Supporting Information

Iron-Catalyzed Aerobic Oxidative Functionalization of sp^3C-H Bonds: a Versatile Strategy for the Construction of *N*-Heterocycles

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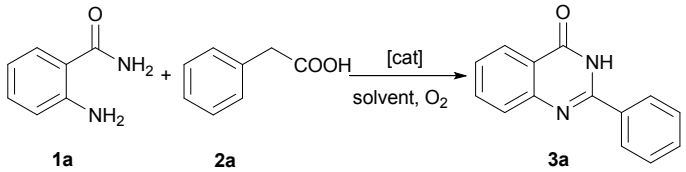
1. General remarks

All manipulations were carried out under air atmosphere unless otherwise specified. The reactions were monitored by GC and GC-MS. The ^{1}H NMR and ^{13}C NMR spectra were recorded on a Brucker ADVANCE III spectrometer at 400 MHz and 100 MHz, respectively. HI-MS was recorded on MAT 95 XP. Flash column chromatography was performed using silica gel 300-400 mesh, GC-MS results were recorded on GC-MS QP2010, and GC analysis was performed on GC 7820A. Amines **1** were purchased from Energy Chemical, Alfa Aesar, Aladdin or Maya Reagent, arylacetic acid **2** were purchased from Aladdin.

2. General experimental procedure for the synthesis of *N*-heterocycle derivatives

A 10 ml Schlenk-type tube equipped with a magnetic stir bar was charged with substrate amine **1** (0.2 mmol) carboxylic acid derivatives **2** (0.22 mmol) and $FeCl_3$ (10 mol%). The reaction tube was evacuated and back-filled with O_2, under oxygen atmospheres, DMF (1 mL) was added at room temperature, then the reaction mixture was stirred at 100 ºC for 12-18 h. The reaction was monitored by GC or GC-MS. After completion of the reaction, the resulting solution was cooled to room temperature, and neutralized with saturated $NaHCO_3$ solution. The product was extracted with EtOAc or $CHCl_3$, dried over anhydrous Na_2SO_4 and concentrated in vacuo. The crude product was purified by flash column chromatography on silica gel to give analytically pure product.

3. Optimization of the reaction conditions[a]

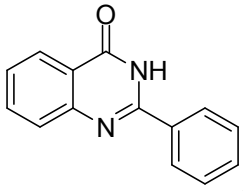


1a **2a** **3a**

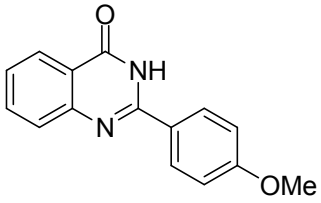
Entry	Cat	Solvent	Yield[b] (%)
1	Fe_2O_3	DMF	60
2	$FeCl_2.H_2O$	DMF	88
3	$FeSO_4.7H_2O$	DMF	30
4	ferrocene	DMF	50
5	Ferrous acetylacetonate	DMF	53
6	$FeBr_3$	DMF	86
7	$FeCl_3$	DMF	92
8	-	DMF	-
9	$PdCl_2$	DMF	-
10	$NiCl_2.6H_2O$	DMF	-
11	$CuCl_2$	DMF	-
12	$FeCl_3$	DMSO	-
13	$FeCl_3$	dioxane	-
14	$FeCl_3$	CH_3CN	-
15	$FeCl_3$	toluene	-
16	$FeCl_3$	EtOAc	-
17	$FeCl_3$	NMP	-
18	$FeCl_3$	*p*-xylene	-
19[c]	$FeCl_3$	DMF	-
21[d]	$FeCl_3$	DMF	-
21[e]	$FeCl_3$	DMF	-
22[f]	$FeCl_3$	DMF	93

[a]Reaction conditions: **1a** (0.2 mmol), **2a** (0.22 mmol), catalyst (0.02 mmol), O_2 (1 atm) in a Schlenk tube (10 mL), 100 °C, 12 h. [b] GC yields based on **1a** using dodecane as an internal standard. [c] 0.5 mmol *mCPBA* (*m*-chloroperbenzoic acid) or $K_2S_2O_8$ was employed as oxidant under N_2 (1 atm) atmosphere. [d]0.5 mmol TBHP (*tert*-butylhydroperoxide) or DTBP was used as oxidant under N_2 (1 atm) atmosphere. [e]80 °C. [f]120 °C.

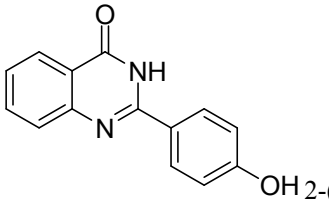
4. ^{1}H NMR and ^{13}C NMR data of products



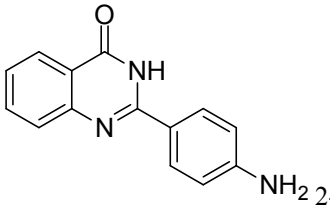
2-phenylquinazolin-4(3*H*)-one **(3a)**[1]**:** Eluent: petroleum ether/ethyl acetate (10:1), white solid, m.p: 236-238 ºC. ^{1}H NMR (400 MHz, DMSO-*d*): δ 12.56 (s, br, 1H), 8.17 (t, *J* = 8.6 Hz, 3H), 7.82 (t, *J* = 7.2 Hz, 1H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.51 (q, *J* = 9.0 Hz, 4H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 162.8, 152.8, 149.1, 135.0, 133.2, 131.8, 129.1, 128.3, 128.2, 127.0, 126.3, 121.4. GC-MS: m/z = 222.



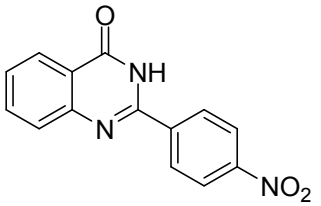
2-(4-methoxyphenyl)quinazolin-4(3*H*)-one **(3b)**[1]: Eluent: petroleum ether/ethyl acetate (10:1), white solid, mp: 248-251 °C. ^{1}H NMR (400 MHz, DMSO-*d*): δ 12.41 (s, br, 1H), 8.18 (d, *J* = 8.4 Hz, 2H), 8.12 (d, *J* = 7.6 Hz, 1H), 7.80 (t, *J* = 7.4 Hz, 1H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.47 (t, *J* = 7.2 Hz, 1H), 7.07 (d, *J* = 8.4 Hz, 1H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 162.8, 162.3, 152.3, 149.4, 135.0, 129.9, 127.8, 126.6, 126.3, 125.3, 121.2, 114.5, 55.9. GC-MS: m/z = 252.



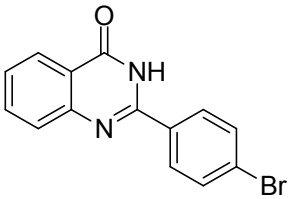
2-(4-hydroxyphenyl)quinazolin-4(3*H*)-one **(3c)**[2]**:** Eluent: petroleum ether/ethyl acetate (3:1), yellow solid, mp: >300ºC. ^{1}H NMR (400 MHz, DMSO-d_6): δ 12.29 (s, br, 1H), 10.20 (s, br, 1H), 8.10 (s, 3H), 7.77 (s, 1H), 7.67 (s, 1H), 7.45 (s, 1H), 6.91 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 162.8, 161.0, 152.6, 149.5, 134.9, 130.1, 127.6, 126.34, 126.28, 123.7, 121.0, 115.8. HRMS (EI): calcd for $C_{14}H_{10}N_2O_2$: 238.0742; found: 238.0740.



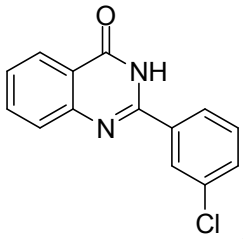
2-(4-aminophenyl)quinazolin-4(3*H*)-one **(3d)**[4]**:** Eluent: petroleum ether/ethyl acetate (3:1), yellow solid, m.p: >300 ºC. ^{1}H NMR (400 MHz, DMSO-d_6): δ 12.07 (s, br, 1H), 8.08 (d, *J* = 7.6Hz, 1H), 7.95 (d, *J* = 8.0 Hz, 2H), 7.75 (t, *J* = 7.4 Hz, 1H), 7.61 (d, *J* = 8.4 Hz, 1H), 7.40 (t, *J* = 7.4 Hz, 1H), 6.63 (d, *J* = 8.0 Hz, 2H), 5.84 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 162.9, 152.9, 152.6, 149.9, 134.9, 129.6, 127.4, 126.3, 125.8, 120.8, 119.2, 113.5. HRMS (EI): calcd for $C_{14}H_{11}N_3O$: 237.0902; found: 237.0901.



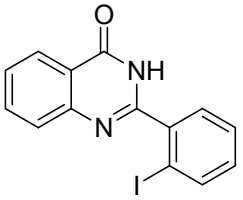
2-(4-nitrophenyl)quinazolin-4(3*H*)-one (**3e**)[2]: Eluent: petroleum ether/ethyl acetate (2:1), white solid, m.p.>300ºC. ^{1}H NMR (400 MHz, DMSO-d_6): δ 12.83 (s, br, 1H), 8.39 (q, *J* = 6.6 Hz, 4H), 8.18 (d, *J* = 8.0 Hz, 1H), 7.88 (t, *J* = 7.2 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.58 (t, *J* = 7.2 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ. 162.6, 151.9, 149.0, 135.1, 132.4, 132.1, 130.3, 127.9, 127.3, 126.4, 125.7, 121.5. GC-MS: m/z =267.



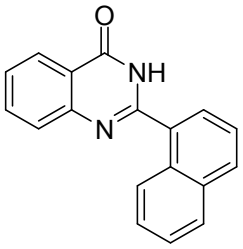
2-(4-bromophenyl)quinazolin-4(3*H*)-one **(3f)**[2]**:** Eluent: petroleum ether/ethyl acetate (10:1), white solid, m.p: 294-296 ºC. ^{1}H NMR (400 MHz, DMSO-d_6): δ 12.61 (s, br, 1H), 8.13 (t, *J* = 9.4 Hz, 3H), 7.82 (d, *J* = 6.8 Hz, 1H), 7.75 (d, *J* = 7.2 Hz, 3H), 7.53 (d, *J* = 6.4 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6,): δ 162.6, 151.9, 149.0, 135.2, 132.4, 132.1, 130.3, 128.0, 127.3, 126.4, 125.7, 121.5. GC-MS: m/z = 299.



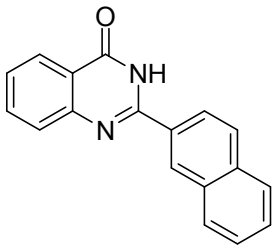
2-(3-chlorophenyl)quinazolin-4(3*H*)-one **(3g)**[2]**:** Eluent: petroleum ether/ethyl acetate (5:1), white solid, m.p: 296-197 ºC. ^{1}H NMR (400 MHz, DMSO-d_6): δ 12.63 (s, br, 1H), 8.24 (s, 1H), 8.15 (d, *J* = 6.4 Hz, 2H), 7.85 (t, *J* = 7.6 Hz, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.65 (d, *J* = 7.6 Hz, 1H), 7.53-7.60 (m, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 163.6, 152.9, 150.0, 136.2, 133.4, 133.1, 131.3, 129.0, 128.3, 127.4, 126.7, 122.5. GC-MS: m/z = 256.



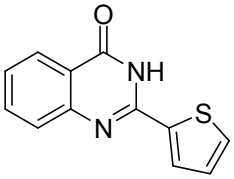
2-(2-iodophenyl)quinazolin-4(3*H*)-one (**3h**)[2] Eluent: petroleum ether/ethyl acetate (5:1), yellow solid, m.p: 216-217 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.62 (s, br, 1H), 8.24 (s, 1H), 8.17 (s 2H), 7.85 (t, *J* = 7.6 Hz, 1H), 7.84 (d, *J* = 7.2 Hz, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.52-7.60 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.6, 151.5, 135.22, 135.18, 133.9, 131.6, 131.0, 127.9, 127.5, 126.9, 126.3, 121.5. GC-MS: m/z = 347.



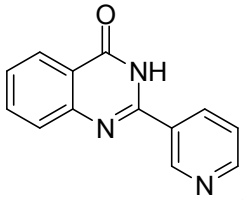
2-(naphthalen-1-yl)quinazolin-4(3*H*)-one **(3i)**[3]**:** Eluent: petroleum ether/ethyl acetate (4:1), white solid, m.p: 286-287 ºC. ^{1}H NMR (400 MHz, DMSO-d_6): δ 12.68 (s, br, 1H), 8.22 (d, *J* = 8.0 Hz, 1H), 8.17 (d, *J* = 7.6 Hz, 1H), 8.12 (d, *J* = 8.0 Hz, 1H), 8.04 (d, *J* = 7.2 Hz, 1H), 7.87 (t, *J* = 7.4 Hz, 1H), 7.79 (d, *J* = 7.2 Hz, 1H), 7.73 (d, *J* = 8.4 Hz, 1H), 7.64 (t, *J* = 8.2 Hz, 1H), 7.56-7.60 (m, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 162.4, 154.1, 149.2, 135.0, 133.6, 132.2, 130.9, 130.7, 128.8, 128.2, 127.9, 127.6, 127.3, 126.9, 126.3, 125.7, 125.6, 121.7. GC-MS: m/z = 272.



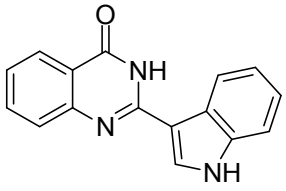
2-(naphthalen-2-yl)quinazolin-4(3*H*)-one **(3j)**[3]: Eluent: petroleum ether/ethyl acetate (10:1), white solid, m.p: 213-215 ºC:. ^{1}H NMR (400 MHz, DMSO-d_6): δ 12.69 (s, br, 1H), 8.22 (d, J = 8.0 Hz, 1H), 8.16 (d, J = 7.2 Hz, 1H), 8.11 (d, J = 8.4 Hz, 1H), 8.04 (d, J = 7.2 Hz, 1H), 7.87 (t, J = 7.2 Hz, 1H), 7.79 (d, J = 6.8 Hz, 1H), 7.73 (d, J = 8.0 Hz, 1H), 7.65 (t, J = 8.8 Hz, 1H), 7.56-7.60 (m, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 162.4, 154.1, 149.2, 135.0, 133.6, 132.2, 130.9, 130.7, 128.8, 128.2, 127.9, 127.6, 127.3, 126.9, 126.3, 125.7, 125.6, 121.7. GC-MS: m/z = 272.



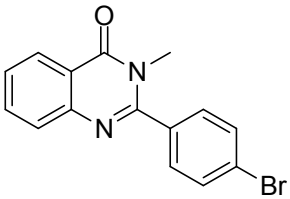
2-(thiophen-2-yl)quinazolin-4(3*H*)-one **(3k)**[1]**:** Eluent: petroleum ether/ethyl acetate (20:1), white solid, m.p: 277-278 ºC. ^{1}H NMR (400 MHz, DMSO-d_6): ^{1}H NMR (400 MHz, DMSO-d_6): δ 12.65 (s, br, 1H), 8.22 (d, *J* = 3.6 Hz, 1H), 8.11 (d, *J* = 8.0 Hz, 1H), 7.85 (d, *J* = 4.8 Hz, 1H), 7.80 (t, *J* = 7.6 Hz, 1H), 7.64 (d, *J* = 8.4 Hz, 1H), 7.48 (t, *J* = 7.4 Hz, 1H), 7.23 (t, *J* = 4.2 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 162.3, 149.0, 148.3, 137.8, 135.2, 132.6, 129.9, 129.0, 127.4, 126.8, 126.5, 121.3. GC-MS: m/z = 228.



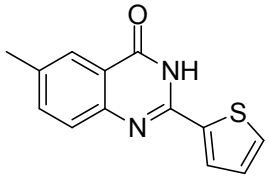
2-(pyridin-3-yl)quinazolin-4(3*H*)-one **(3l)**[1]**:** Eluent: petroleum ether/ethyl acetate (10:1), white solid, m.p: 273-274 ºC. ^{1}H NMR (400 MHz, DMSO-d_6): δ 12.7 (s, 1H), 9.25 (s, 1H), 8.71 (d, *J* = 4.0 Hz, 1H), 8.43 (d, *J* = 8.0 Hz, 1H), 8.12 (d, *J* = 8.0 Hz, 1H), 7.81 (t, *J* = 7.6 Hz, 1H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.48-7.56 (m, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 162.6, 152.3, 151.2, 149.2, 135.9, 135.2, 129.2, 127.9, 127.4, 126.3, 124.0, 121.6. GC-MS: m/z = 223.



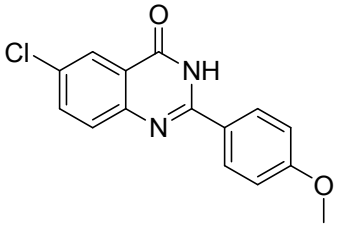
2-(1H-indol-3-yl)quinazolin-4(3*H*)-one **(3m)**[5] Eluent: petroleum ether/ethyl acetate (10:1), faint yellow solid, m.p: >300 ºC. ^{1}H NMR (400 MHz, DMSO-d_6): δ 12.16 (s, br, 1H), 11.88 (s, 1H), 8.70 (d, *J* = 6.8 Hz, 1H), 8.56 (s, 1H), 8.10 (d, *J* = 8.0 Hz, 1H), 7.78 (t, *J* = 7.6 Hz, 1H), 7.73 (d, *J* = 8.4 Hz, 1H), 7.48 (d, *J* = 6.8 Hz, 1H), 7.41 (t, *J* = 7.2 Hz, 1H), 7.20-7.24 (m, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 162.6, 150.8, 150.2, 137.3, 134.9, 129.6, 127.4, 126.2, 126.0, 125.6, 123.1, 122.9, 121.4, 120.9, 112.5, 109.1. GC-MS: m/z = 261.



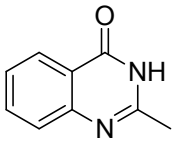
2-(4-bromophenyl)-3-methylquinazolin-4(3*H*)-one **(3n)**[6]**:** Eluent: petroleum ether/ethyl acetate (20:1), white solid, m.p: >300 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.22 (d, *J* = 7.2 Hz, 1H), 7.60-7.66 (m, 4H), 7.41 (d, *J* = 7.6 Hz, 3H), 3.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.5, 155.0, 147.1, 134.4, 134.2, 132.1, 129.8, 127.4, 127.2, 126.6, 124.5, 120.4, 34.2. GC-MS: m/z = 315.



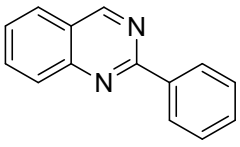
6-methyl-2-(thiophen-2-yl)quinazolin-4(3*H*)-one **(3o):** Eluent: petroleum ether/ethyl acetate (30:1), white solid, m.p.:266-267 ºC. ^{1}H NMR (400 MHz, DMSO-d_6): 12.56 (s, br, 1H), 8.18 (s, 1H), 7.90 (s, 1H), 7.82 (d, *J* = 4.8 Hz, 1H), 7.59 (d, *J* = 8.4 Hz, 1H), 7.53 (d, *J* = 8.0 Hz, 1H), 7.21 (s, 1H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 162.2, 147.5, 147.0, 137.9, 136.5, 136.4, 132.3, 129.5, 128.9, 127.3, 125.9, 121.0, 21.3. HRMS (EI): calcd for $C_{13}H_{10}N_2OS$: 242.0514; found: 242.0513.



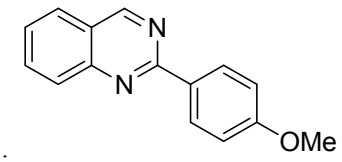
6-chloro-2-(4-methoxyphenyl)quinazolin-4(3*H*)-one **(3p)**[7]**:** Eluent: petroleum ether/ethyl acetate (20:1), white solid, m.p: >300 °C. ^{1}H NMR (400 MHz, $CDCl_3$): 12.58 (s, br, 1H), 8.18 (s, 2H), 8.05 (s, 1H), 7.82 (s, 1H), 7.72 (s, 1H), 7.09 (s, 2H), 3.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.5, 161.8, 152.8, 148.2, 135.1, 130.7, 130.0, 125.3, 124.9, 122.4, 114.5. GC-MS: m/z = 286.



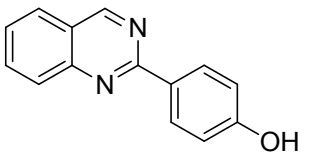
2-methylquinazolin-4(3H)-one (**3q**)[1]: Eluent: petroleum ether/ethyl acetate (5:1), m.p.: 235-239 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.22 (s, br, 1H), 8.28 (d, *J* = 8.0 Hz, 1H), 7.77 (t, *J* = 7.6 Hz, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 1H), 2.61 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.4, 153.4, 149.4, 134.9, 127.0, 126.4, 126.2, 120.2, 22.1. GC-MS: m/z = 160.



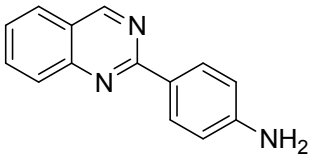
2-phenylquinazoline (**4a**)[10] Eluent: petroleum ether/ethyl acetate (50:1), white solid, m.p: 98-100 °C. ^{1}H NMR (400 MHz, $CDCl_3$): 9.41 (s, 1H), 8.64 (d, *J* = 7.2 Hz, 2H), 8.06 (d, *J* = 8.4 Hz, 1H), 7.83 (d, *J* = 7.6 Hz, 2H), 7.54 (d, *J* = 7.2 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): 160.8, 160.3, 150.6, 137.9, 133.9, 130.5, 128.49, 128.45, 127.1, 126.9, 123.4. GC-MS: m/z = 206



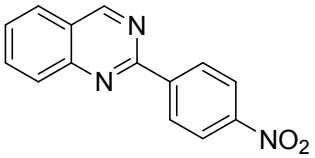
. 2-(4-methoxyphenyl)quinazoline (**4b**)[10] Eluent: petroleum ether/ethyl acetate (20:1), white solid, m.p. 96-98 °C.:. ^{1}H NMR (400 MHz, $CDCl_3$): 9.40 (s, 1H), 8.57 (d, *J* = 7.6 Hz, 2H), 8.03 (d, *J* = 8.4 Hz, 1H), 7.86 (d, *J* = 8.0 Hz, 2H), 7.55 (t, *J* = 7.2 Hz, 1H), 7.04 (d, *J* = 7.2 Hz, 2H), 3.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 161.8, 160.9, 160.4, 150.8, 134.0, 130.7, 130.2, 128.4, 127.2, 126.8, 123.3, 114.0, 55.4. GC-MS: m/z = 236.



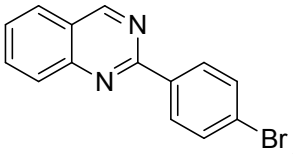
4-(quinazolin-2-yl)phenol (**4c**) Eluent: petroleum ether/ethyl acetate (10:1), yellow solid, m.p: 155-157 °C ^{1}H NMR (400 MHz, DMSO-d_6)): 10.03 (s, 1H), 9.60 (s, 1H), 8.41 (d, *J* = 8.4 Hz, 2H), 8.08 (d, *J* = 8.0 Hz, 1H), 7.97 (d, *J* = 2.8 Hz, 2H), 7.63-7.67 (m, 1H), 6.93 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): 161.5, 160.6, 160.5, 150.4, 135.1, 130.4, 128.9, 128.2, 128.1, 127.4, 123.4, 115.9. HRMS (EI): calcd for $C_{14}H_{10}N_2O$: 222.0793; found: 222.0786.



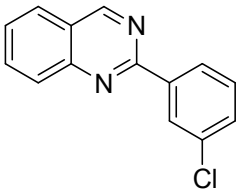
4-(quinazolin-2-yl)aniline (**4d**) Eluent: petroleum ether/ethyl acetate (20:1), yellow solid, m.p: 176-178 °C:. ^{1}H NMR (400 MHz, $CDCl_3$): 9.52 (s, 1H), 8.28 (d, *J* =8.4 Hz, 2H), 8.03 (d, *J* = 8.0 Hz, 1H), 7.90 (q, *J* = 5.6 Hz, 2H), 7.56-7.60 (m, 1H), 6.70 (d, *J* = 8.4 Hz, 2H), 5.71 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): 161.2, 161.0, 152.1, 150.6, 134.8, 130.2, 128.1, 127.8, 126.7, 125.1, 123.1, 113.9. HRMS (EI): calcd for $C_{14}H_{11}N_3$: 221.0953; found: 221.0947.



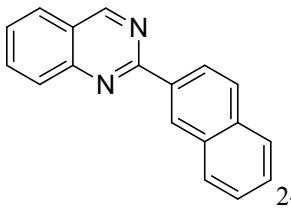
2-(4-nitrophenyl)quinazoline (**4e**)[10] Eluent: petroleum ether/ethyl acetate (15:1), white solid, m.p: 219-220 °C. ^{1}H NMR (400 MHz, $CDCl_3$): 9.50 (s, 1H), 8.80 (s, 2H), 8.36 (s, 2H), 8.12 (s, 1H), 7.97 (s, 2H), 7.70 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): 160.7, 158.8, 150.6, 149.2, 143.8, 134.6, 129.4, 128.8, 128.3, 127.2, 123.9, 123.7. GC-MS: m/z = 251.



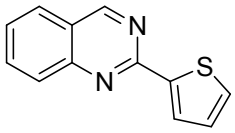
2-(4-bromophenyl)quinazoline (**4f**)[10] Eluent: petroleum ether/ethyl acetate (20:1), white solid, m.p: 157-159 °C. ^{1}H NMR (400 MHz, $CDCl_3$): 9.43 (s, 1H), 8.48 (d, J = 7.2 Hz, 2H), 8.05 (d, J = 8.4 Hz, 1H), 7.90 (t, J = 7.4 Hz, 2H), 7.60-7.66 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 160.5, 160.1, 150.6, 136.9, 134.2, 131.8, 130.1, 128.6, 127.5, 127.1, 125.4, 123.6. GC-MS: m/z = 283.



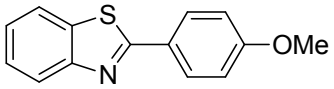
2-(3-chlorophenyl)quinazoline (**4g**)[10]. Eluent: petroleum ether/ethyl acetate (20:1), white solid, m.p. 149-150 °C. ^{1}H NMR (400 MHz, $CDCl_3$): 9.40 (s, 1H), 8.57 (s, 1H), 8.44 (d, J = 3.2 Hz, 1H), 8.03 (d, J = 8.8 Hz, 1H), 7.87 (t, J = 8.6 Hz, 2H), 7.58 (t, J = 7.4 Hz, 1H), 7.41 (s, 2H), 7.19 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): 159.6, 158.8, 149.7, 138.9, 133.8, 133.3, 129.5, 128.8, 127.70, 127.67, 126.6, 126.1, 125.6, 122.8. GC-MS: m/z = 240.



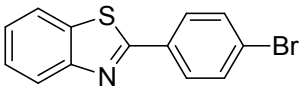
2-(naphthalen-2-yl)quinazoline (**4h**)[11] Eluent: petroleum ether/ethyl acetate (30:1), white solid, m.p:120-121 °C. ^{1}H NMR (400 MHz, $CDCl_3$): 9.60 (s, 1H), 8.71 (t, J = 4.6 Hz, 1H), 8.16-8.19 (m, 2H), 7.93-8.03 (m, 4H), 7.69 (t, J = 7.6 Hz, 1H), 7.62 (t, J = 7.6 Hz, 1H), 7.53-7.56 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): 163.5, 160.5, 150.6, 136.3, 134.4, 134.2, 131.2, 130.4, 129.6, 128.7, 128.6, 127.8, 127.2, 126.9, 125.9, 125.4, 123.2, 114.9. GC-MS: m/z = 256.



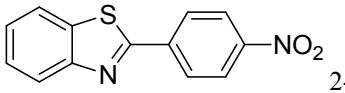
2-(thiophen-2-yl)quinazoline (**4i**)[10] Eluent: petroleum ether/ethyl acetate (20:1), faint yellow solid, m.p: 130-131 °C. ^{1}H NMR (400 MHz, $CDCl_3$): 9.35 (s, 1H), 8.15 (d, J = 3.6 Hz, 1H), 8.01 (d, J = 8.8 Hz, 1H), 8.86-8.89 (m, 2H), 7.67 (d, J = 8.0 Hz, 2H), 7.51 (d, J = 4.8 Hz, 1H), 7.19 (t, J = 4.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$)): 160.5, 157.8, 150.6, 143.8, 134.4, 129.9, 129.3, 128.4, 128.2, 127.3, 127.0, 123.4. GC-MS: m/z = 212.



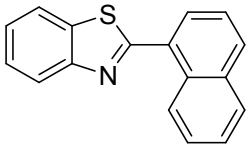
2-(4-methoxyphenyl)benzo[*d*]thiazole (**5a**)[8]**:** Eluent: petroleum ether/ethyl acetate (50:1), white solid, m.p. 123-125 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.03 (d, J = 7.2 Hz, 3H), 7.86 (d, J = 7.6 Hz, 1H), 7.47 (t, J = 7.4 Hz, 1H), 7.35 (t, J = 7.4 Hz, 1H), 6.99 (d, J = 7.2 Hz, 1H), 3.87 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.9, 161.9, 154.2, 134.9, 129.1, 126.4, 126.2, 124.8, 122.8, 121.5, 114.4, 55.5. GC-MS: m/z = 241.



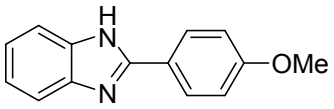
2-(4-bromophenyl)benzo[*d*]thiazole (**5b**)[8]**:** Eluent: petroleum ether/ethyl acetate (50:1), white solid, m.p. 129-131 °C: ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.06 (d, J = 8.0 Hz, 1H), 7.93 (d, J = 8.4 Hz, 2H), 7.88 (J = 8.0 Hz, 1H), 7.60 (d, J = 8.4 Hz, 2H), 7.49 (t, J = 7.6 Hz, 1H), 7.39 (t, J = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.7, 154.1, 135.0, 132.5, 132.3, 128.9, 126.5, 125.5, 125.48, 125.4, 123.3, 121.7. GC-MS: m/z = 290.



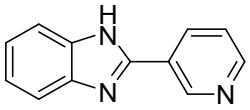
2-(4-nitrophenyl)benzo[*d*]thiazole (**5c**)[8]**:** Eluent: petroleum ether/ethyl acetate (50:1), white solid, m.p. m.p. 141-143 °C: ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.35 (d, *J* = 8.0 Hz, 2H), 8.26 (d, *J* = 7.6 Hz, 2H), 8.12 (d, *J* = 8.4 Hz, 1H), 7.95 (d, *J* = 8.0 Hz, 1H), 7.60 (t, *J* = 7.2 Hz, 1H), 7.54 (t, *J* = 7.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ. 165.3, 153.9, 149.2, 138.8, 135.6, 128.8, 127.6, 126.9, 125.1, 123.9, 123.1. GC-MS: m/z = 256.



2-(naphthalen-1-yl)benzo[*d*]thiazole (**5d**)[8]**:** Eluent: petroleum ether/ethyl acetate (50:1), white solid, m.p. 126-127 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.96 (d, *J* = 8.4 Hz, 1H), 8.22 (d, *J* = 8.0 Hz, 1H), 7.93-8.01 (m, 4H), 7.64 (t, *J* = 7.6 Hz, 1H), 7.55-7.59 (m, 3H), 7.46 (t, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.6, 154.1, 135.4, 133.9, 131.0, 130.8, 130.6, 129.4, 128.4, 127.6, 126.5, 126.2, 125.8, 125.3, 124.9, 123.5, 121.4. GC-MS: m/z = 261.



2-(4-methoxyphenyl)-1H-benzo[*d*]imidazole (**5e**)[9]**:** Eluent: petroleum ether/ethyl acetate (50:1), white solid, m.p:223-225 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 12.93 (s, br, 1H), 7.76 (d, *J* = 7.2 Hz, 2H), 7.67 (s, 1H), 7.53 (d, *J* = 5.2 Hz, 1H), 7.46 (t, *J* =7.8 Hz, 1H), 7.21 (s, 2H), 7.05 (d, *J* = 8.0 Hz, 1H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 160.1, 151.5, 131.9, 130.6, 123.1, 122.2, 119.3, 119.2, 116.3, 111.8. GC-MS: m/z = 224.



2-(pyridin-3-yl)-1H-benzo[*d*]imidazole (**5f**)[9]**:** Eluent: petroleum ether/ethyl acetate (50:1), white solid, m.p: 224-246 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 13.12 (s, br, 1H), 9.36 (s, 1H), 8.68 (t, *J* = 2.4 Hz, 1H), 8.50 (d, *J* = 8.0 Hz, 1H), 7.64 (s, 2H), 7.57-7.60 (m, 1H), 7.24 (t, *J* = 3.0 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 150.9, 149.3, 147.9, 134.2, 126.6, 124.5, 122.9. GC-MS: m/z = 195.

5. References

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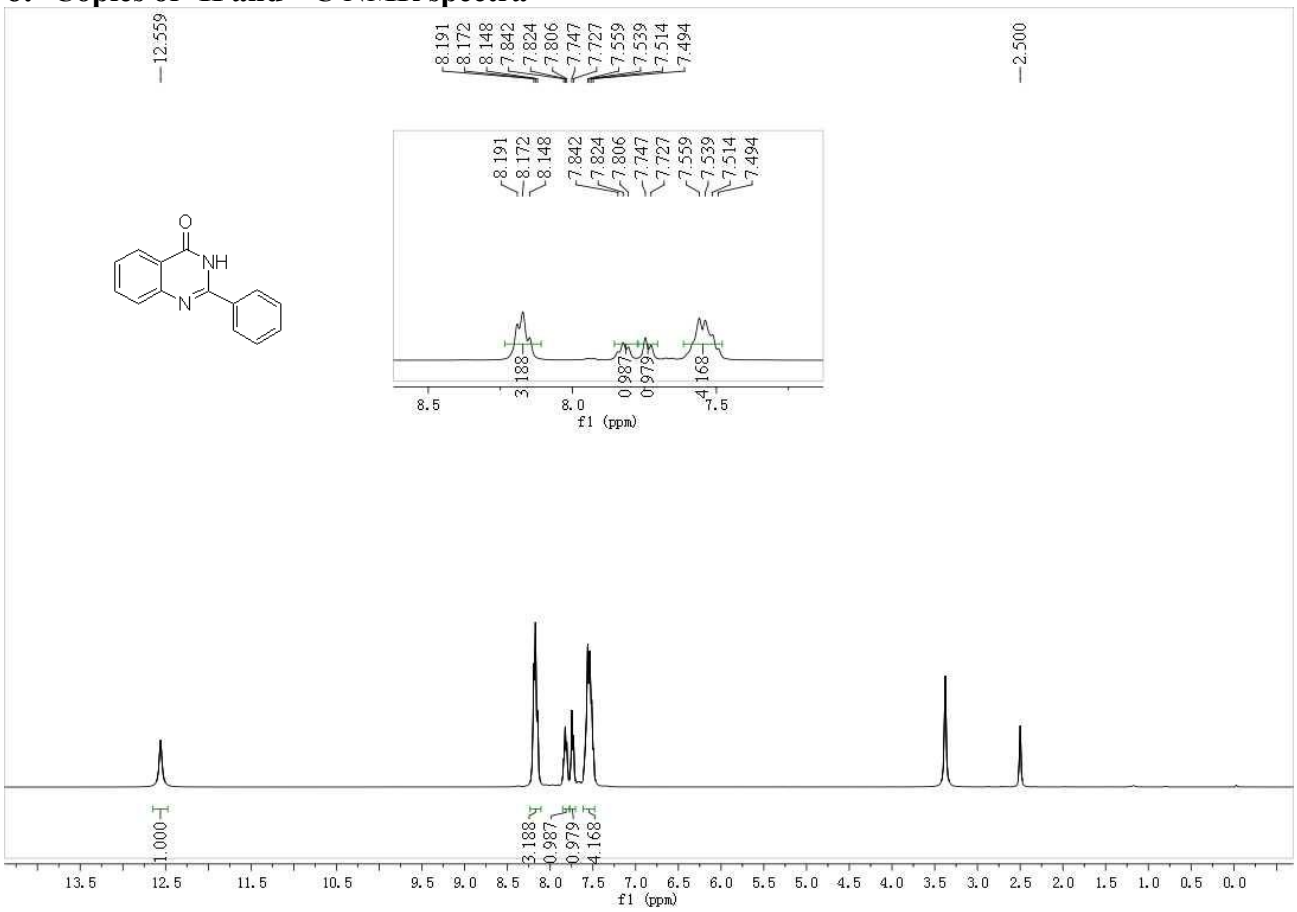
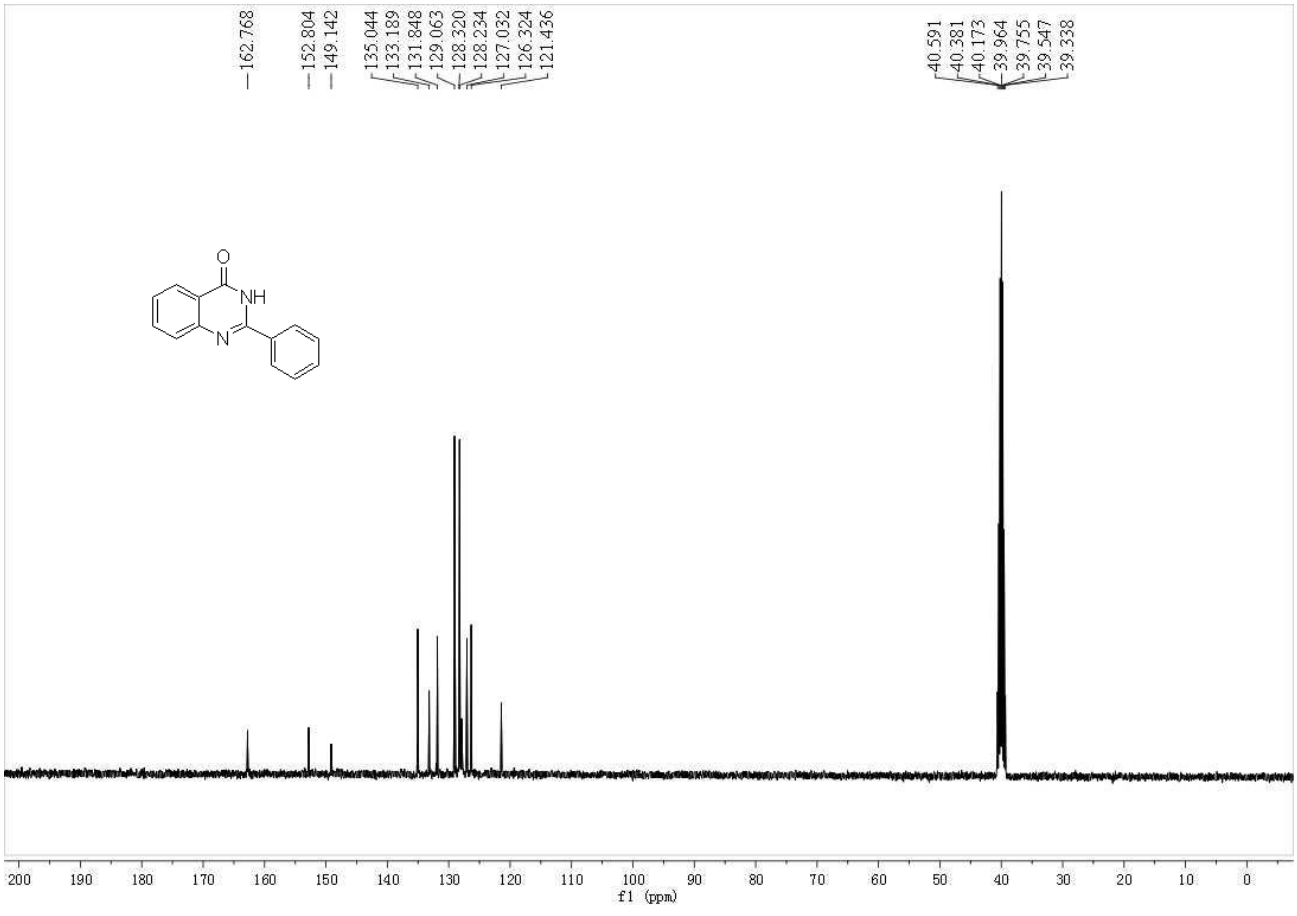
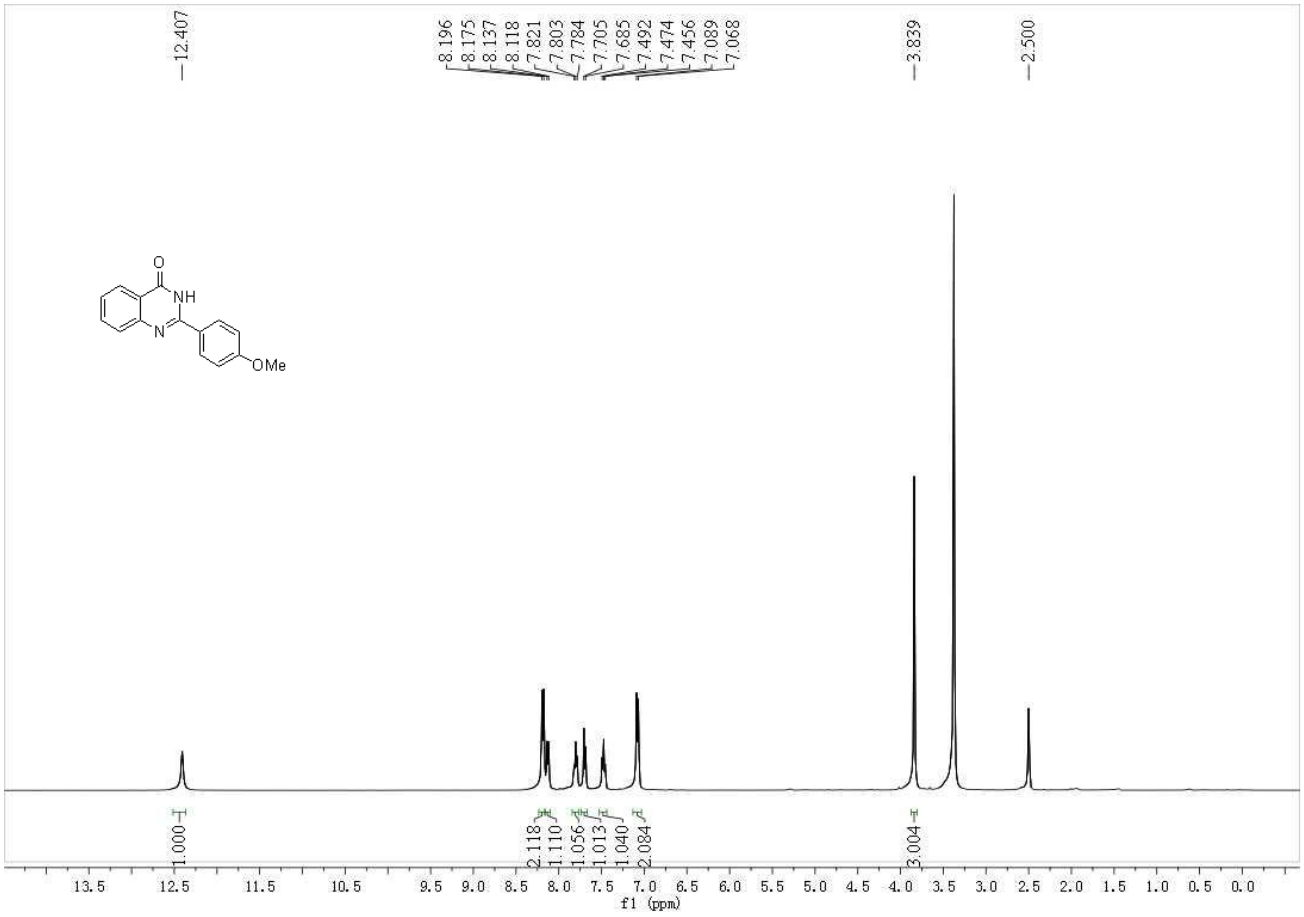
6. Copies of ^{1}H and ^{13}C NMR spectra



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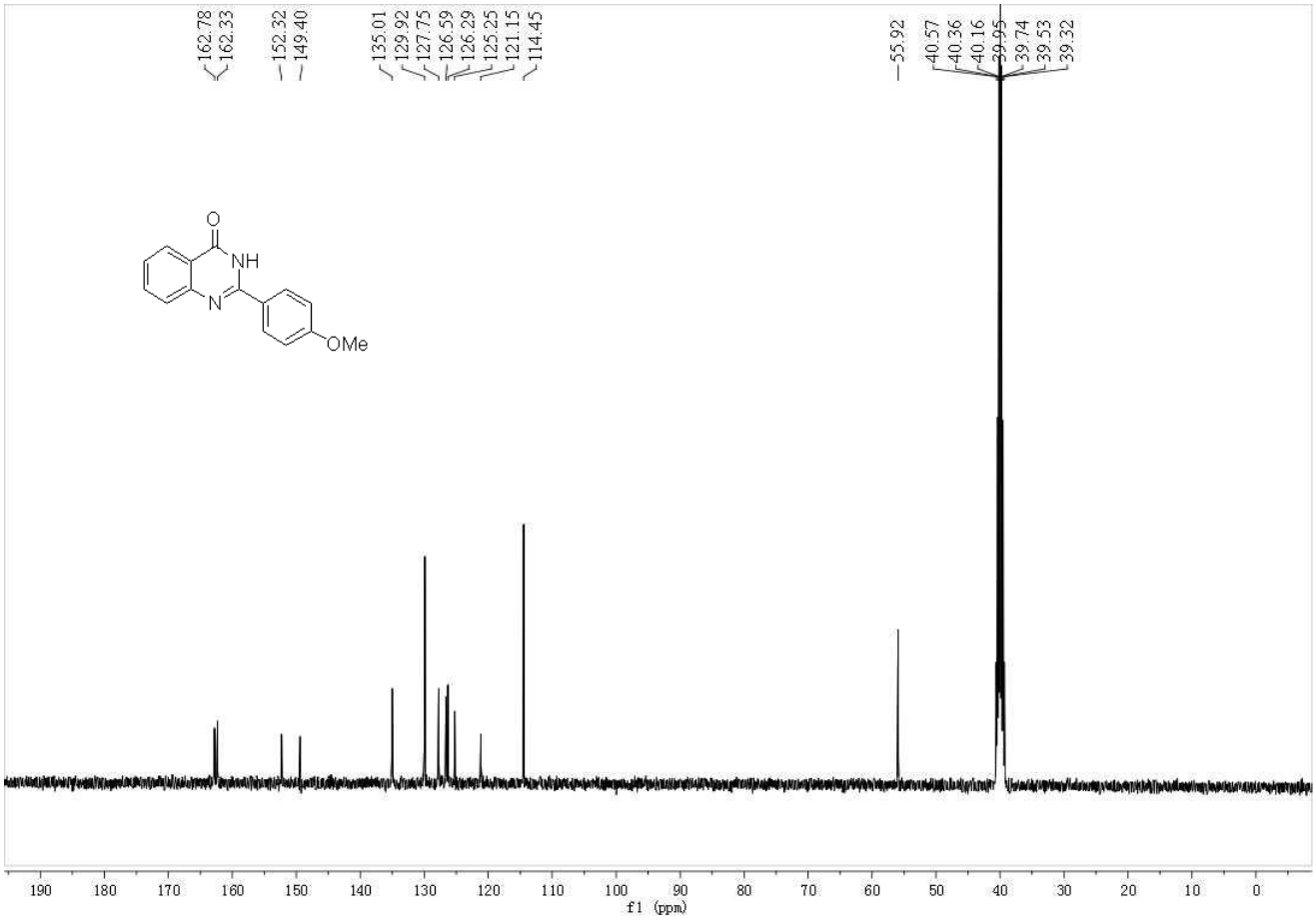
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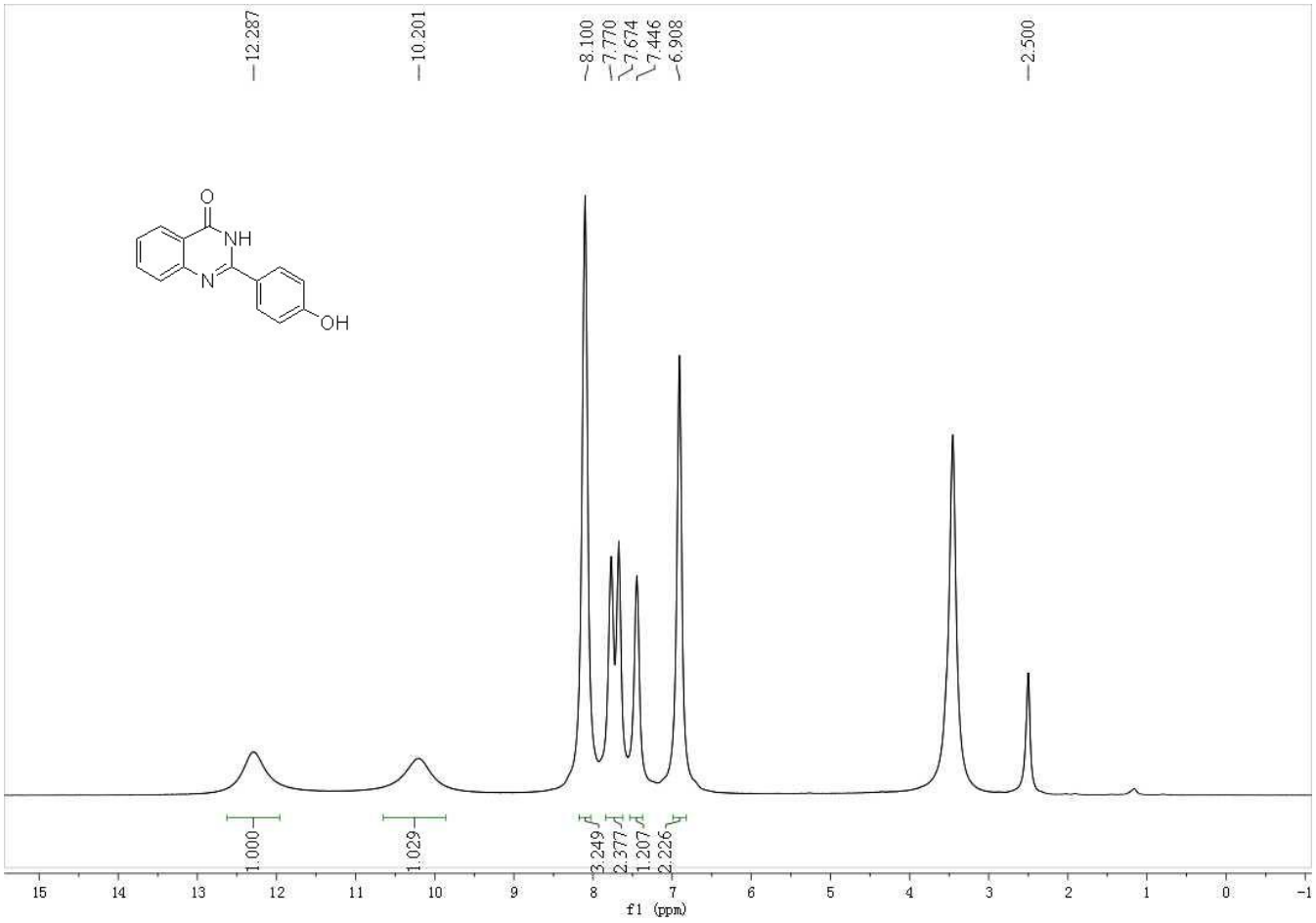
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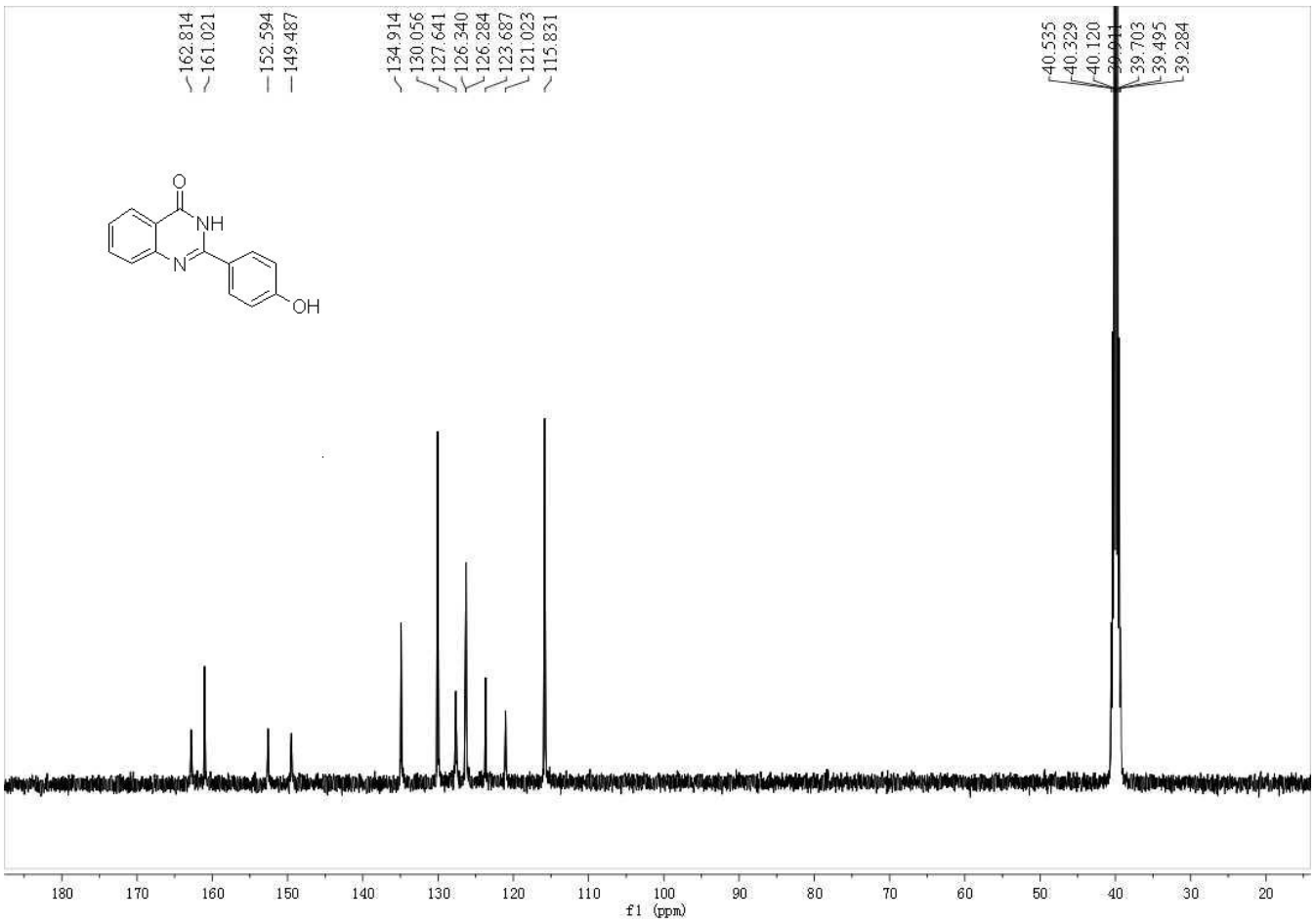
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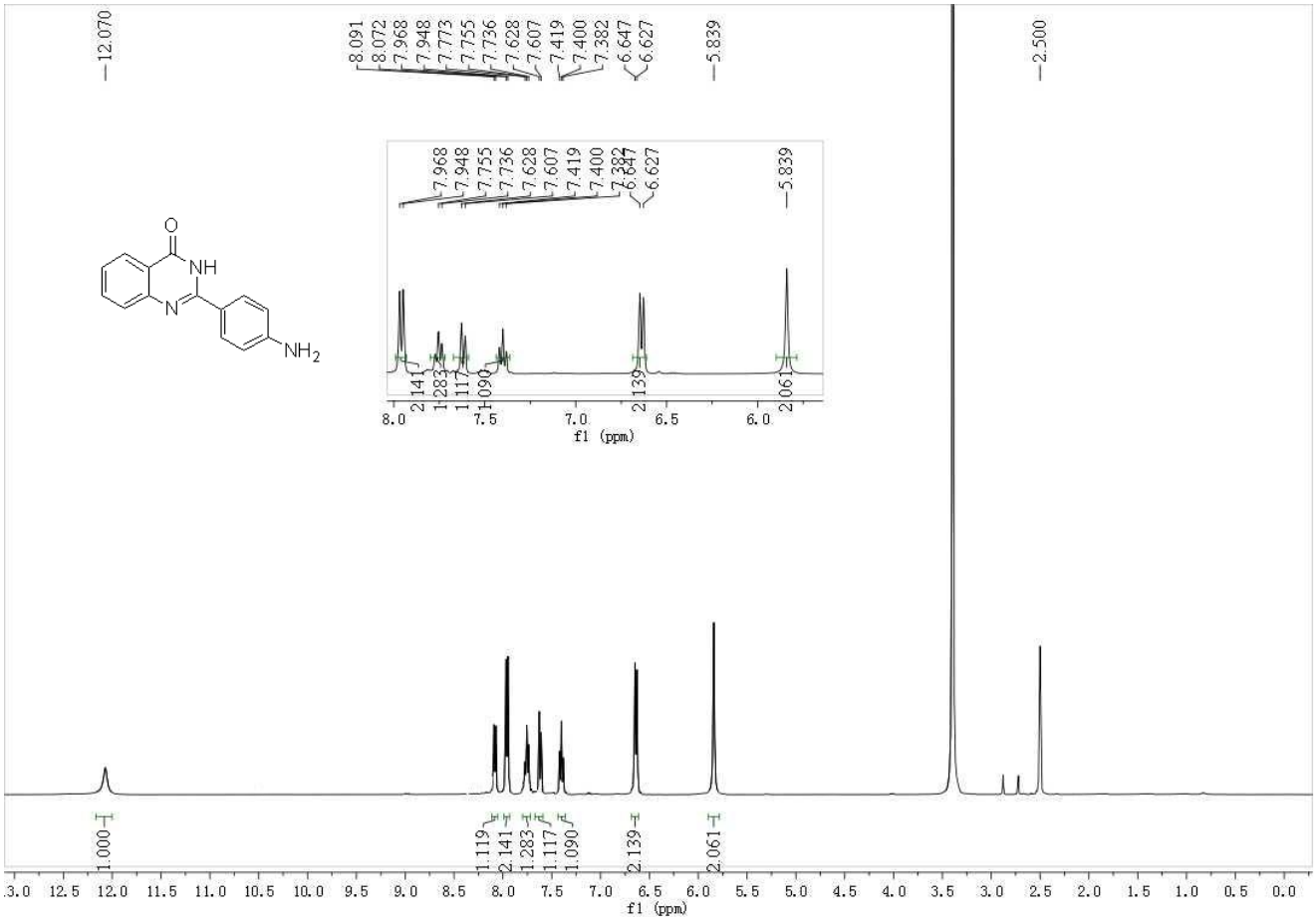
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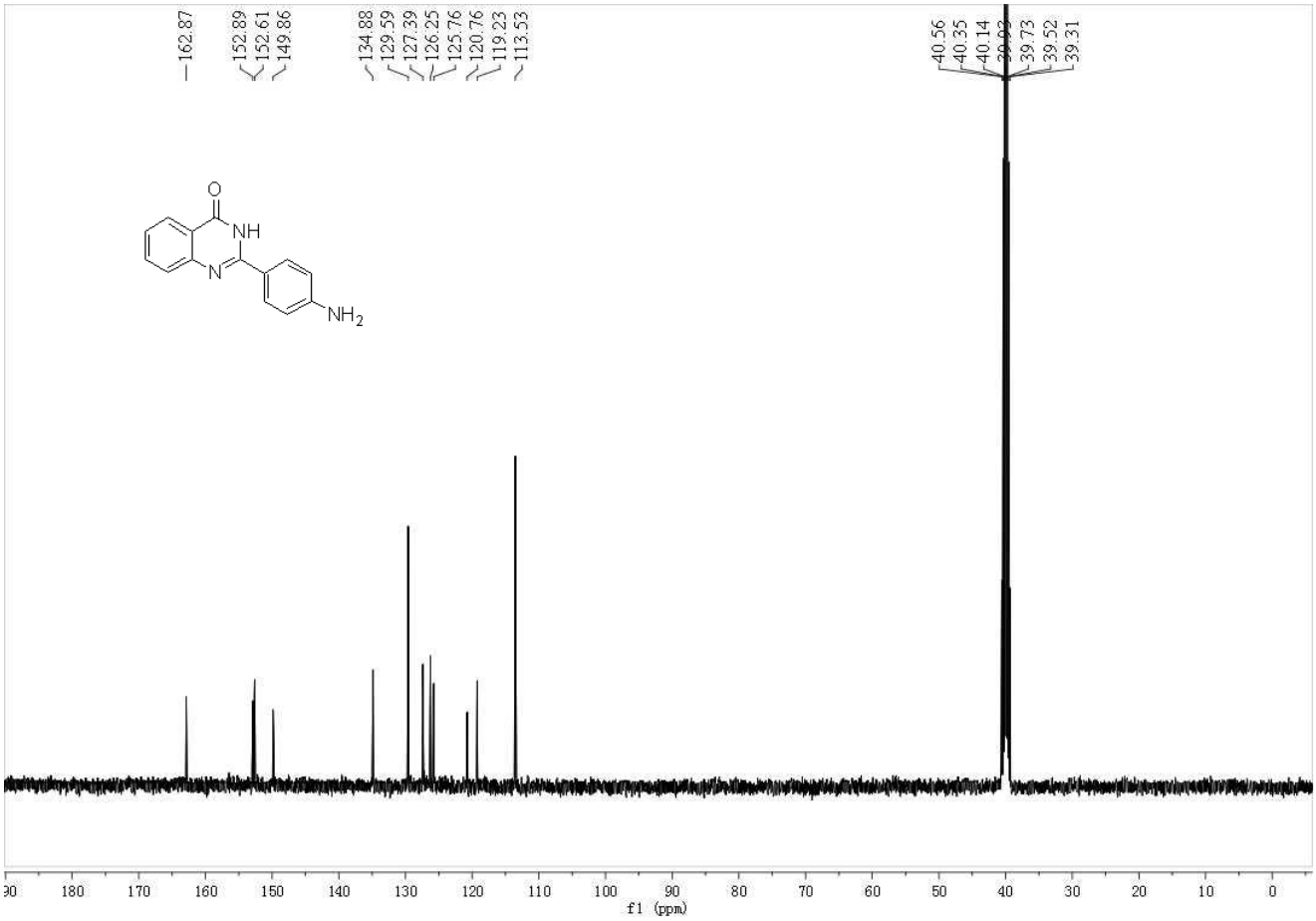
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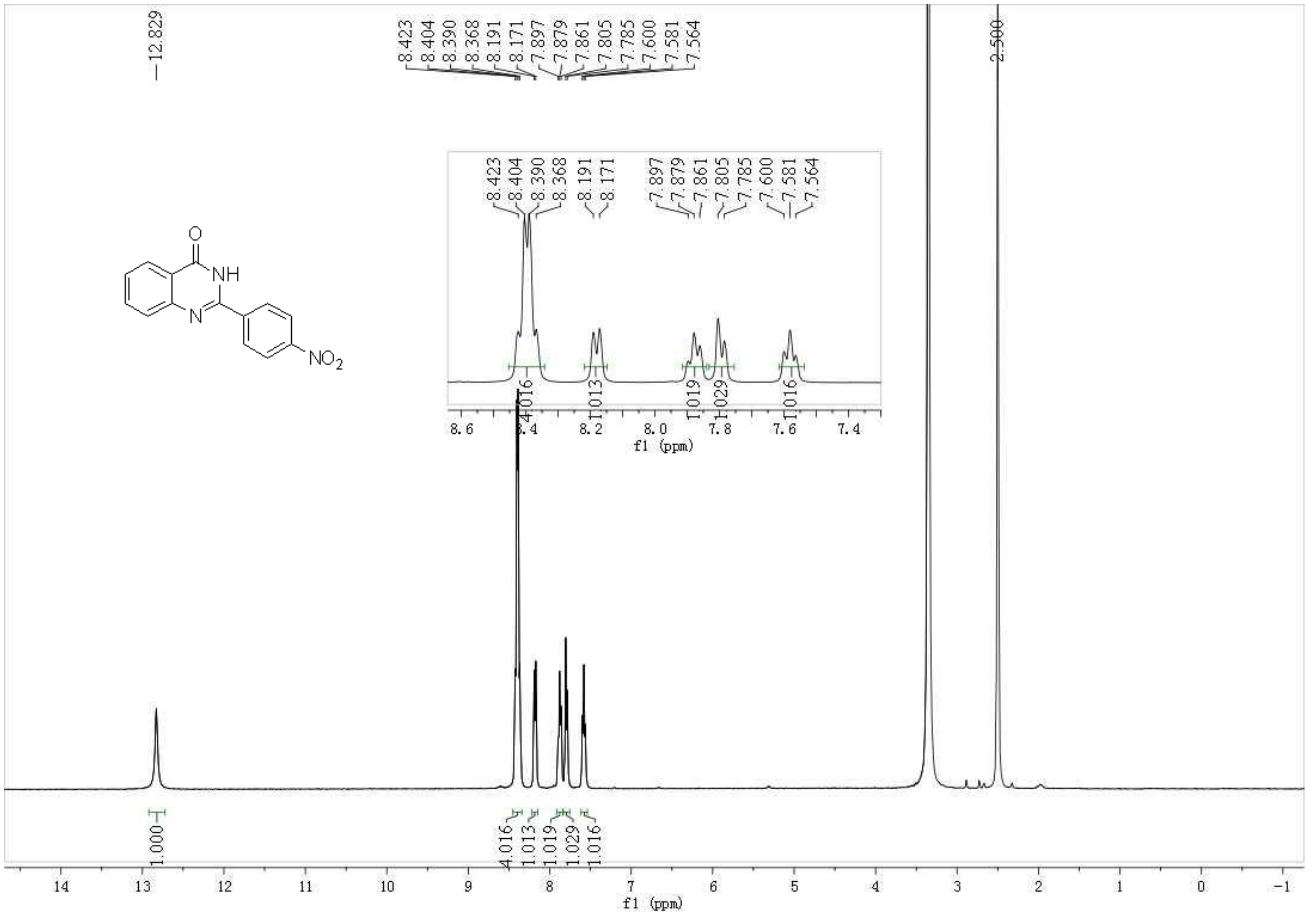
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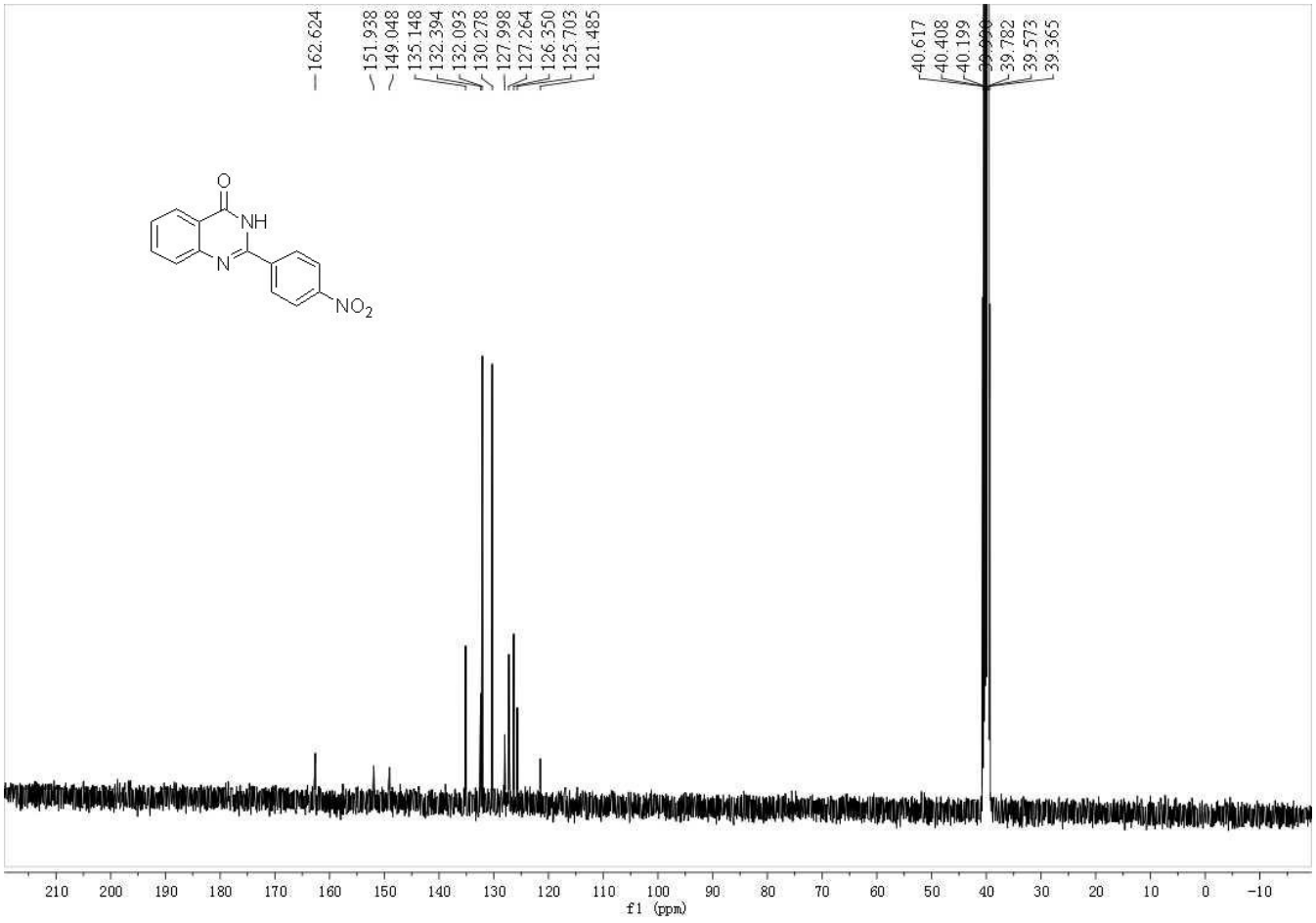
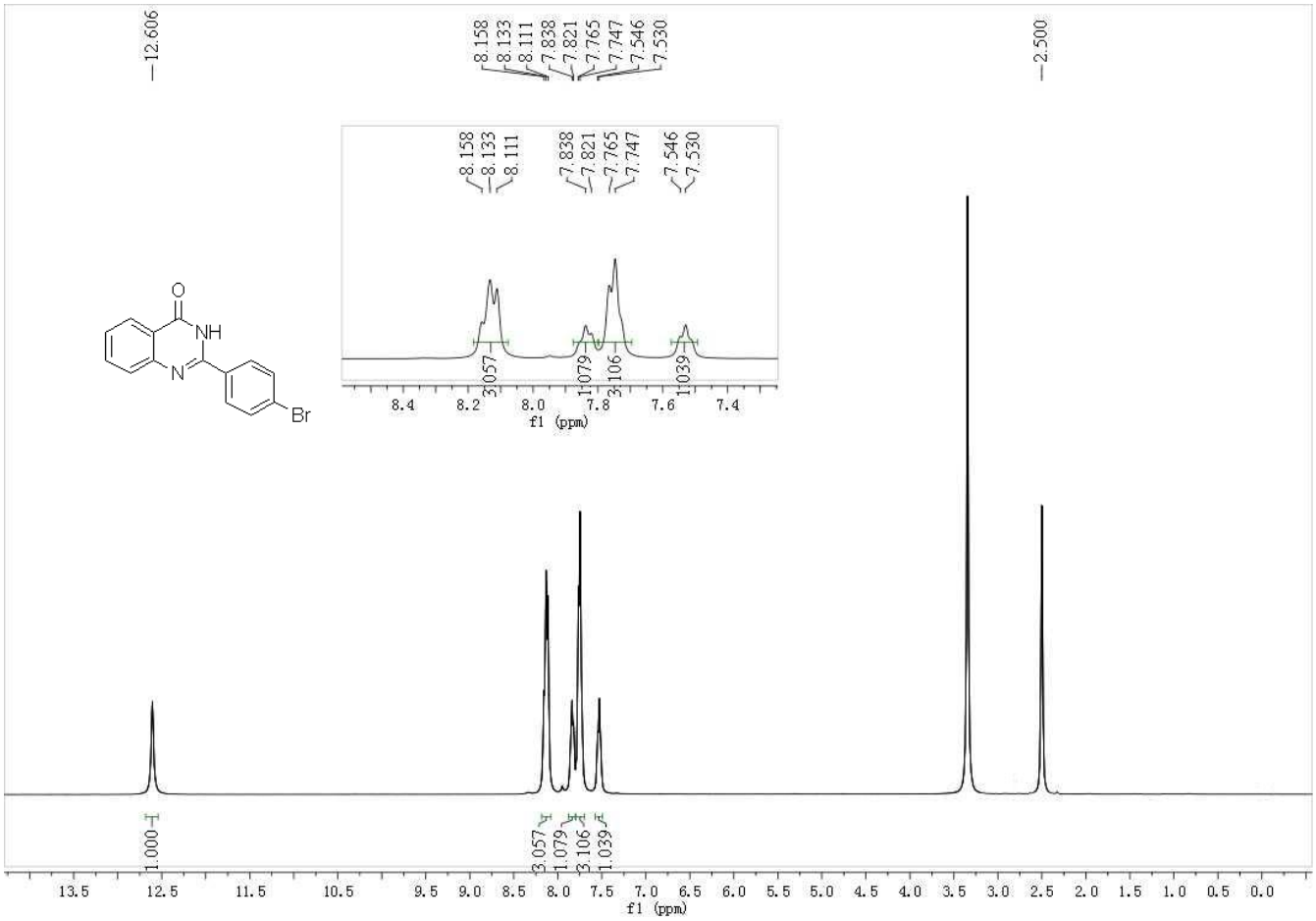
N
O
NO2
1.000
4.016
1.013
1.019
1.029
1.016
f1 (ppm)


162.624
151.938
149.048
135.148
132.394
132.093
130.278
127.998
127.264
126.350
125.703
121.485
40.617
40.408
40.199
39.782
39.573
39.365
NH
N
O
NO2
f1 (ppm)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8.133
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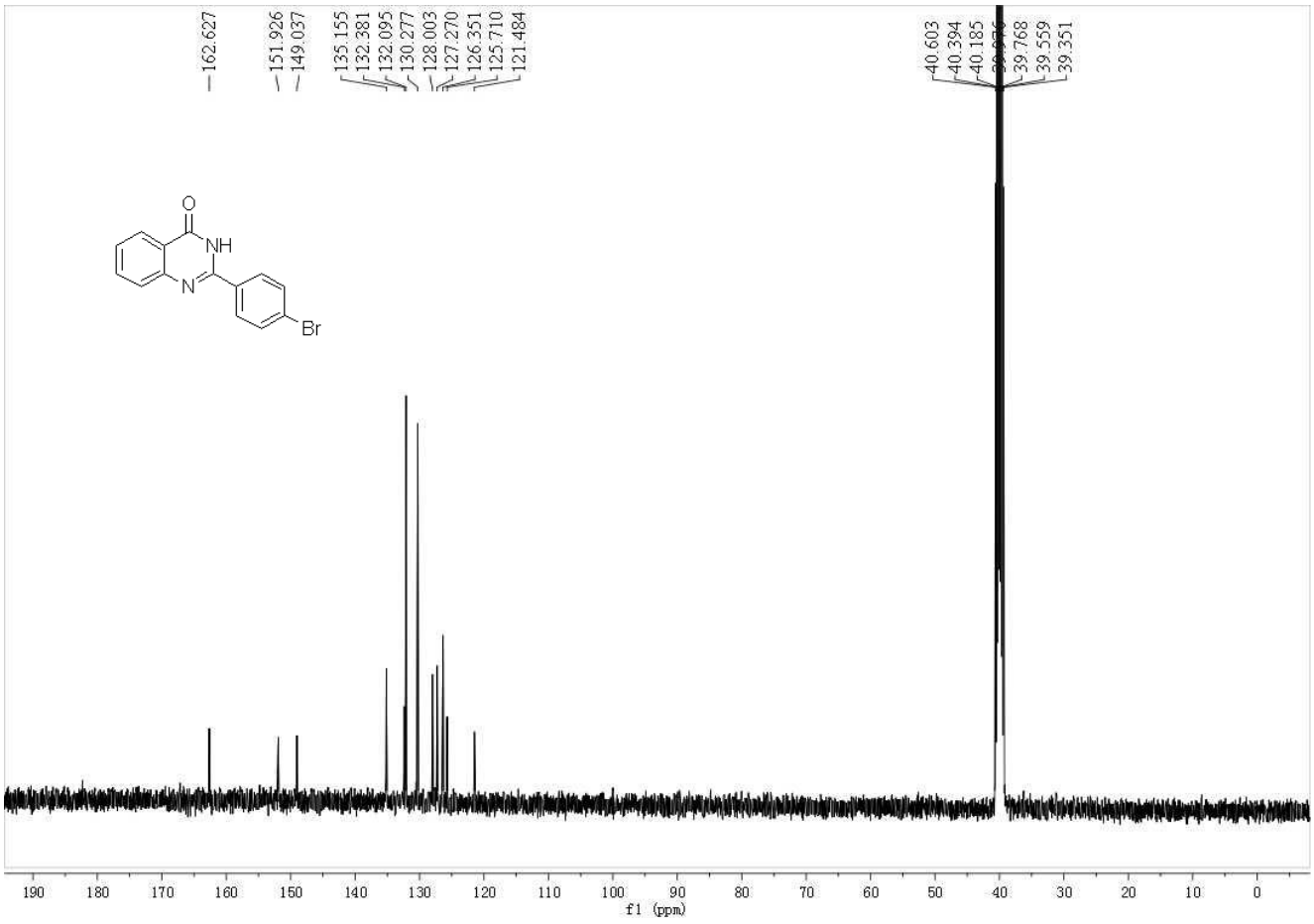
7.821
7.765
7.747
7.546
7.530
2.500
O
NH
N
Br
1.000
3.057
1.079
3.106
1.039
f1 (ppm)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130.277
128.003
127.270
126.351
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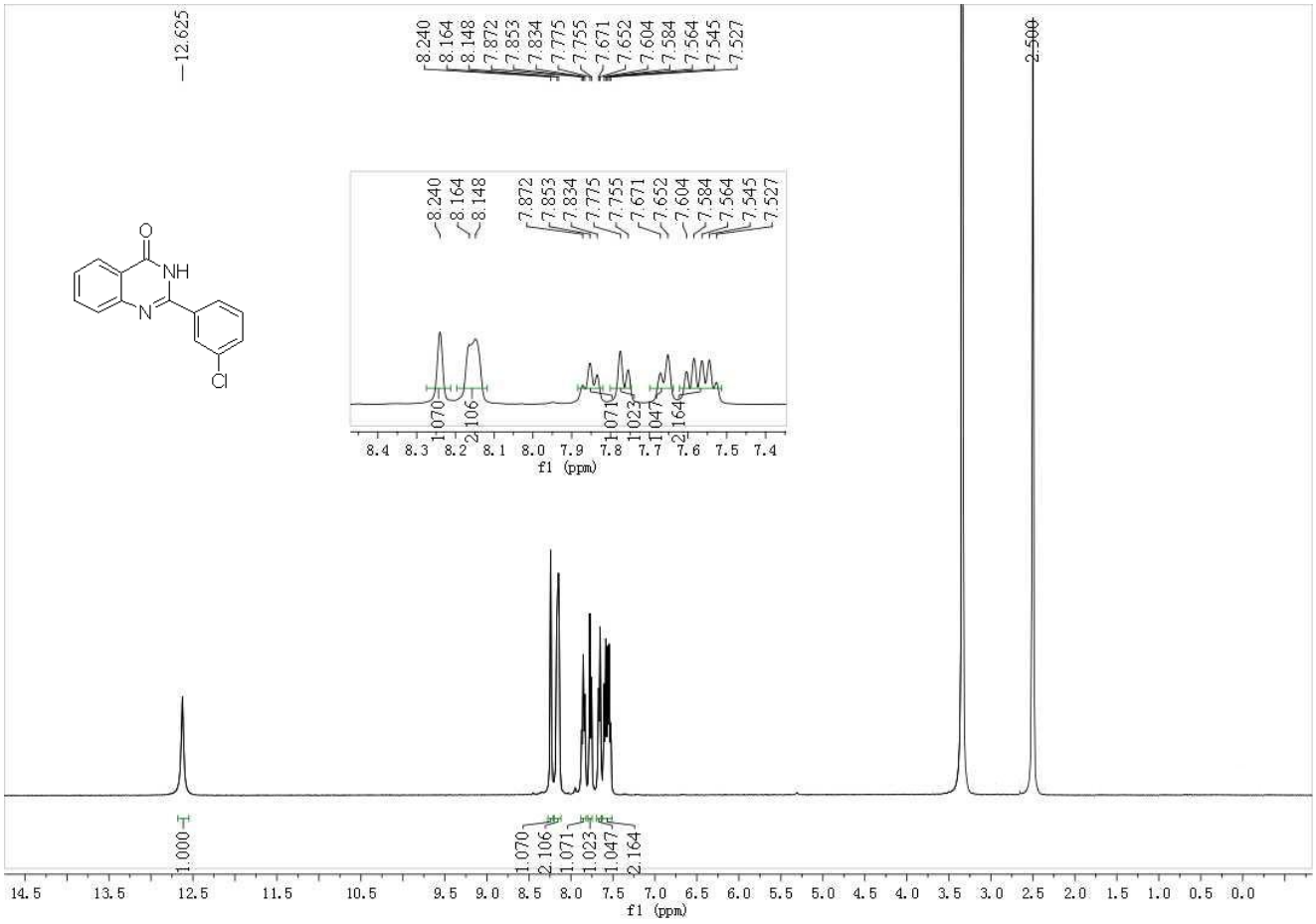
40.603
40.394
40.185
39.768
39.559
39.351
O
NH
N
Br
f1 (ppm)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8.164
8.148
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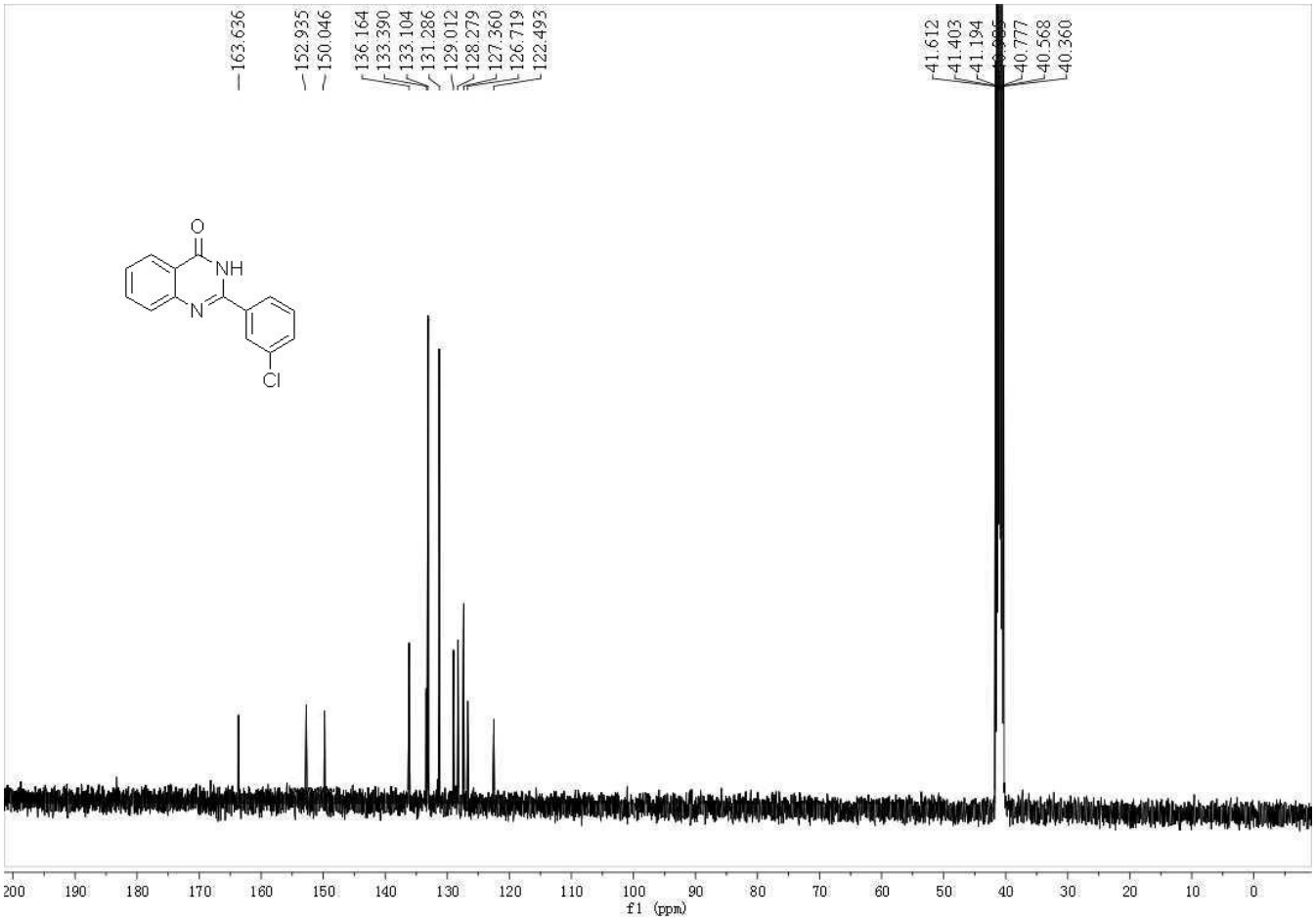
7.853
7.834
7.775
7.755
7.671
7.652
7.604
7.584
7.564
7.545
7.527
2.500
O
NH
N
Cl
1.000
1.070
2.106
1.071
1.023
1.047
2.164
f1 (ppm)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150.046
136.164
133.390
133.104
131.286
129.012
128.279
127.360
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41.403
41.194
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40.568
40.360
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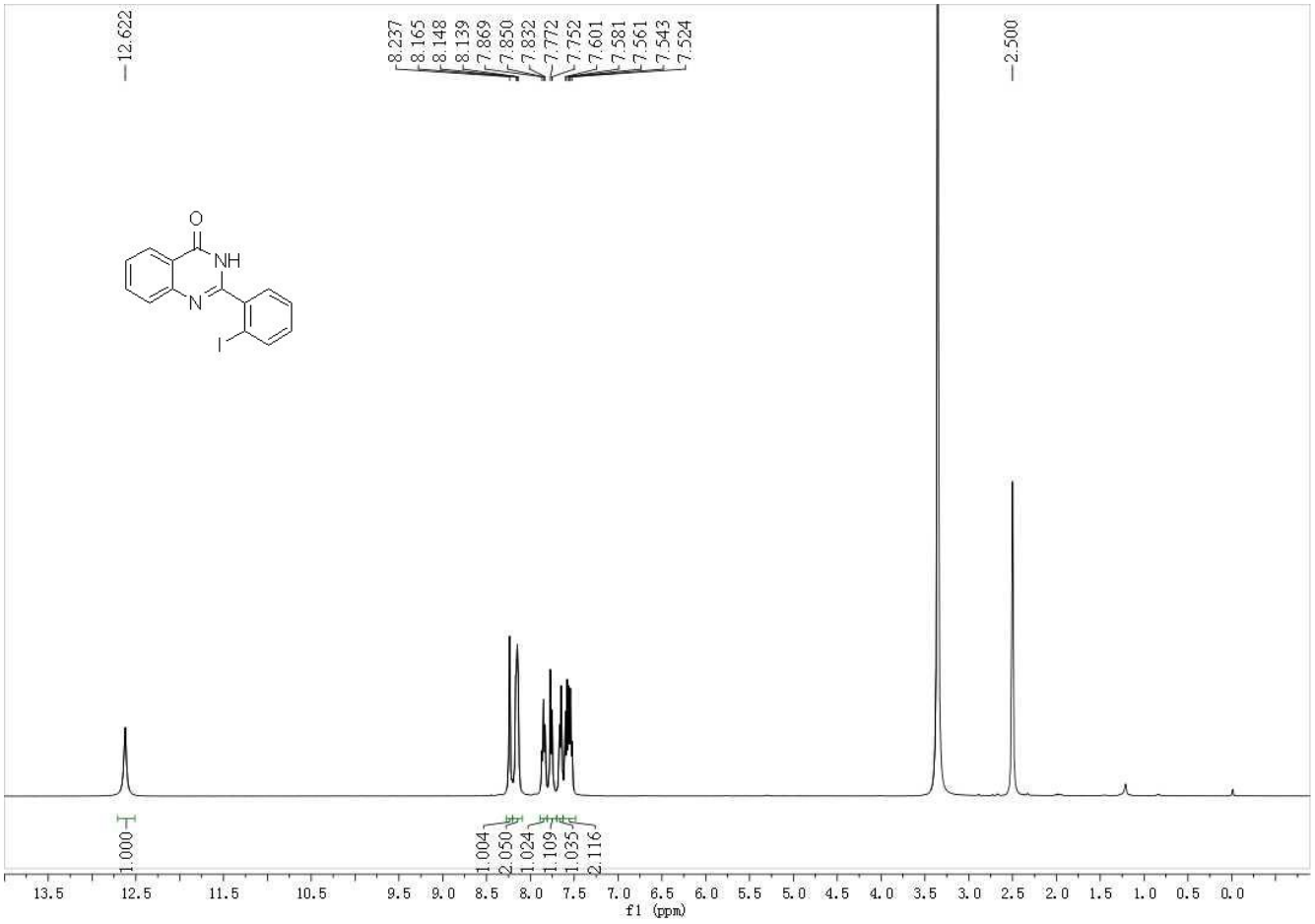
NH
N
Cl
f1 (ppm)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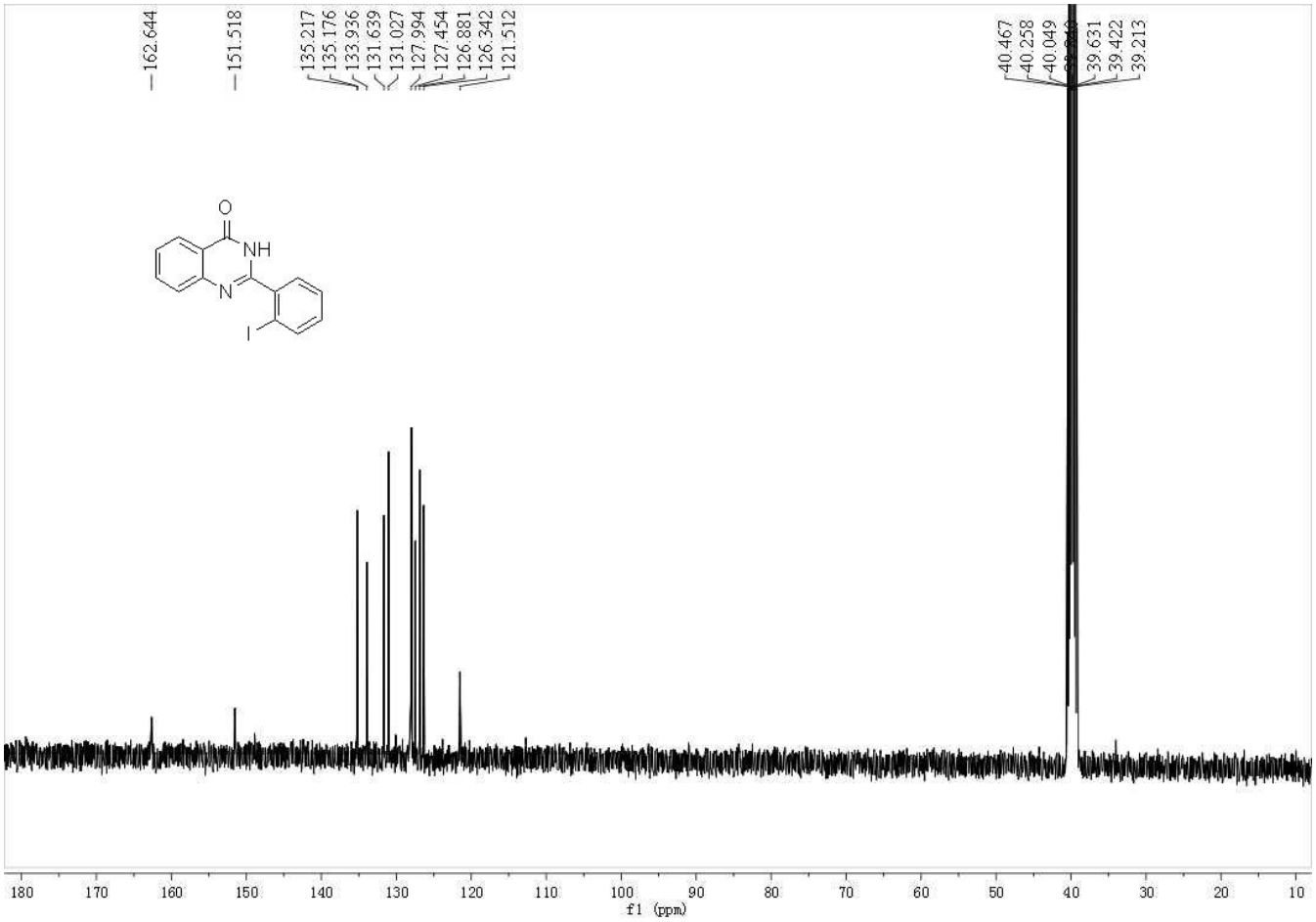
8.165
8.148
8.139
7.869
7.850
7.832
7.772
7.752
7.601
7.581
7.561
7.543
7.524
2.500
O
NH
N
I
1.000
1.004
2.050
1.024
1.109
1.035
2.116
f1 (ppm)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135.217
135.176
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131.639
131.027
127.994
127.454
126.881
126.342
121.512
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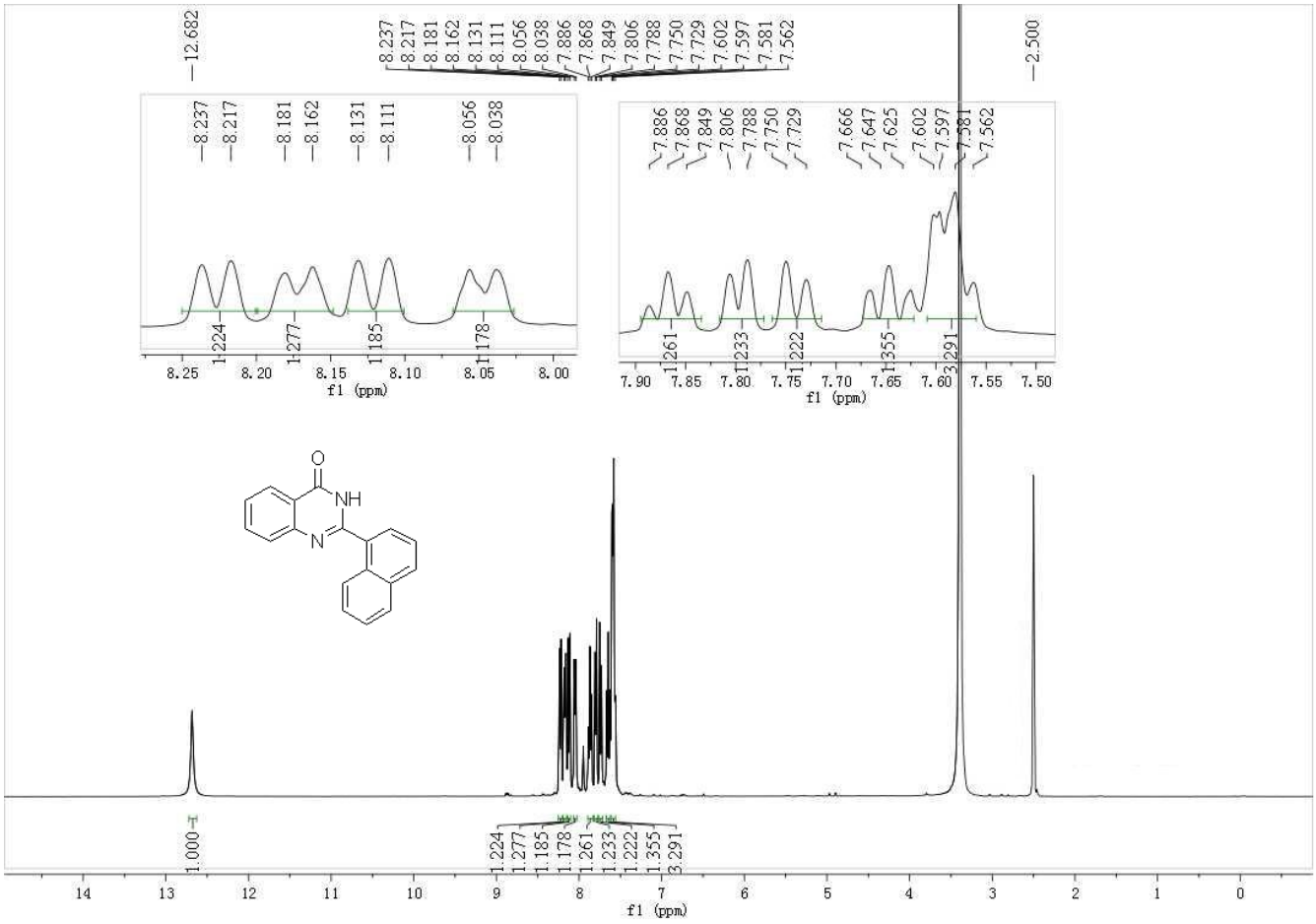
40.258
40.049
39.631
39.422
39.213
O
NH
N
I
f1 (ppm)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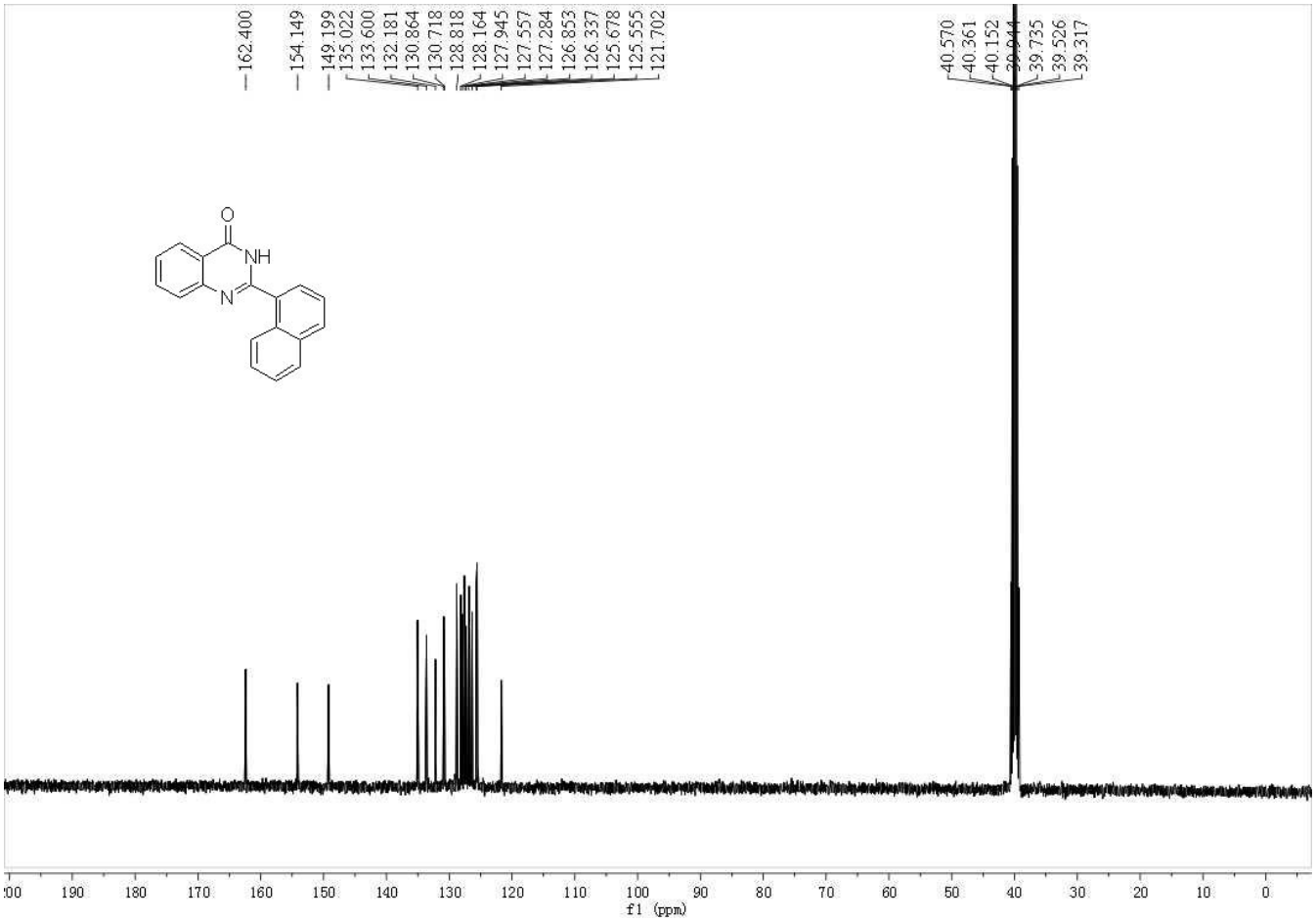
8.237
8.217
8.181
8.162
8.131
8.111
8.056
8.038
7.886
7.868
7.849
7.806
7.788
7.750
7.729
7.602
7.597
7.581
7.562
2.500
7.666
7.647
7.625
1.000
1.224
1.277
1.185
1.178
1.261
1.233
1.222
1.355
3.291
f1 (ppm)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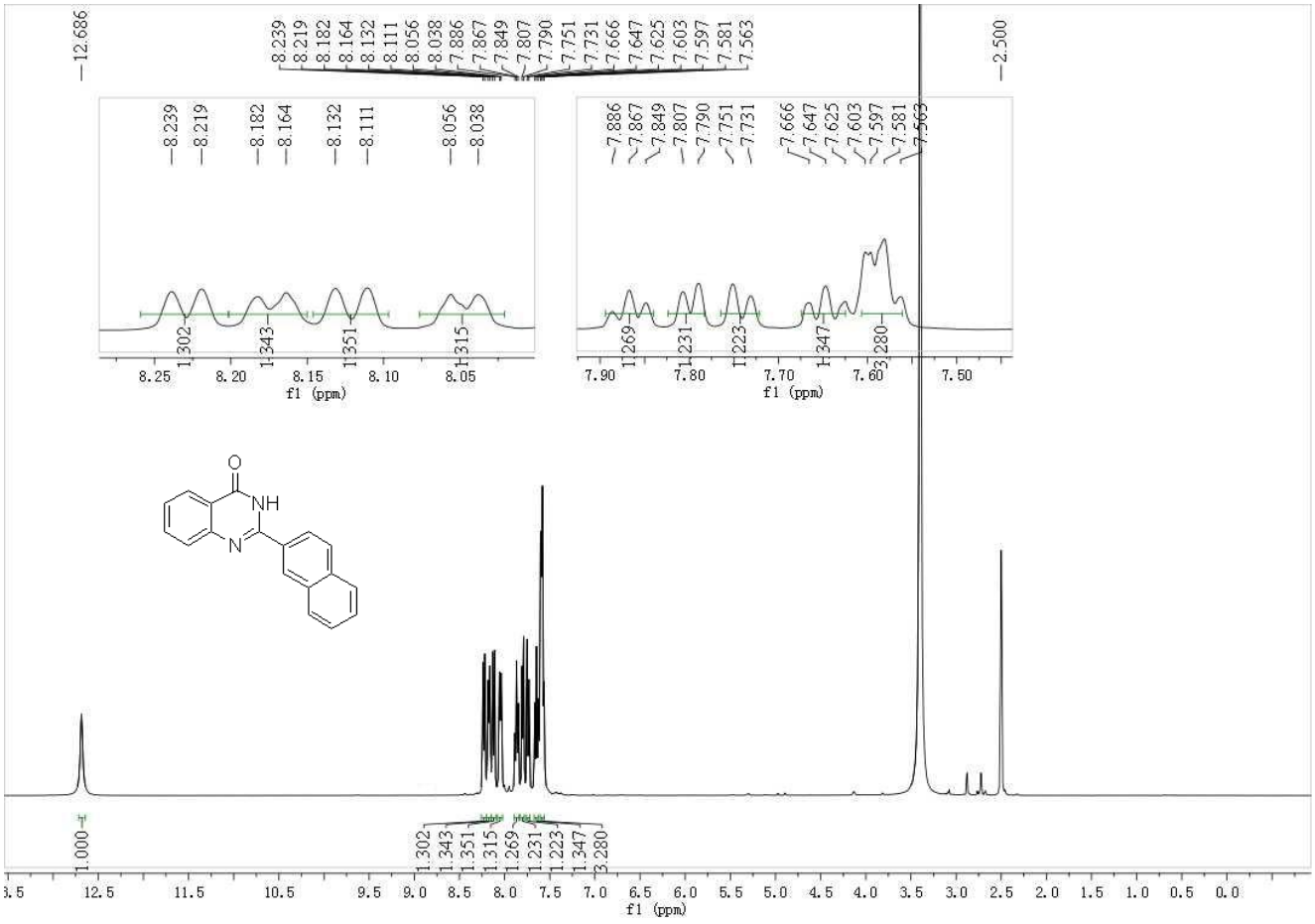
154.149
149.199
135.022
133.600
132.181
130.864
130.718
128.818
128.164
127.945
127.557
127.284
126.853
126.337
125.678
125.555
121.702
40.570
40.361
40.152
39.944
39.735
39.526
39.317
f1 (ppm)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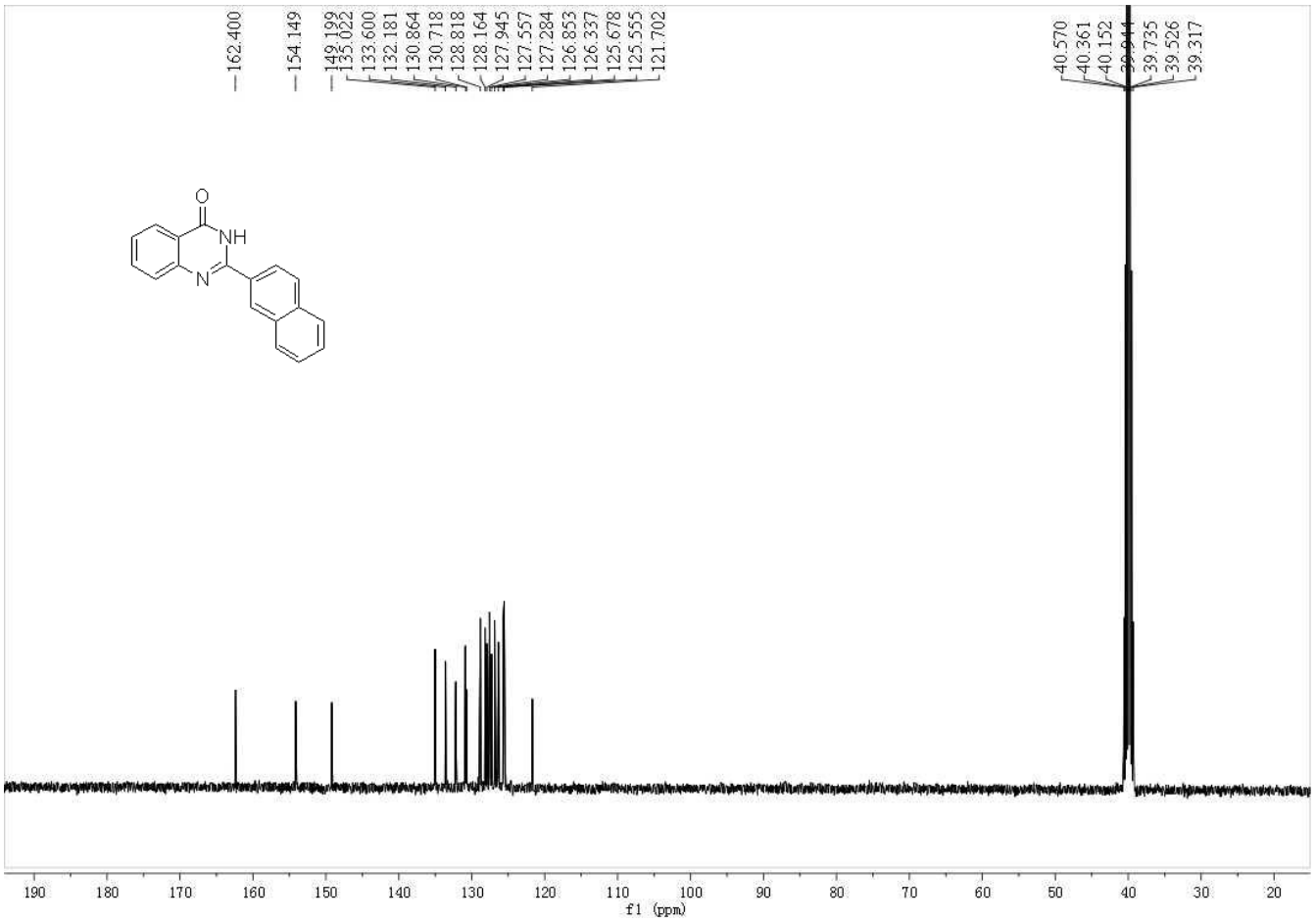
8.182
8.164
8.132
8.111
8.056
8.038
7.886
7.867
7.849
7.807
7.790
7.751
7.731
7.666
7.647
7.625
7.603
7.597
7.581
7.563
2.500
1.000
1.302
1.343
1.351
1.315
1.269
1.231
1.223
1.347
3.280
f1 (ppm)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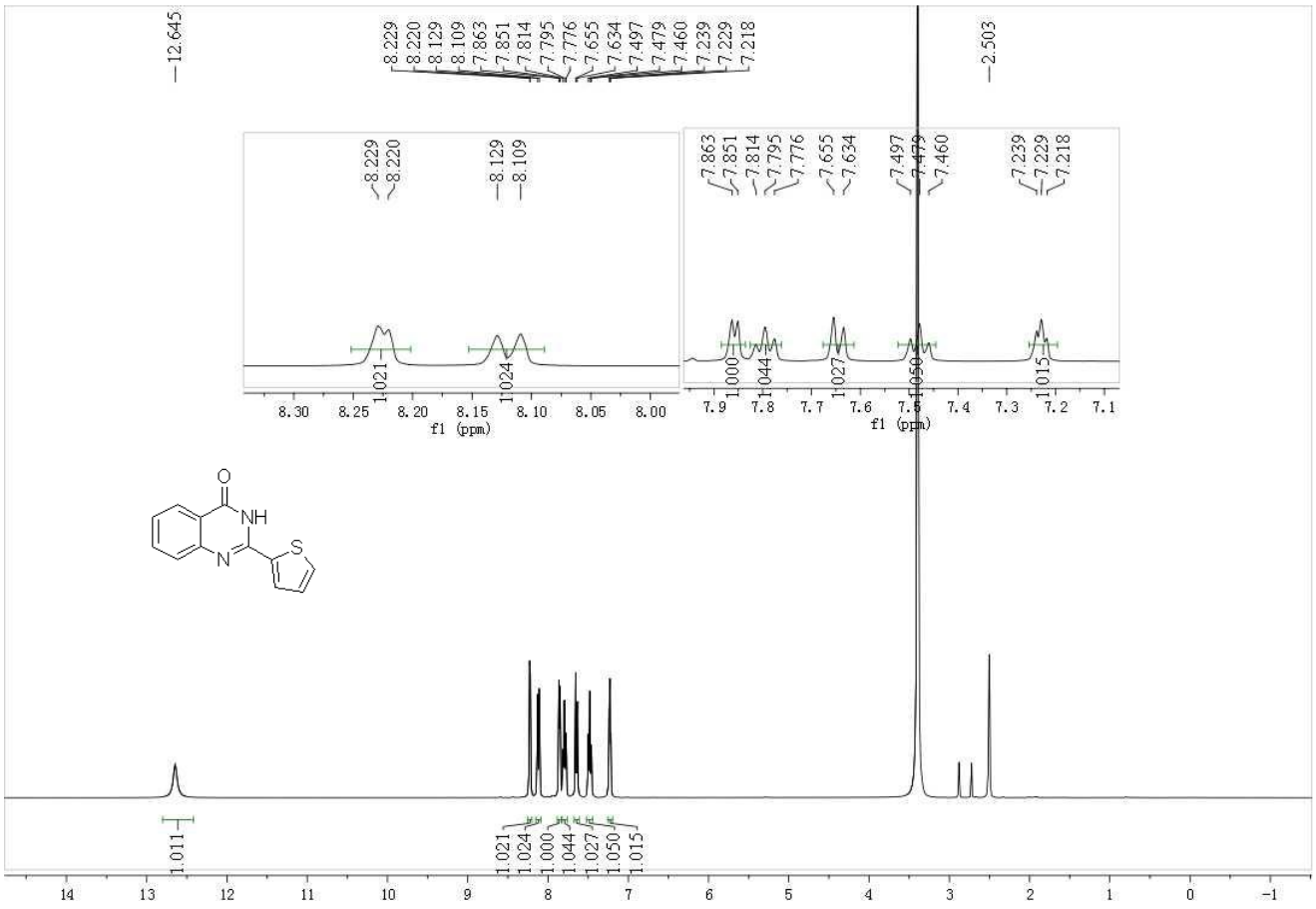
154.149
149.199
135.022
133.600
132.181
130.864
130.718
128.818
128.164
127.945
127.557
127.284
126.853
126.337
125.678
125.555
121.702
40.570
40.361
40.152
39.735
39.526
39.317
f1 (ppm)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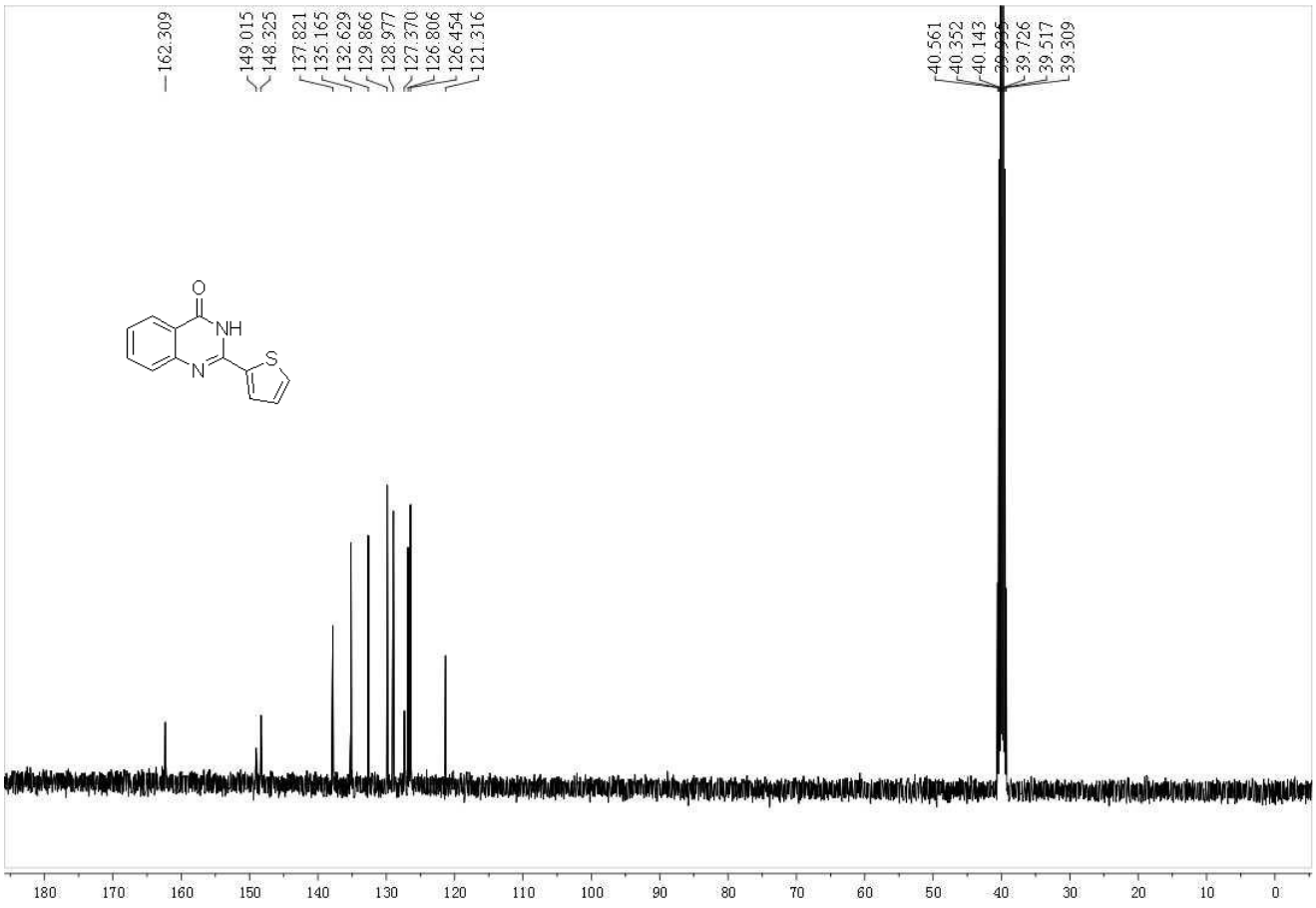
8.220
8.129
8.109
7.863
7.851
7.814
7.795
7.776
7.655
7.634
7.497
7.479
7.460
7.239
7.229
7.218
2.503
1.011
1.021
1.024
1.000
1.044
1.027
1.050
1.015
f1 (ppm)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137.821
135.165
132.629
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128.977
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126.806
126.454
121.316
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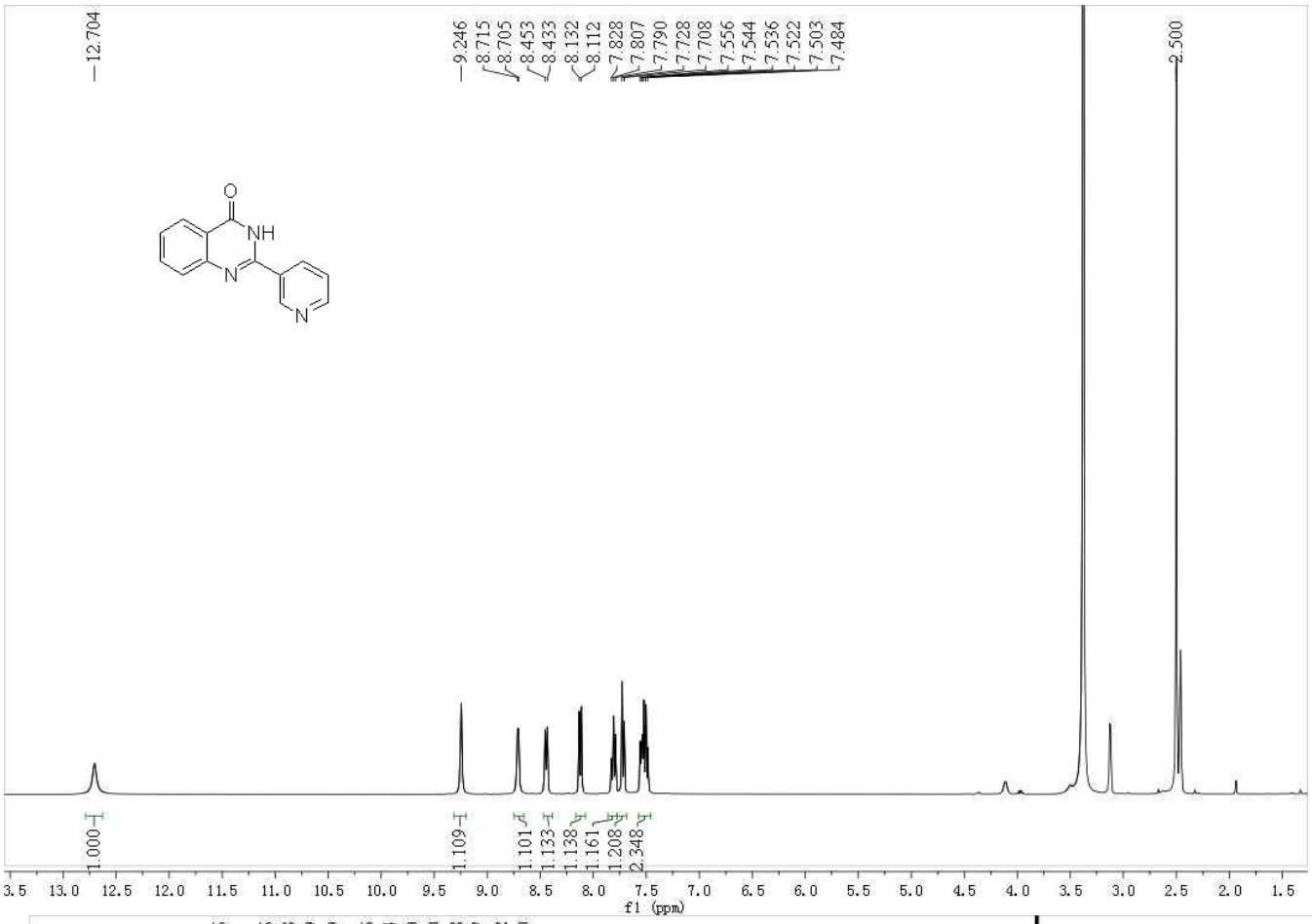
40.352
40.143
39.726
39.517
39.309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9.246
8.715
8.705
8.453
8.433
8.132
8.112
7.828
7.807
7.790
7.728
7.708
7.556
7.544
7.536
7.522
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7.484
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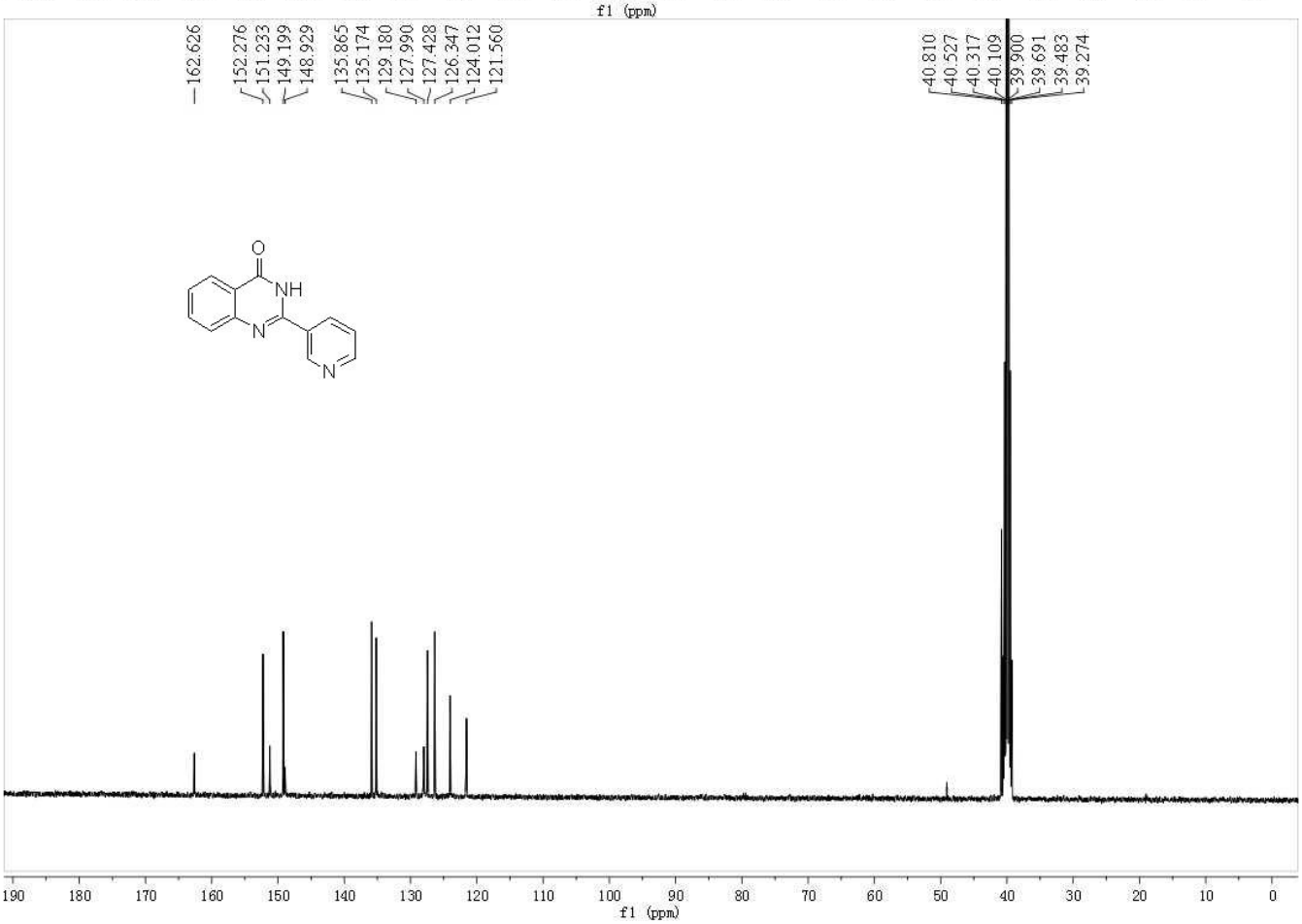
1.000
1.109
1.101
1.133
1.138
1.161
1.208
2.348
f1 (ppm)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151.233
149.199
148.929
135.865
135.174
129.180
127.990
127.428
126.347
124.012
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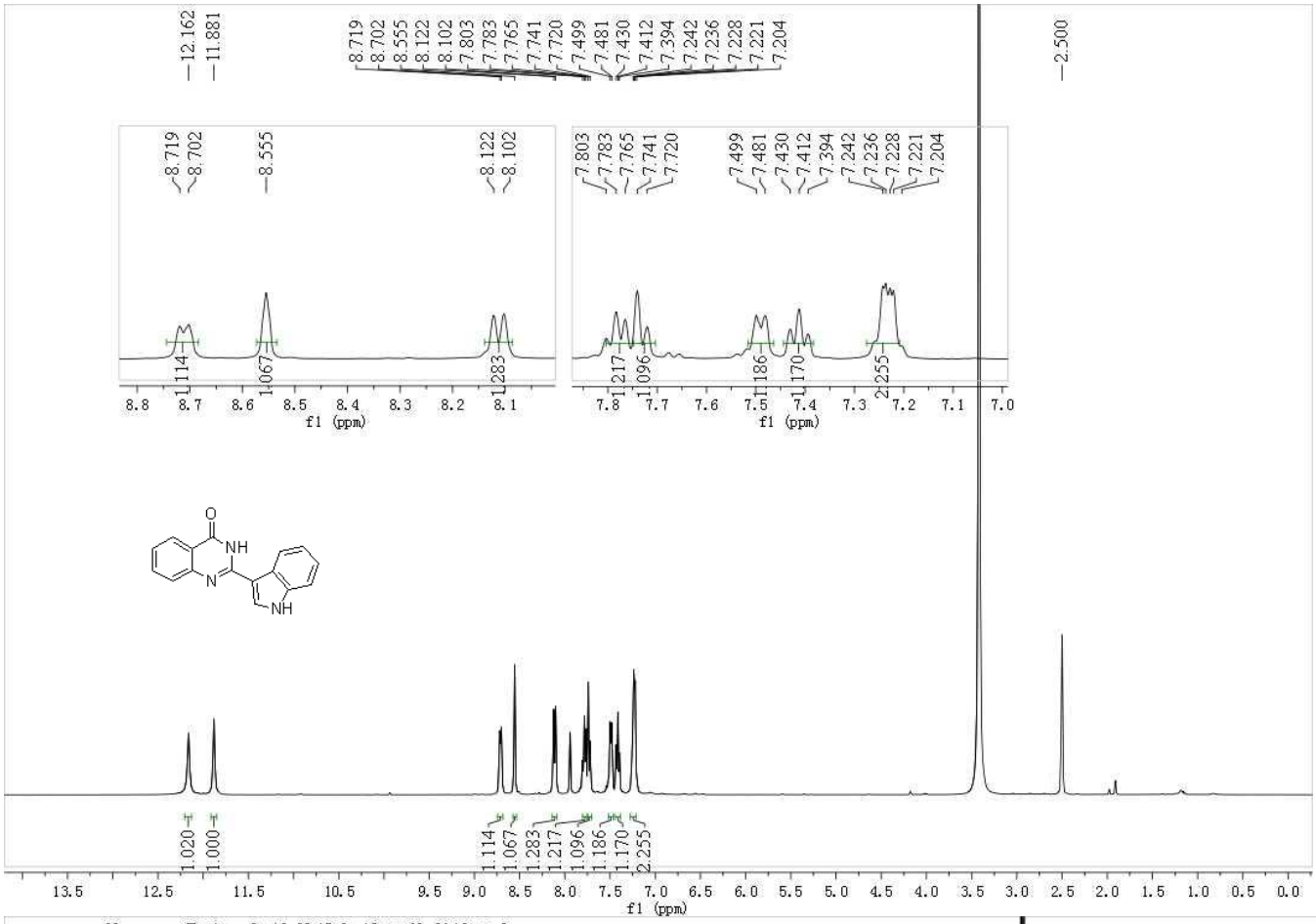
40.810
40.527
40.317
40.109
39.900
39.691
39.483
39.274
f1 (ppm)


12.162
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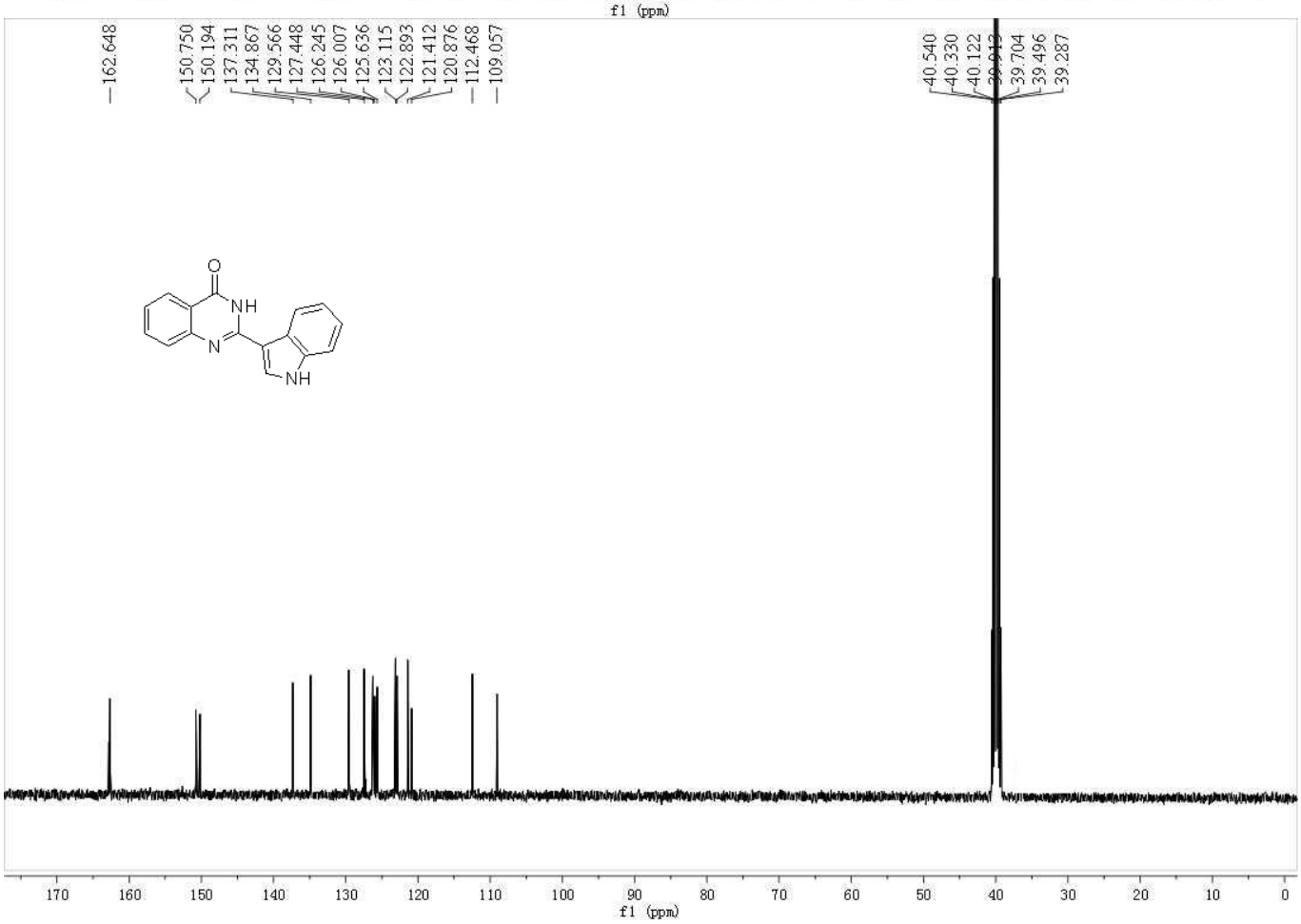
8.719
8.702
8.555
8.122
8.102
7.803
7.783
7.765
7.741
7.720
7.499
7.481
7.430
7.412
7.394
7.242
7.236
7.228
7.221
7.204
2.500
1.114
1.067
1.283
1.217
1.096
1.186
1.170
2.255
f1 (ppm)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137.311
134.867
129.566
127.448
126.245
126.007
125.636
123.115
122.893
121.412
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112.468
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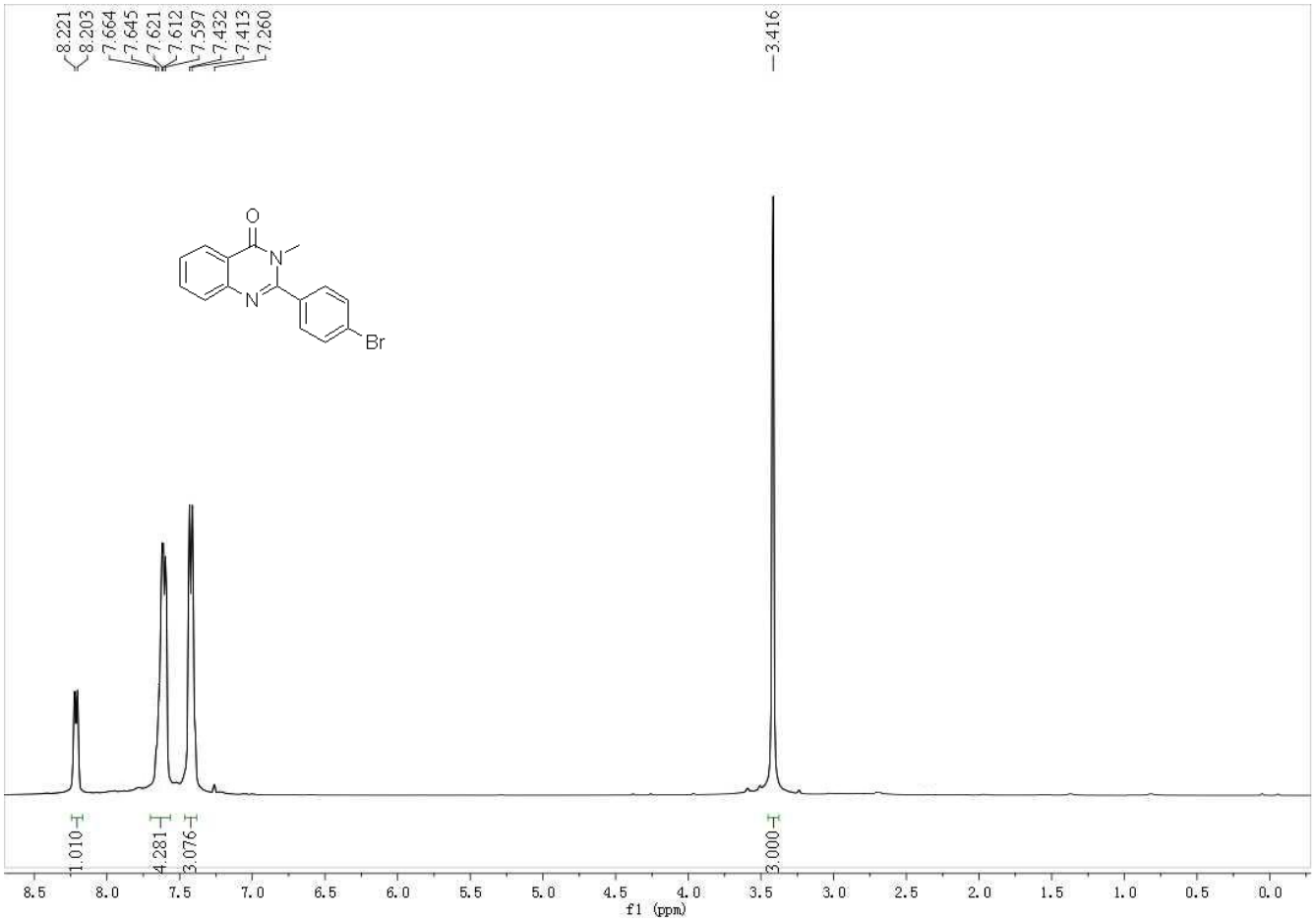
40.540
40.330
40.122
39.704
39.496
39.287
f1 (ppm)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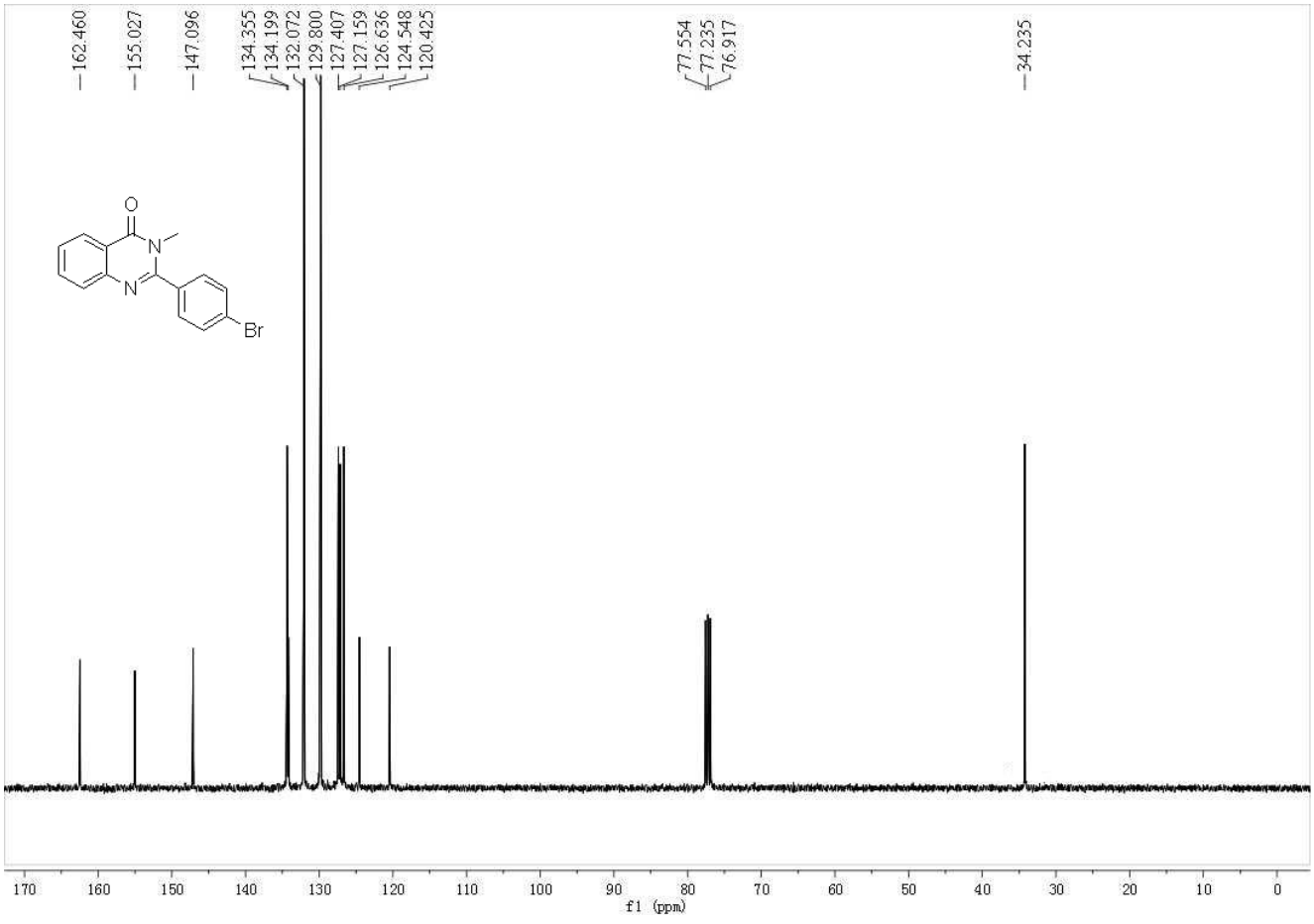
8.203
7.664
7.645
7.621
7.612
7.597
7.432
7.413
7.260
3.416
O
N
N
Br
1.010
4.281
3.076
3.000
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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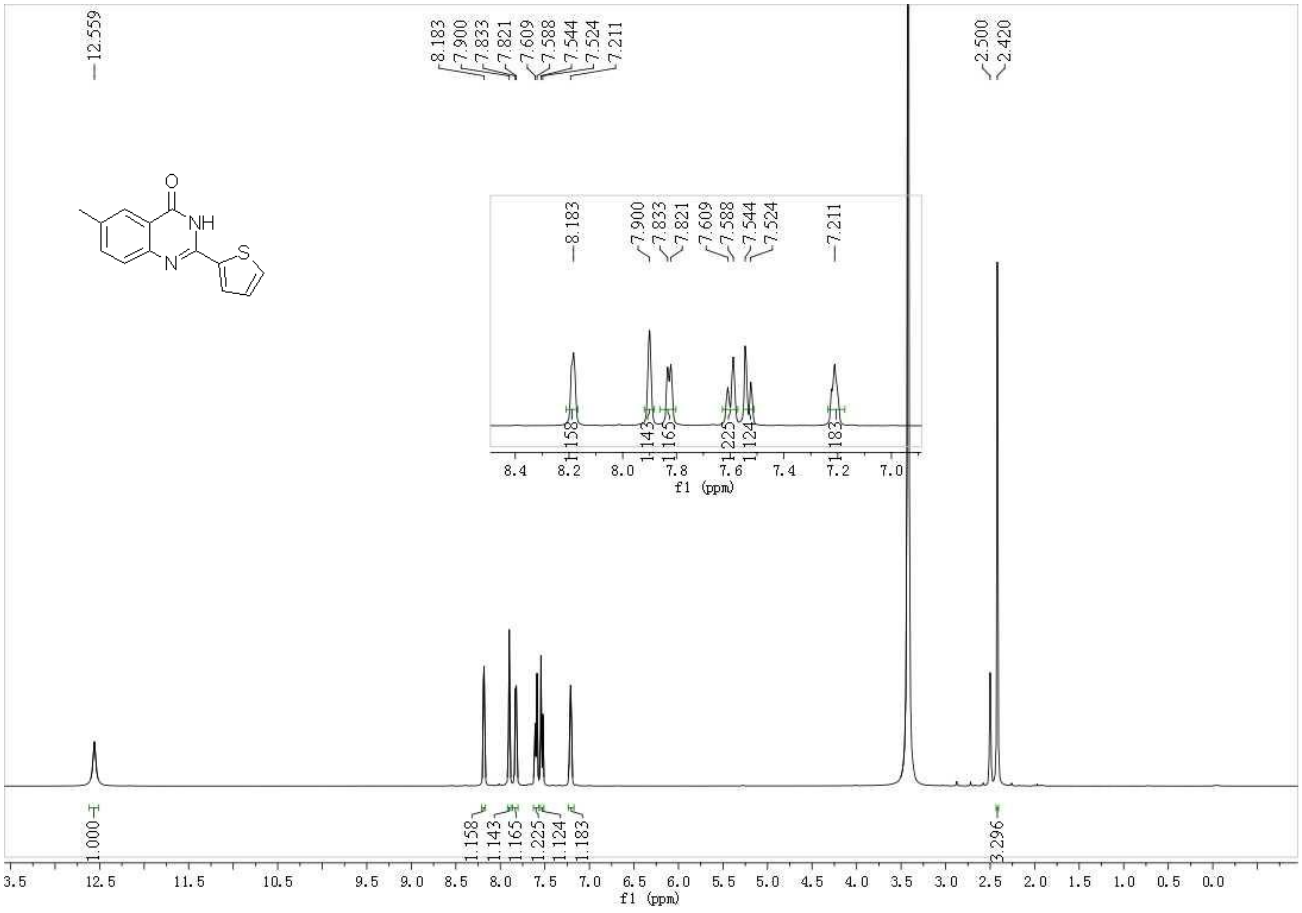
132.072
129.800
127.407
127.159
126.636
124.548
120.425
77.554
77.235
76.917
34.235
O
N
N
Br
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.833
7.821
7.609
7.588
7.544
7.524
7.211
2.500
2.420
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NH
N
S
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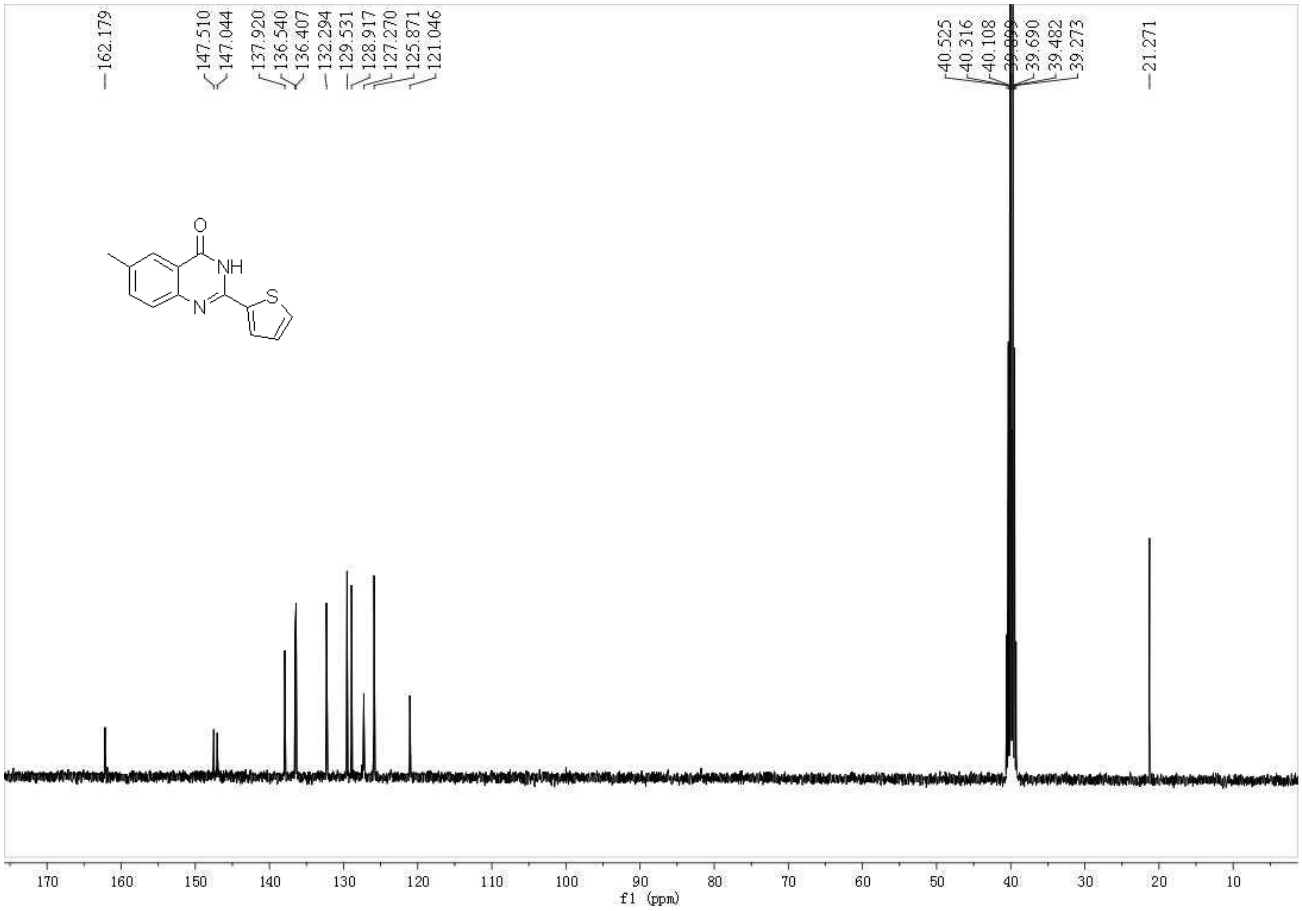
1.143
1.165
1.225
1.124
1.183
3.296
f1 (ppm)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147.044
137.920
136.540
136.407
132.294
129.531
128.917
127.270
125.871
121.046
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40.108
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39.482
39.273
21.271
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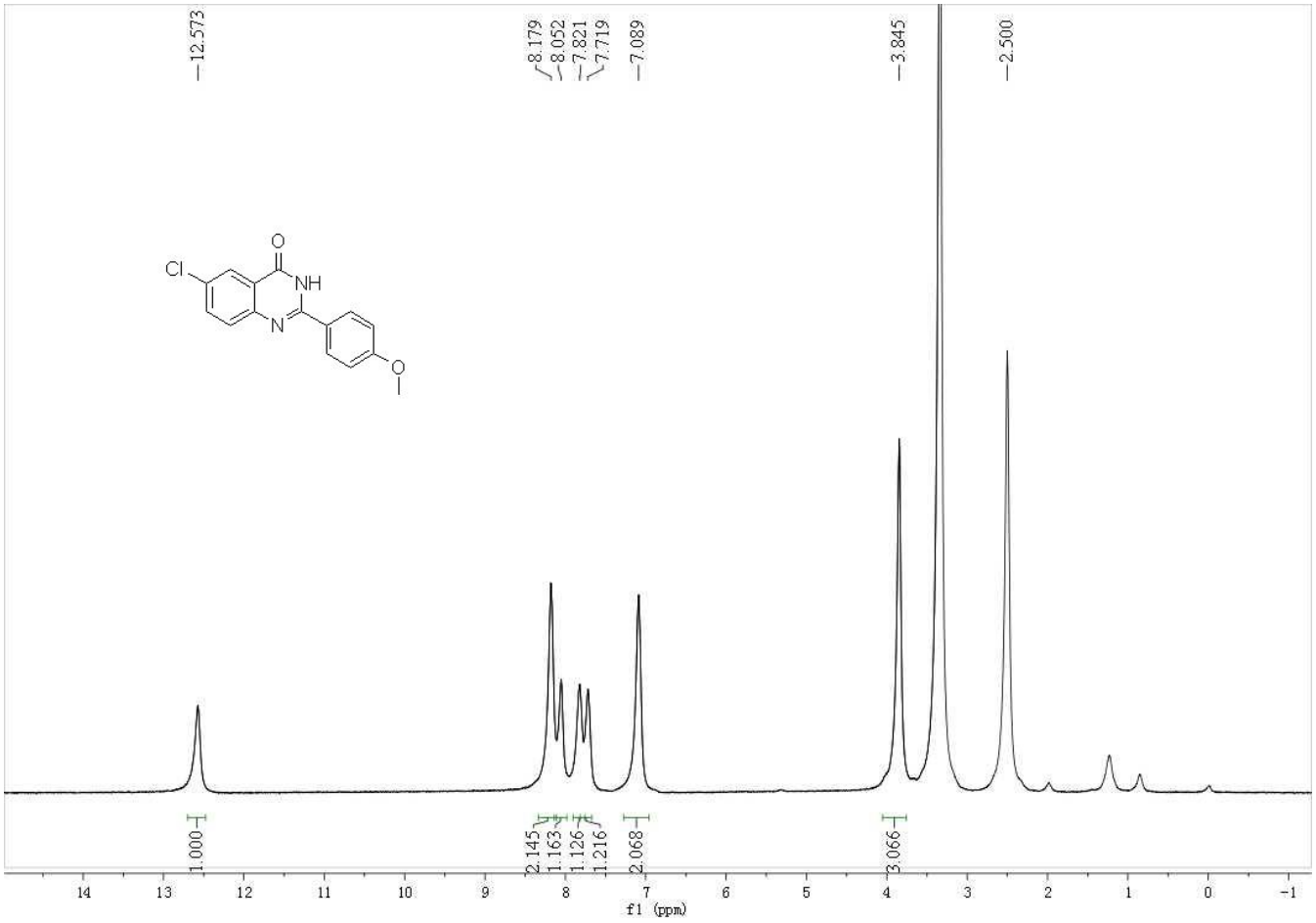
NH
N
S
f1 (ppm)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7.821
7.719
7.089
3.845
2.500
Cl
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NH
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O
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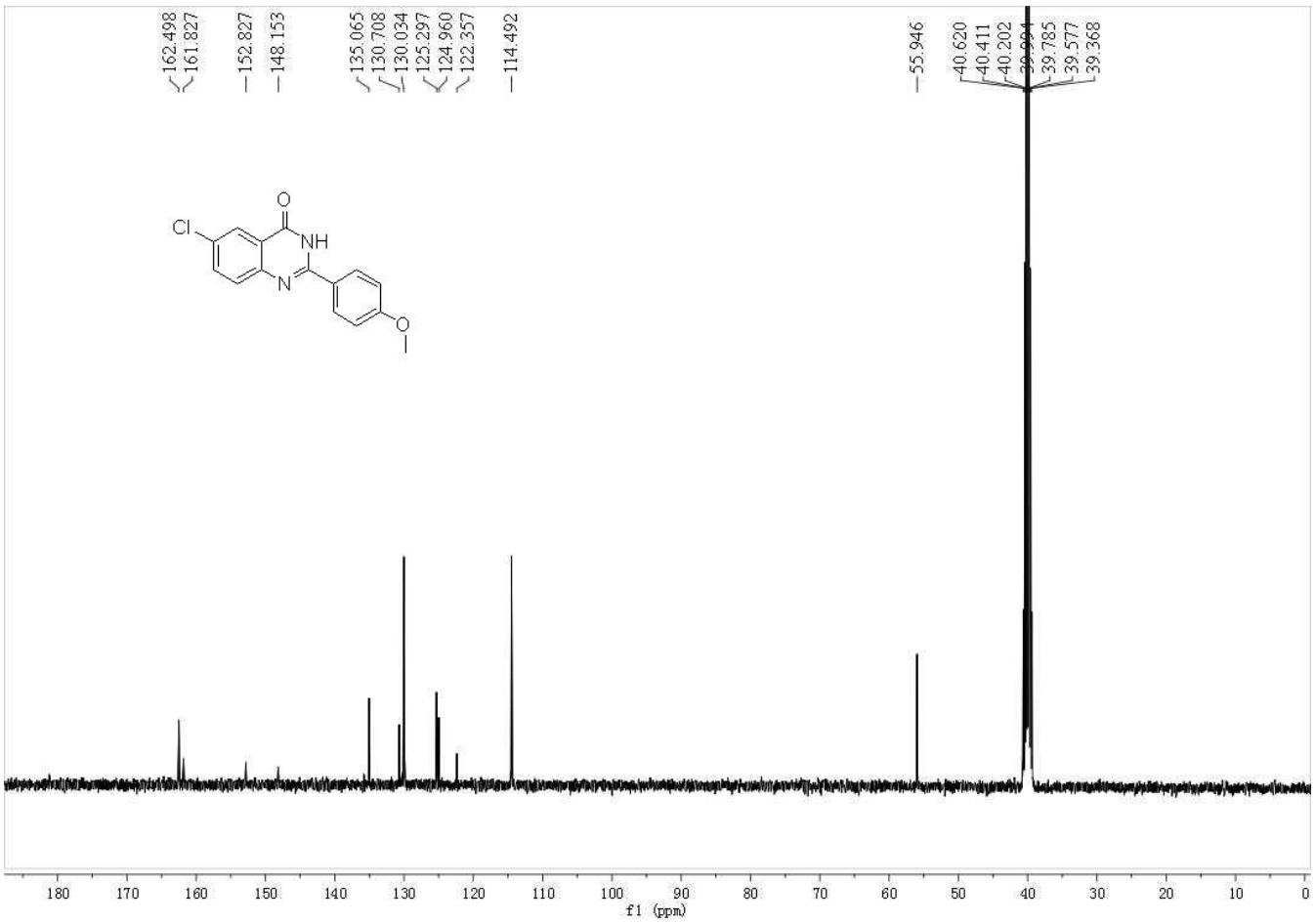
1.163
1.126
1.216
2.068
3.066
f1 (ppm)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148.153
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130.034
125.297
124.960
122.357
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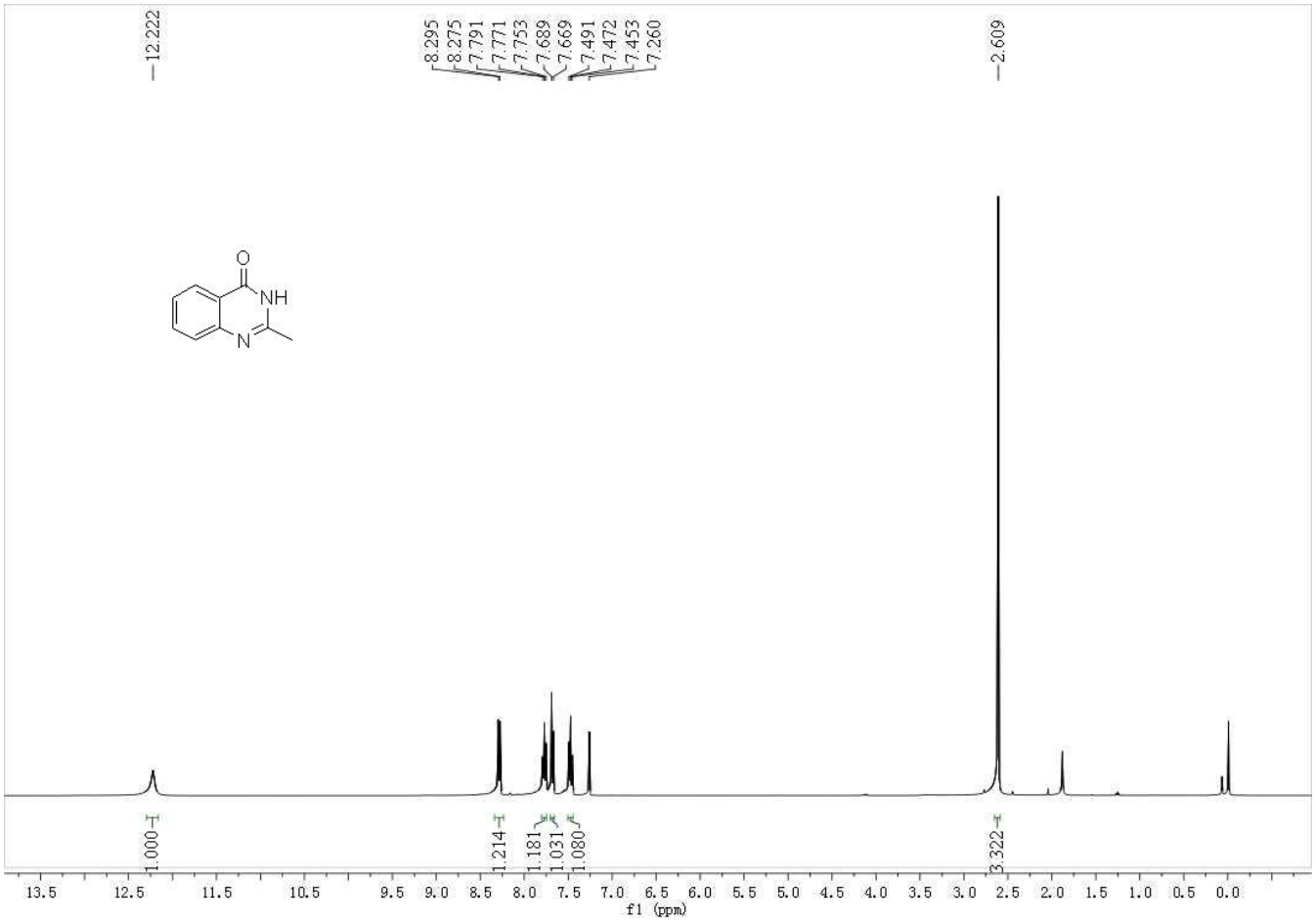
40.411
40.202
39.785
39.577
39.368
Cl
O
NH
N
O
f1 (ppm)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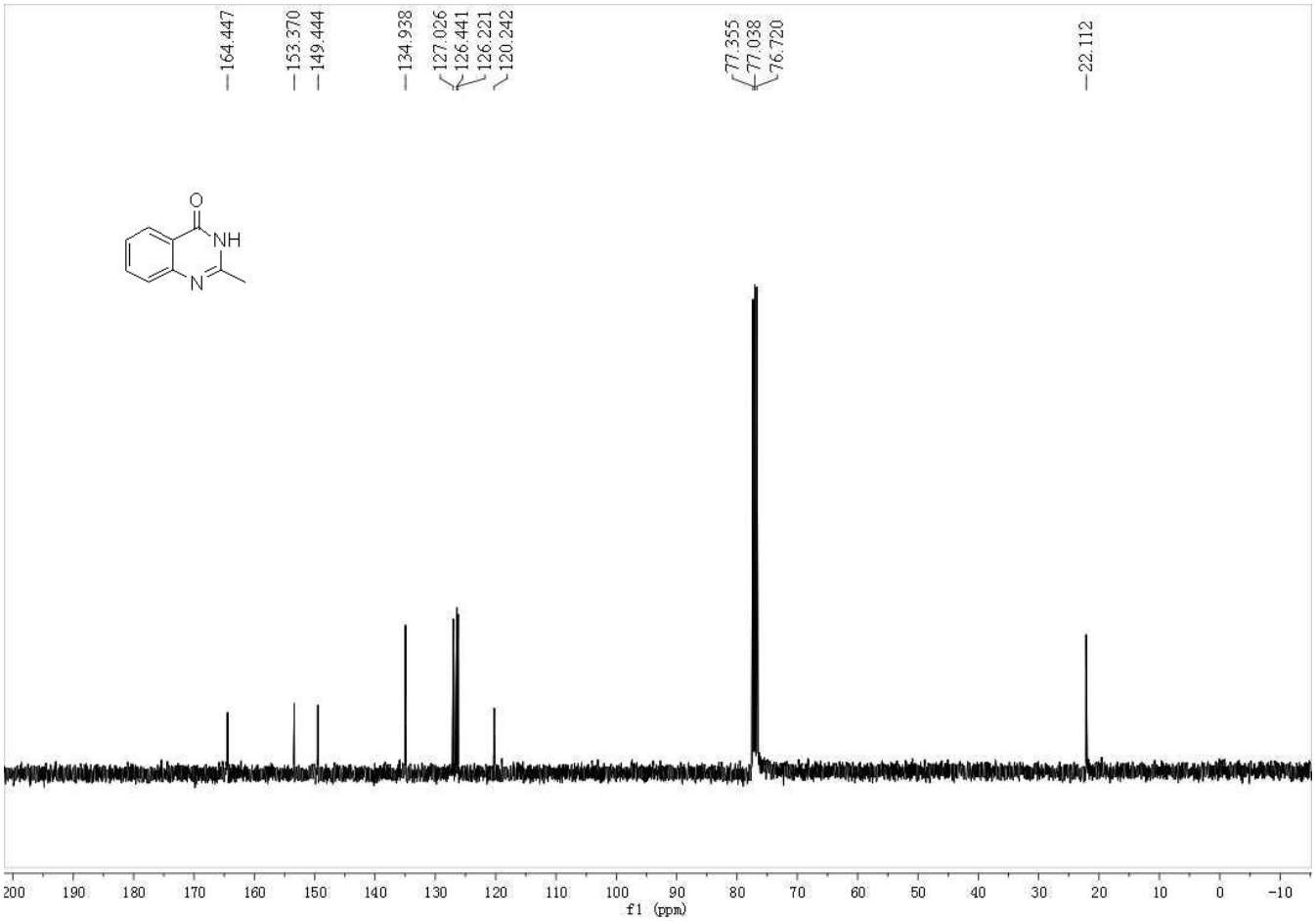
7.771
7.753
7.689
7.669
7.491
7.472
7.453
7.260
2.609
O
NH
N
1.000
1.214
1.181
1.031
1.080
3.322
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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153.370
149.444
134.938
127.026
126.441
126.221
120.242
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77.038
76.720
22.112
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NH
N
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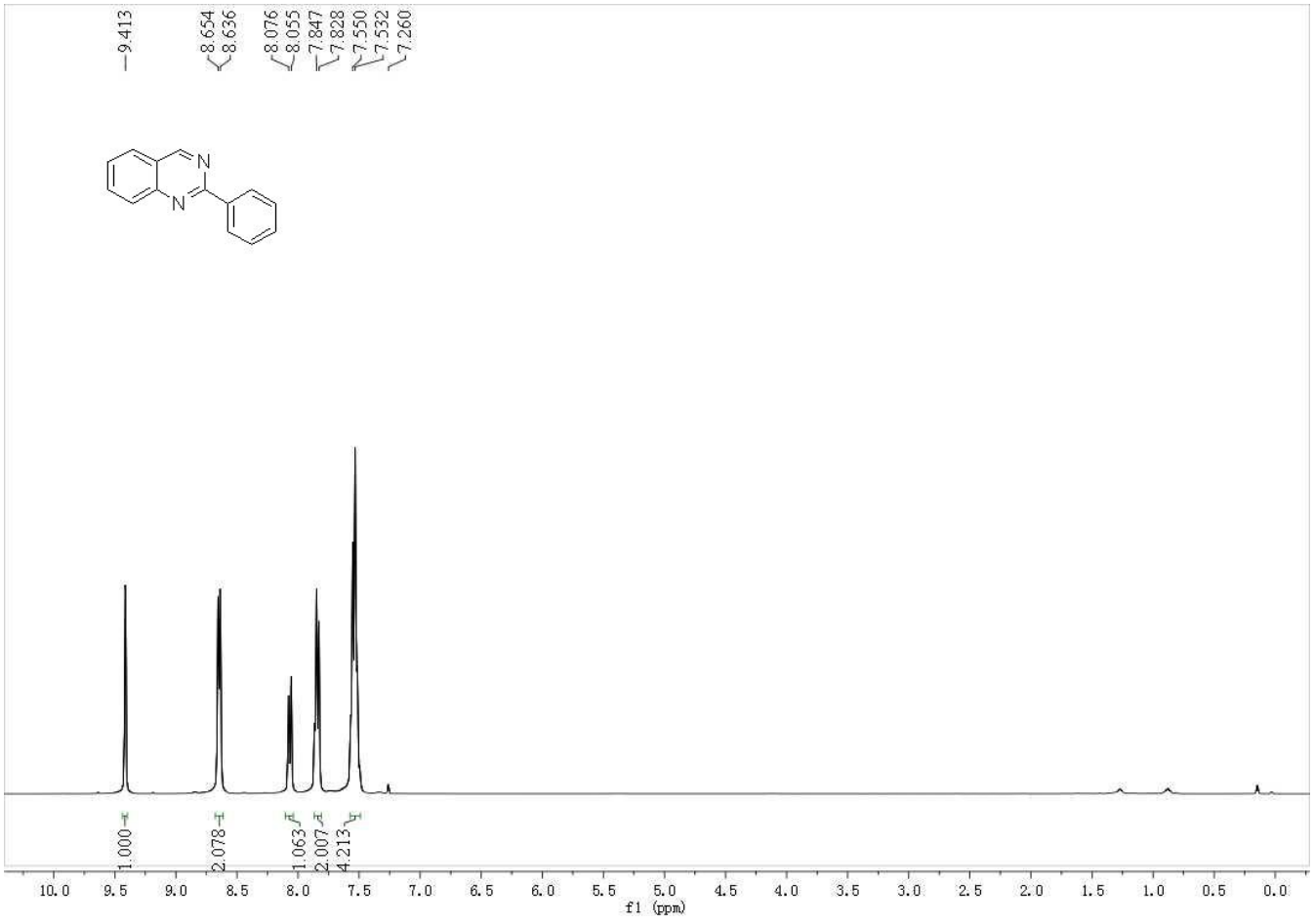
f1 (ppm)


9.413
8.654
8.636
8.076
8.055
7.847
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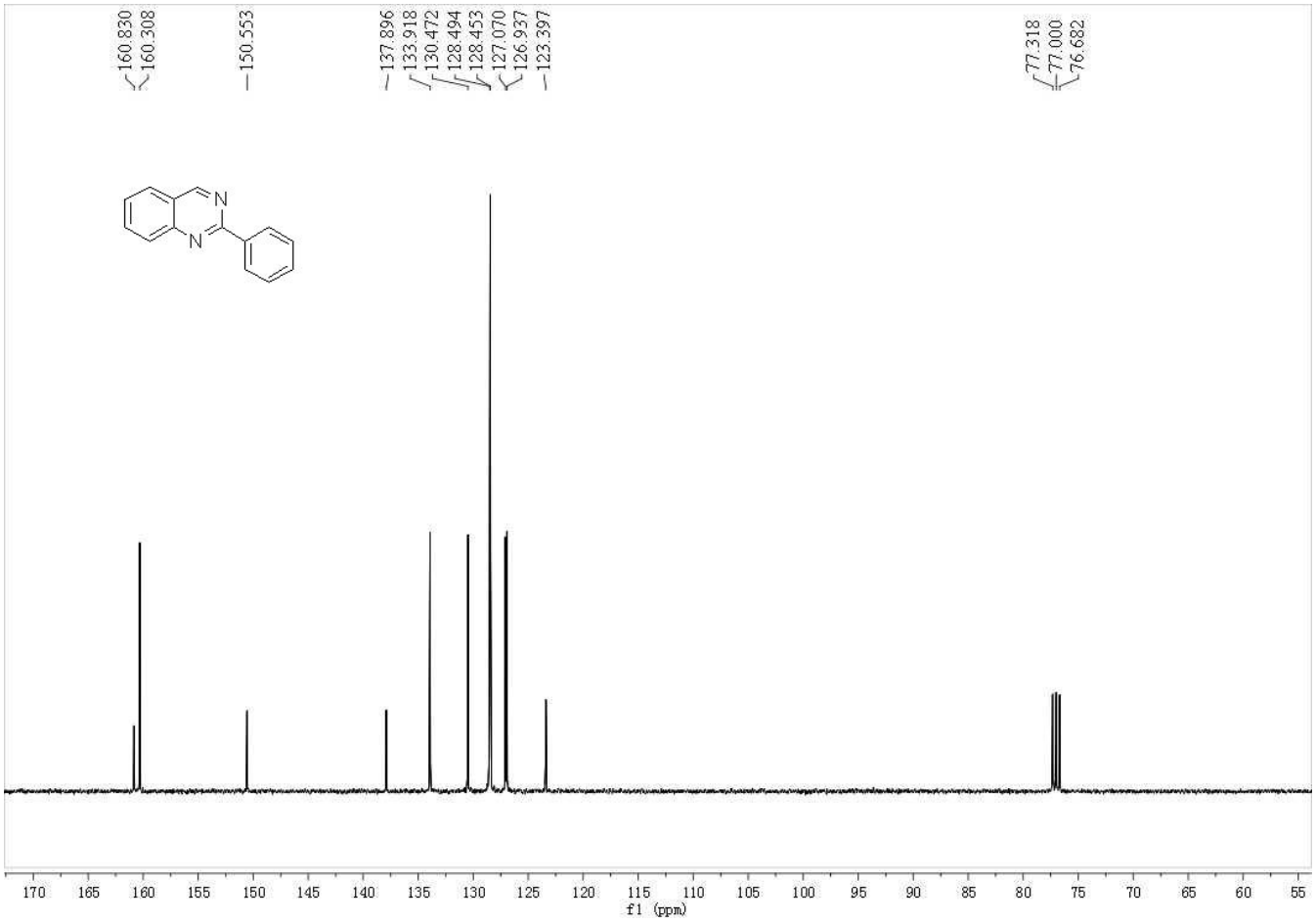
7.550
7.532
7.260
1.000
2.078
1.063
2.007
4.213
f1 (ppm)


160.830
160.308
150.553
137.896
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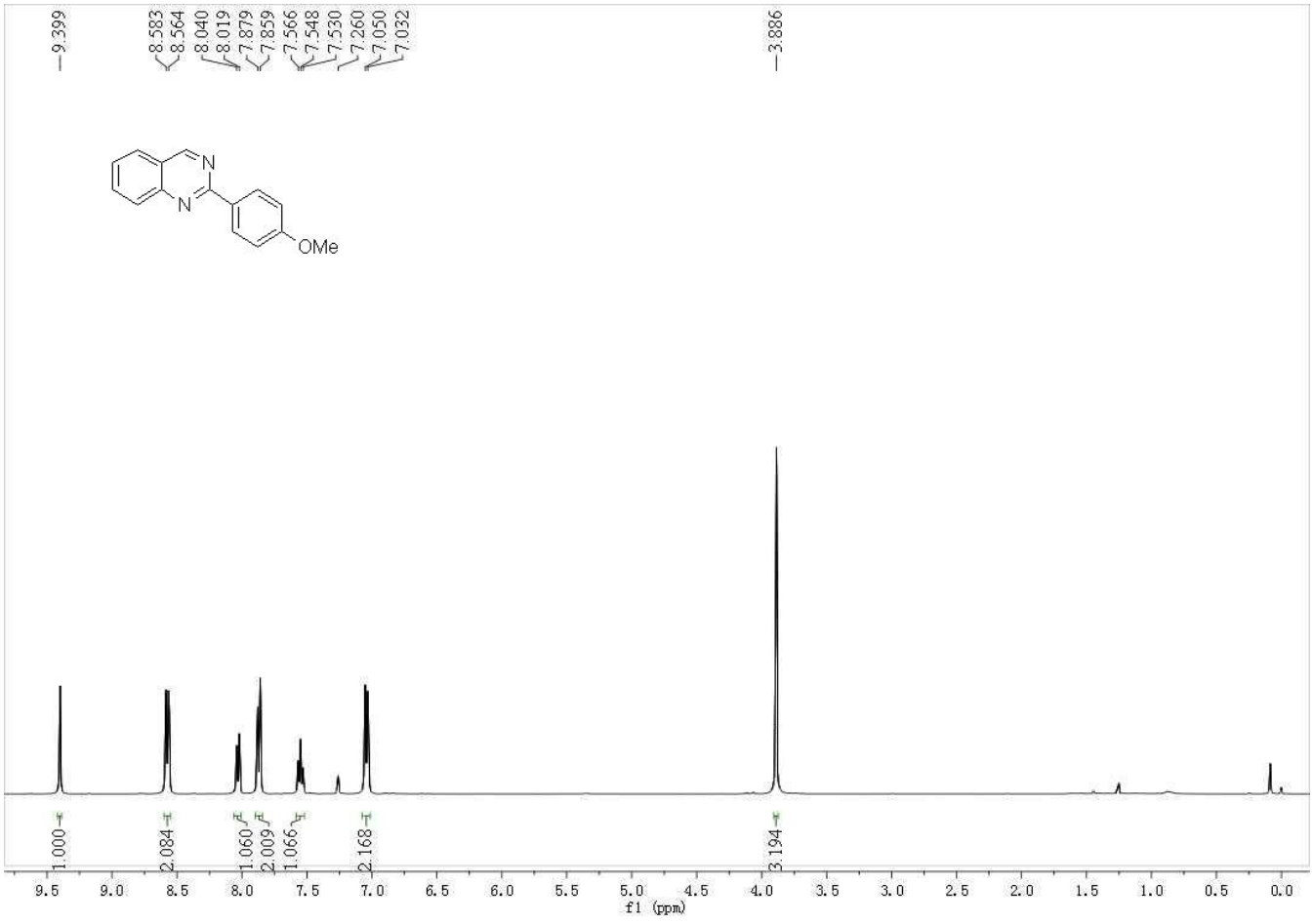
130.472
128.494
128.453
127.070
126.937
123.397
77.318
77.000
76.682
f1 (ppm)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8.564
8.040
8.019
7.879
7.859
7.566
7.548
7.530
7.260
7.050
7.032
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N
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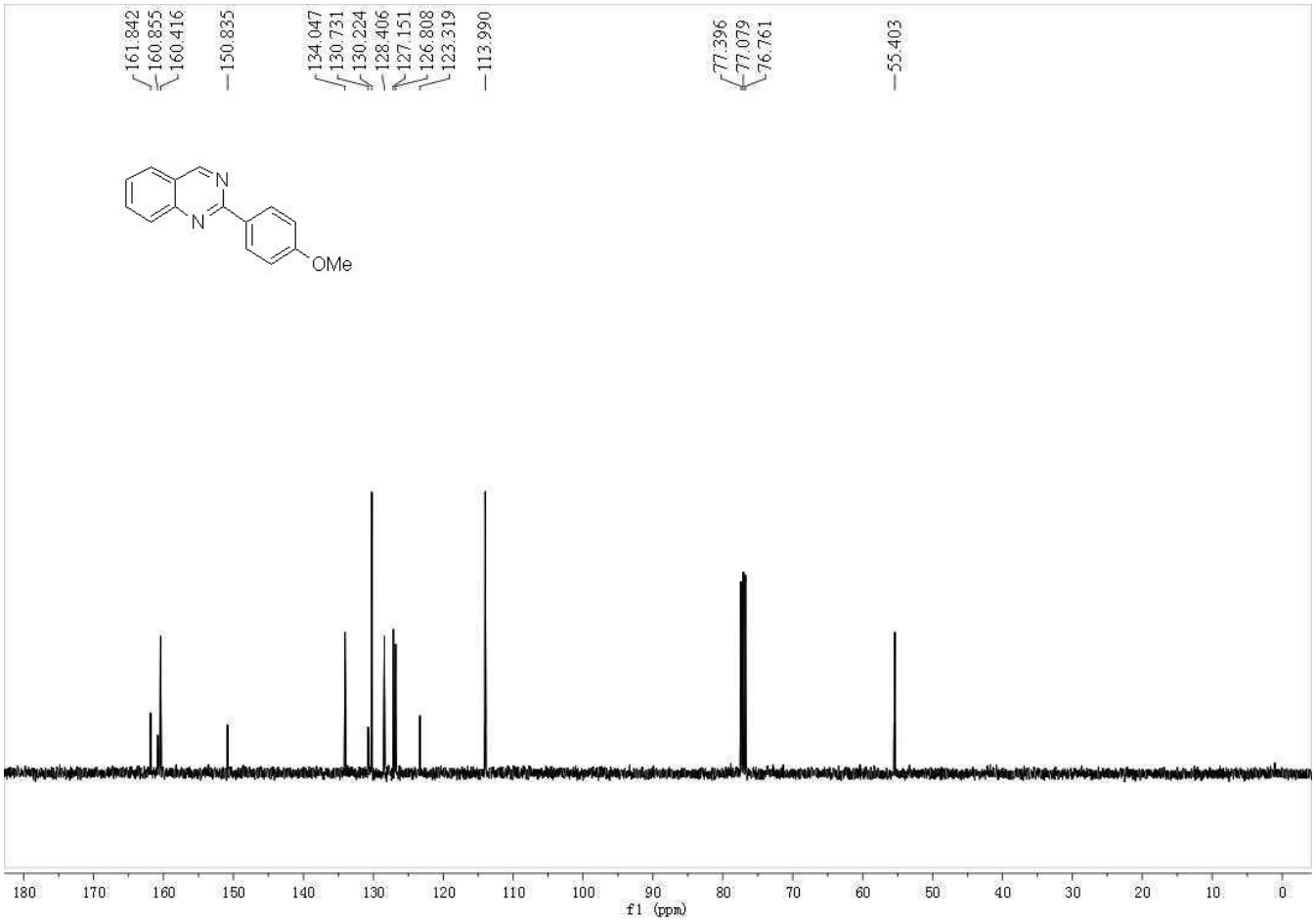
1.060
2.009
1.066
2.168
3.194
f1 (ppm)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150.835
134.047
130.731
130.224
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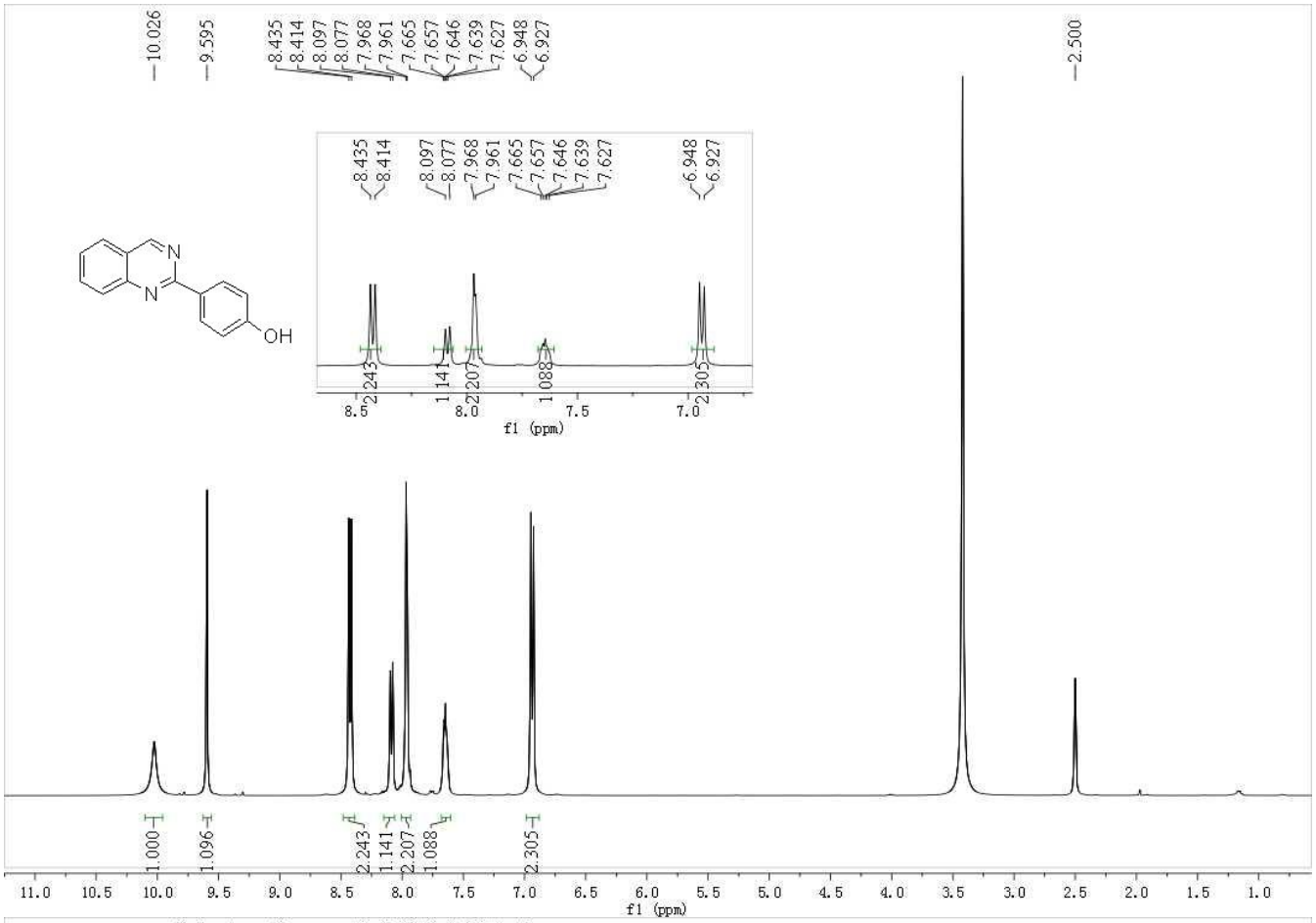
77.079
76.761
55.403
N
N
OMe
f1 (ppm)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9.595
8.435
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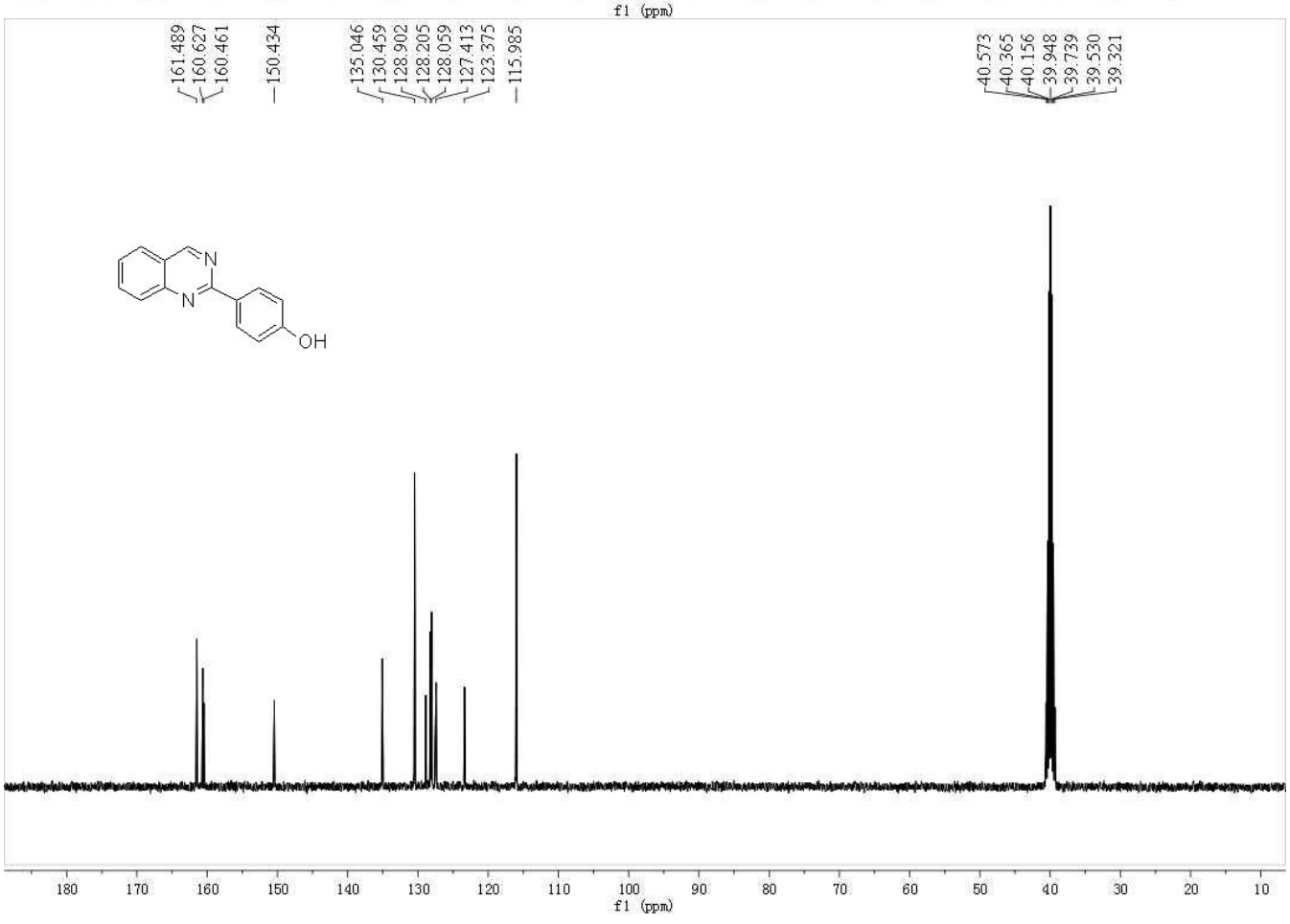
8.097
8.077
7.968
7.961
7.665
7.657
7.646
7.639
7.627
6.948
6.927
2.500
N
N
OH
1.000
1.096
2.243
1.141
2.207
1.088
2.305
f1 (ppm)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128.902
128.205
128.059
127.413
123.375
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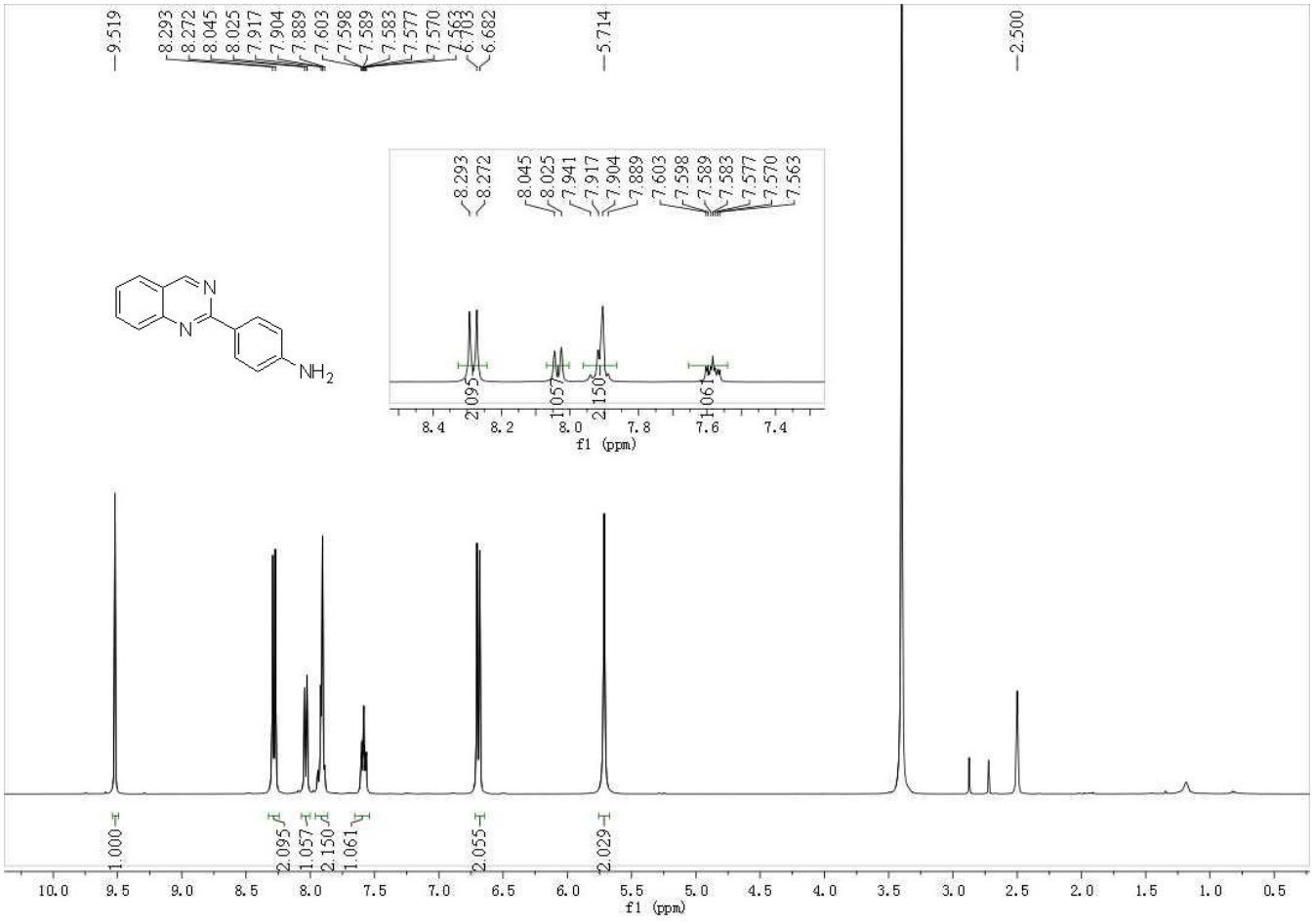
40.365
40.156
39.948
39.739
39.530
39.321
N
N
OH
f1 (ppm)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8.272
8.045
8.025
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7.889
7.603
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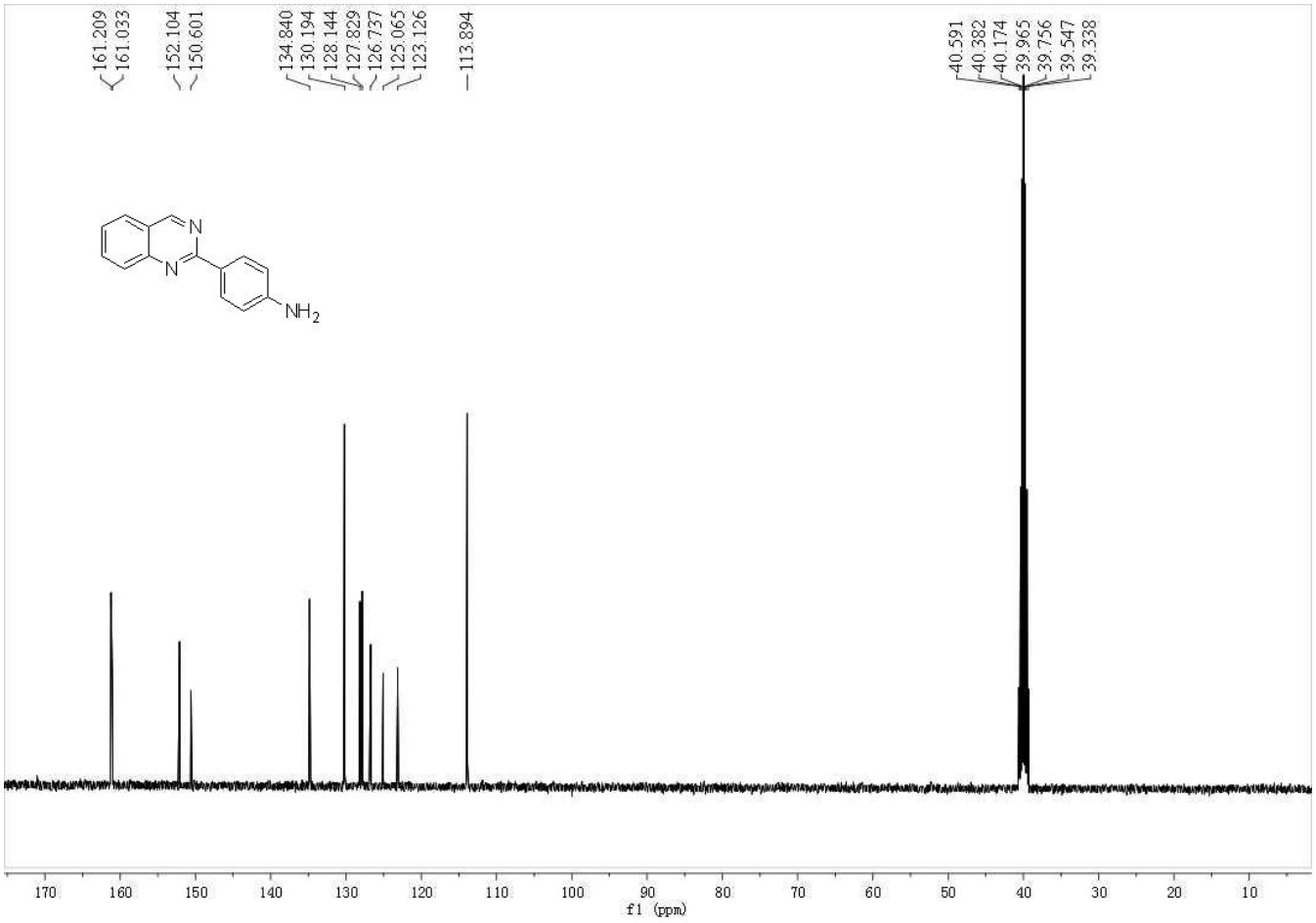
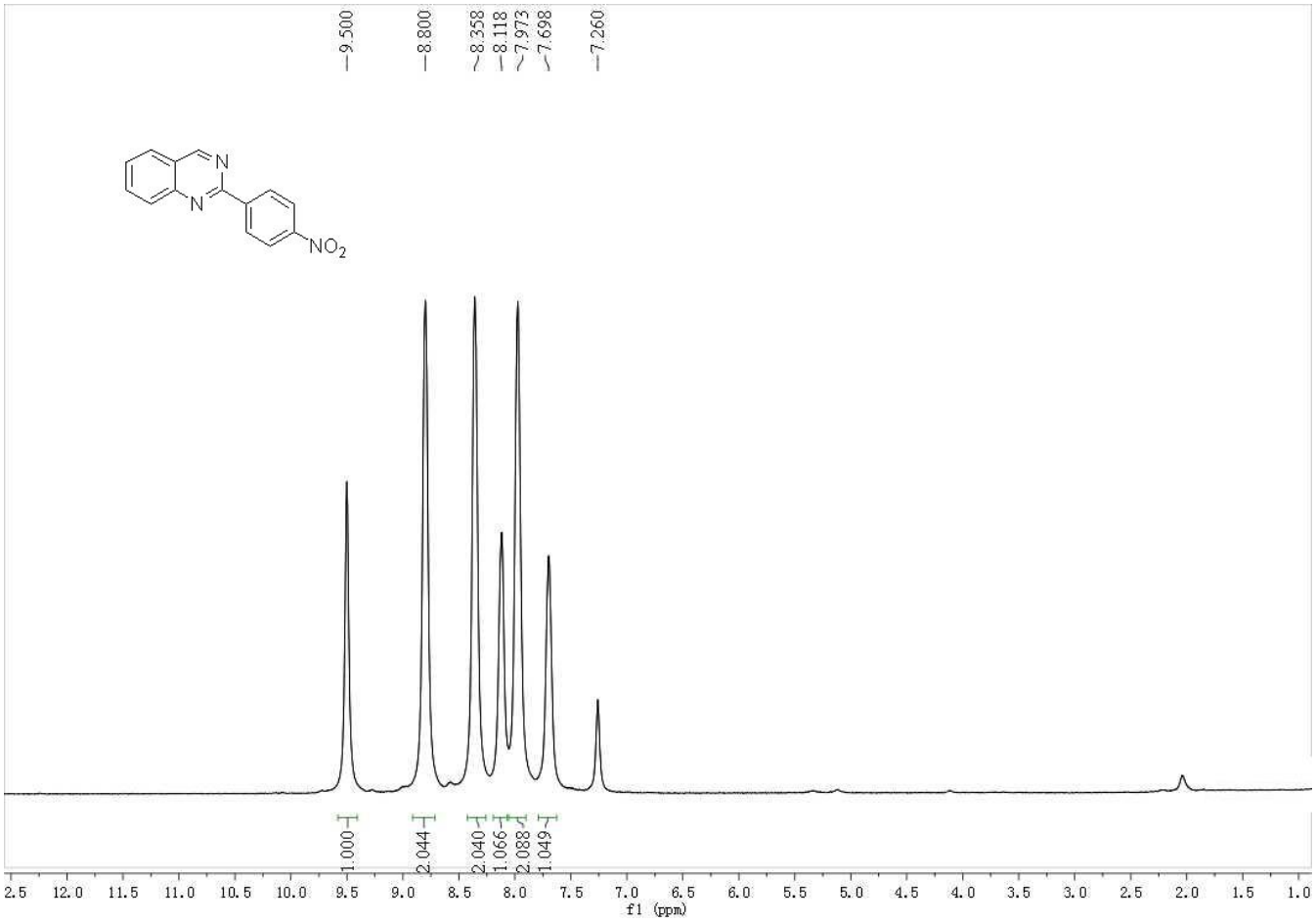
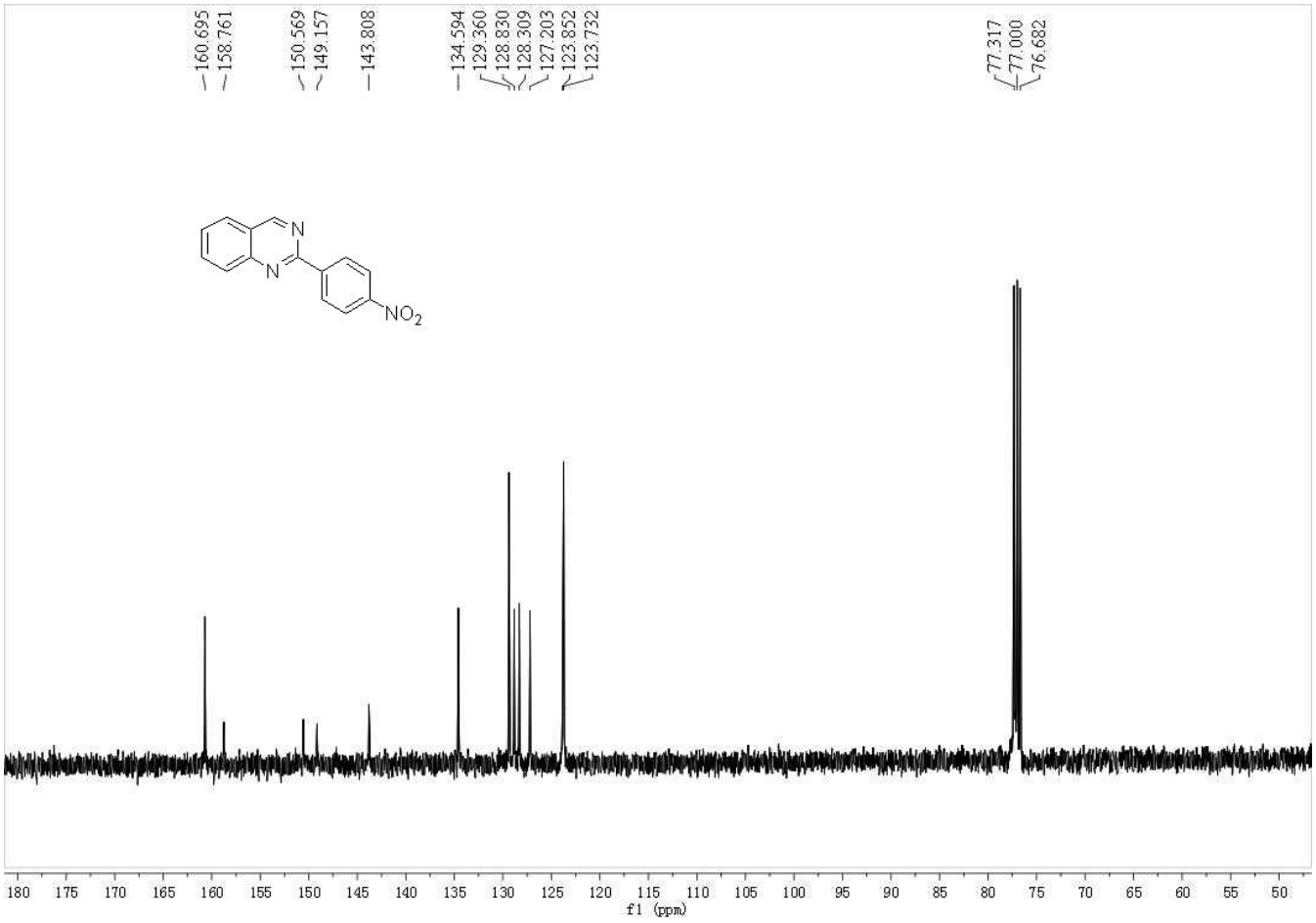
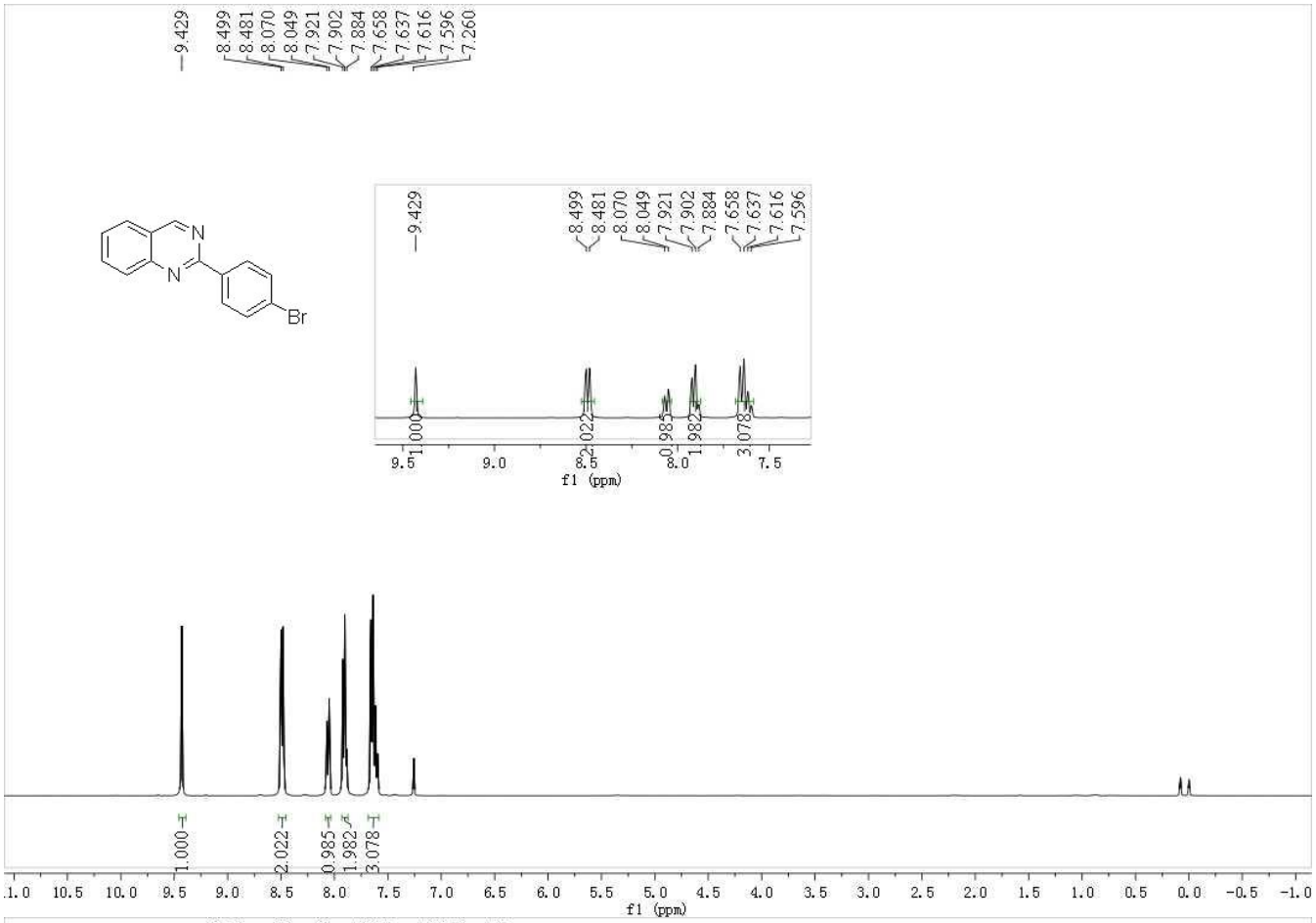
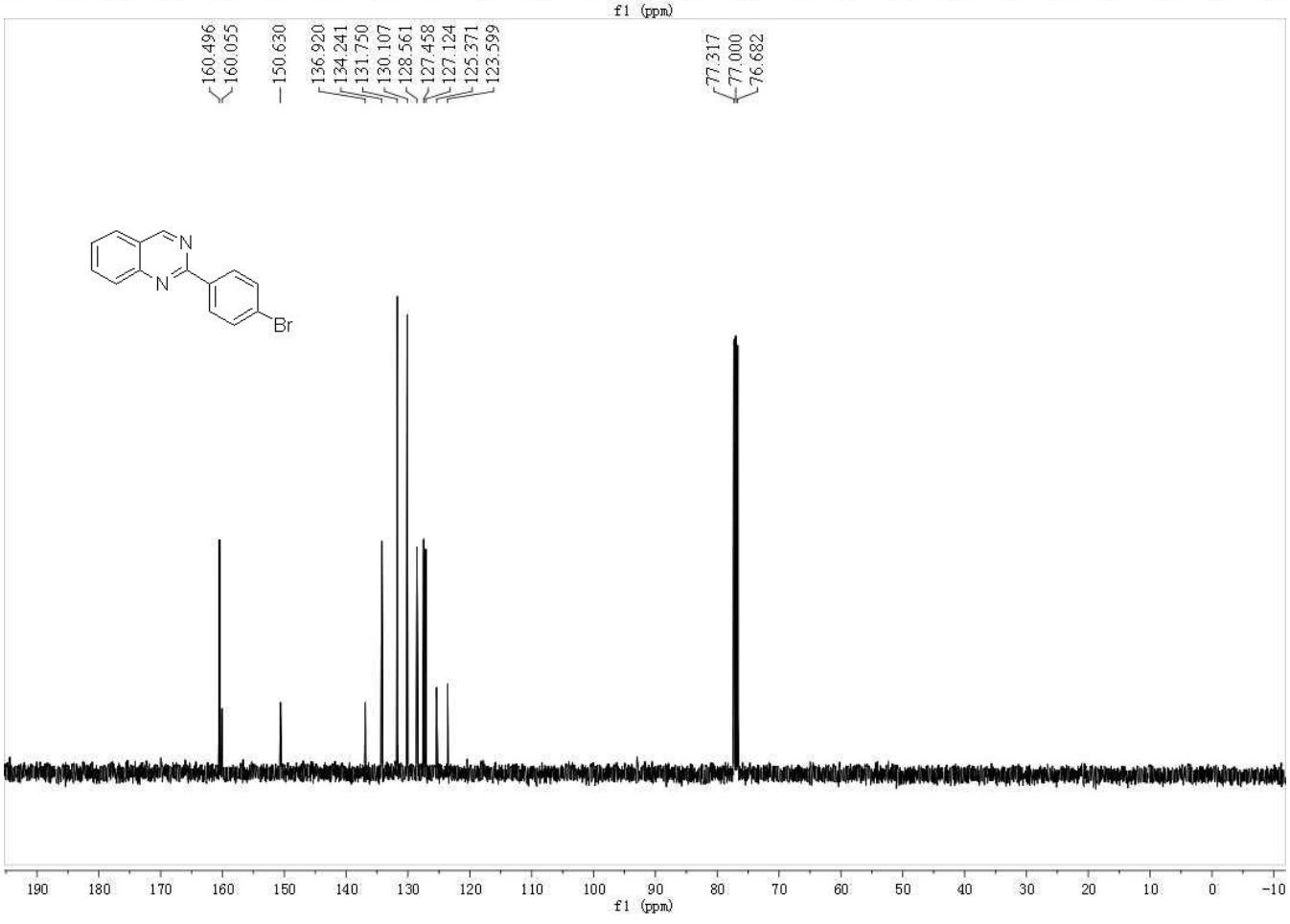
7.589
7.583
7.577
7.570
7.563
6.703
6.682
5.714
2.500
NH2
1.000
2.095
1.057
2.150
1.061
2.055
2.029
f1 (ppm)

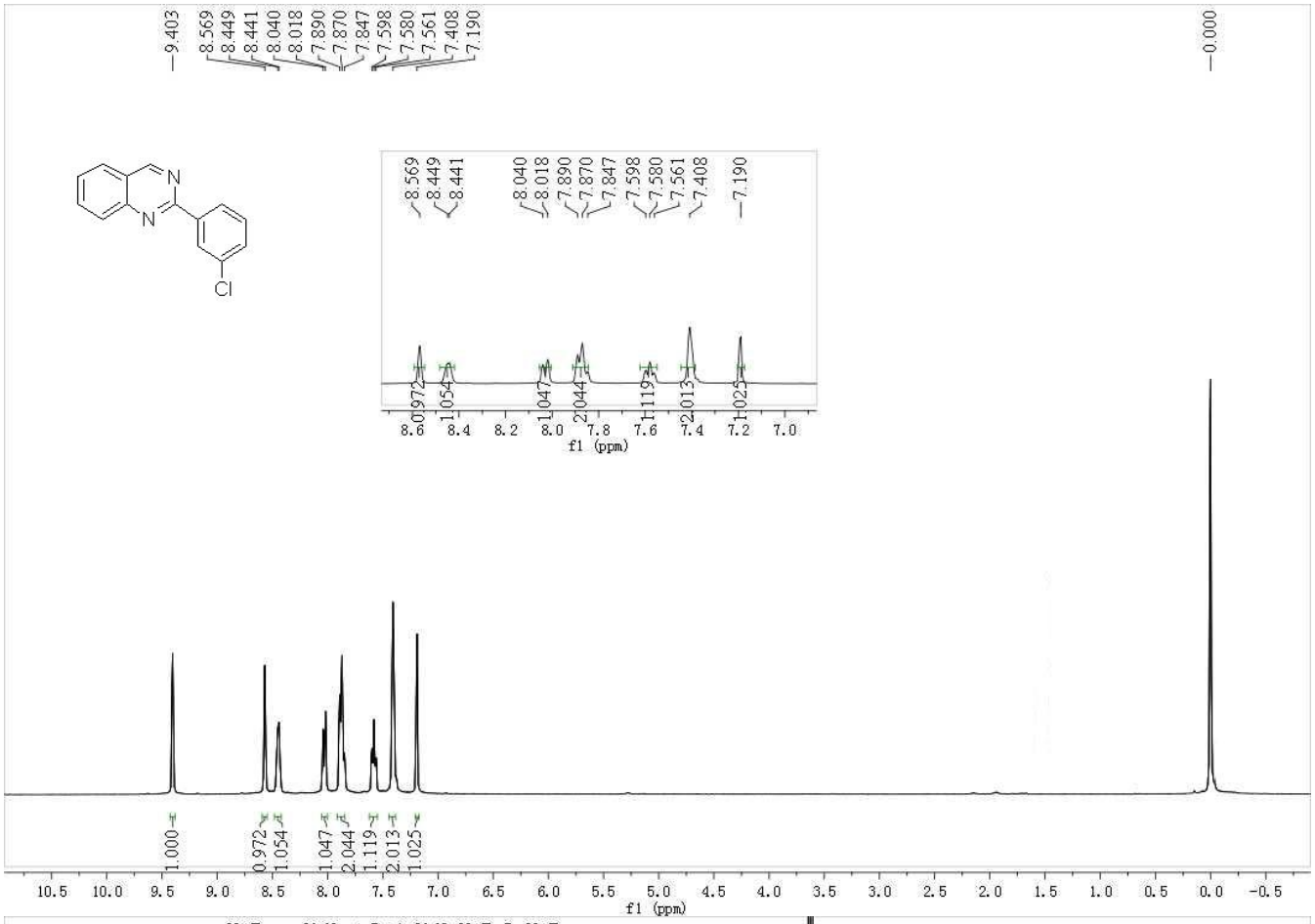

161.209
161.033
152.104
150.601
134.840
130.194
128.144
127.829
126.737
125.065
123.126
113.894
40.591
40.382
40.174
39.965
39.756
39.547
39.338
NH2
f1 (ppm)

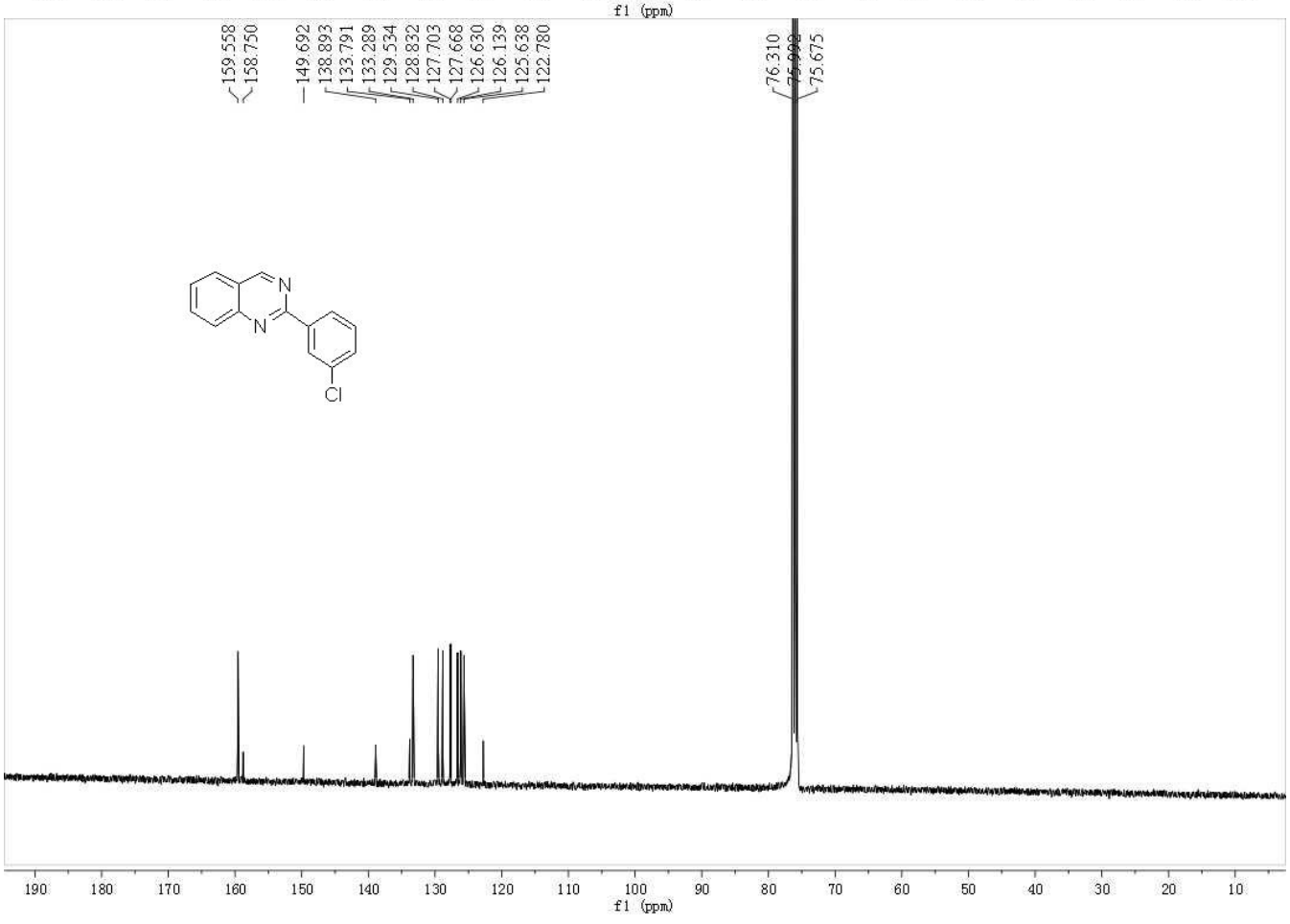

9.500
8.800
8.358
8.118
7.973
7.698
7.260
1.000
2.044
2.040
1.066
2.088
1.049
f1 (ppm)

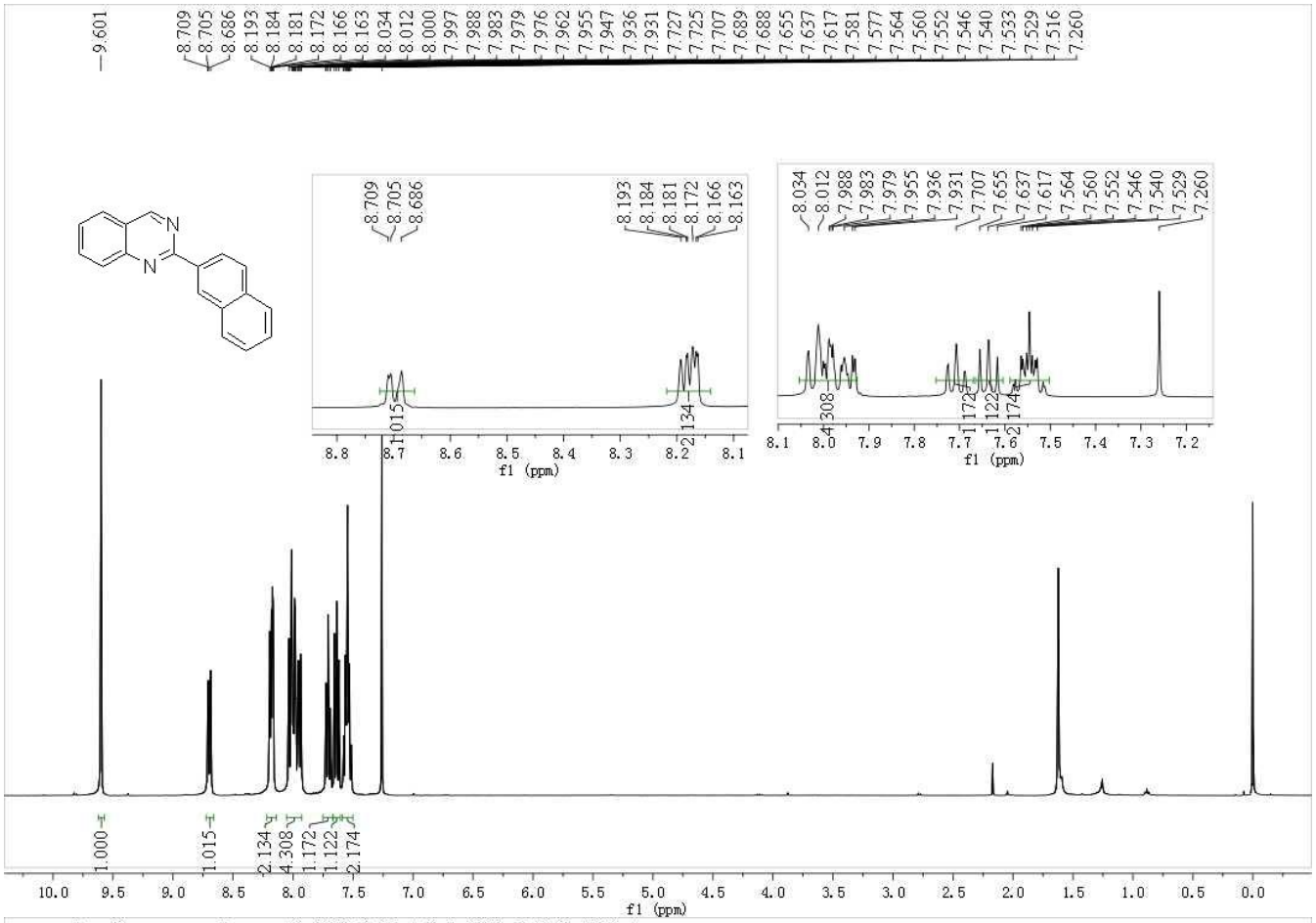

160.695
158.761
150.569
149.157
143.808
134.594
129.360
128.830
128.309
127.203
123.852
123.732
77.317
77.000
76.682
f1 (ppm)

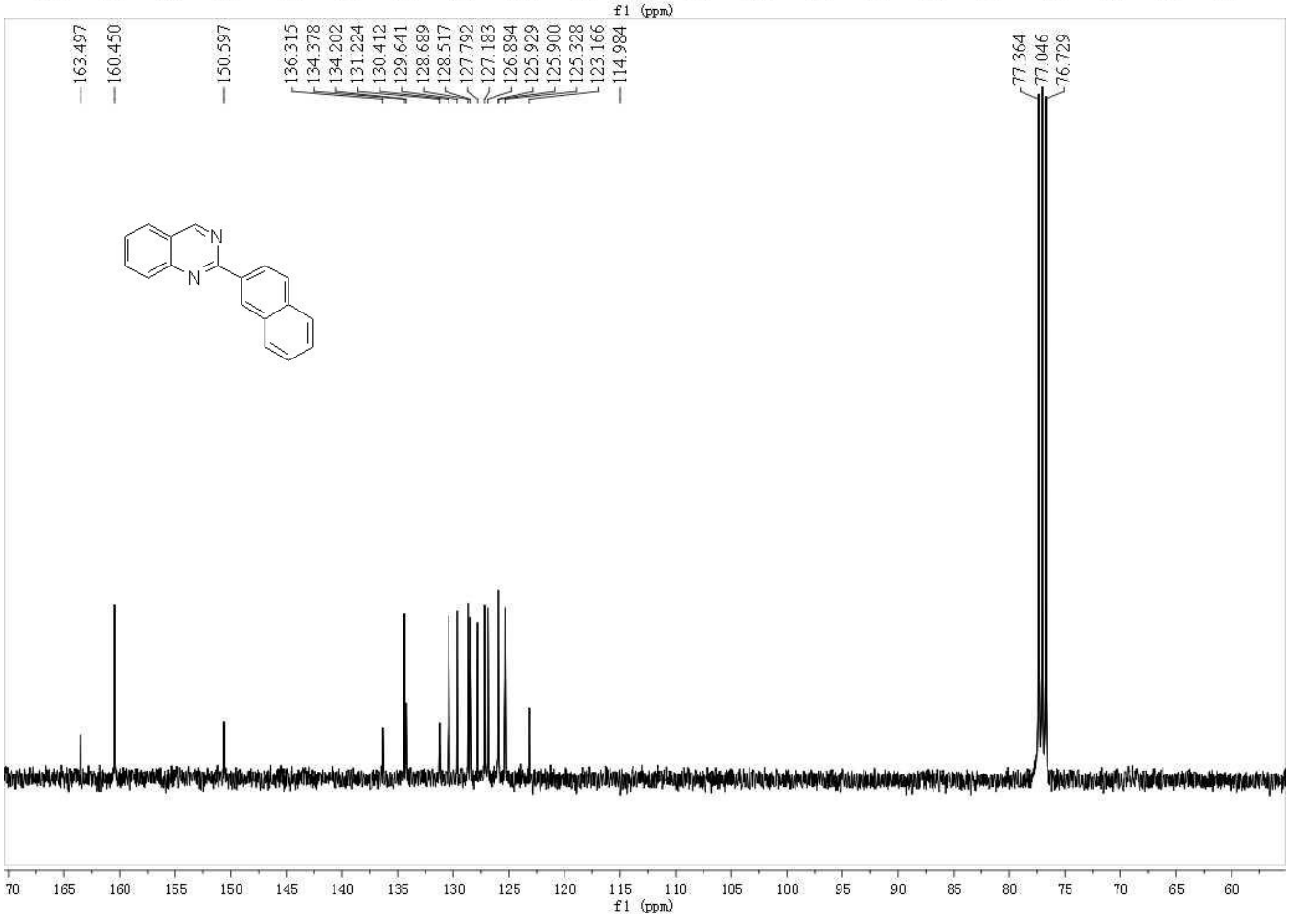

9.429
8.499
8.481
8.070
8.049
7.921
7.902
7.884
7.658
7.637
7.616
7.596
7.260
N
N
Br
1.000
2.022
0.985
1.982
3.078
f1 (ppm)

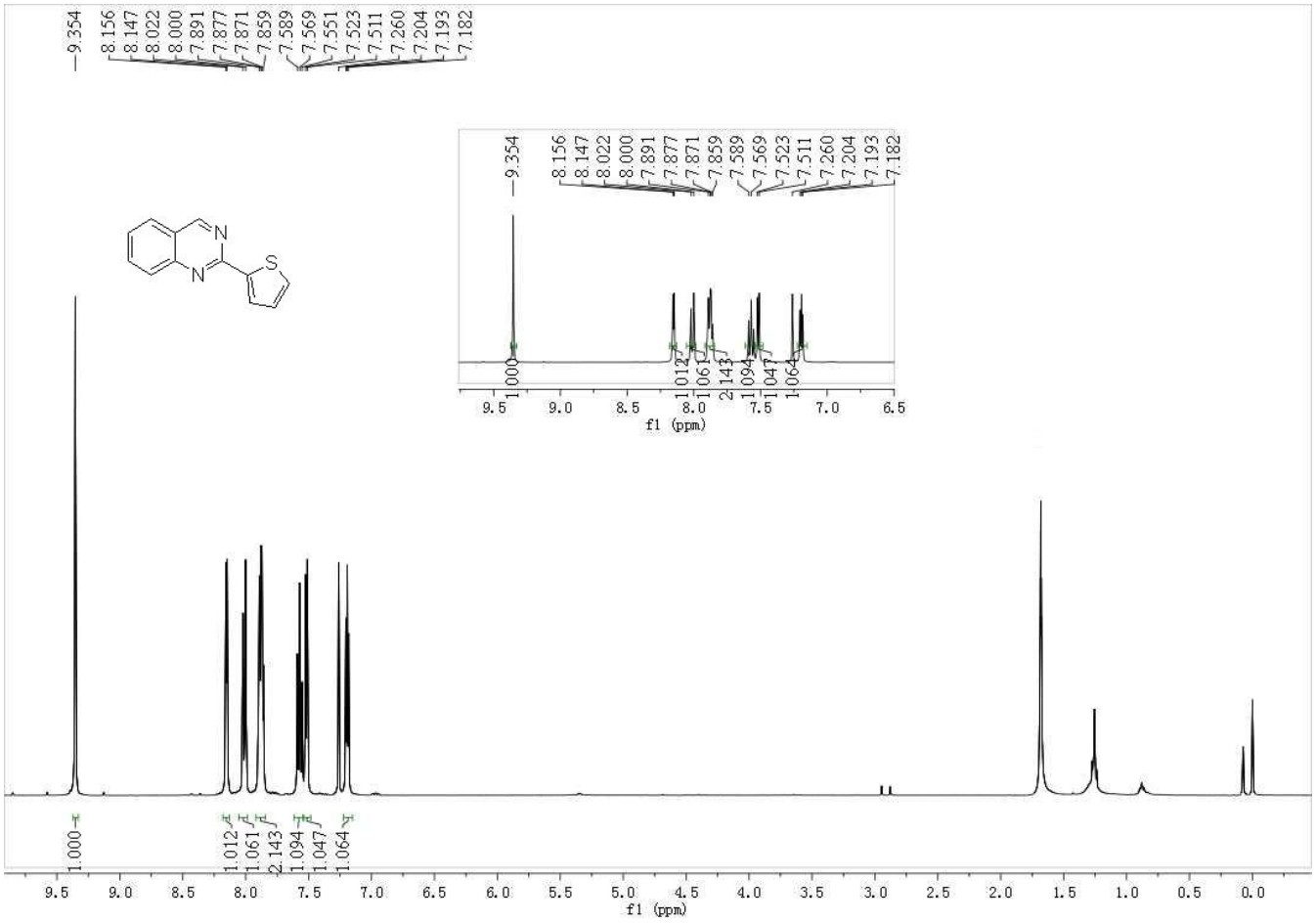

160.496
160.055
150.630
136.920
134.241
131.750
130.107
128.561
127.458
127.124
125.371
123.599
77.317
77.000
76.682
N
N
Br
f1 (ppm)

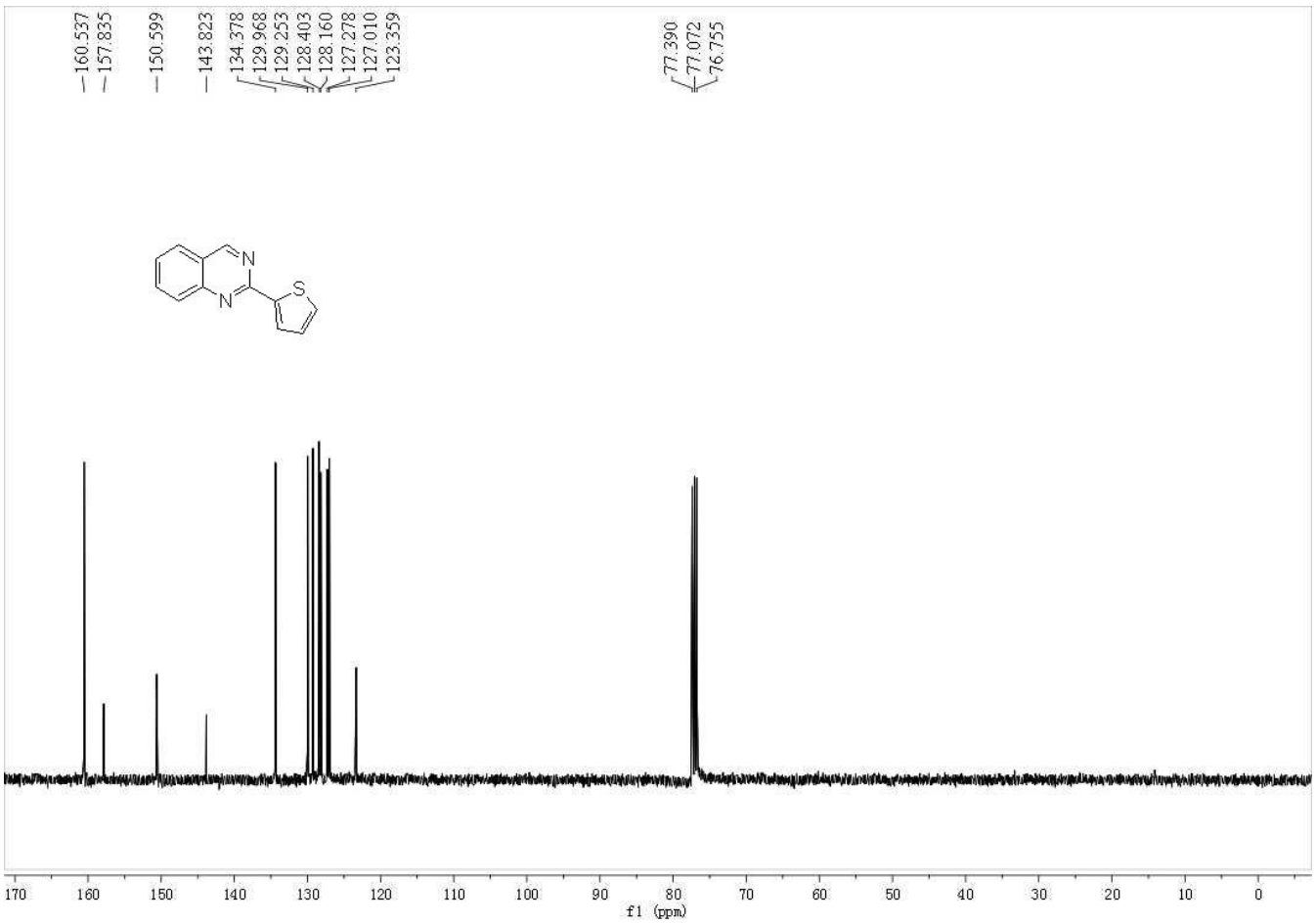

9.403
8.569
8.449
8.441
8.040
8.018
7.890
7.870
7.847
7.598
7.580
7.561
7.408
7.190
0.000
Cl
1.000
0.972
1.054
1.047
2.044
1.119
2.013
1.025
f1 (ppm)

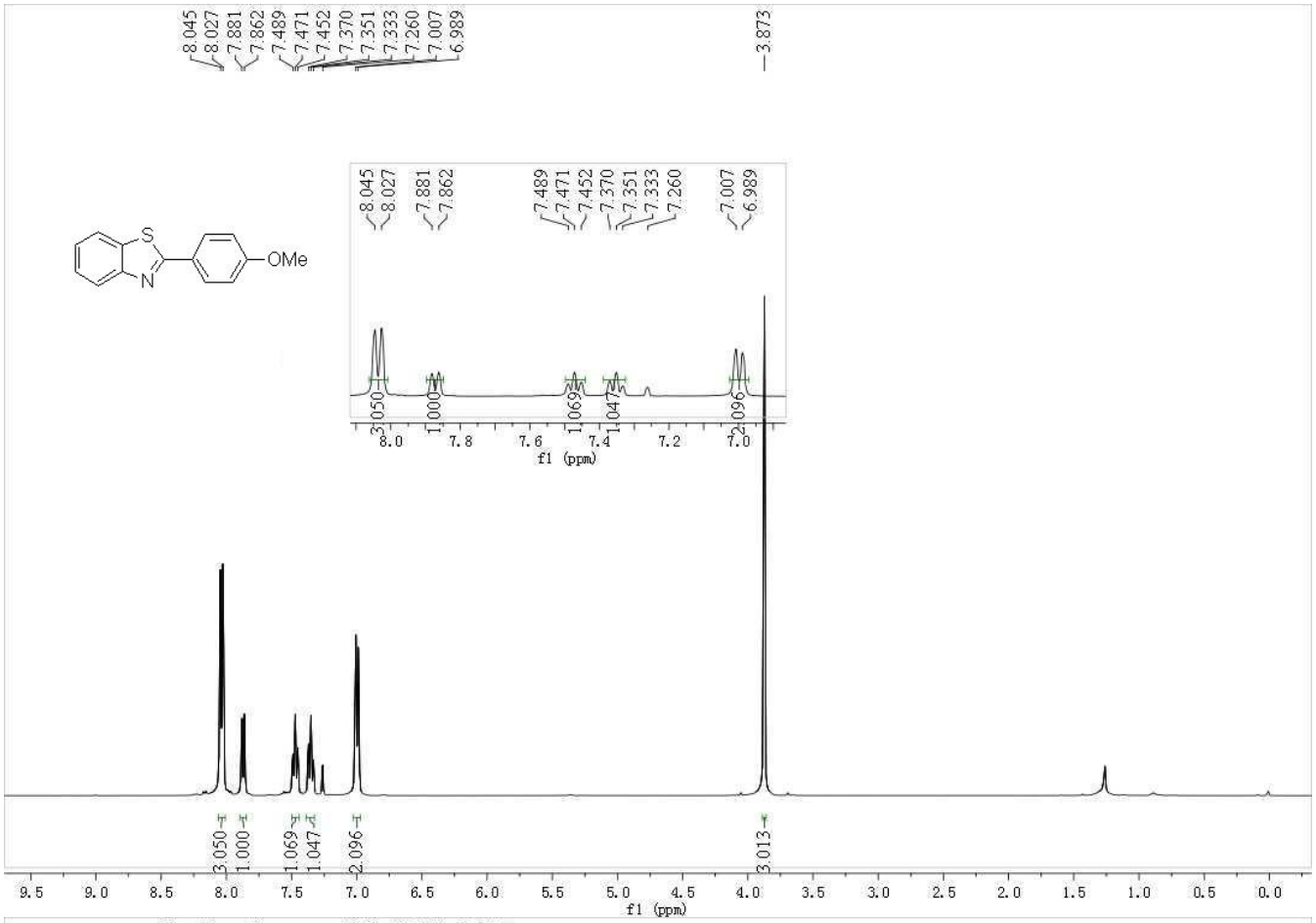

159.558
158.750
149.692
138.893
133.791
133.289
129.534
128.832
127.703
127.668
126.630
126.139
125.638
122.780
76.310
75.675
Cl
f1 (ppm)

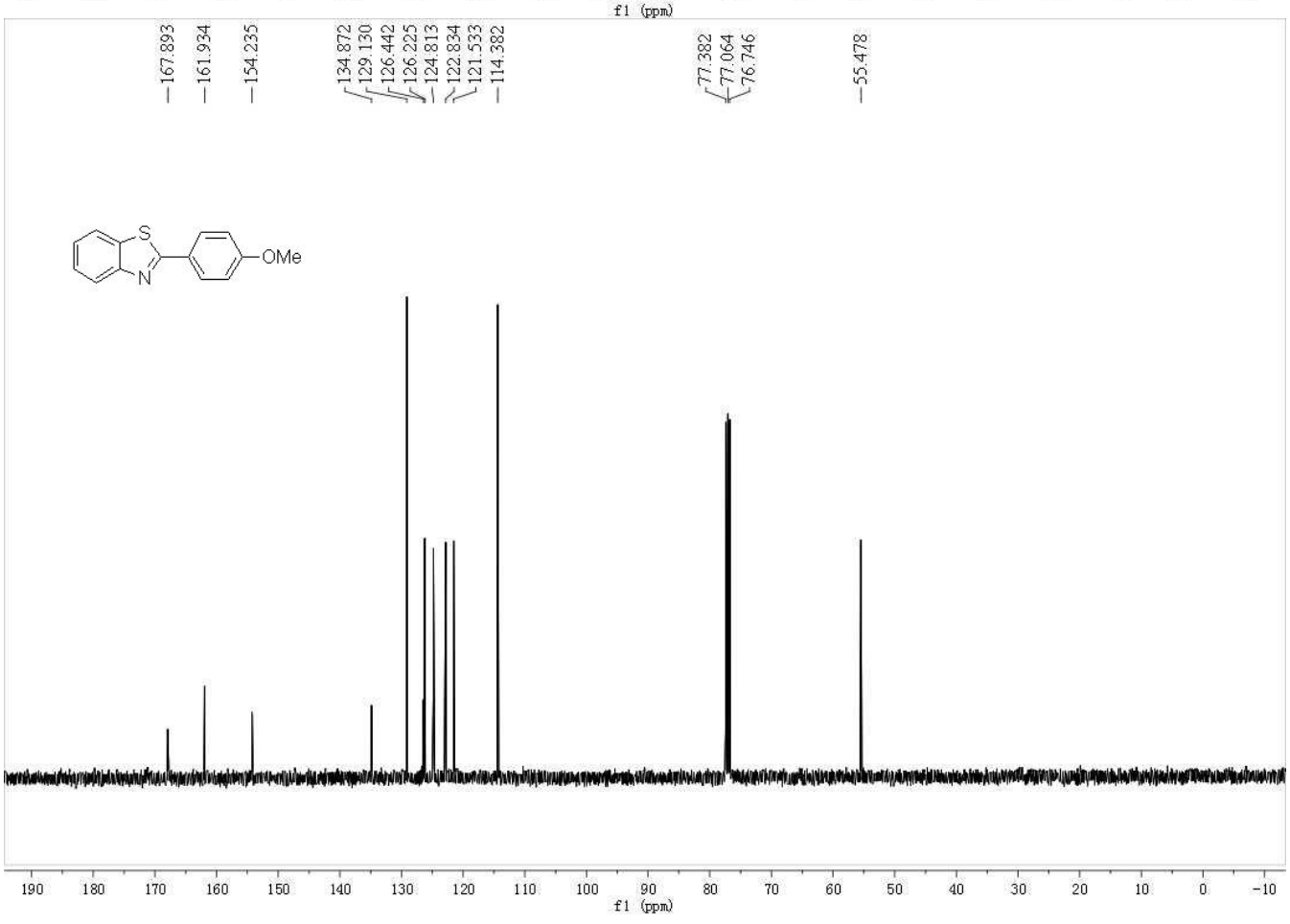

9.601
8.709
8.705
8.686
8.193
8.184
8.181
8.172
8.166
8.163
8.034
8.012
8.000
7.997
7.988
7.983
7.979
7.976
7.962
7.955
7.947
7.936
7.931
7.727
7.725
7.707
7.689
7.688
7.655
7.637
7.617
7.581
7.577
7.564
7.560
7.552
7.546
7.540
7.533
7.529
7.516
7.260
1.000
1.015
2.134
4.308
1.172
1.122
2.174
f1 (ppm)

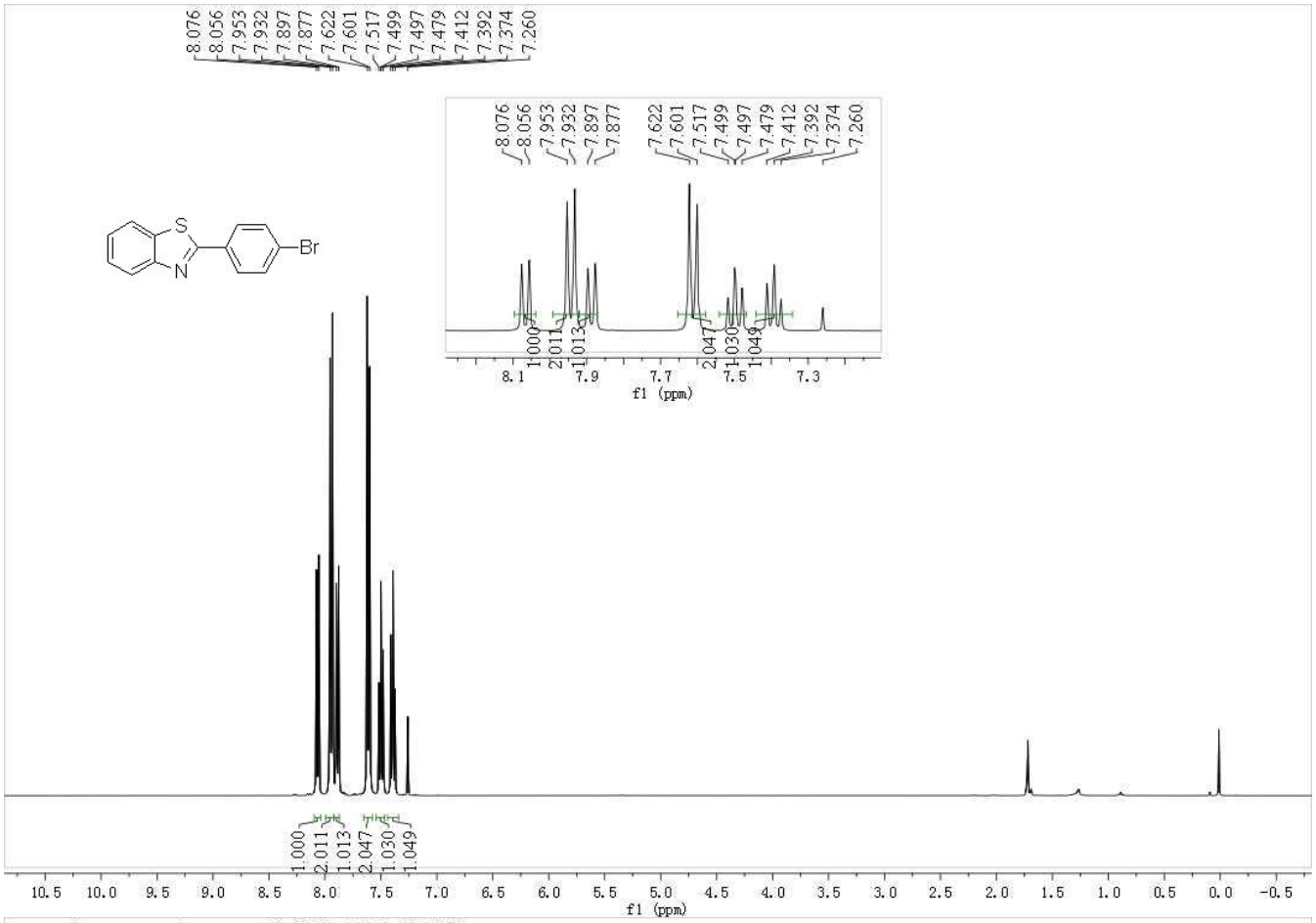

163.497
160.450
150.597
136.315
134.378
134.202
131.224
130.412
129.641
128.689
128.517
127.792
127.183
126.894
125.929
125.900
125.328
123.166
114.984
77.364
77.046
76.729
f1 (ppm)

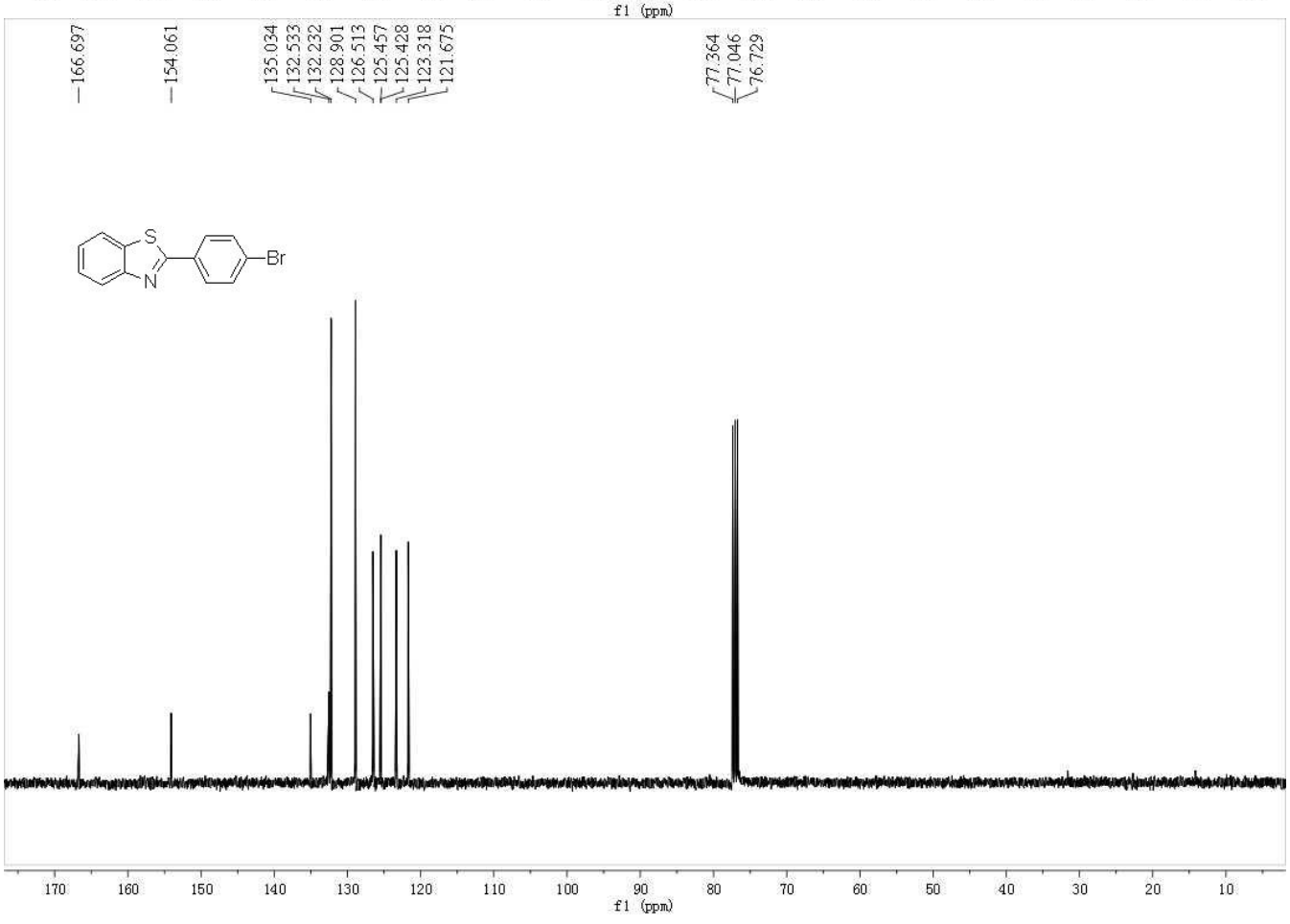

9.354
8.156
8.147
8.022
8.000
7.891
7.877
7.871
7.859
7.589
7.569
7.551
7.523
7.511
7.260
7.204
7.193
7.182
1.000
1.012
1.061
2.143
1.094
1.047
1.064
f1 (ppm)

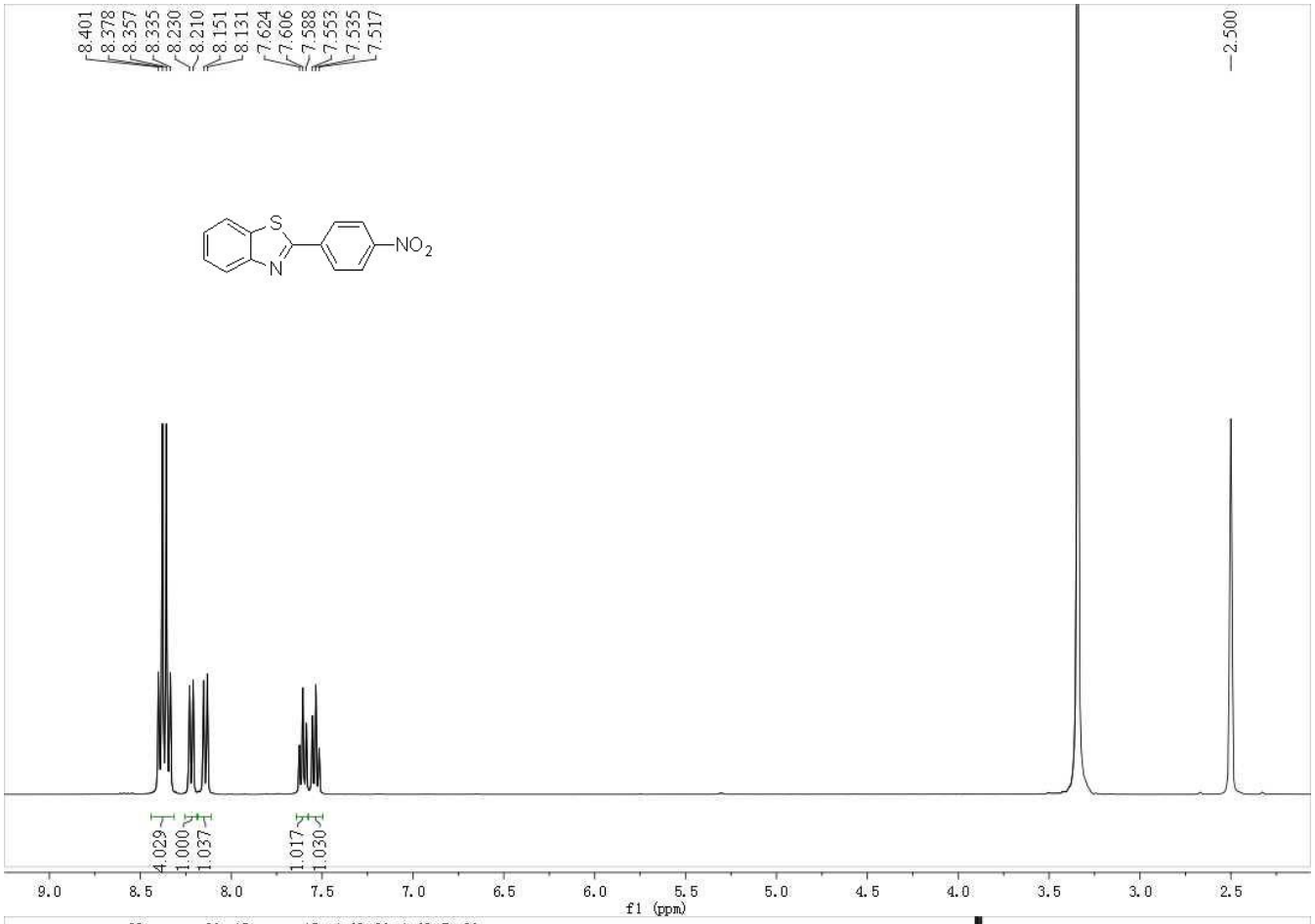

160.537
157.835
150.599
143.823
134.378
129.968
129.253
128.403
128.160
127.278
127.010
123.359
77.390
77.072
76.755
f1 (ppm)

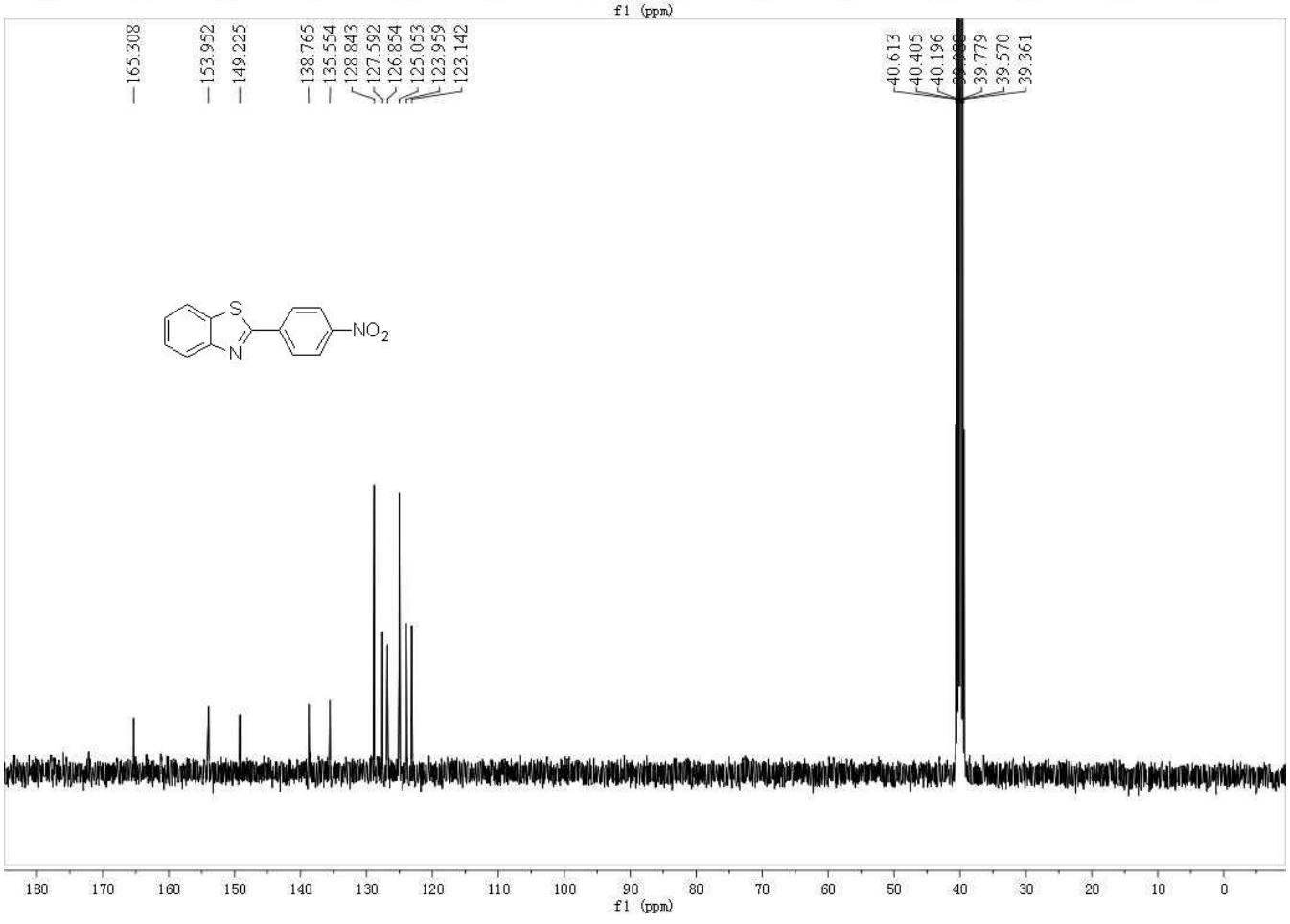

8.045
8.027
7.881
7.862
7.489
7.471
7.452
7.370
7.351
7.333
7.260
7.007
6.989
3.873
OMe
3.050
1.000
1.069
1.047
2.096
3.013
f1 (ppm)

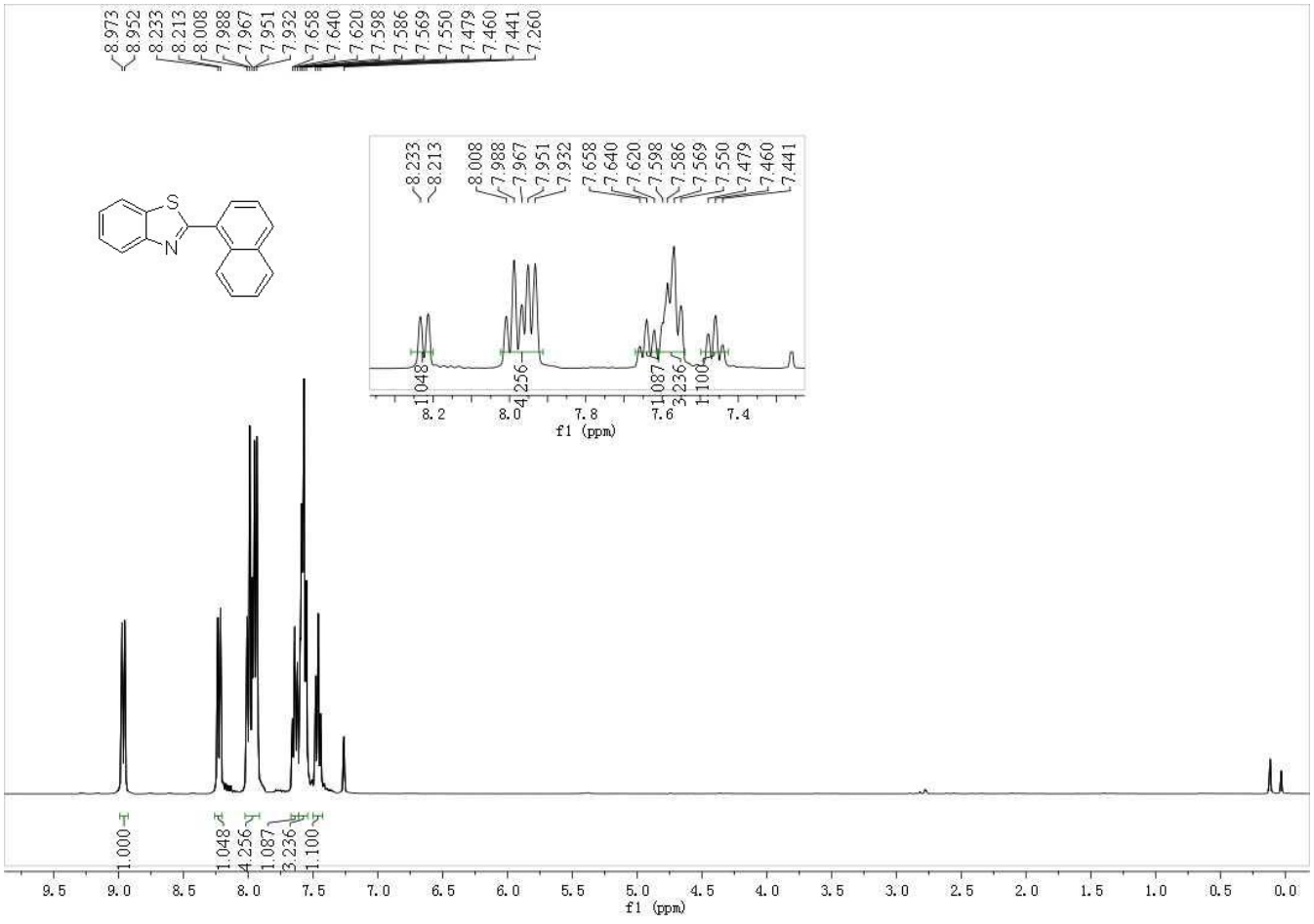

167.893
161.934
154.235
134.872
129.130
126.442
126.225
124.813
122.834
121.533
114.382
77.382
77.064
76.746
55.478
OMe
f1 (ppm)

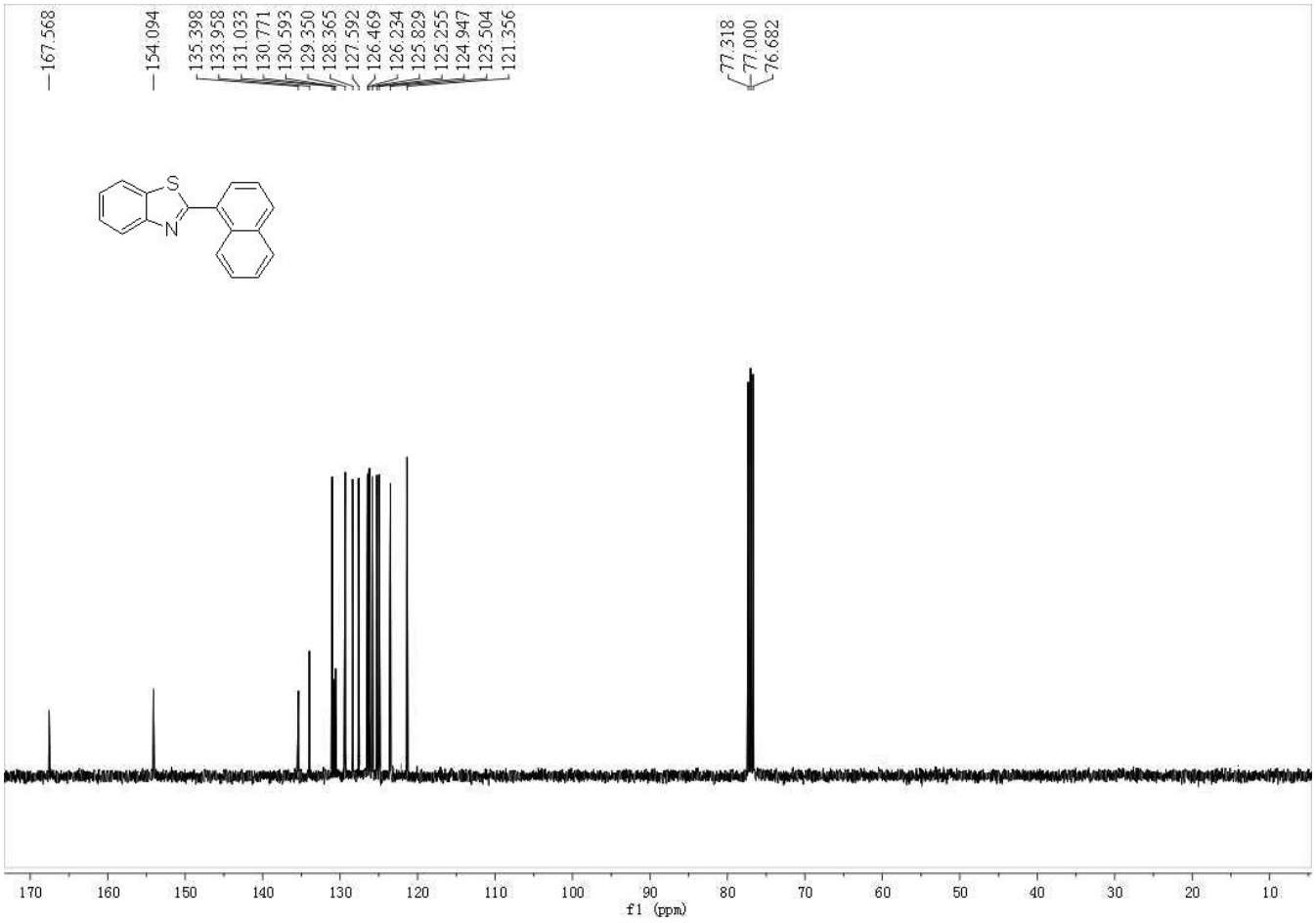

8.076
8.056
7.953
7.932
7.897
7.877
7.622
7.601
7.517
7.499
7.497
7.479
7.412
7.392
7.374
7.260
S
N
Br
1.000
2.011
1.013
2.047
1.030
1.049
f1 (ppm)

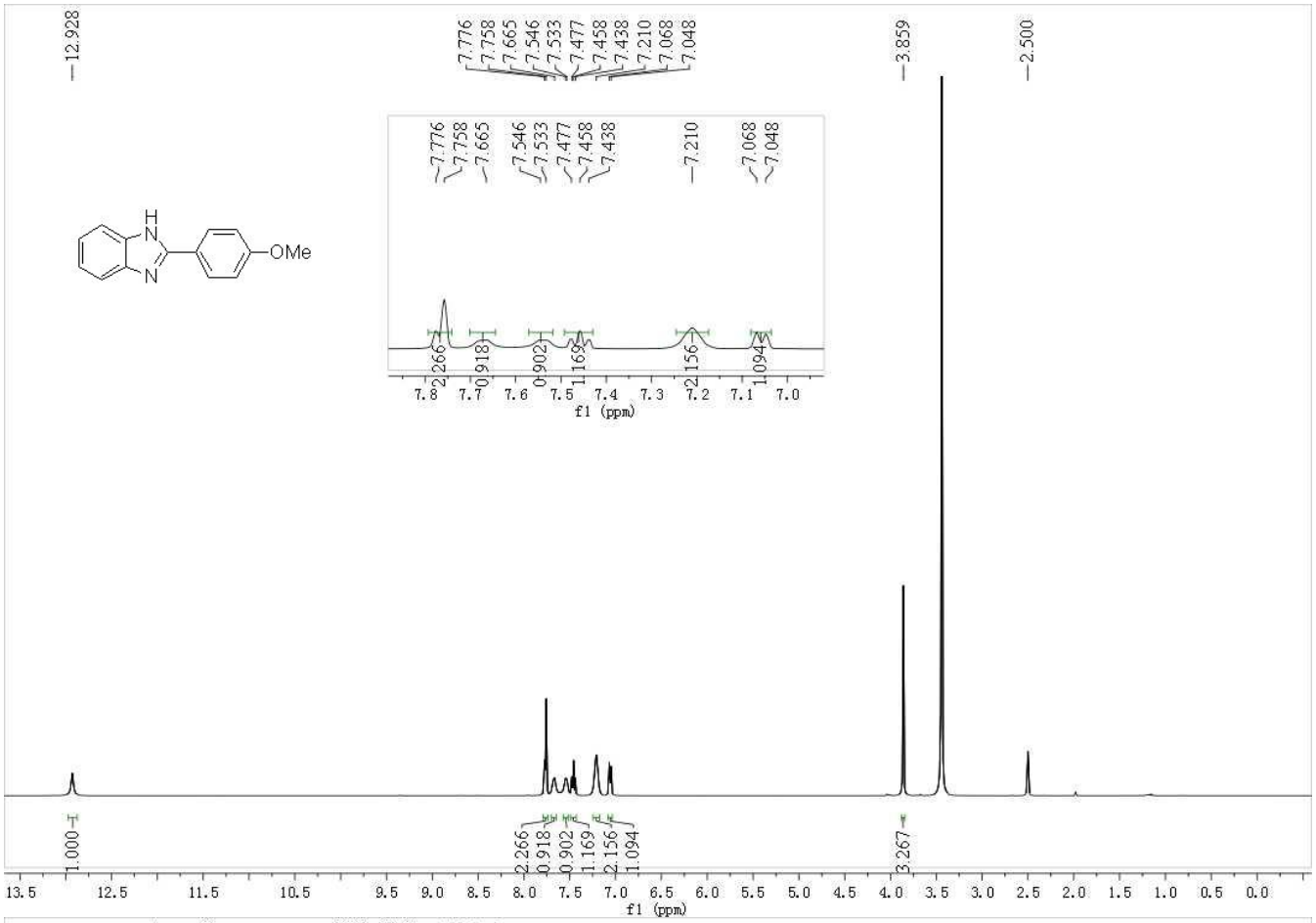

166.697
154.061
135.034
132.533
132.232
128.901
126.513
125.457
125.428
123.318
121.675
77.364
77.046
76.729
S
N
Br
f1 (ppm)

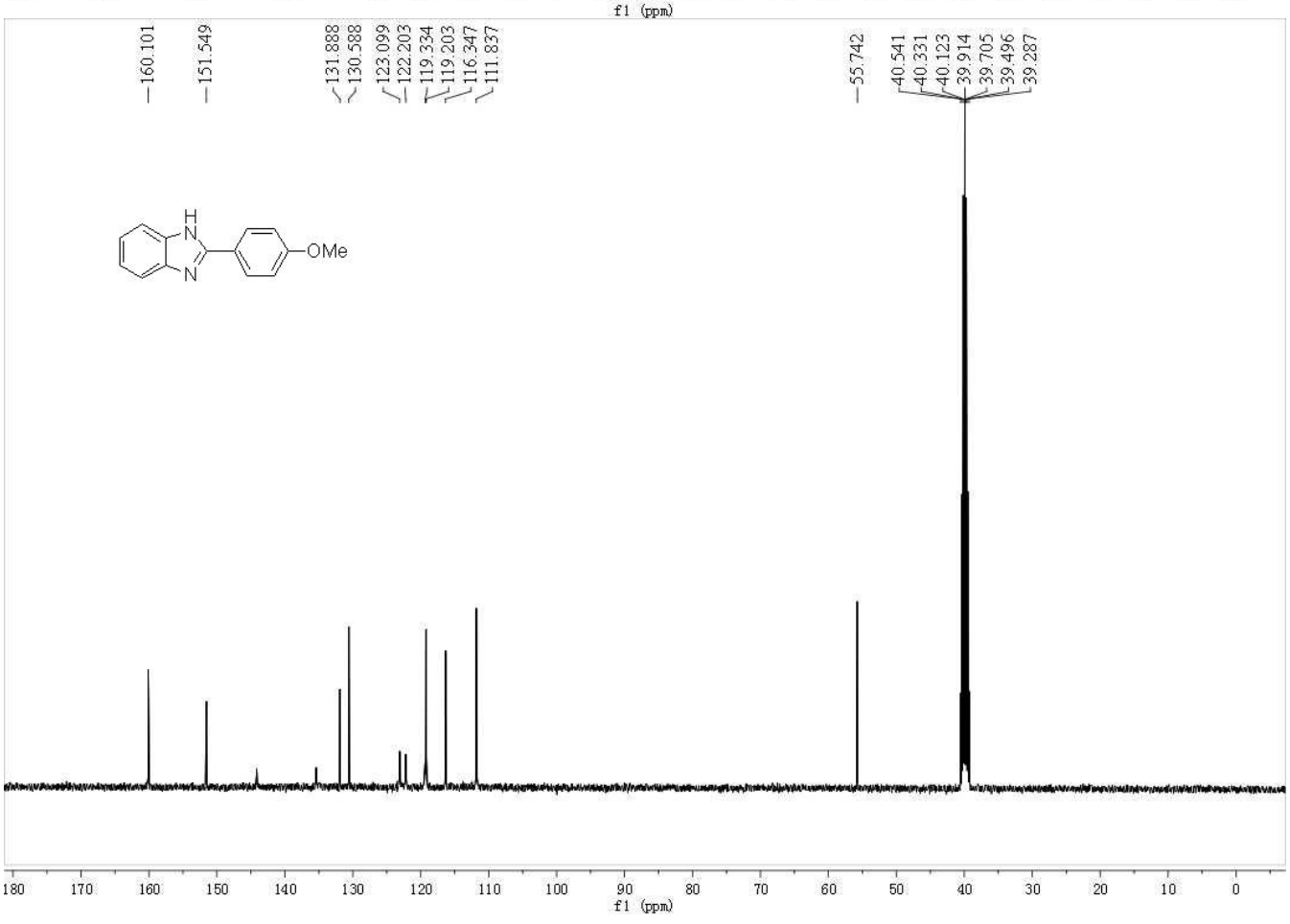

8.401
8.378
8.357
8.335
8.230
8.210
8.151
8.131
7.624
7.606
7.588
7.553
7.535
7.517
2.500
S
N
NO2
4.029
1.000
1.037
1.017
1.030
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
f1 (ppm)

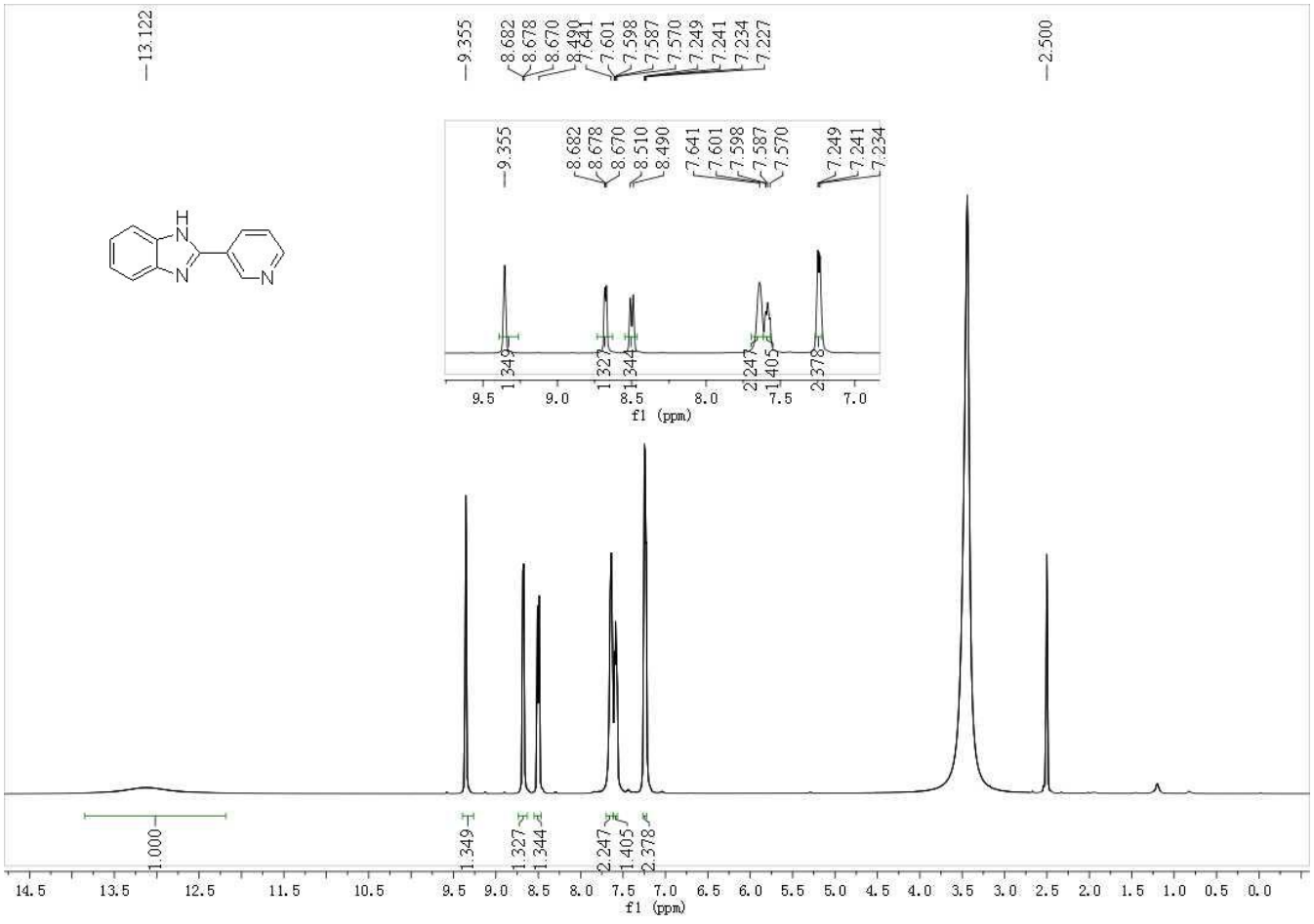

165.308
153.952
149.225
138.765
135.554
128.843
127.592
126.854
125.053
123.959
123.142
40.613
40.405
40.196
39.779
39.570
39.361
S
N
NO2
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

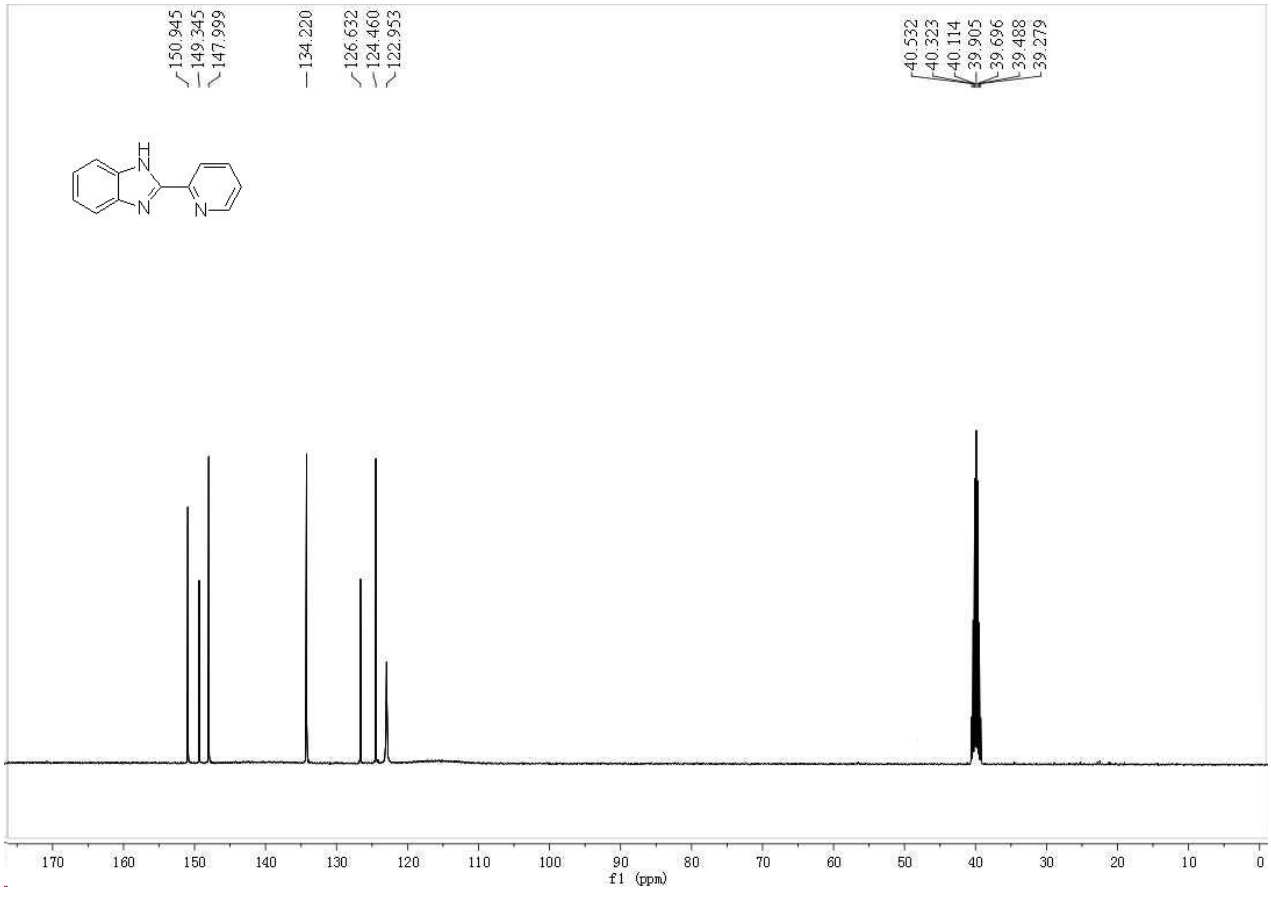

8.973
8.952
8.233
8.213
8.008
7.988
7.967
7.951
7.932
7.658
7.640
7.620
7.598
7.586
7.569
7.550
7.479
7.460
7.441
7.260
1.000
1.048
4.256
1.087
3.236
1.100
f1 (ppm)


167.568
154.094
135.398
133.958
131.033
130.771
130.593
129.350
128.365
127.592
126.469
126.234
125.829
125.255
124.947
123.504
121.356
77.318
77.000
76.682
f1 (ppm)


12.928
7.776
7.758
7.665
7.546
7.533
7.477
7.458
7.438
7.210
7.068
7.048
3.859
2.500
OMe
1.000
2.266
0.918
0.902
1.169
2.156
1.094
3.267
f1 (ppm)


160.101
151.549
131.888
130.588
123.099
122.203
119.334
119.203
116.347
111.837
55.742
40.541
40.331
40.123
39.914
39.705
39.496
39.287
OMe
f1 (ppm)


13.122
9.355
8.682
8.678
8.670
8.490
7.641
7.601
7.598
7.587
7.570
7.249
7.241
7.234
7.227
2.500
1.000
1.349
1.327
1.344
2.247
1.405
2.378
f1 (ppm)


150.945
149.345
147.999
134.220
126.632
124.460
122.953
40.532
40.323
40.114
39.905
39.696
39.488
39.279
f1 (ppm)