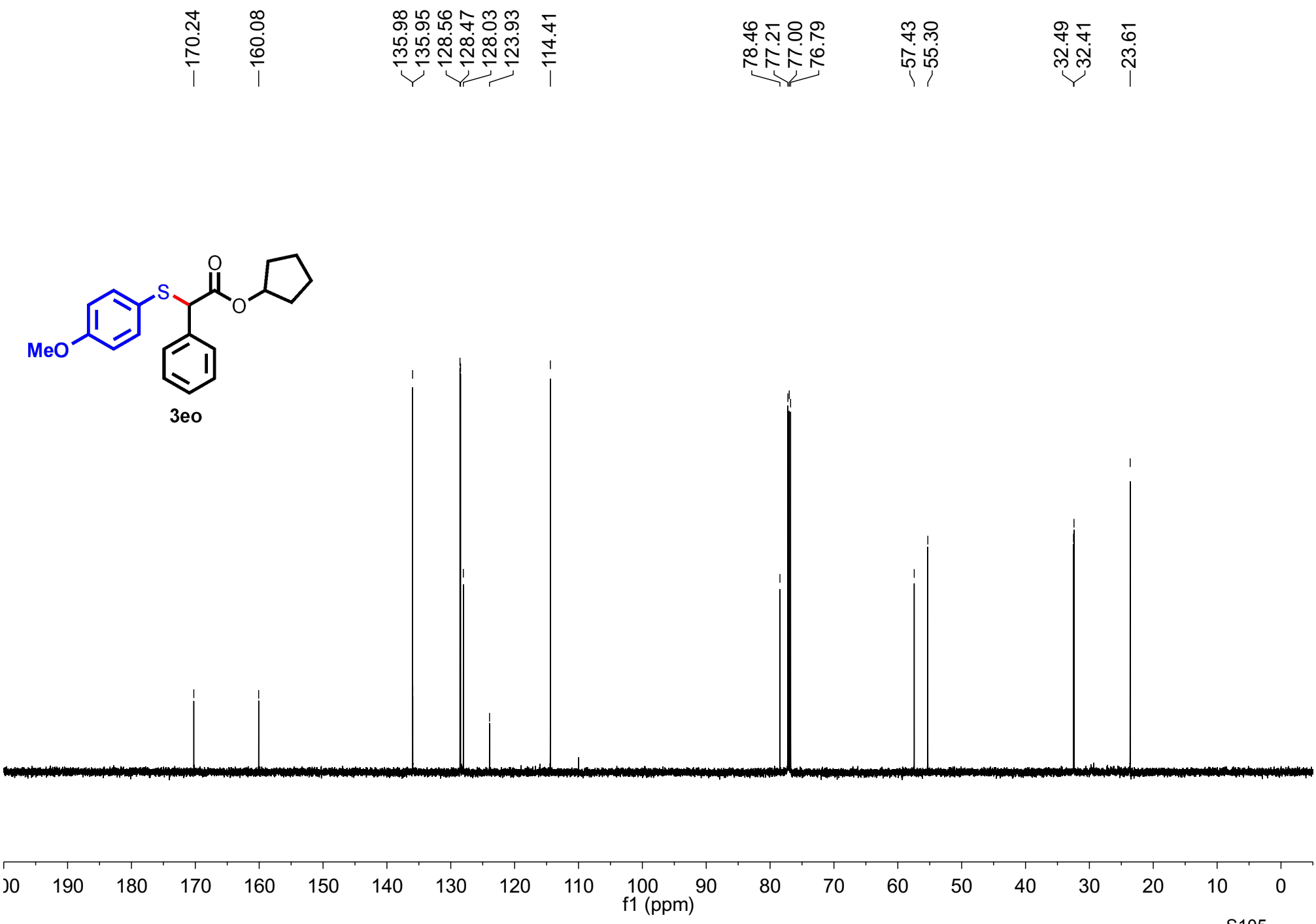
5.01
2.08
1.00
1.02
3.03
2.11
6.02
f1 (ppm)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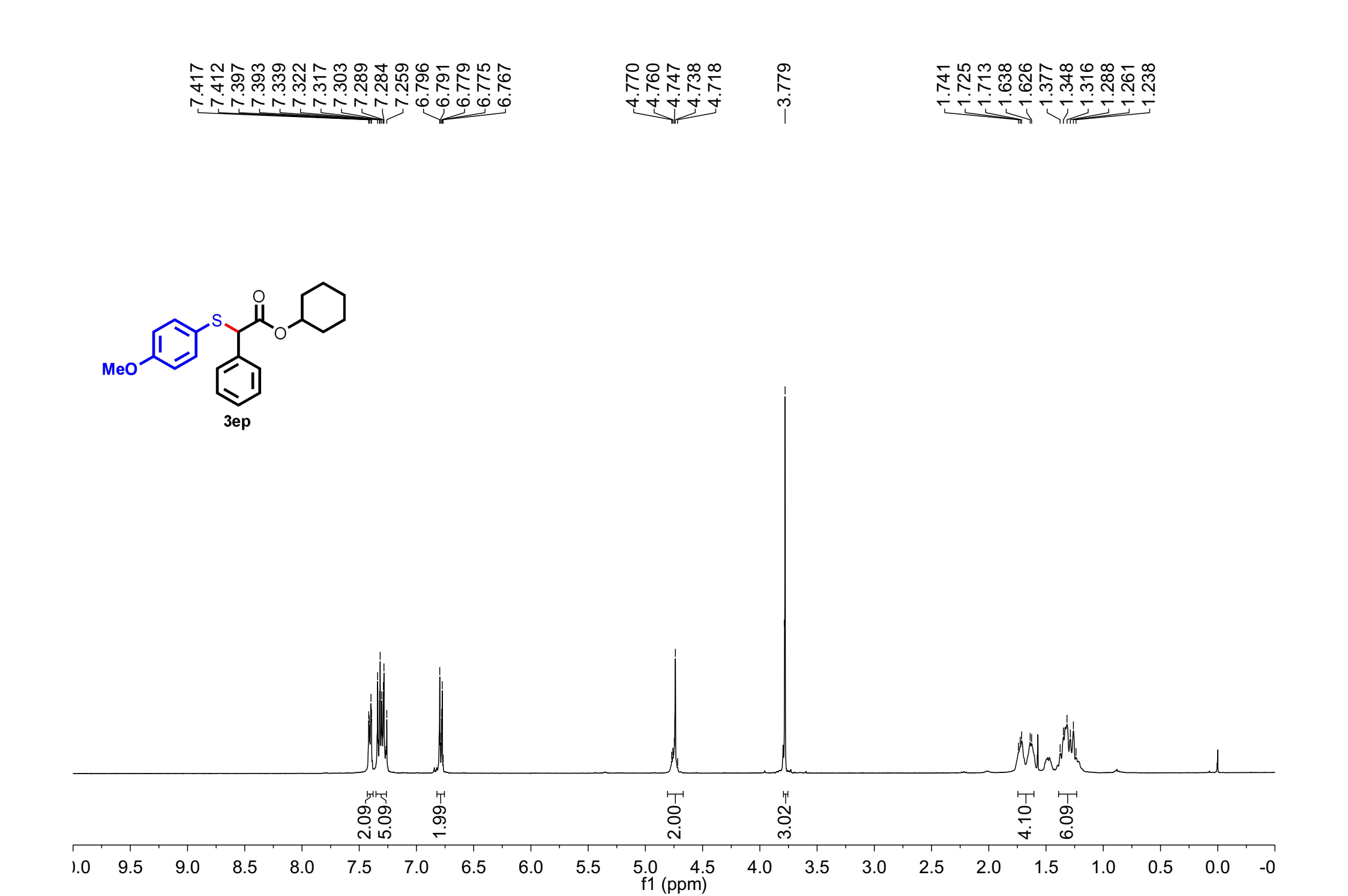
55.30
32.49
32.41
23.61
MeO
S
O
O
3eo
f1 (ppm)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6.791
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6.775
6.767
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4.718
3.779
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1.725
1.713
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1.626
1.377
1.348
1.316
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1.261
1.238
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3ep
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3.02
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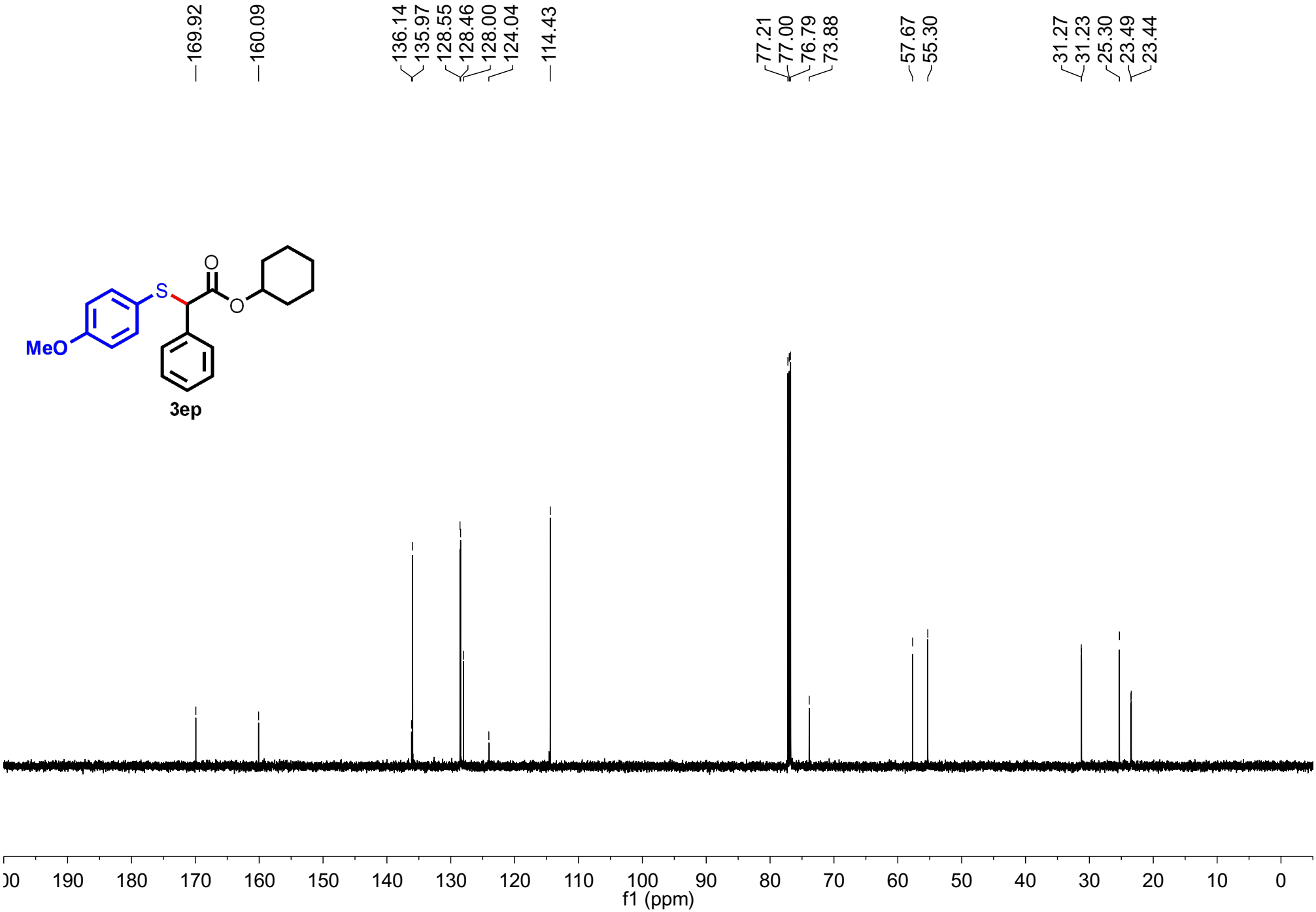
6.09
f1 (ppm)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76.79
73.88
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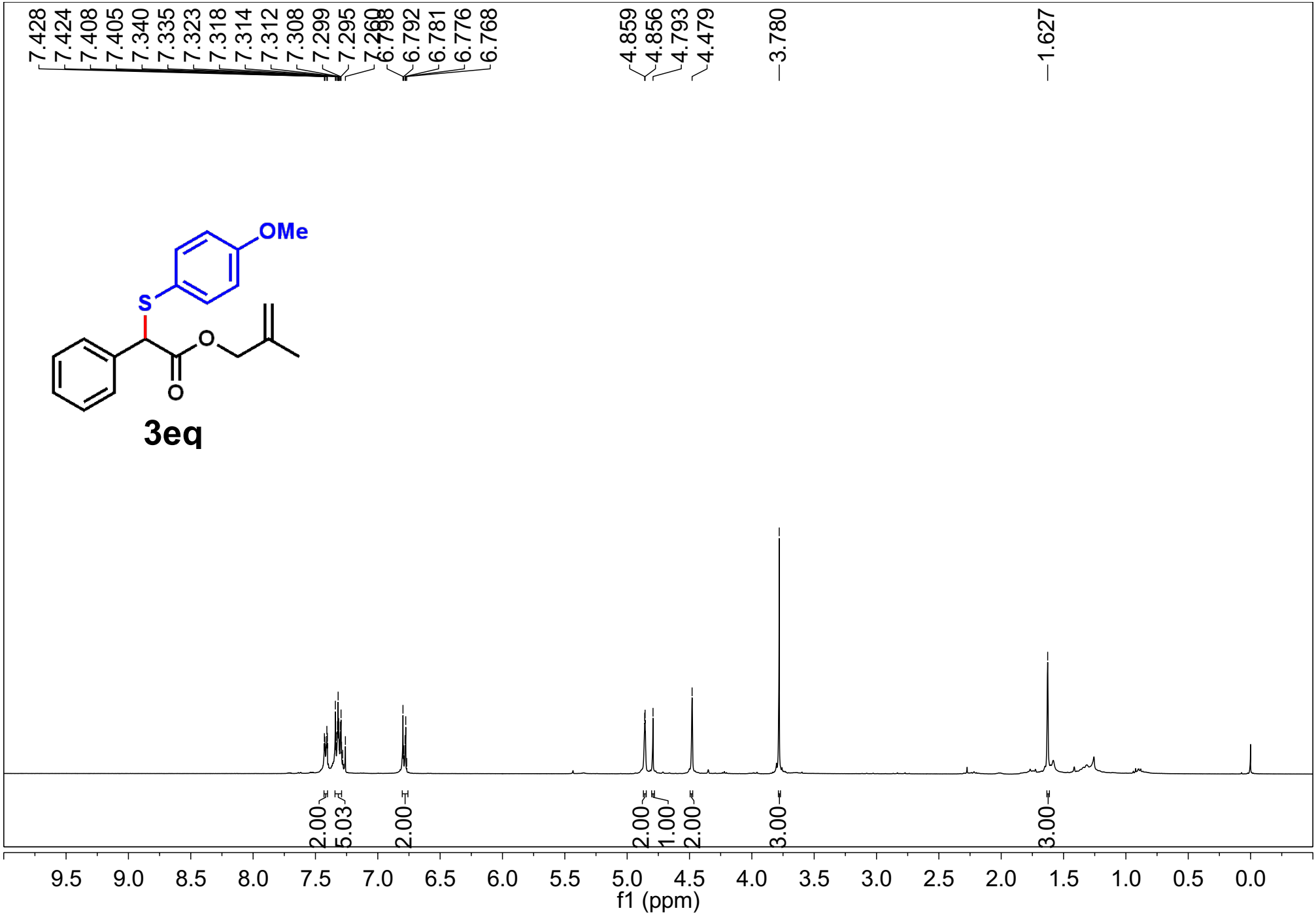
31.23
25.30
23.49
23.44
MeO
S
O
O
3ep
f1 (ppm)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6.792
6.781
6.776
6.768
4.859
4.856
4.793
4.479
3.780
1.627
OMe
S
O
O
3eq
2.00
5.03
2.00
2.00
1.00
2.00
3.00
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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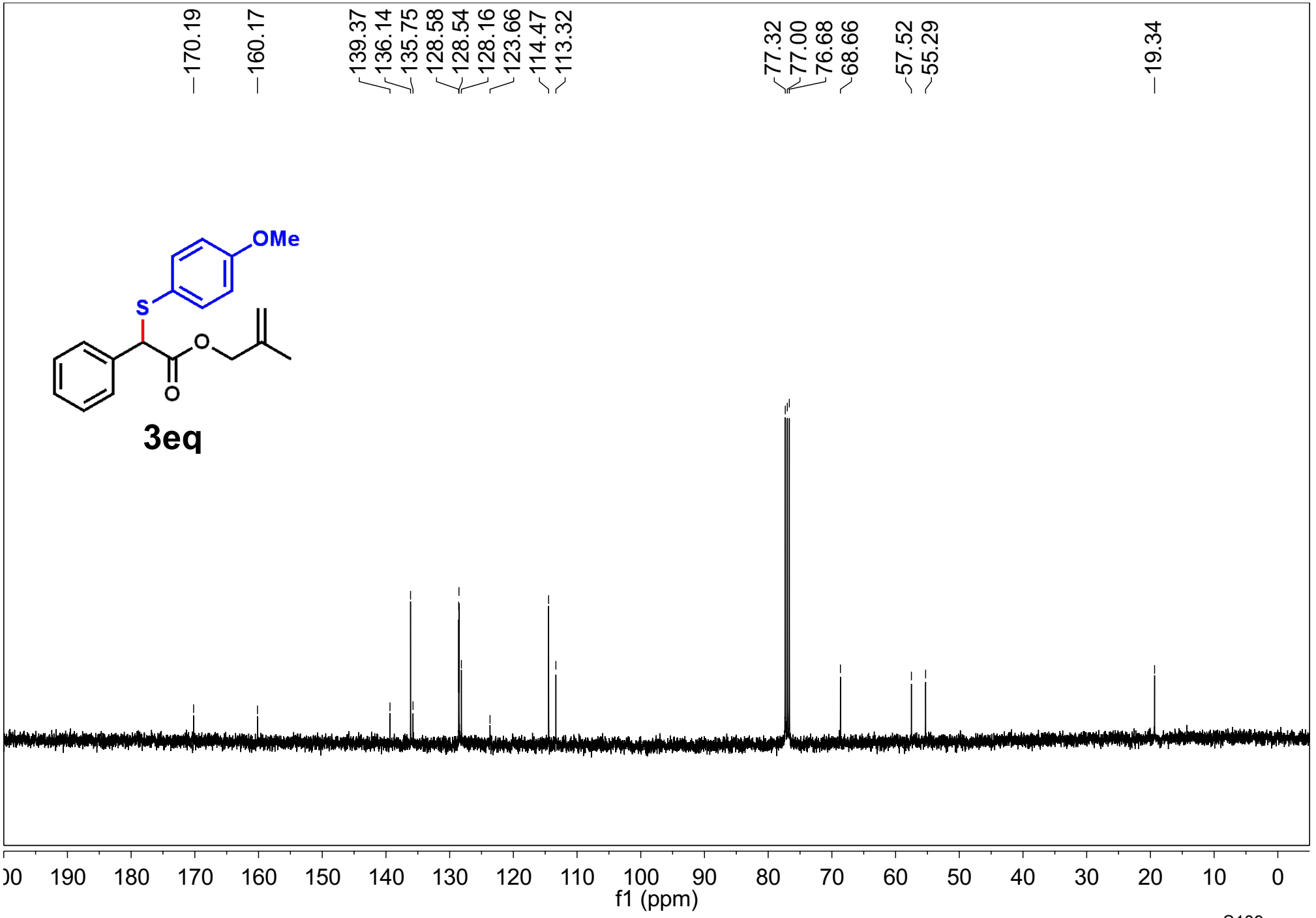
f1 (ppm)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113.32
77.32
77.00
76.68
68.66
57.52
55.29
19.34
OMe
S
O
O
3eq
190
180
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110
100
90
80
70
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50
40
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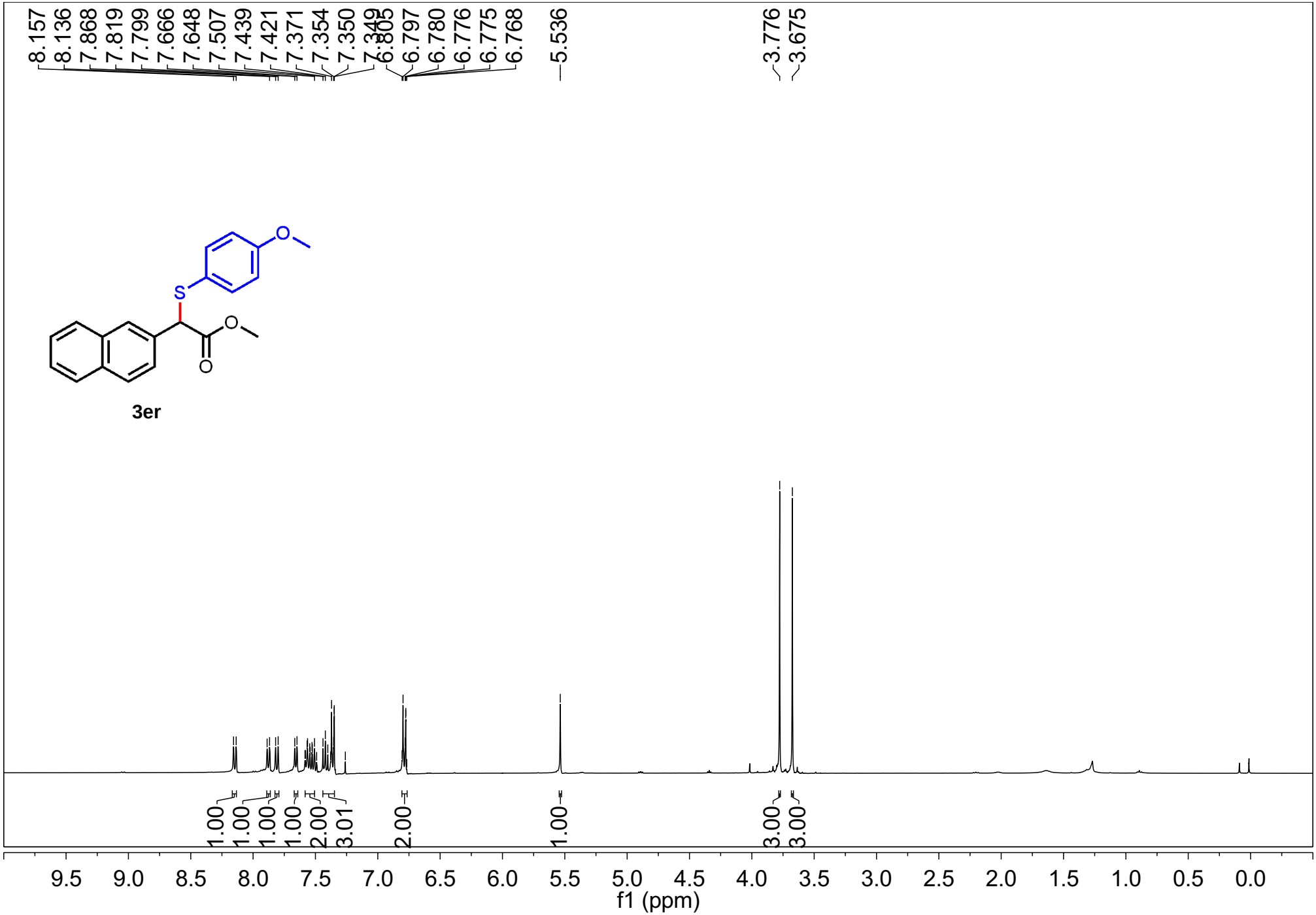
0
f1 (ppm)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7.350
7.349
6.805
6.797
6.780
6.776
6.775
6.768
5.536
3.776
3.675
O
S
O
O
3er
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1.00
1.00
1.00
2.00
3.01
2.00
1.00
3.00
3.00
9.5
9.0
8.5
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7.5
7.0
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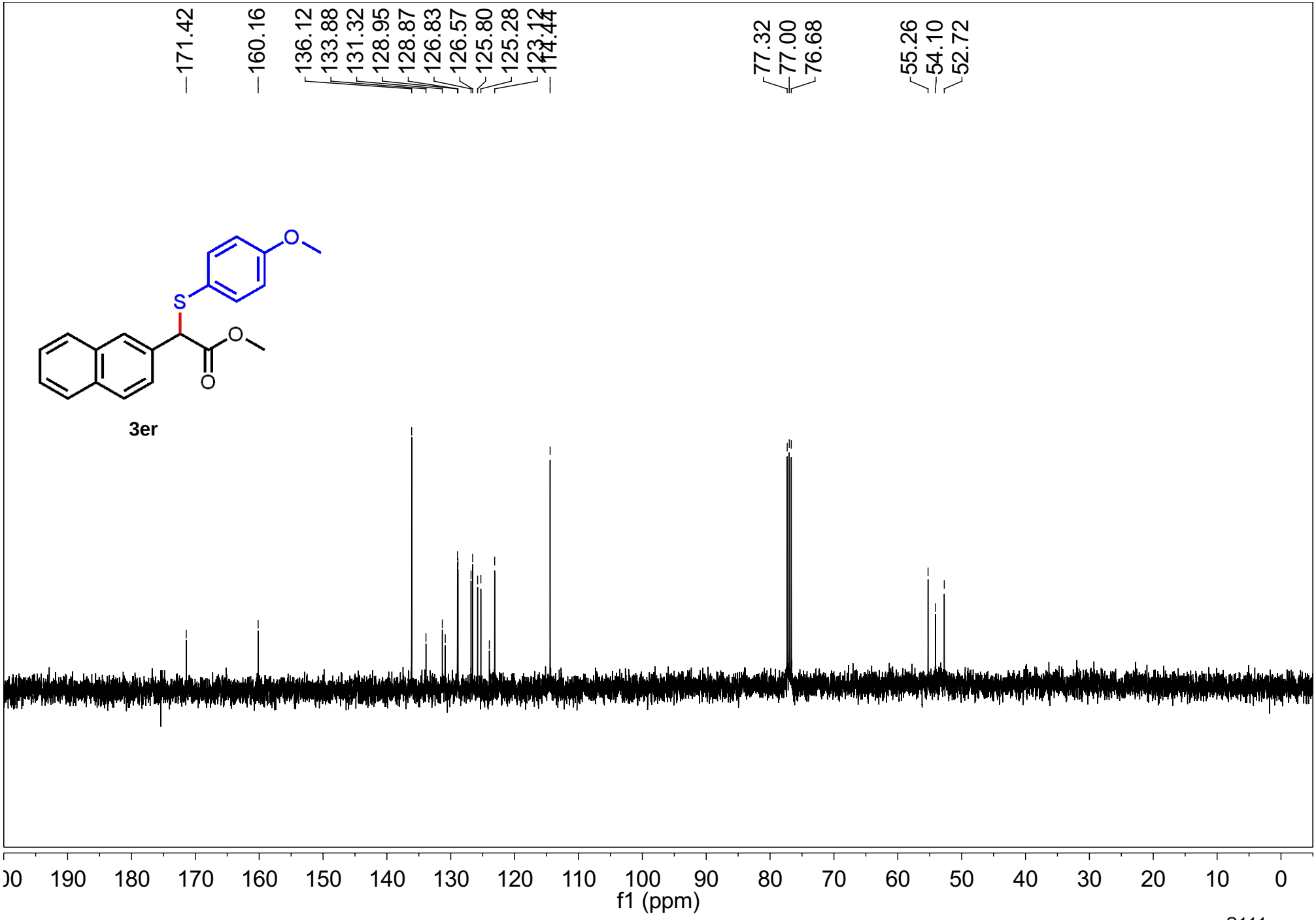
f1 (ppm)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123.12
114.44
77.32
77.00
76.68
55.26
54.10
52.72
O
S
O
O
3er
190
180
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90
80
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50
40
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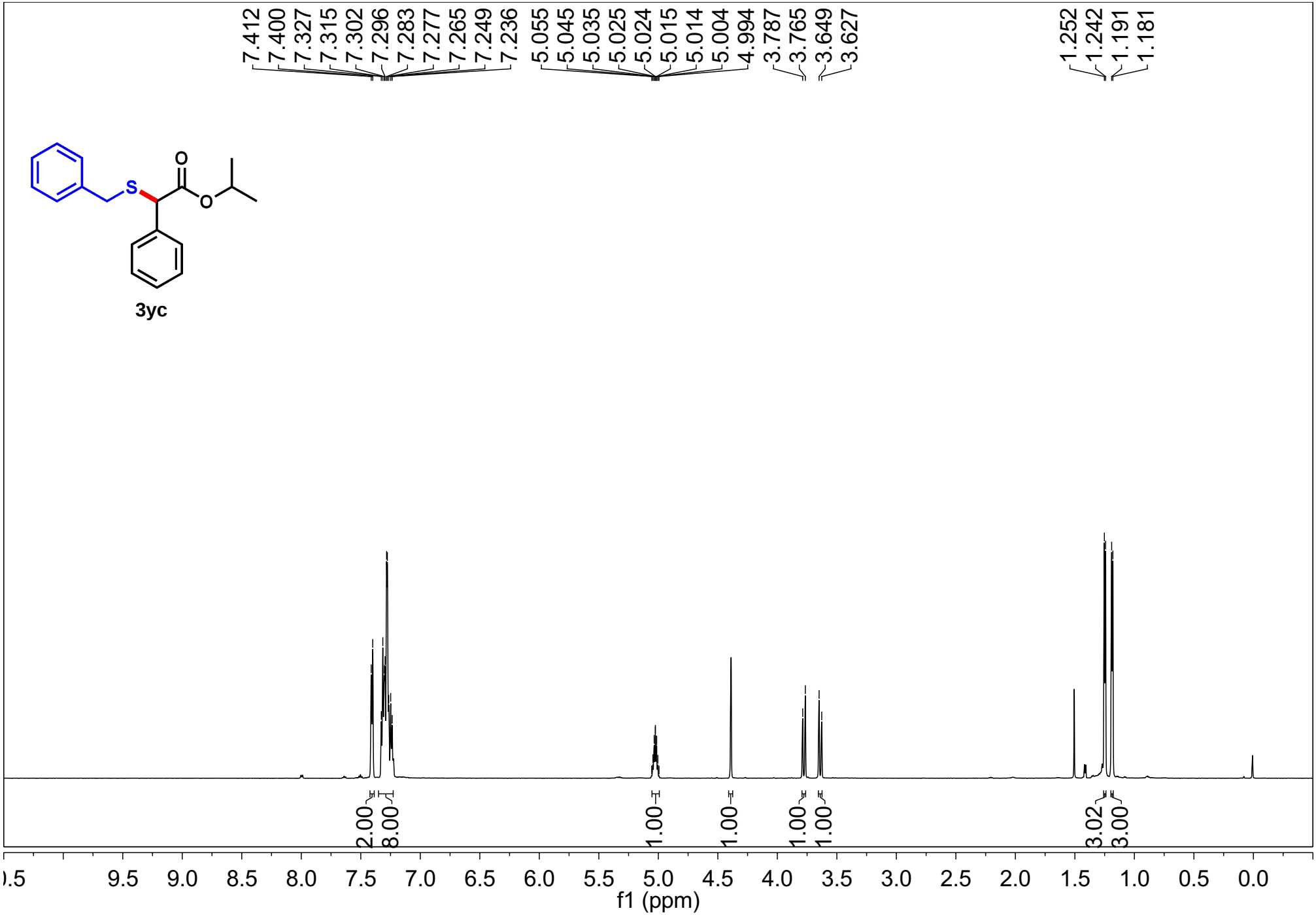
10
0
f1 (ppm)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5.025
5.024
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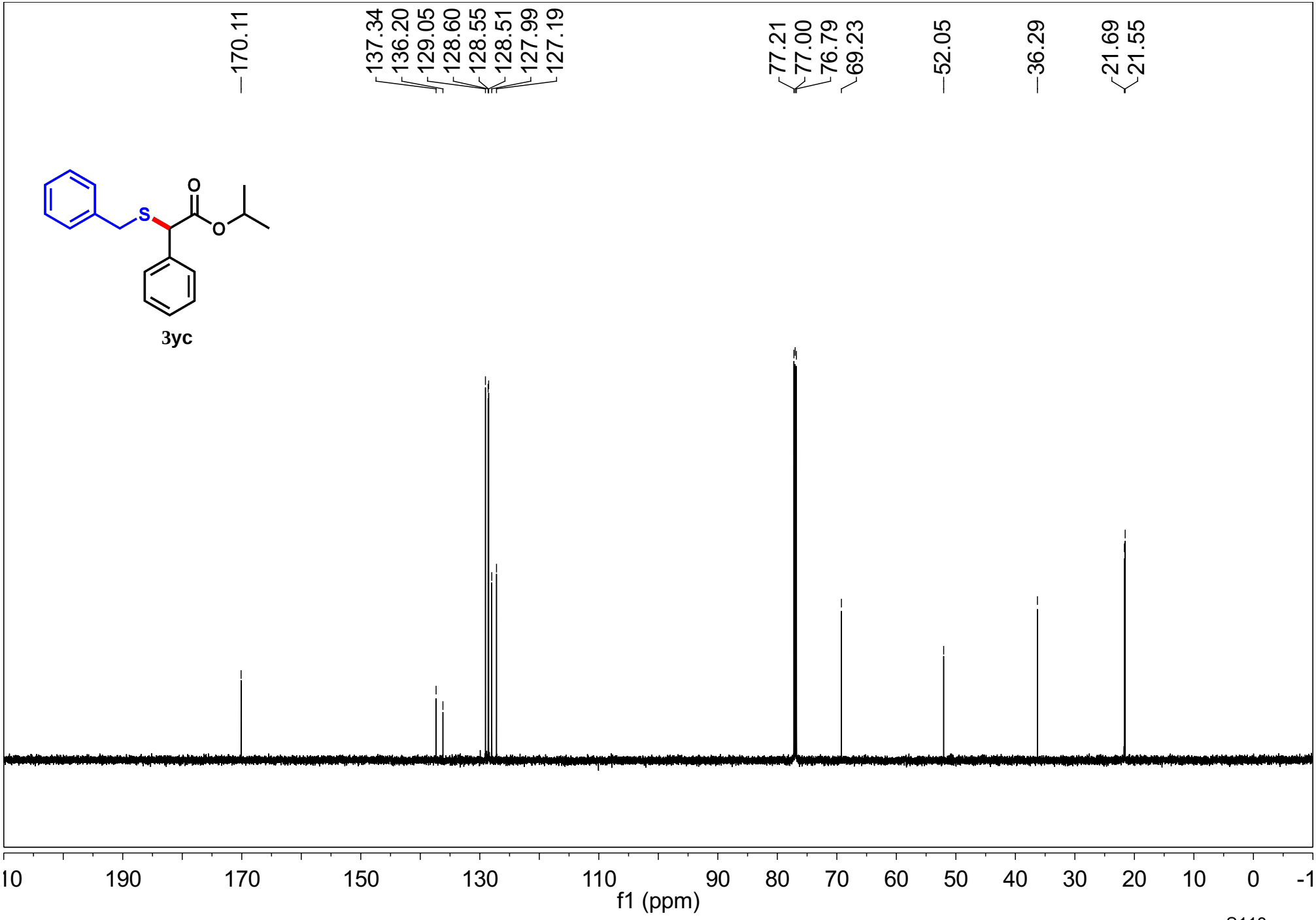
5.004
4.994
3.787
3.765
3.649
3.627
1.252
1.242
1.191
1.181
S
O
O
3yc
2.00
8.00
1.00
1.00
1.00
1.00
3.02
3.00
f1 (ppm)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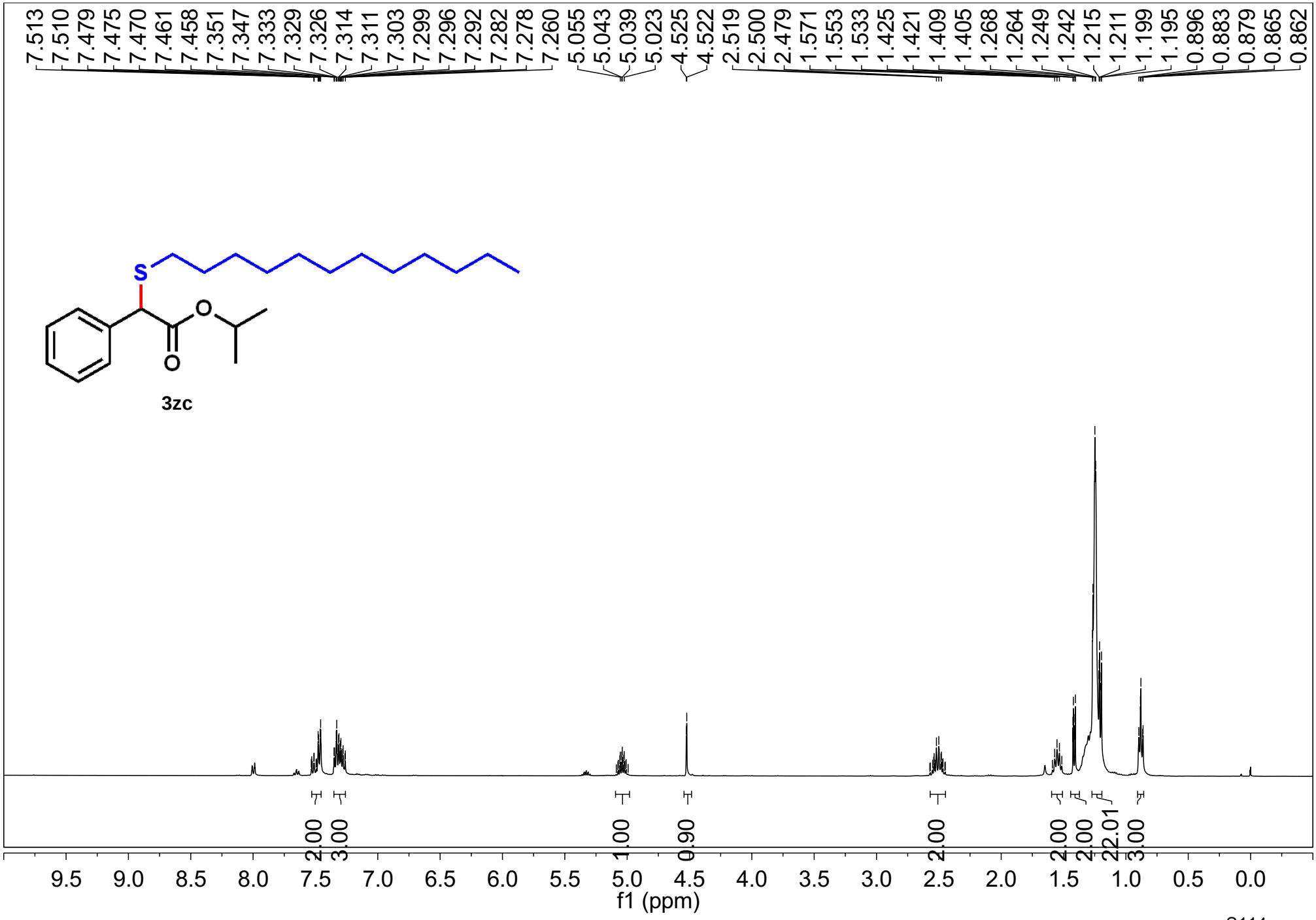
137.34
136.20
129.05
128.60
128.55
128.51
127.99
127.19
77.21
77.00
76.79
69.23
52.05
36.29
21.69
21.55
O
S
O
3yc
10
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)


7.513
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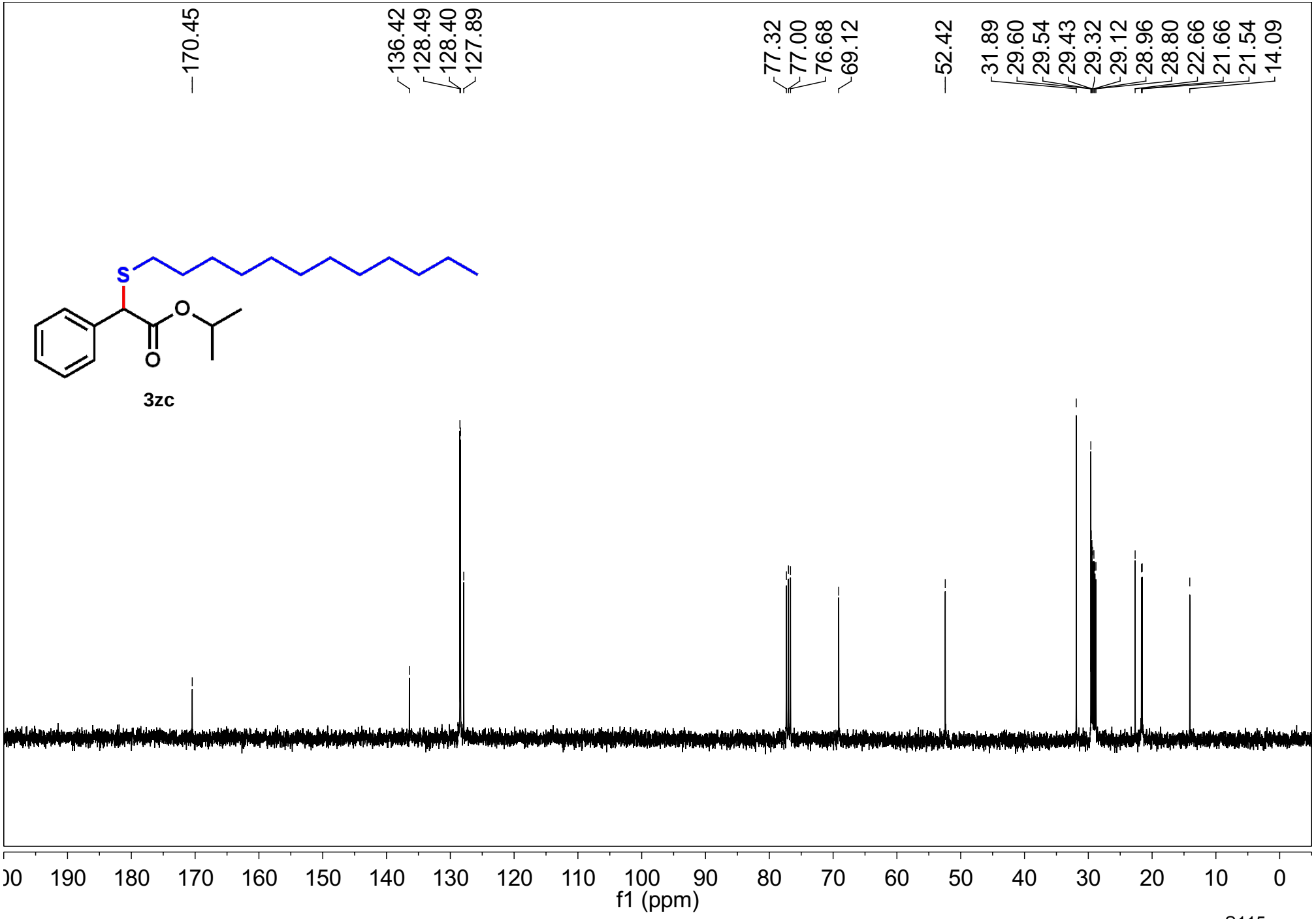
7.475
7.470
7.461
7.458
7.351
7.347
7.333
7.329
7.326
7.314
7.311
7.303
7.299
7.296
7.292
7.282
7.278
7.260
5.055
5.043
5.039
5.023
4.525
4.522
2.519
2.500
2.479
1.571
1.553
1.533
1.425
1.421
1.409
1.405
1.268
1.264
1.249
1.242
1.215
1.211
1.199
1.195
0.896
0.883
0.879
0.865
0.862
S
O
O
3zc
2.00
3.00
1.00
0.90
2.00
2.00
2.00
22.01
3.00
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)


170.45
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128.49
128.40
127.89
77.32
77.00
76.68
69.12
52.42
31.89
29.60
29.54
29.43
29.32
29.12
28.96
28.80
22.66
21.66
21.54
14.09
S
O
O
3zc
f1 (ppm)