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Supporting information

Efficient Synthesis of Chiral Benzofuryl β-Amino Alcohols via Catalytic Asymmetric Henry Reaction

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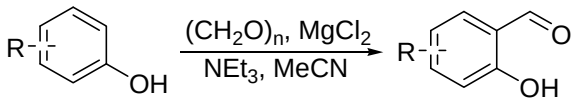
I. General methods

Unless otherwise noted, all the reagents and solvents were commercially available and used as received without any further purification. Tetrahydrofuran (THF) was distilled from sodium wires prior to use. Dichloromethane (DCM), *N*,*N*'-dimethylformide (DMF) and acetonitrile were distilled from calcium hydride prior to use. ^{1}H and ^{13}C NMR spectra were determined in deuterated solvents on a Bruker av500 NMR spectrometer. Chemical shifts were reported in delta (δ) units, parts per million (ppm) downfield from TMS.

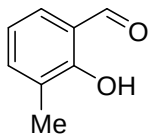
II. Experimental procedures and characterization data

Synthesis of substituted salicylaldehyde[1]



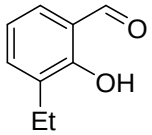
To a solution of phenolic derivative (50.0 mmol), magnesium chloride (7.17 g, 75.0 mmol) in dry acetonitrile (130 mL) was added triethylamine (27.2 mL, 112.5 mmol). The mixture was stirred at room temperature for 15 min, and then was added dry parafomaldehyde (7.50 g, 250.0 mmol) in one portion. The mixture was heated to reflux until the starting material consumed (as monitored by TLC), cooled to ambient temperature, and quenched with diluted HCl (3N) until pH = 2. The resulting solution was extracted with ethyl acetate (3 × 50 mL), and the combined organic layers were washed with brine, dried over sodium sulfate, filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel eluting with petroleum ether-ethyl acetate to give the desired product.

2-Hydroxy-3-methylbenzaldehyde (3b)



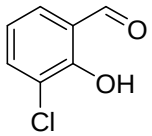
Colorless oil, 6.27 g, 92%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 11.28 (s, 1H), 9.89 (s, 1H), 7.43-7.39 (m, 2H), 6.94 (t, J = 7.55 Hz, 1H), 2.29 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 196.7, 160.0, 137.8, 131.4, 126.8, 120.0, 119.45, 15.0.

2-Hydroxy-3-ethylbenzaldehyde (3c)



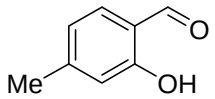
Colorless oil, 7.13 g, 95%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 11.30 (s, 1H), 9.90 (s, 1H), 7.46-7.40 (m, 2H), 6.98 (t, J = 7.55 Hz, 1H), 2.72 (q, J = 7.55 Hz, 2H), 1.26 (t, J = 7.55 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 196.8, 159.7, 136.3, 132.8, 131.4, 120.2, 119.5, 22.2, 13.7.

3-Chloro-2-hydroxybenzaldehyde (3d)



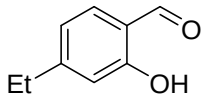
Yellow oil, 5.38 g, 69%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 11.50 (s, 1H), 9.92 (s, 1H), 7.64 (ddd, J = 0.50, 1.60, 2.10 Hz, 1H), 7.53 (dd, J = 1.60, 7.75 Hz, 1H), 7.02 (t, J = 7.60 Hz, 1H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 196.1, 157.2, 136.9, 132.1, 122.2, 121.4, 120.2.

2-Hydroxy-4-methylbenzaldehyde (3e)



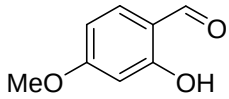
Colorless solid, 6.00 g, 88%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 11.05 (s, 1H), 9.84 (s, 1H), 7.44 (d, J = 7.85 Hz, 1H), 6.87-6.79 (m, 2H), 2.40 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 195.8, 161.7, 148.9, 133.6, 121.1, 118.7, 117.7, 22.2.

2-Hydroxy-4-ethylbenzaldehyde (3f)



Colorless oil, 7.06 g, 94%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 11.07 (s, 1H), 9.85 (s, 1H), 7.47 (d, J = 7.85 Hz, 1H), 6.89-6.86 (m, 1H), 6.85-6.83 (m, 1H), 2.68 (q, J = 7.60 Hz, 2H), 1.27 (t, J = 7.60 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 195.8, 161.9, 155.0, 133.7, 120.0, 118.9, 116.5, 29.4, 14.7.

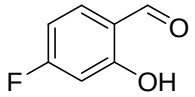
2-Hydroxy-4-methoxybenzaldehyde (3g)



Colorless oil, 6.77 g, 89%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 11.51 (s, 1H), 9.74 (s, 1H), 7.45 (d, J = 8.70 Hz, 1H), 6.56 (dd, J = 2.30, 8.70 Hz, 1H), 6.45 (d, J = 2.30 Hz, 1H), 3.88

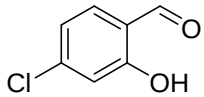
(s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 194.4, 166.8, 164.5, 135.3, 115.2, 108.3, 100.7, 55.7.

4-Fluoro-2-hydroxybenzaldehyde (3h)



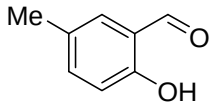
Colorless solid, 3.16 g, 45%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 11.38 (s, 1H), 9.85 (s, 1H), 7.61-7.56 (m, 1H), 6.78-6.72 (m, 1H), 6.69 (dd, J = 2.34, 10.36 Hz, 1H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 195.2, 168.0 (d, $J_{C\text{-}F}$ = 258.7 Hz), 164.1 (d, $J_{C\text{-}F}$ = 14.7 Hz), 136.1 (d, $J_{C\text{-}F}$ = 12.4 Hz), 117.9 (d, $J_{C\text{-}F}$ = 1.9 Hz), 108.2 (d, $J_{C\text{-}F}$ = 23.3 Hz), 104.6 (d, $J_{C\text{-}F}$ = 24.6 Hz).

4-Chloro-2-hydroxybenzaldehyde (3i)



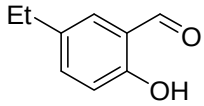
Colorless solid, 3.44 g, 44%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 11.18 (s, 1H), 9.88 (s, 1H), 7.53-7.50 (m, 1H), 7.05-7.00 (m, 2H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 195.6, 162.2, 143.2, 134.6, 120.6, 119.3, 117.9.

2-Hydroxy-5-methylbenzaldehyde (3j)



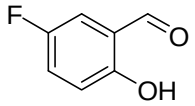
Yellow oil, 6.20 g, 91%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 10.84 (s, 1H), 9.87 (s, 1H), 7.38-7.33 (m, 2H), 6.93-6.90 (m, 1H), 2.36 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 196.5, 159.5, 138.0, 133.4, 129.1, 120.4, 117.4, 20.2.

2-Hydroxy-5-ethylbenzaldehyde (3k)



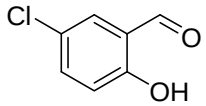
Colorless oil, 6.90 g, 92%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 10.86 (s, 1H), 9.89 (s, 1H), 7.41-7.35 (m, 2H), 6.93 (d, J = 8.35 Hz, 1H), 2.66 (q, J = 7.60 Hz, 2H), 1.26 (t, J = 7.60 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 196.6, 159.7, 137.0, 135.6, 132.2, 120.4, 117.4, 27.7, 15.5.

5-Fluoro-2-hydroxybenzaldehyde (3l)



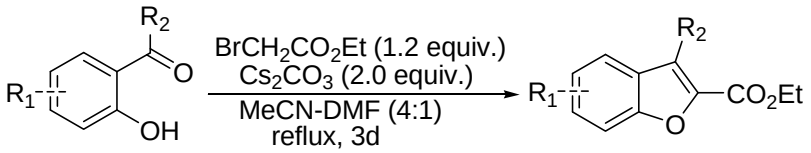
Colorless solid, 3.51 g, 25%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 10.80 (s, 1H), 9.87 (s, 1H), 7.32-7.25 (m, 2H), 7.01-6.97 (m, 1H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 195.5, 157.8 (d, $J_{C\text{-}F}$ = 1.4 Hz), 155.6 (d, $J_{C\text{-}F}$ = 240.6 Hz), 124.6 (d, $J_{C\text{-}F}$ = 23.8 Hz), 120.0 (d, $J_{C\text{-}F}$ = 6.1 Hz), 119.2 (d, $J_{C\text{-}F}$ = 7.0 Hz), 118.0 (d, $J_{C\text{-}F}$ = 12.6 Hz).

5-Chloro-2-hydroxybenzaldehyde (3m)



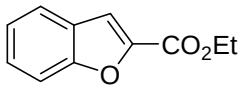
Yellow solid, 2.82 g, 36%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 10.93 (s, 1H), 9.86 (s, 1H), 7.55 (d, J = 2.60 Hz, 1H), 7.49 (dd, J = 2.60, 8.85 Hz, 1H), 6.98 (d, J = 8.85 Hz, 1H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 195.5, 160.1, 136.9, 132.5, 124.7, 121.1, 119.4.

Synthesis of ethyl benzofuran-2-carboxylate



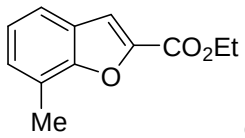
A solution of salicylaldehyde (20.0 mmol) or *o*-hydroxyphenyl ketone (20.0 mmol), ethyl bromoacetate (24.0 mmol) and cesium carbonate (40.0 mmol) in MeCN/DMF (4:1, 80 mL) was refluxed for 72 hours. The insoluble solid was filtered, washed with ethyl acetate and the combined filtrate was concentrated under reduced pressure. The residue was diluted with water (100 mL), extracted with diethyl ether (3 × 50 mL), and the combined filtrate was washed with brine, dried over sodium sulfate, filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel eluting with petroleum ether-ethyl acetate to give the desired product.

Ethyl benzofuran-2-carboxylate (4a)



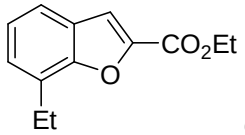
Yellow oil, 2.97 g, 78%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 7.70 (d, J = 7.85 Hz, 1H), 7.61 (dd, J = 0.65, 8.40 Hz, 1H), 7.55 (d, J = 0.85 Hz, 1H), 7.49-7.44 (m, 1H), 7.34-7.30 (m, 1H), 4.47 (q, J = 7.15 Hz, 2H), 1.45 (t, J = 7.15 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 159.6, 155.7, 145.7, 127.5, 127.0, 123.7, 122.8, 113.8, 112.3, 61.5, 14.3.

Ethyl 7-methylbenzofuran-2-carboxylate (4b)



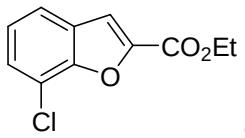
Colorless oil, 2.37 g, 58%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 7.54-7.50 (m, 2H), 7.27-7.24 (m, 1H), 7.22 (t, J = 7.50 Hz, 1H), 4.44 (q, J = 7.10 Hz, 2H), 2.61 (s, 3H), 1.45 (t, J = 7.10 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 159.7, 155.0, 145.5, 128.2, 126.5, 123.8, 122.7, 120.1, 114.1, 61.4, 15.1, 14.3.

Ethyl 7-ethylbenzofuran-2-carboxylate (4c)



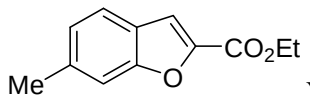
Colorless oil, 2.70 g, 62%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 7.55-7.50 (m, 2H), 7.31-7.28 (m ,1H), 7.25 (t, J = 7.50 Hz, 1H), 4.46 (q, J = 7.10 Hz, 2H), 3.03 (q, J = 7.60 Hz, 2H), 1.45 (t, J = 7.10 Hz, 3H), 1.39 (t, J = 7.60 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 159.7, 154.5, 145.4, 128.9, 126.7, 126.4, 123.9, 120.2, 114.1, 61.3, 22.6, 14.3, 14.0.

Ethyl 7-chlorobenzofuran-2-carboxylate (4d)



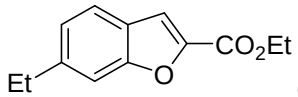
Colorless oil, 2.42 g, 54%; ^{1}H NMR ($CDCl_3$, 400MHz) δ 7.60 (dd, J = 1.02, 7.85Hz, 1H), 7.57 (s, 1H), 7.47 (dd, J = 1.02, 7.75 Hz, 1H), 7.26 (t, J = 7.80 Hz, 1H), 4.48(dq, J = 7.14 Hz, 2H), 1.46 (t, J =7.14 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 140.0, 135.0, 130.3, 129.1, 126.2, 124.0, 80.9, 70.3.

Ethyl 6-methylbenzofuran-2-carboxylate (4e)



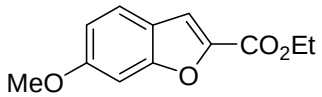
Yellow solid, 2.57 g, 63%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 7.56 (d, J = 8.05 Hz, 1H), 7.50 (d, J = 0.95 Hz, 1H), 7.41-7.39 (m, 1H), 7.16-7.13 (m, 1H), 4.45 (q, J = 7.10 Hz, 2H), 2.51 (s, 3H), 1.44 (t, J = 7.10 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 159.7, 156.2, 145.2, 138.3, 125.4, 124.5, 122.2, 113.8, 112.3, 61.3, 21.9, 14.3.

Ethyl 6-ethylbenzofuran-2-carboxylate (4f)



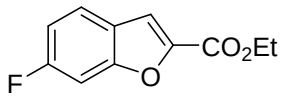
Colorless oil, 2.84 g, 65%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 7.58 (d, J = 8.10 Hz, 1H), 7.50 (d, J = 0.95 Hz, 1H),7.44 (m, 1H), 7.17 (dd, J = 1.40, 8.05 Hz, 1H), 4.45 (q, J = 7.15 Hz, 2H), 2.80 (q, J = 7.60 Hz, 2H), 1.44 (t, J = 7.15 Hz, 3H), 1.31 (t, J = 7.60 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 159.7, 156.3, 145.3, 144.8, 124.7, 124.4, 122.3, 113.8, 111.0, 61.3, 29.2, 15.7, 14.3.

Ethyl 6-methoxybenzofuran-2-carboxylate (4g)



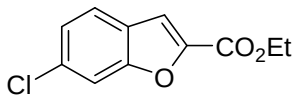
Colorless solid, 2.51 g, 57%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 7.54 (d, J = 8.70 Hz, 1H), 7.48 (d, J = 0.95 Hz, 1H), 7.08 (d, J = 1.95 Hz, 1H), 6.95 (dd, J = 9.28, 13.56 Hz, 1H), 4.44 (q, J = 7.15 Hz, 2H), 3.88 (s, 3H), 1.44 (t, J = 7.15 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 160.5, 159.6, 157.1, 145.0, 123.0, 120.2, 114.0(1), 113.9(5), 95.7, 61.2, 55.6, 14.4.

Ethyl 6-fluorobenzofuran-2-carboxylate (4h)



Colorless solid, 2.38 g, 57%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 7.63 (dd, J = 5.40, 8.70 Hz, 1H), 7.52 (d, J = 1.00 Hz, 1H), 7.33-7.29 (m, 1H), 7.10 (ddd, J = 2.30, 8.75, 9.05 Hz, 1H), 4.46 (q, J = 7.15 Hz, 2H), 1.44 (t, J = 7.15 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 162.6 (d, $J_{C\text{-}F}$ = 247.4 Hz), 159.2, 155.7 (d, $J_{C\text{-}F}$ = 13.9 Hz), 146.6 (d, $J_{C\text{-}F}$ = 4.4 Hz), 123.4 (d, $J_{C\text{-}F}$ = 10.4 Hz), 123.2 (d, $J_{C\text{-}F}$ = 1.5 Hz), 113.5, 112.7 (d, $J_{C\text{-}F}$ = 24.6 Hz), 99.7 (d, $J_{C\text{-}F}$ = 26.8 Hz), 61.5, 14.3.

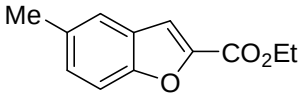
Ethyl 6-chlorobenzofuran-2-carboxylate (4i)



Colorless solid, 2.33 g, 52%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 7.63-7.59 (m, 2H), 7.51 (d, J = 0.90 Hz, 1H), 7.31 (dd, J = 1.65, 8.50 Hz, 1H), 4.46 (q, J = 7.10 Hz, 2H), 1.45 (t, J = 7.10 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 159.2, 155.6, 146.4, 133.5, 125.6, 124.8,

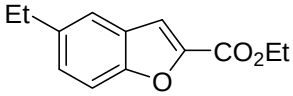
123.3, 113.4, 112.7, 61.7, 14.3.

Ethyl 5-methylbenzofuran-2-carboxylate (4j)



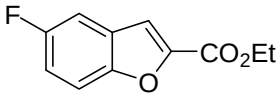
Colorless solid, 2.45 g, 60%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 7.50-7.45 (m, 3H), 7.29-7.25 (m, 1H), 4.46 (q, J = 7.10 Hz, 2H), 2.47 (s, 3H), 1.45 (t, J = 7.10 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 159.7, 154.2, 145.8, 133.3, 129.1, 127.1, 122.3, 113.5, 111.8, 61.4, 21.2, 14.3.

Ethyl 5-ethylbenzofuran-2-carboxylate (4k)



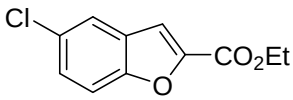
Colorless oil, 2.79 g, 64%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 7.51-7.48 (m, 3H), 7.30 (dd, J = 1.80, 8.55 Hz, 1H), 4.46 (q, J = 7.10 Hz, 2H), 2.77 (q, J = 7.60 Hz, 2H), 1.45 (t, J = 7.10 Hz, 3H), 1.30 (t, J = 7.60 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 159.7, 154.4, 145.8, 139.9, 128.1, 127.1, 121.1, 113.7, 111.9, 61.4, 28.7, 16.0, 14.3.

Ethyl 5-fluorobenzofuran-2-carboxylate (4l)



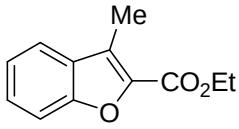
Colorless solid, 2.12 g, 51%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 7.55 (dd, J = 4.10, 9.10 Hz, 1H), 7.50 (d, J = 0.90 Hz, 1H), 7.34 (dd, J = 2.55, 8.15 Hz, 1H), 7.19 (td, J = 2.65, 9.05 Hz, 1H), 4.47 (q, J = 7.15 Hz, 2H), 1.45 (t, J = 7.15 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 159.4 (d, $J_{C\text{-}F}$ = 240.9 Hz), 159.2, 151.9, 147.3, 127.6 (d, $J_{C\text{-}F}$ = 11.0 Hz), 115.7 (d, $J_{C\text{-}F}$ = 26.8 Hz), 113.5 (d, $J_{C\text{-}F}$ = 4.3 Hz), 113.2 (d, $J_{C\text{-}F}$ = 9.5 Hz), 107.8 (d, $J_{C\text{-}F}$ = 24.9 Hz), 61.6, 14.2.

Ethyl 5-chlorobenzofuran-2-carboxylate (4m)



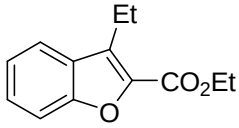
Colorless solid, 3.23 g, 72%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 7.67 (dd, J = 0.45, 2.15 Hz, 1H), 7.53 (dt, J = 0.60, 8.80 Hz, 1H), 7.47 (d, J = 0.90 Hz, 1H), 7.42 (dd, J = 2.15, 8.85 Hz, 1H), 4.47 (q, J = 7.15 Hz, 2H), 1.45 (t, J = 7.15 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 159.1, 153.9, 147.0, 129.4, 128.2, 127.8, 122.1, 113.4, 112.9, 61.7, 14.3.

Ethyl 3-methylbenzofuran-2-carboxylate(4n)



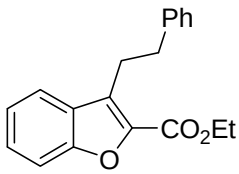
Colorless solid, 2.45 g, 61%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 7.67-7.63 (ddd, J = 0.75, 1.15, 7.90 Hz, 1H), 7.56 (dt, J = 0.74, 8.43 Hz, 1H), 7.48-7.44 (m, 1H), 7.34-7.30 (m, 1H), 4.48 (q, J = 7.14 Hz, 2H), 2.61 (s, 3H), 1.45 (t, J = 7.14 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 160.5, 154.3, 140.9, 129.0, 127.7, 125.6, 123.1, 121.0, 112.1, 61.1, 14.4, 9.3.

Ethyl 3-ethylbenzofuran-2-carboxylate (4o)



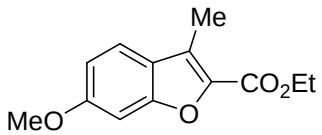
Colorless oil, 2.84 g, 65%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 7.68 (dd, J = 0.73, 1.17, 7.89 Hz, 1H), 7.53 (dt, J = 0.79, 8.41 Hz, 1H), 7.48-7.44 (m, 1H), 7.33-7.29 (m, 1H), 4.48 (q, J = 7.14 Hz, 2H), 3.12 (q, J = 7.60 Hz, 2H), 1.46 (t, J = 7.14 Hz, 3H), 1.33 (t, J = 7.60 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 160.4, 154.5, 140.3, 131.7, 128.2, 127.6, 123.1, 121.1, 112.3, 61.1, 17.6, 14.4, 14.3.

Ethyl 3-phenethylbenzofuran-2-carboxylate (4p)



Colorless oil, 3.53 g, 60%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 7.61-7.55 (m, 2H), 7.48-7.44 (m, 1H), 7.32-7.27 (m, 3H), 7.26-7.20 (m, 3H), 4.46 (q, J = 7.15 Hz, 2H), 3.44-3.36 (m, 2H), 3.03-2.98 (m, 2H), 1.47 (t, J = 7.15 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 160.3, 154.5, 141.3, 141.0, 129.3, 128.5, 128.4, 128.3, 127.7, 126.2, 123.2, 121.1, 112.3, 61.2, 36.1, 26.5, 14.5.

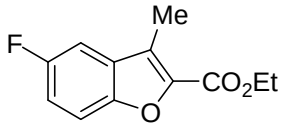
Ethyl 6-methoxy-3-methylbenzofuran-2-carboxylate (4q)



Colorless solid, 3.18 g, 66%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 7.49 (dd,

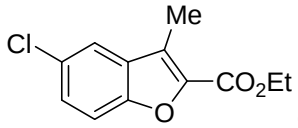
J = 8.65 Hz, 1H), 7.03 (d, J = 2.10 Hz, 1H), 6.94 (dd, J = 1.95, 8.65 Hz, 1H), 4.45 (q, J = 7.13 Hz, 2H), 3.87 (s, 3H), 2.57 (s, 3H), 1.45 (t, J = 7.13 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 160.7, 160.5, 155.7, 140.3, 126.0, 122.4, 121.3, 113.26, 95.5, 60.8, 55.6, 14.4, 9.4.

Ethyl 5-fluoro-3-methylbenzofuran-2-carboxylate (4r)



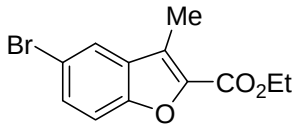
Colorless solid, 2.31 g, 52%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 7.49 (dd, J = 3.98, 9.00 Hz, 1H), 7.53 (dd, J = 5.75, 8.15 Hz, 1H), 7.18 (td, J = 2.63, 9.01 Hz, 1H), 4.47 (q, J = 7.14 Hz, 2H), 2.57 (s, 3H), 1.46 (t, J = 7.14 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 169.2 (d, $J_{C\text{-}F}$ = 189.3 Hz), 150.5, 142.4, 129.8 (d, $J_{C\text{-}F}$ = 8.1 Hz), 125.3 (d, $J_{C\text{-}F}$ = 3.6 Hz), 115.9 (d, $J_{C\text{-}F}$ = 21.2 Hz), 113.0 (d, $J_{C\text{-}F}$ = 7.4 Hz), 106.2 (d, $J_{C\text{-}F}$ = 19.6 Hz), 61.2, 14.3, 9.3.

Ethyl 5-chloro-3-methylbenzofuran-2-carboxylate (4s)



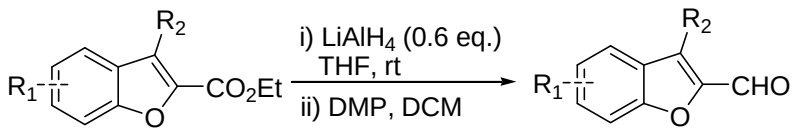
Colorless solid, 2.95 g, 62%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 7.67 (dd, J = 0.40, 2.05 Hz, 1H), 7.48 (dd, J = 0.42, 8.81 Hz, 1H), 7.40 (dd, J = 2.11, 8.80 Hz, 1H), 4.47 (q, J = 7.14 Hz, 2H), 2.57 (s, 3H), 1.46 (t, J = 7.14 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 160.1, 152.5, 142.1, 130.3, 128.8, 127.9, 124.8, 120.5, 113.2, 61.3, 14.3, 9.2.

Ethyl 5-bromo-3-methylbenzofuran-2-carboxylate (4t)



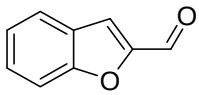
Colorless solid, 3.16 g, 56%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 7.77 (d, J = 1.96 Hz, 1H), 7.54 (dd, J = 2.00, 8.80 Hz, 1H), 7.43 (d, J = 8.80 Hz, 1H), 4.47 (q, J = 7.15 Hz, 2H), 2.57 (s, 3H), 1.46 (t, J = 7.15 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 160.1, 153.0, 142.0, 131.0, 130.6, 124.7, 123.7, 116.2, 113.7, 61.3, 14.4, 9.3

Synthesis of benzofuran-2-carbaldehyde



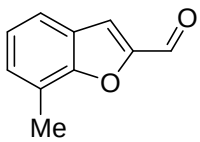
To a suspension of $LiAlH_4$ (0.23 g, 6.0 mmol) in THF (12 mL) was dropwise added a solution of ethyl benzofuran-2-carboxylate (10.0 mmol) in THF (10 mL). The solution was stirred at room temperature for 3 h, cooled with an ice-bath, and carefully quenched with saturated aqueous potassium carbonate (1.0 mL). The resulting suspension was filtered, washed with ethyl acetate (2 × 10 mL), and the combined organic layers were dried over sodium sulfate, filtered and concentrated under reduced pressure. The residue was dissolved in DCM (20 mL), and then Dess-Martin periodinane (DMP, 10.0 mmol) was added. After completion of the reaction (as monitored by TLC), the white suspension was filtered through celite pad and washed with DCM. The combined filtrate was quenched with water, extracted with DCM (2 × 10 mL), and the combined organic layers were washed with brine, dried over sodium sulfate, filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel eluting with ethyl acetate-petroleum ether to give the desired product.

Benzofuran-2-carbaldehyde (5a)



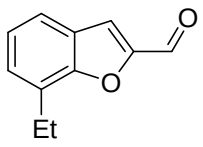
Yellow oil, 0.88 g, 60%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 9.89 (s, 1H), 7.77 (ddd, J = 0.75, 1.15, 8.00 Hz, 1H), 7.77 (dq, J = 0.85, 8.45 Hz, 1H), 7.59 (d, J = 0.95 Hz, 1H), 7.54 (ddd, J = 1.26, 5.61, 8.45 Hz, 1H), 7.36 (ddd, J = 0.94, 7.18, 8.02 Hz, 1H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 179.7, 156.2, 152.7, 129.2, 126.7, 124.2, 123.7, 117.9, 112.6.

7-Methylbenzofuran-2-carbaldehyde (5b)



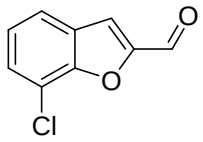
Yellow solid, 1.09 g, 68%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 9.90 (s, 1H), 7.61-7.58 (m, 1H), 7.58 (s, 1H), 7.35-7.32 (m, 1H), 7.26 (t, J = 7.60 Hz, 1H), 2.61 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 179.8, 155.5, 152.6, 129.8, 126.2, 124.3, 123.1, 121.0, 118.2, 15.0.

7-Ethylbenzofuran-2-carbaldehyde (5c)



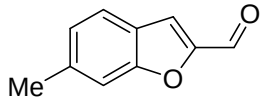
Yellow solid, 1.15 g, 66%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 9.90 (s, 1H), 7.60 (dd, J = 1.20, 7.85 Hz, 1H), 7.58 (s, 1H), 7.38-7.35 (m, 1H), 7.30 (t, J = 7.70 Hz, 1H), 3.02 (q, J = 7.60 Hz, 2H), 1.39 (t, J = 7.60 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 179.8, 155.1, 152.6, 129.4, 128.1, 126.4, 124.4, 121.0, 118.0, 22.7, 14.0.

7-Chlorobenzofuran-2-carbaldehyde (5d)



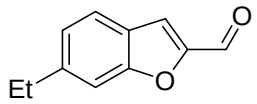
Yellow solid, 1.01 g, 56%; ^{1}H NMR ($CDCl_3$, 400MHz) δ 9.95 (s, 1H), 7.67 (dd, J = 1.00, 7.90 Hz, 1H), 7.61 (s, 1H), 7.54 (dd, J = 1.05, 7.80 Hz, 1H), 7.31 (t, J = 7.85 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 179.7, 153.1, 152.0, 128.9, 128.2, 125.0, 122.1, 118.1, 116.7.

6-Methylbenzofuran-2-carbaldehyde (5e)



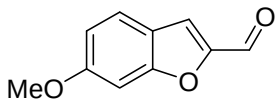
Yellow solid, 1.01 g, 63%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 9.84 (s, 1H), 7.63 (d, J = 8.10 Hz, 1H), 7.52 (d, J = 0.95 Hz, 1H), 7.41-7.39 (m, 1H), 7.18 (ddd, J = 0.50, 1.25, 1.70 Hz, 1H), 2.52 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 179.5, 156.8, 152.5, 140.4, 126.0, 124.3, 123.1, 118.2, 112.5, 22.1.

6-Ethylbenzofuran-2-carbaldehyde (5f)



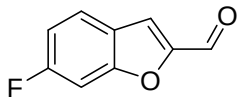
Yellow oil, 1.13 g, 65%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 9.84 (s, 1H), 7.66 (d, J = 8.15 Hz, 1H), 7.54 (d, J = 1.00 Hz, 1H), 7.44-7.42 (m, 1H), 7.22 (dd, J = 1.40, 8.10 Hz, 1H), 2.82 (q, J = 7.60 Hz, 2H), 1.32 (t, J = 7.60 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 179.5, 156.9, 152.6, 146.8, 1254.0, 124.5, 123.2, 118.1, 111.3, 29.4, 15.6.

6-Methoxybenzofuran-2-carbaldehyde (5g)



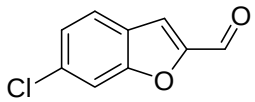
Colorless solid, 1.03 g, 58%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 9.77 (s, 1H), 7.62 (d, J = 8.65 Hz, 1H), 7.51 (d, J = 0.95 Hz, 1H), 7.06 (d, J = 1.95 Hz, 1H), 6.993 (dd, J = 2.20, 8.70 Hz, 1H), 3.91 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 178.7, 161.8, 158.0, 152.5, 124.0, 120.0, 118.8, 114.9, 95.5, 55.7.

6-Fluorobenzofuran-2-carbaldehyde (5h)



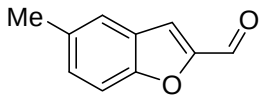
Yellow solid, 0.82 g, 50%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 9.85 (s, 1H), 7.73 (dd, J = 5.40, 8.70 Hz, 1H), 7.56 (d, J = 0.95 Hz, 1H), 7.33-7.30 (m, 1H), 7.14 (ddd, J = 1.80, 8.85, 9.15 Hz, 1H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 179.1, 163.6 (d, $J_{C\text{-}F}$ = 251.2 Hz), 156.5 (d, $J_{C\text{-}F}$ = 13.9 Hz), 153.6 (d, $J_{C\text{-}F}$ = 4.3 Hz), 124.6 (d, $J_{C\text{-}F}$ = 10.5 Hz), 123.0 (d, $J_{C\text{-}F}$ = 1.5 Hz), 117.5, 113.5 (d, $J_{C\text{-}F}$ = 25.0 Hz), 100.0 (d, $J_{C\text{-}F}$ = 26.7 Hz).

6-Chlorobenzofuran-2-carbaldehyde (5i)



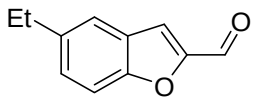
Yellow solid, 1.01 g, 56%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 9.88 (s, 1H), 7.69 (dd, J = 0.35, 8.45 Hz, 1H), 7.64-7.62 (m, 1H), 7.55 (d, J = 1.00 Hz, 1H), 7.35 (dd, J = 1.75, 8.45 Hz, 1H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 179.5, 156.2, 153.3, 135.1, 125.4, 125.3, 124.3, 117.1, 113.1.

5-Methylbenzofuran-2-carbaldehyde (5j)



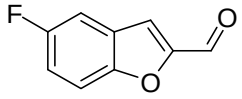
Yellow solid, 0.98 g, 61%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 9.86 (s, 1H), 7.54-7.52 (m, 1H), 7.51-7.48 (m, 2H), 7.35 (dd, J = 1.65, 8.80 Hz, 1H), 2.48 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 179.7, 154.9, 152.9, 133.9, 130.9, 126.8, 123.1, 117.6, 112.2, 21.3.

5-Ethylbenzofuran-2-carbaldehyde (5k)



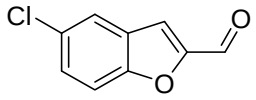
Yellow oil, 1.05 g, 60%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 9.86 (s, 1H), 7.55 (dd, J = 0.75, 1.70 Hz, 1H), 7.54-7.51 (m, 2H), 7.38 (dd, J = 1.75, 8.70 Hz, 1H), 2.78 (q, J = 7.65 Hz, 2H), 1.31 (t, J = 7.65 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 179.7, 155.0, 152.9, 140.4, 129.9, 126.8, 121.8, 117.7, 112.3, 28.7, 16.0.

5-Fluorobenzofuran-2-carbaldehyde (5l)



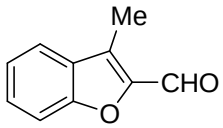
Yellow solid, 0.95 g, 58%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 9.89 (s, 1H), 7.58 (dd, J = 3.95, 9.05 Hz, 1H), 7.55 (d, J = 0.90 Hz, 1H), 7.42 (dd, J = 2.55, 7.95 Hz, 1H), 7.27 (td, J = 2.65, 9.00 Hz, 1H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 179.7, 159.6 (d, $J_{C\text{-}F}$ = 242.0 Hz), 154.0, 152.5, 127.3 (d, $J_{C\text{-}F}$ = 11.0 Hz), 117.5 (d, $J_{C\text{-}F}$ = 26.9 Hz), 117.2, 113.7 (d, $J_{C\text{-}F}$ = 9.5 Hz), 108.5 (d, $J_{C\text{-}F}$ = 25.0 Hz).

5-Chlorobenzofuran-2-carbaldehyde (5m)



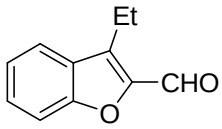
Yellow solid, 1.08 g, 60%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 9.90 (s, 1H), 7.74 (dd, J = 0.45, 2.10 Hz, 1H), 7.55 (dt, J = 0.70, 8.85 Hz, 1H), 7.52 (d, J = 0.90 Hz, 1H), 7.49 (dd, J = 2.15, 8.90 Hz, 1H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 179.7, 154.5, 153.7, 129.9, 129.5, 127.9, 123.0, 116.5, 113.8.

3-Methylbenzofuran-2-carbaldehyde (5n)



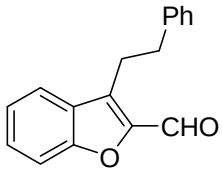
Colorless solid, 1.01 g, 63%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 10.05 (s, 1H), 7.73-7.69 (m, 1H), 7.58-7.51 (m, 2H), 7.37-7.33 (m, 1H), 2.64 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 179.6, 155.3, 148.1, 129.3, 128.6, 123.6, 121.8, 112.5, 8.3.

3-Ethylbenzofuran-2-carbaldehyde (5o)



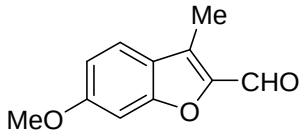
Yellow oil, 1.05 g, 60%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 10.05 (s, 1H), 7.76-7.74 (m, 1H), 7.59-7.57 (m, 1H), 7.55-7.51 (m, 1H), 7.37-7.33 (m, 1H), 3.13 (q, J = 7.63 Hz, 2H), 1.41 (t, J = 7.63 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 179.5, 155.5, 147.5, 134.8, 129.2, 127.7, 123.6, 122.0, 112.6, 16.9, 15.1.

3-Phenethylbenzofuran-2-carbaldehyde (5p)



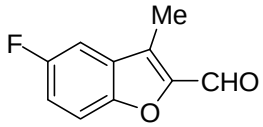
Colorless solid, 1.56 g, 62%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 9.68 (s, 1H), 7.69-7.66 (m, 1H), 7.60-7.57 (m, 1H), 7.56-7.52 (m, 1H), 7.36-7.32 (m, 1H), 7.31-7.26 (m, 2H), 7.25-7.21 (m, 1H), 7.15-7.12 (m, 2H), 3.38 (t, J = 7.51 Hz, 2H), 3.06 (t, J = 7.51 Hz, 2H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 179.4, 155.4, 148.4, 140.3, 131.7, 129.2, 128.6, 128.6, 127.8, 126.6, 123.7, 121.9, 112.7, 36.3, 25.7.

6-Methoxy-3-methylbenzofuran-2-carbaldehyde (5q)



Yellow solid, 1.30 g, 68%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 9.93 (s, 1H), 7.55 (d, J = 8.70 Hz, 1H), 7.00 (d, J = 2.11 Hz, 1H), 6.97 (dd, J = 2.11, 8.68 Hz, 1H), 3.89 (s, 3H), 2.59 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 178.2, 162.0, 157.0, 148.0, 129.6, 122.1, 121.9, 114.1, 95.3, 55.7, 8.3.

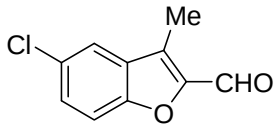
5-Fluoro-3-methylbenzofuran-2-carbaldehyde (5r)



Yellow solid, 0.98 g, 55%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 10.04 (s, 1H), 7.51 (dd, J = 3.98, 9.04 Hz, 1H), 7.34 (dd, J = 2.58, 7.94 Hz, 1H), 7.26 (td, J = 2.63, 8.99 Hz, 1H), 2.61 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 179.7, 165.3 (d, $J_{C\text{-}F}$ = 241.5 Hz), 151.5, 149.4, 129.4

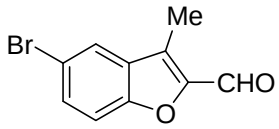
(d, $J_{C\text{-}F}$ = 10.1 Hz), 127.9, 117.5 (d, $J_{C\text{-}F}$ = 26.9 Hz), 113.5 (d, $J_{C\text{-}F}$ = 9.4 Hz), 106.7 (d, $J_{C\text{-}F}$ = 24.5 Hz), 8.3.

5-Chloro-3-methylbenzofuran-2-carbaldehyde (5s)



Colorless solid, 1.13 g, 58%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 10.04 (s, 1H), 7.67 (dd, J = 0.72, 1.88 Hz, 1H), 7.50 (dd, J = 0.71, 8.83 Hz, 1H), 7.47 (dd, J = 1.91, 8.85 Hz, 1H), 2.61 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 179.7, 153.5, 149.0, 129.9, 129.5, 129.3, 127.3, 121.2, 113.6, 8.3.

5-Bromo-3-methylbenzofuran-2-carbaldehyde (5t)

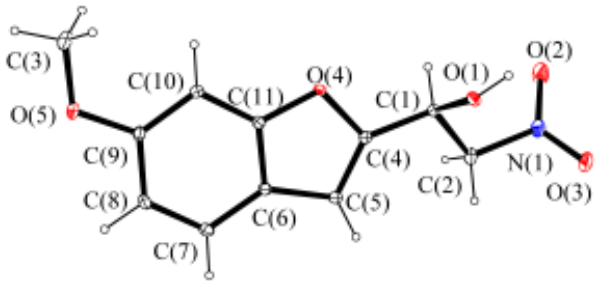


Colorless solid, 1.24 g, 52%; ^{1}H NMR ($CDCl_3$, 500MHz) δ 10.05 (s, 1H), 7.84 (d, J = 1.98 Hz, 1H), 7.61 (dd, J = 2.00, 8.82 Hz, 1H), 7.45 (d, J = 8.81 Hz, 1H), 2.61 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 179.7, 153.8, 148.8, 132.1, 130.5, 127.1, 124.4, 116.7, 114.0, 8.3.

III. Single crystal X-ray analysis data

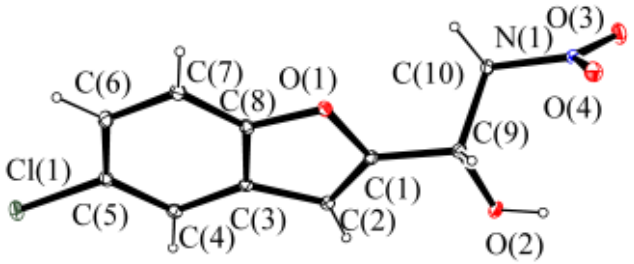
Diffraction data of **6g** (CCDC 1508863) was collected on Oxford Gemini Diffractometer with graphite monochromate Mo-Kα (λ = 0.71073 Å) radiation at 173 K. Diffraction data of **6m** (CCDC 1508862) was collected on Bruker Smart Apex CCD Diffractometer with graphite monochromate Cu-Kα (λ =1.54184 Å) radiation at 173 K. Empirical absorption corrections were applied using the SADABS program. The structures were solved by direct methods and refined by full-matrix least-squares on F^2 by using the Shelxtl crystallographic software package. Hydrogen atoms were included at geometrically calculated positions with thermal parameters derived from the parent atoms.

S3.1 Crystal structure, data and structure refinement of compound **6g**



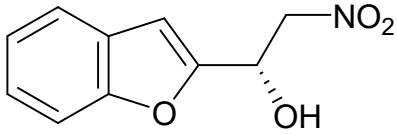
empirical formula	$C_{11}H_{11}NO_5$
fw (g/mol)	237.21
temperature (K)	173(2)
wavelength (Å)	0.71073
space group	$P2_1$
a (Å)	7.993(4)
b (Å)	12.540(5)
c (Å)	10.604 (4)
V (Å^3)	1036.6(8)
Z	2
F(000)	496
D_c (g/mL)	1.520
crystal size (mm^3)	0.20 × 0.10 × 0.10
θ range (deg)	1.97-29.08
data/restraints/param	4338/3/315
GOF on F^2	1.015
R_1 [$I > 2\sigma(I)$]	0.0657
wR_2 [$I > 2\sigma(I)$]	0.1411
R_1 (all data)	0.0865
wR_2 (all data)	0.1532
largest diff/hole(e/Å^3)	0.252/-0.227

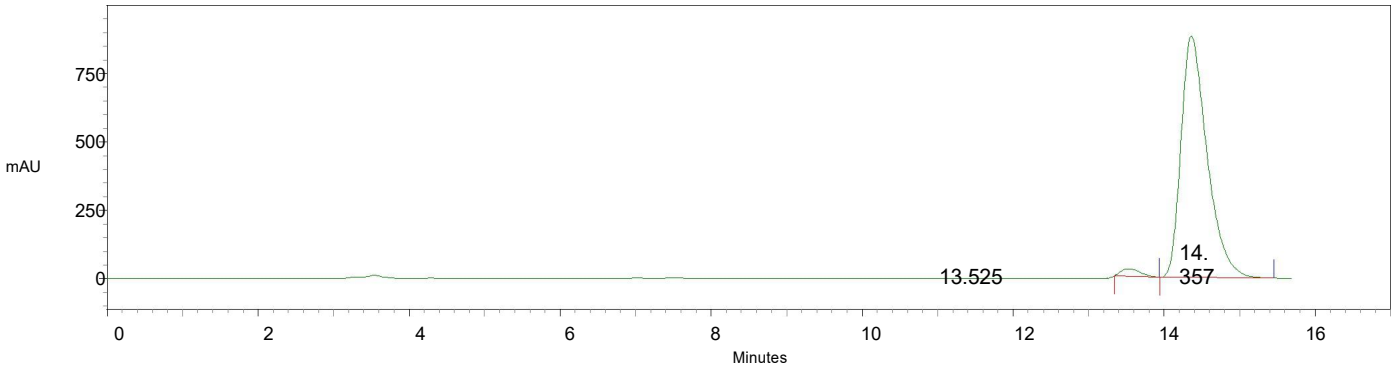
S3.2 Crystal structure, data and structure refinement of compound **6m**



empirical formula	$C_{10}H_8ClNO_4$
fw (g/mol)	241.62
temperature (K)	173(2)
wavelength (Å)	1.54184
space group	$P2_12_12_1$
a (Å)	5.5571(2)
b (Å)	5.6305(2)
c (Å)	32.3624 (10)
V (Å^3)	1012.60(6)
Z	4
F(000)	496
D_c (g/mL)	1.585
crystal size (mm^3)	0.20 × 0.10 × 0.08
θ range (deg)	5.47-62.12
data/restraints/param	1590/2/148
GOF on F^2	1.046
R_1 [$I > 2\sigma(I)$]	0.0217
wR_2 [$I > 2\sigma(I)$]	0.0544
R_1 (all data)	0.0232
wR_2 (all data)	0.0549
largest diff/hole(e/Å^3)	0.113/-0.172

Column: Chiralpak AD-H+G
Mobile Phase: Hex/i-PrOH= 90/10(v/v)
Flow Rate: 1.0 mL/min
Sample Name: 6a

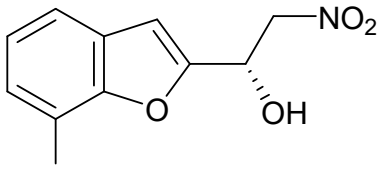


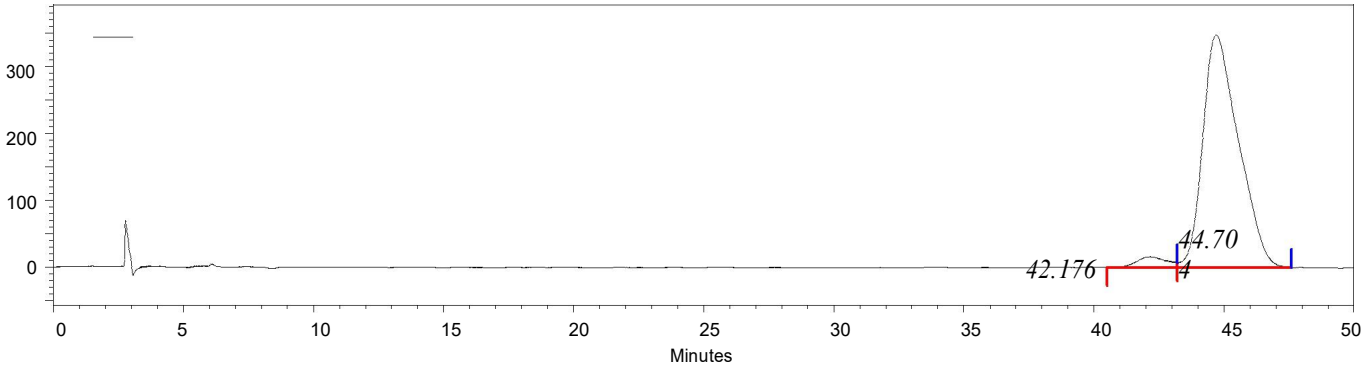


Detector λ：245 nm

Pk#	Retention Time/*min*	Area	Area Percent	Resolution
1	13.525	474358	2.19	0.00
2	14.357	21204625	97.81	1.50
Totals		21678983	100.00	

Column: Chiralpak AD-H+G
Mobile Phase: Hex/EtOH=98/2(v/v)
Flow Rate:1.2 mL/min
Sample Name: 6b

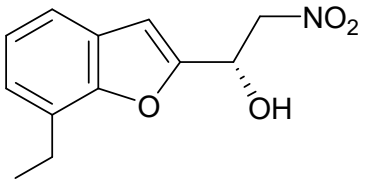


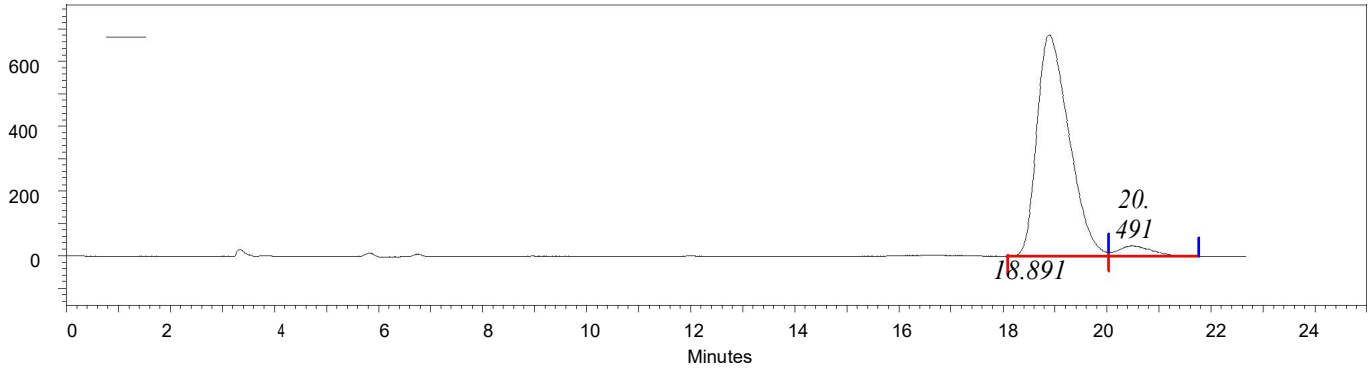


Detector λ：246 nm

Pk#	Retention Time/*min*	Area	Area Percent	Resolution
1	42.176	1256493	3.64	0.00
2	44.704	33289109	96.36	0.00
Totals		34545602	100.00	

Column: Chiralpak AD-H+G
Mobile Phase:Hex/EOH=95/5(v/v)
Flow Rate: 1.0 mL/min
Sample Name: 6c

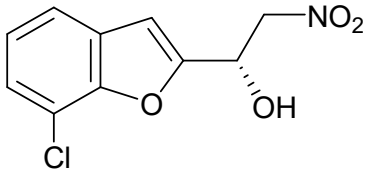


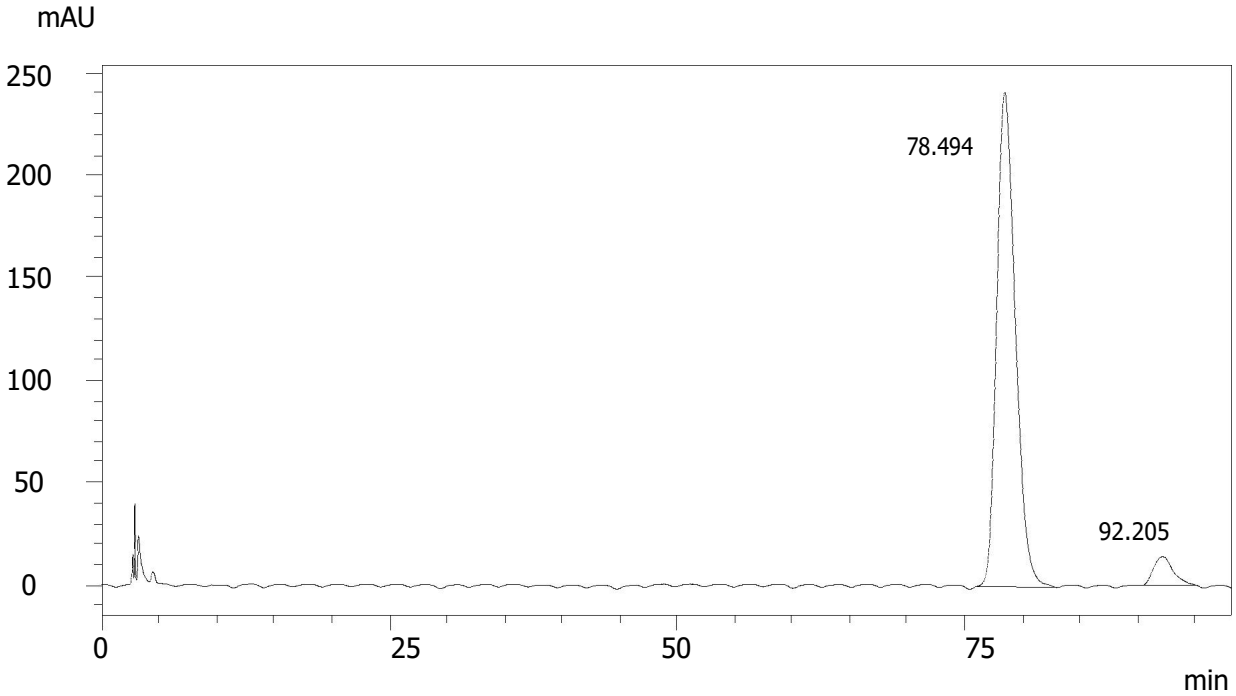


Detector λ：245 nm

Pk#	Retention Time/*min*	Area	Area Percent	Resolution
1	18.891	29328701	95.18	0.00
2	20.491	1483956	4.82	1.28
Totals		30812657	100.00	

Column: Chirlapak AD-H+G
Mobile Phase: Hex/i-PrOH=98.5/1.5(v/v)
Flow Rate:1.2mL/min
Sample Name: 6d

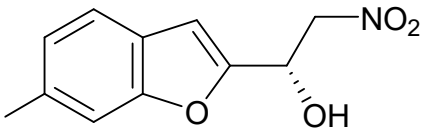


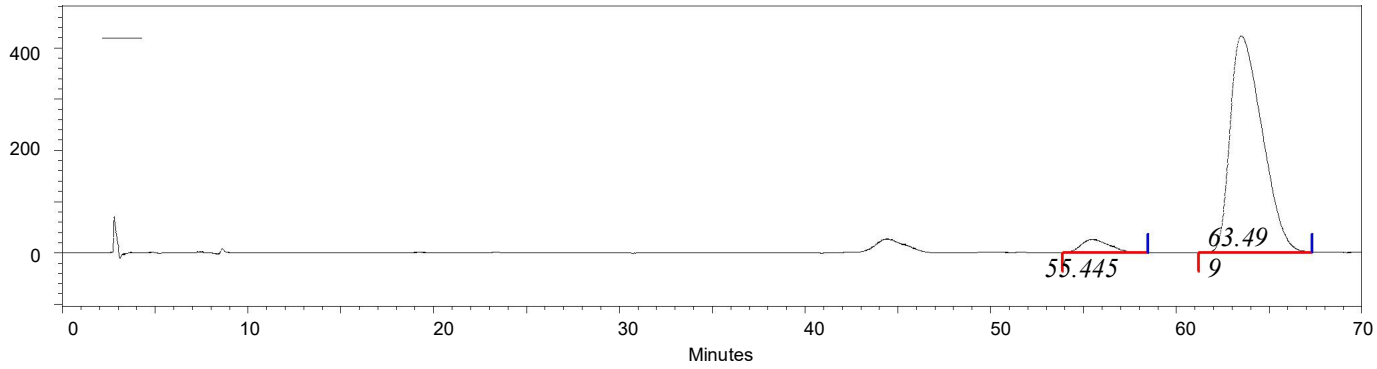


Detector λ：210 nm

Pk#	Retention Time/min	Area	Area Percent	Resolution
1	78.494	27295814	94.261	0.0
2	92.205	1661785	5.739	4.564
Totals		28957599	100.000	

Column: Chiralpak AD-H+G
Mobile Phase: Hex/i-PrOH=98/2(v/v)
Flow Rate: 1.2 mL/min
Sample Name: 6e

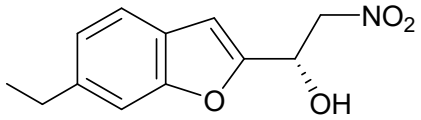


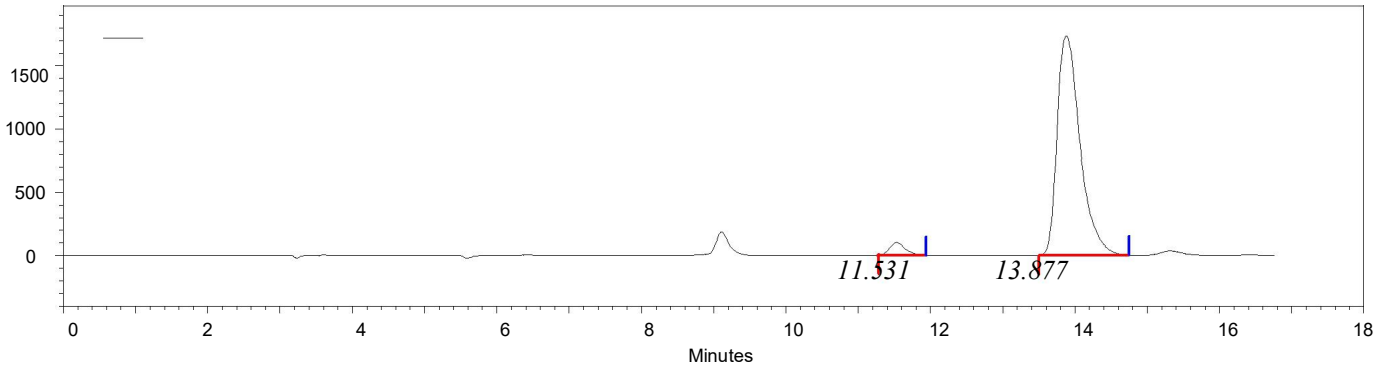


Detector λ：246 nm

Pk#	Retention Time/*min*	Area	Area Percent	Resolution
1	55.445	2771969	5.17	0.00
2	63.499	50848551	94.83	2.41
Totals		53620520	100.00	

Column: Chirlapak AD-H+G
Mobile Phase:Hex/i-PrOH=90/10(v/v)
Flow Rate: 1.0mL/min
Sample Name: 6f

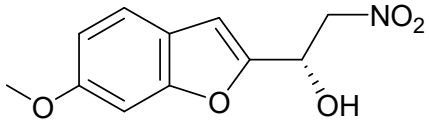


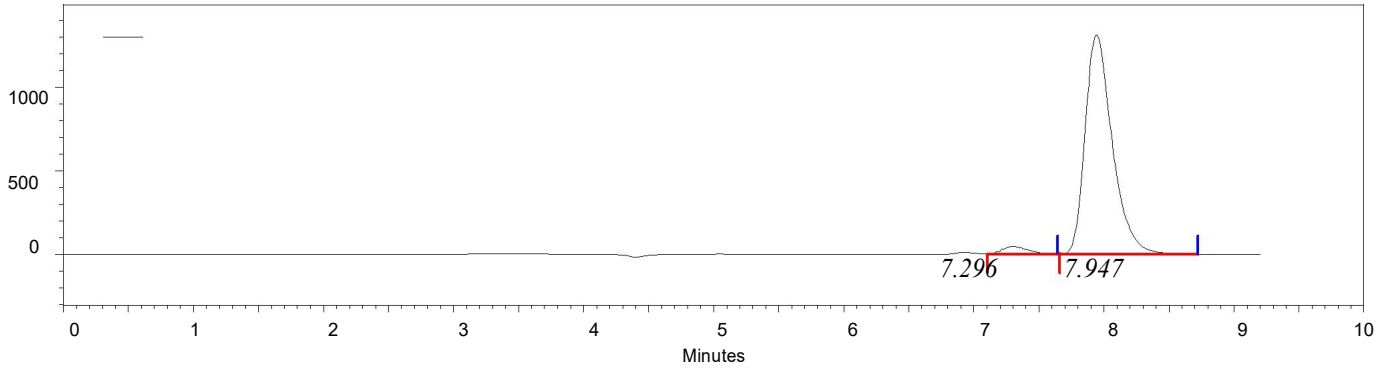


Detector λ：250 nm

Pk#	Retention Time/*min*	Area	Area Percent	Resolution
1	11.531	1487156	3.76	0.00
2	13.877	38110954	96.24	4.99
Totals		39598110	100.00	

Column: Chirlapak AD-H+G
Mobile Phase:Hex/IPA=70/30(v/v)
Flow Rate:1.0mL/min
Sample Name: 6g

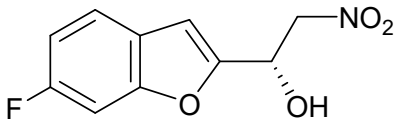


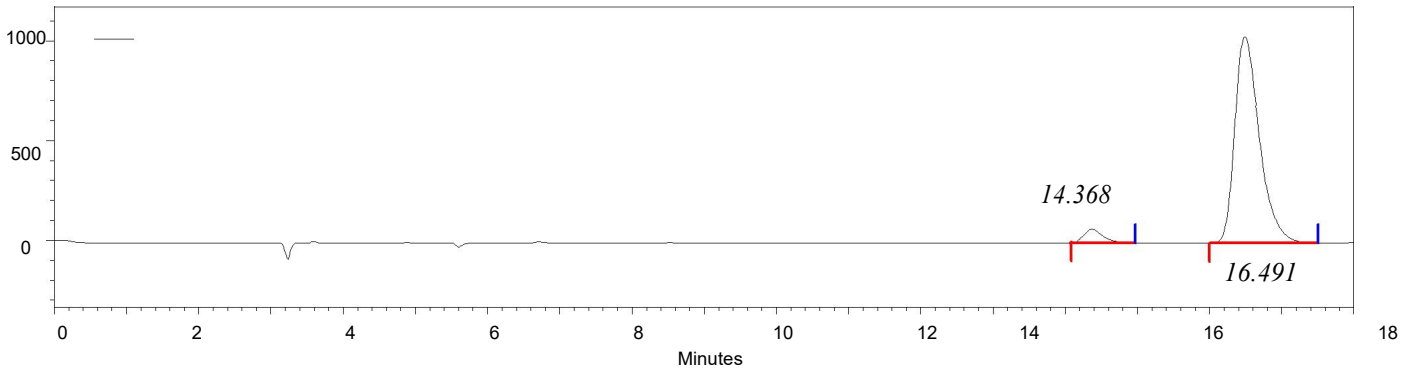


Detector λ：260 nm

Pk#	Retention Time/*min*	Area	Area Percent	Resolution
1	7.296	607152	3.08	0.00
2	7.947	19085930	96.92	1.76
Totals		19693082	100.00	

Column: Chiralpak AD-H+G
Mobile Phase: Hex/i-PrOH=90/10(v/v)
Flow Rate: 1.0mL/min
Sample Name: 6h

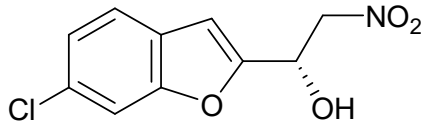


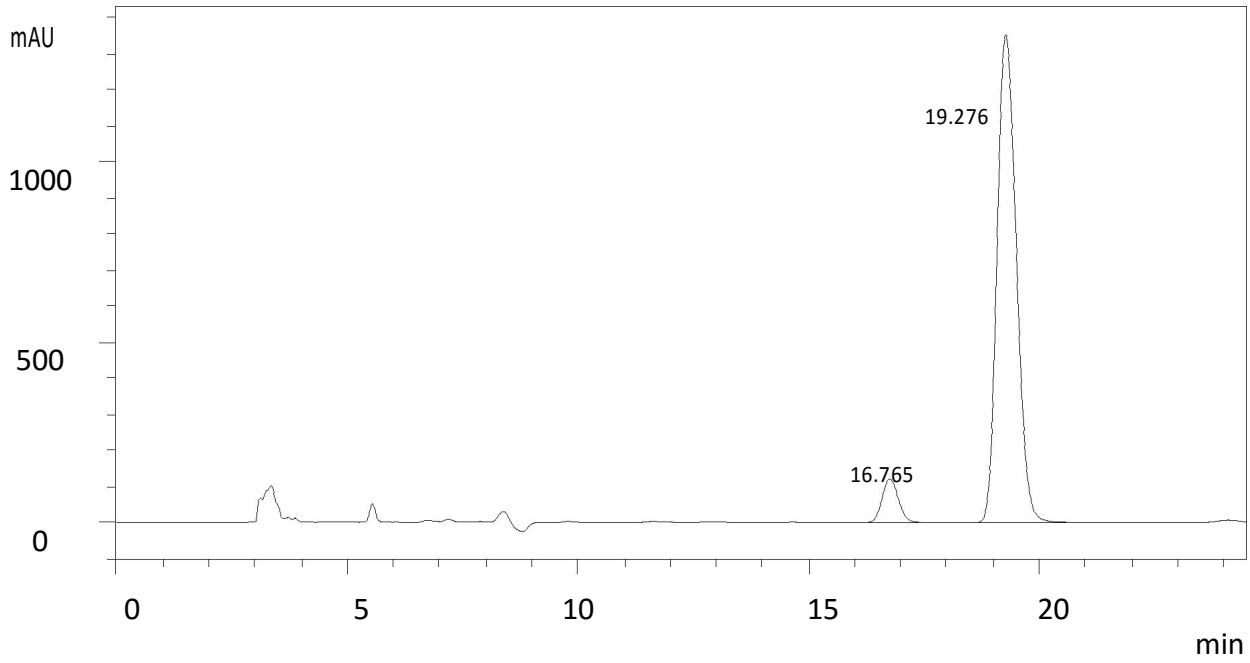


Detector λ：241 nm

Pk#	Retention Time/*min*	Area	Area Percent	Resolution
1	14.368	1252787	4.87	0.00
2	16.491	24480698	95.13	3.89
Totals		25733485	100.00	

Column: Chirlapak AD-H+G
Mobile Phase: Hex/i-PrOH=90/10(v/v)
Flow Rate:1.0mL/min
Sample Name: 6i

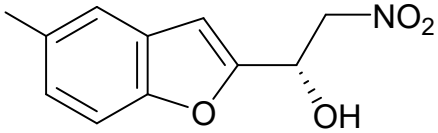


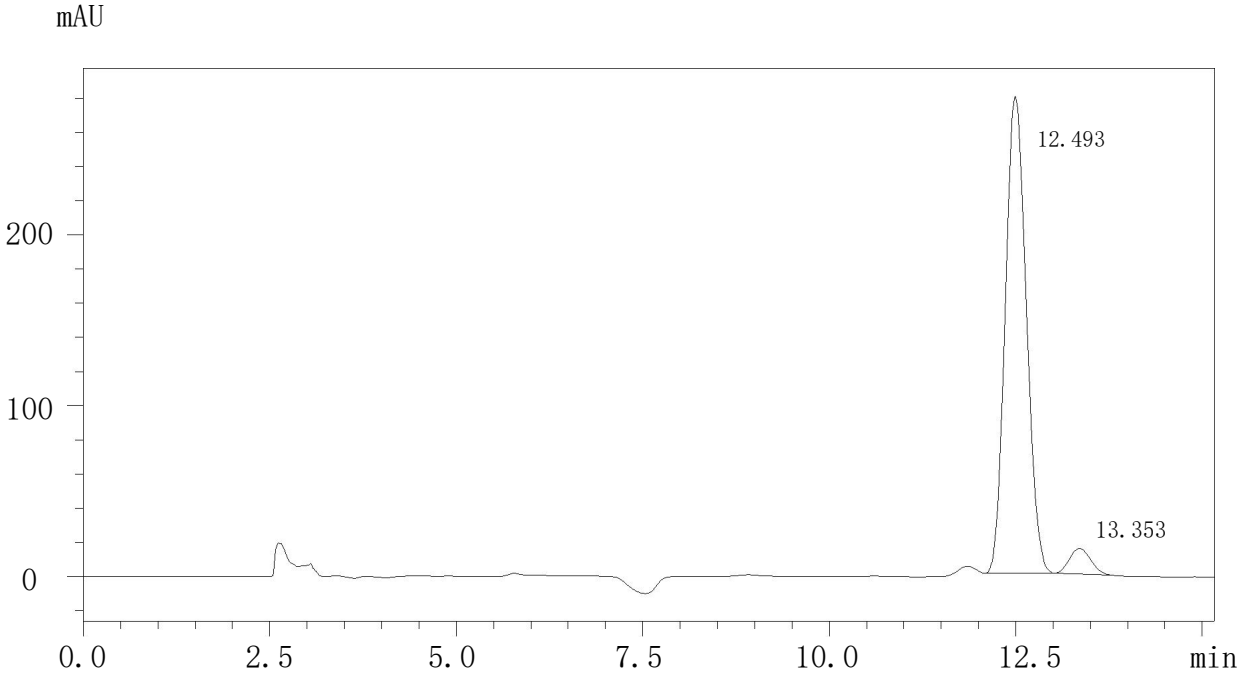


Detector λ：208nm

Pk#	Retention Time/min	Area	Area Percent	Resolution
1	16.765	2964966	7.014	0.0
2	19.276	39305290	92.986	3.533
Totals		42270255	100.000	

Column: Chiralpak AD-H+G
Mobile Phase: Hex/i-POH= 90/10(v/v)
Flow Rate: 1.2 mL/min
Sample Name: 6j

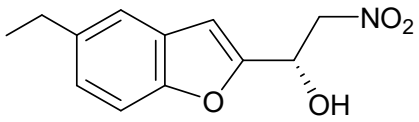


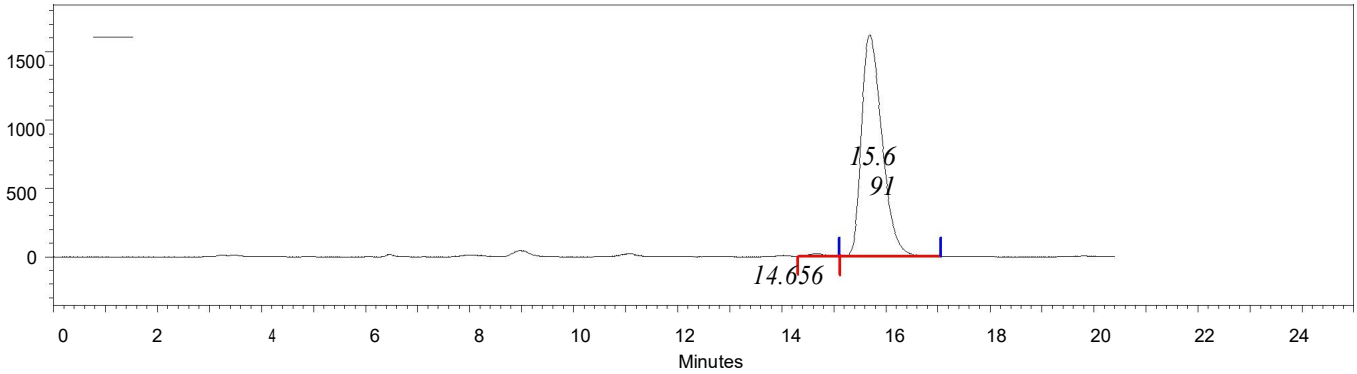


Detector λ: 245 nm

Pk#	Retention Time/*min*	Area	Area Percent	Resolution
1	12.493	5459468	94.83	0.00
2	13.353	297649	5.17	1.612
Totals		5757116	100.00	

Column: Chirlapak AD-H+G
Mobile Phase:Hex/i-PrOH=90/10(v/v)
Flow Rate:1.2 mL/min
Sample Name: 6k

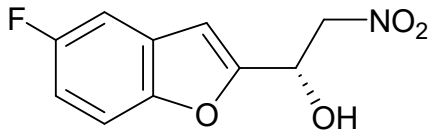


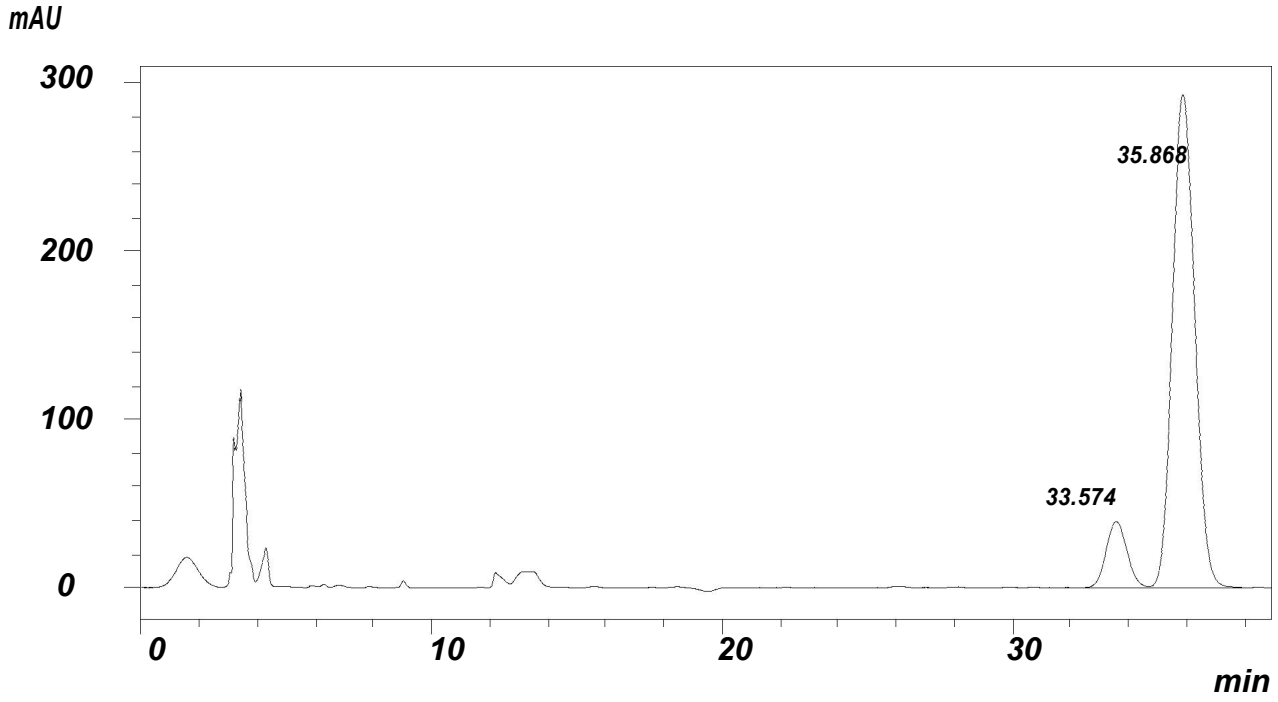


Detector λ：245 nm

Pk#	Retention Time/*min*	Area	Area Percent	Resolution
1	14.656	387364	0.86	0.00
2	15.691	44647852	99.14	1.58
Totals		45035216	100.00	

Column: Chiralpak AD-H+G
Mobile Phase: Hex/i-PrOH=90/10(v/v)
Flow Rate: 1.0mL/min
Sample Name: 6l

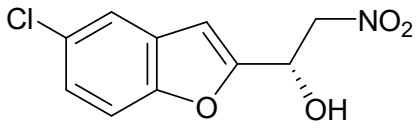


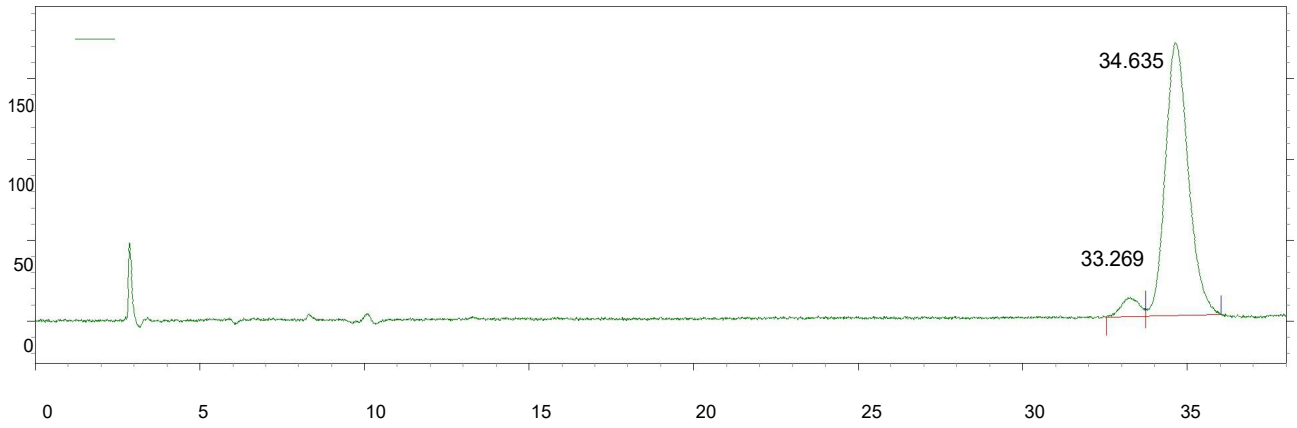


Detector λ：208 nm

Pk#	Retention Time/min	Area	Area Percent	Resolution
1	33.574	1960929	11.136	0.0
2	35.868	15648215	88.864	1.676
Totals		17609144	100.000	

Column: Chiralpak AD-H+G
Mobile Phase: Hex/i-PrOH=95/5(v/v)
Flow Rate: 1.2mL/min
Sample Name: 6m

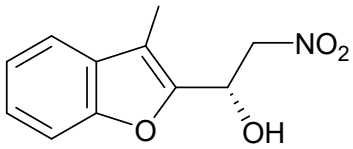


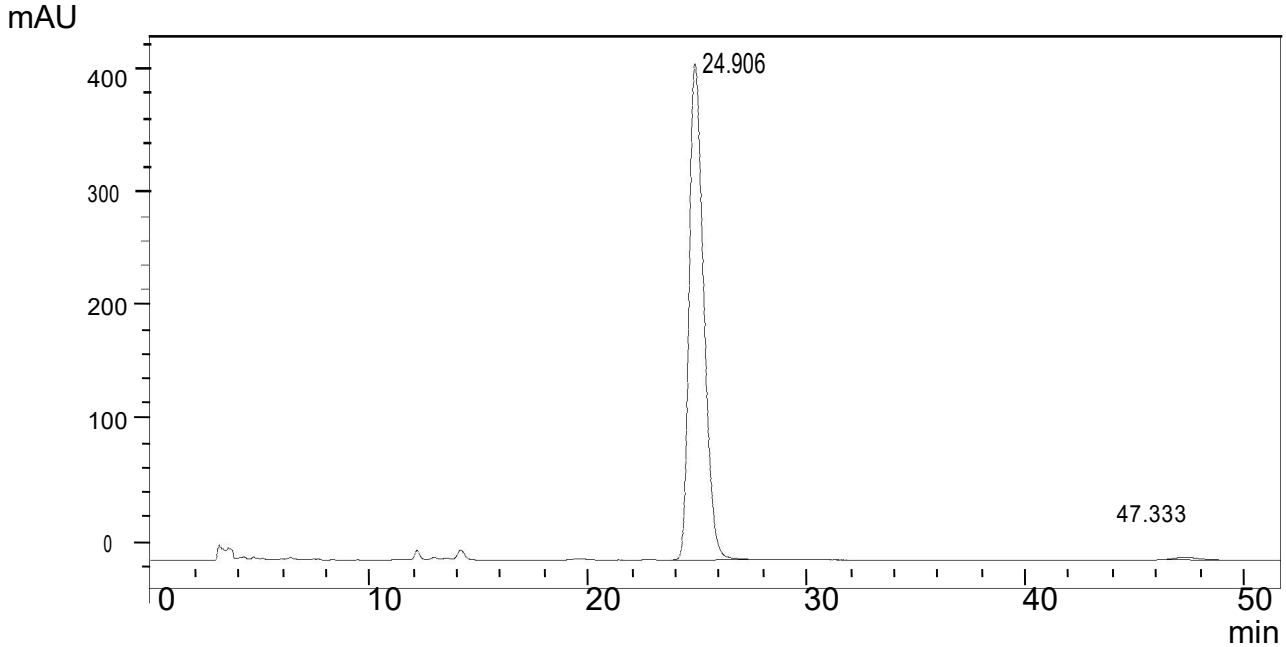


Detector λ：213nm

Pk#	Retention Time/*min*	Area	Area Percent	Resolution
1	33.269	460838	5.296	0.00
2	34.635	8240094	94.704	1.20
Totals		8700932	100.000	

Column: Chirlapak OD-H+G
Mobile Phase: Hex/i-PrOH=90/10(v/v)
Flow Rate:1.0mL/min
Sample Name: 6n

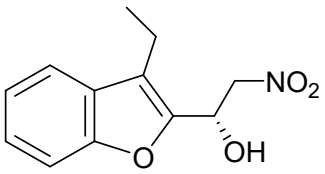


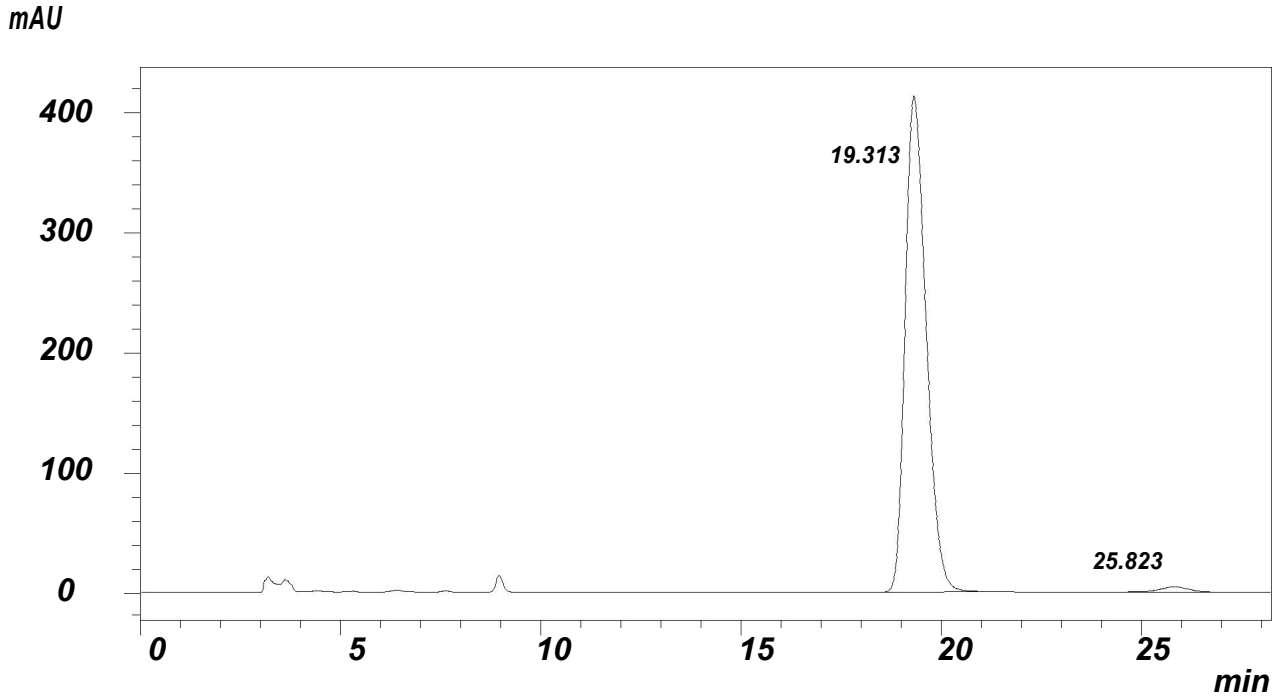


Detector λ：250nm

Pk#	Retention Time/min	Area	Area Percent	Resolution
1	24.906	18660815	99.202	0.0
2	47.333	150127	0.798	13.600
Totals		18810941	100.000	

Column: Chirlapak OD-H+G
Mobile Phase: Hex/i-PrOH=90/10(v/v)
Flow Rate:1.0mL/min
Sample Name: 6o

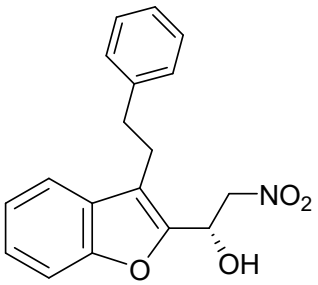


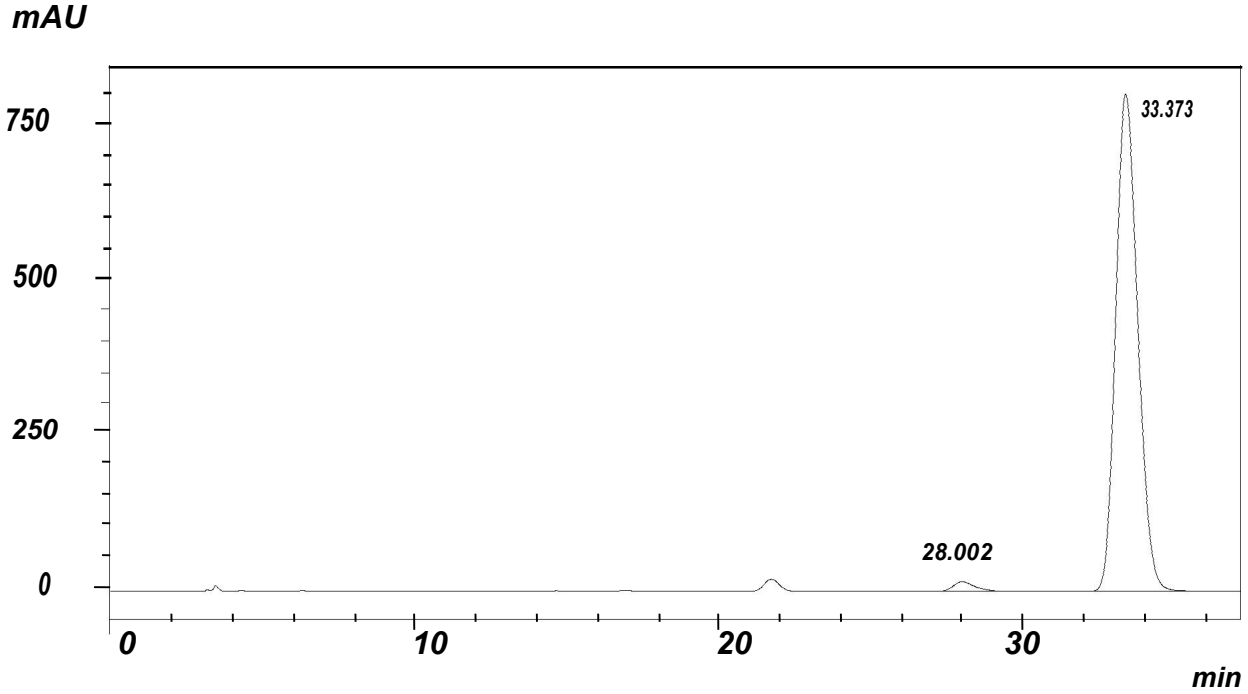


Detector λ：250nm

Pk#	Retention Time/min	Area	Area Percent	Resolution
1	19.313	15040875	98.563	0.0
2	25.823	219232	1.437	5.881
Totals		15260107	100.000	

Column: Chirlapak AD-H+G
Mobile Phase: Hex/i-PrOH=95/5(v/v)
Flow Rate:1.0mL/min
Sample Name: 6p

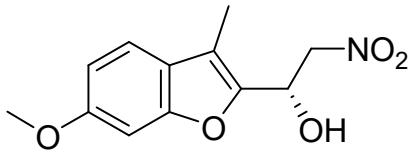


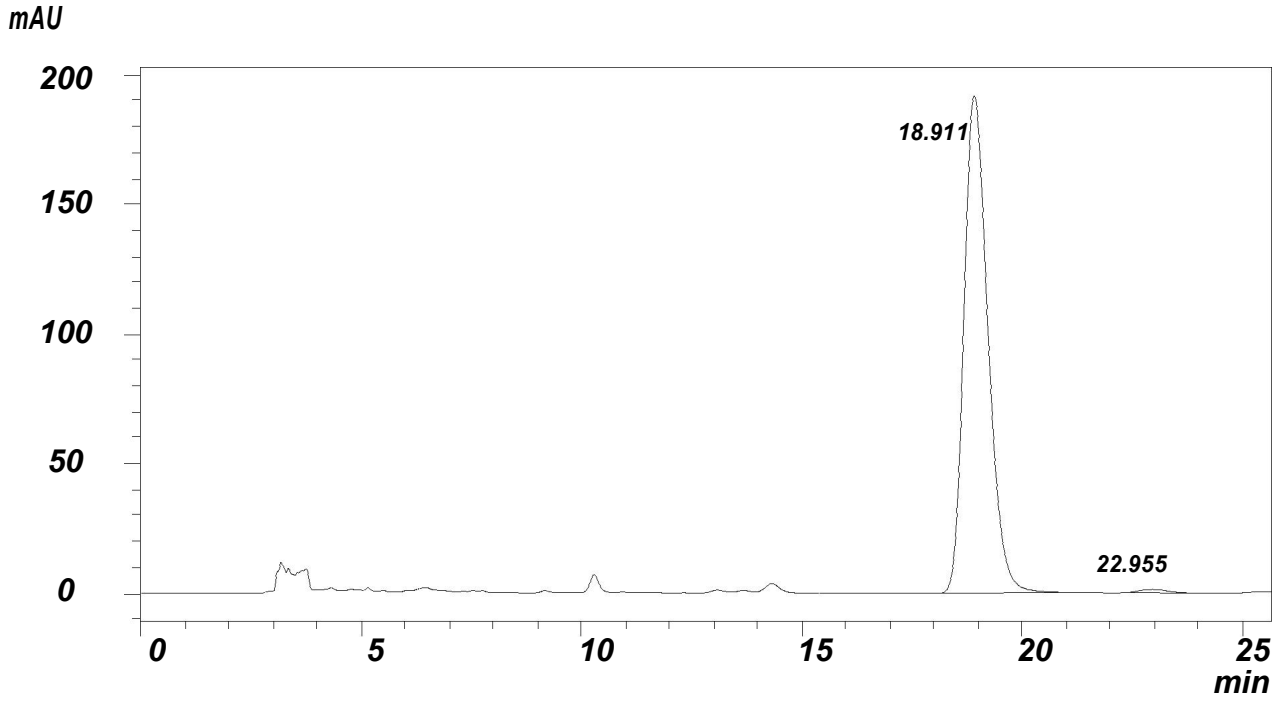


Detector λ：254 nm

Pk#	Retention Time/min	Area	Area Percent	Resolution
1	28.002	759723	1.867	0.0
2	33.373	39938463	98.133	4.125
Totals		40698186	100.000	

Column: Chirlapak OD-H+G
Mobile Phase: Hex/i-PrOH=90/10(v/v)
Flow Rate:1.0mL/min
Sample Name: 6q

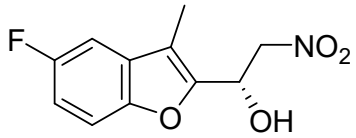


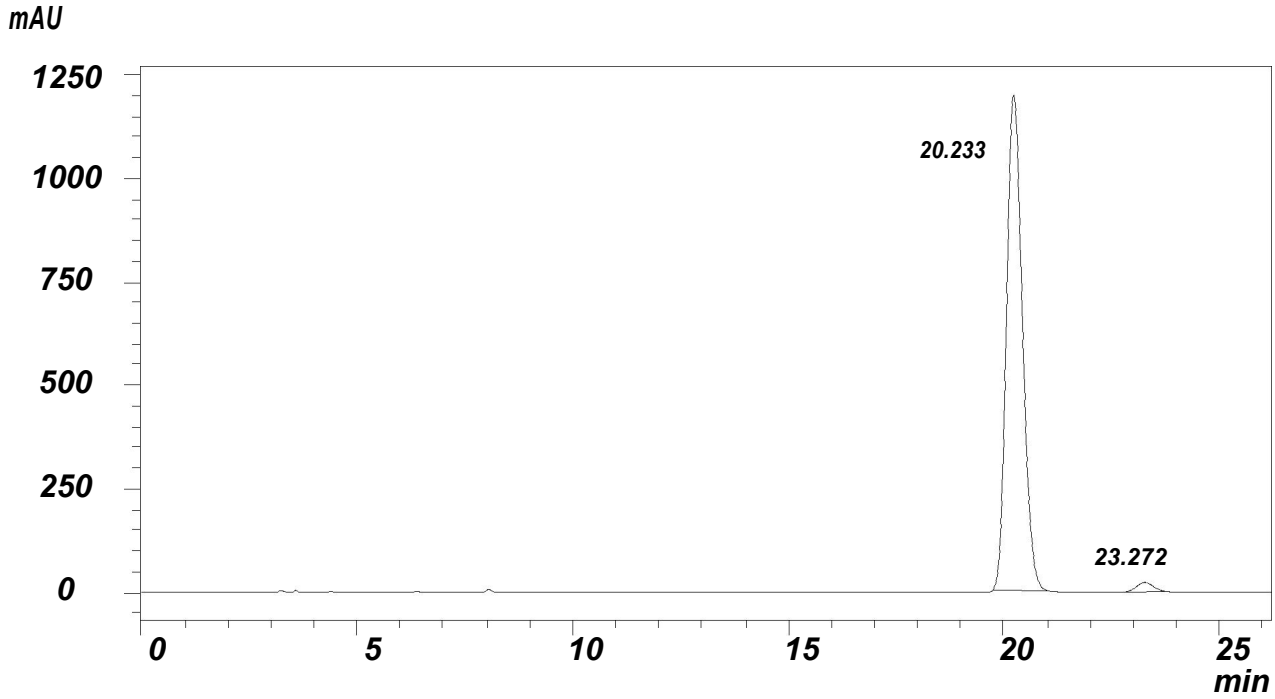


Detector λ：250 nm

Pk#	Retention Time/min	Area	Area Percent	Resolution
1	18.911	7252507	99.161	0.0
2	22.955	61380	0.839	3.761
Totals		7313887	100.000	

Column: Chirlapak AD-H+G
Mobile Phase: Hex/i-PrOH=95/5(v/v)
Flow Rate:1.0mL/min
Sample Name: 6r

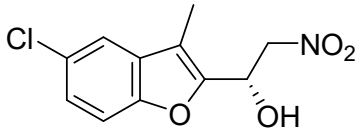


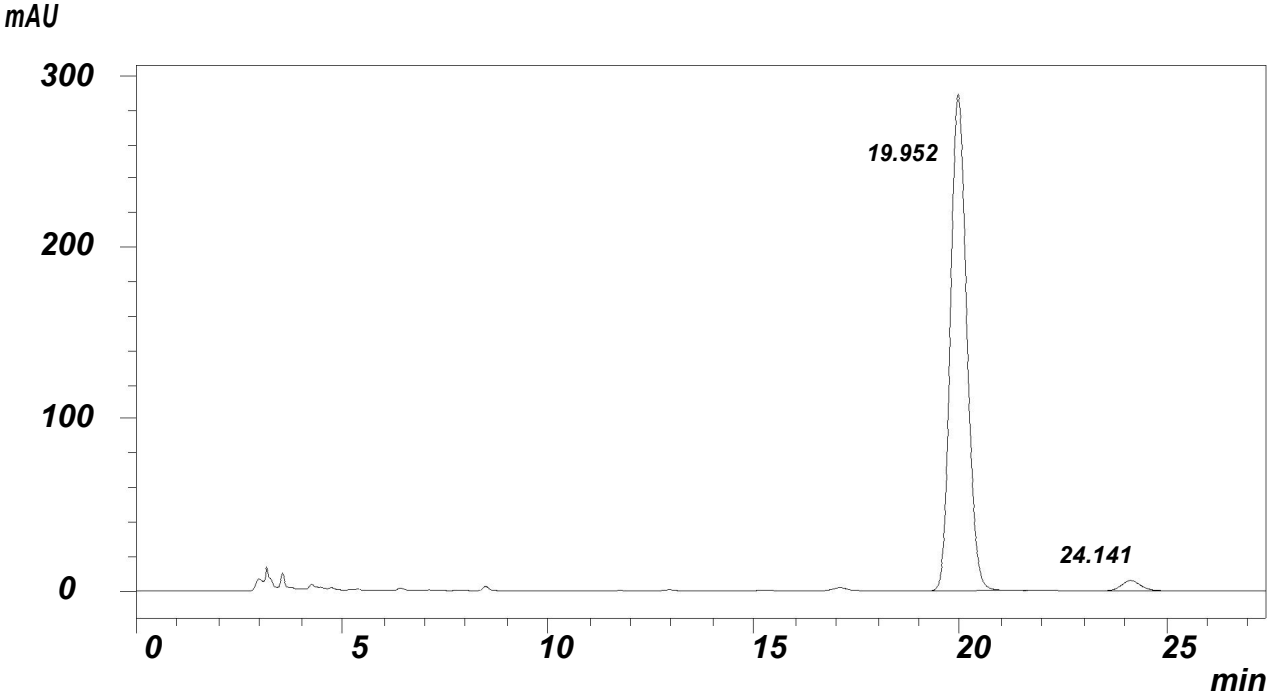


Detector λ: 254 nm

Pk#	Retention Time/min	Area	Area Percent	Resolution
1	20.233	30666404	98.046	0.0
2	23.272	611216	1.954	4.281
Totals		31277620	100.000	

Column: Chirlapak AD-H+G
Mobile Phase: Hex/i-PrOH=95/5(v/v)
Flow Rate:1.0mL/min
Sample Name: 6s

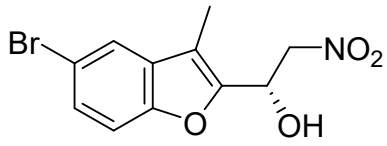


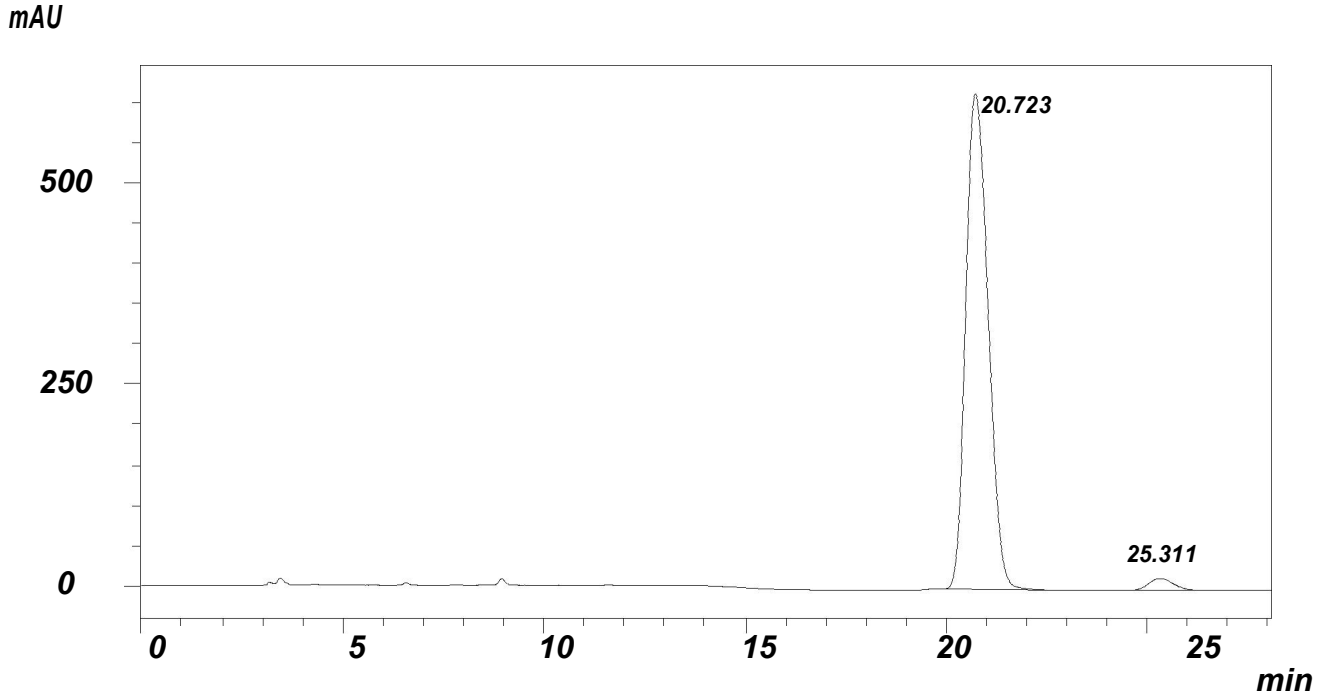


Detector λ：254 nm

Pk#	Retention Time/min	Area	Area Percent	Resolution
1	19.952	7962737	97.692	0.0
2	24.141	188111	2.308	5.328
Totals		8150848	100.000	

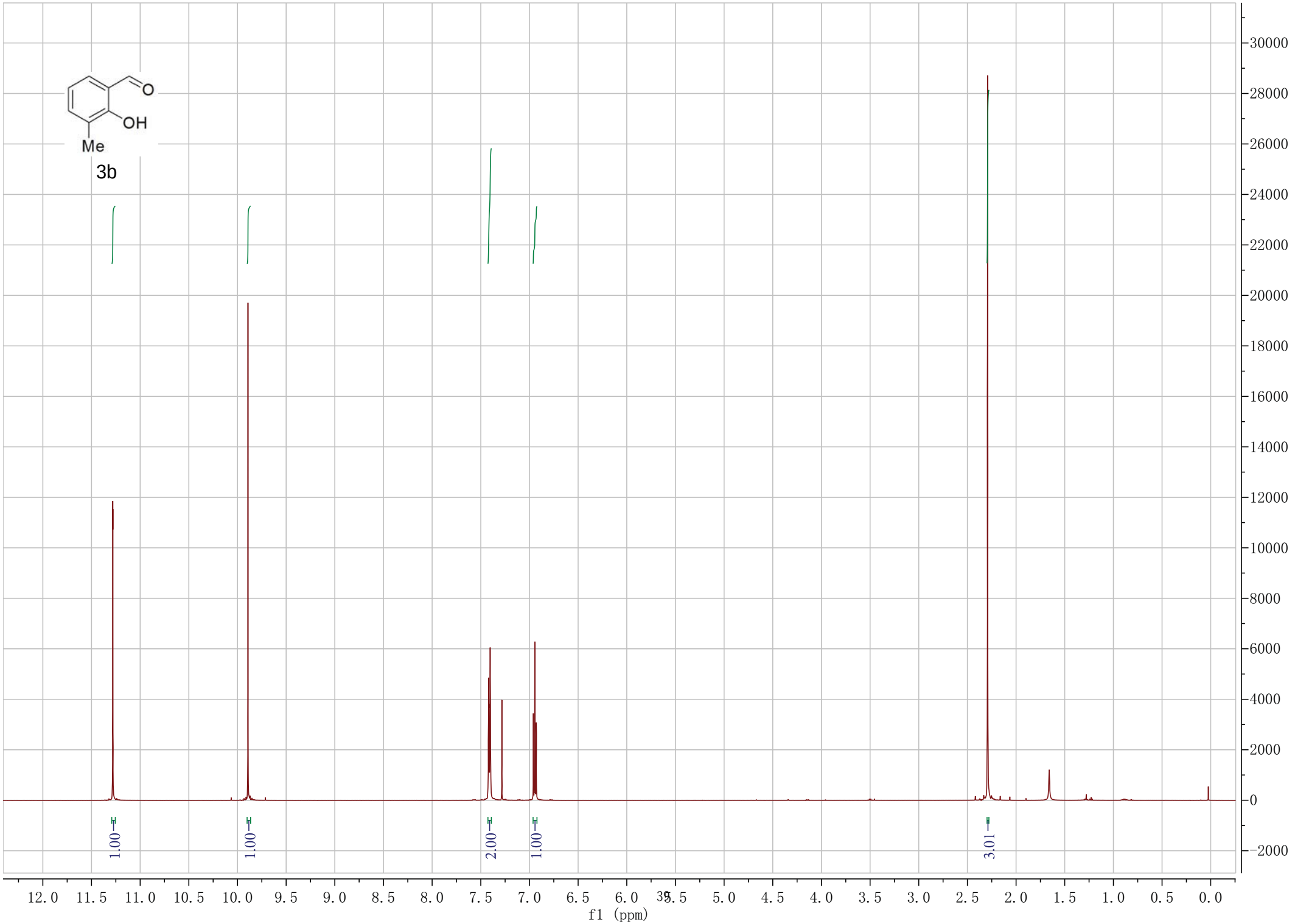
Column: Chirlapak AD-H+G
Mobile Phase: Hex/i-PrOH=95/5(v/v)
Flow Rate:1.0mL/min
Sample Name: 6t

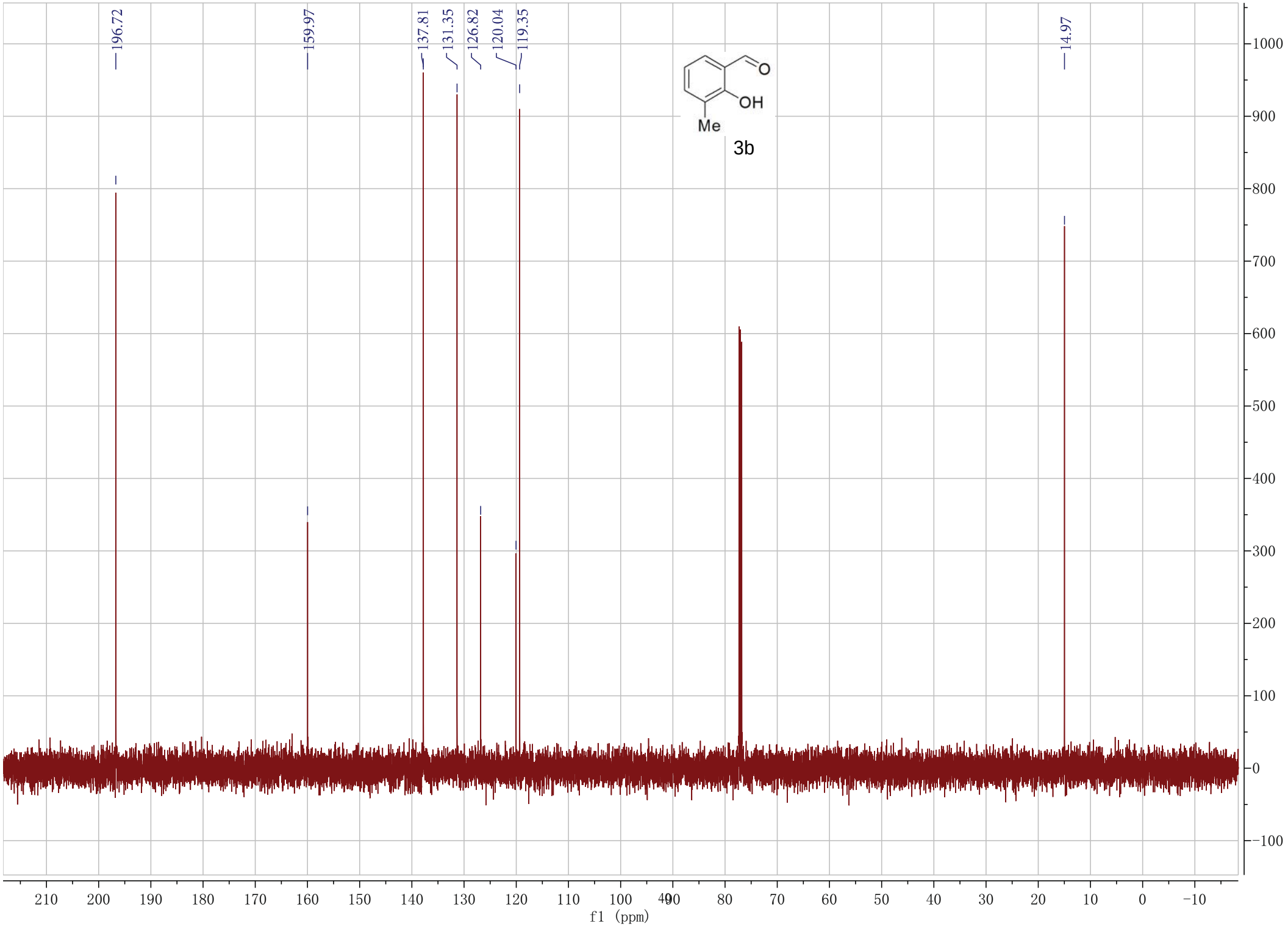


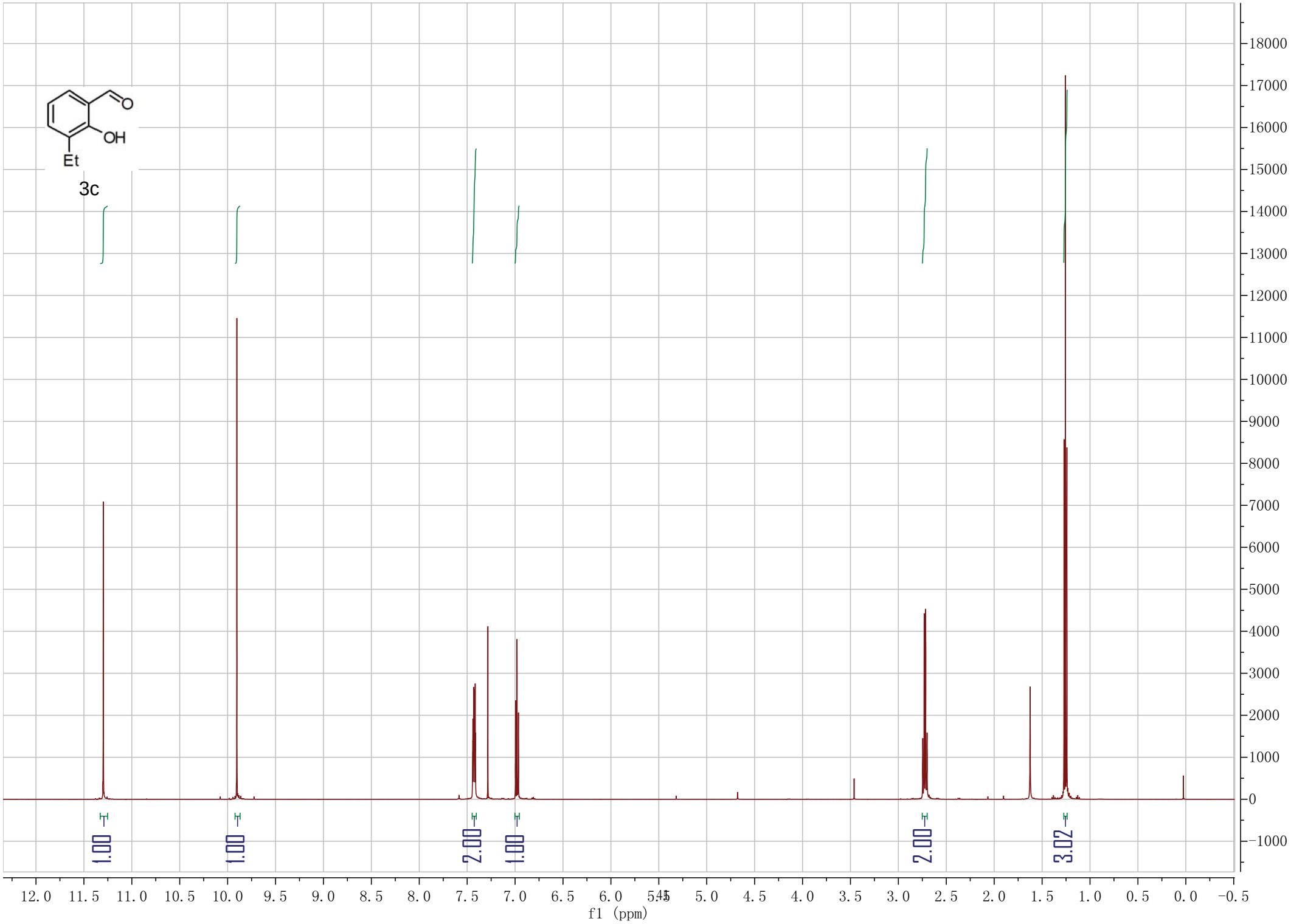


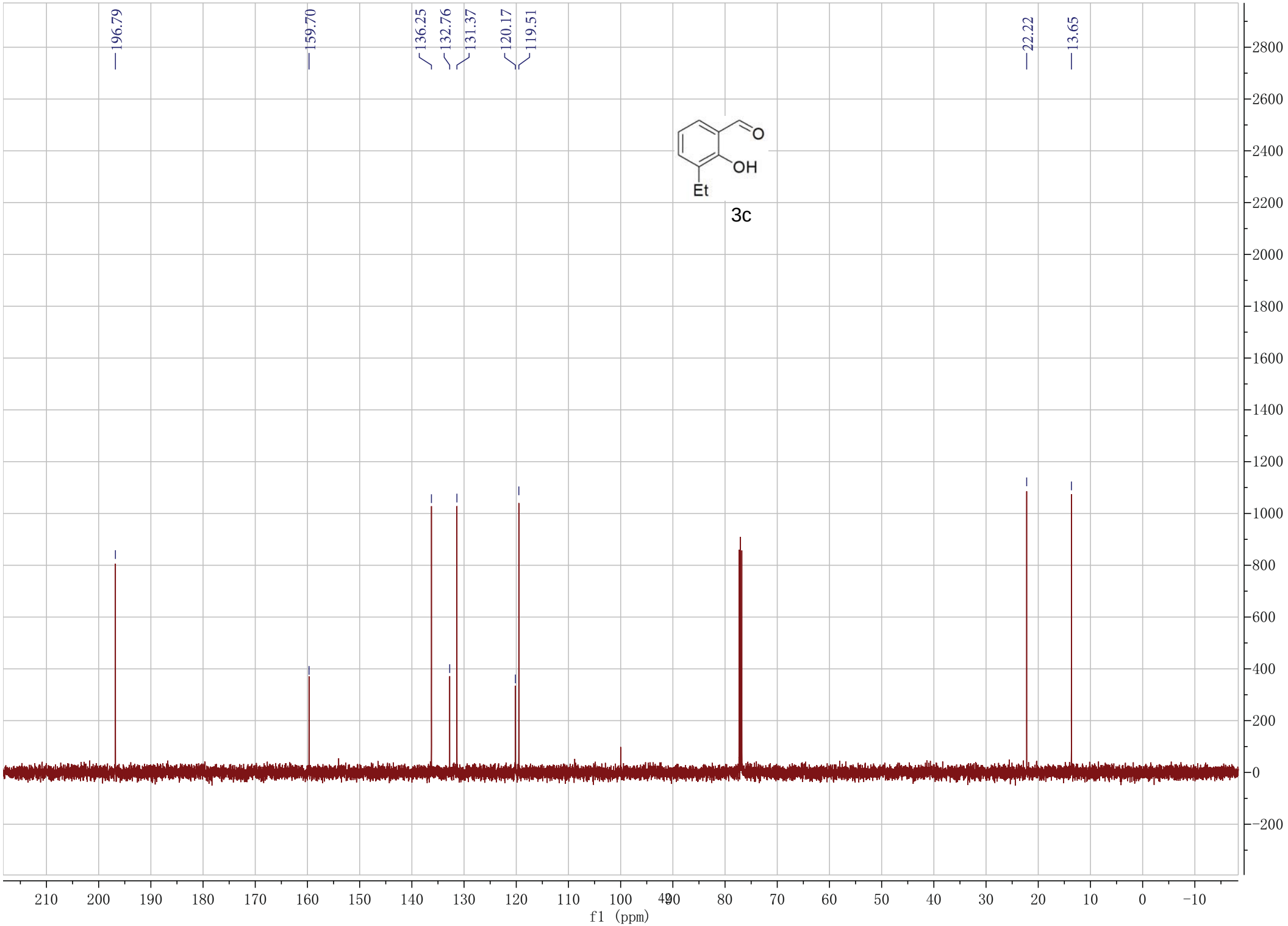
Detector λ: 254 nm

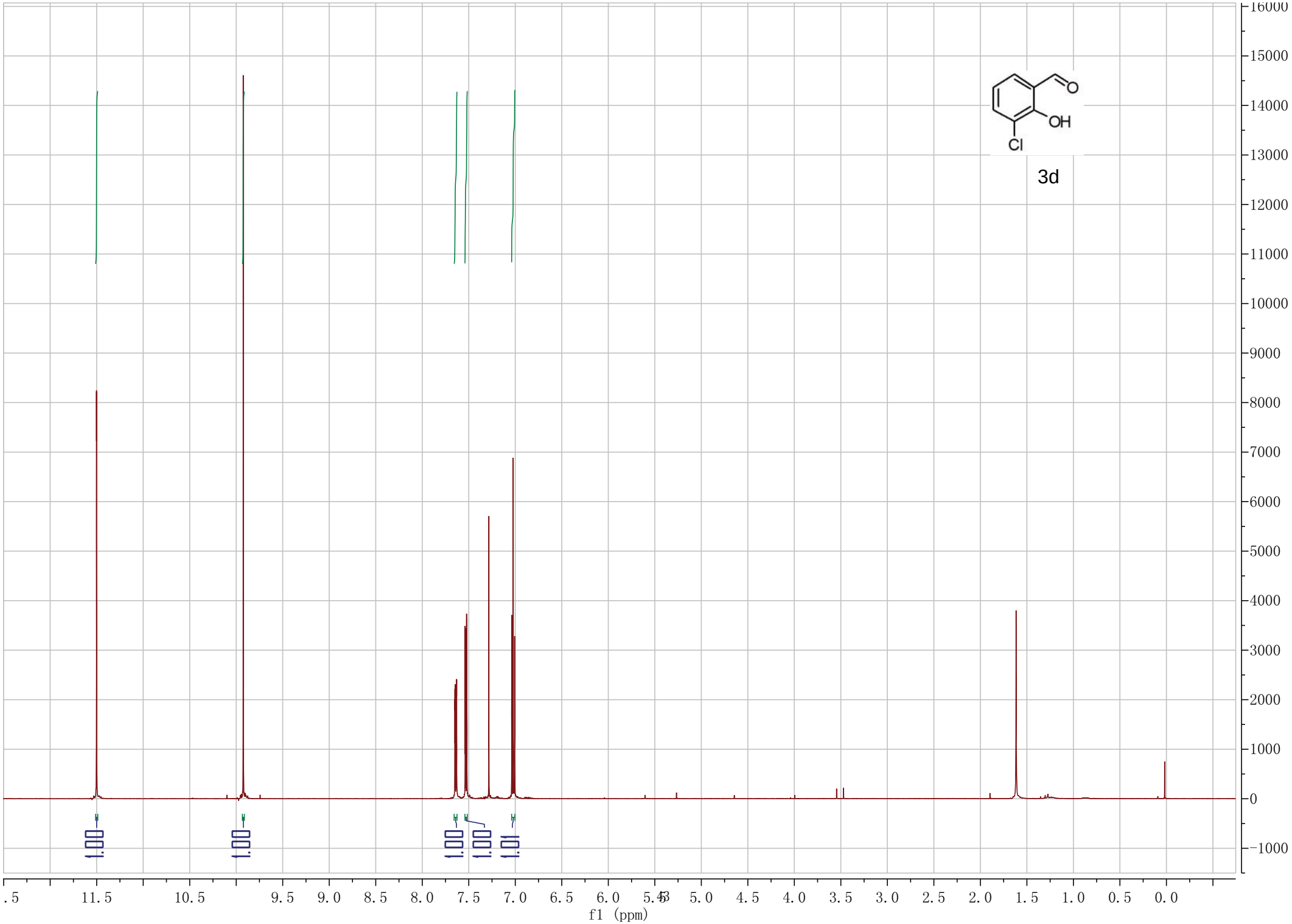
Pk#	Retention Time/min	Area	Area Percent	Resolution
1	20.723	23786140	97.387	0.0
2	25.311	638252	2.613	4.232
Totals		24424392	100.000	

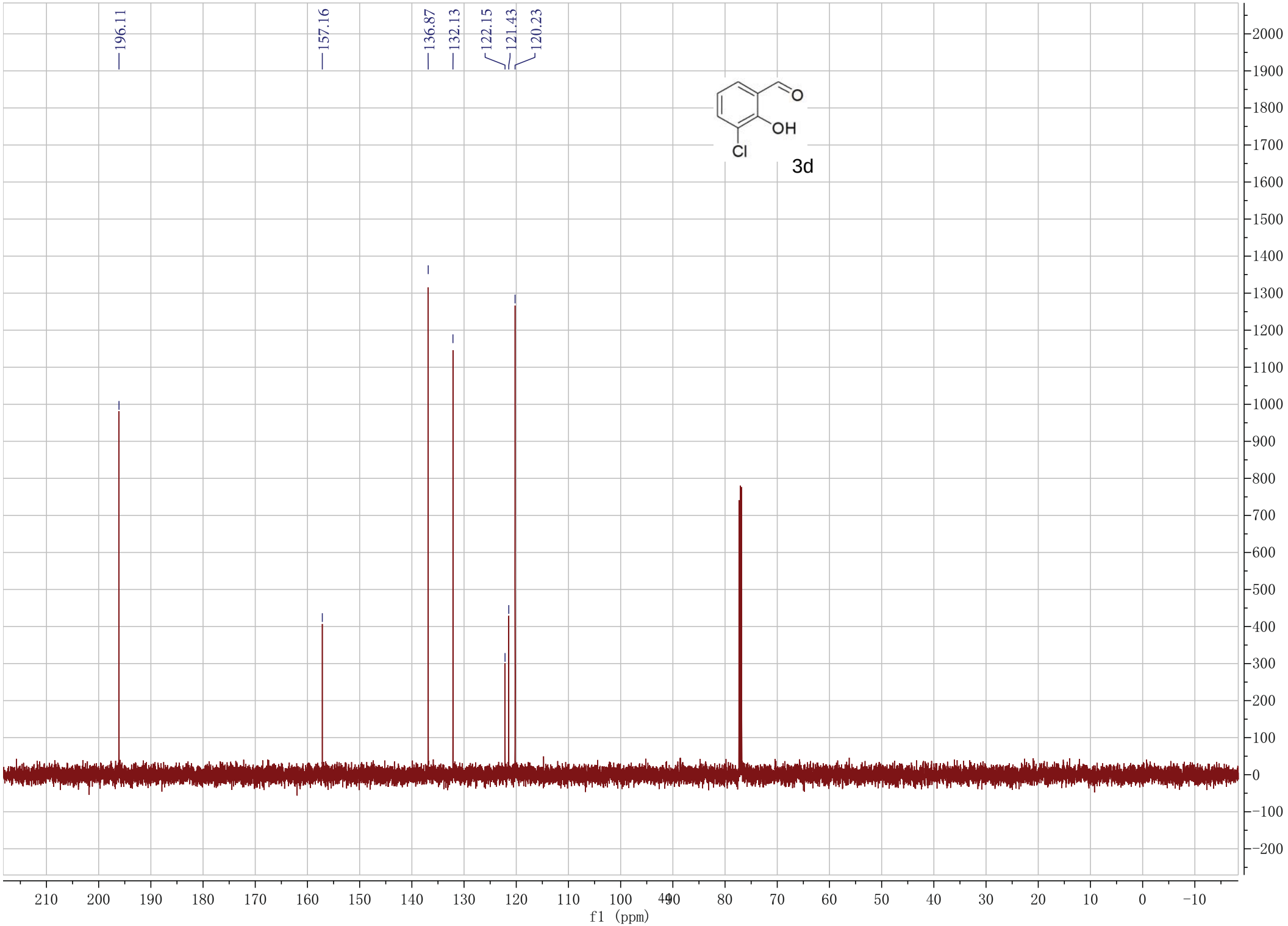

O
OH
Me
3b
1.00
1.00
2.00
1.00
3.01
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

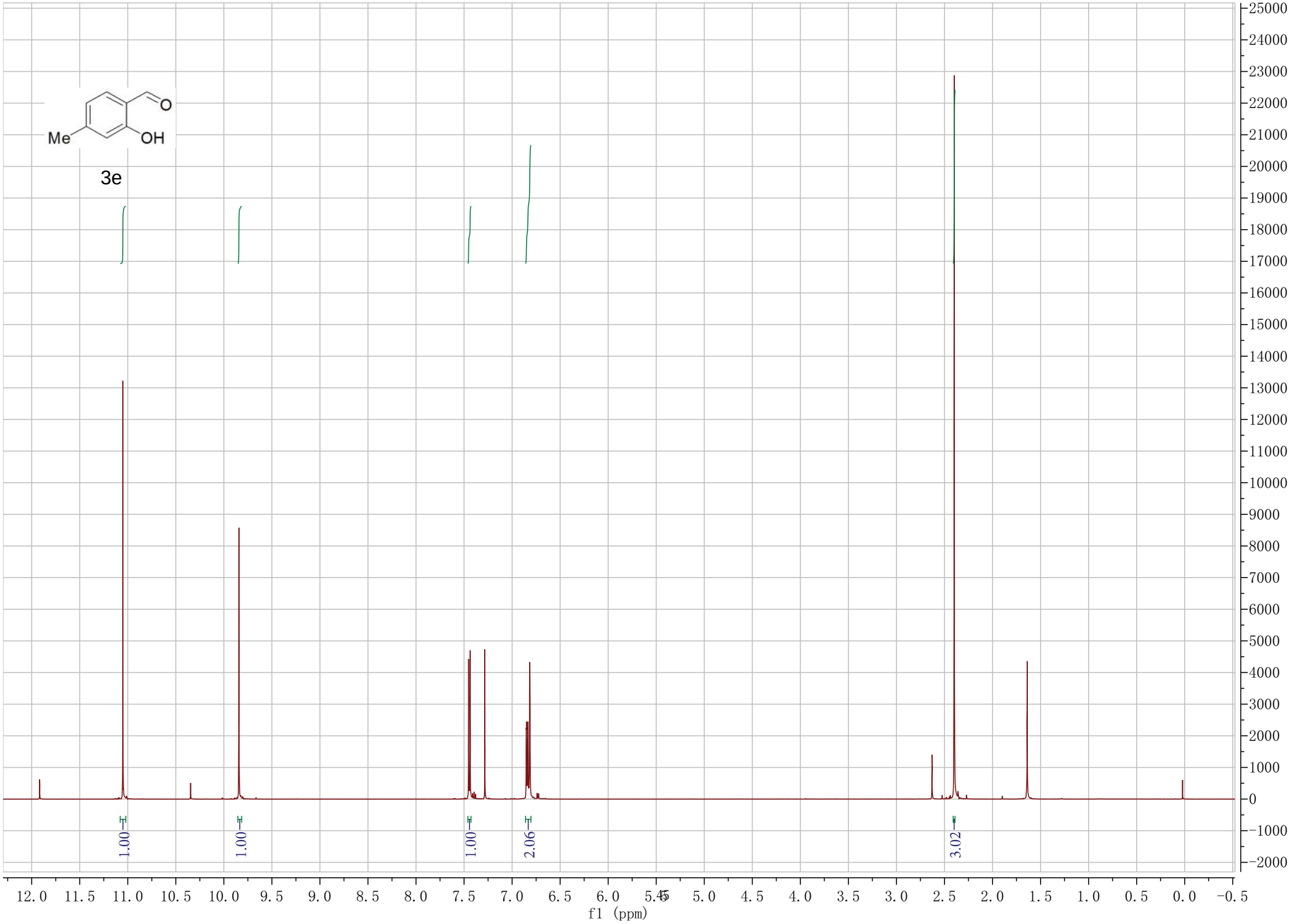

196.72
159.97
137.81
131.35
126.82
120.04
119.35
14.97
O
OH
Me
3b
f1 (ppm)

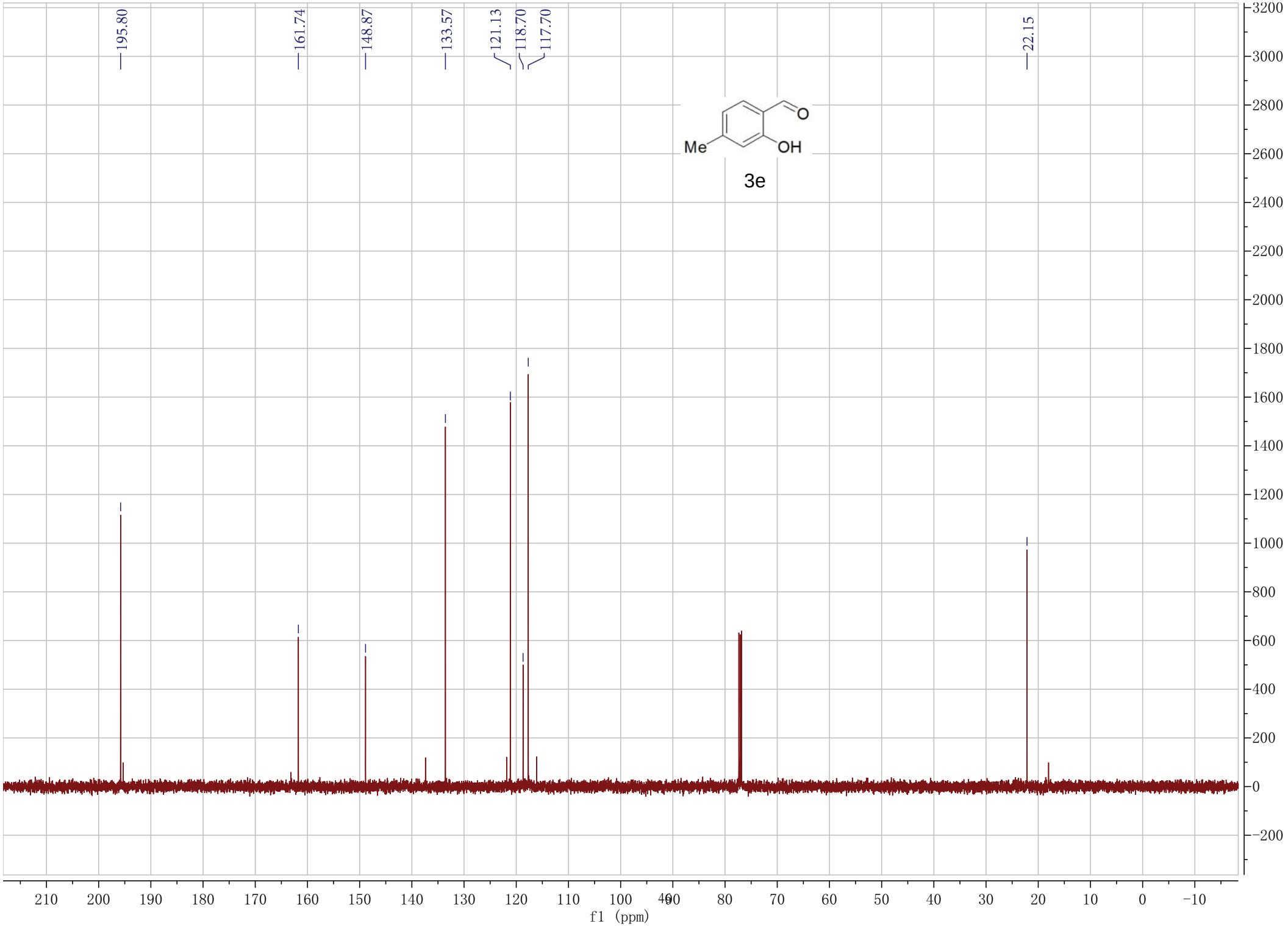

O
OH
Et
3c
1.00
1.00
2.00
1.00
2.00
3.02
f1 (ppm)

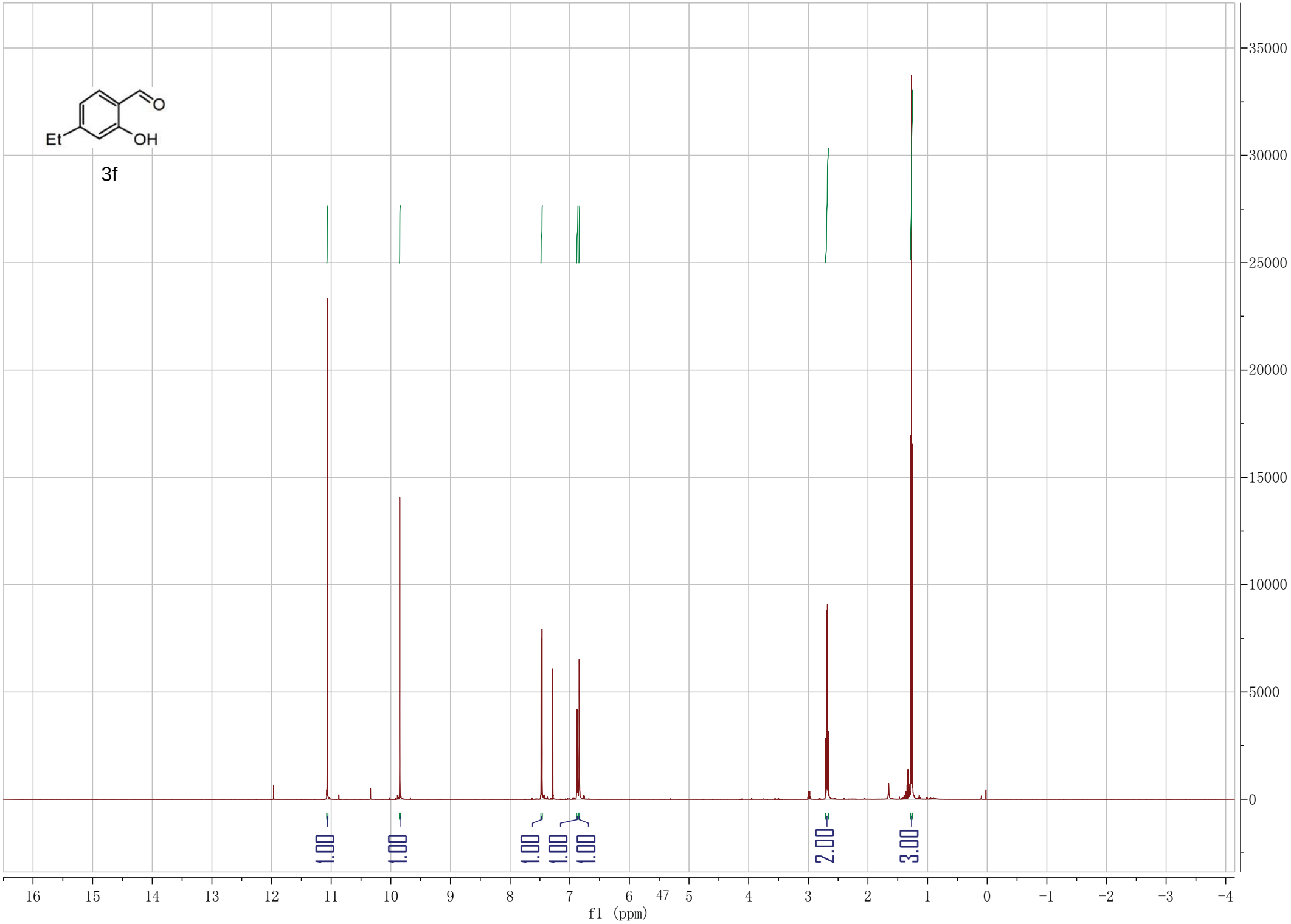

196.79
159.70
136.25
132.76
131.37
120.17
119.51
22.22
13.65
O
OH
Et
3c
f1 (ppm)

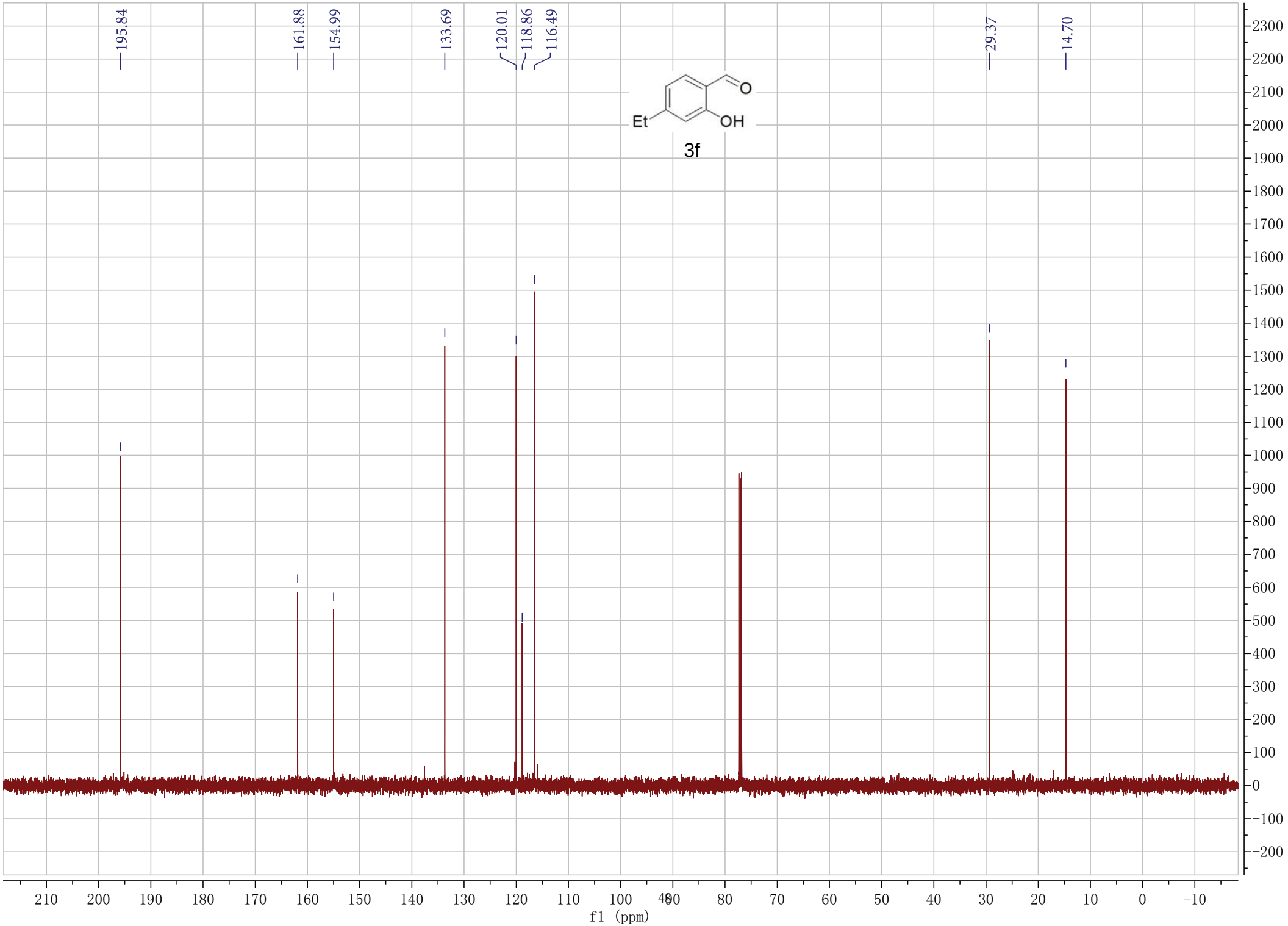

3d
f1 (ppm)

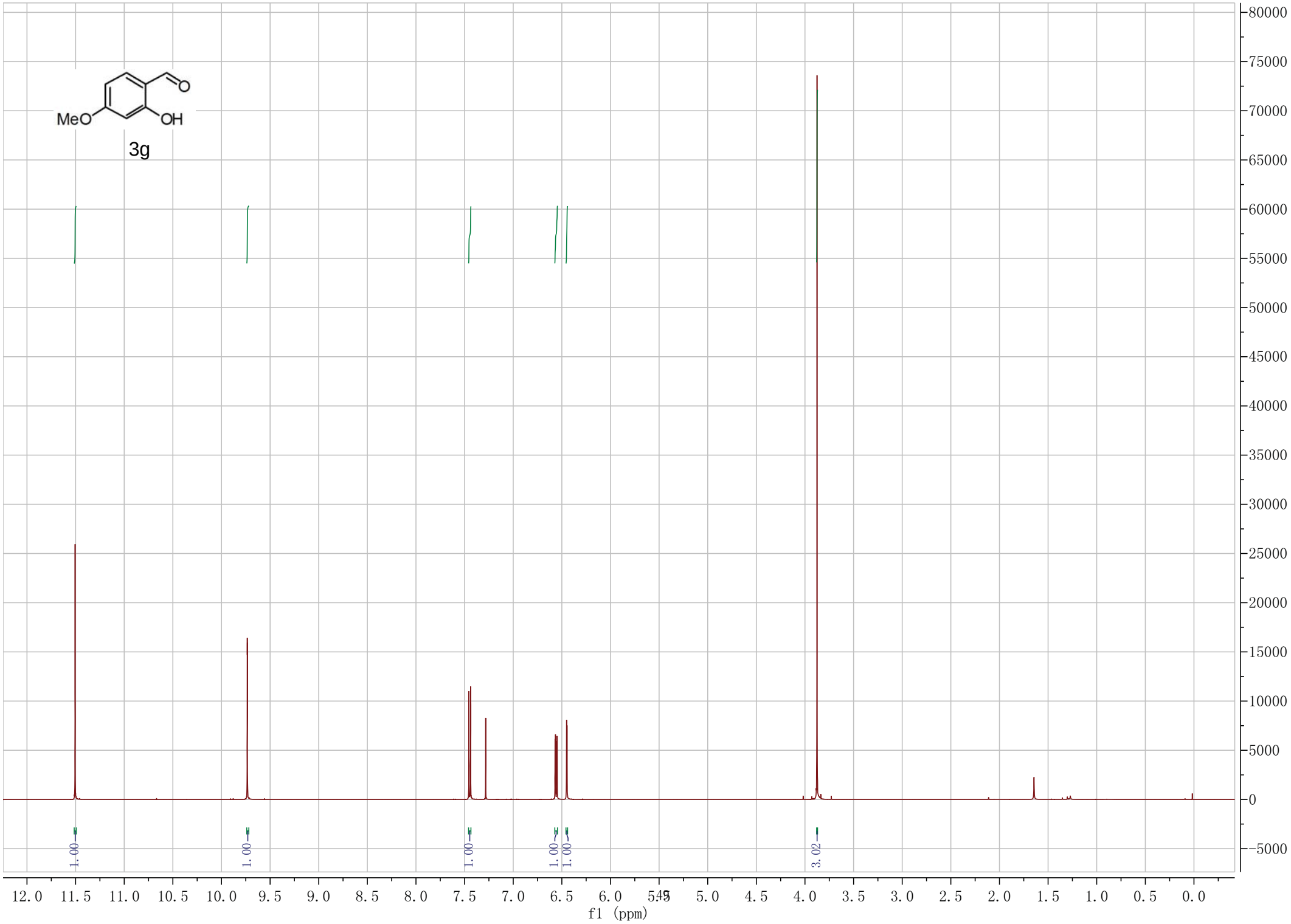

196.11
157.16
136.87
132.13
122.15
121.43
120.23
O
OH
Cl
3d
f1 (ppm)

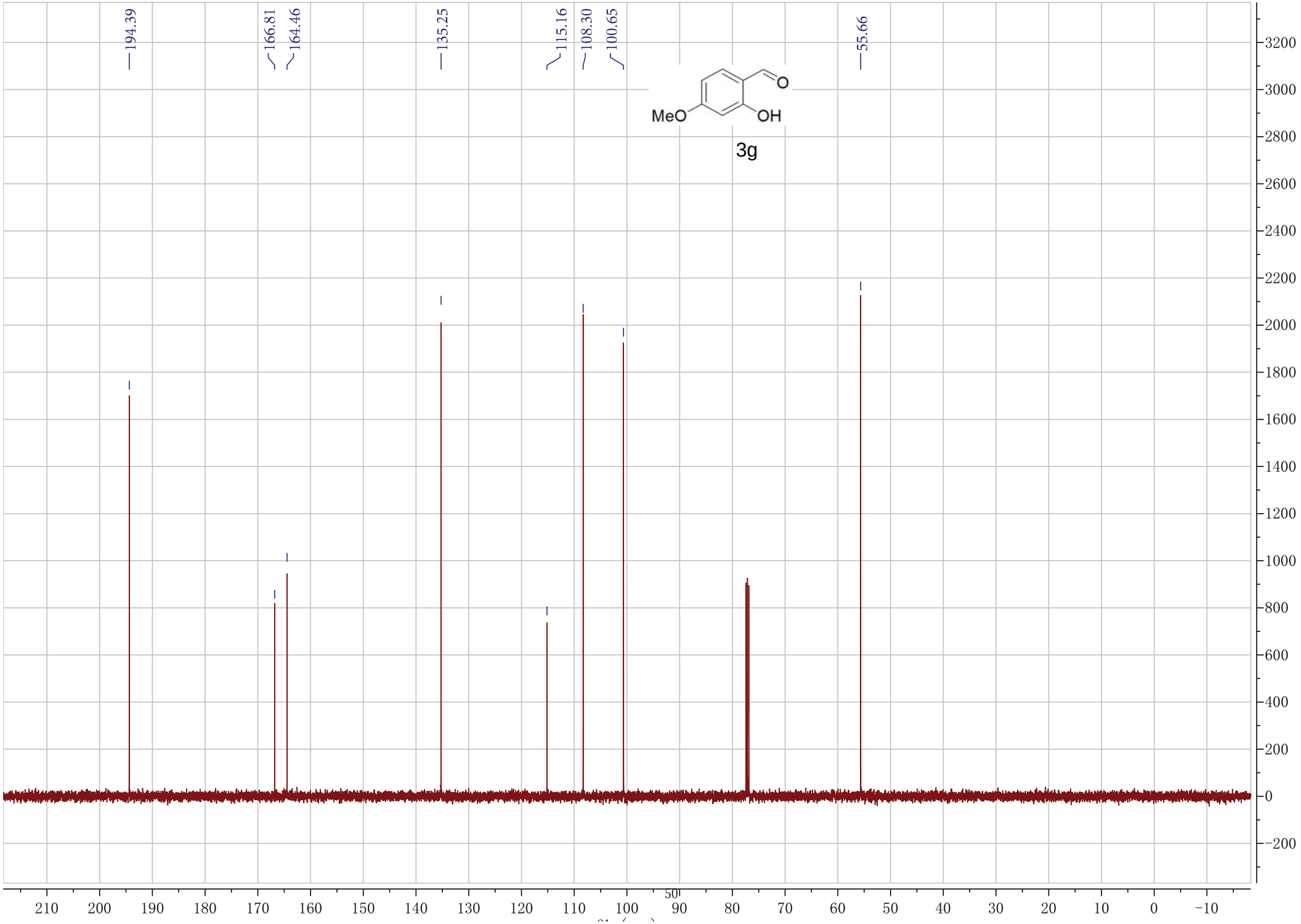

Me
OH
O
3e
1.00
1.00
1.00
2.06
3.02
f1 (ppm)

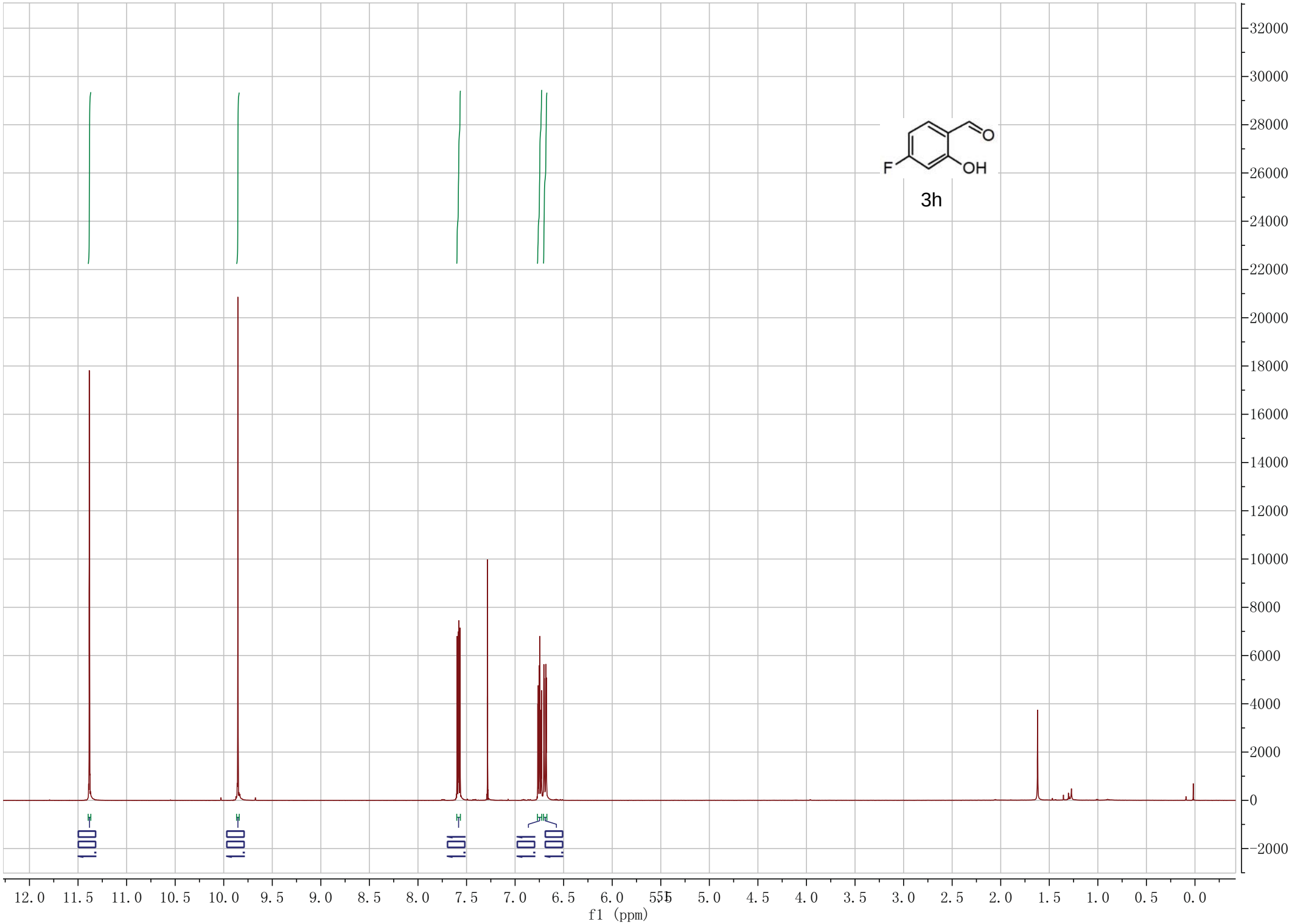

195.80
161.74
148.87
133.57
121.13
118.70
117.70
22.15
Me
OH
O
3e
f1 (ppm)

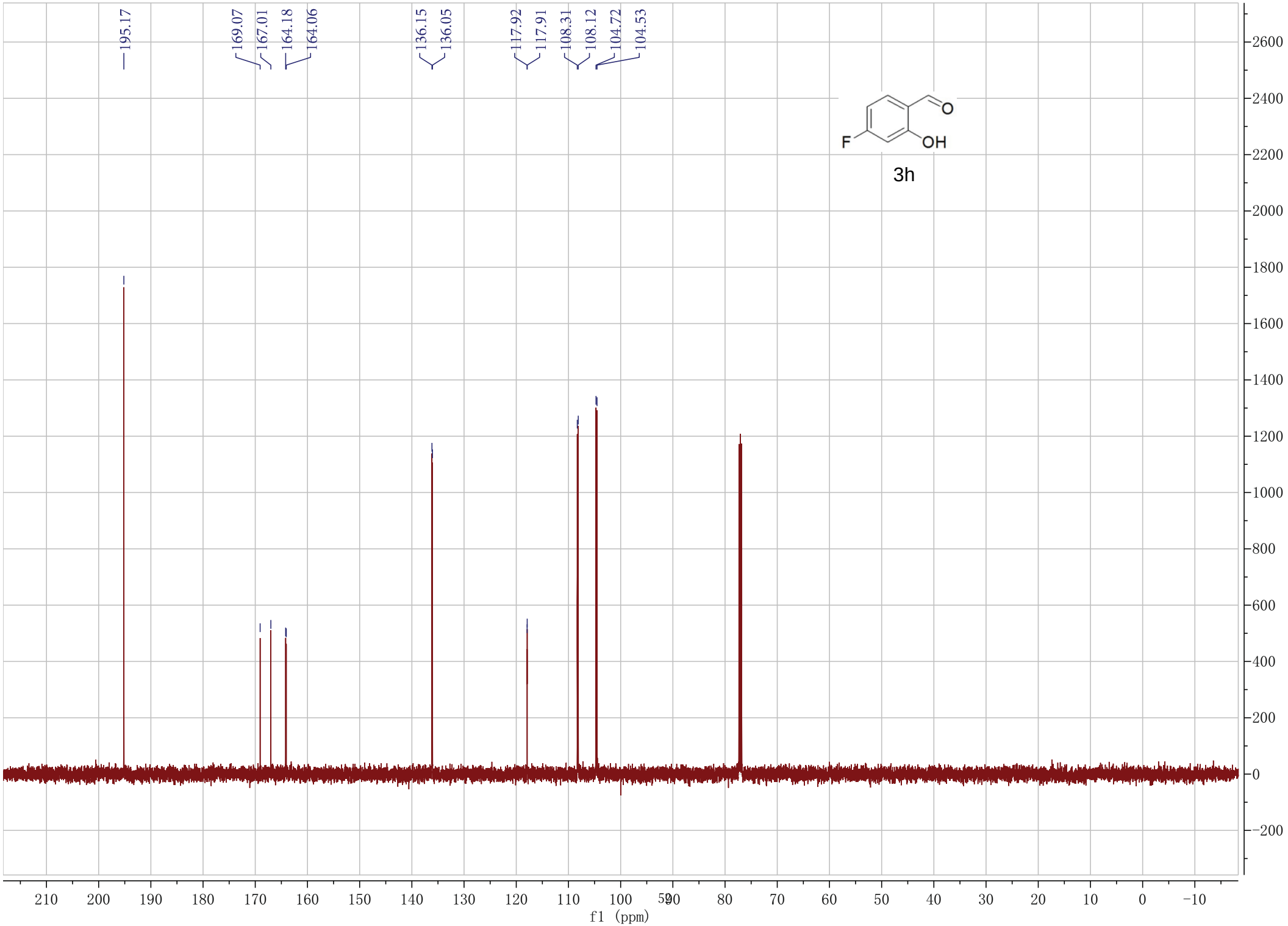

Et
OH
O
3f
1.00
1.00
1.00
1.00
1.00
2.00
3.00
35000
30000
25000
20000
15000
10000
5000
0
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3 −4
f1 (ppm)

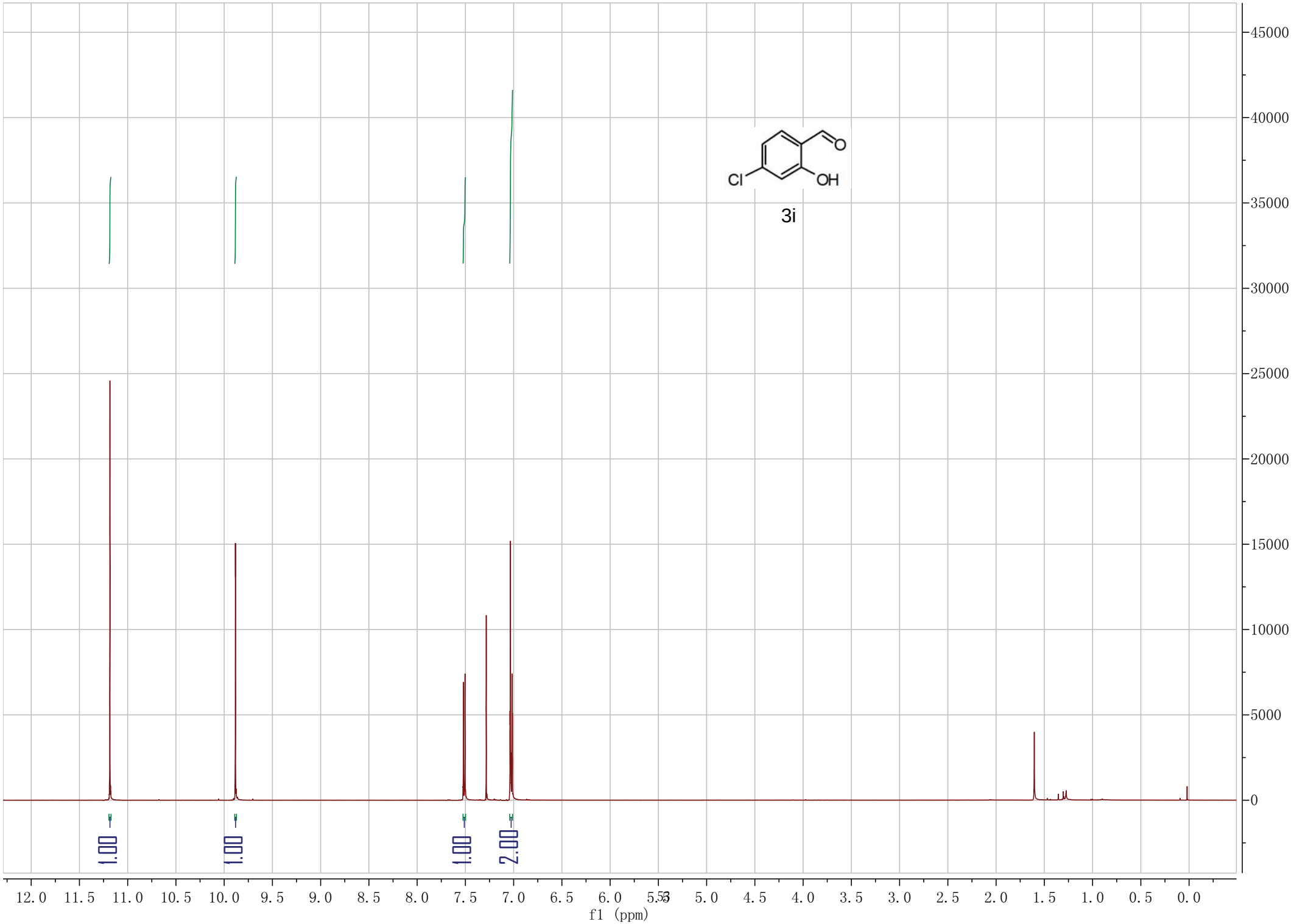

195.84
161.88
154.99
133.69
120.01
118.86
116.49
29.37
14.70
Et
OH
O
3f
f1 (ppm)

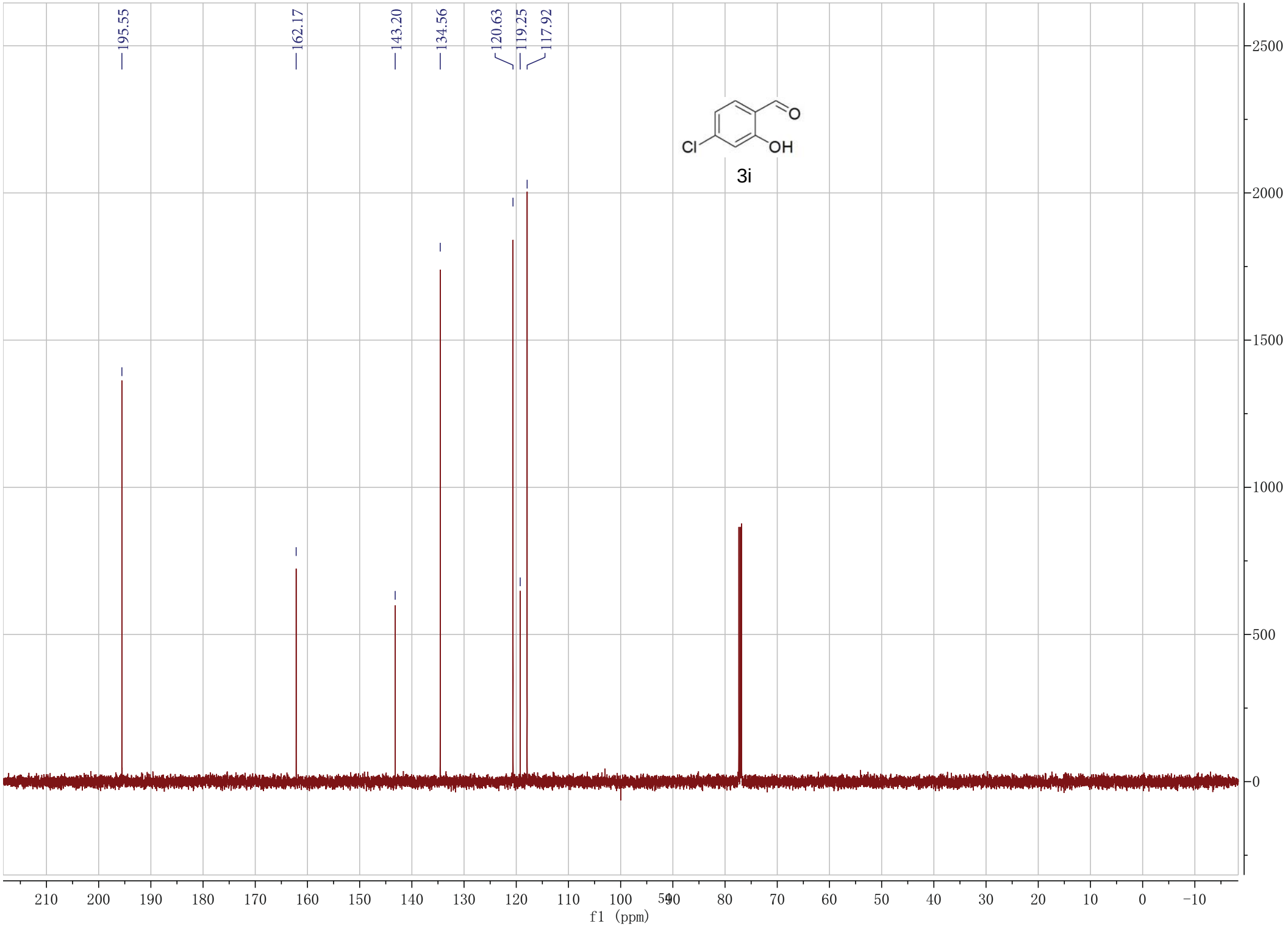

MeO
OH
O
3g
1.00
1.00
1.00
1.00
1.00
3.02
f1 (ppm)

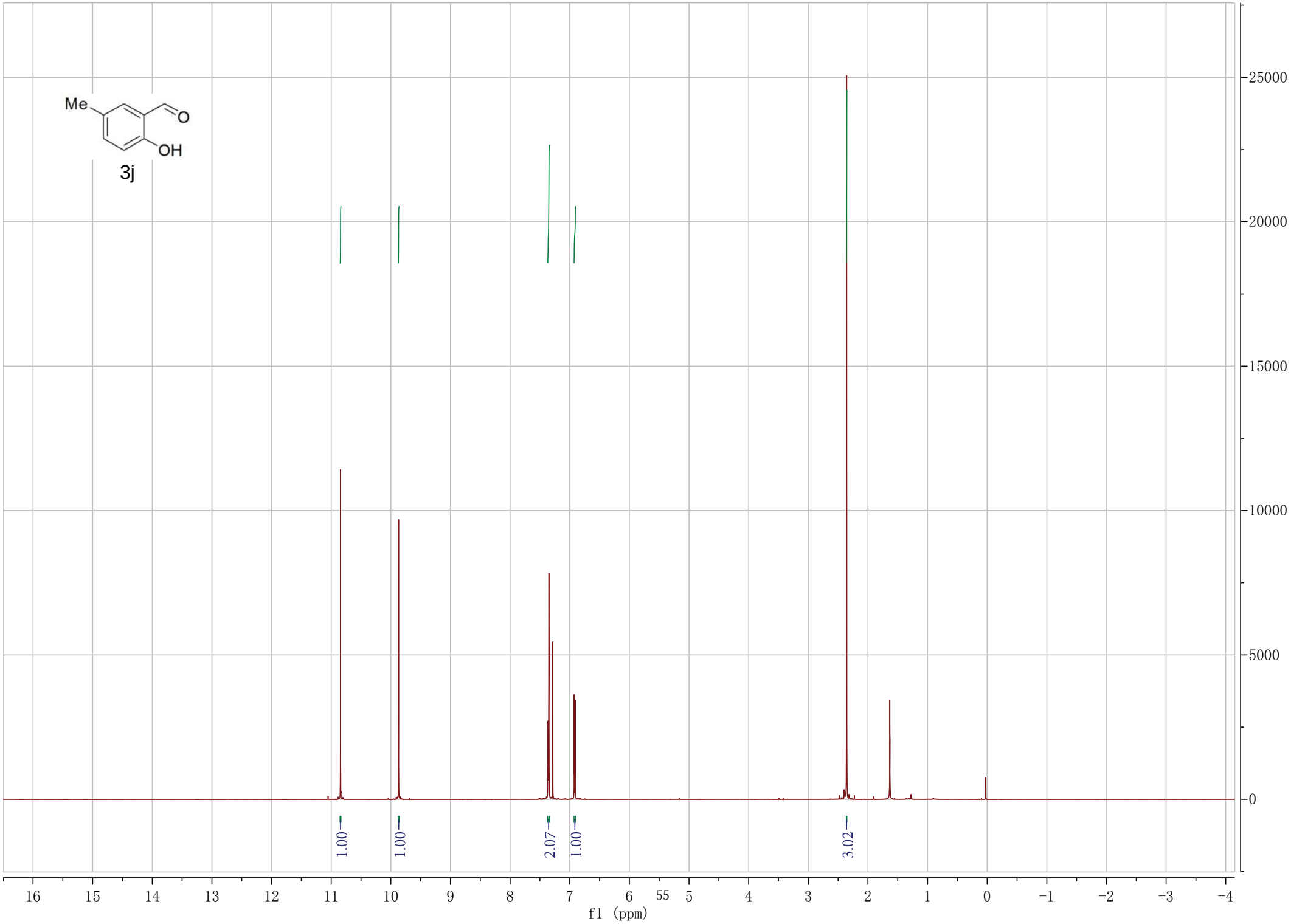

194.39
166.81
164.46
135.25
115.16
108.30
100.65
55.66
MeO
OH
O
3g
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
−200
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10

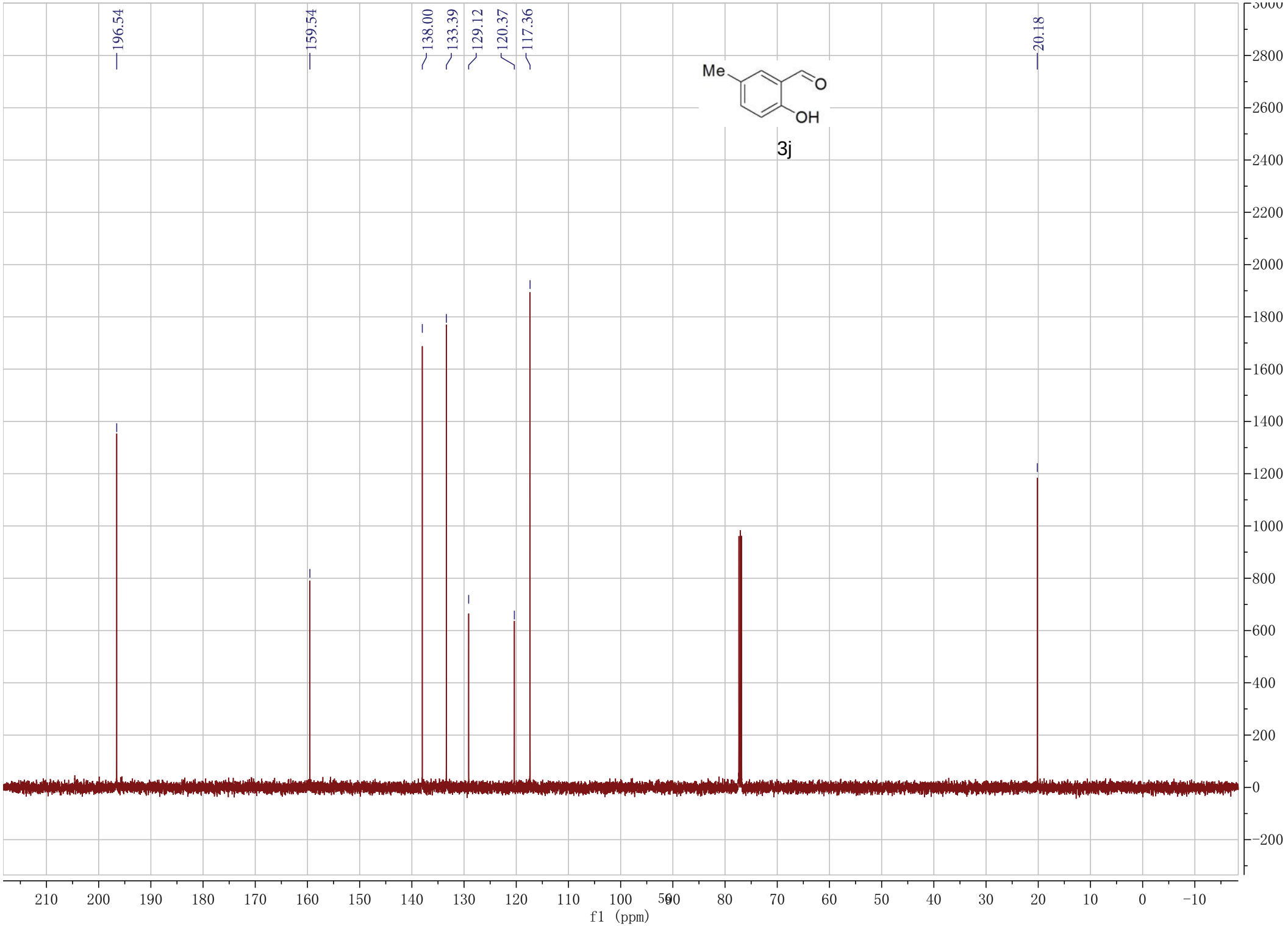

F
OH
O
3h
1.00
1.00
1.01
1.01
1.00
f1 (ppm)

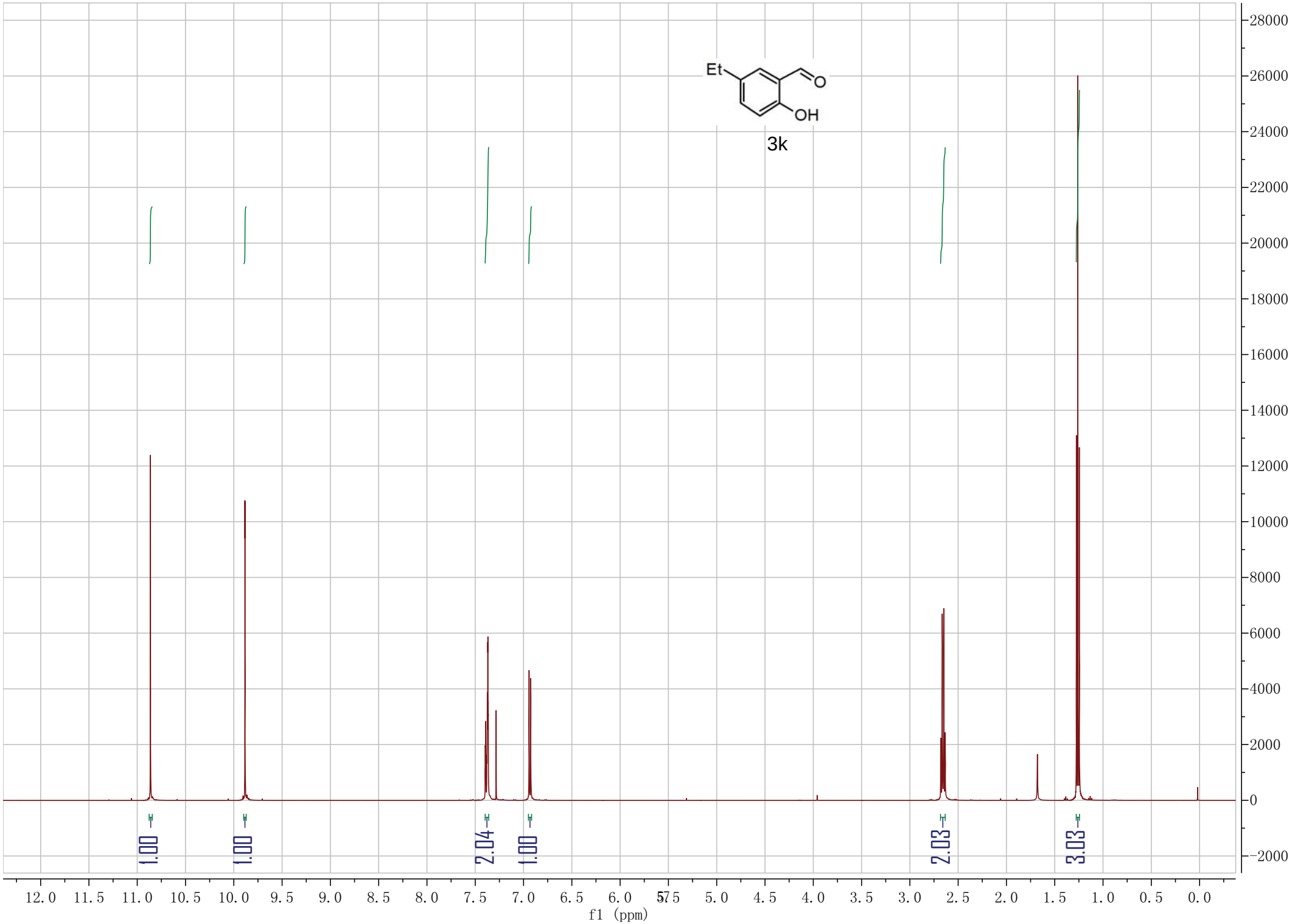

195.17
169.07
167.01
164.18
164.06
136.15
136.05
117.92
117.91
108.31
108.12
104.72
104.53
F
OH
O
3h
f1 (ppm)

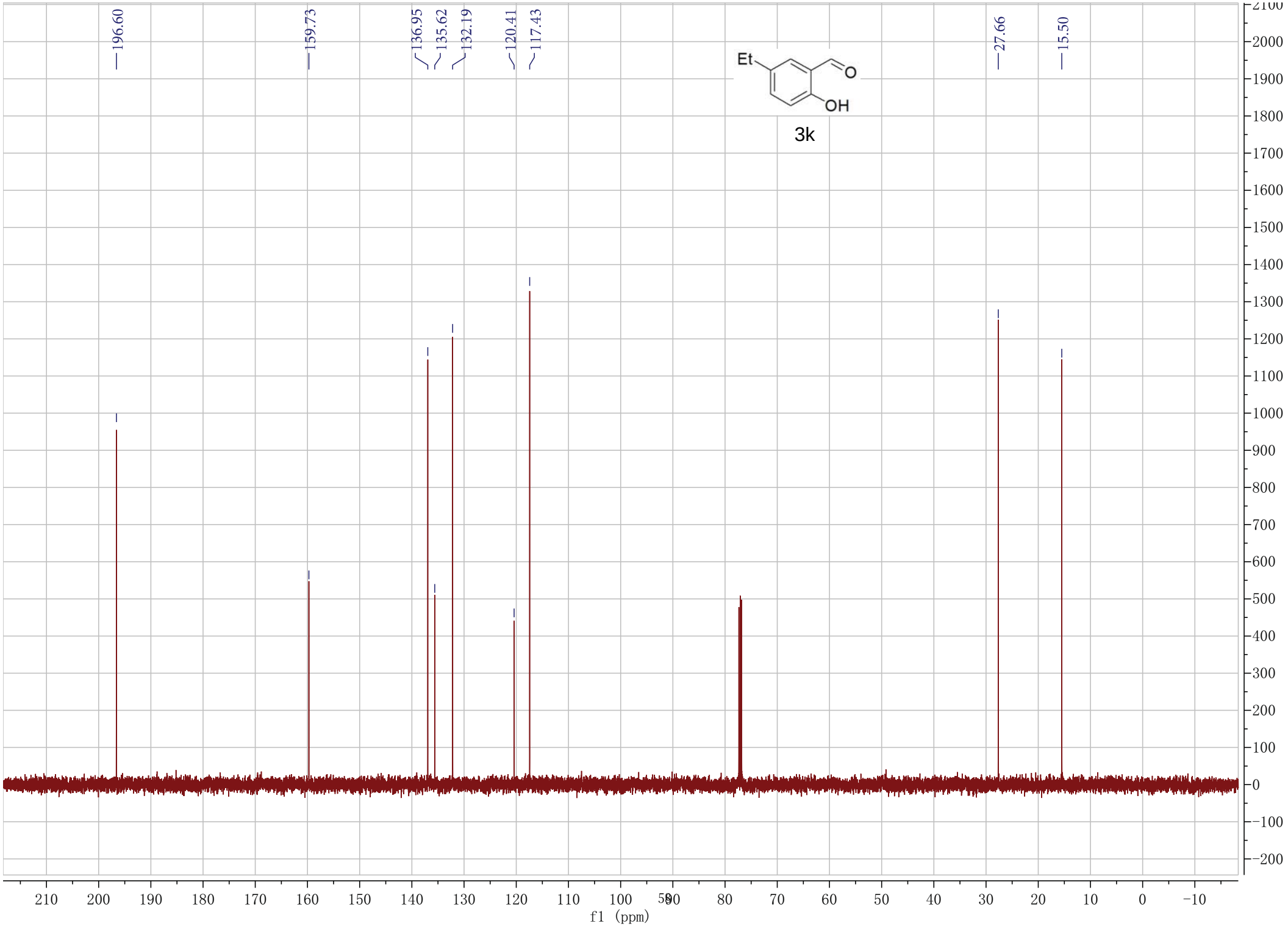

3i
Cl
OH
O
1.00
1.00
1.00
2.00
f1 (ppm)

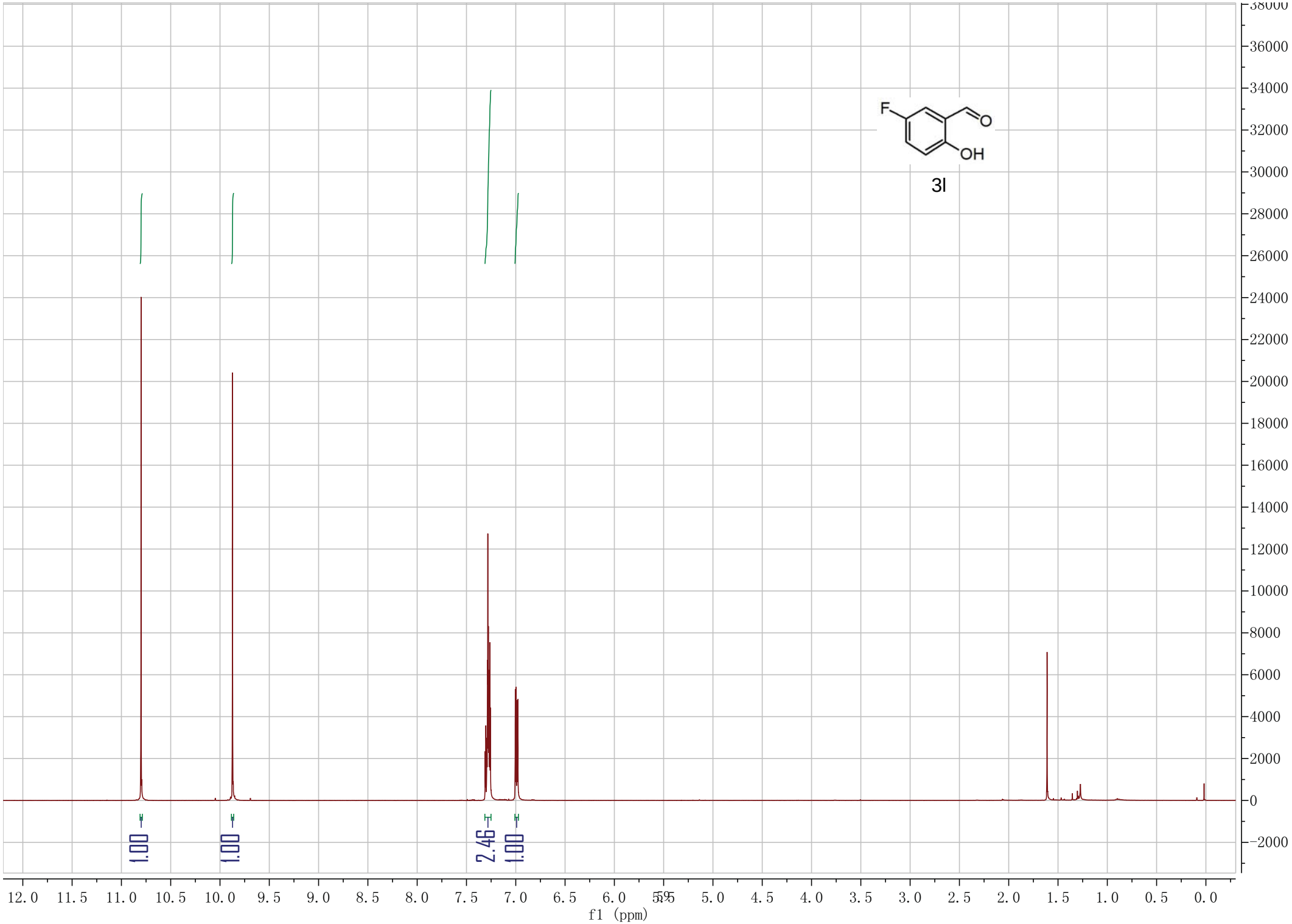

195.55
162.17
143.20
134.56
120.63
119.25
117.92
Cl
OH
O
3i
2500
2000
1500
1000
500
0
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

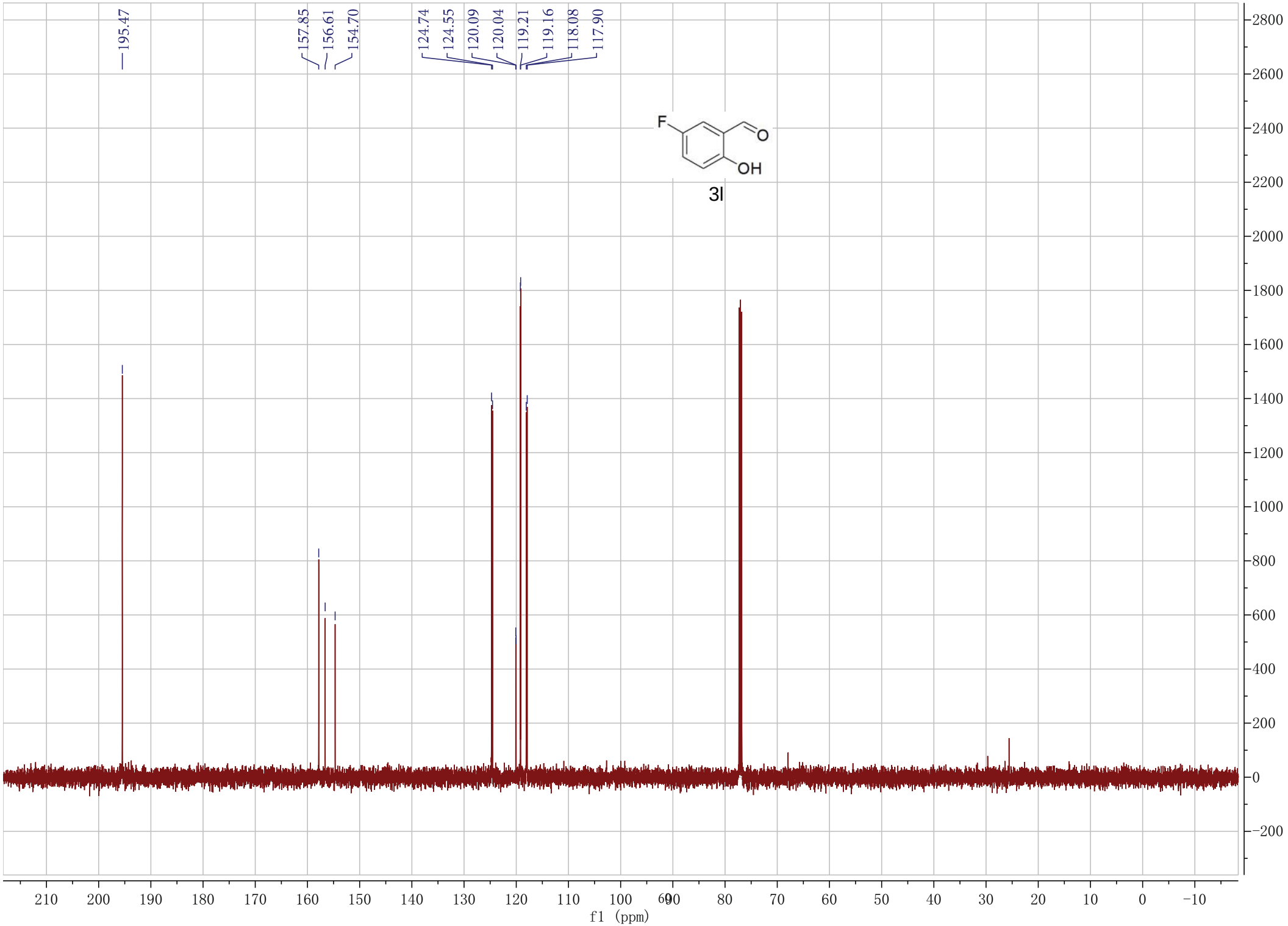

Me
O
OH
3j
1.00
1.00
2.07
1.00
3.02
25000
20000
15000
10000
5000
0
16 15 14 13 12 11 10 9 8 7 6 55 5 4 3 2 1 0 −1 −2 −3 −4
f1 (ppm)

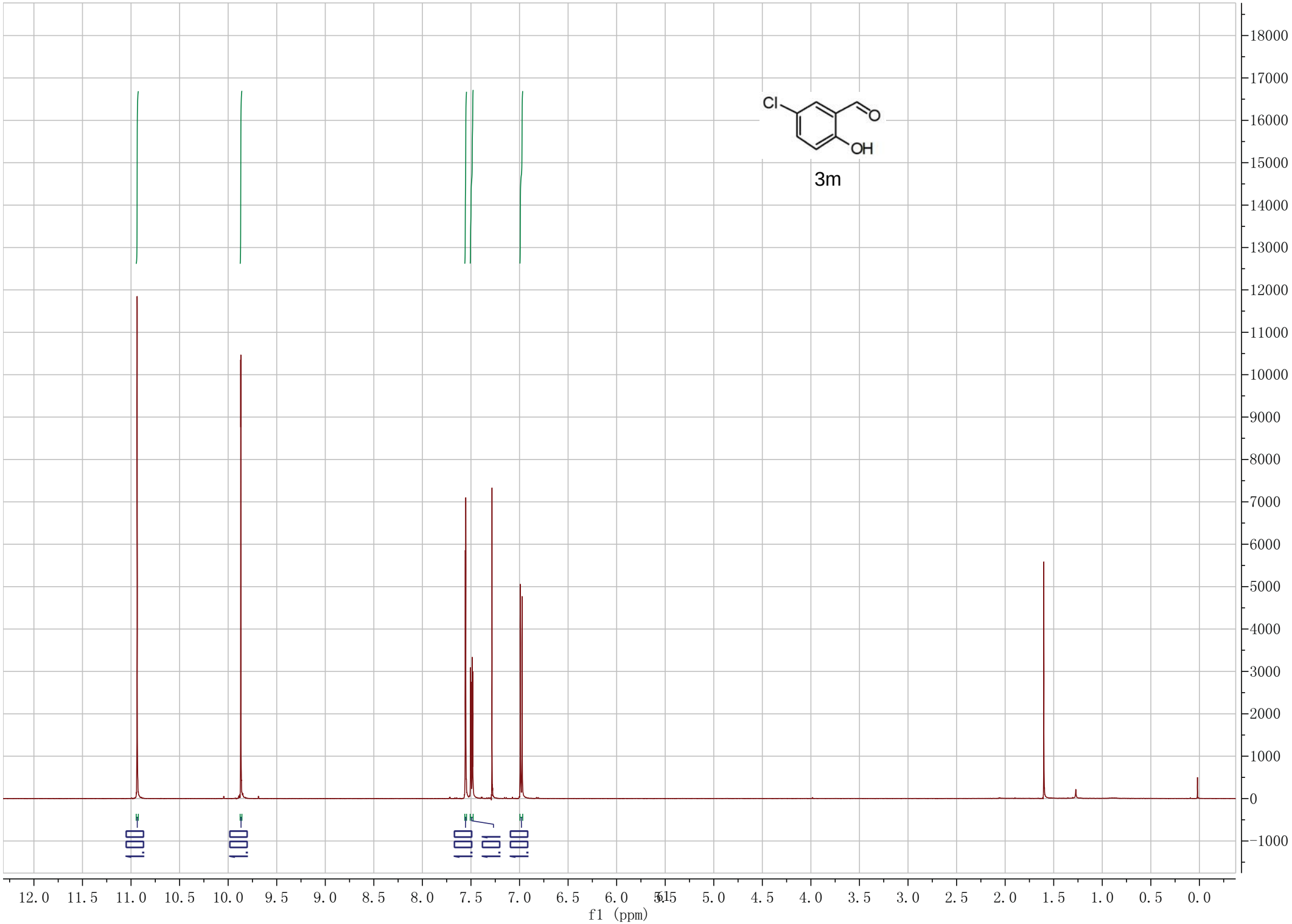

196.54
159.54
138.00
133.39
129.12
120.37
117.36
20.18
Me
O
OH
3j
f1 (ppm)

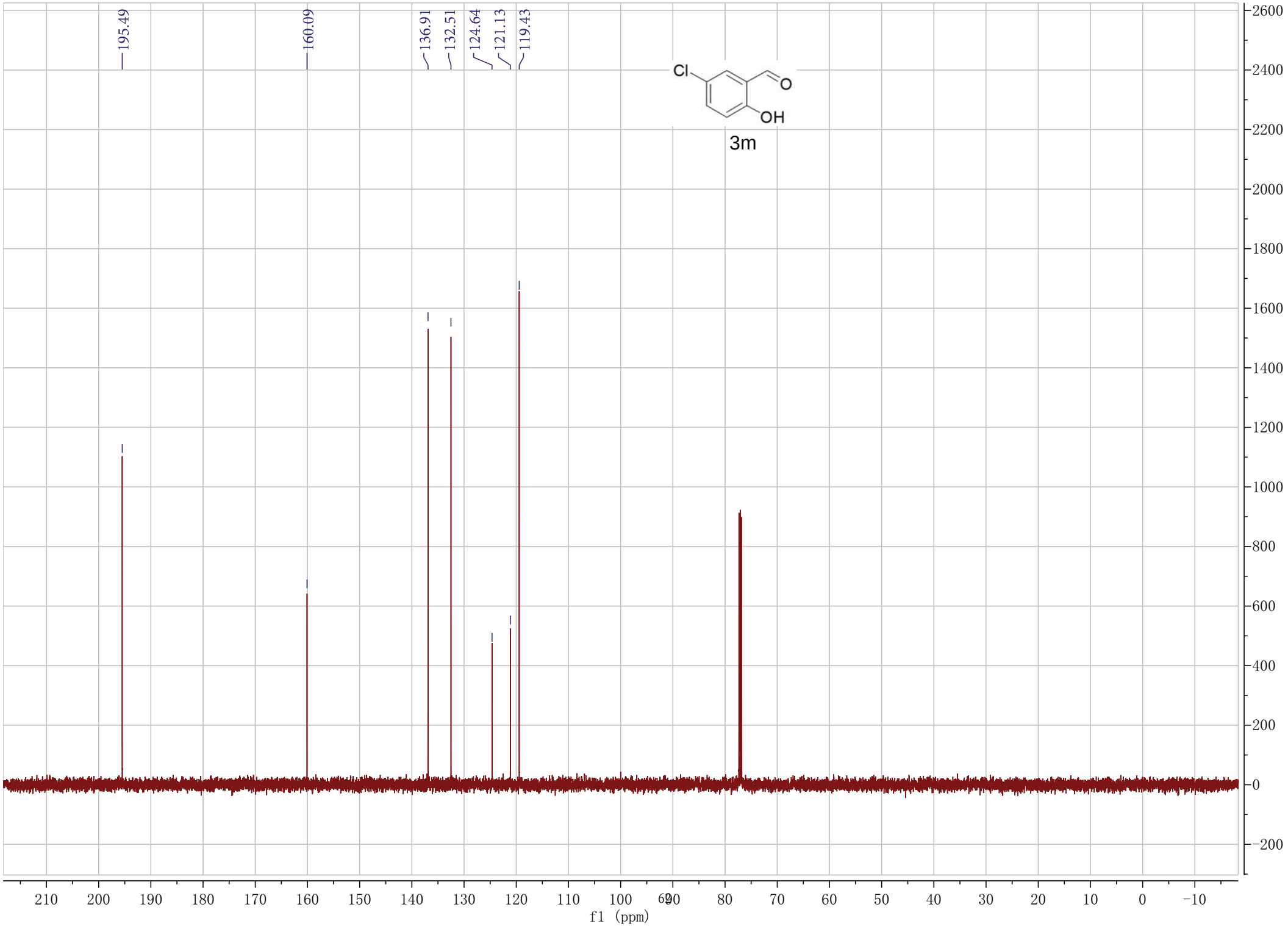

Et
O
OH
3k
1.00
1.00
2.04
1.00
2.03
3.03
f1 (ppm)

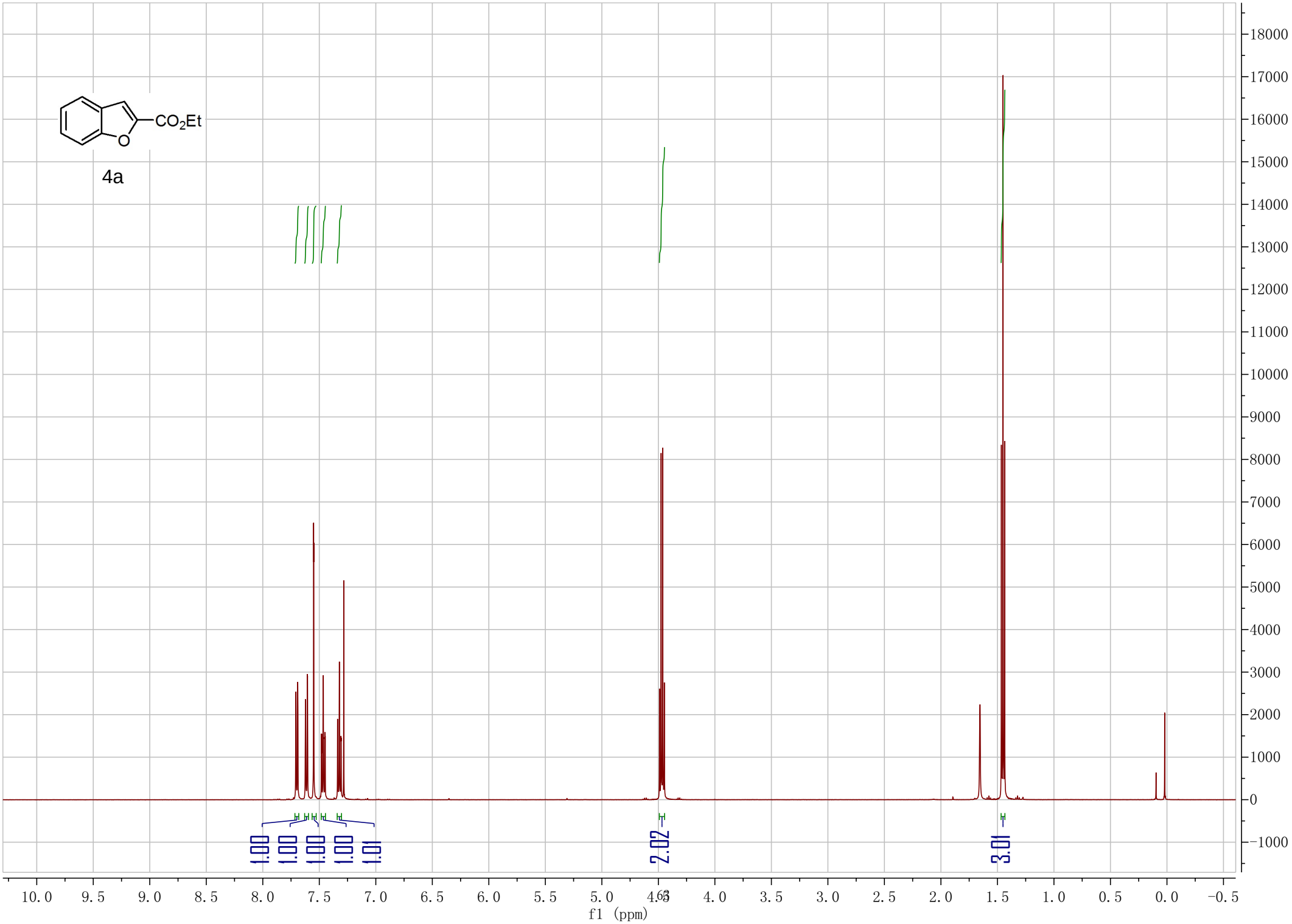

196.60
159.73
136.95
135.62
132.19
120.41
117.43
27.66
15.50
Et
O
OH
3k
f1 (ppm)

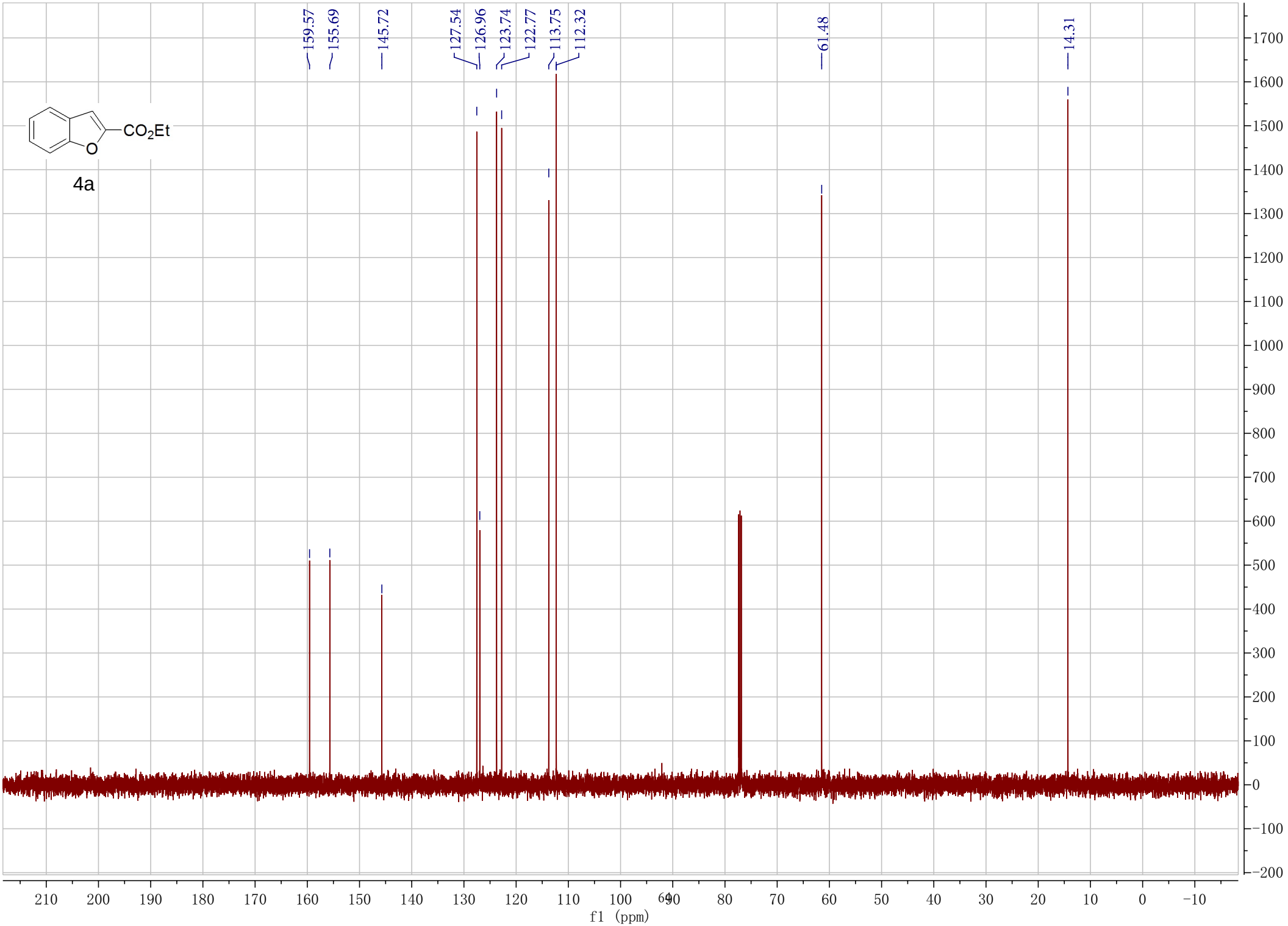

F
O
OH
3l
1.00
1.00
2.46
1.00
f1 (ppm)

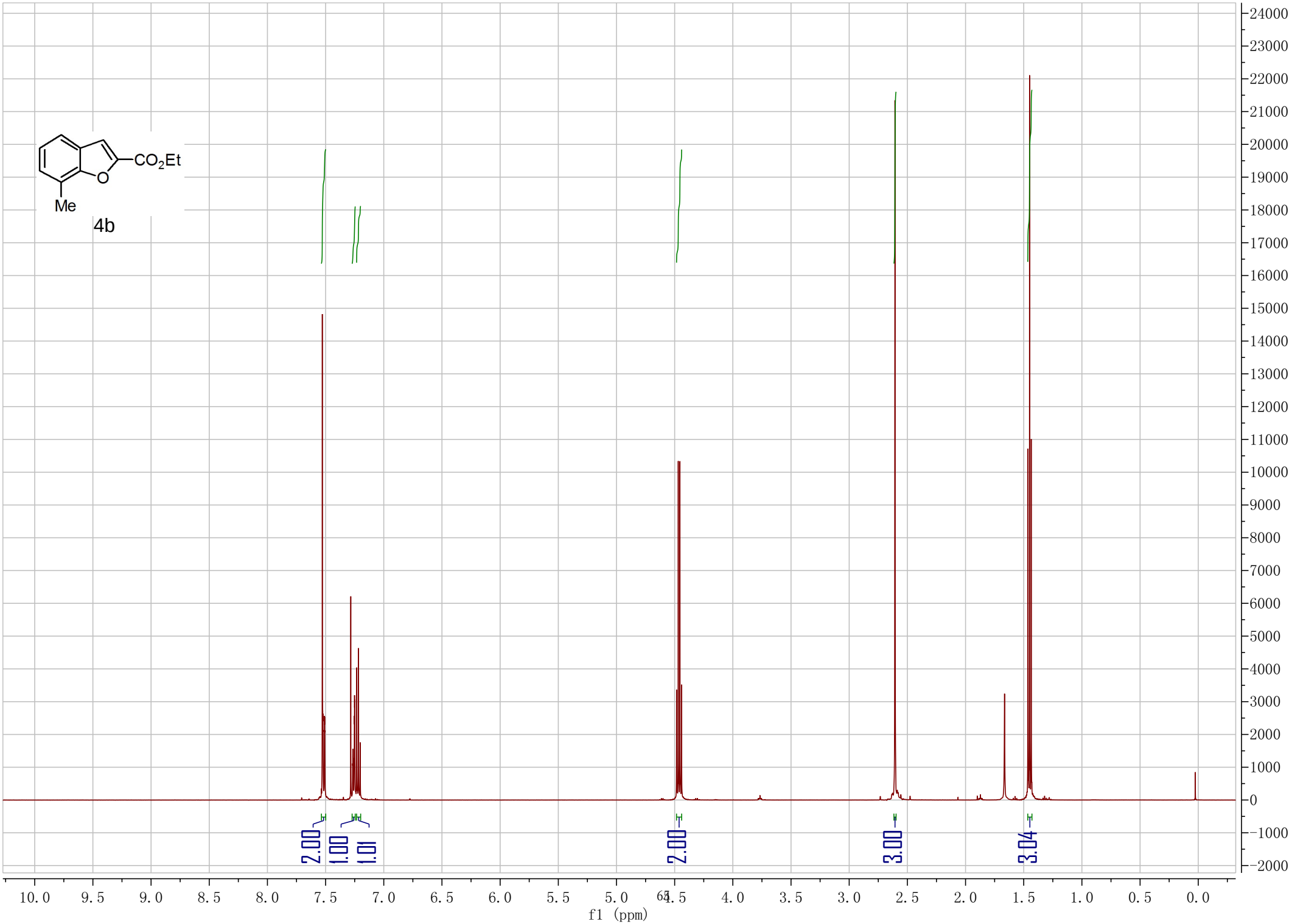

195.47
157.85
156.61
154.70
124.74
124.55
120.09
120.04
119.21
119.16
118.08
117.90
F
O
OH
3l
f1 (ppm)

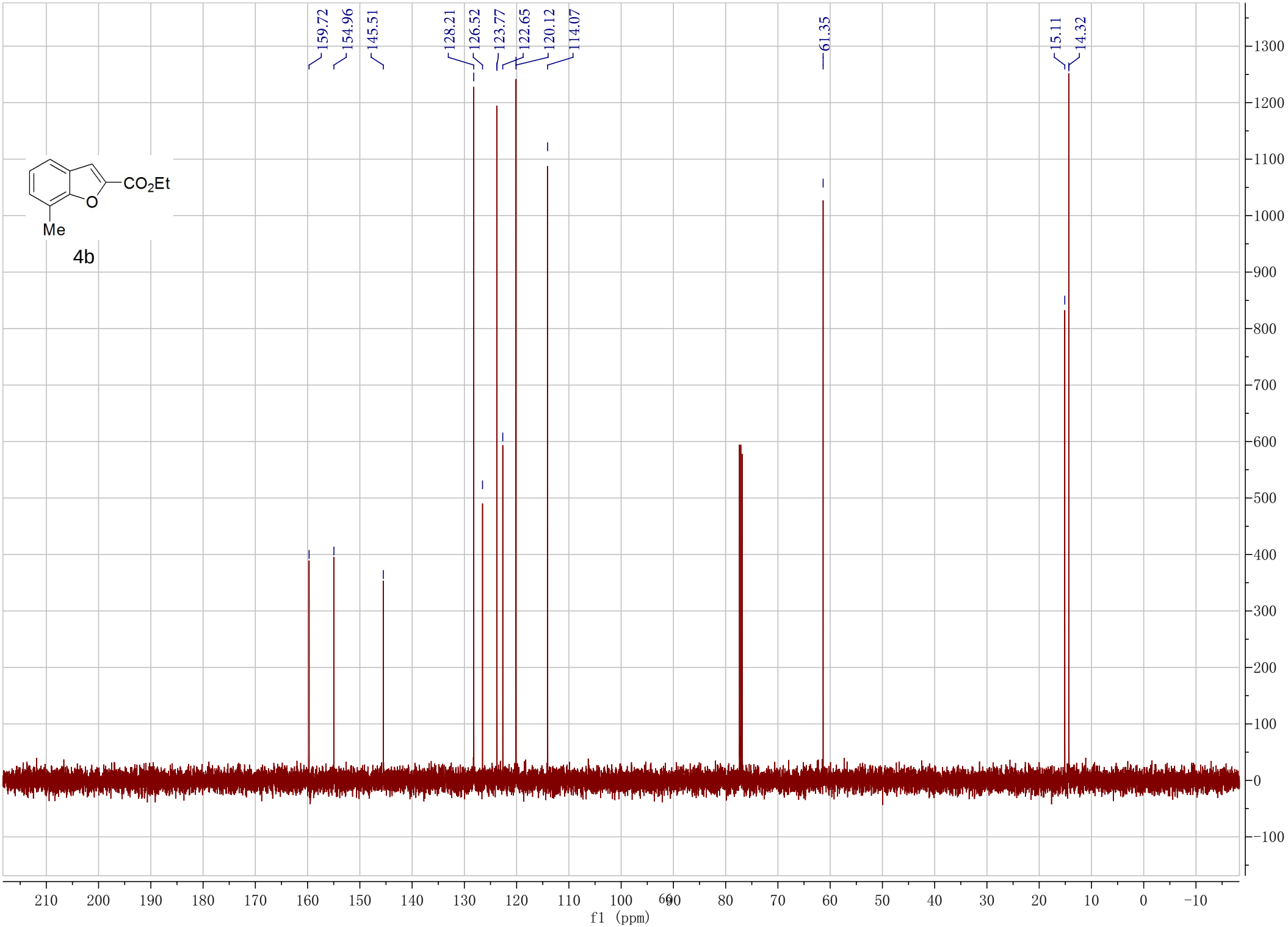

Cl
O
OH
3m
f1 (ppm)

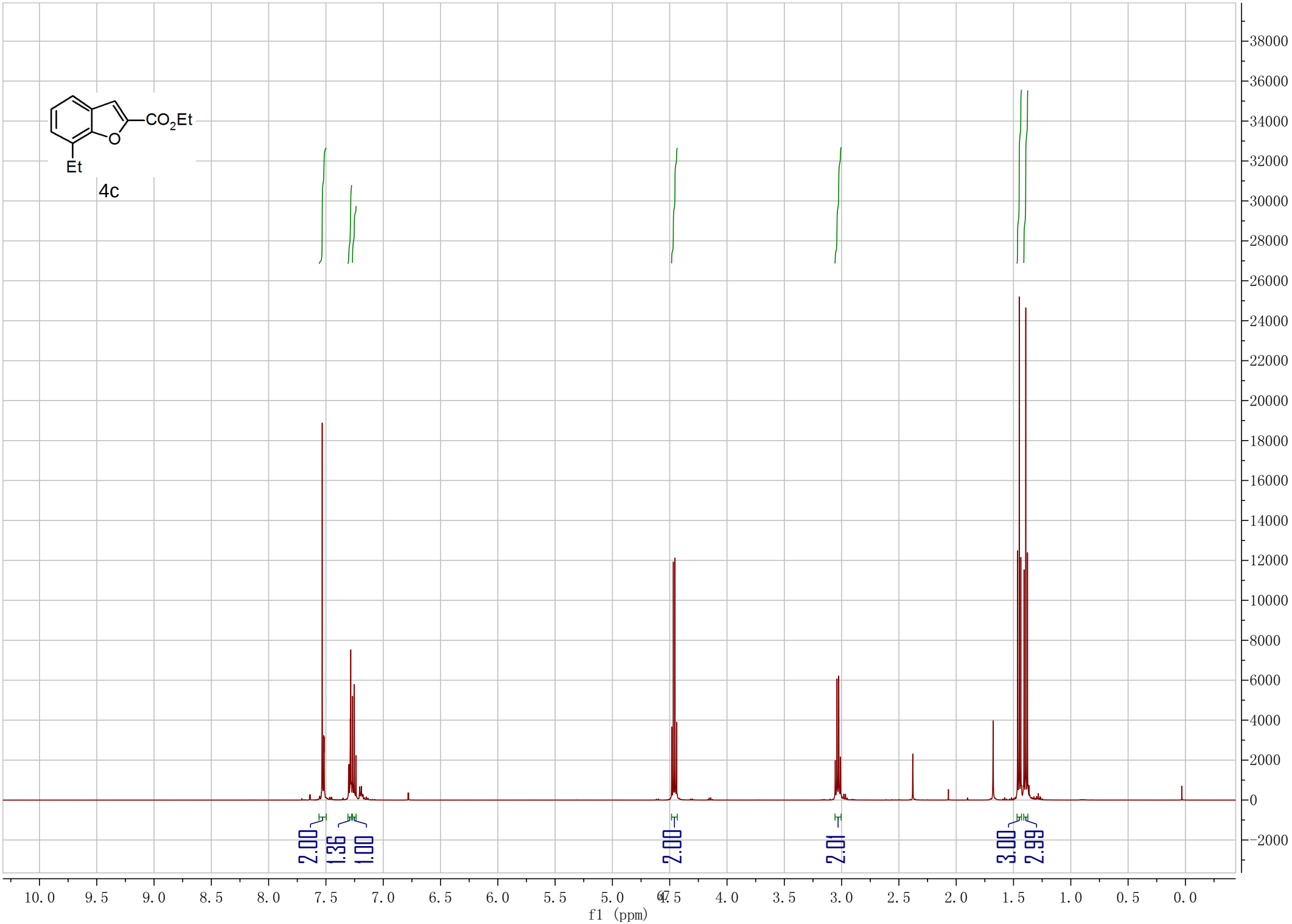

195.49
160.09
136.91
132.51
124.64
121.13
119.43
Cl
O
OH
3m
f1 (ppm)

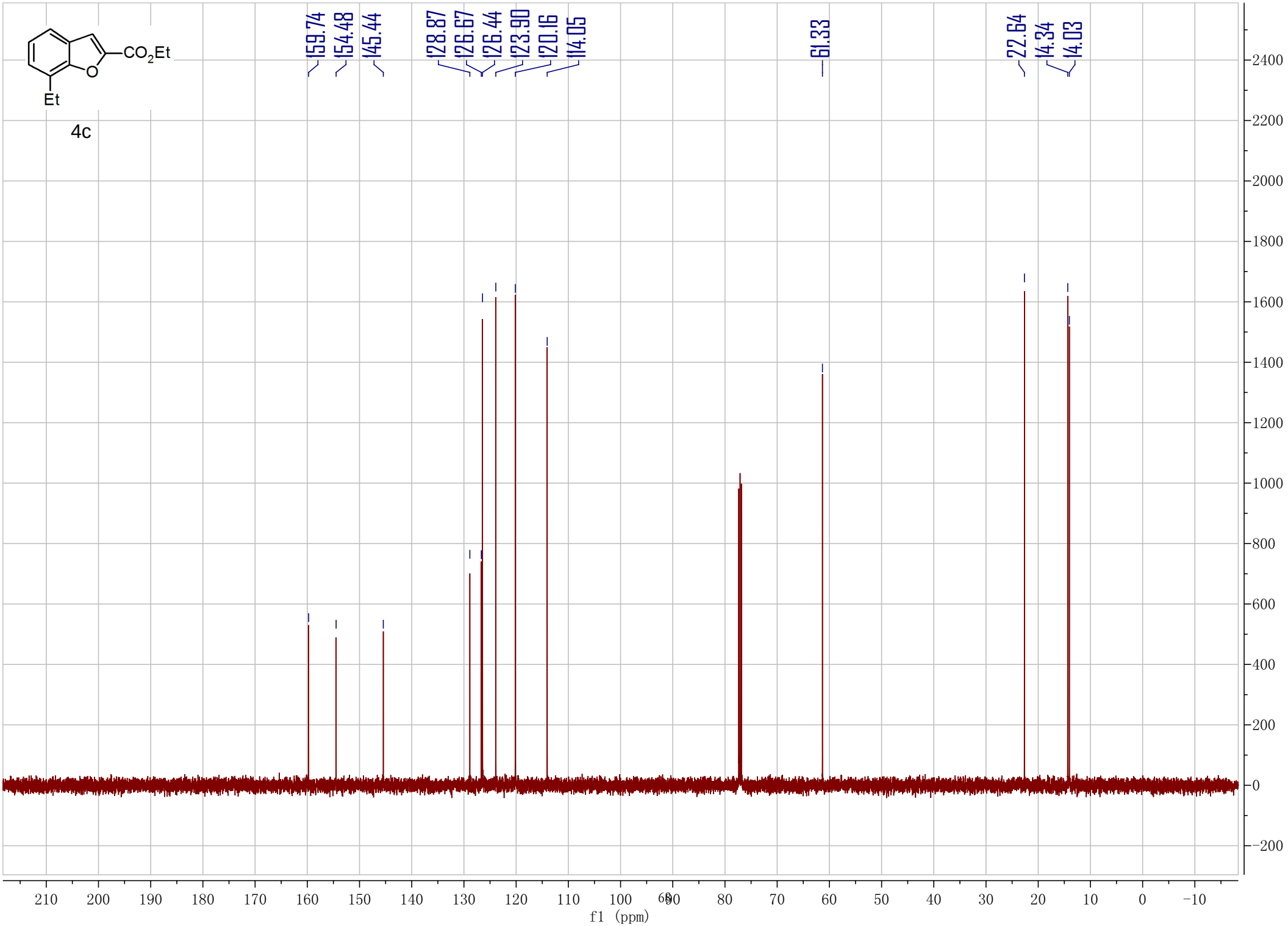

CO2Et
O
4a
1.00
1.00
1.00
1.00
1.01
2.02
3.01
f1 (ppm)

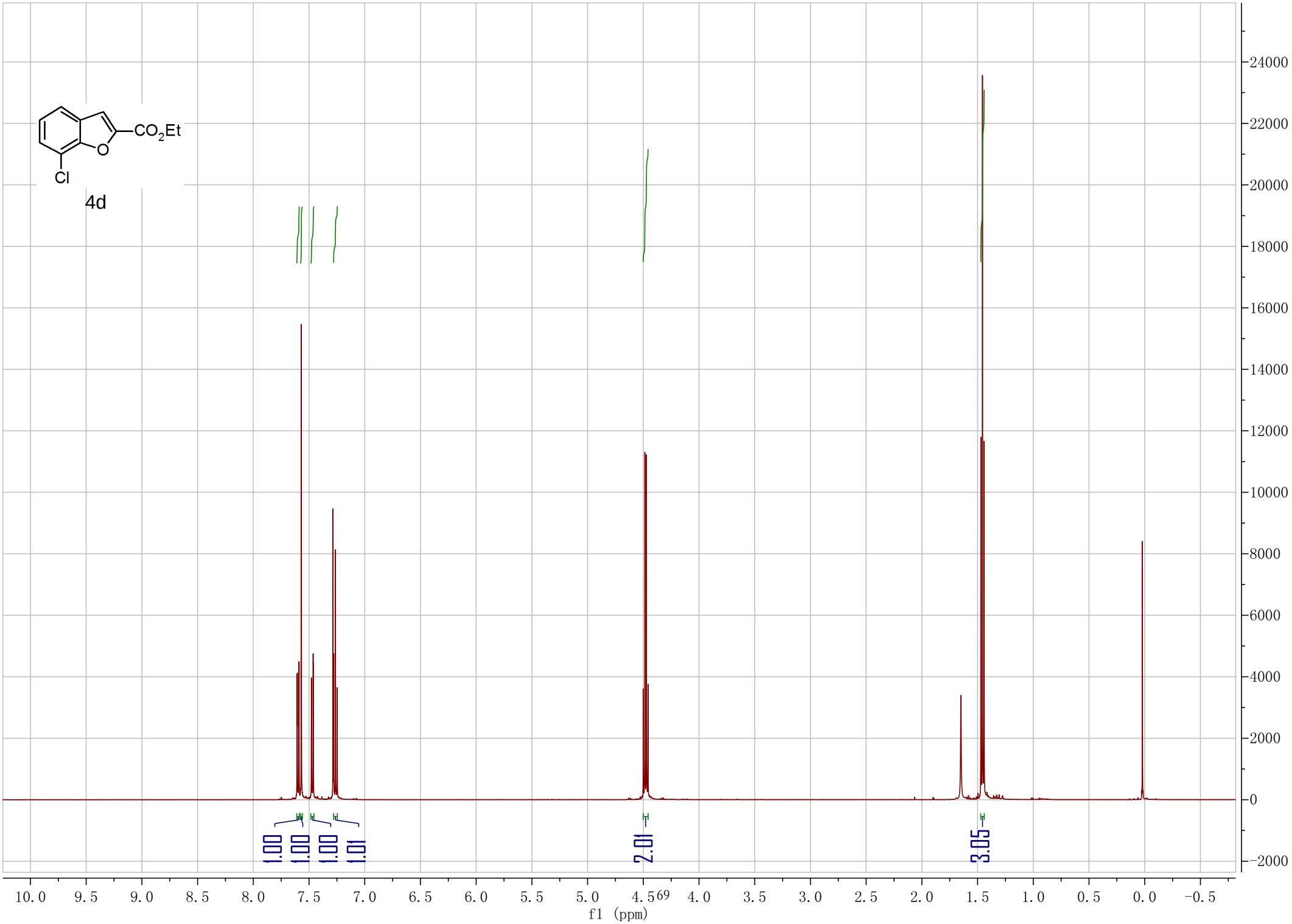

159.57
155.69
145.72
127.54
126.96
123.74
122.77
113.75
112.32
61.48
14.31
CO2Et
O
4a
f1 (ppm)

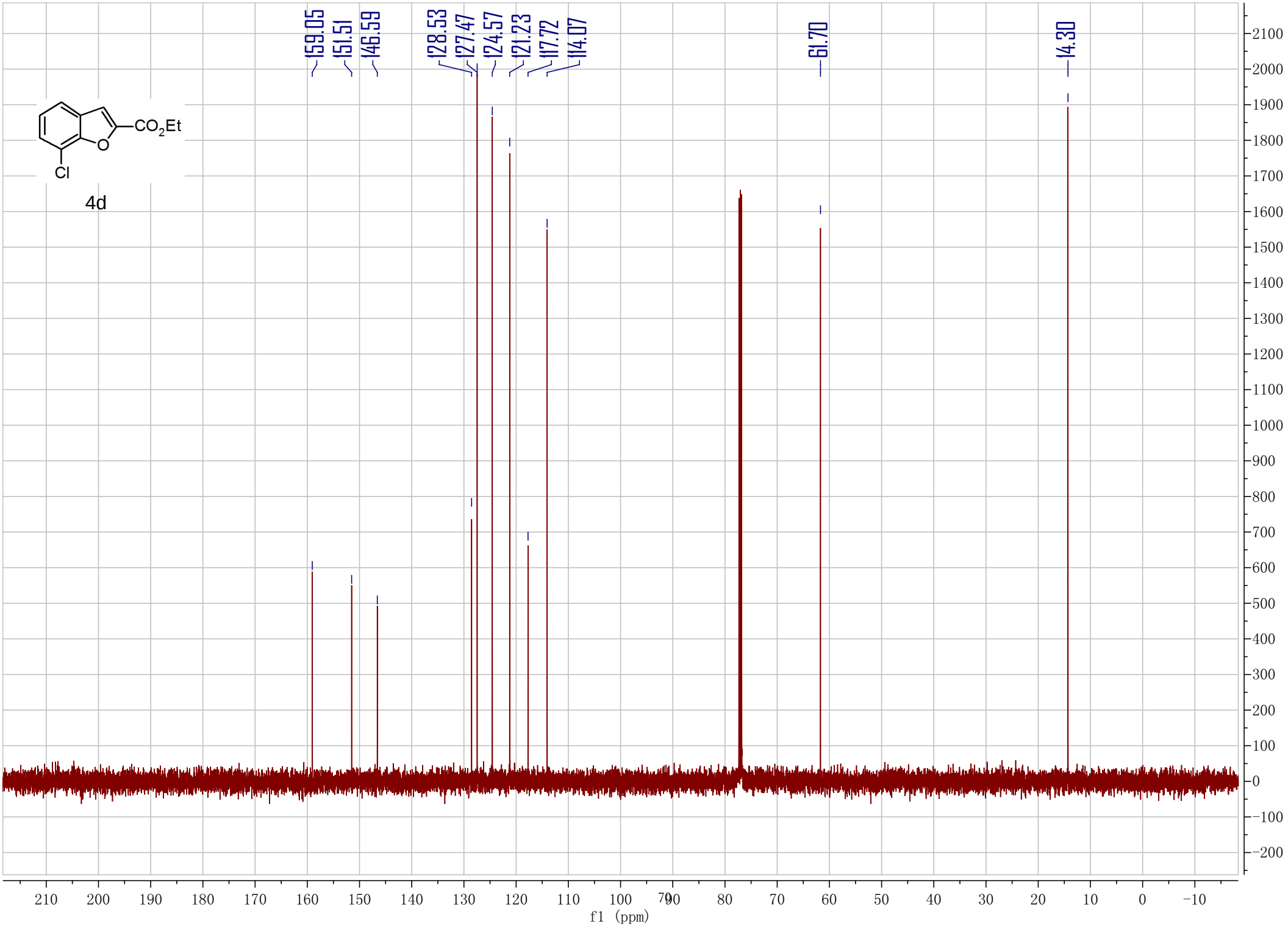

CO2Et
O
Me
4b
2.00
1.00
1.01
2.00
3.00
3.04
f1 (ppm)

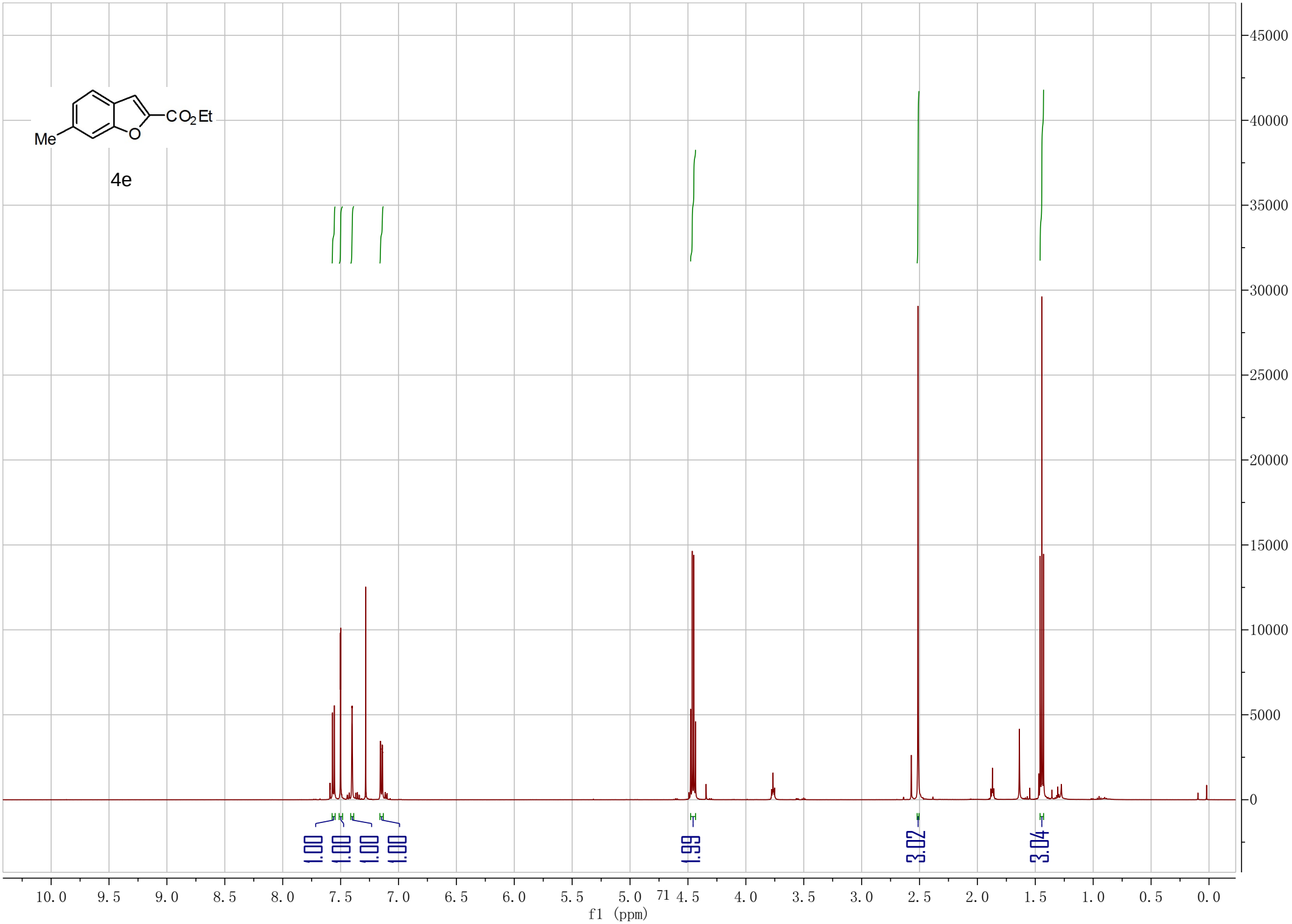

159.72
154.96
145.51
128.21
126.52
123.77
122.65
120.12
114.07
61.35
15.11
14.32
CO2Et
O
Me
4b
f1 (ppm)

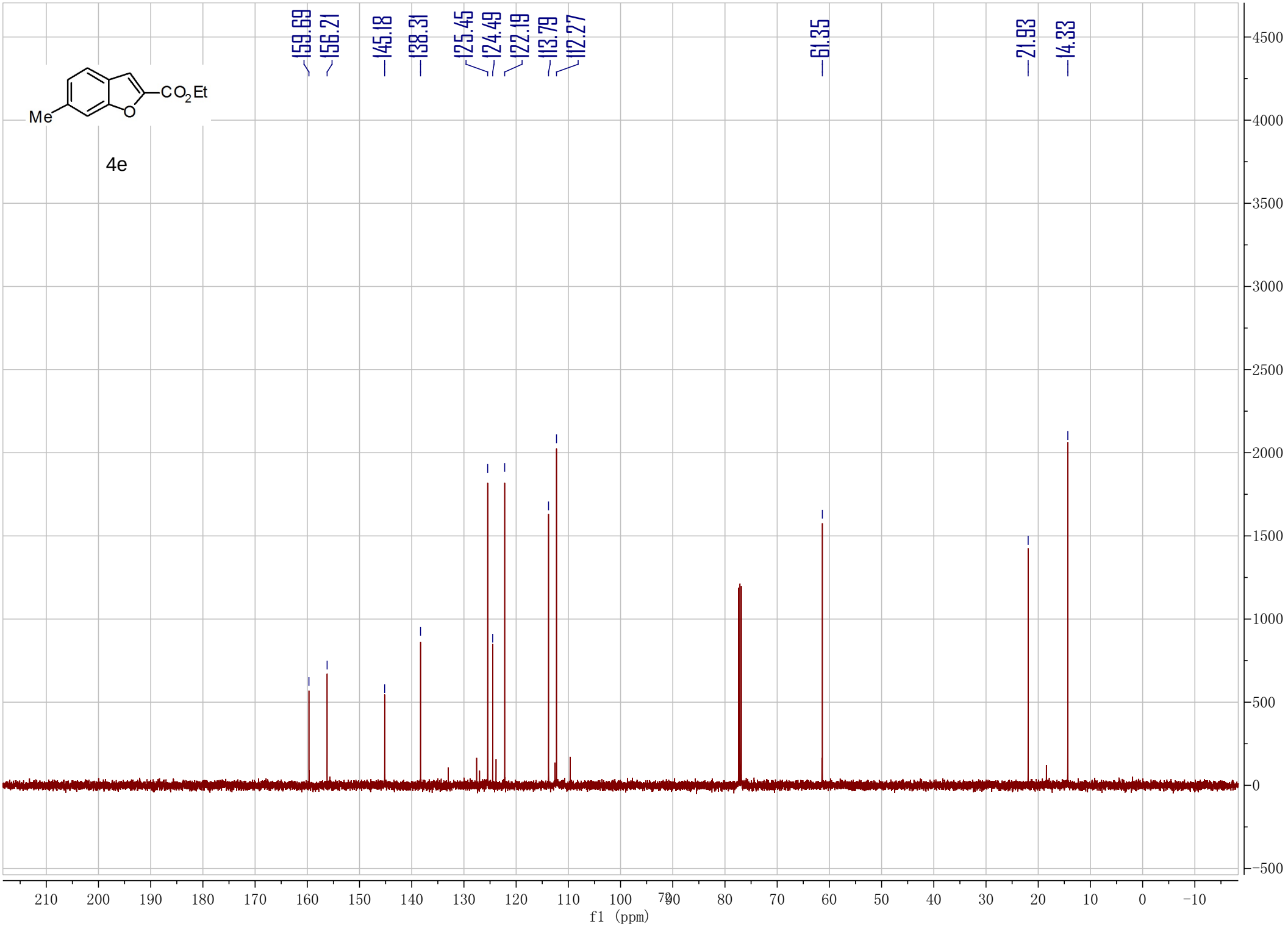

CO2Et
O
Et
4c
2.00
1.36
1.00
2.00
2.01
3.00
2.99
f1 (ppm)

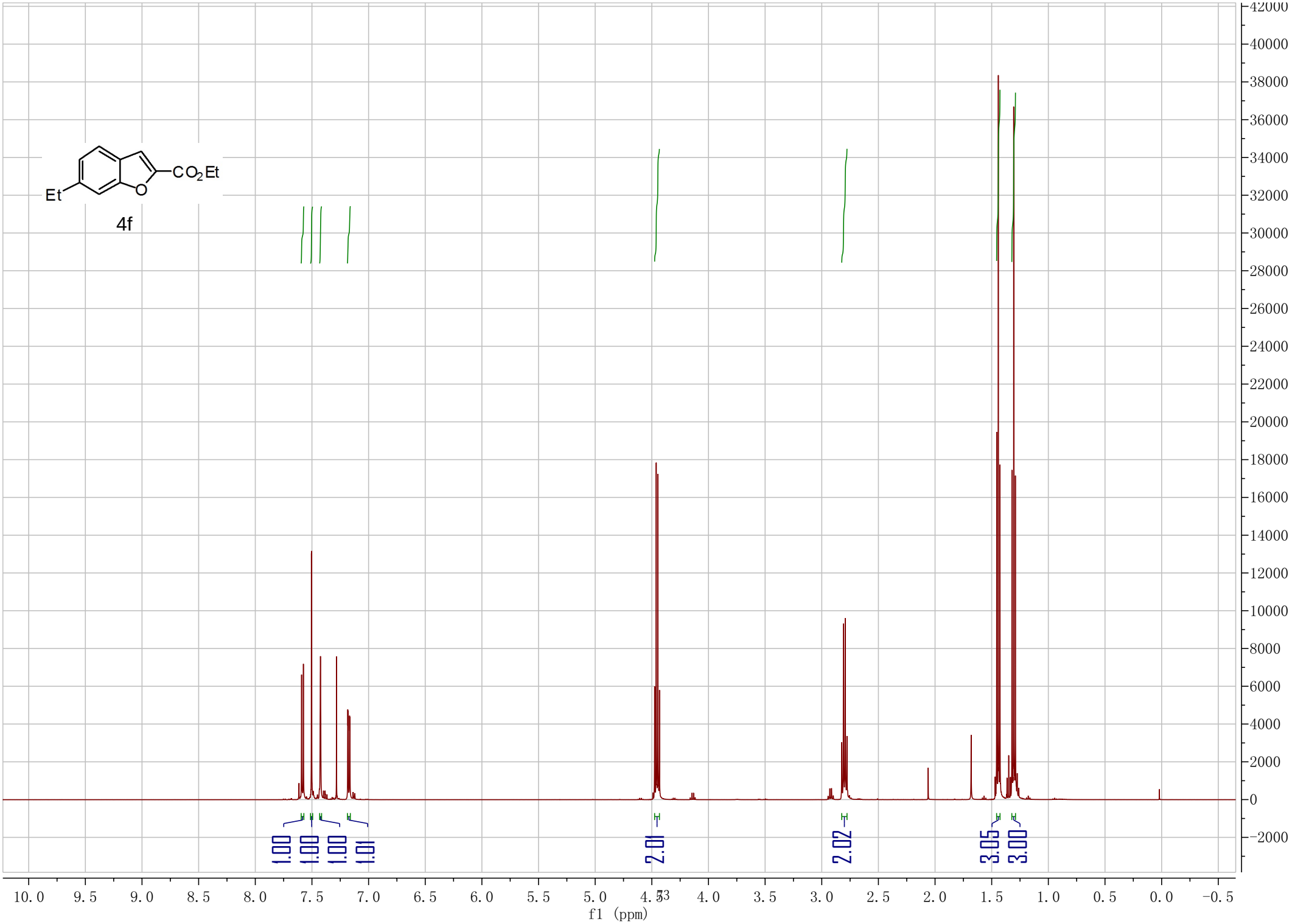

CO2Et
Et
4c
159.74
154.48
145.44
128.87
126.67
126.44
123.90
120.16
114.05
61.33
22.64
14.34
14.03
f1 (ppm)

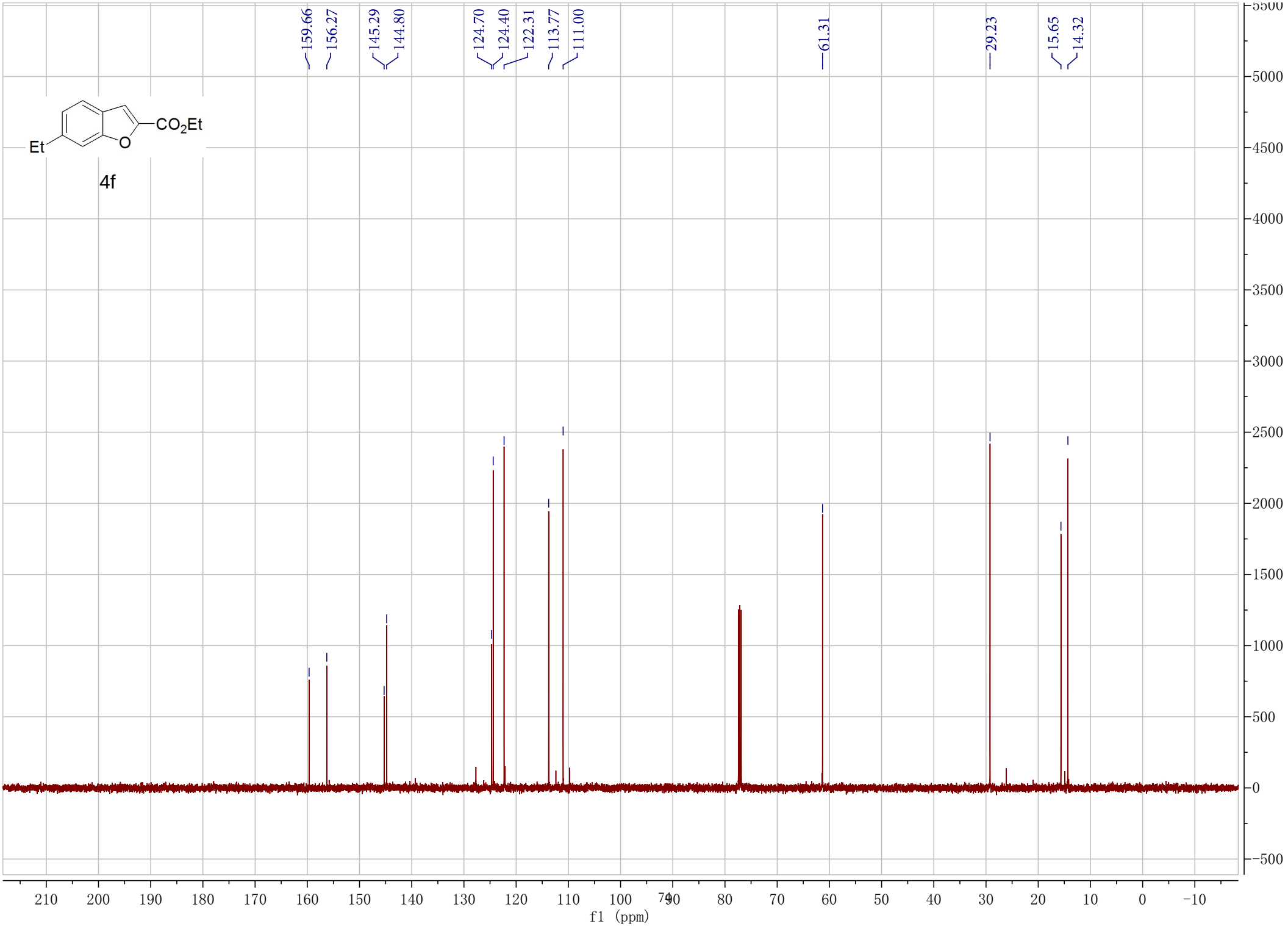

CO2Et
O
Cl
4d
1.00
1.00
1.00
1.01
2.01
3.05
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.569
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

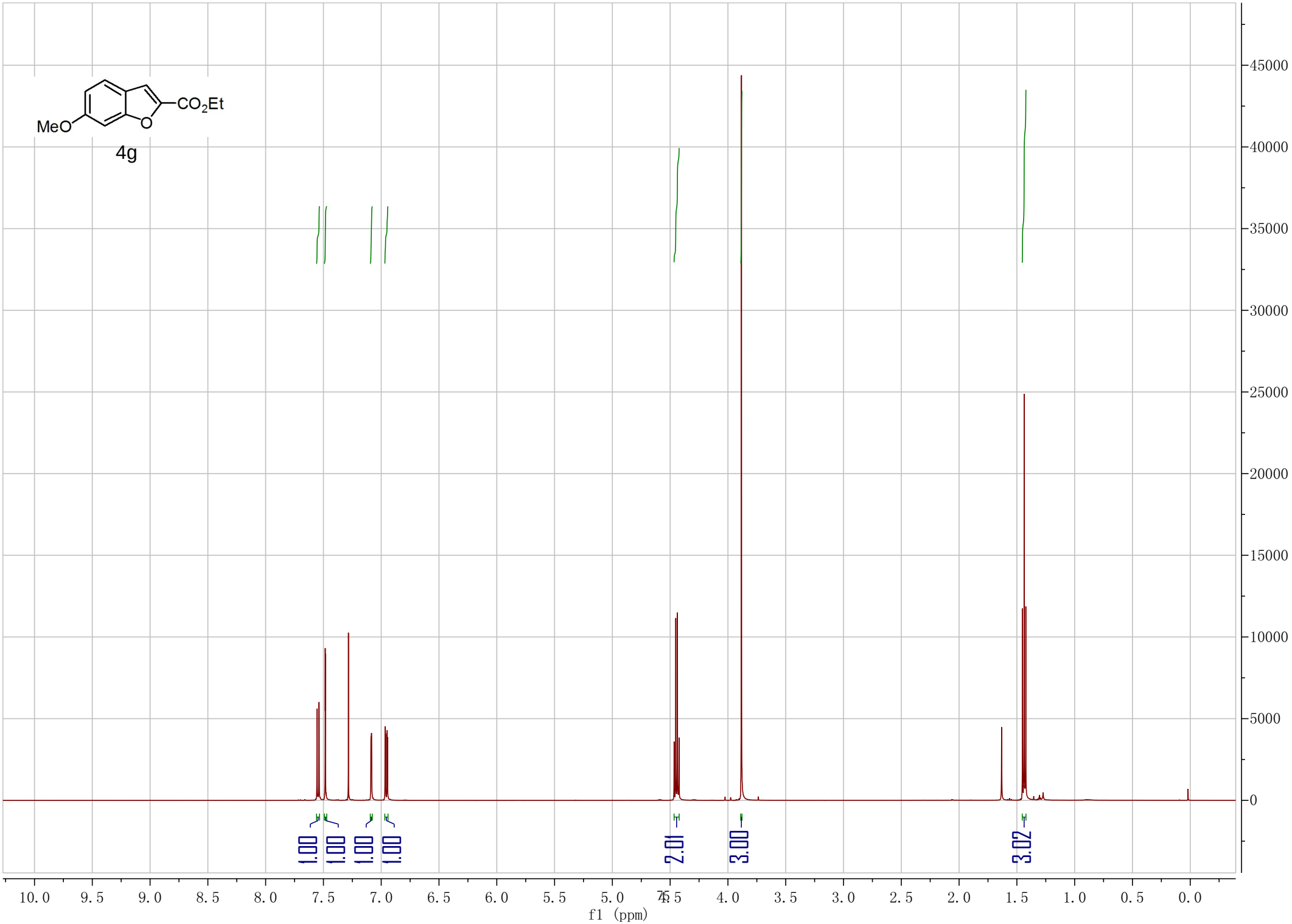

159.05
151.51
146.59
128.53
127.47
124.57
121.23
117.72
114.07
61.70
14.30
CO2Et
O
Cl
4d
f1 (ppm)

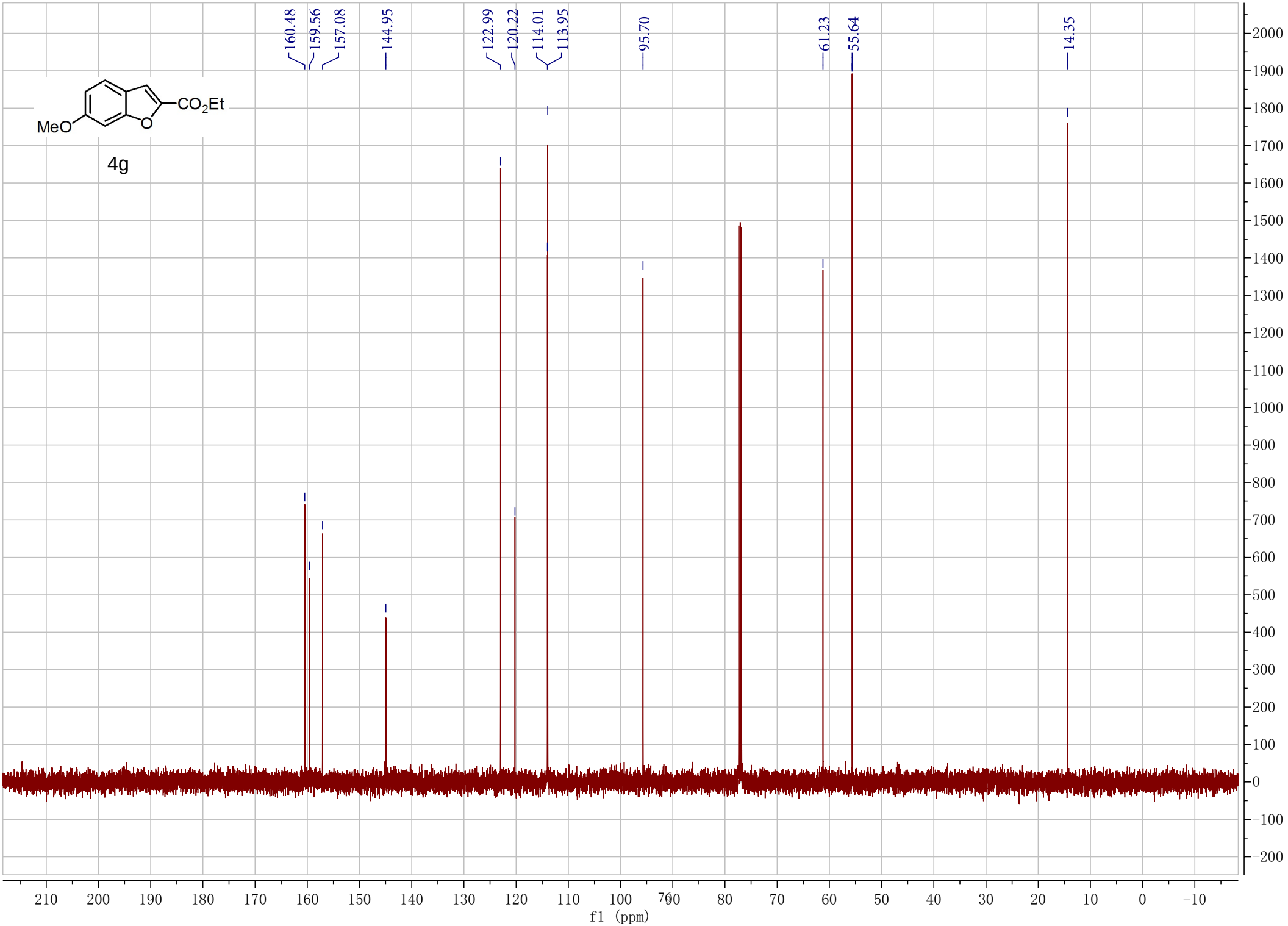

CO2Et
Me
O
4e
1.00
1.00
1.00
1.00
1.99
3.02
3.04
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

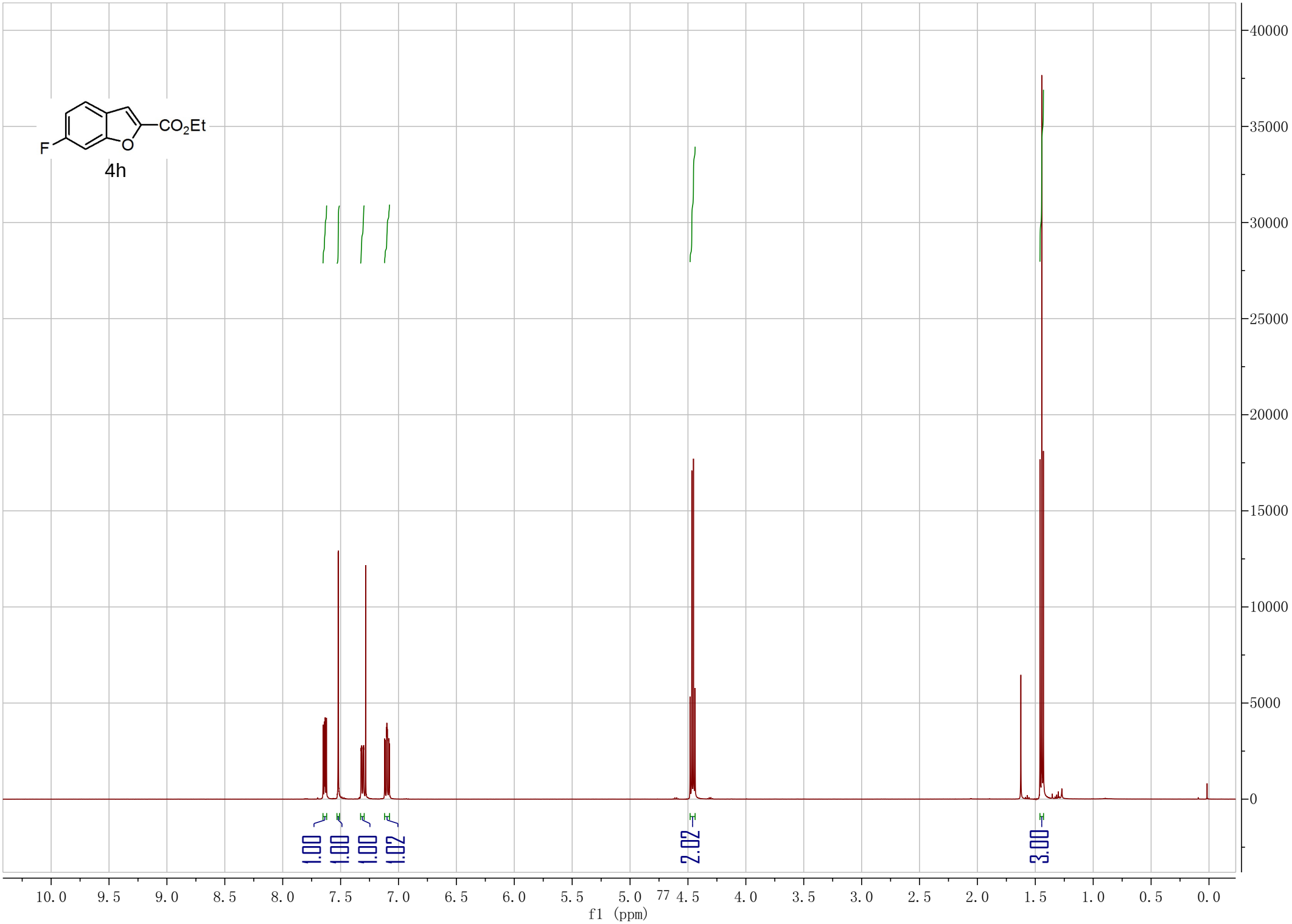

159.69
156.21
145.18
138.31
125.45
124.49
122.19
113.79
112.27
61.35
21.93
14.33
Me
CO2Et
O
4e
f1 (ppm)

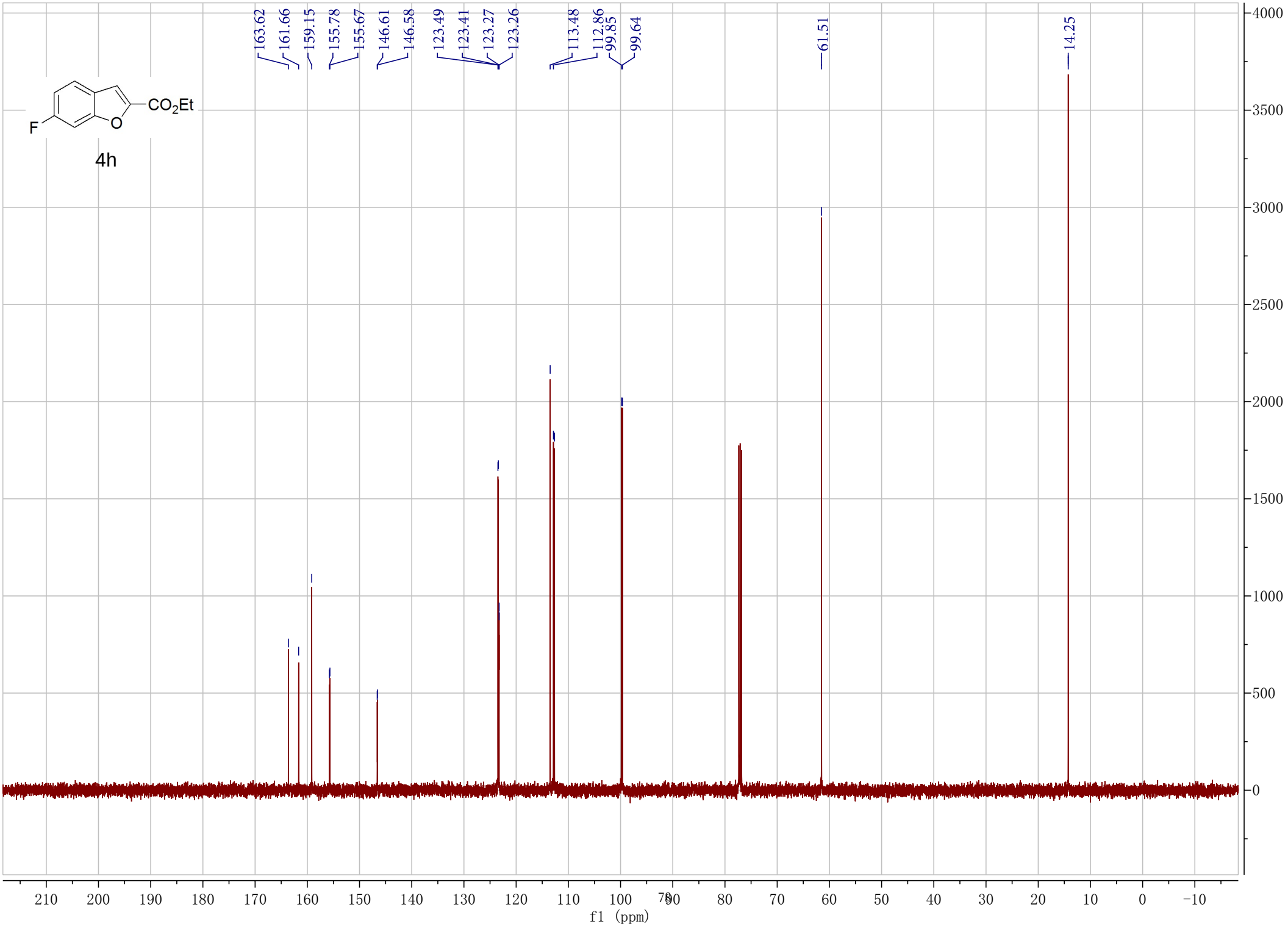

Et
CO2Et
O
4f
1.00
1.00
1.00
1.01
2.01
2.02
3.05
3.00
f1 (ppm)

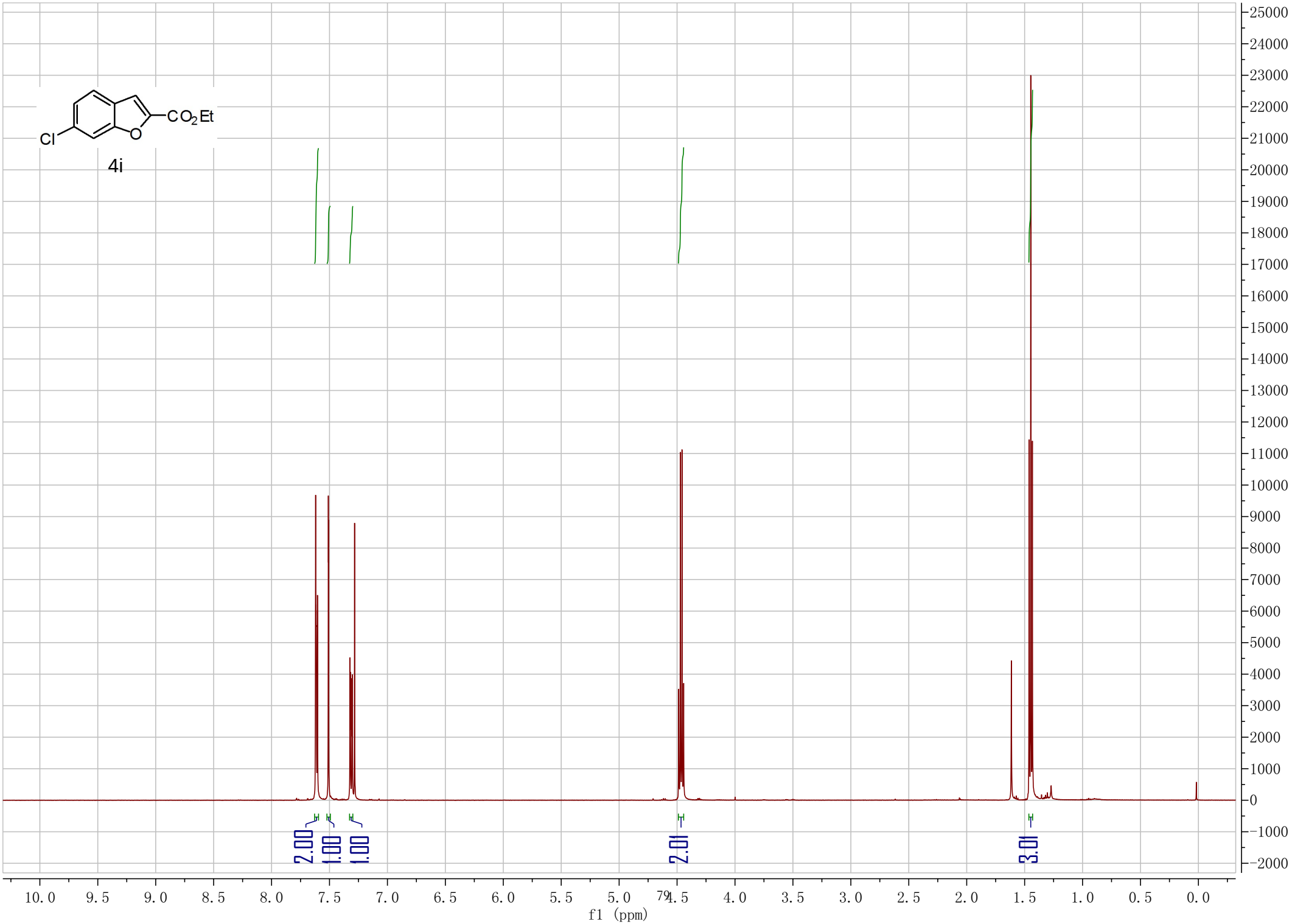

159.66
156.27
145.29
144.80
124.70
124.40
122.31
113.77
111.00
61.31
29.23
15.65
14.32
CO2Et
Et
O
4f
f1 (ppm)

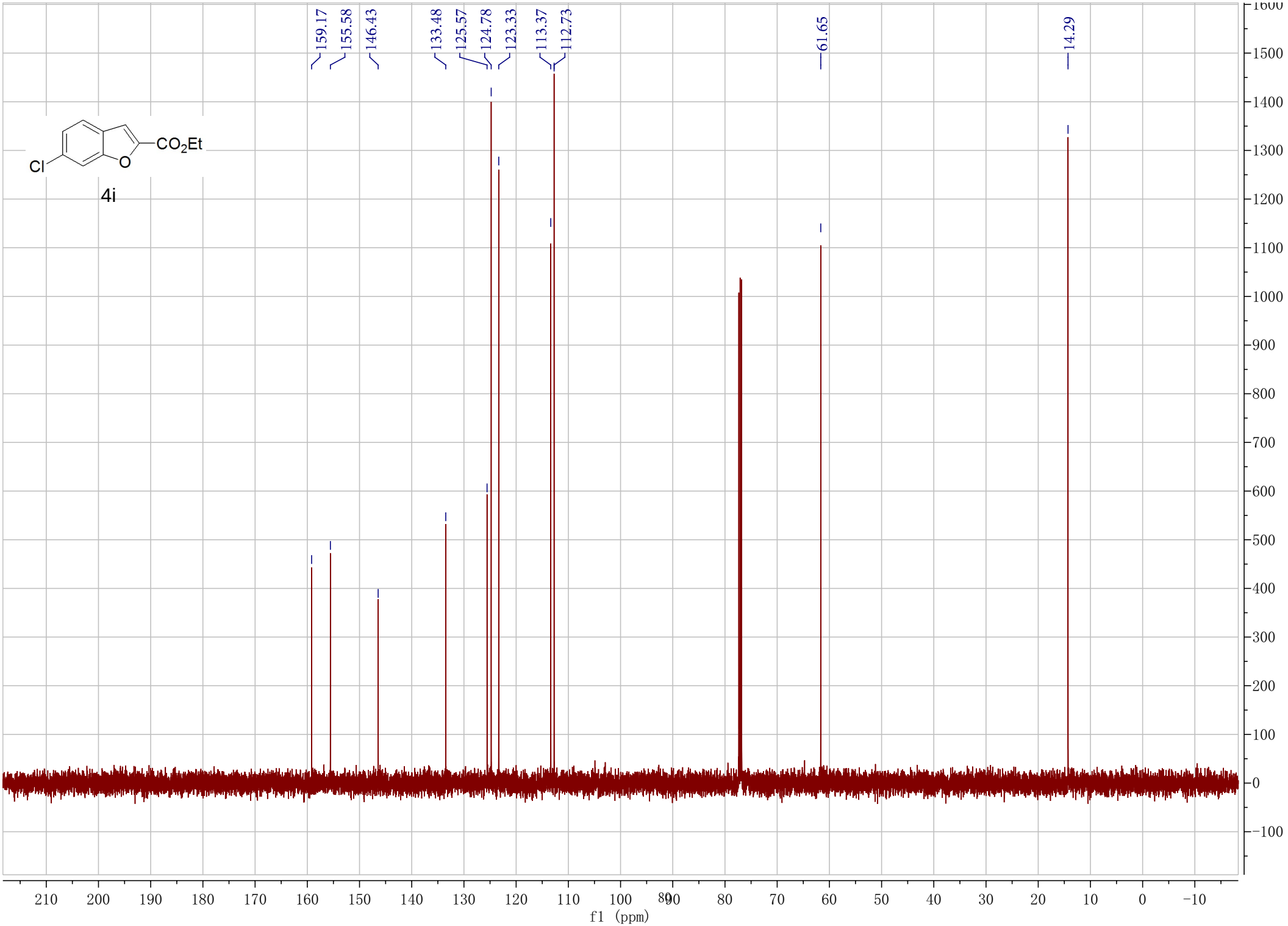

MeO
CO2Et
4g
1.00
1.00
1.00
1.00
2.01
3.00
3.02
f1 (ppm)

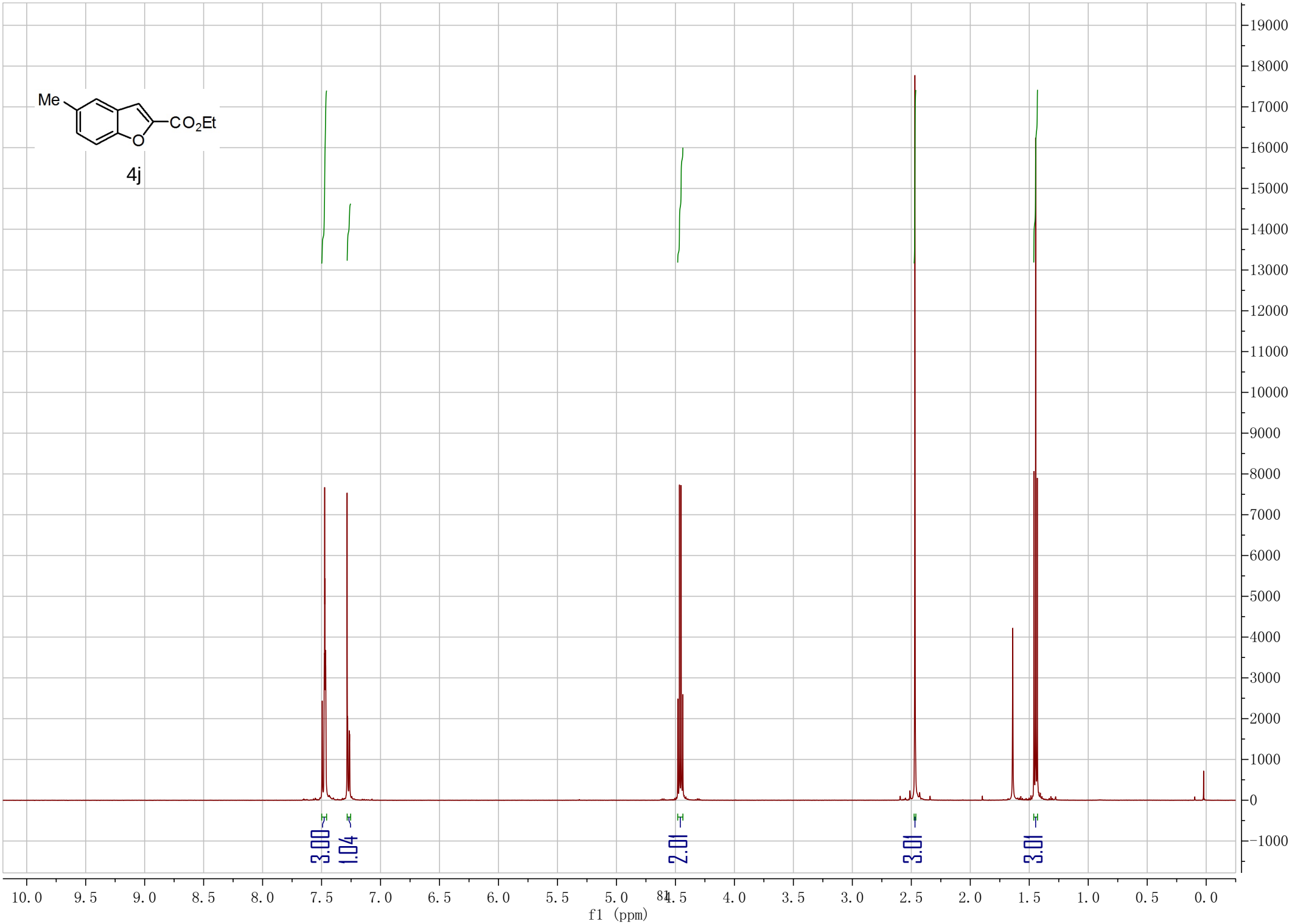

160.48
159.56
157.08
144.95
122.99
120.22
114.01
113.95
95.70
61.23
55.64
14.35
MeO
CO2Et
4g
f1 (ppm)

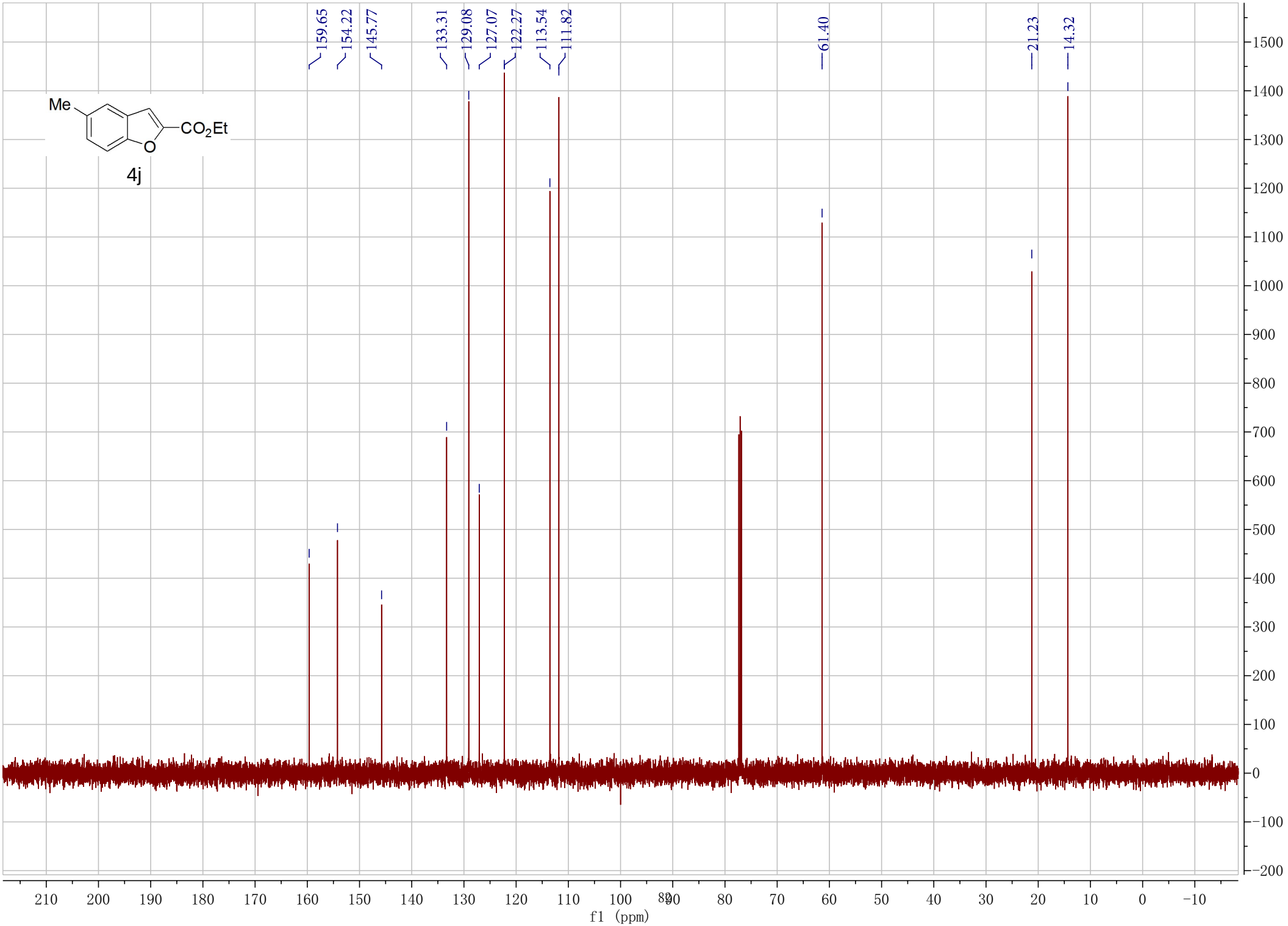

CO2Et
F
O
4h
1.00
1.00
1.00
1.02
2.02
3.00
40000
35000
30000
25000
20000
15000
10000
5000
0
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

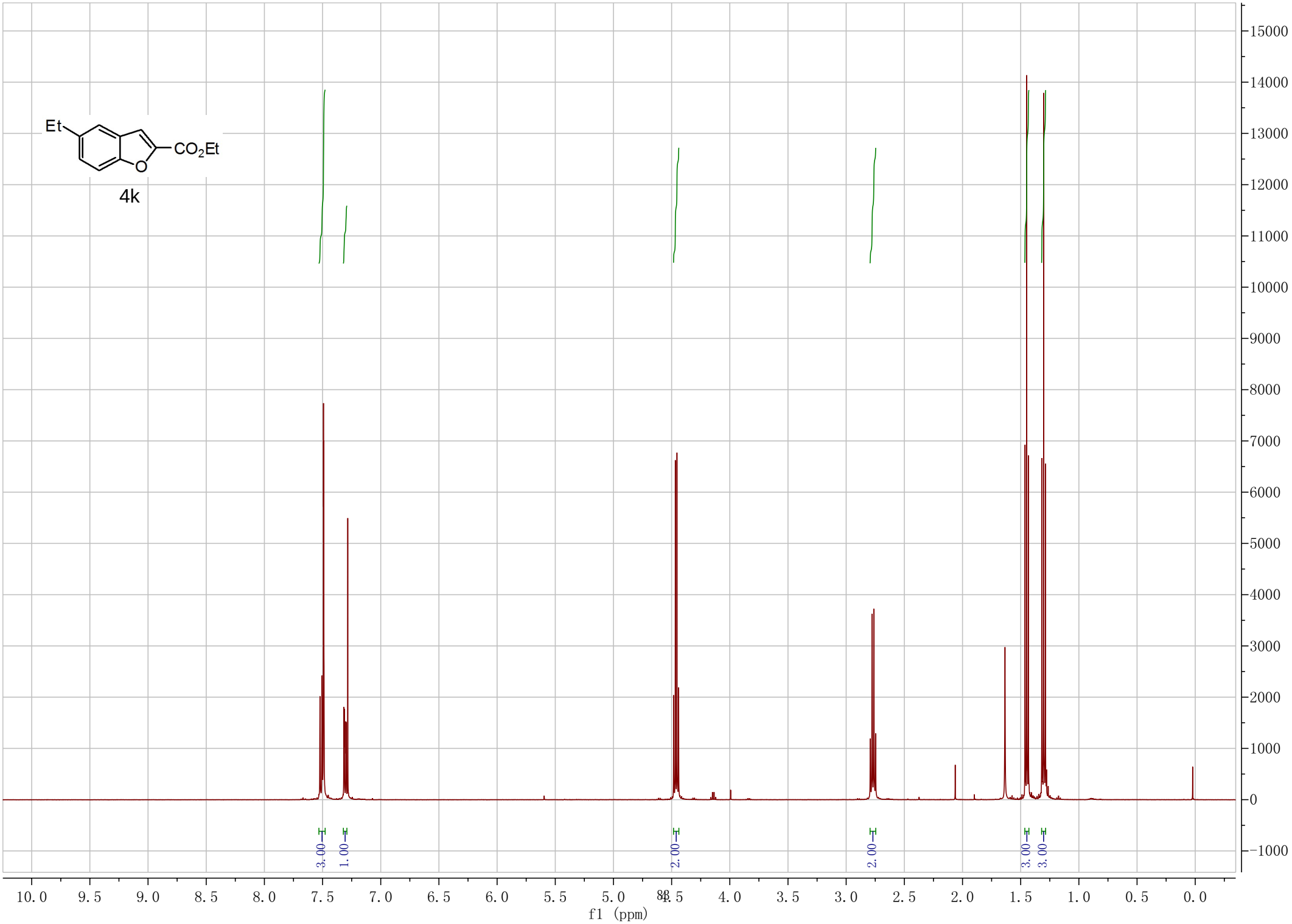

163.62
161.66
159.15
155.78
155.67
146.61
146.58
123.49
123.41
123.27
123.26
113.48
112.86
99.85
99.64
61.51
14.25
CO2Et
F
O
4h
f1 (ppm)

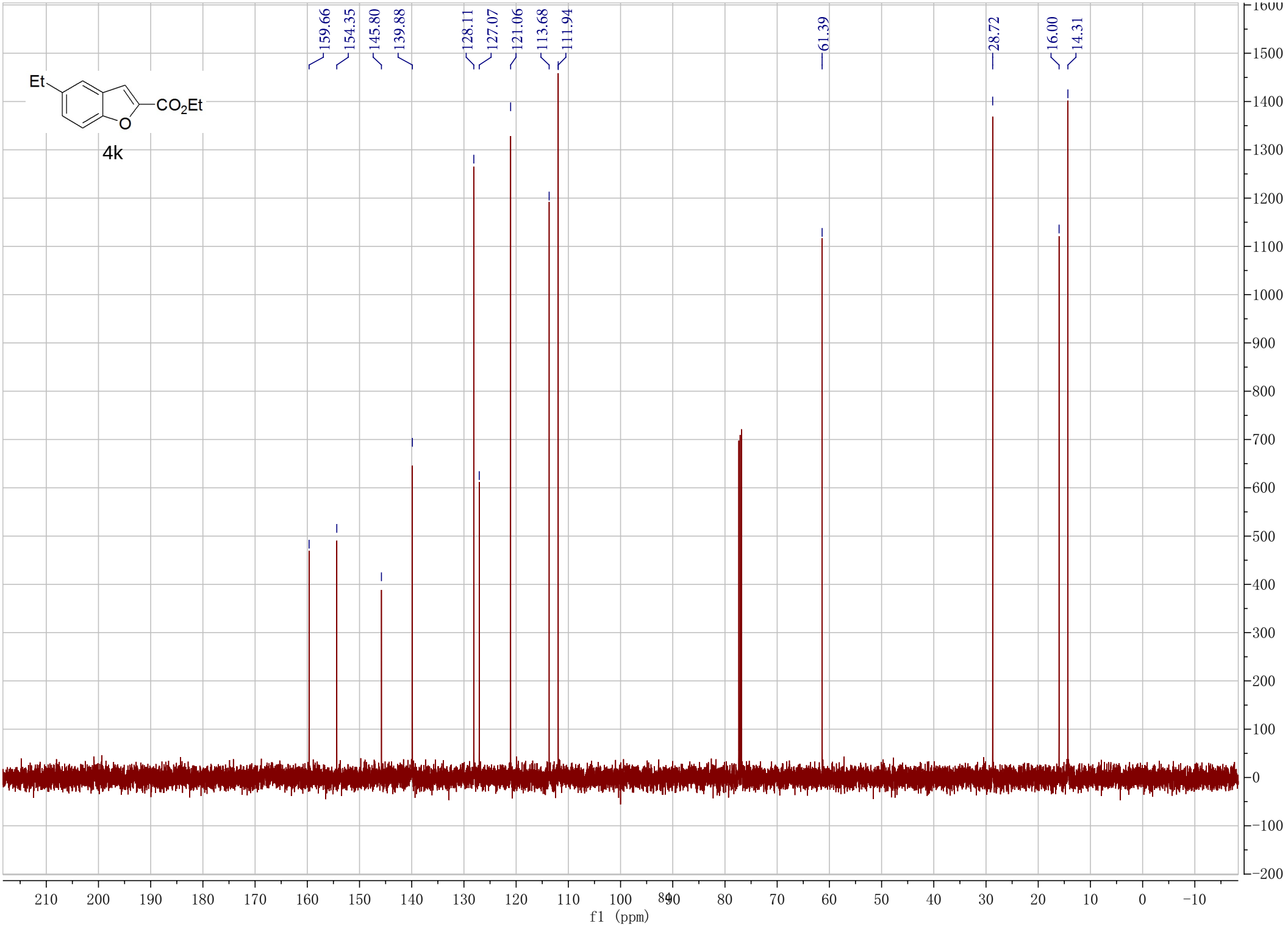

CO2Et
Cl
O
4i
2.00
1.00
1.00
2.01
3.01
f1 (ppm)

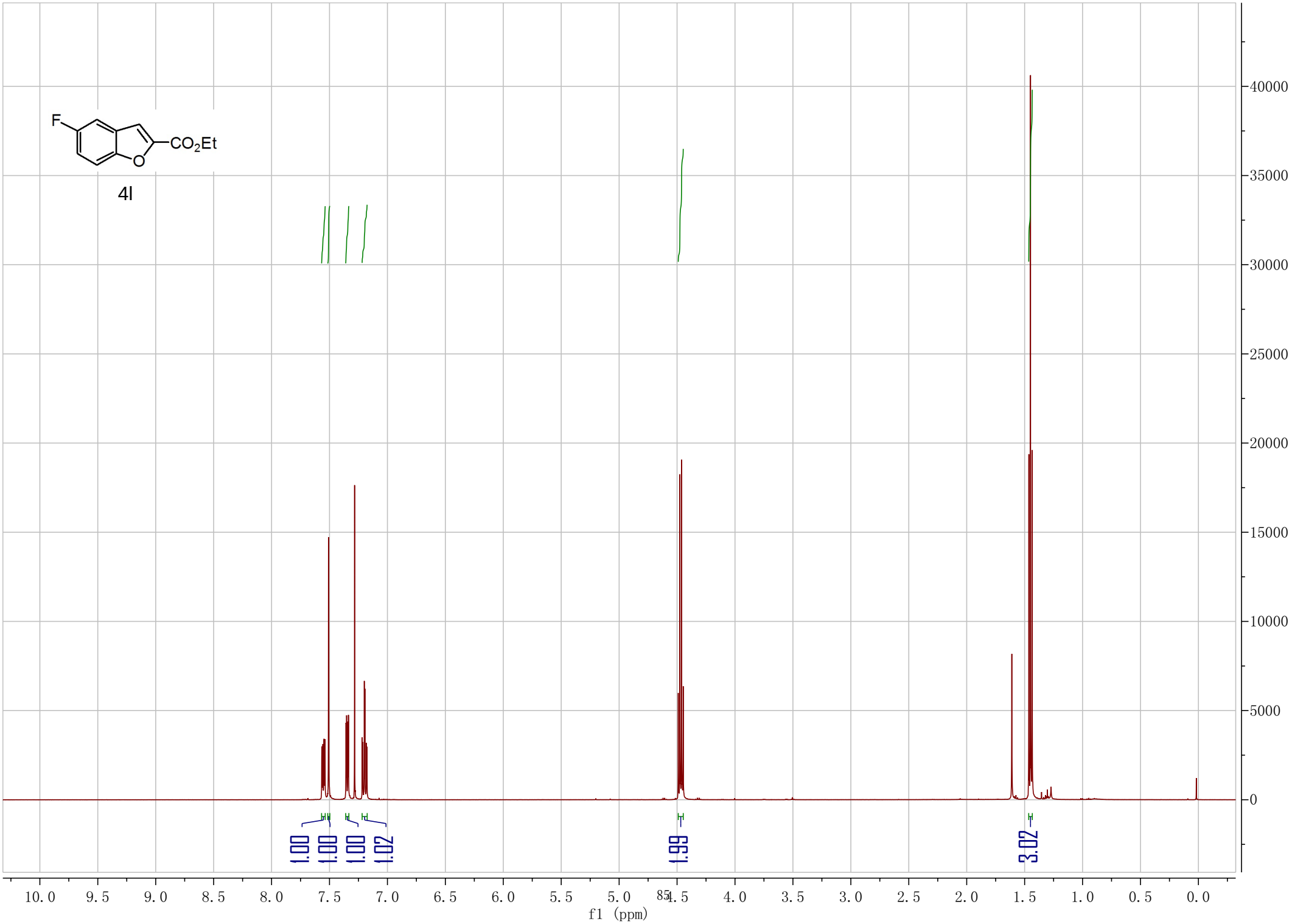

159.17
155.58
146.43
133.48
125.57
124.78
123.33
113.37
112.73
61.65
14.29
CO2Et
Cl
O
4i
f1 (ppm)

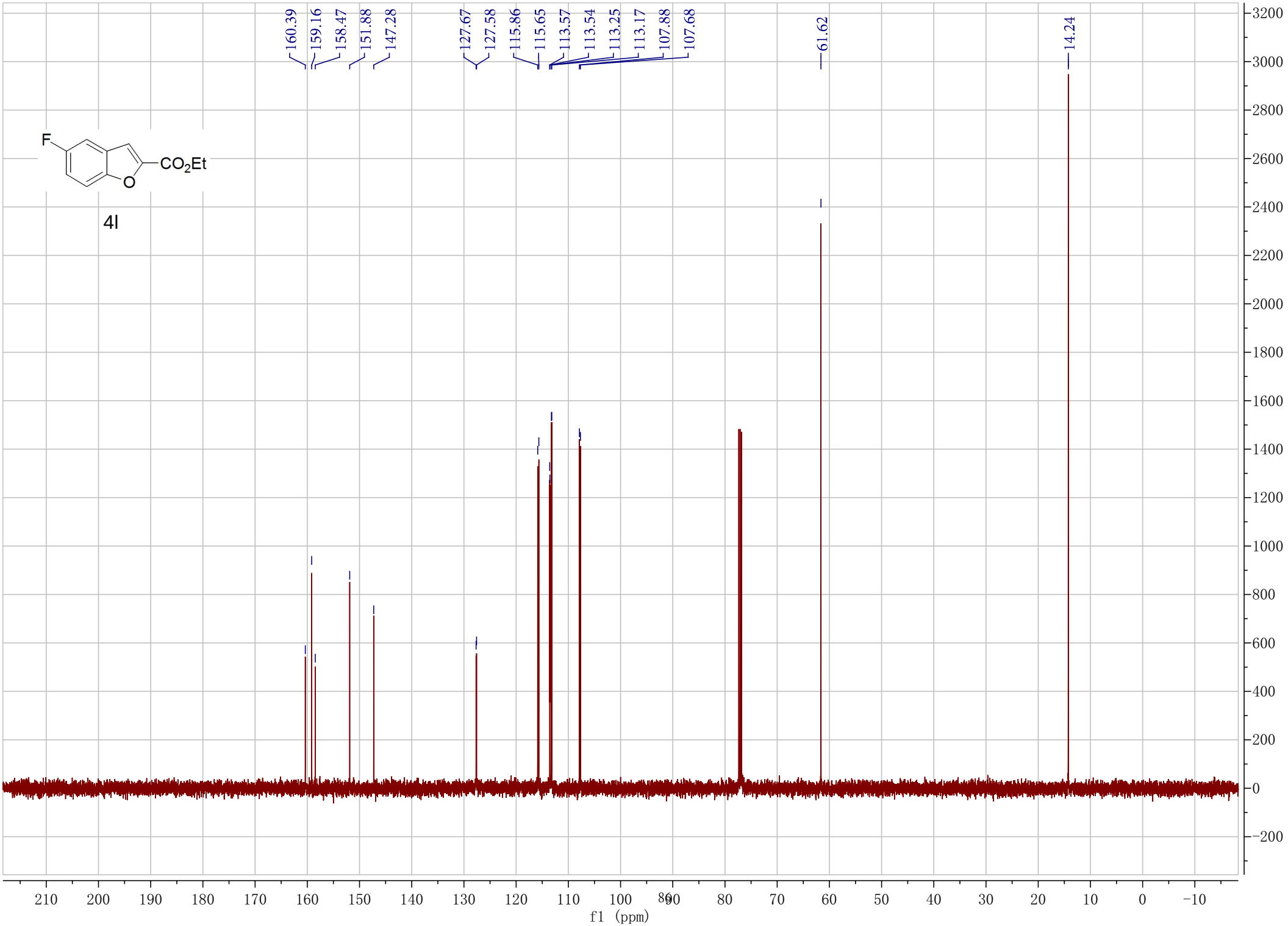

Me
CO2Et
O
4j
3.00
1.04
2.01
3.01
3.01
f1 (ppm)

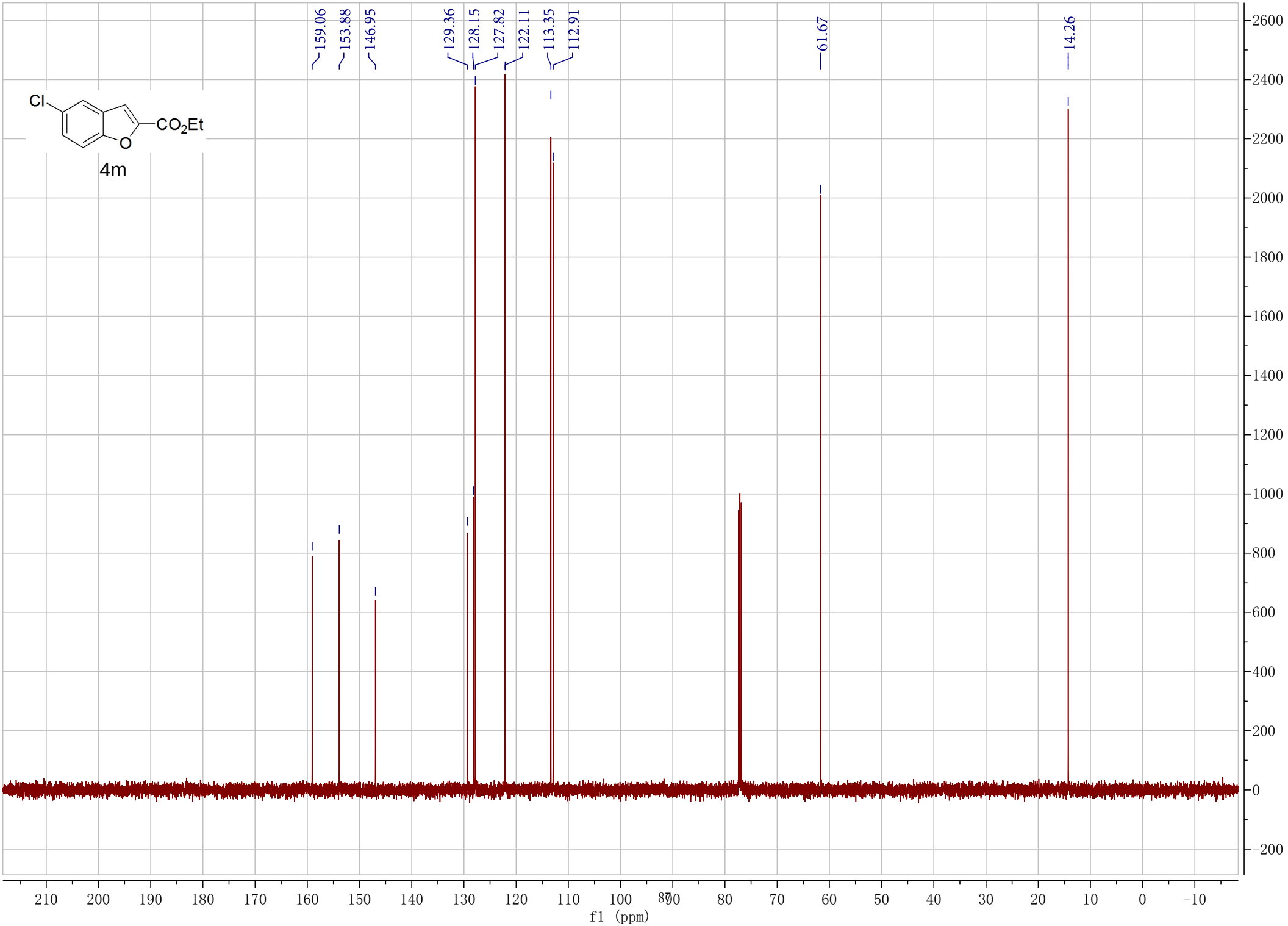

159.65
154.22
145.77
133.31
129.08
127.07
122.27
113.54
111.82
61.40
21.23
14.32
Me
CO2Et
O
4j
f1 (ppm)

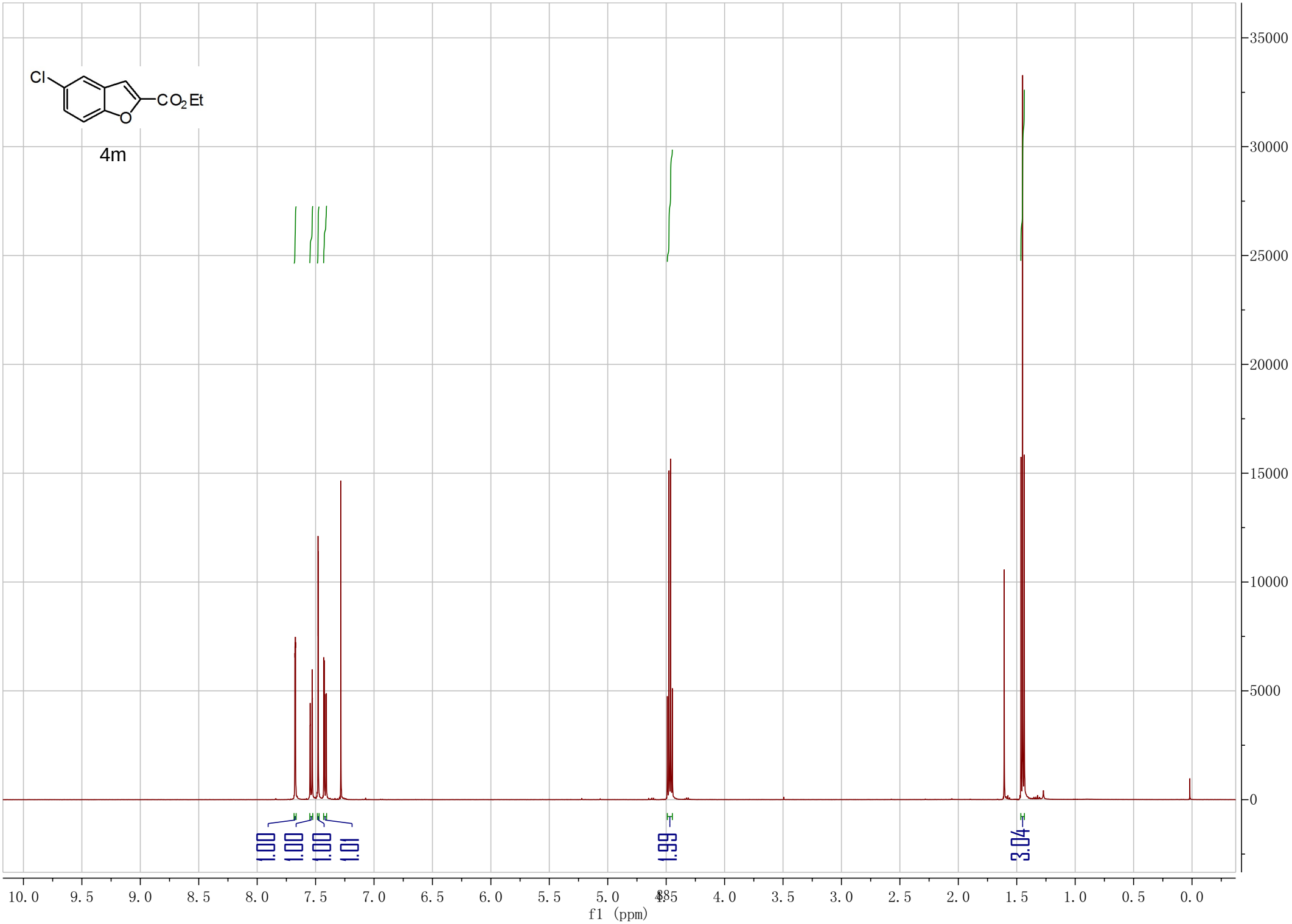

Et
CO2Et
O
4k
3.00
1.00
2.00
2.00
3.00
3.00
f1 (ppm)

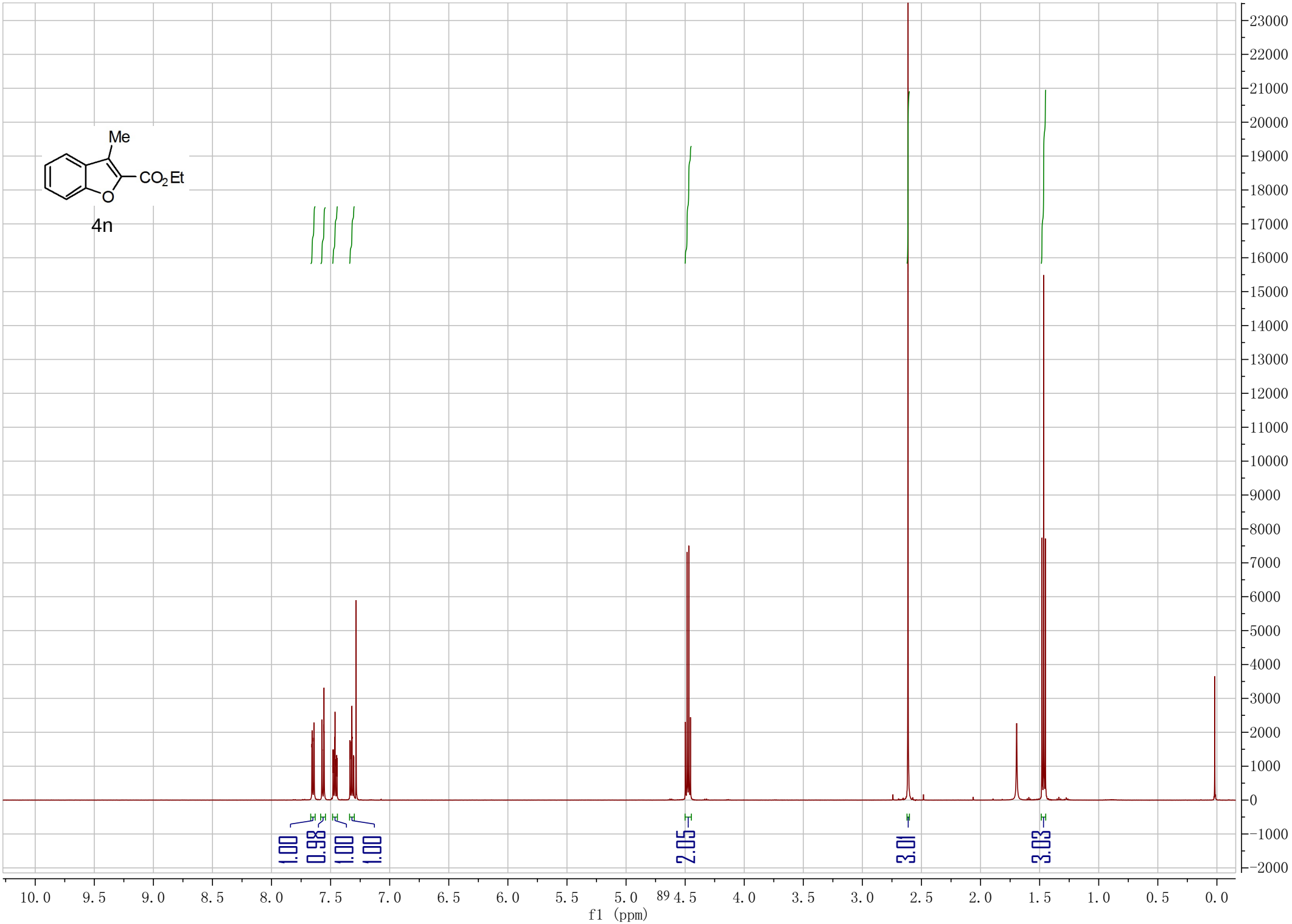

Et
CO2Et
O
4k
159.66
154.35
145.80
139.88
128.11
127.07
121.06
113.68
111.94
61.39
28.72
16.00
14.31
f1 (ppm)

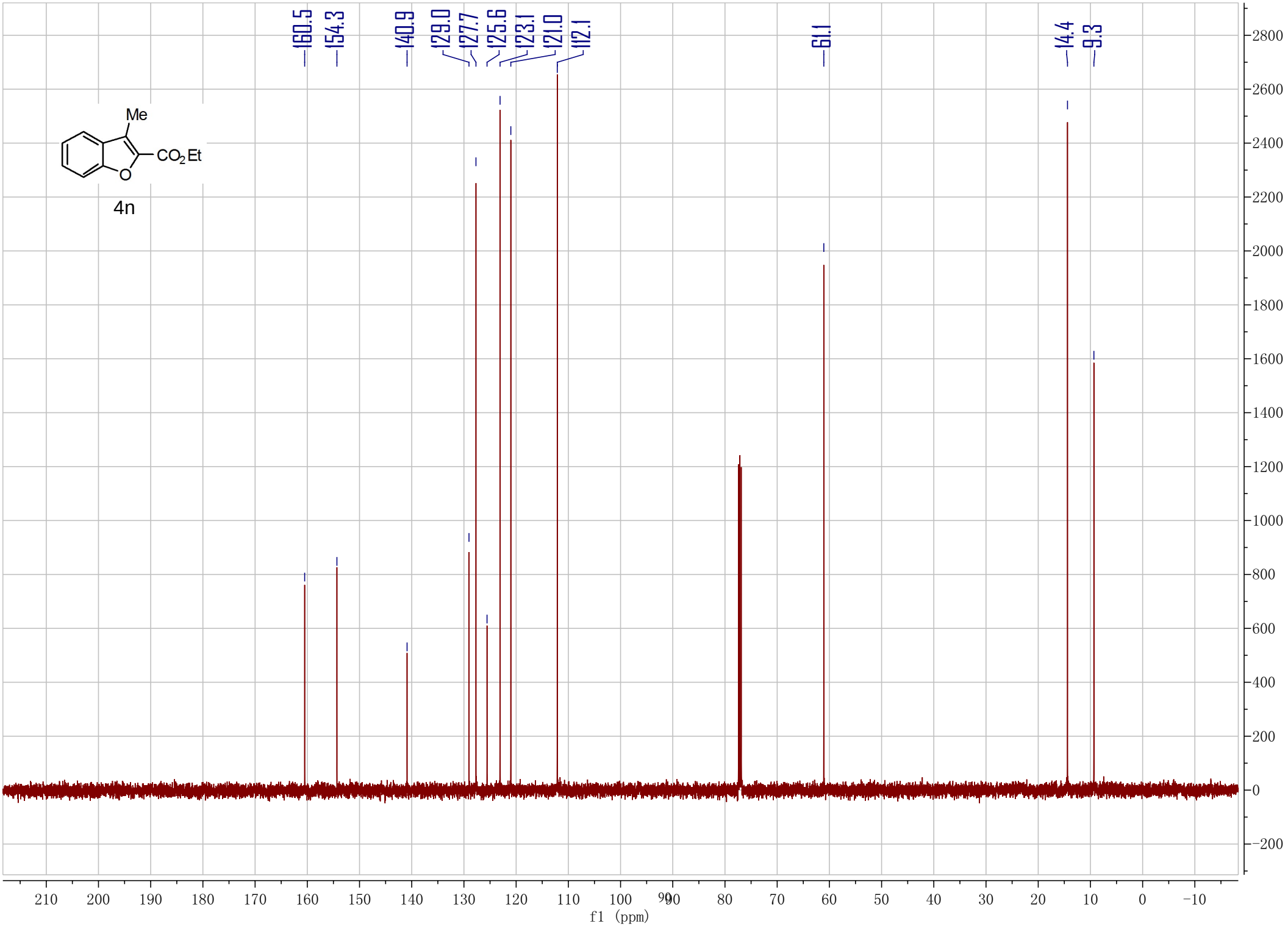

F
CO2Et
O
4l
1.00
1.00
1.00
1.02
1.99
3.02
40000
35000
30000
25000
20000
15000
10000
5000
0
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

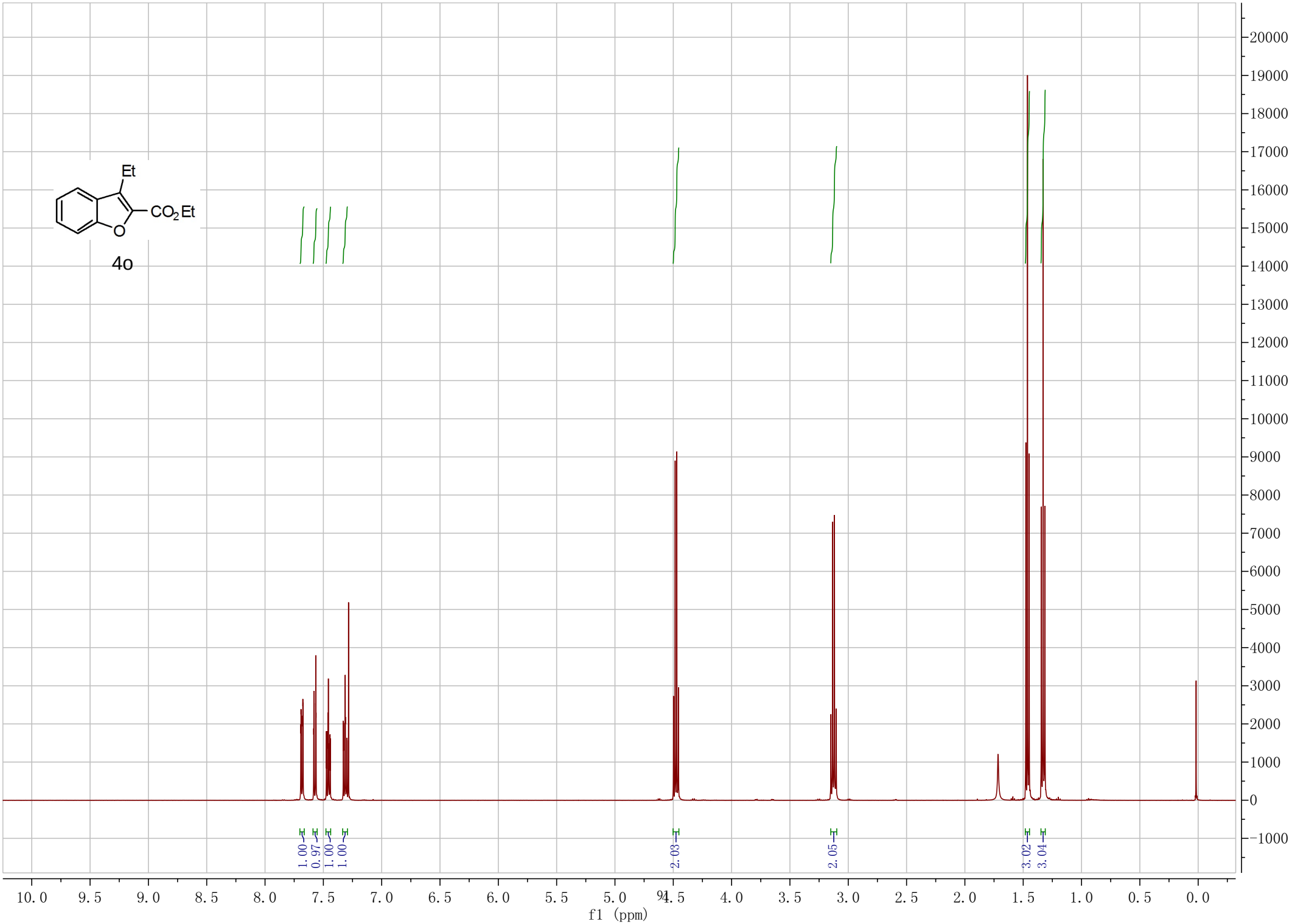

160.39
159.16
158.47
151.88
147.28
127.67
127.58
115.86
115.65
113.57
113.54
113.25
113.17
107.88
107.68
61.62
14.24
F
CO2Et
O
4l
f1 (ppm)

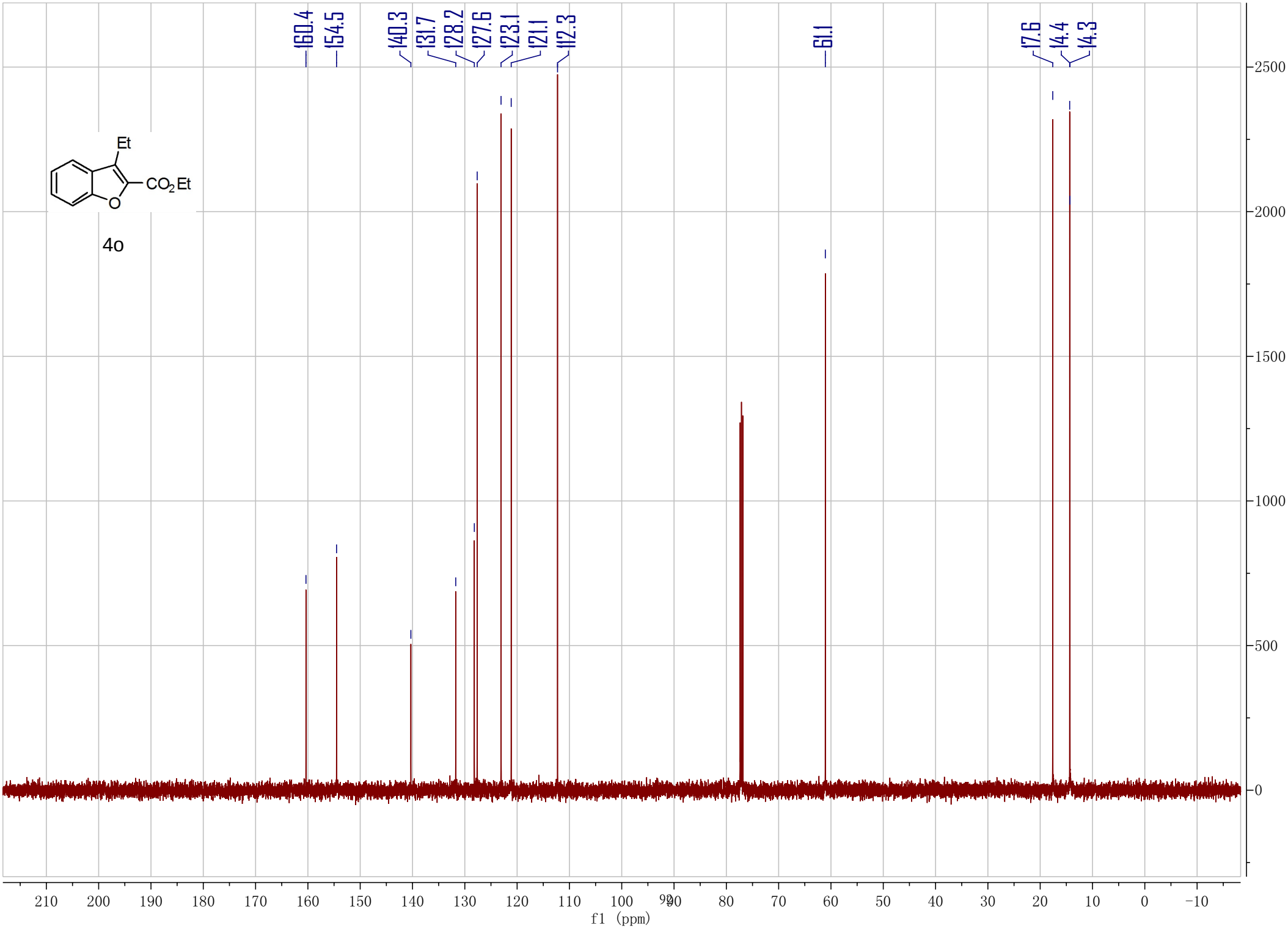

159.06
153.88
146.95
129.36
128.15
127.82
122.11
113.35
112.91
61.67
14.26
Cl
CO2Et
O
4m
f1 (ppm)

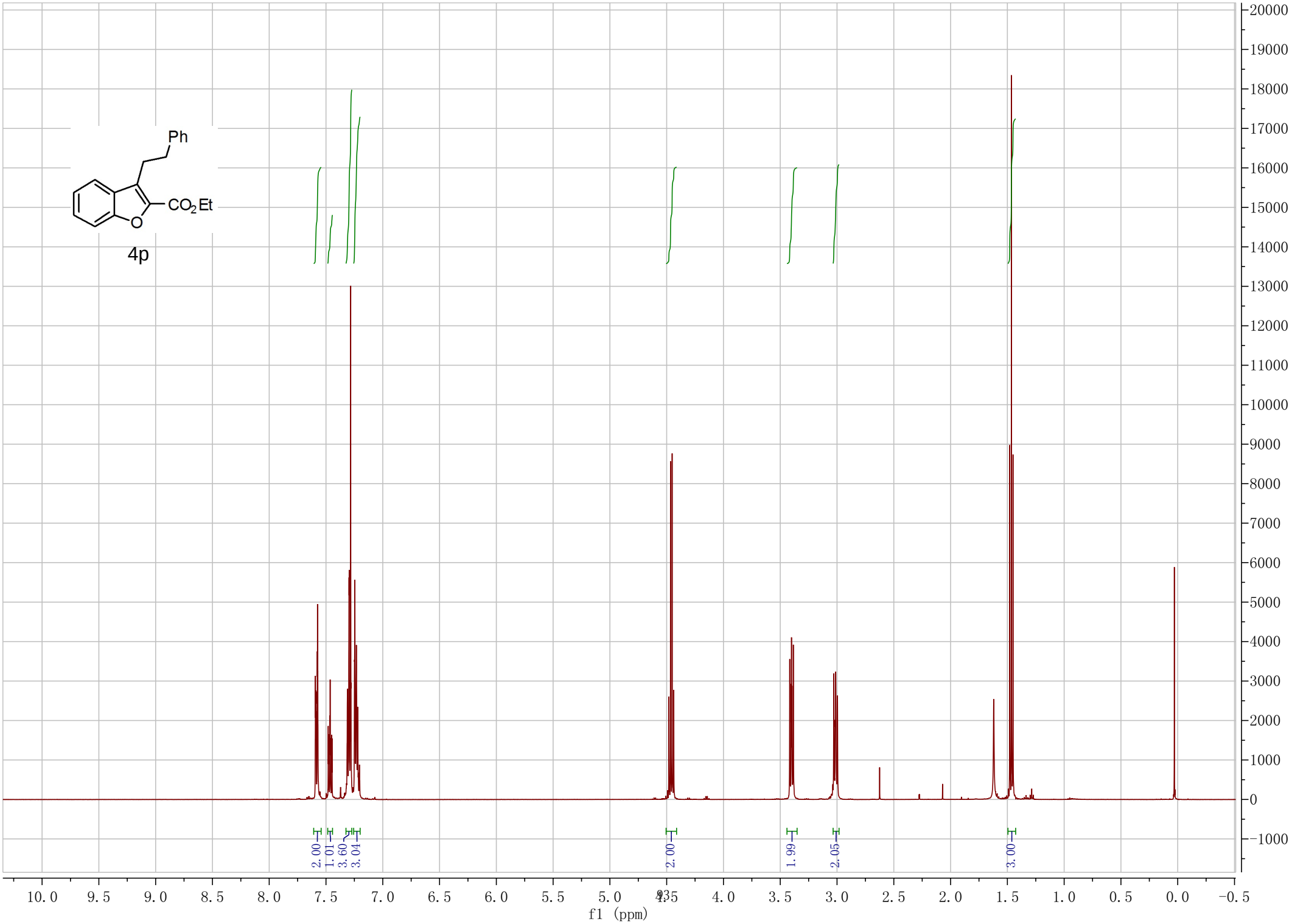

Cl
CO2Et
O
4m
1.00
1.00
1.00
1.01
1.99
3.04
35000
30000
25000
20000
15000
10000
5000
0
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

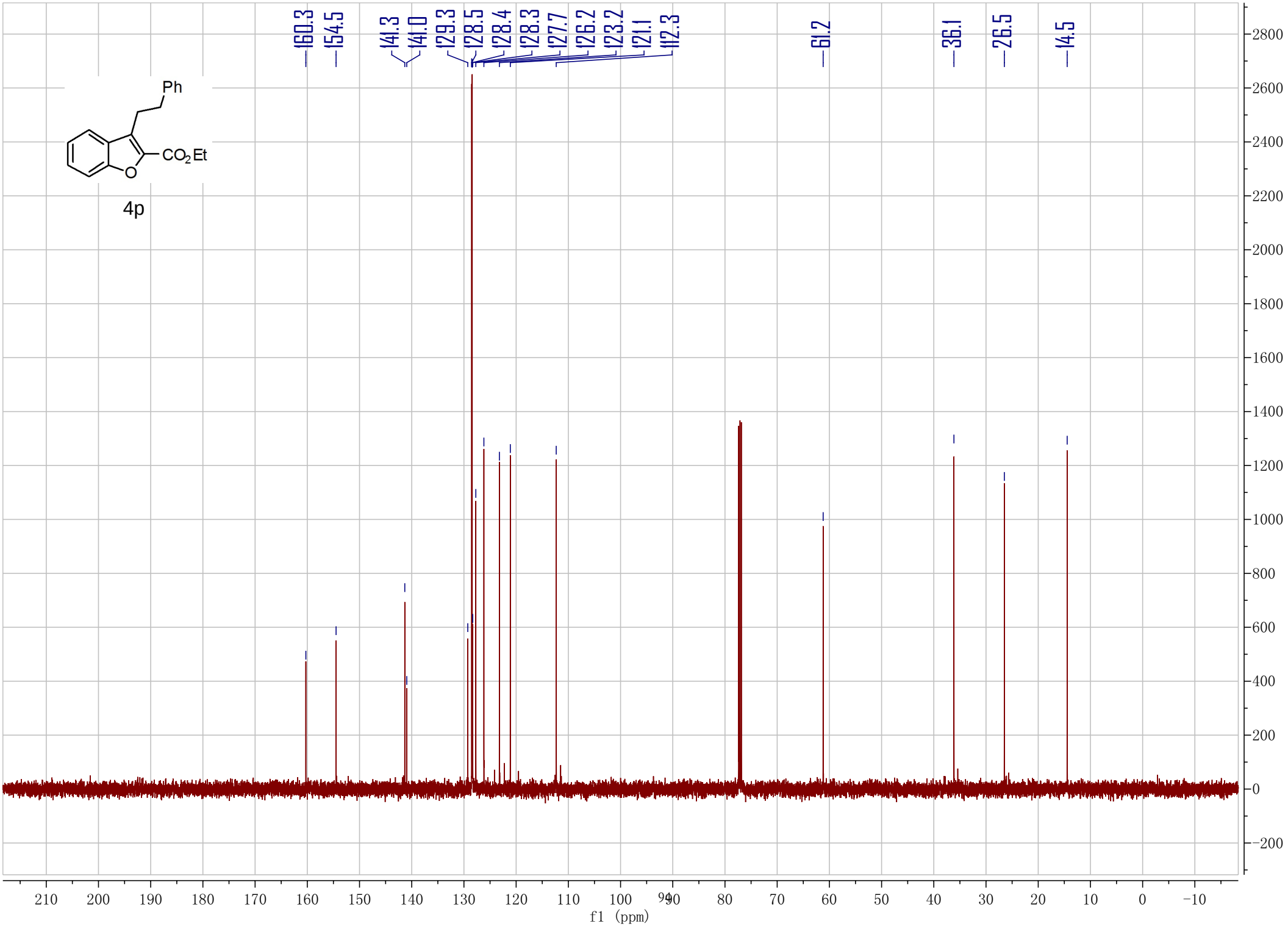

Me
CO2Et
O
4n
1.00
0.98
1.00
1.00
2.05
3.01
3.03
f1 (ppm)

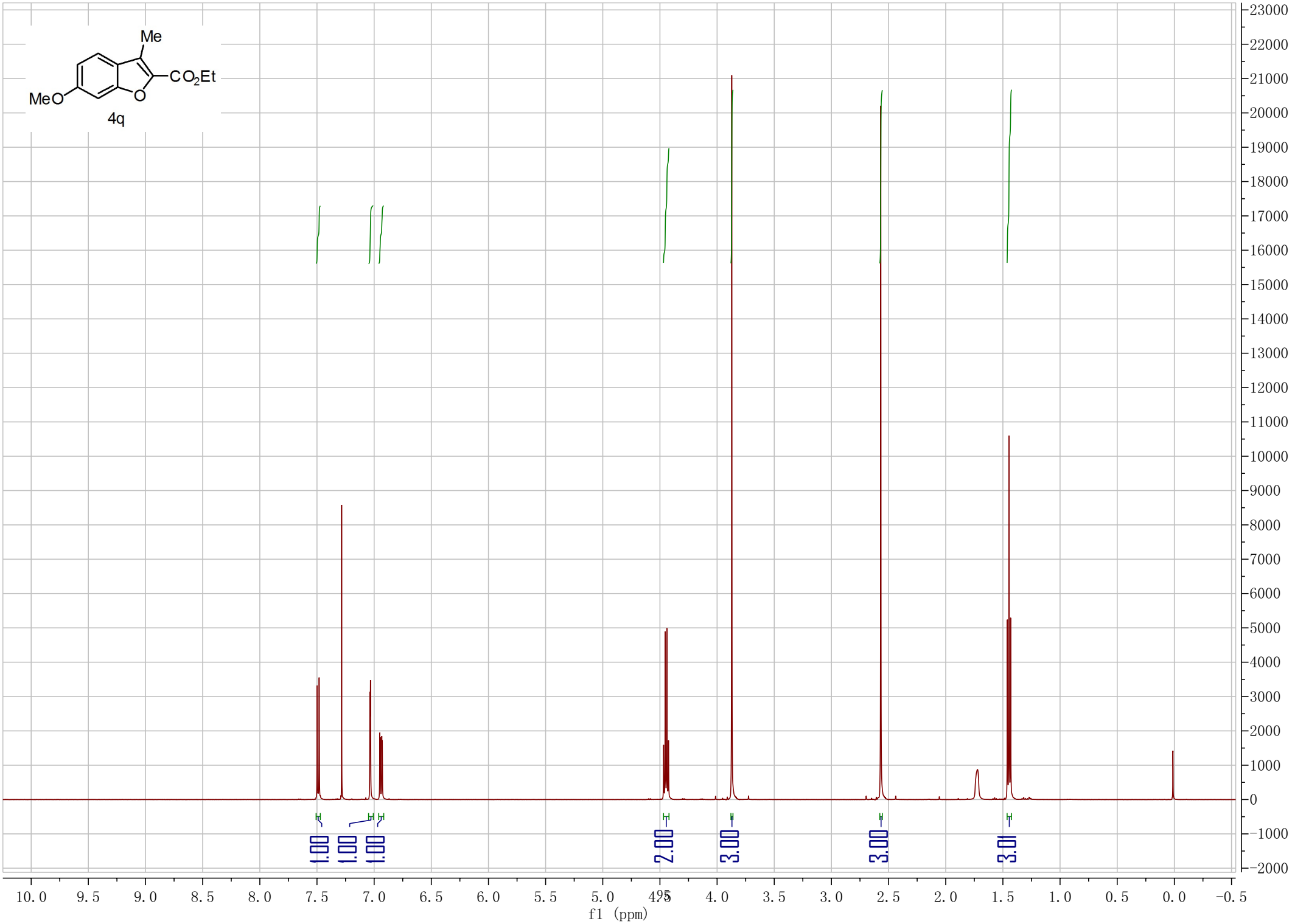

160.5
154.3
140.9
129.0
127.7
125.6
123.1
121.0
112.1
61.1
14.4
9.3
Me
CO2Et
O
4n
f1 (ppm)

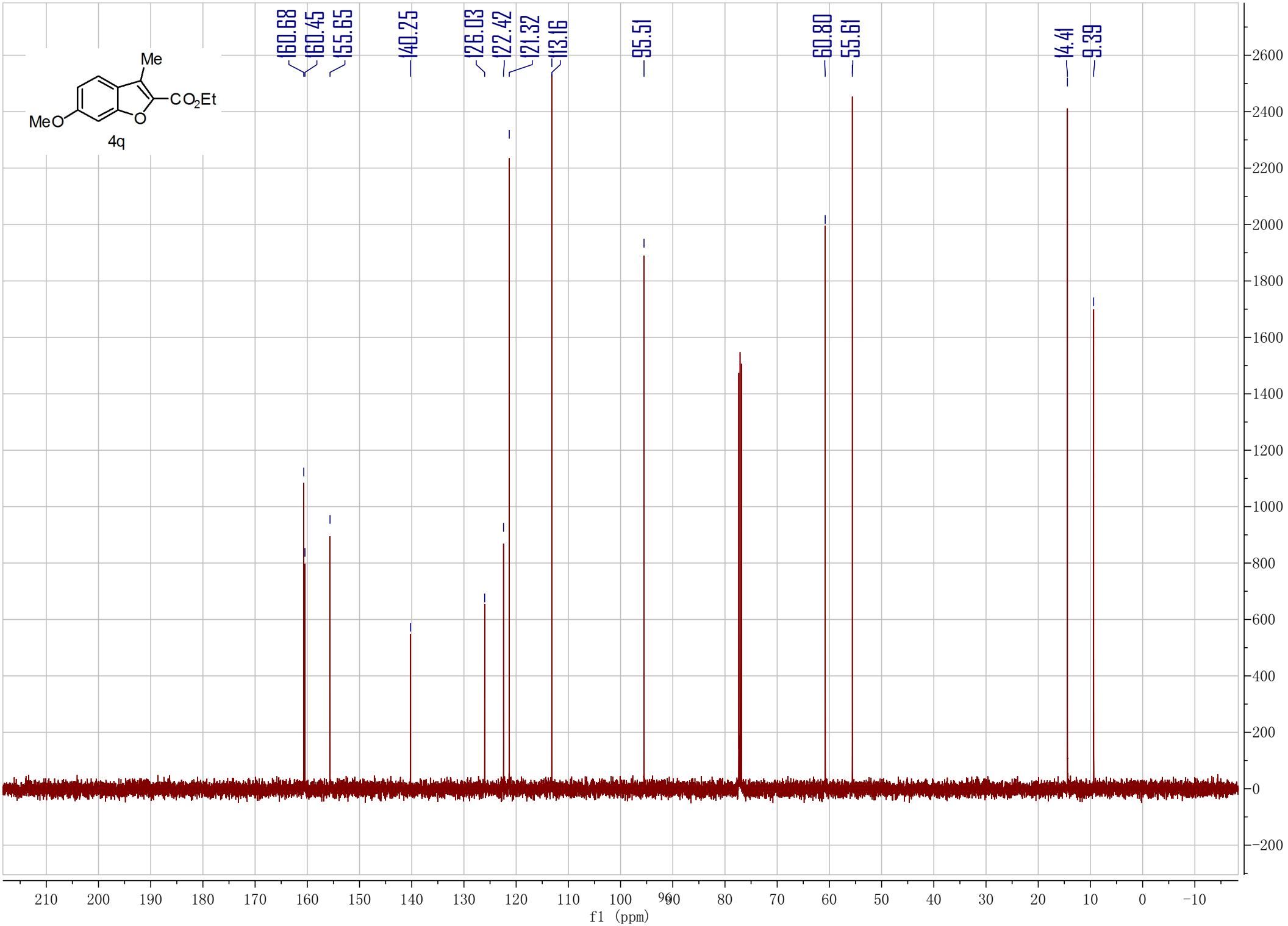

Et
CO2Et
O
4o
1.00
0.97
1.00
1.00
2.03
2.05
3.02
3.04
f1 (ppm)

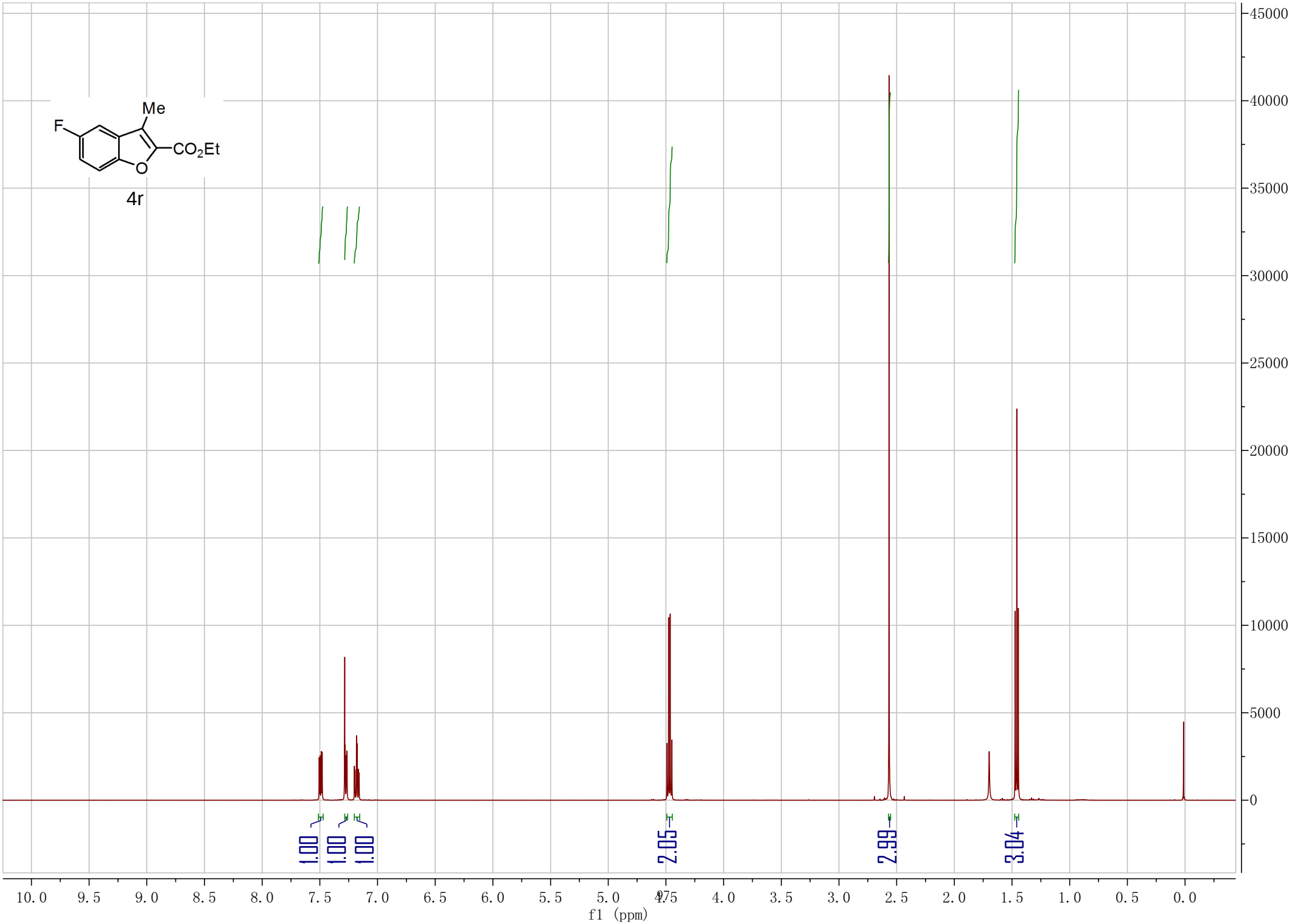

160.4
154.5
140.3
131.7
128.2
127.6
123.1
121.1
112.3
61.1
17.6
14.4
14.3
Et
CO2Et
O
4o
2500
2000
1500
1000
500
0
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

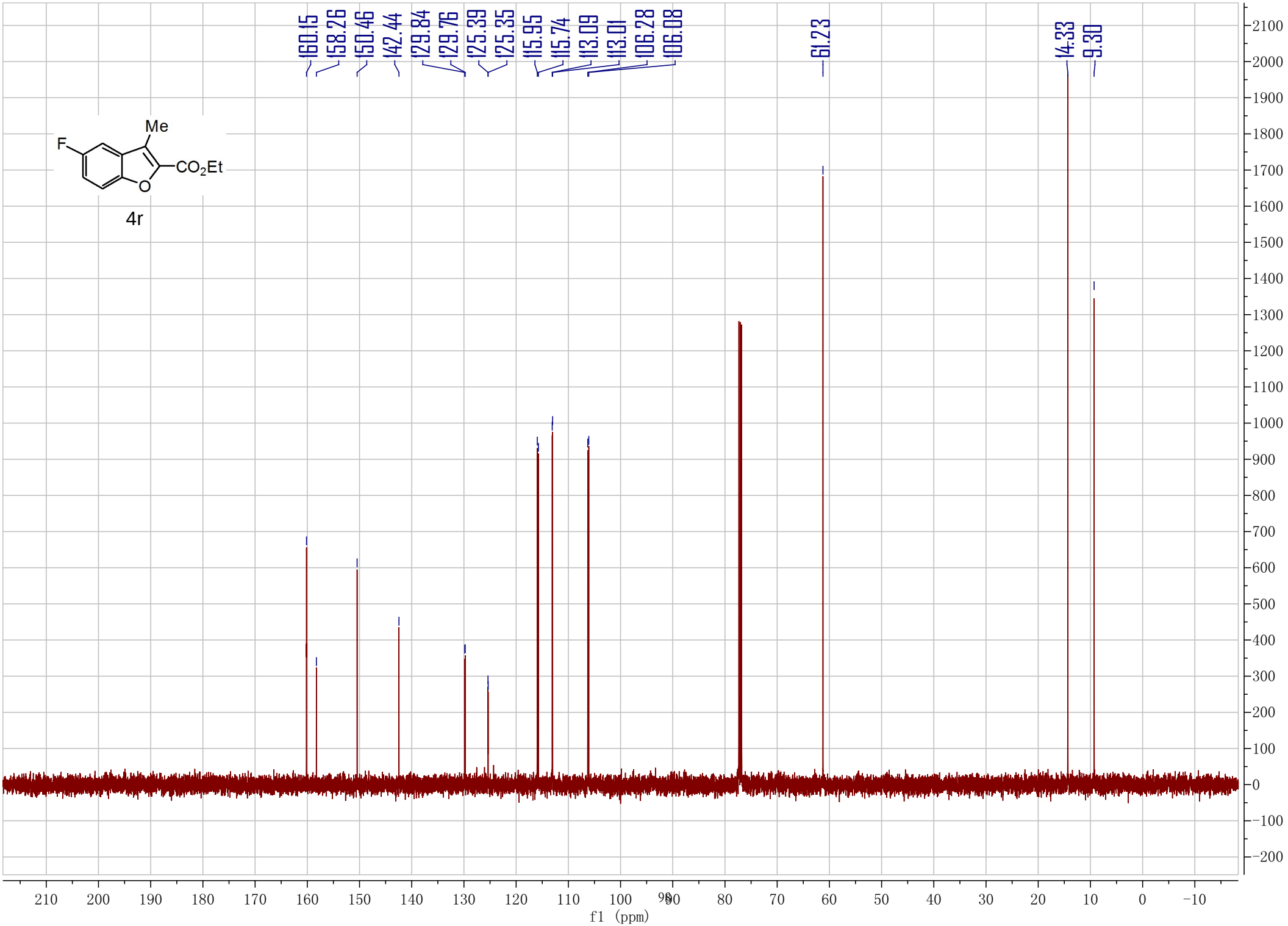

Ph
CO2Et
O
4p
2.00
1.01
3.60
3.04
2.00
1.99
2.05
3.00
f1 (ppm)

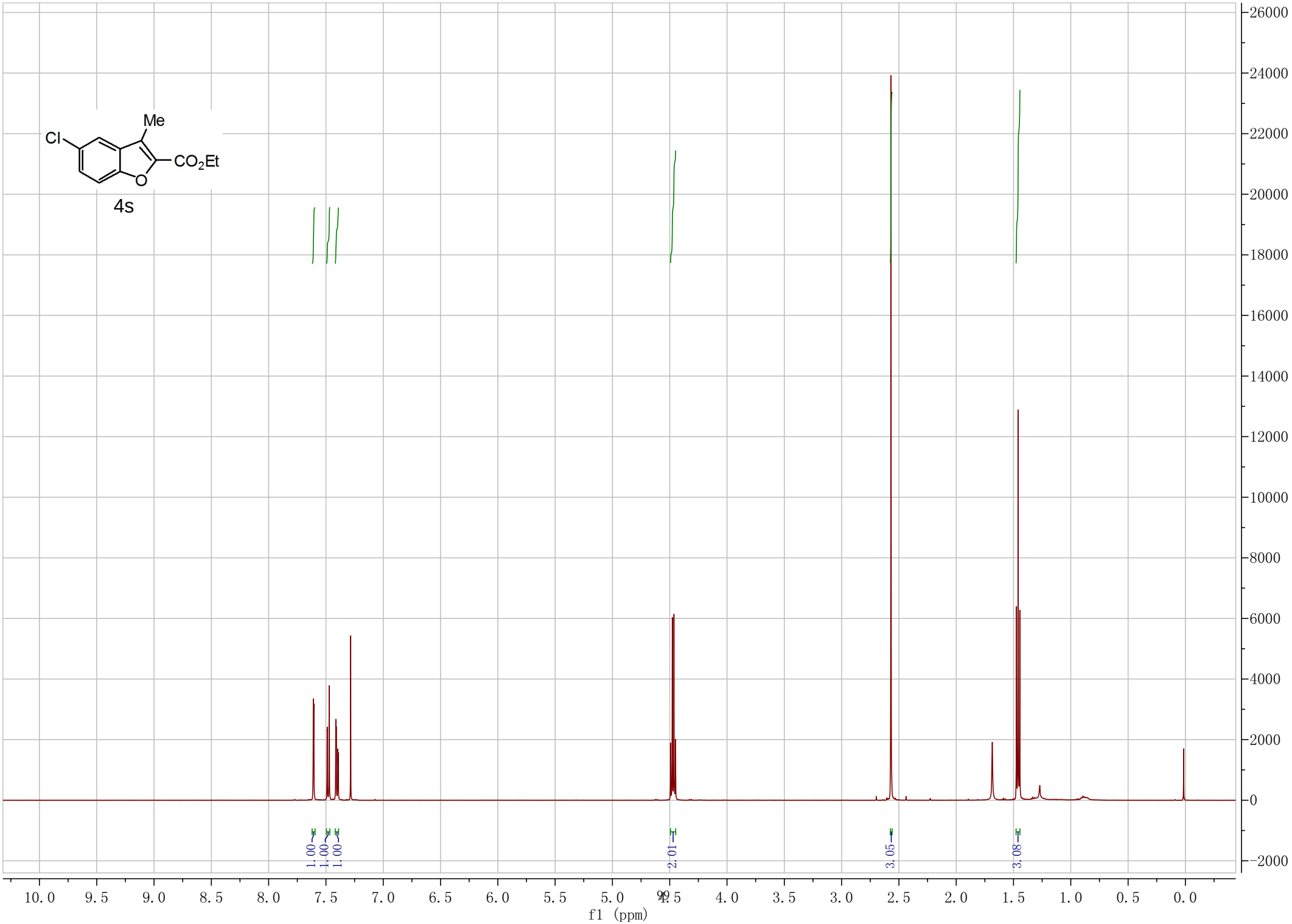

160.3
154.5
141.3
141.0
129.3
128.5
128.4
128.3
127.7
126.2
123.2
121.1
112.3
61.2
36.1
26.5
14.5
Ph
CO2Et
O
4p
f1 (ppm)

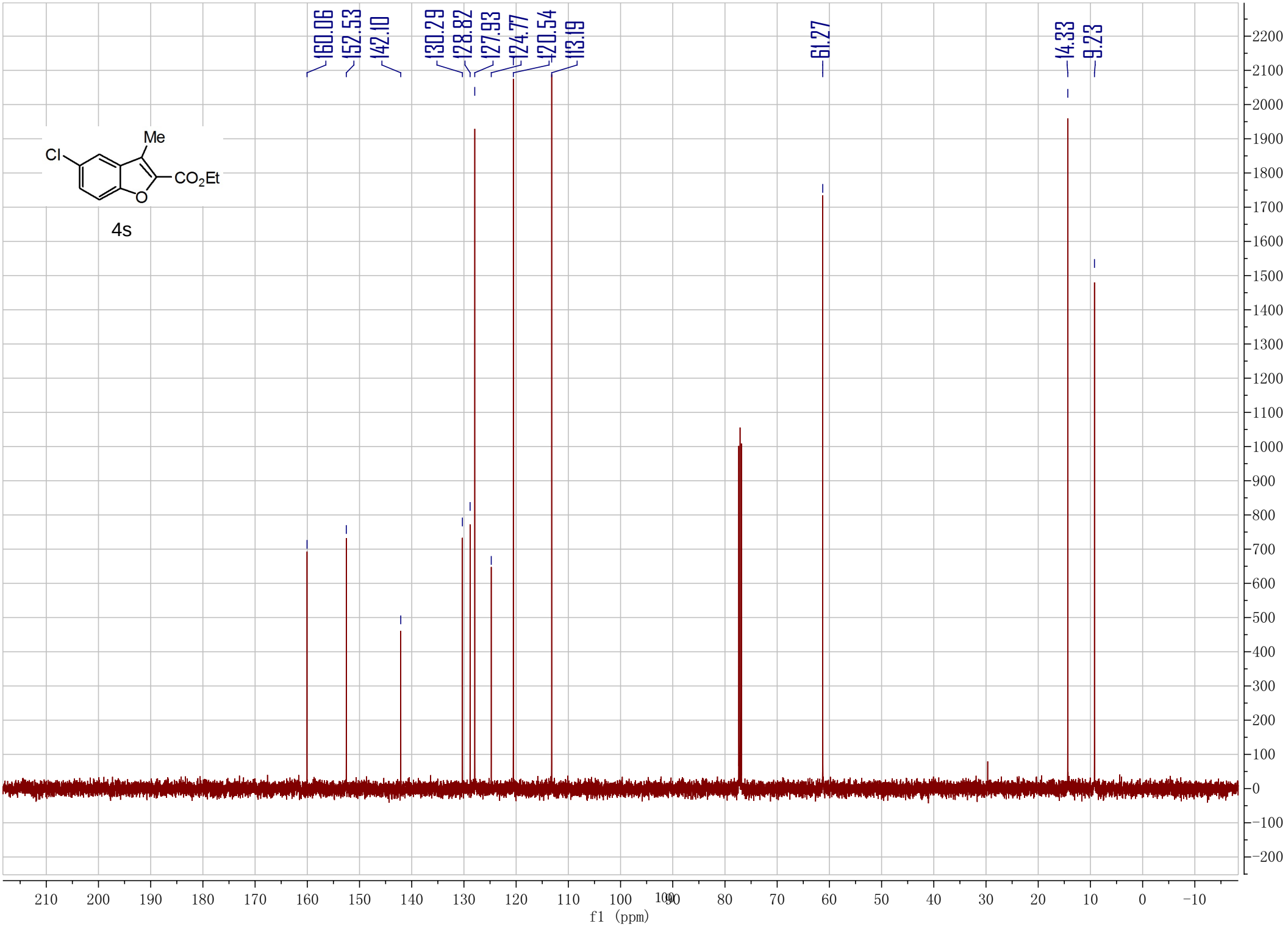

Me
CO2Et
MeO
O
4q
1.00
1.00
1.00
2.00
3.00
3.00
3.01
f1 (ppm)


Me
CO2Et
MeO
O
4q
160.68
160.45
155.65
140.25
126.03
122.42
121.32
113.16
95.51
60.80
55.61
14.41
9.39
f1 (ppm)

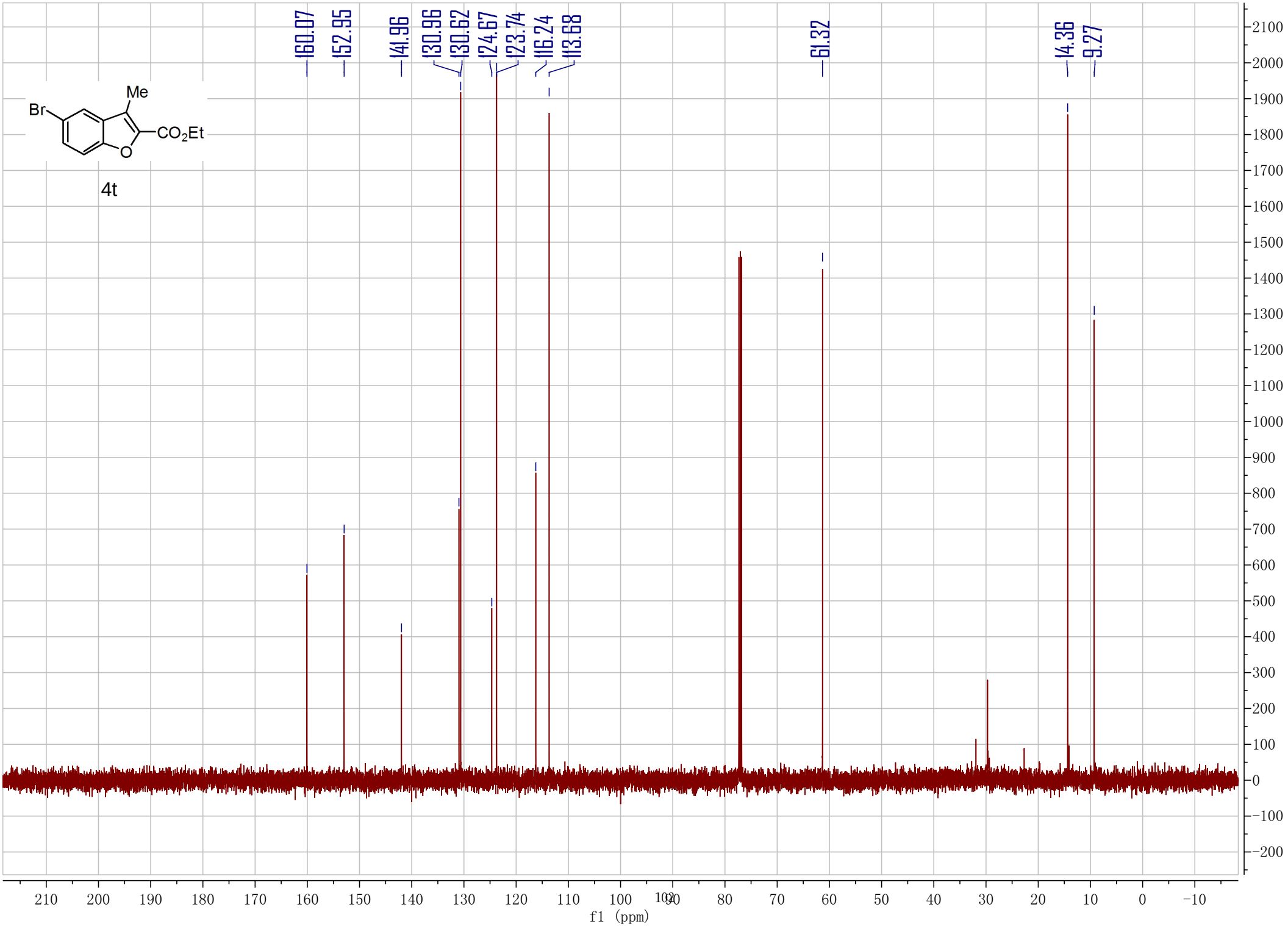

Me
F
CO2Et
O
4r
1.00
1.00
1.00
2.05
2.99
3.04
f1 (ppm)

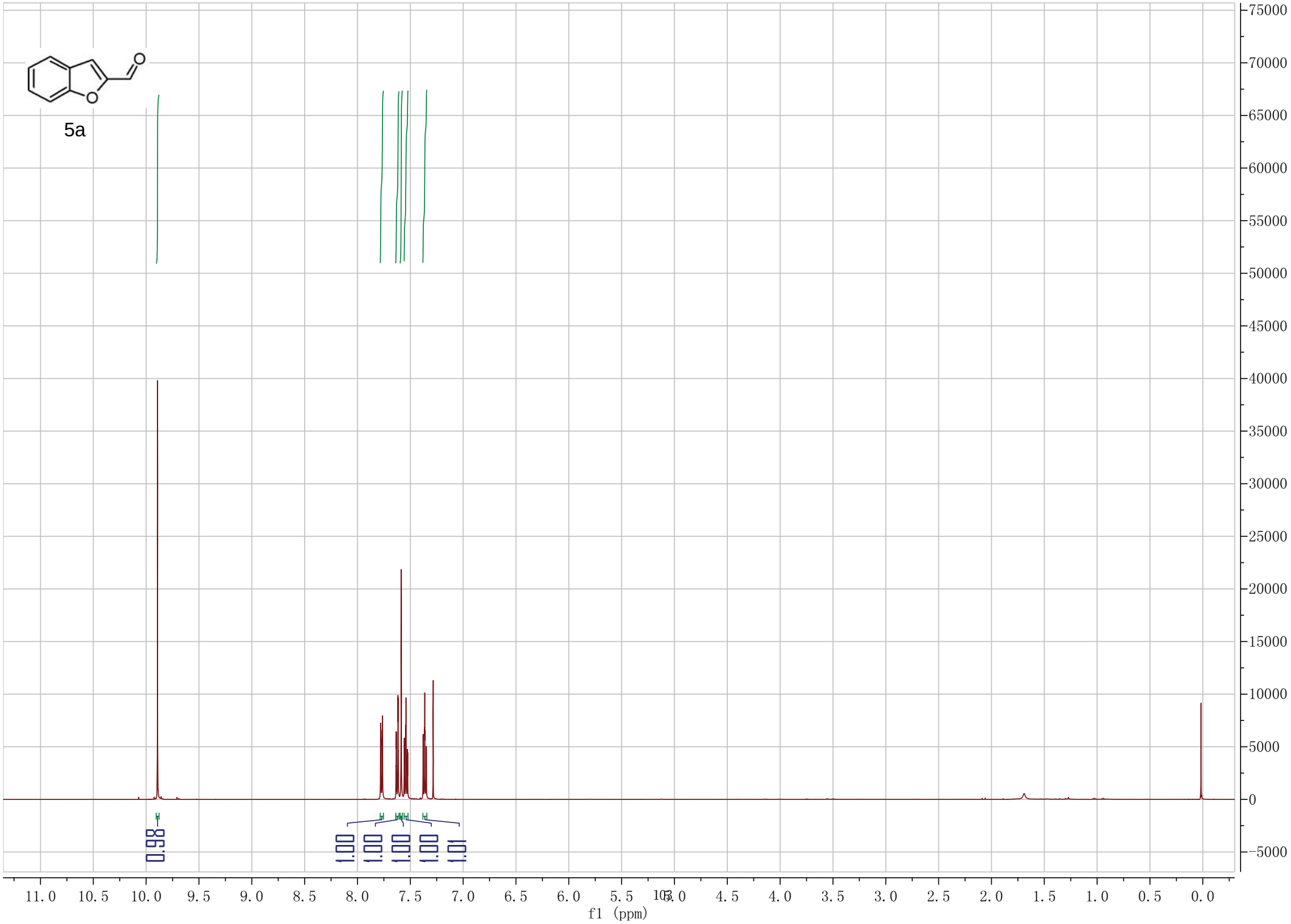

160.15
158.26
150.46
142.44
129.84
129.76
125.39
125.35
115.95
115.74
113.09
113.01
106.28
106.08
61.23
14.33
9.30
Me
F
CO2Et
O
4r
f1 (ppm)

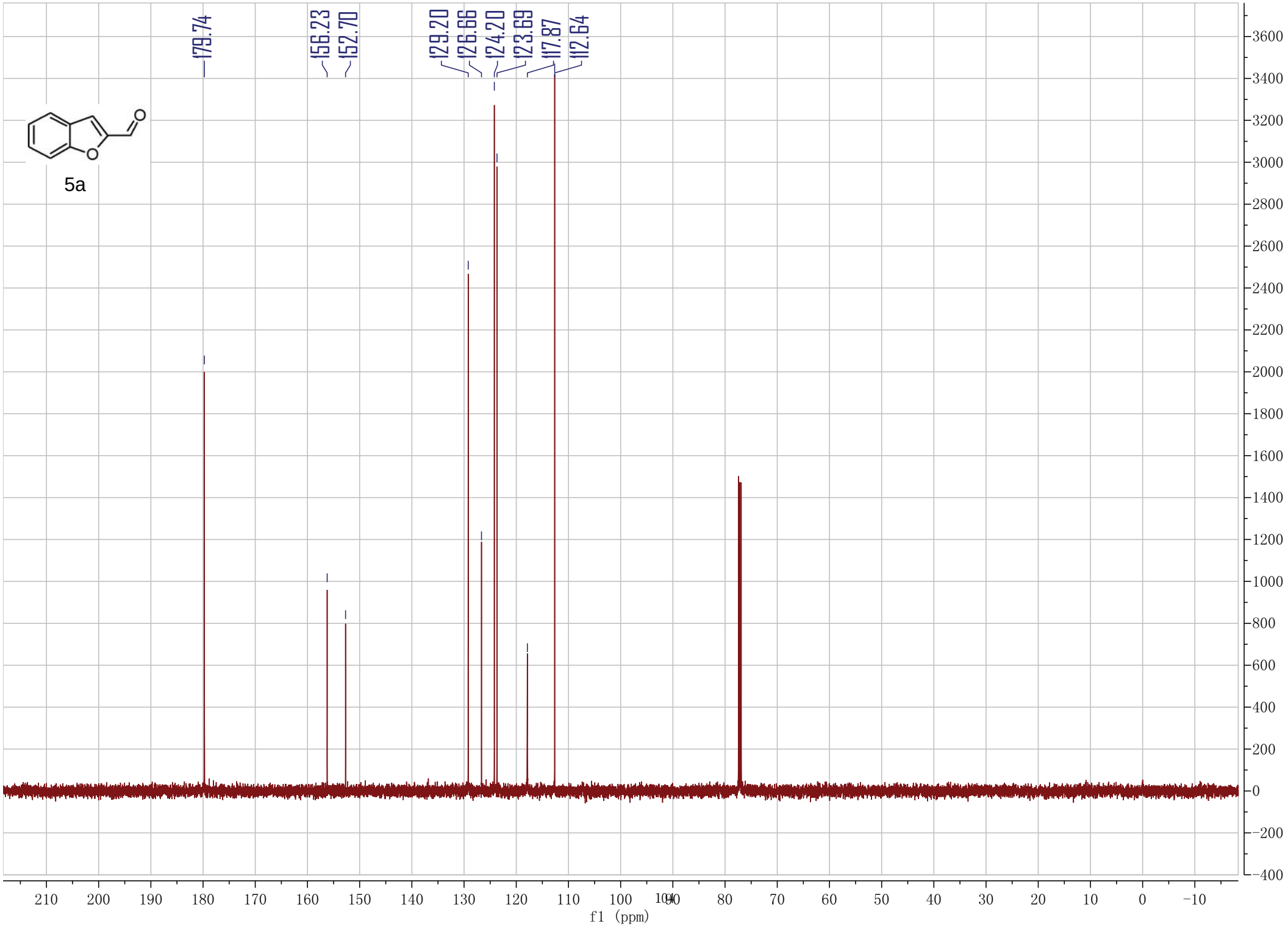

Me
Cl
CO2Et
O
4s
1.00
1.00
1.00
2.01
3.05
3.08
f1 (ppm)

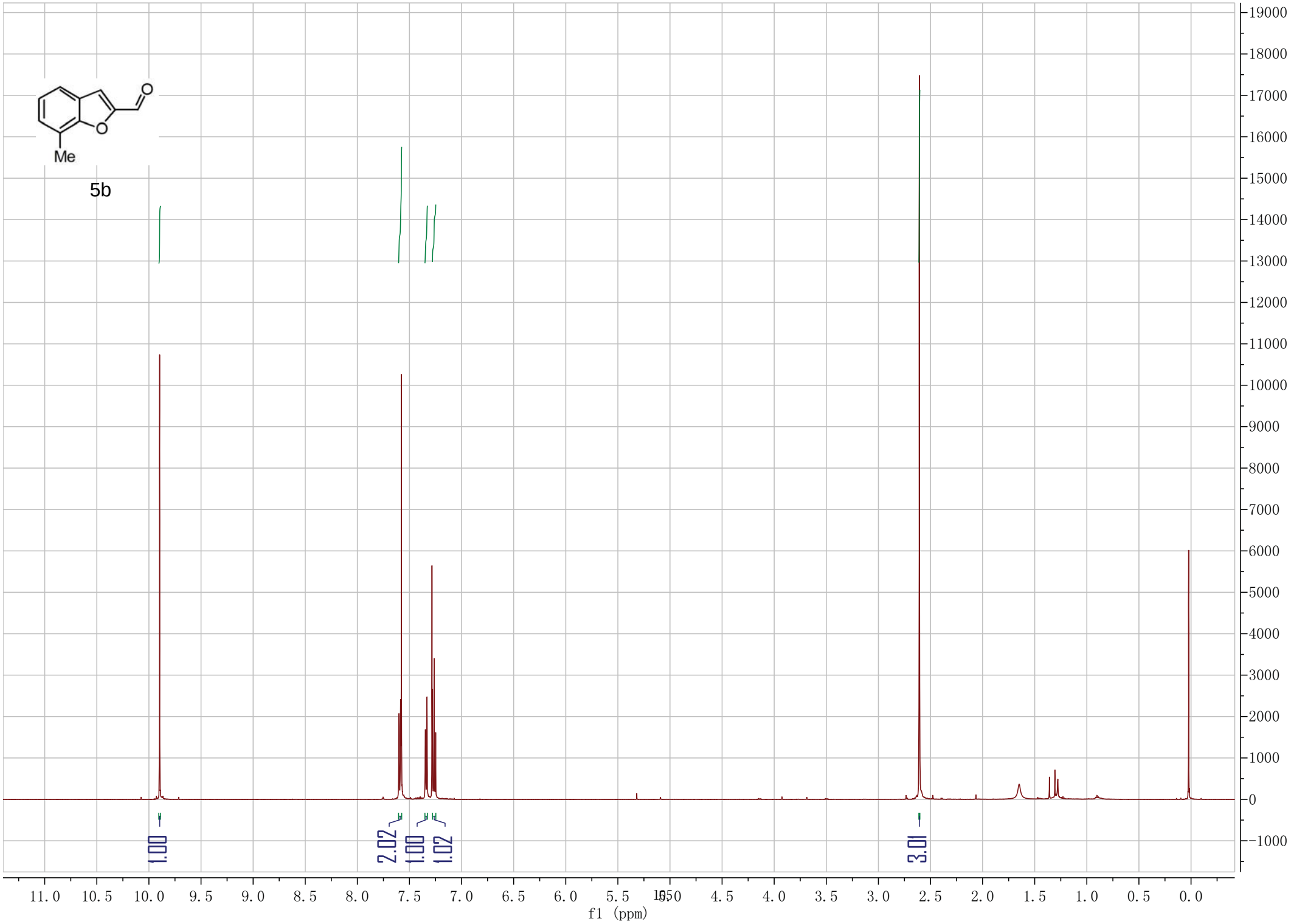

160.06
152.53
142.10
130.29
128.82
127.93
124.77
120.54
113.19
61.27
14.33
9.23
Me
Cl
CO2Et
O
4s
f1 (ppm)

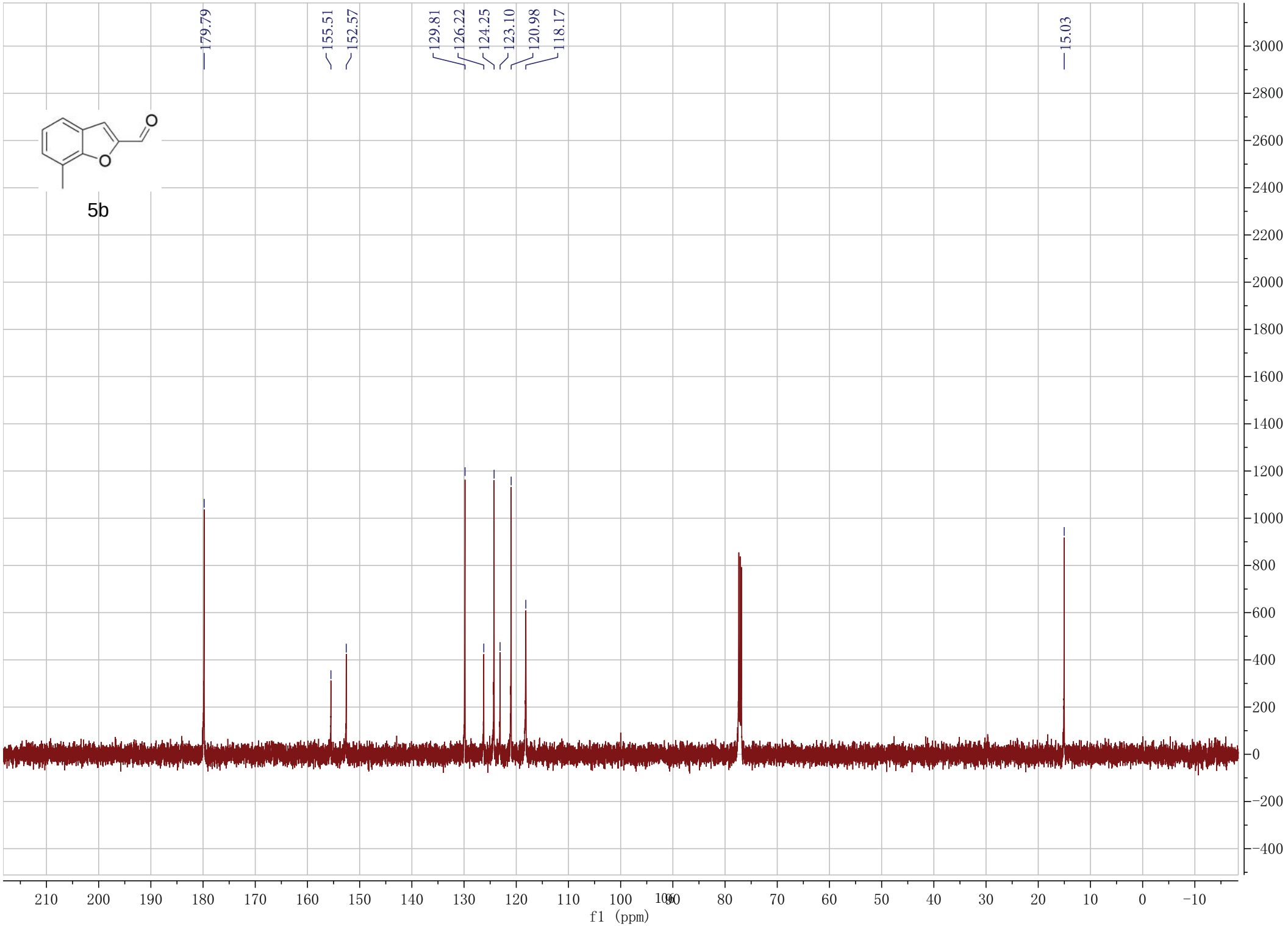
Me
Br
CO2Et
O
4t
0.97
0.99
0.99
2.03
3.00
3.07
f1 (ppm)


160.07
152.95
141.96
130.96
130.62
124.67
123.74
116.24
113.68
61.32
14.36
9.27
Br
Me
CO2Et
O
4t
f1 (ppm)

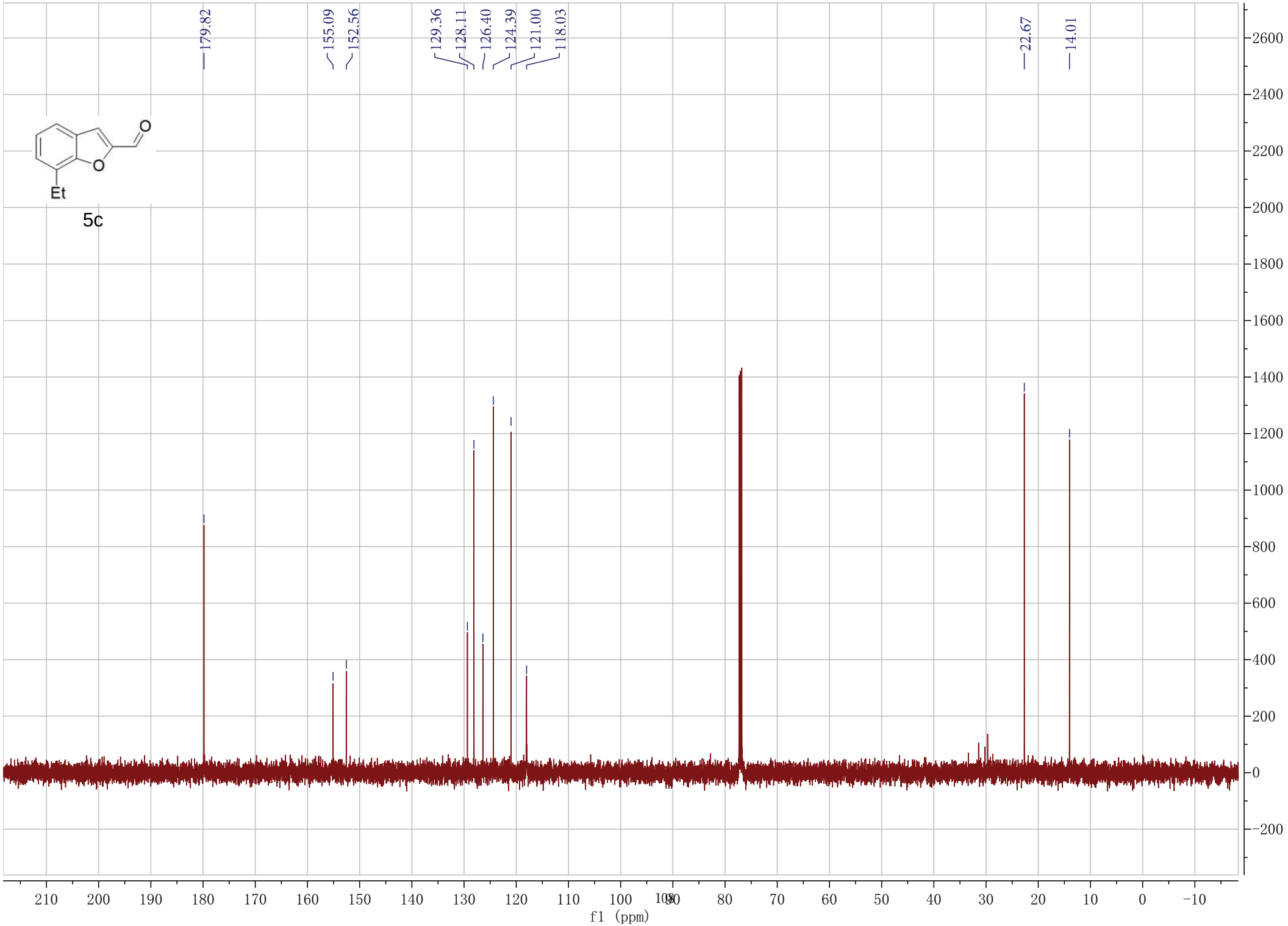

5a
0.98
1.00
1.00
1.00
1.00
1.01
f1 (ppm)

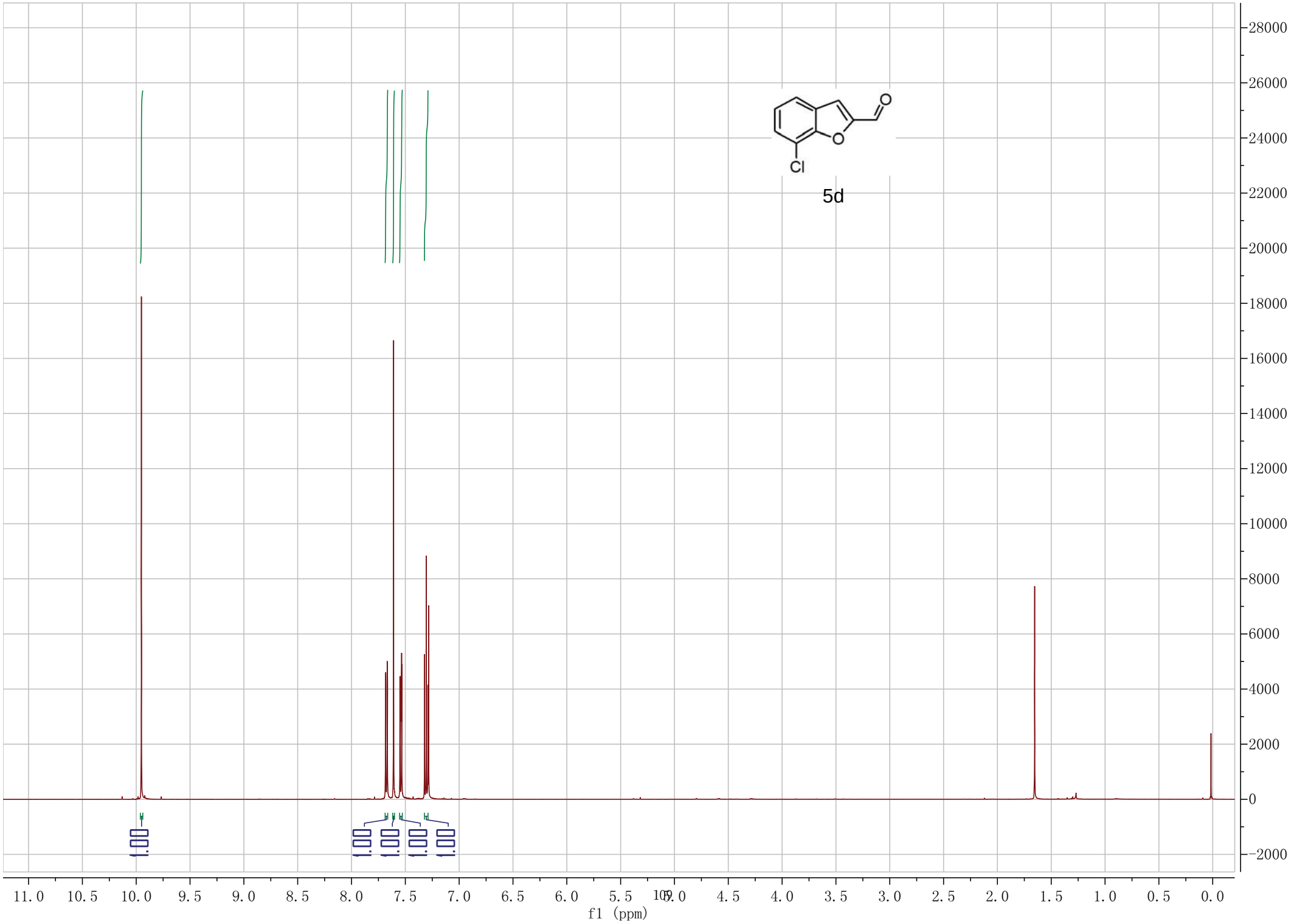

179.74
156.23
152.70
129.20
126.66
124.20
123.69
117.87
112.64
5a
f1 (ppm)

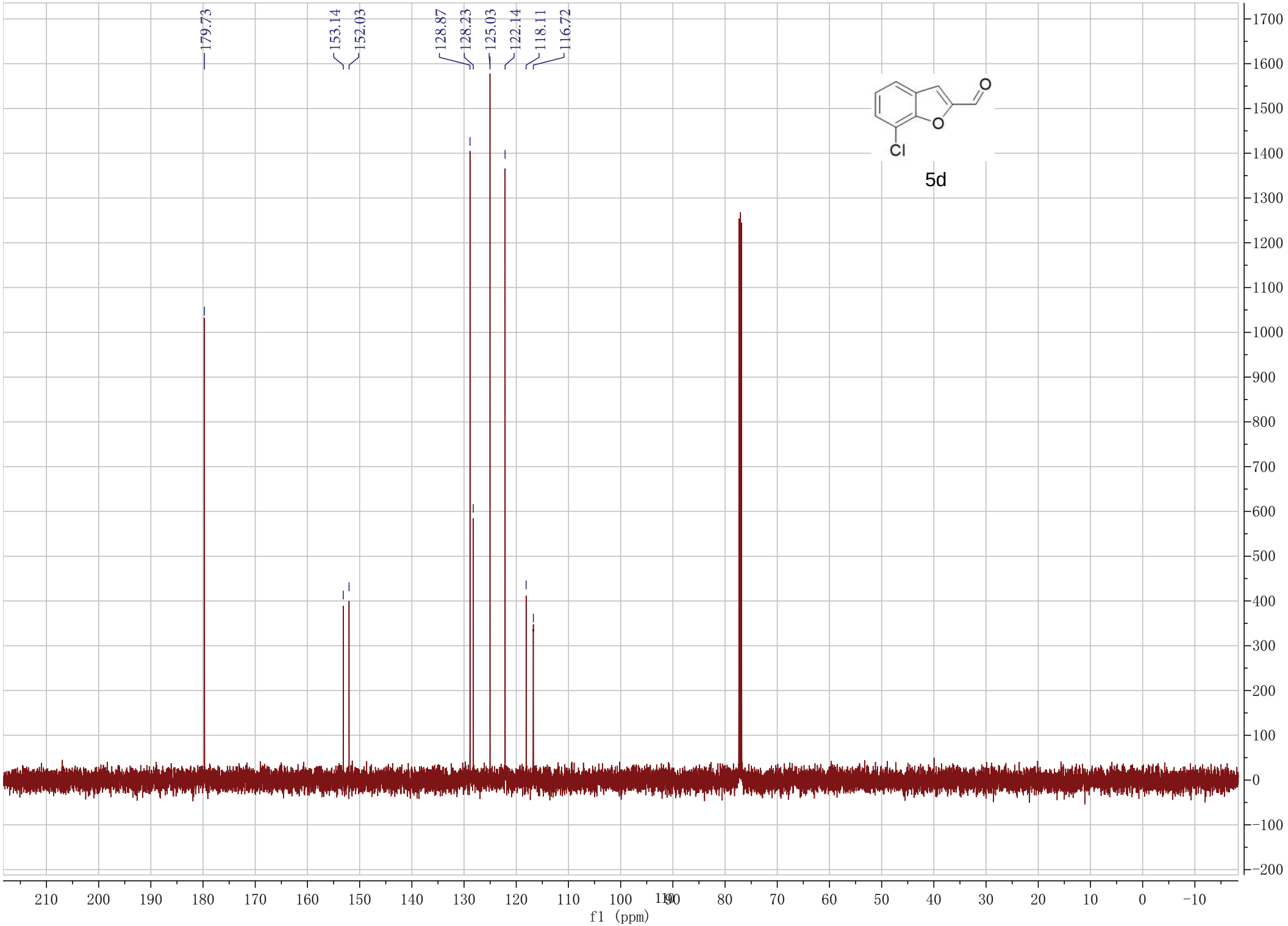

Me
5b
1.00
2.02
1.00
1.02
3.01
f1 (ppm)

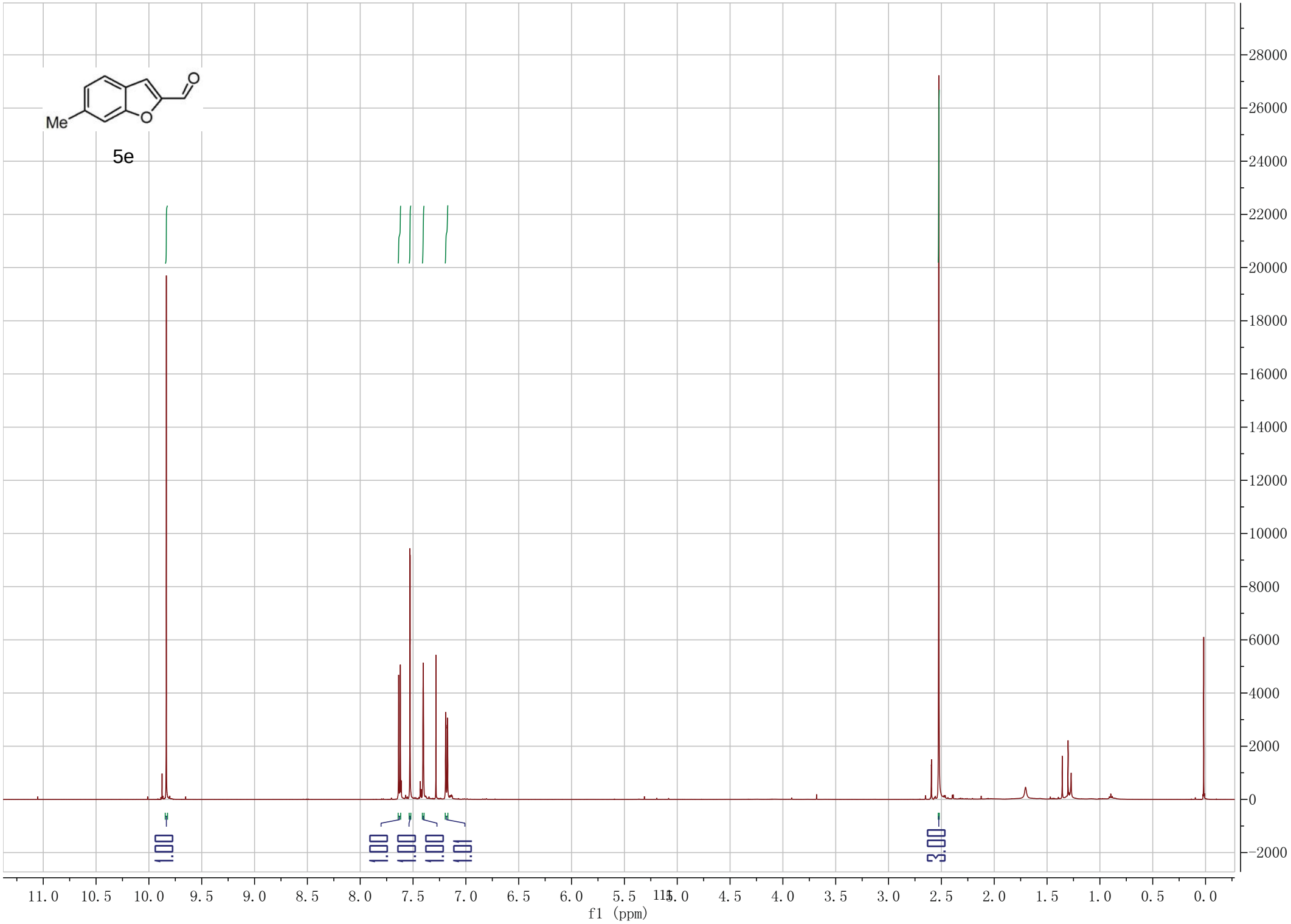

179.79
155.51
152.57
129.81
126.22
124.25
123.10
120.98
118.17
15.03
5b
f1 (ppm)

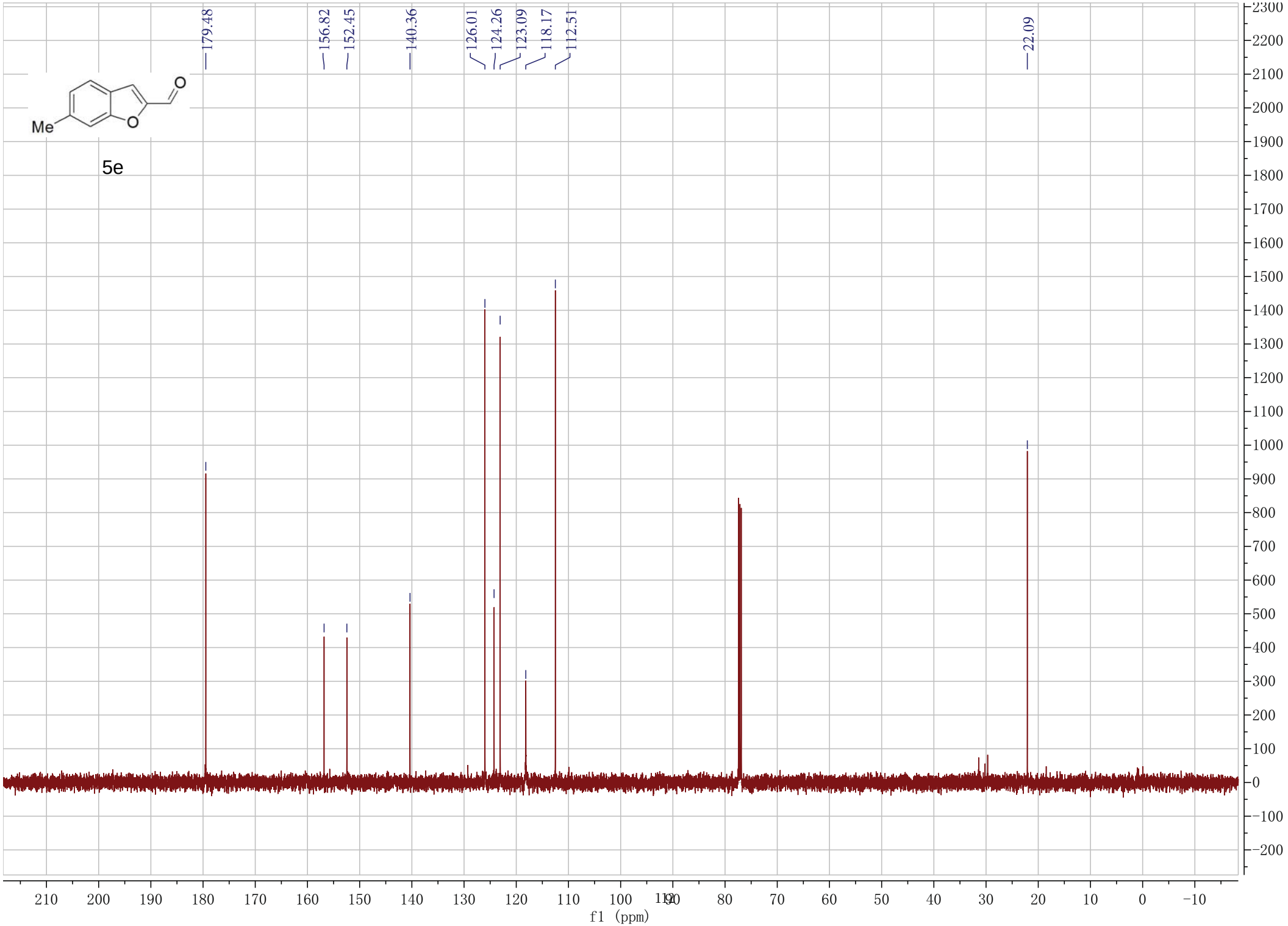
Et
5c
1.00
1.01
0.99
1.03
1.53
2.04
3.06
f1 (ppm)

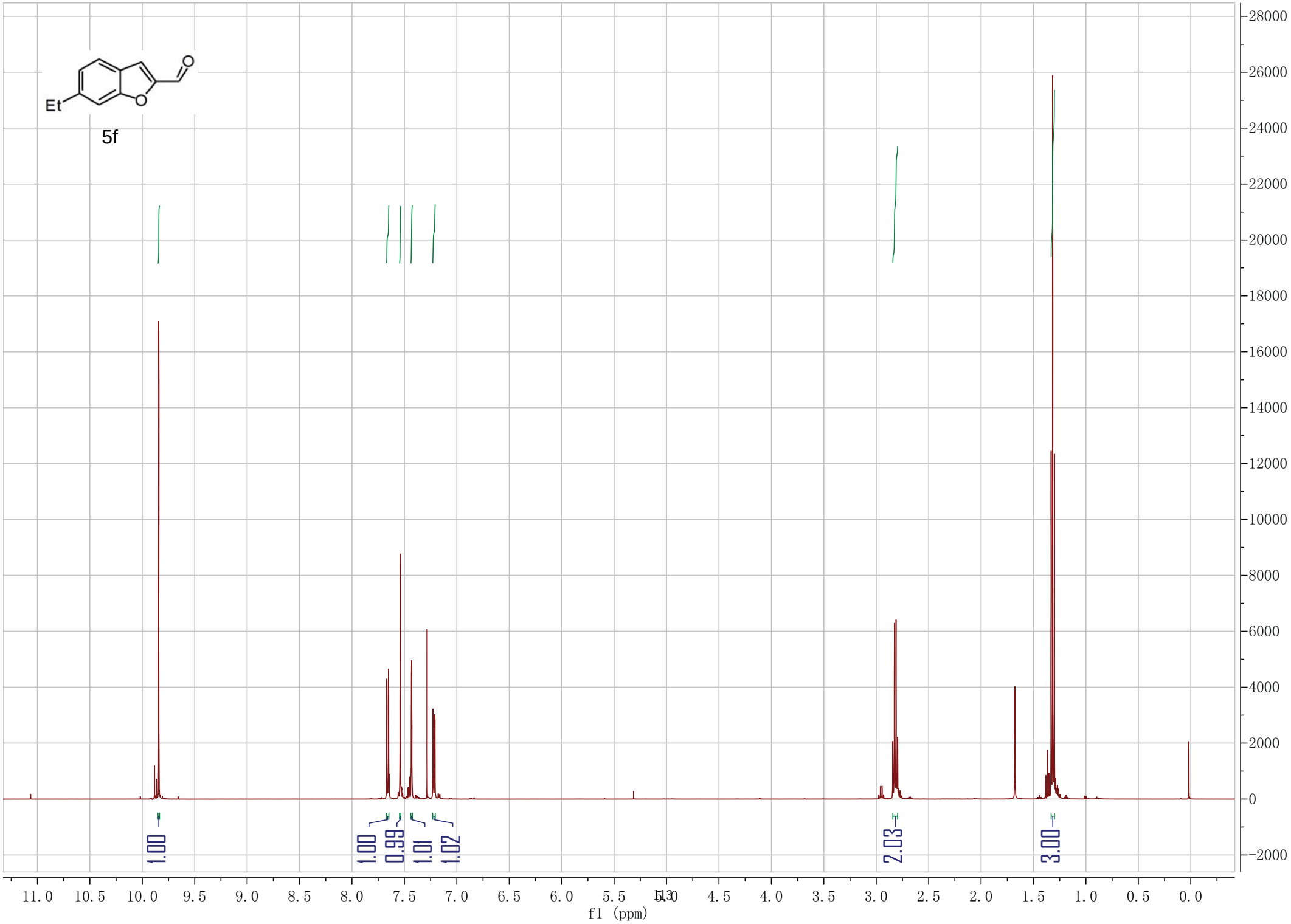

179.82
155.09
152.56
129.36
128.11
126.40
124.39
121.00
118.03
22.67
14.01
O
O
Et
5c
f1 (ppm)

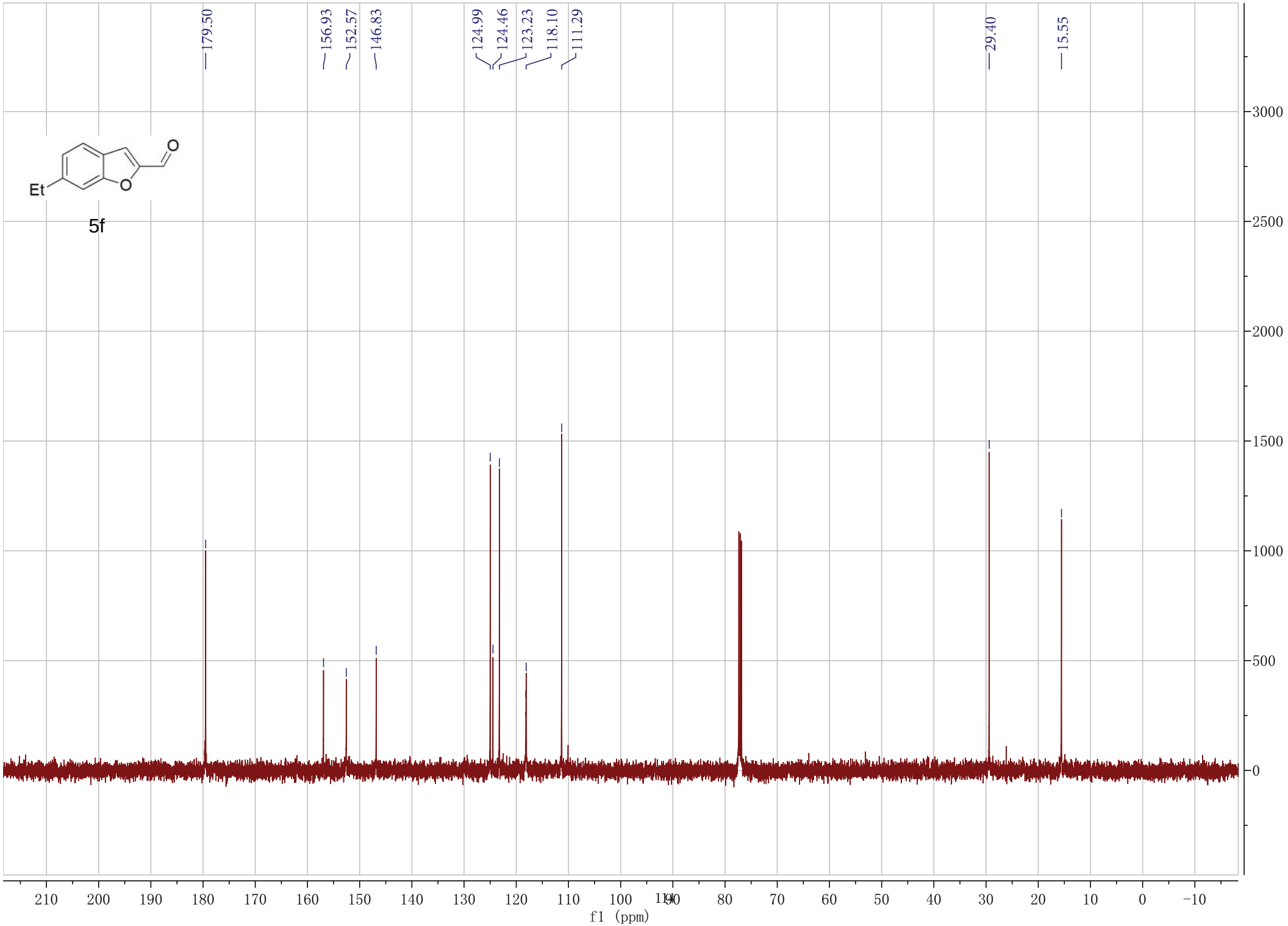

5d
Cl
O
O
f1 (ppm)

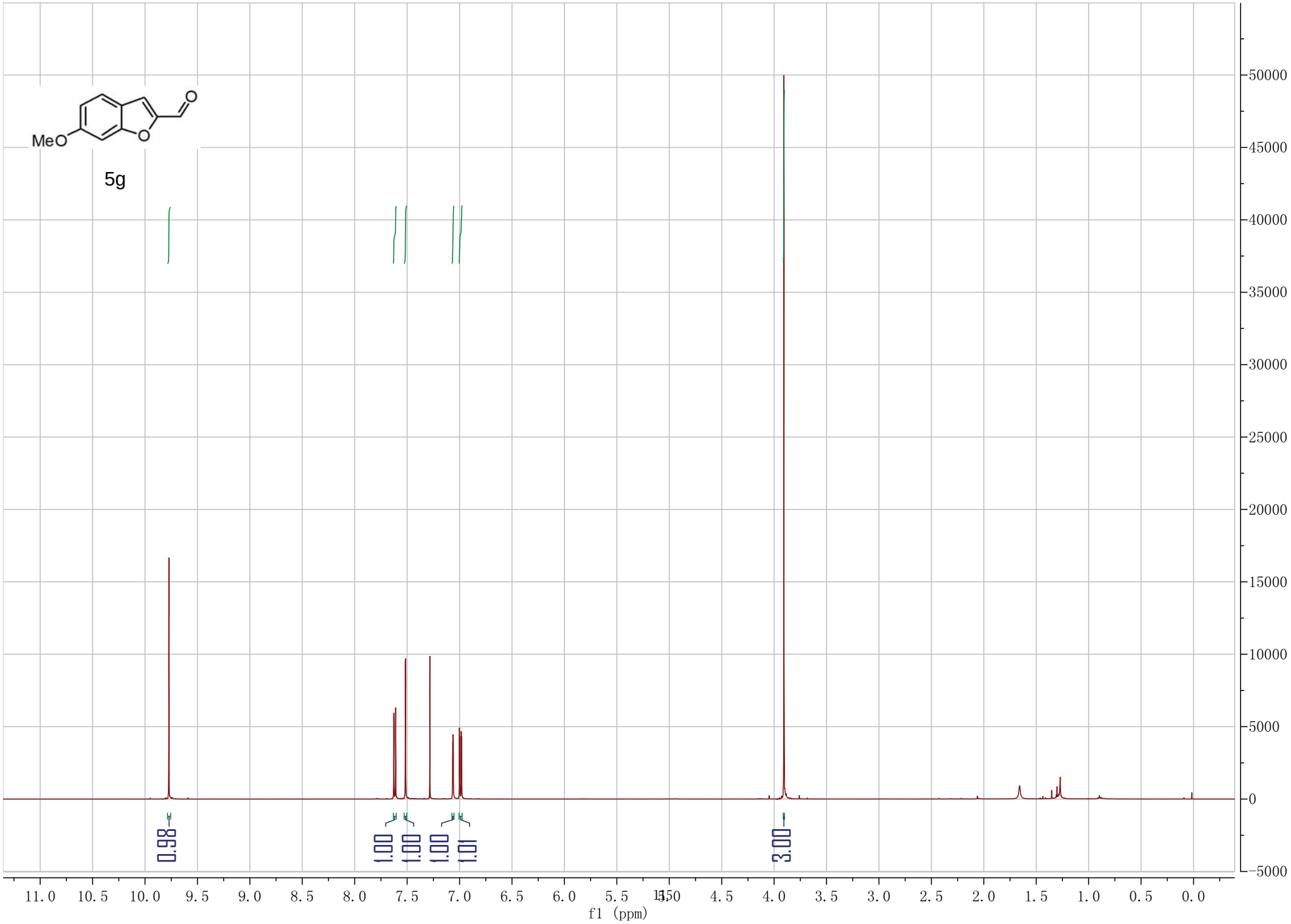

179.73
153.14
152.03
128.87
128.23
125.03
122.14
118.11
116.72
O
O
Cl
5d
f1 (ppm)

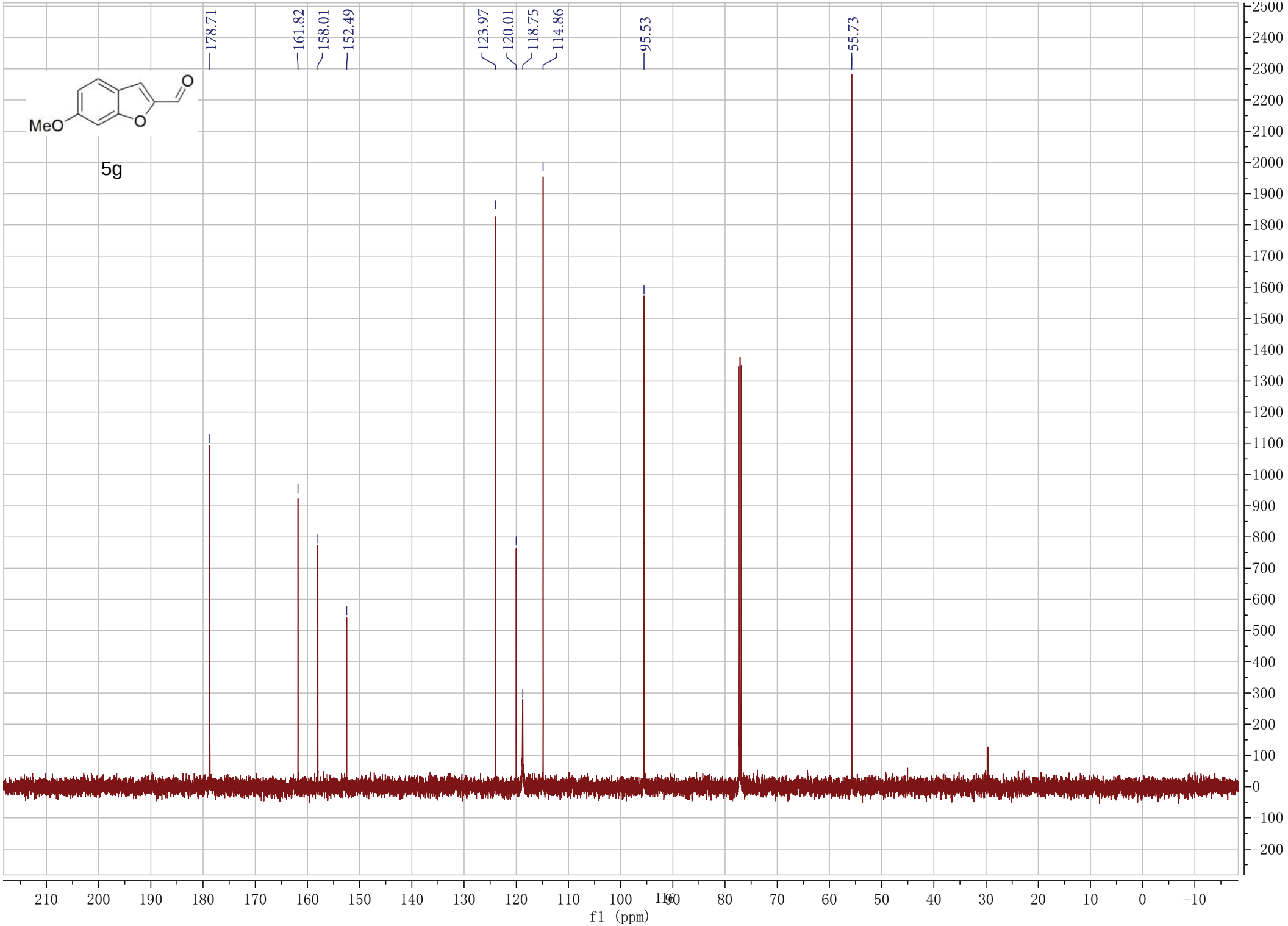

Me
5e
1.00
1.00
1.00
1.00
1.01
3.00
f1 (ppm)

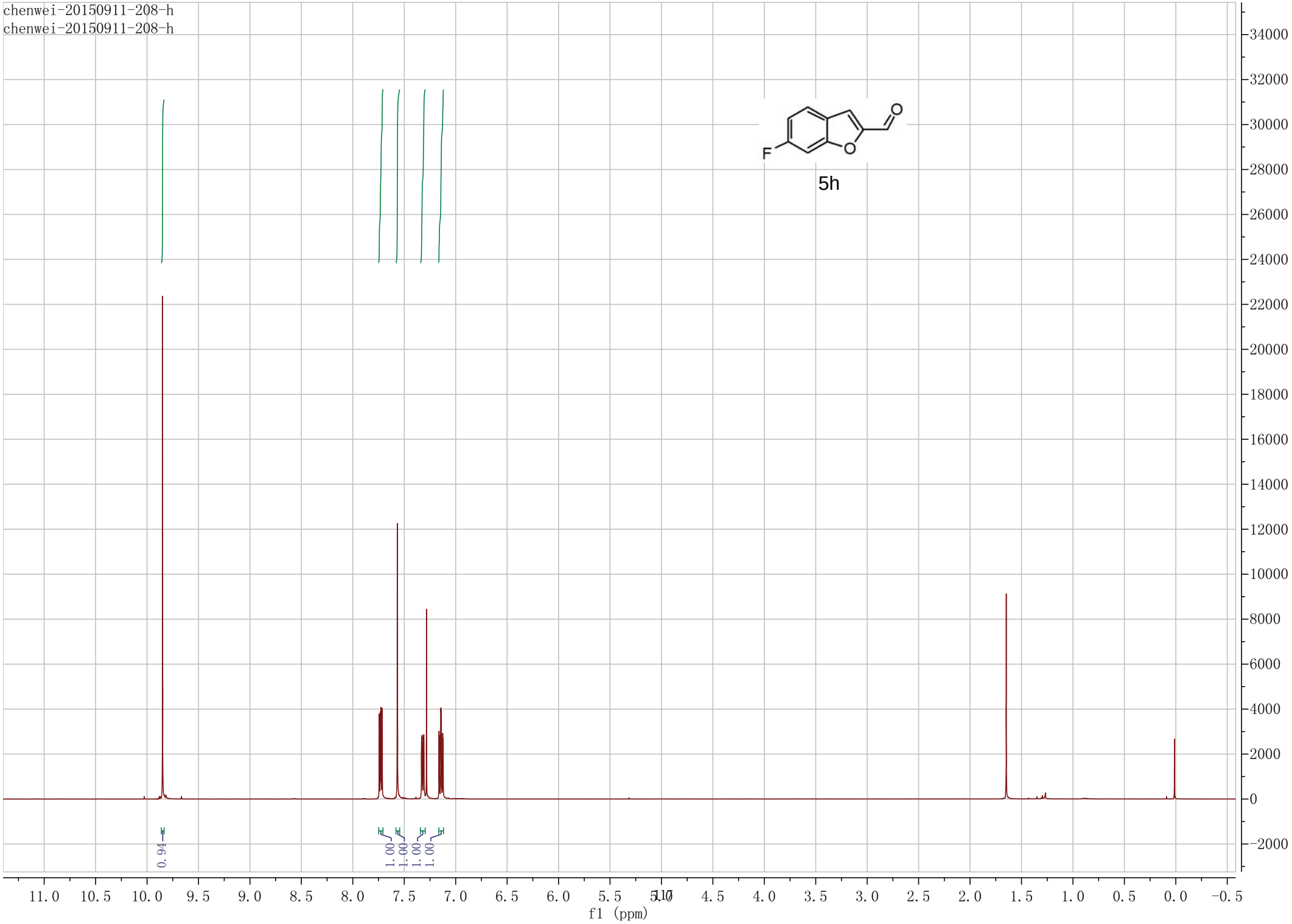

179.48
156.82
152.45
140.36
126.01
124.26
123.09
118.17
112.51
22.09
Me
O
O
5e
f1 (ppm)

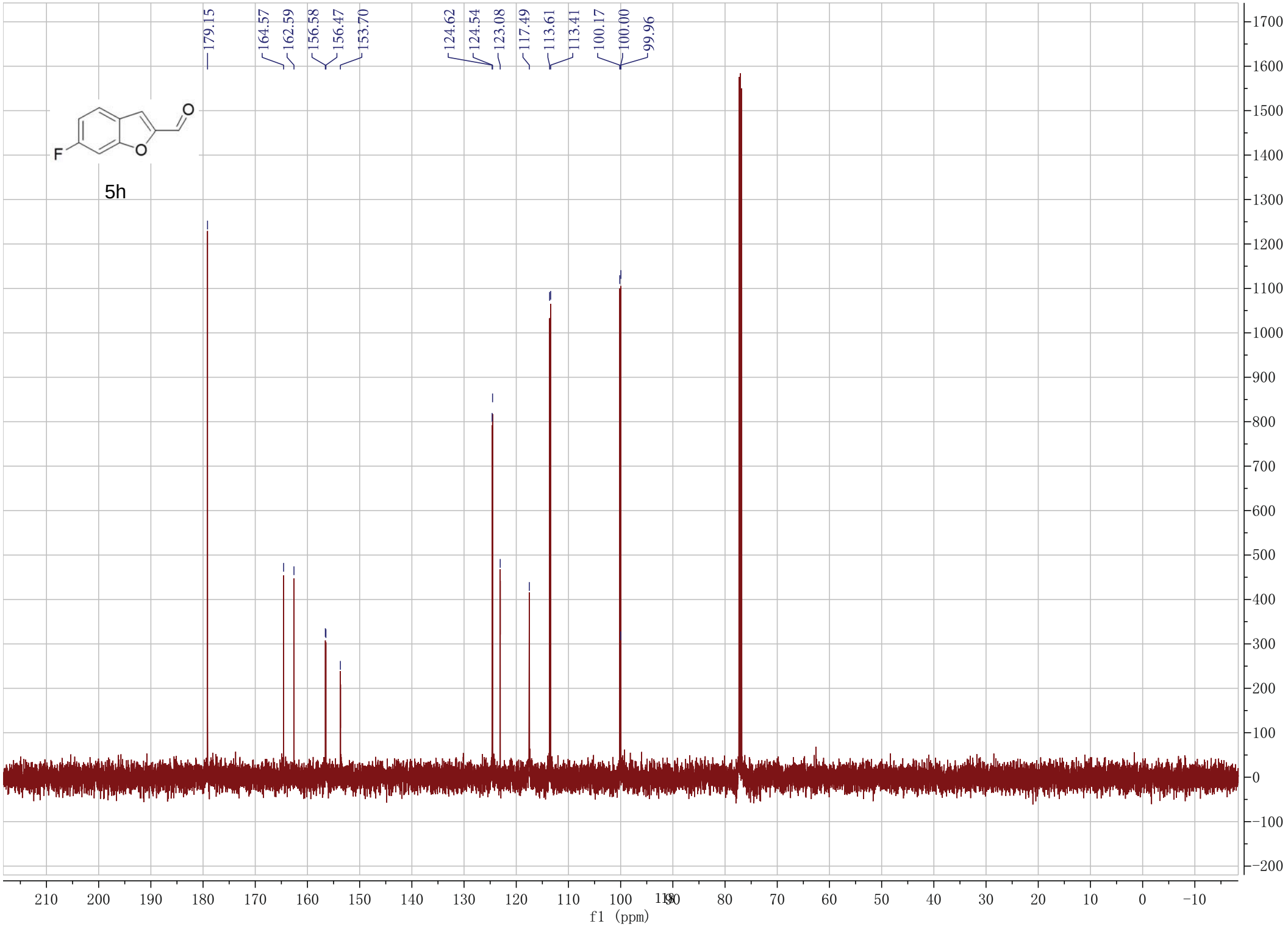

Et
O
O
5f
1.00
1.00
0.99
1.01
1.02
2.03
3.00
f1 (ppm)

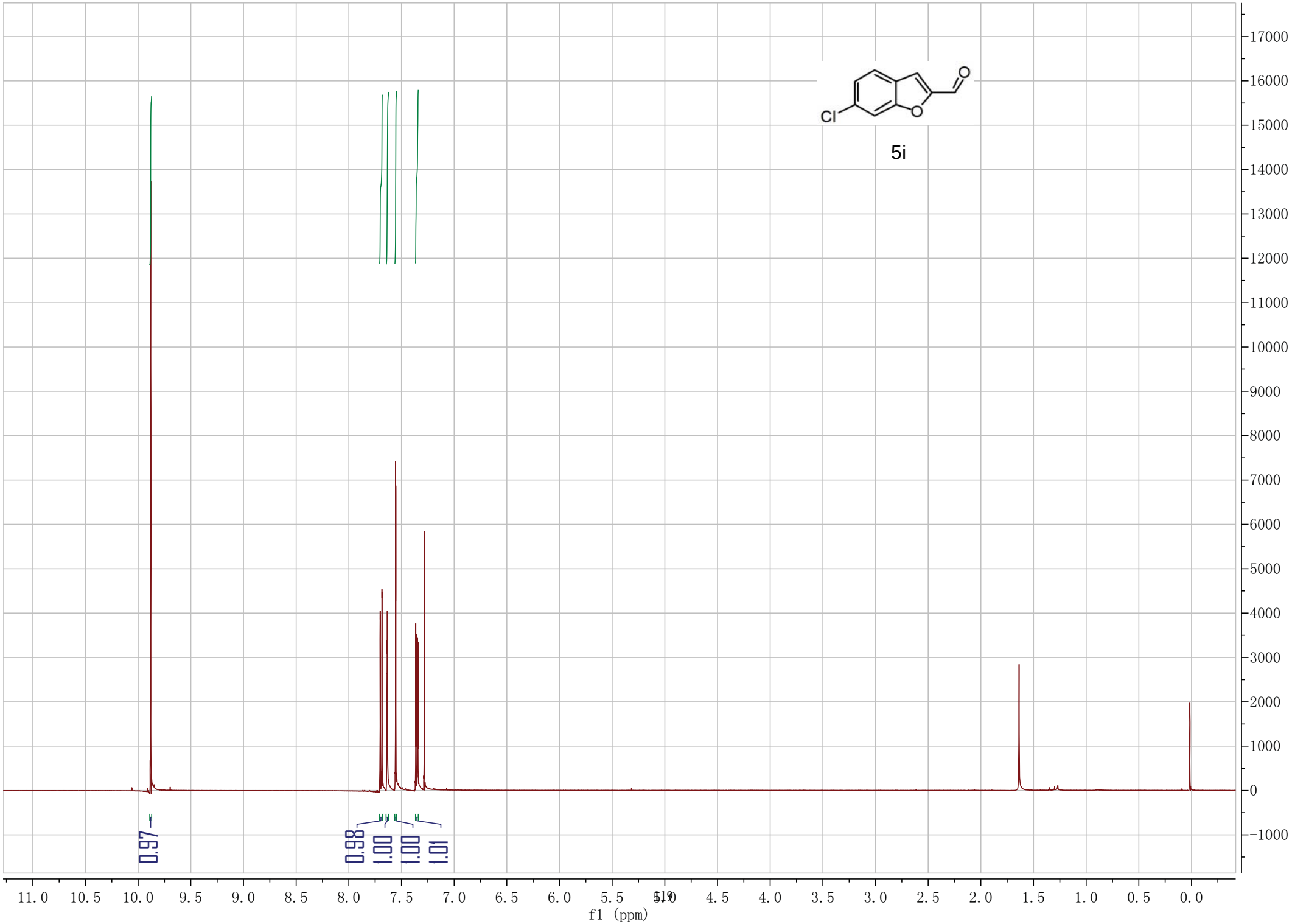

179.50
156.93
152.57
146.83
124.99
124.46
123.23
118.10
111.29
29.40
15.55
Et
O
O
5f
3000
2500
2000
1500
1000
500
0
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

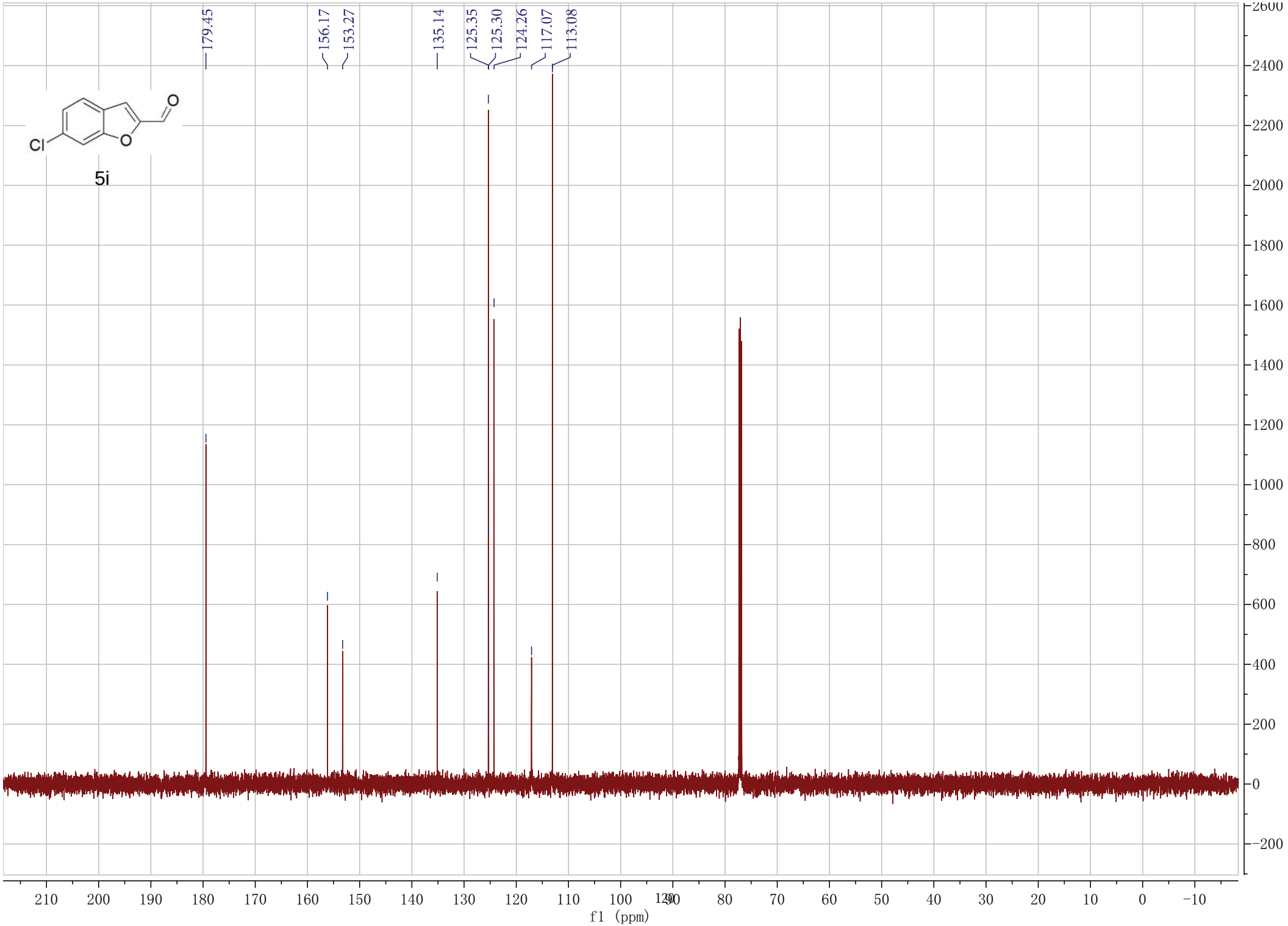

MeO
O
O
5g
0.98
1.00
1.00
1.00
1.01
3.00
f1 (ppm)

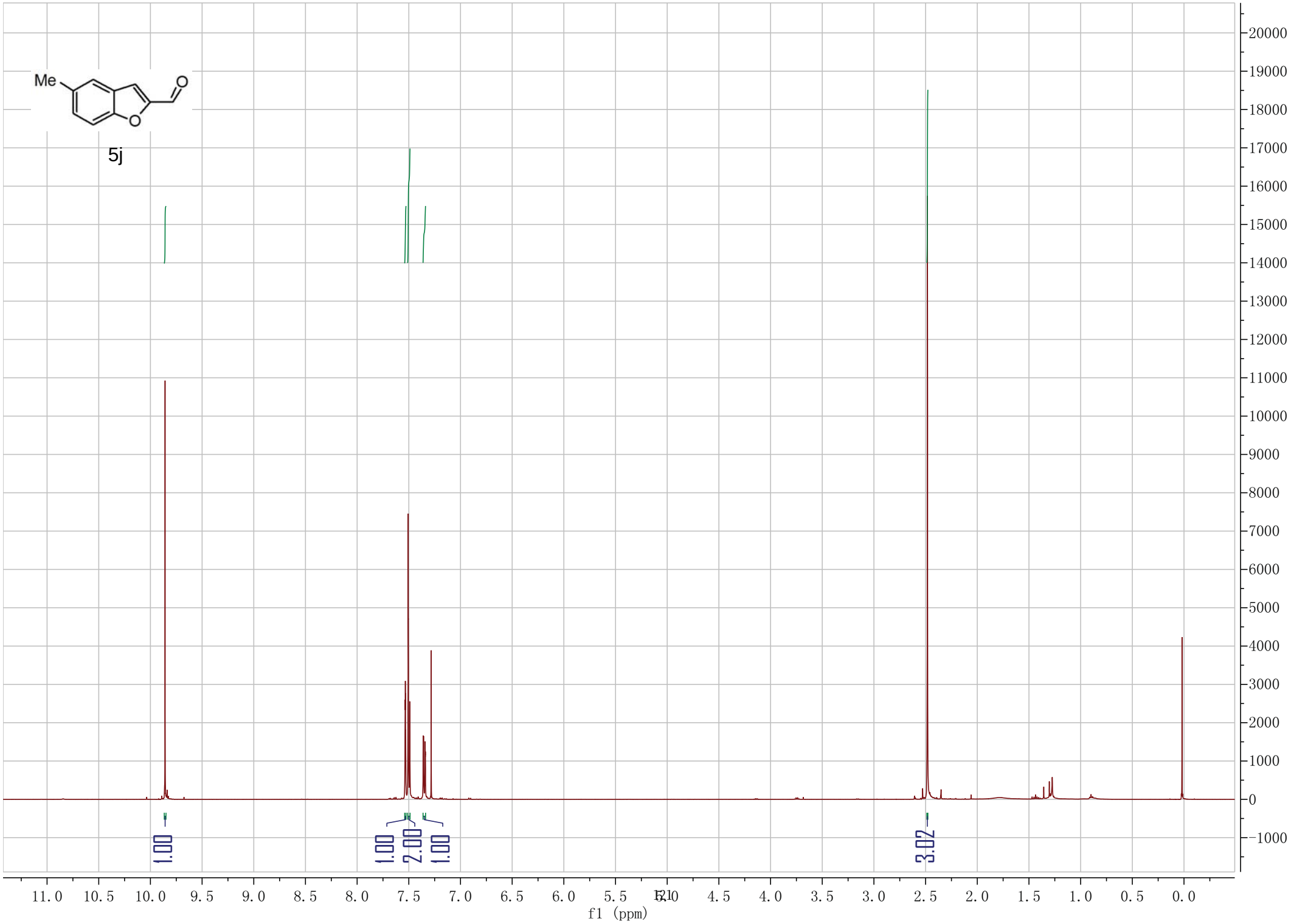

178.71
161.82
158.01
152.49
123.97
120.01
118.75
114.86
95.53
55.73
MeO
O
O
5g
f1 (ppm)

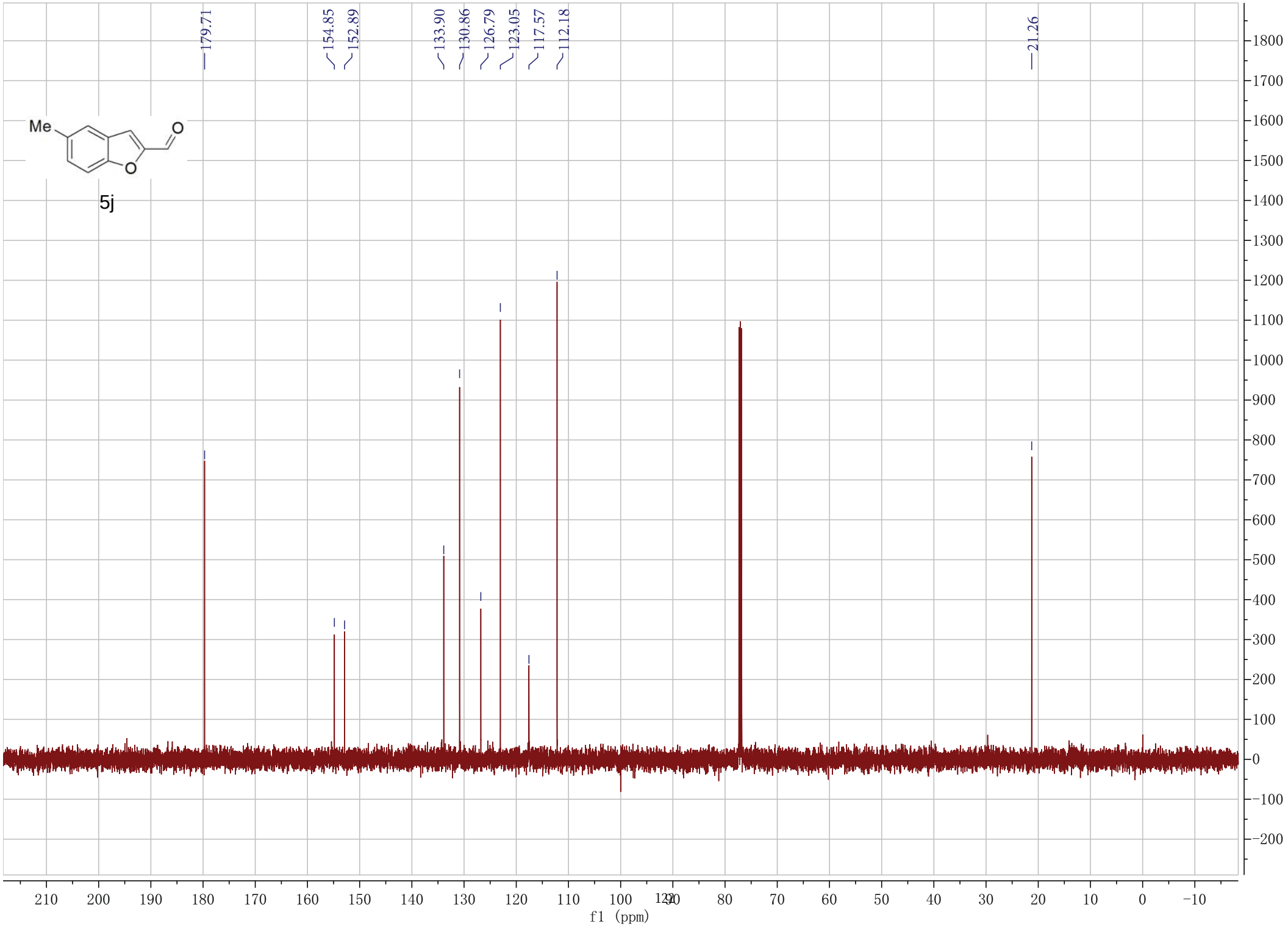

chenwei-20150911-208-h
chenwei-20150911-208-h
F
O
O
5h
0.94
1.00
1.00
1.00
1.00
f1 (ppm)

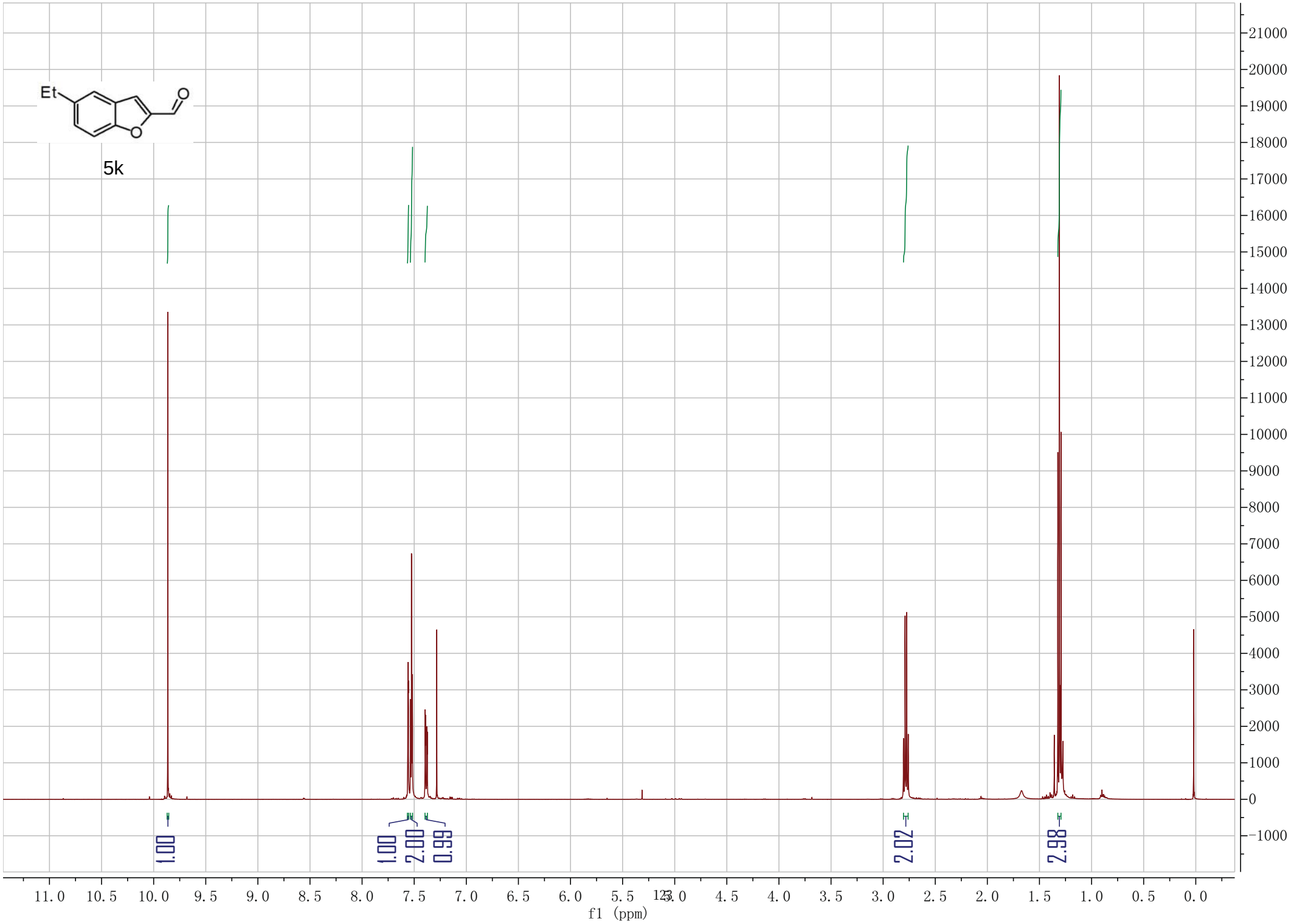

179.15
164.57
162.59
156.58
156.47
153.70
124.62
124.54
123.08
117.49
113.61
113.41
100.17
100.00
99.96
F
O
O
5h
f1 (ppm)

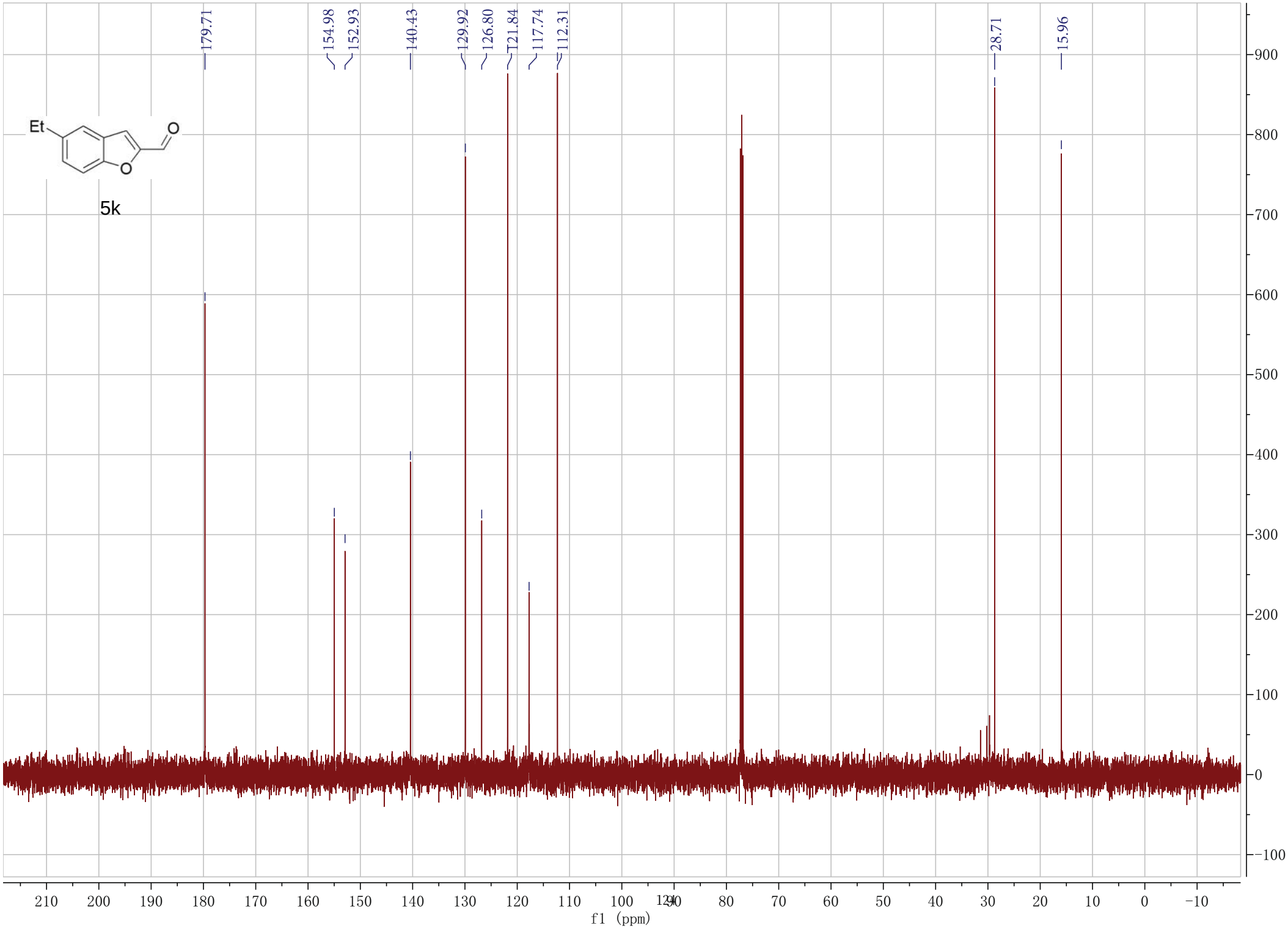

5i
Cl
O
O
0.97
0.98
1.00
1.00
1.01
f1 (ppm)

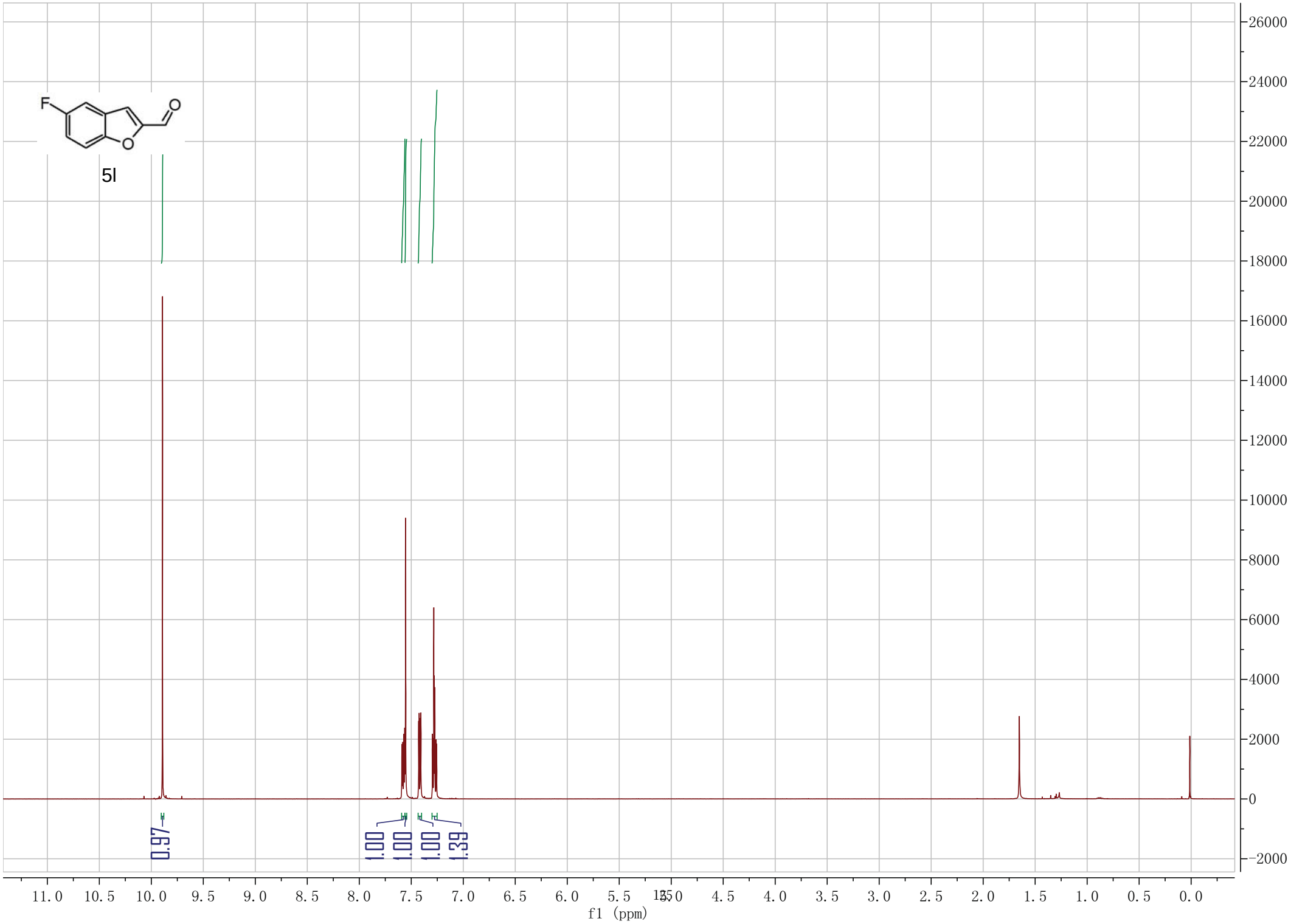

179.45
156.17
153.27
135.14
125.35
125.30
124.26
117.07
113.08
Cl
O
O
5i
f1 (ppm)

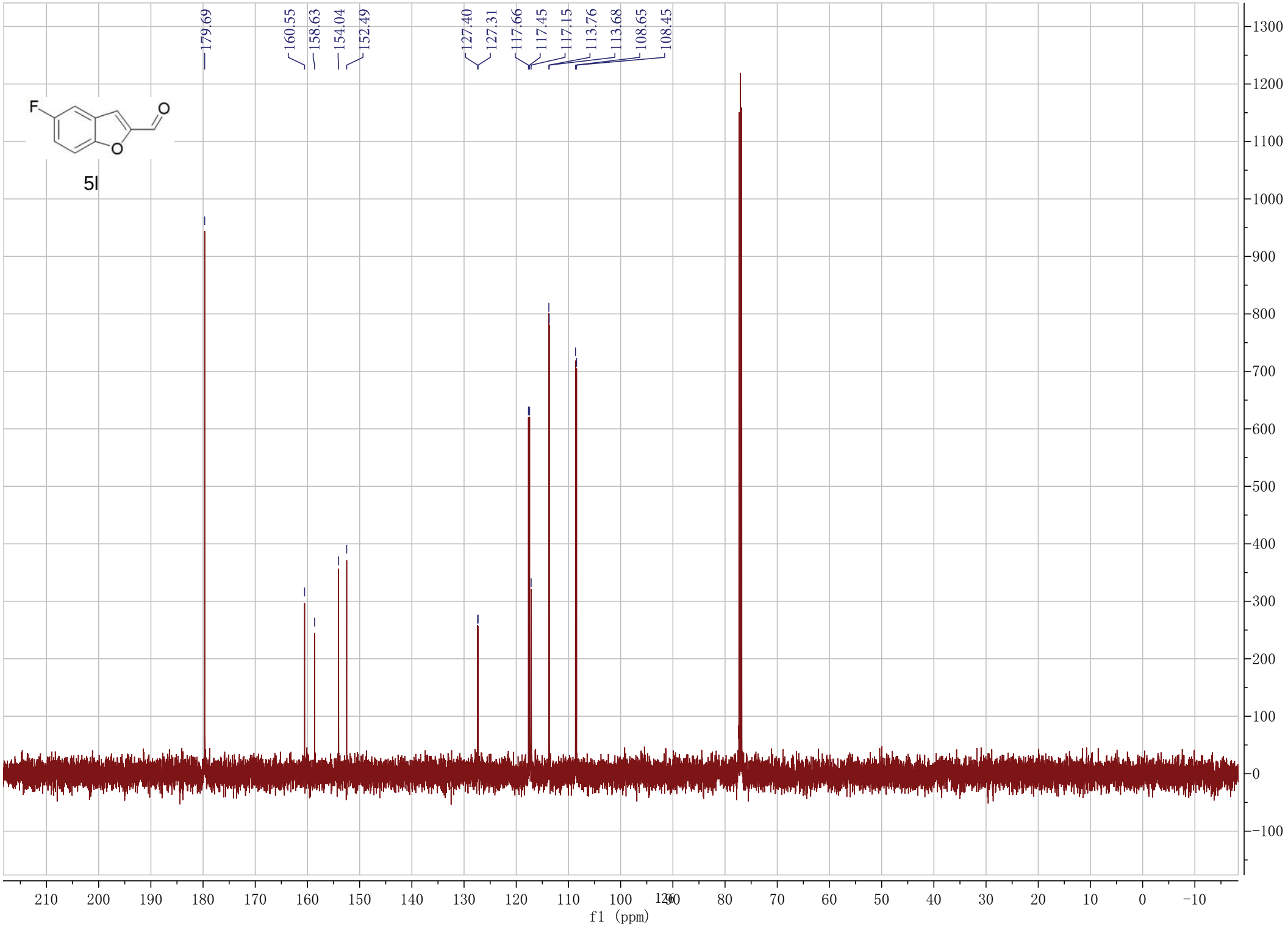

Me
O
O
5j
1.00
1.00
2.00
1.00
3.02
f1 (ppm)

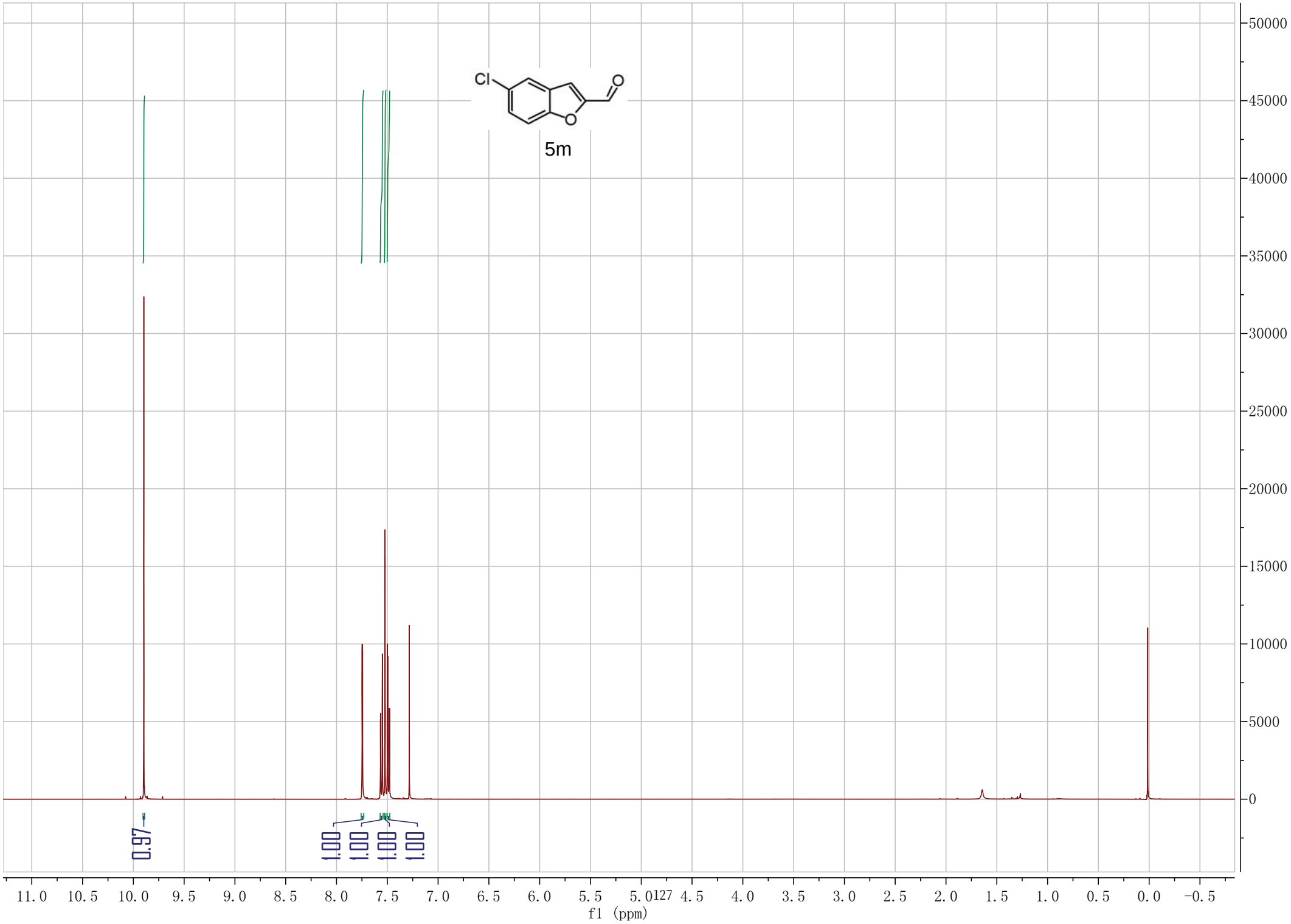

179.71
154.85
152.89
133.90
130.86
126.79
123.05
117.57
112.18
21.26
Me
O
O
5j
f1 (ppm)

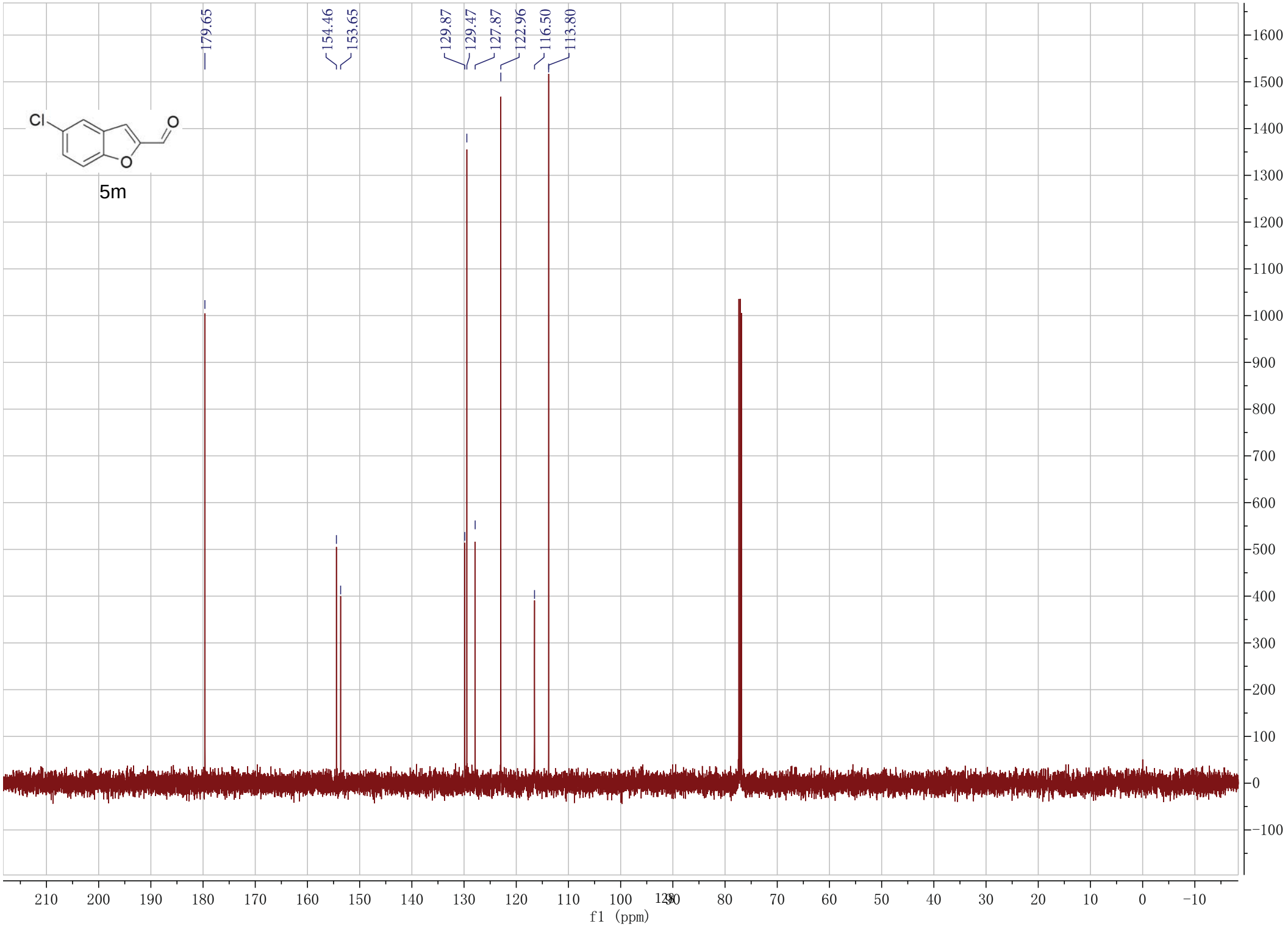

Et
O
O
5k
1.00
1.00
2.00
0.99
2.02
2.98
f1 (ppm)

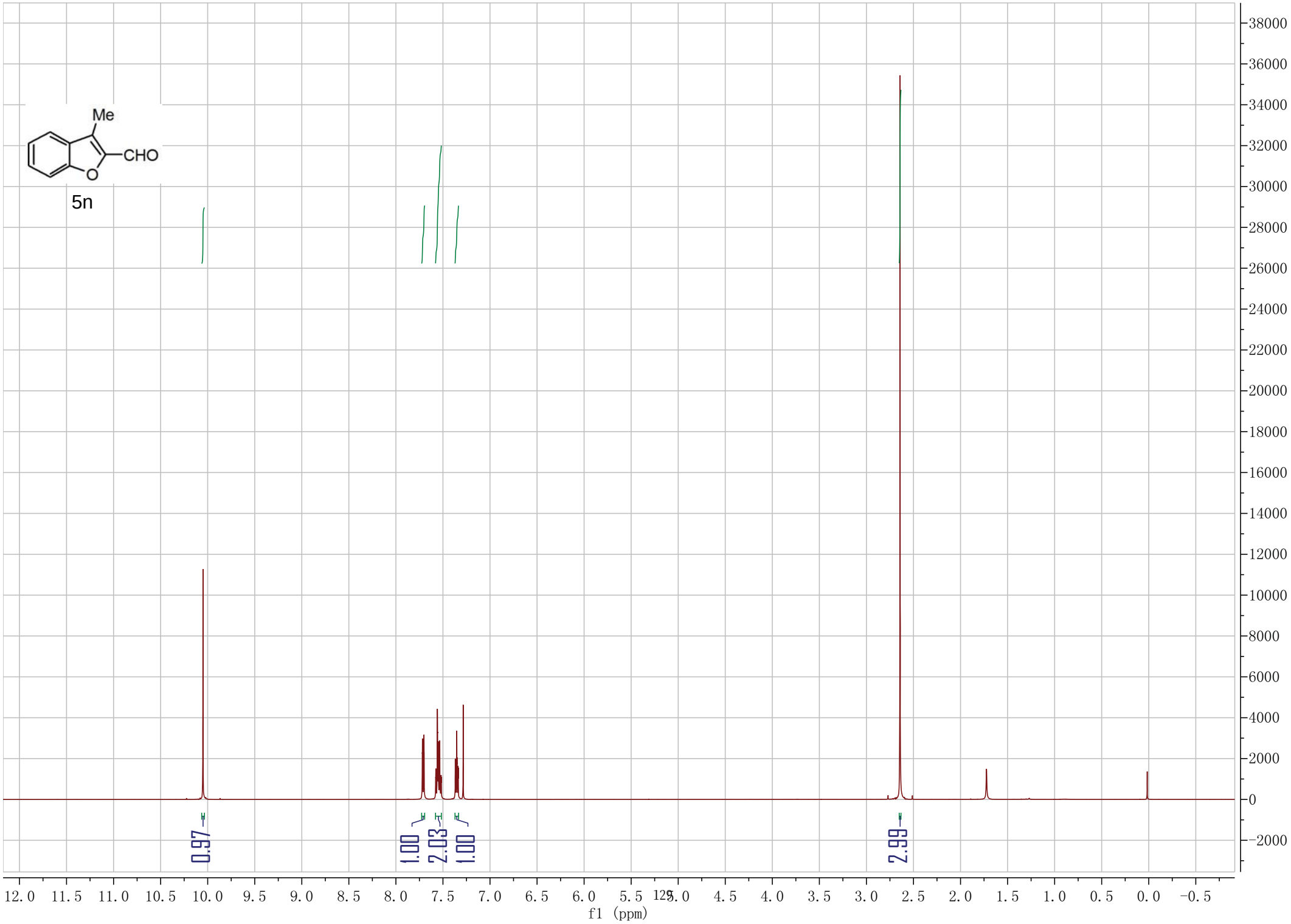

179.71
154.98
152.93
140.43
129.92
126.80
121.84
117.74
112.31
28.71
15.96
Et
O
O
5k
f1 (ppm)

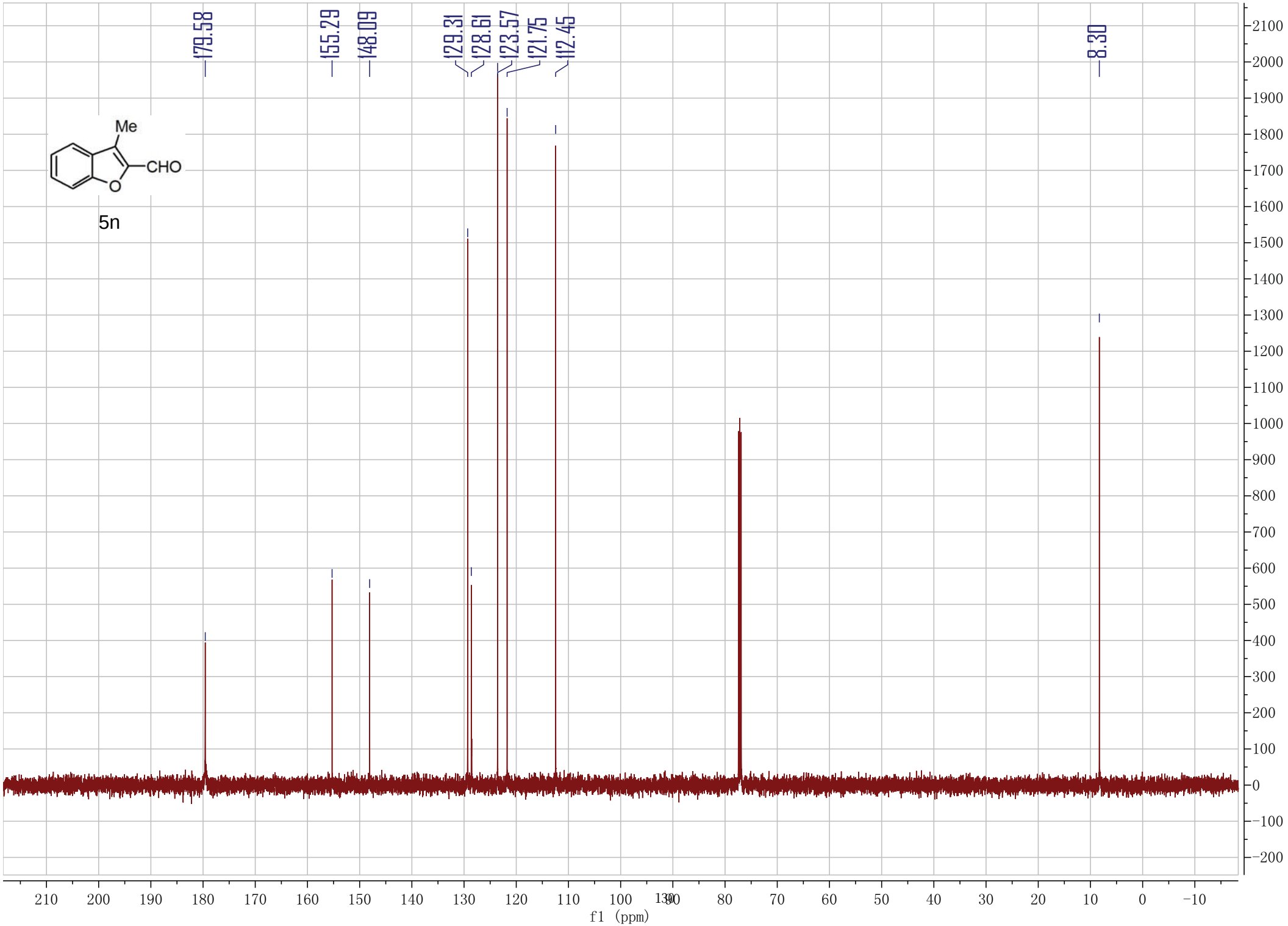

F
O
O
5l
0.97
1.00
1.00
1.00
1.39
f1 (ppm)

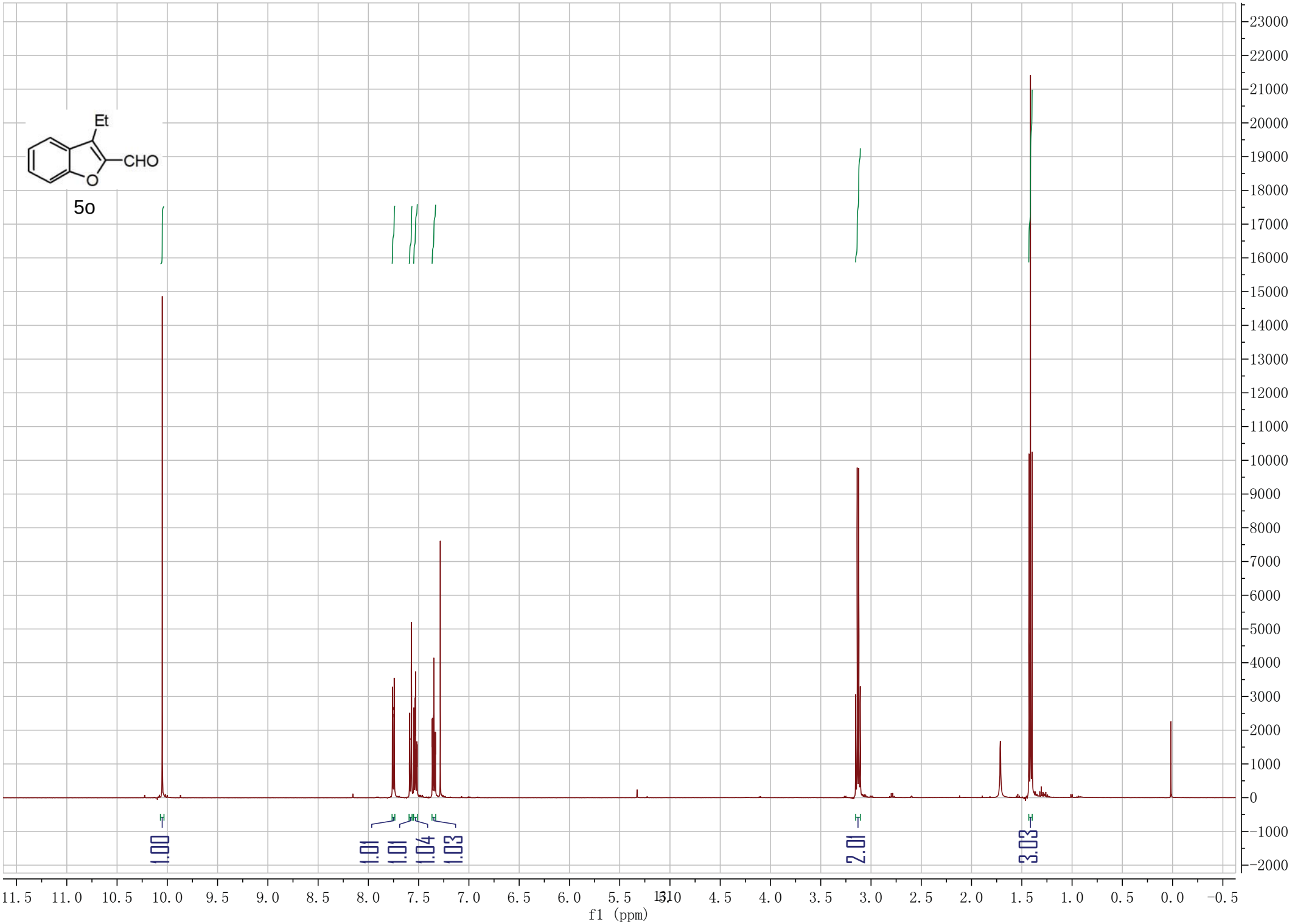

179.69
160.55
158.63
154.04
152.49
127.40
127.31
117.66
117.45
117.15
113.76
113.68
108.65
108.45
F
O
O
5l
f1 (ppm)

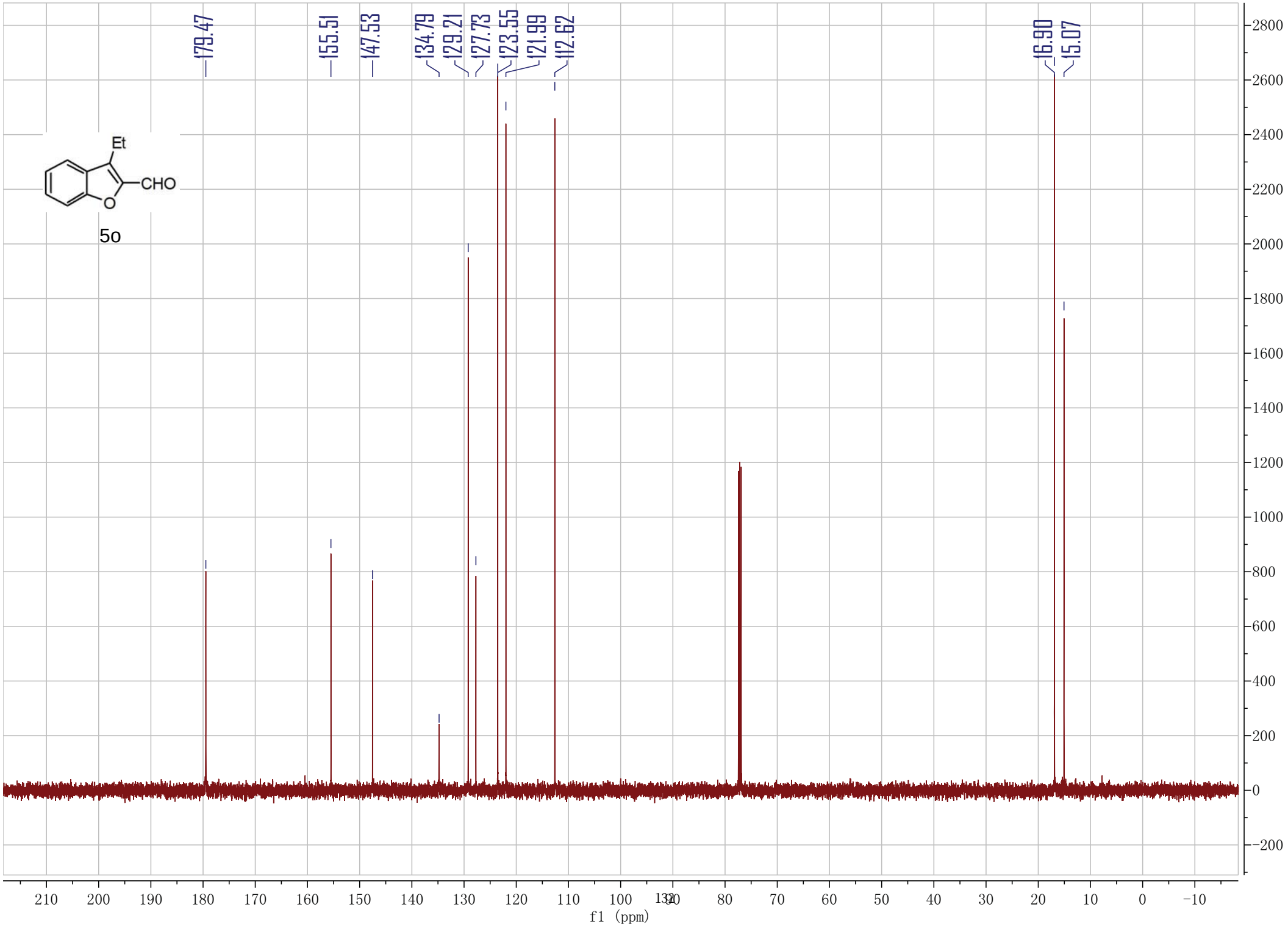

Cl
O
O
5m
0.97
1.00
1.00
1.00
1.00
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0127 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

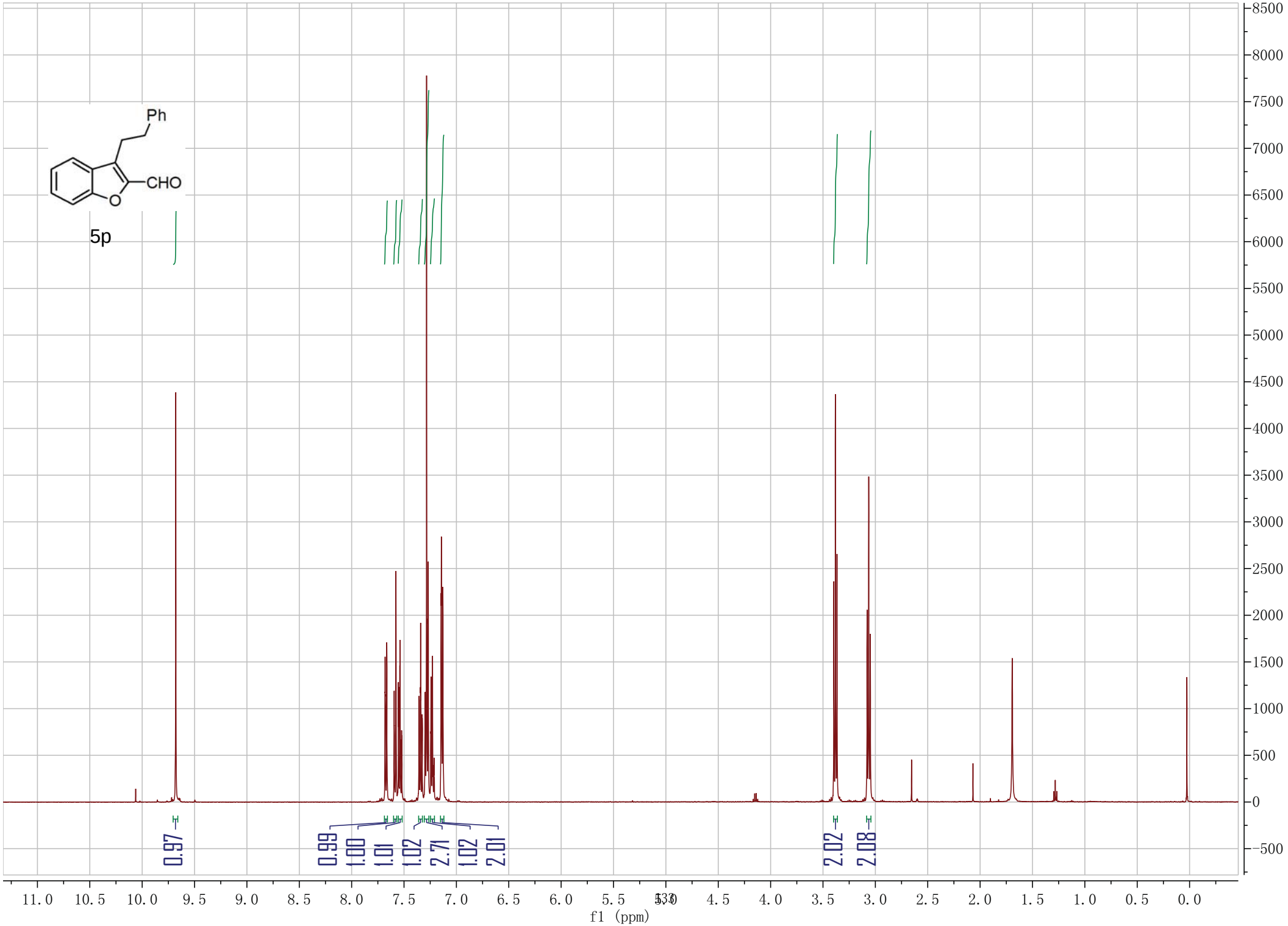

179.65
154.46
153.65
129.87
129.47
127.87
122.96
116.50
113.80
Cl
O
O
5m
f1 (ppm)

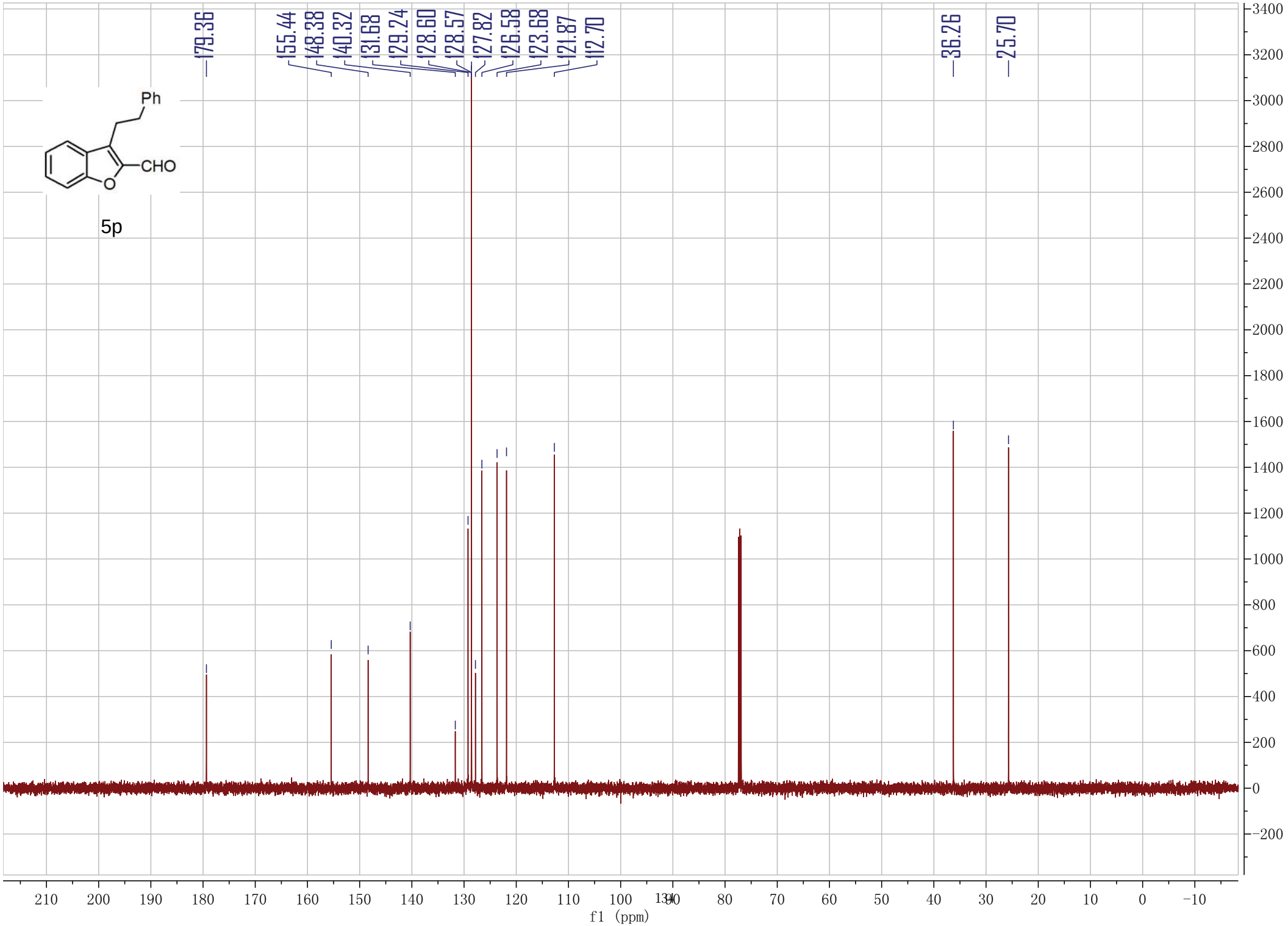

Me
CHO
O
5n
0.97
1.00
2.03
1.00
2.99
f1 (ppm)


179.58
155.29
148.09
129.31
128.61
123.57
121.75
112.45
8.30
Me
CHO
O
5n
f1 (ppm)

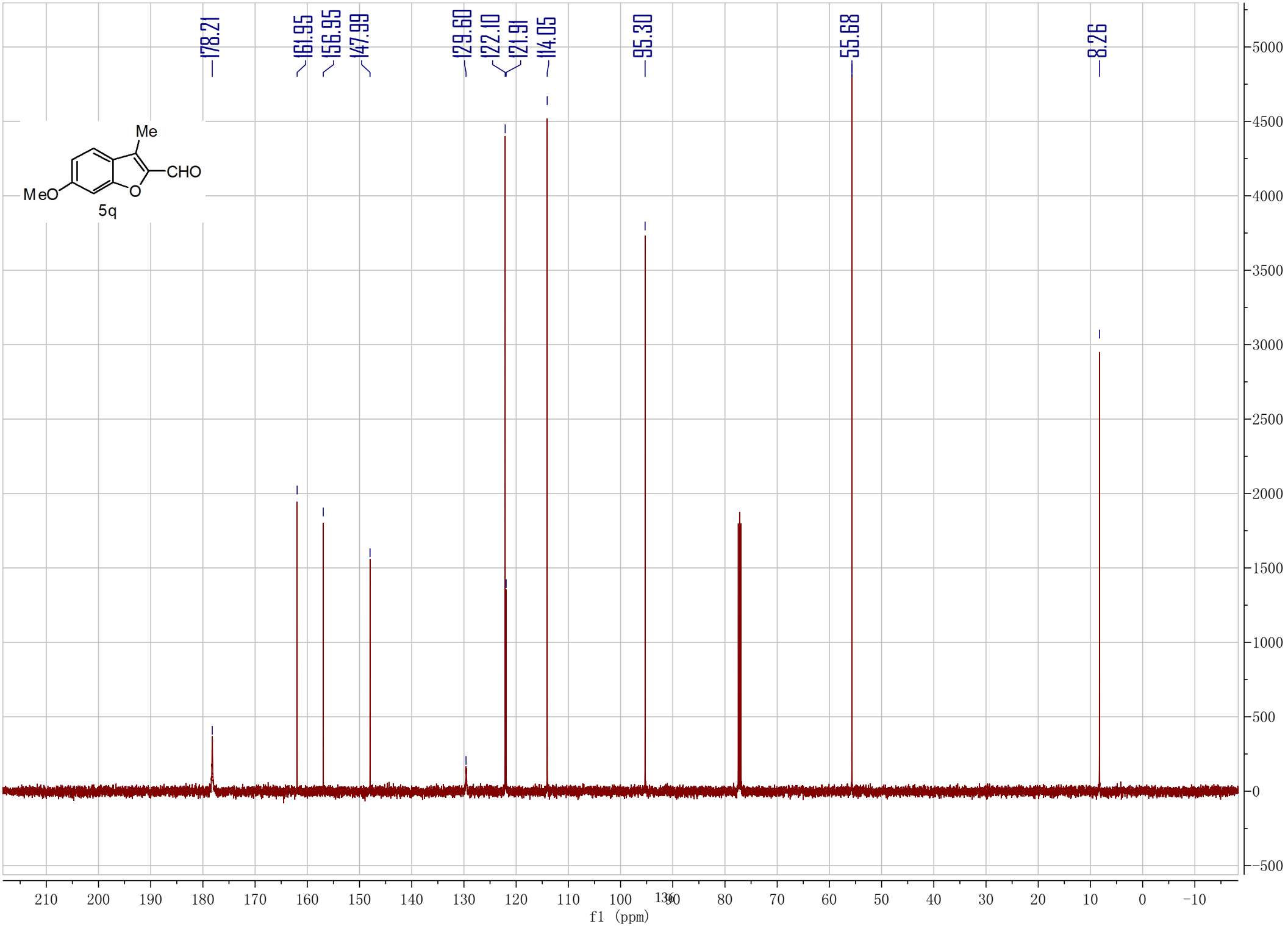

Et
CHO
O
5o
1.00
1.01
1.01
1.04
1.03
2.01
3.03
f1 (ppm)


179.47
155.51
147.53
134.79
129.21
127.73
123.55
121.99
112.62
16.90
15.07
Et
CHO
O
5o
f1 (ppm)

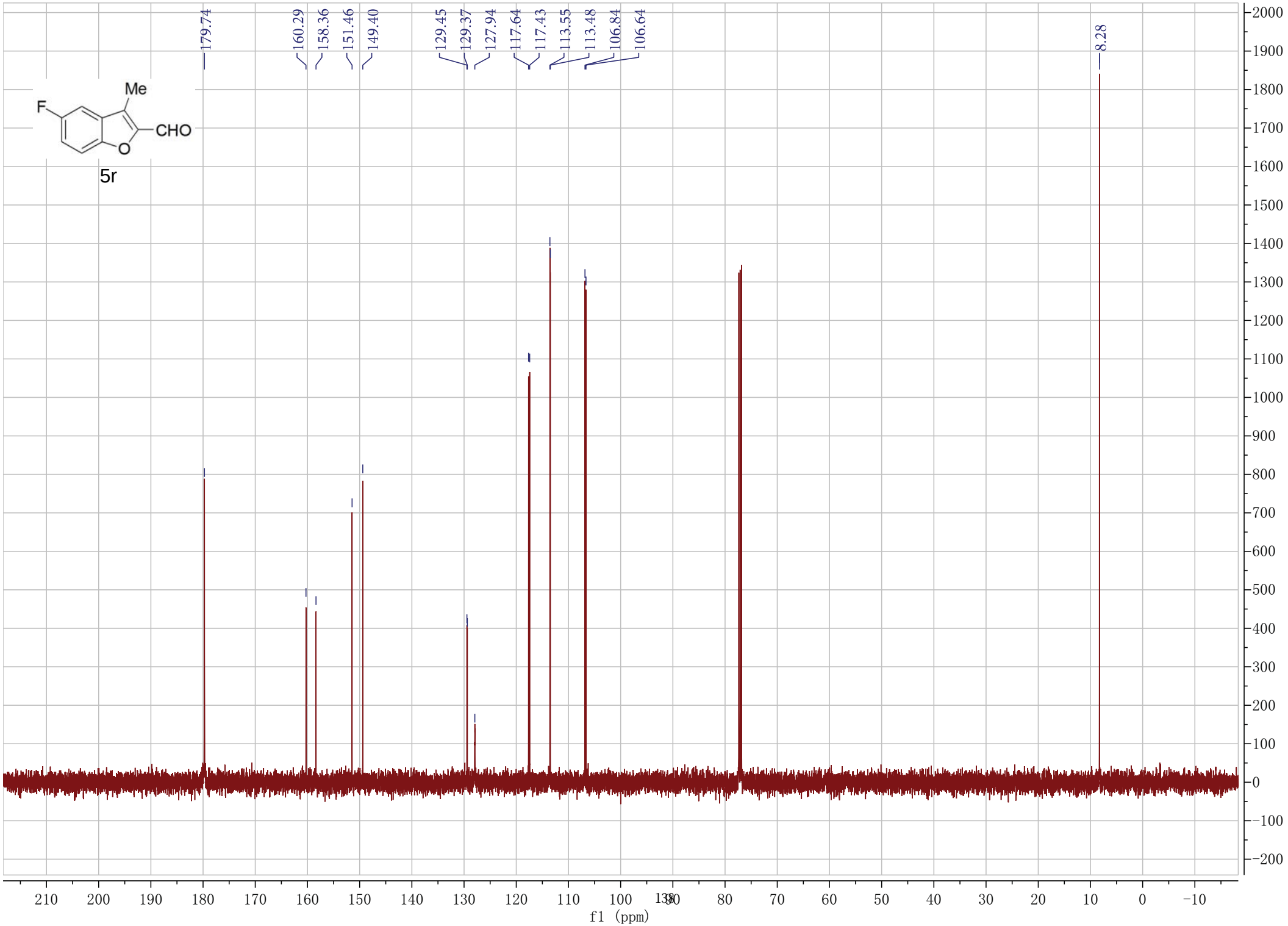

Ph
CHO
O
5p
0.97
0.99
1.00
1.01
1.02
2.71
1.02
2.01
2.02
2.08
f1 (ppm)

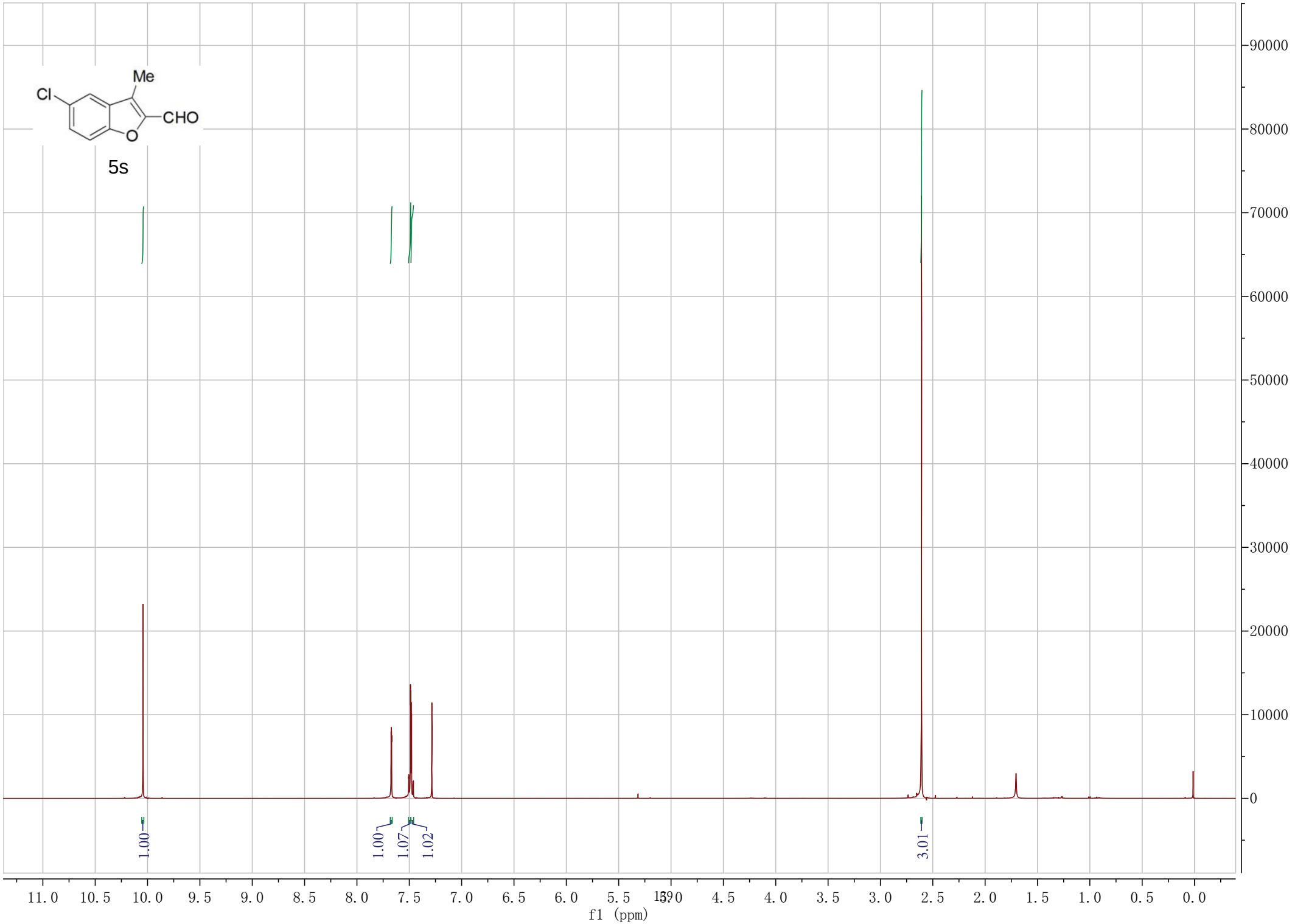

179.36
155.44
148.38
140.32
131.68
129.24
128.60
128.57
127.82
126.58
123.68
121.87
112.70
36.26
25.70
Ph
CHO
O
5p
f1 (ppm)

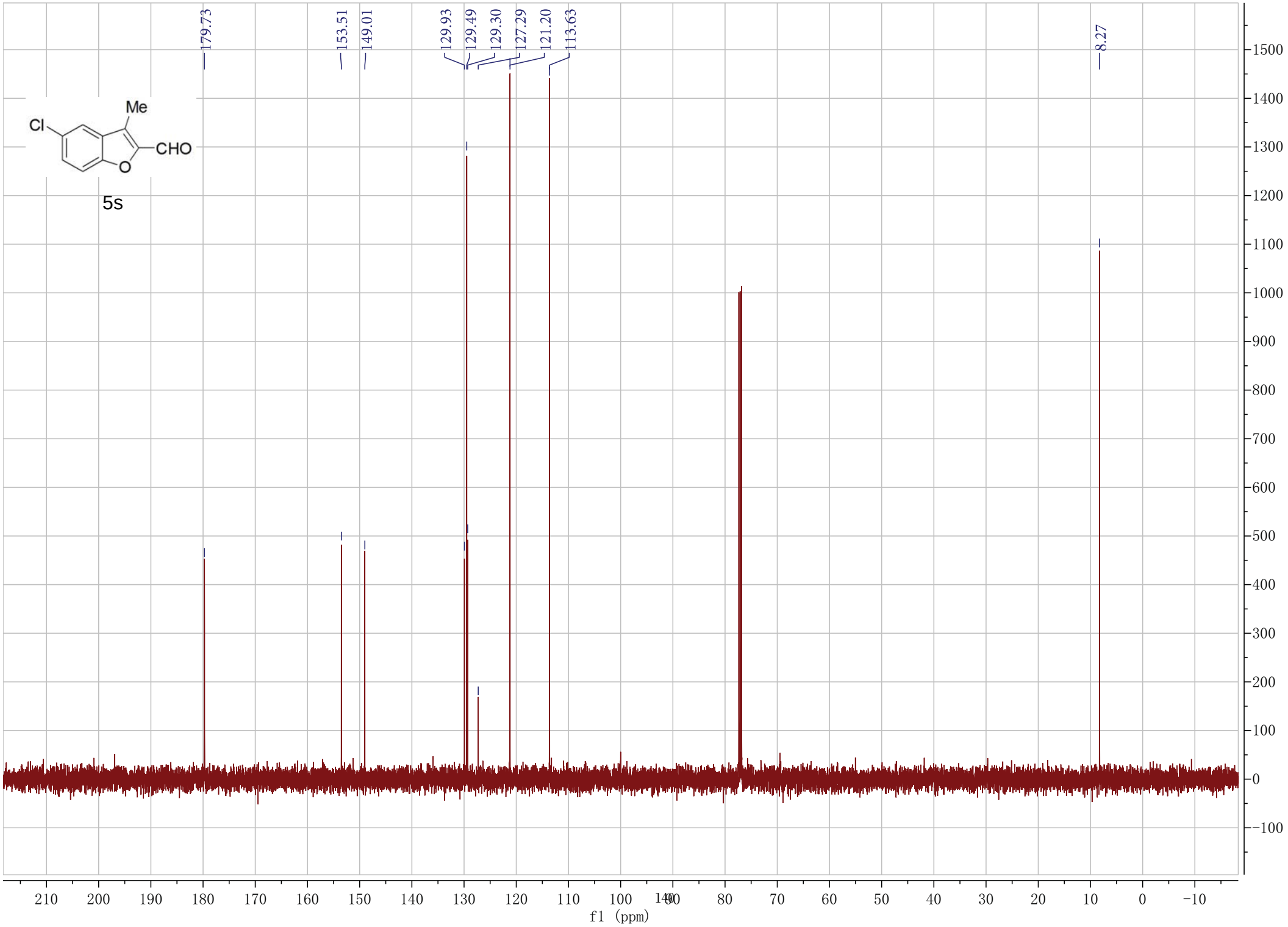
Me
CHO
MeO
O
5q
1.00
1.00
1.00
1.00
2.99
3.00
f1 (ppm)

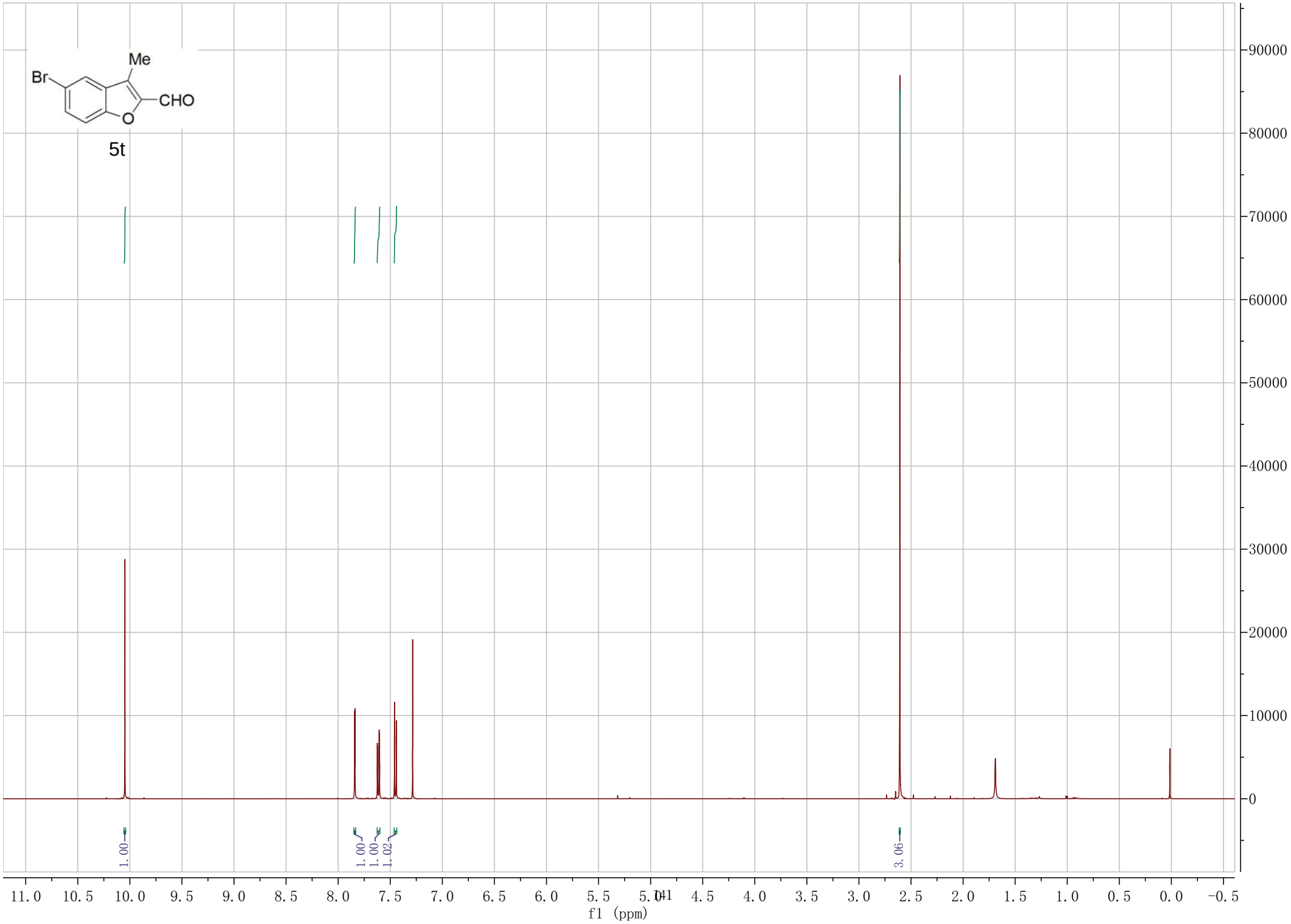

178.21
161.95
156.95
147.99
129.60
122.10
121.91
114.05
95.30
55.68
8.26
Me
CHO
MeO
O
5q
f1 (ppm)

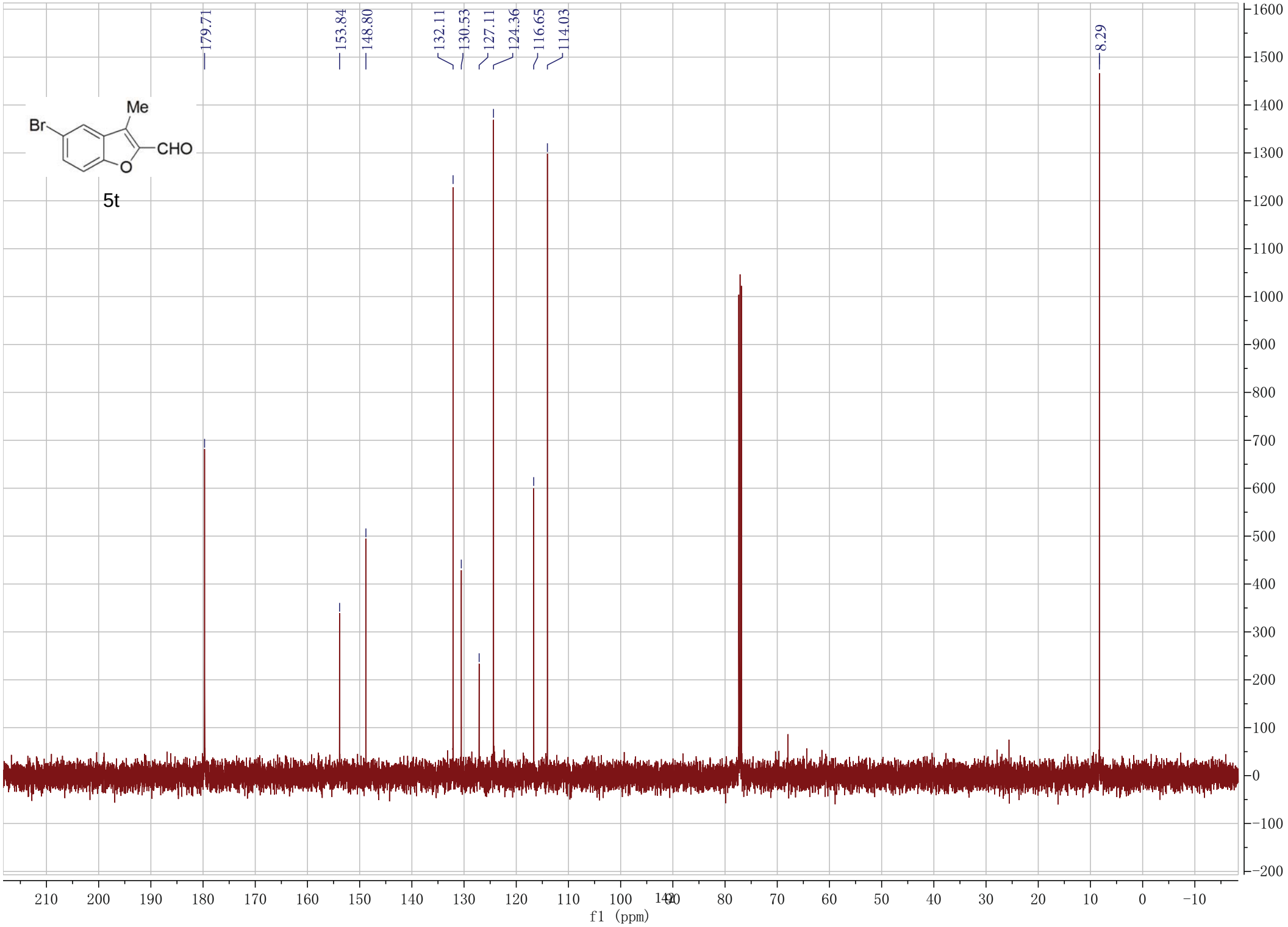
Me
F
CHO
O
5r
1.00
1.01
1.02
1.01
3.01
f1 (ppm)


179.74
160.29
158.36
151.46
149.40
129.45
129.37
127.94
117.64
117.43
113.55
113.48
106.84
106.64
8.28
Me
F
CHO
O
5r
f1 (ppm)

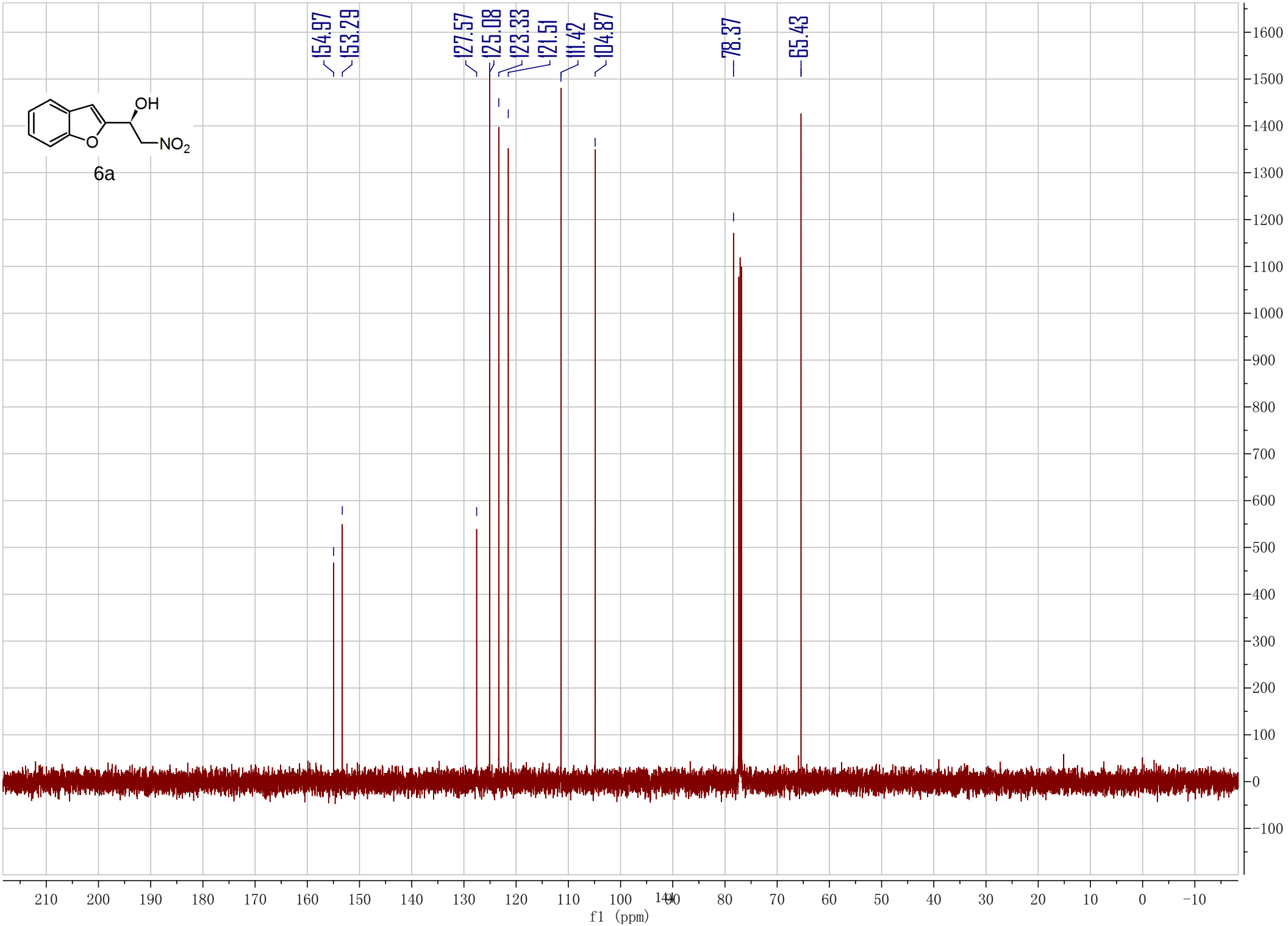

Me
Cl
CHO
O
5s
1.00
1.00
1.07
1.02
3.01
f1 (ppm)

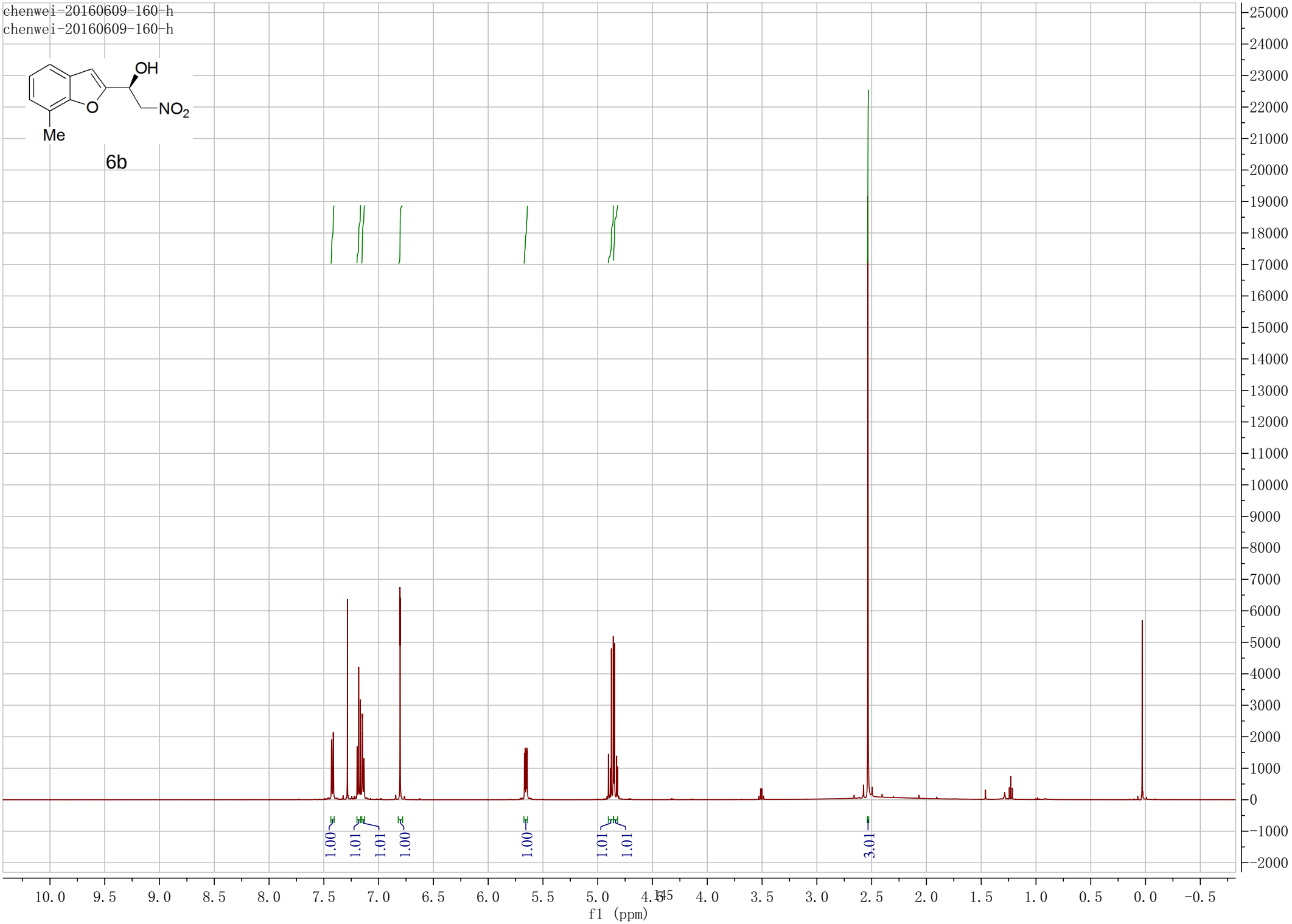

179.73
153.51
149.01
129.93
129.49
129.30
127.29
121.20
113.63
8.27
Me
Cl
CHO
O
5s
f1 (ppm)

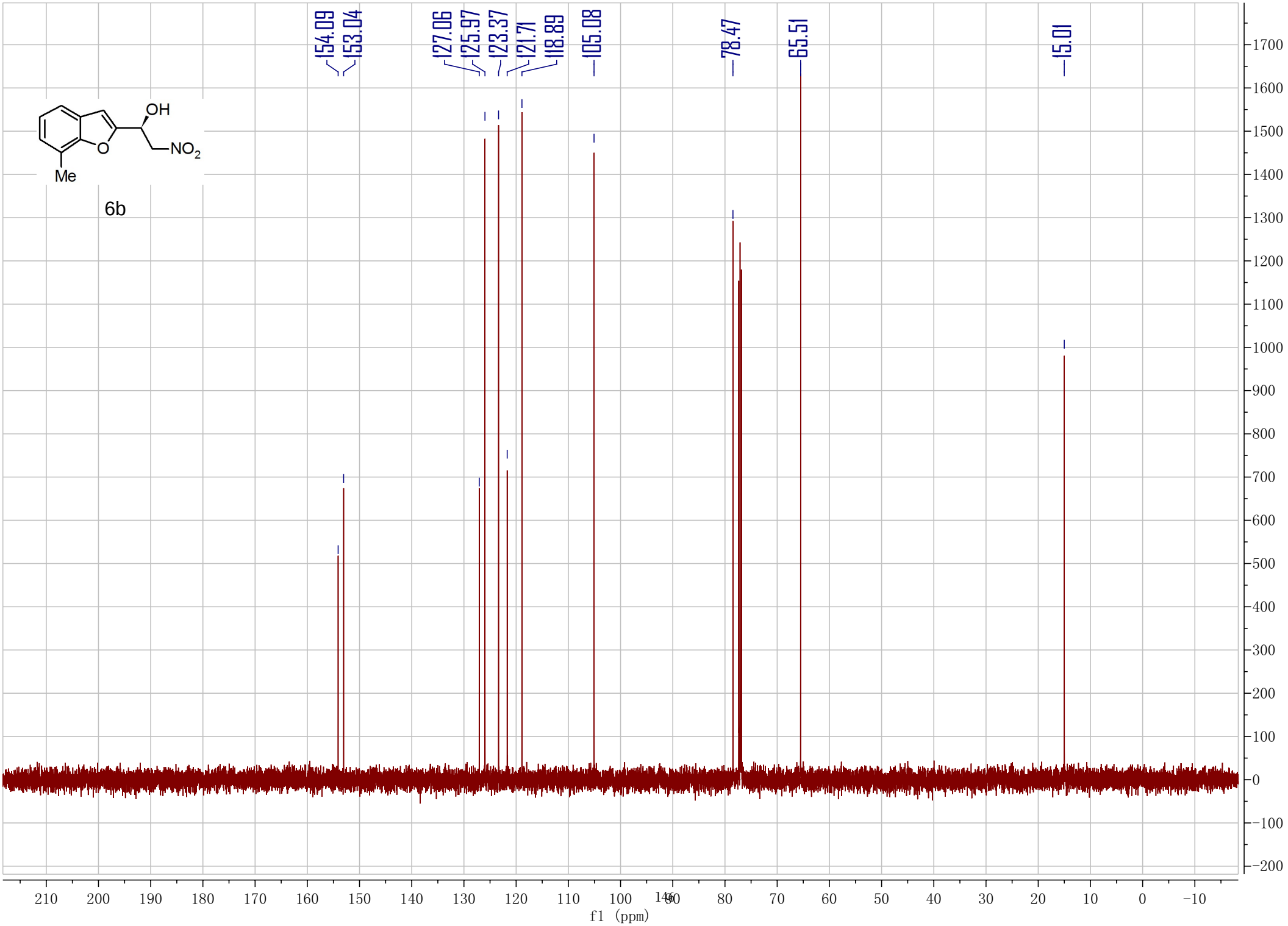

Me
Br
CHO
O
5t
1.00
1.00
1.00
1.02
3.06
f1 (ppm)

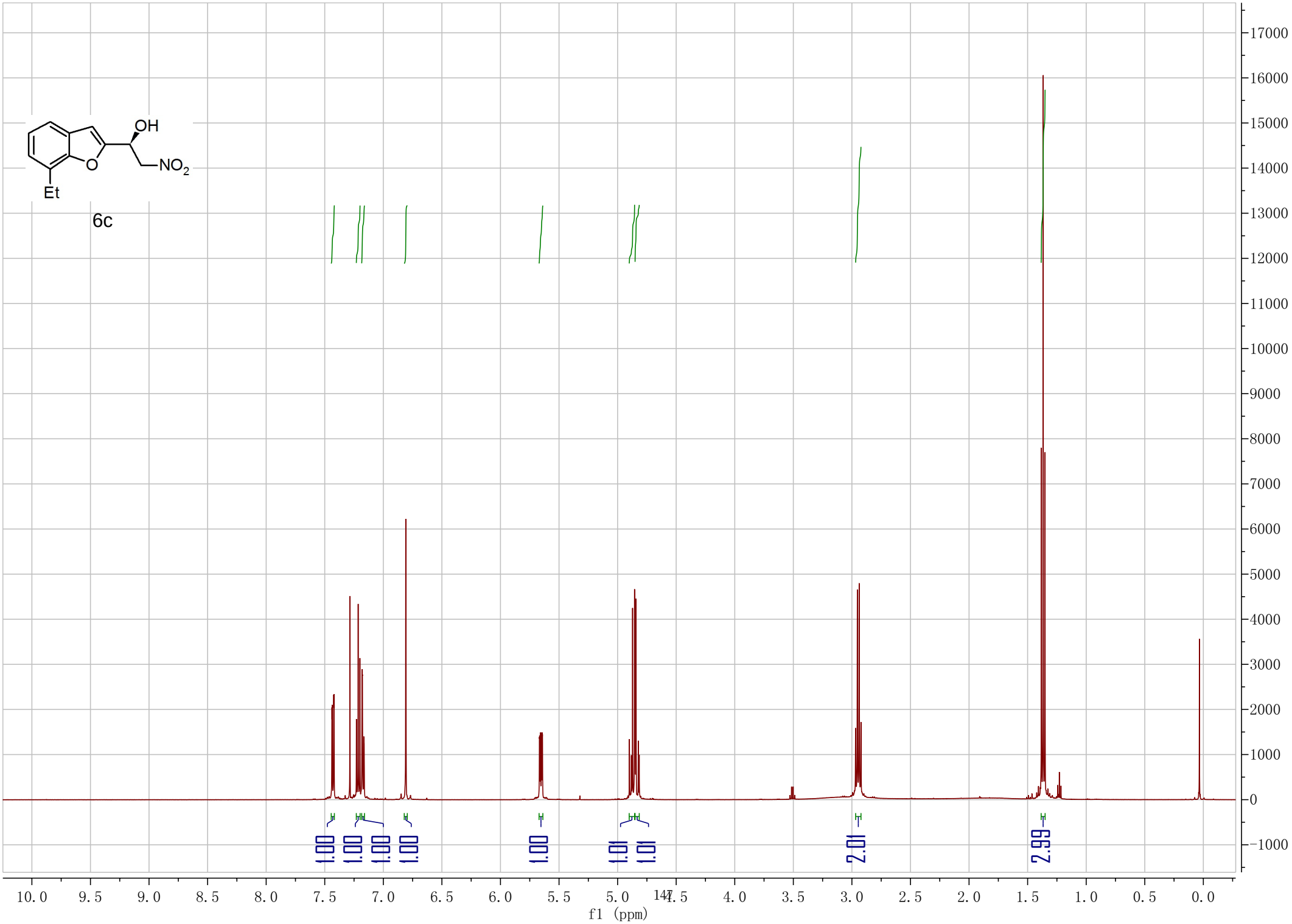

179.71
153.84
148.80
132.11
130.53
127.11
124.36
116.65
114.03
8.29
Me
Br
CHO
O
5t
f1 (ppm)

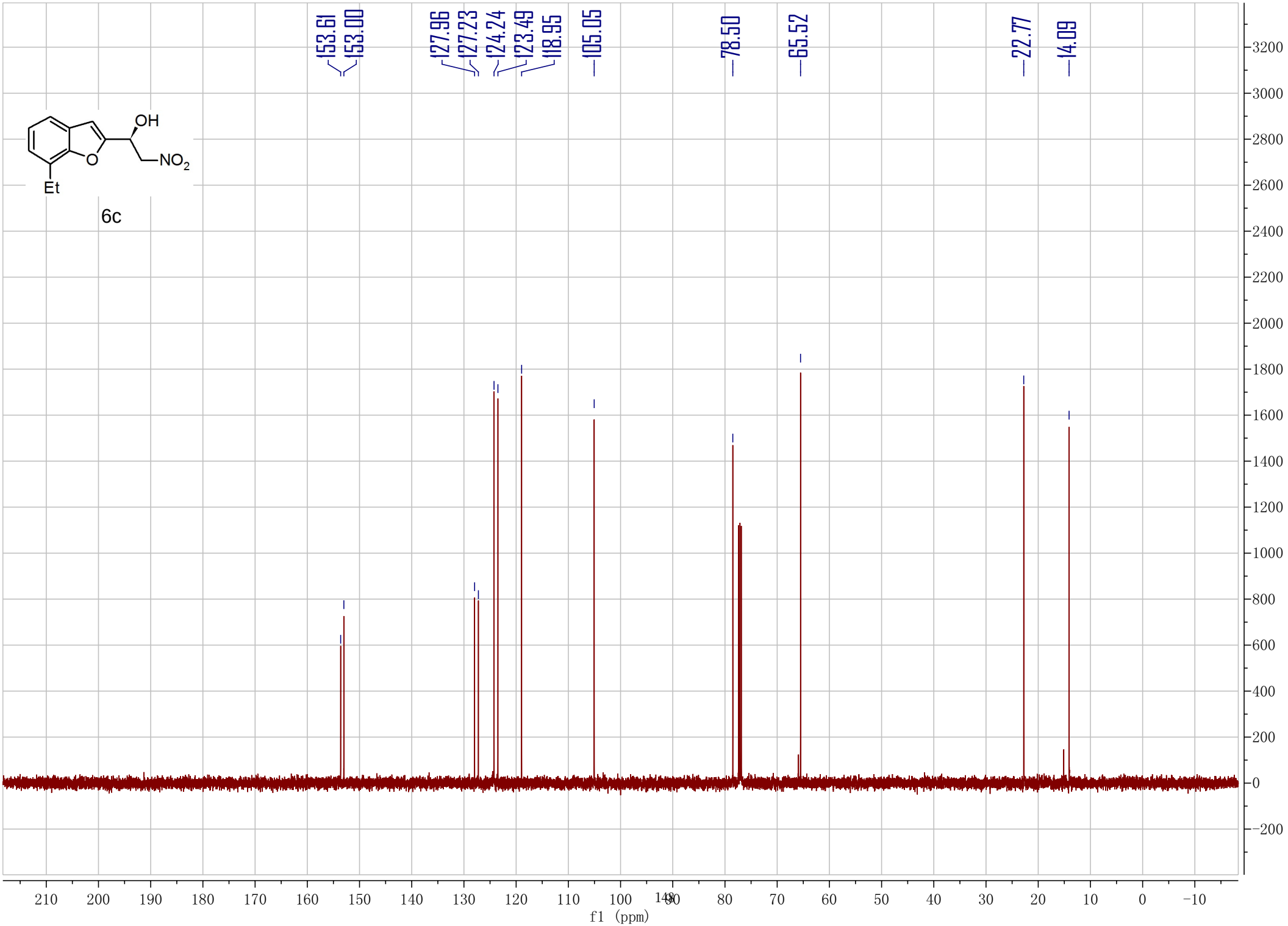
OH
O
NO2
6a
1.00
1.00
1.01
0.38
0.67
1.00
1.00
1.01
1.01
1.01
f1 (ppm)

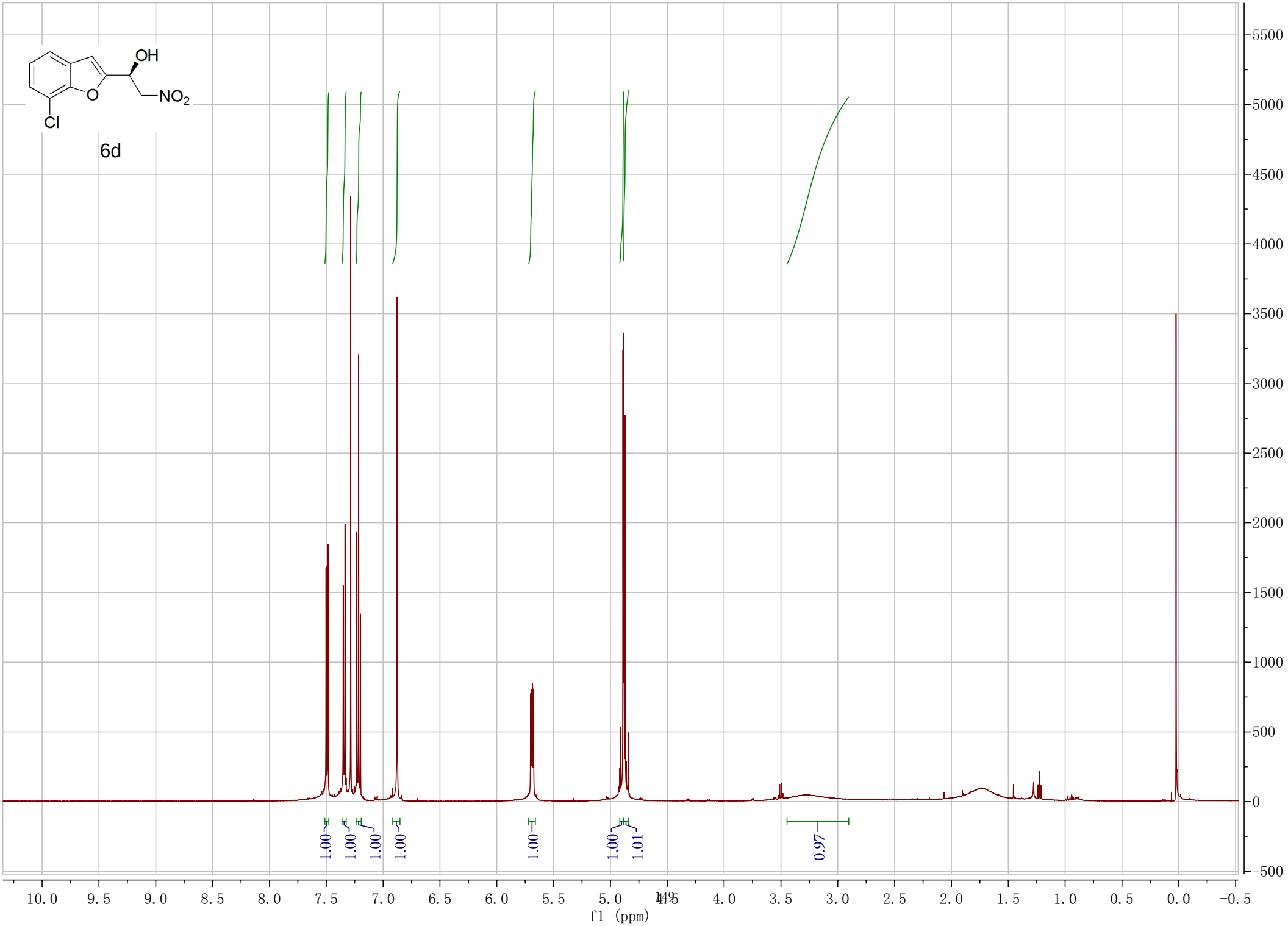

154.97
153.29
127.57
125.08
123.33
121.51
111.42
104.87
78.37
65.43
OH
O
NO2
6a
f1 (ppm)

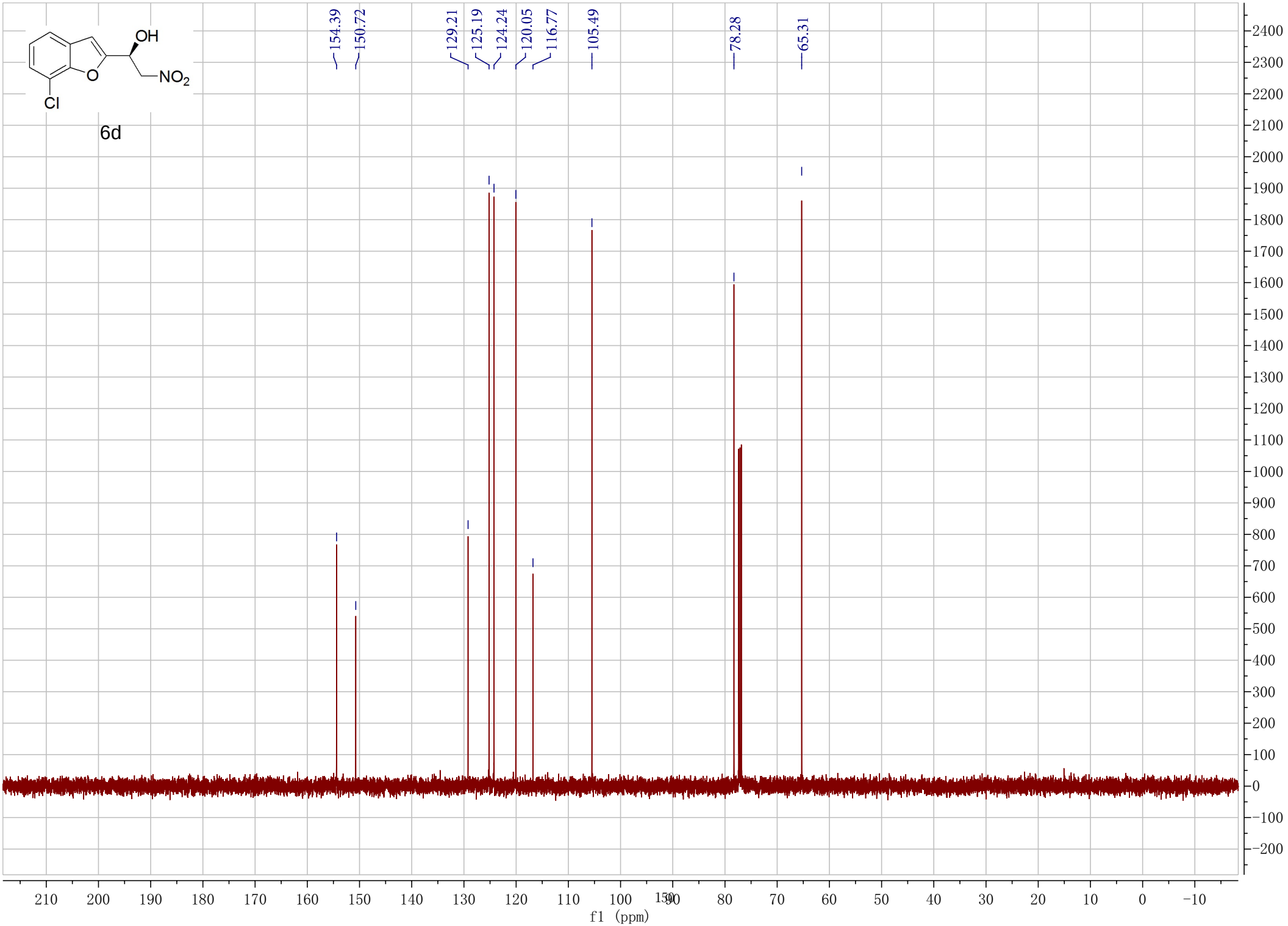

chenwei-20160609-160-h
chenwei-20160609-160-h
OH
O
NO2
Me
6b
1.00
1.01
1.01
1.00
1.00
1.01
1.01
3.01
f1 (ppm)


154.09
153.04
127.06
125.97
123.37
121.71
118.89
105.08
78.47
65.51
15.01
OH
NO2
Me
6b
f1 (ppm)

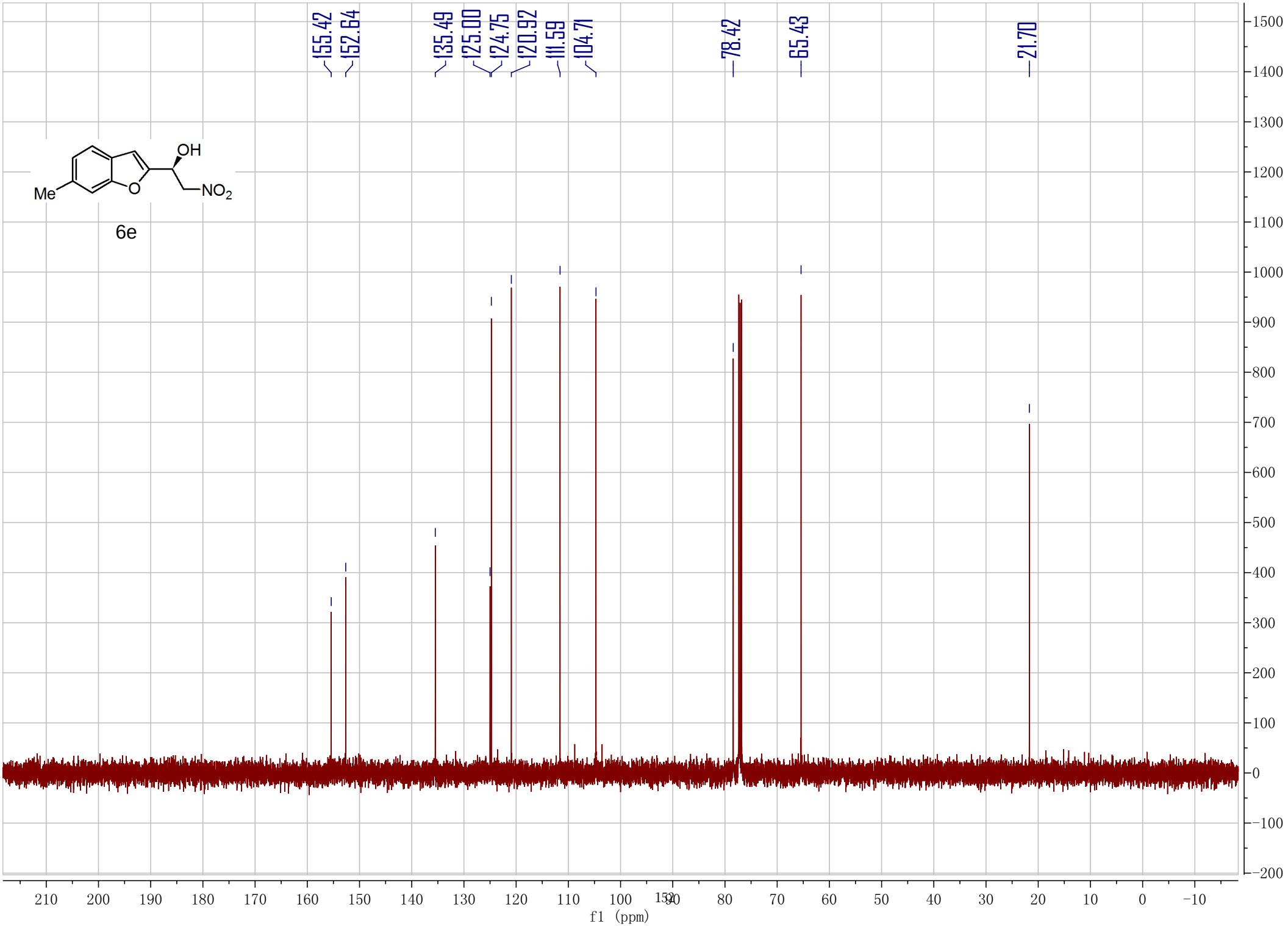

OH
NO2
Et
6c
1.00
1.00
1.00
1.00
1.00
1.01
1.01
2.01
2.99
f1 (ppm)

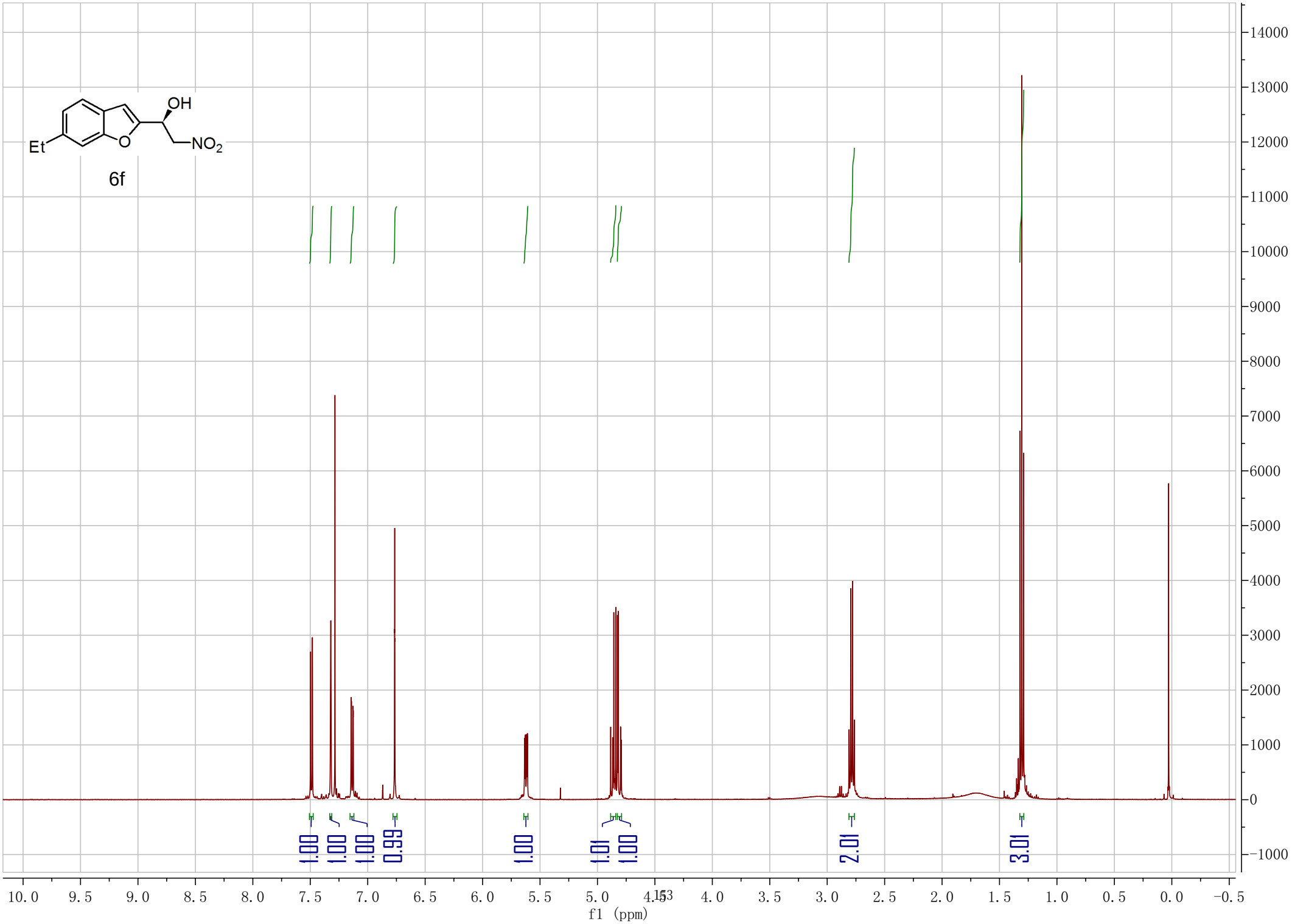

153.61
153.00
127.96
127.23
124.24
123.49
118.95
105.05
78.50
65.52
22.77
14.09
OH
NO2
Et
6c
f1 (ppm)

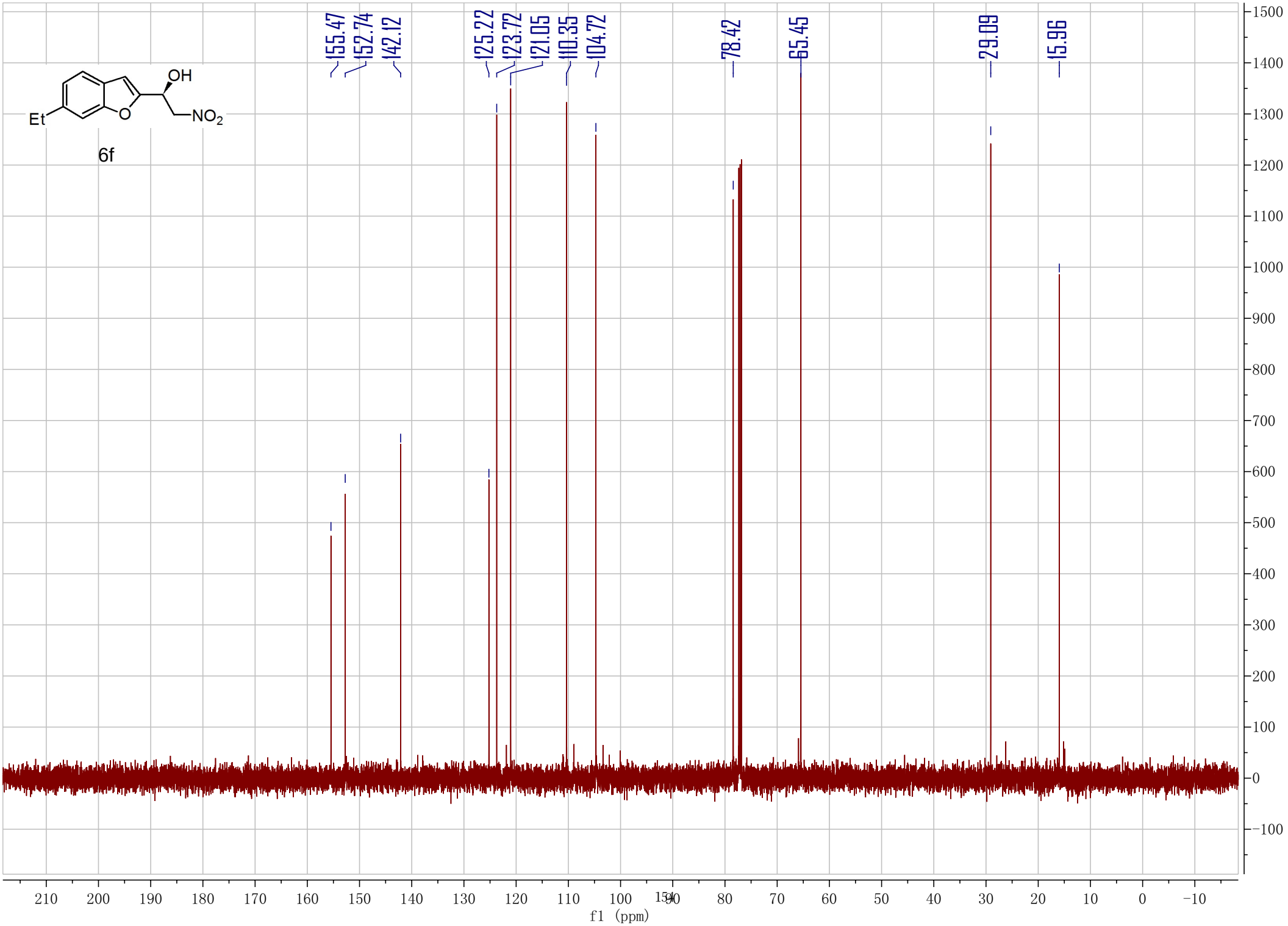

OH
O
NO2
Cl
6d
1.00
1.00
1.00
1.00
1.00
1.00
1.01
0.97
f1 (ppm)

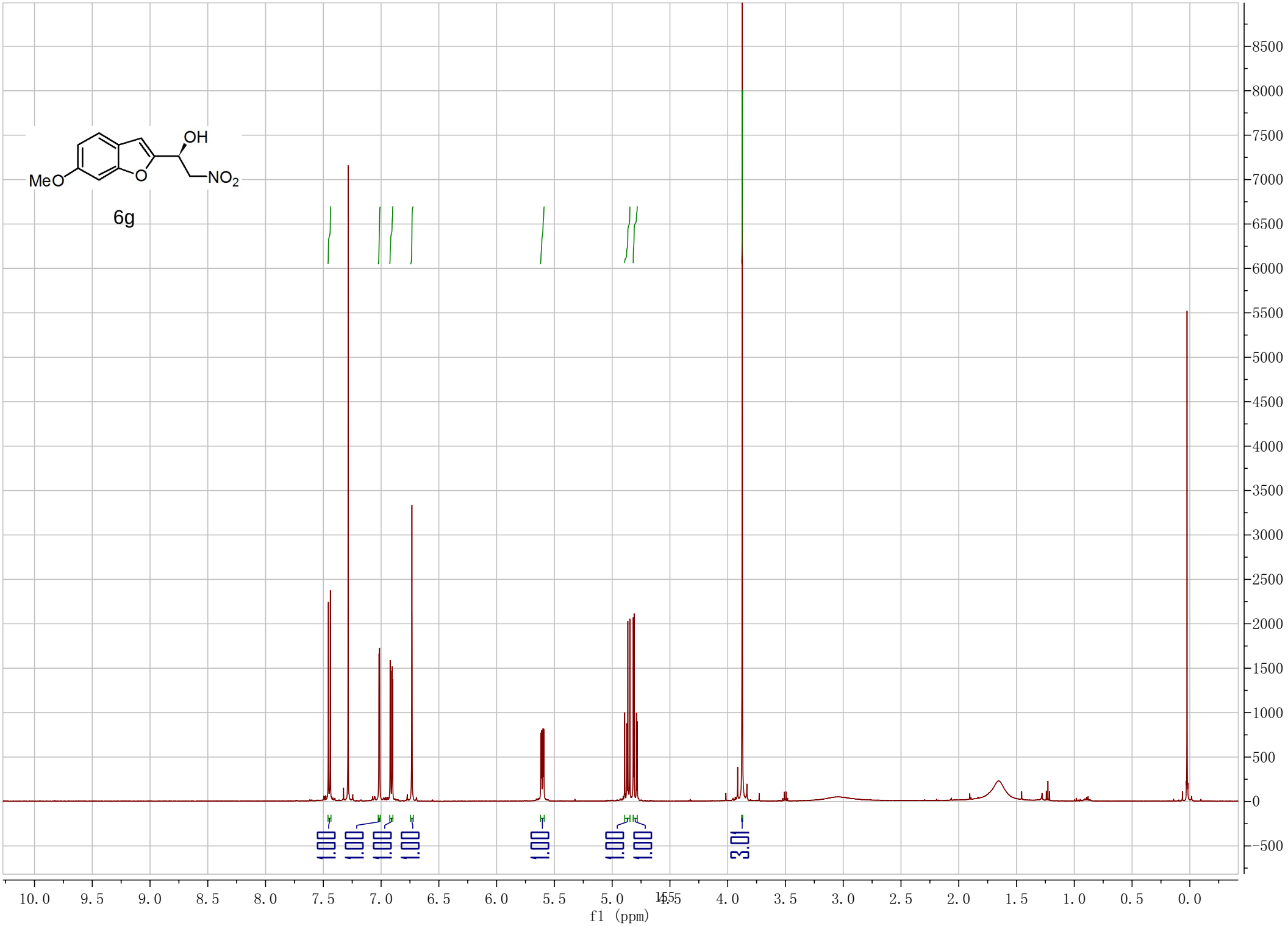

OH
O
NO2
Cl
6d
154.39
150.72
129.21
125.19
124.24
120.05
116.77
105.49
78.28
65.31
f1 (ppm)

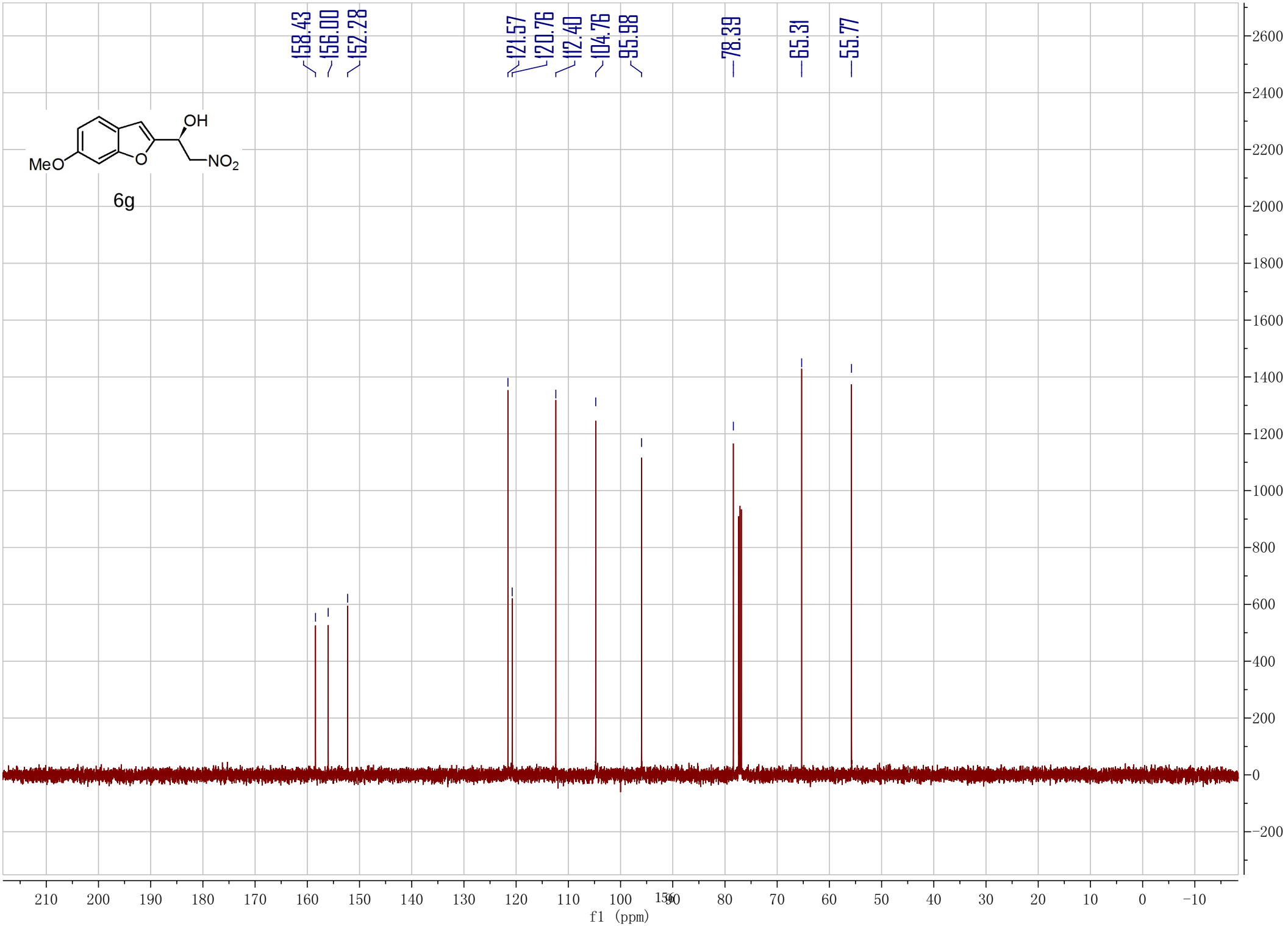
OH
Me
O
NO2
6e
1.00
1.00
1.00
1.00
1.00
1.00
1.00
3.00
f1 (ppm)

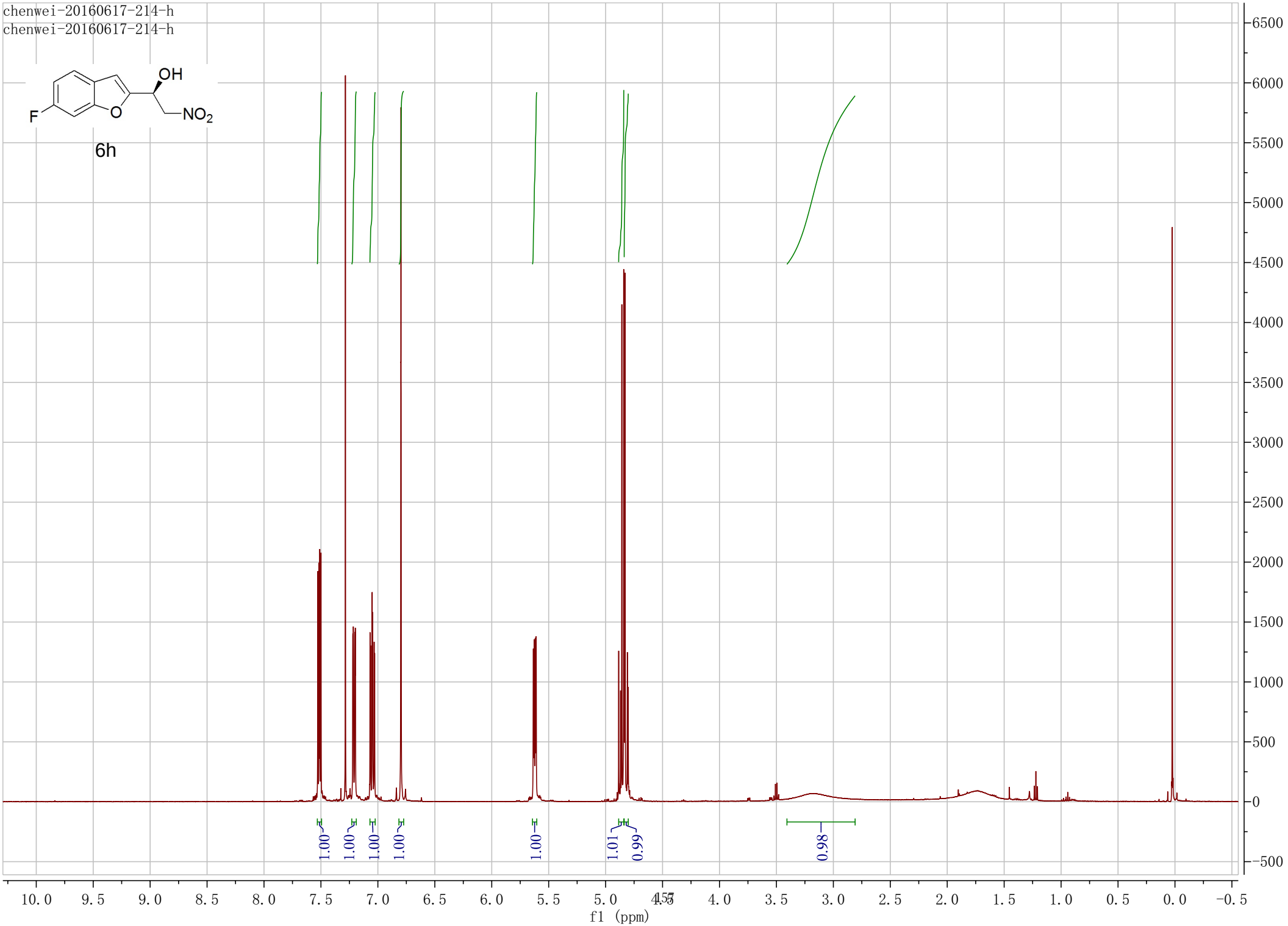

155.42
152.64
135.49
125.00
124.75
120.92
111.59
104.71
78.42
65.43
21.70
OH
Me
O
NO2
6e
f1 (ppm)

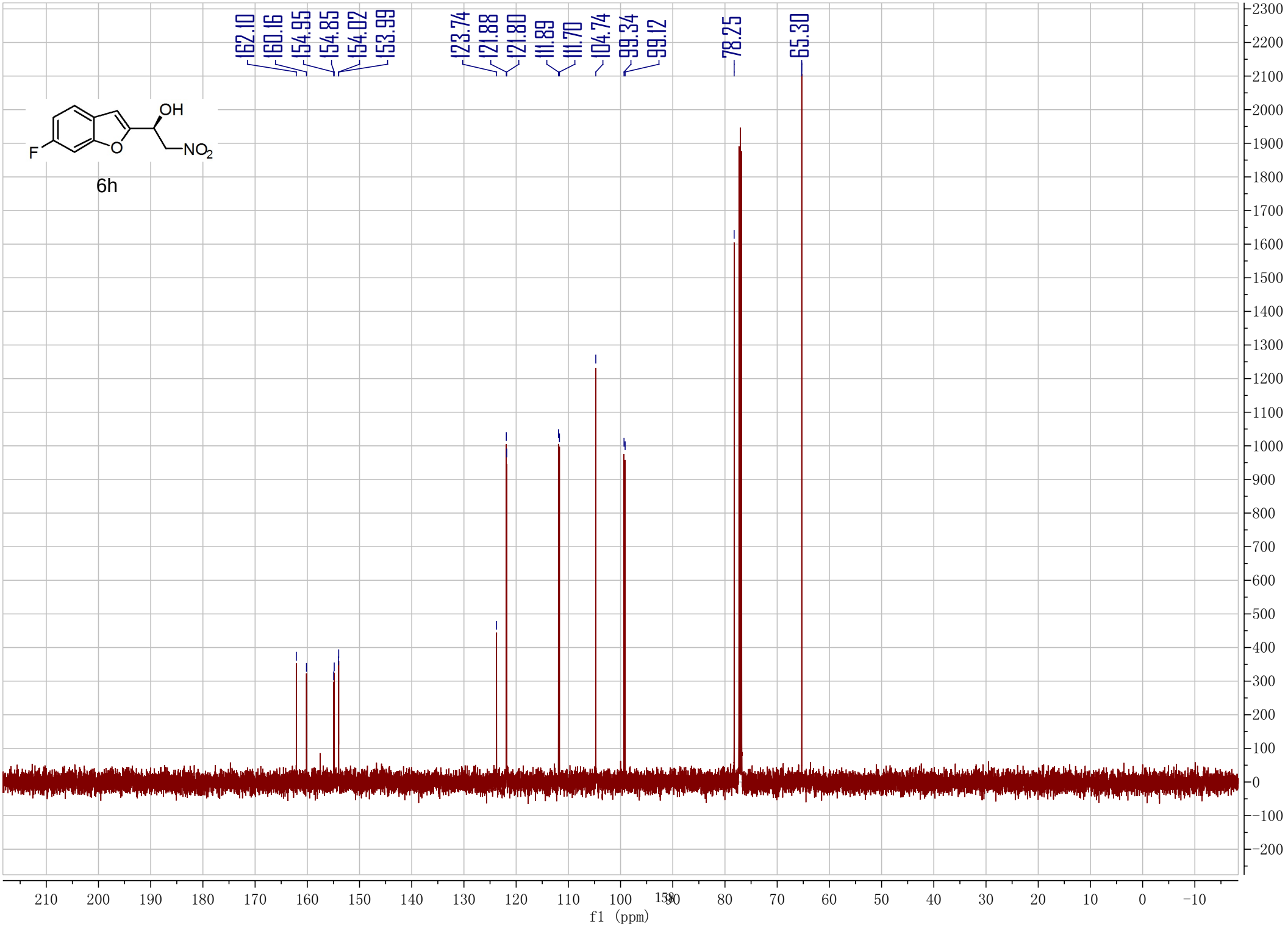

OH
Et
O
NO2
6f
1.00
1.00
1.00
0.99
1.00
1.01
1.00
2.01
3.01
f1 (ppm)

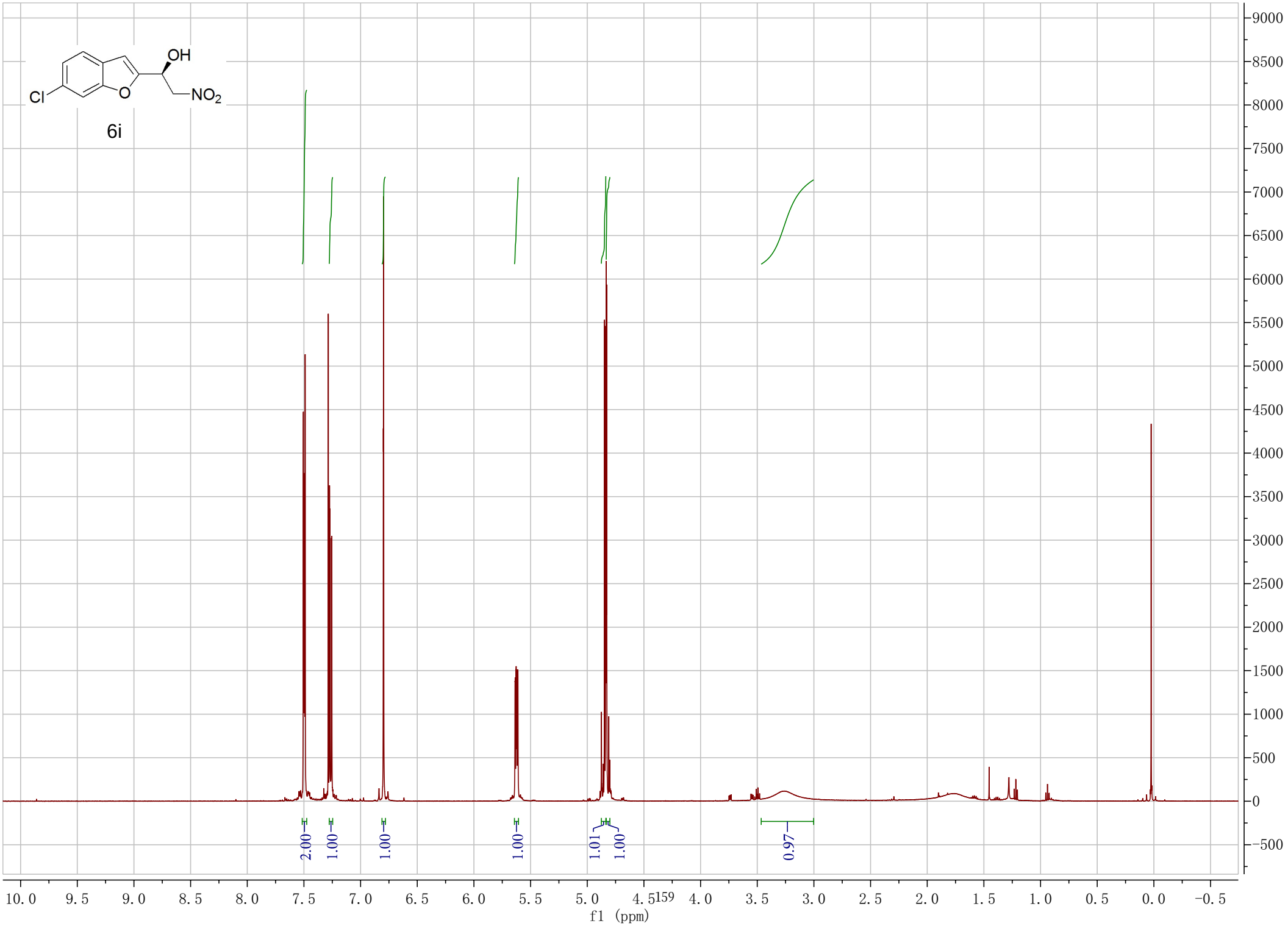

155.47
152.74
142.12
125.22
123.72
121.05
110.35
104.72
78.42
65.45
29.09
15.96
OH
Et
O
NO2
6f
f1 (ppm)

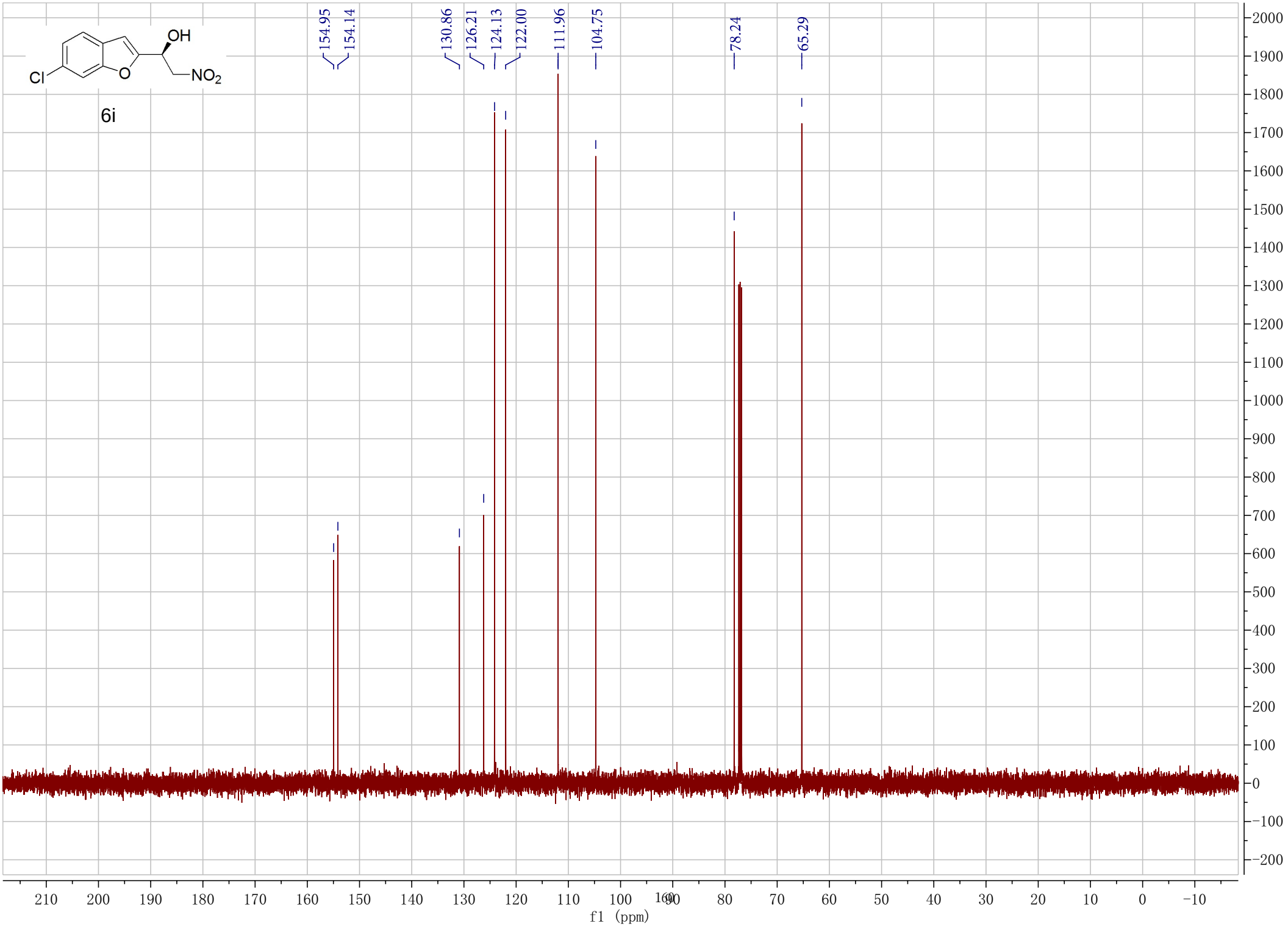

OH
MeO
O
NO2
6g
1.00
1.00
1.00
1.00
1.00
1.00
1.00
3.01
f1 (ppm)

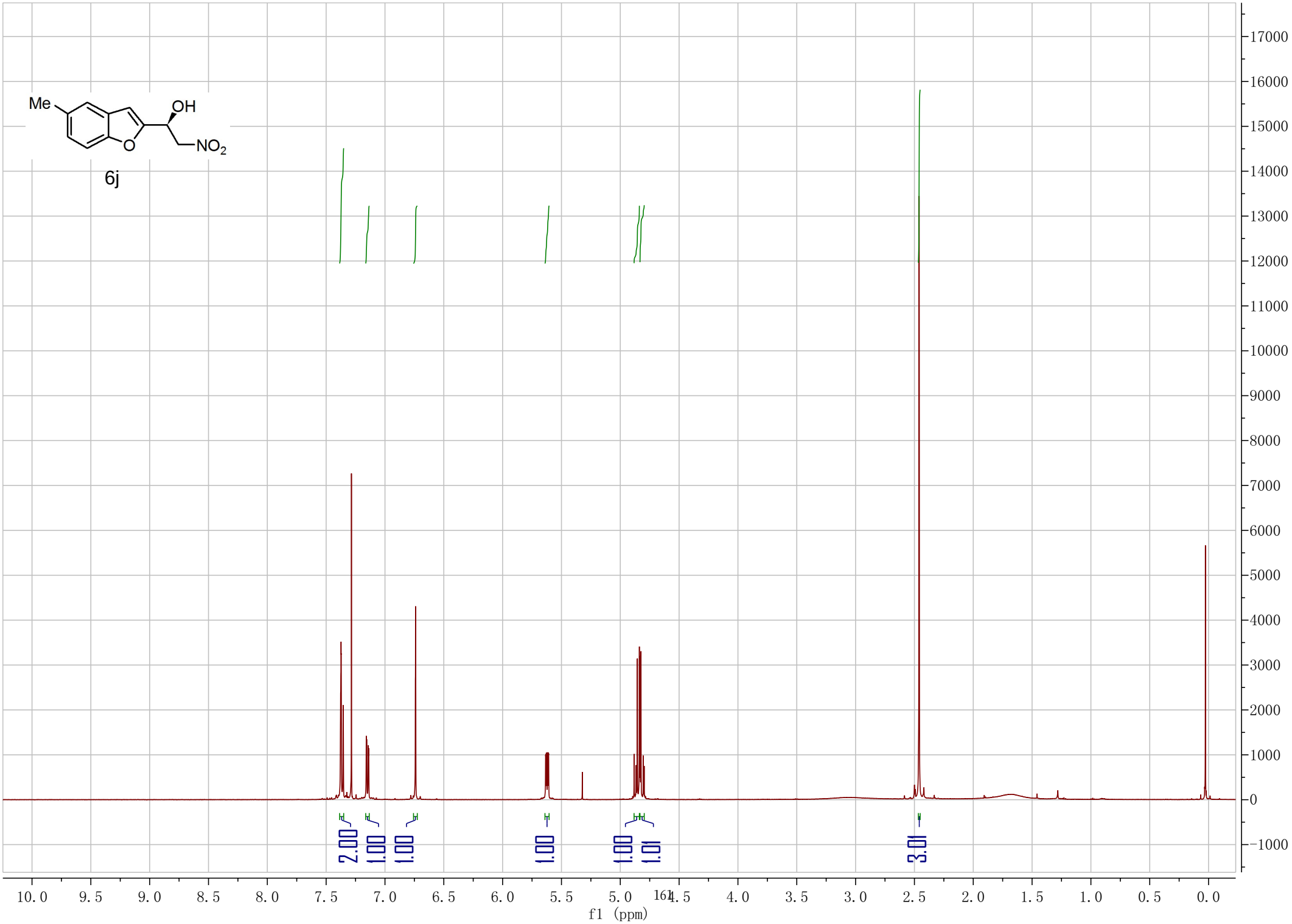

158.43
156.00
152.28
121.57
120.76
112.40
104.76
95.98
78.39
65.31
55.77
OH
MeO
O
NO2
6g
f1 (ppm)

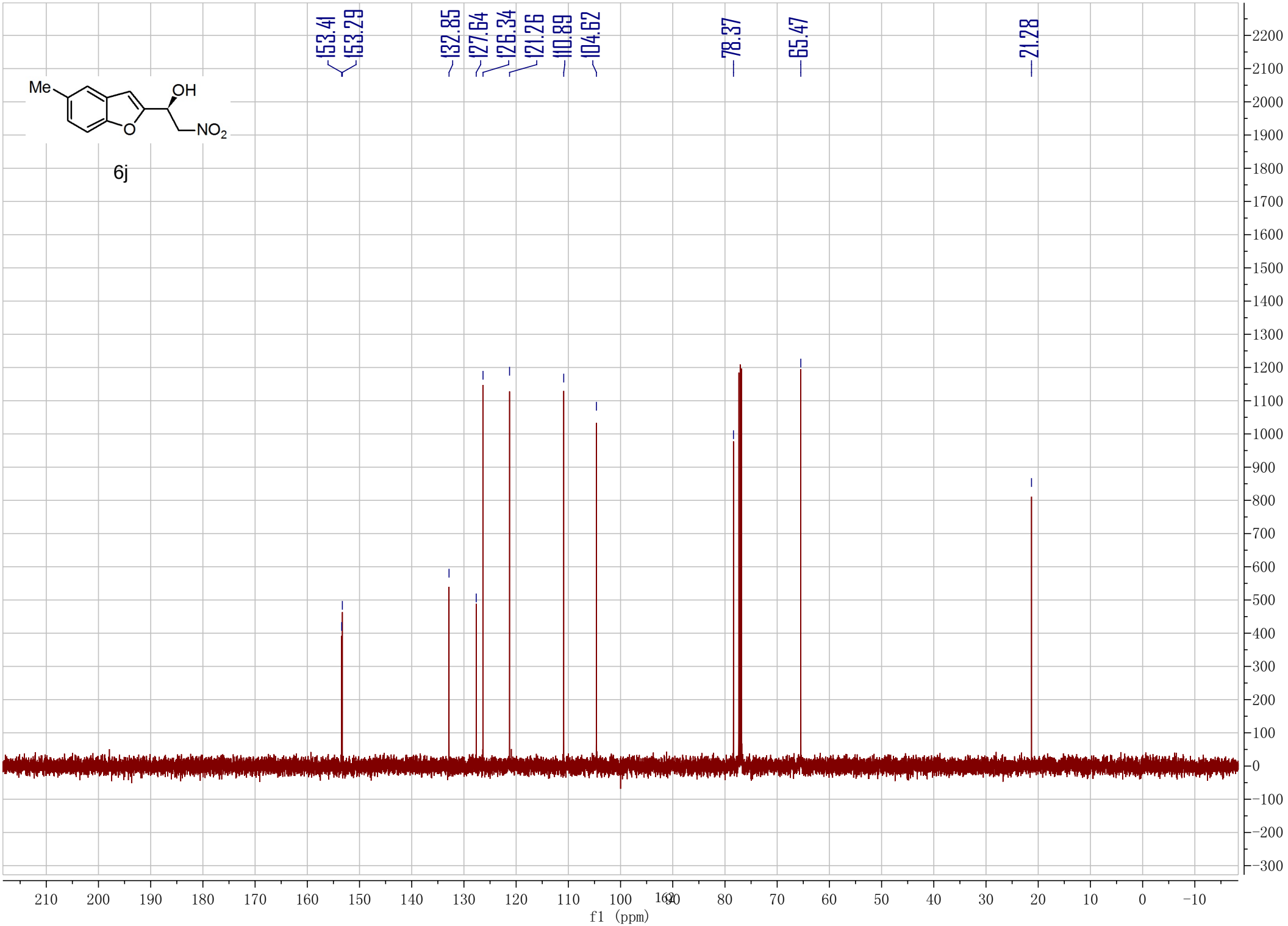

chenwei-20160617-214-h
chenwei-20160617-214-h
OH
F
O
NO2
6h
1.00
1.00
1.00
1.00
1.00
1.01
0.99
0.98
f1 (ppm)

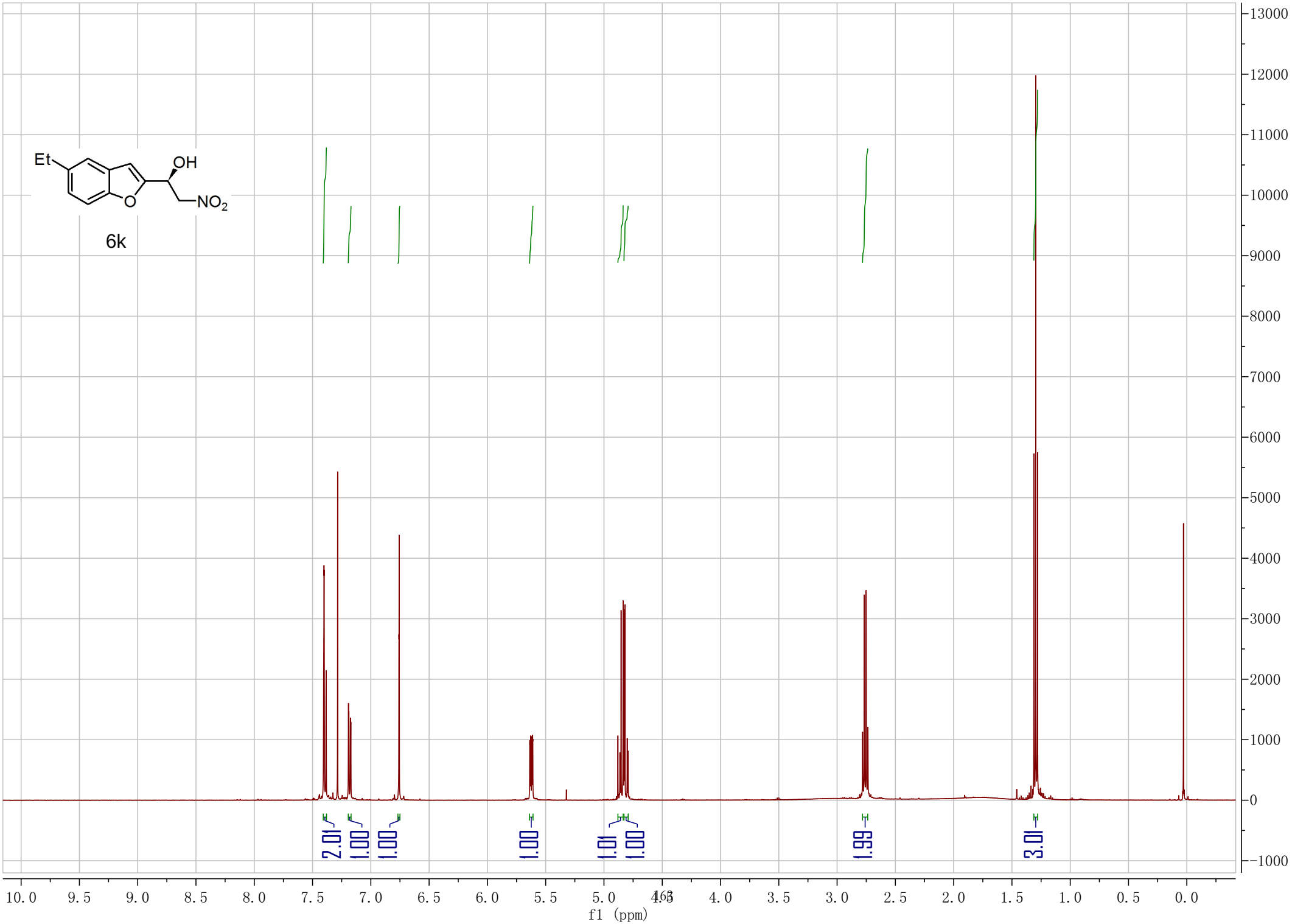

162.10
160.16
154.95
154.85
154.02
153.99
123.74
121.88
121.80
111.89
111.70
104.74
99.34
99.12
78.25
65.30
OH
F
O
NO2
6h
f1 (ppm)

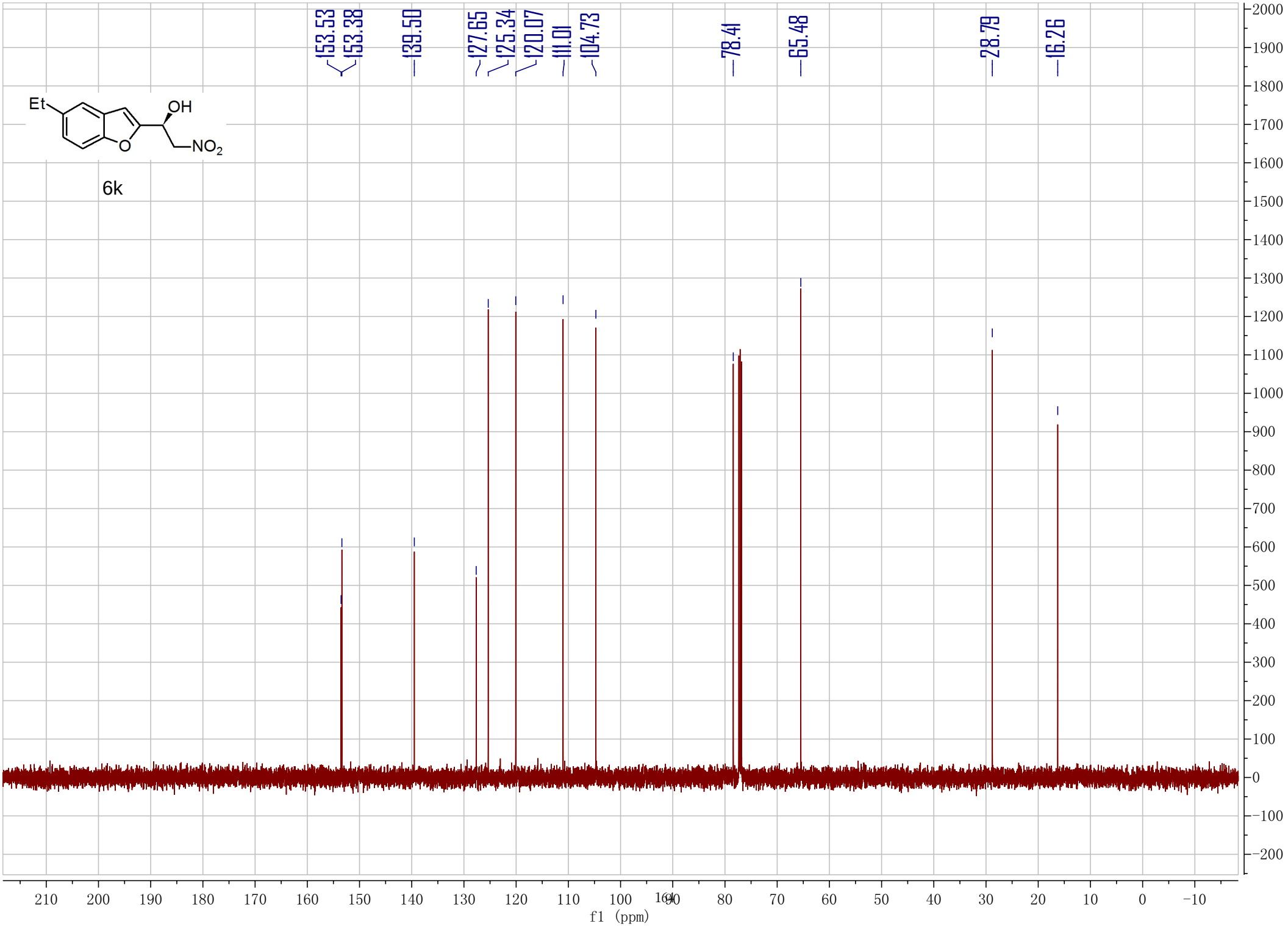

OH
Cl
O
NO2
6i
2.00
1.00
1.00
1.00
1.01
1.00
0.97
f1 (ppm)

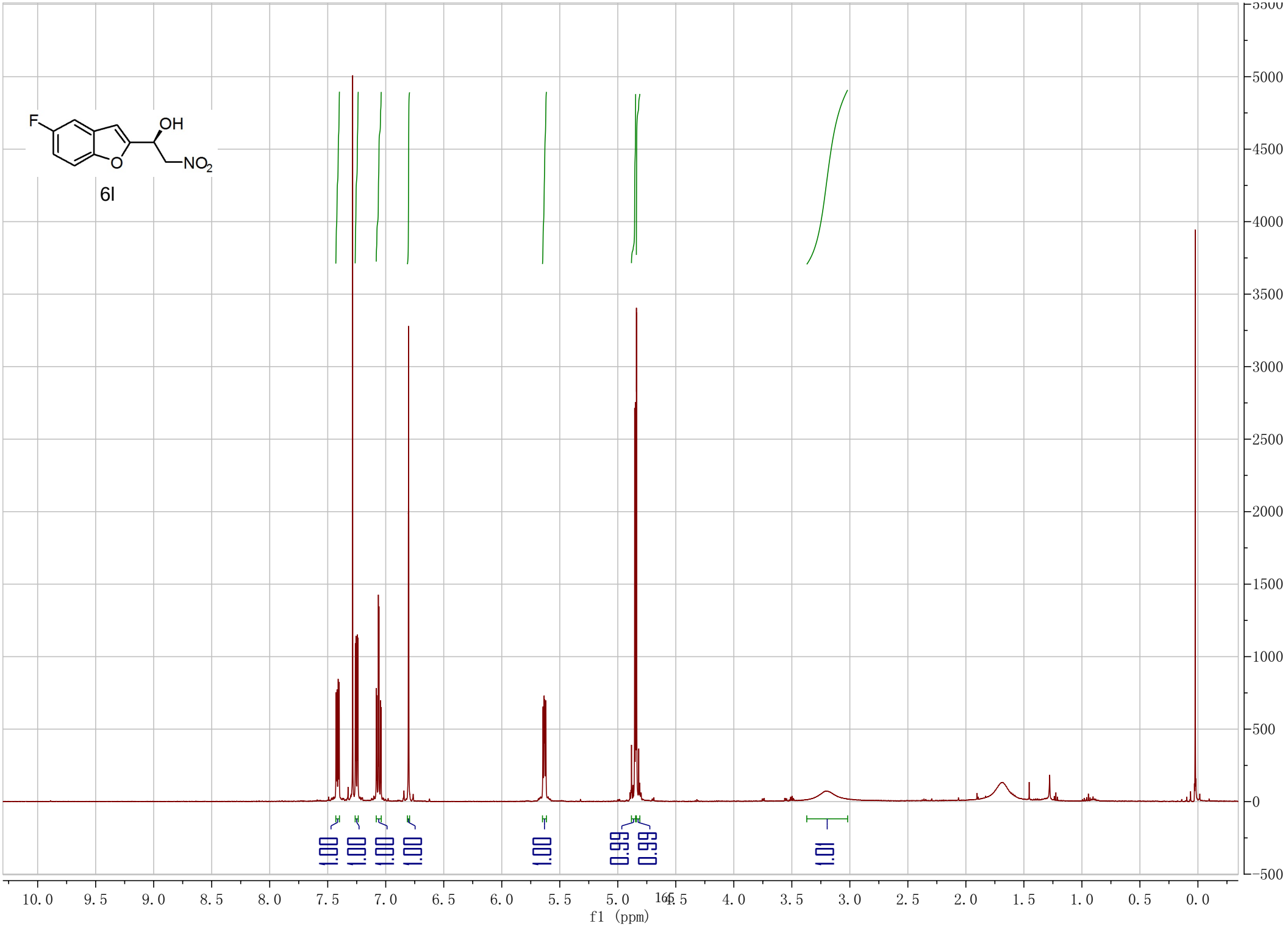

OH
Cl
O
NO2
6i
154.95
154.14
130.86
126.21
124.13
122.00
111.96
104.75
78.24
65.29
f1 (ppm)

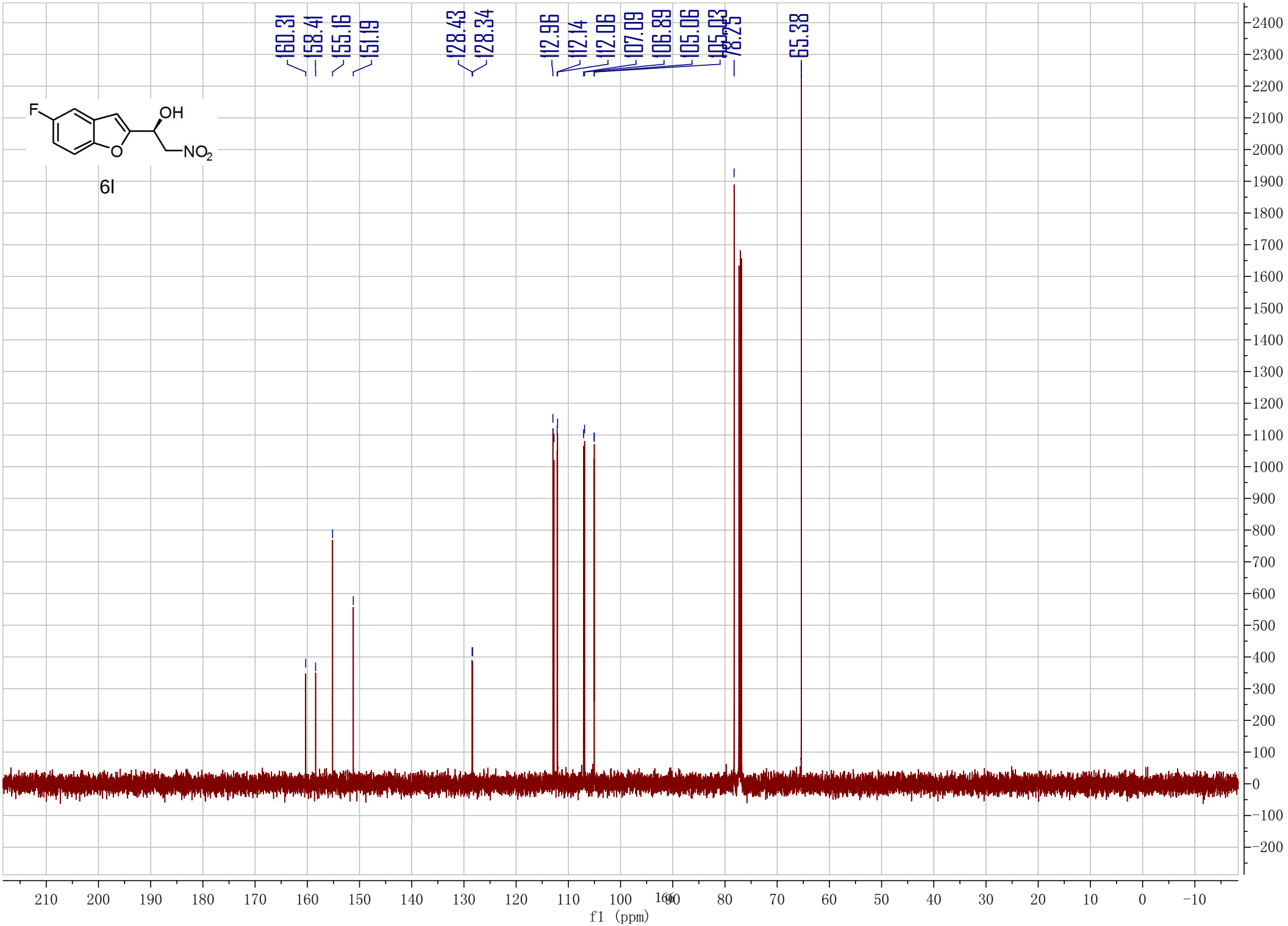

Me
OH
O
NO2
6j
2.00
1.00
1.00
1.00
1.00
1.01
3.01
f1 (ppm)

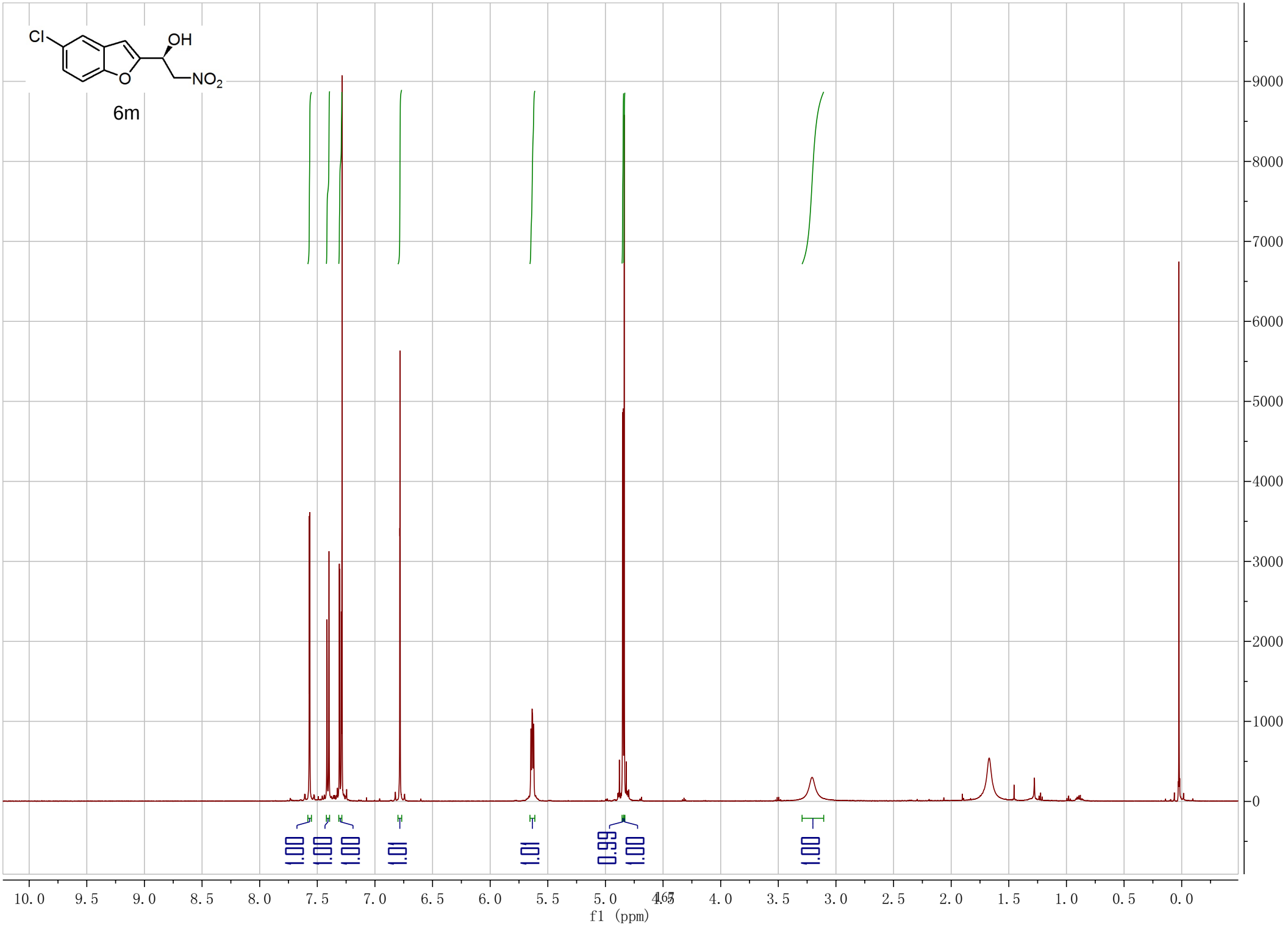

153.41
153.29
132.85
127.64
126.34
121.26
110.89
104.62
78.37
65.47
21.28
Me
OH
O
NO2
6j
f1 (ppm)

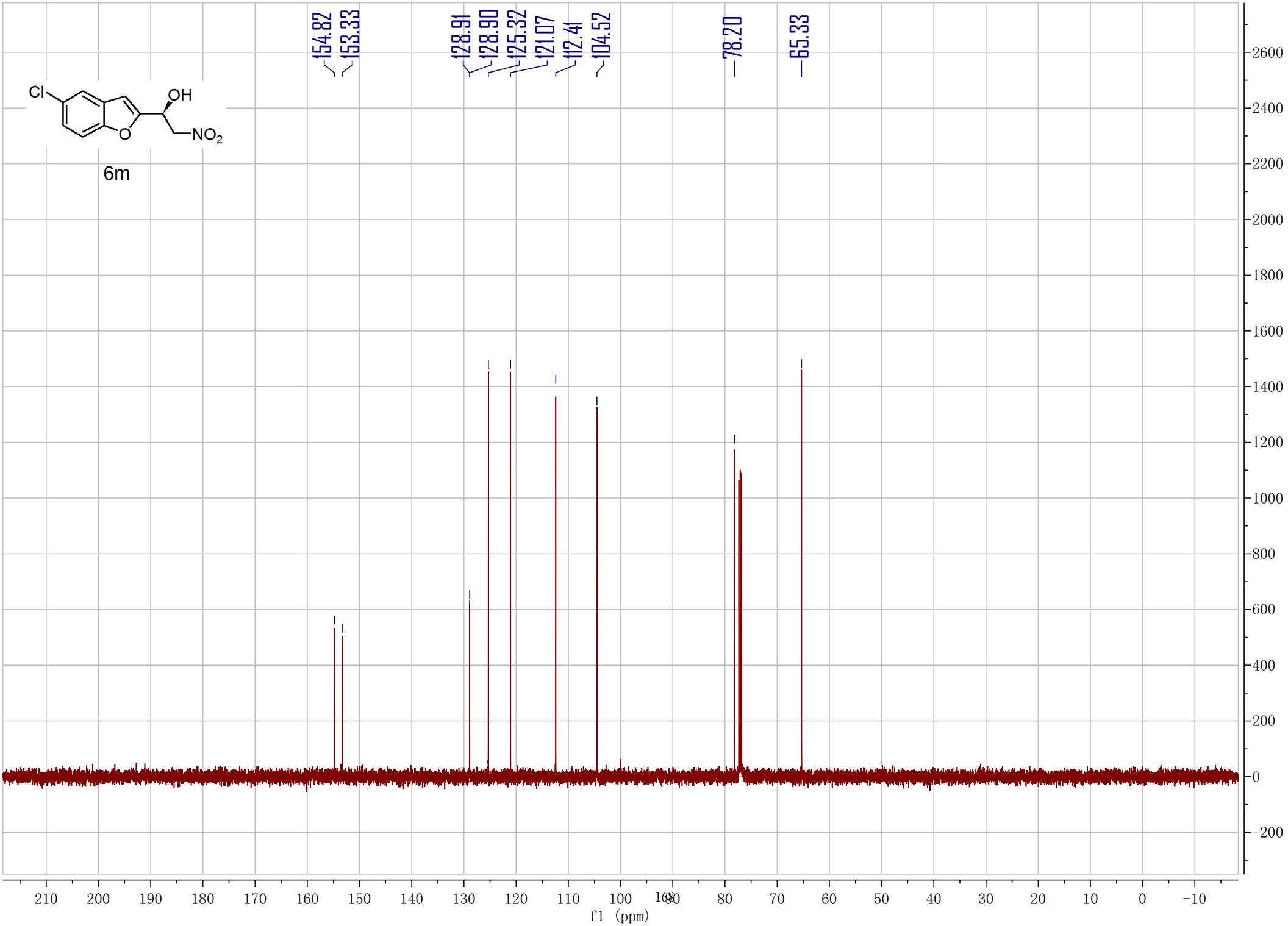

Et
OH
O
NO2
6k
2.01
1.00
1.00
1.00
1.01
1.00
1.99
3.01
f1 (ppm)

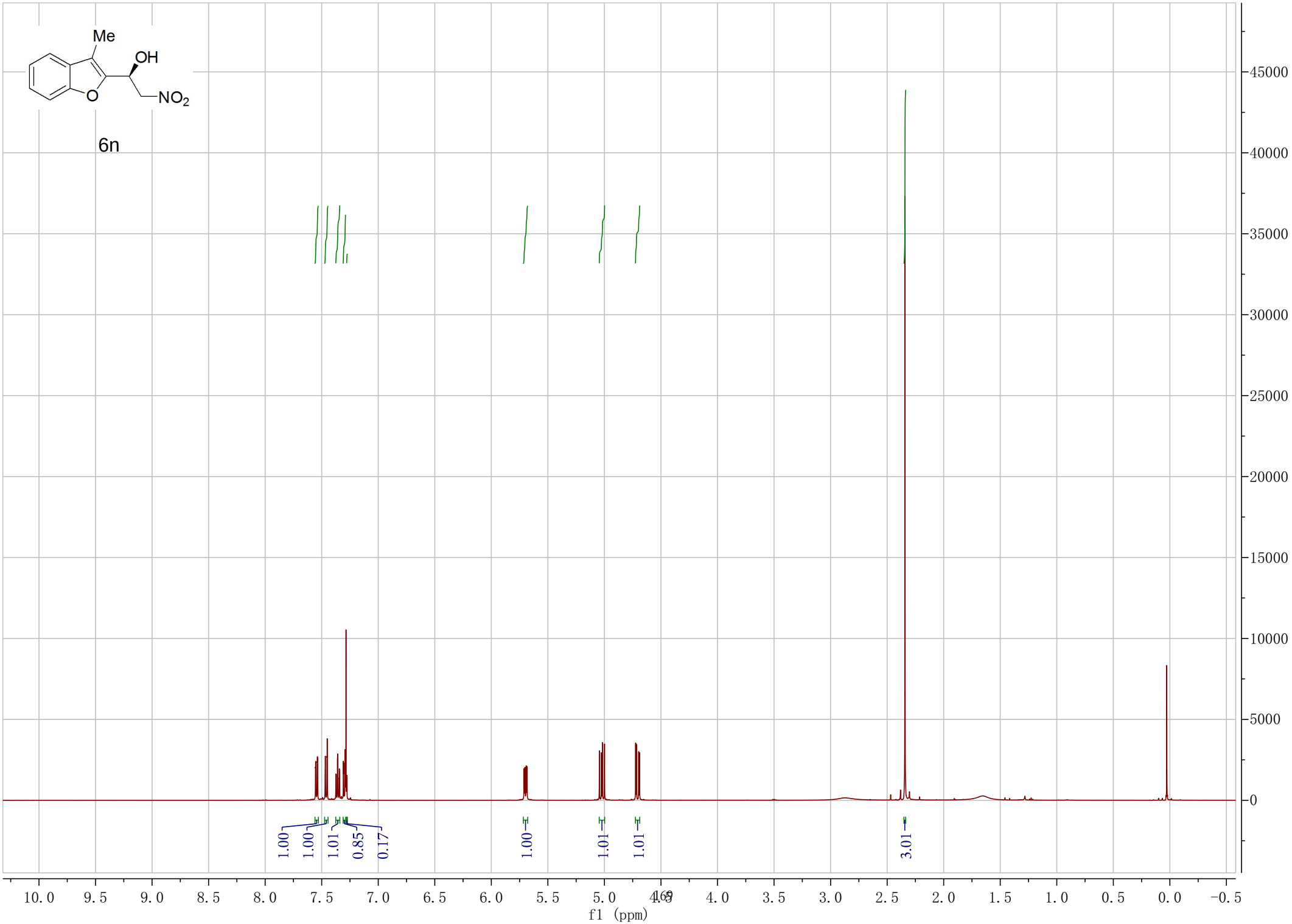

153.53
153.38
139.50
127.65
125.34
120.07
111.01
104.73
78.41
65.48
28.79
16.26
Et
OH
O
NO2
6k
f1 (ppm)

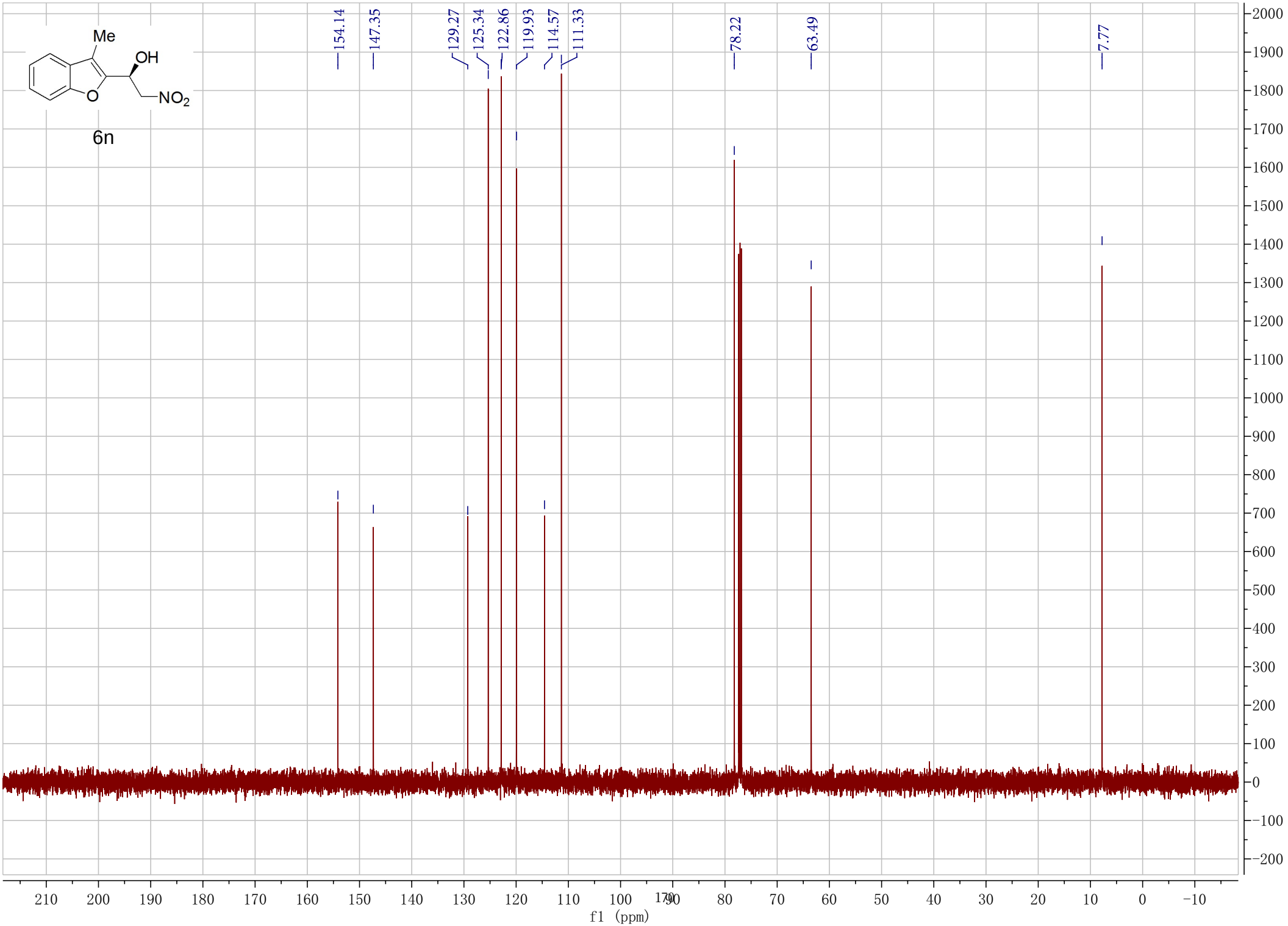

F
OH
O
NO2
6l
1.00
1.00
1.00
1.00
1.00
0.99
0.99
1.01
f1 (ppm)


160.31
158.41
155.16
151.19
128.43
128.34
112.96
112.14
112.06
107.09
106.89
105.06
105.03
78.25
65.38
F
OH
O
NO2
6l
f1 (ppm)

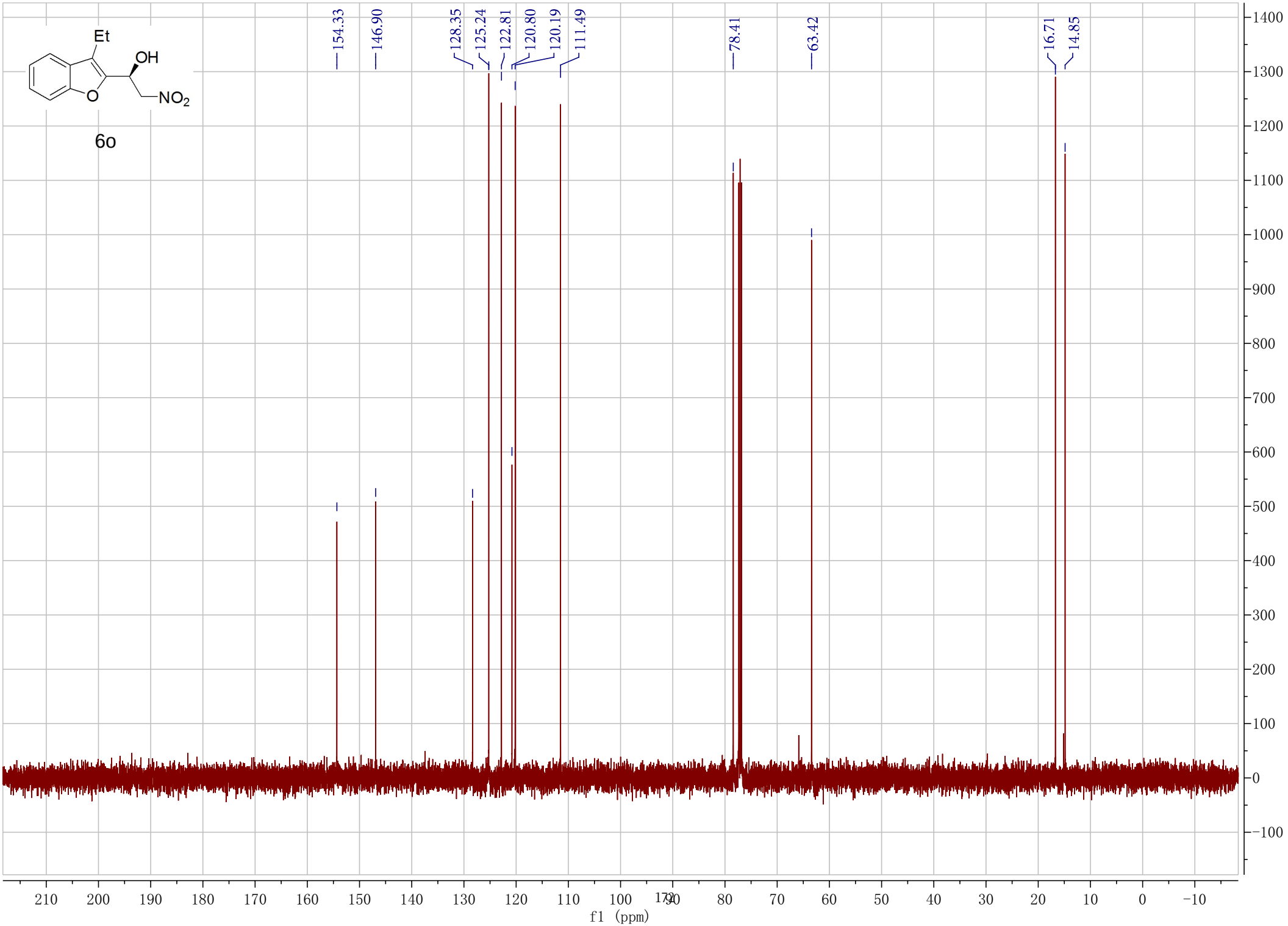

Cl
OH
O
NO2
6m
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
1.00
1.00
1.00
1.01
1.01
0.99
1.00
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

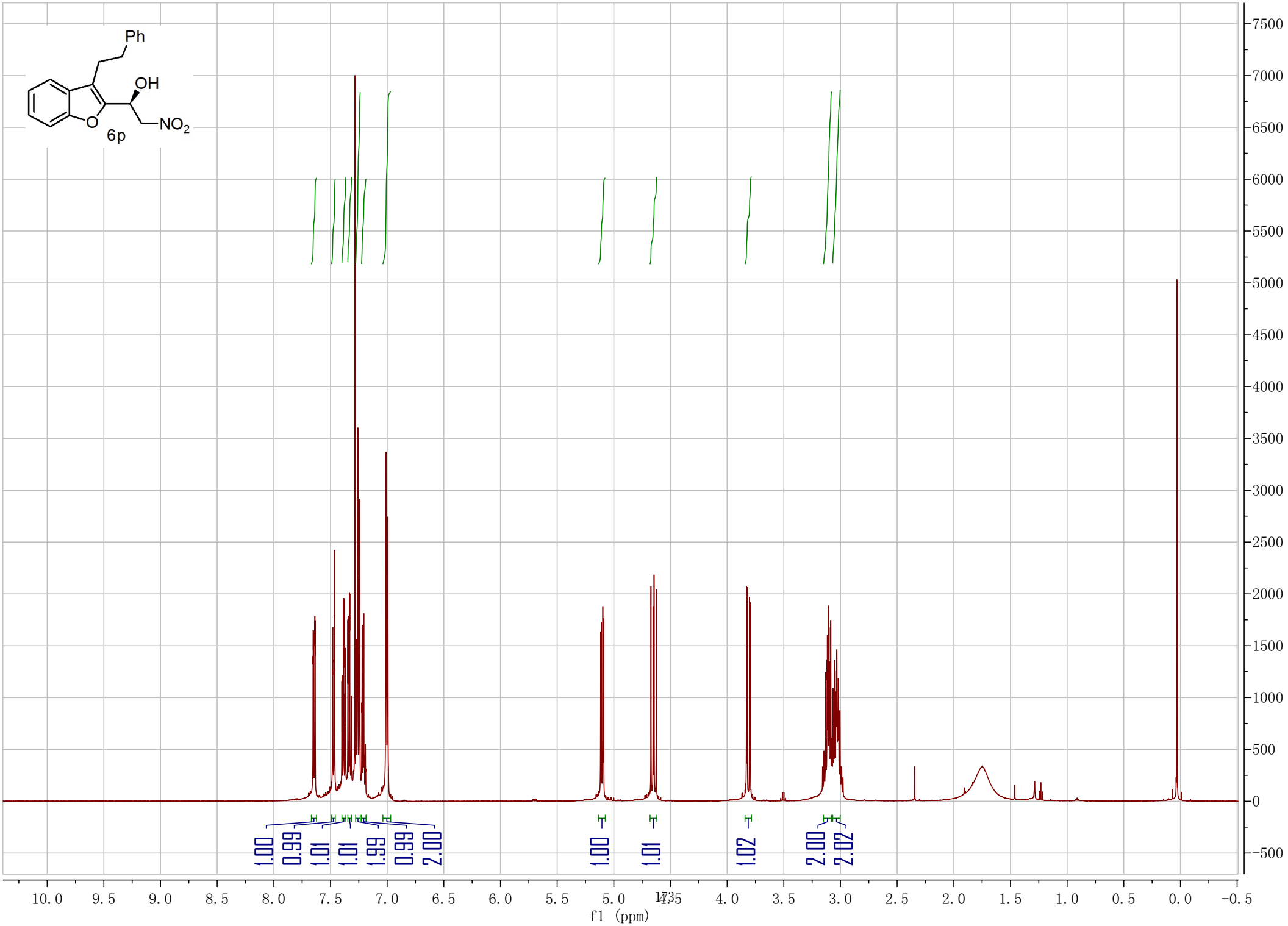

154.82
153.33
128.91
128.90
125.32
121.07
112.41
104.52
78.20
65.33
Cl
OH
O
NO2
6m
f1 (ppm)

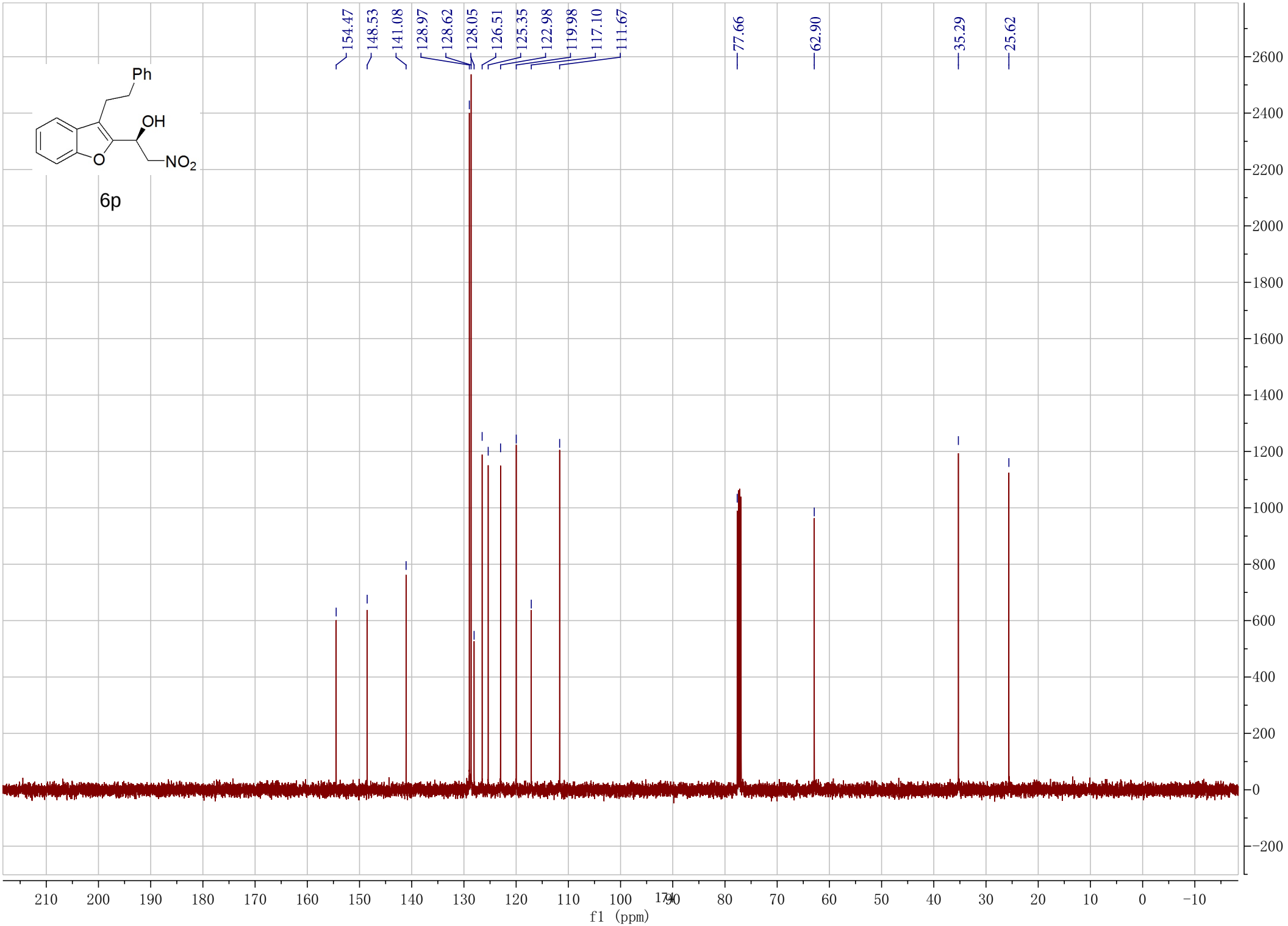

Me
OH
O
NO2
6n
1.00
1.00
1.01
0.85
0.17
1.00
1.01
1.01
3.01
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


Me
OH
O
NO2
6n
154.14
147.35
129.27
125.34
122.86
119.93
114.57
111.33
78.22
63.49
7.77
f1 (ppm)

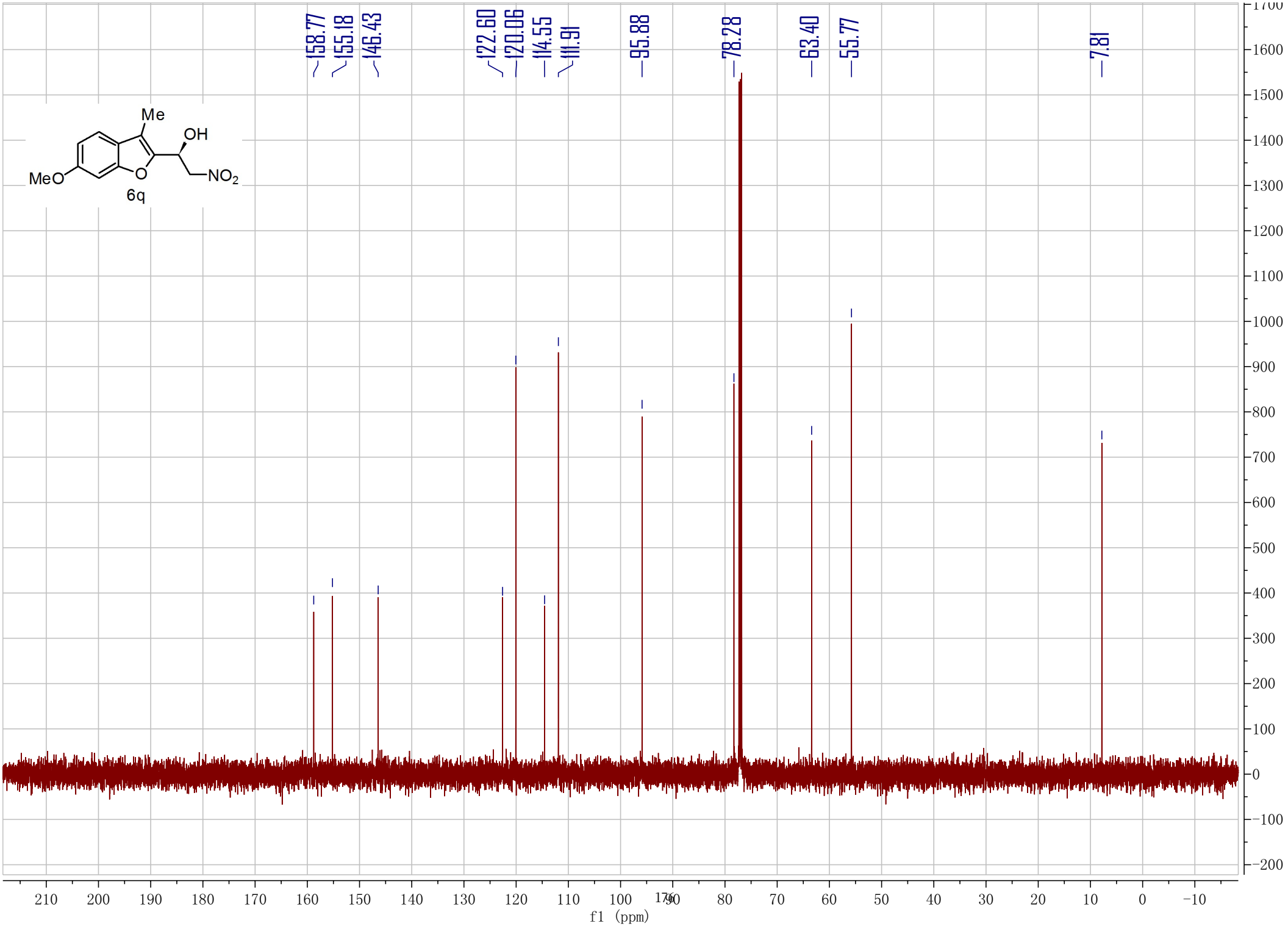
Et
OH
NO2
O
6o
1.00
0.99
1.01
1.39
1.00
1.00
1.00
1.00
1.00
3.00
f1 (ppm)

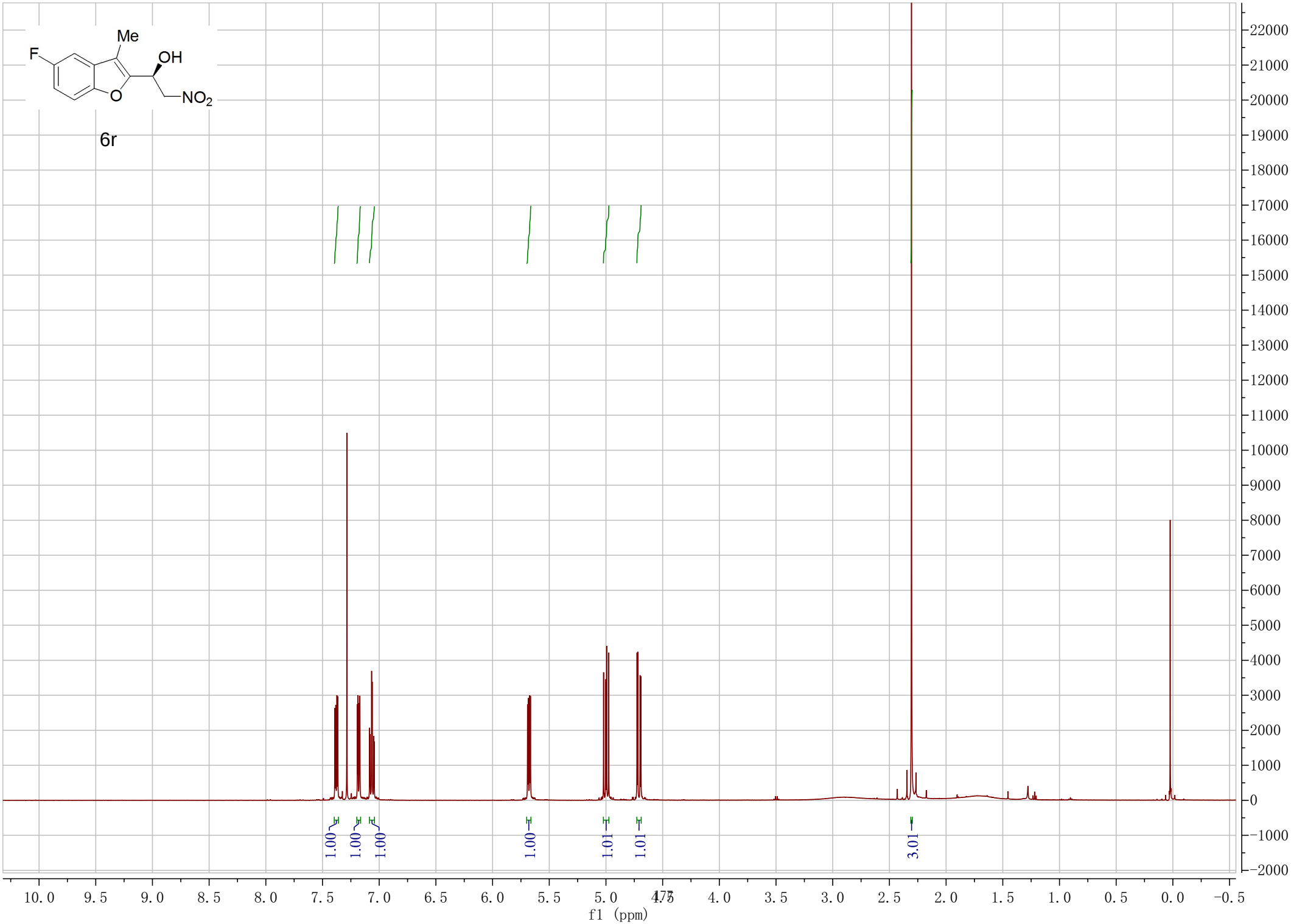

Et
OH
O
NO2
6o
154.33
146.90
128.35
125.24
122.81
120.80
120.19
111.49
78.41
63.42
16.71
14.85
f1 (ppm)

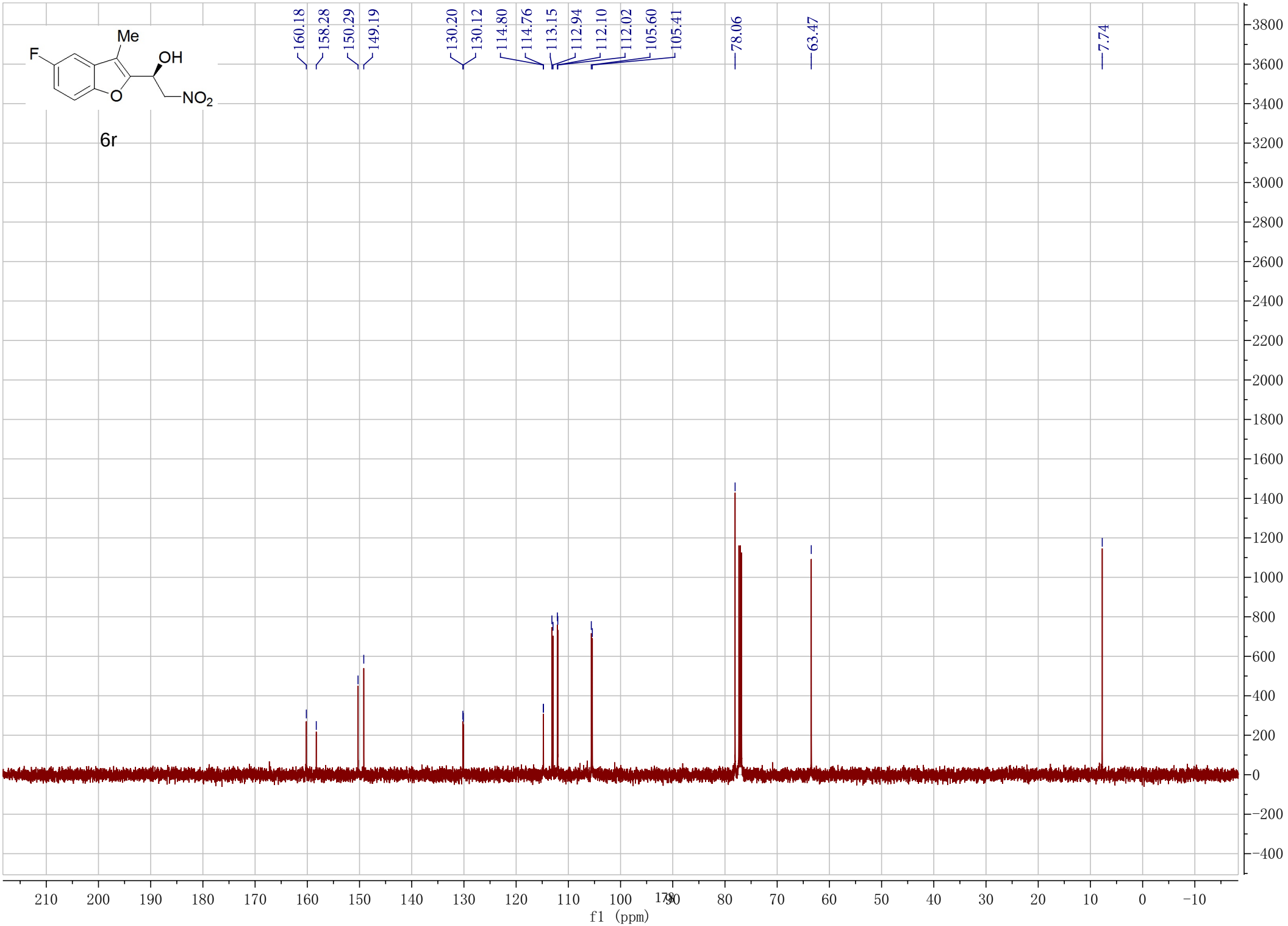

Ph
OH
NO2
6p
1.00
0.99
1.01
1.01
1.99
0.99
2.00
1.00
1.01
1.02
2.00
2.02
f1 (ppm)

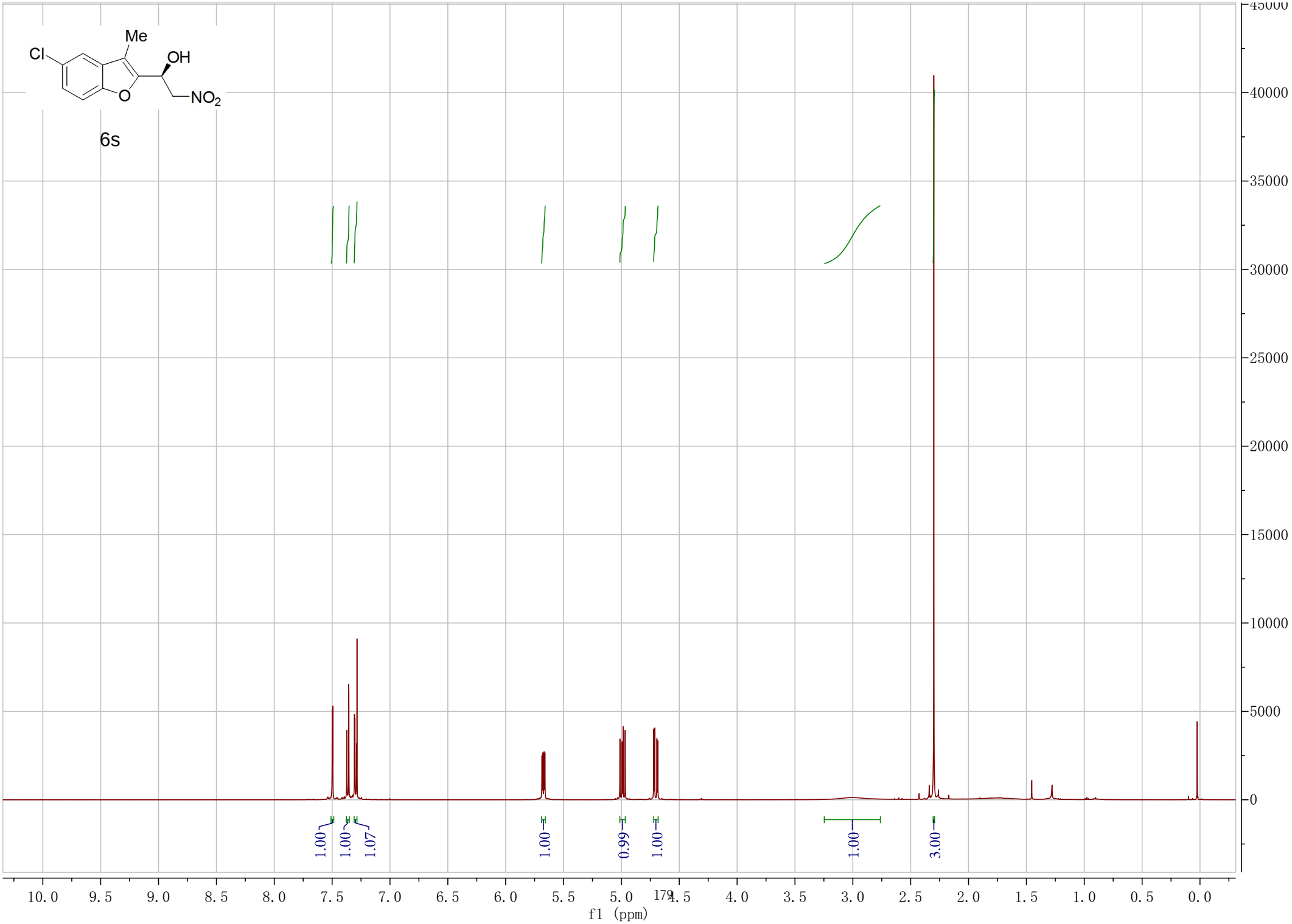

Ph
OH
O
NO2
6p
154.47
148.53
141.08
128.97
128.62
128.05
126.51
125.35
122.98
119.98
117.10
111.67
77.66
62.90
35.29
25.62
f1 (ppm)

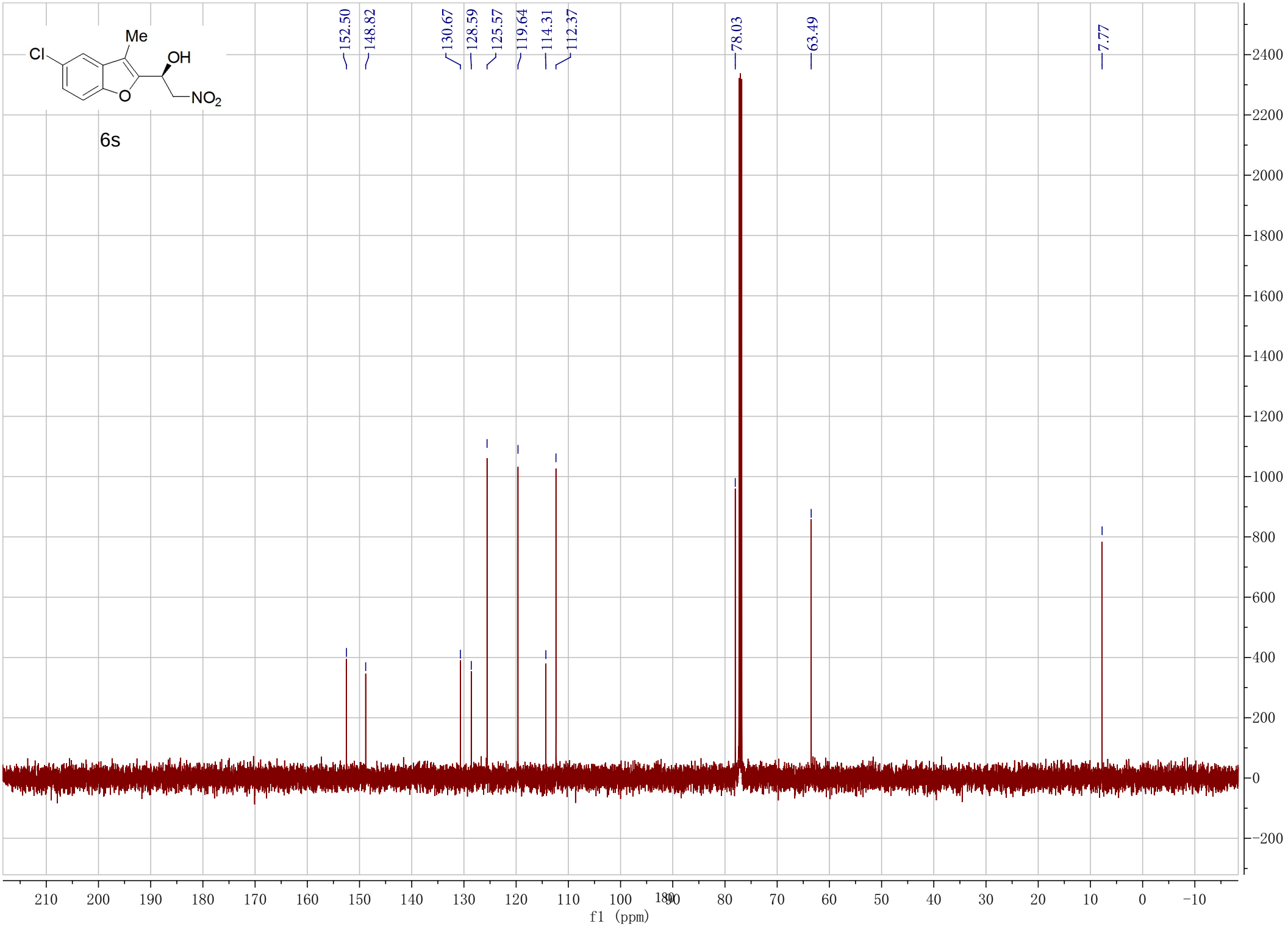
Me
OH
MeO
O
NO2
6q
1.00
1.00
1.01
1.00
1.02
1.01
3.01
3.01
f1 (ppm)

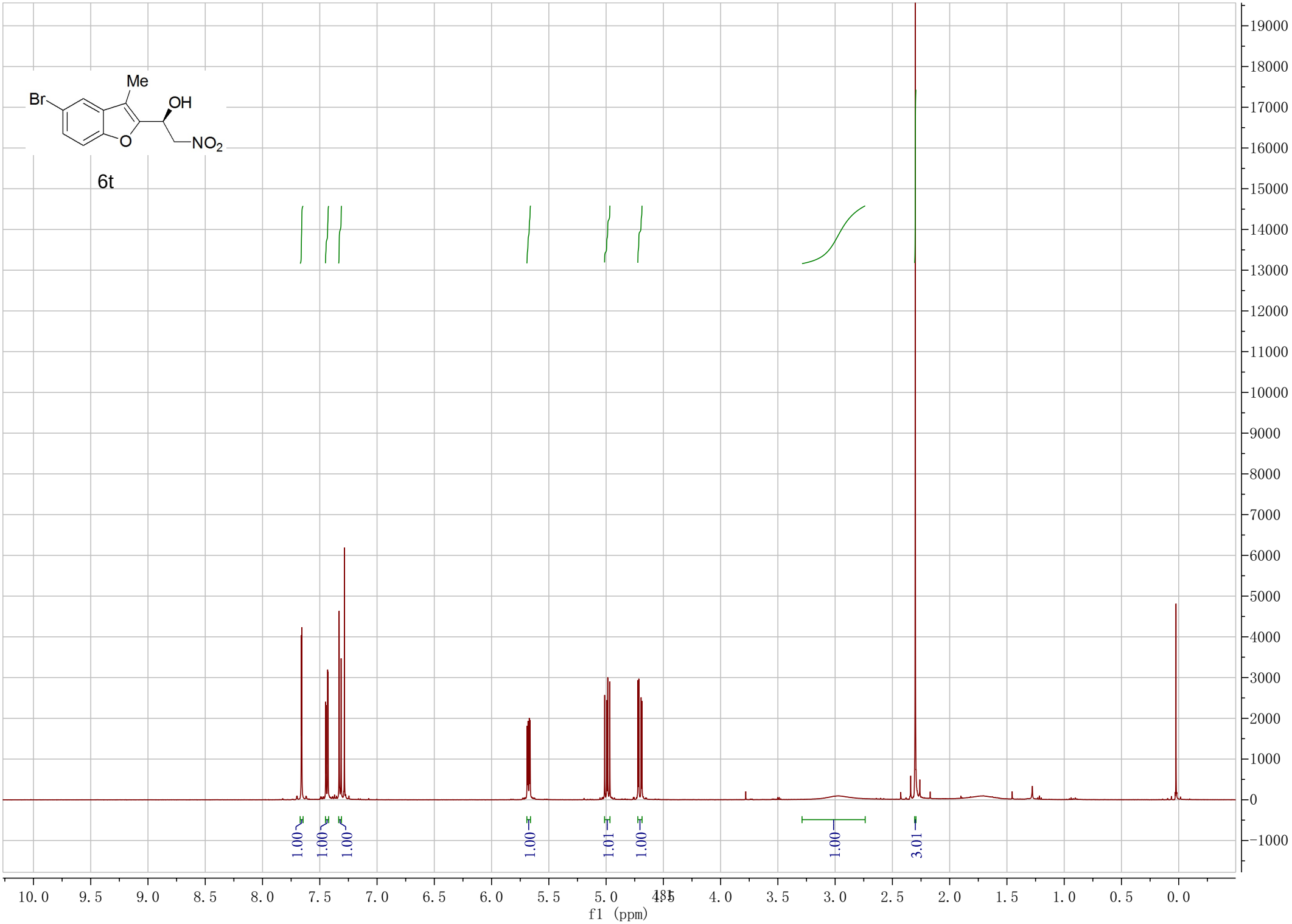

158.77
155.18
146.43
122.60
120.06
114.55
111.91
95.88
78.28
63.40
55.77
7.81
Me
OH
MeO
O
NO2
6q
f1 (ppm)

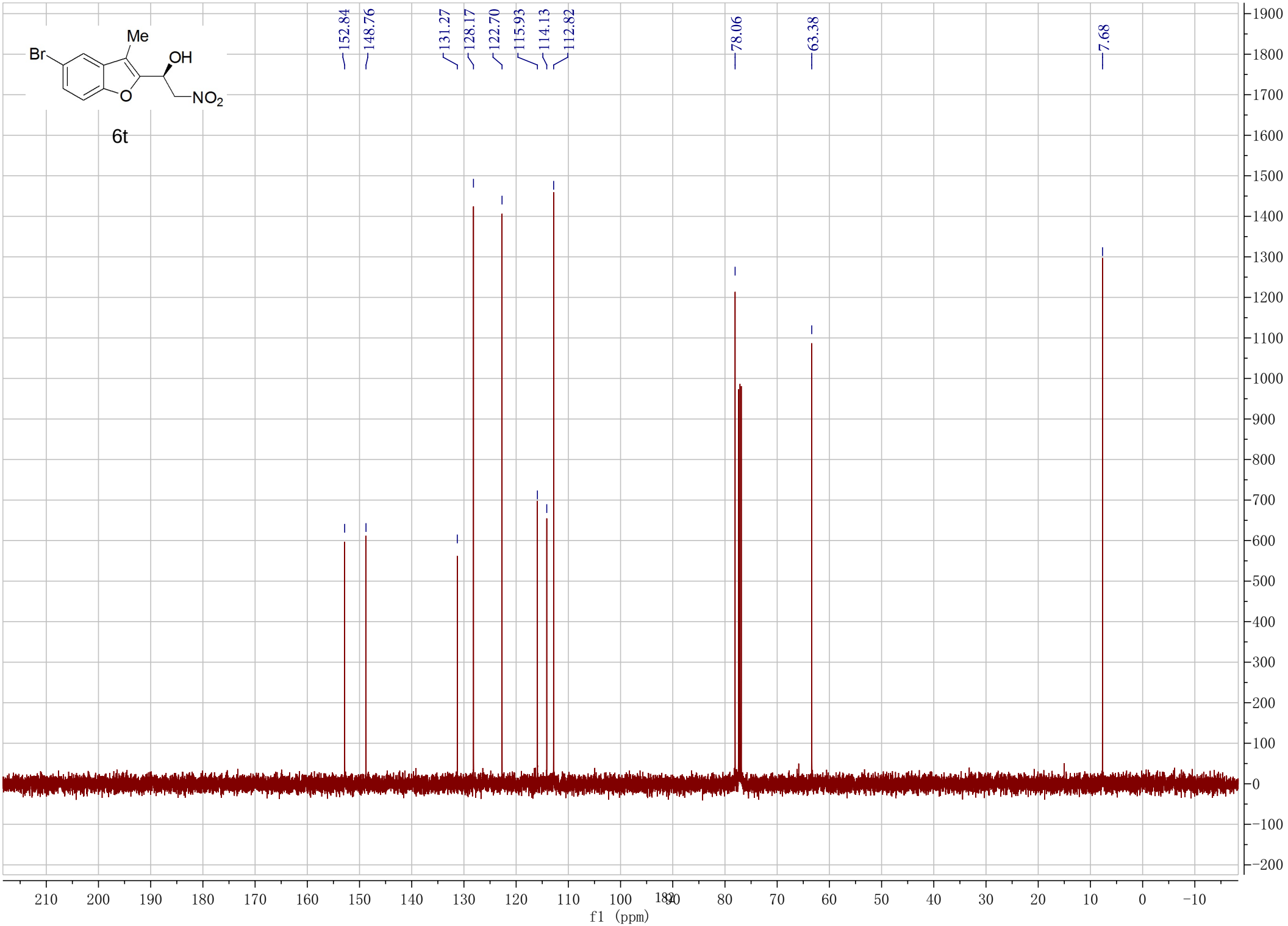

Me
F
OH
O
NO2
6r
1.00
1.00
1.00
1.00
1.01
1.01
3.01
f1 (ppm)

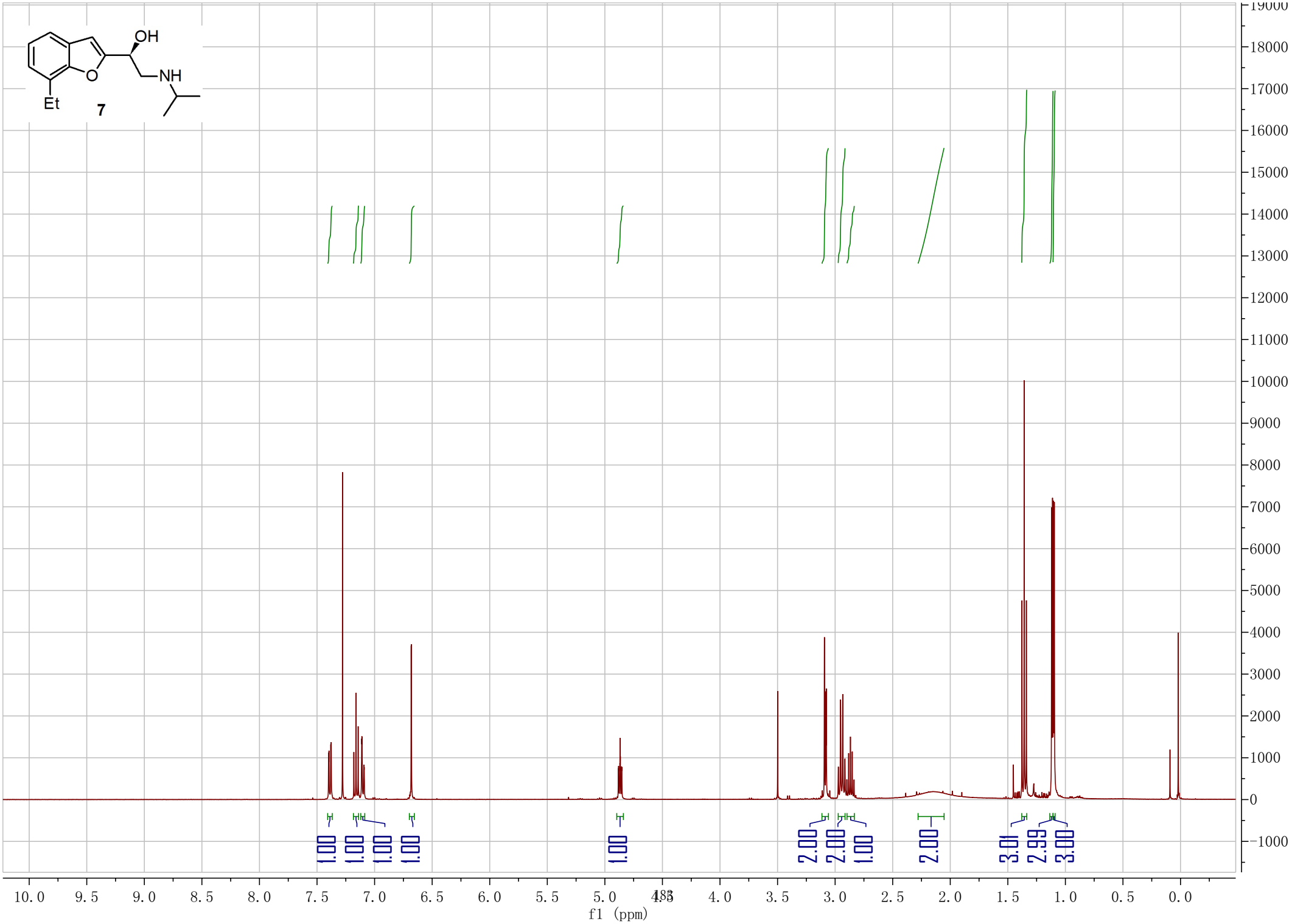

Me
F
OH
O
NO2
6r
160.18
158.28
150.29
149.19
130.20
130.12
114.80
114.76
113.15
112.94
112.10
112.02
105.60
105.41
78.06
63.47
7.74
f1 (ppm)

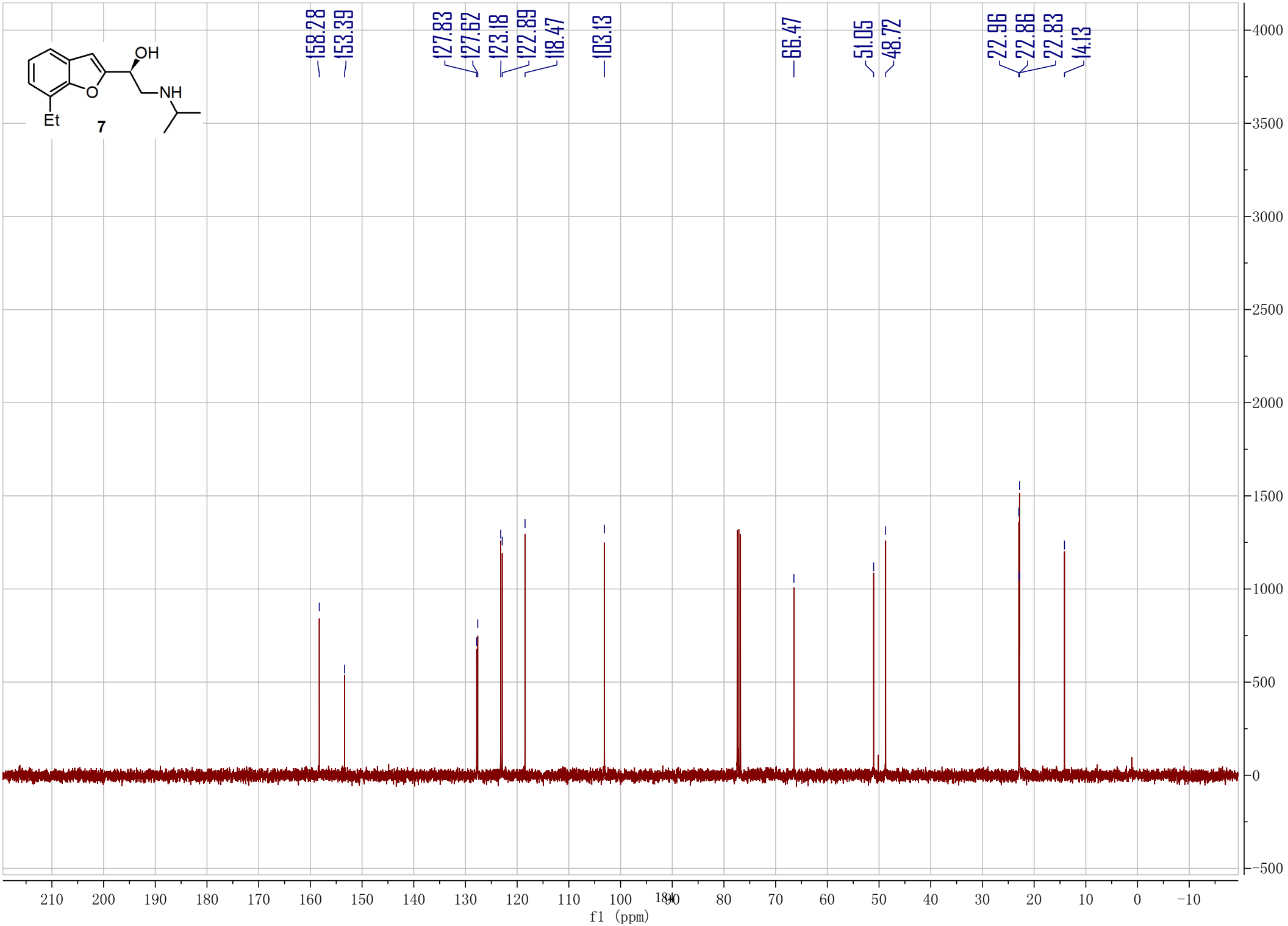

Me
Cl
OH
O
NO2
6s
1.00
1.00
1.07
1.00
0.99
1.00
1.00
3.00
f1 (ppm)


Me
Cl
OH
O
NO2
6s
152.50
148.82
130.67
128.59
125.57
119.64
114.31
112.37
78.03
63.49
7.77
f1 (ppm)

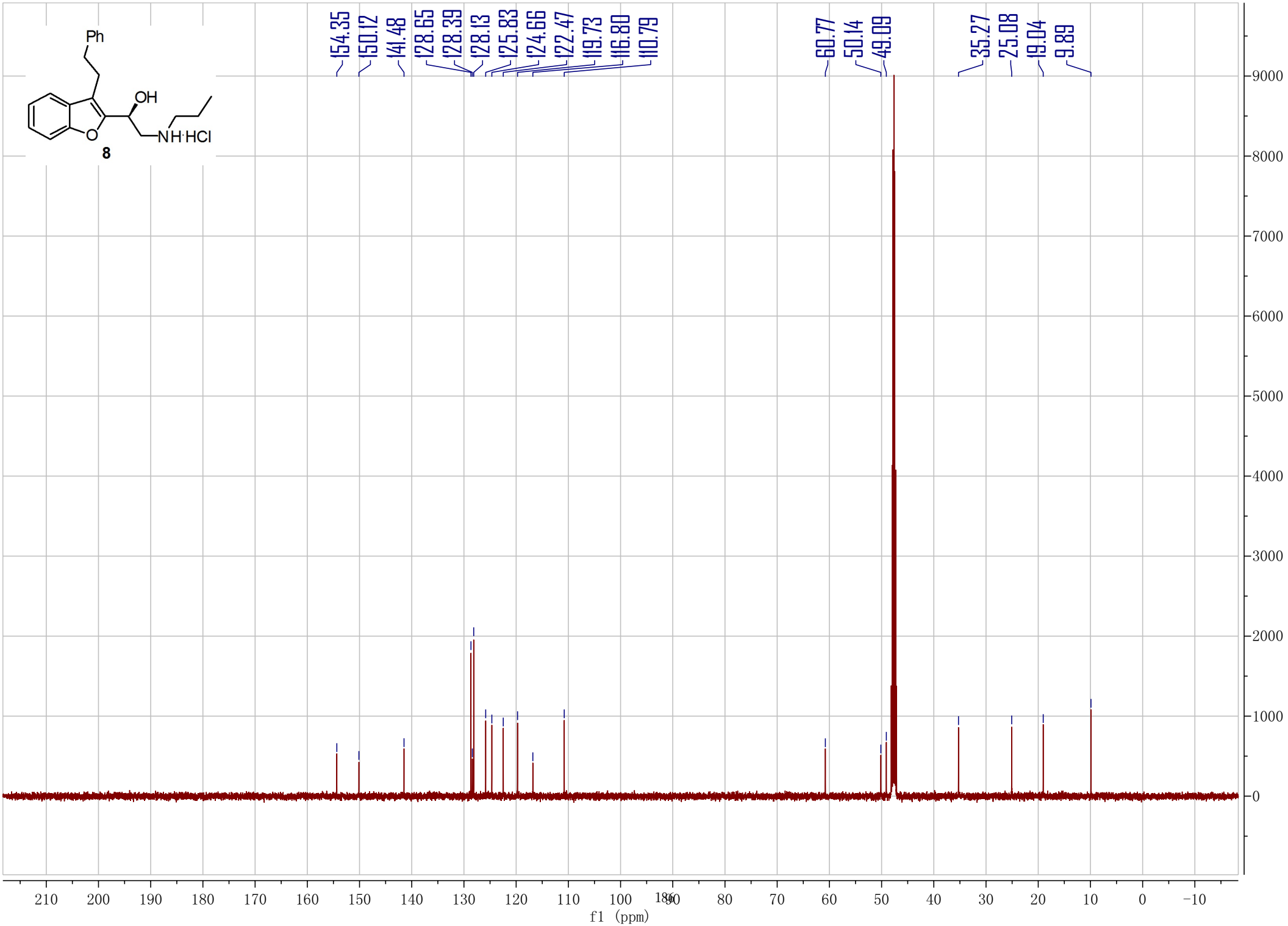

Me
Br
OH
O
NO2
6t
1.00
1.00
1.00
1.00
1.01
1.00
1.00
3.01
f1 (ppm)


Me
Br
OH
O
NO2
6t
152.84
148.76
131.27
128.17
122.70
115.93
114.13
112.82
78.06
63.38
7.68
f1 (ppm)


OH
NH
O
Et
7
1.00
1.00
1.00
1.00
1.00
2.00
2.00
1.00
2.00
3.01
2.99
3.00
f1 (ppm)


OH
NH
O
Et
7
158.28
153.39
127.83
127.62
123.18
122.89
118.47
103.13
66.47
51.05
48.72
22.96
22.86
22.83
14.13
4000
3500
3000
2500
2000
1500
1000
500
0
−500
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)

Ph
OH
NH·HCl
8
1.00
1.00
1.00
3.01
1.00
2.00
1.00
2.01
2.02
3.02
1.01
2.01
3.01
f1 (ppm)


Ph
OH
NH·HCl
8
154.35
150.12
141.48
128.65
128.39
128.13
125.83
124.66
122.47
119.73
116.80
110.79
60.77
50.14
49.09
35.27
25.08
19.04
9.89
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
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)