Suppplementary Information

$PhI(OAc)_2$ oxidative C5 halogenation of quinolines using Copper halides under mild conditions

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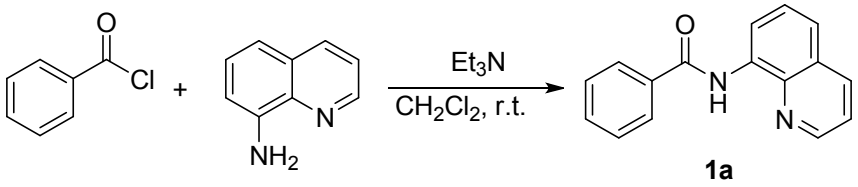
Table of Contents

1. *General information*

All of the reactions were carried out in oven-dried tube. Products were purified by flash chromatography on 200–300 mesh silica gels. Analytical TLC was performed with Merck silica gel 60 F254 plates, and the products were visualized by UV detection. Unless otherwise noted, chemical shifts (δ) are reported in ppm using TMS as internal standard; ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectras were recorded in $CDCl_3$ (δ = 77.00 ppm). The high resolution mass spectra (HRMS) were recorded on an FT-ICR mass spectrometer using electrospray ionization (ESI). Melting points were determined on a microscopic apparatus. Copies of ^{1}H NMR and ^{13}C NMR spectra are provided. Commercially available reagents were used without further purification.

2. *Typical Experimental Procedure*

(A) Synthesis of starting materials



1a

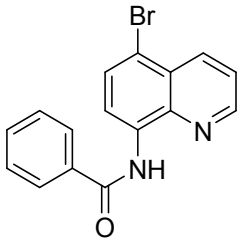
To a 100 ml single neck flask charged with CH_2Cl_2 (30 mL) was added 8-aminoquinoline (10 mmol) and triethylamine (15 mmol) and stirred at room temperature for 5 min, then the reaction solution was cooled in an ice bath. The acid chloride (11 mmol) was added dropwise (if solid, it was dissolved with CH_2Cl_2). The reaction solution was stirred overnight. When it was completed (Monitored by TLC), the mixture was filtered through a pad of Celite, the solid was washed with CH_2Cl_2 (25 mL), and the organic layer was washed with 1 M $NaHCO_3$ aqueous solution (3 × 15 mL), then the organic layer was dried with Na_2SO_4, filtered, and roto-evaporated. The product was purified by silica gel column with PE/EtOAc (20/1) to give the desired amide product **1**.

(B) Typical Experimental Procedure for the $PhI(OAc)_2$ oxidative C5 halogenation of quinolines using Copper halides:

An oven-dried tube with a magnetic stir bar was charged with the quinolines **1** (0.2 mmol) , copper halides (1.0 equiv.), $PhI(OAc)_2$ (2.0 equiv.) , NH_2SO_3H (1.0 equiv.) and DCE (1 ml). Then the reaction mixture was stirred at room temperature under air for indicated time (Table

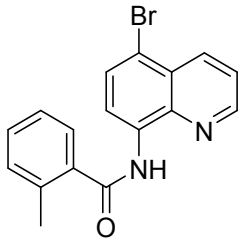
2) until complete consumption of starting material as monitored by TLC. After the reaction was finished, the mixture was concentrated in vacuum, and the residues were purified by silica gel column chromatography (hexane/ethyl acetate = 20:1) to afford the desired product .

3. Spectroscopic Data.



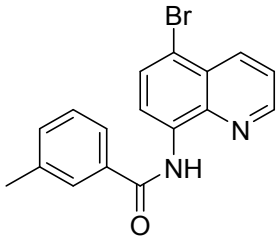
2a

N-(5-bromoquinolin-8-yl)benzamide 2a; White solid (m=61mg, 98%); m.p. 122-124 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.63 (s, 1H), 8.88 – 8.73 (m, 2H), 8.45 (dd, *J* = 8.5, 1.5 Hz, 1H), 8.09 – 7.99 (m, 2H), 7.78 (d, *J* = 8.4 Hz, 1H), 7.59 – 7.49 (m, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.17, 148.62, 139.21, 135.81, 134.68, 134.33, 131.91, 130.80, 128.74, 127.16, 127.05, 122.60, 116.83, 114.30. HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{16}H_{11}BrN_2OH^+$ 327.0127, found 327.0126



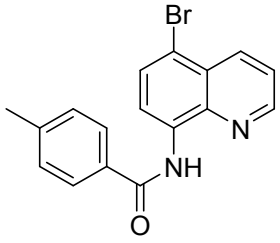
2b

N-(5-bromoquinolin-8-yl)-2-methylbenzamide 2b; White solid (m=46mg, 70%); m.p. 120-123 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 10.19 (s, 1H), 8.84 (d, *J*=8.4, 1H), 8.79 (dd, *J*=4.2, 1.5, 1H), 8.54 (dd, *J*=8.5, 1.5, 1H), 7.85 (d, *J*=8.4, 1H), 7.68 (d, *J*=7.7, 1H), 7.56 (dd, *J*=8.5, 4.2, 1H), 7.45 – 7.37 (m, 1H), 7.33 (t, *J*=7.6, 2H), 2.60 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.11, 148.73, 139.27, 136.77, 136.28, 135.97, 134.63, 131.43, 130.91, 130.48, 127.23, 127.21, 126.03, 122.70, 116.96, 114.46，18.68; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{17}H_{13}BrN_2OH^+$ 341.0283, found 341.0282.



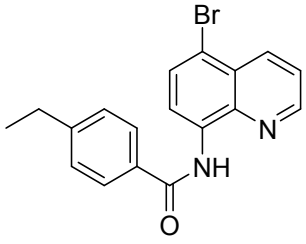
2c

N-(5-bromoquinolin-8-yl)-3-methylbenzamide 2c; White solid (m=64mg, 98%); m.p. 90-93 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.61 (s, 1H), 8.84 – 8.75 (m, 2H), 8.47 (dd, *J* = 8.5, 1.6 Hz, 1H), 7.89 – 7.75 (m, 3H), 7.52 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.44 – 7.33 (m, 2H), 2.46 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.45, 148.64, 139.28, 138.63, 135.83, 134.72, 134.44, 132.69, 130.84, 128.59, 127.95, 127.09, 124.10, 122.60, 116.88, 114.24, 21.43; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{17}H_{13}BrN_2OH^+$ 341.0283, found 341.0283



2d

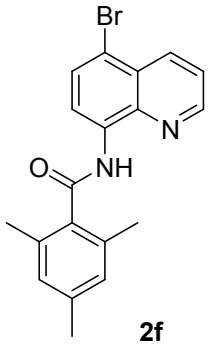
N-(5-bromoquinolin-8-yl)-4-methylbenzamide 2d; White solid (m=65mg, 99%); m.p. 158-160 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.61 (s, 1H), 8.84 – 8.74 (m, 2H), 8.46 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.93 (d, *J* = 8.2 Hz, 2H), 7.78 (d, *J* = 8.4 Hz, 1H), 7.51 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.31 (d, *J* = 8.0 Hz, 2H), 2.43 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.19, 148.60, 142.45, 139.27, 135.81, 134.49, 131.89, 130.84, 129.40, 127.19, 127.08, 122.58, 116.79, 114.12, 21.50; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{17}H_{13}BrN_2OH^+$ 341.0283, found 341.0282



2e

N-(5-bromoquinolin-8-yl)-4-ethylbenzamide 2e; White solid (m=50mg, 73%); m.p. 138-139 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.70 (s, 1H), 8.87 (dd, *J* = 4.2, 1.5 Hz,

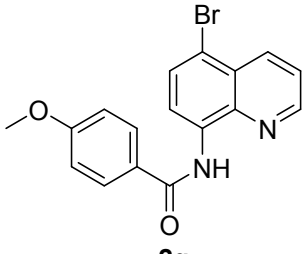
1H), 8.84 (d, *J* = 8.4 Hz, 1H), 8.55 (dd, *J* = 8.5, 1.5 Hz, 1H), 8.00 (d, *J* = 8.2 Hz, 2H), 7.85 (d, *J* = 8.4 Hz, 1H), 7.59 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.38 (d, *J* = 8.2 Hz, 2H), 2.75 (q, *J* = 7.6 Hz, 2H), 1.30 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.43, 148.77, 148.70, 139.39, 135.99, 134.58, 132.22, 130.97, 128.32, 127.37, 127.21, 122.70, 116.90, 114.21, 28.86, 15.35; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{18}H_{15}BrN_2OH^+$ 355.0440, found 355.0441



2f

N-(5-bromoquinolin-8-yl)-2,4,6-trimethylbenzamide 2f; White solid (m=50mg, 71%); m.p. 132-134 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.90 (s, 1H), 8.89 (d, *J* = 8.4 Hz, 1H), 8.74 (dd, *J* = 4.2, 1.5 Hz, 1H), 8.54 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.86 (d, *J* = 8.4 Hz, 1H), 7.55 (dd, *J* = 8.5, 4.2 Hz, 1H), 6.93 (s, 2H), 2.39 (d, *J* = 3.8 Hz, 6H), 2.33 (s, 3H);

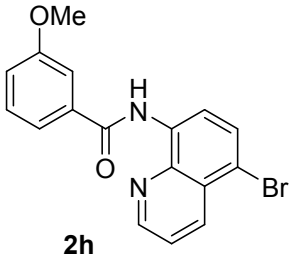
^{13}C NMR (101 MHz, $CDCl_3$) δ 169.10, 148.71, 140.71，139.21, 138.91, 135.92, 135.10, 134.51, 134.38, 130.89, 128.83, 128.45, 127.24, 122.67, 117.13, 114.54, 21.14, 20.05, 19.40; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{19}H_{17}BrN_2OH^+$ 369.0596, found 369.0595



2g

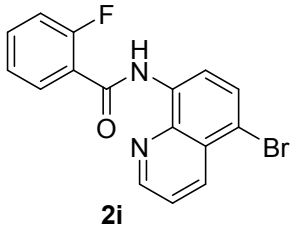
N-(5-bromoquinolin-8-yl)-4-methoxybenzamide 2g; White solid (m=42mg, 61%); m.p. 122-124 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.64 (s, 1H), 8.86 (dd, *J* = 4.2, 1.5 Hz, 1H), 8.81 (d, *J* = 8.4 Hz, 1H), 8.54 (dd, *J* = 8.5, 1.5 Hz, 1H), 8.07 – 8.00 (m, 2H),

7.83 (d, *J* = 8.4 Hz, 1H), 7.58 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.08 – 6.99 (m, 2H), 3.90 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.91, 162.61, 148.65, 139.40, 135.98, 134.67, 130.99, 129.15, 127.21, 127.09, 122.66, 116.81, 114.04, 114.01, 55.47; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{17}H_{13}BrN_2O_2H^+$ 357.0232, found 357.0232



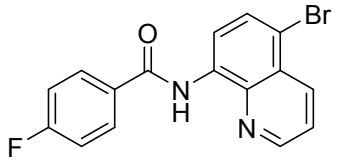
2h

N-(5-bromoquinolin-8-yl)-3-methoxybenzamide 2h; White solid (m= 36mg, 51%); m.p. 108-110^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.69 (s, 1H), 8.86 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.82 (d, *J* = 8.4 Hz, 1H), 8.54 (dd, *J* = 8.5, 1.6 Hz, 1H), 7.85 (d, *J* = 8.4 Hz, 1H), 7.65 – 7.55 (m, 3H), 7.46 (t, *J* = 8.1 Hz, 1H), 7.13 (ddd, *J* = 8.2, 2.6, 1.0 Hz, 1H), 3.92 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.19, 159.99, 148.75, 139.37, 136.28, 135.96, 134.43, 130.92, 129.79, 127.20, 122.71, 119.00, 118.11, 116.97, 114.42, 112.67, 55.49; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{17}H_{13}BrN_2O_2H^+$ 357.0232, found 357.0237.



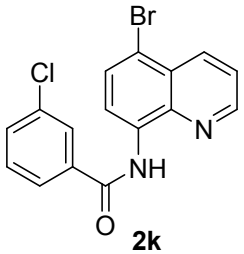
2i

N-(5-bromoquinolin-8-yl)-2-fluorobenzamide 2i; White solid (m= 44 mg, 64%); m.p. 150-151^{o}C; ^{1}H NMR (300 MHz, CDCl3) δ 11.13 (d, *J* = 12.5 Hz, 1H), 888 – 8.84 (m, 2H), 8.51 (dd, *J* = 8.5, 1.5 Hz, 1H), 8.21 (td, *J* = 7.9, 1.9 Hz, 1H), 7.83 (d, *J* = 8.4 Hz, 1H), 7.58 – 7.51 (m, 2H), 7.33 (ddd, *J* = 8.1, 7.4, 0.8 Hz, 1H), 7.25 (ddd, *J* = 11.9, 6.5, 4.7 Hz, 1H); δ^{13}C NMR (75 MHz, CDCl3) δ161.51, 160.55 (d, *J* = 270.0 Hz), 148.91, 139.41, 135.81, 134.72, 133.73 (d, *J* = 9.0 Hz), 132.03 (d, *J* = 1.5 Hz), 130.85, 127.16, 124.88 (d, *J* = 3.0 Hz), 122.68, 121.72 (d, J = 11.3 Hz), 117.66, 116.32 (d, *J* = 24.0 Hz), 114.78; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{16}H_{10}BrFN_2OH^+$ 345.0033, found 345.0037.



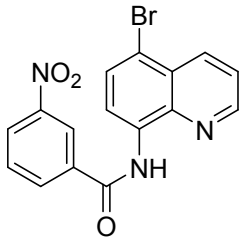
2j

N-(5-bromoquinolin-8-yl)-4-fluorobenzamide 2j; White solid (m= 47 mg, 68%); m.p. 172-174 ^{o}C; ^{1}H NMR (300 MHz, CDCl3) δ 10.63 (s, 1H), 8.85 (dd, *J* = 4.2, 1.5 Hz, 1H), 8.78 (d, *J* = 8.4 Hz, 1H), 8.53 (dd, *J* = 8.5, 1.6 Hz, 1H), 8.09 – 8.06 (m, 2H), 7.83 (d, *J* = 8.4 Hz, 1H), 7.58 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.25 – 7.19 (m, 2H); ^{13}C NMR (75 MHz, CDCl3) δ 165.46 (d, *J* = 252.0 Hz), 164.19, 148.75, 139.32, 136.02, 134.31, 131.01, 130.92, 129.63 (d, *J* = 9.0 Hz), 127.22, 122.73, 116.96, 115.89 (d, *J* = 21.8Hz), 114.50; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{16}H_{10}BrFN_2OH^+$ 345.0033, found 345.0038.



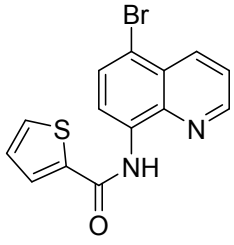
2k

N-(5-bromoquinolin-8-yl)-3-chlorobenzamide 2k：White solid (m=58mg, 83%); m.p. 126-128^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.60 (s, 1H), 8.84 (d, *J* = 3.2 Hz, 1H), 8.75 (d, *J* = 8.4 Hz, 1H), 8.54 – 8.46 (m, 1H), 8.01 (s, 1H), 7.90 (d, *J* = 7.7 Hz, 1H), 7.80 (d, *J* = 8.4 Hz, 1H), 7.60 – 7.50 (m, 2H), 7.46 (t, *J* = 7.8 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.77, 148.80, 139.21, 136.49, 135.96, 135.02, 134.04, 131.97, 130.82, 130.04, 127.62, 127.14, 125.15, 122.74, 117.05, 114.74; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{16}H_{10}BrClN_2OH^+$ 360.9737, found 360.9738



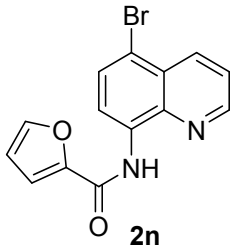
2l

N-(5-bromoquinolin-8-yl)-3-nitrobenzamide 2l: White solid (m=30mg, 41%); m.p. 135-136 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.79 (s, 1H), 8.91 (d, *J* = 2.1 Hz, 2H), 8.81 (d, *J* = 8.4 Hz, 1H), 8.58 (d, *J* = 8.0 Hz, 1H), 8.45 (d, *J* = 8.0 Hz, 1H), 8.40 (d, *J* = 7.7 Hz, 1H), 7.88 (d, *J* = 8.4 Hz, 1H), 7.77 (t, *J* = 8.0 Hz, 1H), 7.63 (dd, *J* = 8.5, 4.2 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.83, 149.07, 148.54, 139.30, 136.55, 136.19, 133.80, 133.07, 130.90, 130.09, 127.32, 126.48, 122.97, 122.34, 117.36, 115.30; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{16}H_{10}BrN_3O_3H^+$ 371.9978, found 371.9977



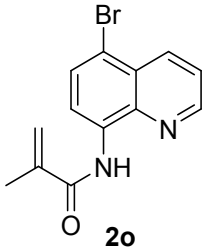
2m

N-(5-bromoquinolin-8-yl)thiophene-2-carboxamide 2m: White solid (m=78mg, 99%); m.p. 134-136 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.53 (s, 1H), 8.85 (dd, *J* = 4.2, 1.4 Hz, 1H), 8.72 (d, *J* = 8.4 Hz, 1H), 8.52 (dd, *J* = 8.5, 1.4 Hz, 1H), 7.86 – 7.77 (m, 2H), 7.61 – 7.54 (m, 2H), 7.18 (dd, *J* = 4.8, 3.9 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.89, 148.75, 139.69, 139.07, 135.95, 134.16, 131.16, 130.90, 128.53, 127.89, 127.17, 122.73, 116.90, 114.39; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{14}H_9BrN_2OSH^+$ 332.9691, found 332.9690



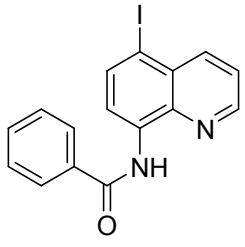
2n

N-(5-bromoquinolin-8-yl)furan-2-carboxamide 2n: White solid (m=40mg, 63%); m.p. 194-197 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.73 (s, 1H), 8.90 (dd, *J* = 4.2, 1.5 Hz, 1H), 8.77 (d, *J* = 8.4 Hz, 1H), 8.54 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.83 (d, *J* = 8.4 Hz, 1H), 7.64 (d, *J* = 0.9 Hz, 1H), 7.59 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.32 (d, *J* = 3.5 Hz, 1H), 6.61 (dd, *J* = 3.5, 1.7 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.26, 148.83, 148.11, 144.61, 139.24, 135.88, 134.07, 130.85, 127.21, 122.71, 117.04, 115.36, 114.54, 112.49; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{14}H_9BrN_2O_2H^+$ 316.9919, found 316.9918.



2o

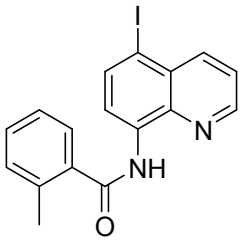
N-(5-bromoquinolin-8-yl)methacrylamide 2o: White solid (m=46mg, 84%); m.p. 128-130 ^{o}C; ^{1}H NMR (400 MHz, DMSO-D_6) δ 10.17 (s, 1H), 8.94 (dd, *J* = 4.2, 1.4 Hz, 1H), 8.52 (d, *J* = 8.4 Hz, 1H), 8.46 (d, *J* = 8.5 Hz, 1H), 7.89 (d, *J* = 8.4 Hz, 1H), 7.76 (dd, *J* = 8.5, 4.2 Hz, 1H), 5.97 (s, 1H), 5.69 – 5.54 (m, 1H), 2.08 (s, 3H); ^{13}C NMR (101 MHz, DMSO-D_6) δ 165.89, 150.19, 140.39, 139.05, 135.90, 134.43, 131.14, 126.94, 124.18, 121.76, 116.97, 114.06, 18.68; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{13}H_{11}BrN_2OH^+$ 291.0127, found 291.0126



3a

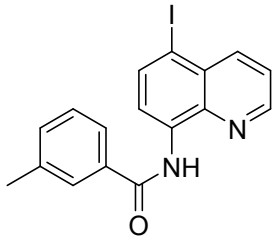
N-(5-iodoquinolin-8-yl)benzamide 3a; White solid (m=72mg, 96%); m.p. 154-157 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.73 (s, 1H), 8.80 (dd, *J* = 4.2, 1.5 Hz, 1H), 8.70 (d, *J* = 8.3 Hz, 1H), 8.37 (dd, *J* = 8.5, 1.6 Hz, 1H), 8.13-8.06 (m, 3H), 7.60-7.52 (m, 4H);^{13}C NMR (75 MHz, $CDCl_3$) δ 165.32, 148.79, 140.68, 139.23, 138.24, 135.40, 134.77,

131.99, 129.57, 128.80, 127.24, 123.17, 117.81, 89.51; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{16}H_{11}IN_2OH^+$ 374.9988, found 374.9987.



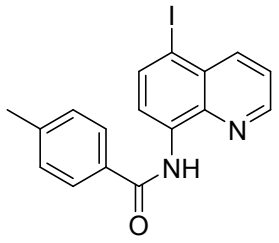
3b

N-(5-iodoquinolin-8-yl)-2-methylbenzamide 3b; White solid (m=66mg, 84%); m.p. 122-124 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 10.21 (s, 1H), 8.76 – 8.67 (m, 2H), 8.39 – 8.34 (m, 1H), 8.12 (d, *J* = 8.3 Hz, 1H), 7.67 (d, *J* = 7.6 Hz, 1H), 7.52 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.40 (d, *J* = 7.9 Hz, 1H), 7.32 (t, *J* = 7.7 Hz, 2H), 2.59 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.07, 148.78, 140.68, 139.14, 138.22, 136.77, 136.26, 135.59, 131.43, 130.47, 129.61, 127.20, 126.01, 123.16, 117.80, 89.56, 20.22; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{17}H_{13}IN_2OH^+$ 389.0145, found 389.0144



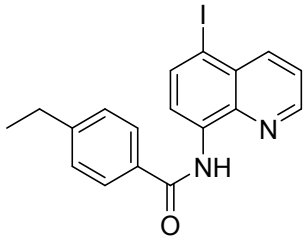
3c

N-(5-iodoquinolin-8-yl)-3-methylbenzamide 3c; White solid (m=60mg, 77%); m.p. 116-118 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 10.66 (s, 1H), 8.78 (dd, *J* = 4.2, 1.5 Hz, 1H), 8.68 (d, *J* = 8.3 Hz, 1H), 8.34 (dd, *J* = 8.5, 1.5 Hz, 1H), 8.09 (d, *J* = 8.3 Hz, 1H), 7.89 – 7.78 (m, 2H), 7.51 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.46 – 7.35 (m, 2H), 2.47 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.52, 148.76, 140.64, 139.23, 138.66, 138.23, 135.46, 134.76, 132.73, 129.54, 128.62, 127.99, 124.15, 123.12, 117.80, 89.40, 21.45; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{17}H_{13}IN_2OH^+$ 389.0145, found 389.0144



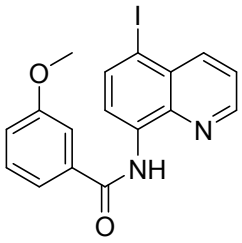
3d

N-(5-iodoquinolin-8-yl)-4-methylbenzamide 3d; White solid (m=60mg, 77%); m.p. 174-176 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.67 (s, 1H), 8.78 (dd, *J* = 4.2, 1.5 Hz, 1H), 8.68 (d, *J* = 8.3 Hz, 1H), 8.34 (dd, *J* = 8.5, 1.5 Hz, 1H), 8.08 (d, *J* = 8.3 Hz, 1H), 7.94 (d, *J* = 8.2 Hz, 2H), 7.51 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.32 (d, *J* = 8.0 Hz, 2H), 2.44 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.28, 148.72, 142.51, 140.63, 139.24, 138.24, 135.52, 131.95, 129.54, 129.44, 127.24, 123.11, 117.73, 89.26, 21.53; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{17}H_{13}IN_2OH^+$ 389.0145, found 389.0144



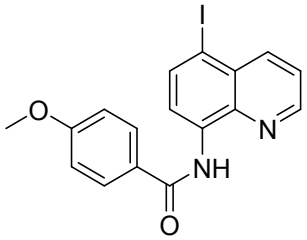
3e

4-ethyl-N-(5-iodoquinolin-8-yl)benzamide 3e; White solid (m=53mg, 65%); m.p. 159-161 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.70 (s, 1H), 8.82 – 8.76 (m, 1H), 8.69 (d, *J* = 8.3 Hz, 1H), 8.35 (dd, *J* = 8.5, 1.2 Hz, 1H), 8.10 (d, *J* = 8.3 Hz, 1H), 7.98 (d, *J* = 8.2 Hz, 2H), 7.53 (dd, *J* = 8.5, 4.1 Hz, 1H), 7.37 (d, *J* = 8.1 Hz, 2H), 2.74 (q, *J* = 7.6 Hz, 2H), 1.29 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (101 MHz, CDCl3) δ 165.36, 148.73, 140.64, 139.21, 138.23, 135.49, 132.16, 130.88, 129.52, 128.78, 128.28, 127.34, 123.14, 117.71, 89.30, 28.83, 15.32; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{18}H_{15}IN_2OH^+$ 403.0301, found 403.0300



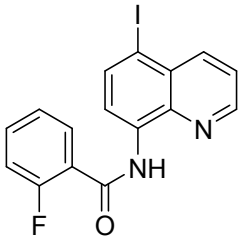
3f

N-(5-iodoquinolin-8-yl)-3-methoxybenzamide 3f; White solid (m=56mg, 81%); m.p. 78-81 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.68 (s, 1H), 8.78 (d, *J* = 4.2 Hz, 1H), 8.66 (t, *J* = 7.5 Hz, 1H), 8.41 – 8.25 (m, 1H), 8.09 (dd, *J* = 8.2, 1.1 Hz, 1H), 7.64 – 7.56 (m, 2H), 7.56 – 7.48 (m, 1H), 7.44 (ddd, *J* = 8.0, 4.6, 1.5 Hz, 1H), 7.11 (dd, *J* = 6.6, 1.7 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.12, 159.96, 148.79, 140.64, 139.21, 138.20, 136.24, 135.36, 129.76, 129.55, 123.15, 118.98, 118.09, 117.78, 112.67, 89.53, 77.32, 77.00, 76.68, 55.47; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{17}H_{13}IN_2O_2H^+$ 405.0094, found 405.0094



3g

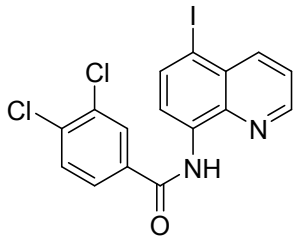
N-(5-iodoquinolin-8-yl)-4-methoxybenzamide 3g; White solid (m=54mg, 66%); m.p. 156-158^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.66 (s, 1H), 8.80 (dd, *J* = 4.2, 1.4 Hz, 1H), 8.69 (d, *J* = 8.3 Hz, 1H), 8.37 (dd, *J* = 8.5, 1.5 Hz, 1H), 8.11 (d, *J* = 8.3 Hz, 1H), 8.07 – 8.01 (m, 2H), 7.54 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.09 – 7.00 (m, 2H), 3.90 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.91, 162.63, 148.73, 140.72, 139.31, 138.32, 135.65, 129.61, 129.17, 127.10, 123.15, 117.70, 114.01, 89.09, 77.32, 77.00, 76.68, 55.47; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{17}H_{13}IN_2O_2H^+$ 405.0094, found 405.0094



3h

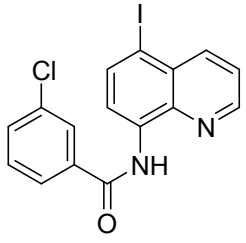
2-fluoro-N-(5-iodoquinolin-8-yl)benzamide 3h; White solid (m=67mg, 85%); m.p. 184-186^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.17 (d, *J* = 12.6 Hz, 1H), 8.83 (dd, *J* = 4.2, 1.5 Hz, 1H), 8.74 (d, *J* = 8.3 Hz, 1H), 8.38 (dd, *J* = 8.5, 1.5 Hz, 1H), 8.21 (td, *J* = 7.9, 1.8 Hz, 1H), 8.12 (d, *J* = 8.3 Hz, 1H), 7.57 – 7.51 (m, 2H), 7.37 – 7.30 (m, 1H), 7.29 – 7.20 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.82, 161.61 (d, *J* = 3 Hz), 159.35, 149.02, 139.43 (d, *J* = 237 Hz), 139.35, 135.75, 133.77 (d, *J* = 9 Hz), 132.07

(d, *J* = 1 Hz), 129.63, 124.91 (d, *J* = 4 Hz), 123.20, 121.79 (d, *J* = 11 Hz) 118.56, 116.35 (d, *J* = 24 Hz), 90.01; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{16}H_{10}FIN_2OH^+$ 392.9894, found 392.9895



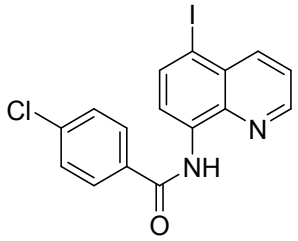
3i

3,4-dichloro-N-(5-iodoquinolin-8-yl)benzamide 3i; White solid (m=50mg, 56%); m.p. 174-177 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.68 (s, 1H), 8.84 (dd, *J* = 4.2, 1.5 Hz, 1H), 8.65 (d, *J* = 8.3 Hz, 1H), 8.41 (dd, *J* = 8.5, 1.5 Hz, 1H), 8.14 (t, *J* = 5.6 Hz, 2H), 7.88 (dd, *J* = 8.3, 2.1 Hz, 1H), 7.63 (d, *J* = 8.3 Hz, 1H), 7.58 (dd, *J* = 8.5, 4.2 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.05, 149.02, 140.88, 139.17, 138.25, 136.55, 134.94, 134.63, 133.45, 130.87, 129.69, 129.56, 126.25, 123.36, 118.05, 90.16; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{16}H_9Cl_2IN_2OH^+$ 442.9209, found 442.9210



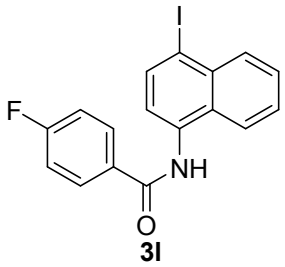
3j

3-chloro-N-(5-iodoquinolin-8-yl)benzamide 3j; White solid (m=44mg, 53%);. m.p. 162-164 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.67 (s, 1H), 8.82 (dd, *J* = 4.2, 1.5 Hz, 1H), 8.65 (d, *J* = 8.3 Hz, 1H), 8.38 (dd, *J* = 8.5, 1.5 Hz, 1H), 8.11 (d, *J* = 8.3 Hz, 1H), 8.03 (t, *J* = 1.8 Hz, 1H), 7.95 – 7.89 (m, 1H), 7.59 – 7.52 (m, 2H), 7.48 (t, *J* = 7.8 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.89, 148.94, 140.78, 139.18, 138.22, 136.57, 135.09, 135.07, 132.02, 130.09, 129.62, 127.67, 125.22, 123.28, 117.98, 89.94; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{16}H_{10}ClIN_2OH^+$ 408.9598, found 408.9598



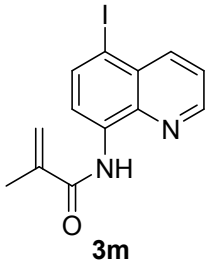
3k

4-chloro-N-(5-iodoquinolin-8-yl)benzamide 3k; White solid (m=51mg, 62%); m.p. 178-181 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.67 (s, 1H), 8.79 (dd, *J* = 4.2, 1.5 Hz, 1H), 8.65 (d, *J* = 8.3 Hz, 1H), 8.37 (dd, *J* = 8.5, 1.5 Hz, 1H), 8.10 (d, *J* = 8.3 Hz, 1H), 8.04 – 7.93 (m, 2H), 7.57 – 7.47 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.17, 148.86, 140.76, 139.16, 138.31, 138.23, 135.16, 133.14, 129.60, 129.07, 128.66, 123.24, 117.87, 89.78; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{16}H_{10}ClIN_2OH^+$ 408.9598, found 408.9599



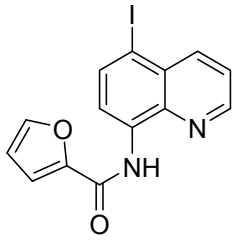
3l

4-fluoro-N-(5-iodoquinolin-8-yl)benzamide 3l; White solid (m=70mg, 89%); m.p. 168-171 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.64 (s, 1H), 8.78 (dd, *J* = 4.2, 1.5 Hz, 1H), 8.64 (d, *J* = 8.3 Hz, 1H), 8.34 (dd, *J* = 8.5, 1.5 Hz, 1H), 8.15 – 8.00 (m, 3H), 7.53 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.25 – 7.15 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.28, 164.12, 163.77, 148.79, 139.46 (d, *J* = 251 Hz), 139.13, 135.22, 130.93 (d, *J* = 4 Hz), 129.63 (d, *J* = 9 Hz), 129.55, 123.19, 117.77, 115.86 (d, *J* = 22 Hz), 89.62; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{16}H_{10}FIN_2OH^+$ 392.9941, found 392.9943.



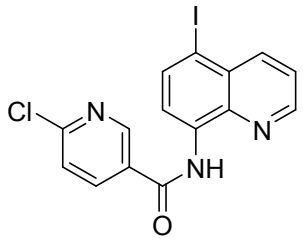
3m

N-(5-iodoquinolin-8-yl)methacrylamide 3m; White solid (m=57mg, 83%); m.p. 76-79 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.32 (s, 1H), 8.74 (dd, *J* = 4.2, 1.5 Hz, 1H), 8.57 (d, *J* = 8.3 Hz, 1H), 8.31 (dd, *J* = 8.5, 1.5 Hz, 1H), 8.05 (d, *J* = 8.3 Hz, 1H), 7.49 (dd, *J* = 8.5, 4.2 Hz, 1H), 6.04 (s, 1H), 5.57 (d, *J* = 0.8 Hz, 1H), 2.18 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.26, 148.70, 140.56, 140.43, 139.10, 138.15, 135.24, 129.45, 123.06, 120.91, 117.67, 89.36, 18.60; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{13}H_{11}IN_2OH^+$ 338.9988, found 338.9987



3n

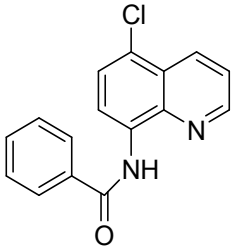
N-(5-iodoquinolin-8-yl)furan-2-carboxamide 3n; White solid (m=69mg, 82%); m.p. 172-175 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.74 (s, 1H), 8.83 (dd, *J* = 4.2, 1.5 Hz, 1H), 8.62 (d, *J* = 8.3 Hz, 1H), 8.36 (dd, *J* = 8.5, 1.5 Hz, 1H), 8.09 (d, *J* = 8.3 Hz, 1H), 7.62 (d, *J* = 0.9 Hz, 1H), 7.54 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.34 – 7.28 (m, 1H), 6.59 (dd, *J* = 3.5, 1.7 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.28, 148.92, 148.11, 144.63, 140.63, 139.12, 138.18, 135.05, 129.61, 123.20, 117.91, 115.41, 112.51, 89.70; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{14}H_9IN_2O_2H^+$ 364.9781, found 364.9782



3o

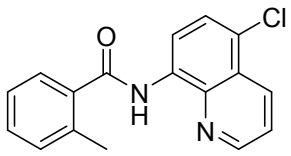
6-chloro-N-(5-iodoquinolin-8-yl)nicotinamide 3o; White solid (m=460mg, 73%); m.p. 132-134 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.72 (s, 1H), 9.08 (d, *J* = 2.5 Hz, 1H), 8.81 (dd, *J* = 4.2, 1.4 Hz, 1H), 8.62 (d, *J* = 8.3 Hz, 1H), 8.40 (dd, *J* = 8.5, 1.4 Hz, 1H), 8.30 (dd, *J* = 8.3, 2.5 Hz, 1H), 8.13 (d, *J* = 8.3 Hz, 1H), 7.58 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.52 (d, *J* = 8.3 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.34, 154.76, 149.06, 148.51, 140.88, 139.03, 138.18, 137.84, 134.68, 129.66, 129.42, 124.53, 123.42,

118.08, 90.44; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{15}H_9ClIN_3OH^+$ 409.9551, found 409.9550



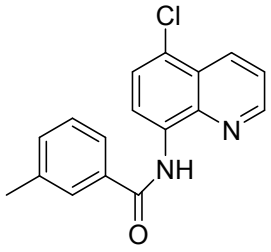
4a

N-(5-chloroquinolin-8-yl)benzamide 4a: white solid (m=50 mg, 88%); m.p.: 134-136 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.68 (s, 1H), 8.88 (dd, *J* = 4.9, 3.5 Hz, 2H), 8.58 (dd, *J* = 8.5, 1.4 Hz, 1H), 8.07 (dd, *J* = 7.9, 1.4 Hz, 2H), 7.65 (d, *J* = 8.4 Hz, 1H), 7.58 (ddd, *J* = 15.9, 9.0, 4.3 Hz, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.36, 148.69, 139.15, 134.75, 133.74, 133.46, 131.98, 128.80, 127.26, 127.23, 125.92, 124.44, 122.38, 116.44.; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{16}H_{11}ClN_2OH^+$: 283.0632, found: 283.0633.



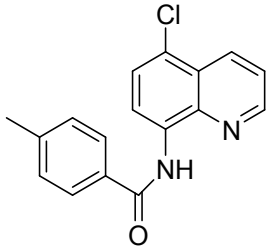
4b

N-(5-chloroquinolin-8-yl)-2-methylbenzamide 4b: white solid (m=38 mg, 64%); m.p.: 140-141 °C; ^{1}H NMR (300 MHz, CDCl3) δ 10.18 (s, 1H), 8.90 (d, *J* = 8.4 Hz, 1H), 8.83 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.59 (dd, *J* = 8.5, 1.6 Hz, 1H), 7.69 (dd, *J* = 10.7, 5.1 Hz, 2H), 7.58 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.45 – 7.40 (m, 1H), 7.33 (dt, *J* = 7.2, 3.5 Hz, 2H), 2.61 (s, 3H); ^{13}C NMR (75 MHz, CDCl3) δ 168.07, 148.69, 139.14, 136.75, 136.31, 133.99, 133.38, 131.41, 130.44, 127.20, 126.01, 124.51, 122.34, 116.40, 20.19; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{17}H_{13}ClN_2OH^+$: 297.0788, found: 297.0790.



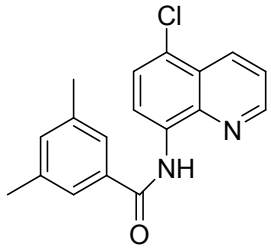
4c

N-(5-chloroquinolin-8-yl)-3-methylbenzamide 4c: white solid (m=45 mg, 76%); m.p.: 104-106 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.67 (s, 1H), 8.91 (dd, *J* = 8.3, 5.0 Hz, 2H), 8.60 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.92 – 7.83 (m, 2H), 7.66 (d, *J* = 8.4 Hz, 1H), 7.61 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.47 – 7.38 (m, 2H), 2.49 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.65, 148.74, 139.27, 138.73, 134.82, 133.88, 133.45, 132.76, 128.67, 128.02, 127.30, 125.97, 124.38, 124.17, 122.39, 116.42, 21.50; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{17}H_{13}ClN_2OH^+$: 297.0788, found:297.0790.



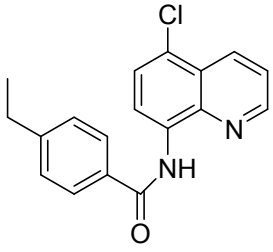
4d

N-(5-chloroquinolin-8-yl)-4-methylbenzamide 4d: white solid (m=41 mg, 70%); m.p.: 135-137 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.65 (s, 1H), 8.87 (d, *J* = 8.5 Hz, 2H), 8.56 (dd, *J* = 8.5, 1.6 Hz, 1H), 7.96 (d, *J* = 8.2 Hz, 2H), 7.63 (d, *J* = 8.4 Hz, 1H), 7.57 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.34 (d, *J* = 8.0 Hz, 2H), 2.45 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.31, 148.65, 142.50, 139.17, 133.86, 133.35, 131.92, 129.45, 127.24, 127.22, 125.88, 124.22, 122.33, 116.26, 21.55; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{17}H_{13}ClN_2OH^+$: 297.0788, found: 297.0789.



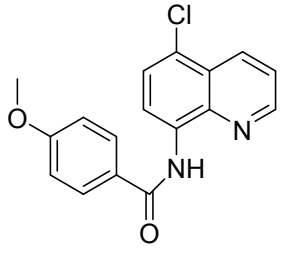
4e

N-(5-chloroquinolin-8-yl)-3,5-dimethylbenzamide 4e: white solid (m=50 mg, 80%); m.p.: 142-144 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.60 (s, 1H), 8.94 – 8.85 (m, 2H), 8.59 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.65 (t, *J* = 4.2 Hz, 3H), 7.59 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.24 (d, *J* = 17.0 Hz, 1H), 2.44 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.87, 148.73, 139.34, 138.52, 134.93, 134.01, 133.62, 133.43, 127.32, 125.99, 125.01, 124.31, 122.34, 116.47, 21.36; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{18}H_{15}ClN_2OH^+$: 311.0945, found: 311.0944.



4f

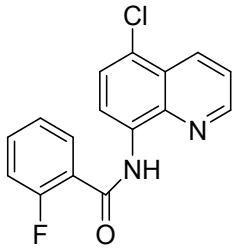
N-(5-chloroquinolin-8-yl)-4-ethylbenzamide 4f: white solid (m=43 mg, 70%); m.p.: 100-102 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.66 (s, 1H), 8.88 (dd, *J* = 5.0, 3.5 Hz, 2H), 8.57 (dd, *J* = 8.5, 1.6 Hz, 1H), 7.99 (d, *J* = 8.3 Hz, 2H), 7.64 (d, *J* = 8.4 Hz, 1H), 7.58 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.37 (d, *J* = 8.3 Hz, 2H), 2.75 (q, *J* = 7.6 Hz, 2H), 1.29 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.40, 148.72, 148.67, 139.22, 133.91, 133.39, 132.21, 128.30, 127.34, 127.27, 125.92, 124.24, 122.35, 116.29, 28.84, 15.34; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{18}H_{15}ClN_2OH^+$: 311.0945, found: 311.0946.



4g

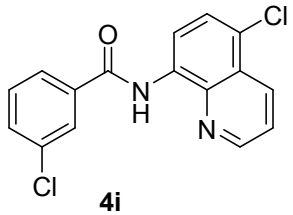
N-(5-chloroquinolin-8-yl)-4-methoxybenzamide 4g : white solid (m=42 mg, 68%); m.p.: 202-204 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.63 (s, 1H), 8.93 – 8.83 (m, 2H), 8.59 (dd, *J* = 8.5, 1.6 Hz, 1H), 8.06 – 8.03 (m, 2H), 7.65 (d, *J* = 8.4 Hz, 1H), 7.60 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.07 – 7.01 (m, 2H), 3.90 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.95, 162.57, 148.66, 139.24, 133.98, 133.43, 129.16, 127.32, 127.06, 125.95, 124.13, 122.36, 116.23, 113.99, 113.69, 55.47; HRMS (EI) $[M+H]^+$ m/z Calcd for

$C_{17}H_{13}ClN_2O_2H^+$: 313.0738, found: 313.0740.



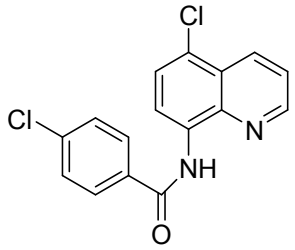
4h

N-(5-chloroquinolin-8-yl)-2-fluorobenzamide 4h: white solid (m=47 mg, 78%); m.p.: 138-140 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 11.12 (d, *J* = 12.9 Hz, 1H), 8.94 – 8.88 (m, 2H), 8.56 (dd, *J* = 8.5, 1.6 Hz, 1H), 8.21 (td, *J* = 7.9, 1.8 Hz, 1H), 7.63 (d, *J* = 8.4 Hz, 1H), 7.60 – 7.50 (m, 2H), 7.37 – 7.29 (m, 1H), 7.28 – 7.21 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.52 (d, *J* = 3.3 Hz), 160.52 (d, *J* = 248 Hz), 148.90, 139.23, 137.40, 134.03, 133.74 (d, *J* = 9.3 Hz), 133.24, 132.01 (d, *J* = 1.8 Hz), 130.19, 127.16, 125.87, 124.89 (d, *J* = 3 Hz), 124.77, 122.36, 121.66 (d, *J* = 11.4 Hz), 117.07, 116.32 (d, *J* = 25 Hz); HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{16}H_{10}ClFN_2OH^+$: 301.0538, found: 301.0536.



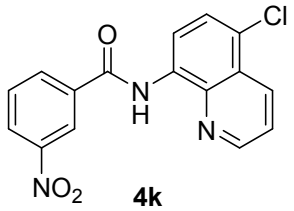
4i

3-chloro-N-(5-chloroquinolin-8-yl)benzamide 4i: white solid (m=42 mg, 67%); m.p.: 130-132 ^oC; ^1H NMR (300 MHz, $CDCl_3$)δ 10.63 (s, 1H), 8.91 (dd, *J* = 4.2, 1.5 Hz, 1H), 8.85 (d, *J* = 8.4 Hz, 1H), 8.60 (dd, *J* = 8.5, 1.6 Hz, 1H), 8.05 (dd, *J* = 2.5, 1.3 Hz, 1H), 7.95 – 7.92 (m, 1H), 7.67 – 7.47 (m, 4H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.90, 148.85, 139.21, 136.62, 135.07, 133.49, 132.00, 130.09, 127.67, 127.23, 125.99, 125.22, 124.84, 122.47, 116.60; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{16}H_{10}Cl_2N_2OH^+$: 317.0242, found: 317.0244.



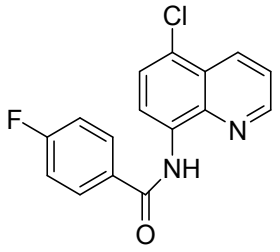
4j

4-chloro-N-(5-chloroquinolin-8-yl)benzamide 4j: white solid (m=52 mg, 83%); m.p.: 160-162 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.66 (s, 1H), 8.91 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.87 (d, *J* = 8.4 Hz, 1H), 8.61 (dd, *J* = 8.5, 1.6 Hz, 1H), 8.07 – 7.98 (m, 2H), 7.67 (d, *J* = 8.4 Hz, 1H), 7.62 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.57 – 7.52 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.21, 148.79, 139.21, 138.30, 133.59, 133.50, 133.21, 129.09, 128.67, 127.26, 125.99, 124.71, 122.45, 116.50; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{16}H_{10}Cl_2N_2OH^+$: 317.0242, found: 317.0240.



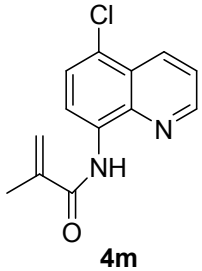
4k

N-(5-chloroquinolin-8-yl)-3-nitrobenzamide 4k: white solid (m=53 mg, 57%); m.p.: 190-192 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.76 (s, 1H), 8.94 – 8.90 (m, 2H), 8.85 (d, *J* = 8.4 Hz, 1H), 8.62 (dd, *J* = 8.5, 1.4 Hz, 1H), 8.47 – 8.39 (m, 2H), 7.77 (t, *J* = 8.0 Hz, 1H), 7.80 – 7.62 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.78, 149.04, 148.52, 139.15, 136.53, 133.59, 133.13, 133.04, 130.06, 127.20, 126.44, 126.02, 125.31, 122.62, 122.33, 116.79; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{16}H_{10}ClN_3O_3H^+$: 328.0483, found: 328.0487.



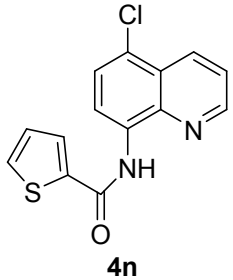
4l

N-(5-chloroquinolin-8-yl)-4-fluorobenzamide 4l: white solid (m=53 mg, 89%); m.p.: 164-166 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.58 (s, 1H), 8.83 (ddd, *J* = 11.3, 6.2, 2.2 Hz, 2H), 8.60 – 8.48 (m, 1H), 8.06 (ddd, *J* = 8.6, 5.2, 1.9 Hz, 2H), 7.64 – 7.52 (m, 2H), 7.21 (td, *J* = 8.6, 1.5 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.03 (d, *J* = 251 Hz), 164.12, 148.71, 139.15, 133.63, 133.40, 130.97 (d, *J* = 3.1 Hz), 129.60 (d, *J* = 9.0 Hz), 127.21, 125.91, 124.53, 122.37, 116.36, 115.85 (d, *J* = 22 Hz); HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{16}H_{10}ClFN_2OH^+$: 301.0538, found: 301.0537.



4m

N-(5-chloroquinolin-8-yl)methacrylamide 4m: white solid (m=40 mg, 81%); m.p.: 83-85 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.31 (s, 1H), 8.86 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.77 (d, *J* = 8.4 Hz, 1H), 8.57 (dd, *J* = 8.5, 1.6 Hz, 1H), 7.65 – 7.54 (m, 2H), 6.04 (s, 1H), 5.57 (d, *J* = 0.9 Hz, 1H), 2.18 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.38, 148.70, 140.54, 139.23, 133.74, 133.39, 127.26, 125.94, 124.35, 122.32, 120.84, 116.36, 18.64; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{13}H_{11}ClN_2OH^+$: 247.0632, found: 247.0631.

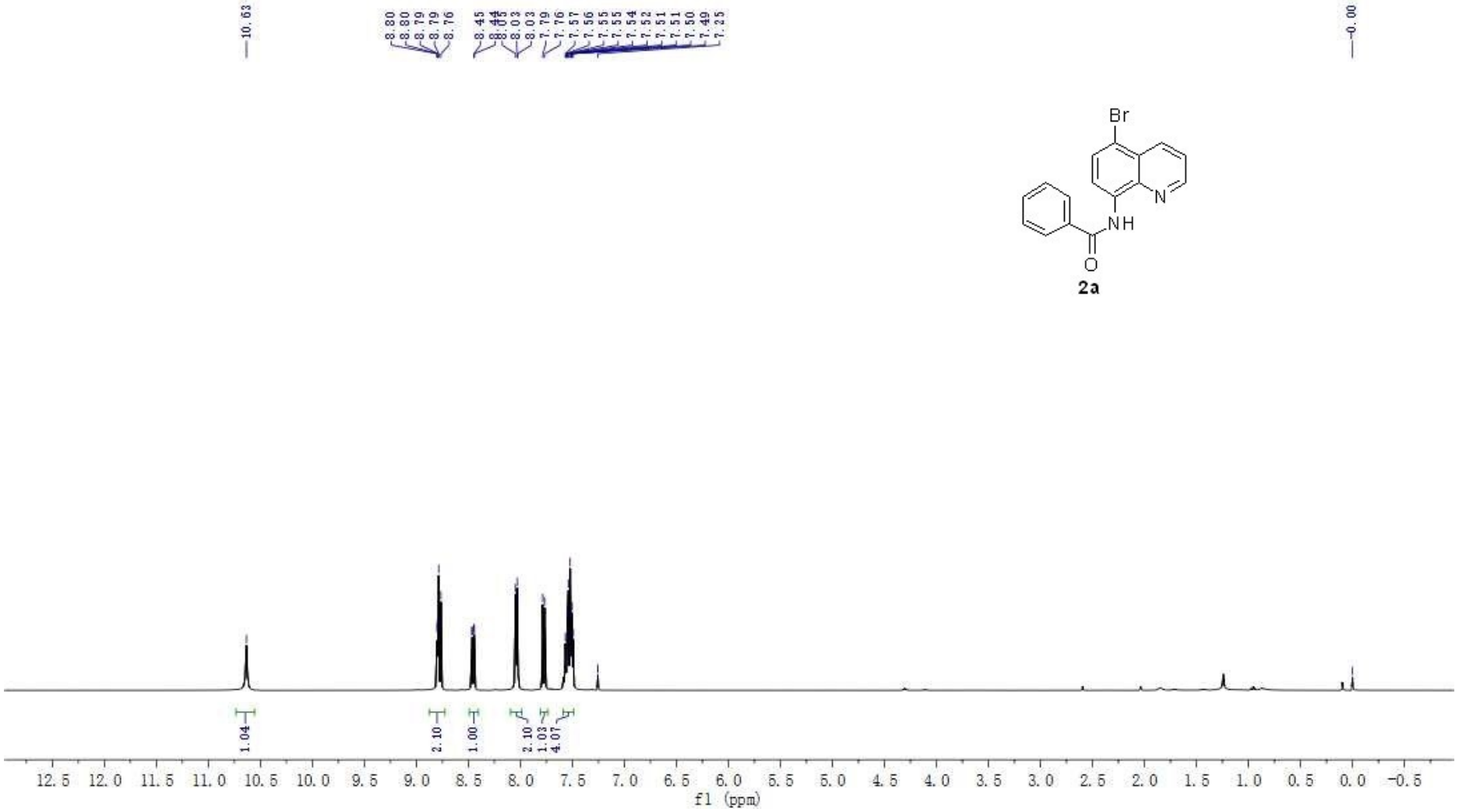


4n

N-(5-chloroquinolin-8-yl)thiophene-2-carboxamide 4n: white solid (m=51 mg, 90%); m.p.: 142-144 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.49 (s, 1H), 8.86 (dd, *J* =

4.2, 1.3 Hz, 1H), 8.76 (d, *J* = 8.4 Hz, 1H), 8.55 (dd, *J* = 8.5, 1.4 Hz, 1H), 7.80 (d, *J* = 3.6 Hz, 1H), 7.64 – 7.54 (m, 3H), 7.20 – 7.15 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 159.86, 148.73, 139.72, 138.94, 133.52, 133.37, 131.09, 128.50, 127.87, 127.23, 125.91, 124.43, 122.38, 116.33; HRMS (EI) $[M+H]^+$ m/z Calcd for $C_{14}H_9ClN_2OSH^+$: 289.0196, found: 289.0197.

4. Copies of ^{1}H NMR and ^{13}C NMR spectra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7.57
7.56
7.55
7.55
7.54
7.52
7.51
7.51
7.50
7.49
7.25
0.00
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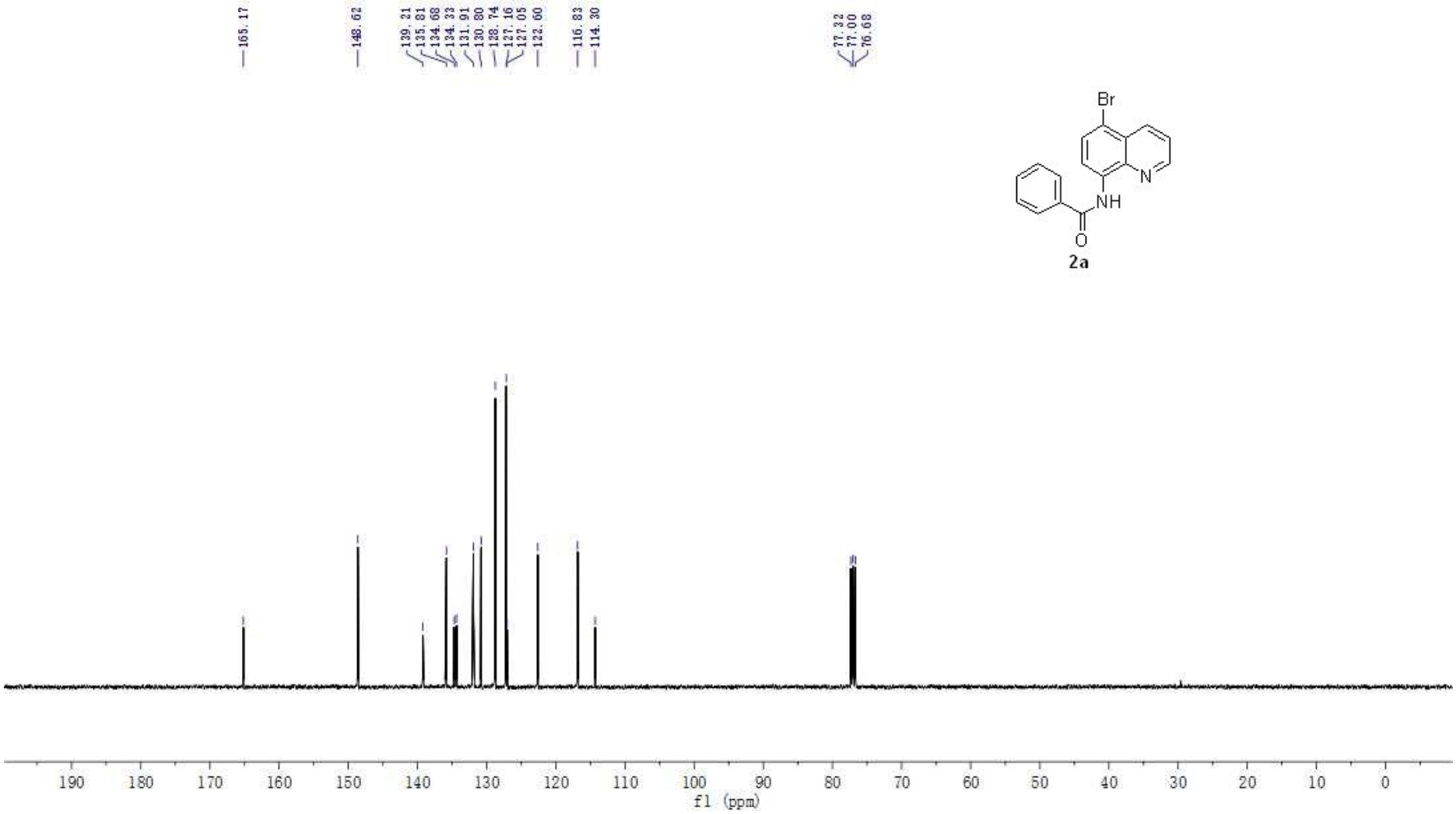
N
NH
O
2a
1.04
2.10
1.00
2.10
1.03
4.07
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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114.30
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77.00
76.68
Br
N
NH
O
2a
190
180
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110
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50
40
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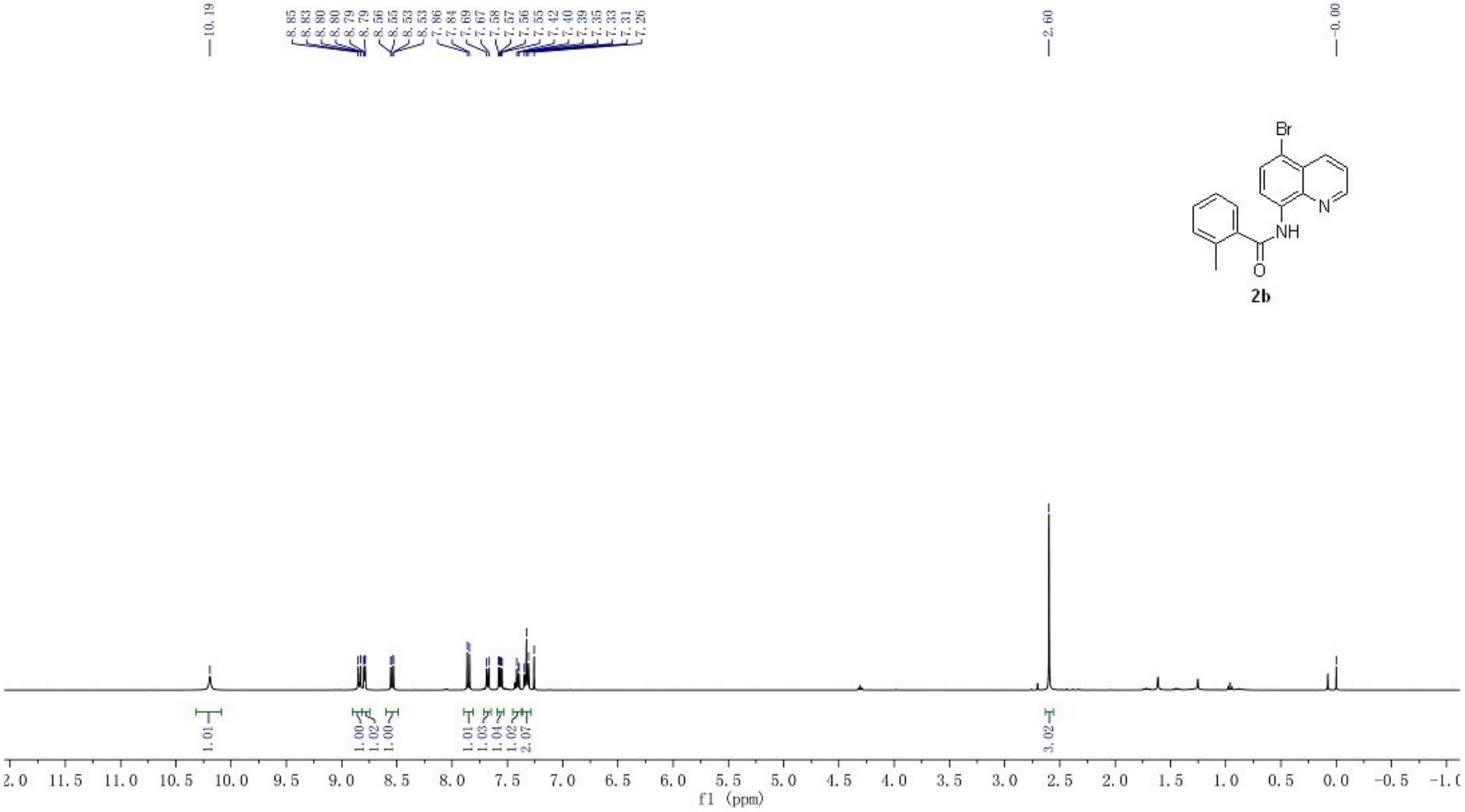
f1 (ppm)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7.58
7.57
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7.35
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1.02
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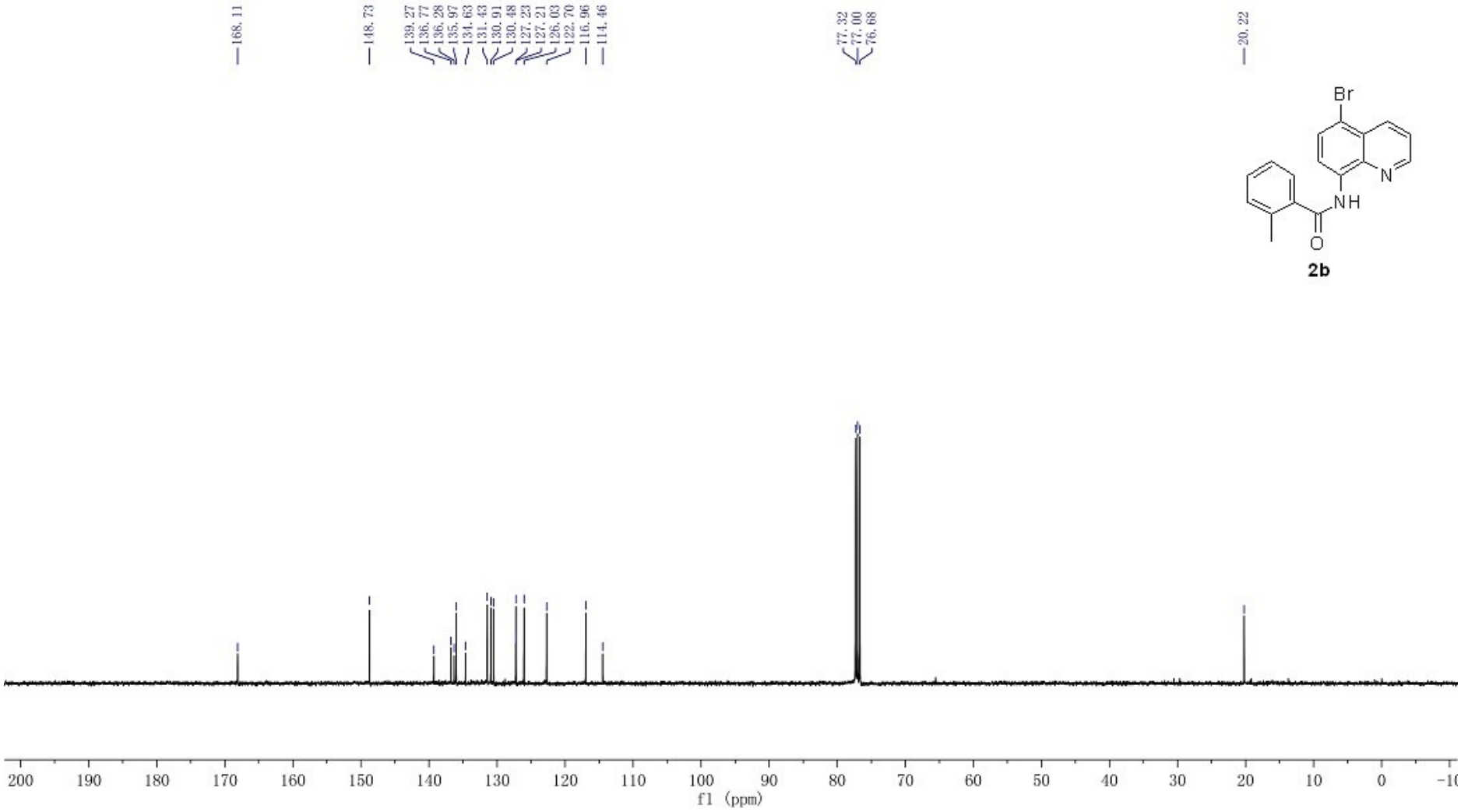
3.02
f1 (ppm)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50
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10
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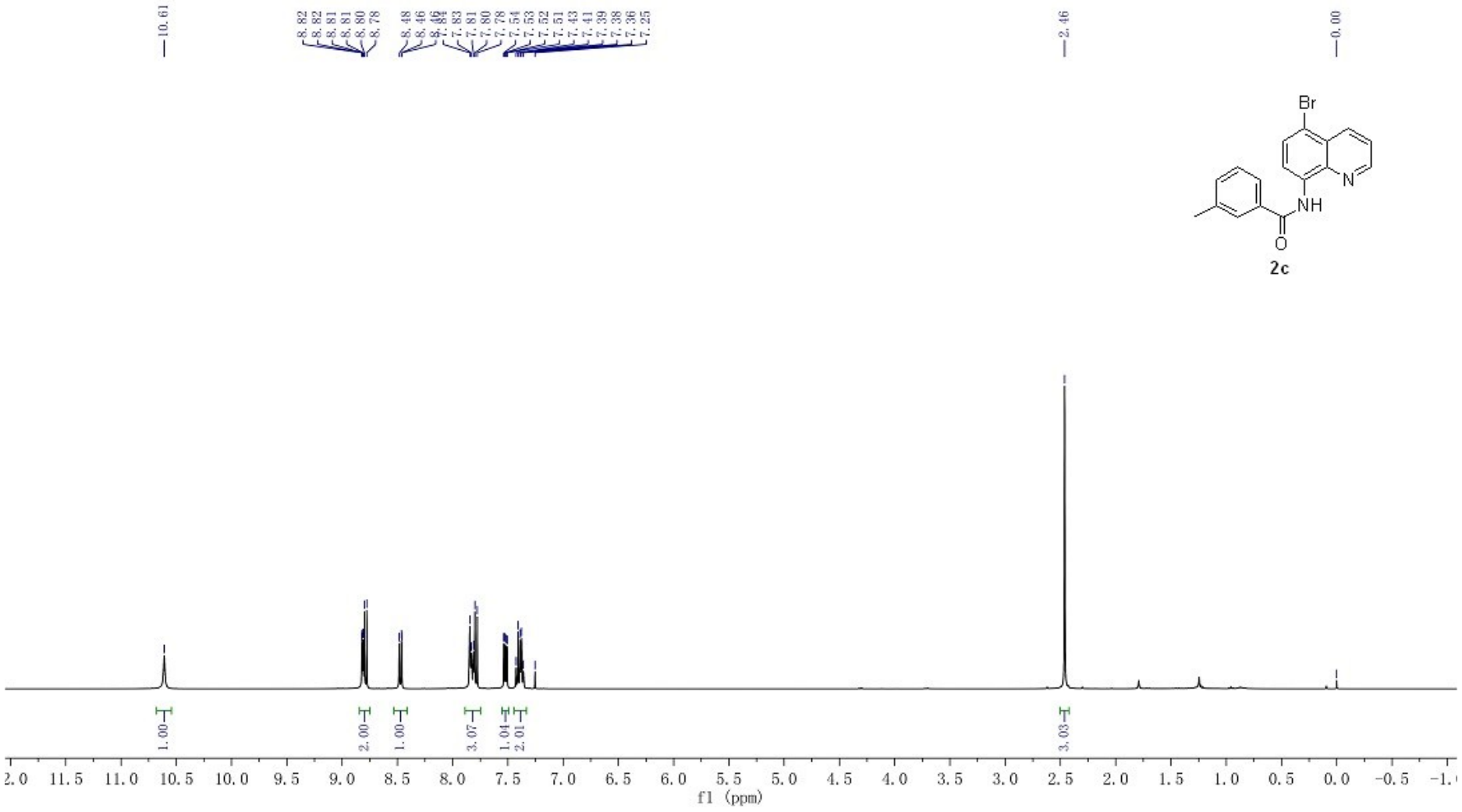
f1 (ppm)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7.54
7.53
7.52
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7.39
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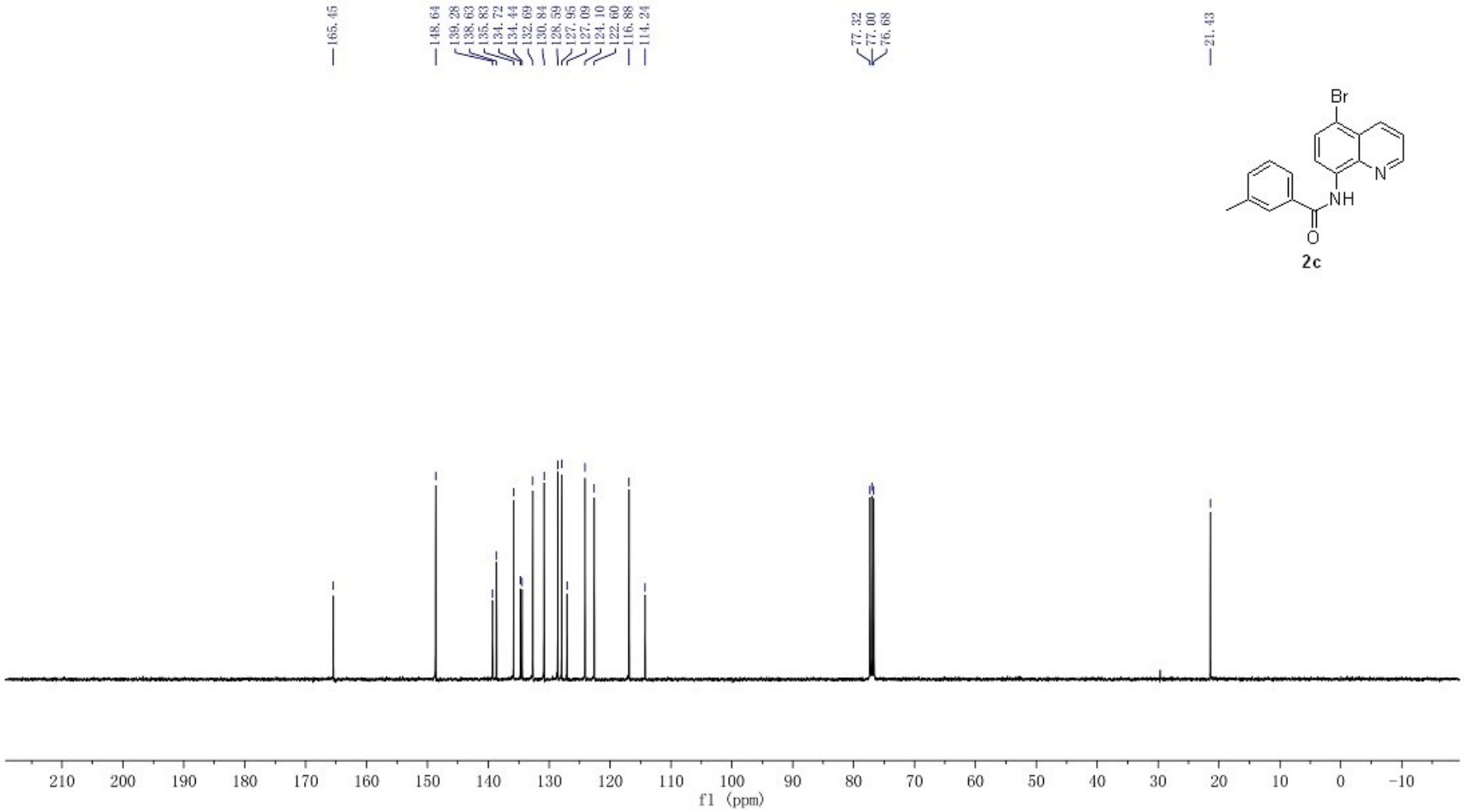
3.03
f1 (ppm)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134.72
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132.69
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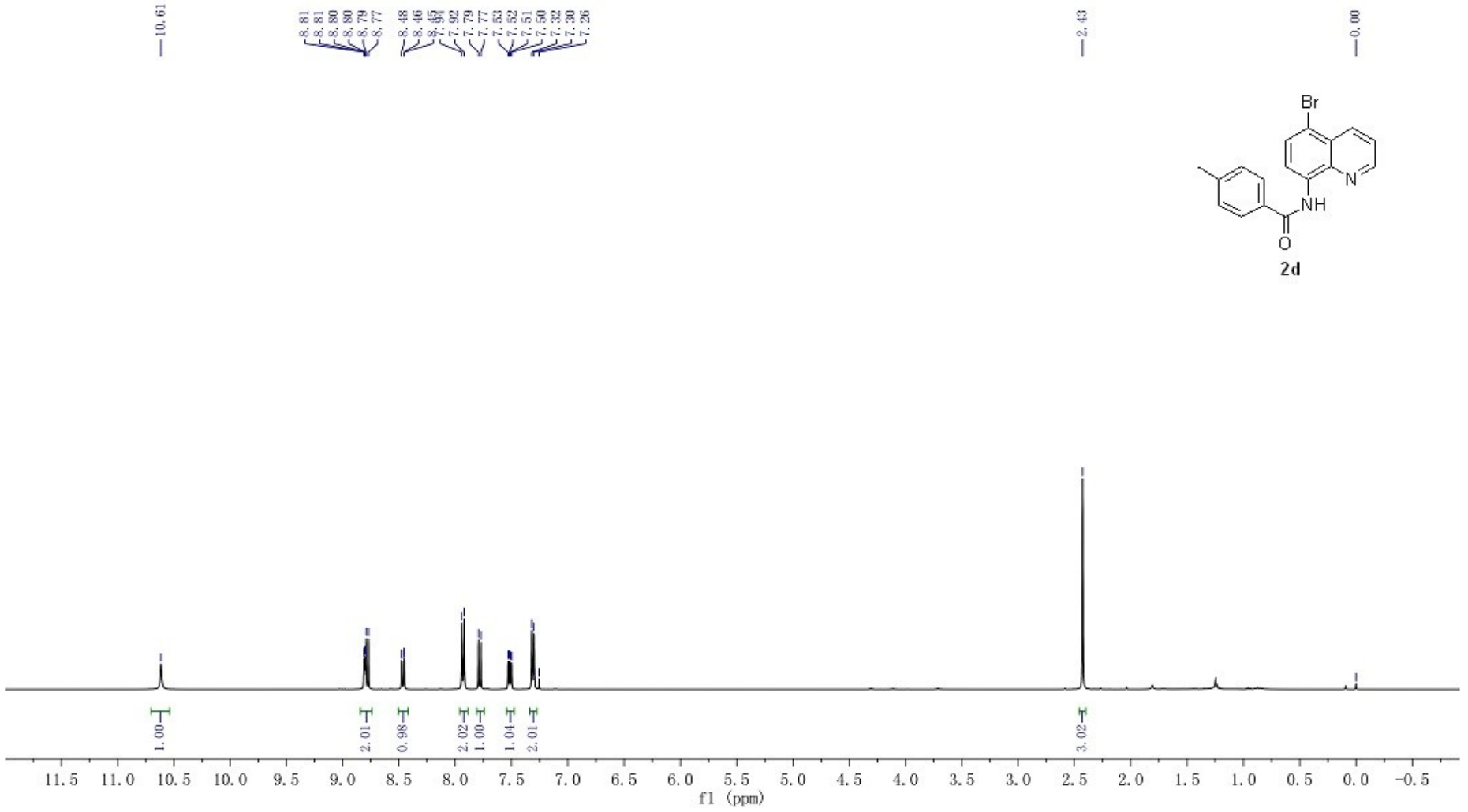
128.59
127.95
127.09
124.10
122.60
116.88
114.24
77.32
77.00
76.68
21.43
Br
N
NH
O
2c
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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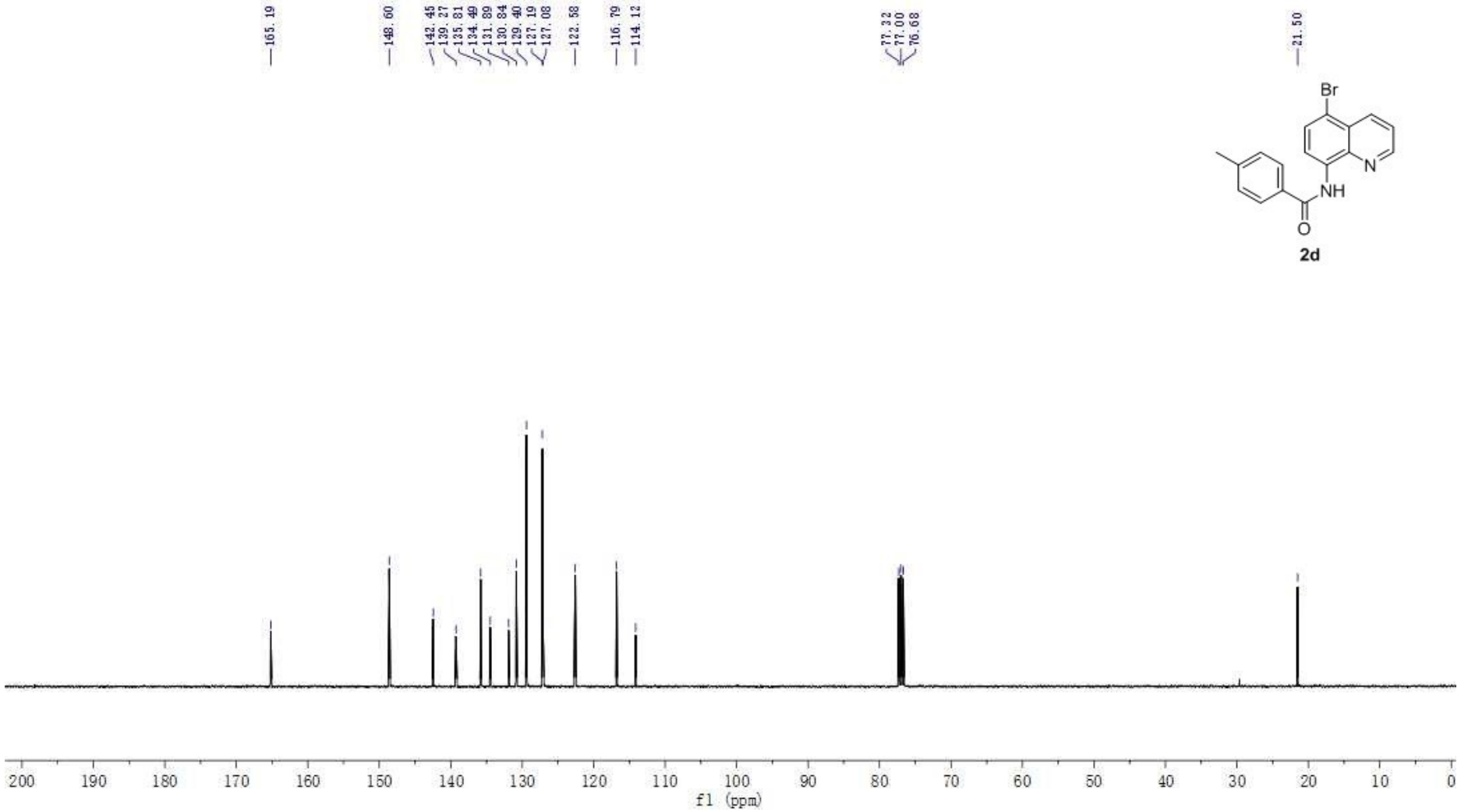
7.52
7.51
7.50
7.32
7.30
7.26
2.43
0.00
Br
N
NH
O
2d
1.00
2.01
0.98
2.02
1.00
1.04
2.01
3.02
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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139.27
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114.12
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77.00
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N
NH
O
2d
200
190
180
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50
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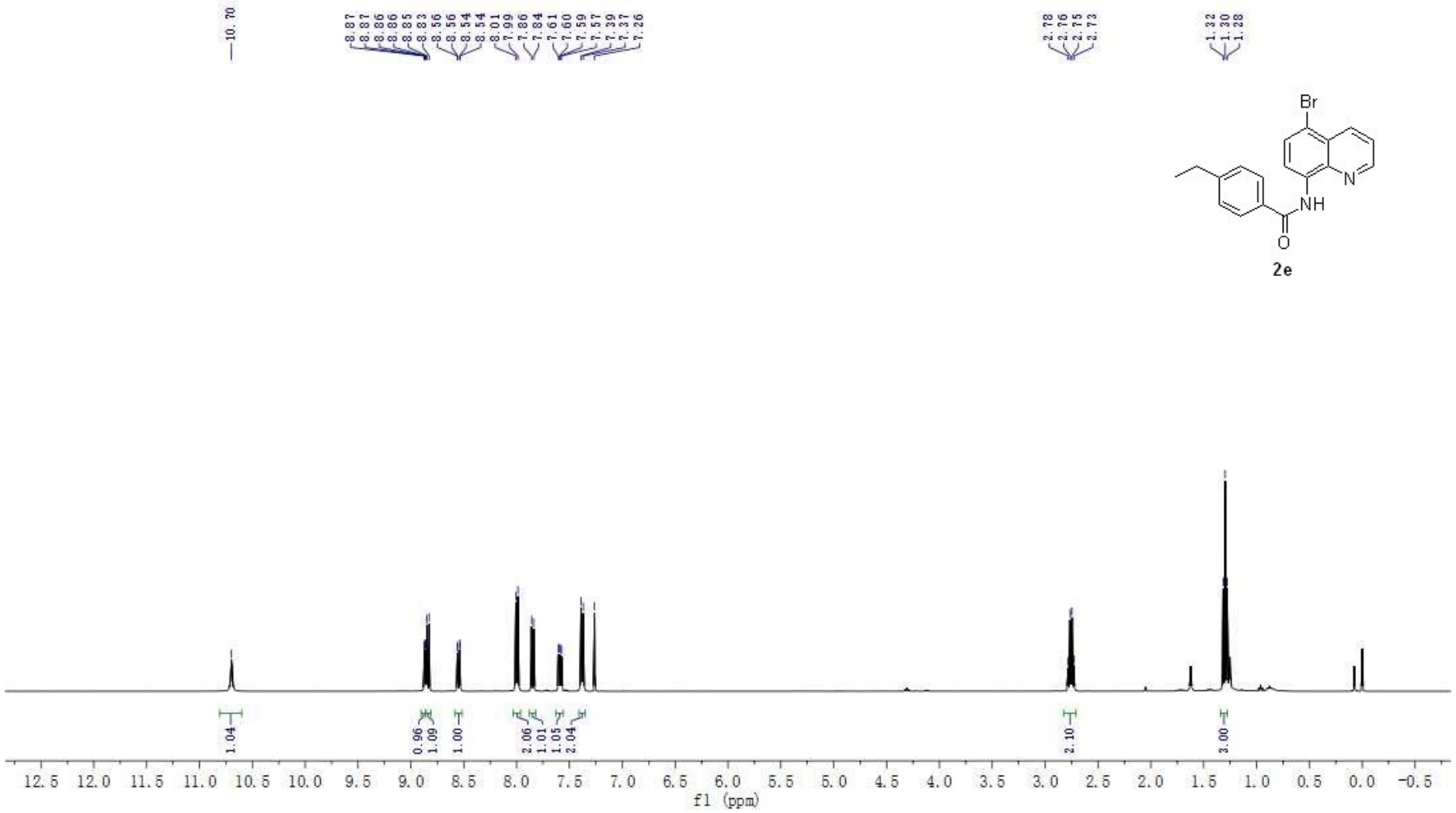
0
f1 (ppm)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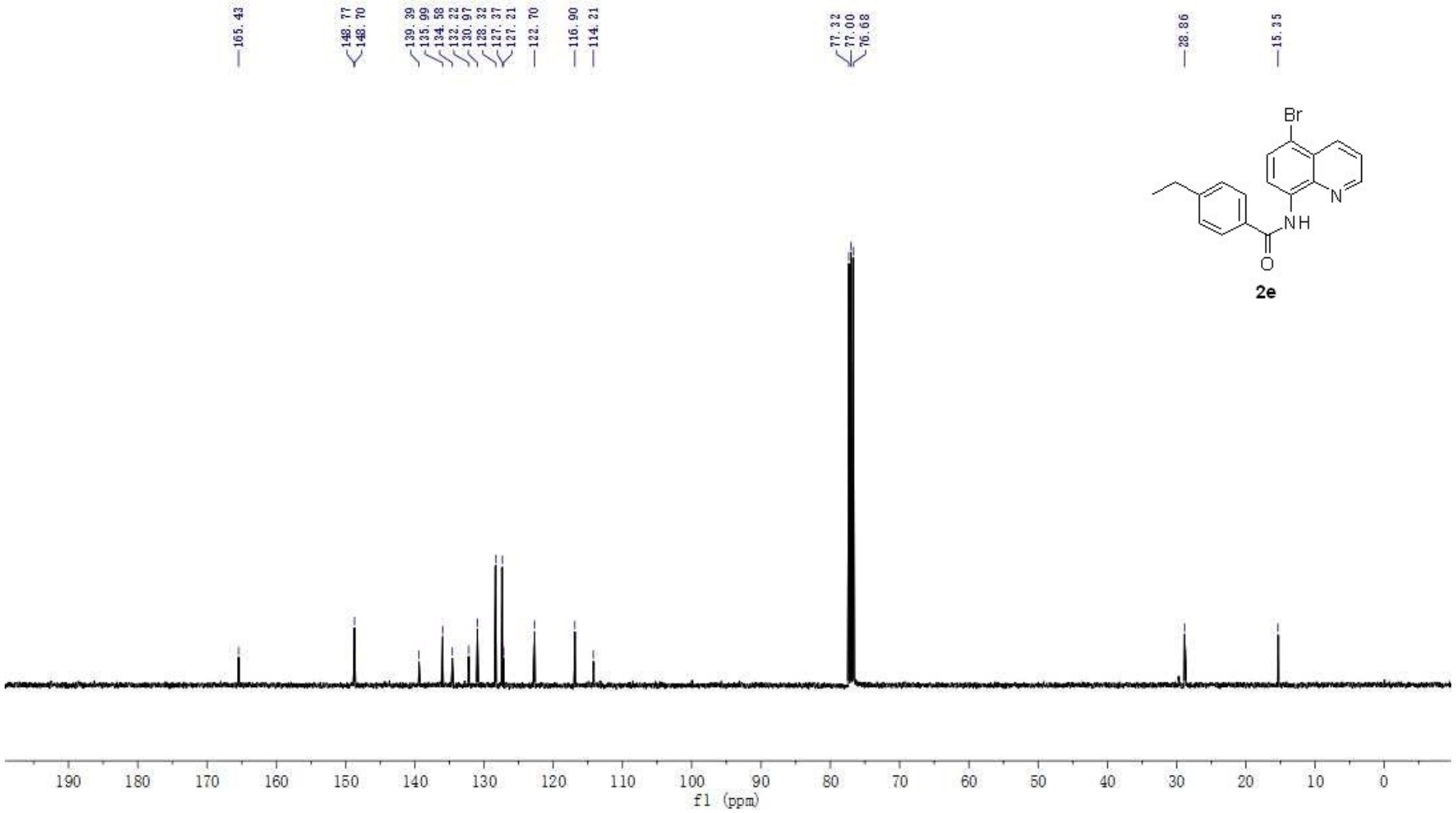
8.86
8.86
8.85
8.83
8.56
8.56
8.54
8.54
8.01
7.99
7.86
7.84
7.61
7.60
7.59
7.57
7.39
7.37
7.26
2.78
2.76
2.75
2.73
1.32
1.30
1.28
Br
N
NH
O
2e
1.04
0.96
1.09
1.00
2.06
1.01
1.05
2.04
2.10
3.00
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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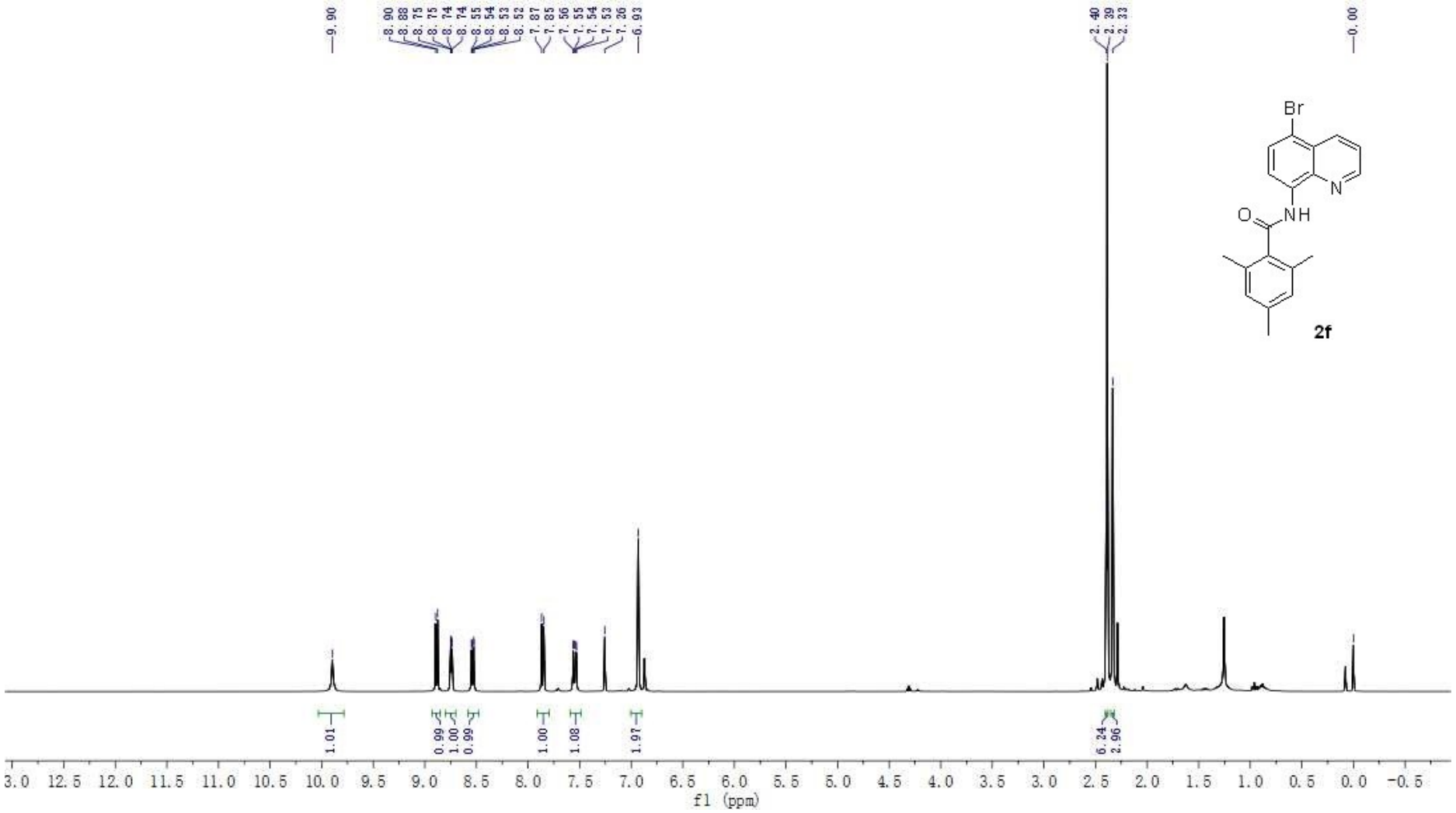
148.77
148.70
139.39
135.99
134.58
132.22
130.97
128.32
127.37
127.21
122.70
116.90
114.21
77.32
77.00
76.68
28.86
15.35
Br
N
NH
O
2e
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.90
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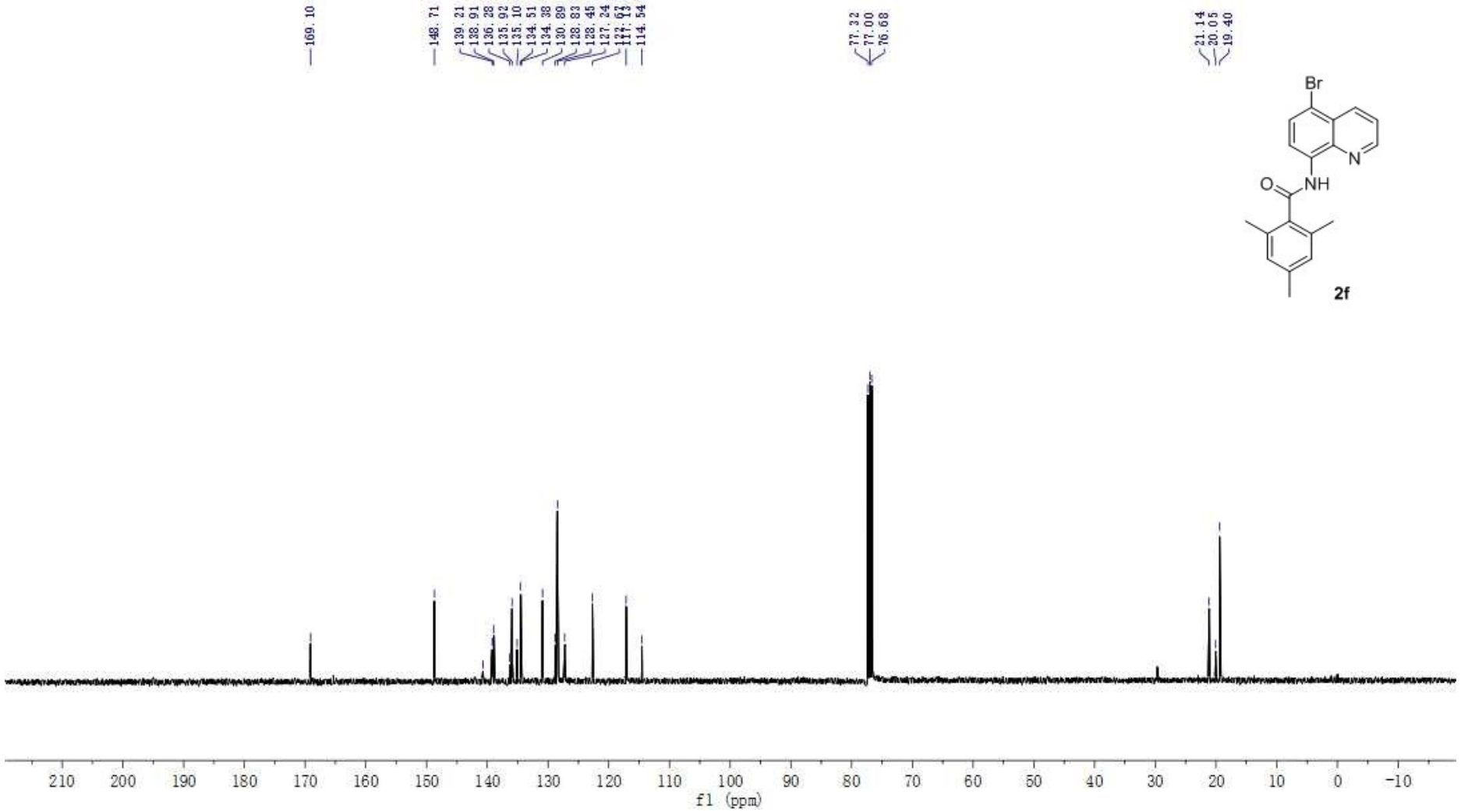
8.74
8.55
8.54
8.53
8.52
7.87
7.85
7.56
7.55
7.54
7.53
7.26
6.93
2.40
2.39
2.33
0.00
Br
N
O
NH
2f
1.01
0.99
1.00
0.99
1.00
1.08
1.97
6.24
2.96
3.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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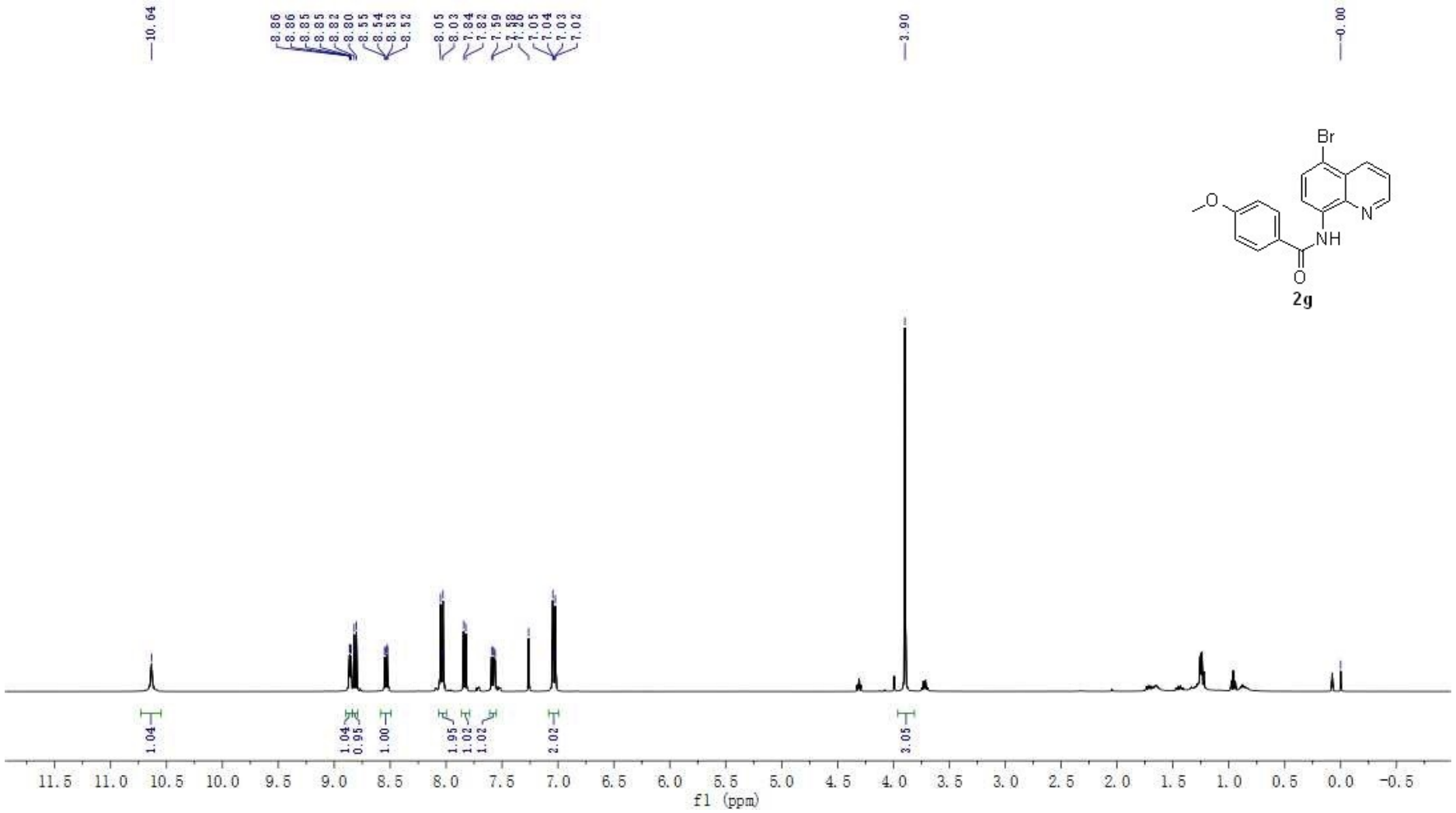
135.92
135.10
134.51
134.38
130.89
128.83
128.45
127.24
114.54
77.32
77.00
76.68
21.14
20.05
19.40
Br
N
O
NH
2f
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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8.86
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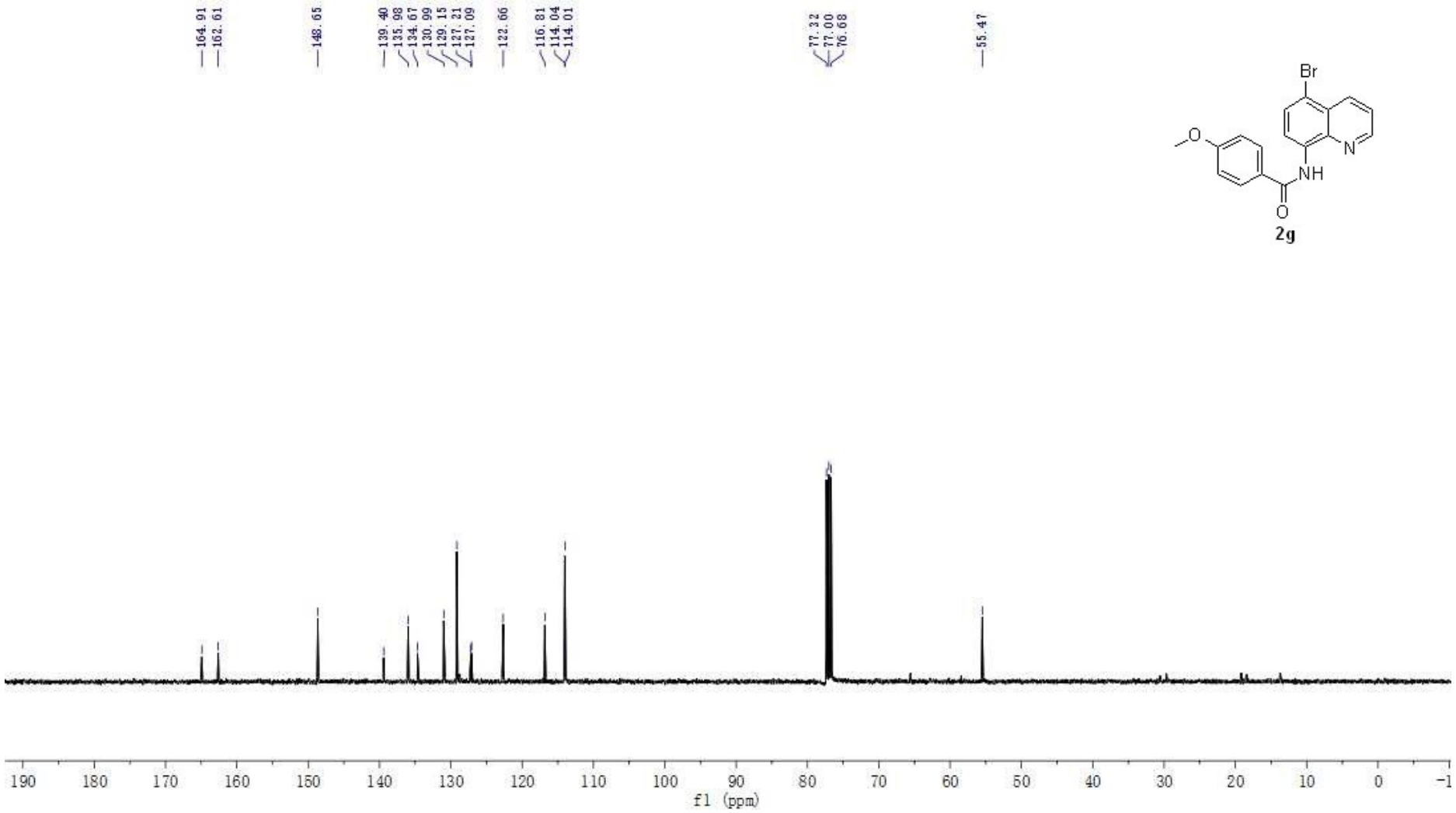
8.55
8.54
8.53
8.52
8.05
8.03
7.84
7.82
7.59
7.58
7.56
7.05
7.04
7.03
7.02
3.90
0.00
Br
O
N
NH
O
2g
1.04
1.04
0.95
1.00
1.95
1.02
1.02
2.02
3.05
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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162.61
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134.67
130.99
129.15
127.21
127.09
122.66
116.81
114.04
114.01
77.32
77.00
76.68
55.47
Br
O
N
NH
O
2g
f1 (ppm)
10.69
8.87
8.87
8.86
8.85
8.84
8.81
8.56
8.55
8.53
8.52
7.86
7.83
7.64
7.64
7.63
7.63
7.62
7.62
7.62
7.61
7.60
7.59
7.57
7.56
7.49
7.46
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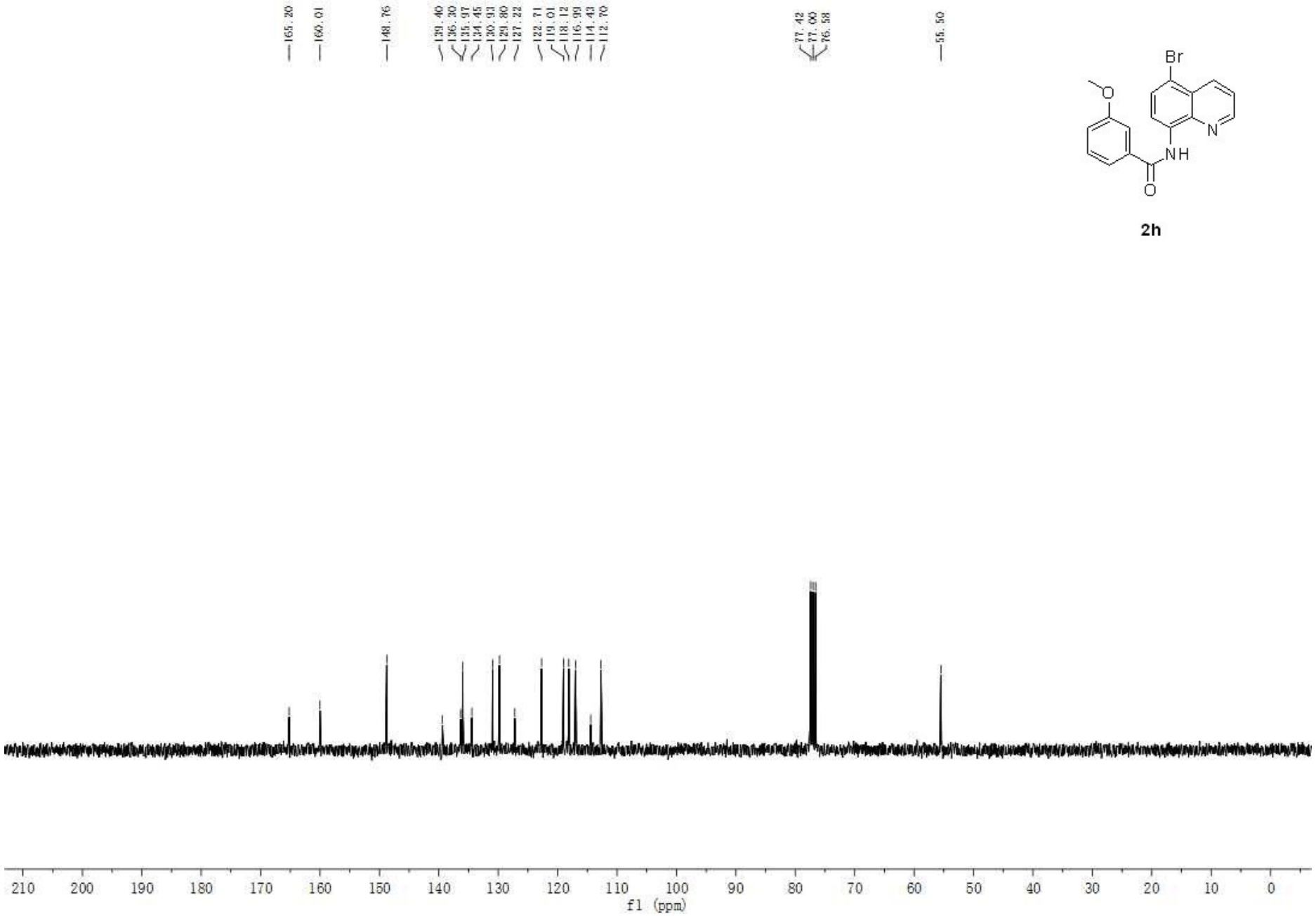
7.12
7.12
7.12
7.11
2.92
0.01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160.01
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139.40
136.30
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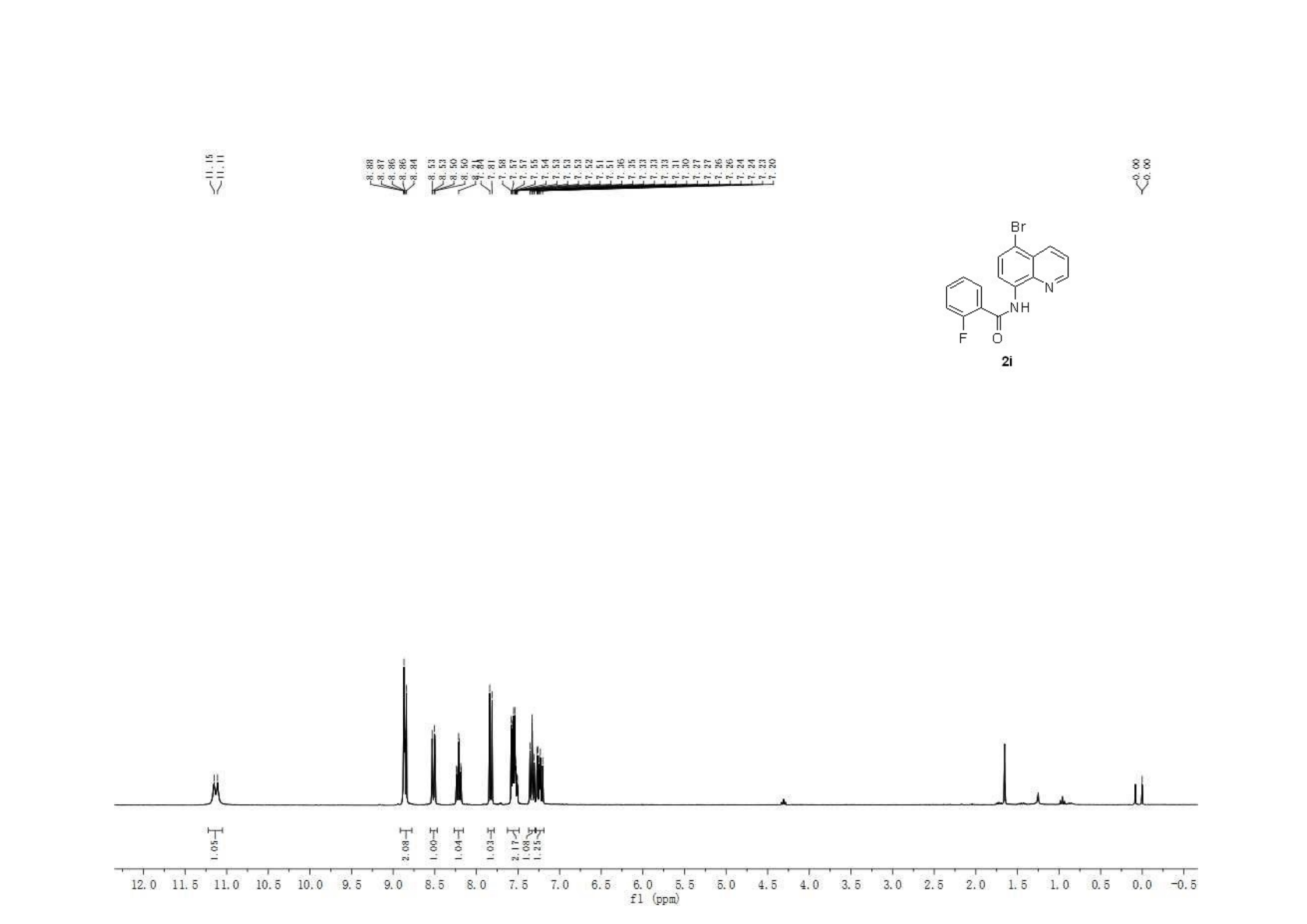
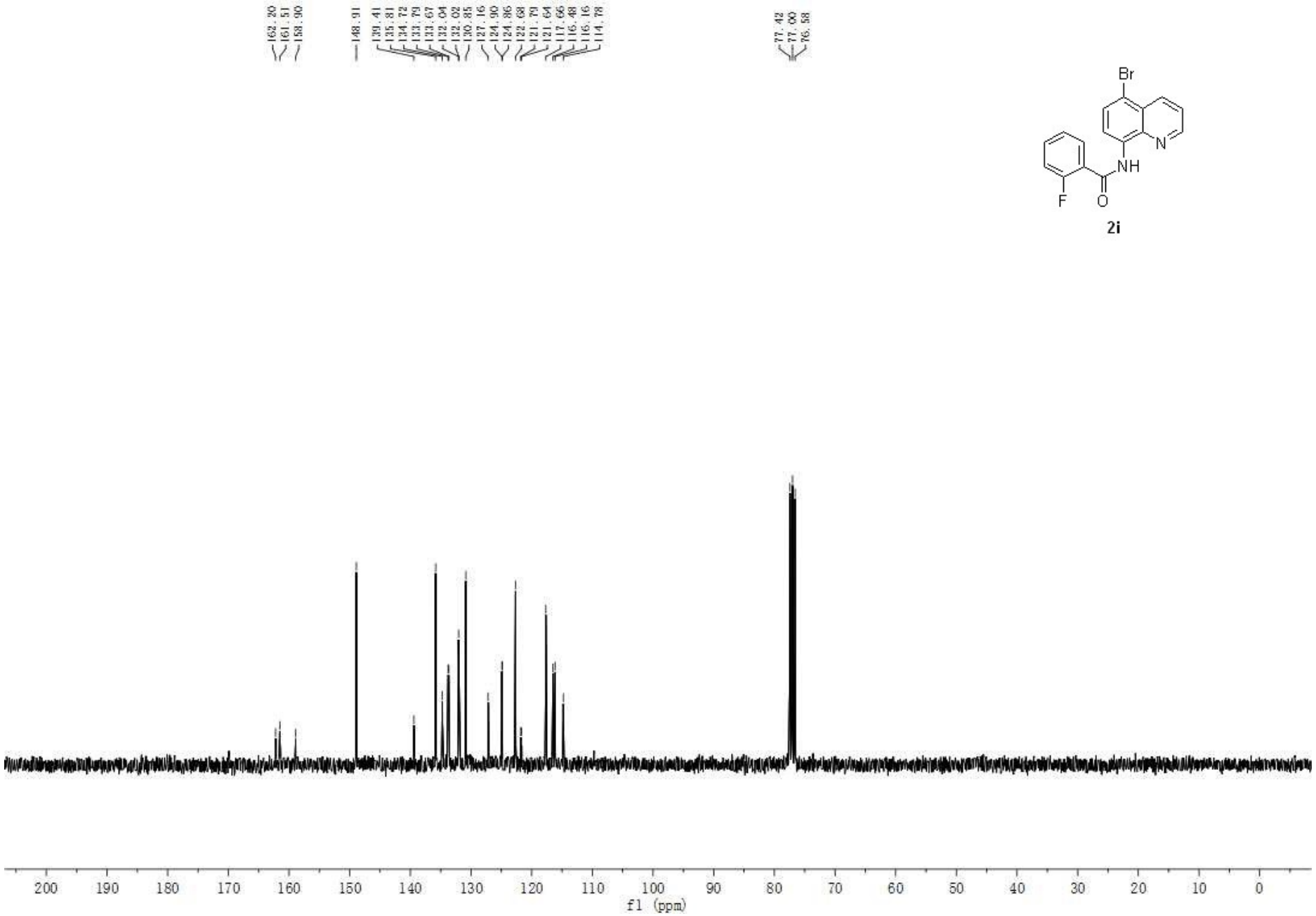
134.45
130.93
129.80
127.22
122.71
119.01
118.12
116.99
114.43
112.70
77.42
77.00
76.58
55.50
Br
O
N
NH
O
2h
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


11.15
11.11
8.88
8.87
8.86
8.86
8.84
8.53
8.53
8.50
8.50
7.81
7.58
7.57
7.57
7.55
7.54
7.53
7.53
7.53
7.52
7.51
7.51
7.36
7.35
7.33
7.33
7.31
7.30
7.27
7.27
7.26
7.26
7.24
7.24
7.23
7.20
0.00
0.00
Br
N
NH
F
O
2i
1.05
2.08
1.00
1.04
1.03
2.17
1.08
1.25
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
-0.5
f1 (ppm)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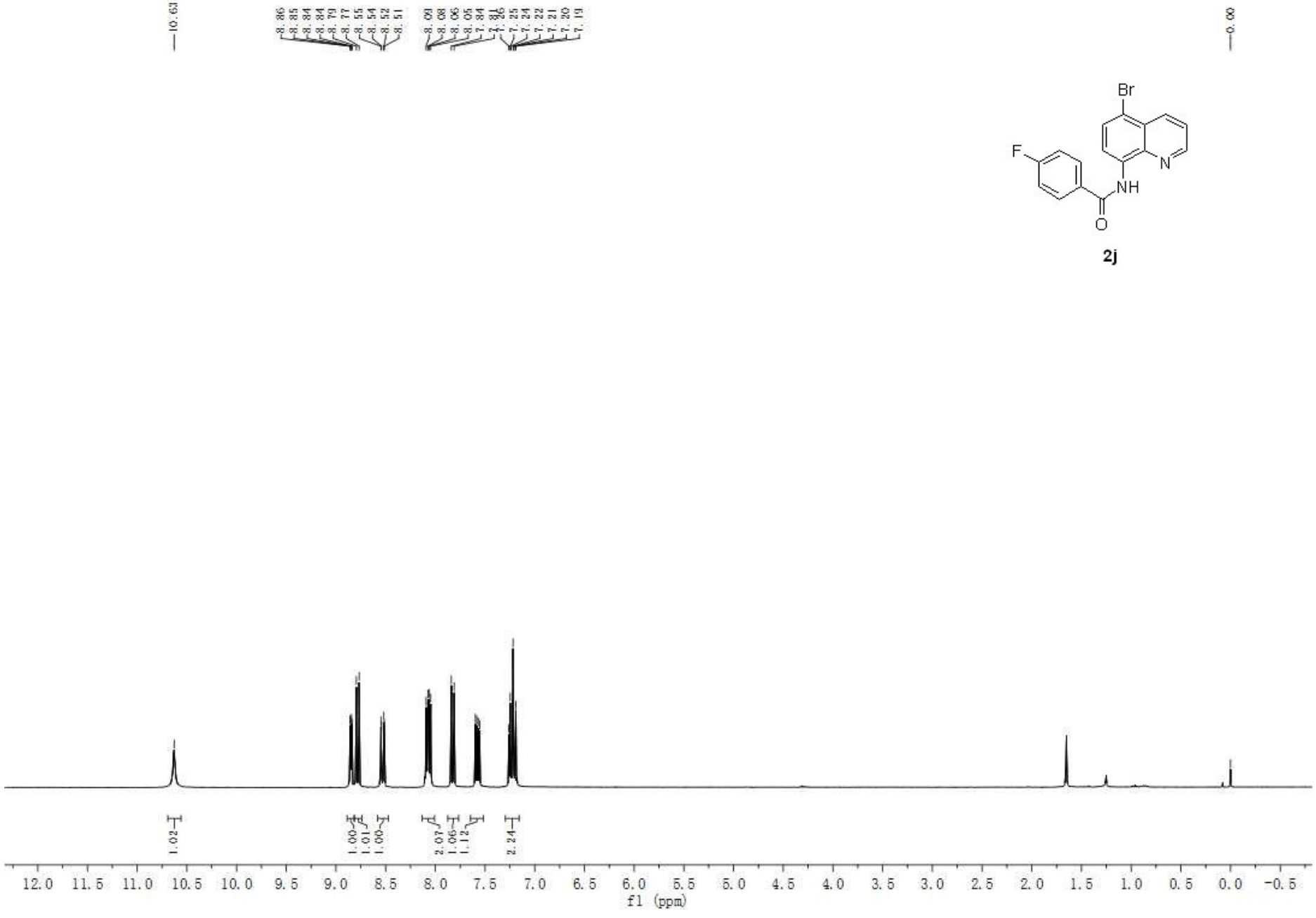
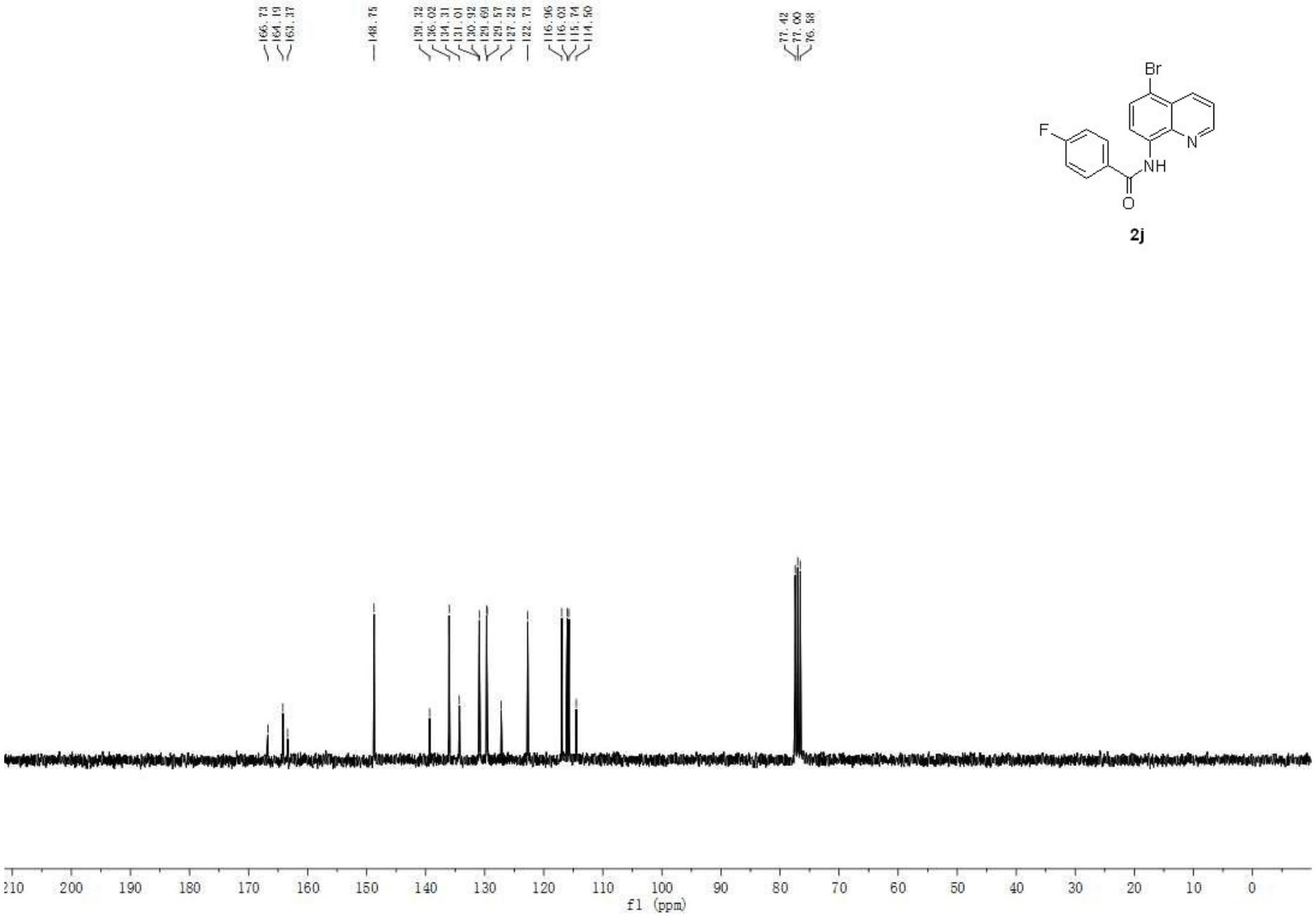
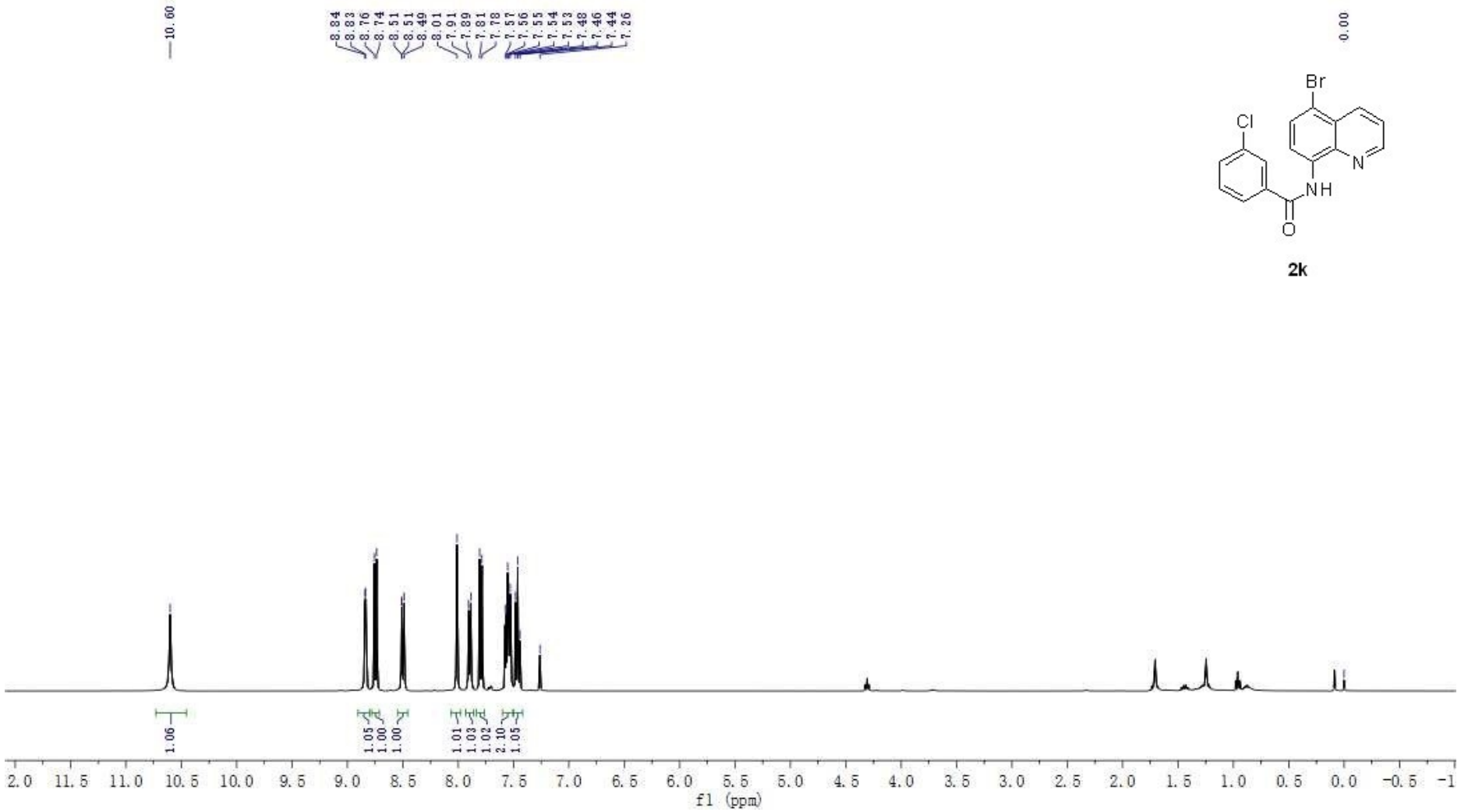
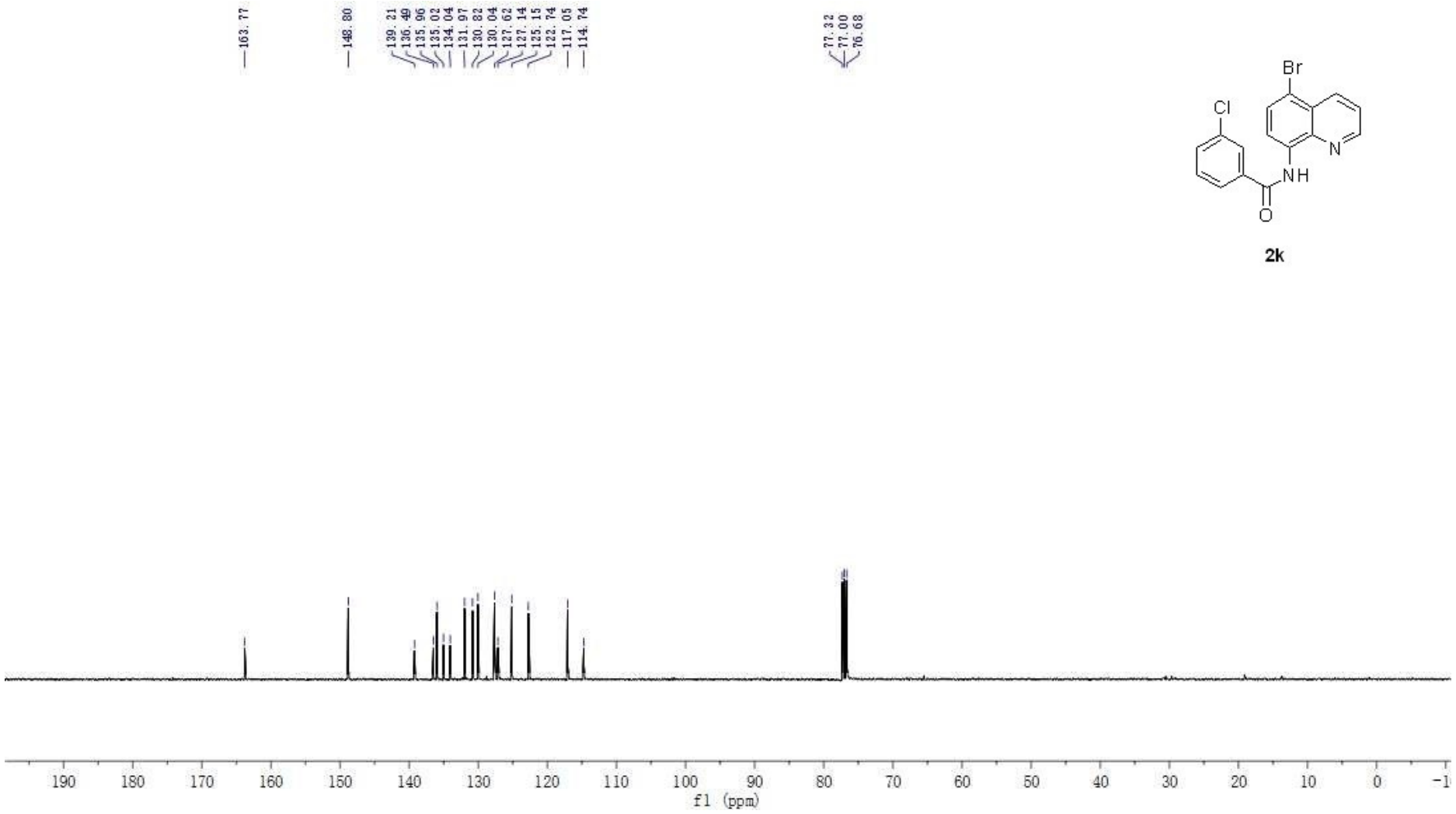
161.51
158.90
148.91
139.41
135.81
134.72
133.79
133.67
132.04
132.02
130.85
127.16
124.90
124.86
122.68
121.79
121.64
117.66
116.48
116.16
114.78
77.42
77.00
76.58
Br
N
NH
F
O
2i
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


10.63
8.86
8.85
8.84
8.84
8.79
8.77
8.55
8.54
8.52
8.51
8.09
8.08
8.06
8.05
7.84
7.81
7.26
7.25
7.24
7.22
7.21
7.20
7.19
0.00
Br
F
N
NH
O
2j
1.02
1.00
1.01
1.00
2.07
1.06
1.12
2.24
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 -0.5
f1 (ppm)


166.73
164.19
163.37
148.75
139.32
136.02
134.31
131.01
130.92
129.69
129.57
127.22
122.73
116.96
116.03
115.74
114.50
77.42
77.00
76.58
Br
F
N
NH
O
2j
f1 (ppm)


10.60
8.84
8.83
8.76
8.74
8.51
8.51
8.49
8.01
7.91
7.89
7.81
7.78
7.57
7.56
7.55
7.54
7.53
7.48
7.46
7.44
7.26
0.00
Br
Cl
N
NH
O
2k
1.06
1.05
1.00
1.00
1.01
1.03
1.02
2.10
1.05
f1 (ppm)


163.77
148.80
139.21
136.49
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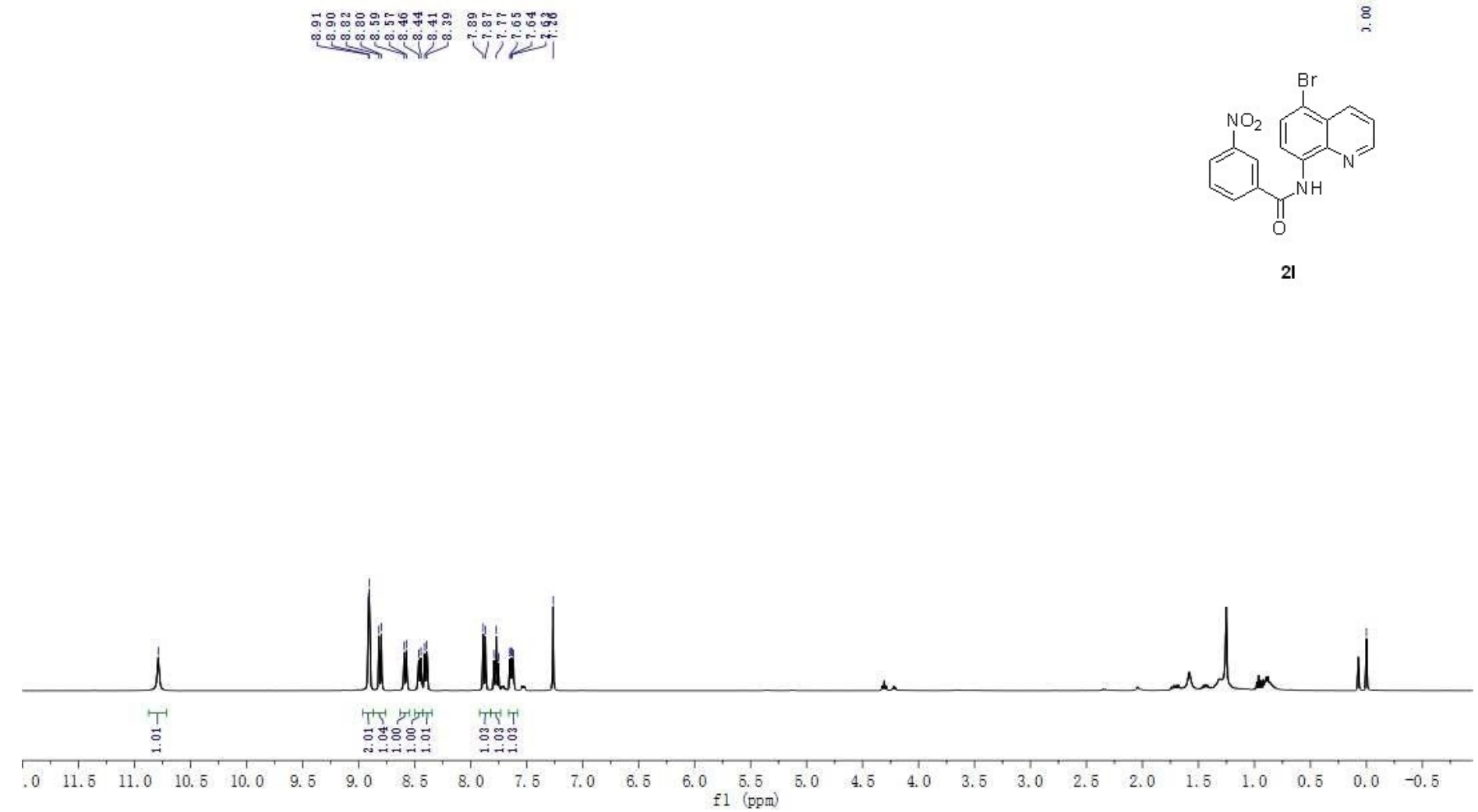
135.02
134.04
131.97
130.82
130.04
127.62
127.14
125.15
122.74
117.05
114.74
77.32
77.00
76.68
Br
Cl
N
NH
O
2k
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)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8.90
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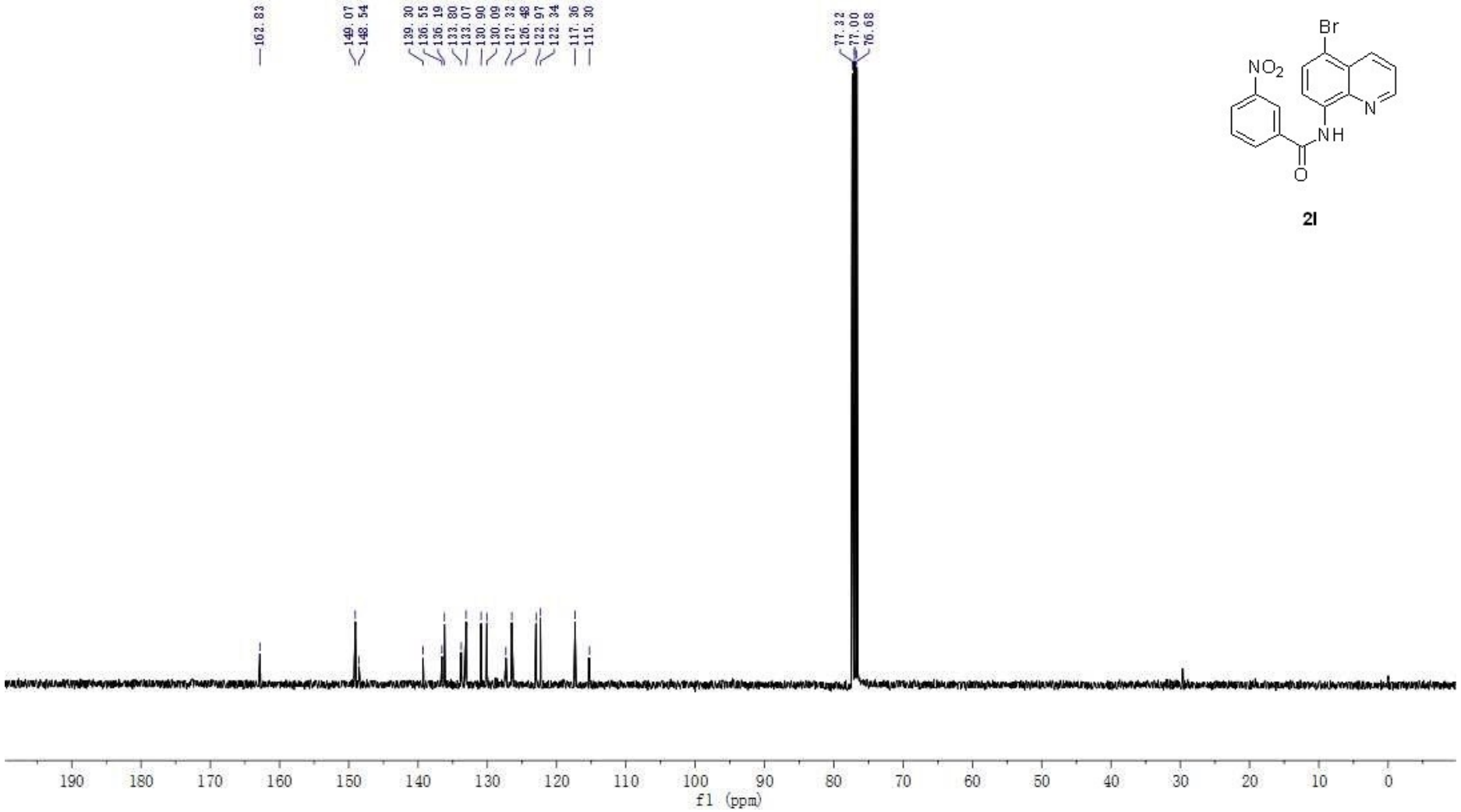
8.80
8.59
8.57
8.46
8.44
8.41
8.39
7.89
7.87
7.77
7.65
7.64
7.63
7.62
3.00
Br
NO2
N
NH
O
1.01
2.01
1.04
1.00
1.00
1.01
1.03
1.03
1.03
f1 (ppm)

2l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149.07
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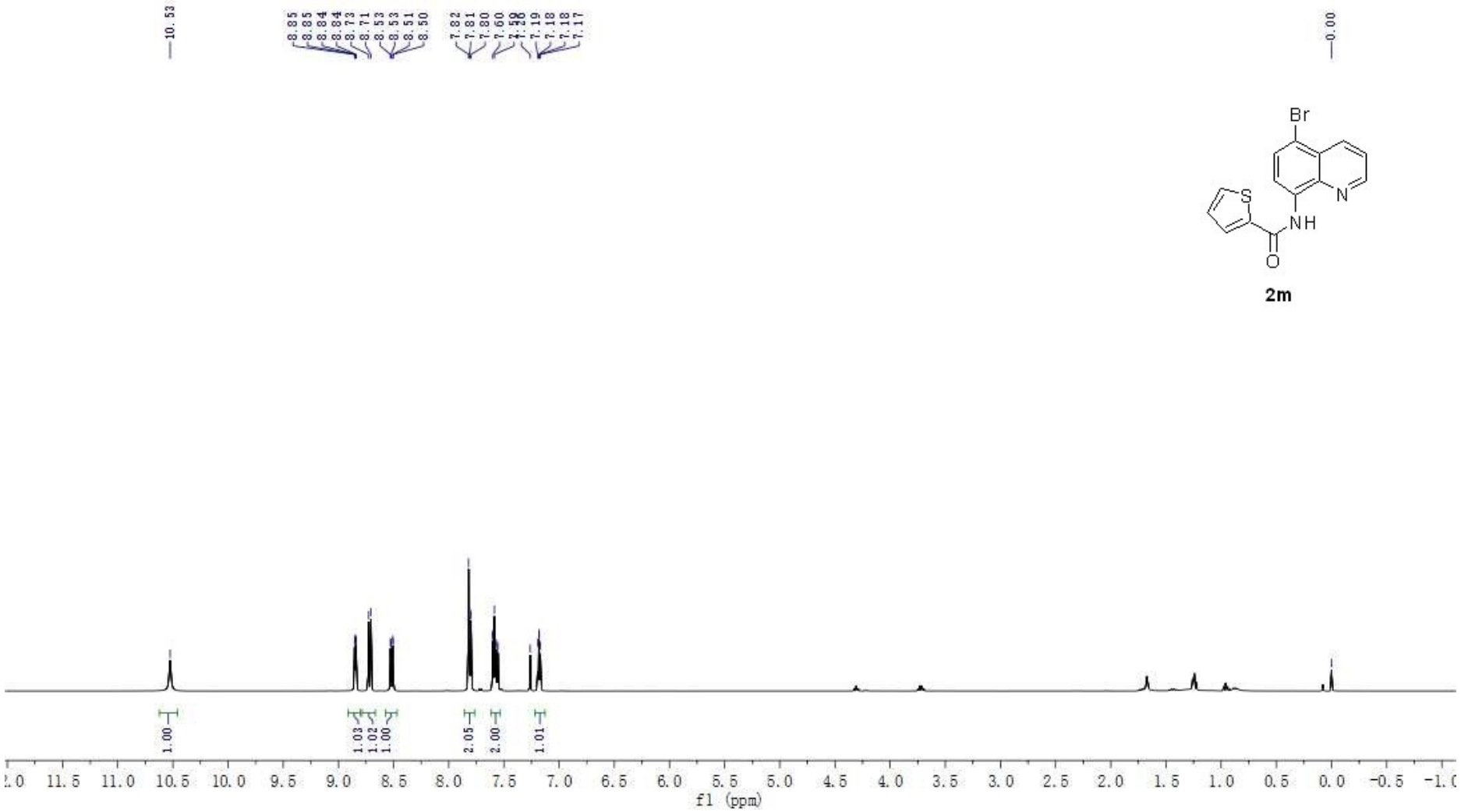
139.30
136.55
136.19
133.80
133.07
130.90
130.09
127.32
126.48
122.97
122.34
117.36
115.30
77.32
77.00
76.68
Br
NO2
N
NH
O
2l
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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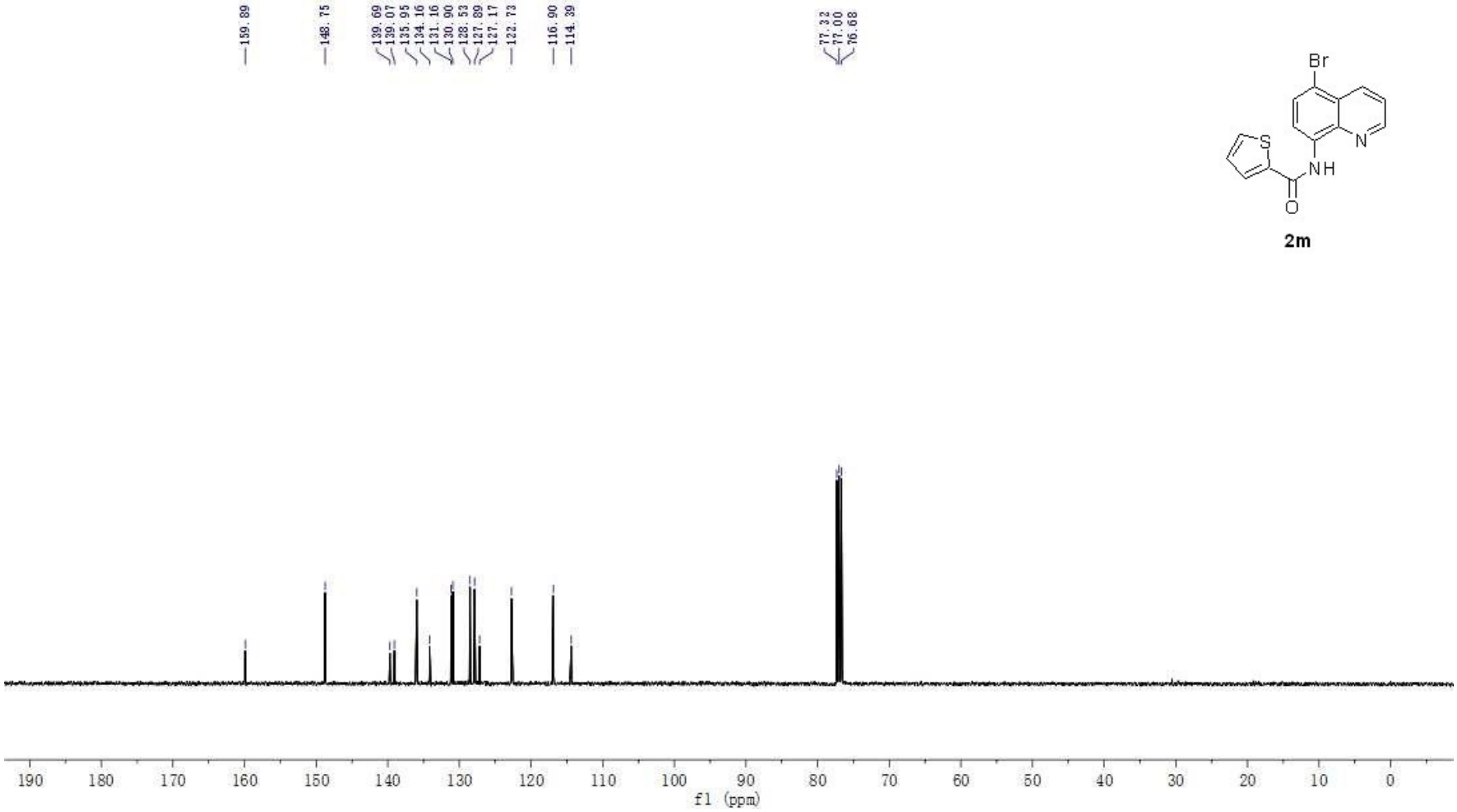
8.85
8.85
8.84
8.84
8.73
8.71
8.53
8.53
8.51
8.50
7.82
7.81
7.80
7.60
7.19
7.18
7.18
7.17
0.00
Br
S
N
NH
O
2m
1.00
1.03
1.02
1.00
2.05
2.00
1.01
f1 (ppm)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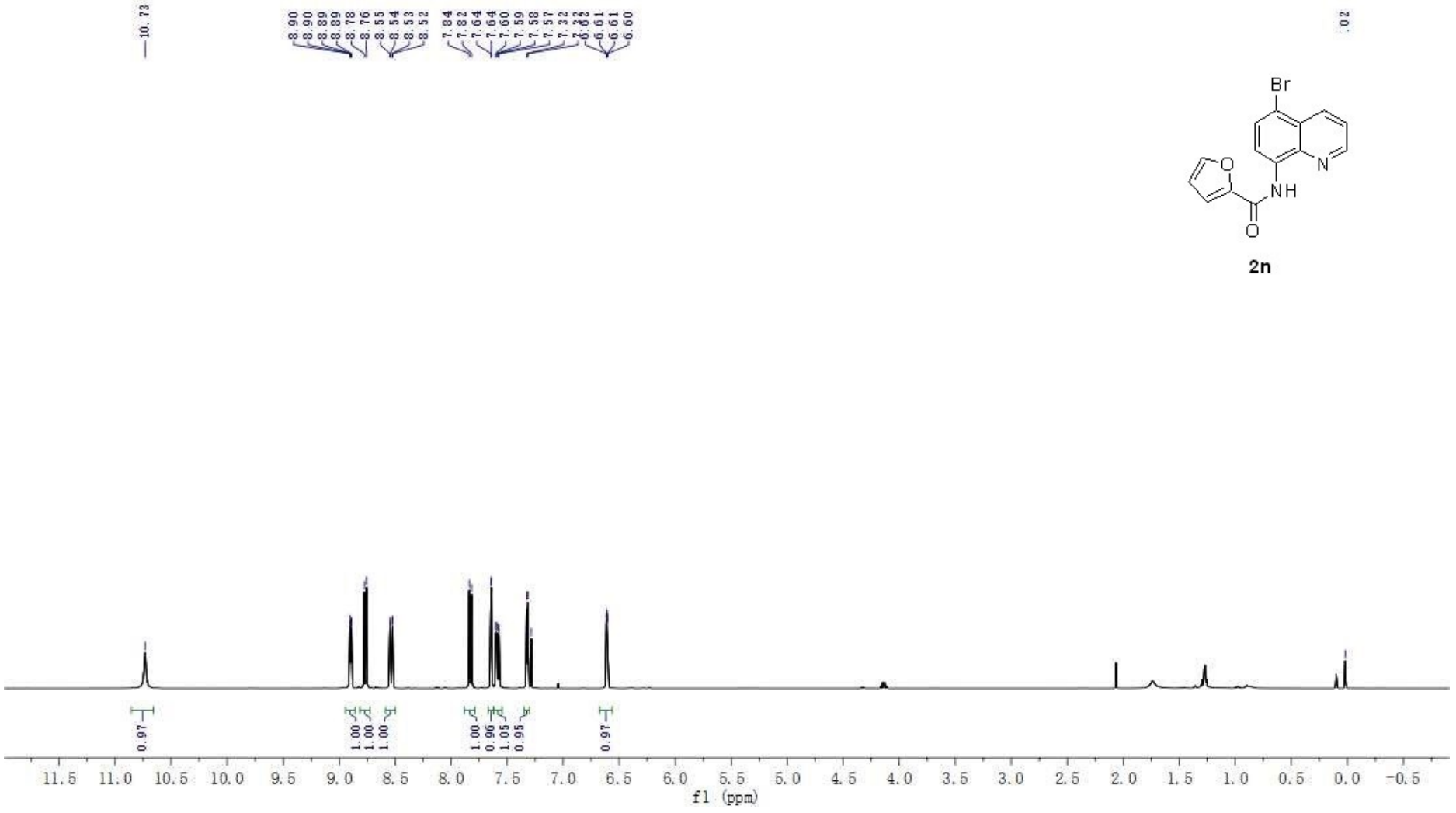
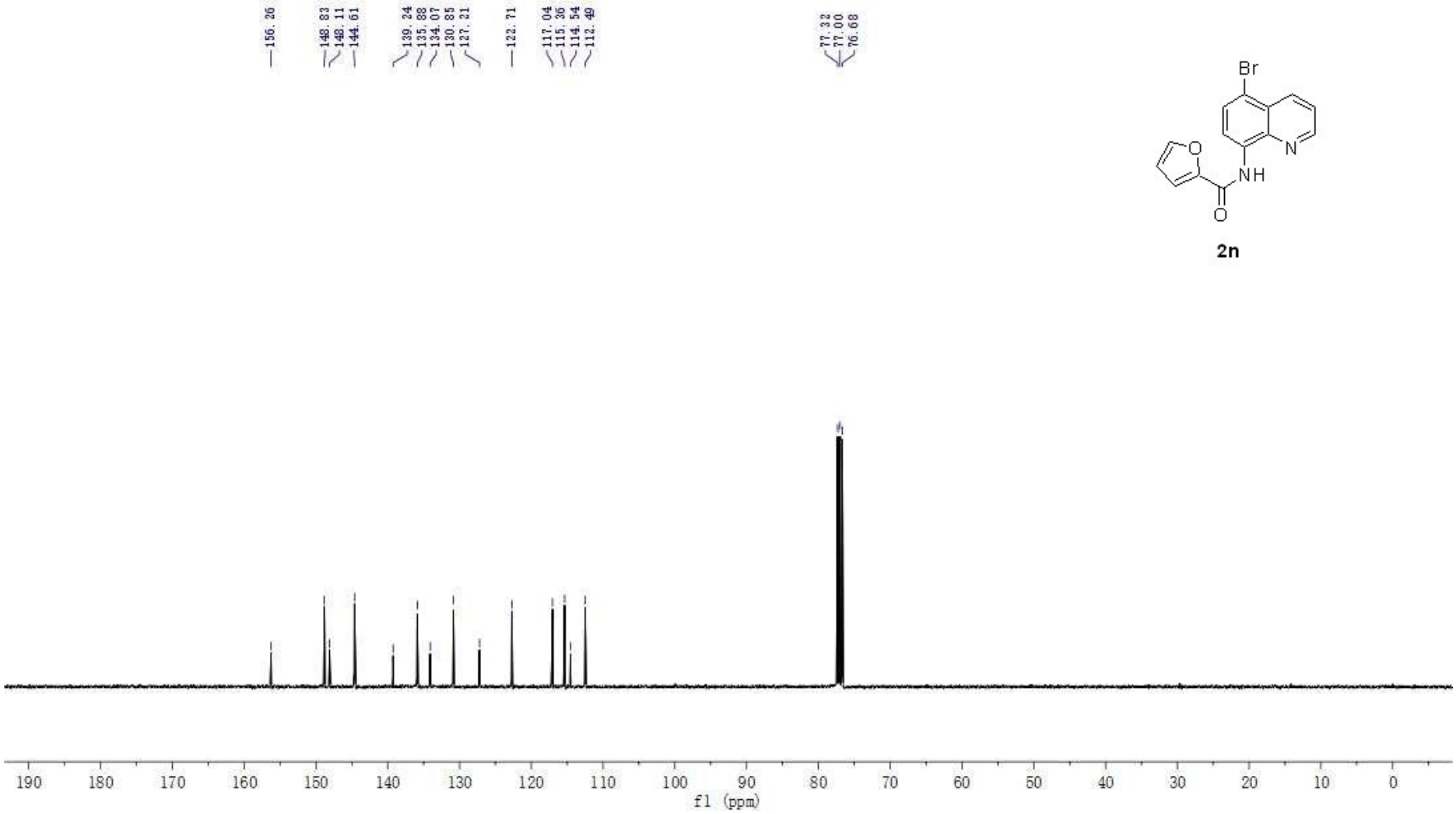
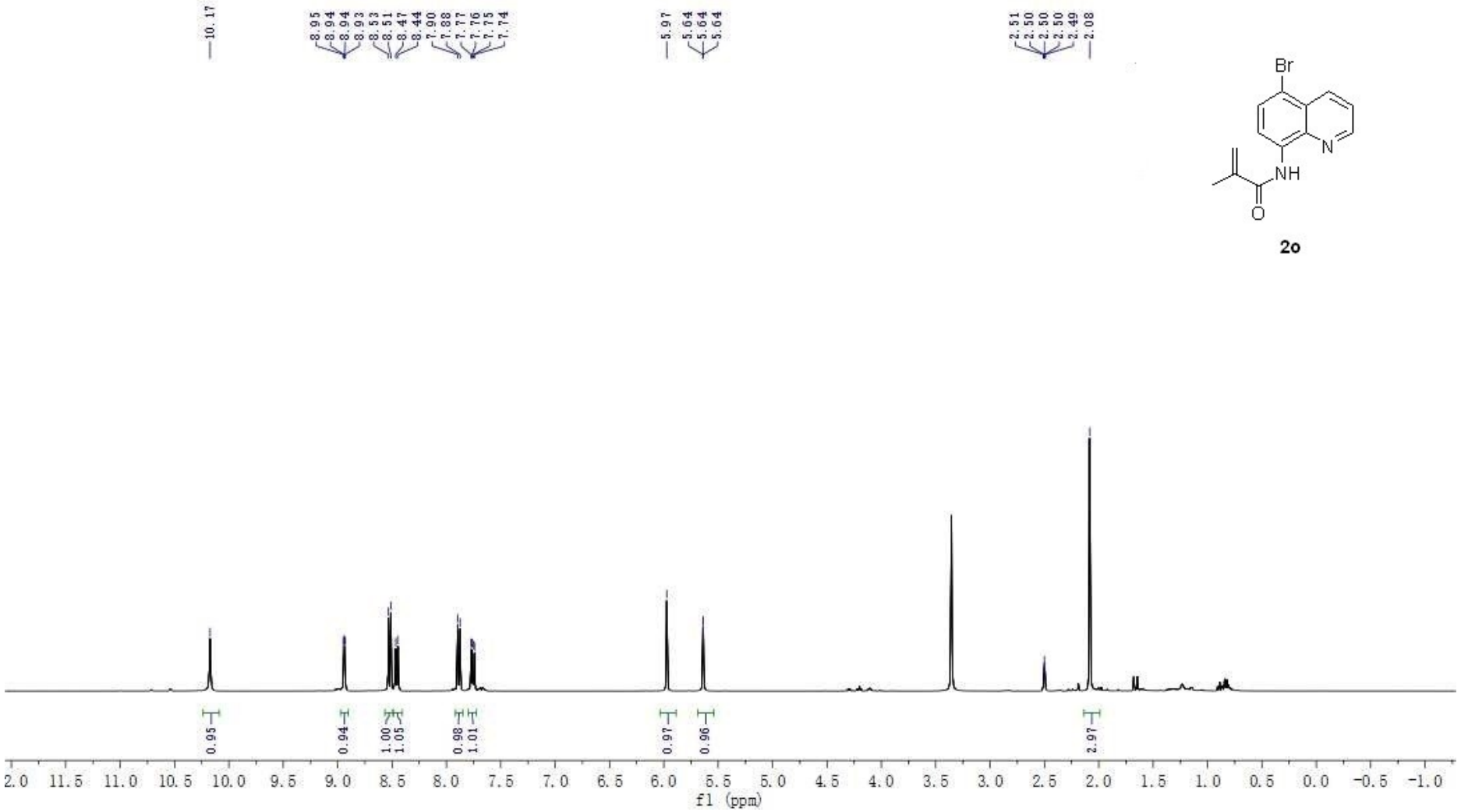
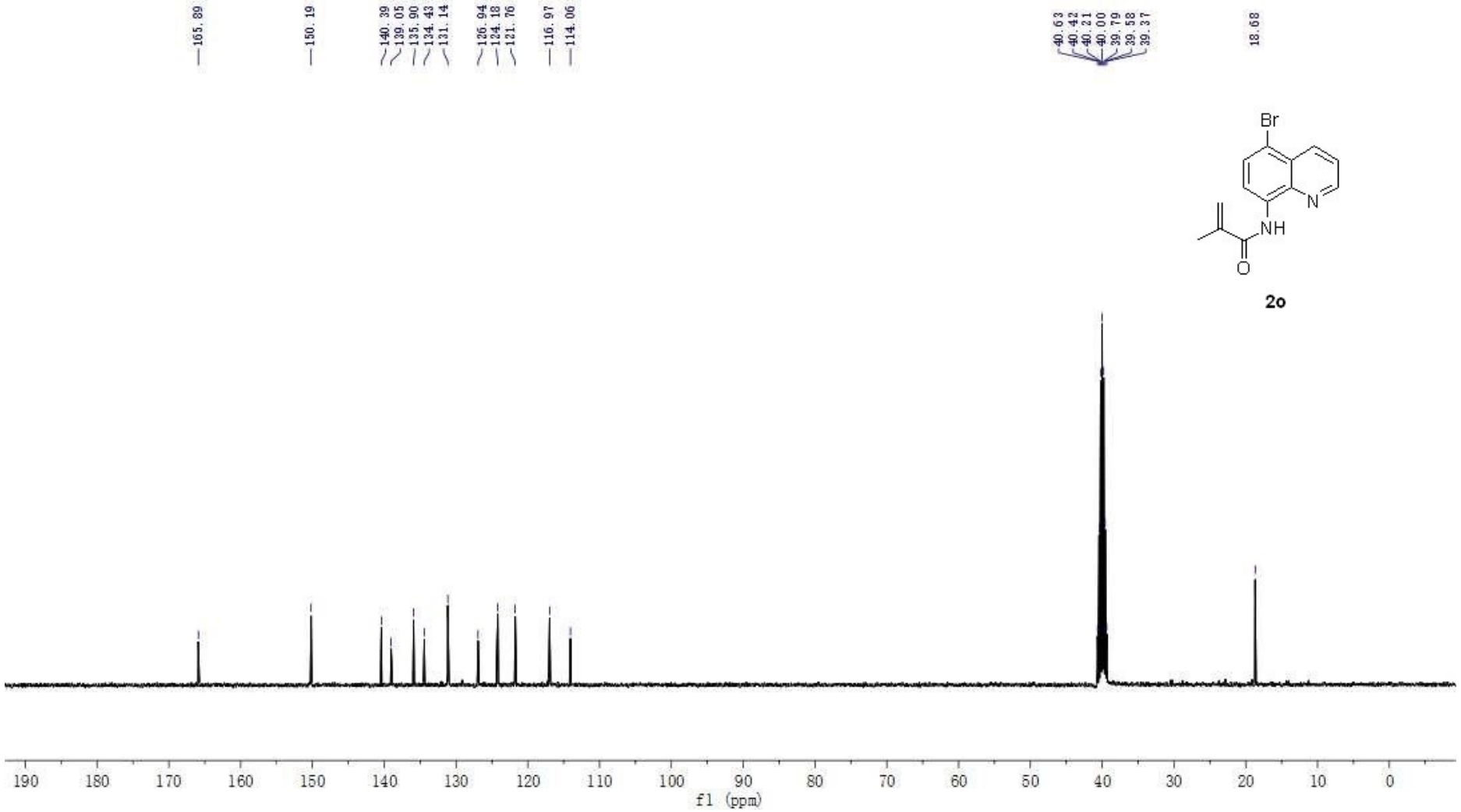
134.16
131.16
130.90
128.53
127.89
127.17
122.73
116.90
114.39
77.32
77.00
76.68
Br
S
N
NH
O
2m
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

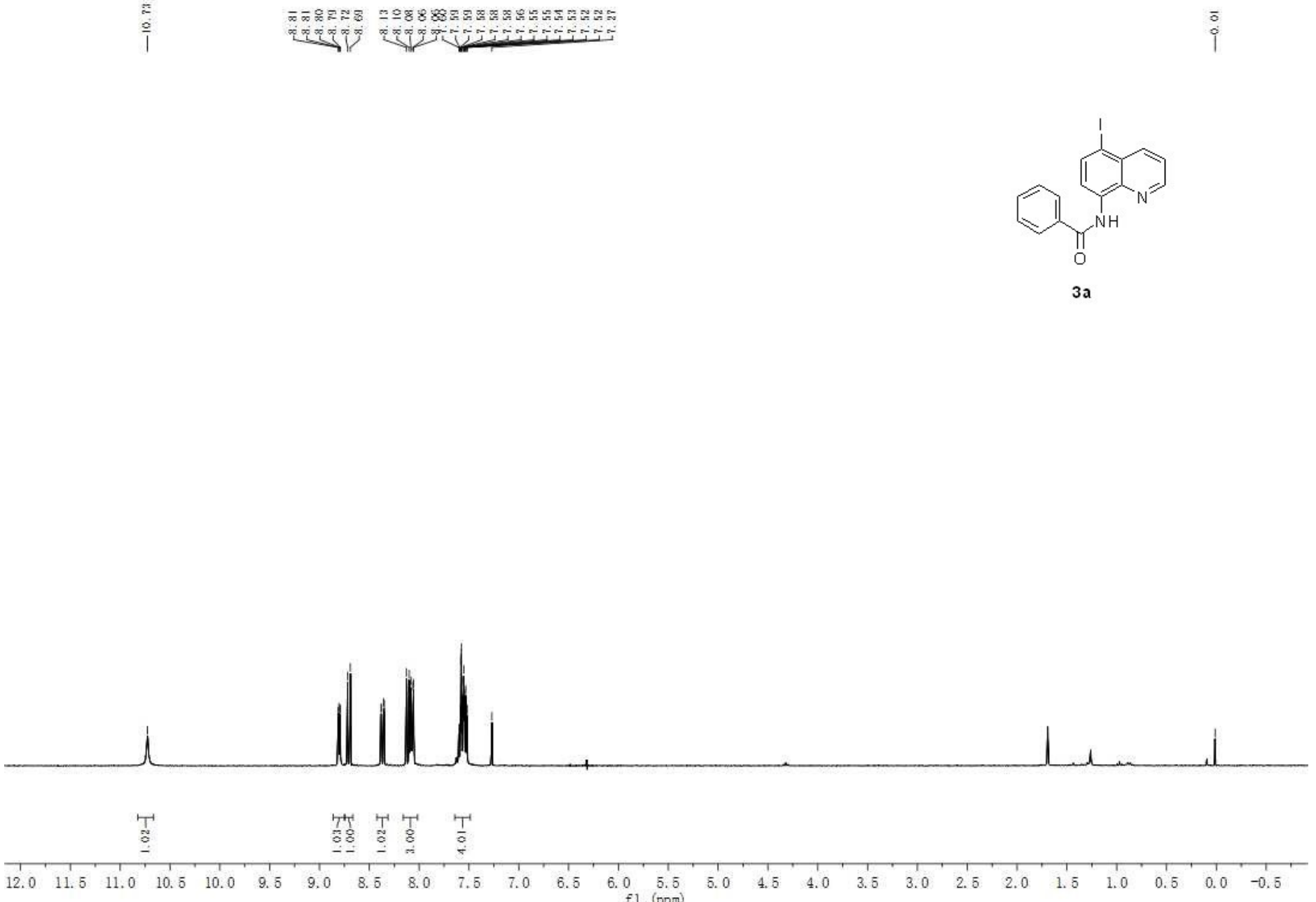

10.73
8.90
8.90
8.89
8.89
8.78
8.76
8.55
8.54
8.53
8.52
7.84
7.82
7.64
7.64
7.60
7.59
7.58
7.57
7.32
6.61
6.61
6.60
Br
N
NH
O
O
2n
0.97
1.00
1.00
1.00
1.00
0.96
1.05
0.95
0.97
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


156.26
148.83
148.11
144.61
139.24
135.88
134.07
130.85
127.21
122.71
117.04
115.36
114.54
112.49
77.32
77.00
76.68
Br
O
N
NH
O
2n
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

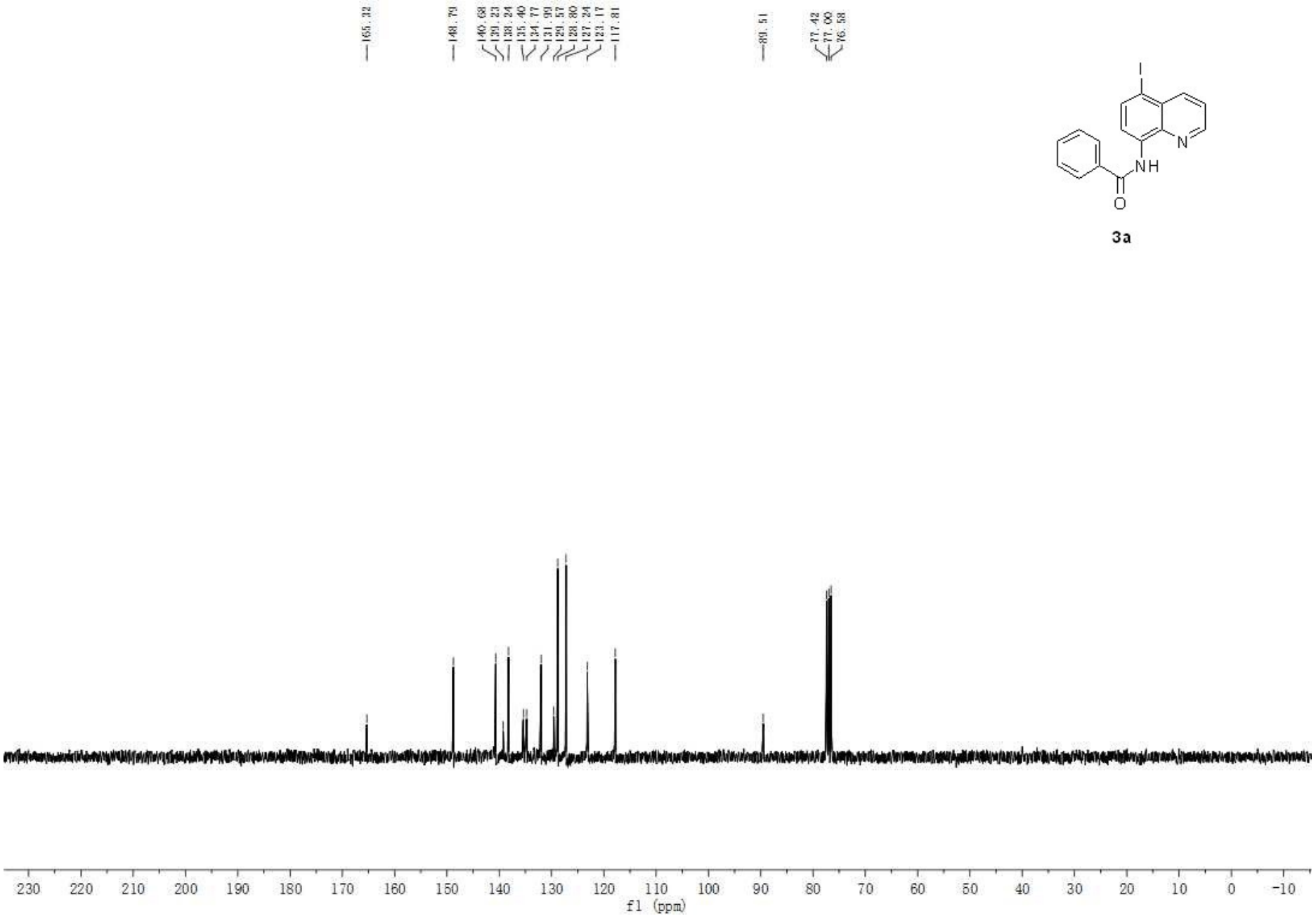

10.17
8.95
8.94
8.94
8.93
8.53
8.51
8.47
8.44
7.90
7.88
7.77
7.76
7.75
7.74
5.97
5.64
5.64
5.64
2.51
2.50
2.50
2.50
2.49
2.08
Br
N
NH
O
0.95
0.94
1.00
1.05
0.98
1.01
0.97
0.96
2.97
f1 (ppm)

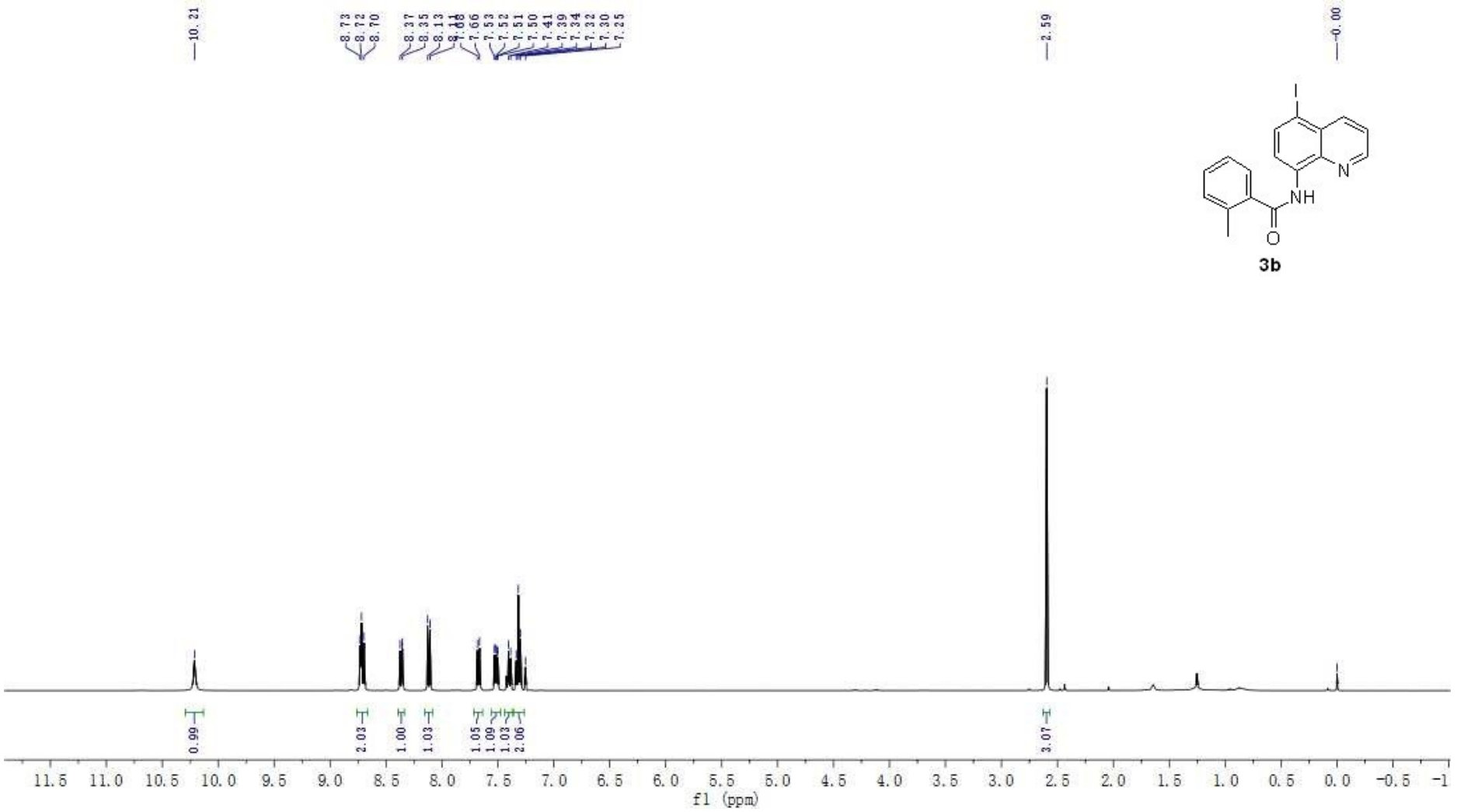
2o

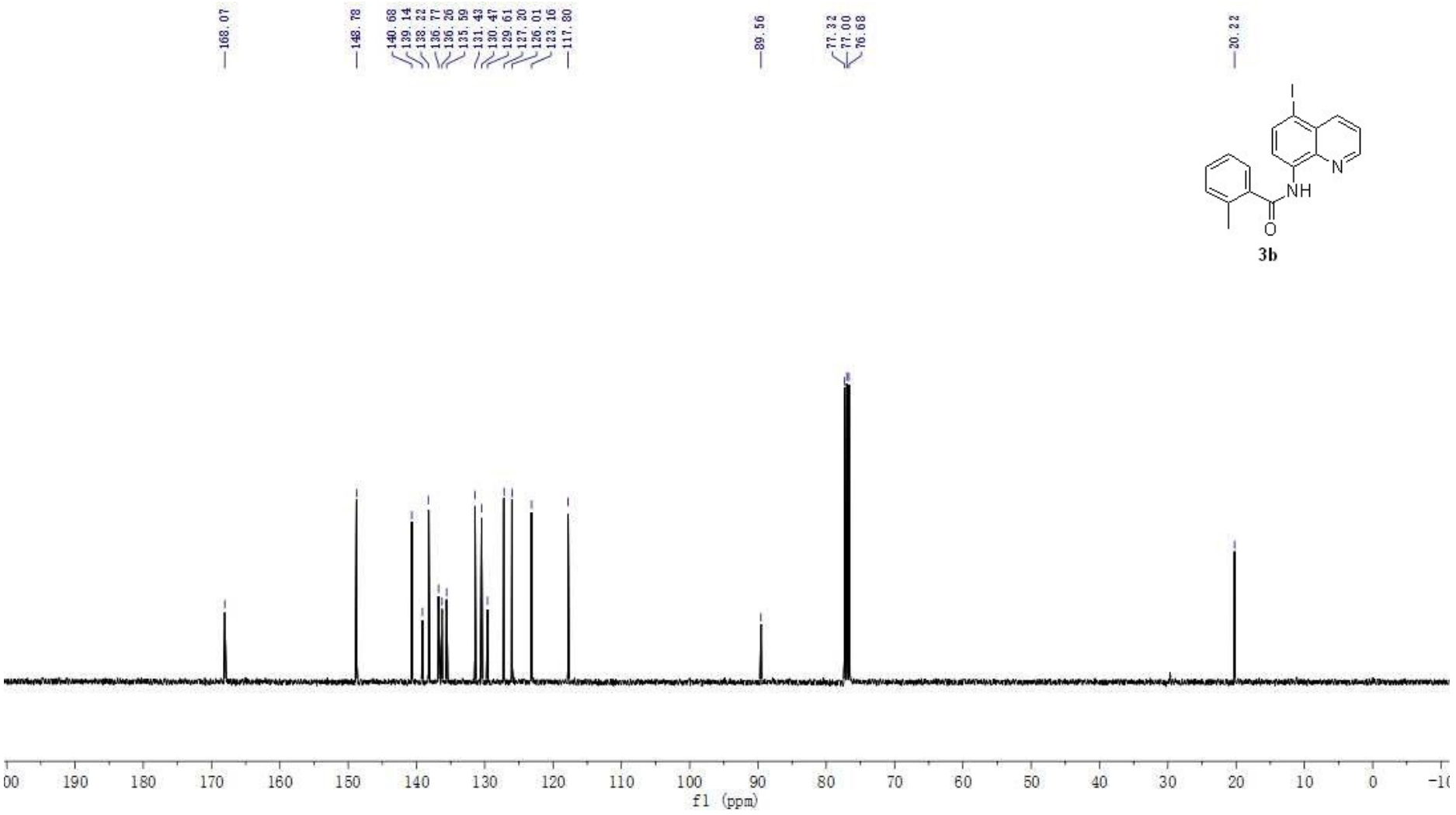

165.89
150.19
140.39
139.05
135.90
134.43
131.14
126.94
124.18
121.76
116.97
114.06
40.63
40.42
40.21
40.00
39.79
39.58
39.37
18.68
Br
N
NH
O
2o
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


10.73
8.81
8.81
8.80
8.79
8.72
8.69
8.13
8.10
8.08
8.05
7.59
7.59
7.58
7.58
7.58
7.56
7.55
7.55
7.54
7.53
7.52
7.52
7.27
0.01
I
N
NH
O
1.02
1.03
1.00
1.02
3.00
4.01
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
-0.5
f1 (ppm)

3a


165.32
148.79
140.68
139.23
138.24
135.46
134.77
131.99
129.57
128.80
127.24
123.17
117.81
89.51
77.42
77.00
76.58
I
N
NH
O
3a
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


10.21
8.73
8.72
8.70
8.37
8.35
8.13
7.66
7.53
7.52
7.51
7.50
7.41
7.39
7.34
7.32
7.30
7.25
2.59
0.00
I
N
NH
O
3b
0.99
2.03
1.00
1.03
1.05
1.09
1.03
2.06
3.07
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 -0.5 -1
f1 (ppm)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140.68
139.14
138.22
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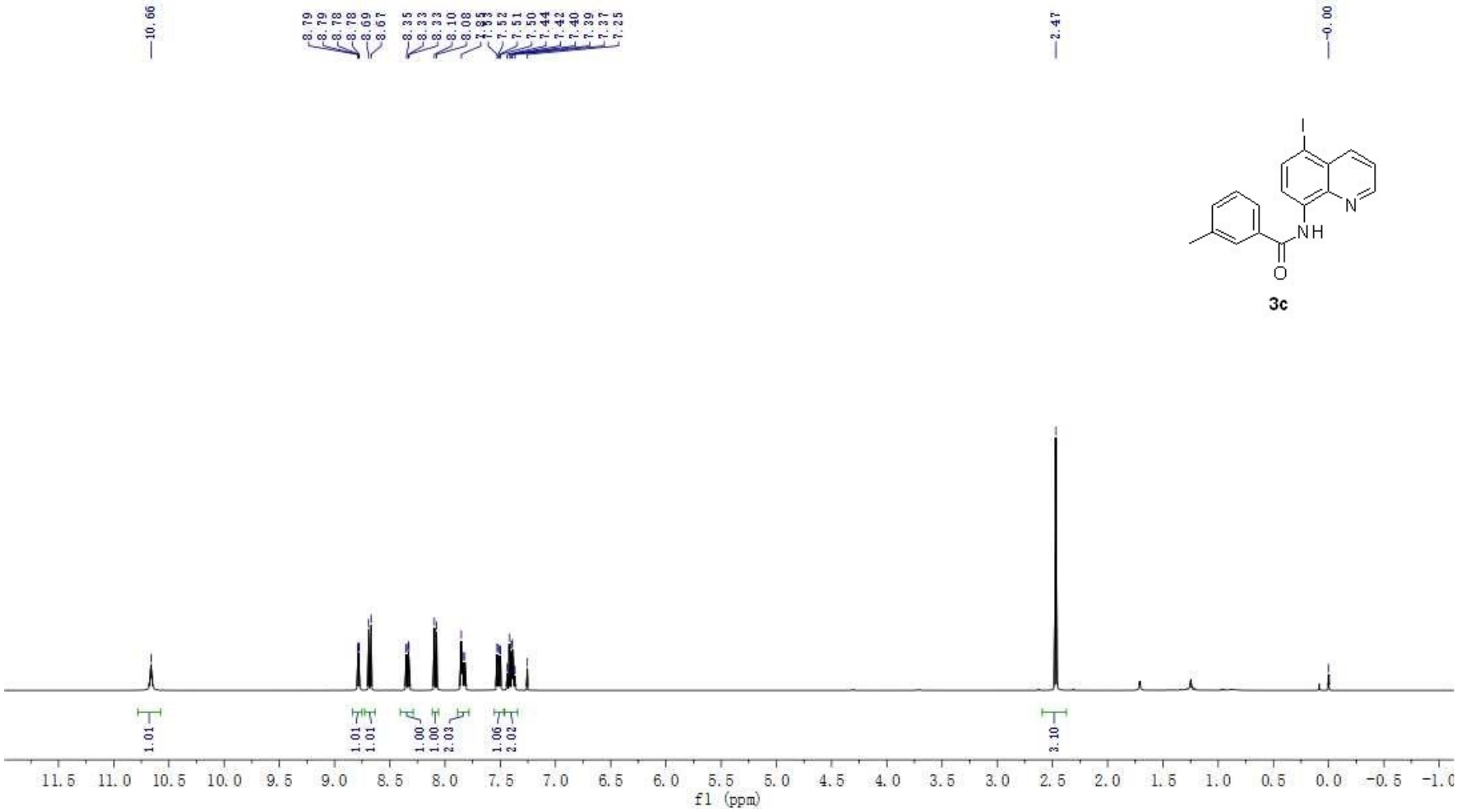
136.26
135.59
131.43
130.47
129.61
127.20
126.01
123.16
117.80
89.56
77.32
77.00
76.68
20.22
I
N
NH
O
3b
f1 (ppm)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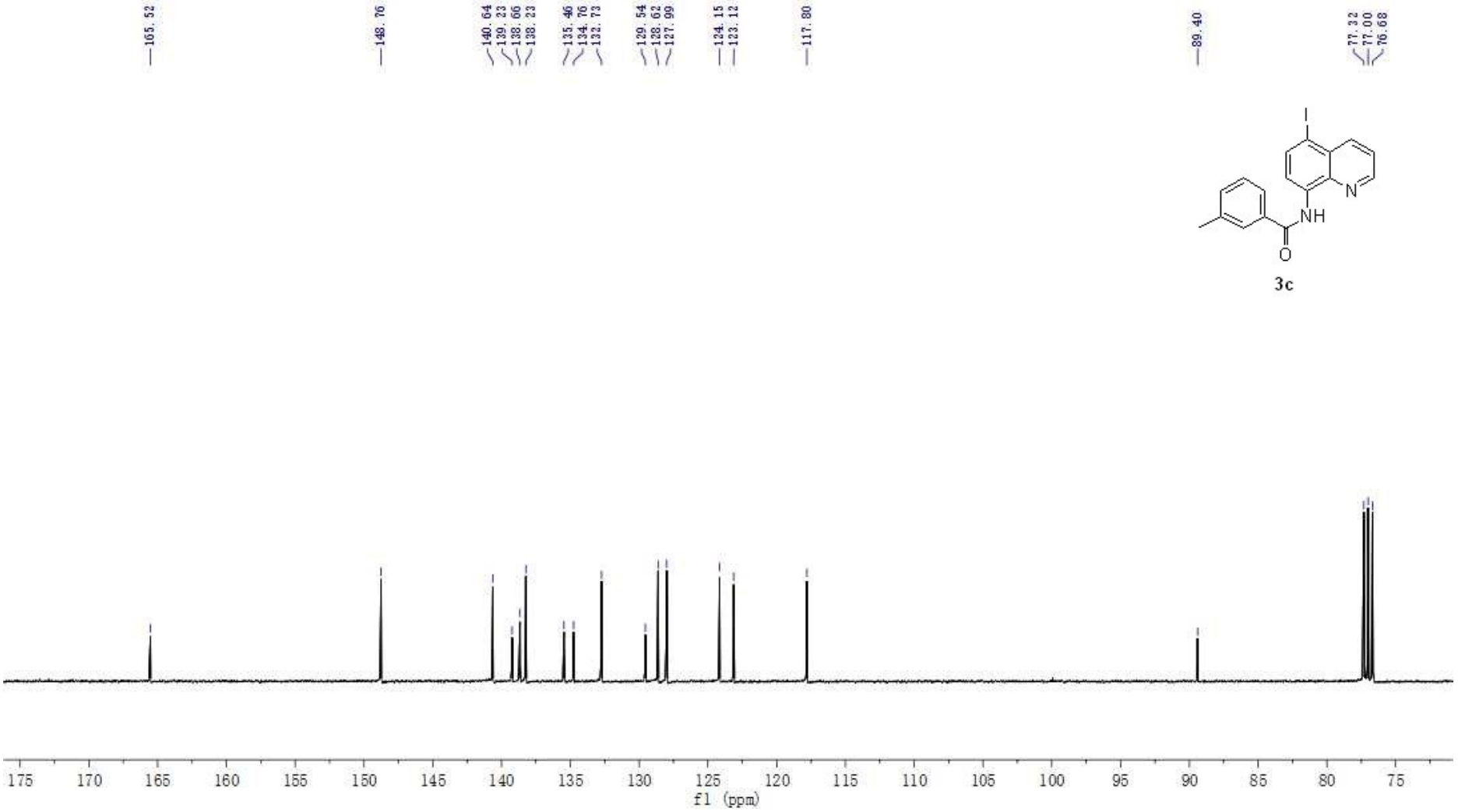
8.35
8.33
8.33
8.10
8.08
7.85
7.83
7.52
7.51
7.50
7.44
7.42
7.40
7.39
7.37
7.25
2.47
0.00
I
N
NH
O
3c
1.01
1.01
1.01
1.00
1.00
2.03
1.06
2.02
3.10
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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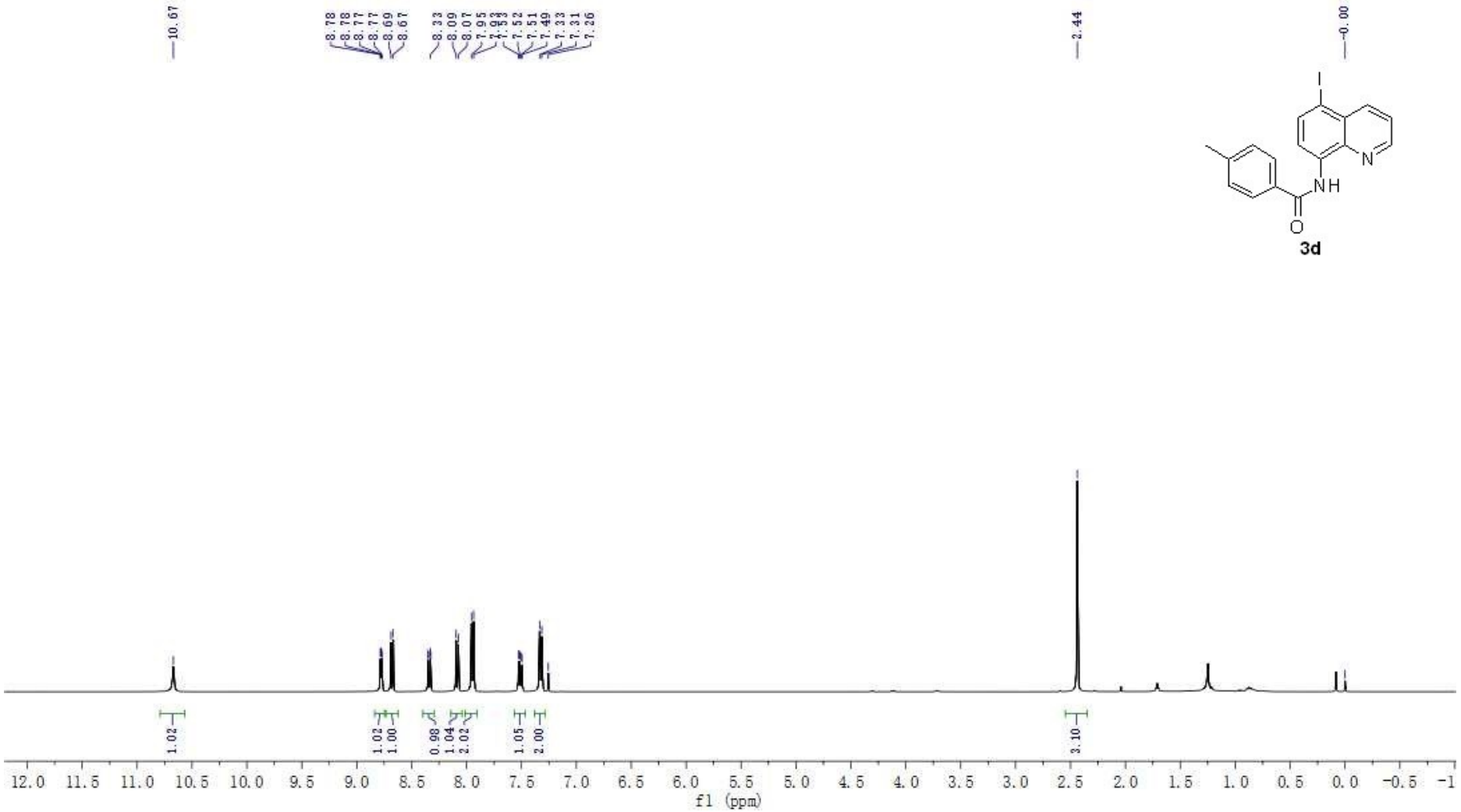
140.64
139.23
138.66
138.23
135.46
134.76
132.73
129.54
128.62
127.99
124.15
123.12
117.80
89.40
77.32
77.00
76.68
I
N
NH
O
3c
175
170
165
160
155
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
f1 (ppm)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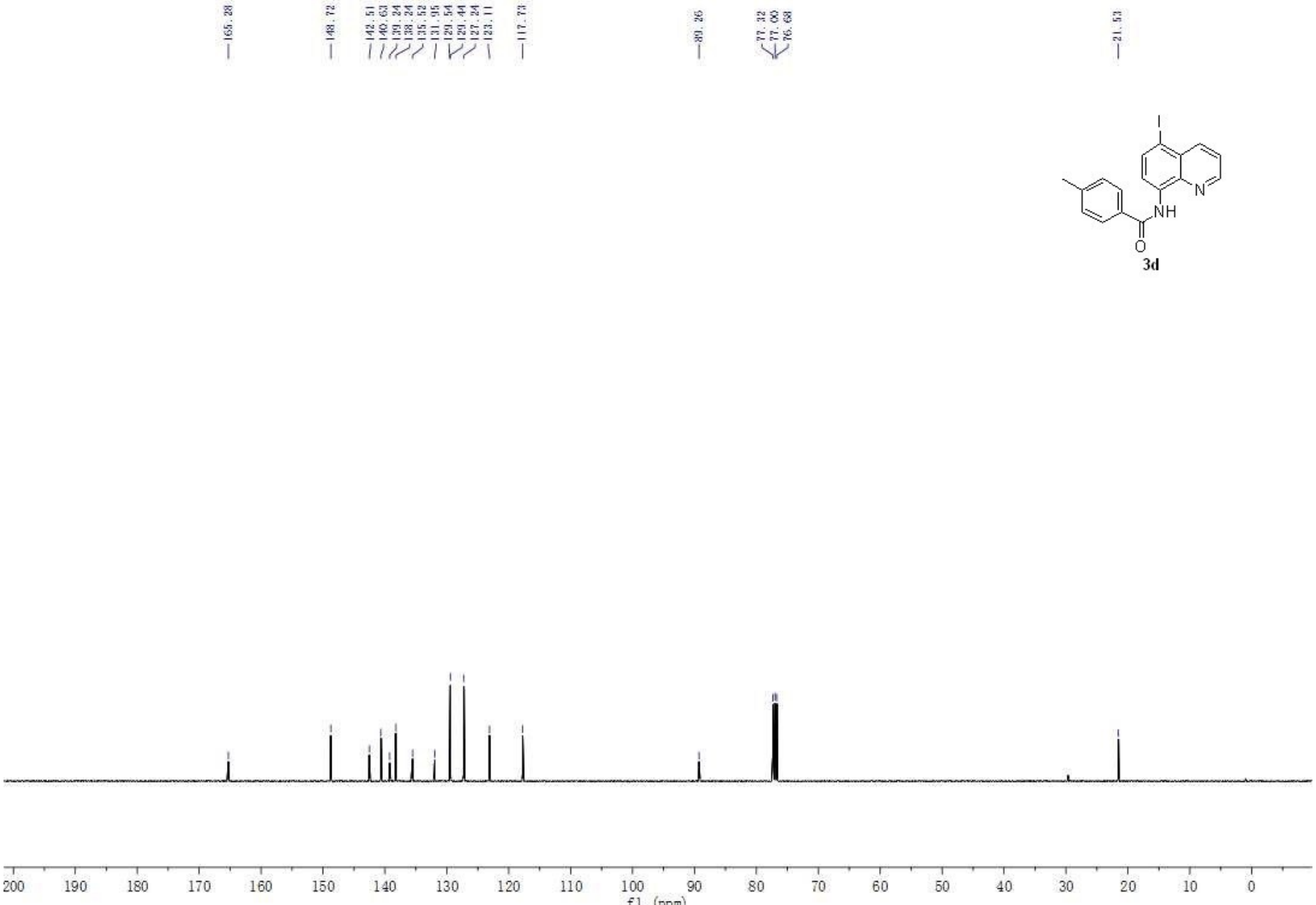
8.67
8.33
8.09
8.07
7.95
7.93
7.52
7.51
7.49
7.33
7.31
7.26
2.44
0.00
I
N
NH
O
3d
1.02
1.02
1.00
0.98
1.04
2.02
1.05
2.00
3.10
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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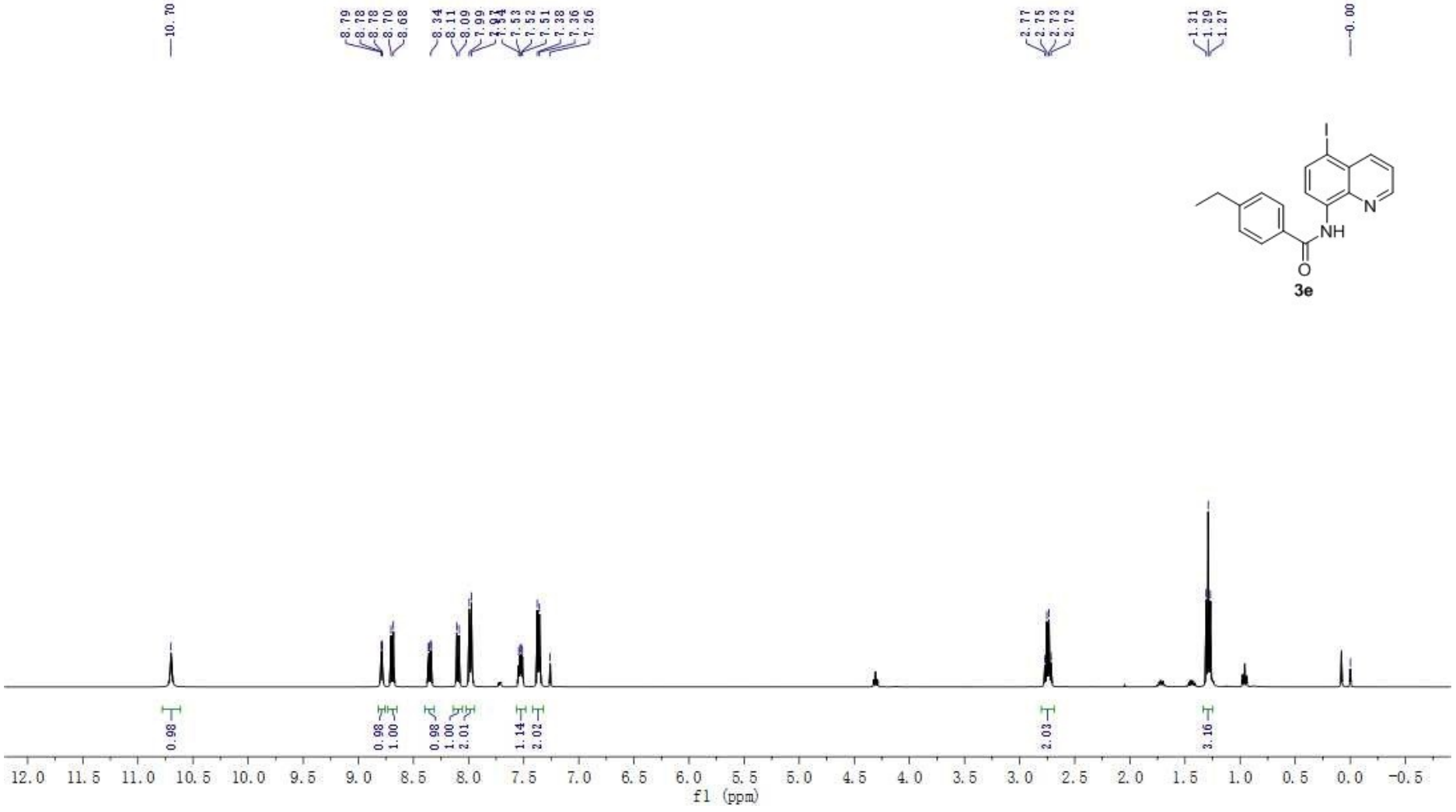
139.24
138.24
135.52
131.95
129.54
129.44
127.24
123.11
117.73
89.26
77.32
77.00
76.68
21.53
I
N
NH
O
3d
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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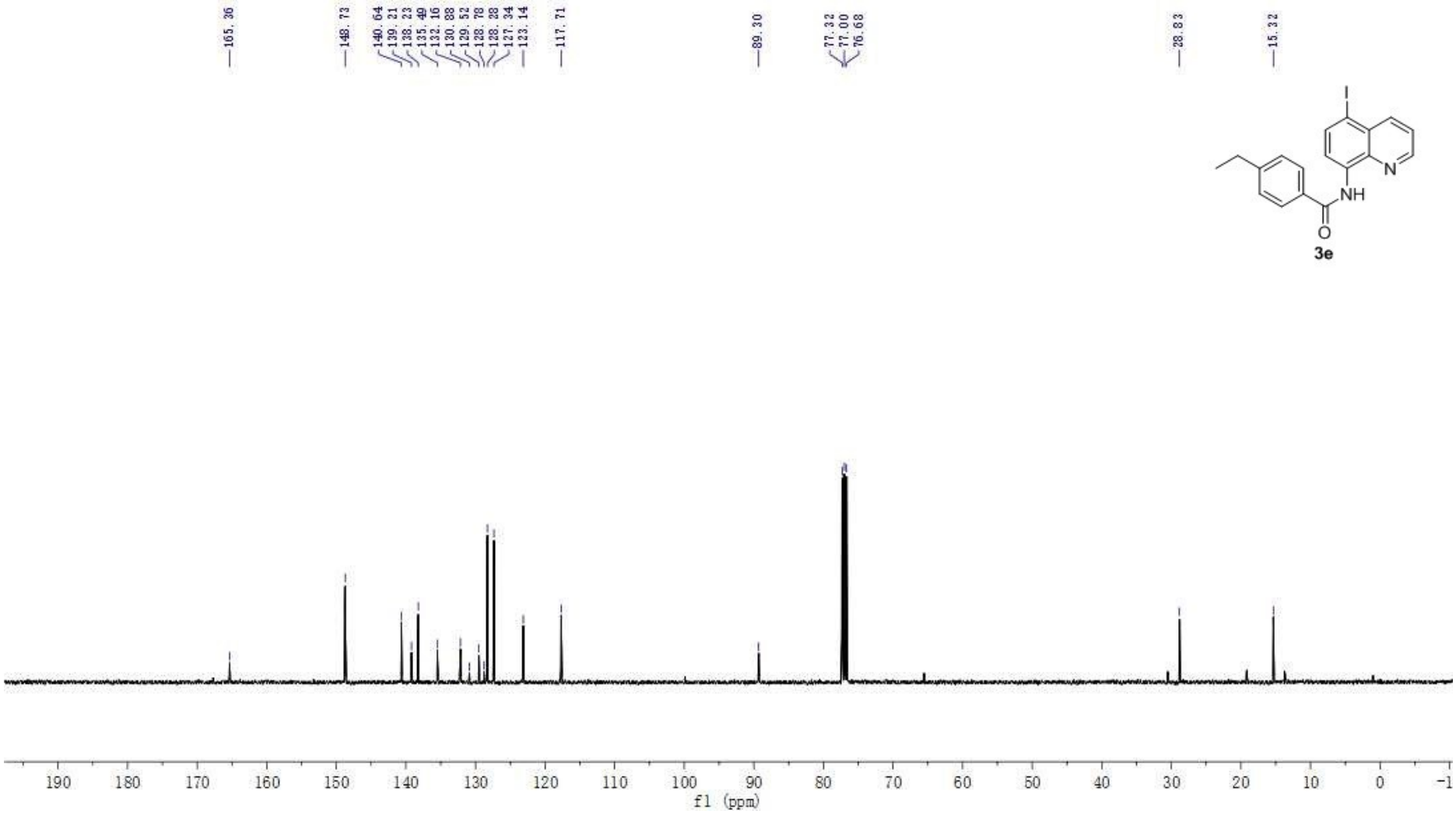
8.79
8.78
8.78
8.70
8.68
8.34
8.11
8.09
7.99
7.97
7.94
7.53
7.52
7.51
7.38
7.36
7.26
2.77
2.75
2.73
2.72
1.31
1.29
1.27
0.00
I
N
NH
O
3e
0.98
0.98
1.00
0.98
1.00
2.01
1.14
2.02
2.03
3.16
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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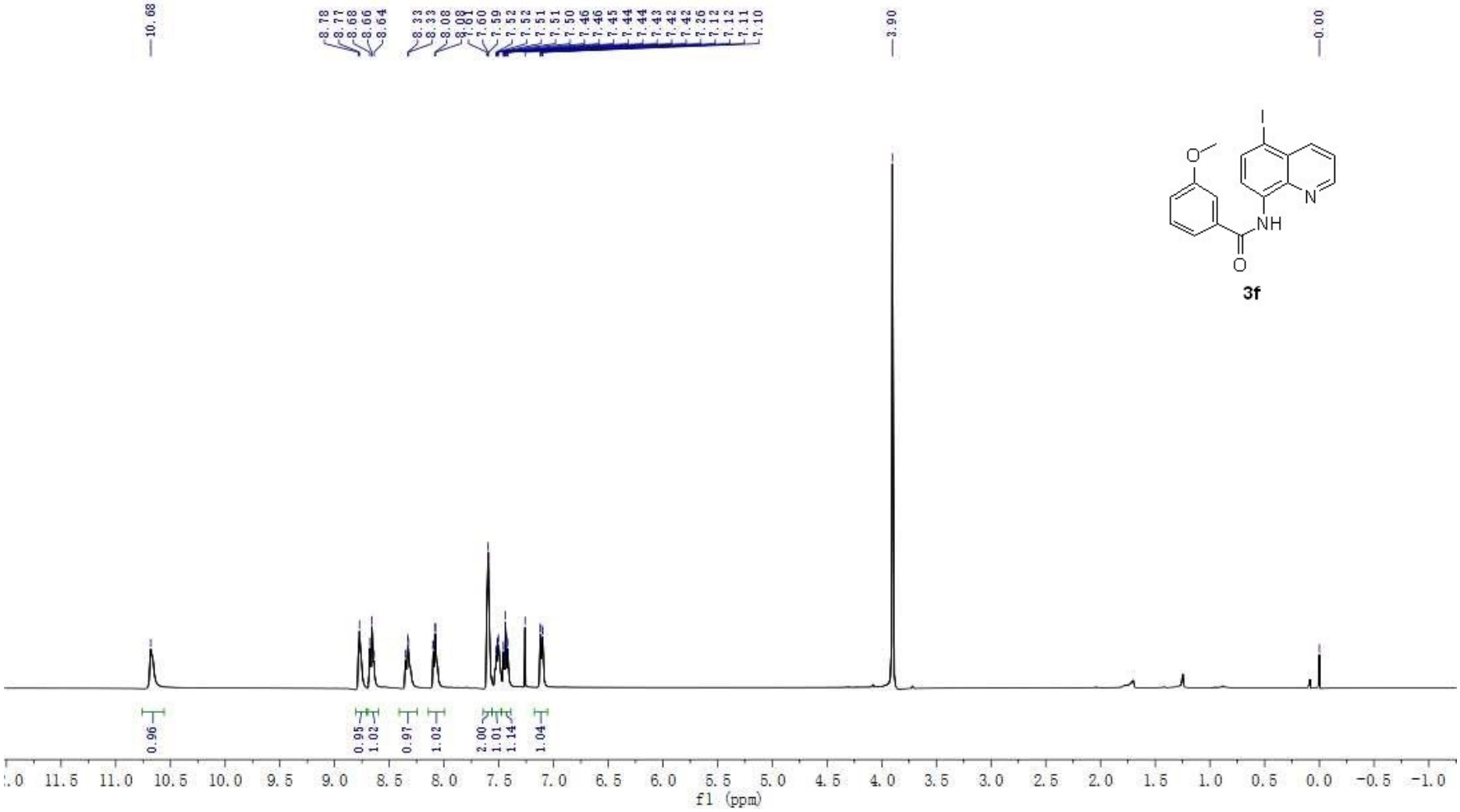
135.49
132.16
130.88
129.52
128.78
128.28
127.34
123.14
117.71
89.30
77.32
77.00
76.68
28.83
15.32
I
N
NH
O
3e
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)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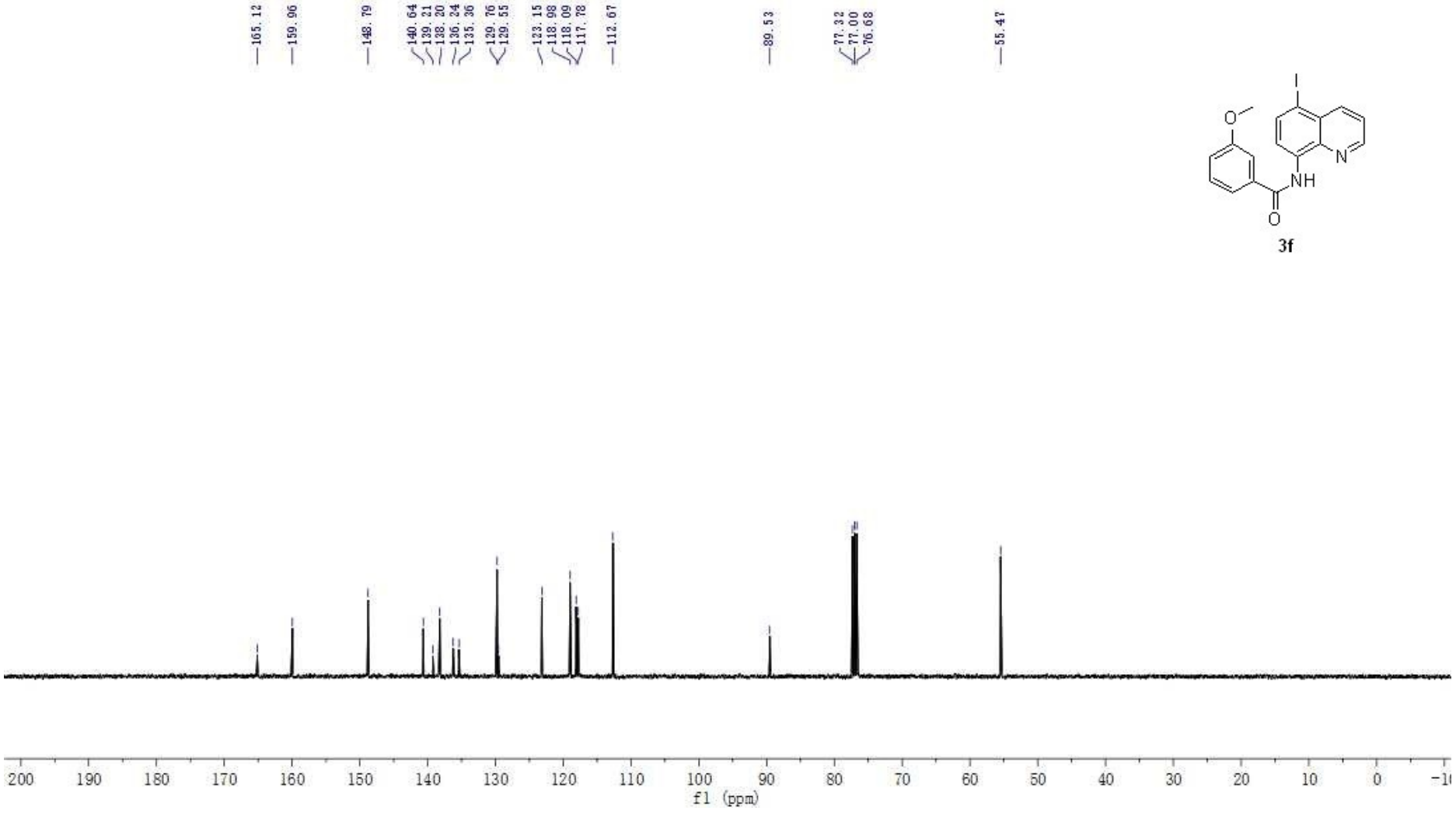
8.78
8.77
8.68
8.66
8.64
8.33
8.33
8.08
8.08
8.01
7.60
7.59
7.52
7.52
7.51
7.51
7.50
7.46
7.46
7.45
7.44
7.44
7.43
7.42
7.42
7.26
7.12
7.11
7.10
3.90
0.00
I
O
N
NH
O
3f
0.96
0.95
1.02
0.97
1.02
2.00
1.01
1.14
1.04
f1 (ppm)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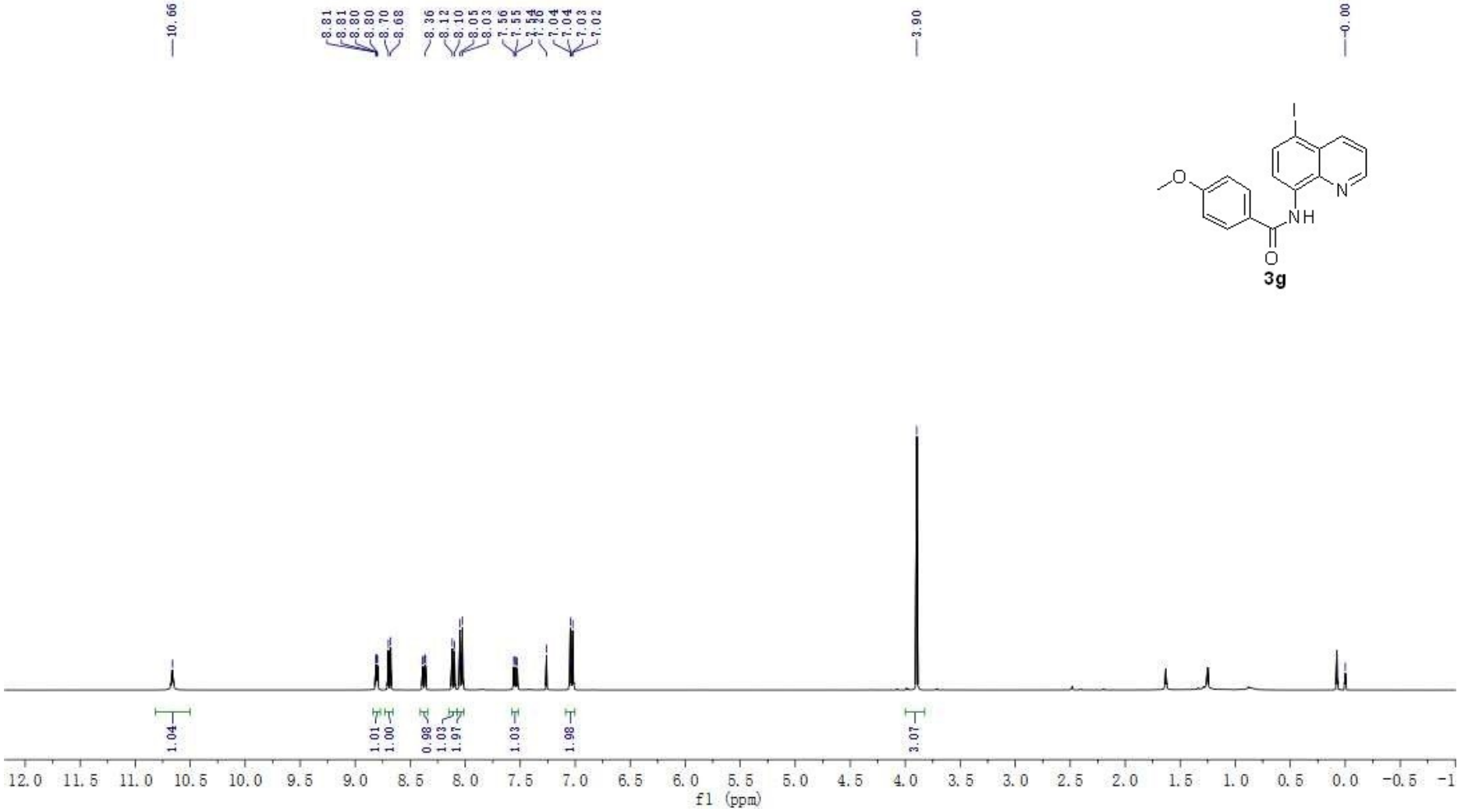
159.96
148.79
140.64
139.21
138.20
136.24
135.36
129.76
129.55
123.15
118.98
118.09
117.78
112.67
89.53
77.32
77.00
76.68
55.47
I
O
N
NH
O
3f
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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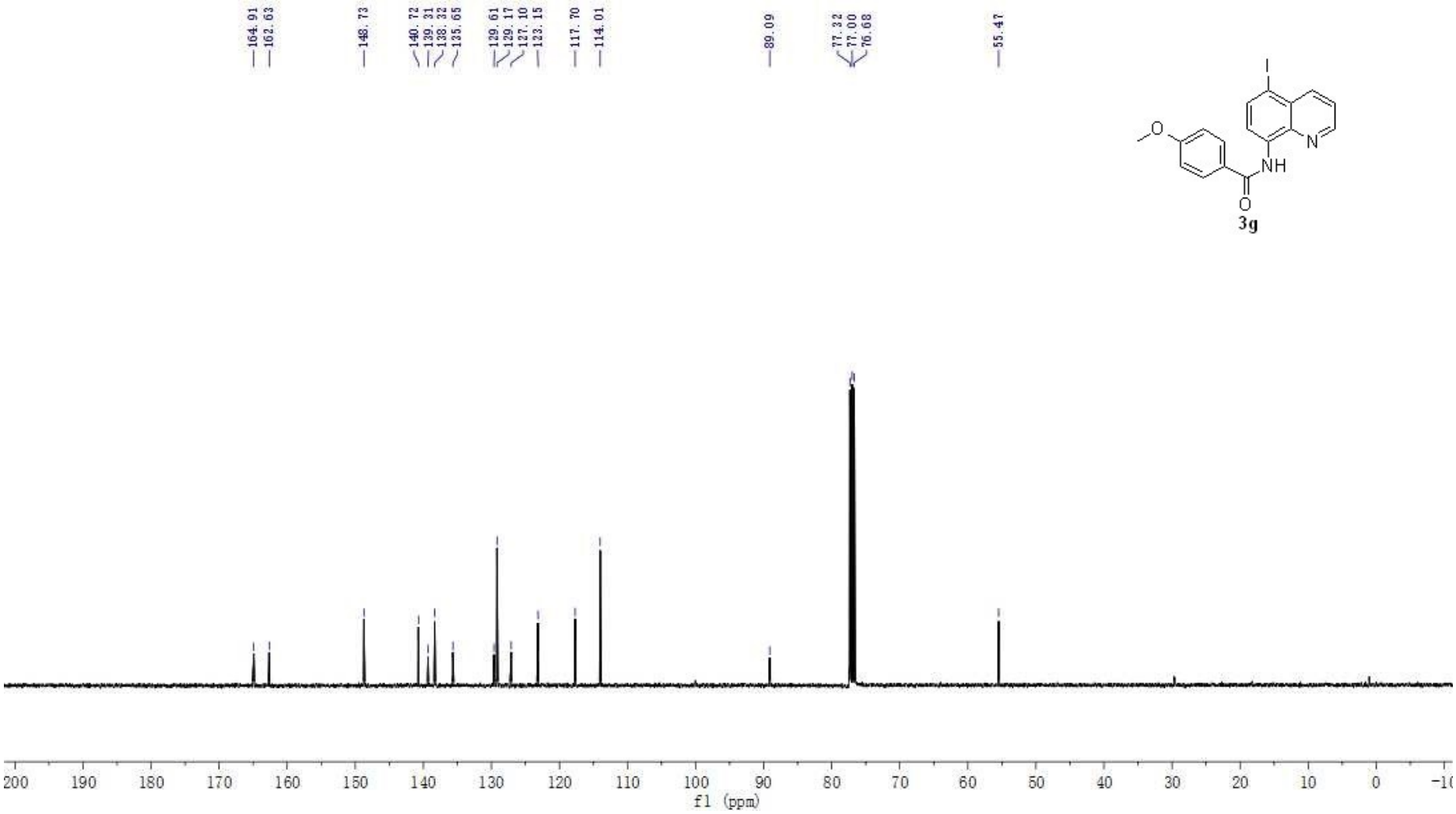
8.81
8.81
8.80
8.80
8.70
8.68
8.36
8.12
8.10
8.05
8.03
7.56
7.55
7.54
7.26
7.04
7.04
7.03
7.02
3.90
0.00
I
O
N
NH
O
3g
1.04
1.01
1.00
0.98
1.03
1.97
1.03
1.98
3.07
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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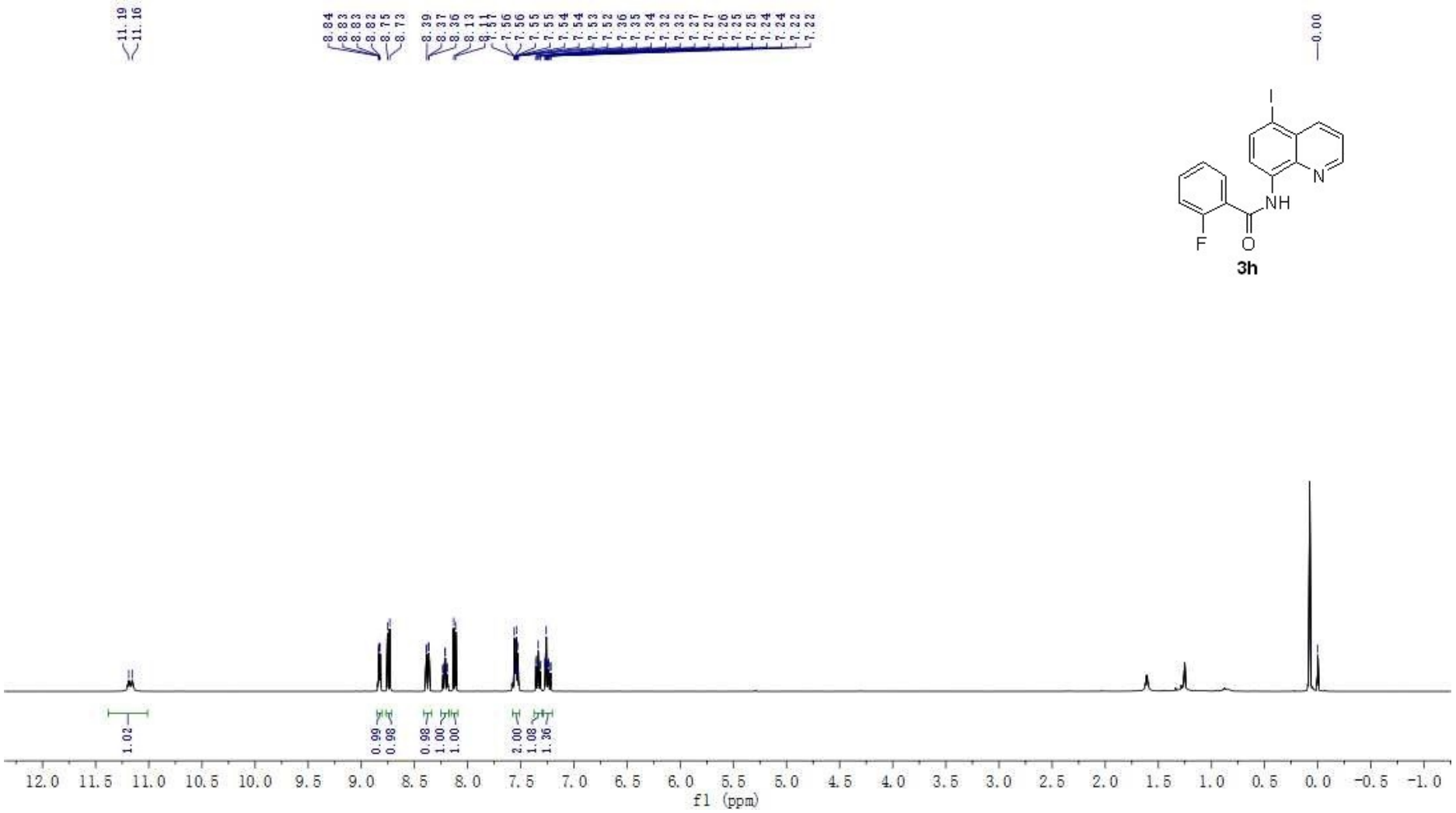
162.63
148.73
140.72
139.31
138.32
135.65
129.61
129.17
127.10
123.15
117.70
114.01
89.09
77.32
77.00
76.68
55.47
I
O
N
NH
O
3g
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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11.16
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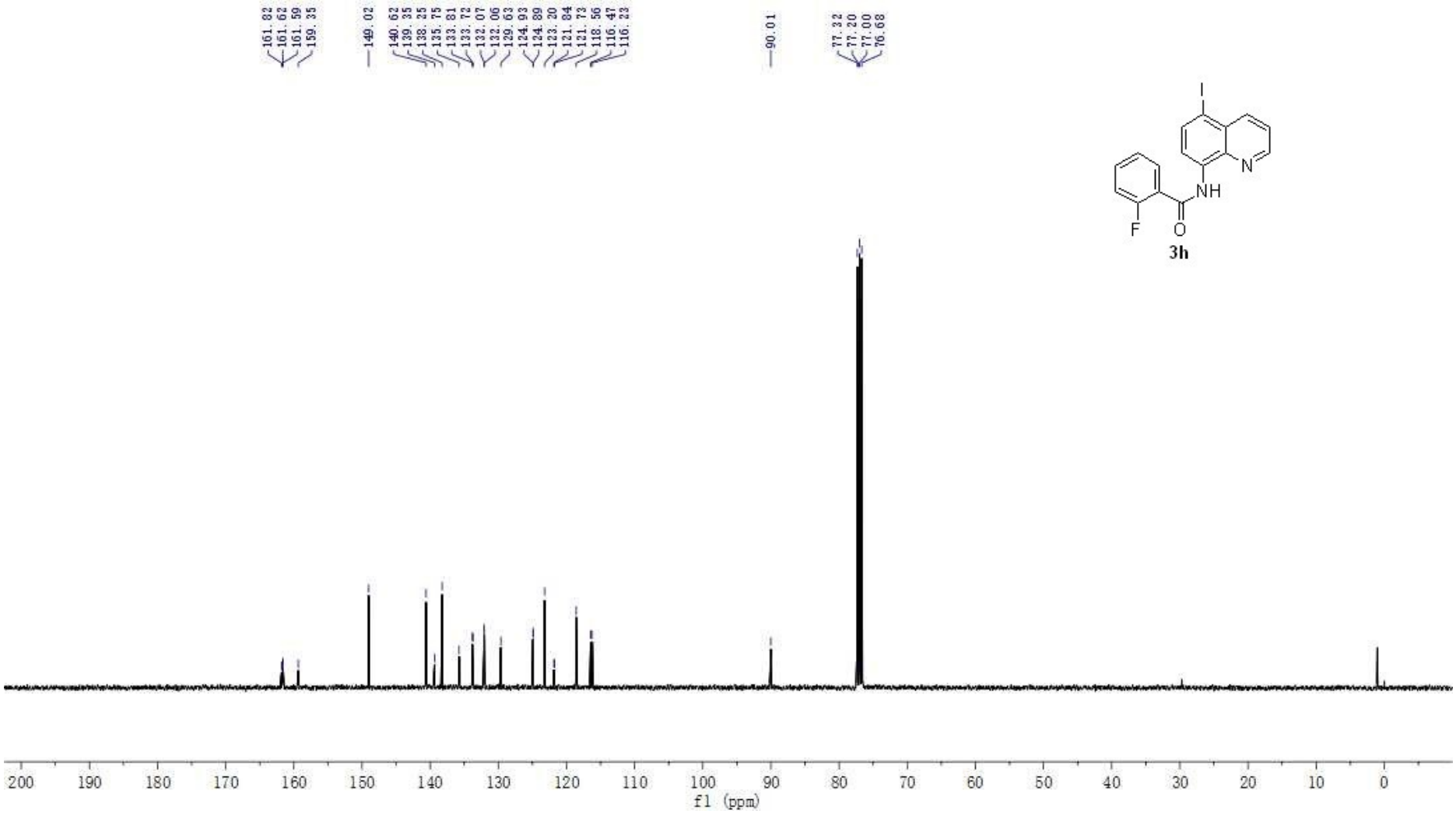
8.83
8.83
8.82
8.75
8.73
8.39
8.37
8.36
8.13
8.11
7.56
7.56
7.55
7.55
7.54
7.54
7.53
7.52
7.36
7.35
7.34
7.32
7.32
7.27
7.27
7.26
7.25
7.25
7.24
7.24
7.22
7.22
0.00
I
N
NH
F
O
3h
1.02
0.99
0.98
0.98
1.00
1.00
2.00
1.08
1.36
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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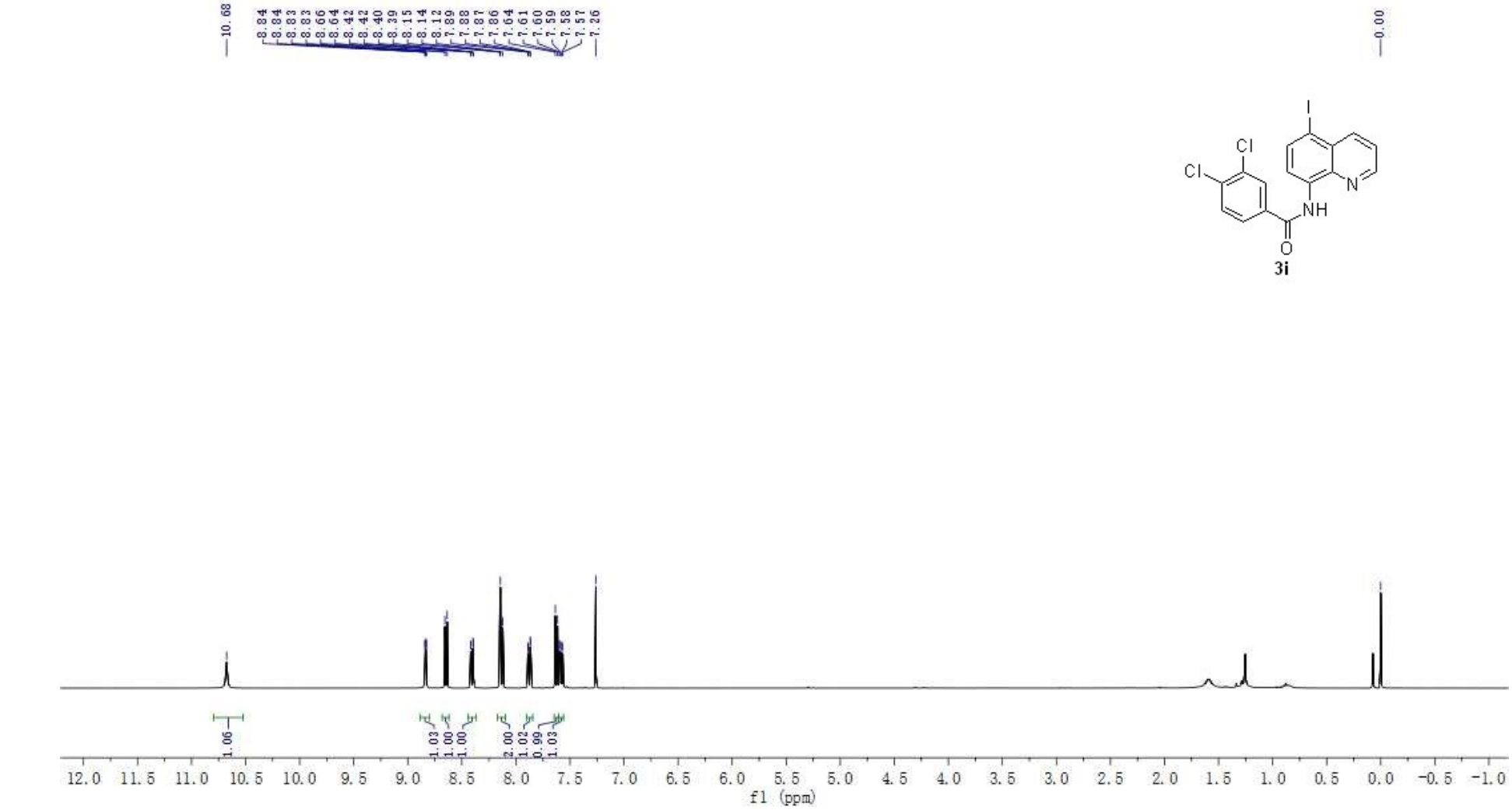
161.59
159.35
149.02
140.62
139.35
138.25
135.75
133.81
133.72
132.07
132.06
129.63
124.93
124.89
123.20
121.84
121.73
118.56
116.47
116.23
90.01
77.32
77.20
77.00
76.68
I
N
NH
F
O
3h
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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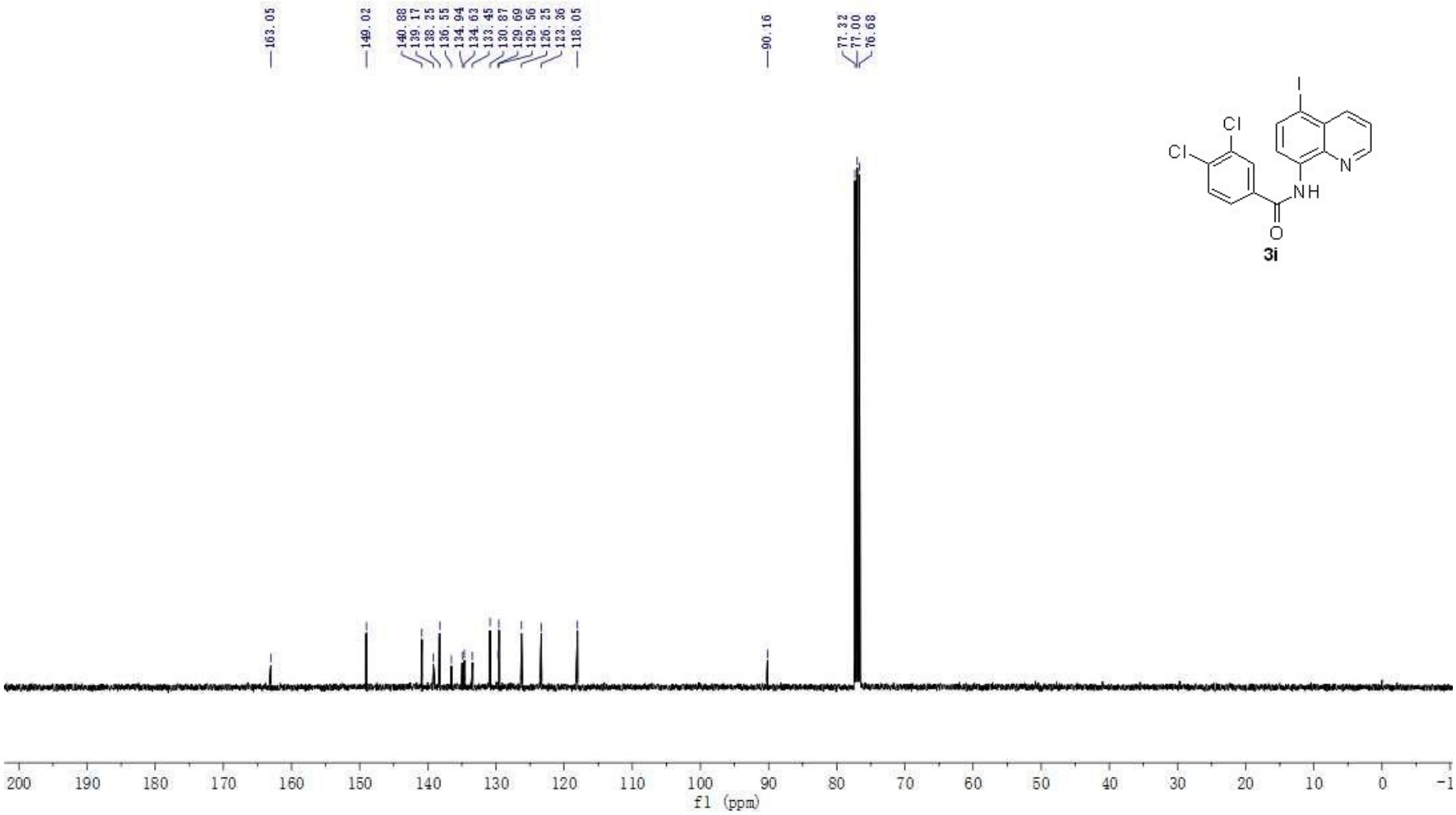
8.84
8.84
8.83
8.83
8.66
8.64
8.42
8.42
8.40
8.39
8.15
8.14
8.12
7.89
7.88
7.87
7.86
7.64
7.61
7.60
7.59
7.58
7.57
7.26
0.00
I
Cl
Cl
N
NH
O
3i
1.06
1.03
1.00
1.00
2.00
1.02
0.99
1.03
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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139.17
138.25
136.55
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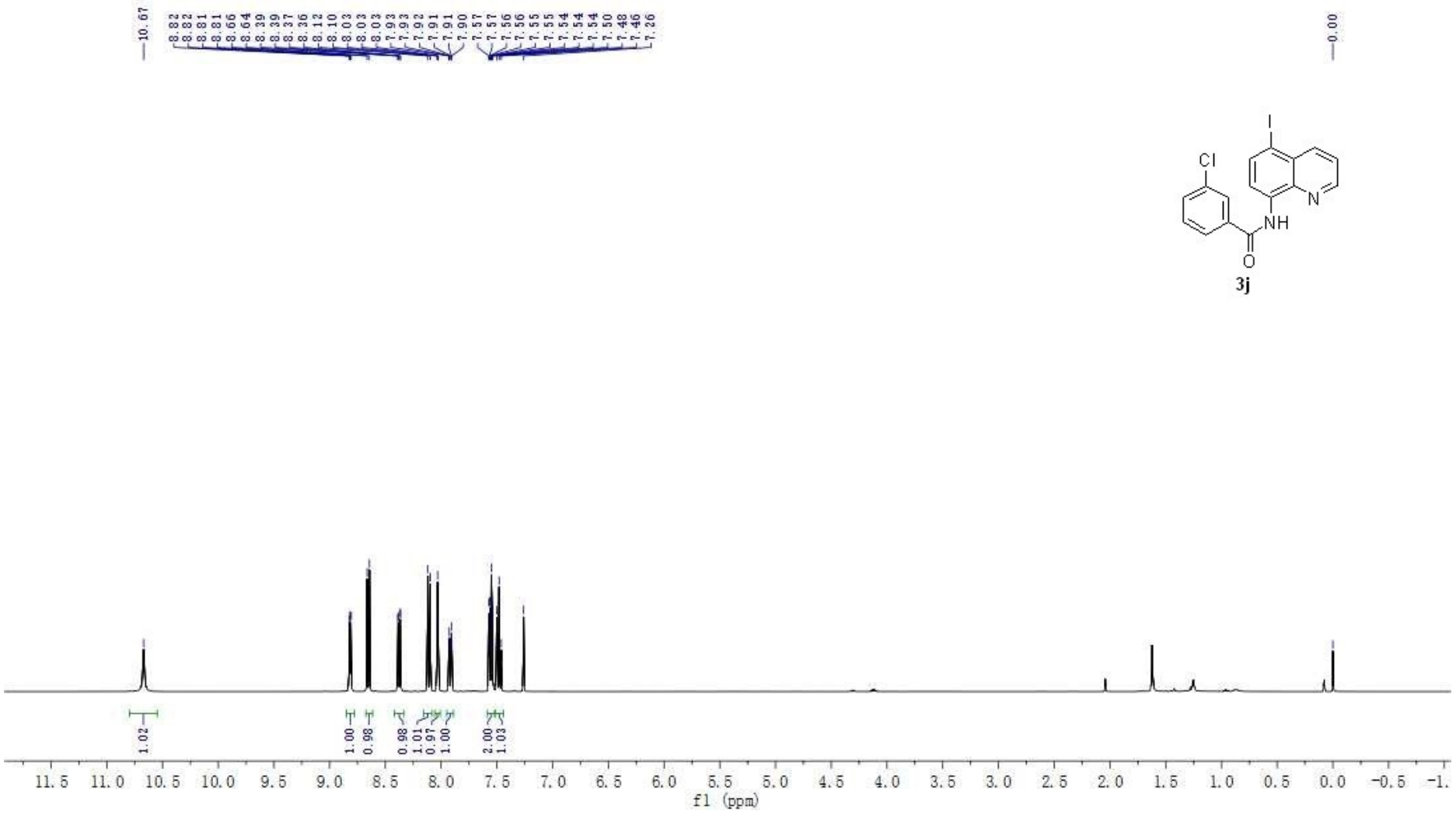
134.63
133.45
130.87
129.69
129.56
126.25
123.36
118.05
90.16
77.32
77.00
76.68
Cl
Cl
I
N
NH
O
3i
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)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8.82
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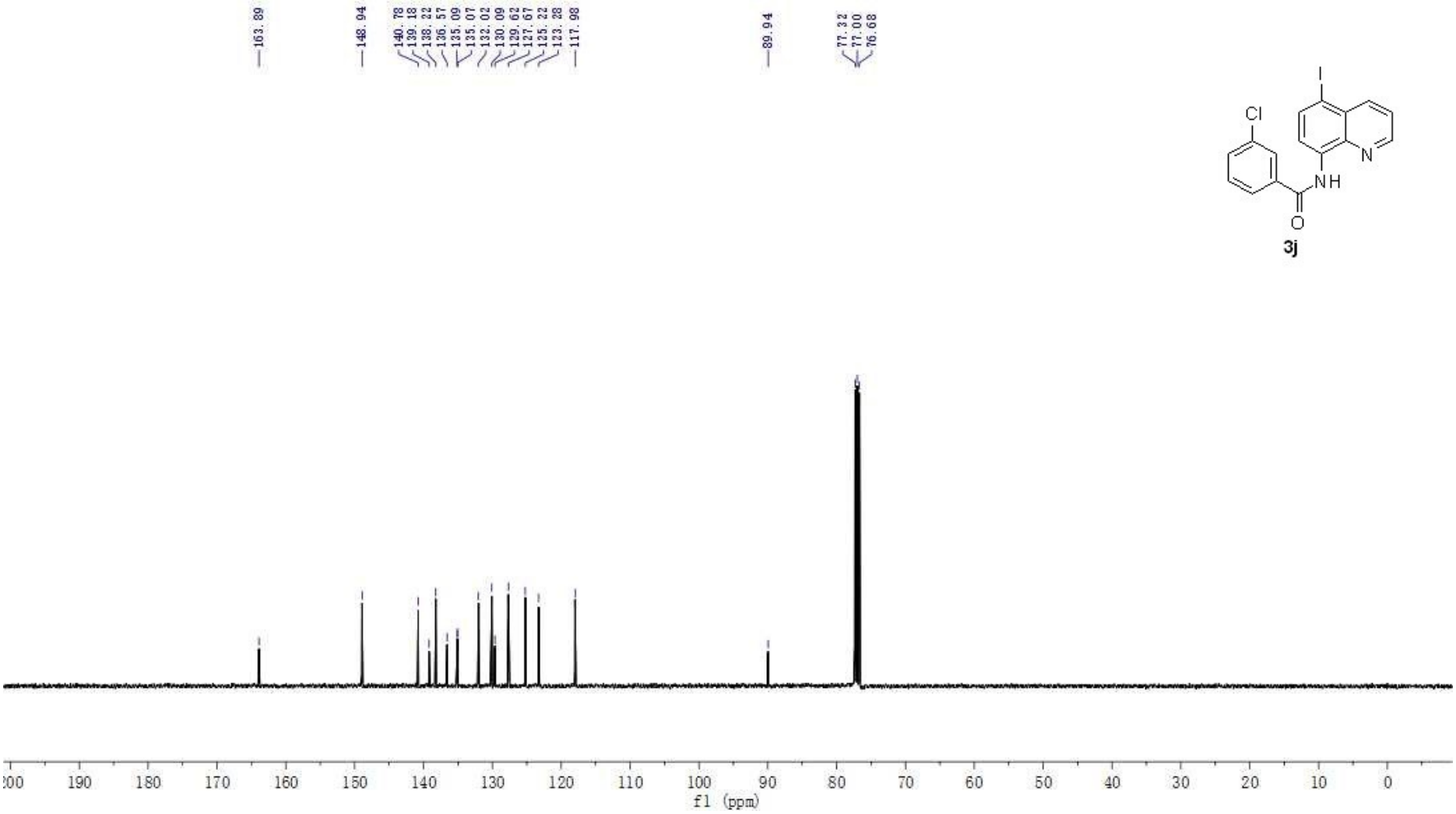
8.39
8.39
8.37
8.36
8.12
8.10
8.03
8.03
8.03
7.93
7.93
7.92
7.91
7.91
7.90
7.57
7.57
7.56
7.56
7.55
7.55
7.54
7.54
7.54
7.50
7.48
7.46
7.26
0.00
I
Cl
N
NH
O
3j
1.02
1.00
0.98
0.98
1.01
0.97
1.00
2.00
1.03
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)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140.78
139.18
138.22
136.57
135.09
135.07
132.02
130.09
129.62
127.67
125.22
123.28
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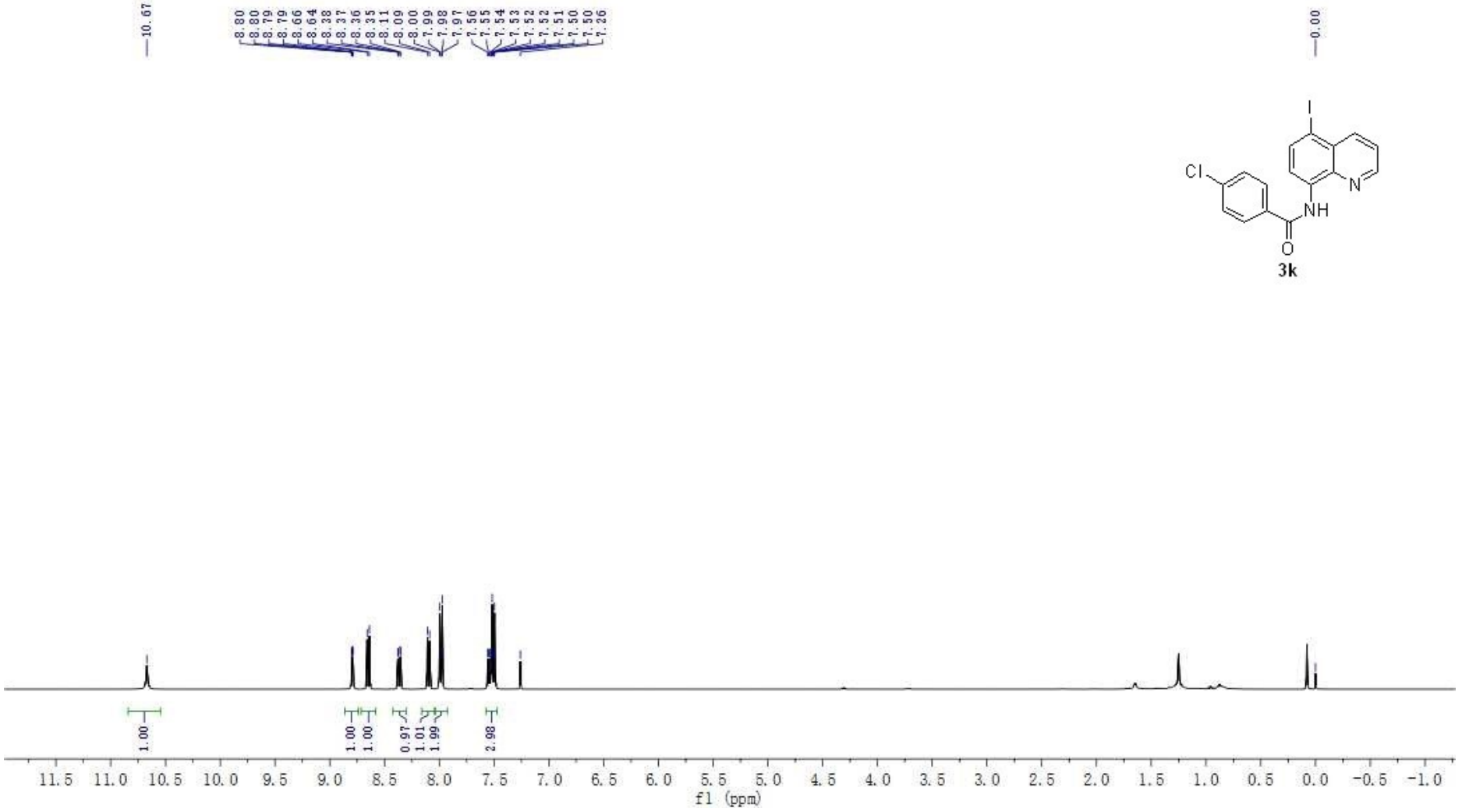
89.94
77.32
77.00
76.68
Cl
I
N
NH
O
3j
f1 (ppm)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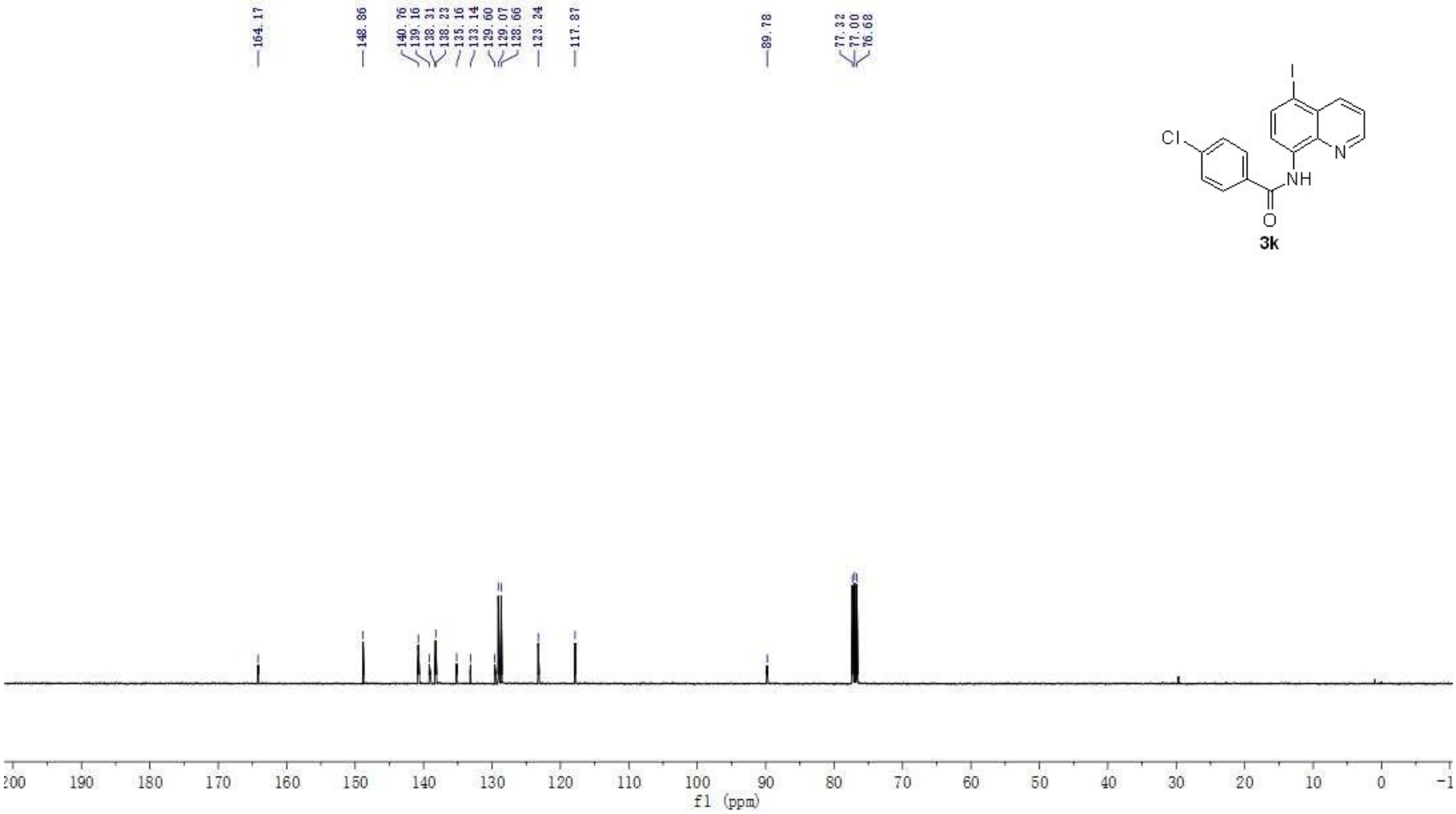
8.64
8.38
8.37
8.36
8.35
8.11
8.09
8.00
7.99
7.98
7.97
7.56
7.55
7.54
7.53
7.52
7.52
7.51
7.50
7.50
7.26
0.00
I
Cl
N
NH
O
3k
1.00
1.00
1.00
0.97
1.01
1.99
2.98
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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139.16
138.31
138.23
135.16
133.14
129.60
129.07
128.66
123.24
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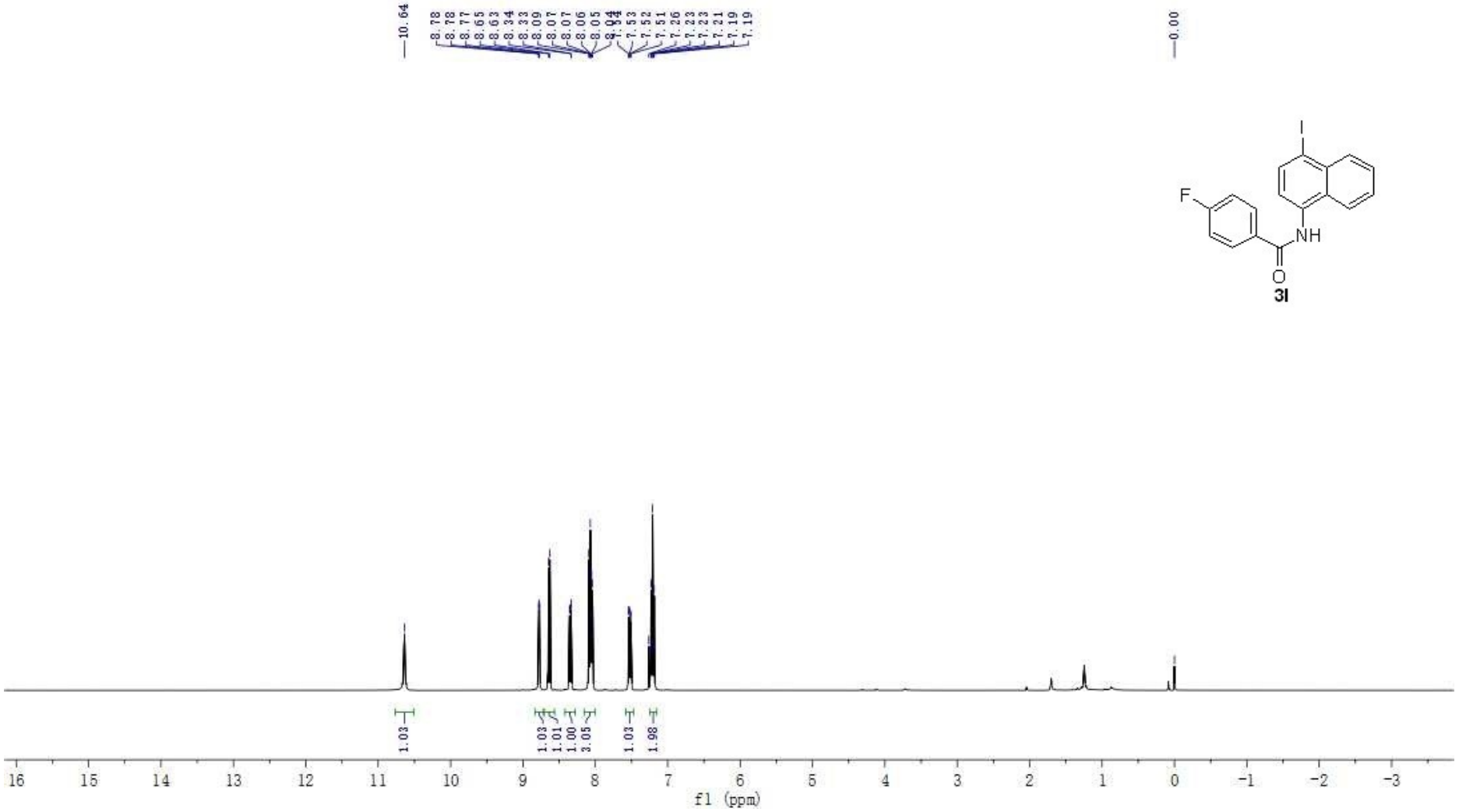
89.78
77.32
77.00
76.68
I
Cl
N
NH
O
3k
f1 (ppm)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8.78
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8.63
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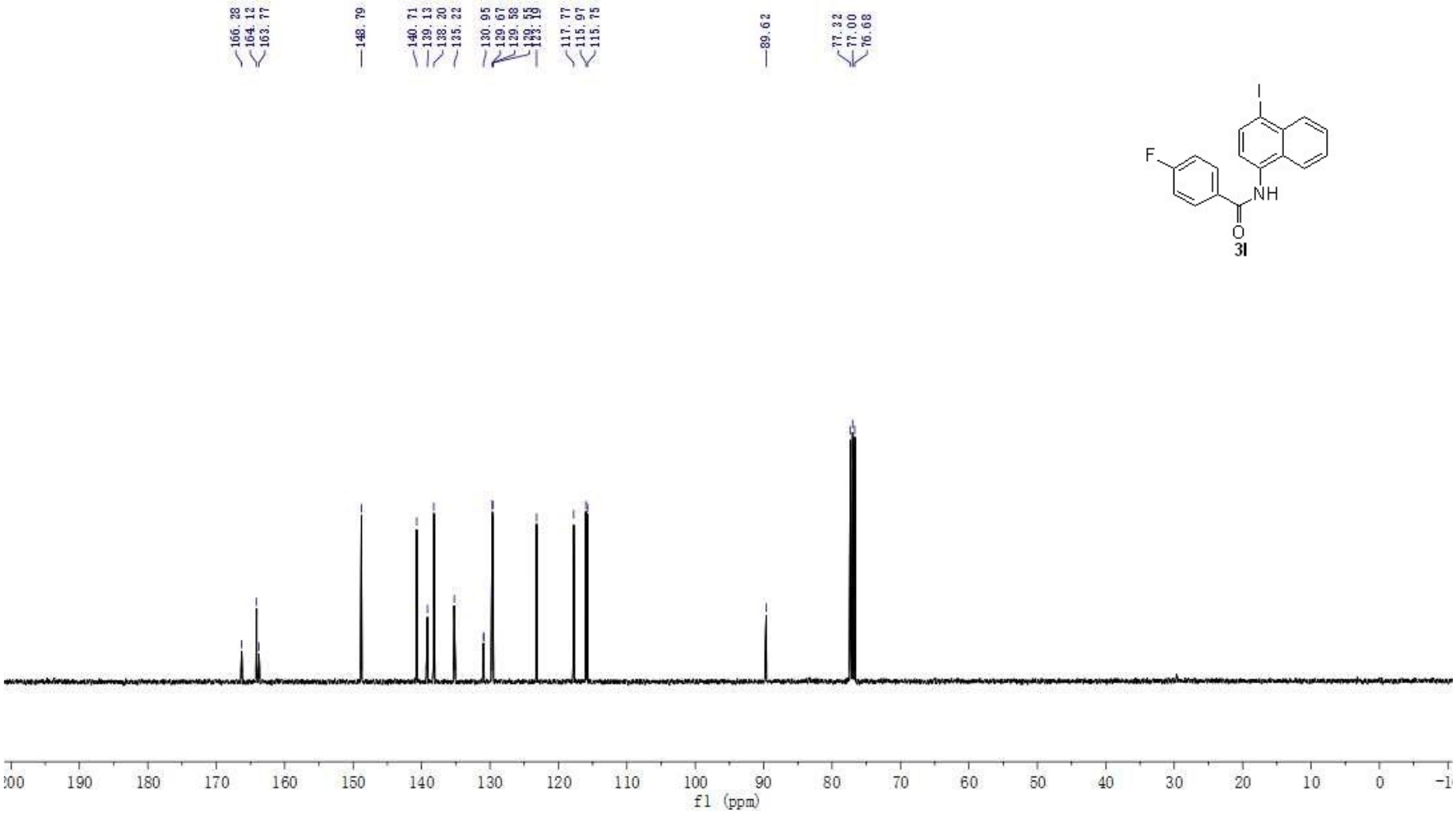
8.33
8.09
8.07
8.07
8.06
8.05
8.04
7.53
7.52
7.51
7.26
7.23
7.23
7.21
7.19
7.19
0.00
I
F
NH
O
3l
1.03
1.03
1.01
1.00
3.05
1.03
1.98
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)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139.13
138.20
135.22
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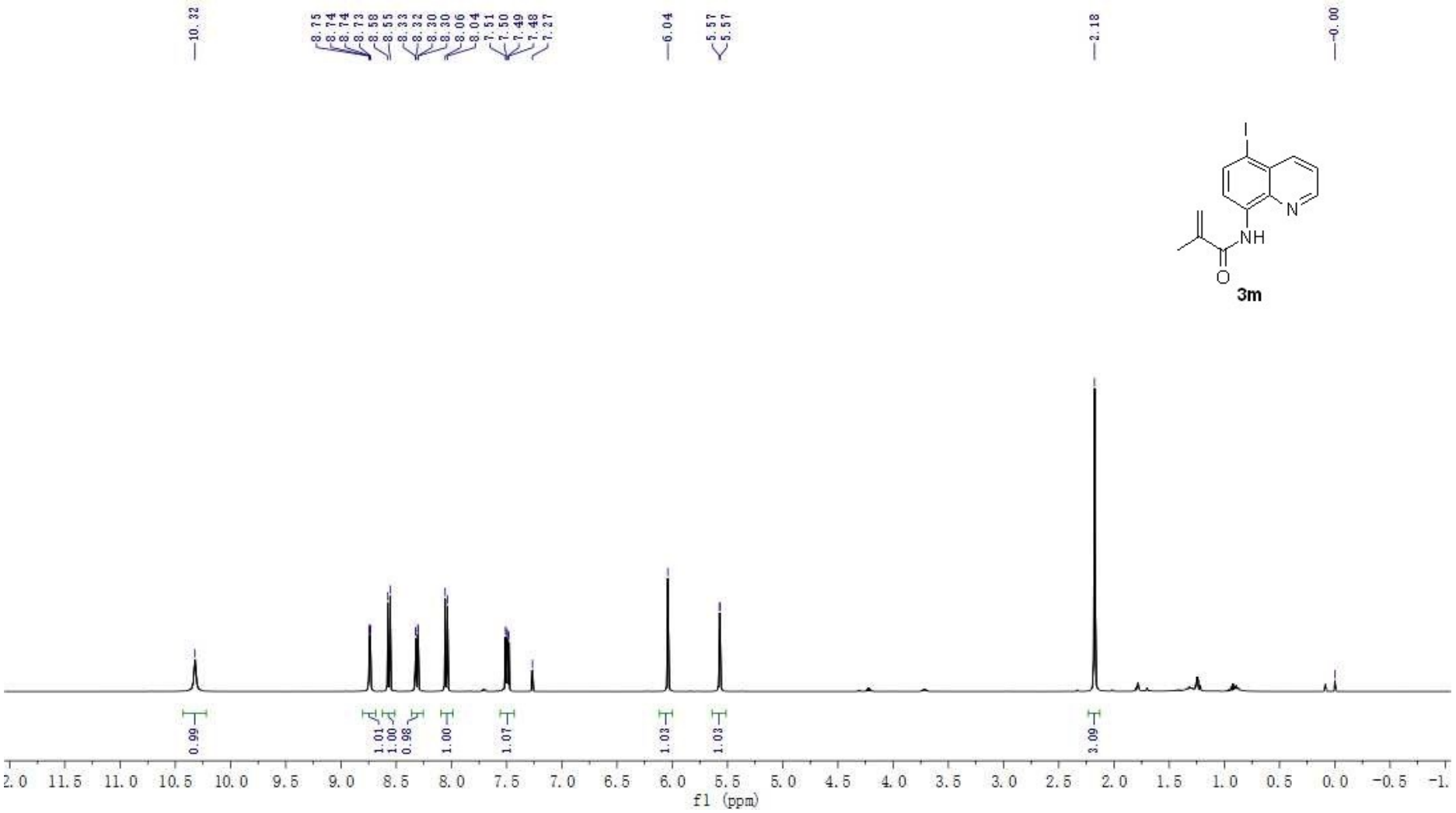
129.67
129.58
117.77
115.97
115.75
89.62
77.32
77.00
76.68
I
F
NH
O
3l
f1 (ppm)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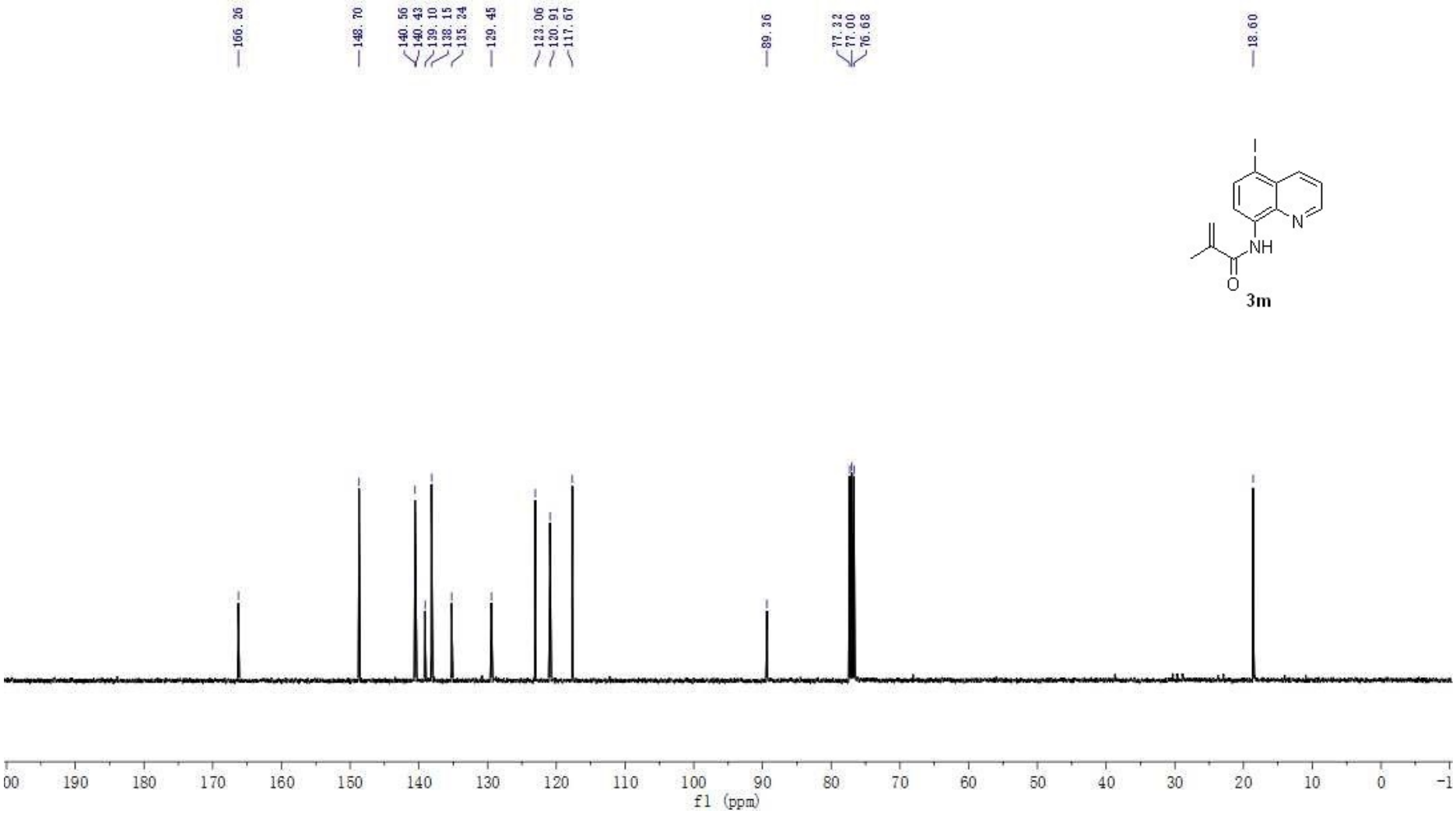
8.74
8.73
8.58
8.55
8.33
8.32
8.30
8.30
8.06
8.04
7.51
7.50
7.49
7.48
7.27
6.04
5.57
5.57
2.18
0.00
I
N
NH
O
3m
0.99
1.01
1.00
0.98
1.00
1.07
1.03
1.03
3.09
f1 (ppm)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138.15
135.24
129.45
123.06
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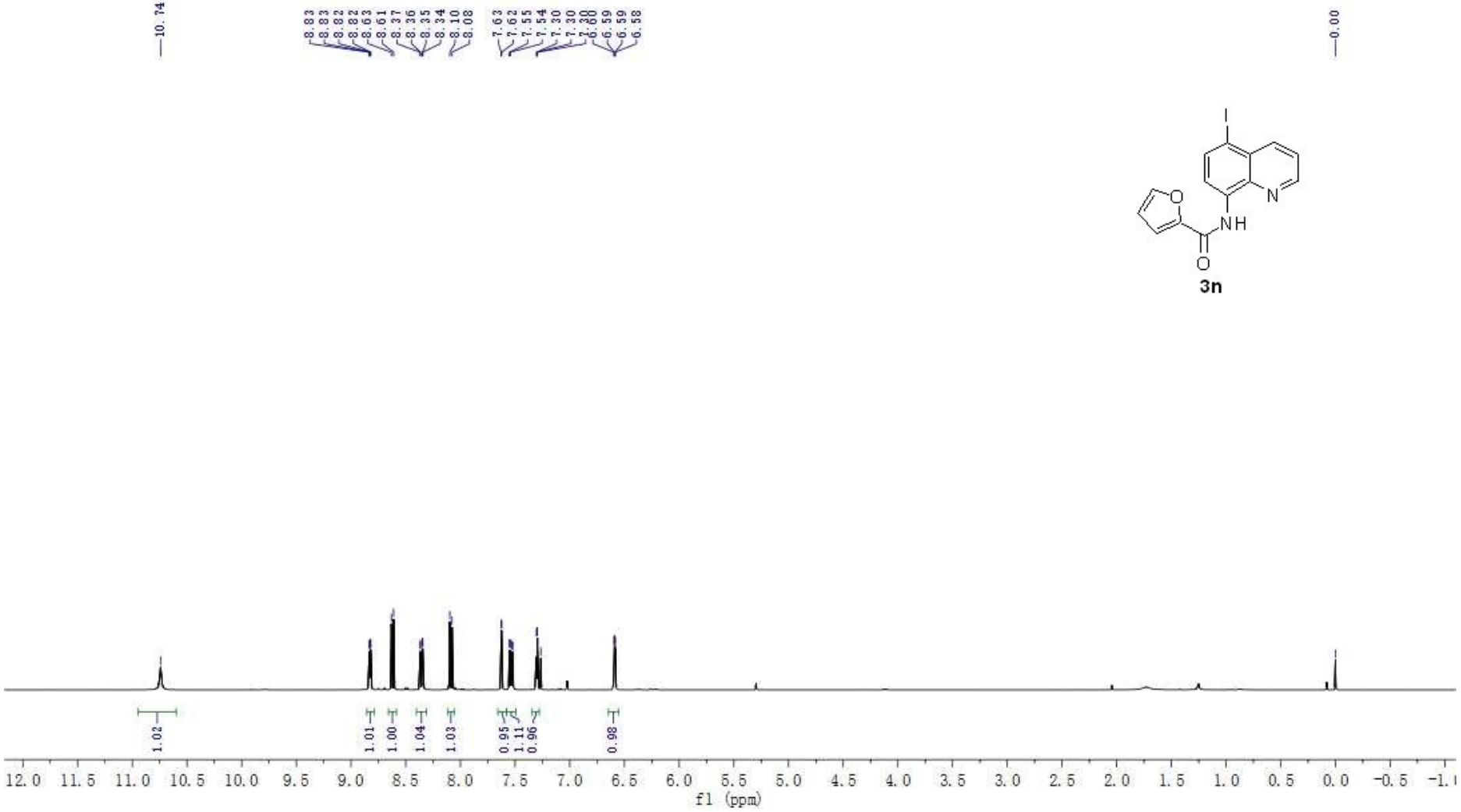
89.36
77.32
77.00
76.68
18.60
I
N
NH
O
3m
f1 (ppm)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8.83
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8.82
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8.37
8.36
8.35
8.34
8.10
8.08
7.63
7.62
7.55
7.54
7.30
7.30
6.59
6.59
6.58
0.00
I
N
O
NH
O
3n
1.02
1.01
1.00
1.04
1.03
0.95
1.11
0.96
0.98
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 -0.5
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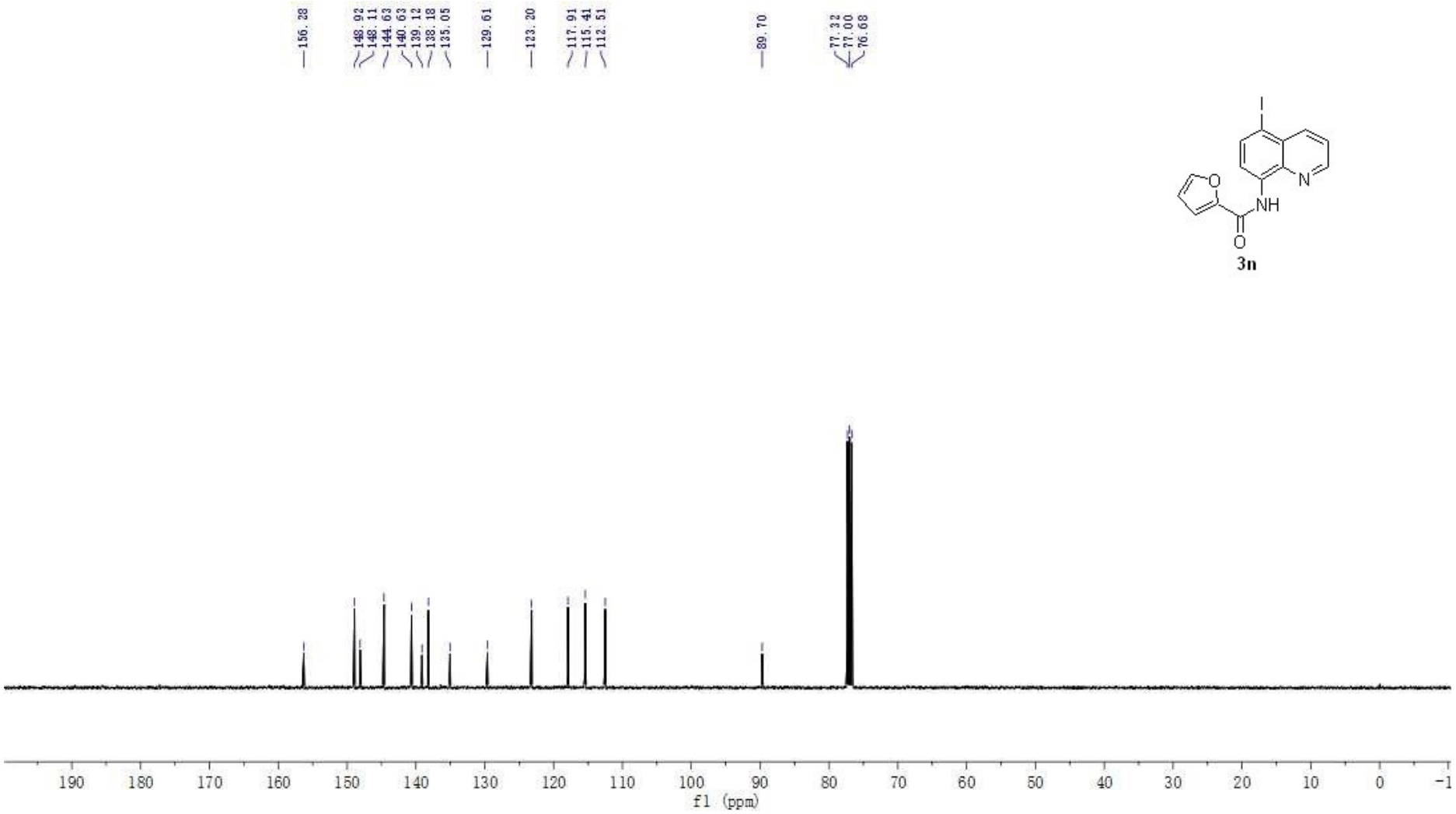
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115.41
112.51
89.70
77.32
77.00
76.68
I
N
NH
O
O
3n
190
180
170
160
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120
110
100
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80
70
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50
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30
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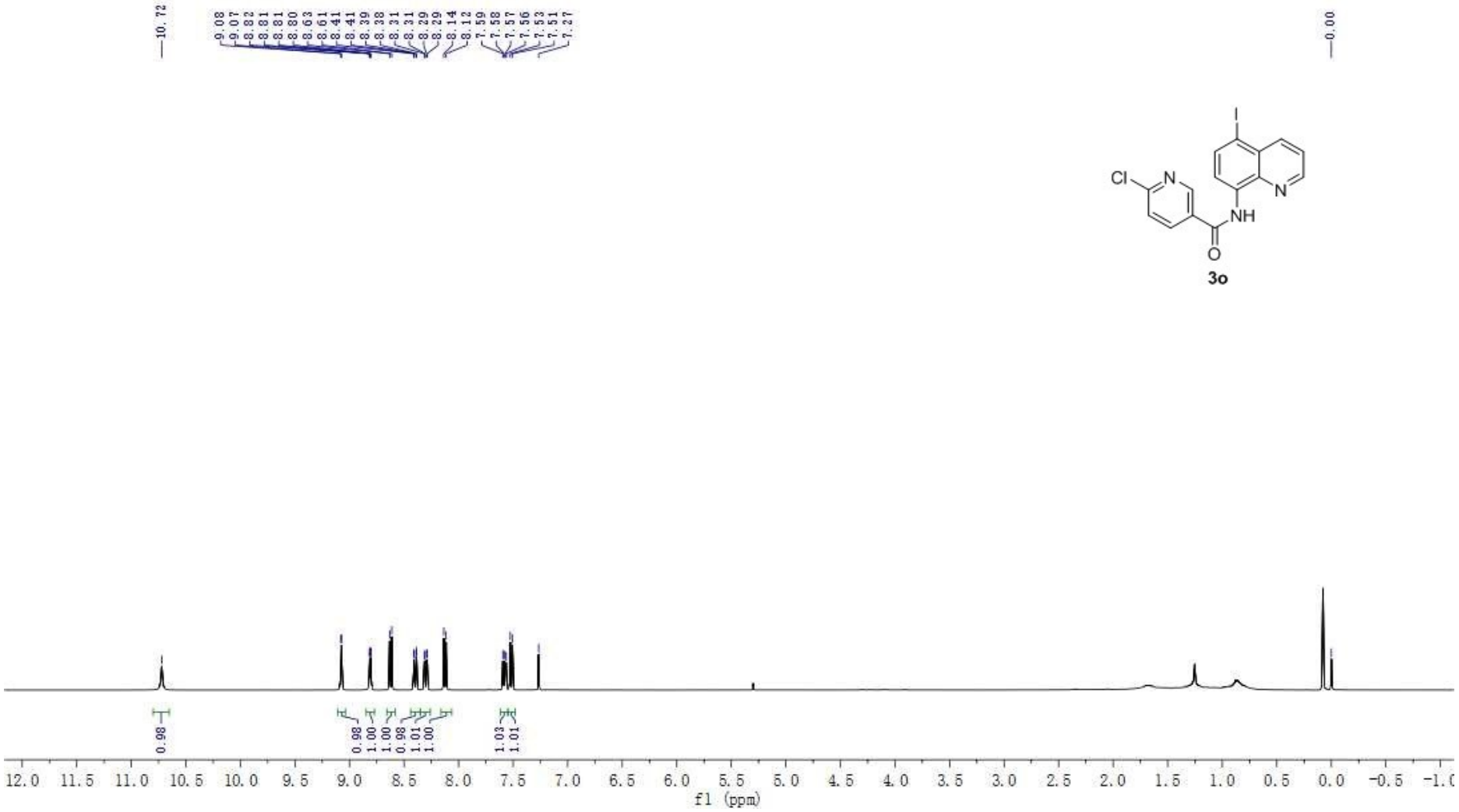
-1
f1 (ppm)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8.41
8.39
8.38
8.31
8.31
8.29
8.29
8.14
8.12
7.59
7.58
7.57
7.56
7.53
7.51
7.27
0.00
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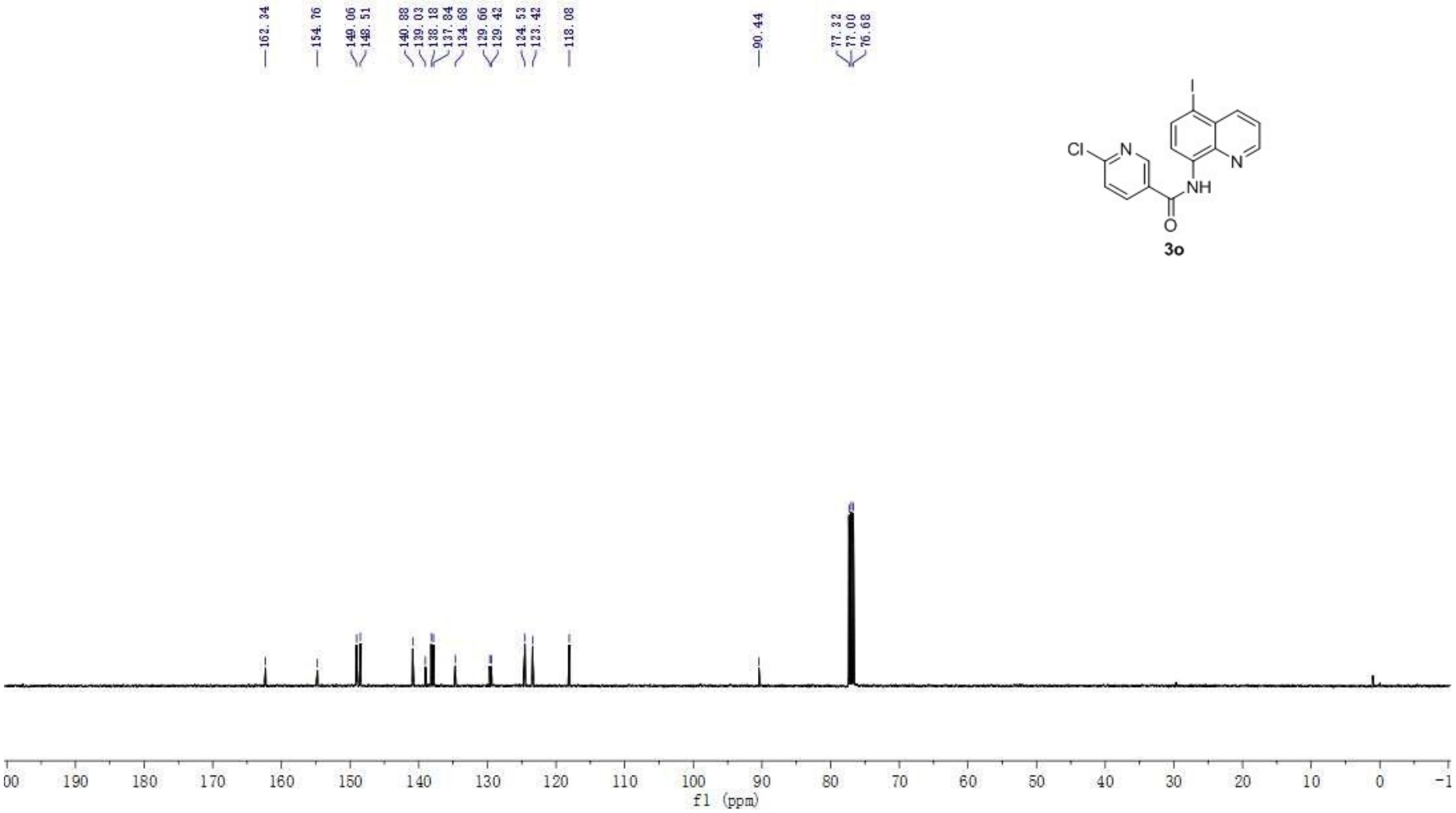
N
NH
O
I
3o
0.98
0.98
1.00
1.00
0.98
1.01
1.00
1.03
1.01
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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129.42
124.53
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77.32
77.00
76.68
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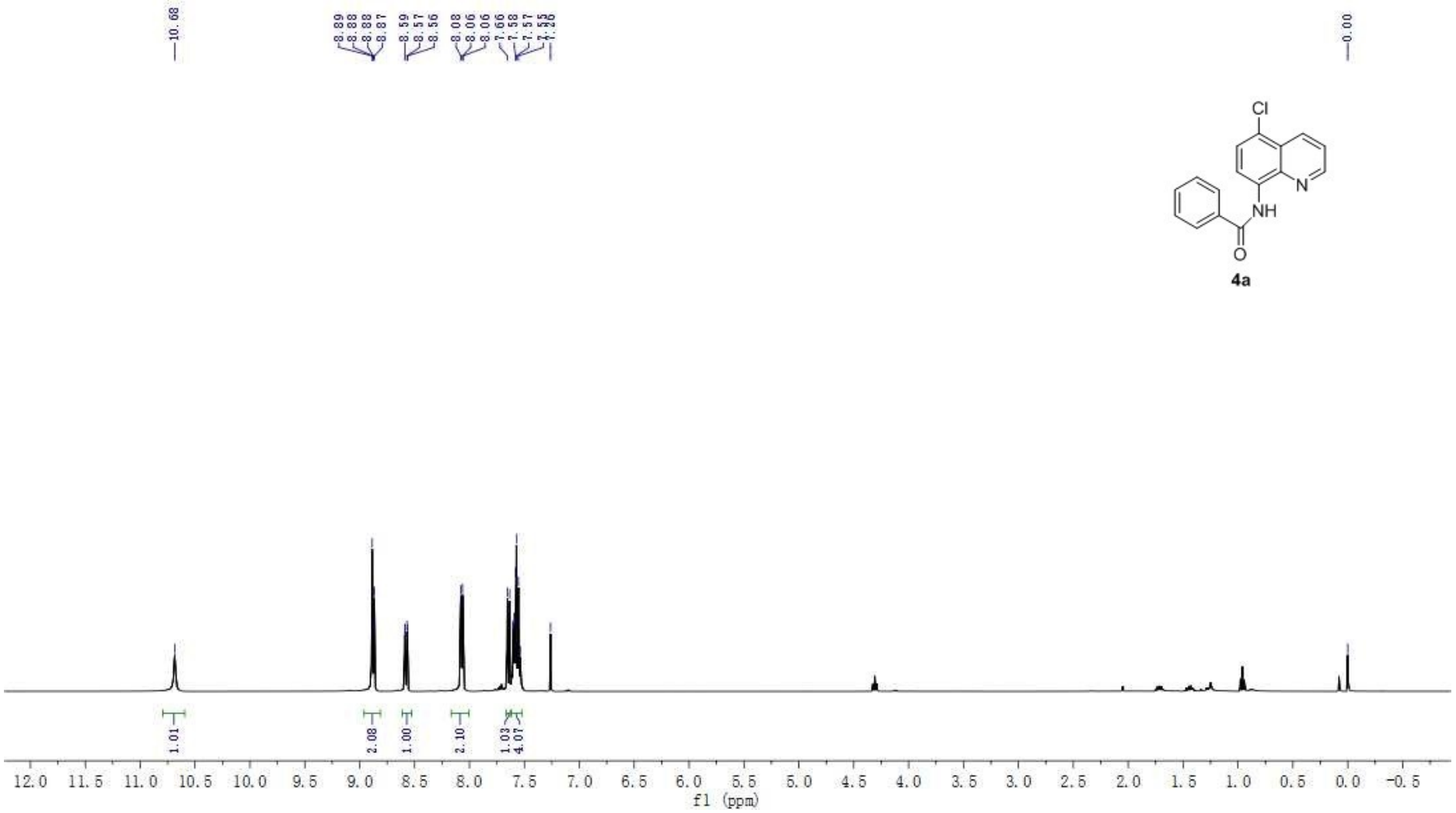
N
I
N
NH
O
3o
f1 (ppm)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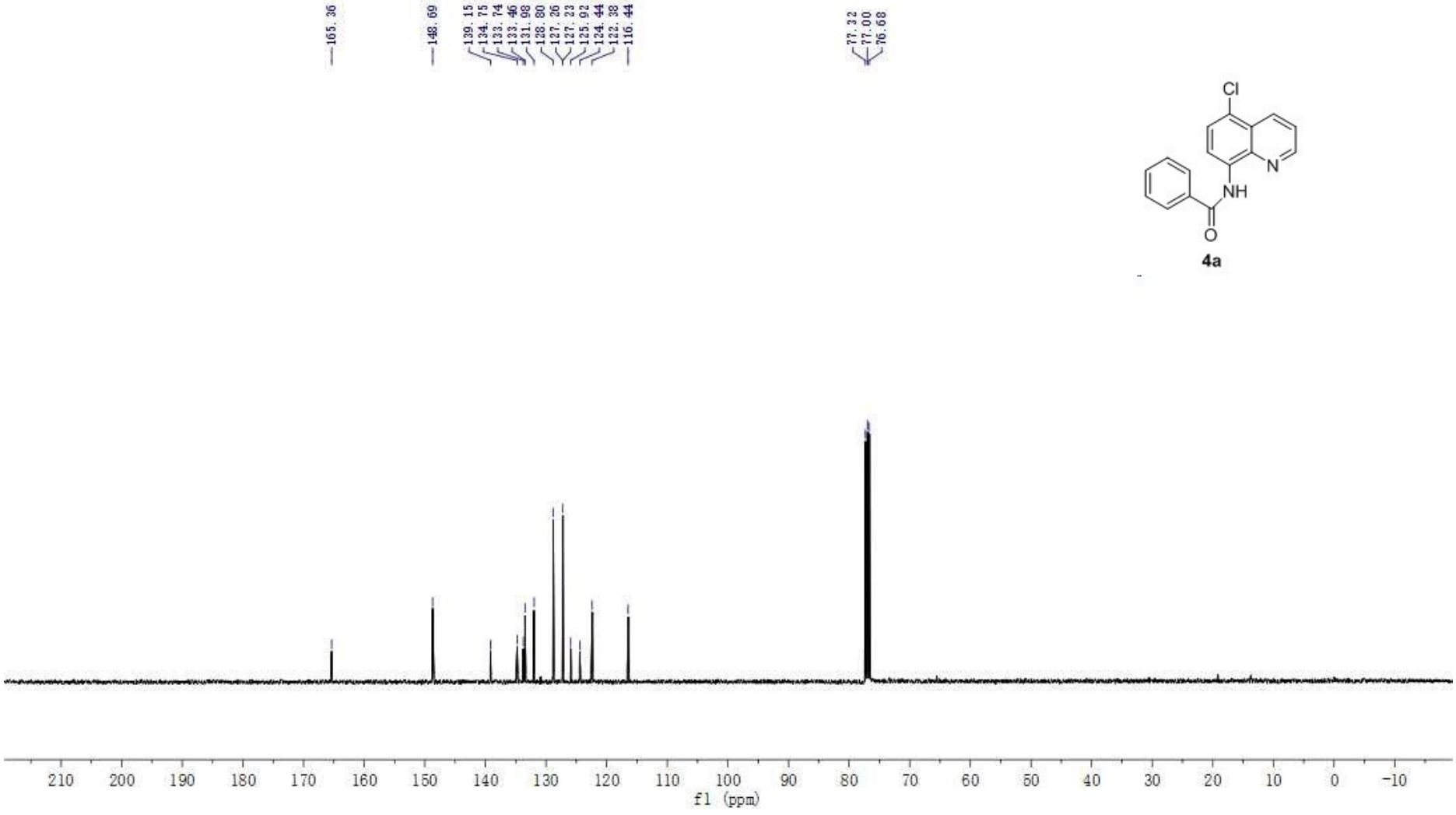
8.56
8.08
8.06
8.06
7.66
7.58
7.57
7.55
7.26
0.00
Cl
N
NH
O
4a
1.01
2.08
1.00
2.10
1.03
4.07
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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125.92
124.44
122.38
116.44
77.32
77.00
76.68
Cl
N
NH
O
4a
210
200
190
180
170
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120
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100
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80
70
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30
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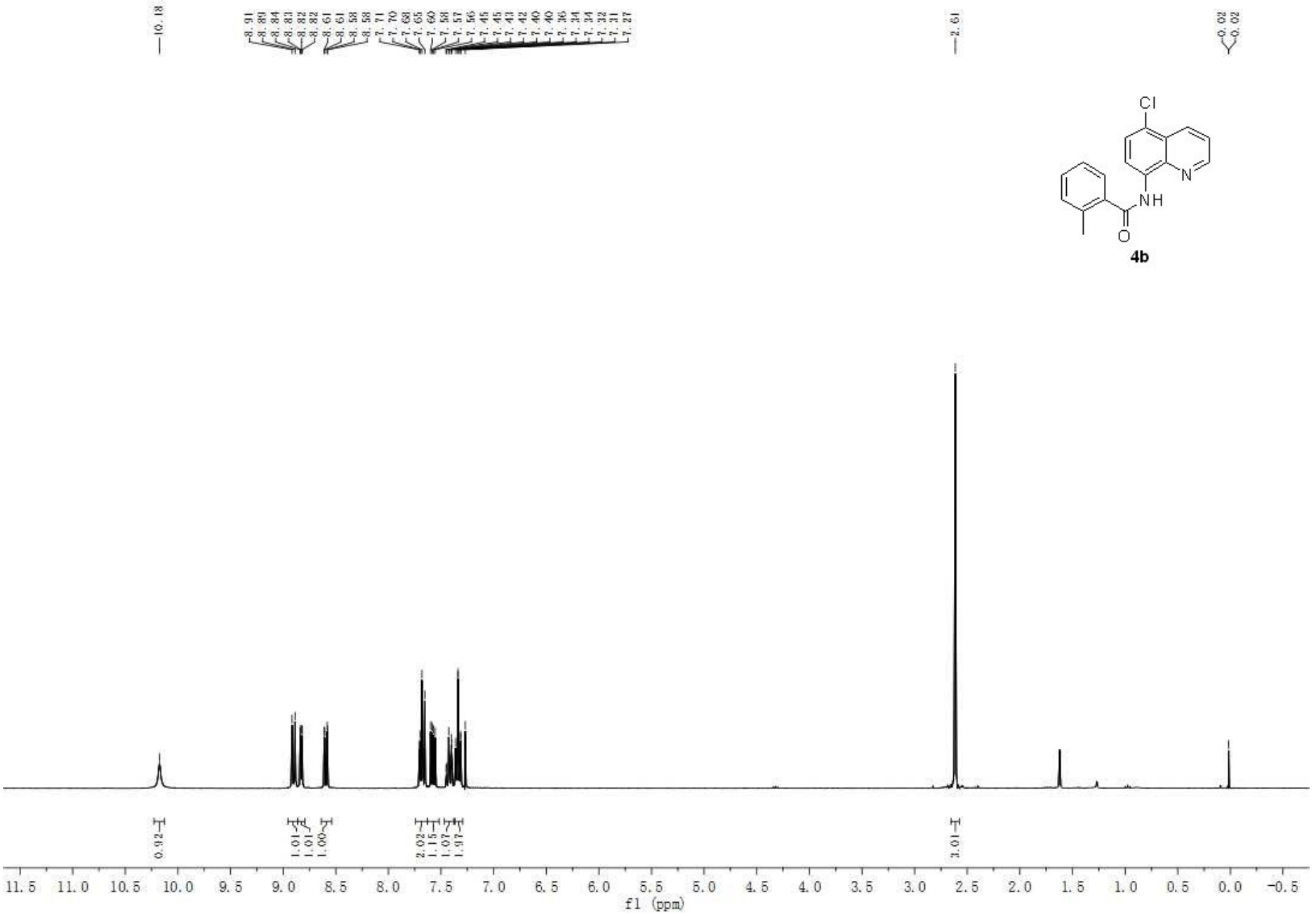
0
-10
f1 (ppm)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7.68
7.65
7.60
7.58
7.57
7.56
7.45
7.45
7.43
7.42
7.40
7.40
7.36
7.34
7.34
7.32
7.31
7.27
2.61
0.02
0.02
Cl
N
NH
O
4b
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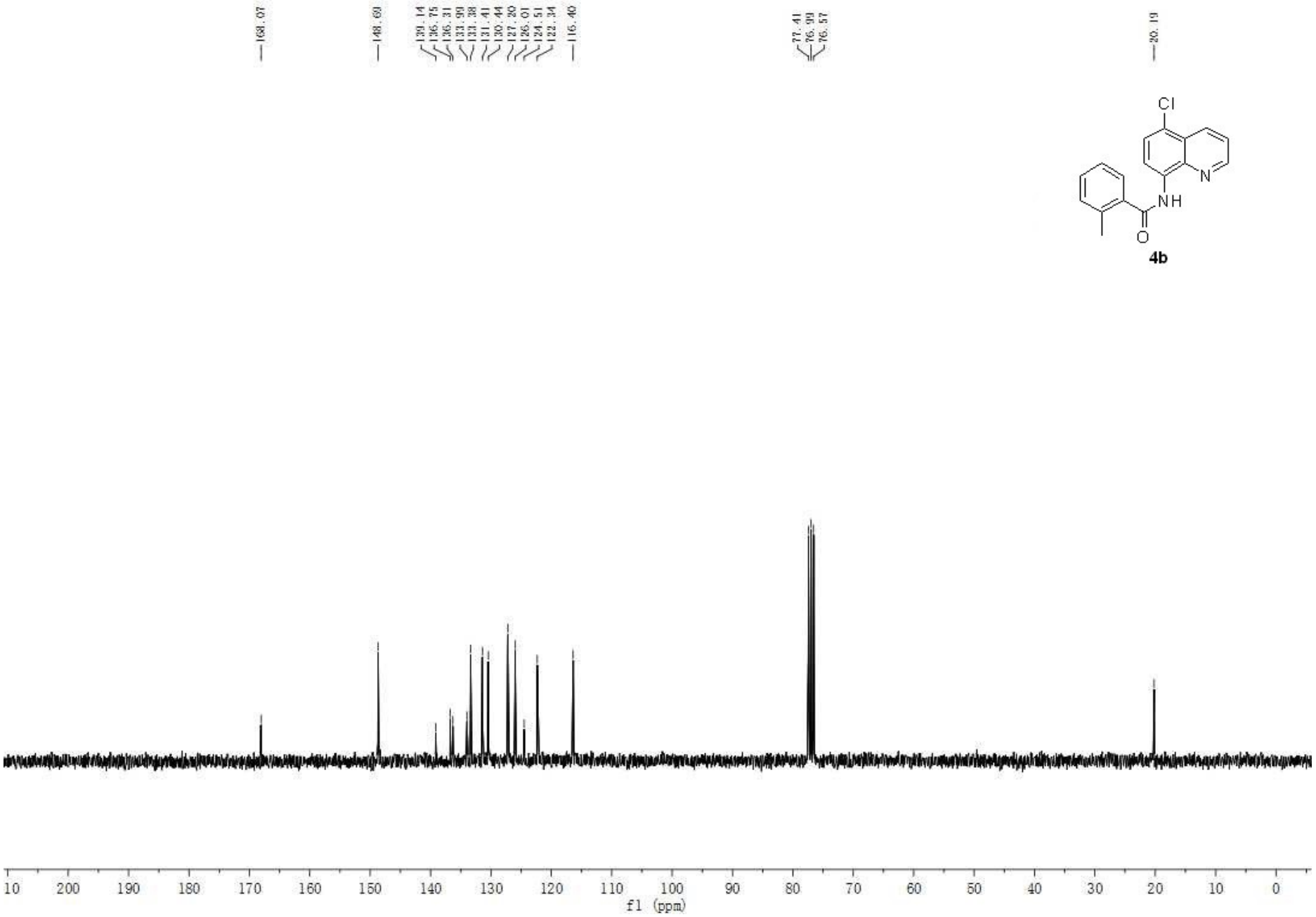
1.01
1.01
1.00
2.02
1.15
1.07
1.97
3.01
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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133.38
131.41
130.44
127.20
126.01
124.51
122.34
116.40
77.41
76.99
76.57
20.19
Cl
N
NH
O
4b
10
200
190
180
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150
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130
120
110
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90
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50
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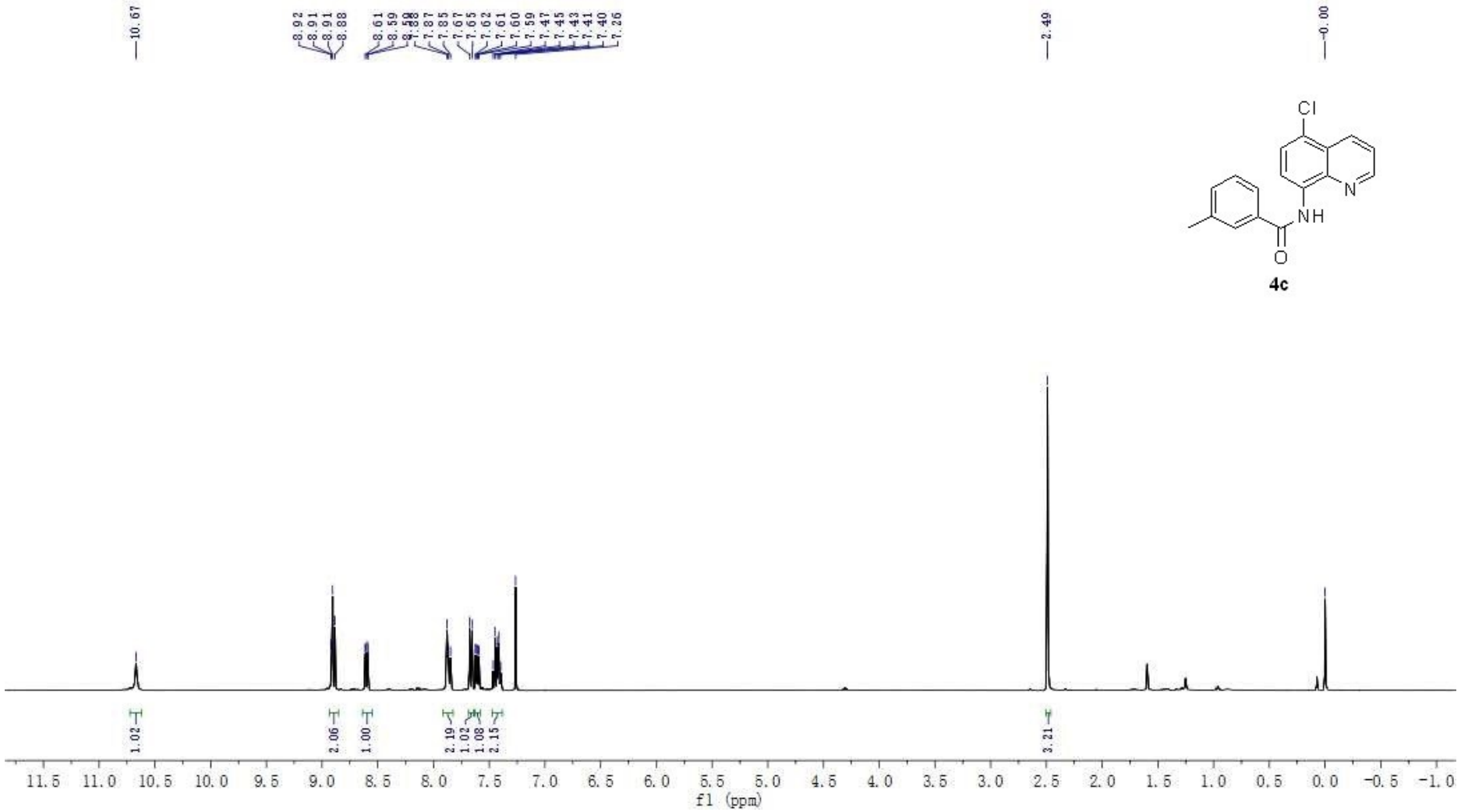
30
20
10
0
f1 (ppm)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8.61
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7.85
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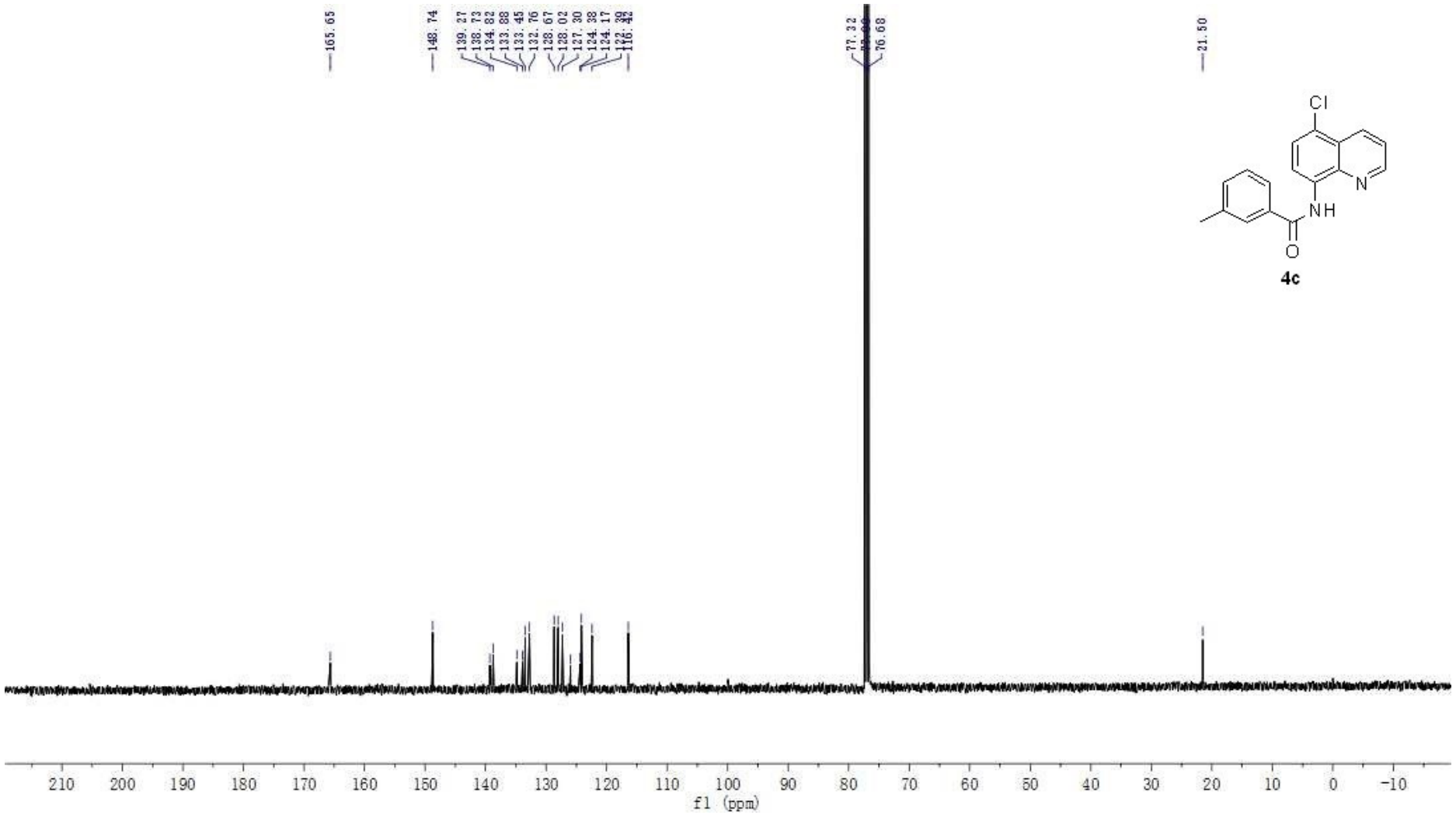
7.61
7.60
7.59
7.47
7.45
7.43
7.41
7.40
7.26
2.49
0.00
Cl
N
NH
O
4c
1.02
2.06
1.00
2.19
1.02
1.08
2.15
3.21
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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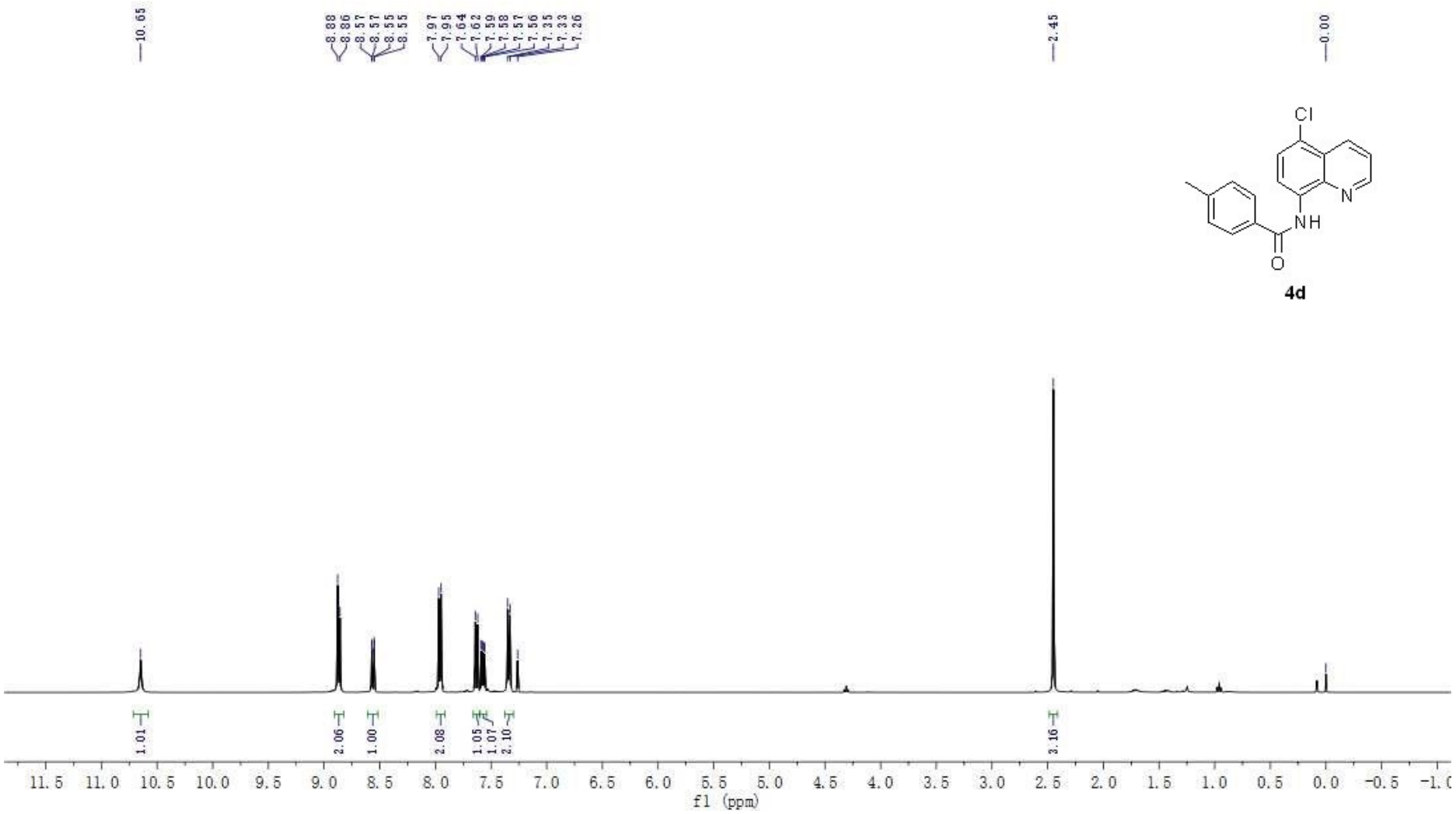
133.88
133.45
132.76
128.67
128.02
127.30
124.38
124.17
122.39
116.42
77.32
76.68
21.50
Cl
N
NH
O
4c
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.62
7.59
7.58
7.57
7.56
7.35
7.33
7.26
2.45
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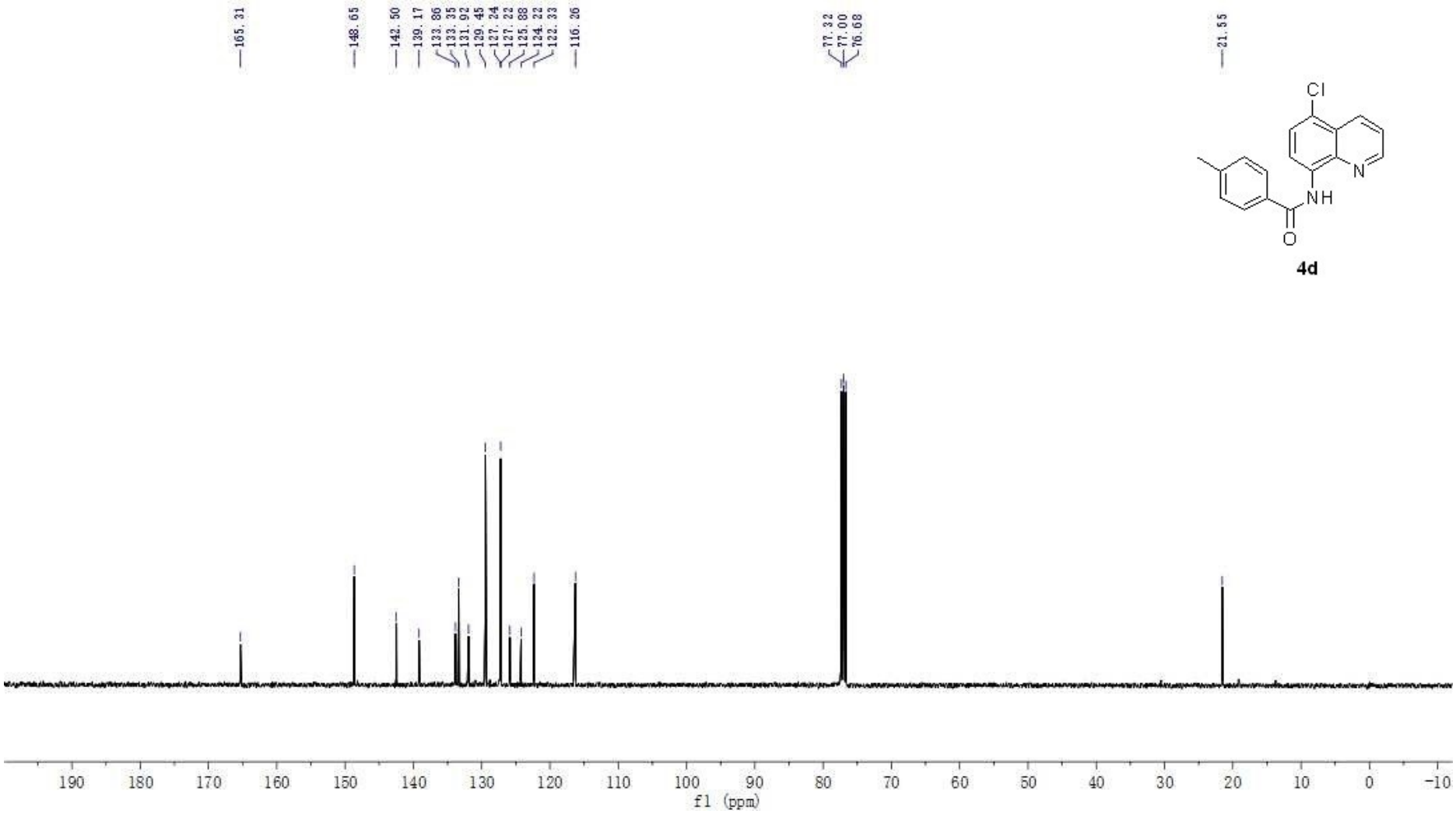
N
NH
O
4d
1.01
2.06
1.00
2.08
1.05
1.07
2.10
3.16
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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133.35
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127.22
125.88
124.22
122.33
116.26
77.32
77.00
76.68
21.55
Cl
N
NH
O
4d
190
180
170
160
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140
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120
110
100
90
80
70
60
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40
30
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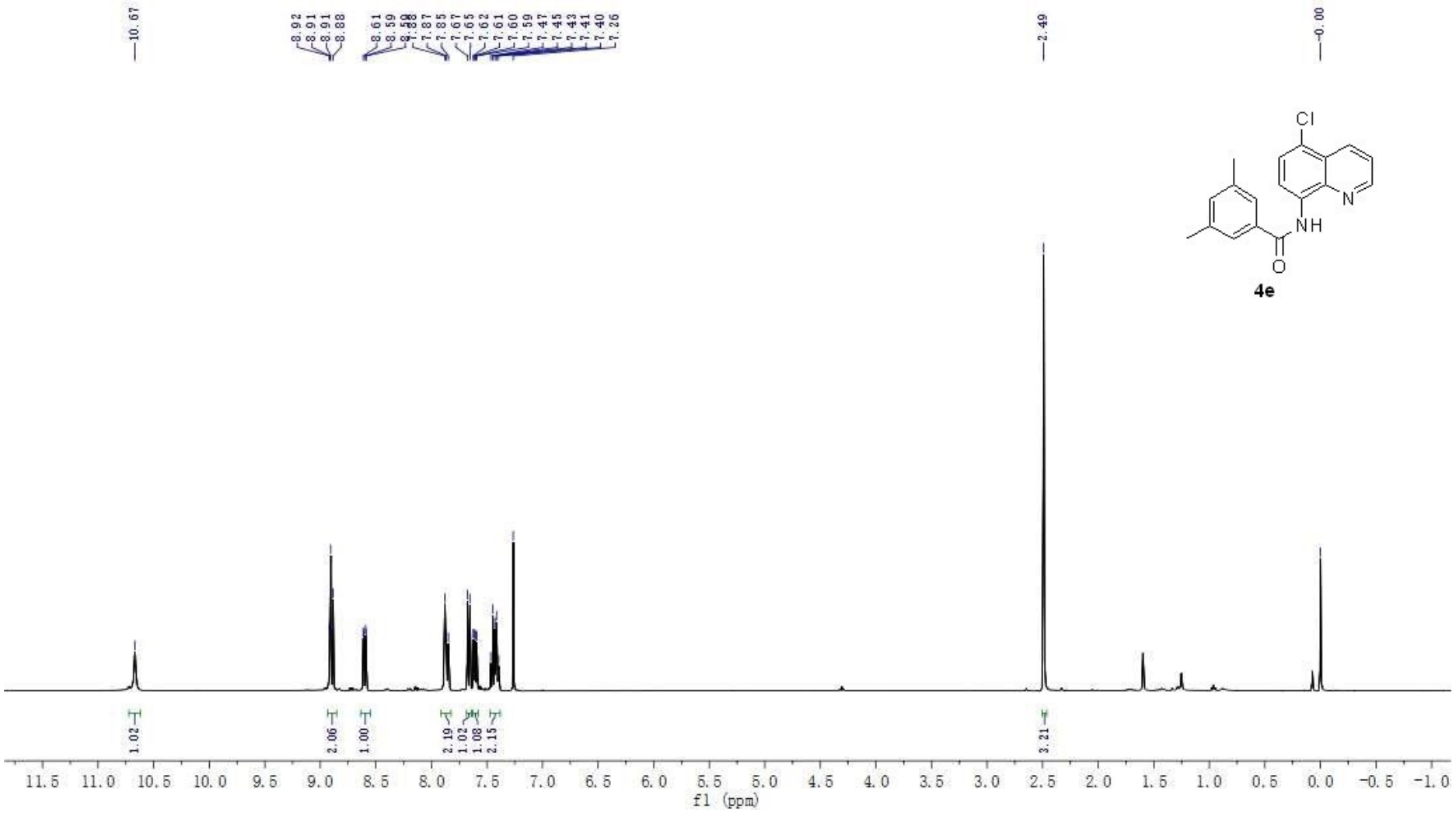
0
-10
f1 (ppm)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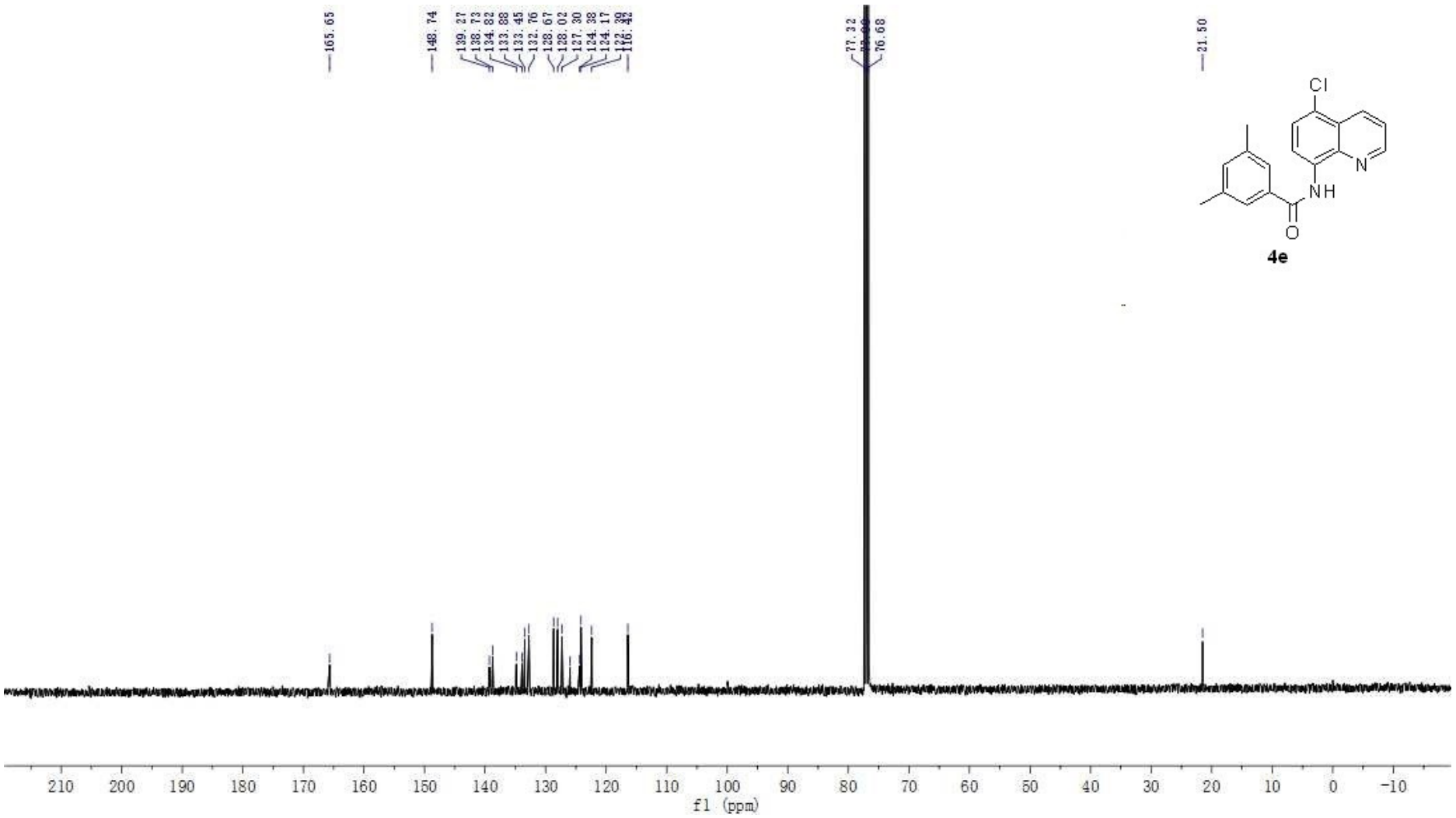
7.62
7.61
7.60
7.59
7.47
7.45
7.43
7.41
7.40
7.26
2.49
0.00
Cl
N
NH
O
4e
1.02
2.06
1.00
2.19
1.02
1.08
2.15
3.21
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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132.76
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128.02
127.30
124.38
124.17
122.39
116.42
77.32
76.68
21.50
Cl
N
NH
O
4e
210
200
190
180
170
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120
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100
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80
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30
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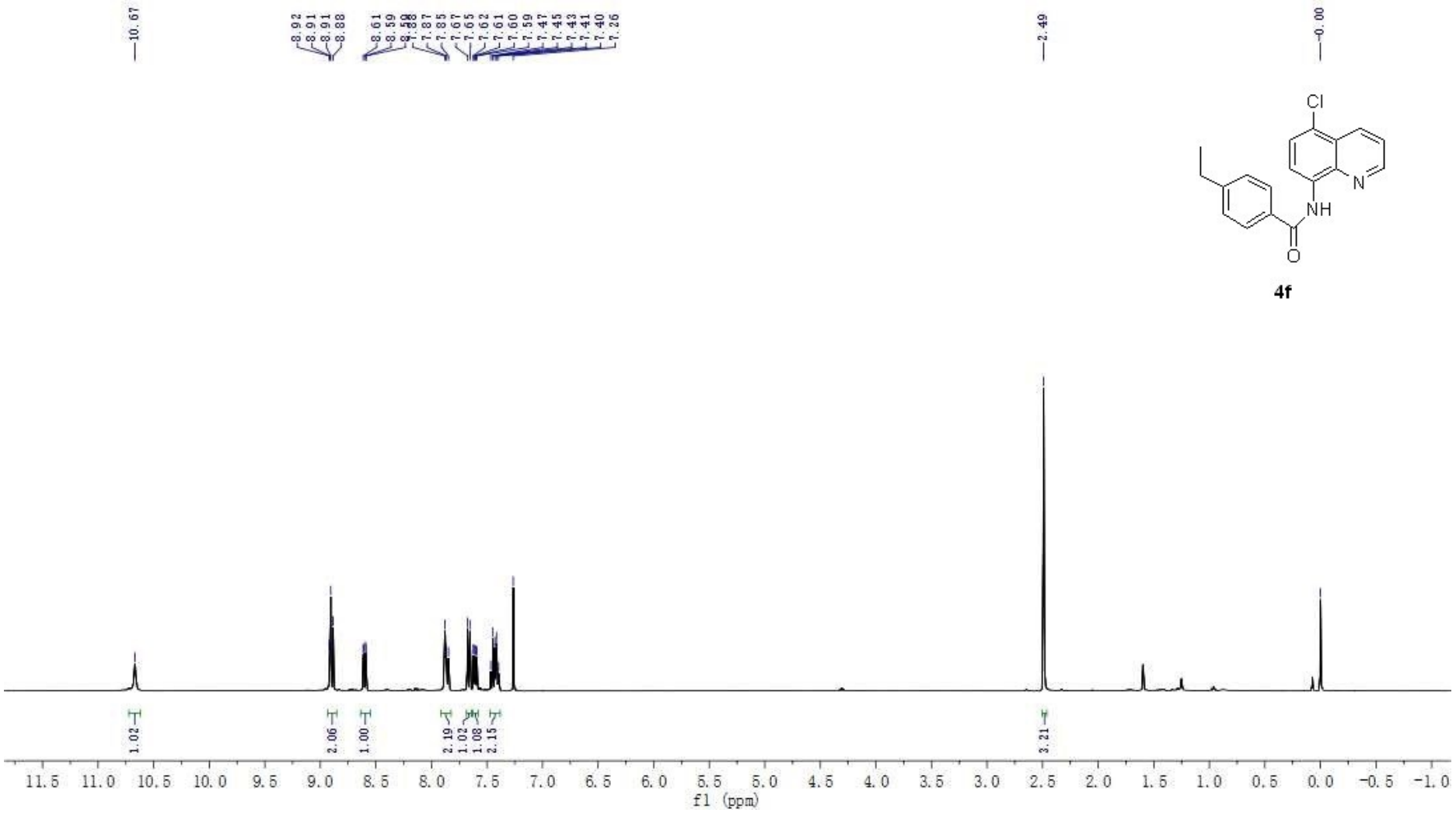
-10
f1 (ppm)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7.59
7.47
7.45
7.43
7.41
7.40
7.26
2.49
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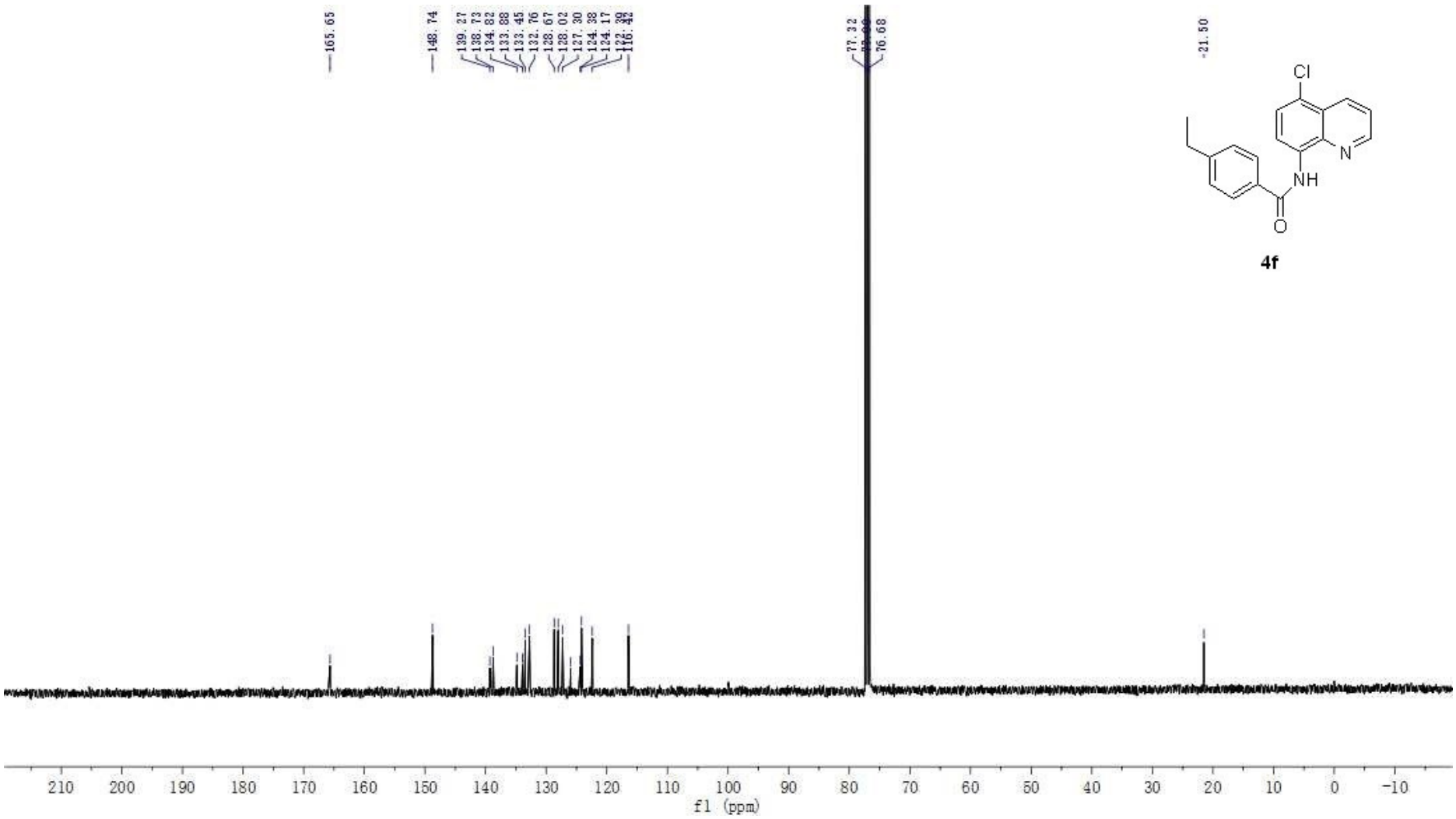
NH
O
4f
1.02
2.06
1.00
2.19
1.02
1.08
2.15
3.21
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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128.02
127.30
124.38
124.17
122.39
116.42
77.32
76.68
21.50
Cl
N
NH
O
4f
210
200
190
180
170
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140
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120
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100
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80
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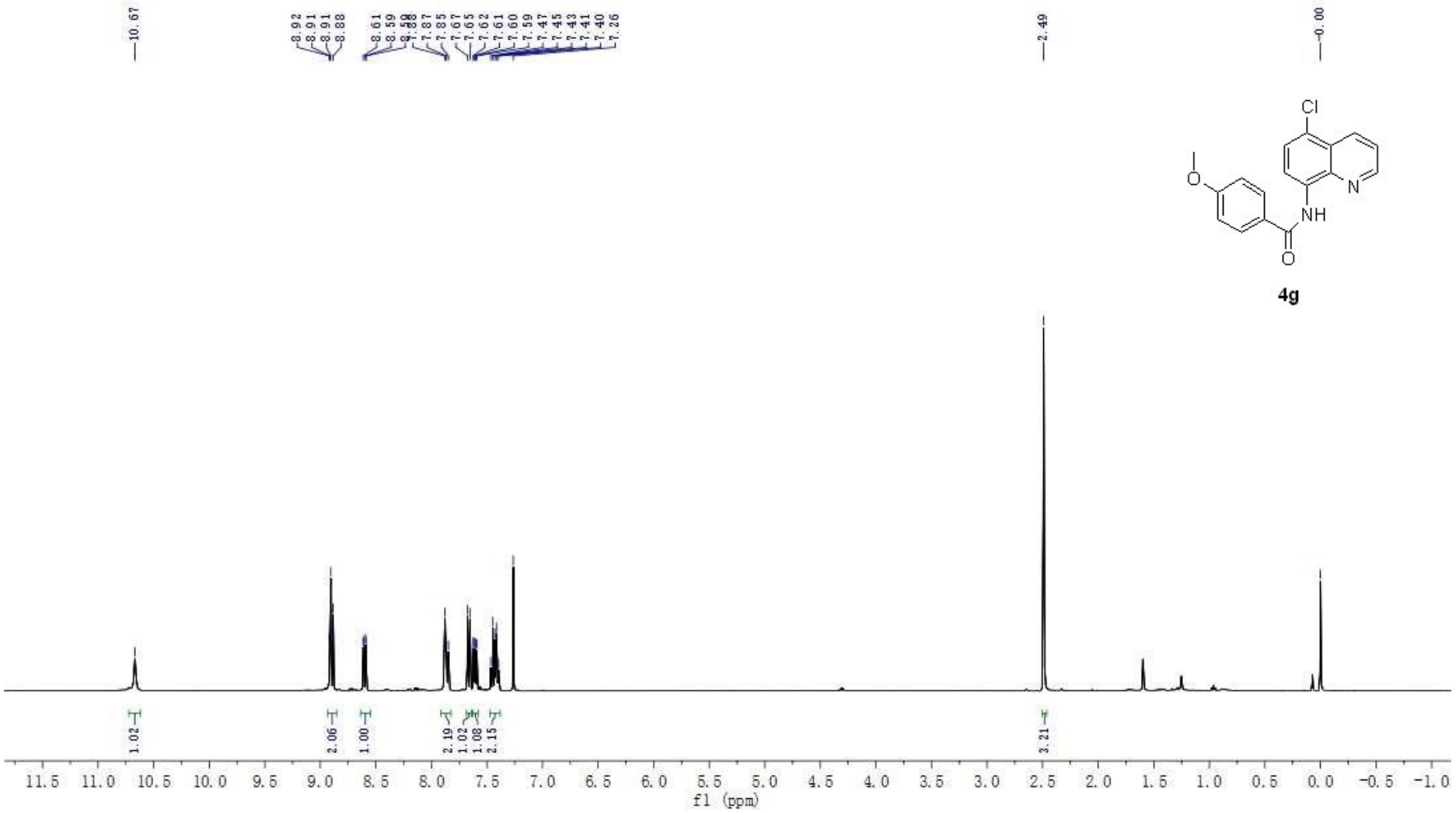
60
50
40
30
20
10
0
-10
f1 (ppm)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7.61
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7.59
7.47
7.45
7.43
7.41
7.40
7.26
2.49
0.00
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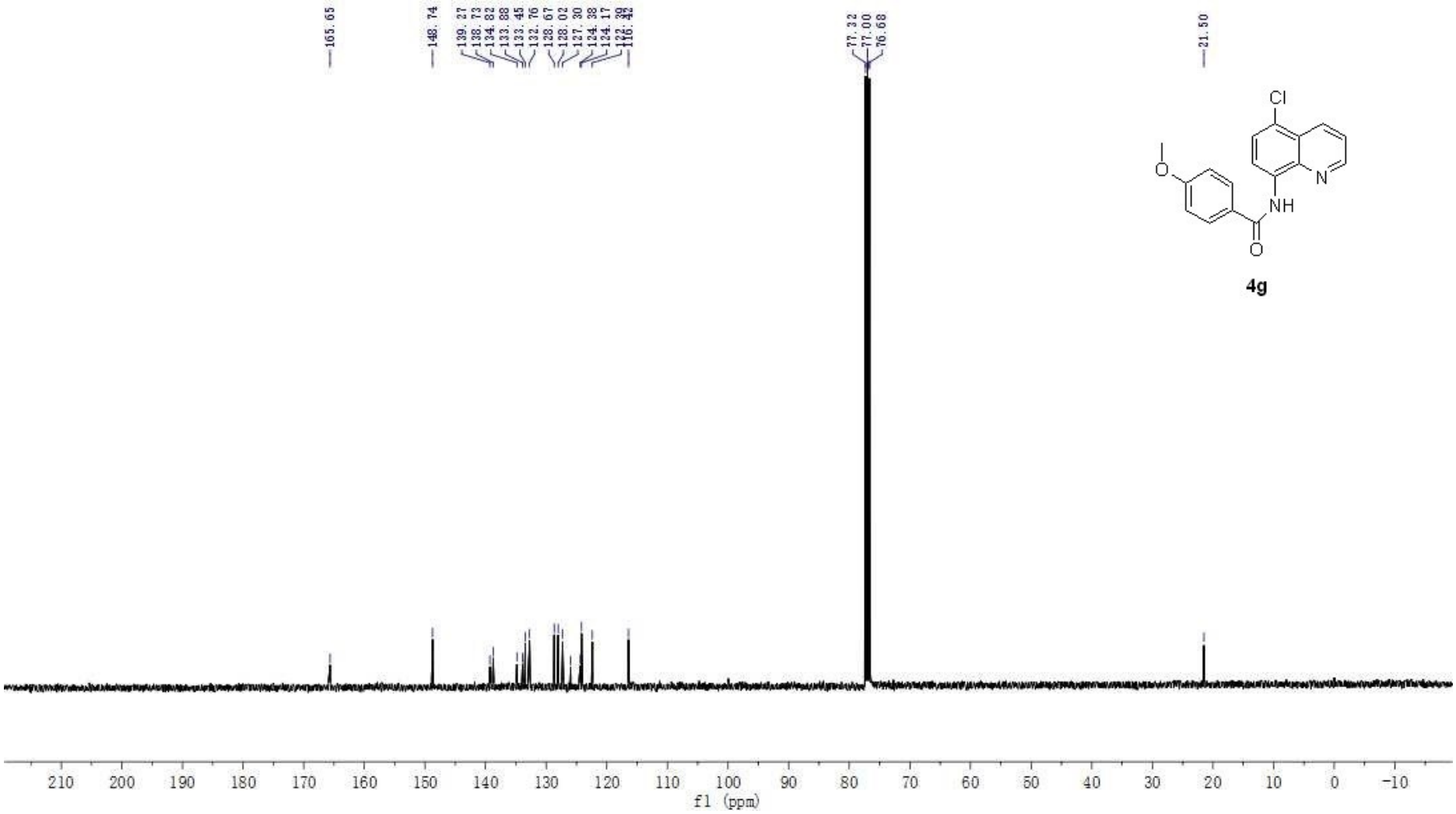
N
NH
O
4g
1.02
2.06
1.00
2.19
1.02
1.08
2.15
3.21
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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127.30
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124.17
122.39
116.42
77.32
77.00
76.68
21.50
Cl
O
N
NH
O
4g
210
200
190
180
170
160
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140
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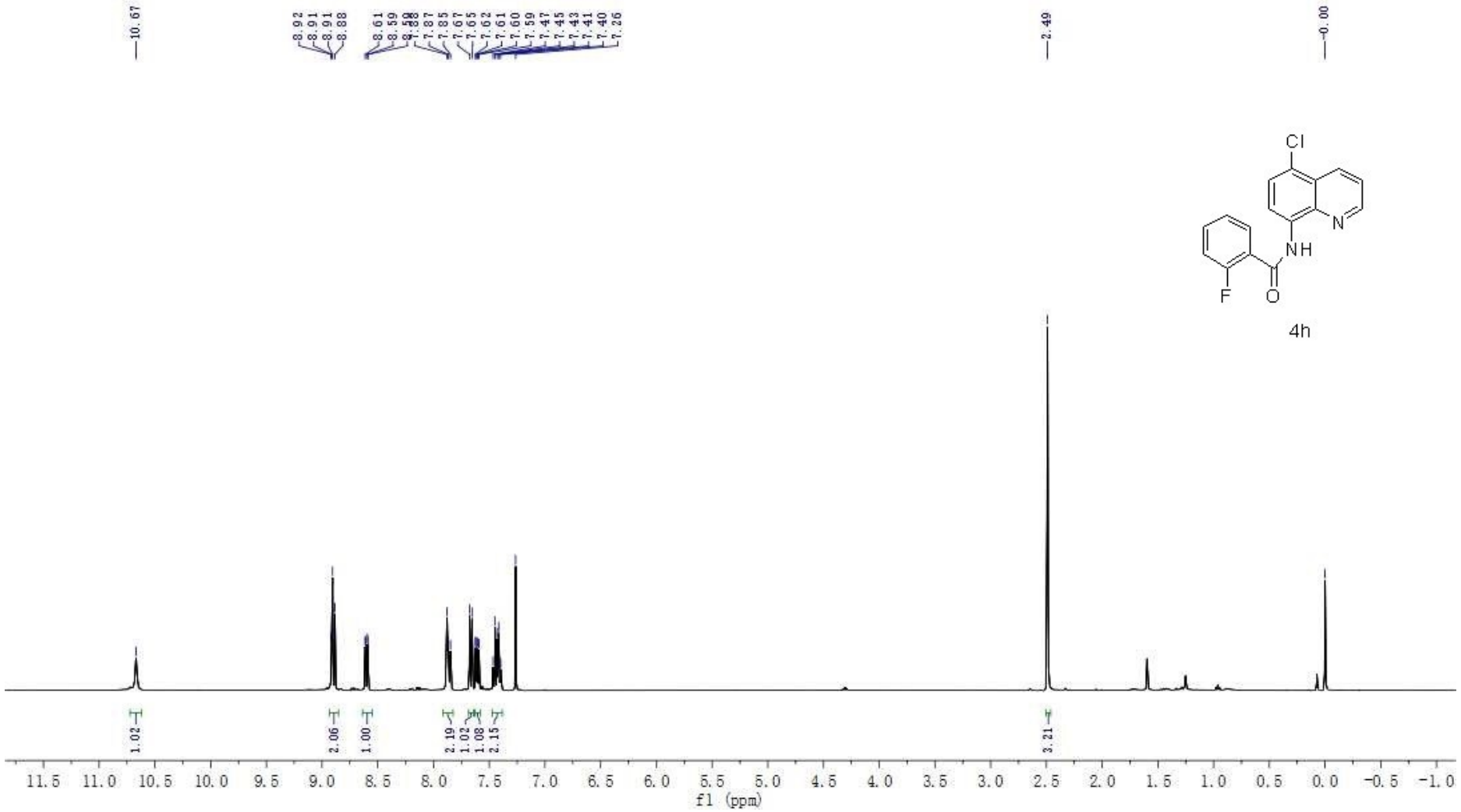
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.65
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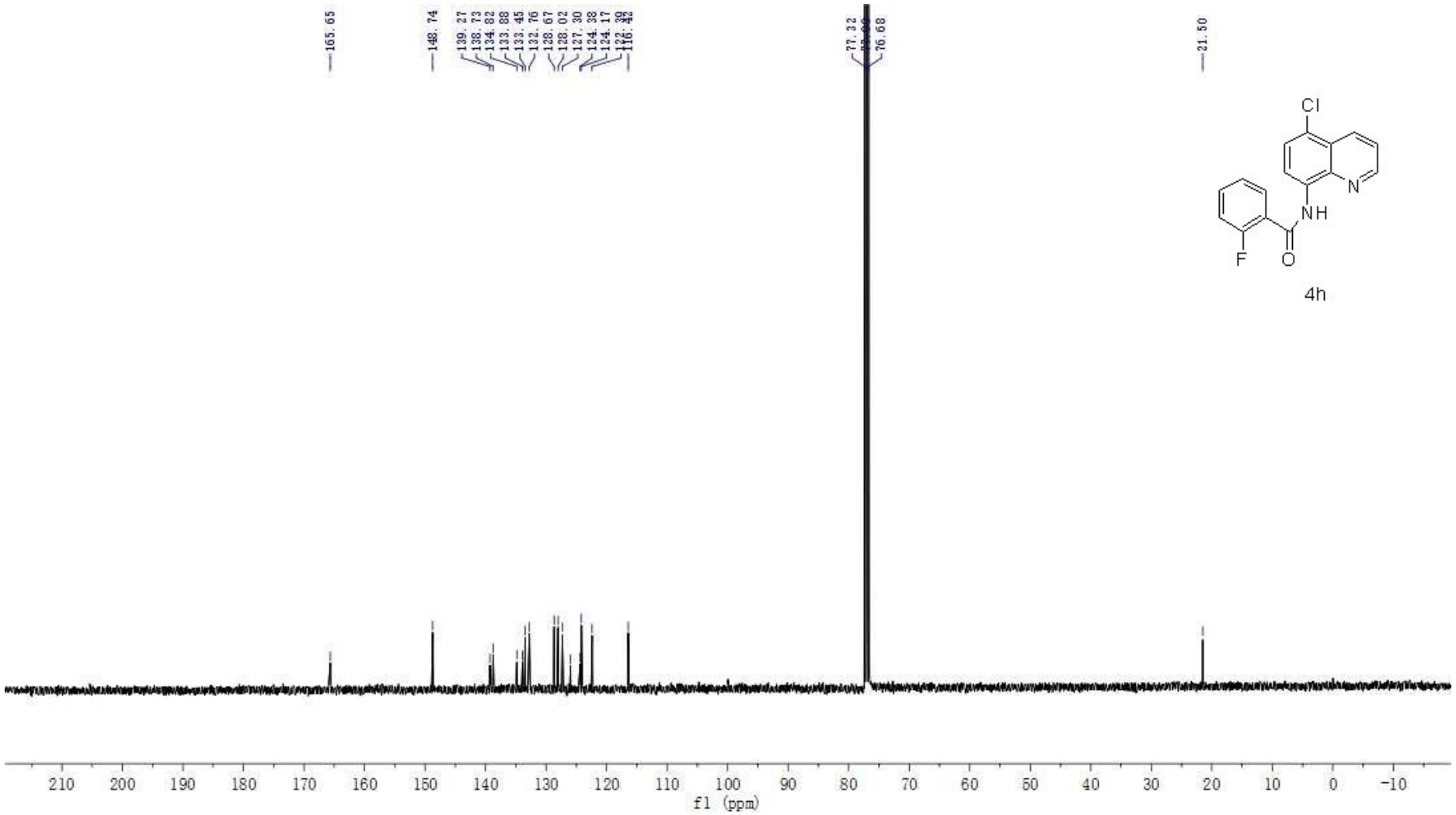
7.61
7.60
7.59
7.47
7.45
7.43
7.41
7.40
7.26
2.49
0.00
Cl
N
NH
F
O
4h
1.02
2.06
1.00
2.19
1.02
1.08
2.15
3.21
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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127.30
124.38
124.17
122.39
116.42
77.32
76.68
21.50
Cl
N
NH
F
O
4h
210
200
190
180
170
160
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140
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120
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100
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80
70
60
50
40
30
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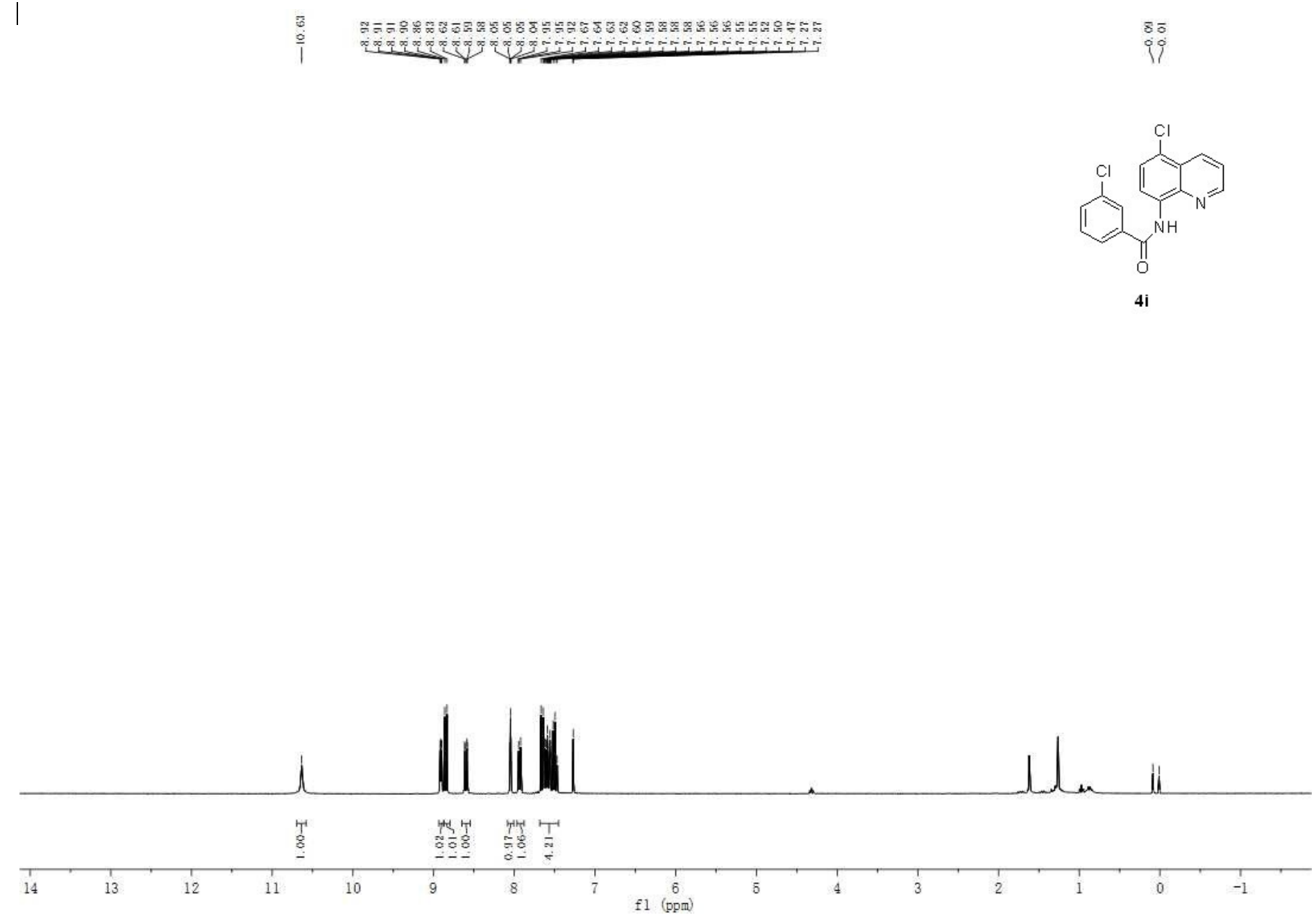
10
0
-10
f1 (ppm)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8.05
8.05
8.04
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7.95
7.92
7.67
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7.63
7.62
7.60
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7.58
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7.58
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7.56
7.55
7.55
7.52
7.50
7.47
7.27
7.27
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0.01
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Cl
N
NH
O
4i
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1.02
1.01
1.00
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1.09
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12
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8
7
6
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4
3
2
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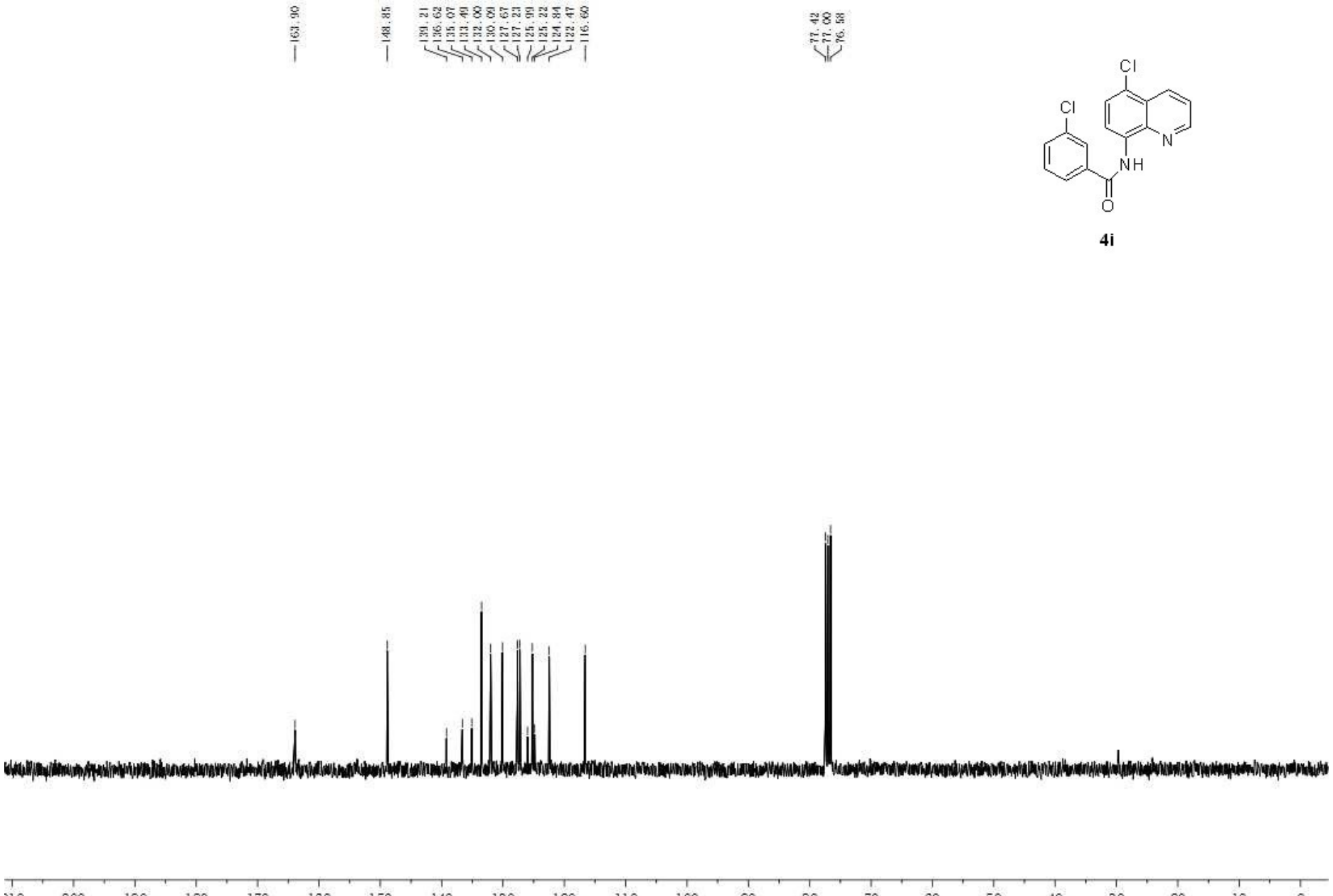
-1
f1 (ppm)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125.22
124.84
122.47
116.60
77.42
77.00
76.58
Cl
Cl
N
NH
O
4i
210
200
190
180
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130
120
110
100
90
80
70
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50
40
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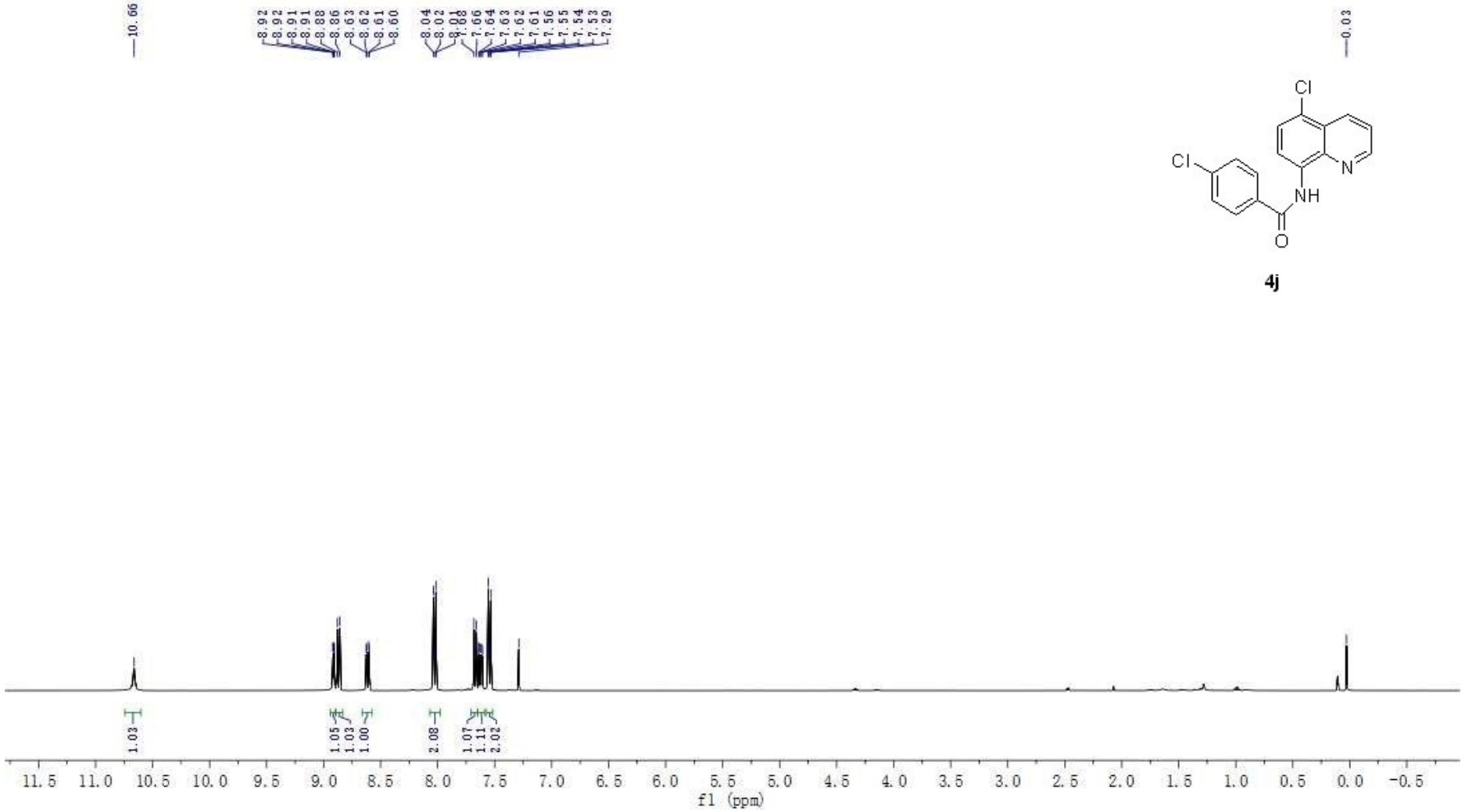
20
10
0
f1 (ppm)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8.63
8.62
8.61
8.60
8.04
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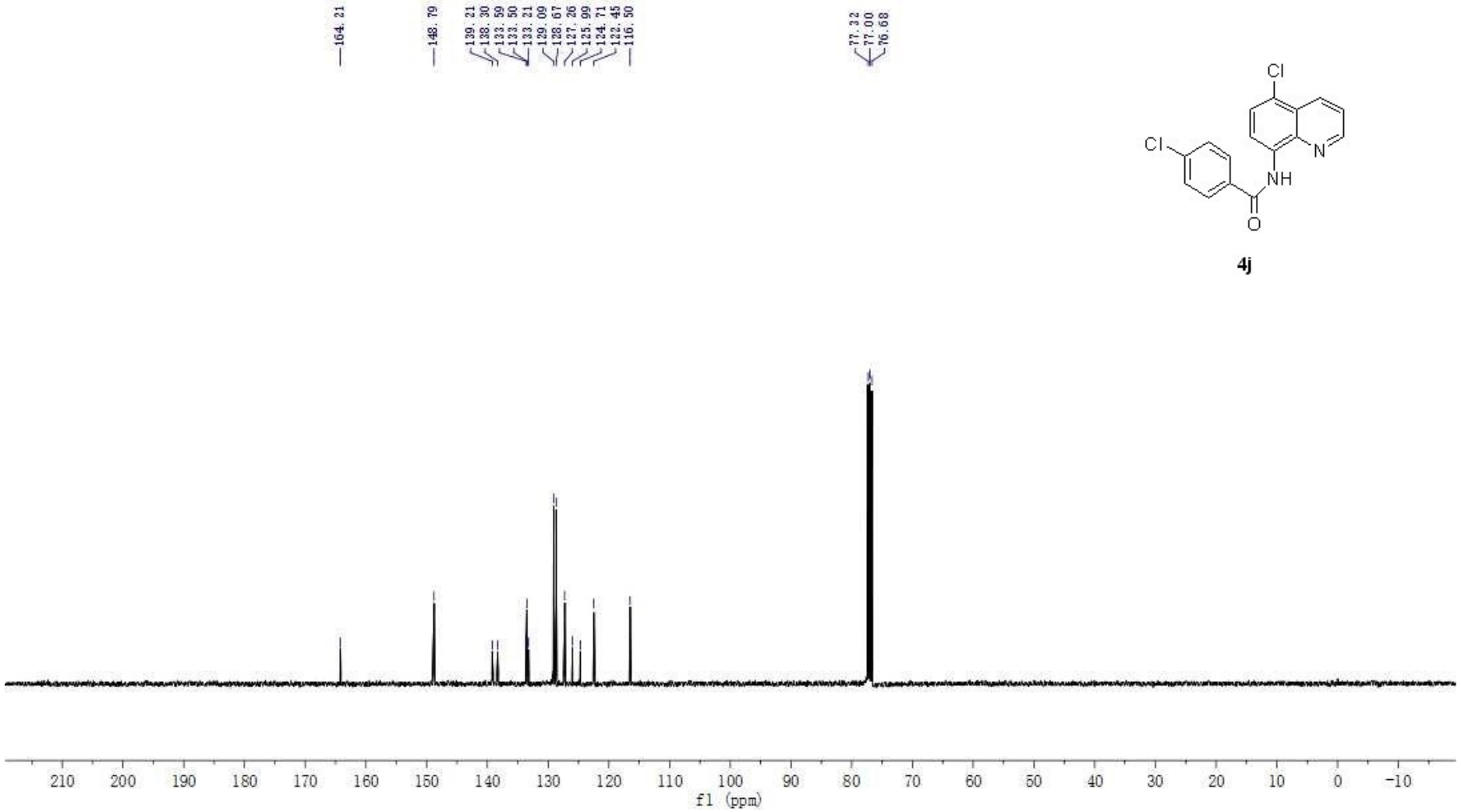
8.01
8.00
7.66
7.64
7.63
7.62
7.61
7.56
7.55
7.54
7.53
7.29
0.03
Cl
Cl
N
NH
O
1.03
1.05
1.03
1.00
2.08
1.07
1.11
2.02
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

4j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133.50
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129.09
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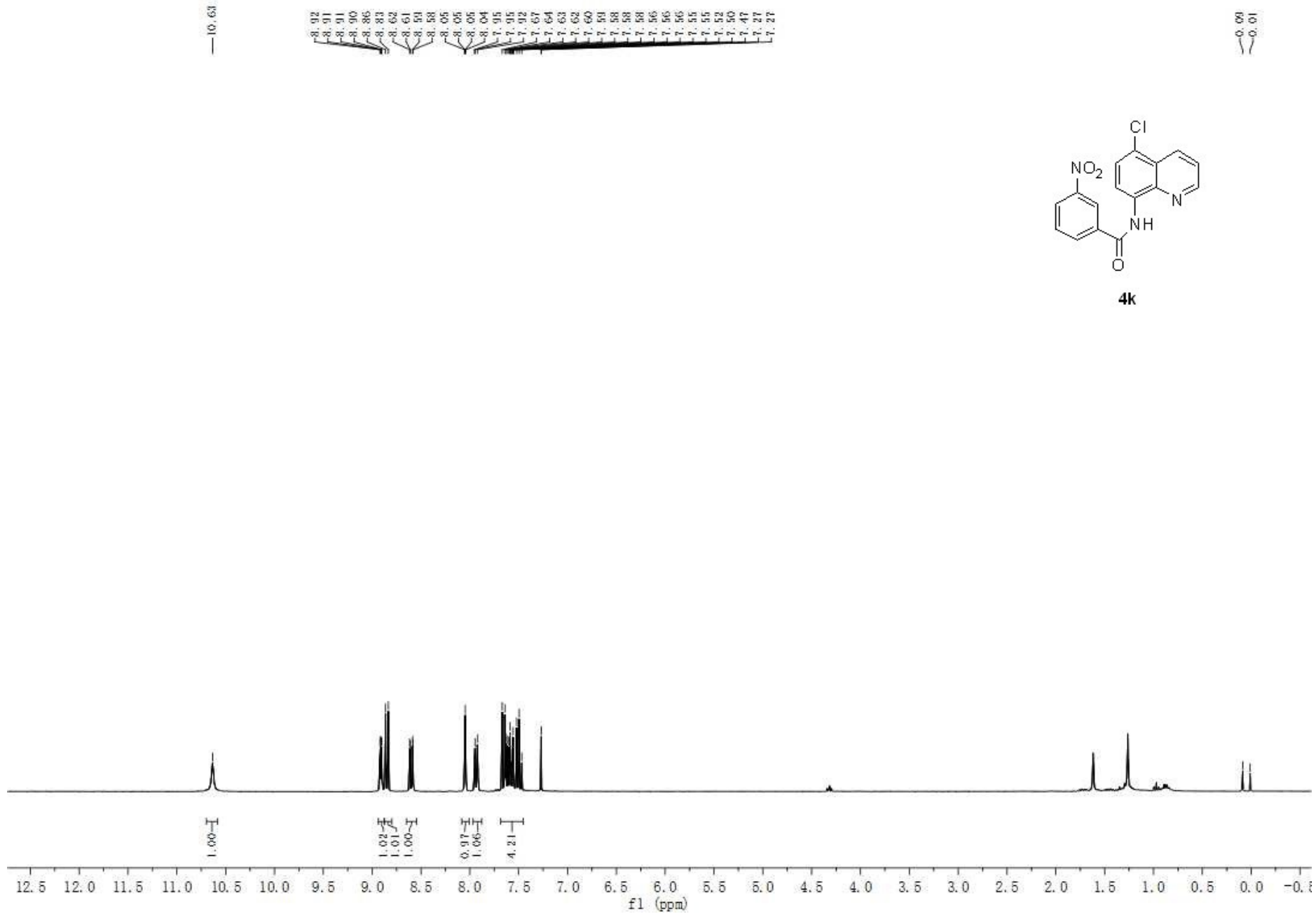
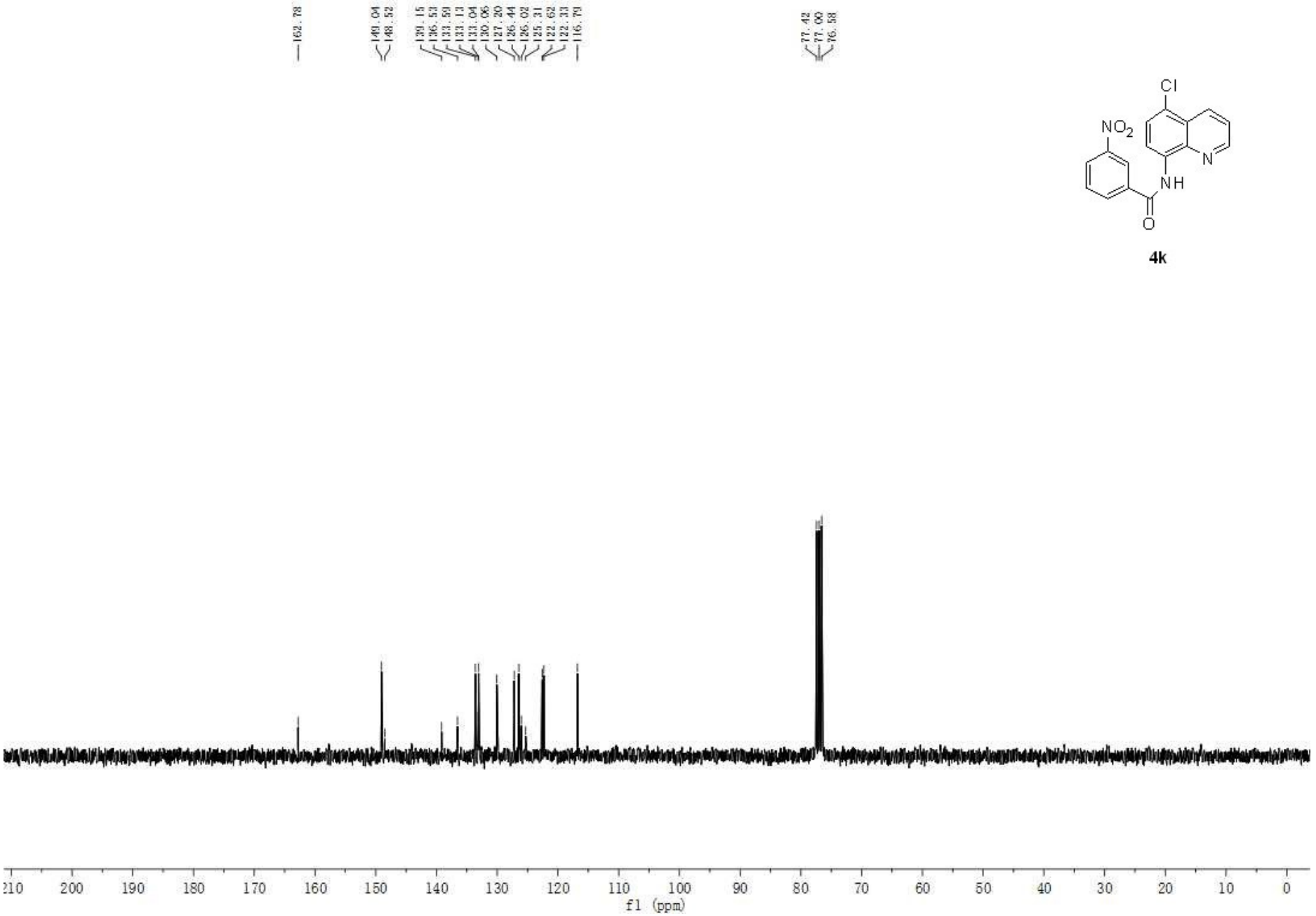
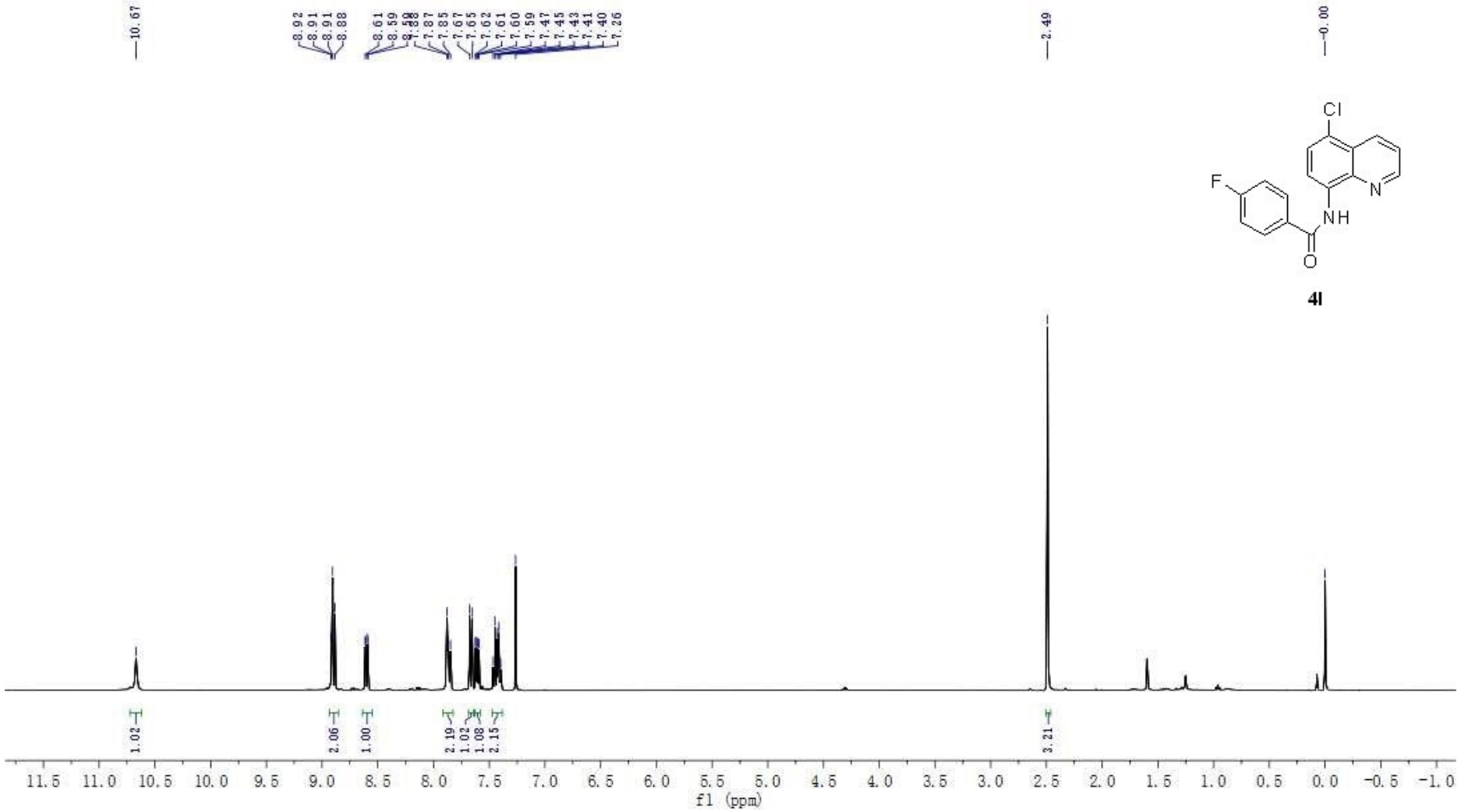
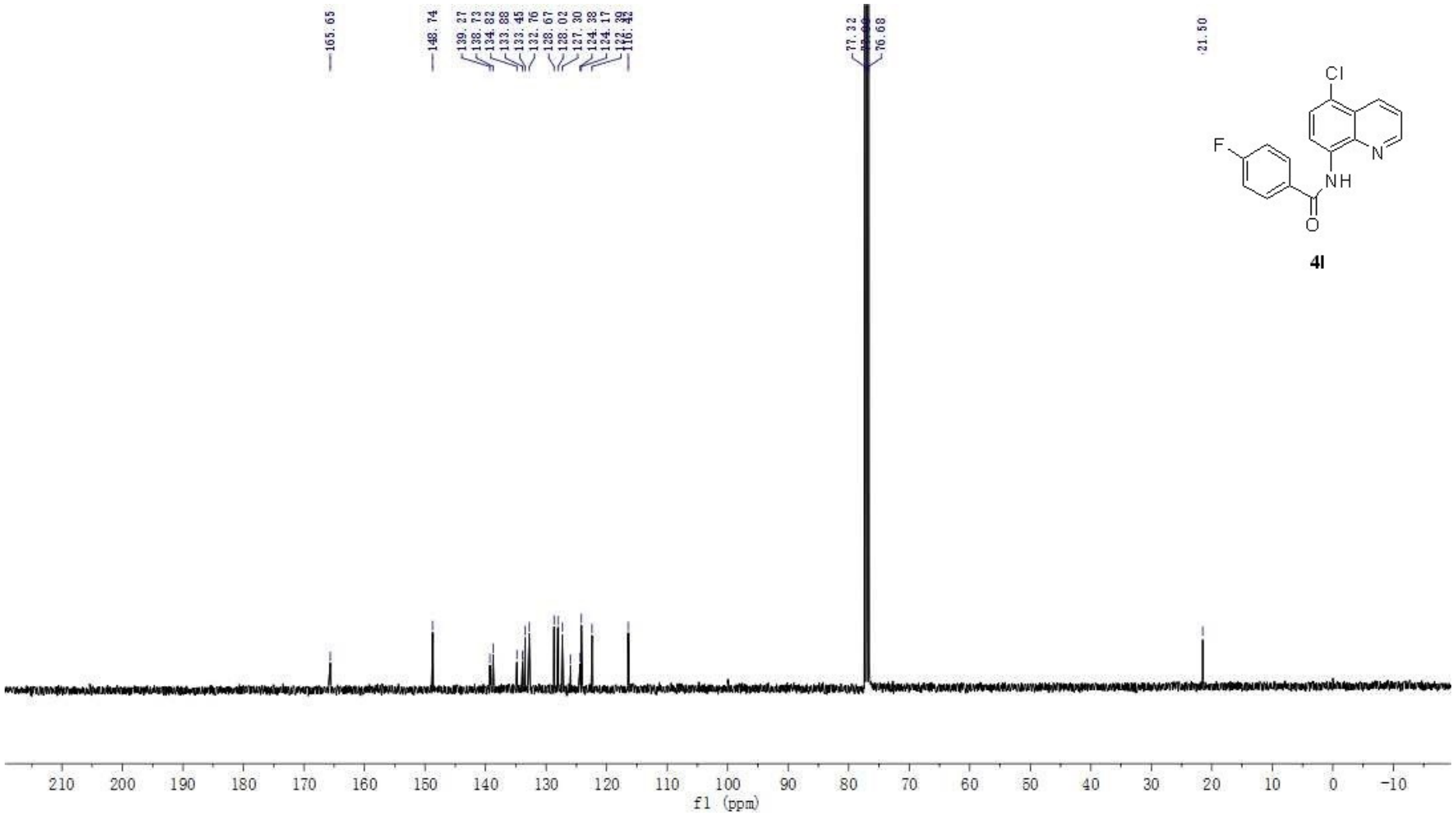
127.26
125.99
124.71
122.45
116.50
77.32
77.00
76.68
Cl
Cl
N
NH
O
4j
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

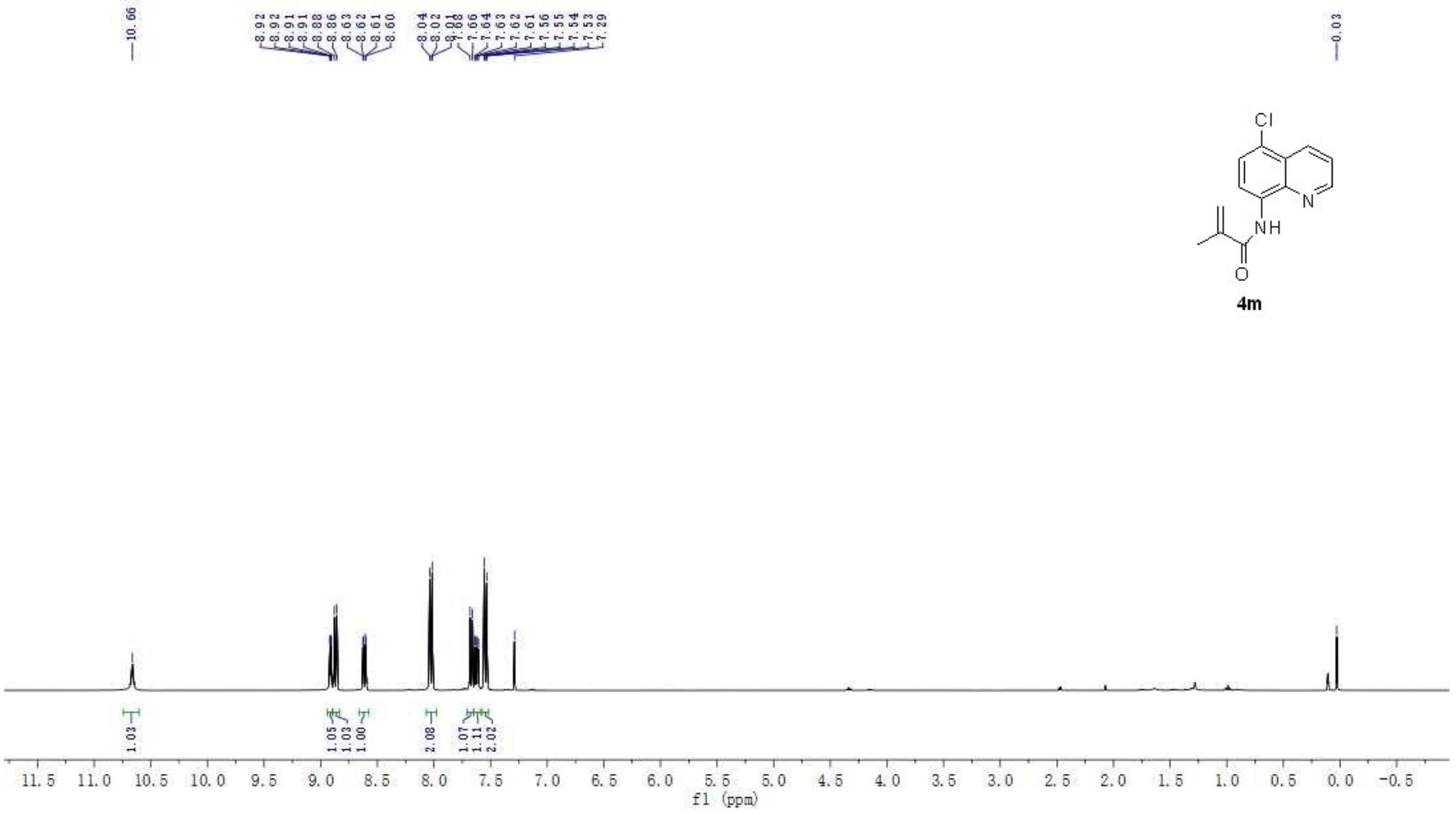

10.63
8.92
8.91
8.91
8.90
8.86
8.83
8.62
8.61
8.59
8.58
8.05
8.05
8.05
8.04
7.95
7.95
7.92
7.67
7.64
7.63
7.62
7.60
7.59
7.58
7.58
7.56
7.56
7.55
7.55
7.52
7.50
7.47
7.27
7.27
0.00
0.01
Cl
NO2
N
NH
O
4k
1.00
1.02
1.01
1.00
0.97
1.06
4.21
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

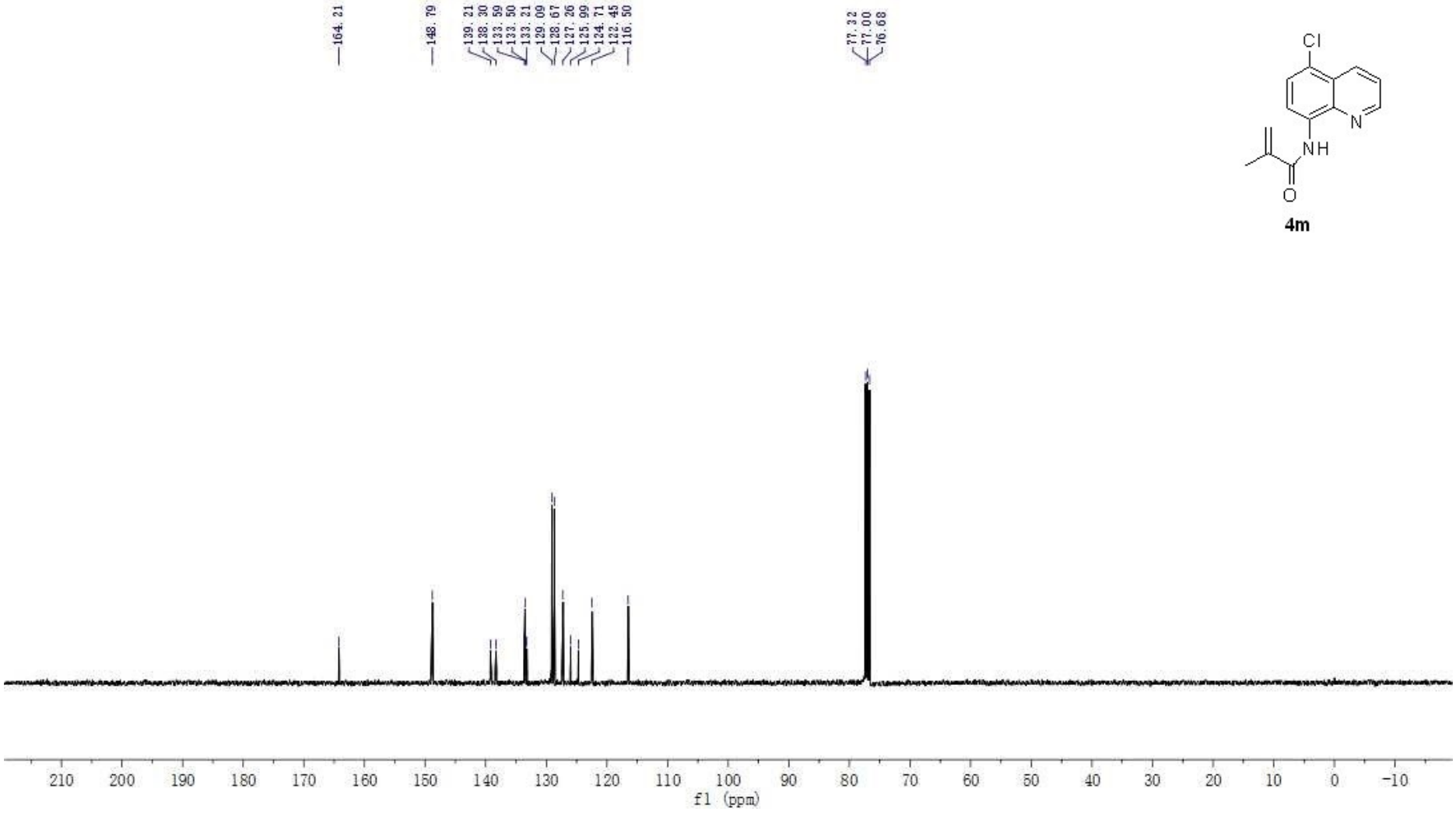

162.78
149.04
148.52
139.15
136.53
133.59
133.13
133.04
130.06
127.20
126.44
126.02
125.31
122.62
122.33
116.79
77.42
77.00
76.58
Cl
NO2
N
NH
O
4k
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

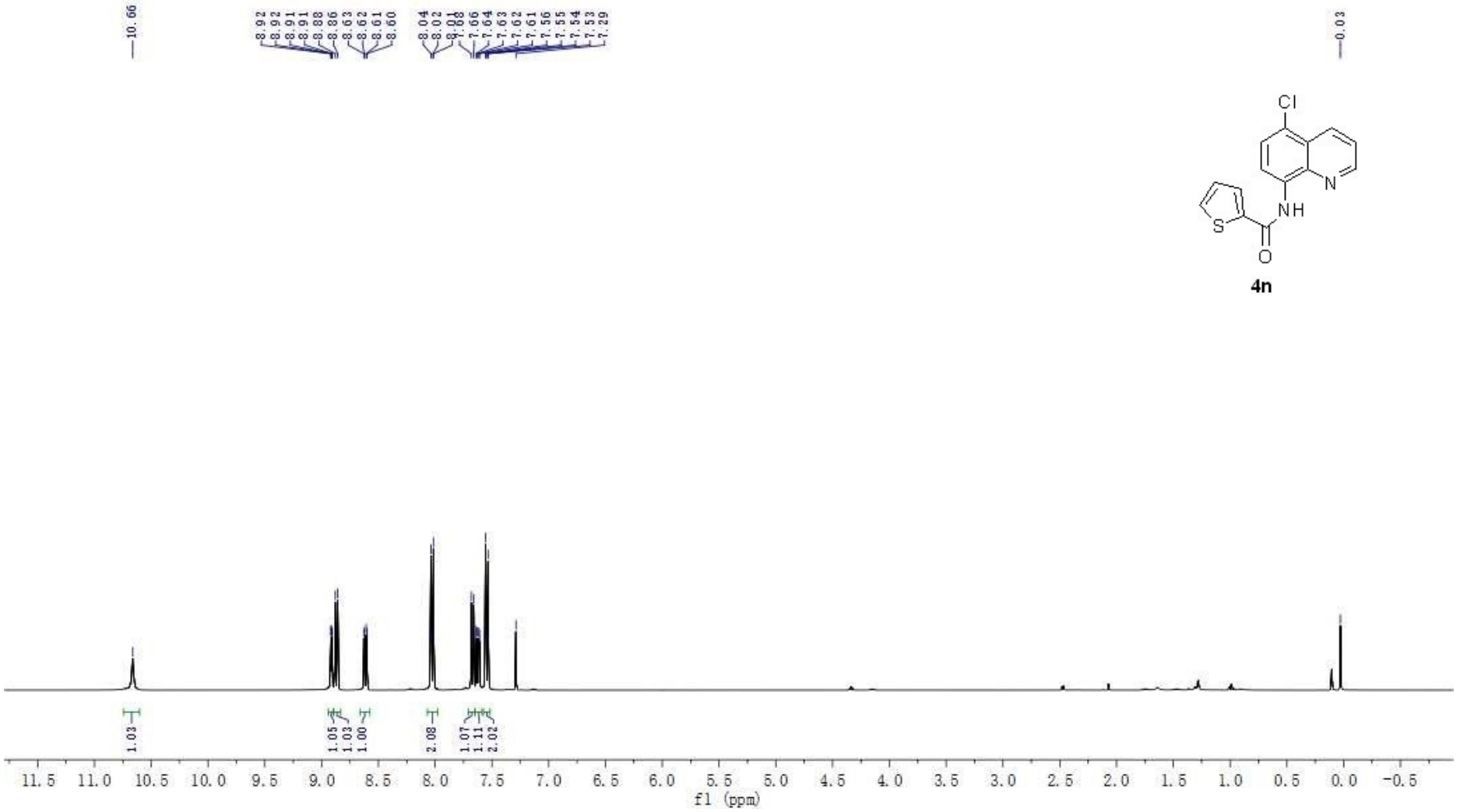

10.67
8.92
8.91
8.91
8.88
8.61
8.59
7.87
7.85
7.67
7.65
7.62
7.61
7.60
7.59
7.47
7.45
7.43
7.41
7.40
7.26
2.49
0.00
Cl
F
N
NH
O
1.02
2.06
1.00
2.19
1.02
1.08
2.15
3.21
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

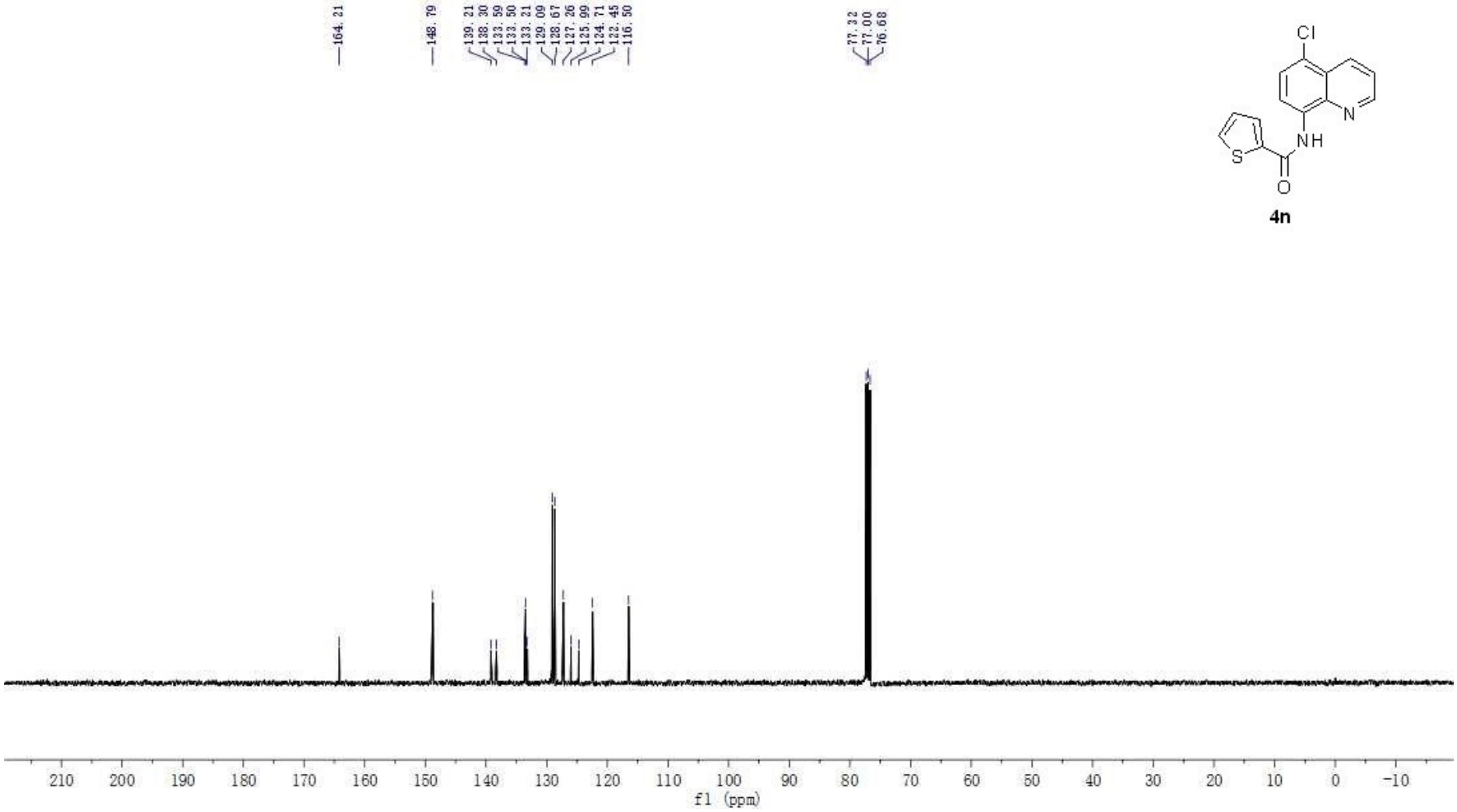
4l


165.65
148.74
139.27
138.73
134.82
133.88
133.45
132.76
128.67
128.02
127.30
124.38
124.17
77.32
76.68
21.50
Cl
F
N
NH
O
4l
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)


10.66
8.92
8.92
8.91
8.91
8.88
8.86
8.63
8.62
8.61
8.60
8.04
8.02
8.01
8.00
7.66
7.64
7.63
7.62
7.61
7.56
7.55
7.54
7.53
7.29
0.03
Cl
N
NH
O
4m
1.03
1.05
1.03
1.00
2.08
1.07
1.11
2.02
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 -0.5
f1 (ppm)


164.21
148.79
139.21
138.30
133.59
133.50
133.21
129.09
128.67
127.26
125.99
124.71
122.45
116.50
77.32
77.00
76.68
Cl
N
NH
O
4m
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)


10.66
8.92
8.92
8.91
8.91
8.88
8.86
8.63
8.62
8.61
8.60
8.04
8.02
8.01
8.00
7.66
7.64
7.63
7.62
7.61
7.56
7.55
7.54
7.53
7.29
0.03
Cl
N
NH
S
O
4n
1.03
1.05
1.03
1.00
2.08
1.07
1.11
2.02
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 -0.5
f1 (ppm)


164.21
148.79
139.21
138.30
133.59
133.50
133.21
129.09
128.67
127.26
125.99
124.71
122.45
116.50
77.32
77.00
76.68
Cl
N
NH
S
O
4n
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)