Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Metal-Free Synthesis of 3-Chalcogenyl Chromones from Alkynyl Aryl Ketones and Diorganyl Diselenides / Disulfides Mediated by PIFA

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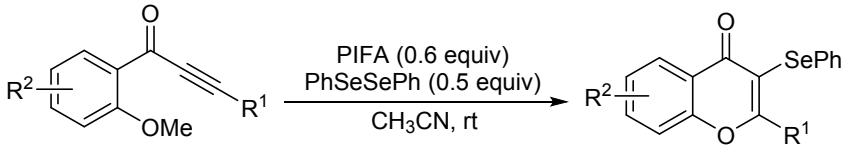
1. General information

^{1}H and ^{13}C NMR spectra were recorded on a 600 MHz spectrometer at 25 ^{o}C. Chemical shifts values are given in ppm and referred as the internal standard to TMS: 0.00 ppm. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, br = broad, m = multiplet). The coupling constants *J*, are reported in Hertz (Hz). High resolution mass spectrometry (HRMS) was obtained on a Q-TOF micro spectrometer. Melting points were determined with a Micromelting point apparatus. TLC plates were visualized by exposure to ultraviolet light.

Reagents and solvents were purchased as reagent grade and were used without further purification. The starting materials **1** were prepared according to literature methods.[1] Flash column chromatography was performed over silica gel (200-300 m) using a mixture of ethyl acetate (EtOAc) and petroleum ether (PE).

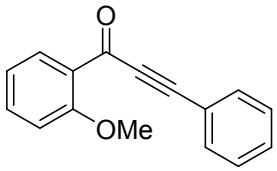
2. General Procedure for the Cyclization Process



1 **2** or **3**

To a solution of PhSeSePh (0.5 mmol) in MeCN (10 mL) was added PIFA (0.6 mmol) at rt. The mixture was stirred for 5 min. Then substrate **1** (1.0 mmol) was added to this solution in one portion and the reaction mixture was stirred for another 15 min until the completion of the starting material (monitored by TLC). The resulting mixture was purified by flash chromatography to afford the corresponding 3-chacogenyl chromone/thiochromones **2** or **3**.

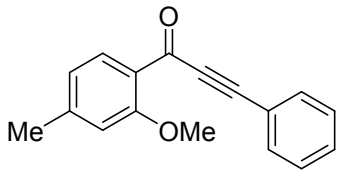
3. Spectral Data of Substrates and Products



1a

1-(2-Methoxyphenyl)-3-(*o*-tolyl)prop-2-yn-1-one (1a)

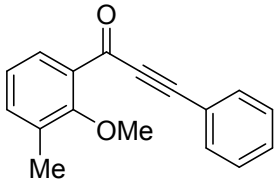
Following the general procedure, **1a** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 1.65 g, 70%, yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.67 – 7.58 (m, 2H), 7.58 – 7.49 (m, 1H), 7.46 – 7.35 (m, 3H), 7.04 (dd, *J* = 17.4, 8.1 Hz, 2H), 3.96 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.8, 159.9, 135.1, 133.0, 132.7, 130.5, 128.6, 126.8, 120.7, 120.4, 112.3, 91.6, 89.2, 56.0. HRMS (ESI) calcd for $C_{16}H_{13}O_2^+$ [M + H^+] 237.0901, found 237.0904.



1b

1-(2-Methoxy-4-methylphenyl)-3-phenylprop-2-yn-1-one (1b)

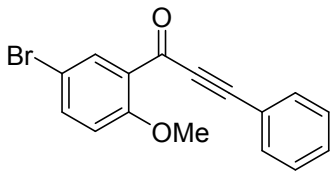
Following the general procedure, **1b** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 1.63 g, 65%, yellow liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.00 (d, *J* = 7.9 Hz, 1H), 7.65 – 7.59 (m, 2H), 7.47 – 7.42 (m, 1H), 7.41 – 7.35 (m, 2H), 6.85 (d, *J* = 7.4 Hz, 1H), 6.81 (s, 1H), 3.94 (s, 3H), 2.41 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 176.2, 160.0, 146.5, 132.9, 130.3, 128.6, 124.3, 121.3, 120.9, 112.9, 91.1, 89.3, 55.9, 22.1. HRMS (ESI) calcd for $C_{17}H_{15}O_2^+$ [M + H^+] 251.1067, found 251.1068



1c

1-(2-Methoxy-3-methylphenyl)-3-phenylprop-2-yn-1-one (1c)

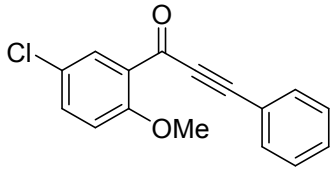
Following the general procedure, **1c** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 1.60 g, 64%, yellow liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.92 (d, *J* = 7.9 Hz, 1H), 7.65 (d, *J* = 7.1 Hz, 2H), 7.45 (t, *J* = 7.8 Hz, 1H), 7.43 – 7.37 (m, 3H), 7.13 (t, *J* = 7.6 Hz, 1H), 3.88 (s, 3H), 2.35 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 177.2, 159.0, 136.6, 133.0, 132.9, 131.0, 130.6, 130.1, 128.6, 123.7, 120.5, 91.5, 89.1, 61.8, 15.9. HRMS (ESI) calcd for $C_{17}H_{15}O_2^+$ [M + H^+] 251.1067, found 251.1070.



1d

1-(5-Bromo-2-methoxyphenyl)-3-phenylprop-2-yn-1-one (1d)

Following the general procedure, **1d** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 2.51 g, 80%, a yellow solid, mp. 86-87 °C ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.13 (t, *J* = 3.1 Hz, 1H), 7.62 (ddd, *J* = 11.6, 6.8, 2.0 Hz, 3H), 7.47 (ddd, *J* = 6.7, 4.0, 1.3 Hz, 1H), 7.43 – 7.37 (m, 2H), 6.91 (dd, *J* = 8.9, 2.3 Hz, 1H), 3.95 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 175.2, 158.8, 137.3, 134.6, 133.1, 130.7, 128.7, 128.4, 120.5, 114.3, 112.7, 92.6, 88.9, 56.3. HRMS (ESI) calcd for $C_{16}H_{12}{}^{79}BrO_2^+$ [M + H^+] 315.0015, found 315.0022.

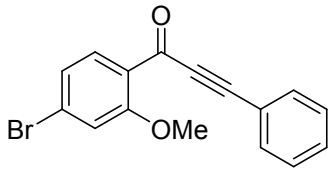


1e

1-(5-Chloro-2-methoxyphenyl)-3-phenylprop-2-yn-1-one (1e)

Following the general procedure, **1e** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 2.21 g, 82%, a yellow solid, mp. 84-85 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.05 – 7.90 (m, 1H), 7.67 – 7.58 (m, 2H), 7.52 – 7.44 (m, 2H), 7.40 (ddd, *J* = 8.3, 2.4, 1.0 Hz, 2H), 6.96 (dd, *J* = 8.9, 2.0 Hz, 1H), 3.95 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 175.3, 158.3, 134.4, 133.1, 131.7, 130.7, 128.7, 127.9, 125.6,

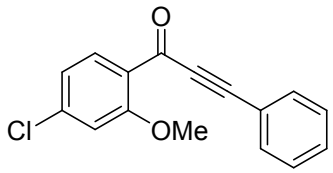
120.5, 113.9, 92.5, 89.0, 56.3. HRMS (ESI) calcd for $C_{16}H_{12}{}^{35}ClO_2^+$ [M + H$^+$] 271.0520, found 271.0522.



1f

1-(4-Bromo-2-methoxyphenyl)-3-phenylprop-2-yn-1-one (1f)

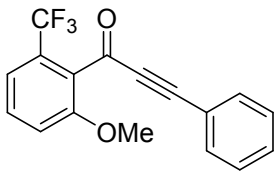
Following the general procedure, **1f** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 2.67 g, 85%, a yellow solid, mp. 86-87 ^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.93 (d, *J* = 8.3 Hz, 1H), 7.62 (d, *J* = 7.9 Hz, 2H), 7.46 (t, *J* = 7.5 Hz, 1H), 7.40 (t, *J* = 7.7 Hz, 2H), 7.20 (d, *J* = 8.4 Hz, 1H), 7.17 (s, 1H), 3.96 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 175.6, 160.1, 133.6, 133.0, 130.6, 129.5, 128.6, 125.8, 123.7, 120.6, 115.9, 92.1, 89.0, 56.3. HRMS (ESI) calcd for $C_{16}H_{12}{}^{79}BrO_2^+$ [M + H$^+$] 315.0015, found 315.0018.



1g

1-(4-Chloro-2-methoxyphenyl)-3-phenylprop-2-yn-1-one (1g)

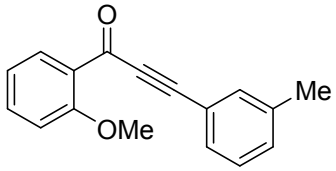
Following the general procedure, **1g** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 2.30 g, 85%, a yellow solid, mp. 65-66 ^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.02 (d, *J* = 9.2 Hz, 1H), 7.62 (d, *J* = 8.1 Hz, 2H), 7.46 (t, *J* = 8.0 Hz, 1H), 7.40 (t, *J* = 7.4 Hz, 2H), 7.04 (d, *J* = 8.4 Hz, 1H), 7.01 (s, 1H), 3.97 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 175.4, 160.3, 141.0, 133.6, 133.0, 130.6, 128.6, 125.4, 120.7, 120.6, 112.9, 92.1, 89.0, 56.2. HRMS (ESI) calcd for $C_{16}H_{12}{}^{35}ClO_2^+$ [M + H$^+$] 271.0520, found 271.0524.



1h

1-(2-Methoxy-6-(trifluoromethyl)phenyl)-3-phenylprop-2-yn-1-one (1h)

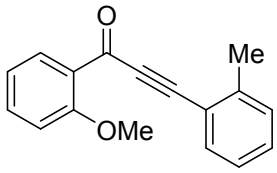
Following the general procedure, **1h** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 2.28 g, 75%, a brown solid, mp. 59-60 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.1 Hz, 1H), 7.63 (dd, *J* = 8.0, 0.9 Hz, 2H), 7.47 (t, *J* = 7.0 Hz, 1H), 7.41 (t, *J* = 7.7 Hz, 2H), 7.31 (d, *J* = 8.1 Hz, 1H), 7.24 (s, 1H), 4.02 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 175.8, 159.5, 136.0 (*J* = 32.5 Hz), 133.1, 132.6, 130.8, 129.7, 128.7, 124.3 (*J* = 271.4 Hz), 120.3, 117.1 (*J* = 3.8 Hz), 109.3, 92.9, 89.0, 56.3. ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.3. HRMS (ESI) calcd for $C_{17}H_{12}F_3O_2^+$ [M + H^+] 305.0784, found 305.0790.



1i

1-(2-Methoxyphenyl)-3-(*m*-tolyl)prop-2-yn-1-one (1i)

Following the general procedure, **1i** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 1.63 g, 65%, yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.59 – 7.47 (m, 1H), 7.46 – 7.37 (m, 2H), 7.31 – 7.21 (m, 1H), 7.10 – 6.95 (m, 2H), 3.94 (s, 3H), 2.34 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.8, 159.8, 138.4, 135.1, 133.5, 132.6, 131.5, 130.1, 128.5, 126.8, 120.5, 120.3, 112.3, 92.0, 89.0, 56.0, 21.2. HRMS (ESI) calcd for $C_{17}H_{15}O_2^+$ [M + H^+] 251.1067, found 251.1070.

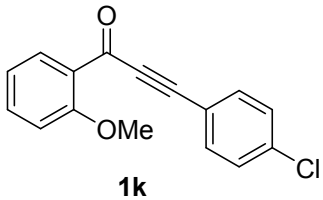


1j

1-(2-Methoxyphenyl)-3-(*o*-tolyl)prop-2-yn-1-one (1j)

Following the general procedure, **1j** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 1.50 g, 60%, yellow liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.08 (d, *J* = 7.8 Hz, 1H), 7.59 (d, *J* = 8.7 Hz, 1H), 7.55 – 7.50 (m, 1H), 7.33 (t, *J* = 8.2 Hz, 1H), 7.25 (d, *J* = 6.2 Hz, 1H), 7.20 (t, *J* = 7.6 Hz, 1H), 7.05 (t, *J* = 7.5 Hz,

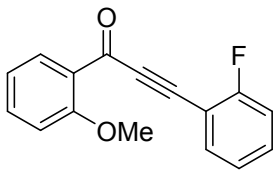
1H), 7.01 (d, *J* = 8.4 Hz, 1H), 3.95 (s, 3H), 2.54 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 176.9, 159.7, 142.0, 134.8, 133.5, 132.5, 130.4, 129.8, 127.1, 125.8, 120.6, 120.3, 112.2, 93.1, 90.7, 55.9, 20.7. HRMS (ESI) calcd for $C_{17}H_{15}O_2^+$ [M + H^+] 251.1067, found 251.1062



1k

3-(4-Chlorophenyl)-1-(2-methoxyphenyl)prop-2-yn-1-one (1k)

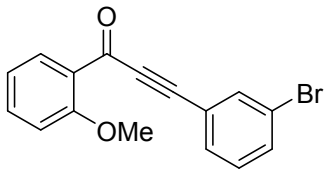
Following the general procedure, **1k** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 1.62 g, 60%, a yellow solid. mp. 66-67 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.08 – 8.02 (m, 1H), 7.59 – 7.51 (m, 3H), 7.40 – 7.34 (m, 2H), 7.08 – 6.98 (m, 2H), 3.96 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 176.4, 159.9, 136.8, 135.1, 134.1, 132.5, 129.1,126.69, 120.4, 119.3, 112.3, 90.1, 89.0, 56.0. HRMS (ESI) calcd for $C_{16}H_{12}{}^{35}ClO_2^+$ [M + H^+] 271.0520, found 271.0524.



1l

3-(2-Fluorophenyl)-1-(2-methoxyphenyl)prop-2-yn-1-one (1l)

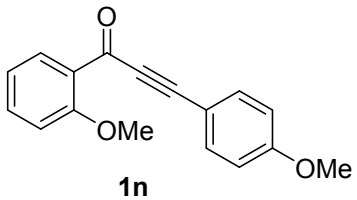
Following the general procedure, **1l** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 1.52 g, 60%, yellow liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.11 (d, *J* = 7.8 Hz, 1H), 7.62 (t, *J* = 8.0 Hz, 1H), 7.54 (t, *J* = 7.8 Hz, 1H), 7.44 (dd, *J* = 14.1, 8.6 Hz, 1H), 7.18 (t, *J* = 7.6 Hz, 1H), 7.14 (t, *J* = 8.8 Hz, 1H), 7.05 (t, *J* = 7.5 Hz, 1H), 7.02 (d, *J* = 8.4 Hz, 1H), 3.96 (s, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 176.3, 164.4 (*J* = 255.0 Hz), 160.1, 135.2, 134.9, 132.7, 132.4 (*J* = 7.5 Hz), 126.5, 124.3 (*J* = 4.5 Hz), 120.4, 115.9 (*J* = 19.5 Hz), 112.2, 109.7 (*J* = 15.0 Hz), 93.7, 84.5, 55.8. ^{19}F NMR (376 MHz, $CDCl_3$) δ -107.3. HRMS (ESI) calcd for $C_{16}H_{12}FO_2^+$ [M + H^+] 255.0816, found 255.0820.



1m

3-(3-Bromophenyl)-1-(2-methoxyphenyl)prop-2-yn-1-one (1m)

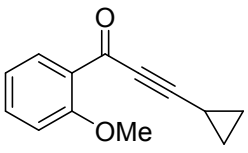
Following the general procedure, **1m** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 1.89 g, 60%, yellow liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.05 (d, *J* = 9.5 Hz, 1H), 7.76 (s, 1H), 7.62 – 7.53 (m, 3H), 7.27 (t, *J* = 7.9 Hz, 1H), 7.06 (t, *J* = 7.9 Hz, 1H), 7.02 (d, *J* = 8.4 Hz, 1H), 3.96 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 176.3, 159.9, 135.4, 135.2, 133.5, 132.5, 131.4, 130.1, 126.6, 122.8, 122.4, 120.4, 112.3, 89.9, 89.3, 56.0. HRMS (ESI) calcd for $C_{16}H_{12}{}^{79}BrO_2^+$ [M + H^+] 315.0015, found 315.0020.



1n

1-(2-Methoxyphenyl)-3-(4-methoxyphenyl)prop-2-yn-1-one (1n)

Following the general procedure, **1n** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 1.60 g, 60%, a yellow solid. mp. 69-70 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.07 (d, *J* = 7.7 Hz, 1H), 7.58 (d, *J* = 8.8 Hz, 2H), 7.55 – 7.49 (m, 1H), 7.04 (t, *J* = 7.5 Hz, 1H), 7.01 (d, *J* = 8.4 Hz, 1H), 6.91 (d, *J* = 8.8 Hz, 2H), 3.96 (s, 3H), 3.84 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 176.8, 161.5, 159.7, 135.0, 134.7, 132.4, 127.1, 120.3, 114.4, 112.6, 112.3, 92.7, 89.2, 56.0, 55.4. HRMS (ESI) calcd for $C_{17}H_{15}O_3^+$ [M + H^+] 267.1016, found 267.1020.

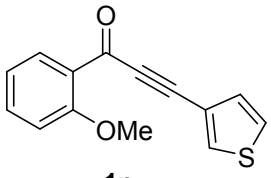


1o

3-Cyclopropyl-1-(2-methoxyphenyl)prop-2-yn-1-one (1o)

Following the general procedure, **1o** was purified by silica gel chromatography

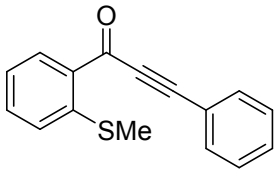
(EtOAc/PE = 5/95). Yield: 1.50 g, 75%, yellow liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.96 (d, *J* = 7.8 Hz, 1H), 7.49 (t, J = 7.9 Hz, 1H), 7.00 (t, *J* = 7.5 Hz, 1H), 6.97 (d, *J* = 8.4 Hz, 1H), 1.49 (m, 1H), 1.04 – 0.98 (m, 2H), 0.96 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 176.7, 159.5, 134.4, 132.5, 126.9, 120.1, 112.1, 99.6, 77.7, 55.7, 9.7. HRMS (ESI) calcd for $C_{13}H_{13}O_2^+$ [M + H$^+$] 201.0910, found 201.0914.



1p

1-(2-Methoxyphenyl)-3-(thiophen-3-yl)prop-2-yn-1-one (1p)

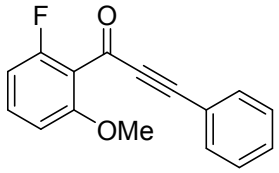
Following the general procedure, **1p** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 1.70 g, 70%, yellow liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.06 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.77 (dd, *J* = 2.9, 1.0 Hz, 1H), 7.58 – 7.46 (m, 1H), 7.34 (dd, *J* = 5.0, 3.0 Hz, 1H), 7.29 – 7.24 (m, 1H), 7.05 (t, *J* = 7.5 Hz, 1H), 7.01 (d, *J* = 8.4 Hz, 1H), 3.95 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 176.7, 159.8, 134.9, 133.4, 132.5, 130.3, 126.8, 126.1, 120.4, 120.0, 112.3, 89.4, 87.0, 55.9. HRMS (ESI) calcd for $C_{14}H_{14}O_2S^+$ [M + H$^+$] 243.0474, found 243.0478.



1q

1-(2-(Methylthio)phenyl)-3-phenylprop-2-yn-1-one (1q)

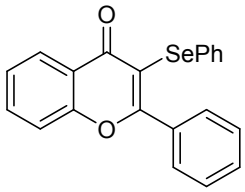
Following the general procedure, **1q** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 1.76 g, 70%, a yellow solid, mp. 73-74 ^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.42 (d, *J* = 9.1 Hz, 1H), 7.66 (d, *J* = 7.1 Hz, 2H), 7.53 (t, *J* = 8.4 Hz, 1H), 7.46 (t, *J* = 7.5 Hz, 1H), 7.41 (t, *J* = 7.5 Hz, 2H), 7.33 (d, *J* = 8.1 Hz, 1H), 7.26 (t, *J* = 7.2 Hz, 1H), 2.46 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 177.6, 144.8, 134.6, 133.3, 133.2, 132.9, 130.6, 128.7, 124.3, 123.3, 120.4, 92.7, 87.2, 15.5. HRMS (ESI) calcd for $C_{16}H_{13}OS^+$ [M + H$^+$] 253.0682, found 253.0686.



1r

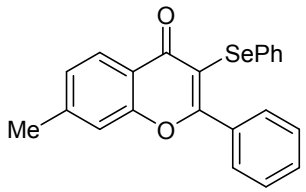
1-(2-Fluoro-6-methoxyphenyl)-3-phenylprop-2-yn-1-one (1r)

Following the general procedure, **1r** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 1.42 g, 56%, yellow liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.2 Hz, 2H), 7.44 (t, *J* = 7.5 Hz, 1H), 7.41 – 7.35 (m, 3H), 6.80 – 6.71 (m, 2H), 3.90 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 174.6, 161.7 (*J* = 252.9 Hz) 158.9 (*J* = 5.9 Hz), 133.1, 132.9 (*J* = 10.9 Hz), 130.7, 128.6, 120.3, 108.6, 108.4, 107.4, 92.0, 89.7, 56.4. ^{19}F NMR (376 MHz, $CDCl_3$) δ -113.7. HRMS (ESI) calcd for $C_{16}H_{12}FO_2^+$ [M + H^+] 255.0816, found 255.0818.



2-Phenyl-3-(phenylselanyl)-4*H*-chromen-4-one (2a)

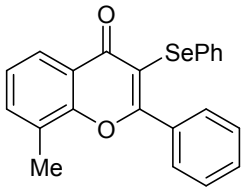
Following the general procedure, **2a** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 336 mg, 89%, a yellow solid, mp. 129-131 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.26 (dd, J = 8.0, 1.7 Hz, 1H), 7.73 – 7.63 (m, 3H), 7.52 – 7.46 (m, 2H), 7.43 (td, J = 7.7, 6.2 Hz, 3H), 7.36 – 7.27 (m, 2H), 7.13 (p, J = 3.9, 3.5 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 176.0, 167.8, 156.0, 134.2, 134.0, 131.4, 131.1, 130.7, 129.3, 129.0, 128.0, 126.8, 126.7, 125.6, 122.5, 117.9, 114.2. HRMS (ESI) calcd for $C_{21}H_{15}O_2Se^+$ [M + H^+] 379.0232, found 379.0230.



7-Methyl-2-phenyl-3-(phenylselanyl)-4*H*-chromen-4-one (2b)

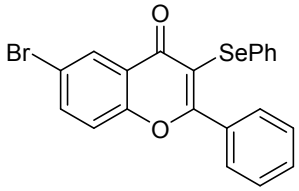
Following the general procedure, **2b** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 341 mg, 87%, a yellow solid, mp. 142-144 °C. 1H NMR

(600 MHz, $CDCl_3$) δ 8.14 (d, *J* = 8.1 Hz, 1H), 7.68 – 7.62 (m, 2H), 7.51 – 7.46 (m, 1H), 7.43 (dd, *J* = 8.3, 6.7 Hz, 2H), 7.31 (dd, *J* = 6.7, 3.0 Hz, 2H), 7.28 (s, 1H), 7.24 (d, *J* = 8.1 Hz, 1H), 7.13 (dd, *J* = 5.0, 1.9 Hz, 3H), 2.49 (s, 3H). ^{13}C NMR (151 MHz, CDCl3) δ 175.8, 167.6, 156.1, 145.4, 134.4, 131.5, 131.0, 130.6, 129.2, 129.0, 128.0, 127.1, 126.6, 126.5, 120.2, 117.6, 114.0, 21.8. HRMS (ESI) calcd for $C_{22}H_{17}O_2Se^+$ [M + H^+] 393.0388, found 393.0392.



8-Methyl-2-phenyl-3-(phenylselanyl)-4*H*-chromen-4-one (2c)

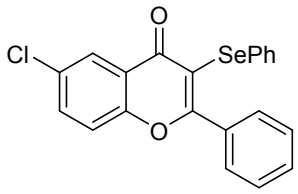
Following the general procedure, **2c** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 328 mg, 84%, a yellow solid, mp. 126-128 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.09 (d, J = 7.8 Hz, 1H), 7.71 (d, *J* = 7.5 Hz, 2H), 7.52 (d, *J* = 7.3 Hz, 1H), 7.48 (d, *J* = 7.2 Hz, 1H), 7.44 (t, *J* = 7.5 Hz, 2H), 7.34 – 7.28 (m, 3H), 7.15 – 7.09 (m, 3H), 2.47 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 176.3, 167.3, 154.5, 134.8, 134.4, 131.5, 131.0, 130.7, 129.4, 129.0, 128.0, 127.4, 126.7, 125.2, 124.3, 122.4, 113.9, 15.6. HRMS (ESI) calcd for $C_{22}H_{17}O_2Se^+$ [M + H^+] 393.0388, found 393.0382.



6-Bromo-2-phenyl-3-(phenylselanyl)-4*H*-chromen-4-one (2d)

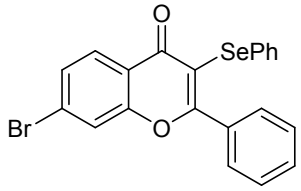
Following the general procedure, **2d** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 429 mg, 94%, a yellow solid, mp. 138-140 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.37 (d, *J* = 2.5 Hz, 1H), 7.76 (dd, *J* = 8.8, 2.5 Hz, 1H), 7.68 – 7.63 (m, 2H), 7.54 – 7.48 (m, 1H), 7.47 – 7.42 (m, 2H), 7.38 (d, *J* = 8.8 Hz, 1H), 7.33 – 7.28 (m, 2H), 7.17 – 7.12 (m, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 174.8, 167.8, 154.8, 136.9, 133.9, 131.3, 130.97, 130.96, 129.3, 129.2, 129.1, 128.1, 127.0, 123.7, 119.9, 118.9, 114.4. HRMS (ESI) calcd for $C_{21}H_{14}{}^{79}BrO_2Se^+$ [M + H^+] 456.9337,

found 456.9342.



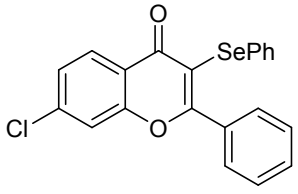
6-Chloro-2-phenyl-3-(phenylselanyl)-4*H*-chromen-4-one (2e)

Following the general procedure, **2e** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 370 mg, 90%, a yellow solid, mp. 128-130 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.21 (d, *J* = 2.5 Hz, 1H), 7.69 – 7.64 (m, 2H), 7.63 (dd, *J* = 8.9, 2.6 Hz, 1H), 7.53 – 7.48 (m, 1H), 7.48 – 7.42 (m, 3H), 7.34 – 7.28 (m, 2H), 7.18 – 7.10 (m, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 174.9, 167.8, 154.3, 134.2, 133.9, 131.5, 131.3, 131.0, 131.0, 129.3, 129.1, 128.1, 127.0, 126.0, 123.3, 119.7, 114.3. HRMS (ESI) calcd for $C_{21}H_{14}{}^{35}ClO_2Se^+$ [M + H$^+$] 412.9842, found 412.9844.



7-Bromo-2-phenyl-3-(phenylselanyl)-4*H*-chromen-4-one (2f)

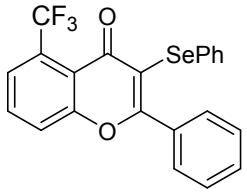
Following the general procedure, **2f** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 429 mg, 94%, a yellow solid, mp. 84-86 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.5 Hz, 1H), 7.68 (d, *J* = 1.8 Hz, 1H), 7.65 (dt, *J* = 7.1, 1.4 Hz, 2H), 7.53 (dd, *J* = 8.5, 1.8 Hz, 1H), 7.52 – 7.47 (m, 1H), 7.44 (dd, *J* = 8.3, 6.7 Hz, 2H), 7.32 – 7.28 (m, 2H), 7.15 – 7.12 (m, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 175.3, 167.5, 156.0, 133.8, 131.3, 131.0, 130.9, 129.3, 129.2, 129.1, 128.2, 128.2, 128.1, 126.9, 121.3, 121.1, 114.7. HRMS (ESI) calcd for $C_{21}H_{14}{}^{79}BrO_2Se^+$ [M + H$^+$] 456.9337, found 456.9334.



7-Chloro-2-phenyl-3-(phenylselanyl)-4*H*-chromen-4-one (2g)

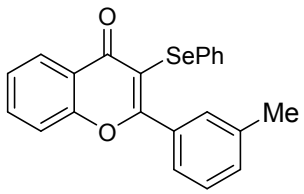
Following the general procedure, **2g** was purified by silica gel chromatography

(EtOAc/PE = 5/95). Yield: 366 mg, 89%, a yellow solid, mp. 97-99 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.18 (d, *J* = 8.6 Hz, 1H), 7.67 – 7.61 (m, 2H), 7.53 – 7.48 (m, 2H), 7.44 (td, *J* = 7.2, 6.7, 1.3 Hz, 2H), 7.39 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.33 – 7.29 (m, 2H), 7.14 (dd, *J* = 4.7, 1.9 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 175.2, 167.6, 156.1, 140.0, 133.8, 131.3, 131.0, 130.9, 129.3, 129.1, 128.1, 128.1, 126.9, 126.4, 120.9, 118.0, 114.7. HRMS (ESI) calcd for $C_{21}H_{14}{}^{35}ClO_2Se^+$ [M + H^+] 412.9842, found 412.9840.



2-Phenyl-3-(phenylselanyl)-5-(trifluoromethyl)-4*H*-chromen-4-one (2h)

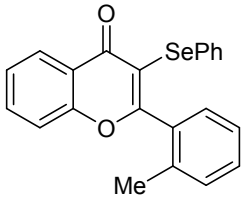
Following the general procedure, **2h** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 418 mg, 94%, a yellow solid, mp. 108-110 °C. 1H NMR (400 MHz, Chloroform-d) δ 8.37 (dd, J = 8.3, 1.0 Hz, 1H), 7.80 (dd, J = 1.6, 0.8 Hz, 1H), 7.71 – 7.63 (m, 3H), 7.56 – 7.49 (m, 1H), 7.49 – 7.43 (m, 2H), 7.34 – 7.29 (m, 2H), 7.17 – 7.12 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.20, 168.10, 155.39, 135.68, 135.35, 133.59, 131.32, 131.15, 130.75, 129.29, 129.16, 128.15, 128.09, 127.07, 124.42, 121.9 (q, J = 4.5 Hz), 116.0 (q, J = 6 Hz), 115.01. ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.1. HRMS (ESI) calcd for $C_{22}H_{14}F_3O_2Se^+$ [M + H^+] 447.0106, found 447.0110.



3-(Phenylselanyl)-2-(*m*-tolyl)-4*H*-chromen-4-one (2i)

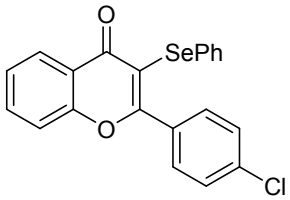
Following the general procedure, **2i** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 321 mg, 82%, a yellow solid, mp. 140-142 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.24 (dd, J = 8.0, 1.7 Hz, 1H), 7.65 (ddd, J = 8.6, 7.1, 1.7 Hz, 1H), 7.45 (ddd, J = 8.2, 6.6, 1.3 Hz, 2H), 7.43 – 7.37 (m, 2H), 7.35 – 7.26 (m, 4H), 7.13 (qd, J = 3.9, 1.7 Hz, 3H), 2.37 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 176.0,

168.0, 156.0, 137.8, 134.2, 134.0, 131.5, 131.5, 131.2, 131.2, 129.7, 129.0, 127.9, 126.7, 126.7, 126.4, 125.6, 122.5, 117.9, 114.2, 21.4. HRMS (ESI) calcd for $C_{22}H_{17}O_2Se^+$ [M + H^+] 393.0388, found 393.0384.



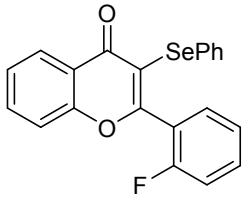
3-(Phenylselanyl)-2-(*o*-tolyl)-4*H*-chromen-4-one (2j）

Following the general procedure, **2j** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 360 mg, 92%, a yellow solid, mp. 58-60 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.14 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.50 (ddd, *J* = 8.7, 7.2, 1.7 Hz, 1H), 7.30 – 7.24 (m, 2H), 7.21 (td, *J* = 7.5, 1.5 Hz, 1H), 7.15 – 7.11 (m, 3H), 7.10 – 7.06 (m, 2H), 7.01 – 6.92 (m, 3H), 2.03 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 175.8, 168.7, 156.2, 136.2, 134.1, 134.0, 132.2, 130.7, 130.3, 130.3, 129.2, 128.9, 127.0, 126.7, 125.7, 125.6, 122.7, 118.0, 116.1, 19.5. HRMS (ESI) calcd for $C_{22}H_{17}O_2Se^+$ [M + H^+] 393.0388, found 393.0390.



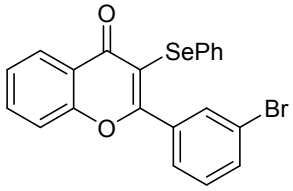
2-(4-Chlorophenyl)-3-(phenylselanyl)-4*H*-chromen-4-one (2k)

Following the general procedure, **2k** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 354 mg, 86%, a yellow solid, mp. 100-102 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.25 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.69 (ddd, *J* = 8.6, 7.1, 1.7 Hz, 1H), 7.63 – 7.59 (m, 2H), 7.47 (dd, *J* = 8.5, 1.0 Hz, 1H), 7.43 (ddd, *J* = 8.1, 7.1, 1.1 Hz, 1H), 7.41 – 7.37 (m, 2H), 7.33 – 7.28 (m, 2H), 7.14 (tt, *J* = 3.8, 2.4 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 175.9, 166.4, 155.9, 137.0, 134.1, 132.5, 131.1, 130.7, 129.1, 128.3, 126.9, 126.8, 125.7, 122.4, 117.9, 114.5. HRMS (ESI) calcd for $C_{21}H_{14}{}^{35}ClO_2Se^+$ [M + H^+] 412.9842, found 412.9846.



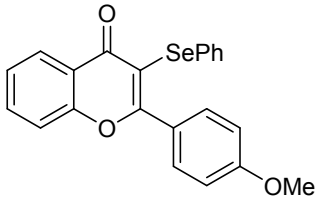
2-(2-Fluorophenyl)-3-(phenylselanyl)-4*H*-chromen-4-one (2l)

Following the general procedure, **2l** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 371 mg, 94%, a yellow solid, mp. 132-134 ^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.24 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.66 (ddd, *J* = 8.7, 7.1, 1.7 Hz, 1H), 7.51 – 7.36 (m, 4H), 7.32 (dd, *J* = 7.4, 2.3 Hz, 2H), 7.21 (td, *J* = 7.6, 1.0 Hz, 1H), 7.16 – 7.08 (m, 4H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 175.5, 163.2, 160 (*J* = 250.0 Hz), 156.2, 134.1, 132.6 (*J* = 9.1 Hz), 131.8, 130.7(*J* = 2.1 Hz), 130.5, 129.0, 127.0, 126.7, 125.7, 123.9 (*J* = 3.7 Hz), 122.7 (*J* = 14.6 Hz), 122.6, 118.0, 117.2, 116.1 (*J* = 21.3 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -111.6 HRMS (ESI) calcd for $C_{21}H_{14}FO_2Se^+$ [M + H^+] 397.0138, found 397.0140.



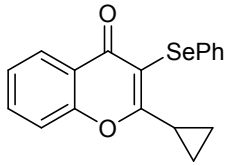
2-(3-Bromophenyl)-3-(phenylselanyl)-4*H*-chromen-4-one (2m)

Following the general procedure, **2m** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 402 mg, 88%, a yellow solid, mp. 146-148 ^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.26 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.76 (t, *J* = 1.8 Hz, 1H), 7.69 (ddd, *J* = 8.7, 7.1, 1.7 Hz, 1H), 7.58 (ddq, *J* = 7.9, 2.0, 1.0 Hz, 2H), 7.47 (dd, *J* = 8.4, 0.9 Hz, 1H), 7.44 (ddd, *J* = 8.1, 7.1, 1.1 Hz, 1H), 7.35 – 7.30 (m, 2H), 7.28 (t, *J* = 7.9 Hz, 1H), 7.19 – 7.12 (m, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 175.9, 165.6, 155.9, 135.9, 134.1, 133.6, 132.0, 131.7, 131.0, 129.5, 129.1, 127.9, 127.1, 126.8, 125.8, 122.4, 122.0, 117.9, 115.2. HRMS (ESI) calcd for $C_{21}H_{14}{}^{79}BrO_2Se^+$ [M + H^+] 456.9337, found 456.9340.



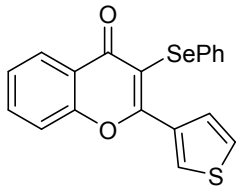
2-(4-Methoxyphenyl)-3-(phenylselanyl)-4*H*-chromen-4-one (2n)

Following the general procedure, **2n** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 367 mg, 90%, a yellow solid, mp. 104-106 ^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.23 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.76 – 7.59 (m, 3H), 7.46 (dd, *J* = 8.5, 1.0 Hz, 1H), 7.39 (ddd, *J* = 8.1, 7.1, 1.1 Hz, 1H), 7.35 – 7.30 (m, 2H), 7.19 – 7.08 (m, 3H), 6.93 (d, *J* = 8.8 Hz, 2H), 3.84 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 176.0, 167.7, 161.6, 155.9, 133.9, 131.6, 131.2, 130.6, 129.1, 126.7, 126.6, 126.4, 125.5, 122.4, 117.8, 113.4, 113.1, 55.5. HRMS (ESI) calcd for $C_{22}H_{17}O_3Se^+$ [M + H^+] 409.0337, found 409.0340.



2-Cyclopropyl-3-(phenylselanyl)-4*H*-chromen-4-one (2o)

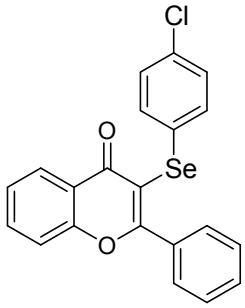
Following the general procedure, **2o** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 310 mg, 91%, a yellow solid, mp. 104-106 ^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.19 (d, *J* = 7.9 Hz, 1H), 7.60 (t, *J* = 7.8 Hz, 1H), 7.44 (d, *J* = 7.2 Hz, 2H), 7.35 (t, *J* = 7.5 Hz, 1H), 7.31 (d, *J* = 8.4 Hz, 1H), 7.18 (dt, *J* = 14.0, 7.0 Hz, 3H), 3.12 – 2.96 (m, 1H), 1.29 (dt, *J* = 7.0, 3.5 Hz, 2H), 1.12 – 1.06 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 174.8, 172.7, 155.1, 133.5, 131.4, 130.6, 129.1, 126.7, 126.6, 125.3, 122.7, 117.2, 112.6, 16.1, 10.0. HRMS (ESI) calcd for $C_{18}H_{15}O_2Se^+$ [M + H^+] 343.0232, found 343.0236.



3-(Phenylselanyl)-2-(thiophen-3-yl)-4H-chromen-4-one (2p)

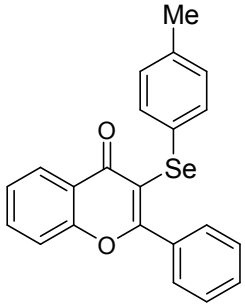
Following the general procedure, **2p** was purified by silica gel chromatography

(EtOAc/PE = 5/95). Yield: 307 mg, 80%, a yellow solid, mp. 118-120 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.23 (dd, *J* = 8.0, 1.6 Hz, 1H), 8.18 (dd, *J* = 3.0, 1.3 Hz, 1H), 7.72 (dd, *J* = 5.1, 1.3 Hz, 1H), 7.68 (ddd, *J* = 8.6, 7.1, 1.6 Hz, 1H), 7.49 (d, *J* = 8.4 Hz, 1H), 7.41 (t, *J* = 7.3 Hz, 1H), 7.38 – 7.33 (m, 3H), 7.21 – 7.08 (m, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 176.0, 162.6, 155.7, 134.6, 134.0, 131.4, 130.8, 130.4, 129.2, 128.5, 126.8, 126.7, 125.6, 125.3, 122.3, 117.7, 112.7. HRMS (ESI) calcd for $C_{19}H_{13}O_2SSe^+$ [M + H^+] 384.9796, found 384.9792.



3-((4-Chlorophenyl)selanyl)-2-phenyl-4*H*-chromen-4-one (2q)

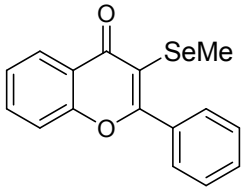
Following the general procedure, **2q** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 362 mg, 88%, a yellow solid, mp. 180-182 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.25 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.70 (ddd, *J* = 8.6, 7.1, 1.7 Hz, 1H), 7.68 – 7.62 (m, 2H), 7.55 – 7.34 (m, 5H), 7.25 (d, *J* = 8.0 Hz, 2H), 7.15 – 7.07 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 175.8, 167.8, 156.0, 134.1, 134.1, 133.0, 132.6, 130.9, 129.4, 129.2, 129.2, 128.1, 126.7, 125.7, 122.4, 117.9, 114.1. HRMS (ESI) calcd for $C_{21}H_{14}{}^{35}ClO_2Se^+$ [M + H^+] 412.9842, found 412.9850.



2-Phenyl-3-(p-tolylselanyl)-4*H*-chromen-4-one (2r)

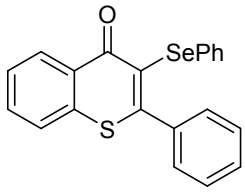
Following the general procedure, **2r** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 376 mg, 96%, a yellow solid, mp. 104-106 °C. 1H NMR (600 MHz, $CDCl_3$) δ 8.25 (dd, J = 8.0, 1.7 Hz, 1H), 7.73 – 7.64 (m, 3H), 7.52 – 7.37

(m, 5H), 7.24 (d, J = 7.8 Hz, 2H), 6.95 (d, J = 7.9 Hz, 2H), 2.24 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 176.0, 167.5, 156.0, 136.8, 134.3, 133.9, 131.6, 130.7, 129.9, 129.3, 128.0, 127.5, 126.7, 125.5, 122.5, 117.9, 114.5, 21.1. HRMS (ESI) calcd for $C_{22}H_{17}O_2Se^+$ [M + H^+] 393.0388, found 393.0384.



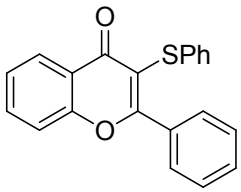
3-(Methylselanyl)-2-phenyl-4*H*-chromen-4-one (2s)

Following the general procedure, **2s** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 300 mg, 95%, yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (dd, J = 8.0, 1.7 Hz, 1H), 7.76 – 7.70 (m, 2H), 7.67 (ddd, J = 8.6, 7.1, 1.7 Hz, 1H), 7.57 – 7.49 (m, 3H), 7.48 – 7.39 (m, 2H), 2.19 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.4, 165.1, 155.9, 134.3, 133.8, 130.8, 129.4, 128.1, 126.3, 125.4, 122.1, 117.9, 113.5, 8.2. HRMS (ESI) calcd for $C_{16}H_{13}O_2Se^+$ [M + H^+] 317.0075, found 317.0080.



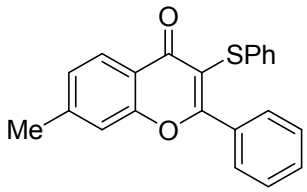
2-Phenyl-3-(phenylselanyl)-4*H*-thiochromen-4-one (2t)

Following the general procedure, **2t** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 267 mg, 67%, a yellow solid, mp. 118-120 ^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.55 (d, J = 8.1 Hz, 1H), 7.62 (t, J = 7.5 Hz, 1H), 7.56 (d, J = 8.4 Hz, 2H), 7.39 (t, J = 7.0 Hz, 1H), 7.33 (p, J = 7.1, 6.5 Hz, 4H), 7.20 (d, J = 7.4 Hz, 2H), 7.08 (dd, J = 13.2, 7.0 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 178.1, 155.9, 138.1, 137.2, 132.0, 132.0, 131.6, 129.8, 129.8, 129.6, 128.8, 128.5, 128.3, 128.2, 128.1, 126.6, 125.5. HRMS (ESI) calcd for $C_{21}H_{15}OSSe^+$ [M + H^+] 395.0003, found 395.0010.



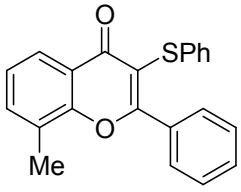
2-Phenyl-3-(phenylthio)-4*H*-chromen-4-one (3a)

Following the general procedure, **3a** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 238 mg, 72%, a yellow solid, mp. 127-129 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.80 – 7.75 (m, 2H), 7.74 – 7.67 (m, 1H), 7.55 – 7.48 (m, 2H), 7.50 – 7.40 (m, 3H), 7.23 – 7.18 (m, 4H), 7.15 – 7.07 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.9, 168.7, 155.9, 136.2, 134.1, 133.1, 131.1, 129.2, 129.0, 128.1, 127.3, 126.7, 125.9, 125.7, 122.8, 118.0, 115.2. HRMS (ESI) calcd for $C_{21}H_{15}O_2S^+$ [M + H^+] 331.0787, found 331.0790.



7-Methyl-2-phenyl-3-(phenylthio)-4*H*-chromen-4-one (3b)

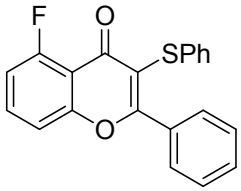
Following the general procedure, **3b** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 245 mg, 82%, a yellow solid, mp. 157-159 ^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.1 Hz, 1H), 7.78 – 7.72 (m, 2H), 7.52 – 7.48 (m, 1H), 7.45 (dd, *J* = 8.3, 6.7 Hz, 2H), 7.31 (s, 1H), 7.24 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.21 – 7.16 (m, 4H), 7.10 (dq, *J* = 5.5, 2.8 Hz, 1H), 2.49 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 175.7, 168.5, 156.0, 145.6, 136.4, 133.2, 131.0, 129.2, 128.9, 128.1, 127.2, 126.4, 125.8, 120.6, 117.8, 115.2, 115.0, 21.9. HRMS (ESI) calcd for $C_{22}H_{17}O_2S^+$ [M + H^+] 345.0944, found 345.0948.



8-Methyl-2-phenyl-3-(phenylthio)-4*H*-chromen-4-one (3c)

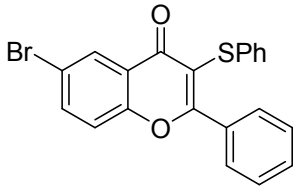
Following the general procedure, **3c** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 245 mg, 71%, a yellow solid, mp. 156-158 ^{o}C. ^{1}H NMR

(600 MHz, $CDCl_3$) δ 8.09 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.88 – 7.77 (m, 2H), 7.56 – 7.50 (m, 2H), 7.49 – 7.44 (m, 2H), 7.32 (t, *J* = 7.6 Hz, 1H), 7.23 – 7.16 (m, 4H), 7.13 – 7.07 (m, 1H), 2.51 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 176.2, 168.2, 154.4, 136.3, 135.0, 133.2, 131.0, 129.3, 128.9, 128.2, 127.5, 127.3, 125.8, 125.3, 124.3, 122.7, 114.9, 15.6. HRMS (ESI) calcd for $C_{22}H_{17}O_2S^+$ [M + H^+] 345.0944, found 345.0946.



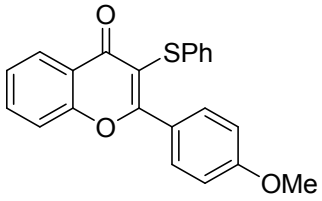
5-Fluoro-2-phenyl-3-(phenylthio)-4*H*-chromen-4-one (3d)

Following the general procedure, **3d** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 254 mg, 73%, a yellow solid, mp. 134-136 °C. ^1H NMR (600 MHz, $CDCl_3$) δ 7.80 – 7.75 (m, 2H), 7.62 (td, *J* = 8.4, 5.4 Hz, 1H), 7.56 – 7.50 (m, 1H), 7.49 – 7.44 (m, 2H), 7.31 (dt, *J* = 8.5, 1.0 Hz, 1H), 7.24 – 7.18 (m, 4H), 7.15 – 7.09 (m, 1H), 7.08 (ddd, *J* = 10.2, 8.2, 1.0 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 173.7, 167.6, 161.6, 159.8, 156.8, 135.8, 134.1 (d, *J* = 10.5 Hz), 132.6, 131.2, 129.2, 129.0, 128.2, 127.8, 126.1, 116.5, 113.9 (d, *J* = 4.5 Hz), 113.4 (d, *J* = 10.5 Hz), 112.5 (d, *J* = 19.5 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -110.1. HRMS (ESI) calcd for $C_{21}H_{14}FO_2S^+$ [M + H^+] 349.0693, found 349.0696.



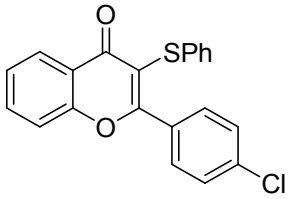
6-Bromo-2-phenyl-3-(phenylthio)-4*H*-chromen-4-one (3e)

Following the general procedure, **3e** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 332 mg, 81%, a yellow solid, mp. 120-122 °C. ^1H NMR (600 MHz, $CDCl_3$) δ 8.35 (d, *J* = 2.4 Hz, 1H), 7.79 – 7.70 (m, 3H), 7.55 – 7.48 (m, 1H), 7.46 (tt, *J* = 6.6, 1.5 Hz, 2H), 7.40 (d, *J* = 8.8 Hz, 1H), 7.23 – 7.16 (m, 4H), 7.14 – 7.07 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 174.6, 168.7, 154.6, 137.1, 135.8, 132.7, 131.3, 129.2, 129.2, 129.0, 128.2, 127.6, 126.1, 124.1, 120.0, 119.1, 115.7. HRMS (ESI) calcd for $C_{21}H_{14}{}^{79}BrO_2S^+$ [M + H^+] 408.9892, found 408.9896.



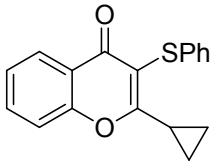
2-(4-Methoxyphenyl)-3-(phenylthio)-4*H*-chromen-4-one (3f)

Following the general procedure, **3f** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 252 mg, 70%, a yellow solid, mp. 100-102 ^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.24 (d, *J* = 7.9 Hz, 1H), 7.80 (d, *J* = 8.8 Hz, 2H), 7.70 (t, *J* = 7.8 Hz, 1H), 7.51 (d, *J* = 8.4 Hz, 1H), 7.42 (t, *J* = 7.1 Hz, 1H), 7.23 – 7.17 (m, 4H), 7.11 (dt, *J* = 8.6, 2.8 Hz, 1H), 6.96 (d, *J* = 8.1 Hz, 2H), 3.86 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 175.92, 168.47, 161.89, 155.81, 136.47, 133.96, 131.19, 128.96, 127.03, 126.65, 125.73, 125.57, 125.28, 122.79, 117.91, 114.03, 113.54, 55.44. HRMS (ESI) calcd for $C_{22}H_{17}O_3S^+$ [M + H^+] 361.0893, found 361.0896.



2-(4-Chlorophenyl)-3-(phenylthio)-4*H*-chromen-4-one (3g)

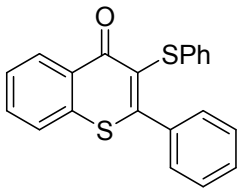
Following the general procedure, **3g** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 223 mg, 61%, a yellow solid, mp. 118-120 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.76 – 7.67 (m, 3H), 7.51 (dd, *J* = 8.4, 0.9 Hz, 1H), 7.49 – 7.37 (m, 3H), 7.24 – 7.18 (m, 4H), 7.16 – 7.09 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.7, 167.4, 155.8, 137.3, 135.9, 134.3, 131.4, 130.6, 129.1, 128.5, 127.2, 126.7, 126.0, 125.9, 122.8, 118.0, 115.4. HRMS (ESI) calcd for $C_{21}H_{14}{}^{35}ClO_2S^+$ [M + H^+] 365.0398, found 365.0394.



2-Cyclopropyl-3-(phenylthio)-4*H*-chromen-4-one (3h)

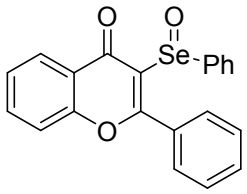
Following the general procedure, **3h** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 235 mg, 80%, a yellow solid, mp. 102-104 ^{o}C. ^{1}H NMR

(400 MHz, $CDCl_3$) δ 8.19 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.63 (ddd, *J* = 8.7, 7.2, 1.7 Hz, 1H), 7.41 – 7.31 (m, 2H), 7.31 – 7.26 (m, 2H), 7.26 – 7.19 (m, 2H), 7.16 – 7.08 (m, 1H), 3.05 (tt, *J* = 8.3, 5.0 Hz, 1H), 1.42 – 1.28 (m, 2H), 1.15 (dt, *J* = 8.3, 3.5 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.8, 174.1, 155.0, 136.1, 133.6, 128.9, 127.3, 126.7, 125.8, 125.4, 123.0, 117.3, 113.7, 14.1, 10.0. HRMS (ESI) calcd for $C_{18}H_{15}O_2S^+$ [M + H^+] 295.0787 found 295.0786.



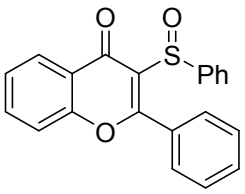
2-Phenyl-3-(phenylthio)-4*H*-thiochromen-4-one (3i)

Following the general procedure, **3i** was purified by silica gel chromatography (EtOAc/PE = 5/95). Yield: 191 mg, 55%, a yellow solid, mp. 140-142 °C. ^1H NMR (600 MHz, $CDCl_3$) δ 8.53 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.63 (t, *J* = 7.4 Hz, 1H), 7.60 – 7.52 (m, 2H), 7.47 – 7.35 (m, 5H), 7.13 (ddd, *J* = 13.9, 8.3, 6.6 Hz, 4H), 7.10 – 7.05 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 177.6, 158.1, 136.9, 136.9, 136.6, 131.8, 130.6, 129.9, 129.9, 128.8, 128.5, 128.4, 128.1, 128.0, 125.8, 125.7. HRMS (ESI) calcd for $C_{21}H_{15}OS_2^+$ [M + H^+] 347.0559, found 347.0562.



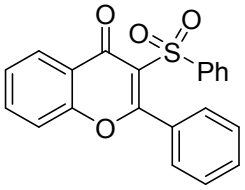
2-Phenyl-3-(phenylseleninyl)-4*H*-chromen-4-one (4)

Following the general procedure, **4** was purified by silica gel chromatography (EtOAc/PE = 40/60). Yield: 354 mg, 90%, a yellow solid, mp. 156-158 °C. ^1H NMR (600 MHz, $CDCl_3$) δ 8.21 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.76 – 7.69 (m, 3H), 7.60 (dd, J = 5.1, 3.3 Hz, 2H), 7.58 – 7.54 (m, 1H), 7.50 – 7.44 (m, 4H), 7.43 – 7.38 (m, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 176.0, 168.8, 156.1, 141.1, 134.7, 131.9, 130.6, 130.1, 129.8, 129.2, 128.1, 126.5, 126.2, 126.1, 125.1, 123.3, 118.2. HRMS (ESI) calcd for $C_{21}H_{15}O_3Se^+$ [M + H^+] 395.0181, found 395.0184.



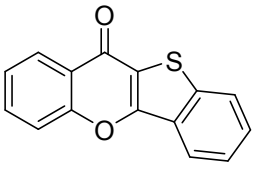
2-Phenyl-3-(phenylsulfinyl)-4*H*-chromen-4-one (5)

Following the general procedure,[2] **5** was purified by silica gel chromatography (EtOAc/PE = 30/70). Yield: 285 mg, 82%, a yellow solid, mp. 206-208 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.13 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.82 (d, *J* = 8.5 Hz, 2H), 7.70 (t, *J* = 7.0 Hz, 1H), 7.67 (d, *J* = 7.3 Hz, 2H), 7.63 (t, *J* = 7.5 Hz, 1H), 7.57 (t, *J* = 7.5 Hz, 2H), 7.50 (d, *J* = 8.3 Hz, 1H), 7.44 (t, *J* = 7.5 Hz, 2H), 7.42 – 7.38 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.96, 169.65, 155.72, 142.95, 134.55, 132.02, 130.84, 130.04, 129.72, 128.70, 128.60, 126.40, 126.14, 125.07, 124.61, 124.32, 118.12. HRMS (ESI) calcd for $C_{21}H_{15}O_3S^+$ [M + H^+] 347.0736, found 347.0740.



2-Phenyl-3-(phenylsulfonyl)-4H-chromen-4-one (7)

Following the general procedure, **7** was purified by silica gel chromatography (EtOAc/PE = 20/80). Yield: 344 mg, 95%, a yellow solid, mp. 220-222 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.12 (d, *J* = 9.5 Hz, 1H), 8.06 (d, *J* = 7.4 Hz, 2H), 7.71 (dd, *J* = 14.8, 8.5 Hz, 3H), 7.64 (t, *J* = 7.5 Hz, 1H), 7.59 – 7.54 (m, 3H), 7.51 – 7.45 (m, 3H), 7.42 (t, *J* = 7.6 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 173.03, 170.08, 155.31, 141.59, 134.82, 133.29, 132.17, 131.58, 129.16, 128.80, 128.46, 128.02, 126.38, 126.26, 124.61, 123.81, 118.10. HRMS (ESI) calcd for $C_{21}H_{15}O_4S^+$ [M + H^+] 363.0686, found 363.0688.



11*H*-Benzo[4,5]thieno[3,2-*b*]chromen-11-one (8)

Following the general procedure,[3] **8** was purified by silica gel chromatography

(EtOAc/PE = 2/98). Yield: 177 mg, 70%, a yellow solid, mp. 201-202 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (d, *J* = 7.9 Hz, 1H), 8.14 (d, *J* = 8.0 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.73 (t, *J* = 8.6 Hz, 1H), 7.64 (d, *J* = 8.4 Hz, 1H), 7.56 (t, *J* = 7.6 Hz, 1H), 7.53 – 7.41 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.39, 156.05, 153.75, 139.96, 133.83, 129.33, 125.99, 125.16, 125.01, 123.81, 122.69, 122.49, 120.78, 118.10. HRMS (ESI) calcd for $C_{15}H_9O_2S^+$ [M + H^+] 253.0318, found 253.0320.

4. Mechanistic Studies

To a solution of PhSeSePh (0.2 mmol) in DCE (10 mL) was added PIFA (0.2 mmol) at rt. The reaction mixture was stirred for 5 min. HRMS analysis of the resulting mixture thus obtained showed some fragmentary peaks including 172.94953 (which was attributed to $PhSeO^-$) and 112.98556 (which was attributed to $CF_3CO_2^-$). The spectra diagrams are shown below.

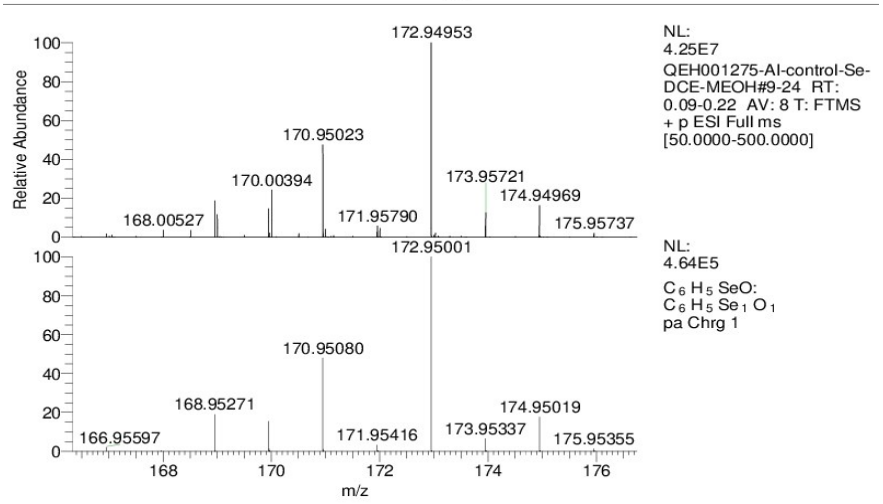


Figure S1 HRMS spectrum of $PhSeO^-$

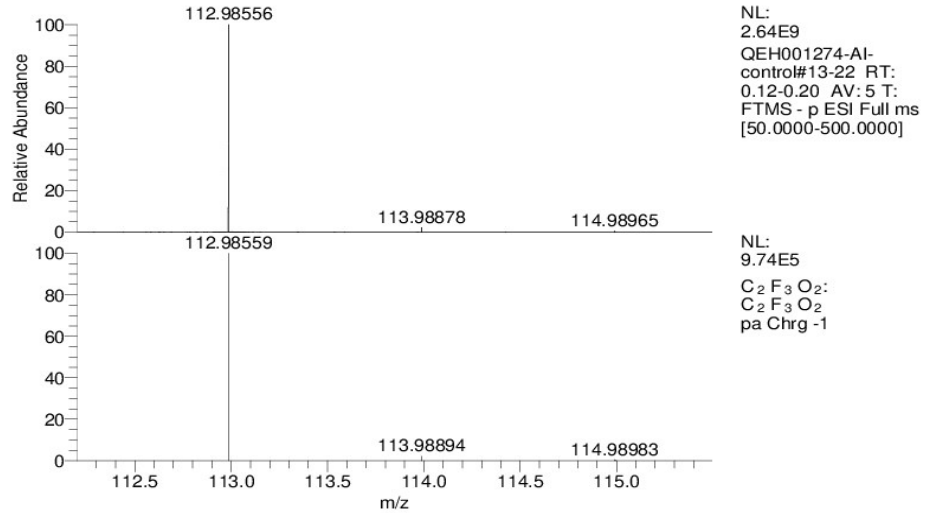


Figure S2 HRMS spectrum of CF_3COO^-

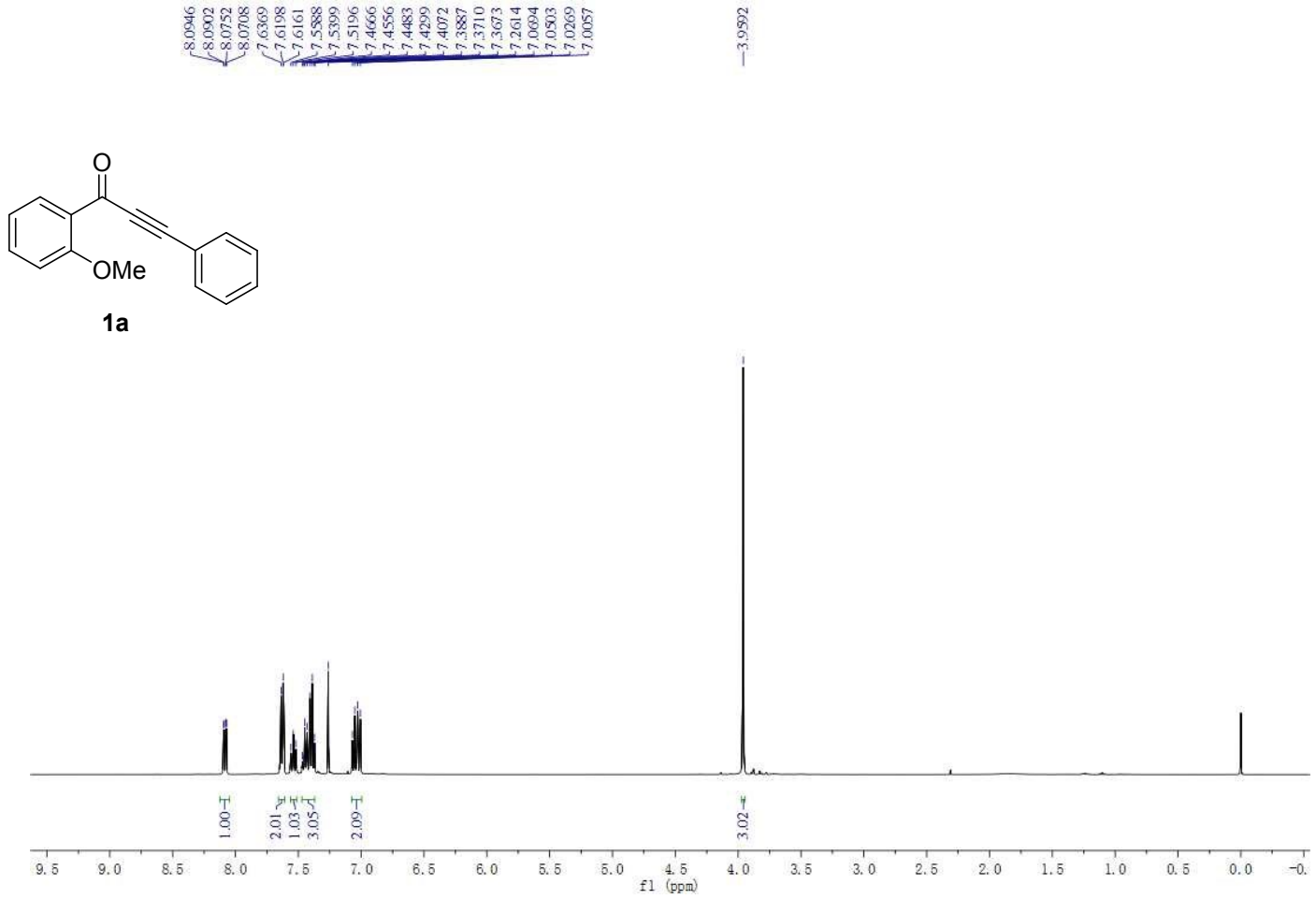
5. References

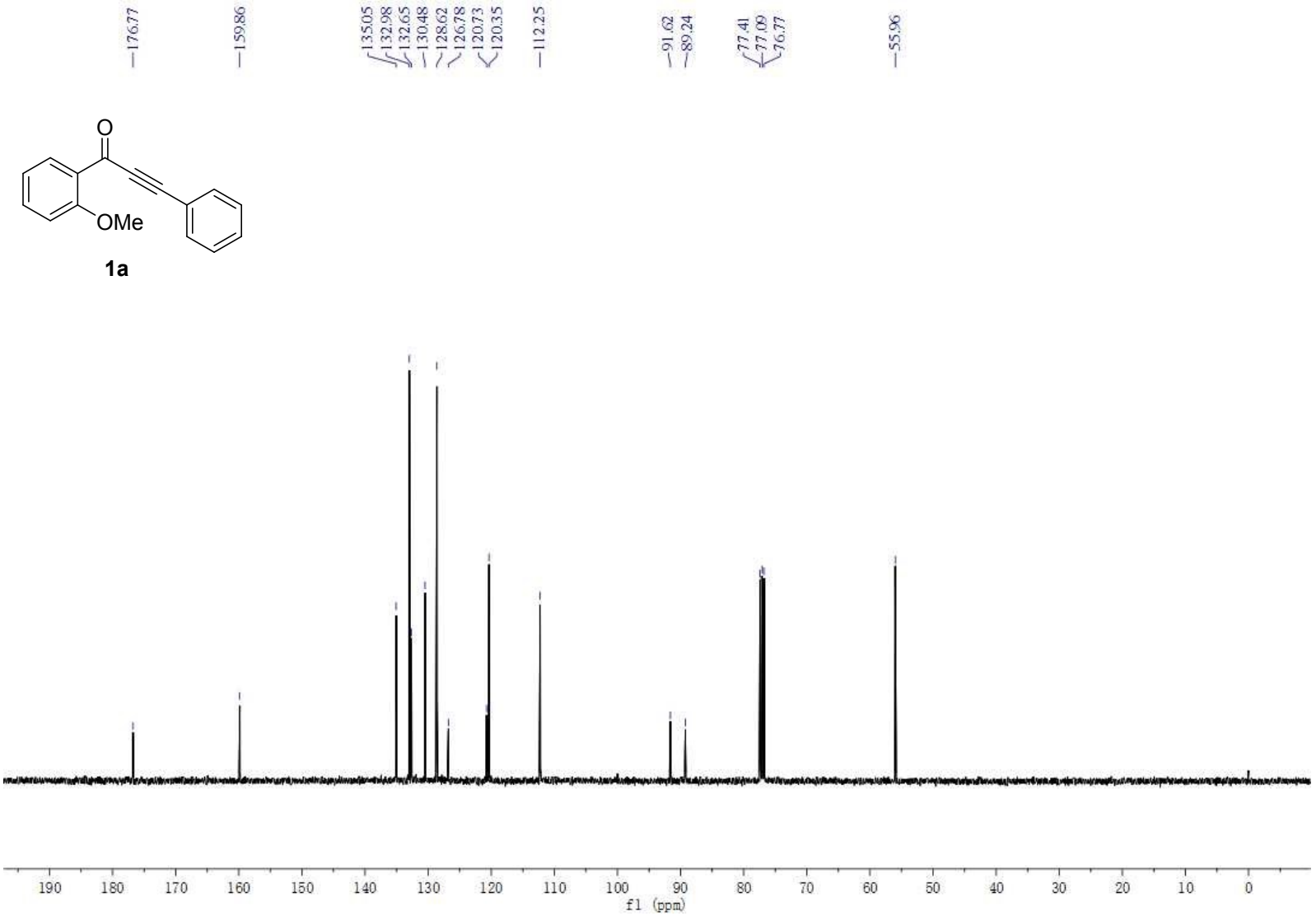
1 (a) A. J. Luxen, L. E. E. Christiaens and M. J. Renson, New synthesis of chalcogenochromones, *J. Organomet. Chem.*, 1985, **287**, 81; (b) J. Liu, W. Wei, T. Zhao, X. Liu, J. Wu, W. Yu and J. Chang, Iodine/Copper Iodide-Mediated C–H functionalization: synthesis of imidazo[1,2-*a*]pyridines and indoles from *N*-aryl enamines, *J. Org. Chem.*, 2016, **81**, 9326.

2 T. Siu and A. K. Yudin, Electrochemical imination of sulfoxides using *N*-aminophthalimide, *Org. Lett.*, 2002, **4**, 1839.

3 M. Tobisu, Y. Masuya, K. Baba and N. Chatani, Palladium(ii)-catalyzed synthesis of dibenzothiophene derivatives via the cleavage of carbon–sulfur and carbon–hydrogen bonds, *Chem. Sci.*, 2016, **7**, 2587.

6. ^{1}H-NMR and ^{13}C-NMR Spectra

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77.09
76.77
55.96
O
OMe
1a
190
180
170
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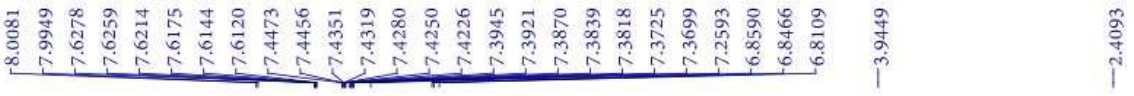
f1 (ppm)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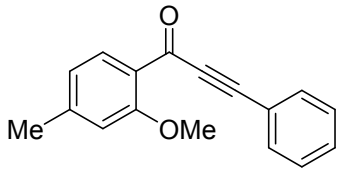
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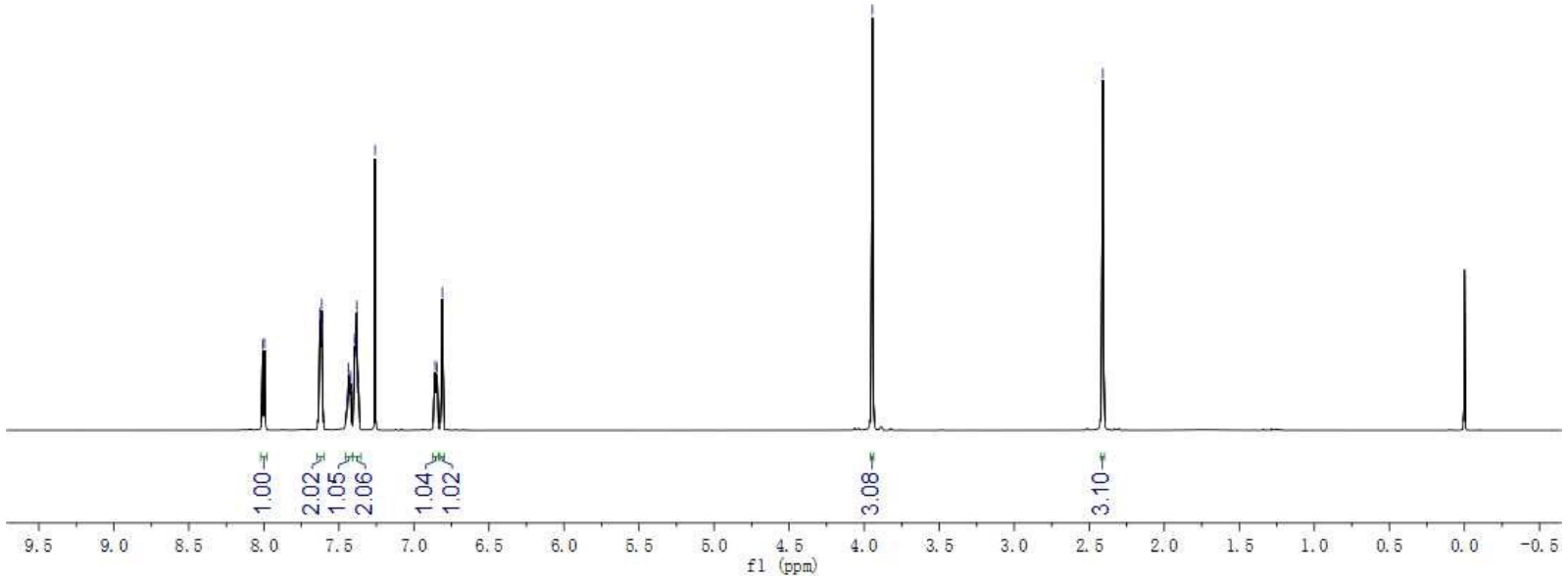
OMe

1b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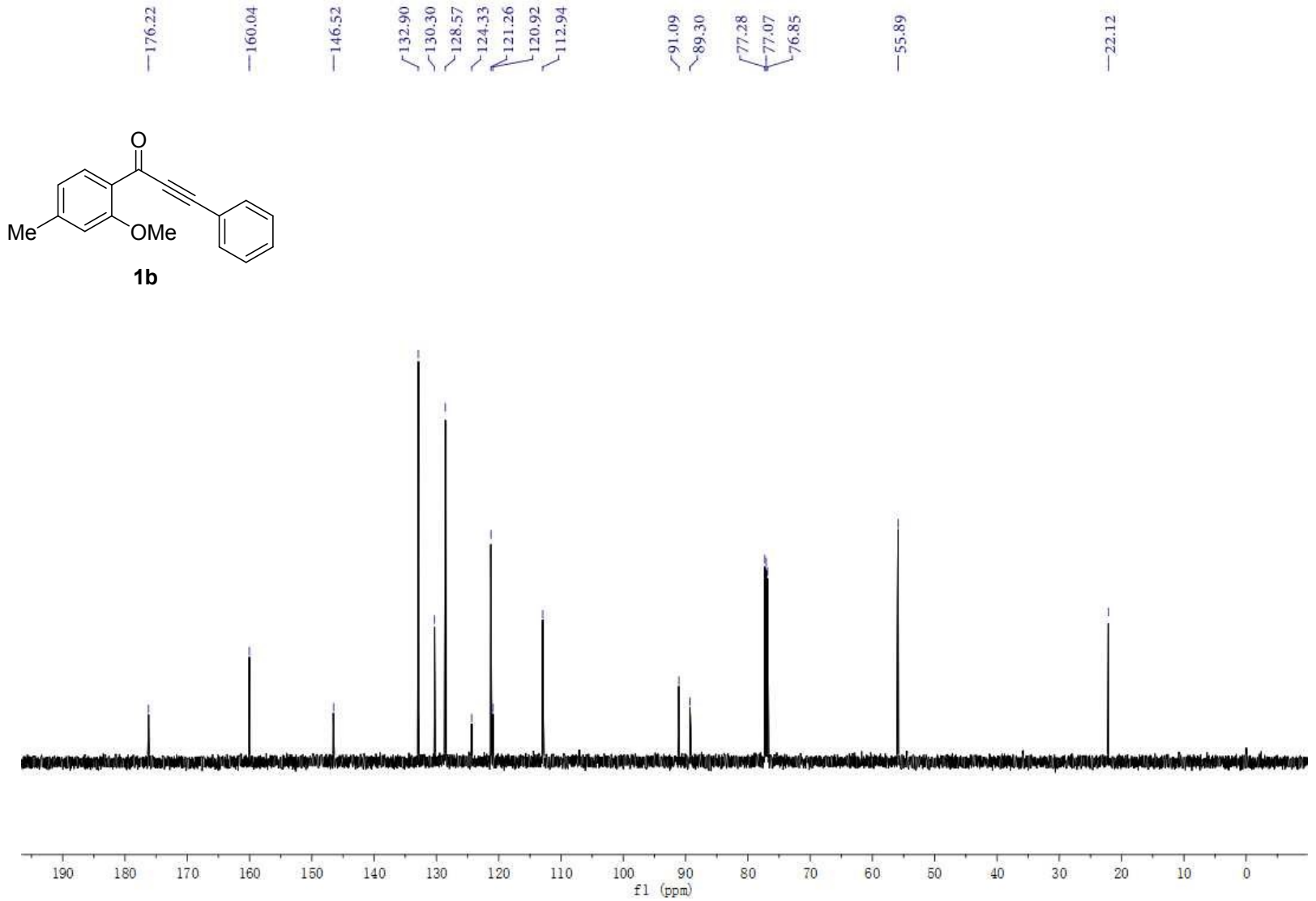
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77.28
77.07
76.85
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22.12
O
Me
OMe
1b
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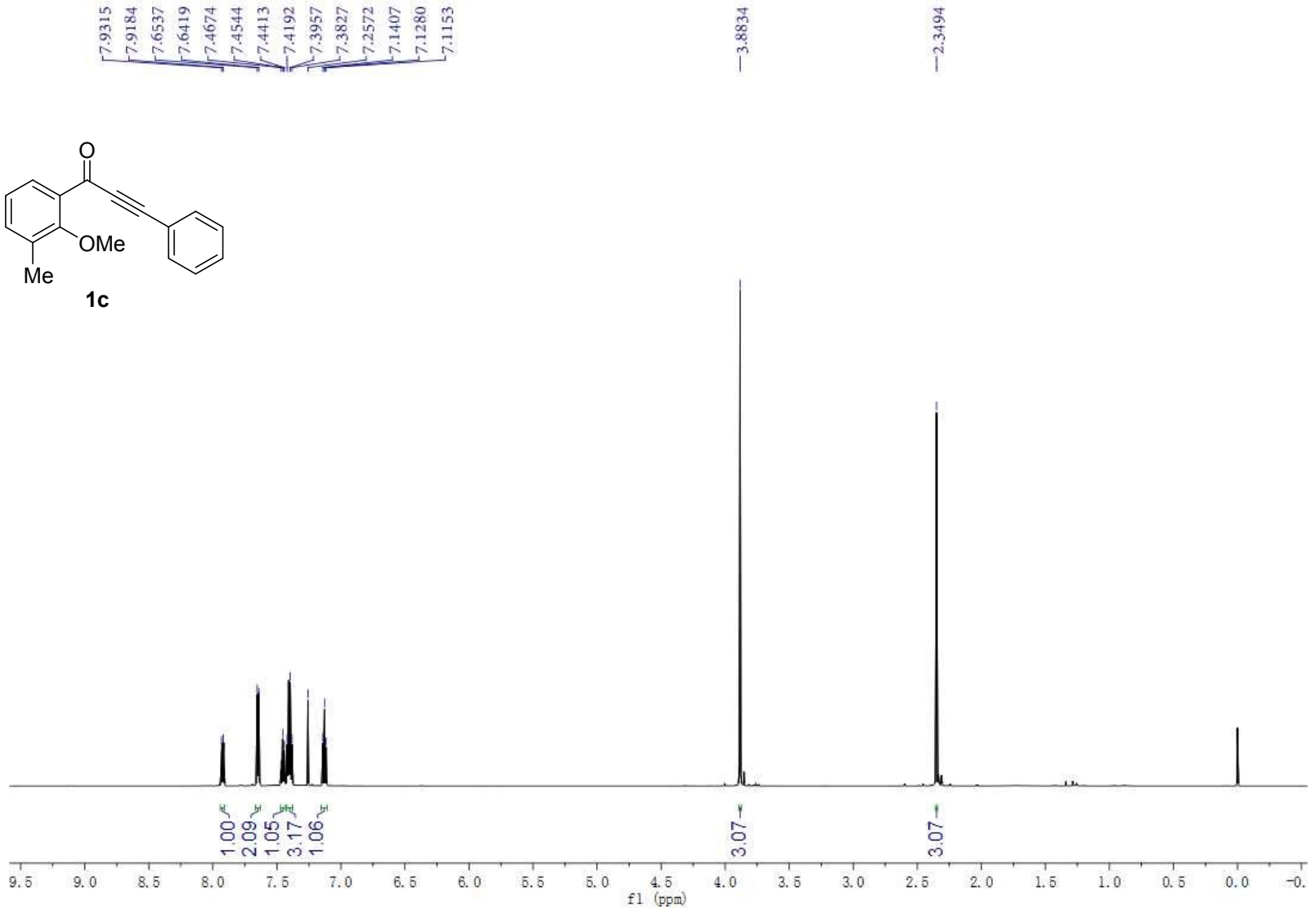
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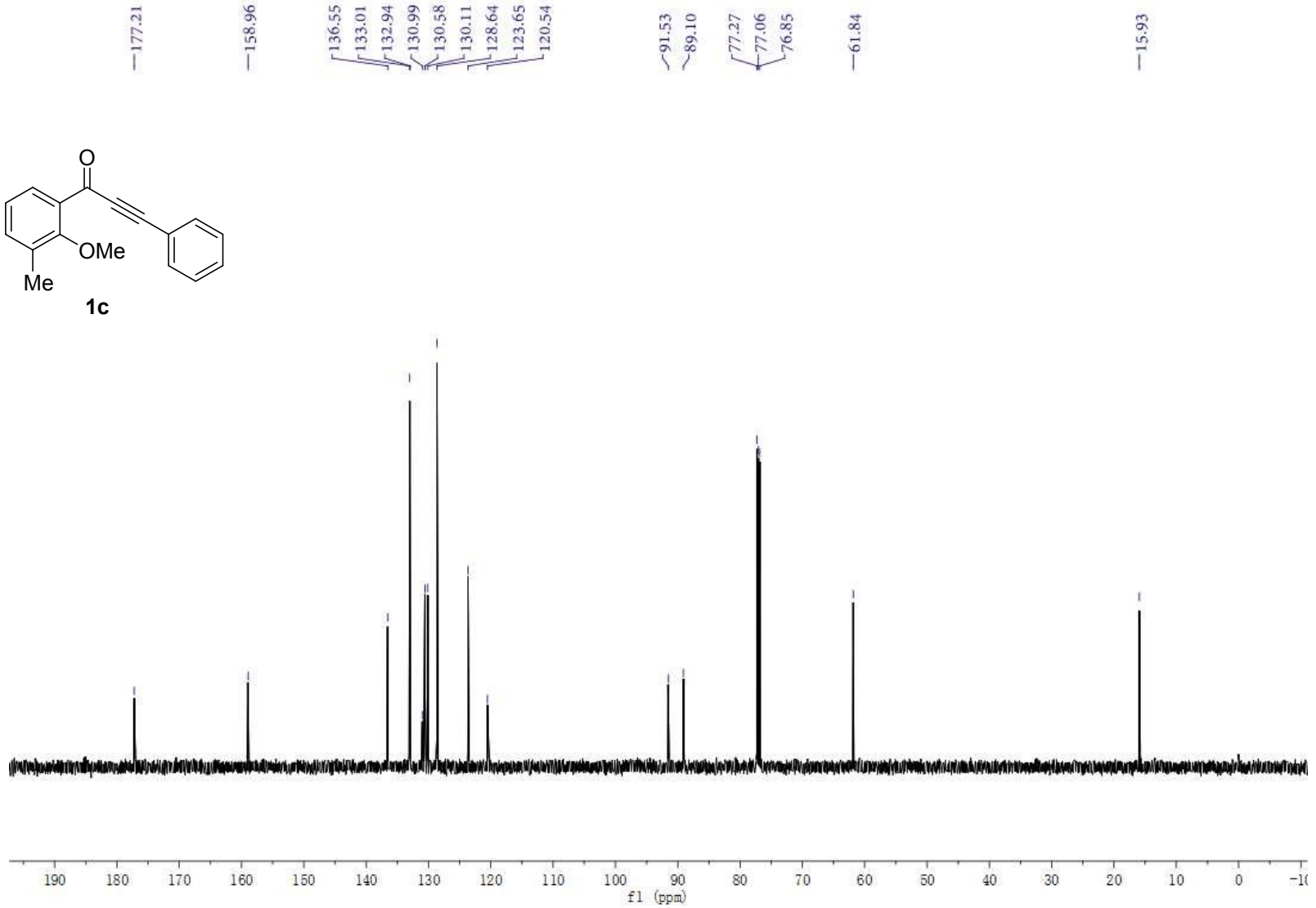
f1 (ppm)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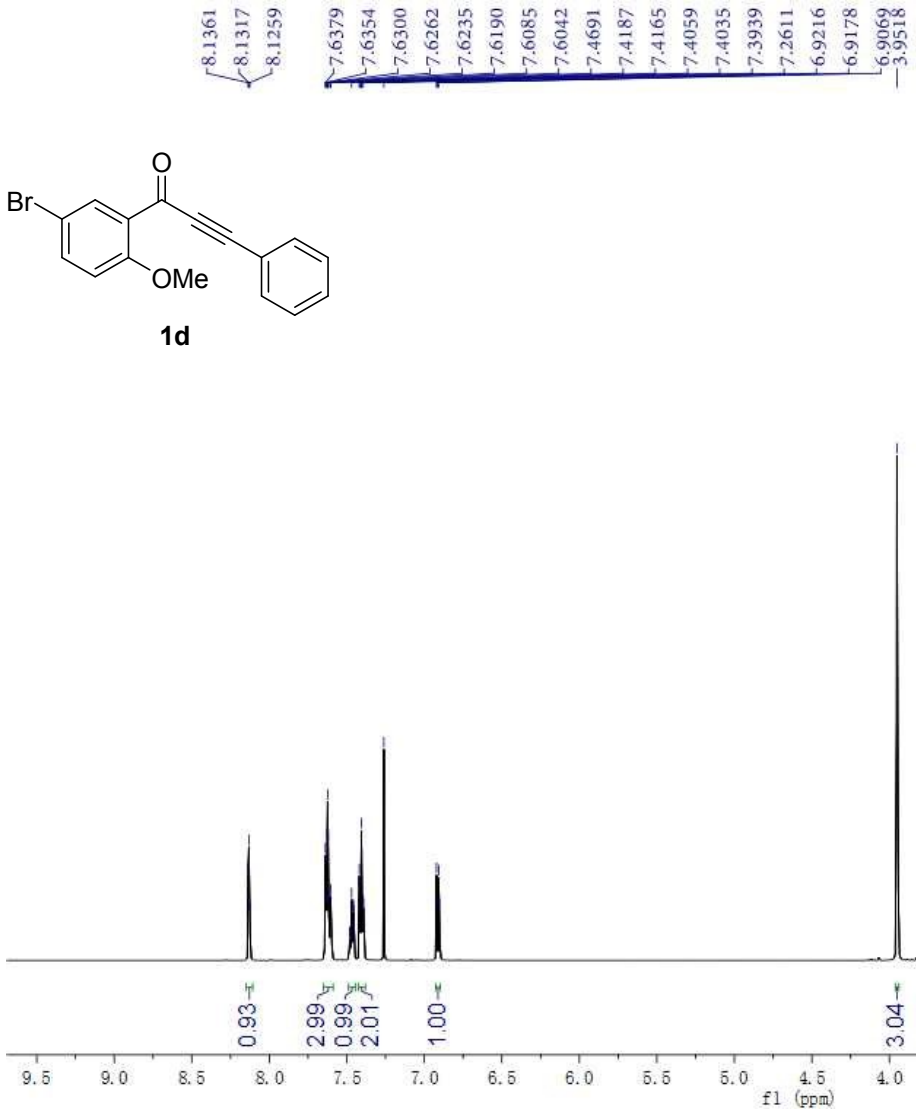
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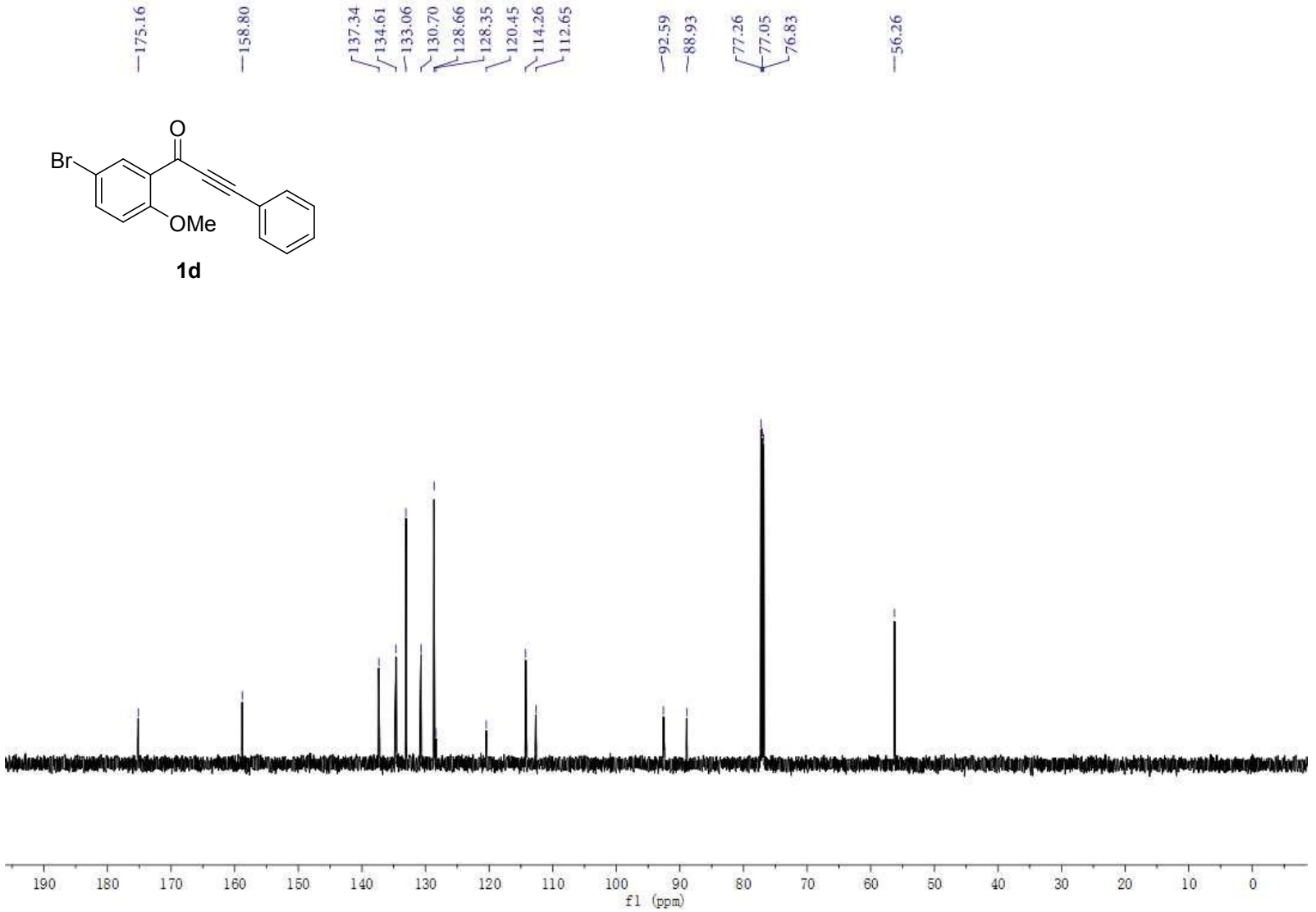
1d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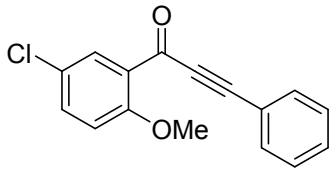
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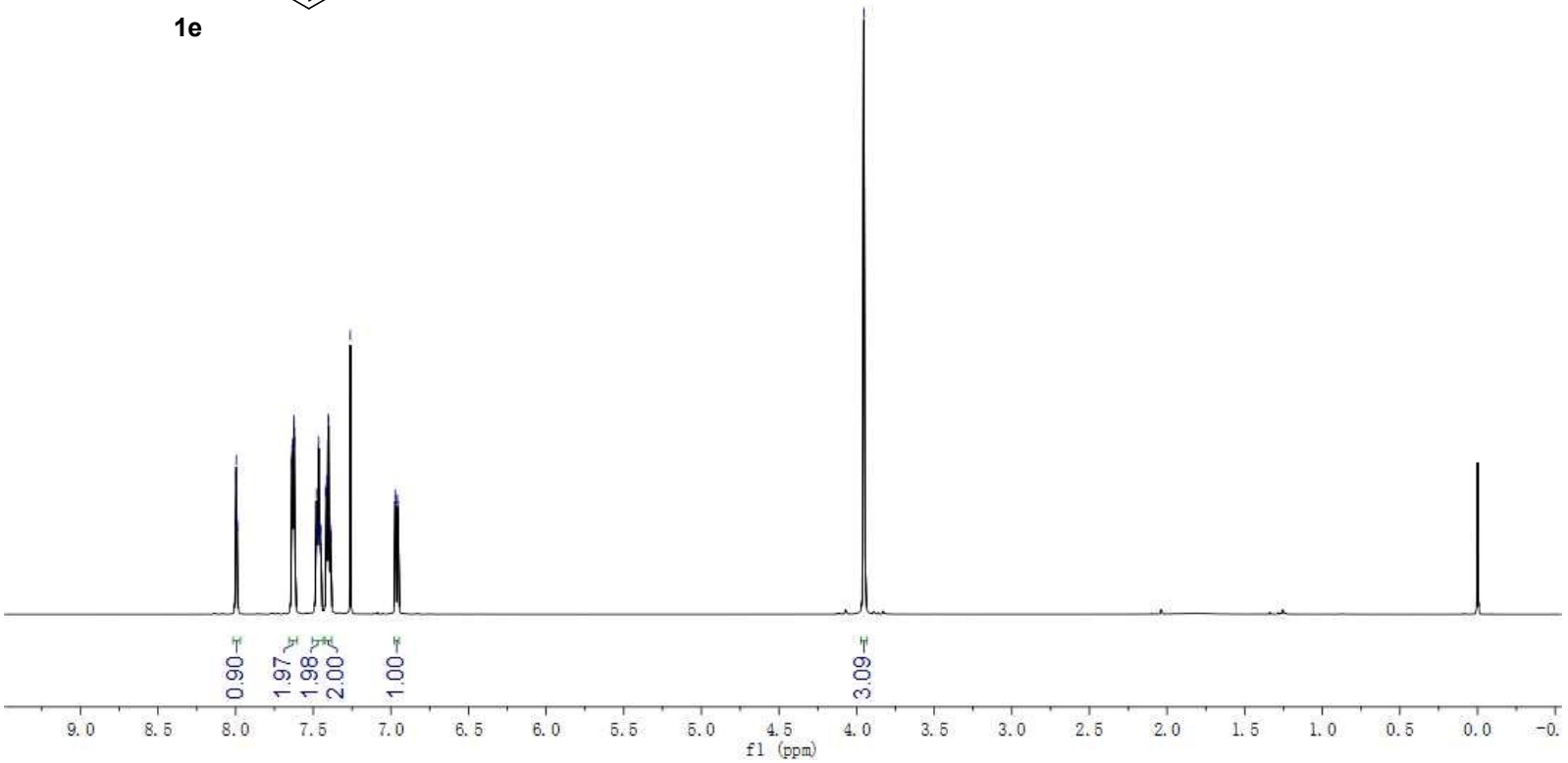
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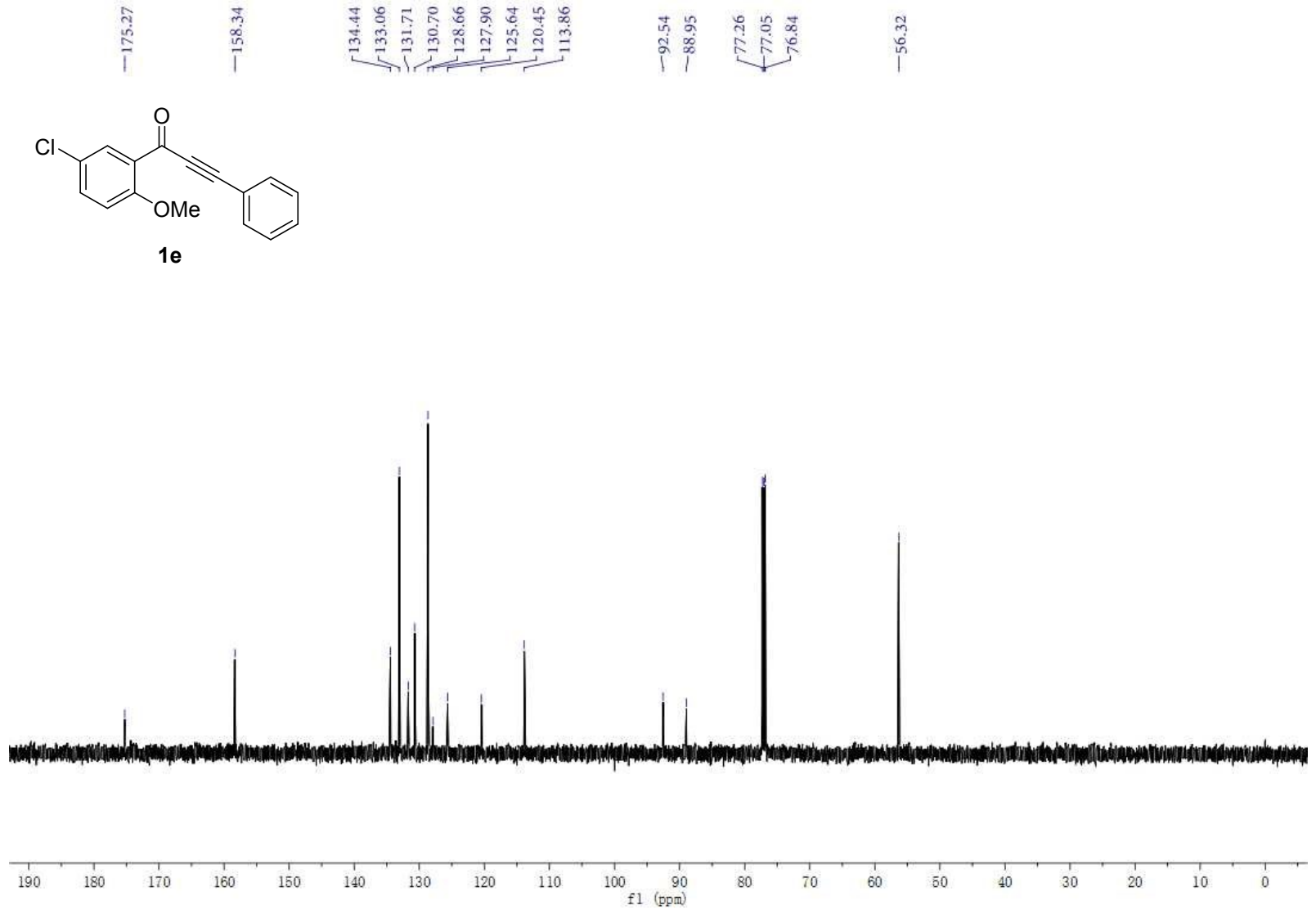
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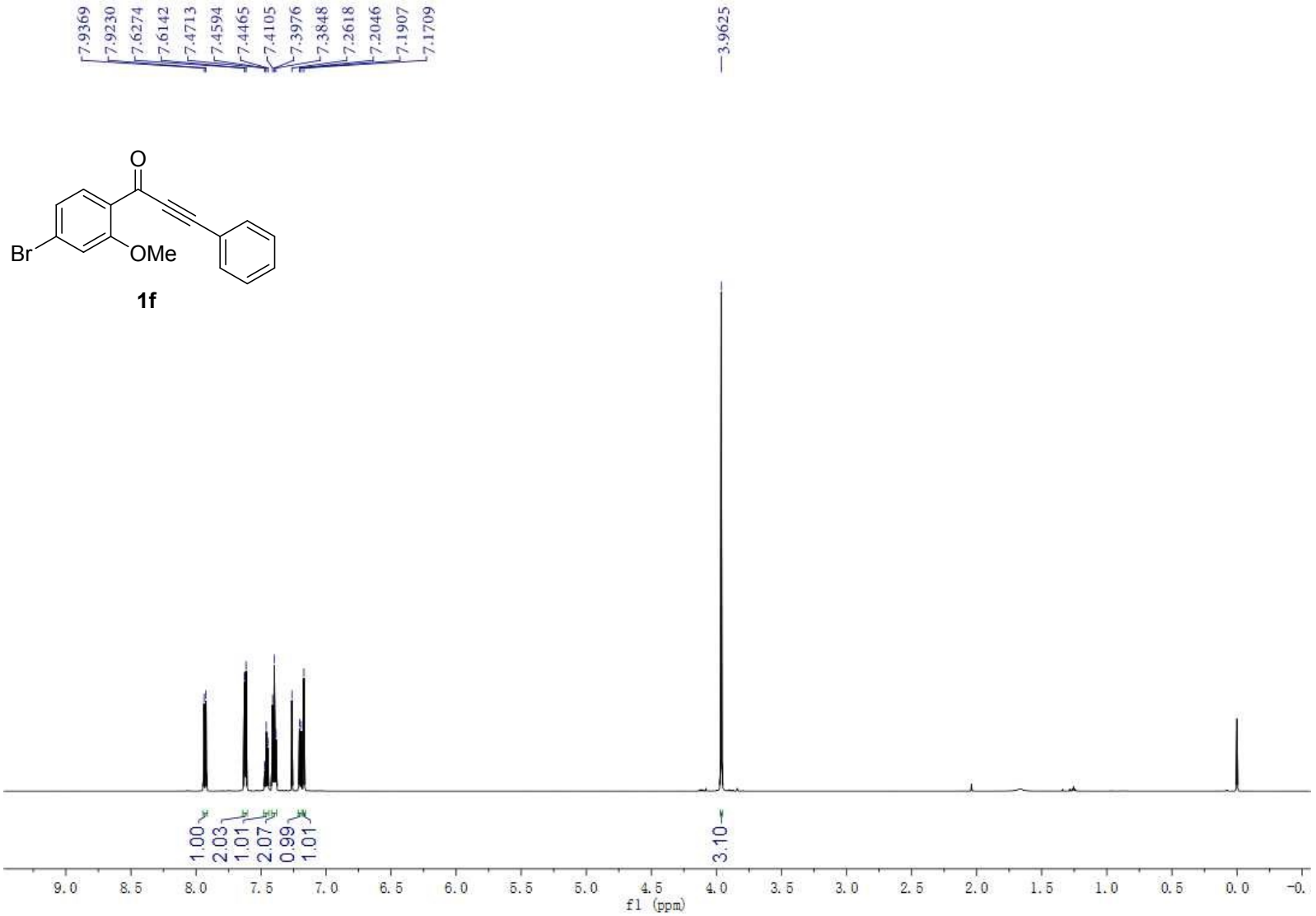
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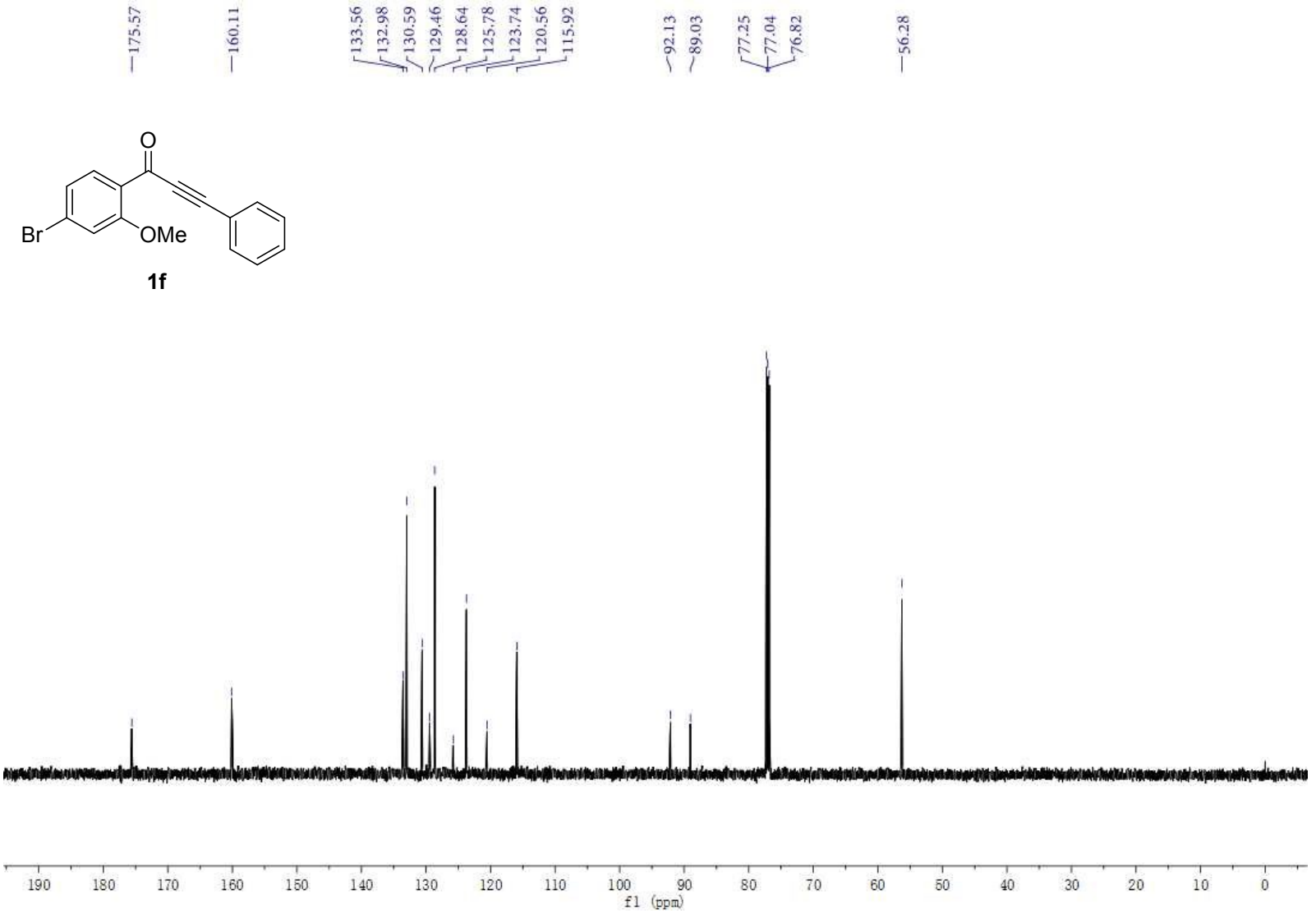
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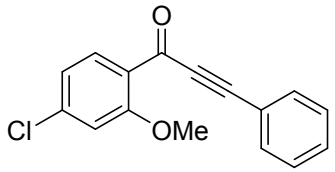
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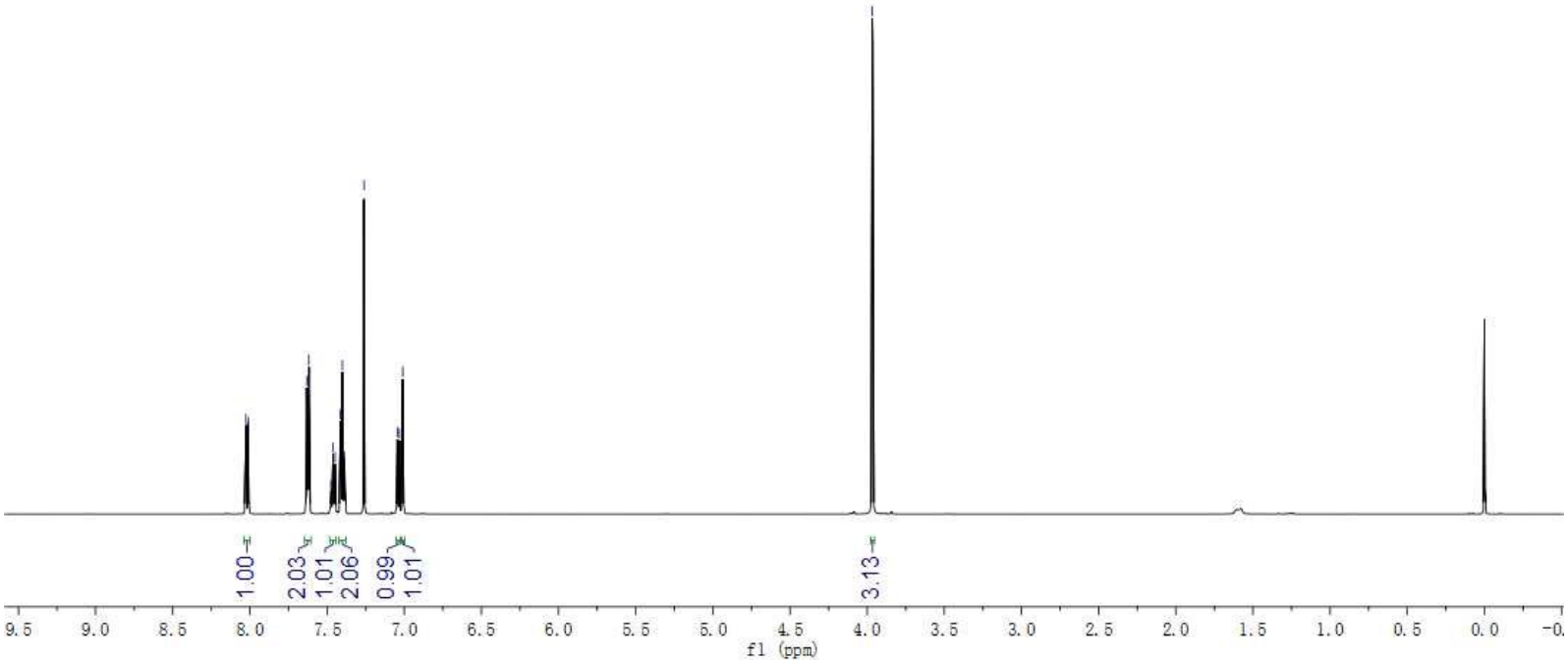
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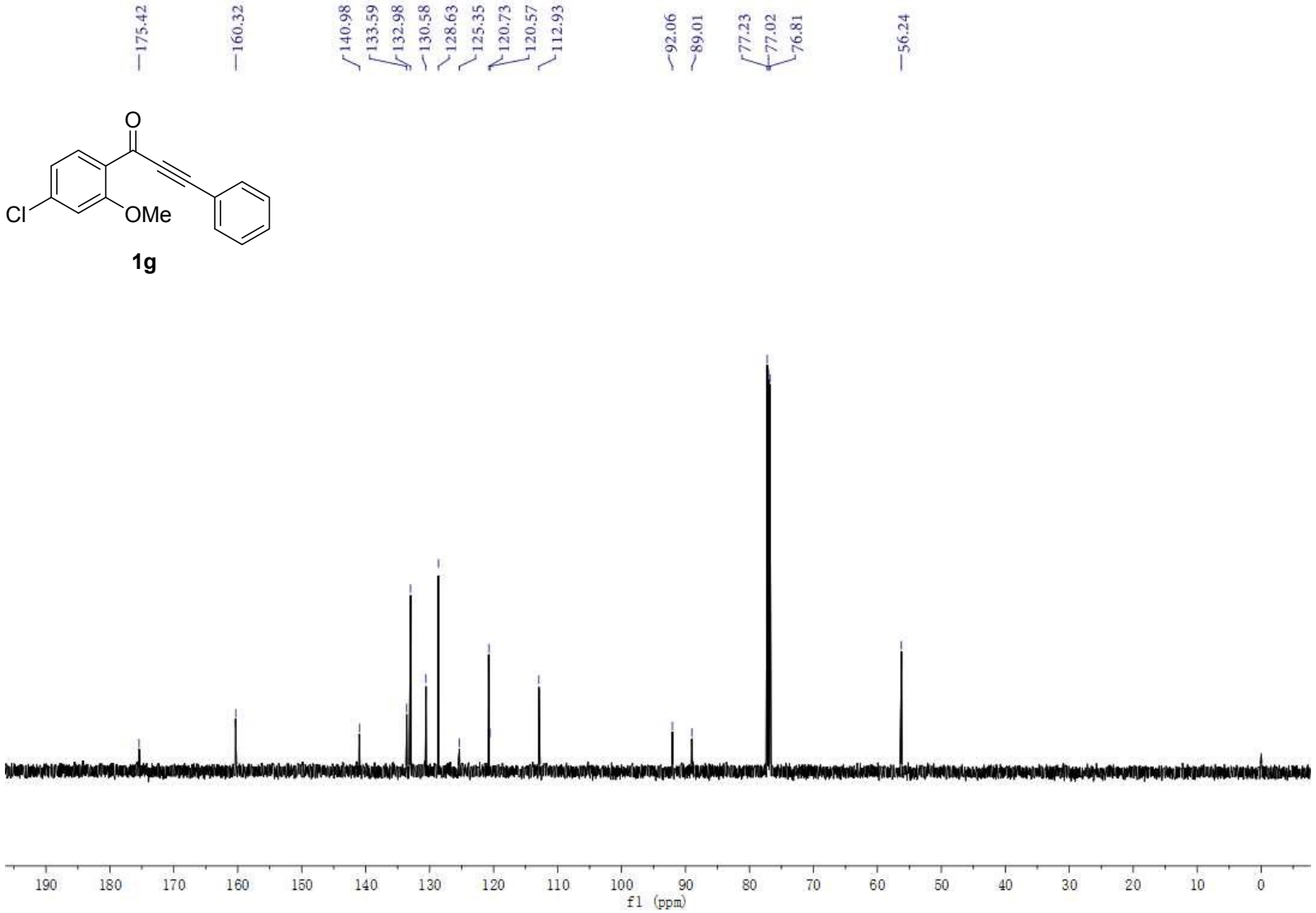
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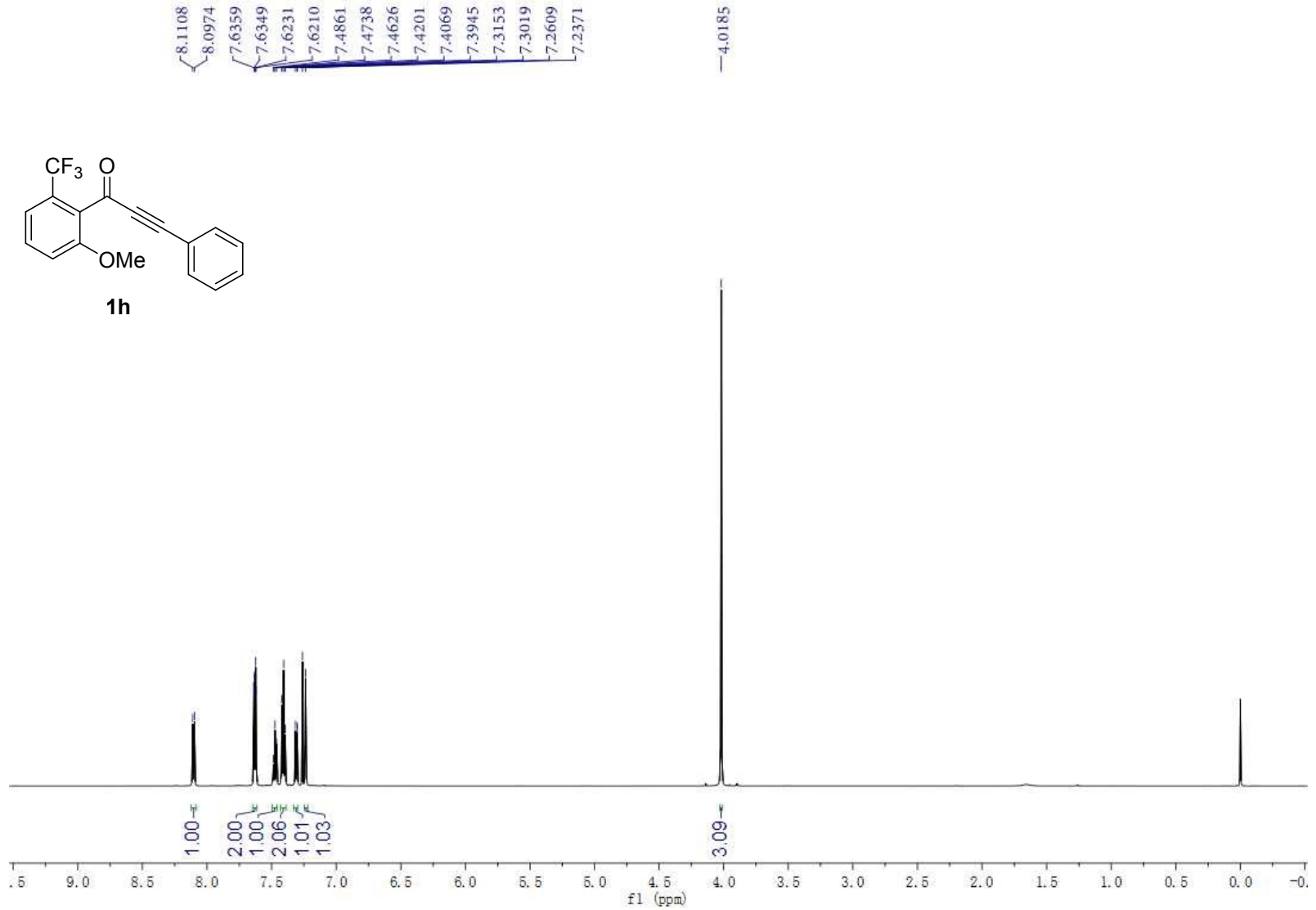
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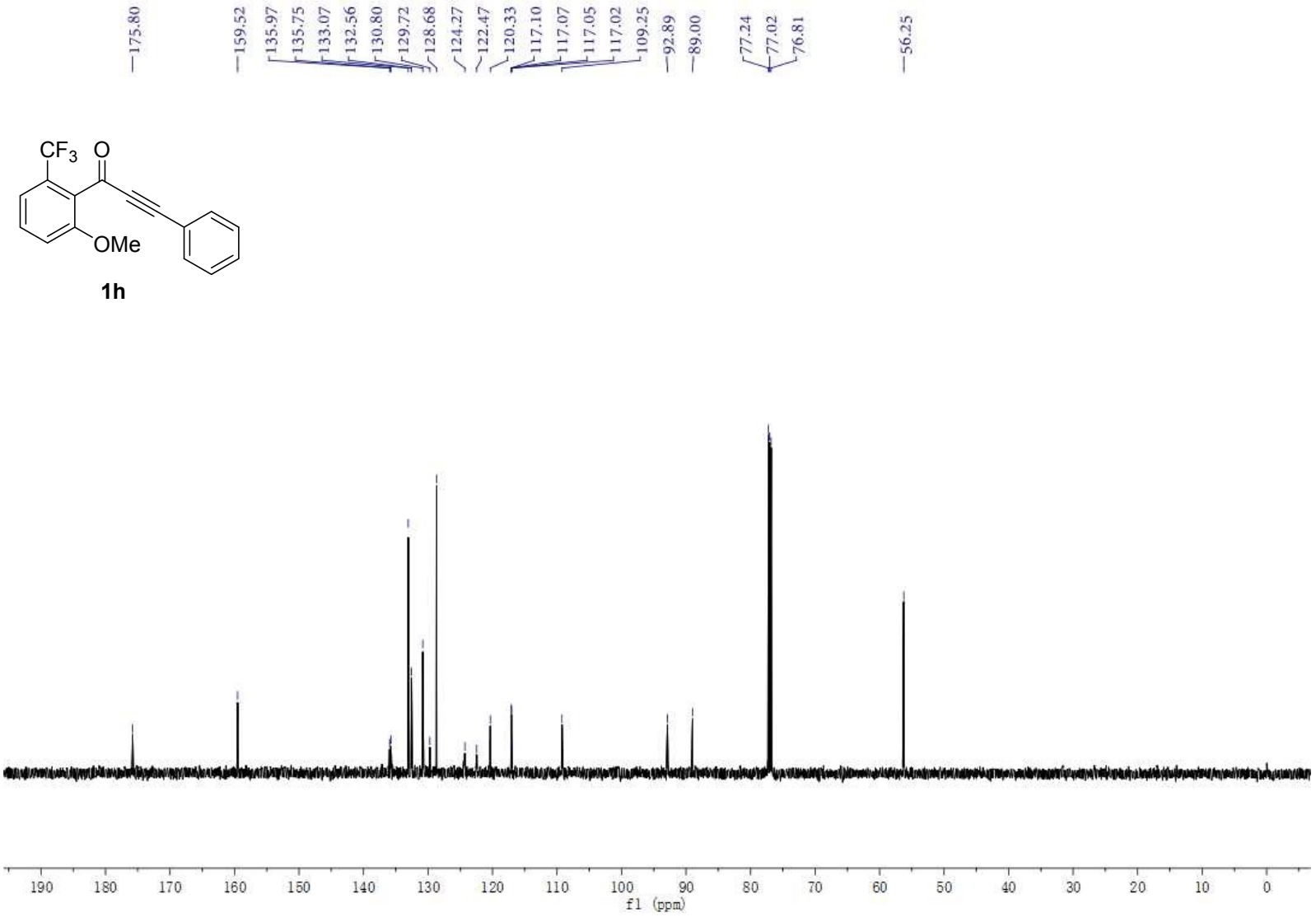
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1h


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7.0112
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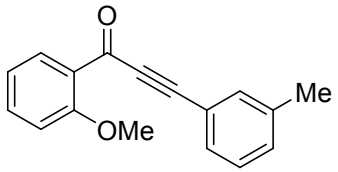
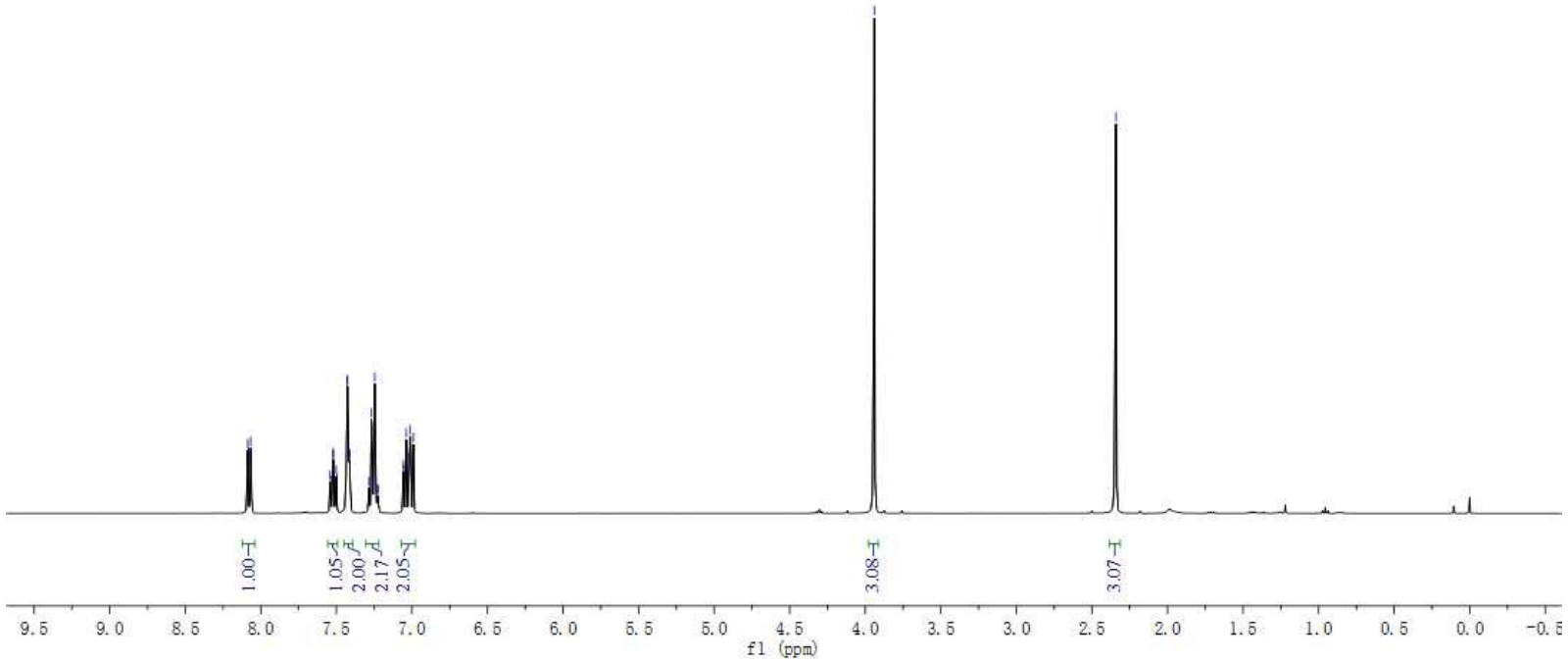
2.3412


O
Me
OMe

1i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3.07
9.5
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8.5
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7.0
6.5
6.0
5.5
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3.5
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2.5
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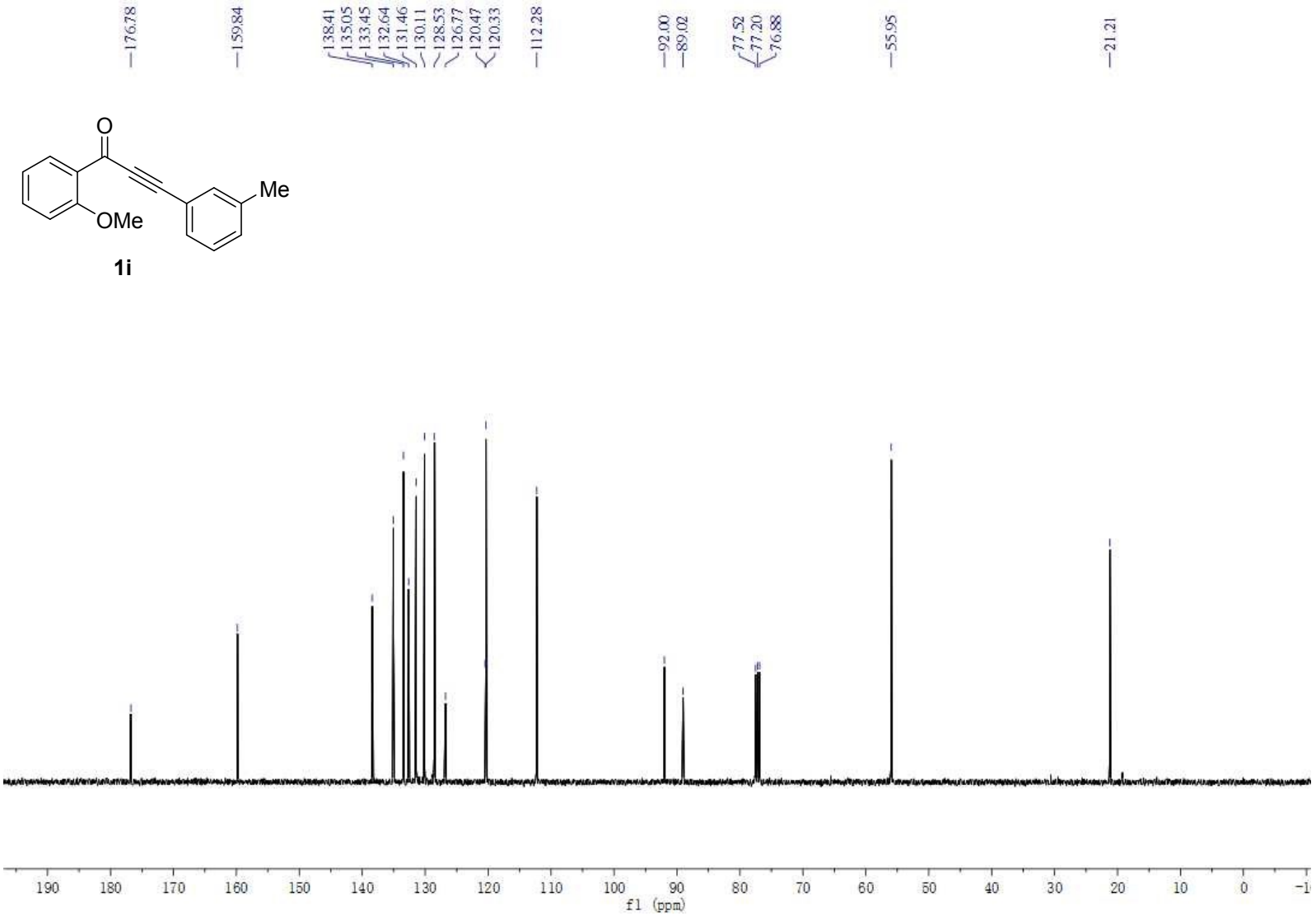
f1 (ppm)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126.77
120.47
120.33
112.28
92.00
89.02
77.52
77.20
76.88
55.95
21.21
O
Me
OMe
1i
190
180
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110
100
90
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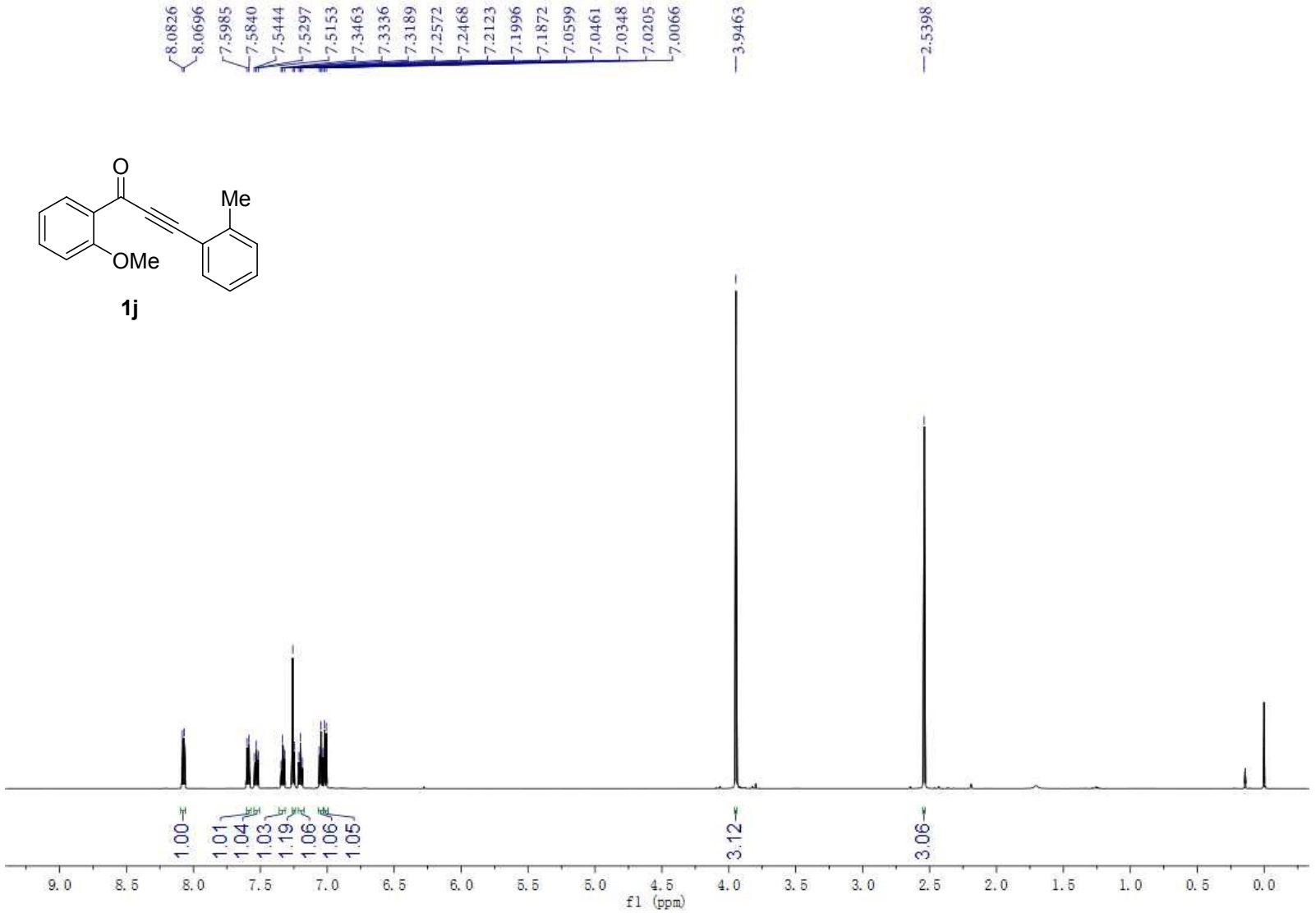
50
40
30
20
10
0
f1 (ppm)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7.2572
7.2468
7.2123
7.1996
7.1872
7.0599
7.0461
7.0348
7.0205
7.0066
3.9463
2.5398
O
Me
OMe
1j
1.00
1.01
1.04
1.03
1.19
1.06
1.06
1.05
3.12
3.06
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.0
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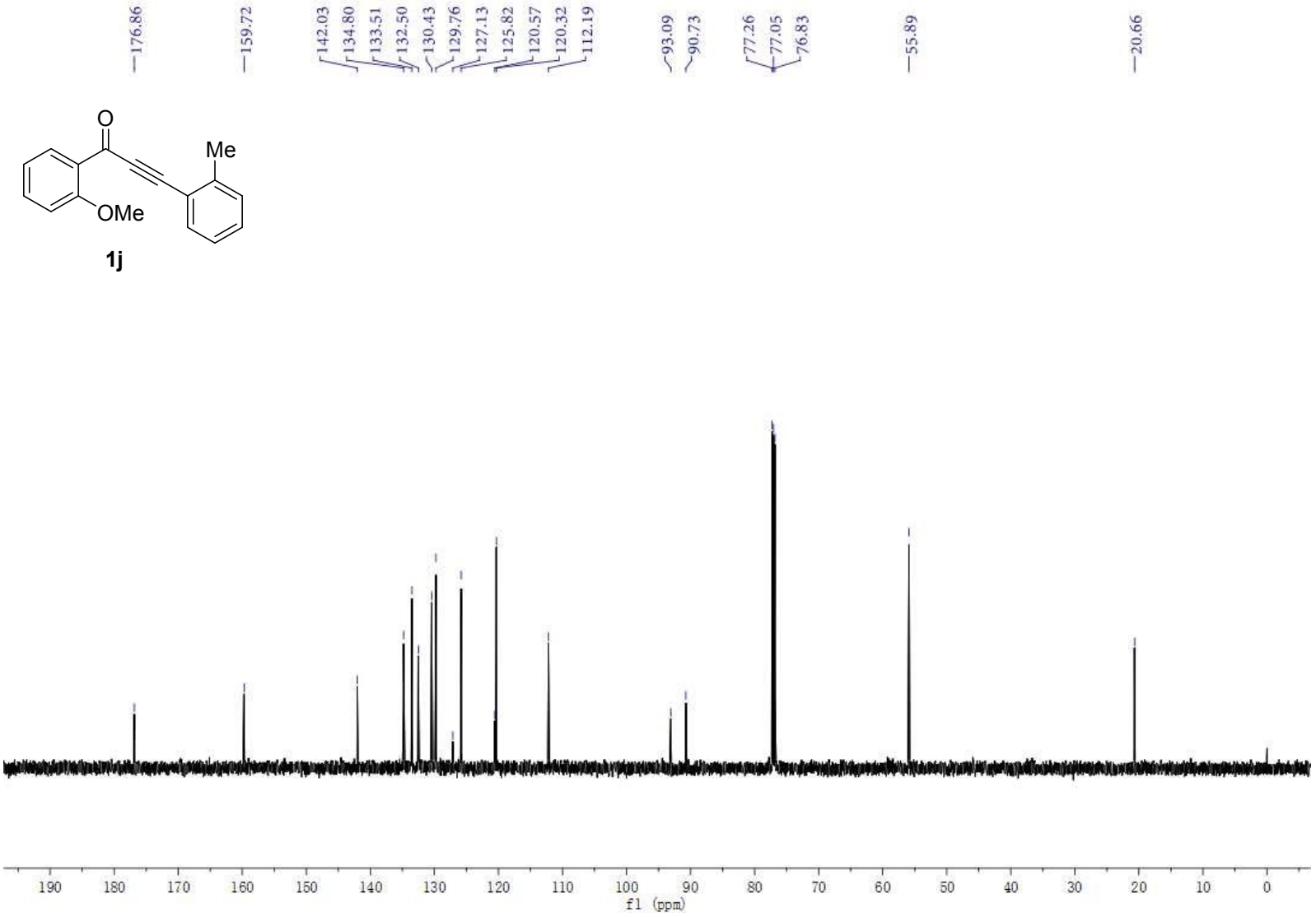
f1 (ppm)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125.82
120.57
120.32
112.19
93.09
90.73
77.26
77.05
76.83
55.89
20.66
O
Me
OMe
1j
190
180
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90
80
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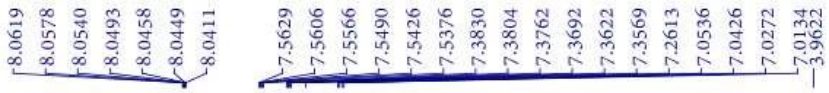
f1 (ppm)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7.5606
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7.5426
7.5376
7.3830
7.3804
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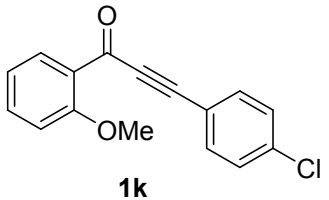
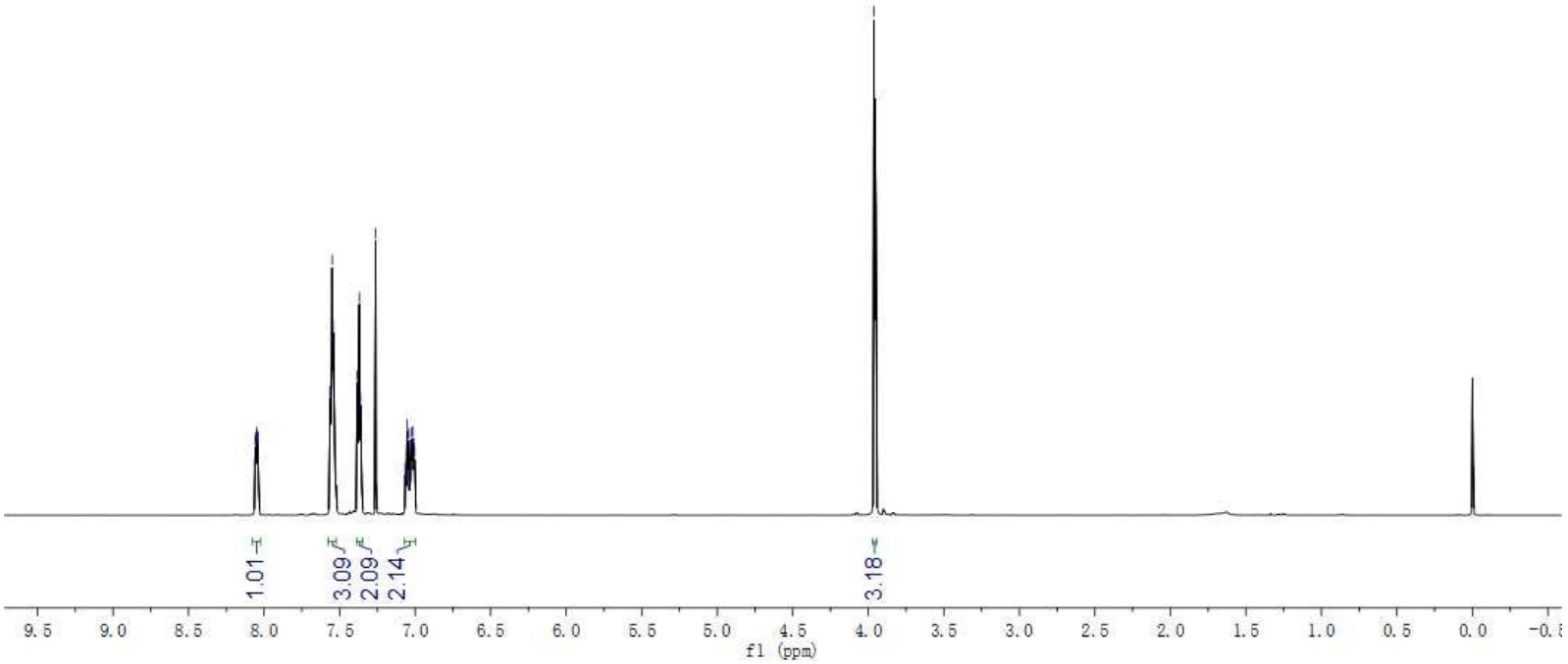
7.2613
7.0536
7.0426
7.0272
7.0134
3.9622


O
OMe
Cl

1k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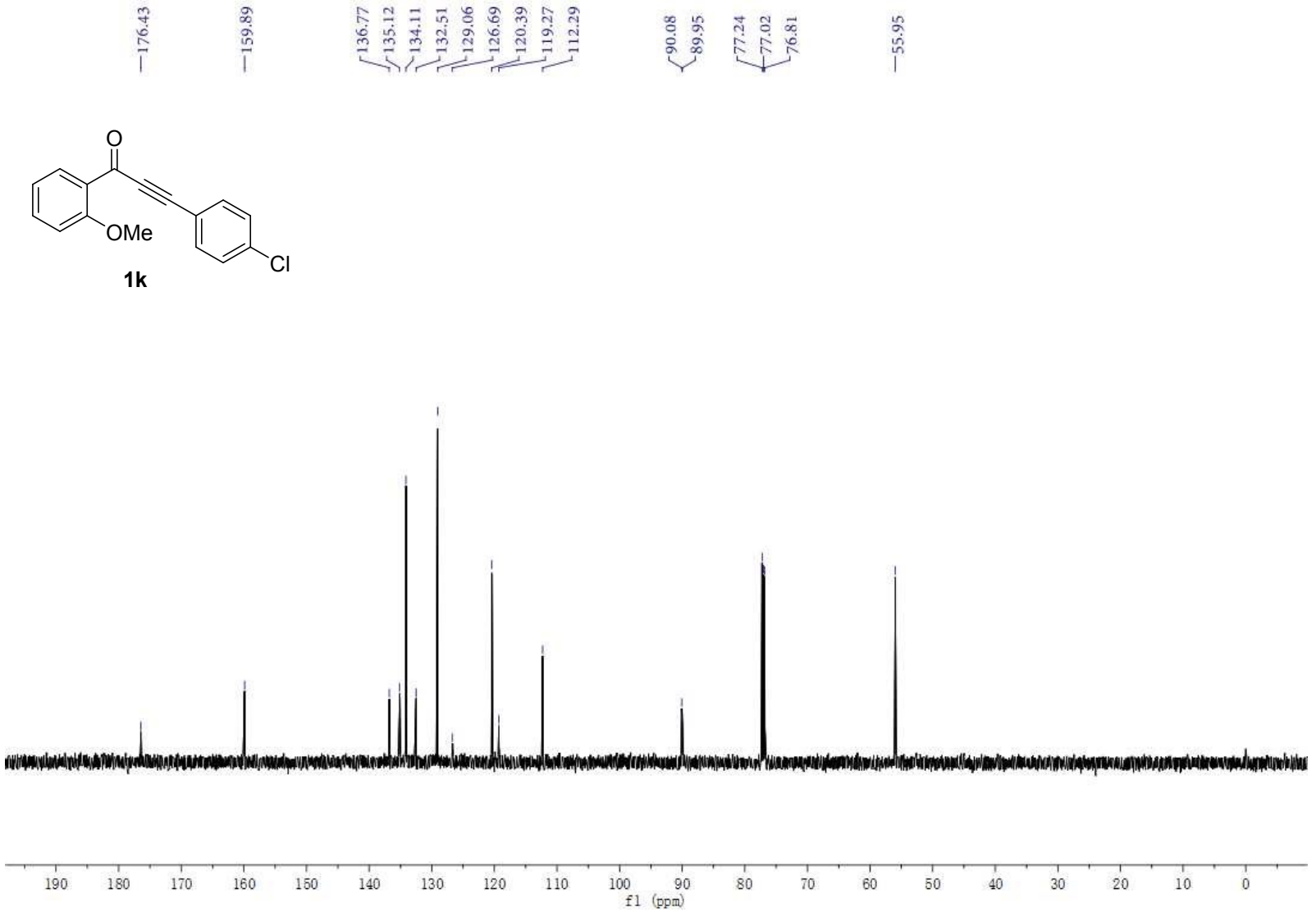
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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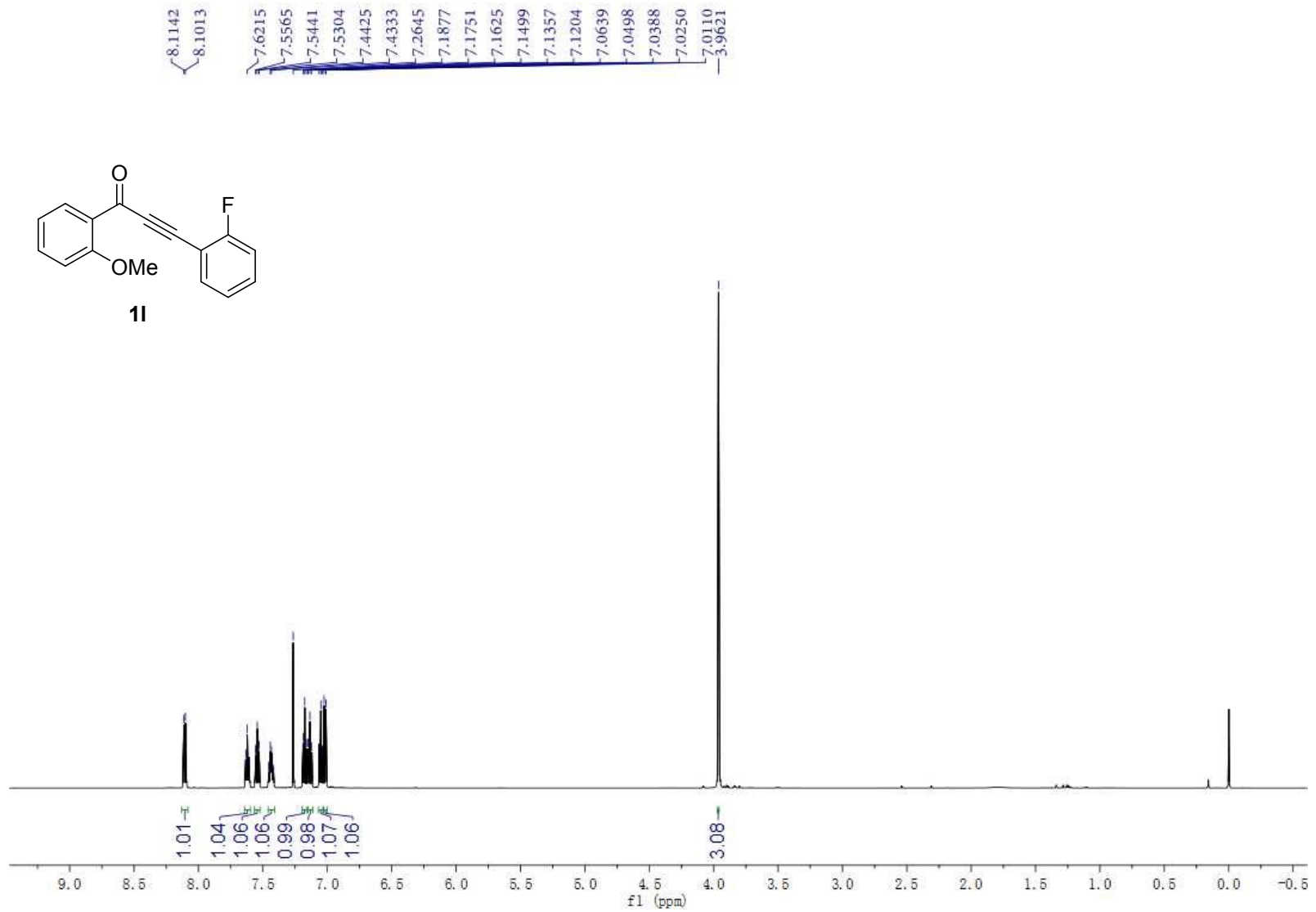
129.06
126.69
120.39
119.27
112.29
90.08
89.95
77.24
77.02
76.81
55.95
O
OMe
Cl
1k
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.5304
7.4425
7.4333
7.2645
7.1877
7.1751
7.1625
7.1499
7.1357
7.1204
7.0639
7.0498
7.0388
7.0250
7.0110
3.9621
O
F
OMe
1.01
1.04
1.06
1.06
0.99
0.98
1.07
1.06
3.08
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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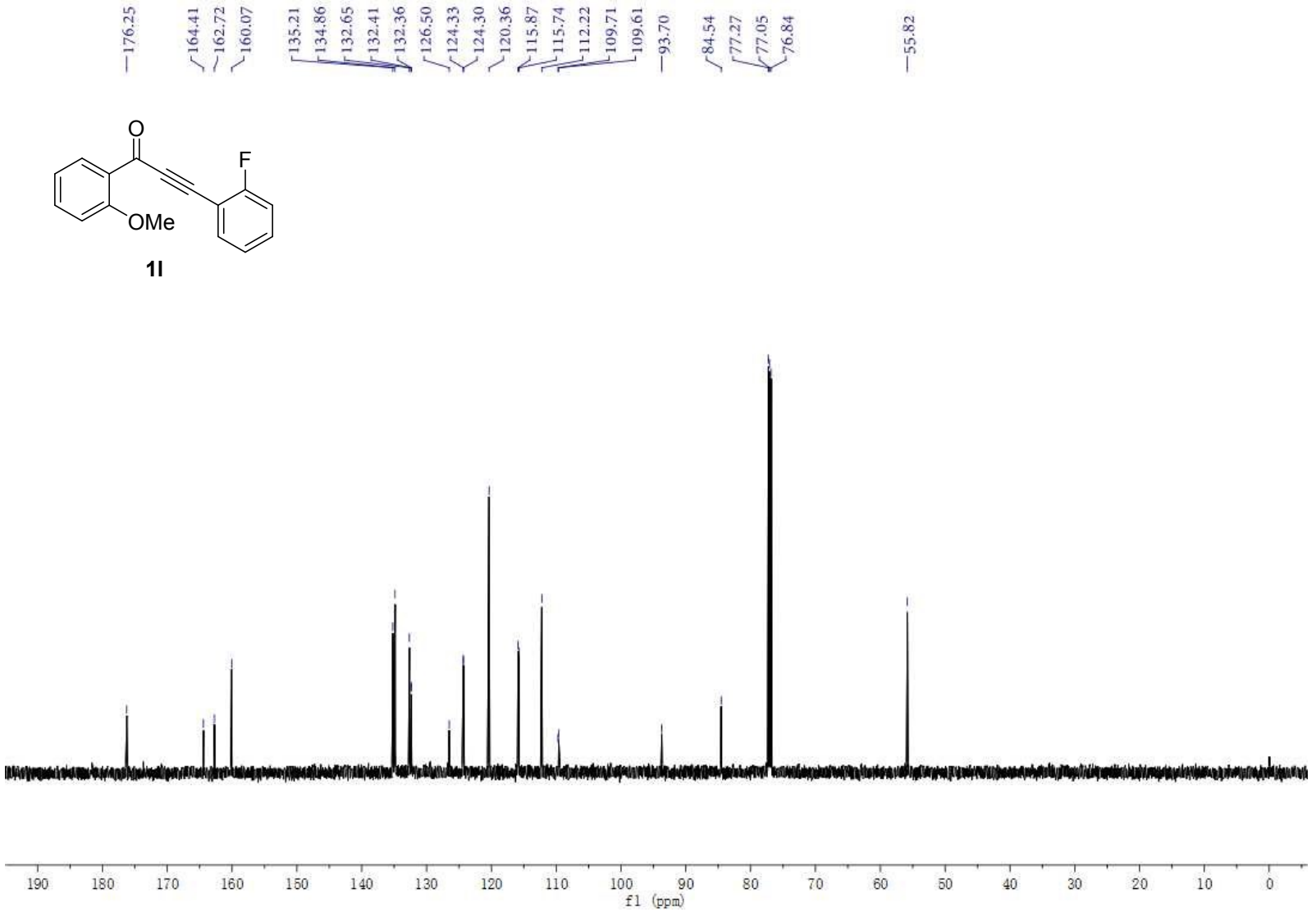
f1 (ppm)

1l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132.41
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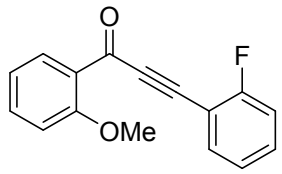
124.33
124.30
120.36
115.87
115.74
112.22
109.71
109.61
93.70
84.54
77.27
77.05
76.84
55.82
O
F
OMe
1l
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


O
F
OMe

1l

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


8.0593
8.0434
7.7562
7.5823
7.5808
7.5792
7.5705
7.5689
7.5673
7.5654
7.5618
7.5598
7.5578
7.5559
7.5526
7.5500
7.5473
7.5449
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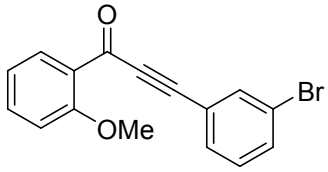
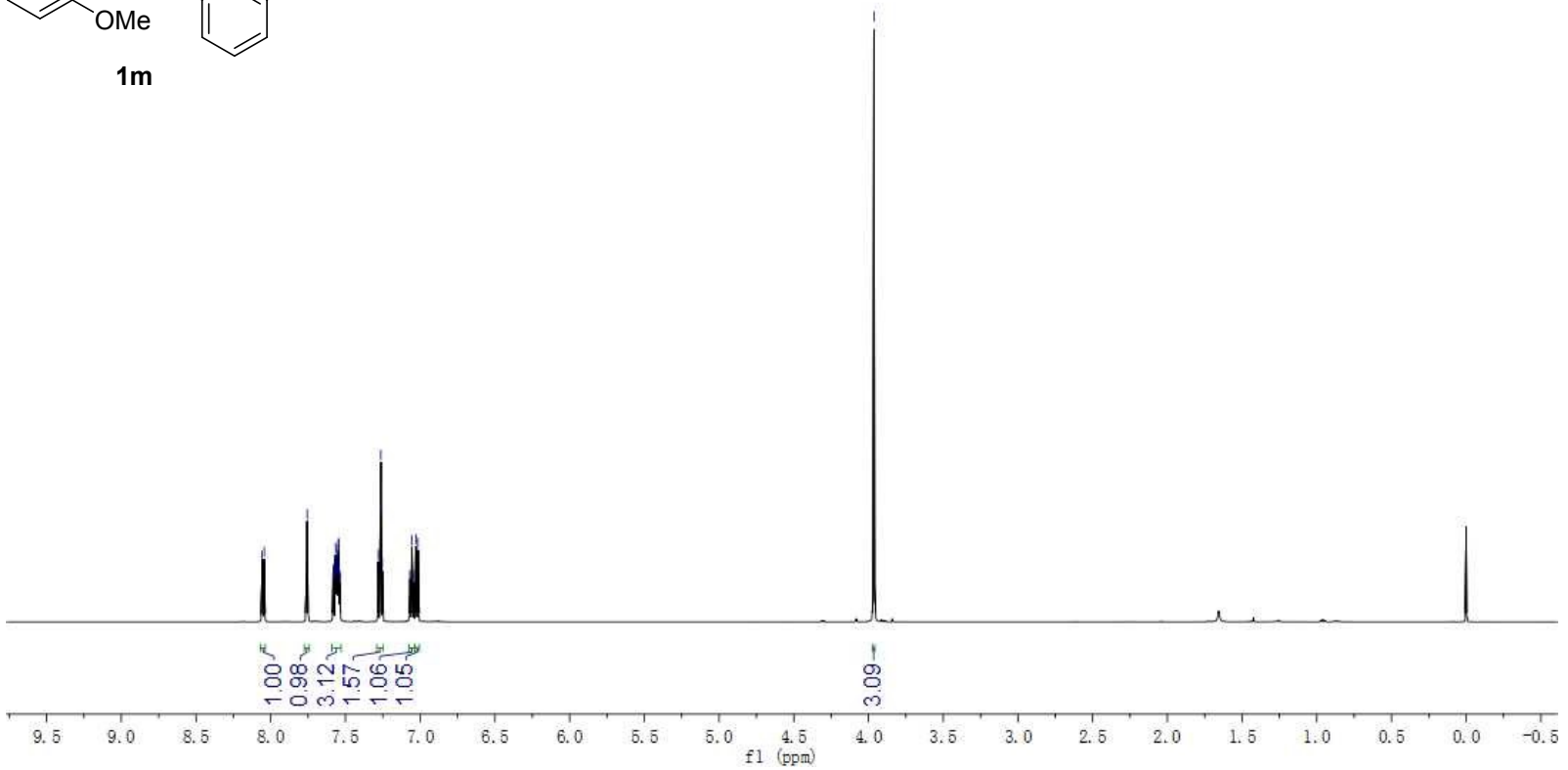
7.0150
3.9638


O
Br
OMe

1m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3.09
9.5
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8.5
8.0
7.5
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6.5
6.0
5.5
5.0
4.5
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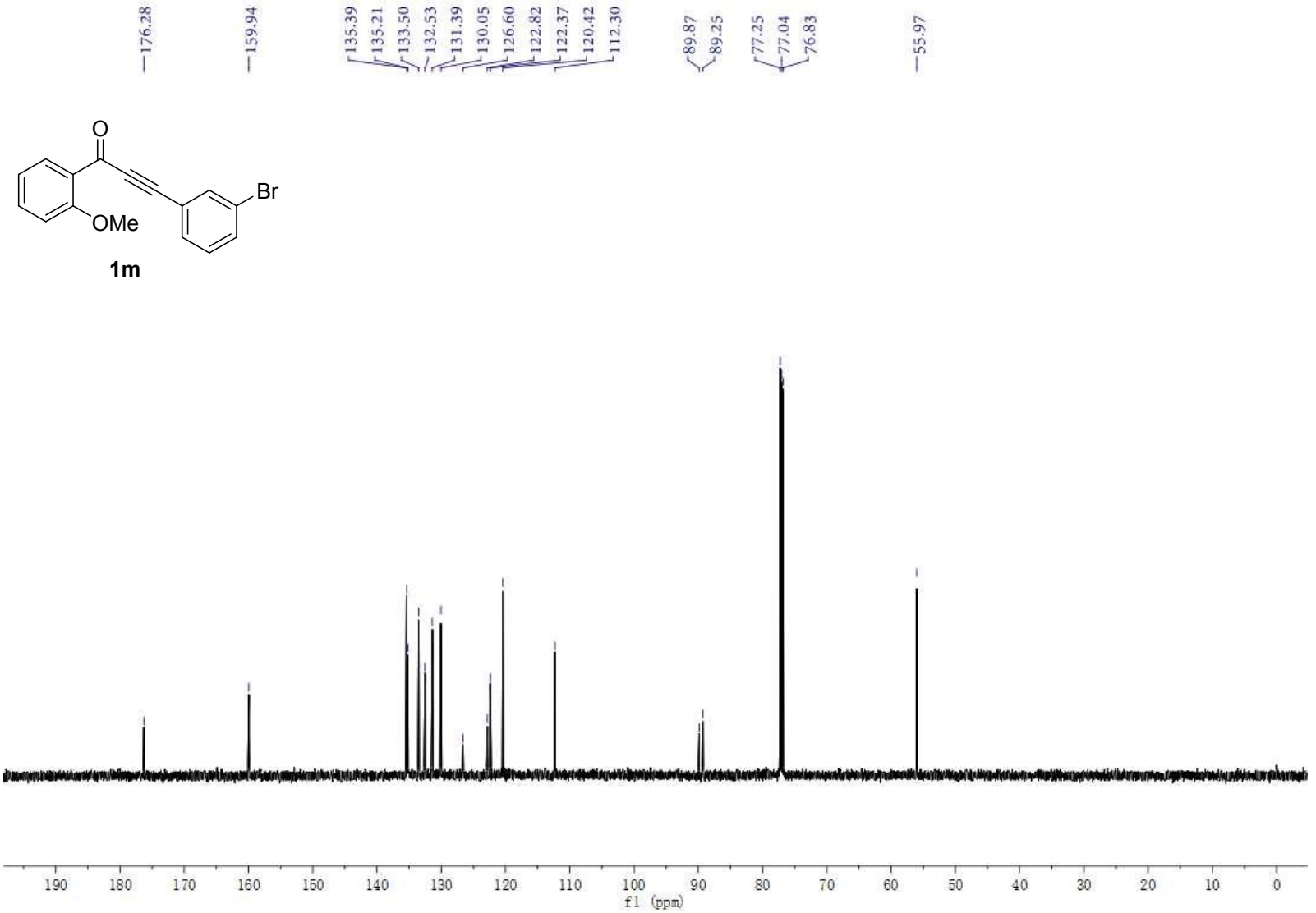
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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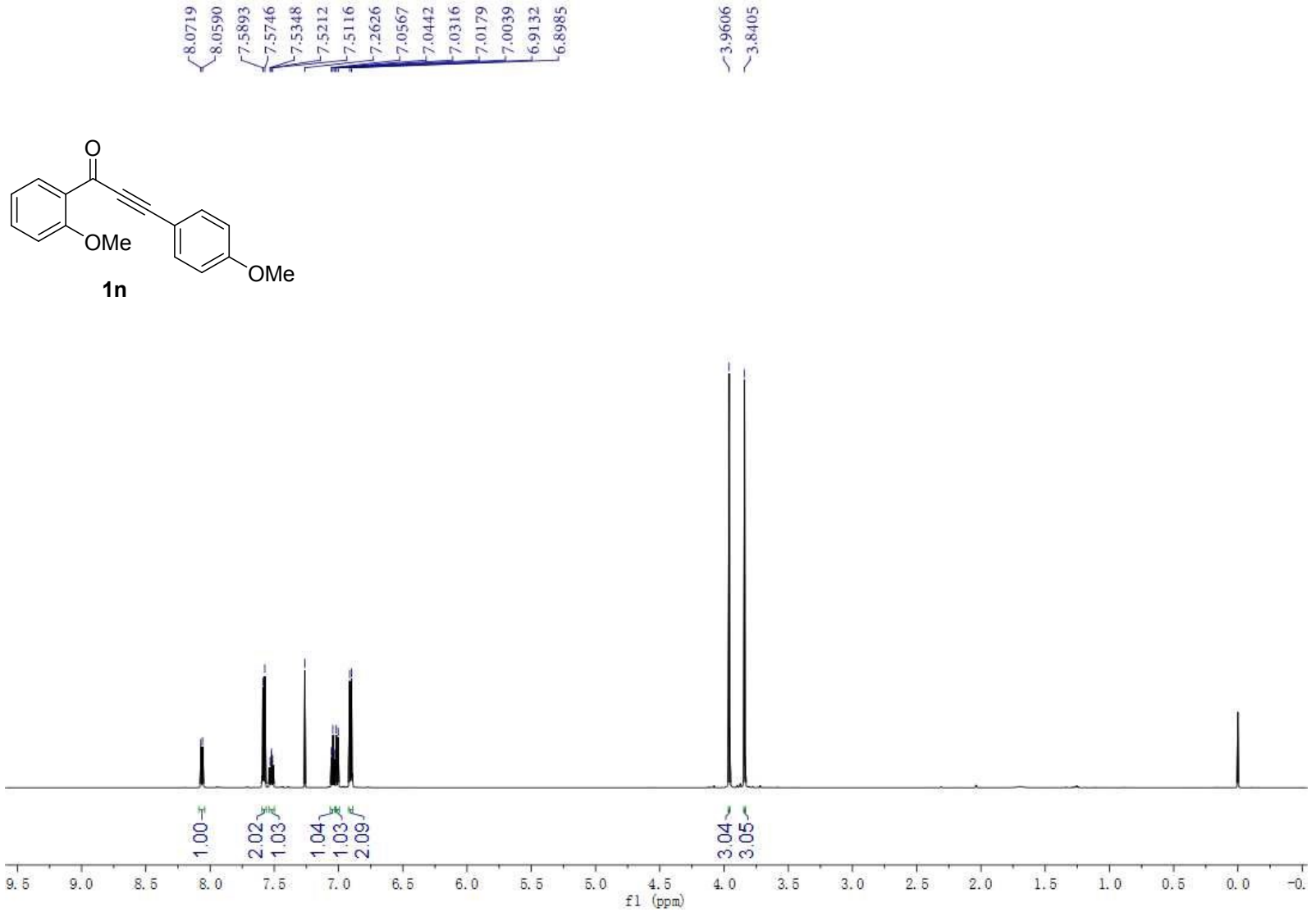
130.05
126.60
122.82
122.37
120.42
112.30
89.87
89.25
77.25
77.04
76.83
55.97
O
Br
OMe
1m
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.0567
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7.0316
7.0179
7.0039
6.9132
6.8985
3.9606
3.8405
O
OMe
OMe
1n
1.00
2.02
1.03
1.04
1.03
2.09
3.04
3.05
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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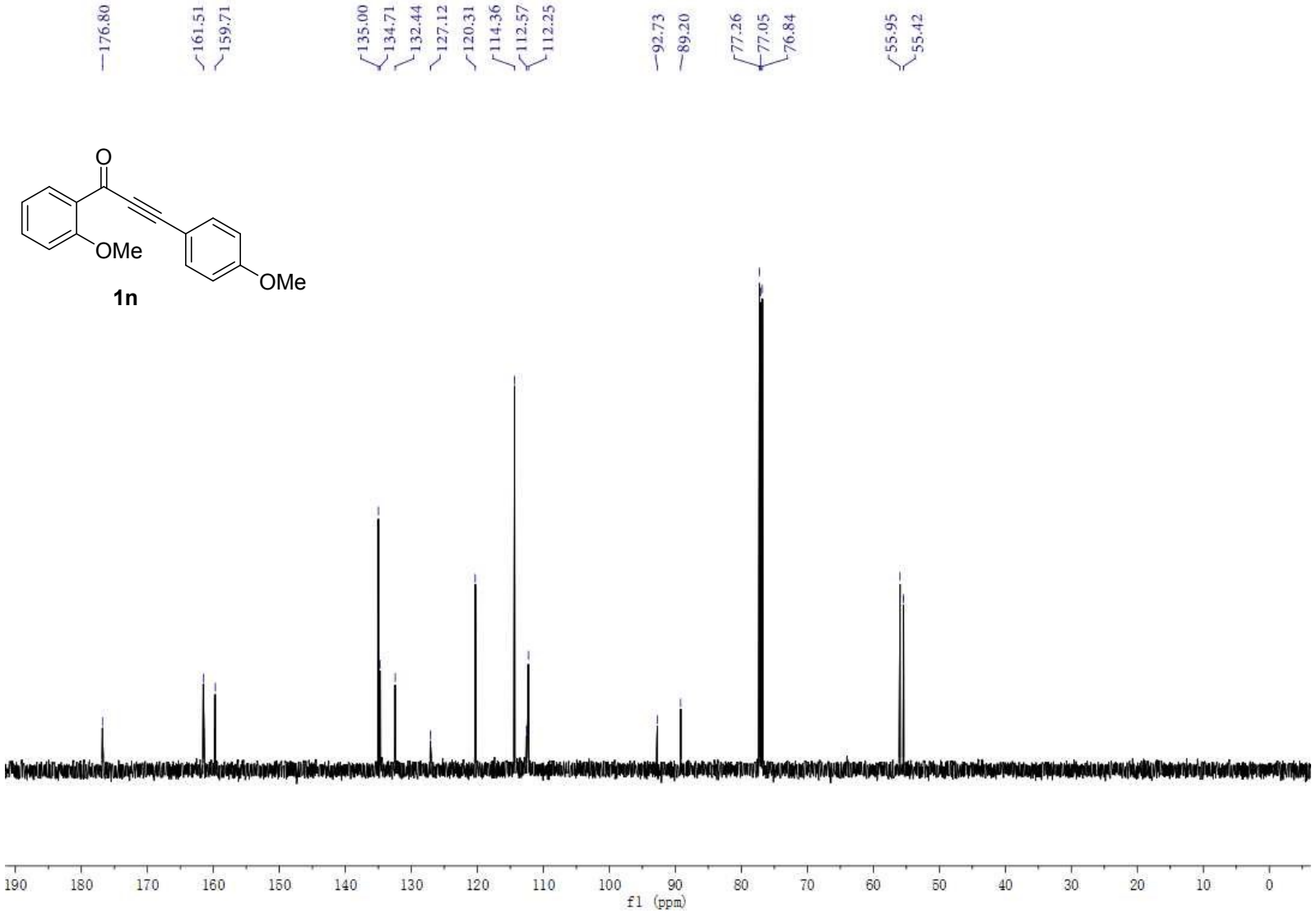
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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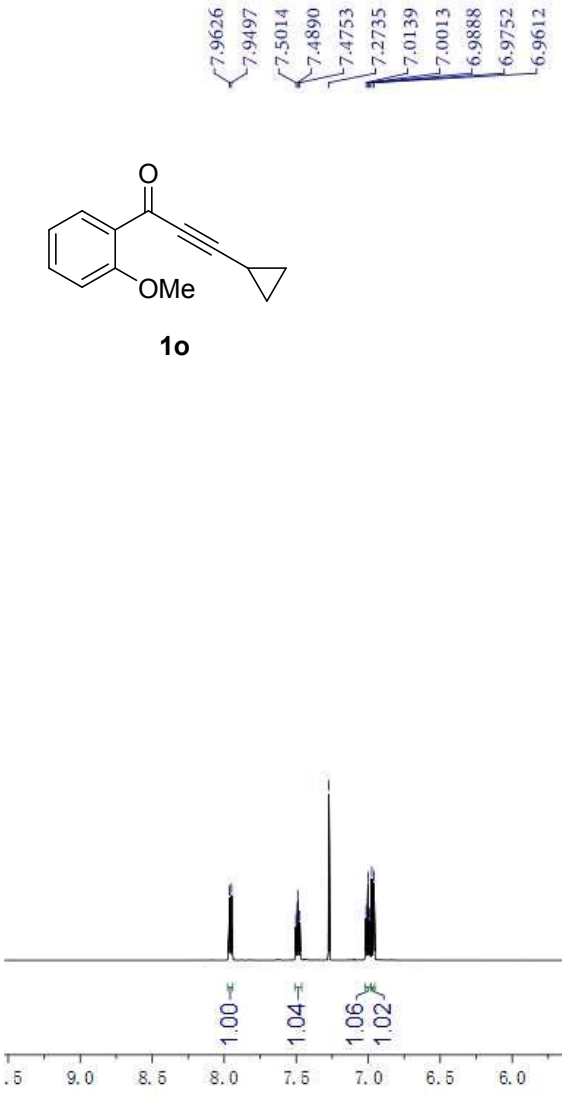
112.57
112.25
92.73
89.20
77.26
77.05
76.84
55.95
55.42
O
OMe
OMe
1n
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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6.9612
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1.4954
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1.4828
1.4788
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1.4652
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1.0103
1.0070
1.0008
0.9968
0.9941
0.9877
0.9721
0.9672
0.9633
0.9592
0.9547
0.9480
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OMe
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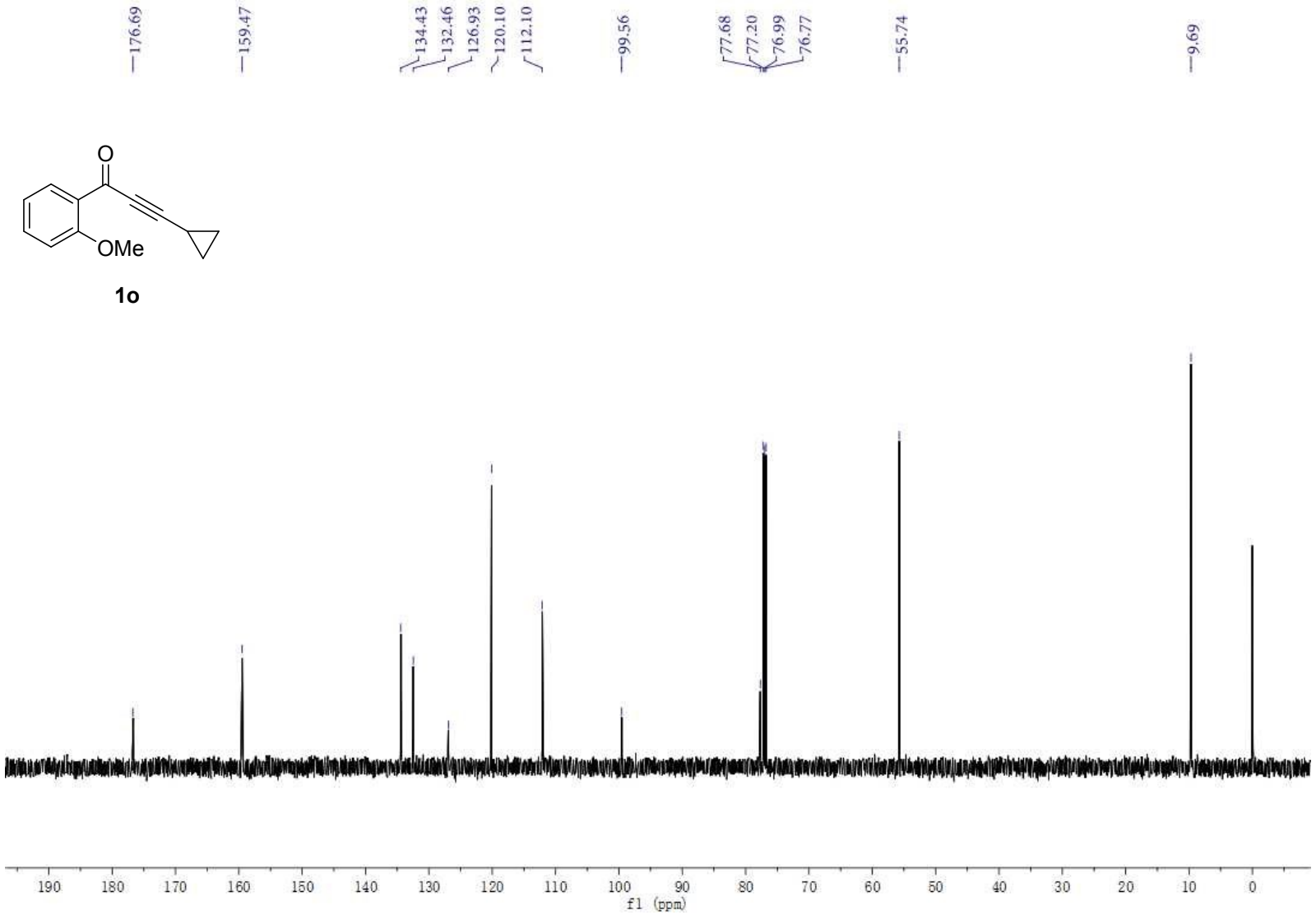
1.04
1.06
1.02
3.13
0.99
2.03
2.07
f1 (ppm)

1o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120.10
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99.56
77.68
77.20
76.99
76.77
55.74
9.69
O
OMe
1o
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.0636
8.0606
8.0506
8.0477
7.7724
7.7707
7.7675
7.7658
7.5431
7.5293
7.5169
7.3467
7.3418
7.3384
7.3334
7.2686
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7.2586
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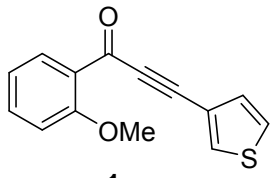
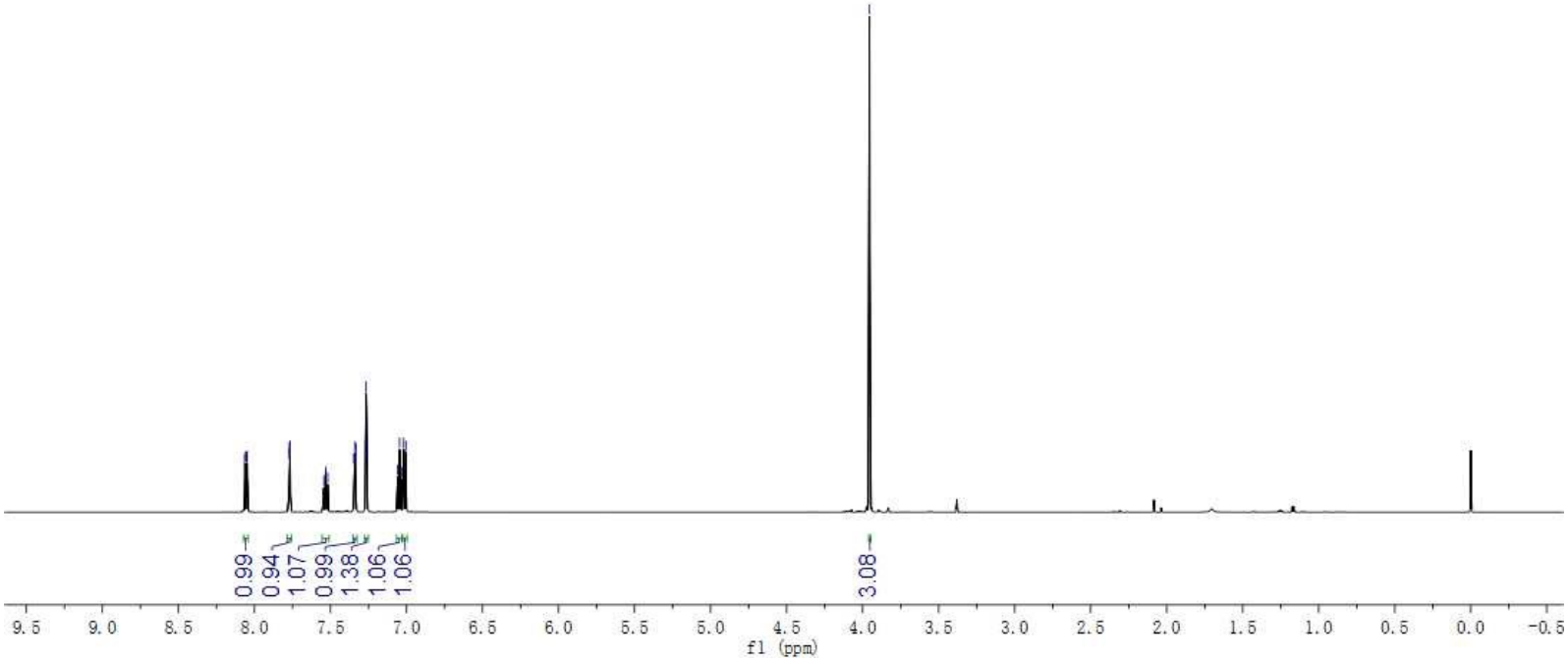
7.0185
7.0045
3.9547


O
OMe
S

1p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3.08
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7.0
6.5
6.0
5.5
5.0
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3.0
2.5
2.0
1.5
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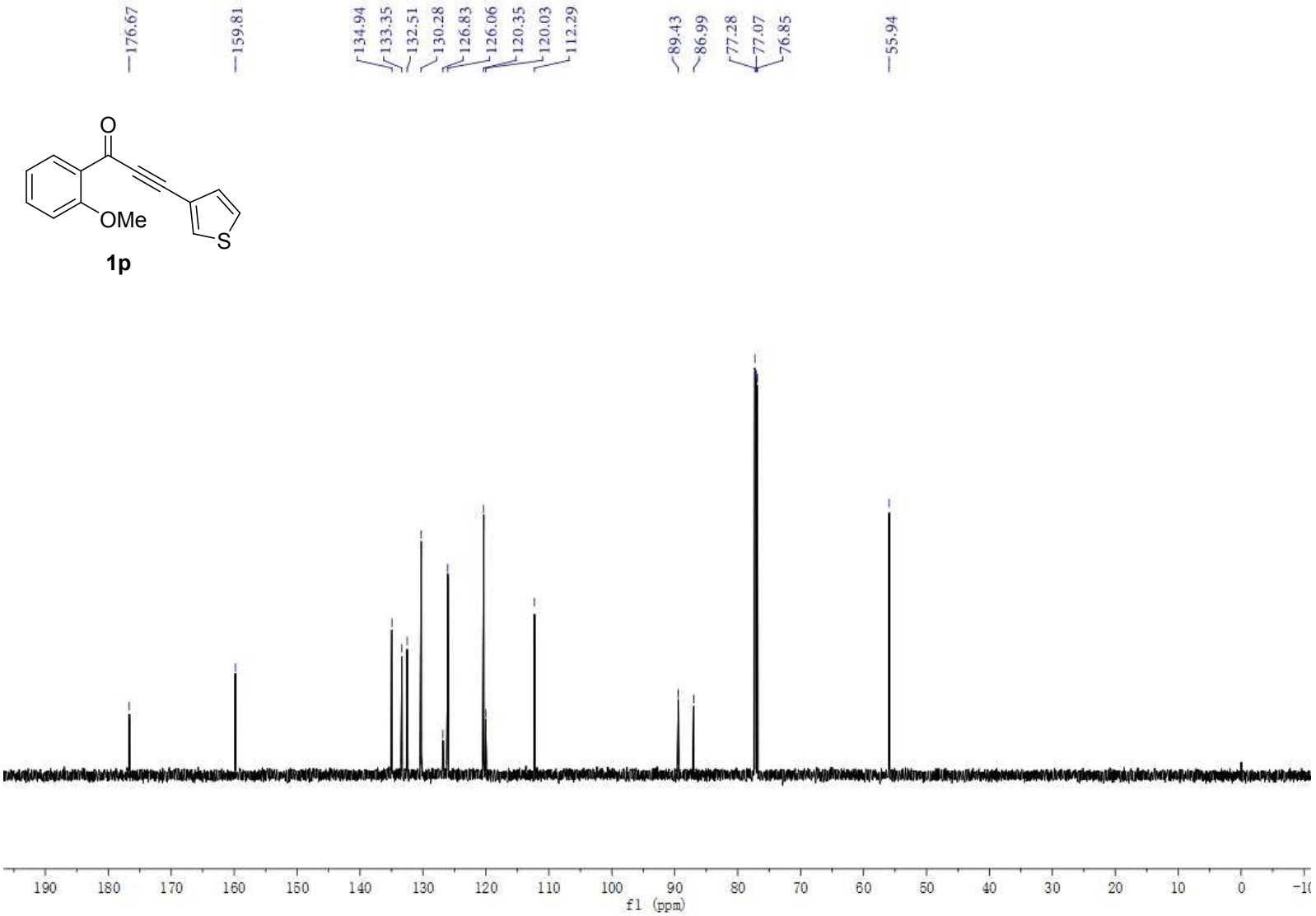
0.5
0.0
-0.5
f1 (ppm)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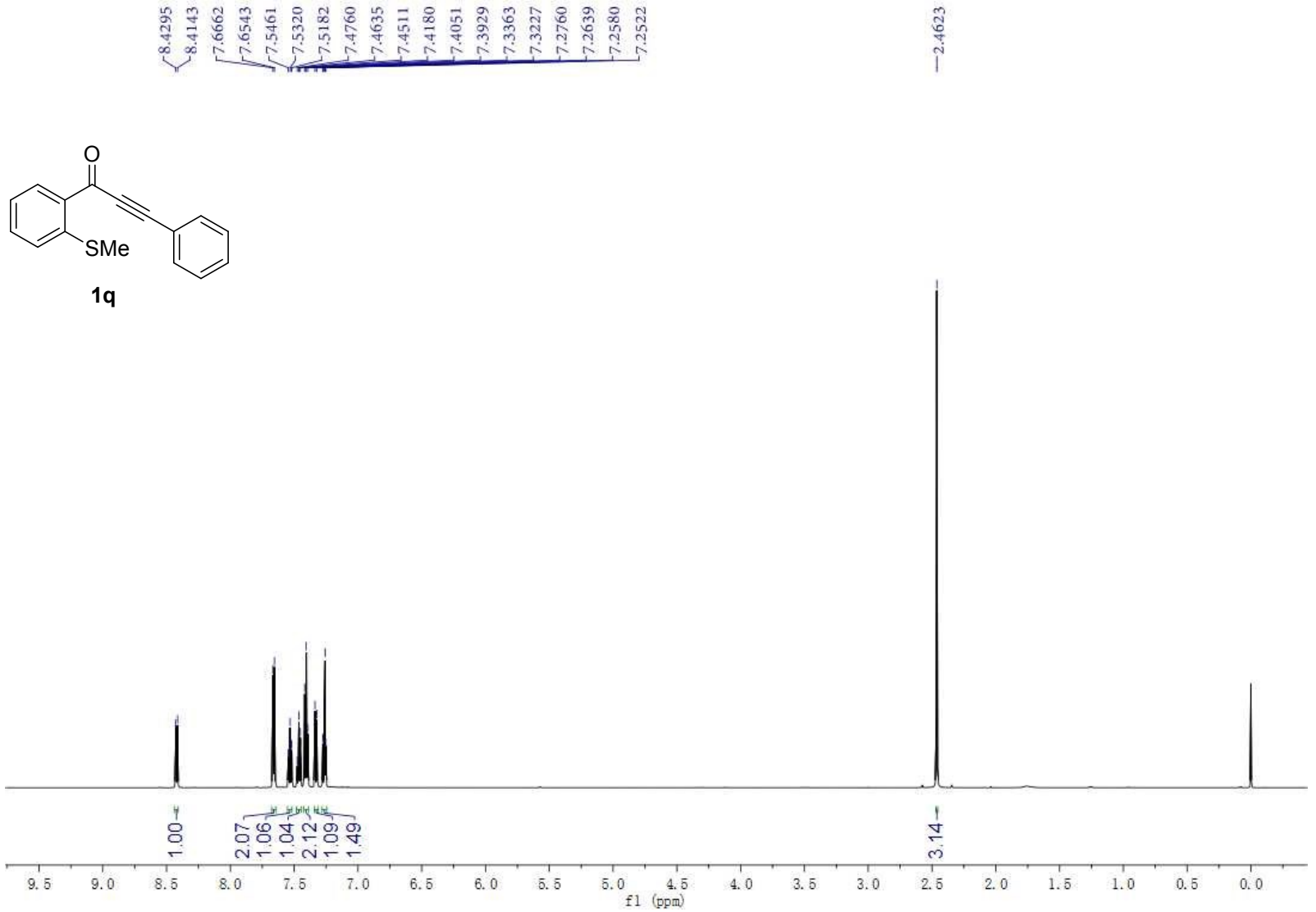
126.06
120.35
120.03
112.29
89.43
86.99
77.28
77.07
76.85
55.94
O
OMe
S
1p
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.5182
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7.4635
7.4511
7.4180
7.4051
7.3929
7.3363
7.3227
7.2760
7.2639
7.2580
7.2522
2.4623
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SMe
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1.06
1.04
2.12
1.09
1.49
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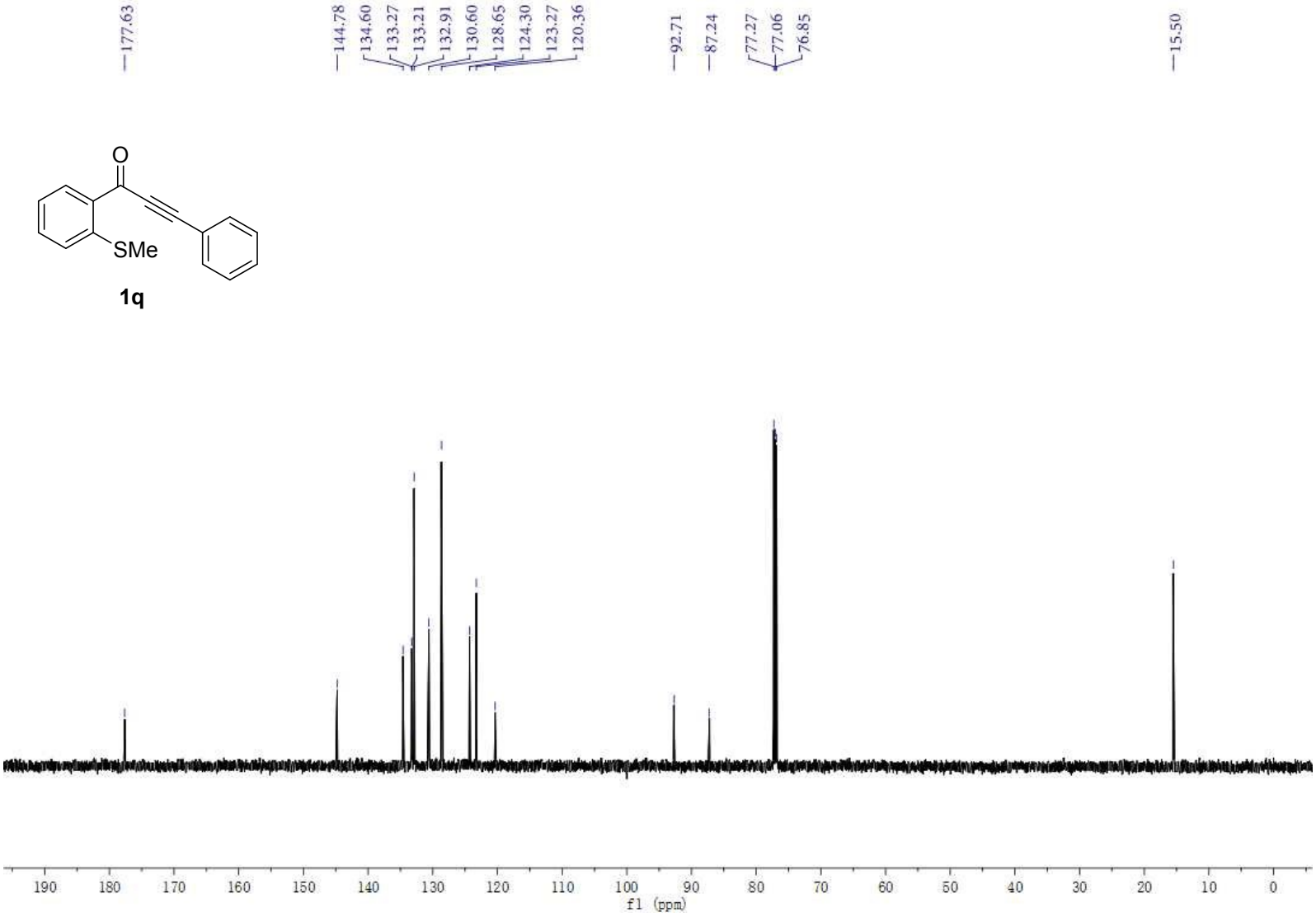
1q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128.65
124.30
123.27
120.36
92.71
87.24
77.27
77.06
76.85
15.50
O
SMe
1q
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.5864
7.5744
7.4427
7.3882
7.3871
7.3836
7.3776
7.3765
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7.3575
6.7771
6.7679
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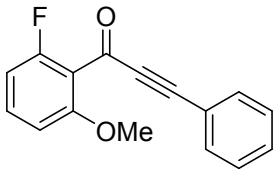
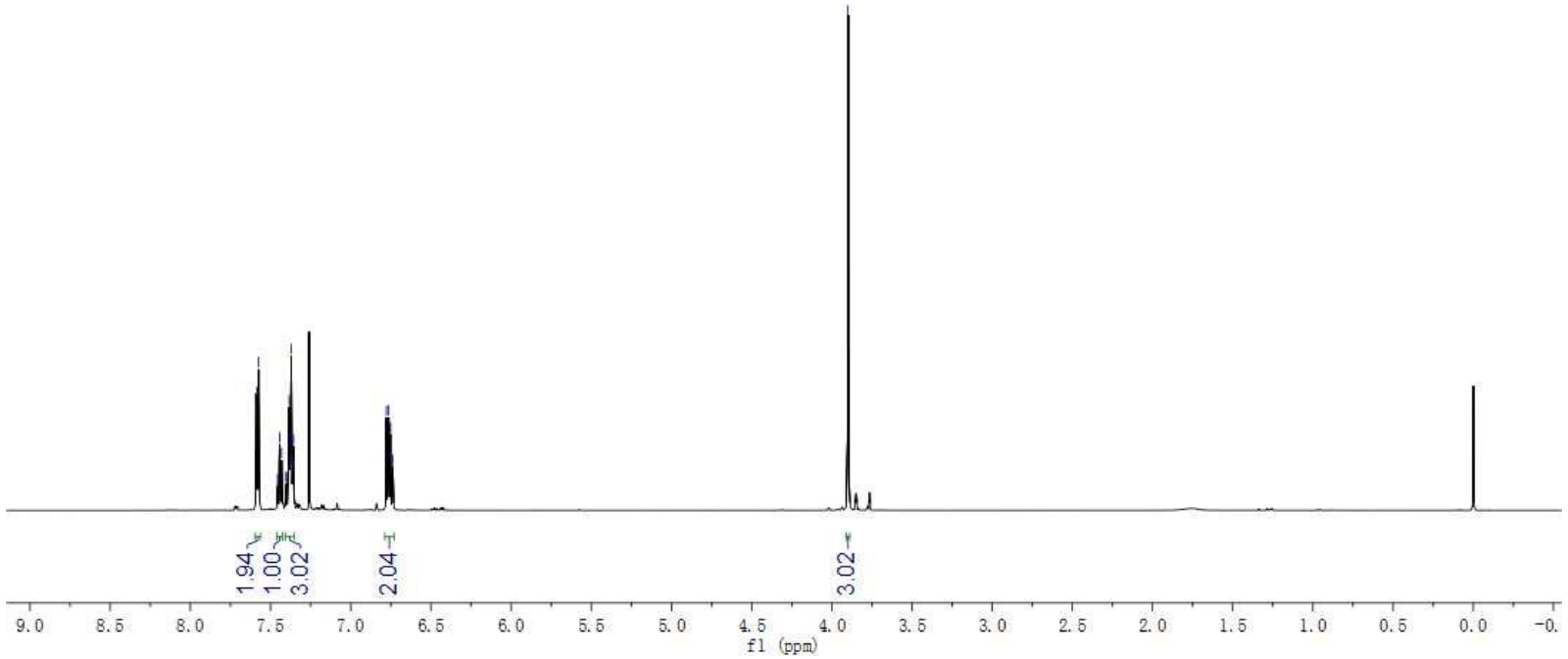
6.7538
6.7525
6.7384
3.8997


F
O
OMe

1r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3.02
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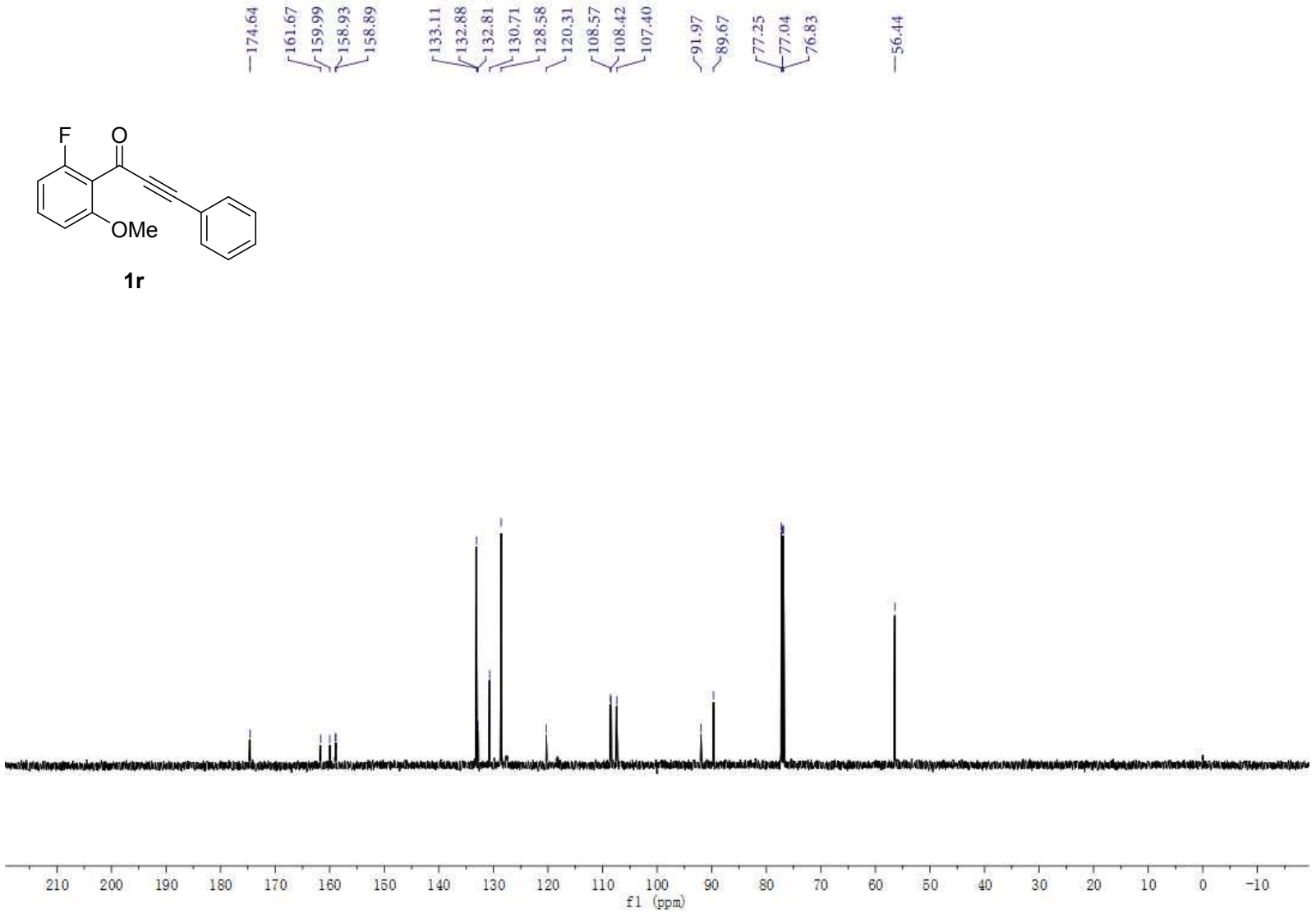
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)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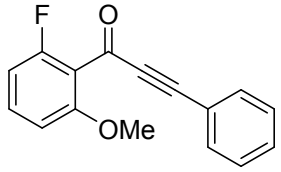
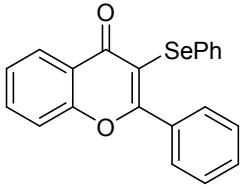
158.89
133.11
132.88
132.81
130.71
128.58
120.31
108.57
108.42
107.40
91.97
89.67
77.25
77.04
76.83
56.44
F
O
OMe
1r
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


F
O
OMe

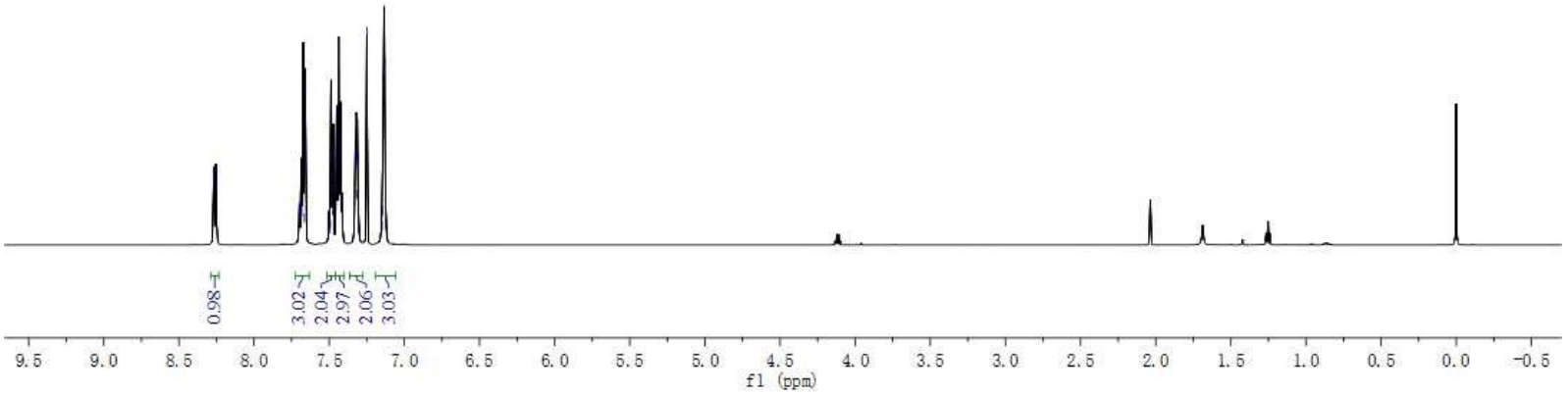
1r

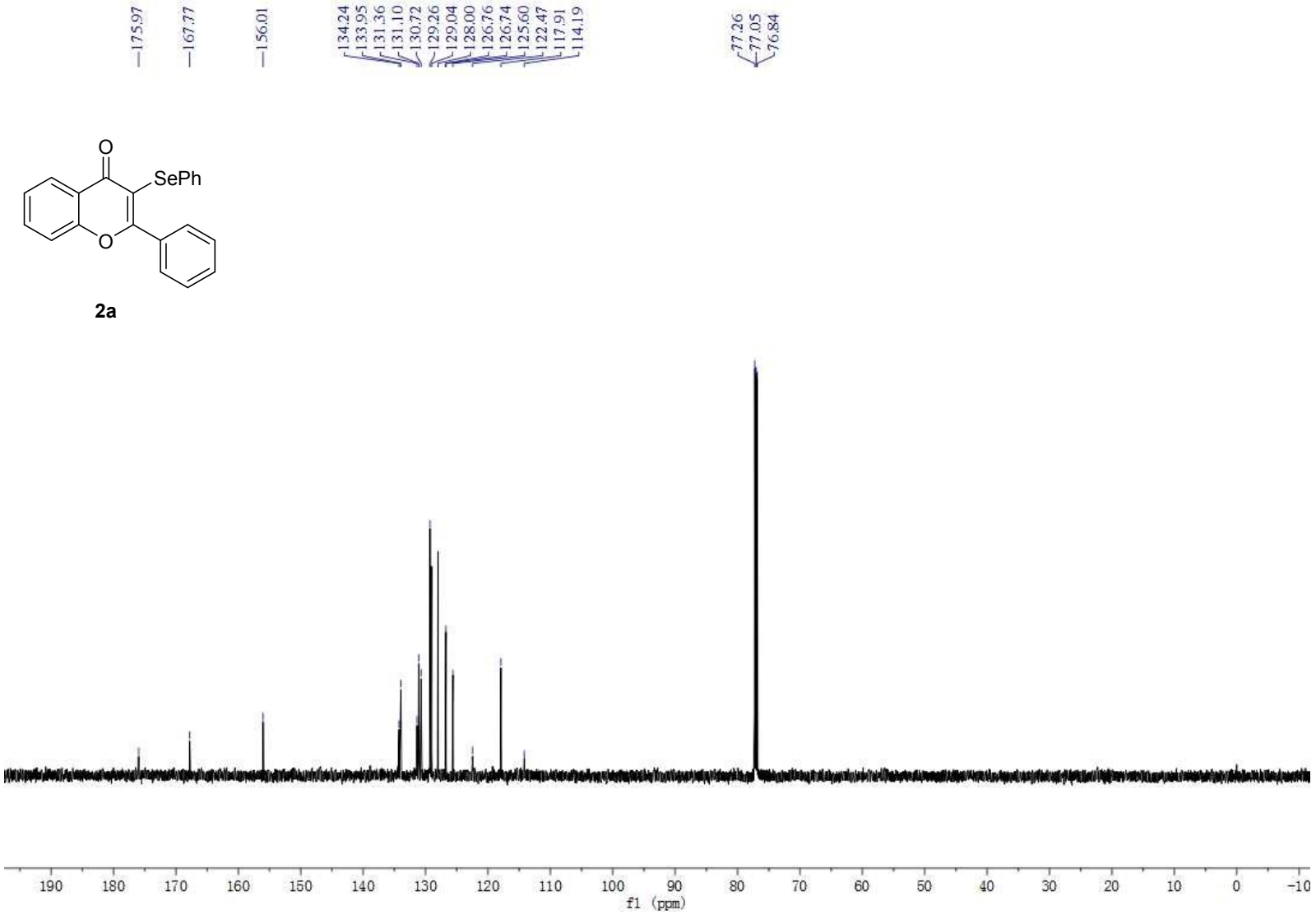
-113.65
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)

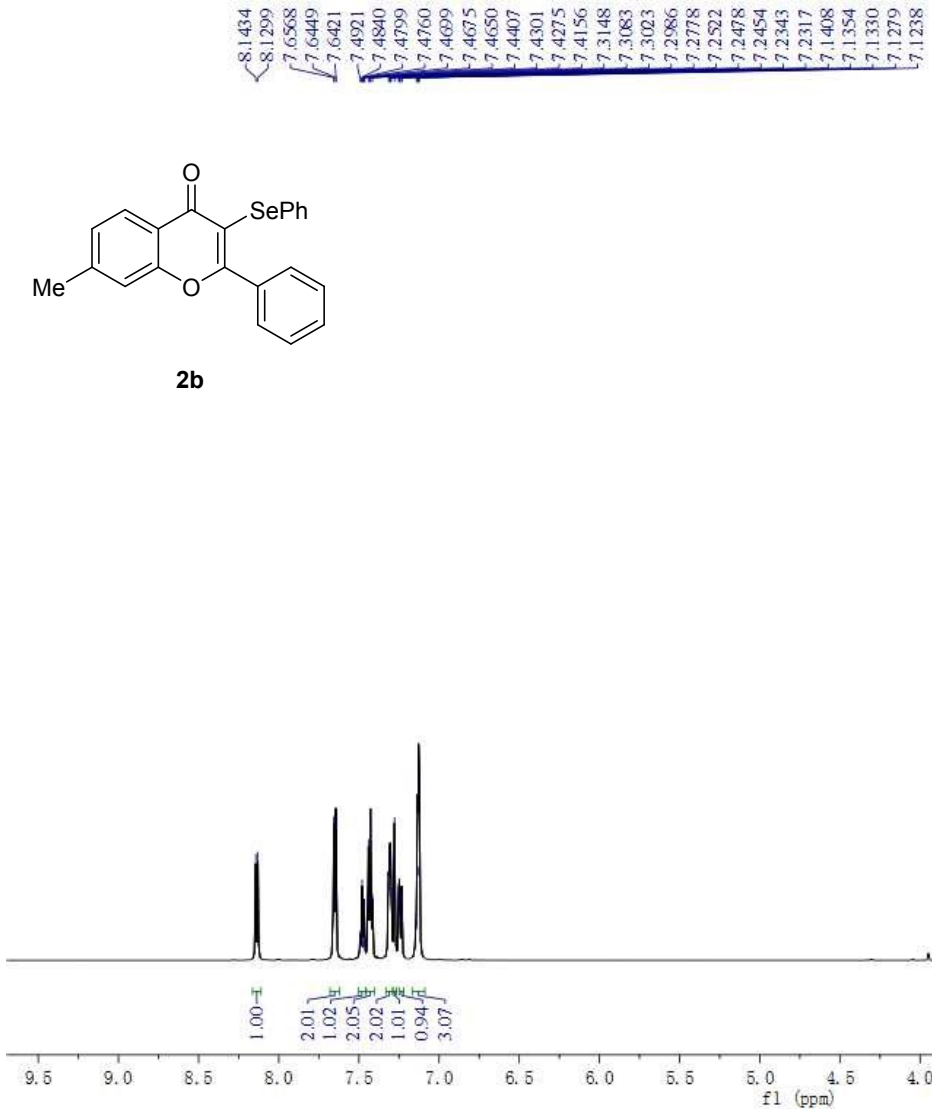

8.2678
8.2651
8.2546
8.2518
7.6994
7.6967
7.6887
7.6852
7.6827
7.6742
7.6726
7.6705
7.6644
7.6609
7.6582
7.5030
7.5008
7.4986
7.4925
7.4881
7.4856
7.4784
7.4761
7.4732
7.4715
7.4495
7.4392
7.4366
7.4270
7.4246
7.4144
7.4128
7.3253
7.3193
7.3176
7.3131
7.3094
7.3034
7.2495
7.1478
7.1456
7.1405
7.1342
7.1298
7.1233


O
SePh
O

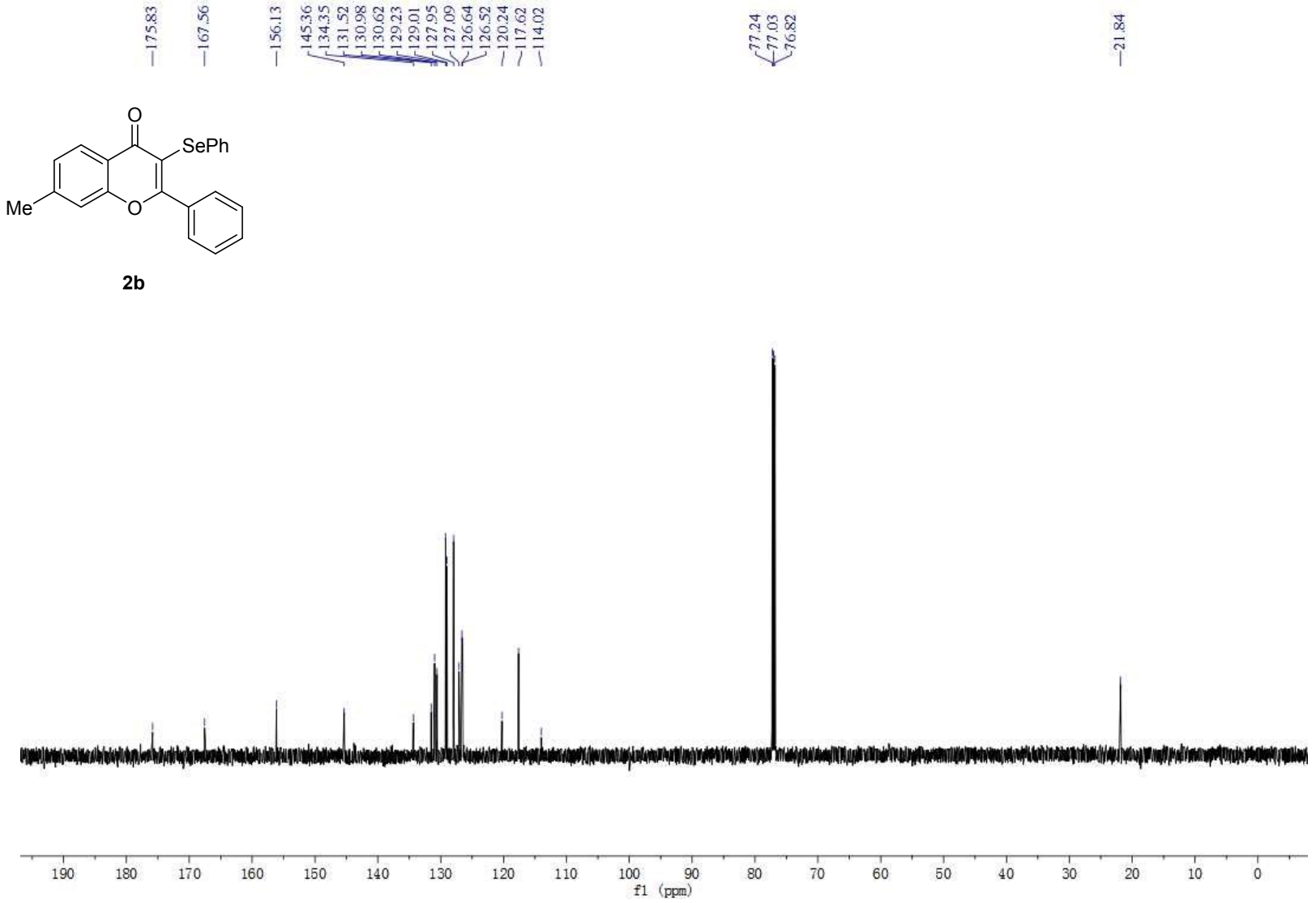
2a

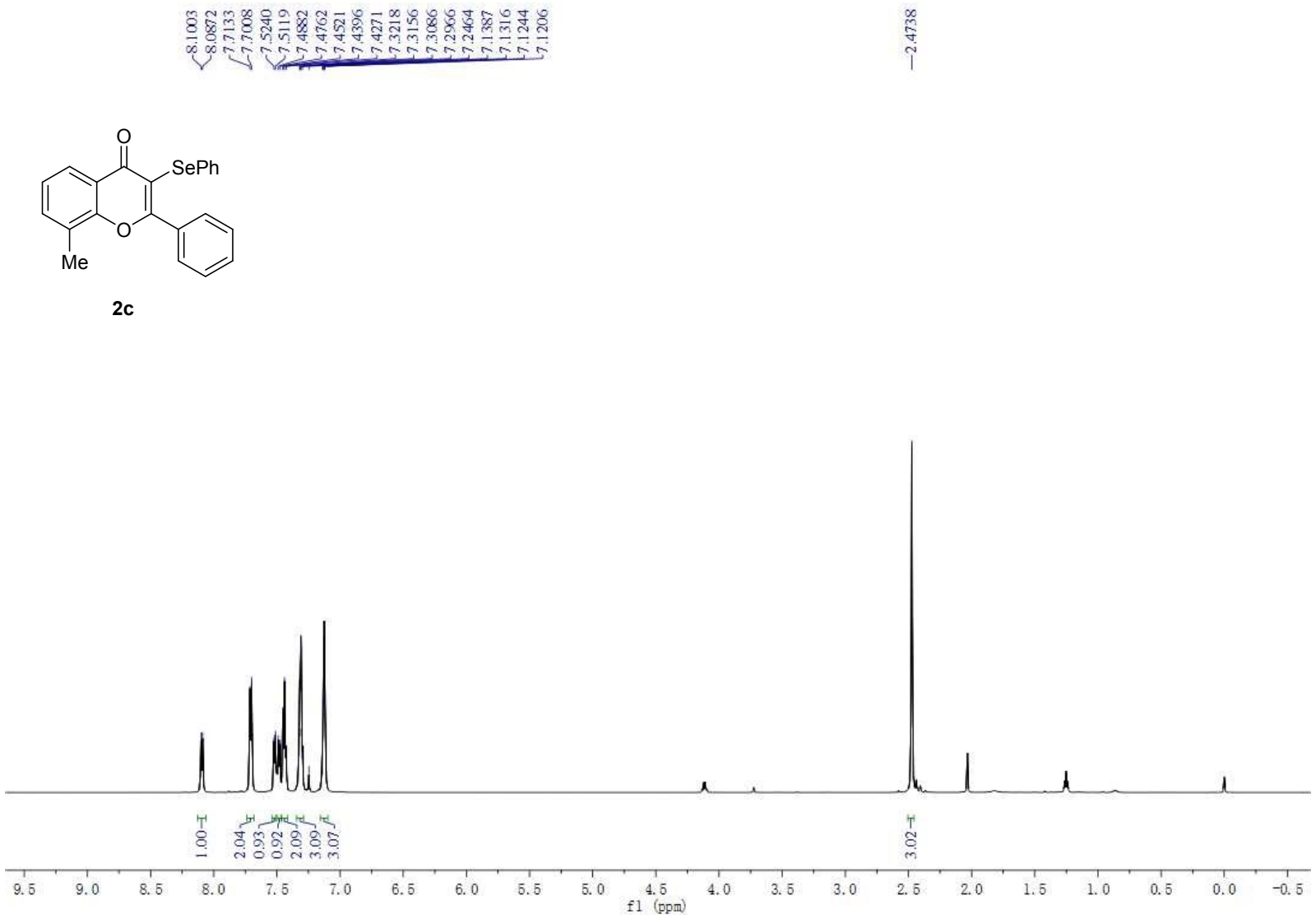

0.98
3.02
2.04
2.97
2.06
3.03
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


175.97
167.77
156.01
134.24
133.95
131.36
131.10
130.72
129.26
129.04
128.00
126.76
126.74
125.60
122.47
117.91
114.19
77.26
77.05
76.84
O
SePh
O
2a
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

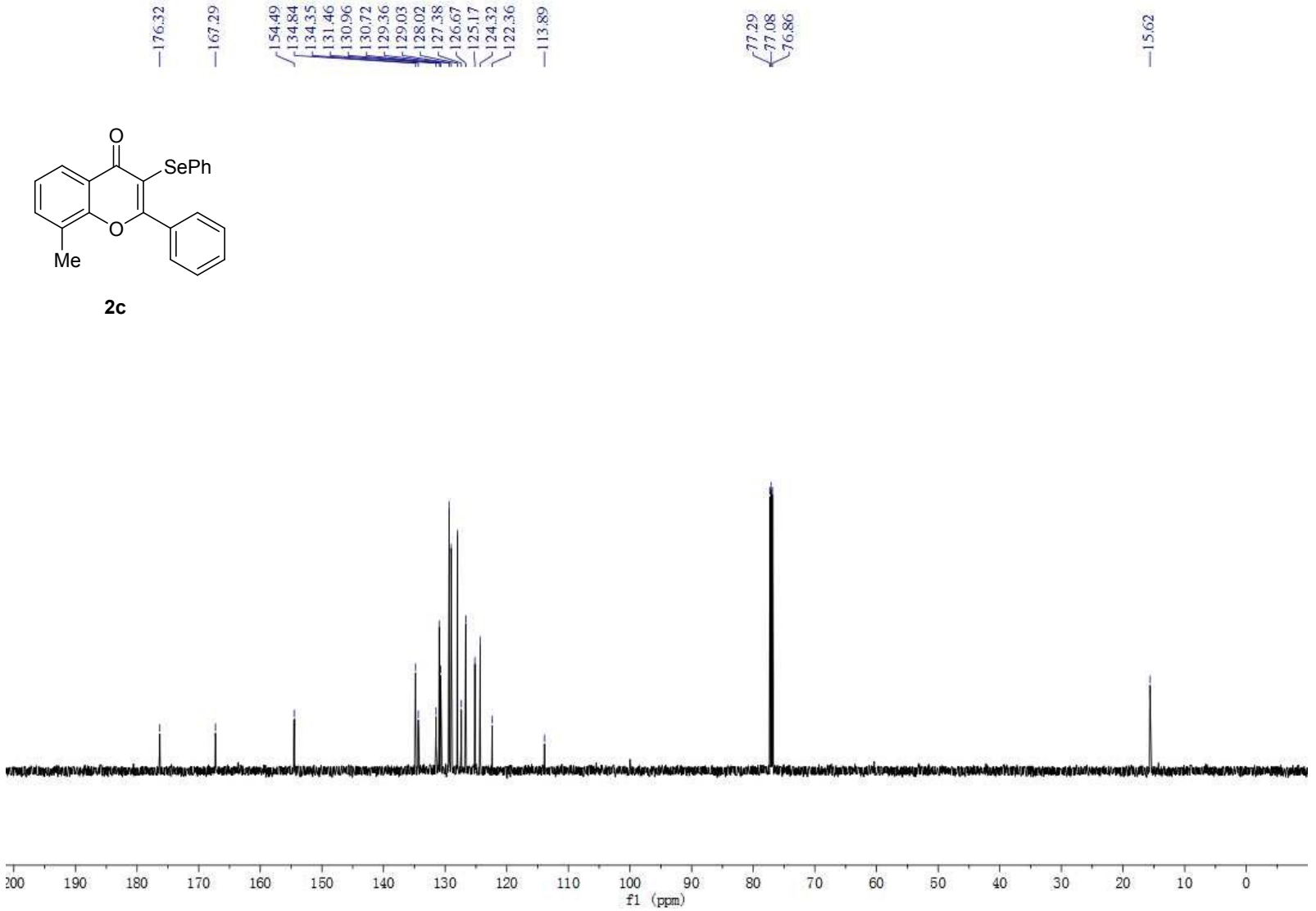

8.1434
8.1299
7.6568
7.6449
7.6421
7.4921
7.4840
7.4799
7.4760
7.4699
7.4675
7.4650
7.4407
7.4301
7.4275
7.4156
7.3148
7.3083
7.3023
7.2986
7.2778
7.2522
7.2478
7.2454
7.2343
7.2317
7.1408
7.1354
7.1330
7.1279
7.1238
2.4859
O
SePh
Me
O
1.00
2.01
1.02
2.05
2.02
1.01
0.94
3.07
3.07
9.5
9.0
8.5
8.0
7.5
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)

2b

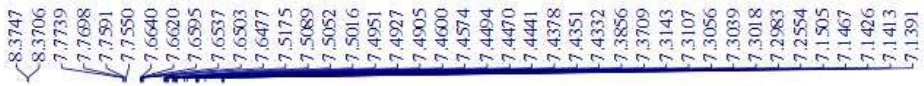

175.83
167.56
156.13
145.36
134.35
131.52
130.98
130.62
129.23
129.01
127.95
127.09
126.64
126.52
120.24
117.62
114.02
77.24
77.03
76.82
21.84
O
SePh
Me
O
2b
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.1003
8.0872
7.7133
7.7008
7.5240
7.5119
7.4882
7.4762
7.4521
7.4396
7.4271
7.3218
7.3156
7.3086
7.2966
7.2464
7.1387
7.1316
7.1244
7.1206
2.4738
O
SePh
O
Me
1.00
2.04
0.93
0.92
2.09
3.09
3.07
3.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

2c


176.32
167.29
154.49
134.84
134.35
131.46
130.96
130.72
129.36
129.03
128.02
127.38
126.67
125.17
124.32
122.36
113.89
77.29
77.08
76.86
15.62
O
SePh
O
Me
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

2c


8.3747
8.3706
7.7739
7.7698
7.7591
7.7550
7.6640
7.6620
7.6595
7.6537
7.6503
7.6477
7.5175
7.5089
7.5052
7.5016
7.4951
7.4927
7.4905
7.4600
7.4574
7.4494
7.4470
7.4441
7.4378
7.4351
7.4332
7.3856
7.3709
7.3143
7.3107
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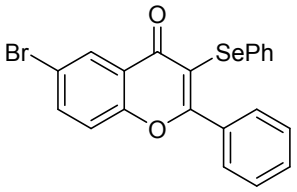
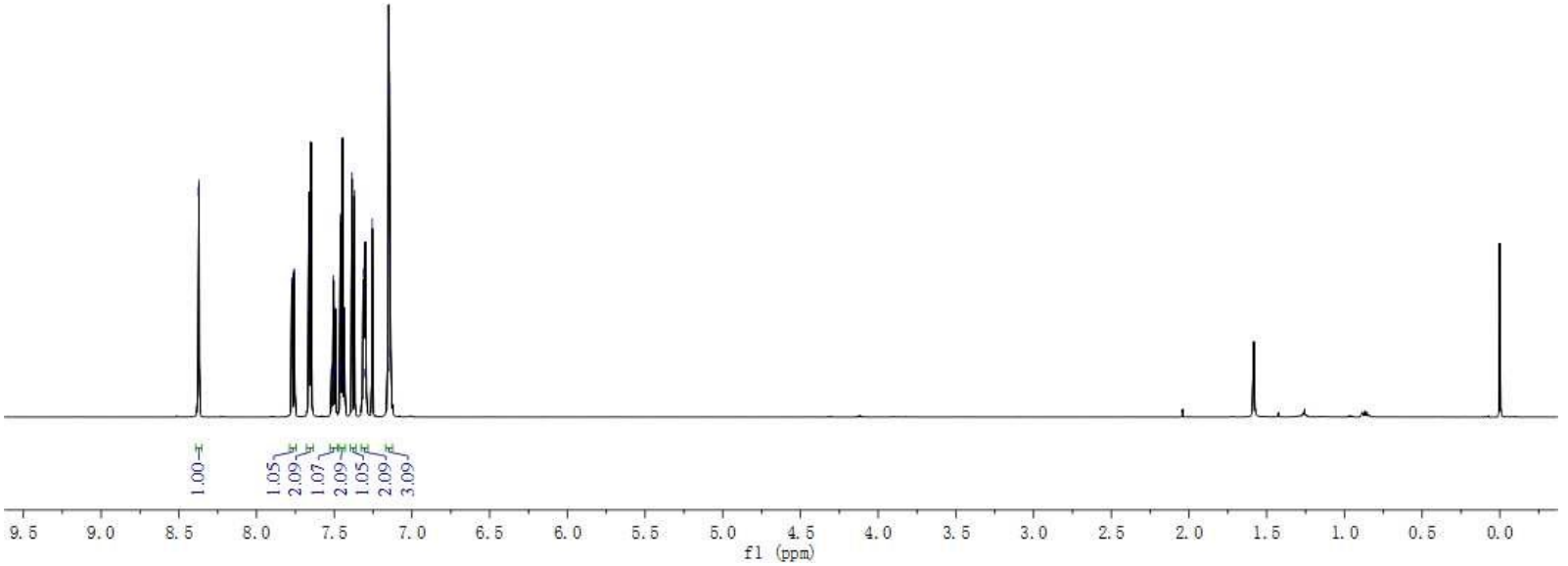
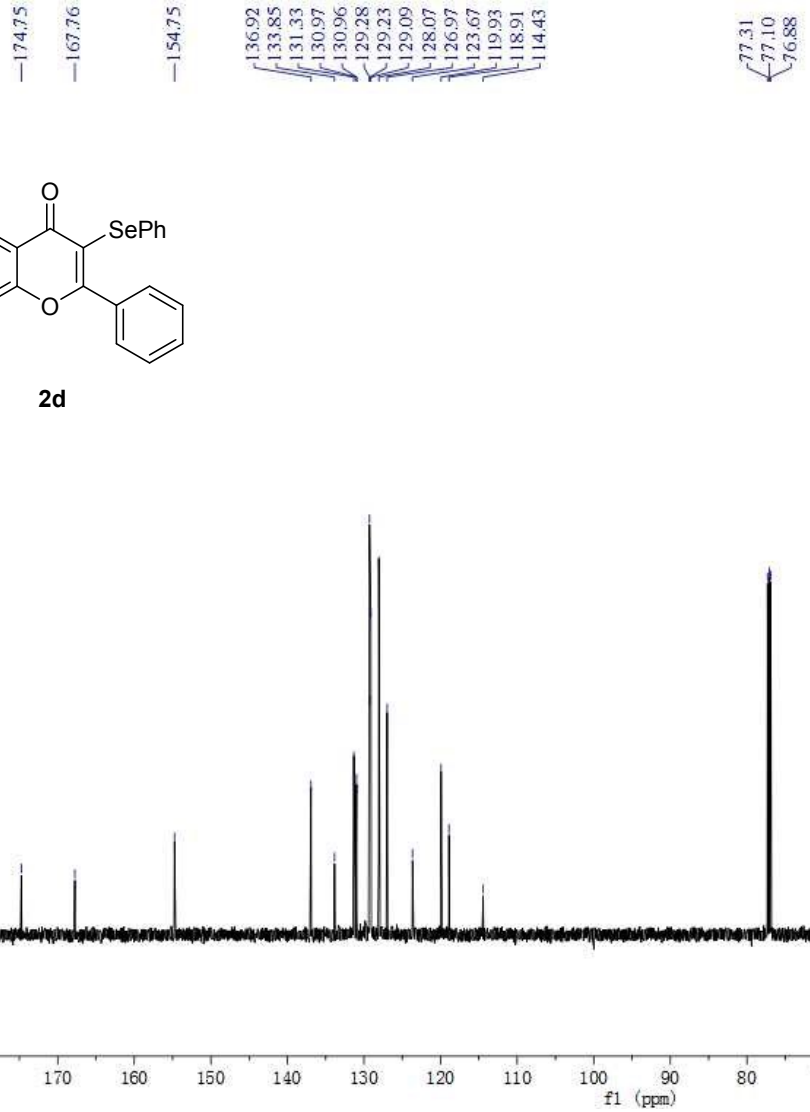
7.1505
7.1467
7.1426
7.1413
7.1391


O
Br
SePh
O

2d


1.00
1.05
2.09
1.07
2.09
1.05
2.09
3.09
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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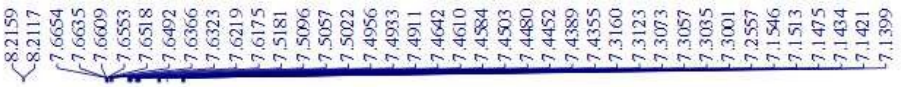
167.76
154.75
136.92
133.85
131.33
130.97
130.96
129.28
129.23
129.09
128.07
126.97
123.67
119.93
118.91
114.43
77.31
77.10
76.88
O
Br
SePh
O
2d
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.2159
8.2117
7.6654
7.6635
7.6609
7.6553
7.6518
7.6492
7.6366
7.6323
7.6219
7.6175
7.5181
7.5096
7.5057
7.5022
7.4956
7.4933
7.4911
7.4642
7.4610
7.4584
7.4503
7.4480
7.4452
7.4389
7.4355
7.3160
7.3123
7.3073
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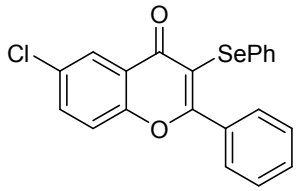
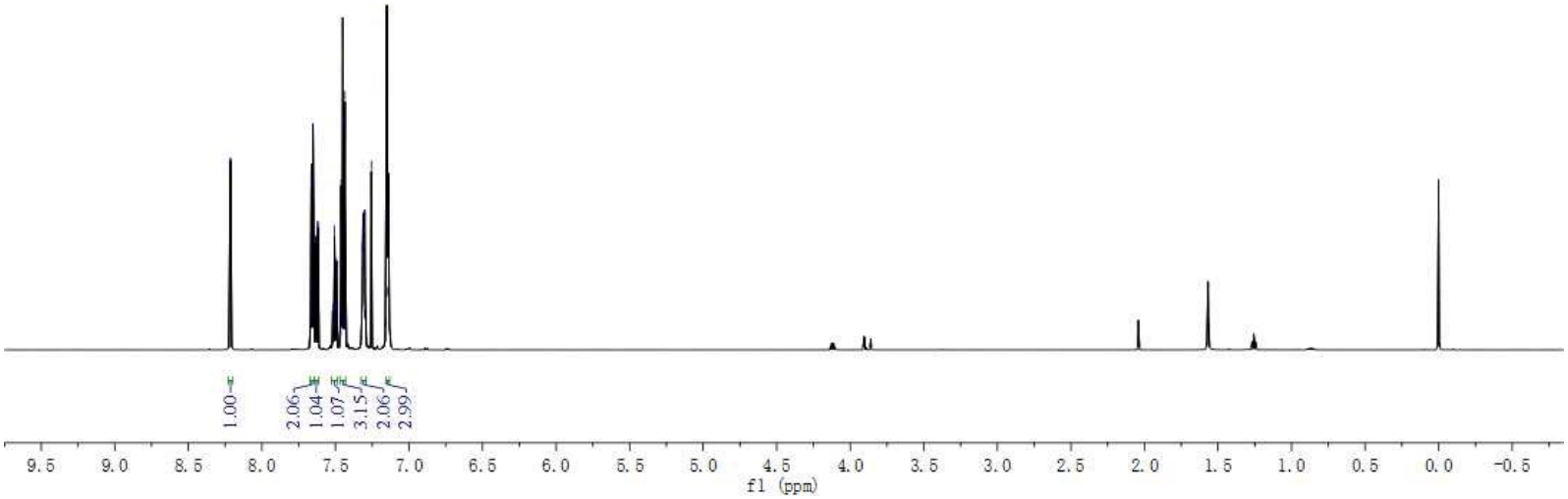
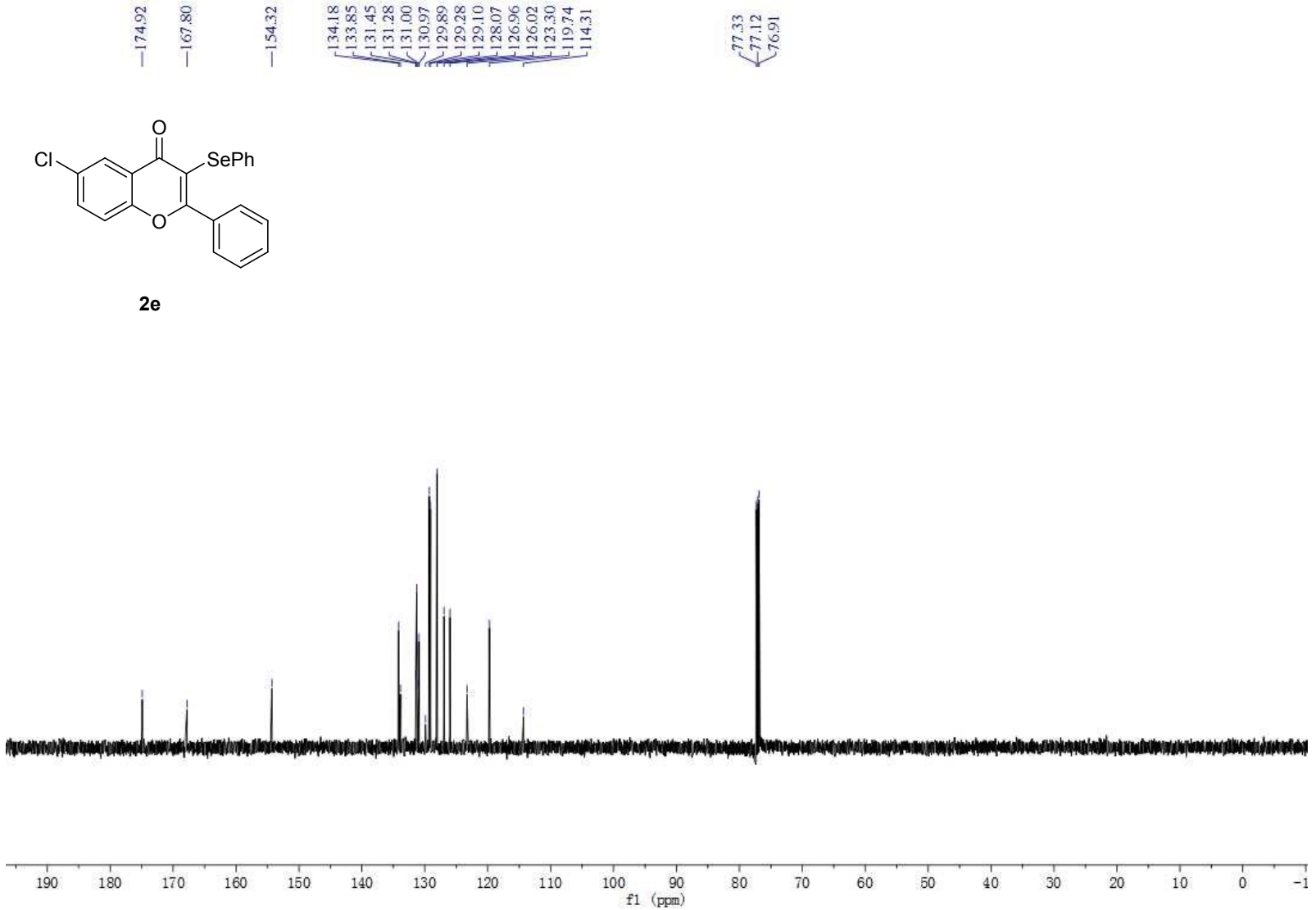
7.1513
7.1475
7.1434
7.1421
7.1399

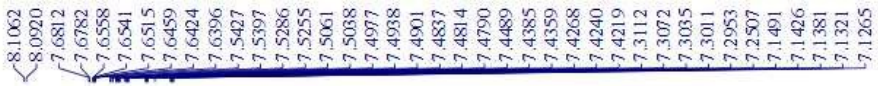

O
Cl
SePh
O

2e


1.00
2.06
1.04
1.07
3.15
2.06
2.99
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


174.92
167.80
154.32
134.18
133.85
131.45
131.28
131.00
130.97
129.89
129.28
129.10
128.07
126.96
126.02
123.30
119.74
114.31
77.33
77.12
76.91
O
Cl
SePh
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

2e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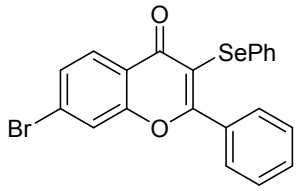
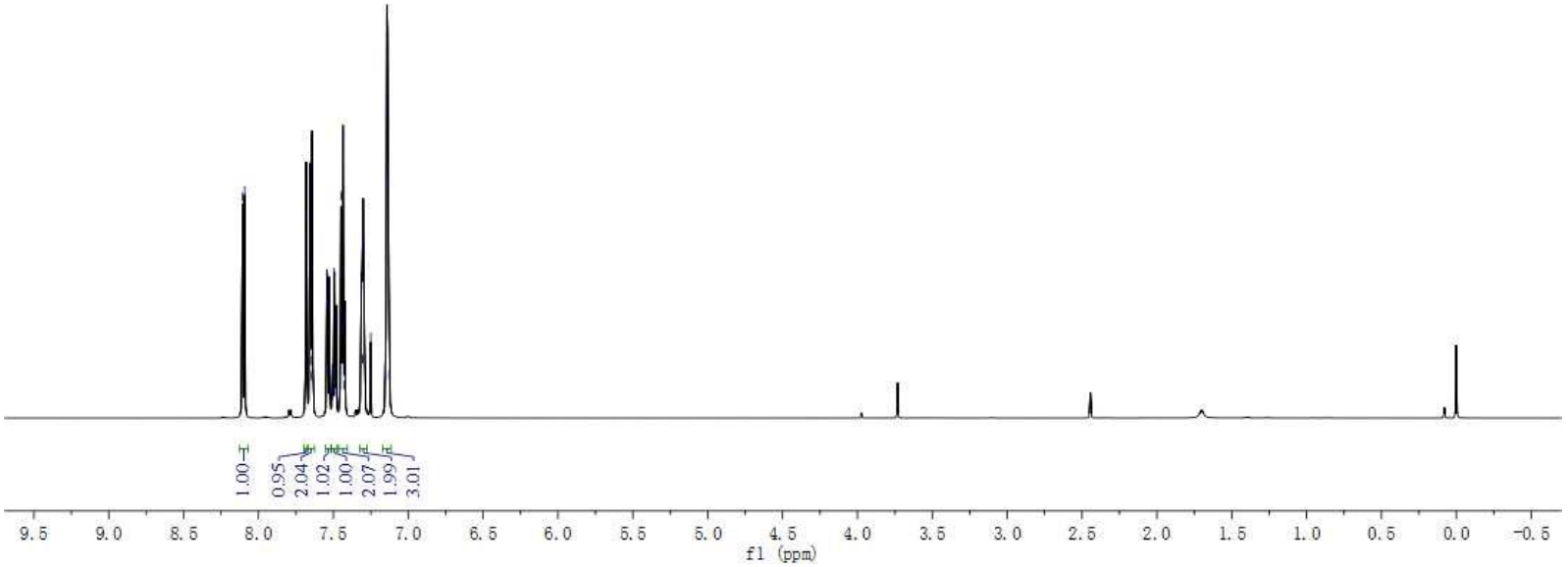
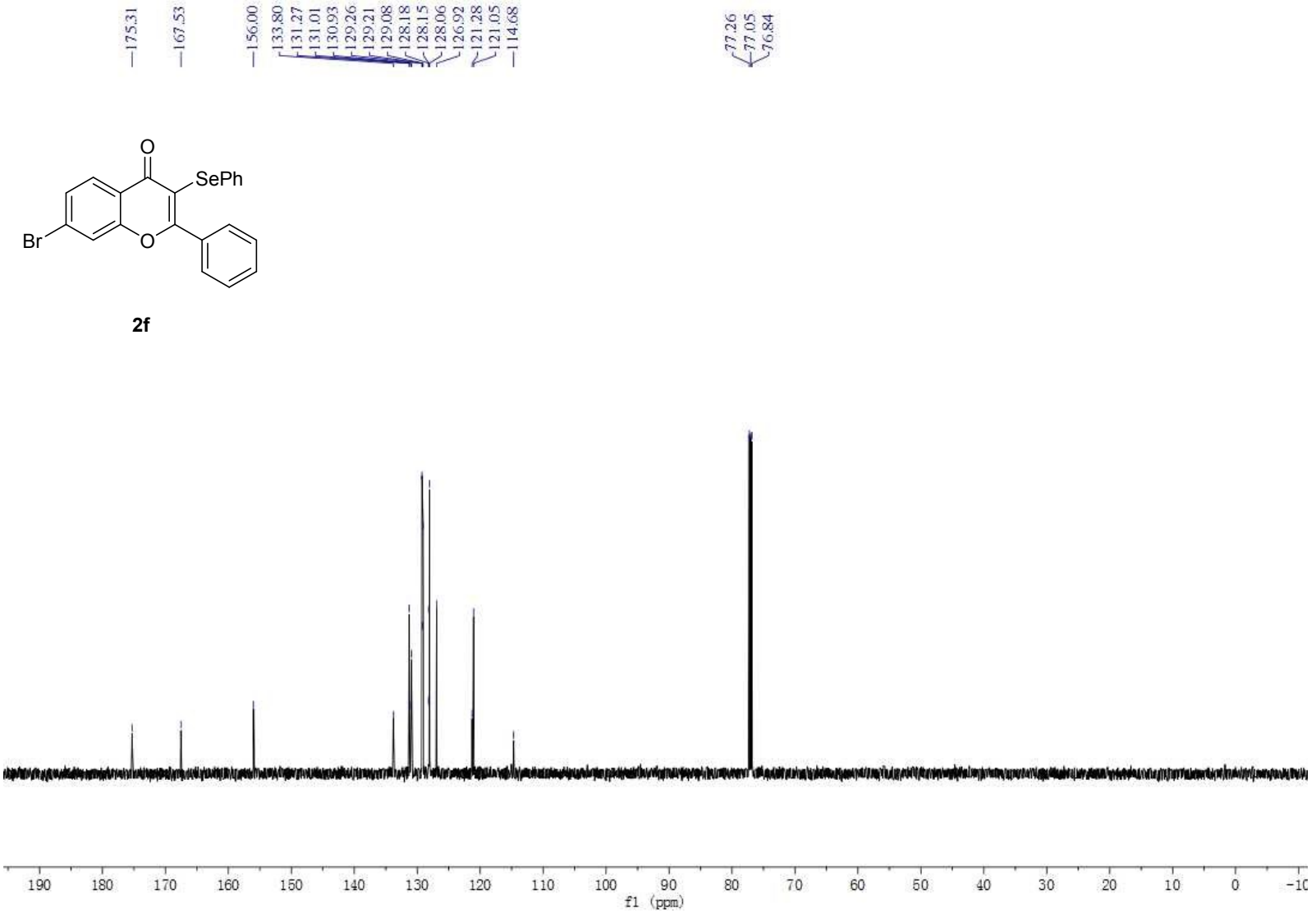
8.0920
7.6812
7.6782
7.6558
7.6541
7.6515
7.6459
7.6424
7.6396
7.5427
7.5397
7.5286
7.5255
7.5061
7.5038
7.4977
7.4938
7.4901
7.4837
7.4814
7.4790
7.4489
7.4385
7.4359
7.4268
7.4240
7.4219
7.3112
7.3072
7.3035
7.3011
7.2953
7.2507
7.1491
7.1426
7.1381
7.1321
7.1265

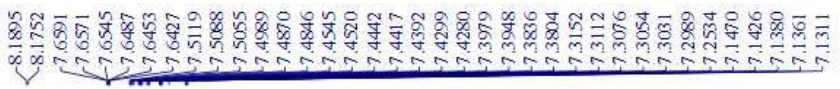

O
SePh
Br
O

2f


1.00
0.95
2.04
1.02
1.00
2.07
1.99
3.01
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


175.31
167.53
156.00
133.80
131.27
131.01
130.93
129.26
129.21
129.08
128.18
128.15
128.06
126.92
121.28
121.05
114.68
77.26
77.05
76.84
O
SePh
Br
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

2f


8.1895
8.1752
7.6591
7.6571
7.6545
7.6487
7.6453
7.6427
7.5119
7.5088
7.5055
7.4989
7.4870
7.4846
7.4545
7.4520
7.4442
7.4417
7.4392
7.4299
7.4280
7.3979
7.3948
7.3836
7.3804
7.3152
7.3112
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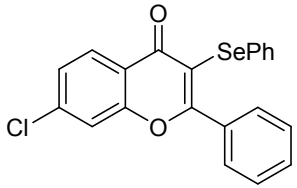
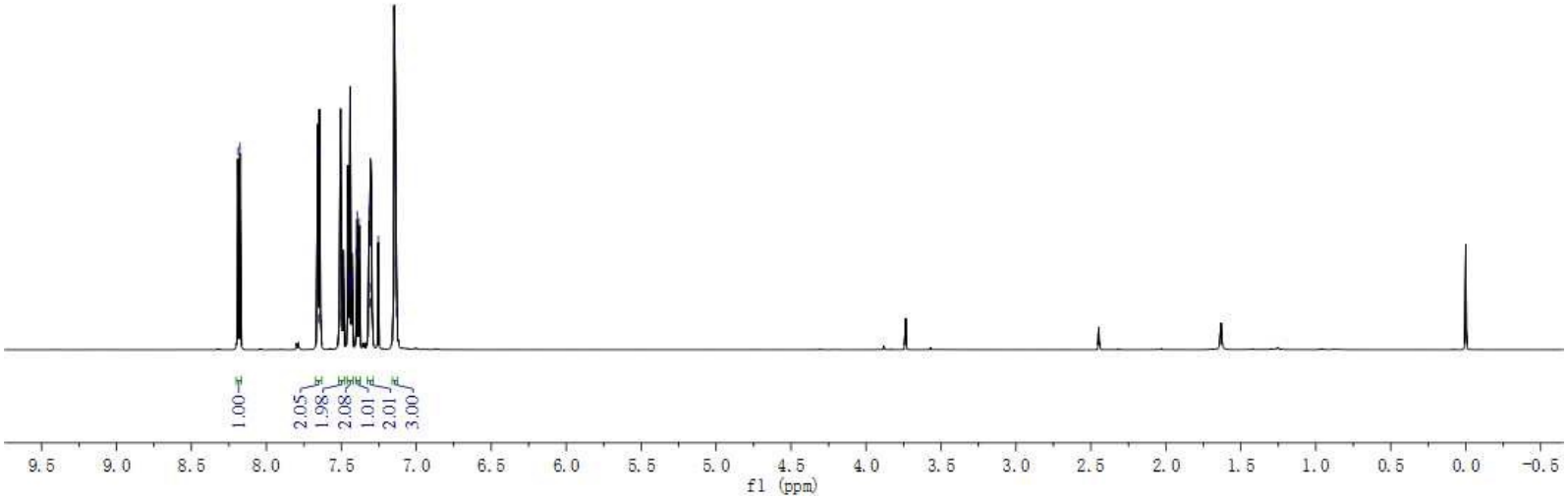
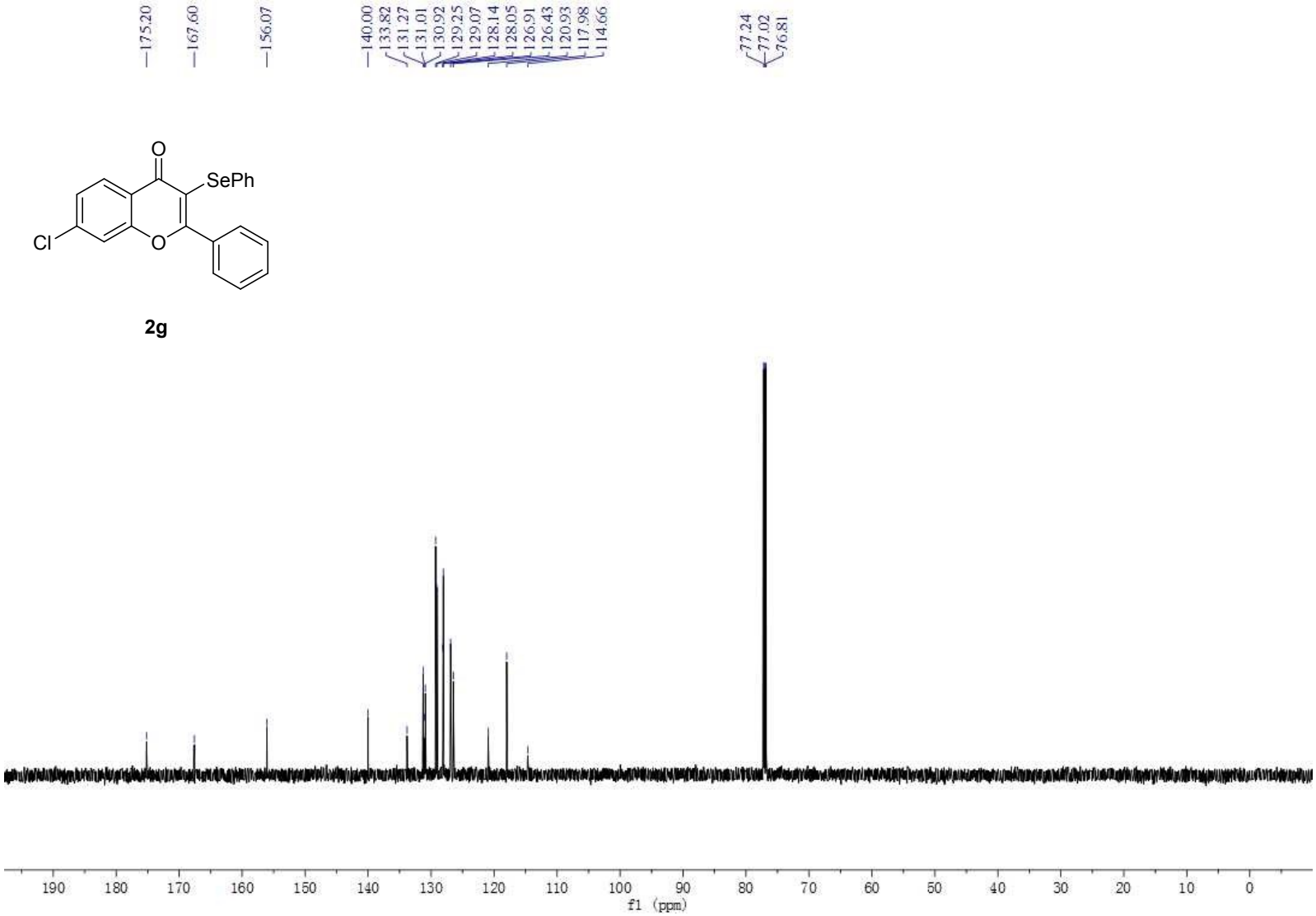
7.1470
7.1426
7.1380
7.1361
7.1311


O
SePh
Cl
O

2g


1.00
2.05
1.98
2.08
1.01
2.01
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
-0.5
f1 (ppm)


175.20
167.60
156.07
140.00
133.82
131.27
131.01
130.92
129.25
129.07
128.14
128.05
126.91
126.43
120.93
117.98
114.66
77.24
77.02
76.81
O
SePh
Cl
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

2g


8.3853
8.3829
8.3646
8.3621
7.8024
7.8007
7.7987
7.7964
7.6941
7.6910
7.6868
7.6791
7.6737
7.6698
7.6666
7.6497
7.6457
7.5413
7.5300
7.5227
7.5166
7.5083
7.5046
7.5008
7.4854
7.4817
7.4796
7.4761
7.4650
7.4609
7.4560
7.4476
7.4435
7.4395
7.3279
7.3240
7.3220
7.3149
7.3125
7.3093
7.3060
7.3036
7.2550
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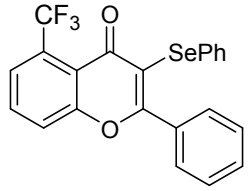
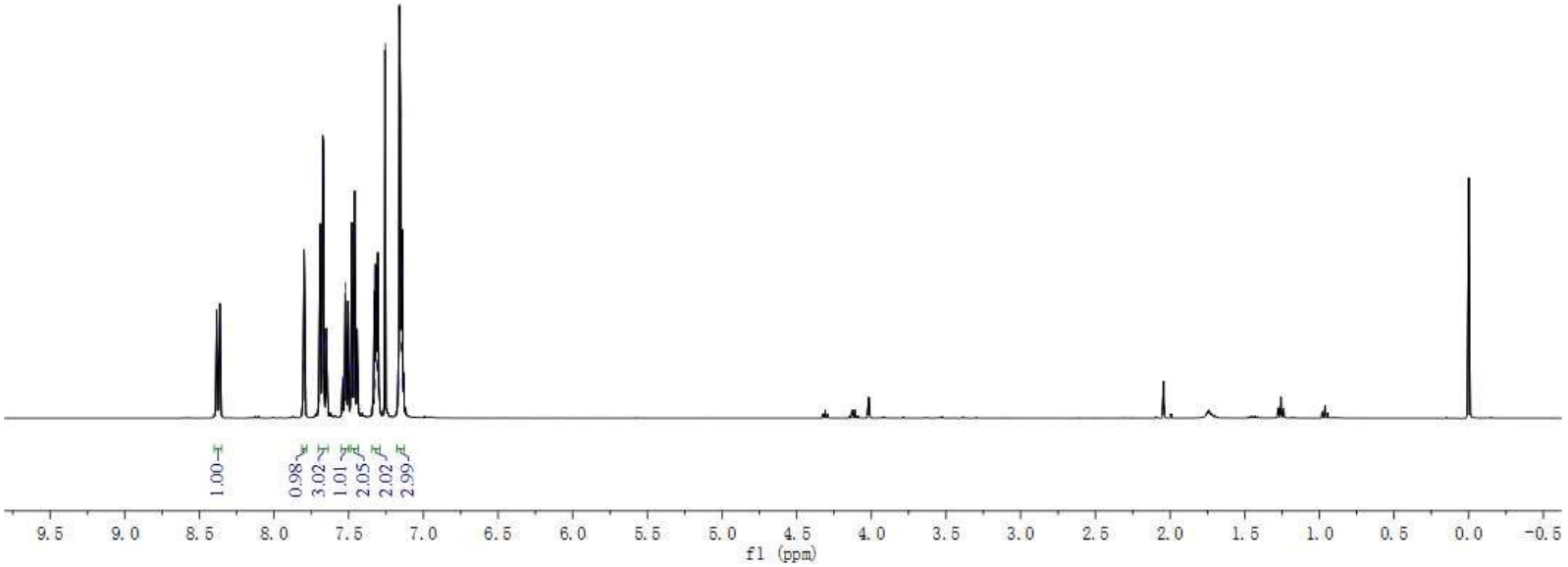
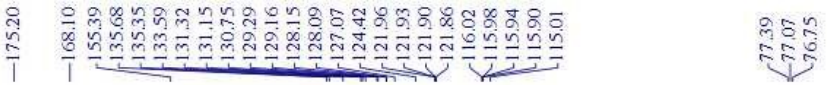
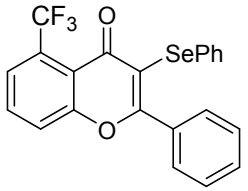
7.1645
7.1597
7.1539
7.1480
7.1457
7.1427
7.1373
7.1340


CF3
O
SePh
O

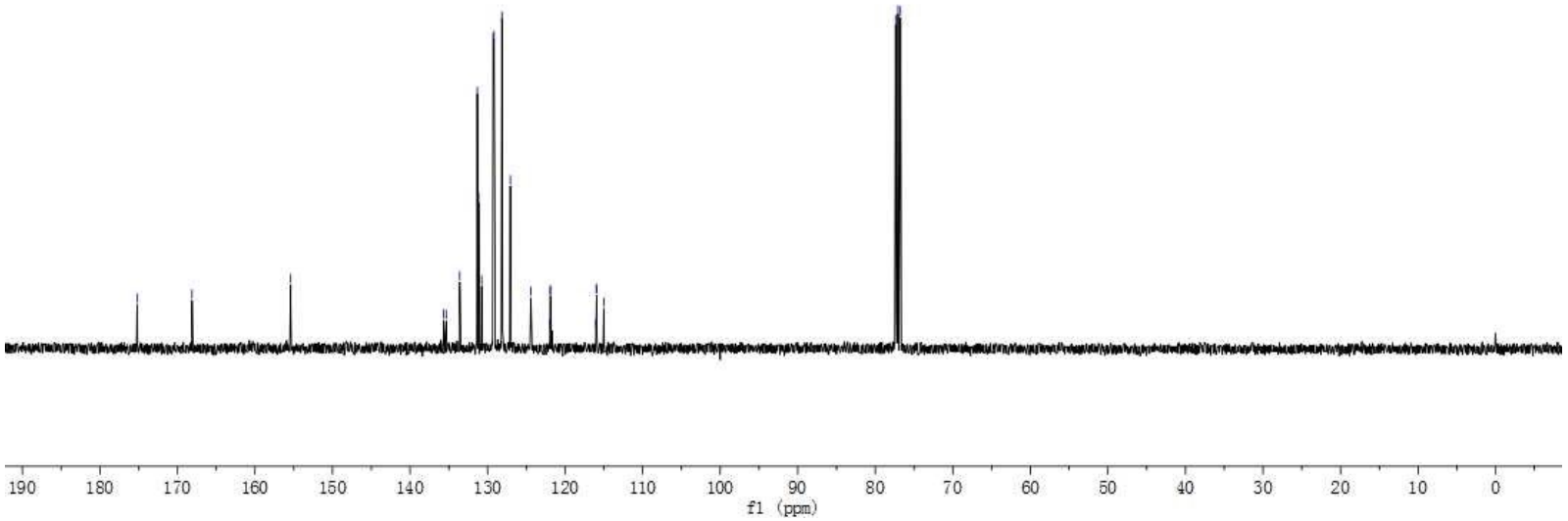
2h

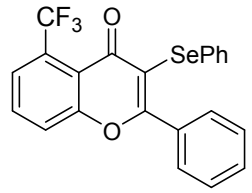

1.00
0.98
3.02
1.01
2.05
2.02
2.99
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


175.20
168.10
155.39
135.68
135.35
133.59
131.32
131.15
130.75
129.29
129.16
128.15
128.09
127.07
124.42
121.96
121.93
121.90
121.86
116.02
115.98
115.94
115.90
115.01
77.39
77.07
76.75


CF3
O
SePh
O

2h

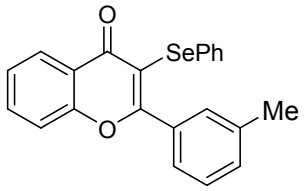

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


CF3
O
SePh
O

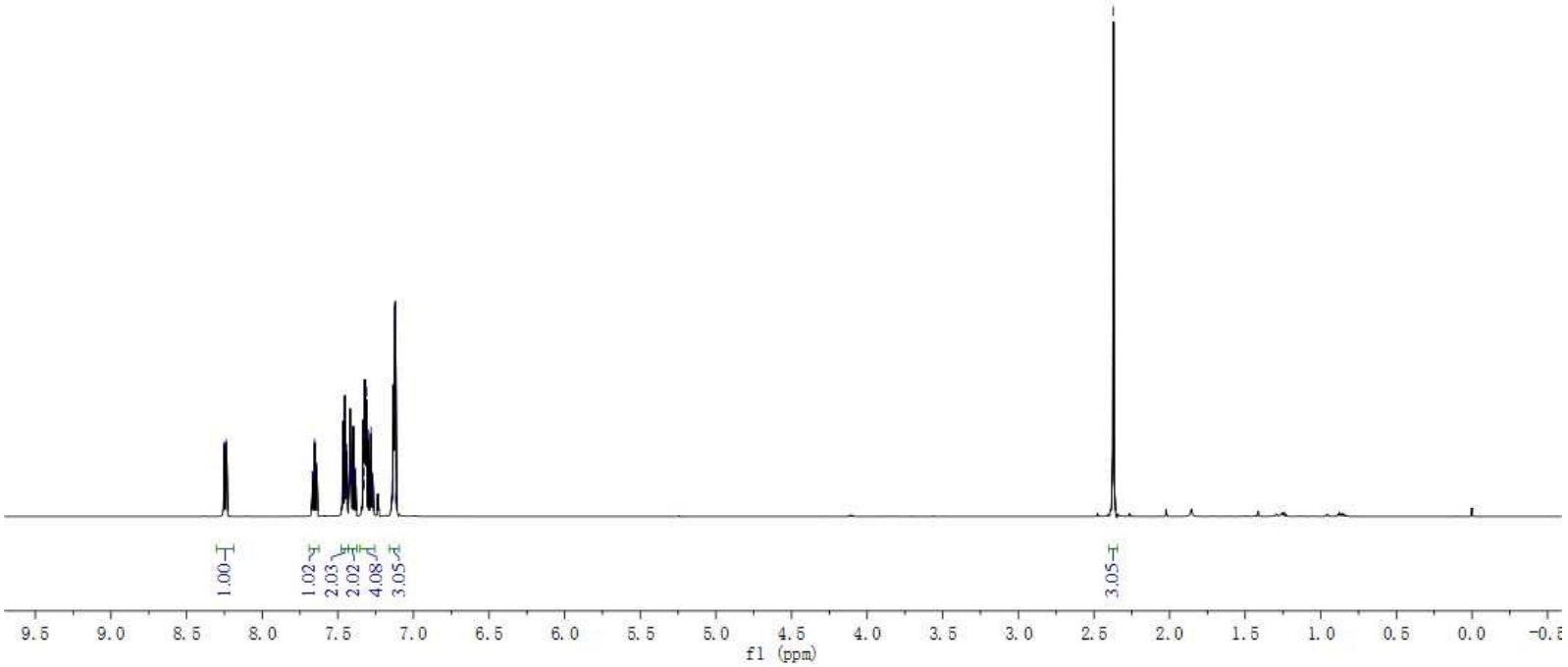
2h

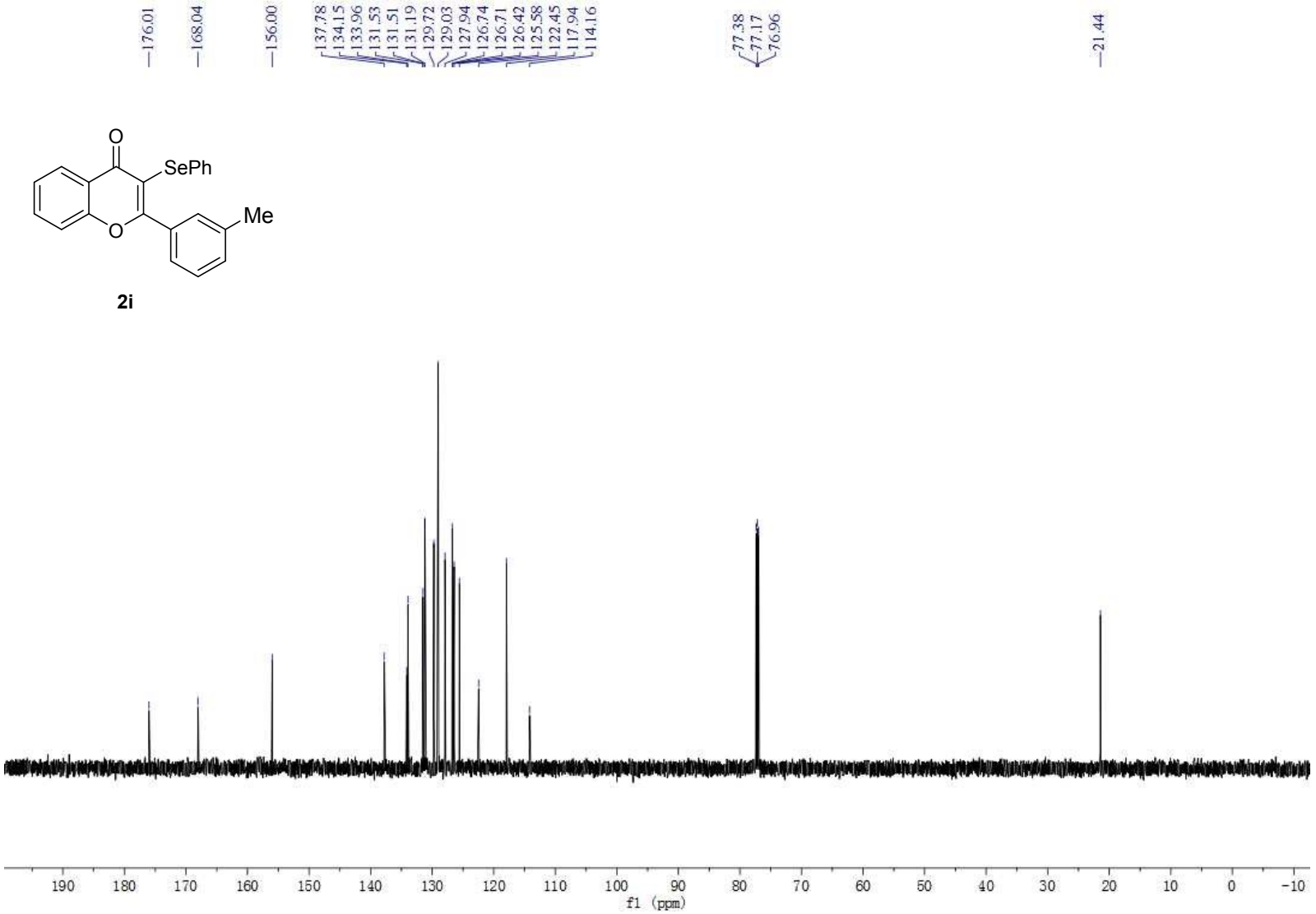
-63.10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)


8.2524
8.2495
8.2391
8.2362
7.6684
7.6655
7.6566
7.6541
7.6515
7.6425
7.6396
7.4670
7.4653
7.4530
7.4513
7.4422
7.4215
7.4185
7.4171
7.4153
7.4099
7.4082
7.3981
7.3964
7.3948
7.3848
7.3830
7.3306
7.3254
7.3230
7.3179
7.3144
7.3097
7.2973
7.2816
7.2687
7.1376
7.1309
7.1279
7.1229
7.1193
2.3712

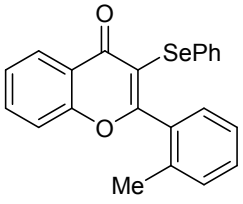

O
SePh
Me
O

2i

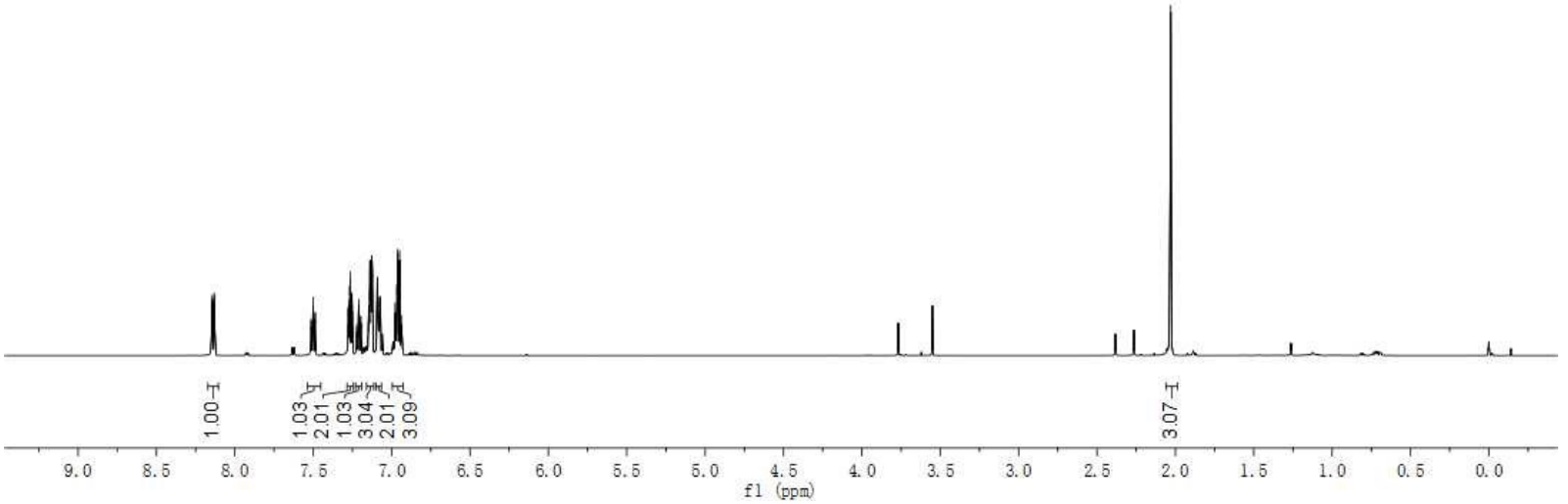

1.00
1.02
2.03
2.02
4.08
3.05
3.05
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

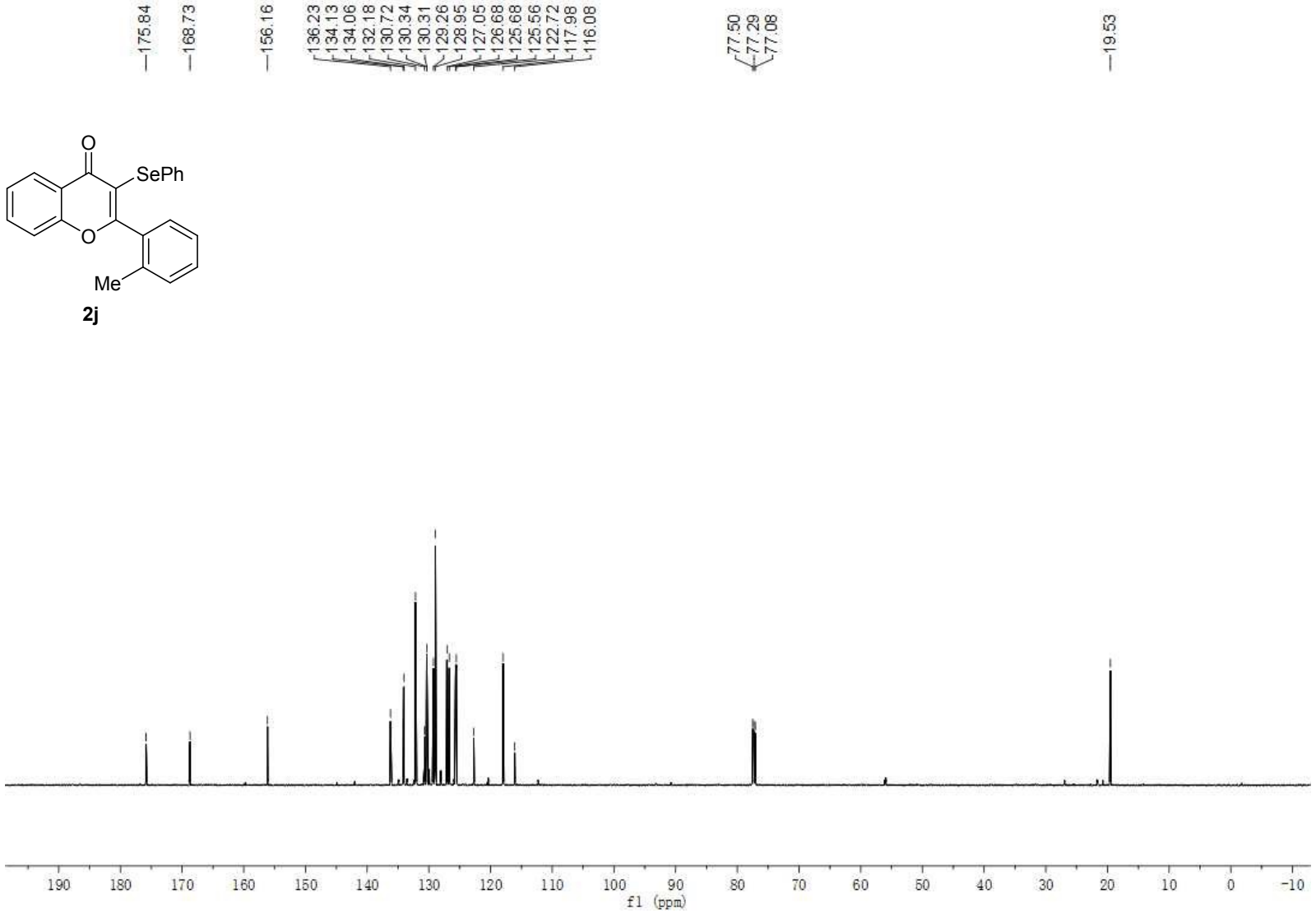

176.01
168.04
156.00
137.78
134.15
133.96
131.53
131.51
131.19
129.72
129.03
127.94
126.74
126.71
126.42
125.58
122.45
117.94
114.16
77.38
77.17
76.96
21.44
O
SePh
O
Me
2i
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.1460
8.1430
8.1322
8.1295
7.5147
7.5119
7.5027
7.5004
7.4977
7.4887
7.4859
7.2748
7.2696
7.2676
7.2627
7.2556
7.2537
7.2509
7.2208
7.2107
7.2082
7.1980
7.1955
7.1460
7.1438
7.1397
7.1373
7.1341
7.1308
7.1265
7.1236
7.0925
7.0903
7.0857
7.0786
7.0737
7.0718
6.9776
6.9691
6.9664
6.9613
6.9583
6.9529
6.9486
2.0303

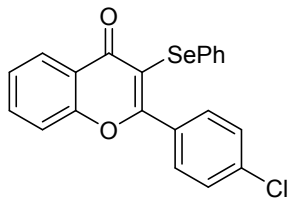

O
SePh
O
Me

2j

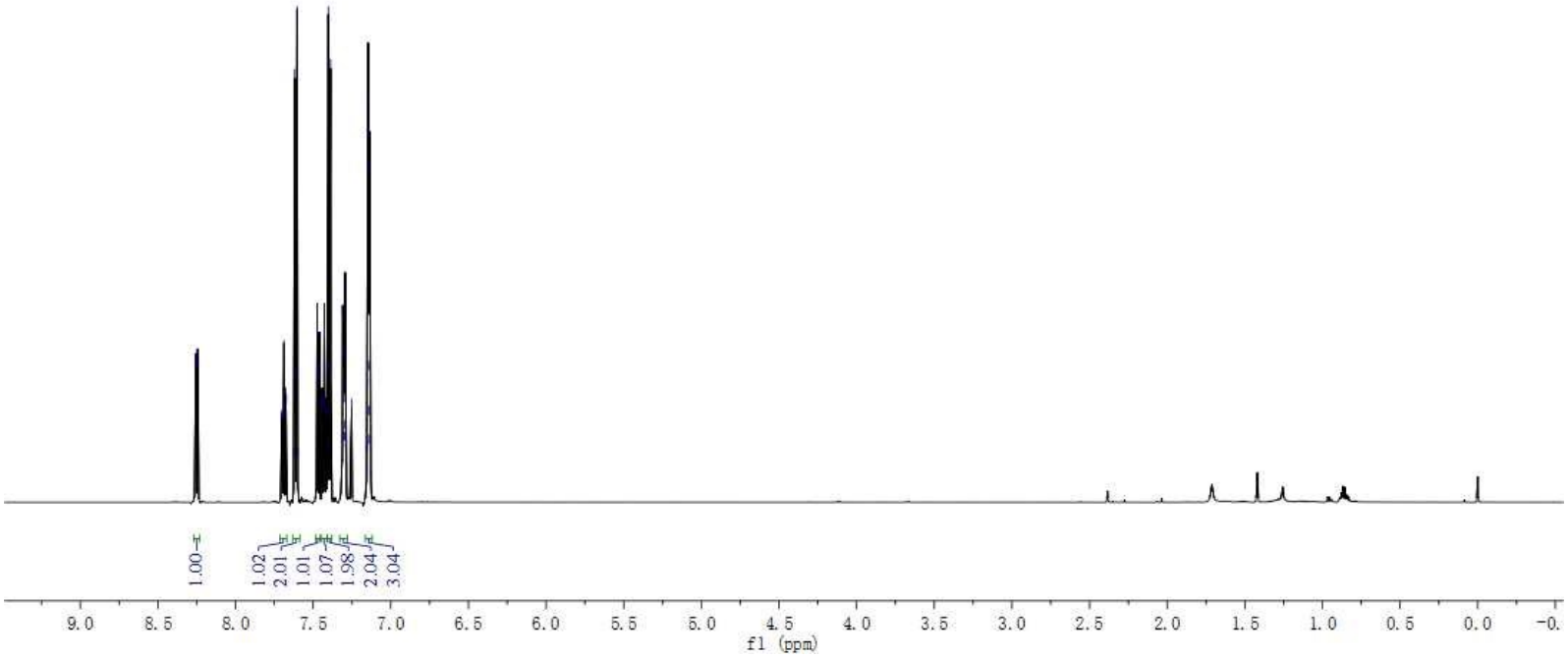

1.00
1.03
2.01
1.03
3.04
2.01
3.09
3.07
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

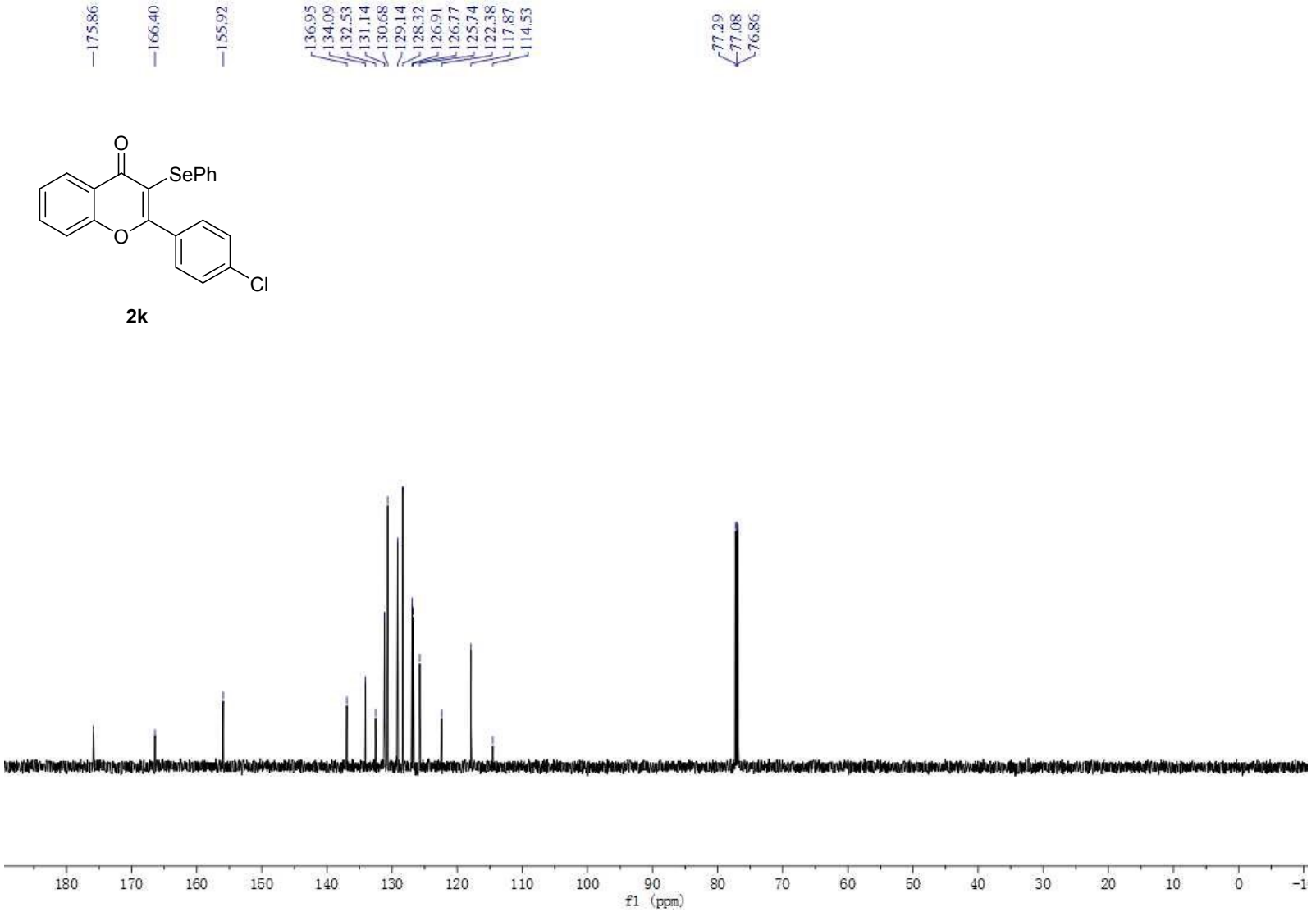

175.84
168.73
156.16
136.23
134.13
134.06
132.18
130.72
130.34
130.31
129.26
128.95
127.05
126.68
125.68
125.56
122.72
117.98
116.08
77.50
77.29
77.08
19.53
O
SePh
O
Me
2j
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.2566
8.2538
8.2432
8.2405
7.7025
7.6997
7.6907
7.6881
7.6856
7.6766
7.6738
7.6228
7.6186
7.6154
7.6077
7.6043
7.6002
7.4749
7.4732
7.4608
7.4592
7.4415
7.4397
7.4296
7.4281
7.4265
7.4163
7.4146
7.4064
7.4022
7.3989
7.3912
7.3879
7.3101
7.3077
7.3055
7.3028
7.3007
7.2995
7.2978
7.2962
7.2941
7.2918
7.2520
7.1530
7.1490
7.1466
7.1442
7.1415
7.1391
7.1380
7.1358
7.1330
7.1317

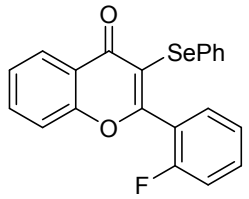

O
SePh
O
Cl

2k

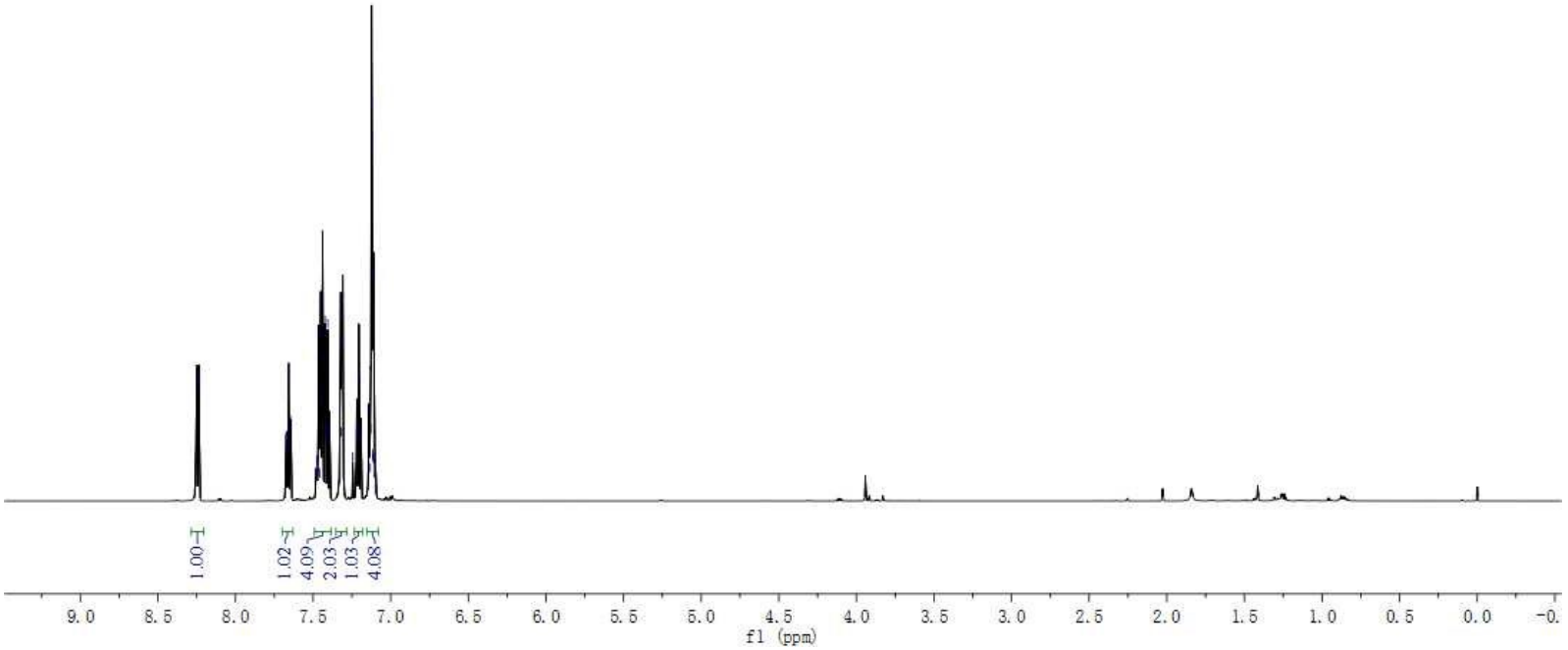

1.00
1.02
2.01
1.01
1.07
1.98
2.04
3.04
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)

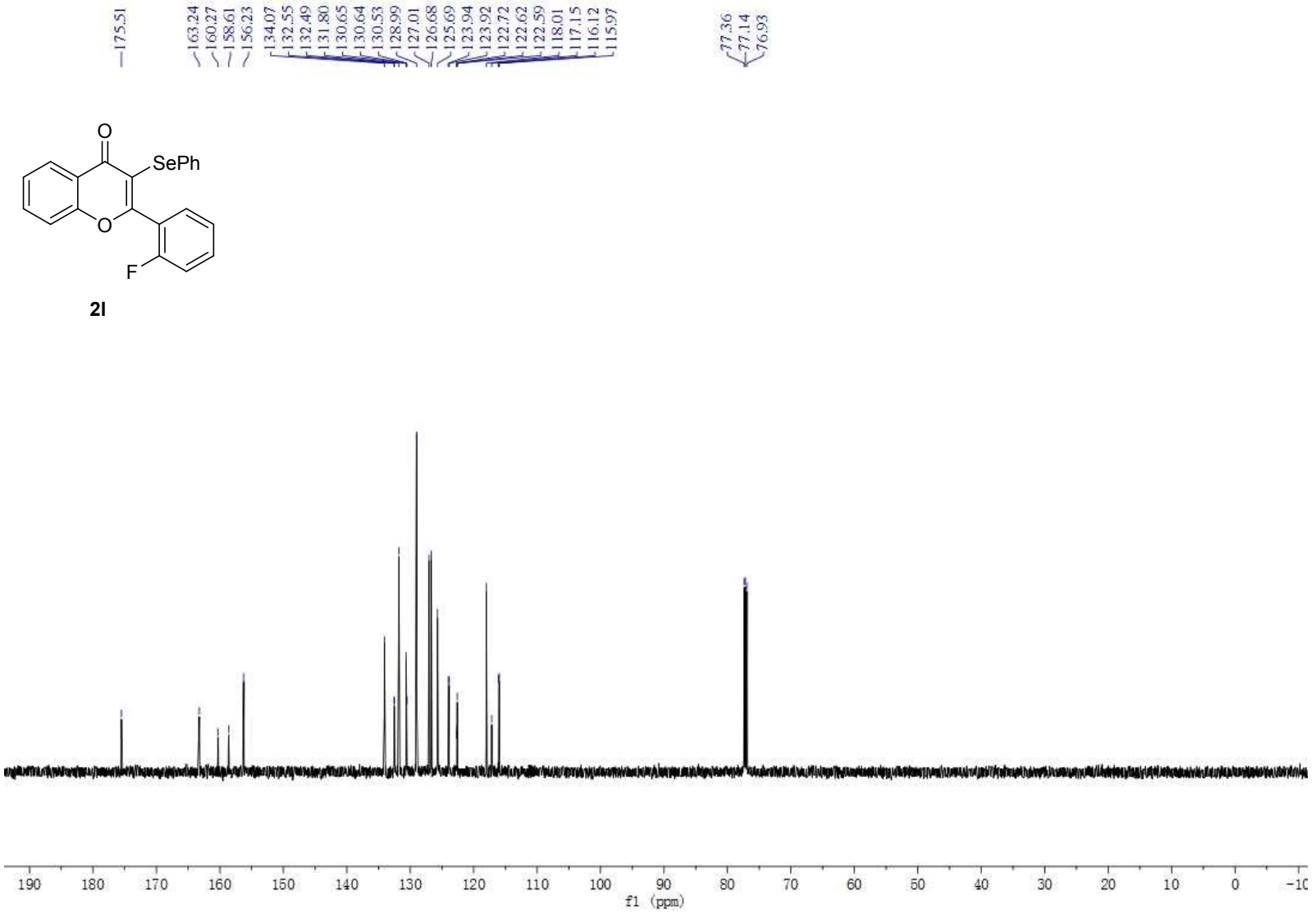

175.86
166.40
155.92
136.95
134.09
132.53
131.14
130.68
129.14
128.32
126.91
126.77
125.74
122.38
117.87
114.53
77.29
77.08
76.86
O
SePh
O
Cl
2k
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)


8.2525
8.2496
8.2391
8.2363
7.6728
7.6699
7.6610
7.6584
7.6558
7.6467
7.6439
7.4792
7.4762
7.4705
7.4673
7.4633
7.4577
7.4534
7.4505
7.4396
7.4377
7.4244
7.4200
7.4184
7.4067
7.3948
7.3932
7.3297
7.3247
7.3214
7.3173
7.3130
7.3086
7.2444
7.2193
7.2177
7.2067
7.2050
7.1940
7.1924
7.1390
7.1324
7.1294
7.1242
7.1212
7.1168
7.1146
7.1117
7.1072
7.1036
7.0996
7.0970


O
SePh
O
F

2l


1.00
1.02
4.09
2.03
1.03
4.08
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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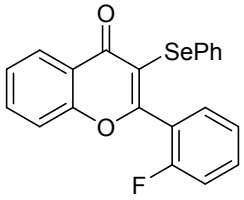
163.24
160.27
158.61
156.23
134.07
132.55
132.49
131.80
130.65
130.64
130.53
128.99
127.01
126.68
125.69
123.94
123.92
122.72
122.62
122.59
118.01
117.15
116.12
115.97
77.36
77.14
76.93
O
SePh
O
F
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

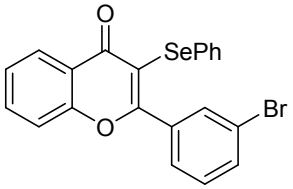
2l


O
SePh
O
F

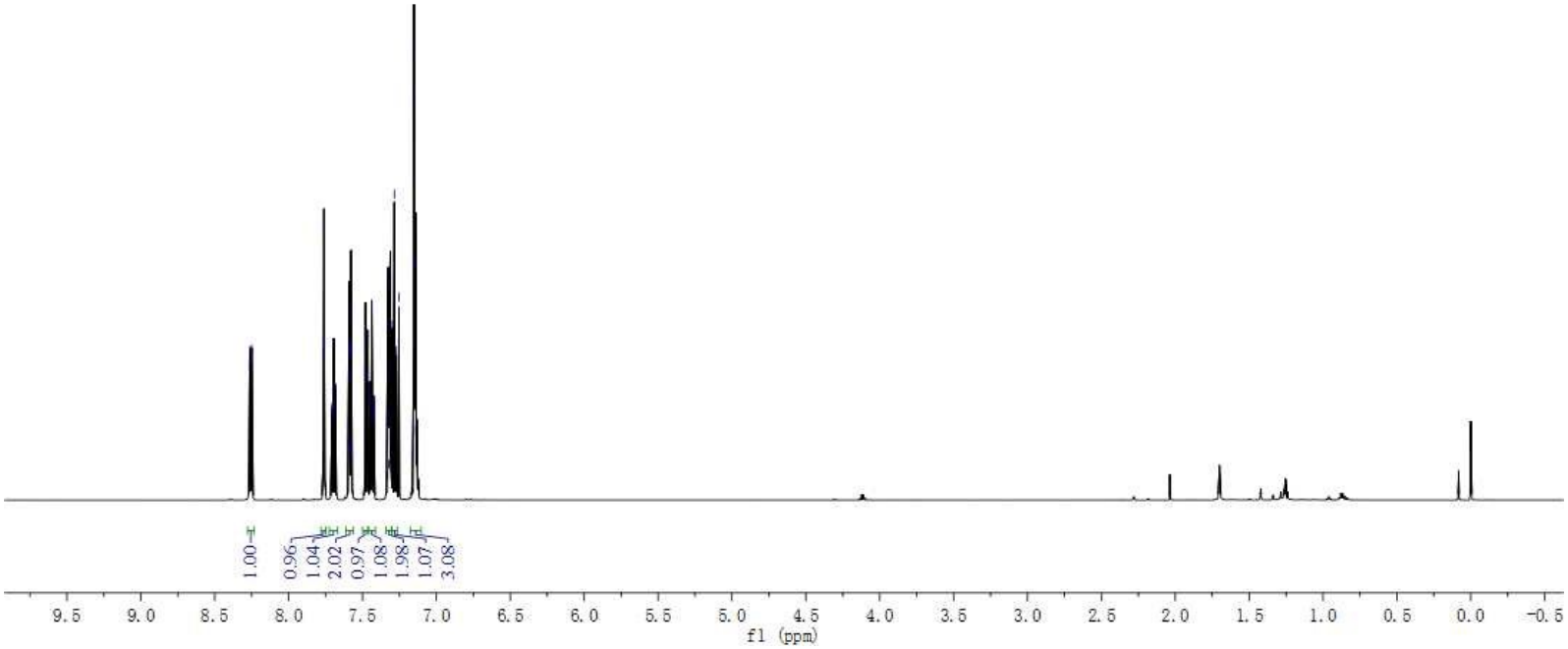
2l

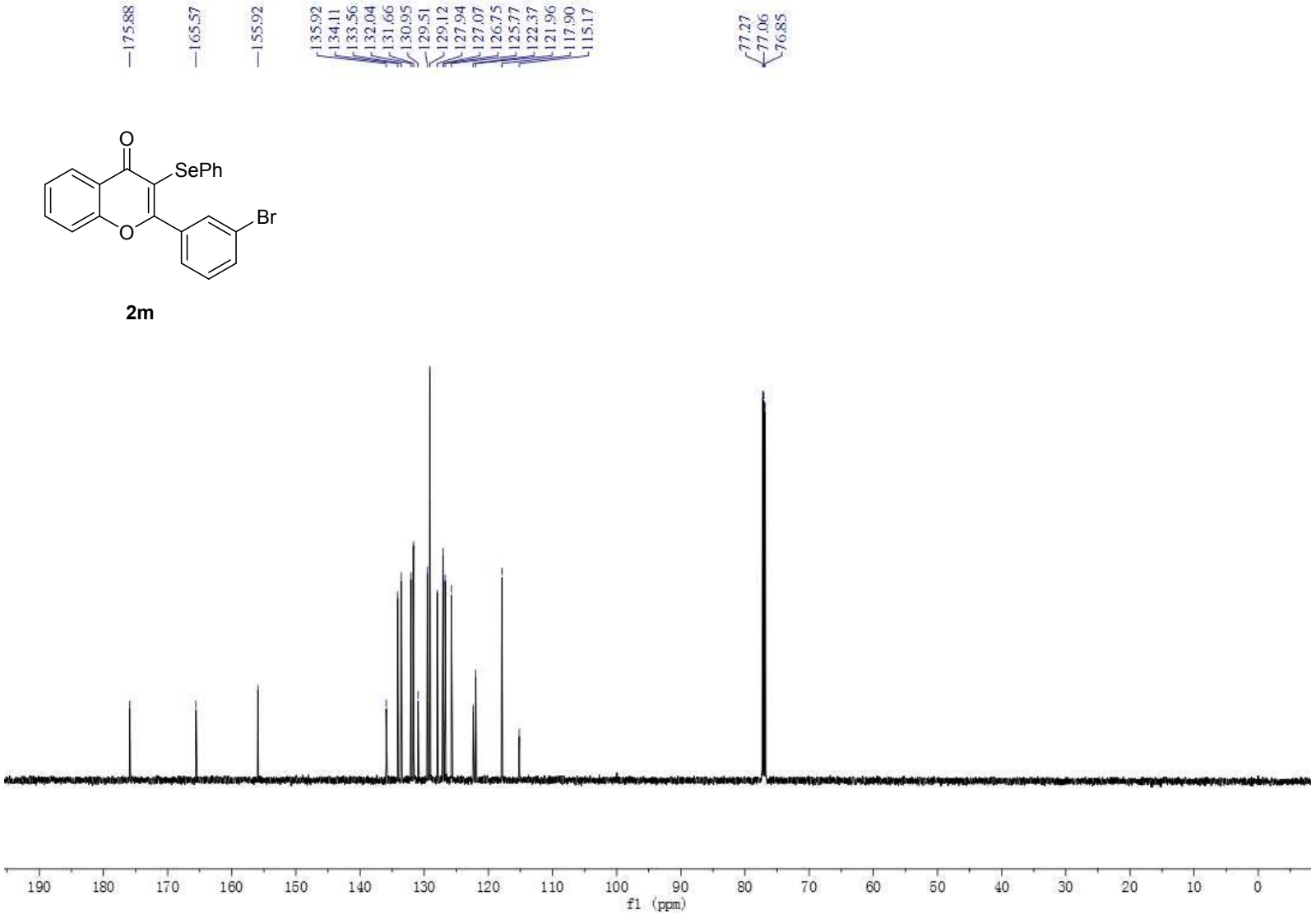
-111.59
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-21
f1 (ppm)


8.2648
8.2621
8.2515
8.2488
7.7630
7.7600
7.7570
7.7090
7.7062
7.6972
7.6947
7.6921
7.6830
7.6802
7.5952
7.5935
7.5913
7.5899
7.5883
7.5866
7.5819
7.5801
7.5782
7.5768
7.5752
7.5734
7.4805
7.4789
7.4665
7.4648
7.4504
7.4486
7.4385
7.4369
7.4352
7.4252
7.4234
7.3299
7.3282
7.3248
7.3222
7.3201
7.3192
7.3175
7.3158
7.3135
7.3122
7.2978
7.2846
7.2714
7.2535
7.1552
7.1528
7.1511
7.1477
7.1426
7.1395
7.1326

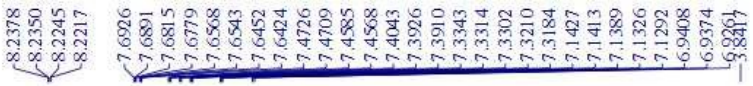

O
SePh
Br
O

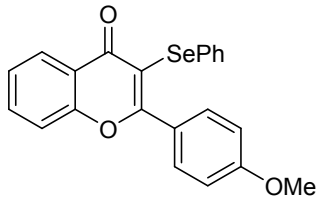
2m


1.00
0.96
1.04
2.02
0.97
1.08
1.98
1.07
3.08
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

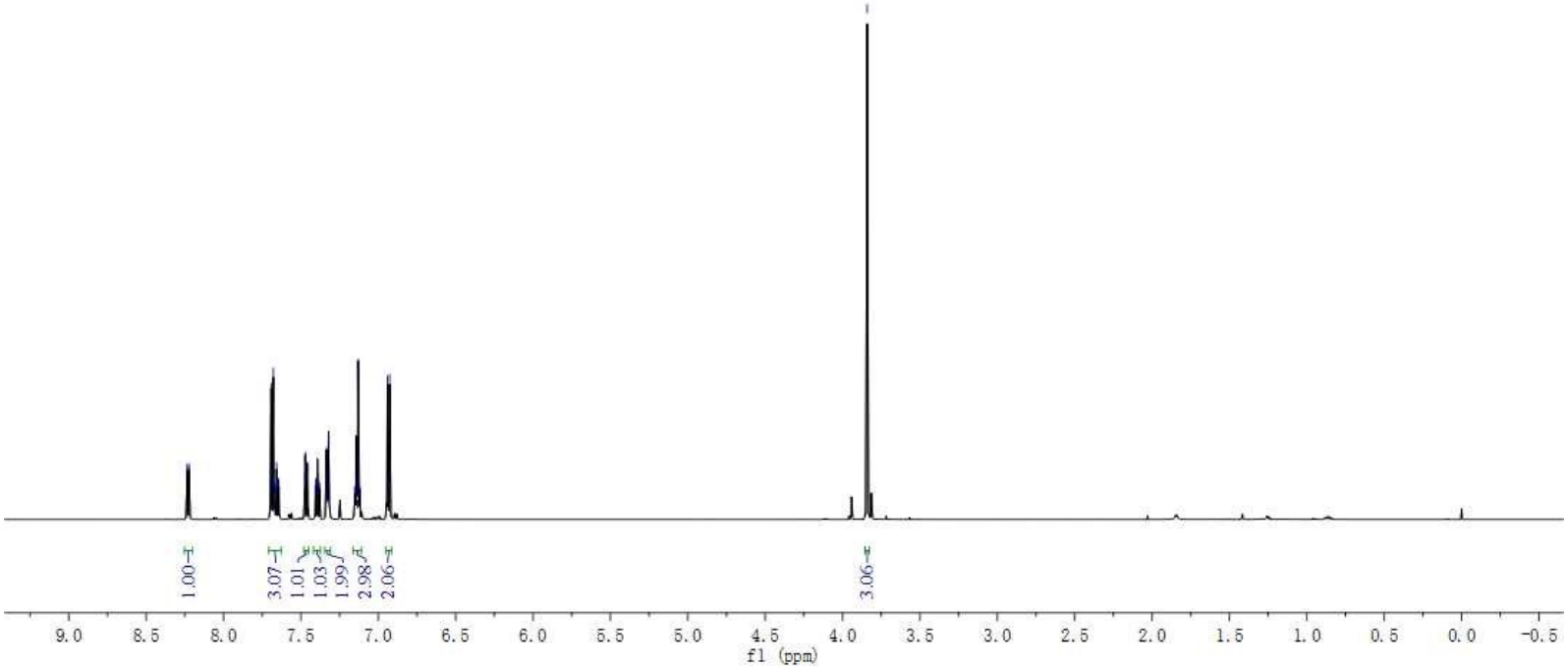

175.88
165.57
155.92
135.92
134.11
133.56
132.04
131.66
130.95
129.51
129.12
127.94
127.07
126.75
125.77
122.37
121.96
117.90
115.17
77.27
77.06
76.85
O
SePh
O
Br
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

2m


8.2378
8.2350
8.2245
8.2217
7.6926
7.6891
7.6815
7.6779
7.6568
7.6543
7.6452
7.6424
7.4726
7.4709
7.4585
7.4568
7.4043
7.3926
7.3910
7.3343
7.3314
7.3302
7.3210
7.3184
7.1427
7.1413
7.1389
7.1326
7.1292
6.9408
6.9374
6.9261
3.8417


O
SePh
O
OMe

2n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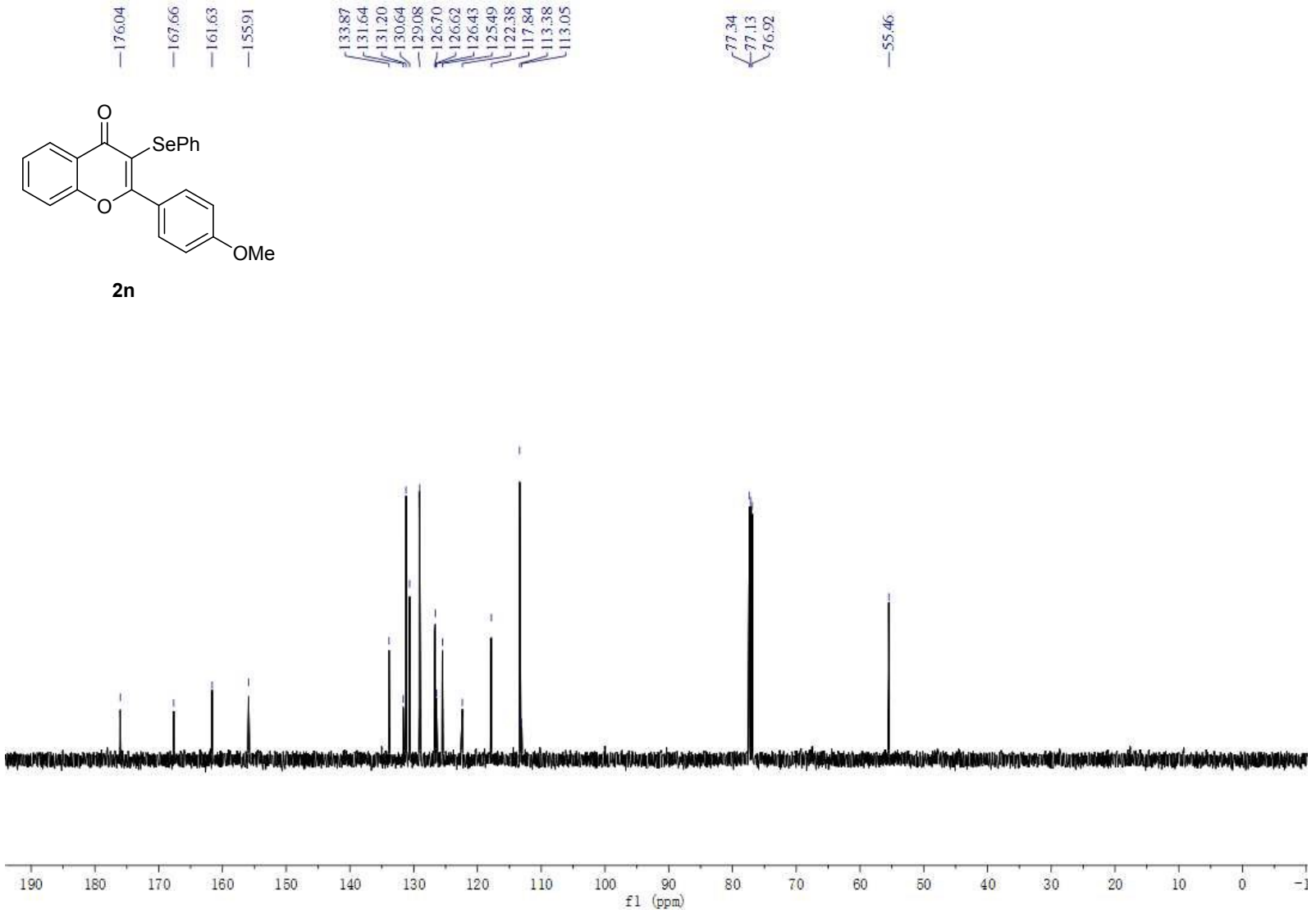
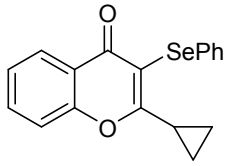
3.07
1.01
1.03
1.99
2.98
2.06
3.06
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

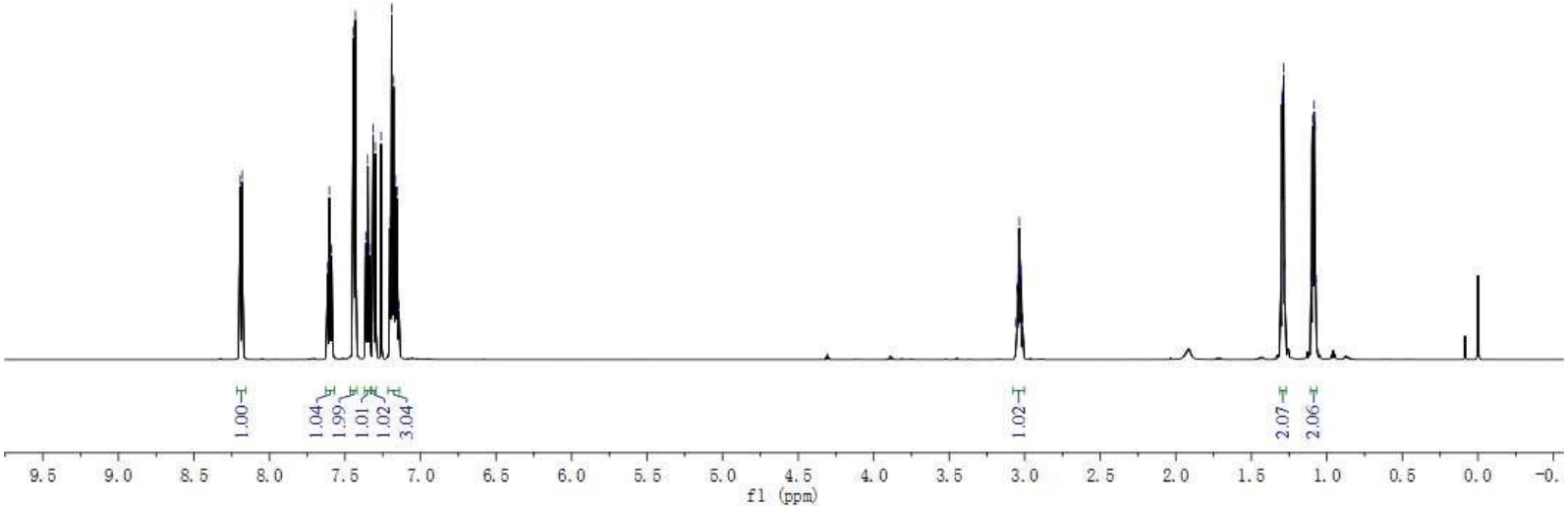

176.04
167.66
161.63
155.91
133.87
131.64
131.20
130.64
129.08
126.70
126.62
126.43
125.49
122.38
117.84
113.38
113.05
77.34
77.13
76.92
55.46
O
SePh
O
OMe
f1 (ppm)

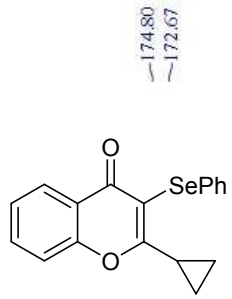
2n


8.1934
8.1802
7.6145
7.6027
7.5886
7.4441
7.4320
7.3625
7.3499
7.3374
7.3134
7.2994
7.2608
7.2022
7.1906
7.1778
7.1664
7.1546
7.1426
3.0583
3.0500
3.0444
3.0363
3.0282
3.0225
3.0142
1.3051
1.2978
1.2933
1.2899
1.2852
1.2782
1.1048
1.0981
1.0933
1.0844
1.0796
1.0722


O
SePh
O

2o

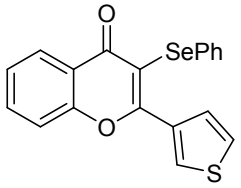

1.00
1.04
1.99
1.01
1.02
3.04
1.02
2.07
2.06
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


O
SePh
O

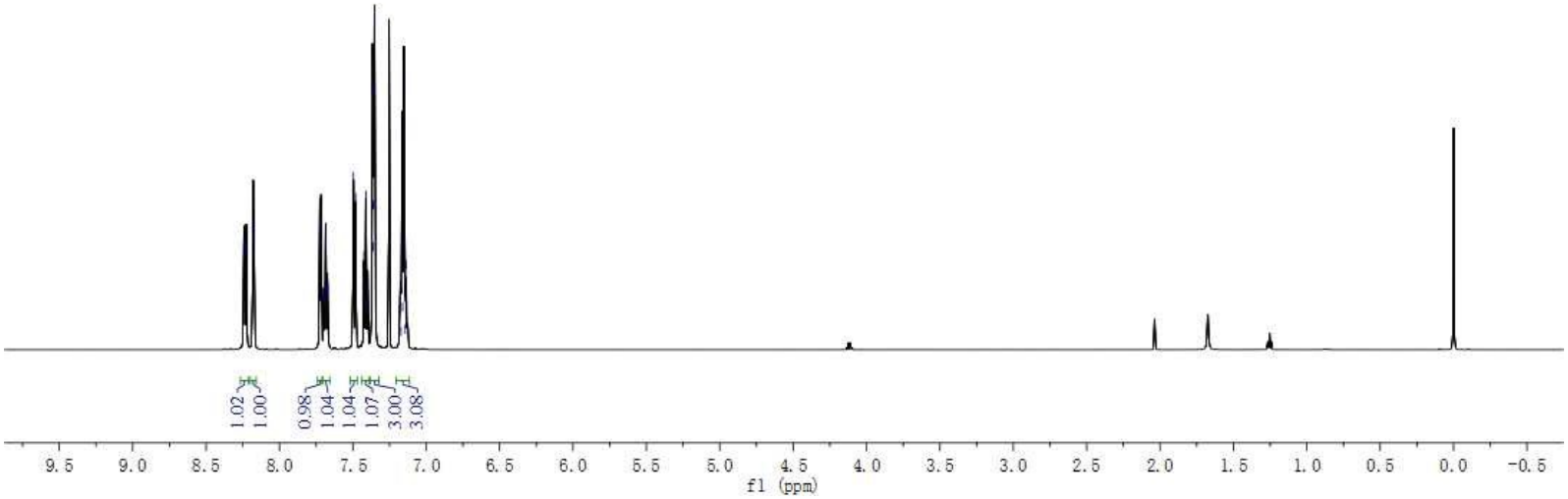
2o

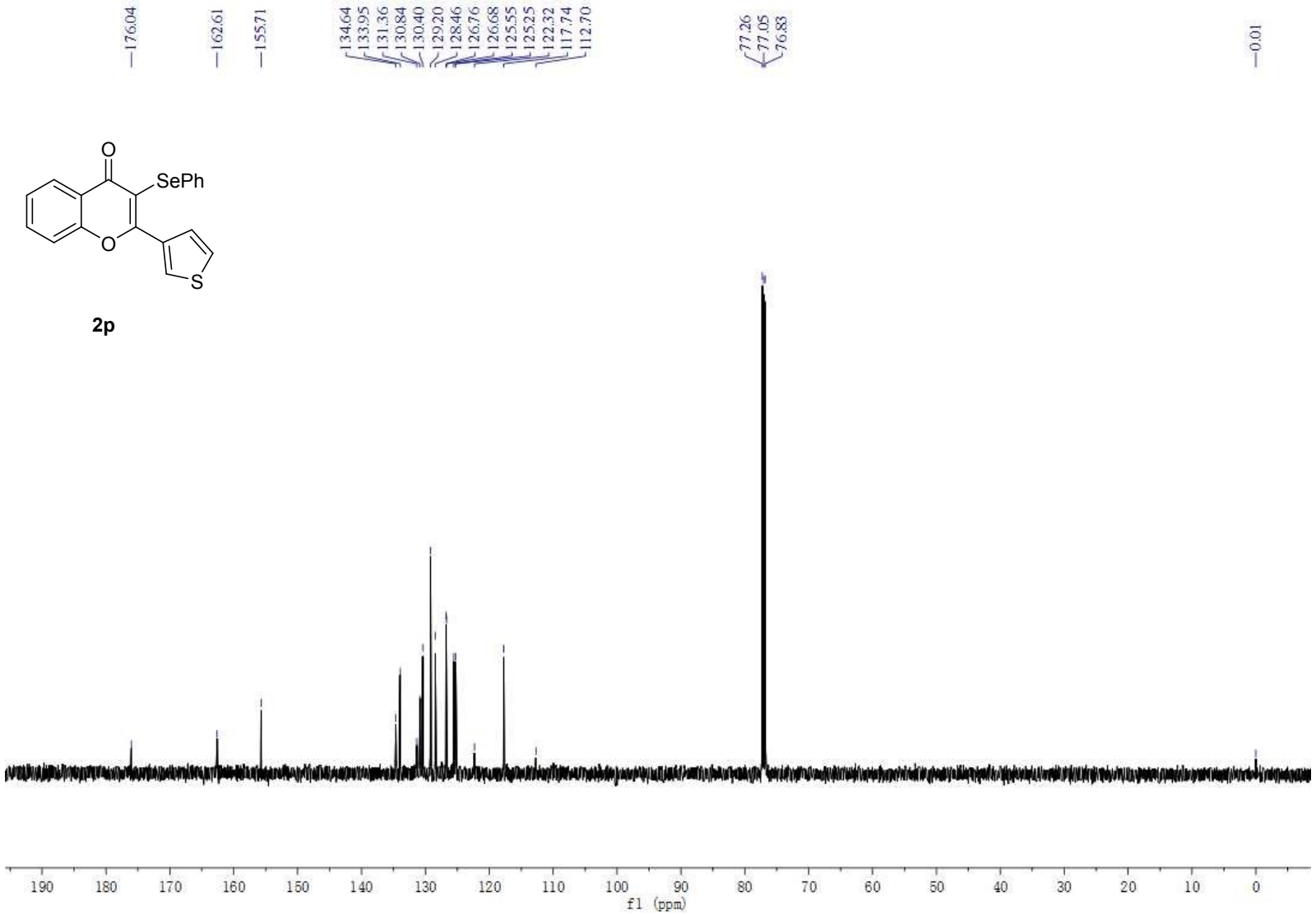
174.80
172.67
155.08
133.45
131.36
130.62
129.11
126.71
126.57
125.28
122.68
117.22
112.63
77.32
77.11
76.90
16.10
9.95
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.2420
8.2393
8.2287
8.2260
8.1811
8.1790
8.1761
8.1740
7.7261
7.7240
7.7175
7.7154
7.6992
7.6965
7.6874
7.6849
7.6824
7.6734
7.6706
7.4961
7.4821
7.4241
7.4115
7.3996
7.3982
7.3657
7.3633
7.3606
7.3566
7.3520
7.1793
7.1752
7.1722
7.1648
7.1608
7.1525
7.1493
7.1469
7.1435
7.1387


O
SePh
O
S

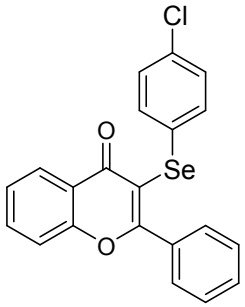
2p


1.02
1.00
0.98
1.04
1.04
1.07
3.00
3.08
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

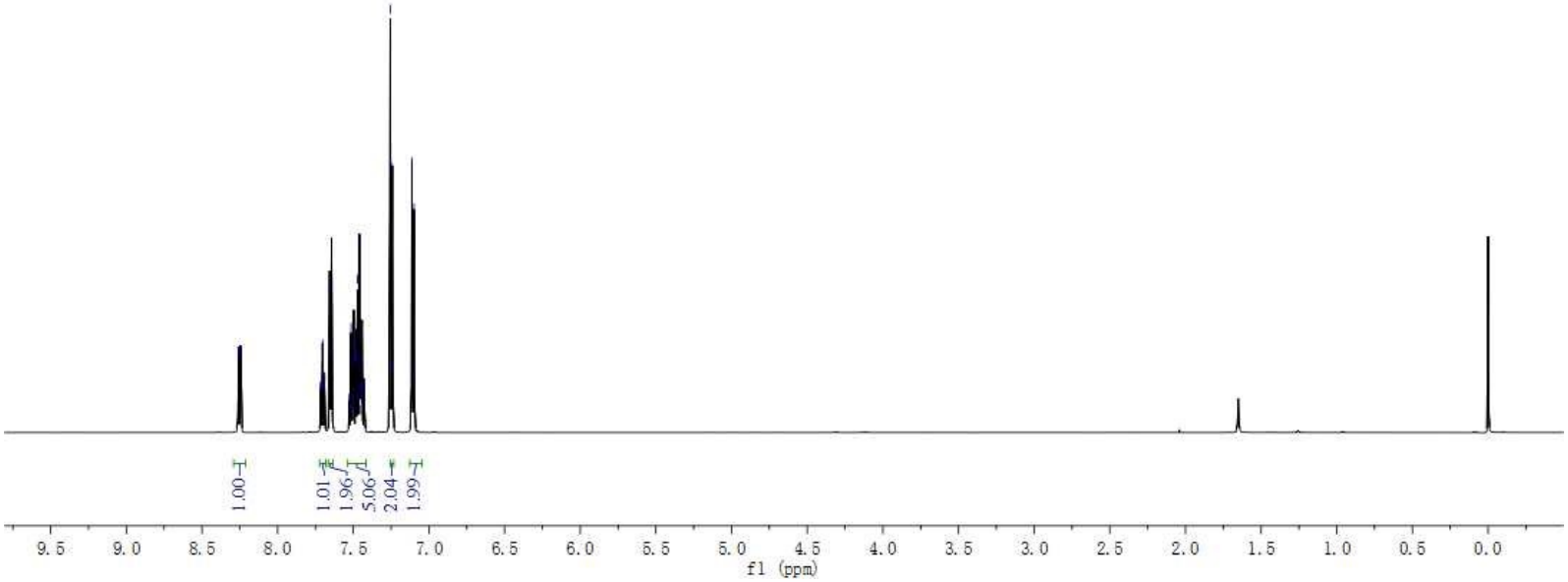

176.04
162.61
155.71
134.64
133.95
131.36
130.84
130.40
129.20
128.46
126.76
126.68
125.55
125.25
122.32
117.74
112.70
77.26
77.05
76.83
0.01
O
SePh
O
S
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

2p


8.2595
8.2567
8.2462
8.2434
7.7167
7.7139
7.7049
7.7023
7.6997
7.6908
7.6880
7.6571
7.6552
7.6436
7.6409
7.5269
7.5184
7.5144
7.5108
7.5044
7.5021
7.4982
7.4965
7.4840
7.4824
7.4730
7.4703
7.4625
7.4600
7.4557
7.4538
7.4509
7.4482
7.4462
7.4438
7.4421
7.4405
7.4304
7.4287
7.2559
7.2458
7.2425
7.1130
7.1096
7.1020
7.0987


Cl
O
Se
O

2q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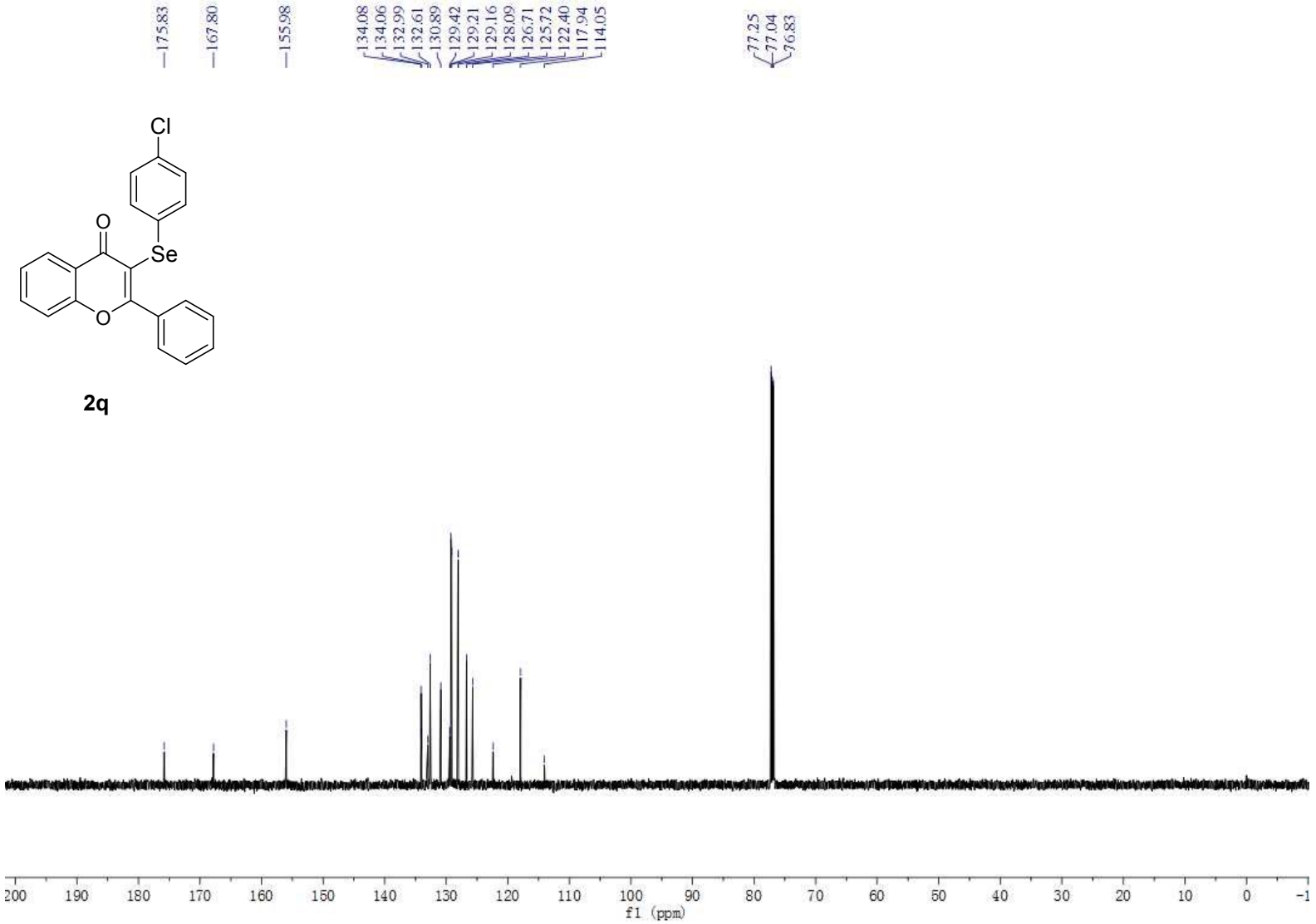
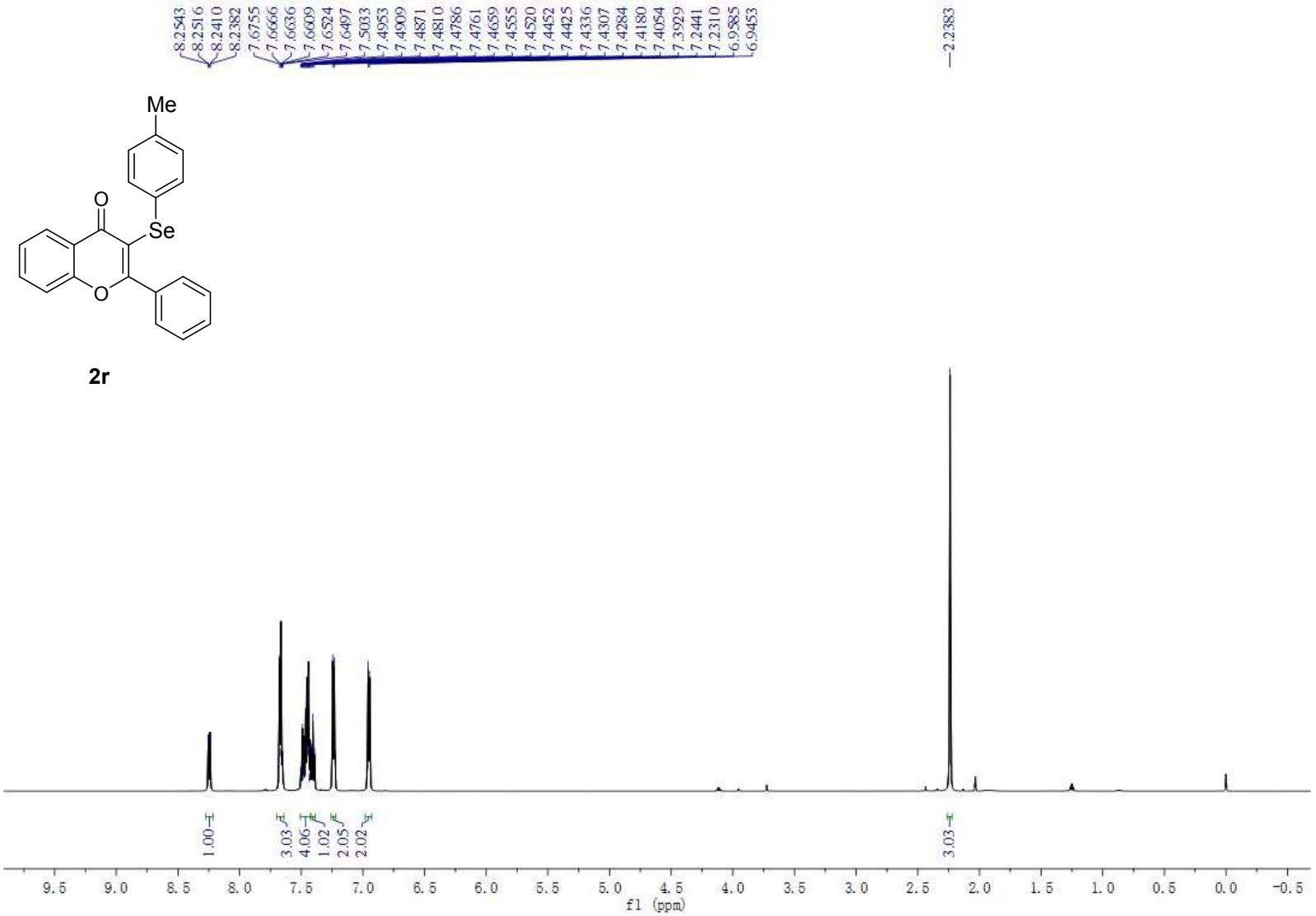
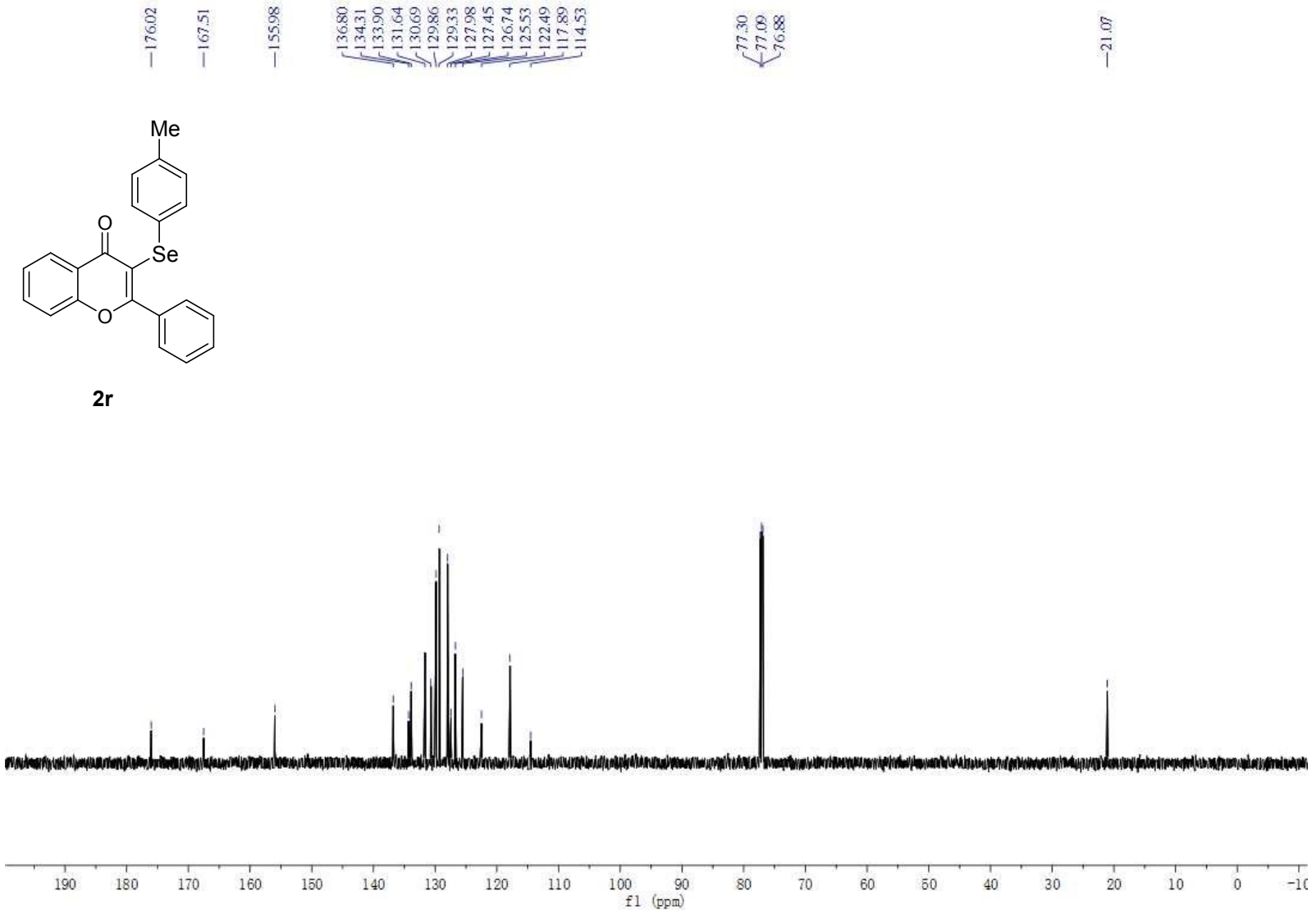
1.01
1.96
5.06
2.04
1.99
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


175.83
167.80
155.98
134.08
134.06
132.99
132.61
130.89
129.42
129.21
129.16
128.09
126.71
125.72
122.40
117.94
114.05
77.25
77.04
76.83
Cl
O
Se
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

2q

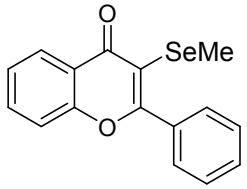

8.2543
8.2516
8.2410
8.2382
7.6755
7.6666
7.6636
7.6609
7.6524
7.6497
7.5033
7.4953
7.4909
7.4871
7.4810
7.4786
7.4761
7.4659
7.4555
7.4520
7.4452
7.4425
7.4336
7.4307
7.4284
7.4180
7.4054
7.3929
7.2441
7.2310
6.9585
6.9453
2.2383
Me
O
Se
O
1.00
3.03
4.06
1.02
2.05
2.02
3.03
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

2r

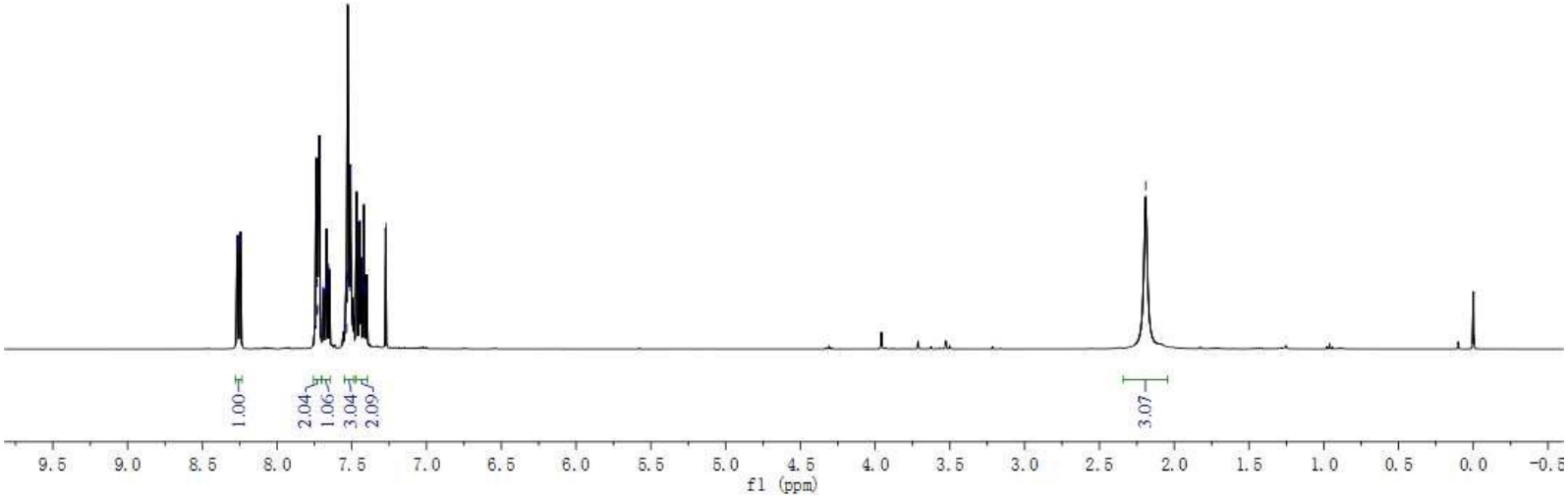

176.02
167.51
155.98
136.80
134.31
133.90
131.64
130.69
129.86
129.33
127.98
127.45
126.74
125.53
122.49
117.89
114.53
77.30
77.00
76.88
21.07
Me
O
Se
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

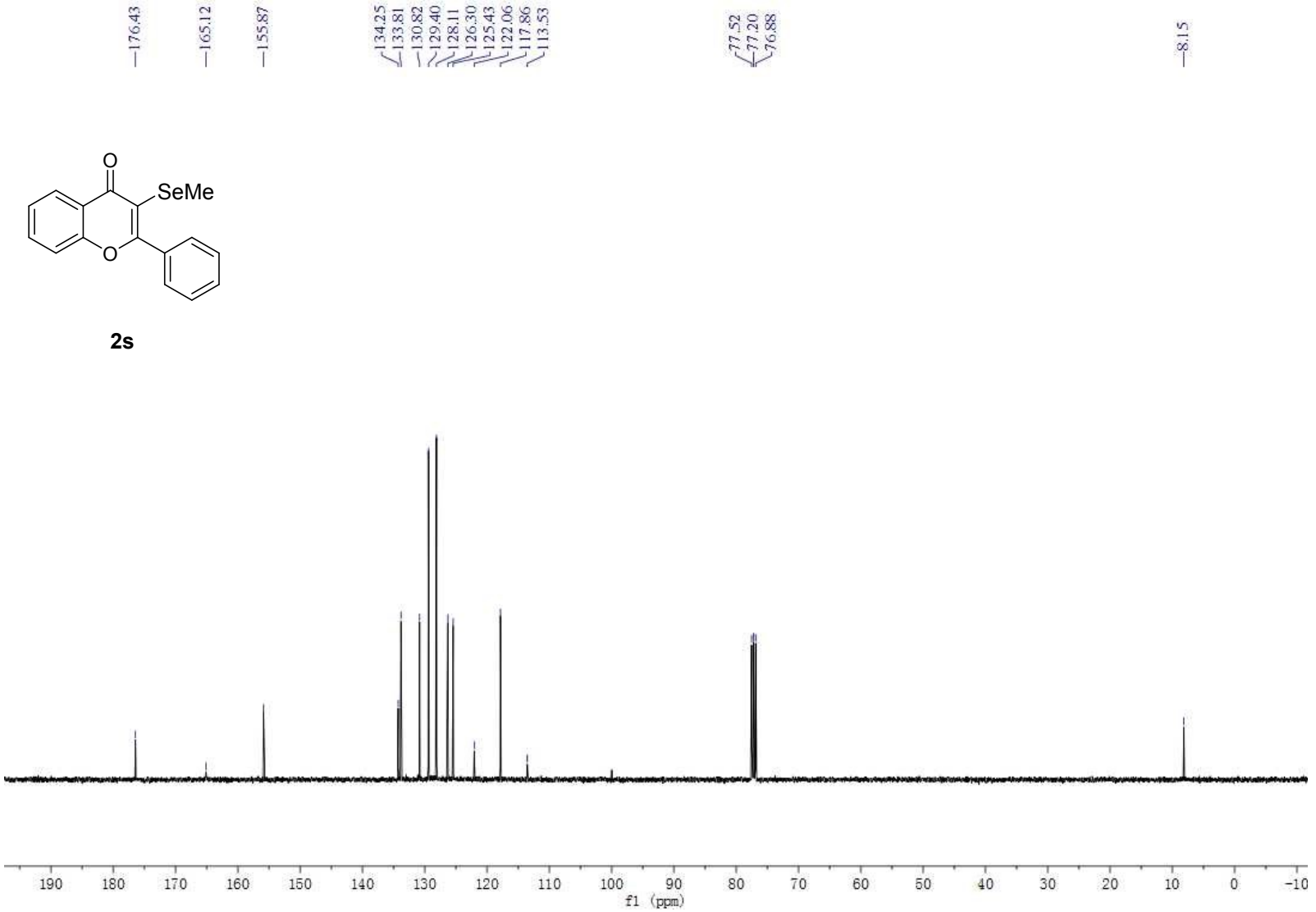
2r


8.2674
8.2632
8.2475
8.2433
7.7408
7.7366
7.7323
7.7299
7.7273
7.7227
7.7168
7.7127
7.6913
7.6871
7.6736
7.6697
7.6658
7.6523
7.6481
7.5428
7.5390
7.5312
7.5277
7.5256
7.5225
7.5197
7.5137
7.5094
7.5004
7.4958
7.4703
7.4679
7.4492
7.4467
7.4386
7.4359
7.4209
7.4185
7.4159
7.4009
7.3983
2.1912

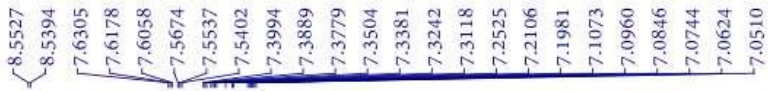

O
SeMe
O

2s


1.00
2.04
1.06
3.04
2.09
3.07
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)


176.43
165.12
155.87
134.25
133.81
130.82
129.40
128.11
126.30
125.43
122.06
117.86
113.53
77.52
77.20
76.88
8.15
O
SeMe
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

2s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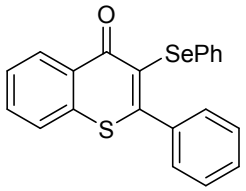
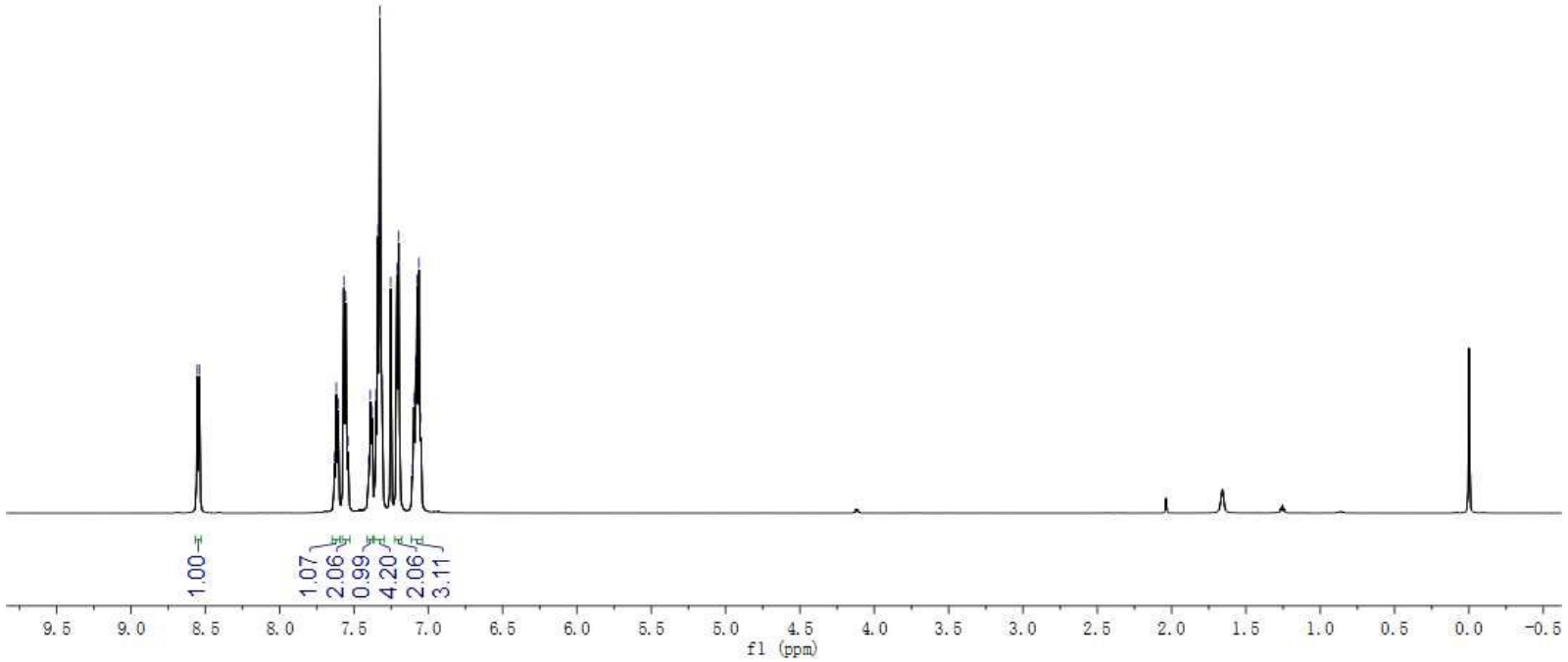
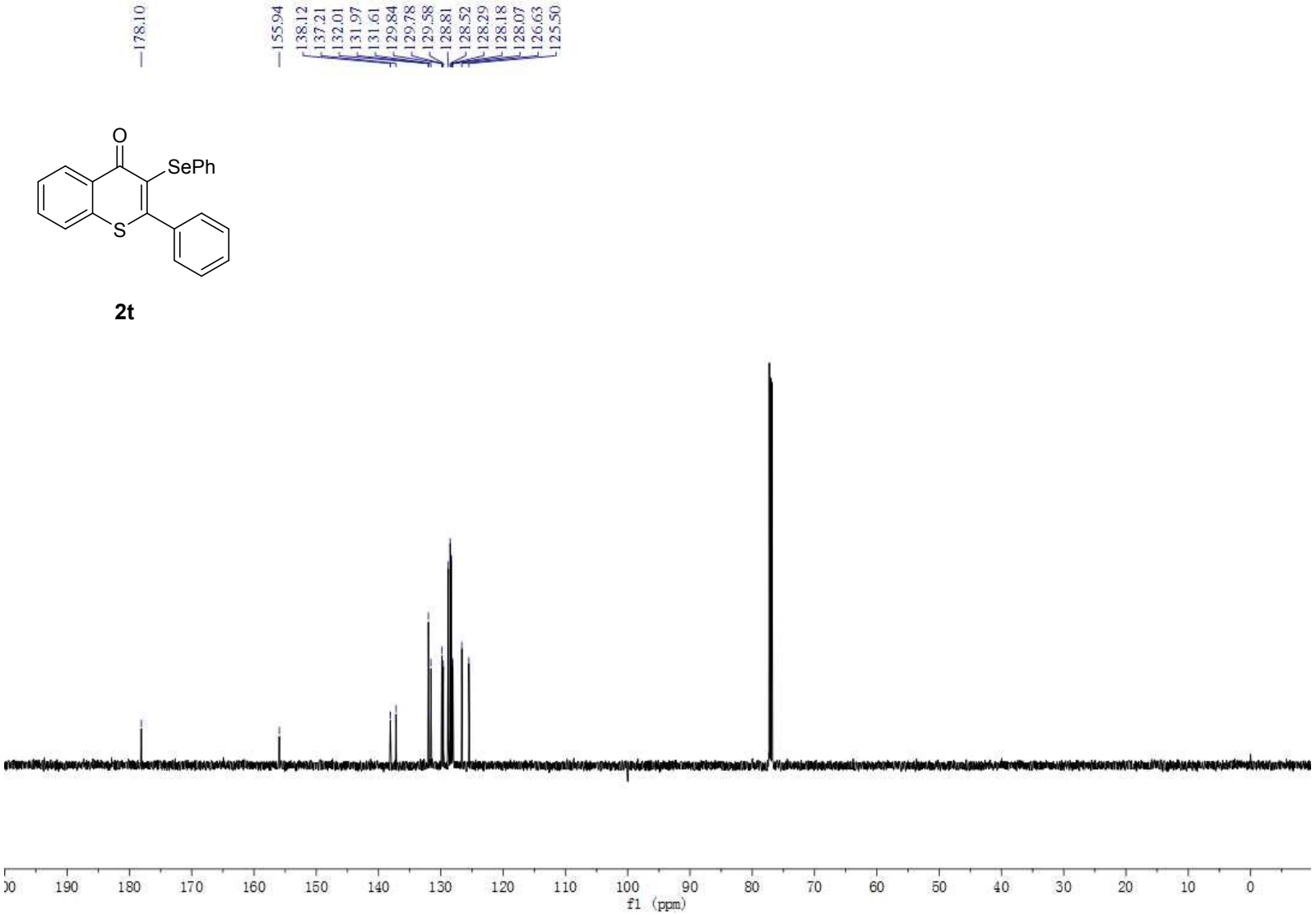
8.5394
7.6305
7.6178
7.6058
7.5674
7.5537
7.5402
7.3994
7.3889
7.3779
7.3504
7.3381
7.3242
7.3118
7.2525
7.2106
7.1981
7.1073
7.0960
7.0846
7.0744
7.0624
7.0510


O
SePh
S

2t


1.00
1.07
2.06
0.99
4.20
2.06
3.11
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


178.10
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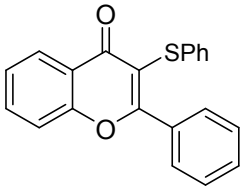
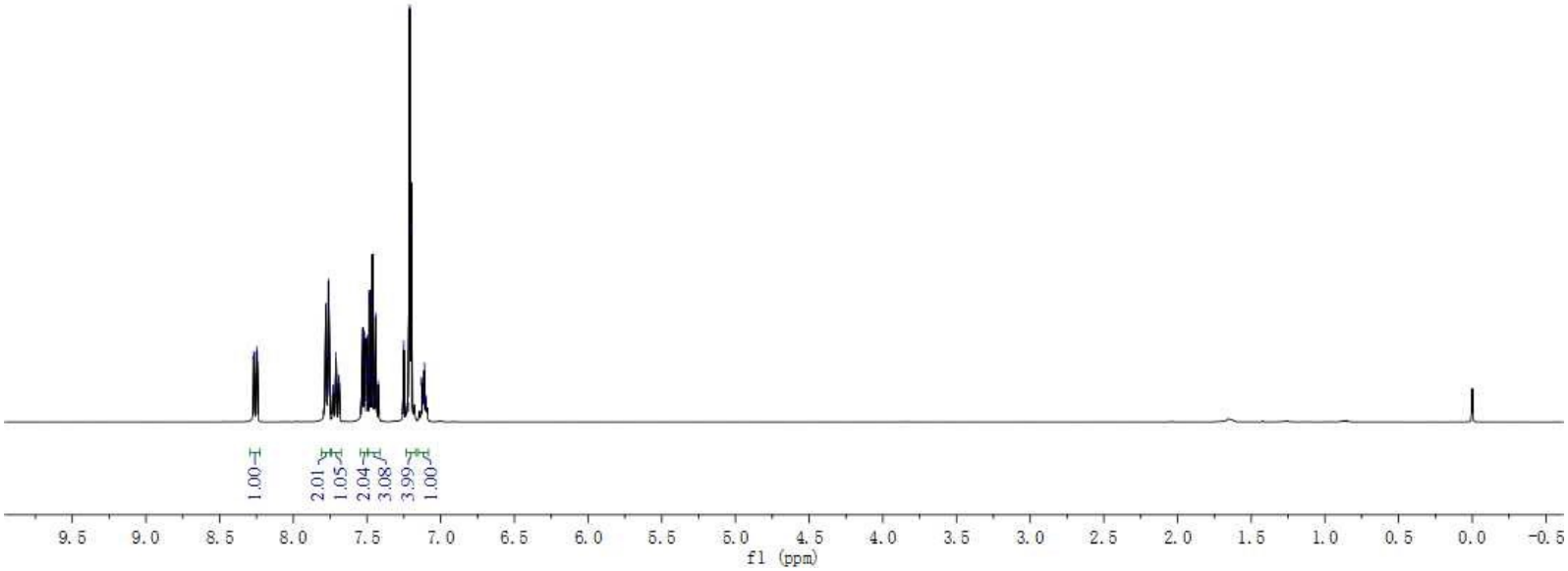
138.12
137.21
132.01
131.97
131.61
129.84
129.78
129.58
128.81
128.52
128.29
128.18
128.07
126.63
125.50
O
SePh
S
f1 (ppm)

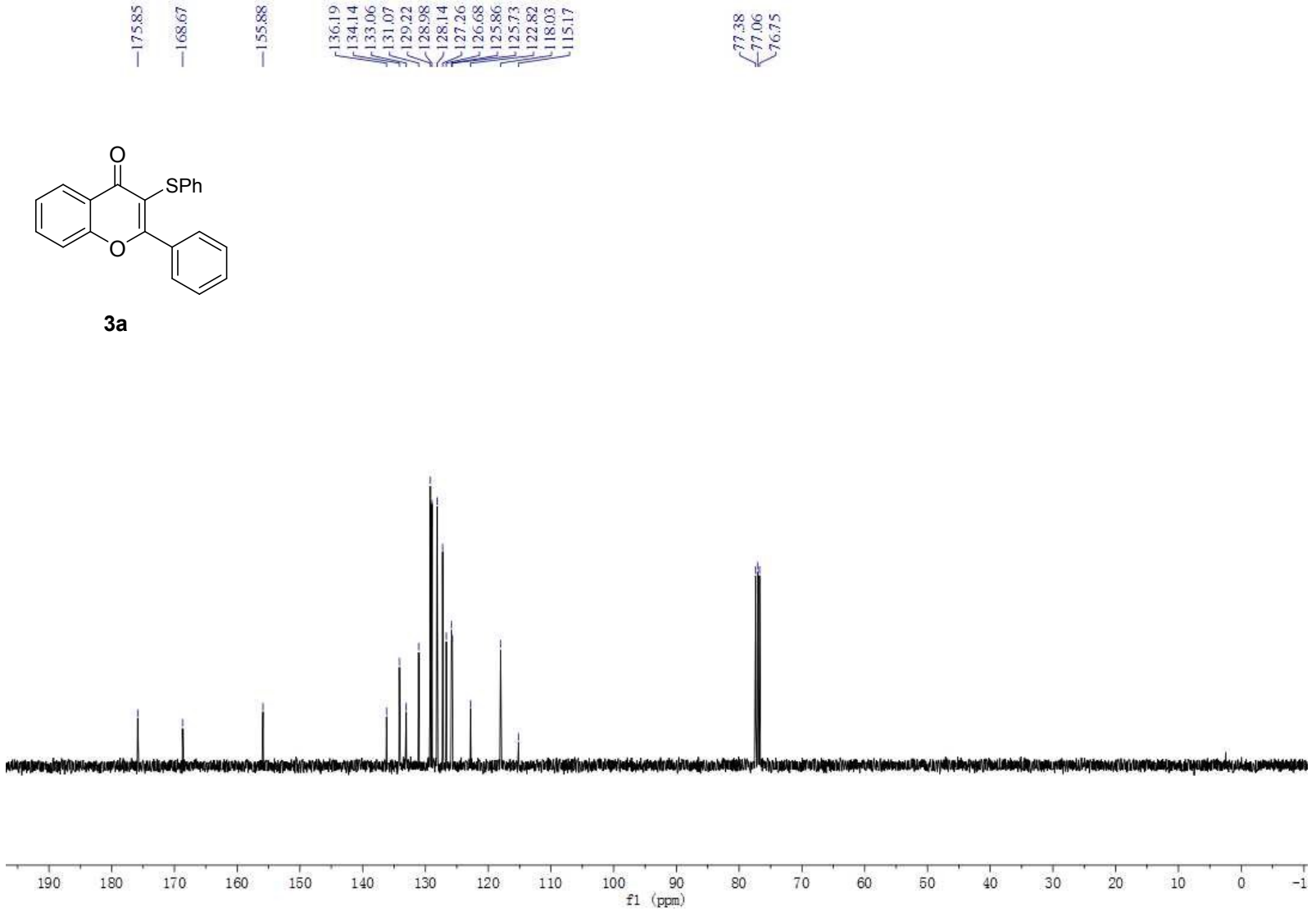
2t


8.2683
8.2643
8.2484
8.2442
7.7817
7.7784
7.7743
7.7668
7.7614
7.7572
7.7322
7.7278
7.7146
7.7106
7.7066
7.6932
7.6880
7.5361
7.5303
7.5275
7.5175
7.5113
7.5090
7.5062
7.5032
7.4995
7.4957
7.4864
7.4827
7.4806
7.4770
7.4665
7.4622
7.4605
7.4572
7.4490
7.4445
7.4405
7.4379
7.4228
7.4202
7.2504
7.2227
7.2196
7.2104
7.2016
7.1983
7.1323
7.1247
7.1205
7.1179
7.1152
7.1108
7.1058
7.1035
7.1017
7.0993
7.0990

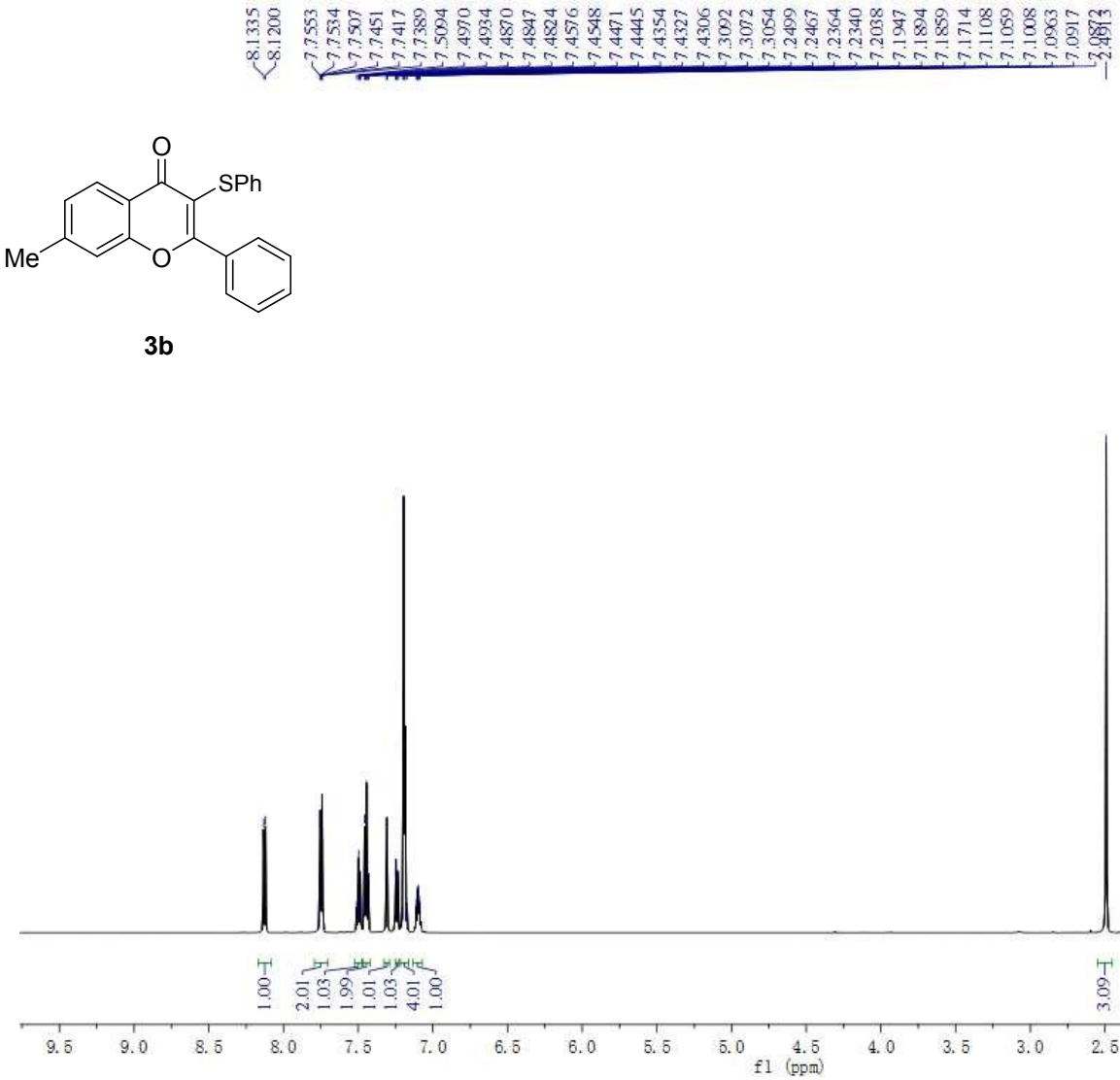

O
SPh
O

3a


1.00
2.01
1.05
2.04
3.08
3.99
1.00
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
-0.5
f1 (ppm)


175.85
168.67
155.88
136.19
134.14
133.06
131.07
129.22
128.98
128.14
127.26
126.68
125.86
125.73
122.82
118.03
115.17
77.38
77.06
76.75
O
SPh
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

3a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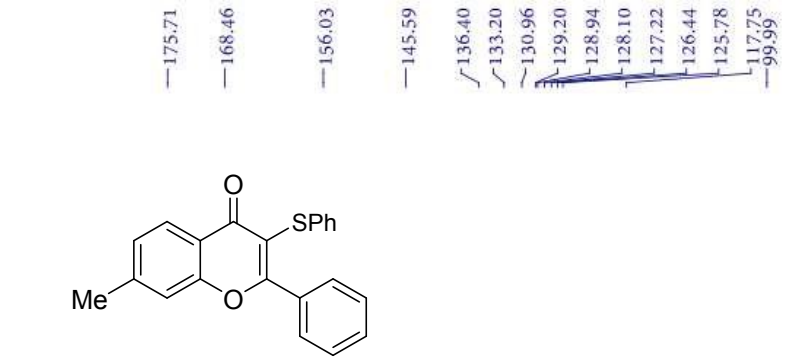
7.7534
7.7507
7.7451
7.7417
7.7389
7.5094
7.4970
7.4934
7.4870
7.4847
7.4824
7.4576
7.4548
7.4471
7.4445
7.4354
7.4327
7.4306
7.3092
7.3072
7.3054
7.2499
7.2467
7.2364
7.2340
7.2038
7.1947
7.1894
7.1859
7.1714
7.1108
7.1059
7.1008
7.0963
7.0917
7.0872
2.4913
O
SPh
Me
O
1.00
2.01
1.03
1.99
1.01
1.03
4.01
1.00
3.09
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)

3b


175.71
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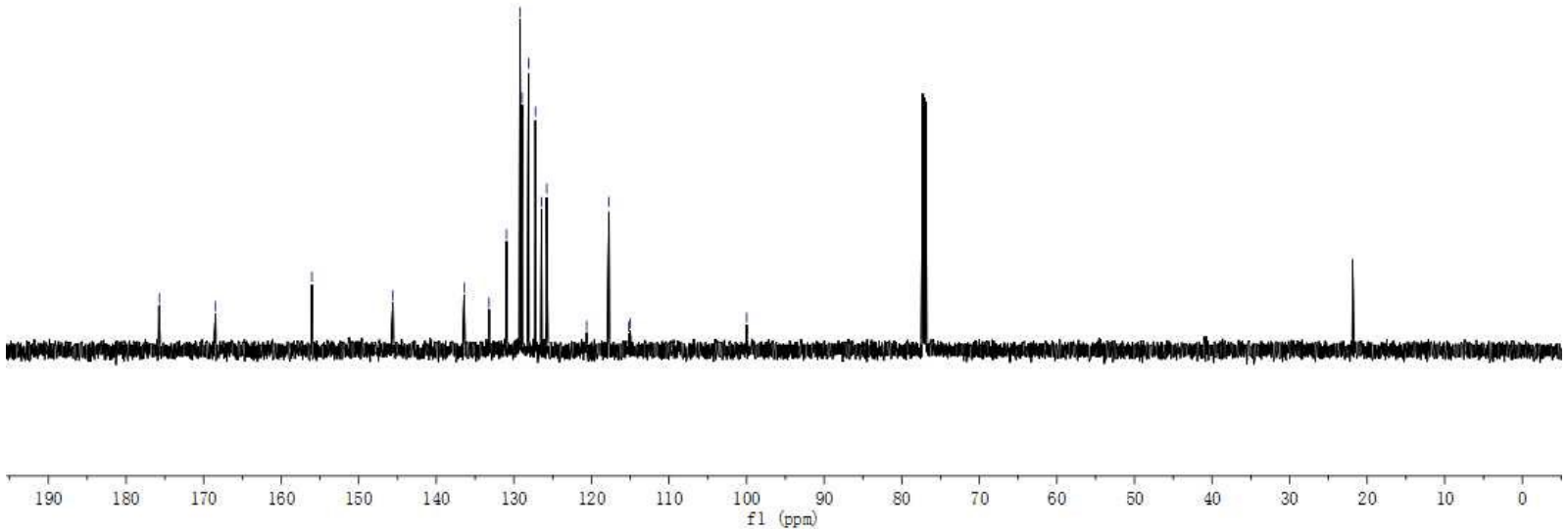
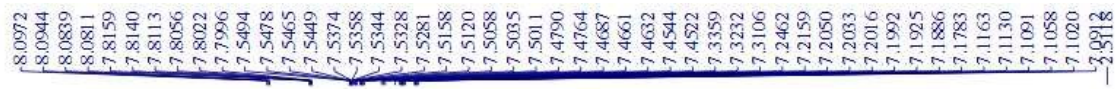
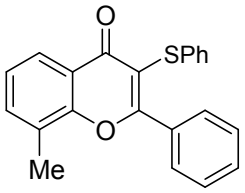
156.03
145.59
136.40
133.20
130.96
129.20
128.94
128.10
127.22
126.44
125.78
117.75
99.99
O
SPh
Me
O

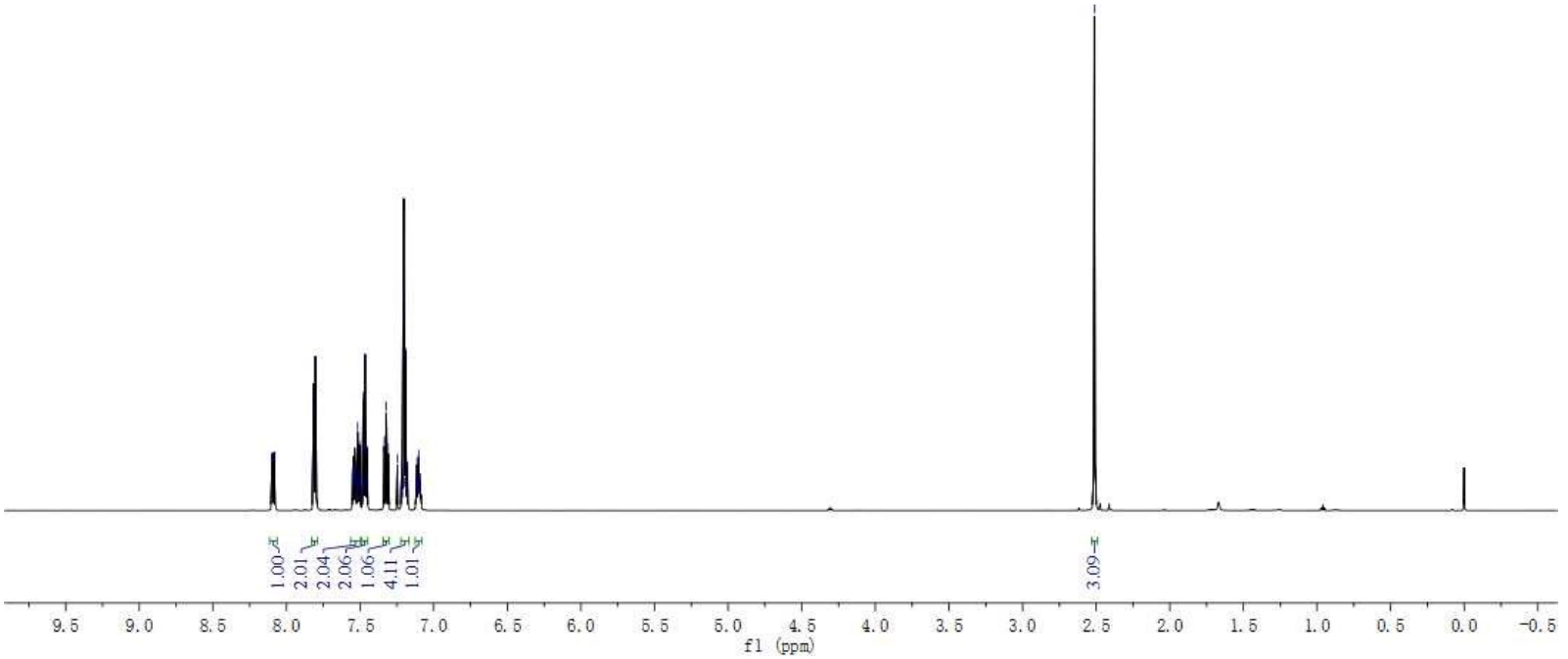
3b

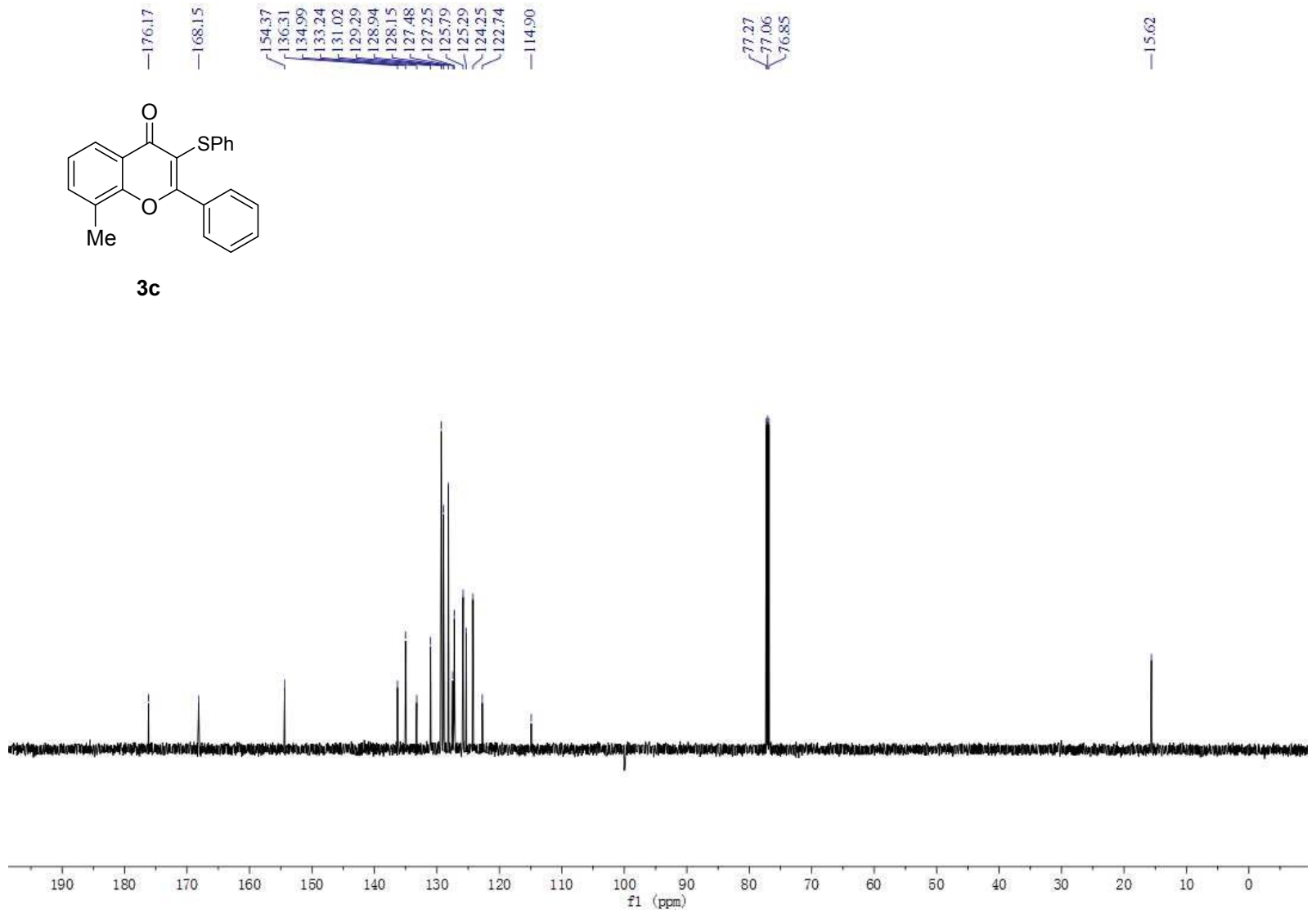

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.0972
8.0944
8.0839
8.0811
7.8159
7.8140
7.8113
7.8056
7.8022
7.7996
7.5494
7.5478
7.5465
7.5449
7.5374
7.5358
7.5344
7.5328
7.5281
7.5158
7.5120
7.5058
7.5035
7.5011
7.4790
7.4764
7.4687
7.4661
7.4632
7.4544
7.4522
7.3359
7.3232
7.3106
7.2462
7.2159
7.2050
7.2033
7.2016
7.1992
7.1925
7.1886
7.1783
7.1163
7.1130
7.1091
7.1058
7.1020
2.5118


O
SPh
O
Me

3c


1.00
2.01
2.04
2.06
1.06
4.11
1.01
3.09
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


176.17
168.15
154.37
136.31
134.99
133.24
131.02
129.29
128.94
128.15
127.48
127.25
125.79
125.29
124.25
122.74
114.90
77.27
77.06
76.85
15.62
O
SPh
O
Me
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

3c


7.7701
7.7681
7.7656
7.7598
7.7564
7.7538
7.6411
7.6321
7.6271
7.6182
7.6132
7.6043
7.5329
7.5307
7.5285
7.5222
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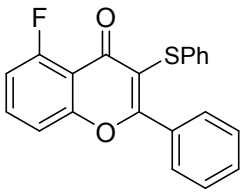
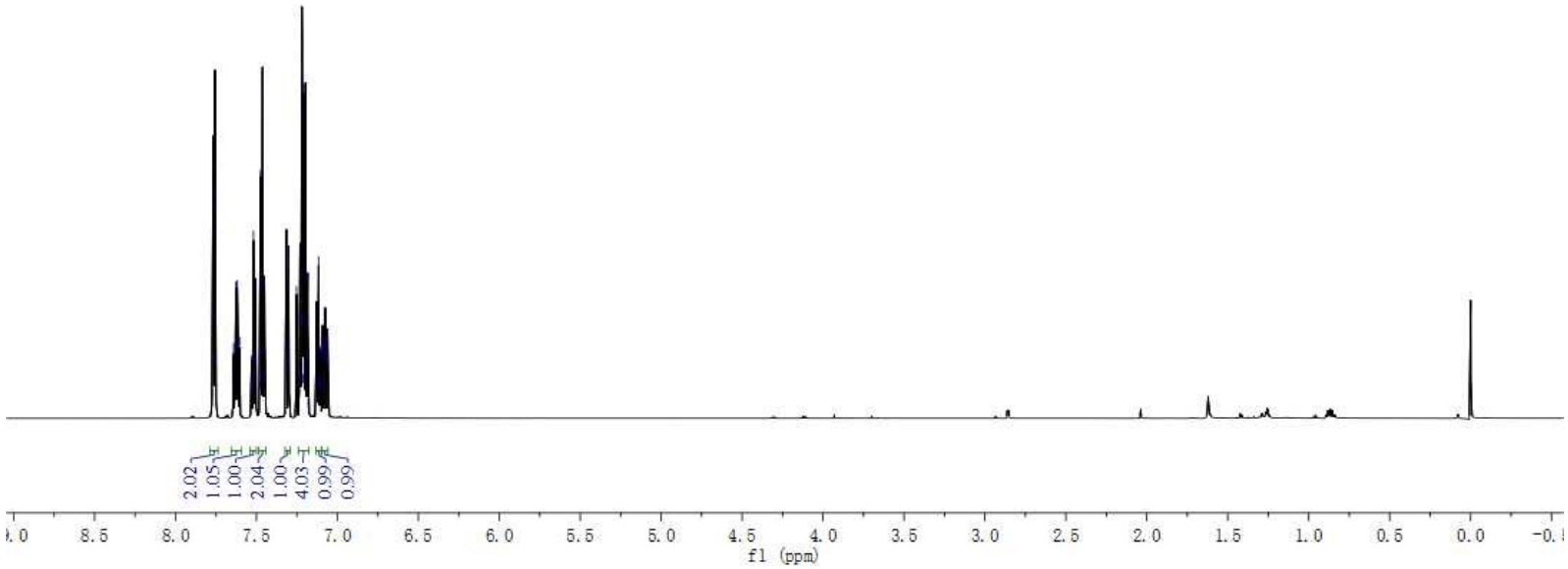
7.5147
7.5083
7.5059
7.5036
7.4786
7.4755
7.4728
7.4649
7.4625
7.4595
7.4533
7.4505
7.4485
7.3173
7.3155
7.3139
7.3031
7.3013
7.2997
7.2523
7.2337
7.2309
7.2276
7.2229
7.2209
7.2193
7.2171
7.2140
7.2093
7.2054
7.2001
7.1982
7.1969
7.1941
7.1865
7.1837
7.1307
7.1282
7.1256
7.1198
7.1165
7.1129
7.1071
7.1047
7.1021
7.0920
7.0904
7.0783
7.0765
7.0747
7.0731
7.0612
7.0595


F
O
SPh
O

3d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1.05
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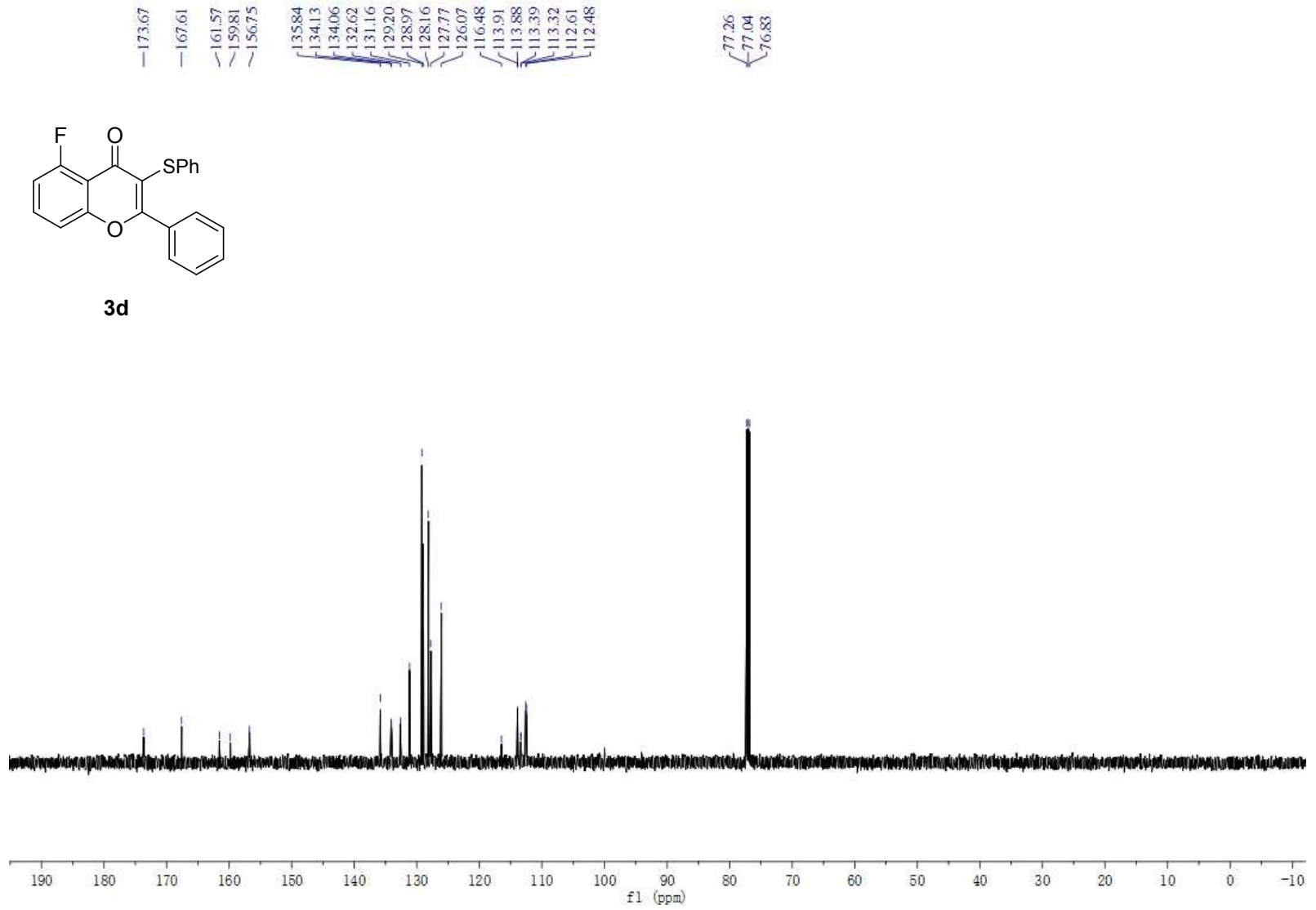
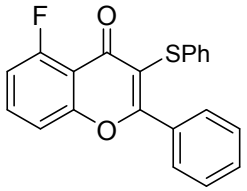
2.04
1.00
4.03
0.99
0.99
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


173.67
167.61
161.57
159.81
156.75
135.84
134.13
134.06
132.62
131.16
129.20
128.97
128.16
127.77
126.07
116.48
113.91
113.88
113.39
113.32
112.61
112.48
77.26
77.04
76.83
F
O
SPh
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

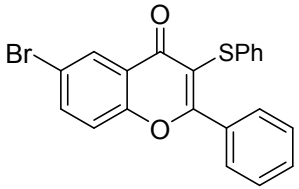
3d


F
O
SPh
O

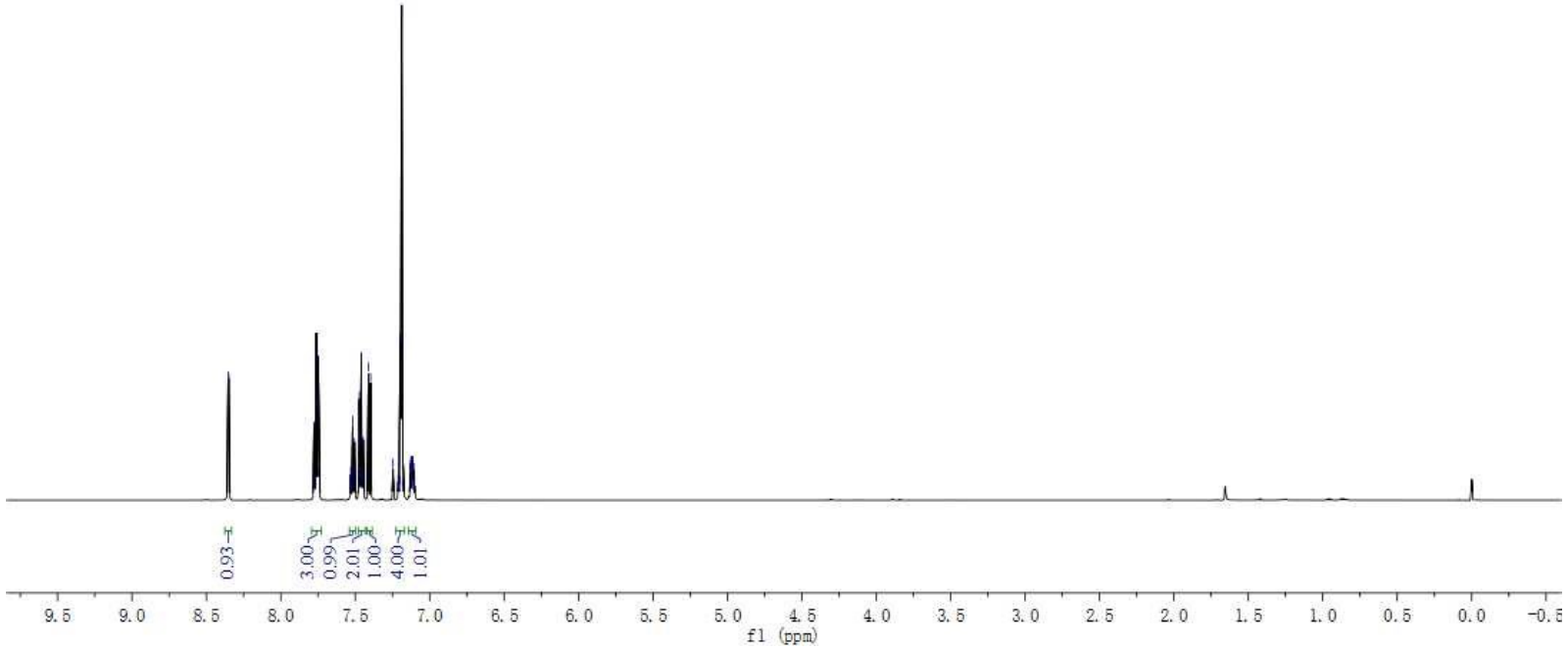
3d

-110.09
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)


8.3538
8.3497
7.7769
7.7728
7.7652
7.7620
7.7598
7.7578
7.7514
7.7481
7.7454
7.5321
7.5299
7.5277
7.5214
7.5177
7.5141
7.5074
7.5052
7.5029
7.4753
7.4722
7.4695
7.4616
7.4591
7.4562
7.4499
7.4471
7.4452
7.4114
7.3967
7.2463
7.2121
7.2106
7.2079
7.2018
7.1976
7.1936
7.1883
7.1825
7.1811
7.1790
7.1304
7.1257
7.1211
7.1183
7.1161
7.1122
7.1102
7.1065
7.1018


O
Br
SPh
O

3e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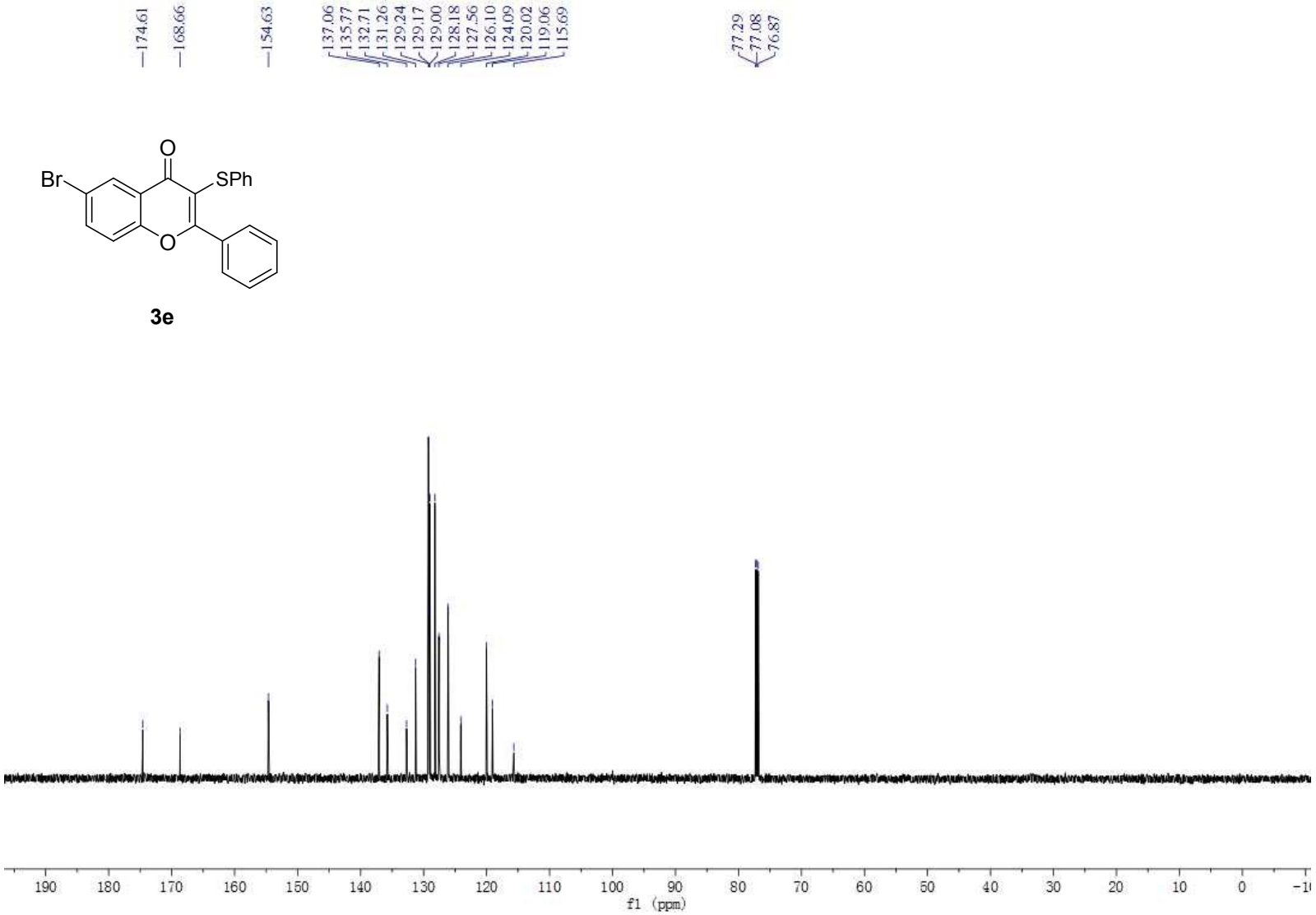
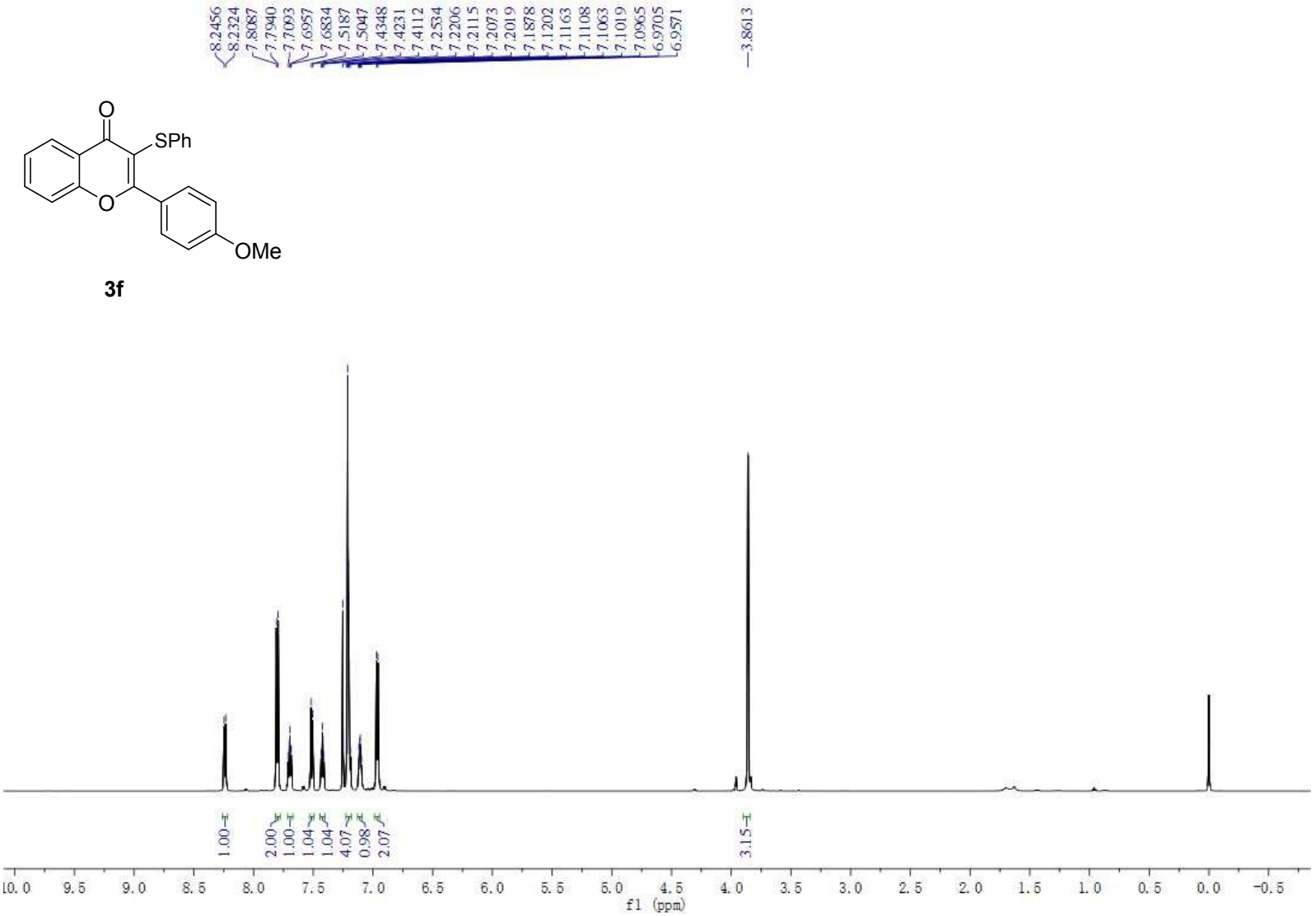
3.00
0.99
2.01
1.00
4.00
1.01
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

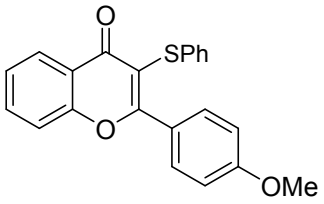

174.61
168.66
154.63
137.06
135.77
132.71
131.26
129.24
129.17
129.00
128.18
127.56
126.10
124.09
120.02
119.06
115.69
77.29
77.08
76.87
O
Br
SPh
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

3e

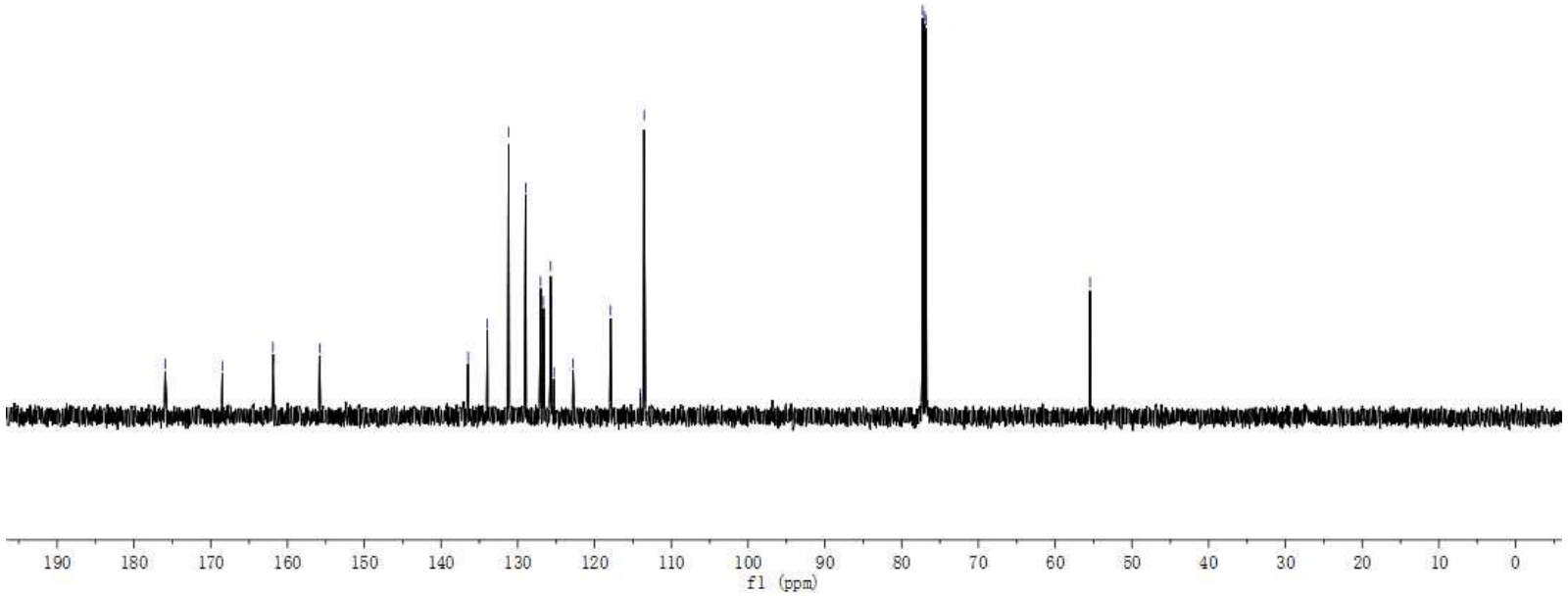

8.2456
8.2324
7.8087
7.7940
7.7093
7.6957
7.6834
7.5187
7.5047
7.4348
7.4231
7.4112
7.2534
7.2206
7.2115
7.2073
7.2019
7.1878
7.1202
7.1163
7.1108
7.1063
7.1019
7.0965
6.9705
6.9571
3.8613
O
SPh
O
OMe
1.00
2.00
1.00
1.04
1.04
4.07
0.98
2.07
3.15
f1 (ppm)

3f

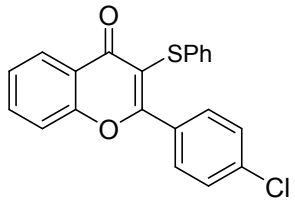

175.92
168.47
161.89
155.81
136.47
133.96
131.19
128.96
127.03
126.65
125.73
125.57
125.28
122.79
117.91
114.02
113.54
77.26
77.05
76.84
55.44


O
SPh
O
OMe

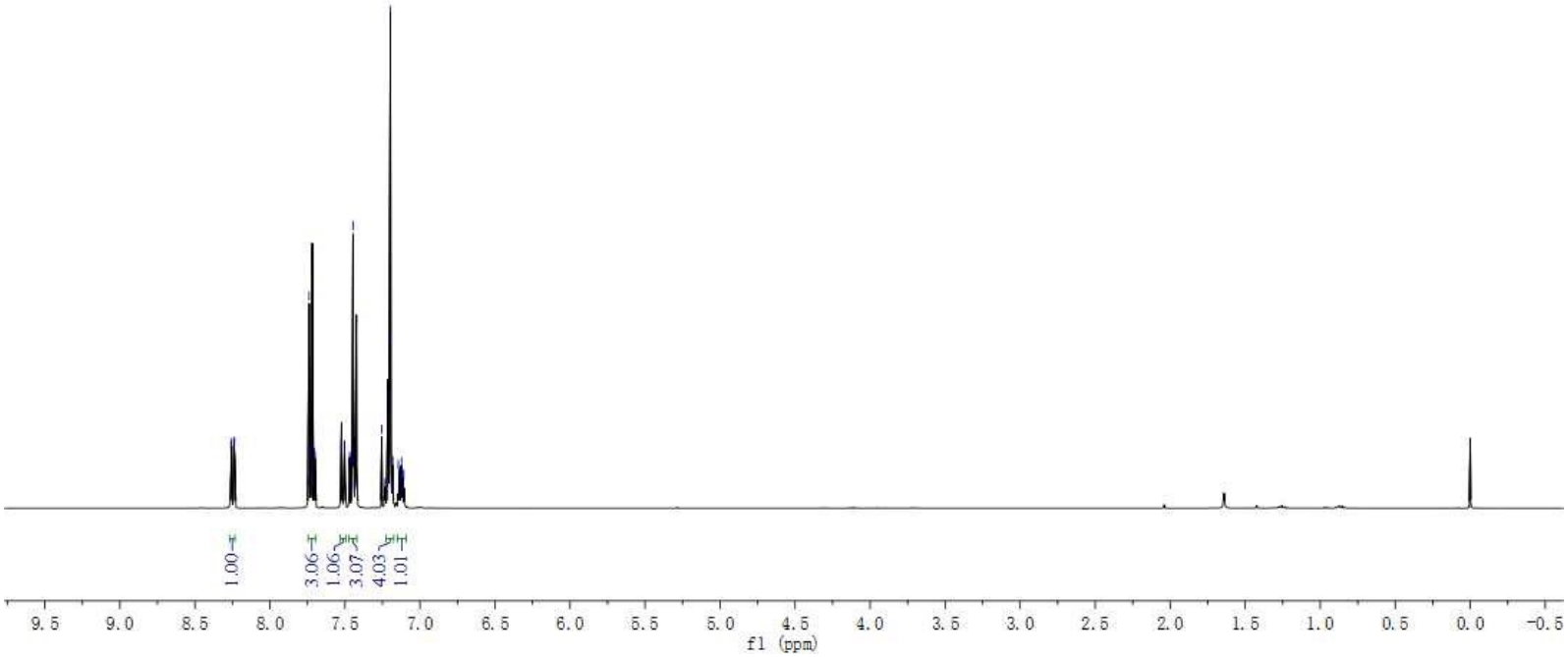
3f

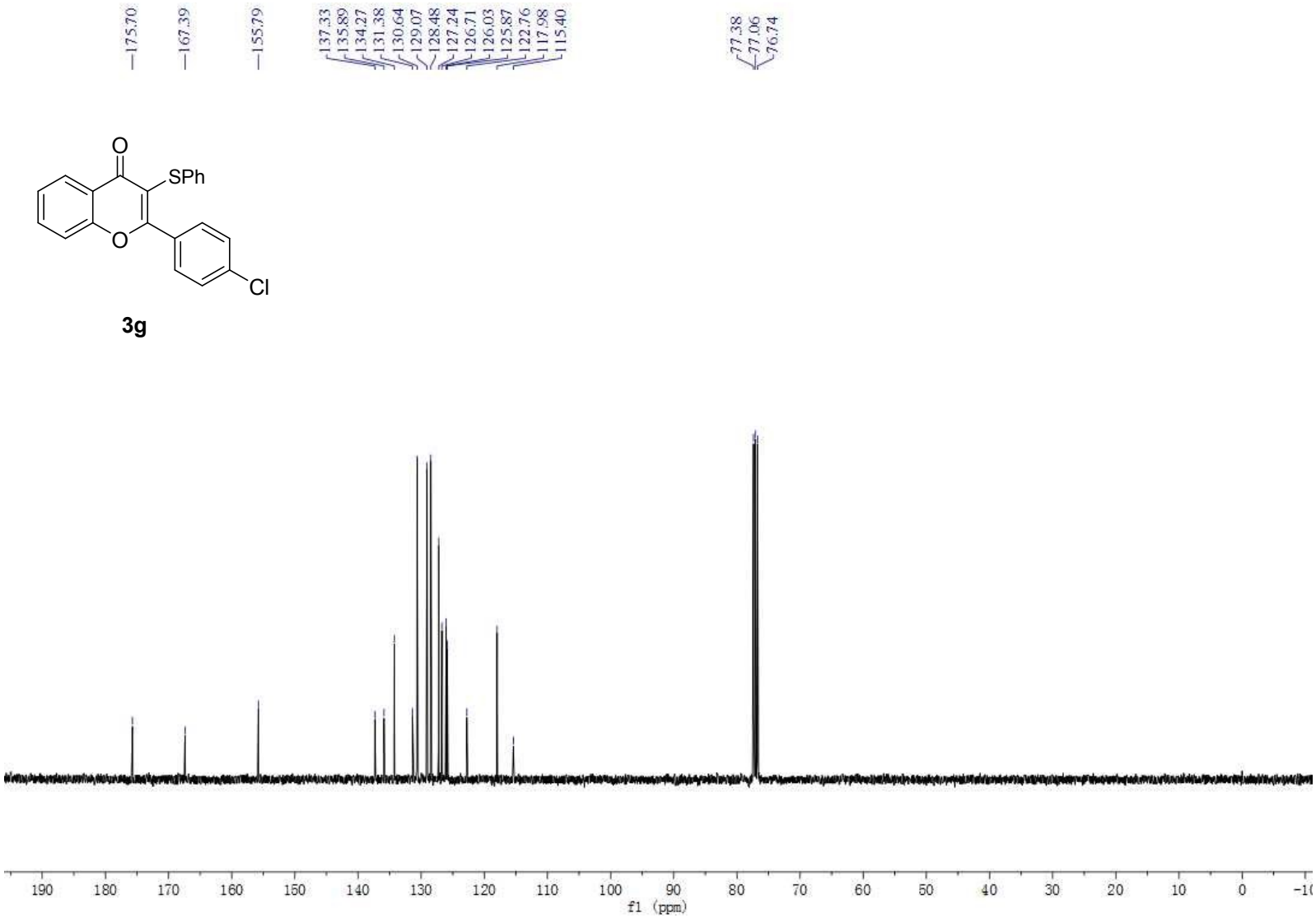

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.2605
8.2563
8.2406
8.2365
7.7428
7.7393
7.7345
7.7248
7.7229
7.7210
7.7177
7.7116
7.7035
7.6992
7.5249
7.5227
7.5039
7.5016
7.4690
7.4663
7.4529
7.4513
7.4490
7.4465
7.4415
7.4300
7.4250
7.4187
7.2546
7.2322
7.2184
7.2129
7.2111
7.2035
7.1970
7.1867
7.1851
7.1816
7.1446
7.1393
7.1374
7.1308
7.1288
7.1259
7.1232
7.1195
7.1153
7.1082

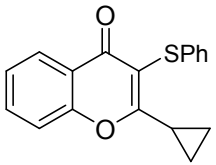

O
SPh
O
Cl

3g

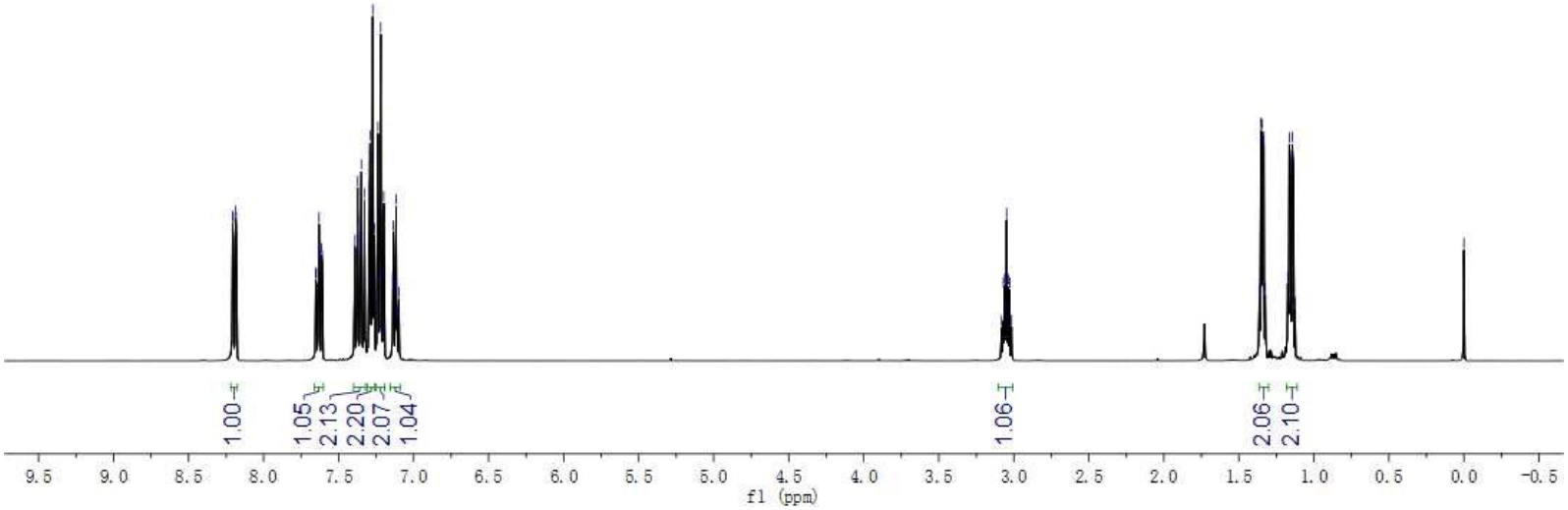

1.00
3.06
1.06
3.07
4.03
1.01
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

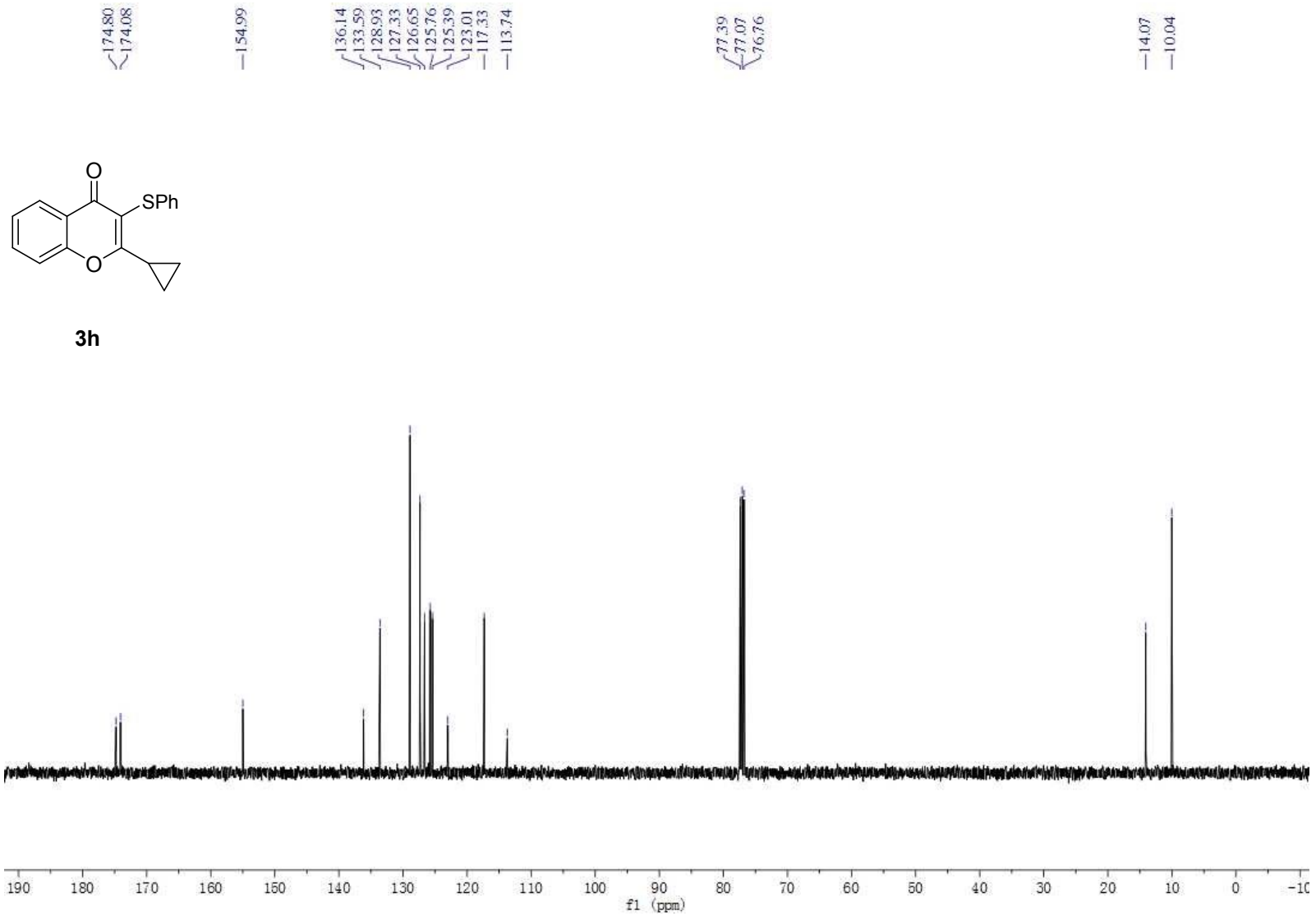

175.70
167.39
155.79
137.33
135.89
134.27
131.38
130.64
129.07
128.48
127.24
126.71
126.03
125.87
122.76
117.98
115.40
77.38
77.06
76.74
O
SPh
O
Cl
3g
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.2067
8.2029
8.1869
8.1830
7.6522
7.6480
7.6342
7.6305
7.6270
7.6132
7.6089
7.3936
7.3910
7.3753
7.3733
7.3714
7.3557
7.3531
7.3484
7.3274
7.2939
7.2904
7.2853
7.2748
7.2724
7.2699
7.2593
7.2377
7.2325
7.2192
7.2155
7.2035
7.1994
7.1382
7.1350
7.1169
3.0604
3.0480
3.0356
1.3524
1.3452
1.3401
1.3330
1.1742
1.1642
1.1569
1.1436
1.1361
0.0000


O
SPh
O

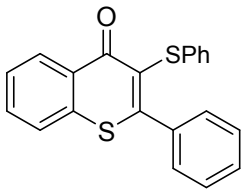
3h


1.00
1.05
2.13
2.20
2.07
1.04
1.06
2.06
2.10
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

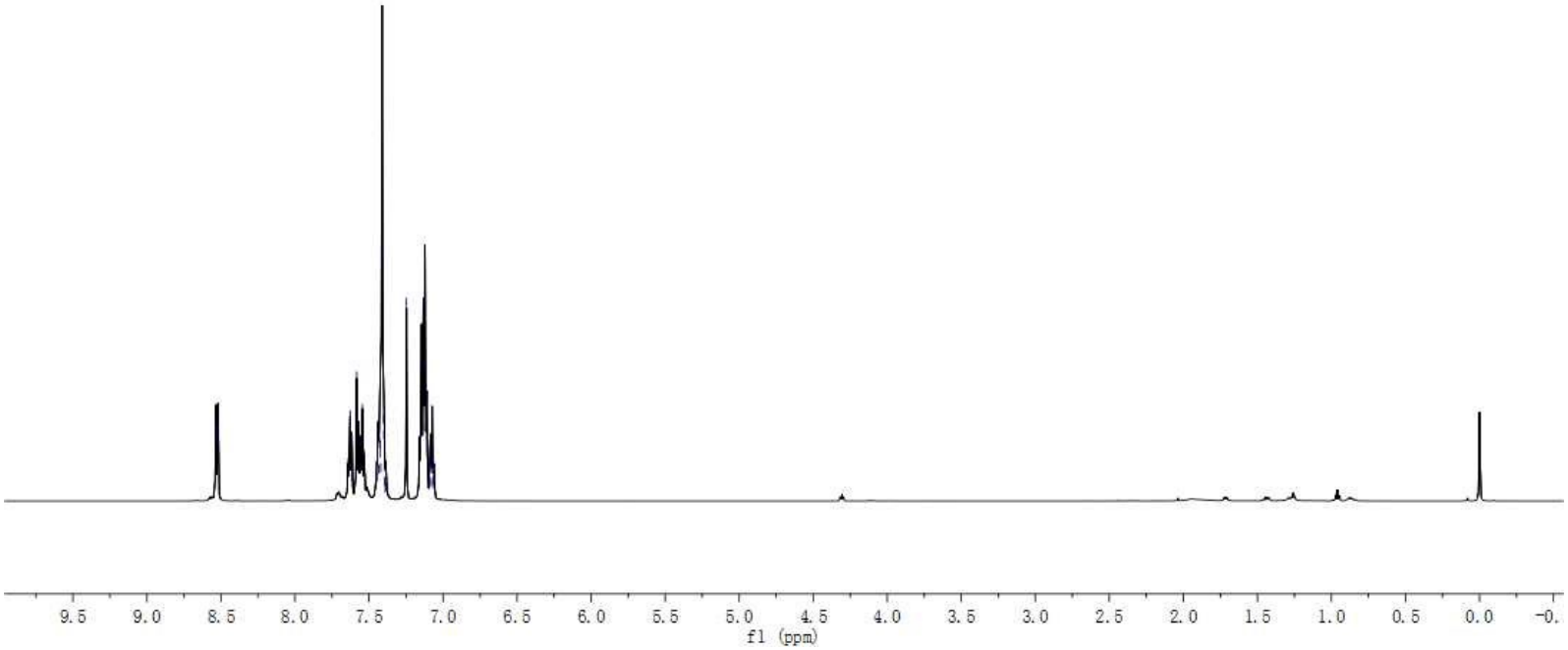

174.80
174.08
154.99
136.14
133.59
128.93
127.33
126.65
125.76
125.39
123.01
117.33
113.74
77.39
77.07
76.76
14.07
10.04
O
SPh
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

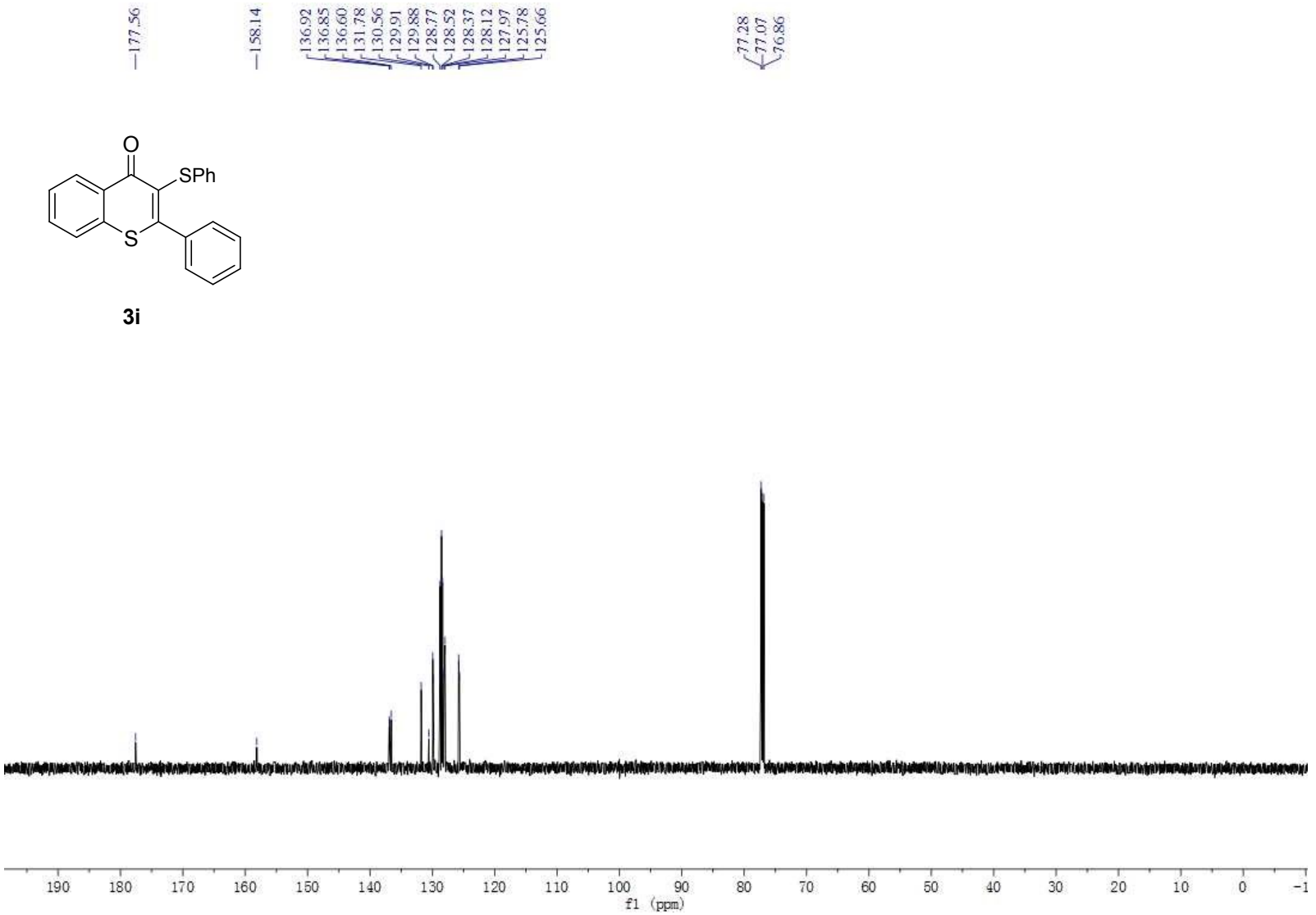
3h


8.5346
8.5323
8.5211
8.5187
7.6411
7.6283
7.6165
7.6138
7.5835
7.5702
7.5579
7.5452
7.5328
7.4500
7.4459
7.4393
7.4341
7.4281
7.4251
7.4226
7.4198
7.4125
7.4100
7.4012
7.3991
7.3960
7.3899
7.3871
7.3847
7.2475
7.1586
7.1479
7.1452
7.1337
7.1249
7.1219
7.1105
7.0874
7.0847
7.0818
7.0763
7.0731
7.0691
7.0644
7.0614


O
SPh
S

3i


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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158.14
136.92
136.85
136.60
131.78
130.56
129.91
129.88
128.77
128.52
128.37
128.12
127.97
125.78
125.66
77.28
77.07
76.86
O
SPh
S
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

3i


8.2145
8.2120
8.2012
8.1986
7.7387
7.7359
7.7322
7.7293
7.7268
7.7226
7.7200
7.7148
7.7129
7.7100
7.6113
7.6026
7.5995
7.5973
7.5762
7.5742
7.5723
7.5617
7.5512
7.5492
7.5472
7.4932
7.4770
7.4708
7.4693
7.4637
7.4574
7.4542
7.4511
7.4456
7.4440
7.4237
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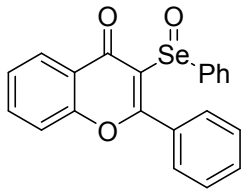
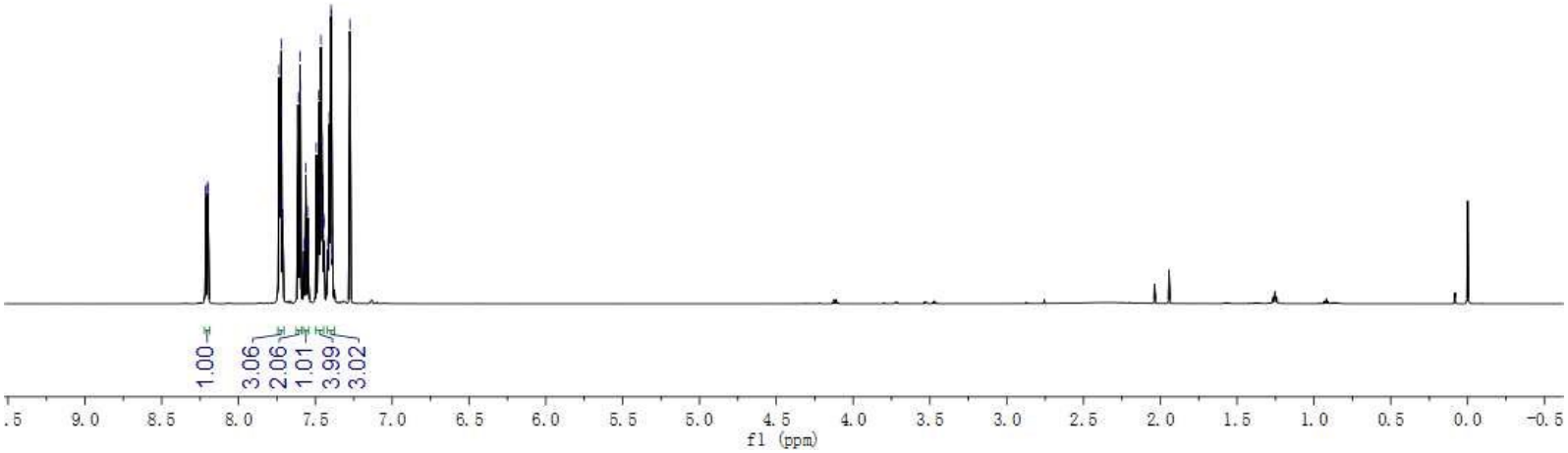
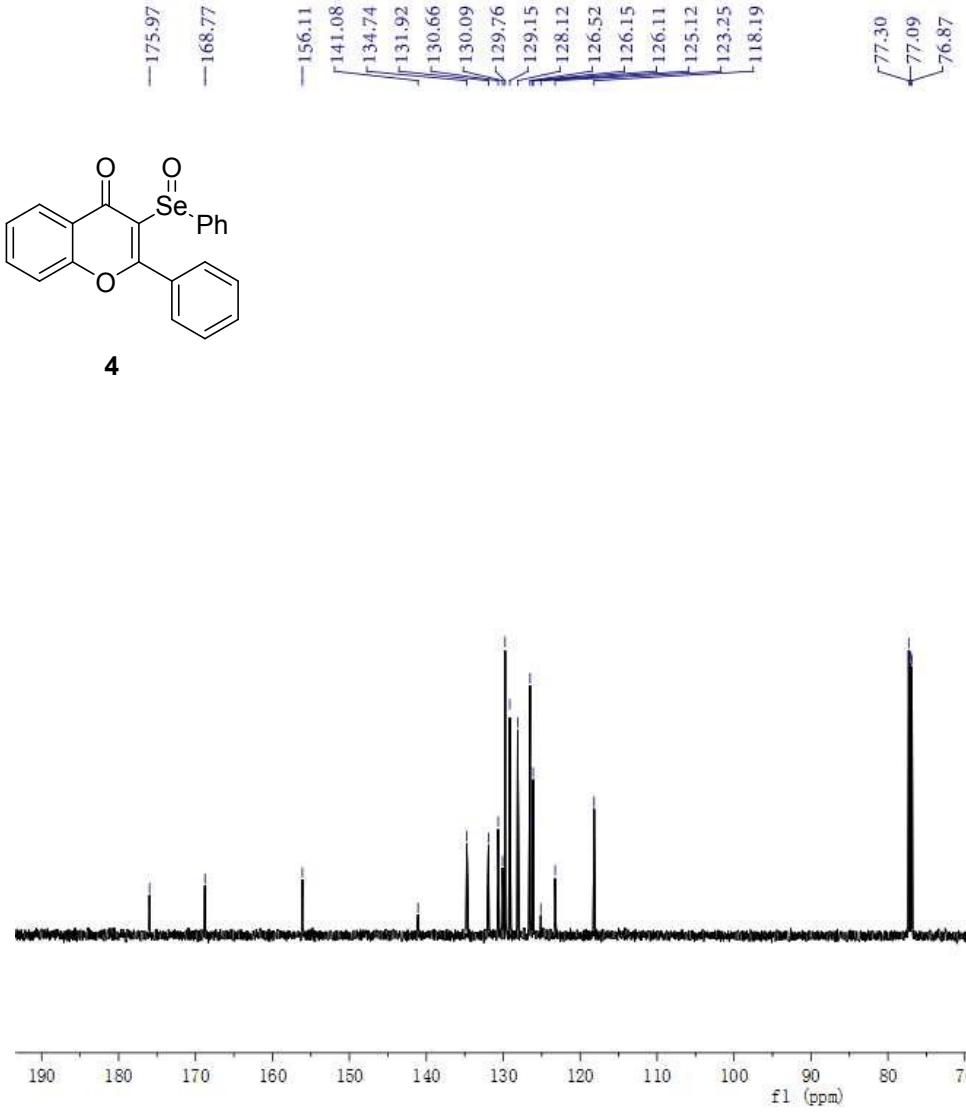
7.4019
7.3984
7.3968
7.3904
7.3875
7.2754


O
O
Se
Ph
O

4


1.00
3.06
2.06
1.01
3.99
3.02
f1 (ppm)


175.97
168.77
156.11
141.08
134.74
131.92
130.66
130.09
129.76
129.15
128.12
126.52
126.15
126.11
125.12
123.25
118.19
77.30
77.09
76.87
O
O
Se
Ph
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

4


8.1369
8.1343
8.1236
8.1210
7.8246
7.8105
7.7146
7.7030
7.6913
7.6749
7.6626
7.6472
7.6348
7.6224
7.5860
7.5730
7.5608
7.5049
7.4910
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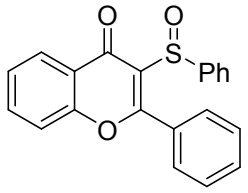
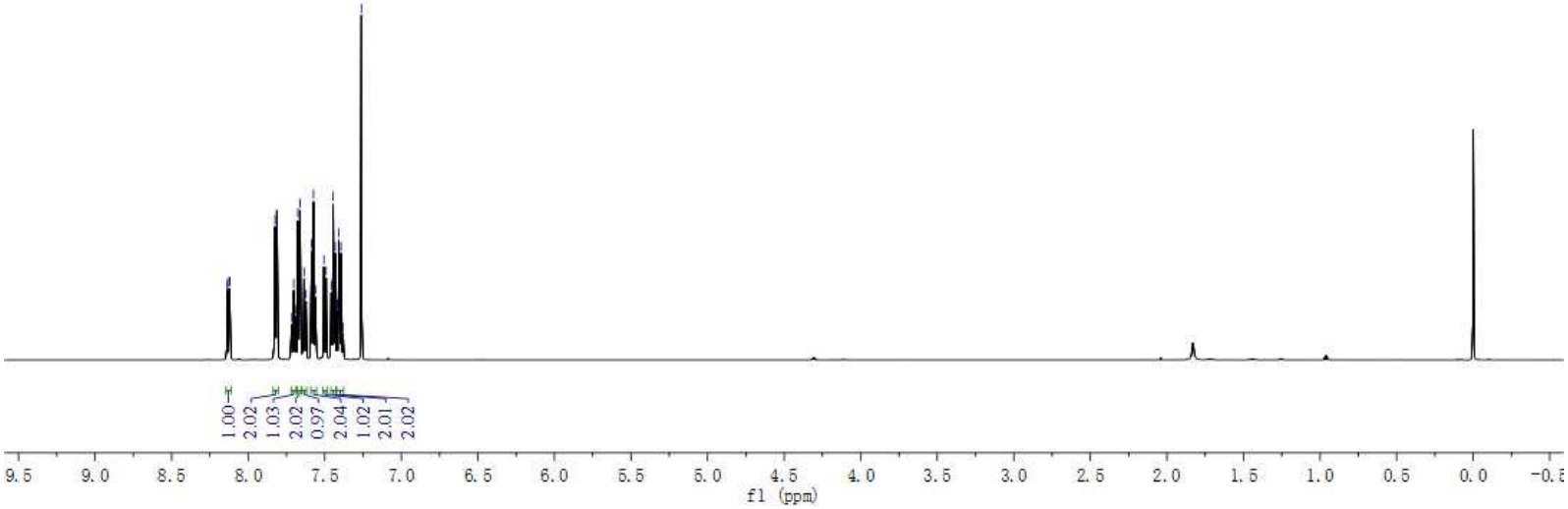
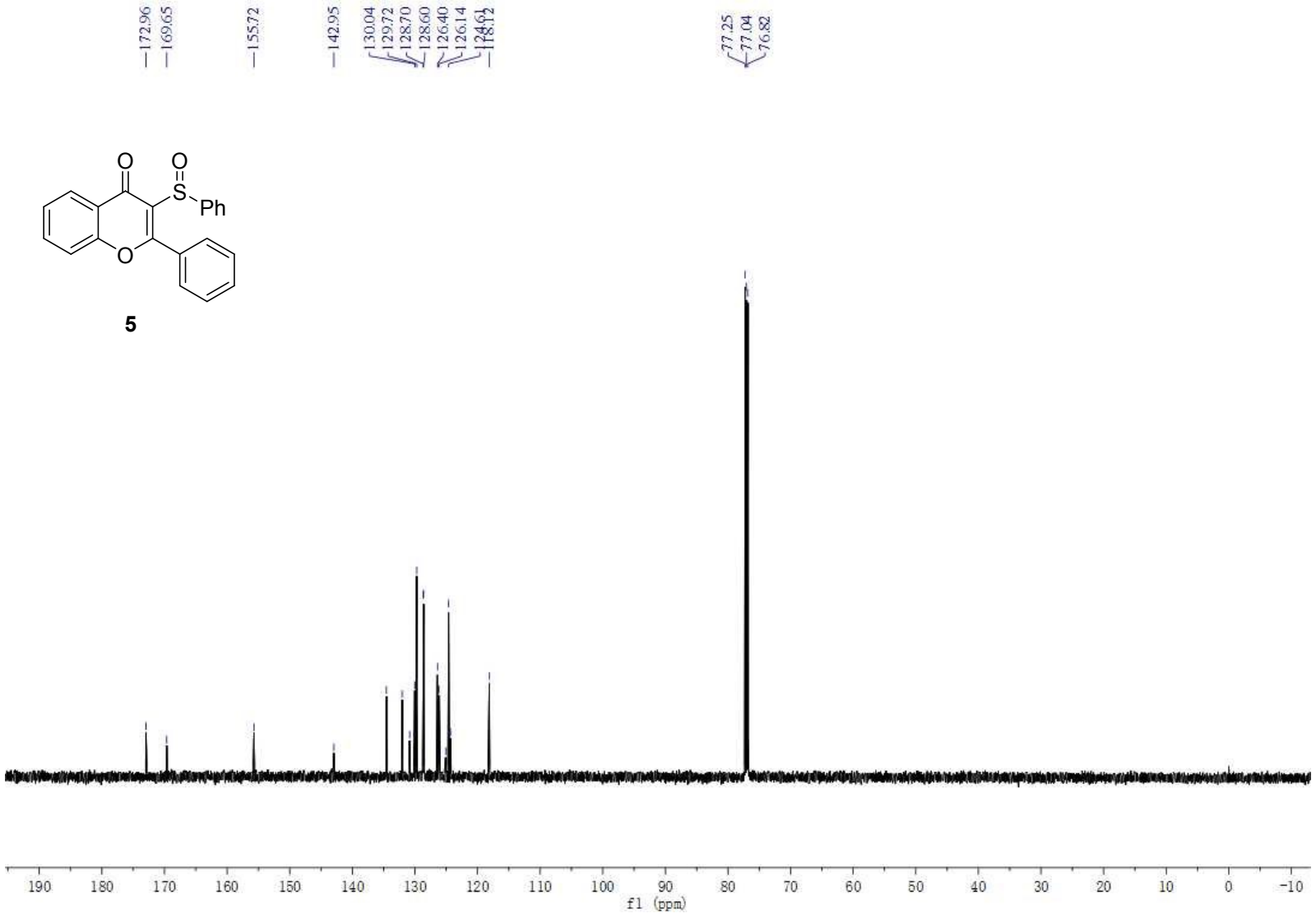
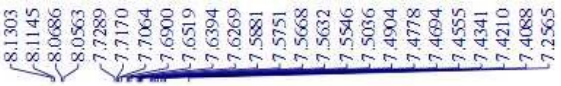
7.4453
7.4323
7.4209
7.4200
7.4076
7.3937
7.3812
7.2607

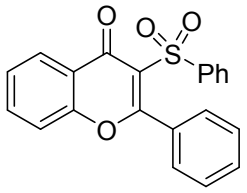

O
O
S
Ph
O

5

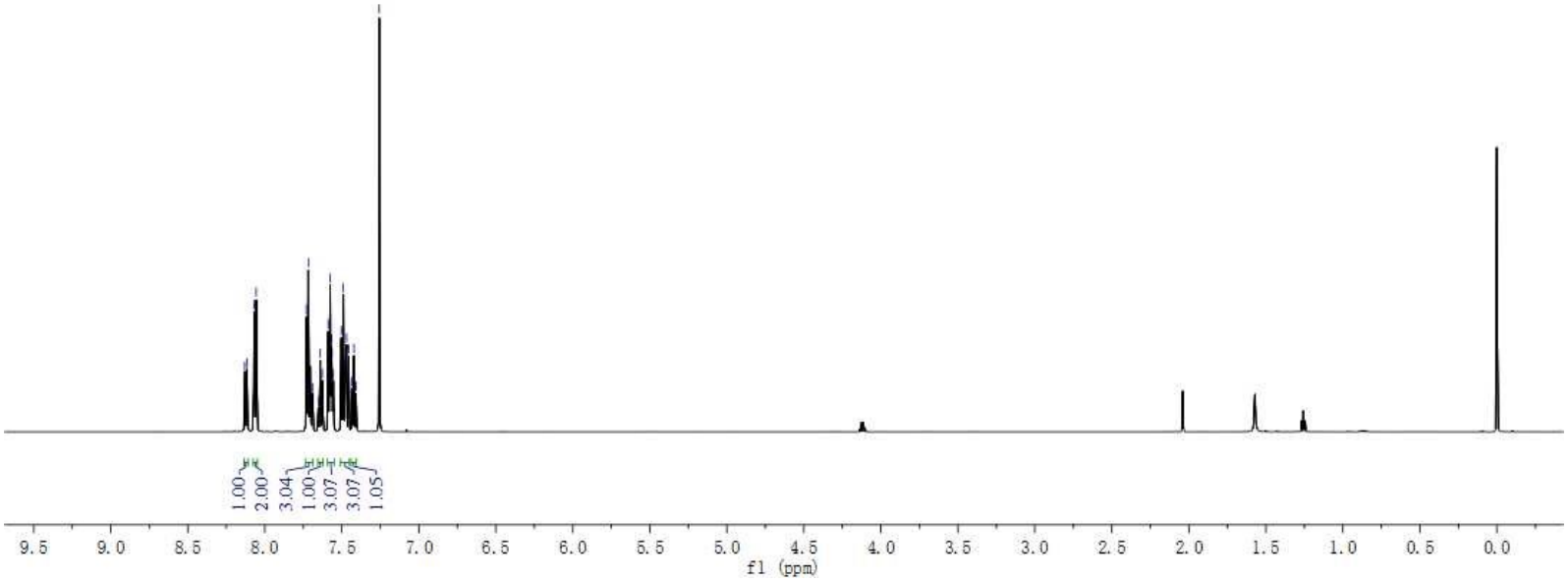

1.00
2.02
1.03
2.02
0.97
2.04
1.02
2.01
2.02
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

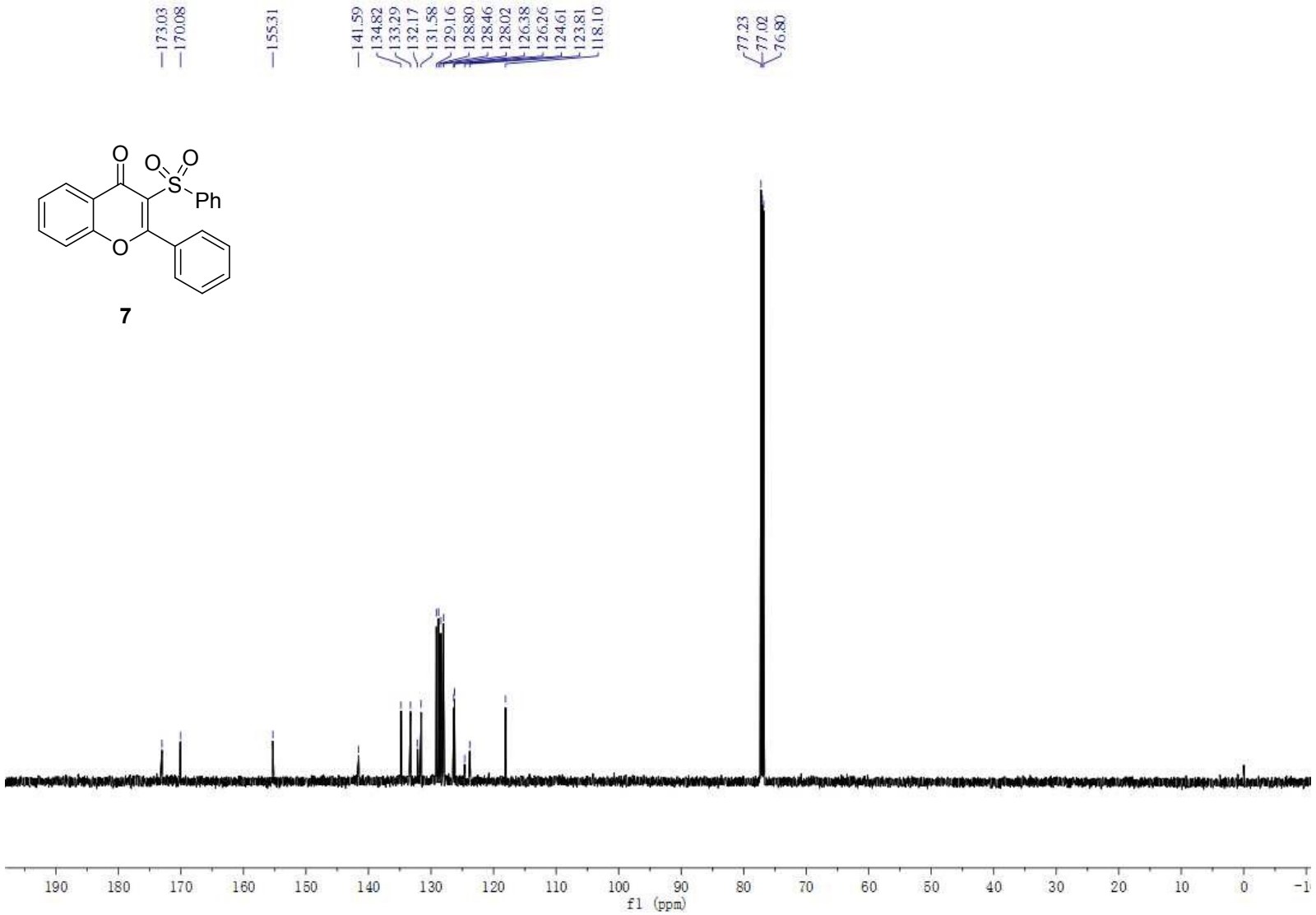

172.96
169.65
155.72
142.95
130.04
129.72
128.70
128.60
126.40
126.14
124.61
118.12
77.25
77.04
76.82
O
O
S
Ph
O
5
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.1303
8.1145
8.0686
8.0563
7.7289
7.7170
7.7064
7.6900
7.6519
7.6394
7.6269
7.5881
7.5751
7.5668
7.5632
7.5546
7.5036
7.4904
7.4778
7.4694
7.4555
7.4341
7.4210
7.4088
7.2565

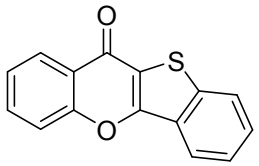

O
O
S
O
Ph
O

7

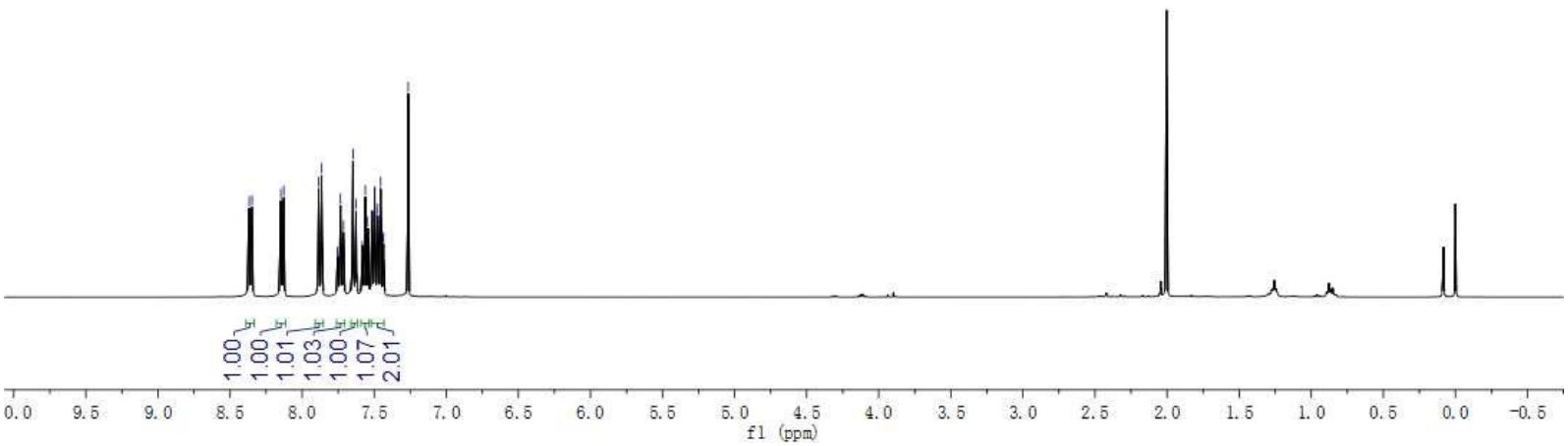

1.00
2.00
3.04
1.00
3.07
3.07
1.05
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

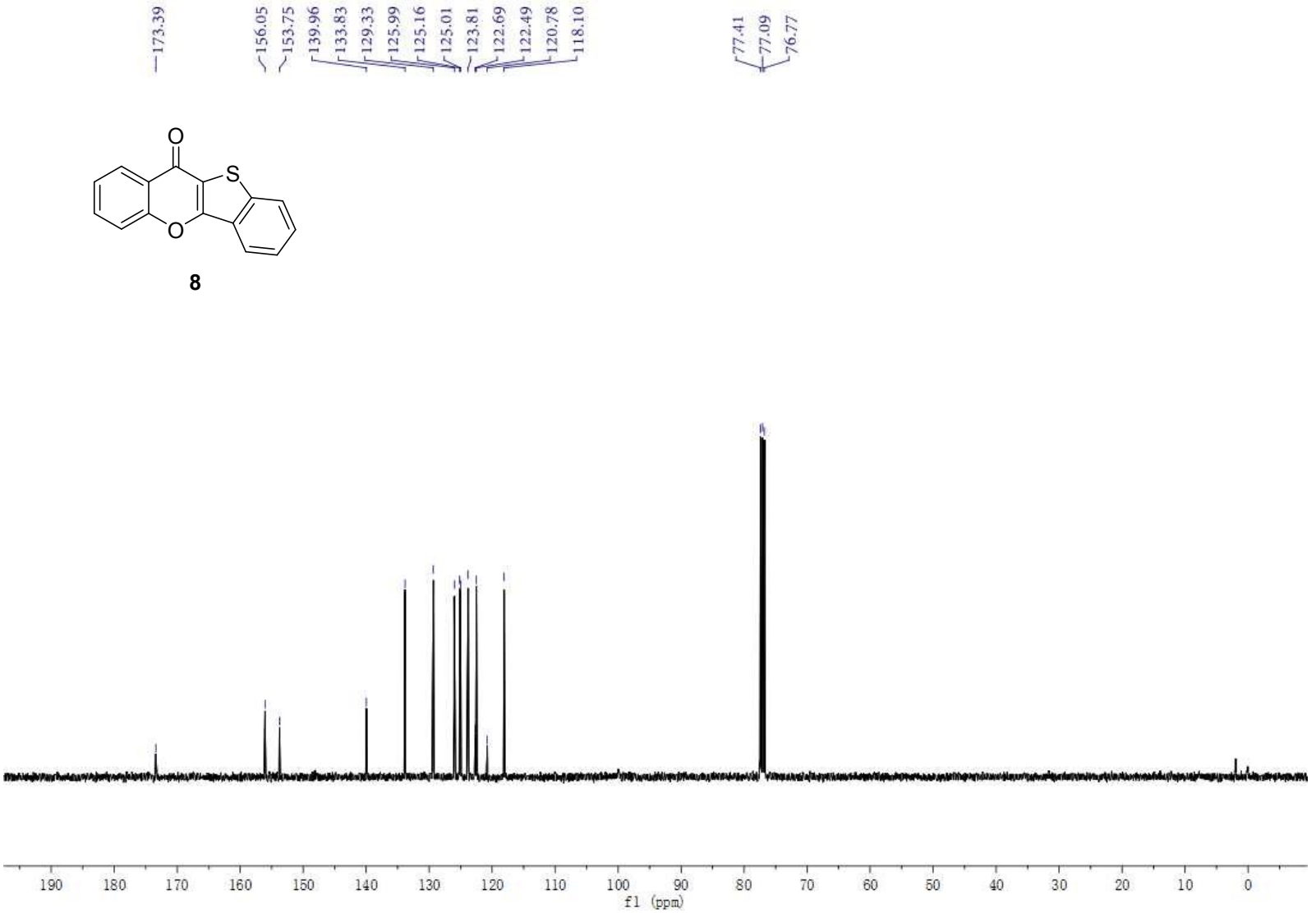

173.03
170.08
155.31
141.59
134.82
133.29
132.17
131.58
129.16
128.80
128.46
128.02
126.38
126.26
124.61
123.81
118.10
77.23
77.02
76.80
O
O
O
S
Ph
O
7
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.3670
8.3472
8.1477
8.1276
7.8848
7.8647
7.7553
7.7339
7.7125
7.6476
7.6266
7.5827
7.5621
7.5449
7.5168
7.4950
7.4753
7.4727
7.4549
7.4374
7.4350
7.2642


O
S
O

8


1.00
1.00
1.01
1.03
1.00
1.07
2.01
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


173.39
156.05
153.75
139.96
133.83
129.33
125.99
125.16
125.01
123.81
122.69
122.49
120.78
118.10
77.41
77.09
76.77
O
S
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

8