Supporting Information

Design, Synthesis and Structural Investigation of a Novel Class of Aggregation-Induced Emission (AIE) Molecular Scaffolds

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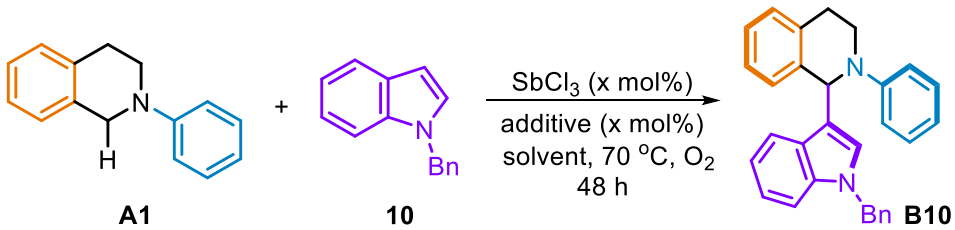
General:

Flash chromatography was carried out with silica gel (200-300 mesh). Analytical TLC was performed with silica gel GF254 plates, and the products were visualized by UV detection. ^{1}H NMR (400 MHz or 600 MHz) and ^{13}C NMR (100 MHz or 150 MHz) spectra were recorded in $CDCl_3$. Chemical shifts (δ) are reported in ppm using TMS as internal standard and spin-spin coupling constants (J) are given in Hz. The high resolution mass spectra (HRMS) were measured on an electrospray ionization (ESI) apparatus using time of flight (TOF) mass spectrometry. UV-visible absorption and fluorescence emission spectra were recorded on commercial spectrophotometers (SHIMADZU UV-2550 and Hitachi F-7000, 200-800 nm scan range) at room temperature. X-ray crystallographic studies were carried out on a Bruker D8 QUEST diffractometer. Data collection for the crystal structure was performed with programs from the SHELXTL-2018 program package and olex2 1.3. All calculations (atom distance and dihedral angle) were performed with programs Diamond package.

Optimization of reaction conditions

1. The reactions between *N*-aryl THIQs and indoles



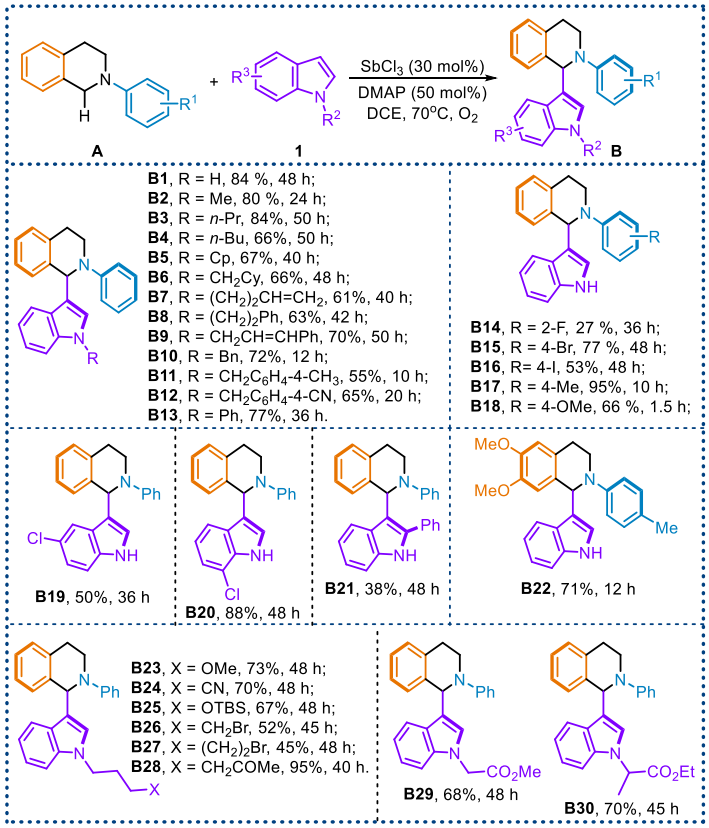
Entry	**A1 : 10**	$SbCl_3$ (x mol %)	Additive (x mol %)	Solvent	Yield (%) [a]
1	1 : 1	30	DMAP (50)	MeCN	40
2	2 : 1	30	DMAP (50)	MeCN	67
3	1 : 2	30	DMAP (50)	MeCN	38
4	2 : 1	40	DMAP (50)	MeCN	66
5	2 : 1	50	DMAP (50)	MeCN	60
6	2 : 1	60	DMAP (50)	MeCN	51
7	2 : 1	20	DMAP (50)	MeCN	30
8	2 : 1	30	DABCO (50)	MeCN	65
9	2 : 1	30	NEt_3 (50)	MeCN	51
10	2 : 1	30	DIPEA (50)	MeCN	62
11	2 : 1	30	K_3PO_4 (50)	MeCN	60
12	2 : 1	30	DMAP (50)	anisole	45
13	**2 : 1**	**30**	**DMAP (50)**	**DCE**	**72**
14	2 : 1	30	DMAP (50)	THF	71
15	2 : 1	30	DMAP (50)	1,4-dioxane	57
16	2 : 1	30	DMAP (50)	DCE	55 [b]
17	2 : 1	30	DMAP (50)	DCE	45 [c]

[a.] Isolated yield; [b.] At 45 °C; [c.] At 80 °C.

Based on our previous studies on $SbCl_3/O_2$ promoted C−H functionalization, the

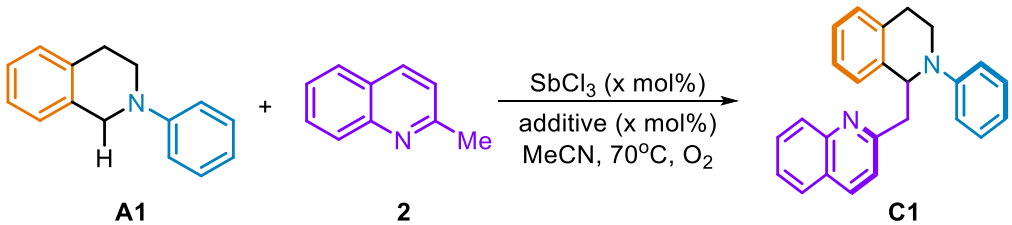
reaction between *N*-aryl THIQ **A1** and *N*-benzyl indole **10** was attempted using DMAP as an additive, and the desired rection proceeded smoothly, affording the target product **B10** in 40% yield (entry 1). Subsequently, optimization of the stoichiometric ratio between the starting materials revealed that a 2:1 ratio of **A1** to **10** provided the highest reaction yield (entries 2-3). Further investigation into the amount of $SbCl_3$ demonstrated that either increasing or decreasing its loading led to diminished product yields (entries 4-7). To enhance the reaction efficiency, a series of basic additives were screened; however, DMAP remained the best choice (entries 8-11). Solvent and temperature studies identified 1,2-dichloroethane (DCE) as the preferred solvent at 70 °C, under which conditions the C−H functionalization product was obtained in an improved yield of 72% (entries 12-17).

Based on the best reaction conditions, 30 α-indolyl THIQs were prepared in high yields, in which various functional groups were smoothly introduced to the aryl rings (Scheme S1).



Scheme S1. Synthesis of the α-(indol-3-yl)-N-aryl THIQs

2. The reactions between *N*-aryl THIQs and 2-methylquinolines



Entry	**A1 : 2**	$SbCl_3$ (x mol %)	Additive (x mol %)	Solvent	Yield (%) [a]

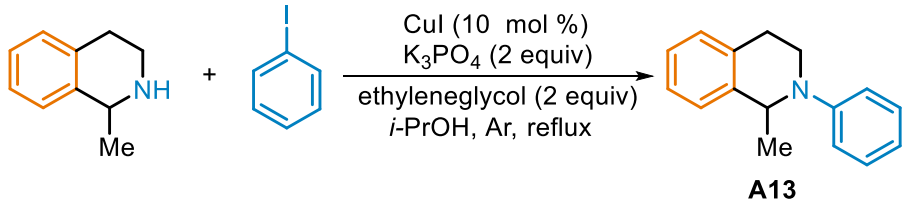
1	1 : 1	50	DMAP (50)	MeCN	29
2	1 : 2	50	DMAP (50)	MeCN	34
3	1 : 2	75	DMAP (50)	MeCN	54
4	1 : 3	75	DMAP (50)	MeCN	70
5	1 : 4	75	DMAP (50)	MeCN	53
6	1 : 3	75	$Cu(OAc)_2$ (50)	MeCN	85
7	1 : 3	75	$NiCl_2$ (50)	MeCN	66
8	1 : 3	75	$FeCl_3$ (50)	MeCN	59
9	1 : 3	75	$CuCl_2$ (50)	MeCN	57
10	1 : 3	75	$AlCl_3$ (50)	MeCN	75
11	1 : 3	75	$InCl_3$ (50)	MeCN	70
12	**1 : 3**	**75**	**$Cu(OAc)_2$ (5)**	**MeCN**	**87**
13	1 : 3	75	$Cu(OAc)_2$ (5)	THF	59
14	1 : 3	75	$Cu(OAc)_2$ (5)	DCE	67
15	1 : 3	75	$Cu(OAc)_2$ (5)	DMSO	23
16	1 : 3	75	$Cu(OAc)_2$ (5)	anisole	73

[a.] Isolated yield.

Building upon the optimized conditions established for the THIQ–indole coupling, DMAP was initially employed as the additive to investigate the reaction with 2-methylquinoline. However, the desired α-quinolinylmethyl product **C1** was obtained in only 29% isolated yield (entry 1). Increasing the stoichiometry of 2-methylquinoline led to a marginal improvement in yield, yet a significant portion of *N*-phenyltetrahydroisoquinoline (**A1**) remained unchanged (entry 2). To address this limitation, the loading of $SbCl_3$ was elevated to 75 mol % while further increasing the equivalents of 2-methylquinoline, ultimately achieving the target product in 70% yield (entries 3-5). Given that the activation of the α-methyl position of 2-methylquinoline via enamine formation is involved in this reaction, we hypothesized that introducing a Lewis acid might enhance the reaction efficiecy. Screening of various Lewis acids revealed $Cu(OAc)_2$ as the most effective additive, delivering the desired product in 85% yield (entries 6-11). Notably, reducing the loading of to $Cu(OAc)_2$ 5 mol % did not significantly diminish the reaction efficiency (entry 12), suggesting that C–H oxidation at the α-position of THIQ plays a pivotal role in this transformation. Finally, a brief solvent evaluation was conducted, and acetonitrile was still the optimal choice for this reaction. Given the similarities of structure and reactivity between 2-methylquinoline and its analogues, the above optimized reaction conditions were directly applied to the coupling of THIQ with 1-methylisoquinoline without further optimization.

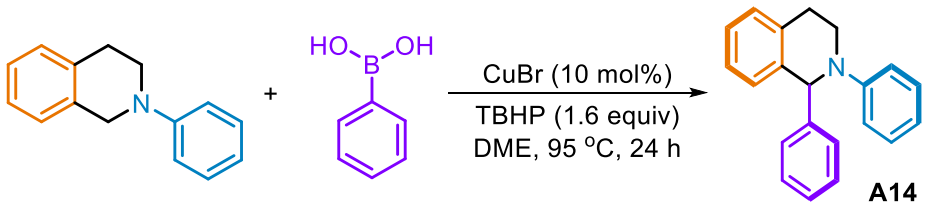
Synthesis of the α-substituted *N*-aryl THIQs

1. Synthesis of the α-methyl- and α-phenyl-*N*-phenyl THIQs



A13

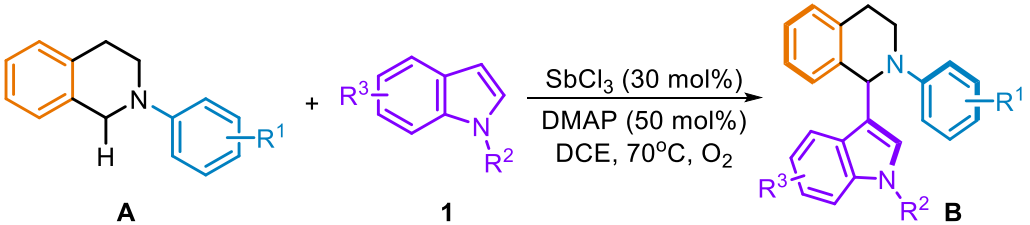
The compound **A13** was synthesized according to the literature as follow: [1] Add CuI (1 mmol) and K_3PO_4 (20 mmol) into a Schlenk-tube. Evacuate the tube and back fill with argon for 3 times, then *i*-PrOH (10 mL), ethyleneglycol (20 mmol), α-methyl-1,2,3,4-tetrahydroisoquinoline (15 mmol) and iodobenzene (10 mmol) were added stepwise room temperature.The reaction mixture was refluxed for 24 hours. After the mixture was cooled to room temperature and diethyl ether (20 mL) and water (20 mL) were added. The resulted mixture was extracted with diethyl ether 3 times and the combined organic extracts was washed with brine and dry over anhydrous $MgSO_4$. After the residue was filtered and concentrated under reduced pressure, the crude product was purified by column chromatography on silica gel using EtOAc/PE.



A14

The compound **A14** was synthesized according to the literature as follow: [2] Weigh CuBr (2.8 mg, 0.02 mmol), 2-phenyl-tetrahydroisoquinoline (0.1 mmol) and phenylboronic acid (0.16 mmol) under air and place the mixture inside a glass vial. Evacuate the vial equipped with a cap under vacuum and back-fill the vial with nitrogen at room temperature. Add DME (500 μL) to the mixture, followed by dropwise addition of TBHP (23 μL, 0.16 mmol). The reaction mixture was stirred at 95 °C for 24 hours and then was extracted with ethyl acetate and filtered through a short layer of silica gel eluting with ethyl acetate. The solvent was removed under reduced pressure. Finally, the residue was purified by column chromatography on silica gel.

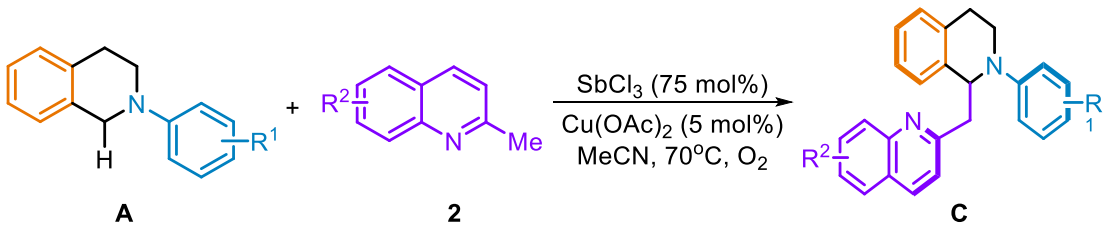
2. Synthesis of the α-(indol-3-yl)-*N*-aryl THIQs



A **1** **B**

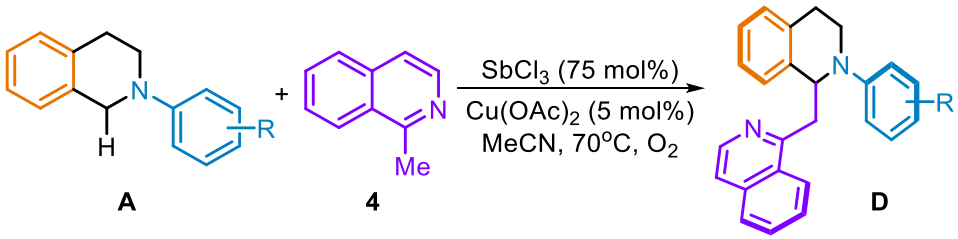
A solution of **A** (0.4 mmol), **1** (0.2 mmol) and DMAP (0.1 mmol) was mixed fully in 2 mL DCE, then $SbCl_3$ (0.06 mmol) was added dropwise under O_2 atmosphere. The reaction solution was stirred at 70 °C (oil bath). After completion monitored by TLC (by UV visualization), the solvent was removed under reduced pressure. The products were separated by TLC eluted with petroleum ether/ethyl acetate (25 : 1) to afford the products **B** in pure form.

3. Synthesis of the α-(quinolin-2-ylmethyl)-*N*-aryl THIQs



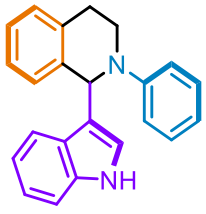
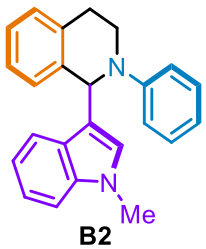
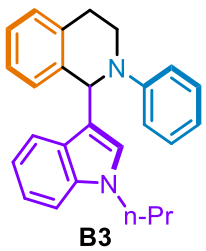
A solution of **A** (0.2 mmol), **1** (0.6 mmol) and $Cu(OAc)_2$ (0.01 mmol) was mixed fully in 2 mL MeCN, then $SbCl_3$ (0.27 mmol) was added dropwise under O_2 atmosphere. The reaction solution was stirred at 70 °C (oil bath). After completion monitored by TLC (by UV visualization), the solvent was removed under reduced pressure. The products were separated by TLC eluted with petroleum ether/ethyl acetate (6 : 1) to afford the products **C** in pure form.

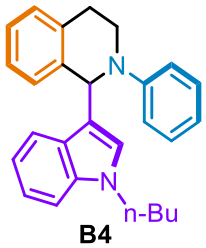
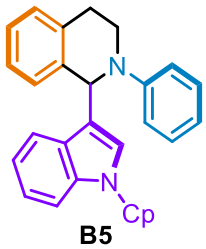
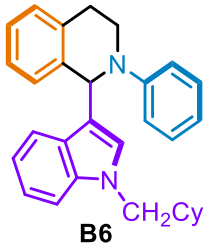
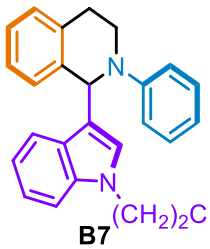
4. Synthesis of the α-(isoquinolin-1-ylmethyl)-*N*-aryl THIQs

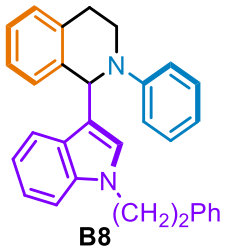
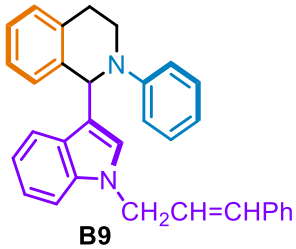
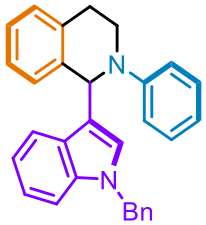
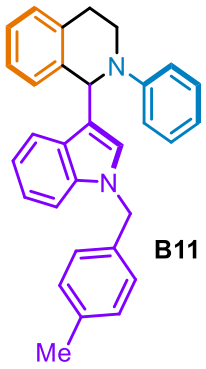
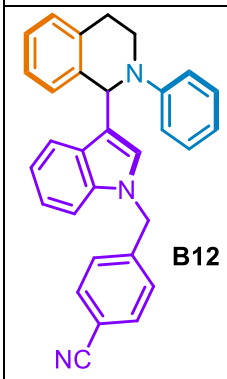


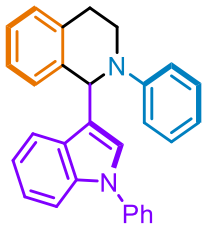
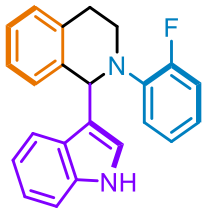
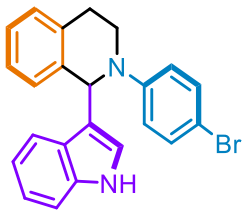
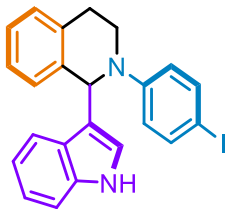
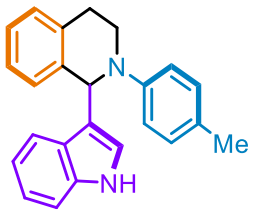
Follow the above experimental procedure 3, and the products **D** was afforded in pure form.

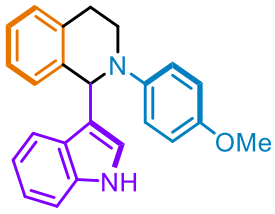
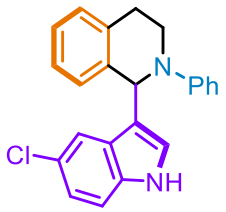
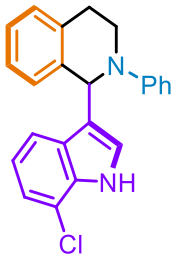
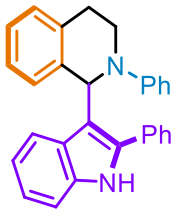
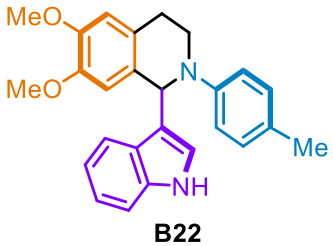
Analytical data for products

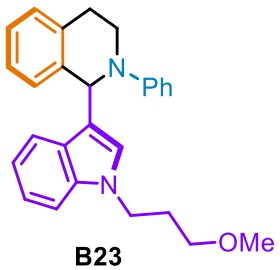
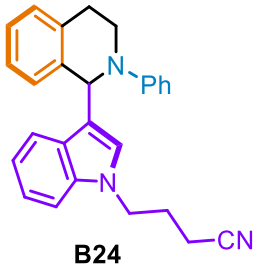
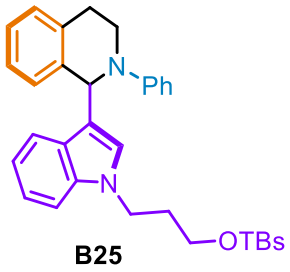
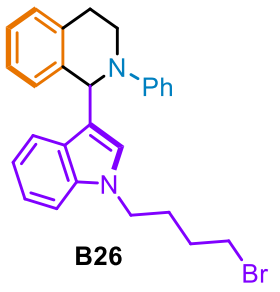
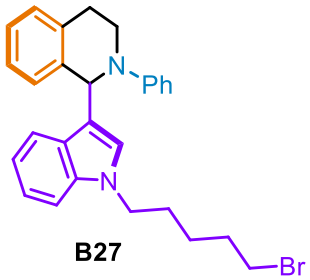
1. Analytical data for α-(indol-3-yl)-*N*-aryl THIQs (B1-B22)	
 B1	**1-(*1H*-Indol-3-yl)-2-phenyl-1,2,3,4-tetrahydroisoquinoline (B1)** [3] Compound **B1** was isolated in 84% yield (54 mg); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.77 (d, *J* = 45.6 Hz, 1H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.39 – 7.12 (m, 7H), 7.06 (d, *J* = 8.1 Hz, 3H), 6.82 (t, *J* = 7.2 Hz, 1H), 6.59 (s, 1H), 6.21 (s, 1H), 3.68 – 3.63 (m, 2H), 3.09 (dt, *J* = 15.6, 7.6 Hz, 1H), 2.88 – 2.80 (m, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 149.7, 137.4, 136.5, 135.5, 129.2, 128.8, 128.0, 126.6, 126.4, 125.7, 124.1, 122.0, 120.0, 119.6, 119.1, 118.1, 115.7, 111.0, 56.6, 42.2, 26.6.
 B2	**1-(1-Methyl-*1H*-indol-3-yl)-2-phenyl-1,2,3,4-tetrahydroisoquinoline (B2)** [4] Compound **B2** was isolated in 80% yield (54 mg); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.69 (d, *J* = 8.0 Hz, 1H), 7.44 – 7.40 (m, 1H), 7.38 – 7.23 (m, 7H), 7.15 – 7.13 (m, 3H), 6.89 (t, *J* = 7.3 Hz, 1H), 6.61 (s, 1H), 6.31 (s, 1H), 3.82 – 3.71 (m, 2H), 3.70 (s, 3H), 3.23 – 3.15 (m, 1H), 2.97 – 2.89 (m, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 149.7, 137.5, 137.3, 135.5, 129.1, 128.7, 128.7, 127.9, 126.8, 126.6, 125.6, 121.6, 120.1, 119.0, 117.9, 117.5, 115.5, 109.1, 56.5, 42.1, 32.6, 26.5.
 B3	**2-Phenyl-1-(1-propyl-1H-indol-3-yl)-1,2,3,4-tetrahydroisoquinoline (B3)** Compound **B3** was isolated in 84% yield (62 mg, pale yellow solid); mp 146-148 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.55 (d, *J* = 8.0 Hz, 1H), 7.36 – 7.18 (m, 8H), 7.08 – 7.02 (m, 3H), 6.80 (t, *J* = 7.2 Hz, 1H), 6.56 (s, 1H), 6.21 (s, 1H), 4.06 – 3.85 (m, 2H), 3.65 (3, 2H), 3.10 (dt, *J* = 15.6, 7.7 Hz, 1H), 2.90 – 2.77 (m, 1H), 1.77 (dd, *J* = 14.5, 7.2 Hz, 2H), 0.86 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 149.8, 137.6, 136.6, 135.6, 129.1, 128.8, 128.0, 128.0,

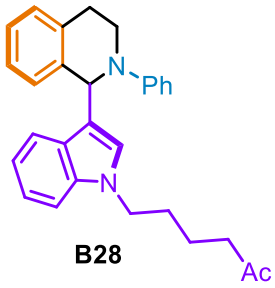
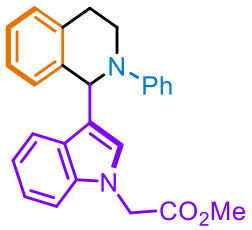
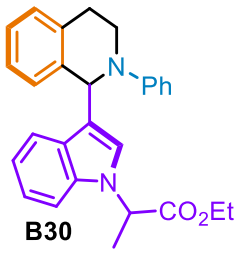
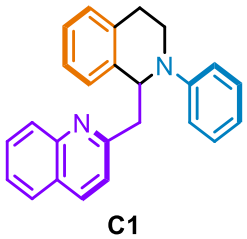
	127.0, 126.5, 125.6, 121.4, 120.2, 118.9, 118.0, 117.3, 115.8, 109.3, 56.7, 47.9, 42.2, 26.6, 23.4, 11.4. **HRMS (ESI-TOF)**: [M + H] $^+$ Calcd for $C_{26}H_{29}N_2^+$, 367.2169; found, 367.2153.
 **B4**	**1-(1-Butyl-1H-indol-3-yl)-2-phenyl-1,2,3,4-tetrahydroisoquinoline (B4)** Compound **B4** was isolated in 66% yield (50 mg, pale yellow solid); mp 143-145 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.53 (d, *J* = 8.0 Hz, 1H), 7.40 – 7.15 (m, 8H), 7.06 – 7.02 (m, 3H), 6.80 (t, *J* = 7.3 Hz, 1H), 6.55 (s, 1H), 6.20 (s, 1H), 4.05 – 3.94 (m, 2H), 3.64 (m, 2H), 3.15 – 2.99 (m, 1H), 2.88 – 2.81 (m, 1H), 1.81 – 1.63 (m, 2H), 1.34 – 1.18 (m, 2H), 0.90 (t, *J* = 7.3 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 149.8, 137.6, 136.5, 135.5, 129.1, 128.8, 128.0, 127.9, 127.0, 126.5, 125.6, 121.4, 120.2, 118.9, 118.0, 117.2, 115.9, 109.3, 56.7, 46.0, 42.2, 32.2, 26.7, 20.1, 13.7; **HRMS (ESI-TOF)**: [M + H] $^+$ Calcd for $C_{27}H_{29}N_2^+$, 381.2325; found, 381.2310.
 **B5**	**1-(1-Cyclopentyl-1H-indol-3-yl)-2-phenyl-1,2,3,4-tetrahydroisoquinoline (B5)** Compound **B5** was isolated in 67% yield (53 mg, pale yellow solid); mp 128-130 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.46 (d, *J* = 8.0 Hz, 1H), 7.33 (d, *J* = 8.3 Hz, 1H), 7.30 – 7.11 (m, 7H), 7.00 (dd, *J* = 13.7, 7.5 Hz, 3H), 6.77 (t, *J* = 7.2 Hz, 1H), 6.60 (s, 1H), 6.17 (s, 1H), 4.76 – 4.55 (m, 1H), 3.67 – 3.49 (m, 2H), 3.17 – 2.97 (m, 1H), 2.90 – 2.68 (m, 1H), 2.21 – 1.99 (m, 2H), 1.89 – 1.61 (m, 6H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 150.0, 137.5, 136.7, 135.5, 129.1, 128.8, 128.1, 127.3, 126.5, 125.7, 124.6, 121.2, 120.2, 119.1, 118.1, 117.3, 116.1, 109.8, 57.0, 56.9, 42.3, 32.4, 32.4, 26.8, 23.9, 23.9; **HRMS (ESI-TOF)**: [M + H] $^+$ Calcd for $C_{28}H_{29}N_2^+$, 393.2325; found, 393.2321.
 **B6**	**1-(1-(Cyclohexylmethyl)-1H-indol-3-yl)-2-phenyl-1,2,3,4-tetrahydroisoquinoline (B6)** Compound **B6** was isolated in 66% yield (56 mg, pale yellow solid); mp 112-114 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.47 (d, *J* = 8.0 Hz, 1H), 7.35 – 7.07 (m, 8H), 7.00 (dd, *J* = 15.4, 8.1 Hz, 3H), 6.78 (t, *J* = 7.2 Hz, 1H), 6.50 (s, 1H), 6.17 (s, 1H), 3.85 – 3.70 (m, 2H), 3.65 – 3.61 (m, 2H), 3.14 – 3.07 (m, 1H), 2.84 (dt, *J* = 16.2, 4.2 Hz, 1H), 1.82 – 1.60 (m, 4H), 1.51 (t, *J* = 10.9 Hz, 2H), 1.20 – 1.12 (m, 3H), 0.95 – 0.87 (m, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 150.0, 137.6, 136.9, 135.5, 129.1, 128.7, 128.7, 128.1, 127.0, 126.5, 125.6, 121.3, 120.2, 118.9, 118.2, 116.8, 116.2, 109.6, 38.6, 30.9, 26.9, 26.3, 25.7; **HRMS (ESI-TOF)**: [M + H] $^+$ Calcd for $C_{30}H_{33}N_2^+$, 421.2638; found, 421.2635.
 **B7**	**1-(1-(But-3-en-1-yl)-1H-indol-3-yl)-2-phenyl-1,2,3,4-tetrahydroisoquinoline (B7)** Compound **B7** was isolated in 61% yield (46 mg, pale yellow solid); mp 146-148 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.56 (d, *J* = 7.9 Hz, 1H), 7.38 – 7.20 (m, 8H), 7.05 (d, *J* = 7.8 Hz, 3H), 6.81 (t, *J* = 6.9 Hz, 1H), 6.56 (s, 1H), 6.21 (s, 1H), 5.70 (dt, *J* = 16.4, 7.0 Hz, 1H), 5.02 (d, *J* = 12.7 Hz, 2H), 4.06 (t, *J* = 7.1 Hz, 2H), 3.65 (m, 2H), 3.19 – 2.99 (m, 1H), 2.84 (m, 1H), 2.49 (q, *J* = 7.0 Hz, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 149.8, 137.5, 136.5, 135.5, 134.5, 129.1, 128.8, 128.0, 127.8, 127.0, 126.6, 125.6, 121.5, 120.2, 119.1, 118.0, 117.5, 117.3, 115.8, 109.2, 56.7, 45.7, 42.2, 34.4, 26.6; **HRMS (ESI-TOF)**: [M + H] $^+$ Calcd for $C_{27}H_{27}N_2^+$, 379.2169; found, 379.2153.

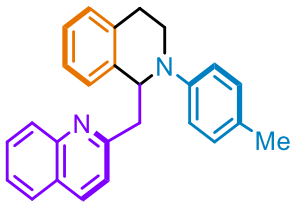
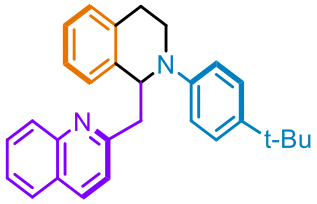
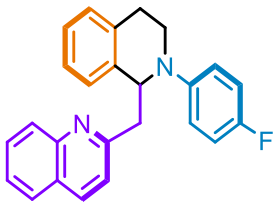
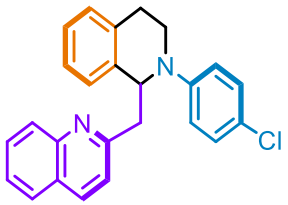
 **B8**	**1-(1-Phenethyl-1H-indol-3-yl)-2-phenyl-1,2,3,4-tetrahydroisoquinoline (B8)** Compound **B8** was isolated in 63% yield (54 mg, pale yellow solid); mp 140-142 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.57 (d, *J* = 7.9 Hz, 1H), 7.35 – 7.09 (m, 11H), 7.08 – 6.92 (m, 5H), 6.78 (t, *J* = 7.2 Hz, 1H), 6.28 (s, 1H), 6.13 (s, 1H), 4.21 (t, *J* = 7.2 Hz, 2H), 3.65 – 3.46 (m, 2H), 3.10 – 2.98 (m, 3H), 2.79 – 2.68 (m, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 149.7, 138.4, 137.4, 136.2, 135.5, 129.1, 128.7, 128.5, 128.1, 128.0, 127.0, 126.5, 125.6, 121.5, 120.3, 119.1, 117.9, 117.4, 115.6, 109.2, 56.5, 47.9, 42.1, 36.5, 26.5; **HRMS (ESI-TOF)**: $[M + H]^+$ Calcd for $C_{31}H_{29}N_2^+$, 429.2325; found, 429.2313.
 **B9**	**1-(1-Cinnamyl-1H-indol-3-yl)-2-phenyl-1,2,3,4-tetrahydroisoquinoline (B9)** Compound **B9** was isolated in 70% yield (62 mg, pale yellow solid); mp 96-98 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.69 (d, *J* = 7.9 Hz, 1H), 7.47 – 7.19 (m, 13H), 7.15 (d, *J* = 7.7 Hz, 3H), 6.88 (t, *J* = 7.2 Hz, 1H), 6.70 (s, 1H), 6.45 (d, *J* = 15.9 Hz, 1H), 6.37 – 6.25 (m, 2H), 4.79 (d, *J* = 5.3 Hz, 2H), 3.88 – 3.66 (m, 2H), 3.24 – 3.10 (m, 1H), 2.92 (m, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 149.7, 137.4, 136.7, 136.1, 135.5, 131.8, 129.1, 128.8, 128.5, 128.0, 127.7, 127.2, 126.6, 126.4, 125.7, 124.9, 121.7, 120.2, 119.3, 118.1, 118.0, 115.8, 109.6, 56.6, 48.2, 42.3, 26.6; **HRMS (ESI-TOF)**: $[M + H]^+$ Calcd for $C_{32}H_{29}N_2^+$, 441.2325; found, 441.2315.
 **B10**	**1-(1-Benzyl-1H-indol-3-yl)-2-phenyl-1,2,3,4-tetrahydroisoquinoline (B10)** [4] Compound **B10** was isolated in 72% yield (60 mg); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.61 (d, *J* = 7.9 Hz, 1H), 7.40 – 6.95 (m, 15H), 6.91 – 6.80 (m, 1H), 6.68 (s, 1H), 6.27 (s, 1H), 5.22 (s, 2H), 3.78 – 3.60 (m, 2H), 3.14 (dt, *J* = 15.6, 7.6 Hz, 1H), 2.88 (dt, *J* = 16.2, 4.3 Hz, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 149.8, 137.5, 137.4, 136.9, 135.5, 129.1, 128.8, 128.6, 128.4, 128.0, 127.4, 127.2, 126.6, 126.3, 125.7, 121.8, 120.3, 119.3, 118.2, 118.1, 116.0, 109.7, 56.8, 49.8, 42.4, 26.7.
 **B11**	**1-(1-(4-Methylbenzyl)-1H-indol-3-yl)-2-phenyl-1,2,3,4-tetrahydroisoquinoline (B11)** Compound **B11** was isolated in 55% yield (47 mg, pale yellow solid); mp 121-123 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.58 (d, *J* = 7.9 Hz, 1H), 7.43 – 6.98 (m, 13H), 6.91 (d, *J* = 7.8 Hz, 2H), 6.83 (t, *J* = 7.2 Hz, 1H), 6.66 (s, 1H), 6.25 (s, 1H), 5.17 (s, 2H), 3.67 (m, 2H), 3.18 – 3.06 (m, 1H), 2.89 – 2.83 (m, 1H), 2.34 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 149.9, 137.4, 137.03, 136.9, 135.5, 134.5, 129.3, 129.1, 128.8, 128.4, 128.0, 127.2, 126.6, 126.3, 125.7, 121.7, 120.2, 119.3, 118.2, 118.0, 116.1, 109.7, 56.8, 49.7, 42.4, 26.8, 21.0; **HRMS (ESI-TOF)**: $[M + H]^+$ Calcd for $C_{31}H_{29}N_2^+$, 429.2325; found, 429.2326.
 **B12**	**4-((3-(2-Phenyl-1,2,3,4-tetrahydroisoquinolin-1-yl)-1H-indol-1-yl)methyl)benzonitrile (B12)** Compound **B12** was isolated in 65% yield (57 mg, pale yellow solid); mp 180-182 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.54 (t, *J* = 8.8 Hz, 3H), 7.31 – 7.11 (m, 7H), 7.10 – 6.94 (m, 6H), 6.80 (t, *J* = 6.9 Hz, 1H), 6.61 (s, 1H), 6.19 (s, 1H), 5.24 (s, 2H), 3.63 (m, 2H), 3.09 (dt, *J* = 14.9, 7.4 Hz, 1H), 2.89 – 2.81 (m, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 149.9, 143.0, 137.2, 136.7, 135.5, 132.5, 129.1, 128.8, 128.0, 128.0, 127.3, 126.9, 126.7, 125.8, 122.2, 120.6, 119.8, 118.9, 118.5, 118.5, 116.3, 111.4, 109.3, 56.8, 49.5, 42.7, 26.9; **HRMS (ESI-TOF)**: $[M + H]^+$ Calcd for $C_{31}H_{26}N_3^+$, 440.2121; found, 440.2114.

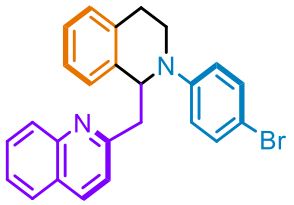
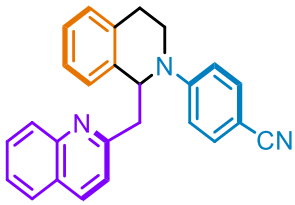
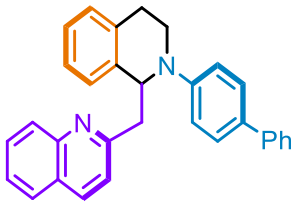
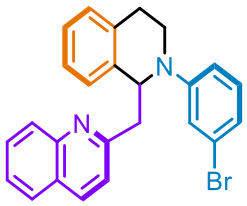
 **B13**	**2-Phenyl-1-(1-phenyl-1H-indol-3-yl)-1,2,3,4-tetrahydroisoquinoline (B13)** Compound **B13** was isolated in 77% yield (62 mg, pale yellow solid); mp 133-135 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.67 (d, *J* = 8.0 Hz, 1H), 7.55 (d, *J* = 8.3 Hz, 1H), 7.50 – 7.37 (m, 5H), 7.34 – 7.16 (m, 7H), 7.11 (dd, *J* = 15.0, 7.9 Hz, 3H), 6.88 – 6.78 (m, 2H), 6.26 (s, 1H), 3.79 – 3.62 (m, 2H), 3.19 – 3.08 (m, 1H), 2.85 (dt, *J* = 16.3, 4.2 Hz, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 149.7, 139.6, 137.0, 136.5, 135.6, 129.5, 129.2, 128.9, 128.1, 127.8, 126.7, 126.3, 125.8, 124.2, 122.5, 120.5, 120.3, 120.2, 118.2, 115.9, 110.4, 56.6, 42.4, 26.5; **HRMS (ESI-TOF):** [M + H] $^+$ Calcd for $C_{29}H_{25}N_2^+$, 401.2012; found, 401.2000.
 **B14**	**2-(2-Fluorophenyl)-1-(1H-indol-3-yl)-1,2,3,4-tetrahydroisoquinoline (B14)** Compound **B14** was isolated in 27% yield (18 mg, pale yellow solid); mp 156-158 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.85 (s, 1H), 7.36 – 7.17 (m, 4H), 7.20 – 7.02 (m, 4H), 6.92 (ddd, *J* = 20.6, 15.2, 7.4 Hz, 3H), 6.79 (t, *J* = 7.8 Hz, 1H), 6.50 (s, 1H), 6.03 (s, 1H), 3.54 (dd, *J* = 11.2, 4.0 Hz, 1H), 3.45 (dd, *J* = 12.4, 5.2 Hz, 1H), 3.07 (ddd, *J* = 16.8, 10.9, 6.1 Hz, 1H), 2.86 (d, *J* = 16.4 Hz, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 156.5 (d, *J* = 246.1 Hz), 139.2 (d, *J* = 8.8 Hz), 137.4, 136.3, 134.9, 128.9, 128.3, 127.0, 126.4, 125.7, 124.6, 124.2 (d, *J* = 3.4 Hz), 122.5, 122.4 (d, *J* = 11.1 Hz), 121.9, 120.2, 119.5, 118.4, 116.0 (d, *J* = 20.8 Hz), 57.2, 43.4, 27.7; **HRMS (ESI-TOF)**: [M + H] $^+$ Calcd for $C_{23}H_{20}FN_2^+$, 343.1605; found, 343.1591.
 **B15**	**2-(4-Bromophenyl)-1-(1H-indol-3-yl)-1,2,3,4-tetrahydroisoquinoline (B15)** [3] Compound **B15** was isolated in 77% yield (62 mg); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.93 (s, 1H), 7.52 (d, *J* = 8.0 Hz, 1H), 7.31 (t, *J* = 8.3 Hz, 4H), 7.22 – 7.10 (m, 4H), 7.04 (t, *J* = 7.5 Hz, 1H), 6.88 (d, *J* = 8.7 Hz, 2H), 6.63 (s, 1H), 6.10 (s, 1H), 3.66 – 3.51 (m, 2H), 3.11 – 2.99 (m, 1H), 2.82 (dt, *J* = 16.2, 4.5 Hz, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 148.7, 137.0, 136.6, 135.3, 131.9, 128.8, 128.0, 126.8, 126.3, 125.8, 124.1, 122.2, 119.9, 119.7, 118.8, 117.3, 111.1, 109.9, 56.6, 42.5, 26.6.
 **B16**	**1-(1H-Indol-3-yl)-2-(4-iodophenyl)-1,2,3,4-tetrahydroisoquinoline (B16)** Compound **B16** was isolated in 53% yield (48 mg, pale yellow solid); mp 76-78 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.95 (s, 1H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.47 (d, *J* = 8.7 Hz, 2H), 7.31 (t, *J* = 6.3 Hz, 2H), 7.22 – 7.12 (m, 4H), 7.05 (t, *J* = 7.5 Hz, 1H), 6.79 (d, *J* = 8.7 Hz, 2H), 6.64 (s, 1H), 6.11 (s, 1H), 3.65 – 3.54 (m, 2H), 3.09 – 2.99 (m, 1H), 2.82 (dt, *J* = 16.3, 4.7 Hz, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 149.2, 137.8, 137.0, 136.6, 135.3, 128.8, 127.9, 126.88, 126.2, 125.9, 124.1, 122.2, 119.9, 119.7, 118.8, 117.6, 111.1, 79.0, 56.4, 42.2, 26.6; **HRMS (ESI-TOF)**: [M + H] $^+$ Calcd for $C_{23}H_{20}IN_2^+$, 451.0666; found, 451.0661.
 **B17**	**1-(1H-Indol-3-yl)-2-(p-tolyl)-1,2,3,4-tetrahydroisoquinoline (B17)** [5] Compound **B17** was isolated in 95% yield (64 mg); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.95 (s, 1H), 7.57 (d, *J* = 8.0 Hz, 1H), 7.28 (d, *J* = 8.0 Hz, 2H), 7.18 (dd, *J* = 13.1, 7.5 Hz, 4H), 7.08 (t, *J* = 9.3 Hz, 3H), 6.98 (d, *J* = 8.3 Hz, 2H), 6.56 (s, 1H), 6.15 (s, 1H), 3.60 (d, *J* = 4.3 Hz, 2H), 3.09 (dt, *J* = 15.9, 7.9 Hz, 1H), 2.84 – 2.77 (m, 1H), 2.30 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 147.8, 137.5, 136.6, 135.5, 129.8, 128.9, 128.2, 127.8, 126.6, 126.6, 125.7, 124.3, 122.0, 120.1, 119.6, 119.2, 116.6, 111.1, 56.9, 42.7, 26.5, 20.5.

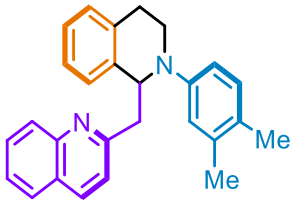
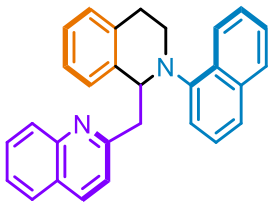
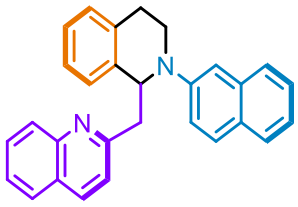
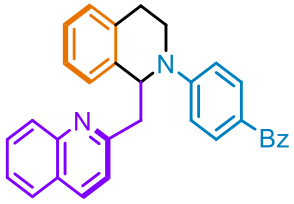
 **B18**	**1-(1H-Indol-3-yl)-2-(4-methoxyphenyl)-1,2,3,4-tetrahydroisoquinoline (B18)** Compound **B18** was isolated in 66% yield (47 mg, pale yellow solid); mp 157-159 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.90 (s, 1H), 7.43 (d, *J* = 8.0 Hz, 1H), 7.29 (d, *J* = 8.1 Hz, 1H), 7.23 – 7.09 (m, 5H), 7.03 – 6.92 (m, 3H), 6.81 (d, *J* = 3.6 Hz, 2H), 6.55 (s, 1H), 5.97 (s, 1H), 3.75 (s, 3H), 3.59 – 3.45 (m, 2H), 3.04 (ddd, *J* = 16.0, 9.9, 5.9 Hz, 1H), 2.80 (dt, *J* = 16.4, 4.1 Hz, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 153.3, 144.7, 137.6, 136.5, 135.4, 128.9, 128.2, 126.8, 126.4, 125.7, 124.3, 122.0, 120.2, 119.6, 119.5, 119.1, 114.4, 110.9, 58.0, 55.6, 43.8, 26.8; **HRMS (ESI-TOF)**: [M + H] $^+$ Calcd for $C_{24}H_{23}N_2O^+$, 355.1805; found, 355.1800.
 **B19**	**1-(5-Chloro-1H-indol-3-yl)-2-phenyl-1,2,3,4-tetrahydroisoquinoline (B19)** Compound **B19** was isolated in 50% yield (36 mg, pale yellow solid); mp 192-194 °C; **^{1}H NMR (400 MHz, *d*$_6$-DMSO)** δ 11.06 (s, 1H), 7.41 (s, 1H), 7.32 (d, *J* = 8.2 Hz, 2H), 7.15 (d, *J* = 8.3 Hz, 5H), 7.01 (t, *J* = 7.6 Hz, 3H), 6.82 (s, 1H), 6.66 (t, *J* = 7.1 Hz, 1H), 6.22 (s, 1H), 3.61 – 3.44 (m, 2H), 3.05 – 2.91 (m, 1H), 2.84 (dt, *J* = 8.8, 4.1 Hz, 1H); **^{13}C NMR (100 MHz, *d*$_6$-DMSO)** δ 149.6, 138.0, 135.4, 135.3, 129.5, 128.9, 128.2, 127.5, 127.0, 126.7, 126.1, 123.6, 121.4, 118.9, 117.8, 115.3, 113.5, 55.6, 42.1, 26.8; **HRMS (ESI-TOF)**: [M + H] $^+$ Calcd for $C_{23}H_{20}ClN_2^+$, 359.1310; found, 359.1303.
 **B20**	**1-(7-Chloro-1H-indol-3-yl)-2-phenyl-1,2,3,4-tetrahydroisoquinoline (B20)** Compound **B20** was isolated in 88% yield (63 mg, pale yellow solid); mp 123-125 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.10 (s, 1H), 7.44 (d, *J* = 8.0 Hz, 1H), 7.22 (ddd, *J* = 18.5, 13.6, 7.7 Hz, 7H), 7.04 (d, *J* = 8.2 Hz, 2H), 6.97 (t, *J* = 7.8 Hz, 1H), 6.82 (t, *J* = 7.2 Hz, 1H), 6.67 (s, 1H), 6.16 (s, 1H), 3.67 – 3.56 (m, 2H), 3.14 – 3.03 (m, 1H), 2.82 (dt, *J* = 16.2, 4.2 Hz, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 149.8, 137.0, 135.5, 133.8, 129.2, 128.9, 128.0, 128.0, 126.8, 125.8, 124.7, 121.5, 120.5, 120.40, 118.8, 118.5, 116.5, 116.2, 56.8, 42.4, 26.7; **HRMS (ESI-TOF)**: [M + H] $^+$ Calcd for $C_{23}H_{20}ClN_2^+$, 359.1310; found, 359.1315.
 **B21**	**2-Phenyl-1-(2-phenyl-1H-indol-3-yl)-1,2,3,4-tetrahydroisoquinoline (B21)** [4] Compound **B21** was isolated in 38% yield (30 mg); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.01 (s, 1H), 7.42 – 7.23 (m, 6H), 7.24 – 6.96 (m, 8H), 6.91 (t, *J* = 7.6 Hz, 1H), 6.77 (dd, *J* = 13.9, 7.5 Hz, 3H), 5.94 (s, 1H), 3.80 – 3.70 (m, 1H), 3.65 (dt, *J* = 12.2, 5.2 Hz, 1H), 3.07 (q, *J* = 4.8 Hz, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 150.7, 138.2, 137.1, 135.8, 135.3, 132.9, 128.8, 128.6, 128.6, 128.5, 128.2, 128.1, 128.0, 126.2, 126.2, 121.9, 120.9, 120.6, 120.4, 119.8, 114.9, 110.6, 57.1, 47.3, 28.4.
 **B22**	**1-(1H-Indol-3-yl)-6,7-dimethoxy-2-(p-tolyl)-1,2,3,4-tetrahydroisoquinoline (B22)** [6] Compound **B22** was isolated in 71% yield (57 mg); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.97 (s, 1H), 7.53 (d, *J* = 7.9 Hz, 1H), 7.31 (d, *J* = 8.1 Hz, 1H), 7.16 (t, *J* = 7.6 Hz, 1H), 7.01 (dt, *J* = 16.3, 8.4 Hz, 5H), 6.74 (s, 1H), 6.60 (d, *J* = 17.6 Hz, 2H), 6.04 (s, 1H), 3.83 (d, *J* = 28.9 Hz, 6H), 3.61 – 3.50 (m, 2H), 2.98 (ddd, *J* = 16.6, 10.3, 6.6 Hz, 1H), 2.58 (d, *J* = 16.1 Hz, 1H), 2.27 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 147.9, 147.7, 147.0, 136.5, 129.7, 129.0, 128.0, 127.5, 126.7, 124.4, 122.1, 120.1, 119.6, 117.1, 111.5, 111.0, 56.3, 55.9, 55.8, 42.3, 25.5, 20.4.

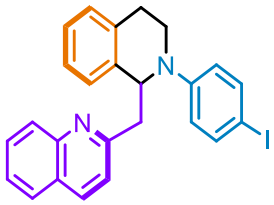
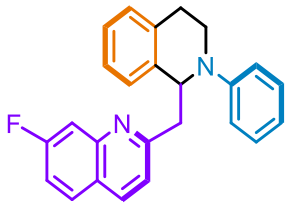
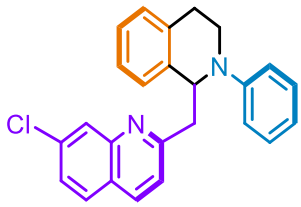
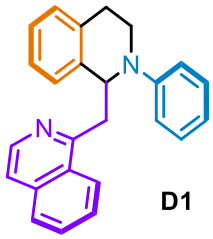
 **B23**	**1-(1-(3-Methoxypropyl)-1H-indol-3-yl)-2-phenyl-1,2,3,4-tetrahydroisoquinoline (B23)** Compound **B23** was isolated in 67% yield (53 mg, pale yellow solid); mp 104-106 °C; **H NMR (400 MHz, $CDCl_3$)** δ 7.56 (d, *J* = 8.0 Hz, 1H), 7.36 – 7.10 (m, 8H), 7.03 (m, 3H), 6.79 (t, *J* = 7.2 Hz, 1H), 6.55 (s, 1H), 6.20 (s, 1H), 4.12 (t, *J* = 6.7 Hz, 2H), 3.72 – 3.56 (m, 2H), 3.23 (s, 3H), 3.19 (t, *J* = 5.8 Hz, 2H), 3.15 – 3.04 (m, 1H), 2.90 – 2.81 (m, 1H), 2.02 – 1.87 (m, 2H); **^{3}C NMR (100 MHz, $CDCl_3$)** δ 149.8, 140.0, 137.6, 136.6, 135.5, 131.8, 129.1, 128.8, 128.2, 128.0, 127.4, 127.0, 126.6, 126.5, 125.6, 121.9, 121.5, 121.2, 120.2, 119.0, 118.9, 118.0, 117.6, 115.8, 114.3, 109.3, 68.9, 58.5, 56.7, 42.6, 42.3, 30.1, 26.7; **HRMS (ESI-TOF)**: [M + H] $^+$ Calcd for $C_{27}H_{29}N_2O^+$, 397.2274; found, 397.2266.
 **B24**	**4-(3-(2-Phenyl-1,2,3,4-tetrahydroisoquinolin-1-yl)-1H-indol-1-yl)butanenitrile (B24)** Compound **B24** is isolated in 70% yield (55 mg, pale yellow solid); mp 174-176 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.49 (d, *J* = 8.0 Hz, 1H), 7.29 – 7.15 (m, 8H), 7.02 (m, 3H), 6.79 (t, *J* = 7.2 Hz, 1H), 6.56 (s, 1H), 6.15 (s, 1H), 4.20 – 4.11 (m, 2H), 3.61 (dd, *J* = 7.5, 4.5 Hz, 2H), 3.12 – 3.03 (m, 1H), 2.92 – 2.79 (m, 1H), 2.12 – 1.98 (m, 4H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 150.0, 137.2, 136.4, 135.4, 129.1, 128.8, 127.9, 127.5, 127.3, 126.7, 125.8, 122.1, 120.6, 119.6, 118.7, 118.5, 118.4, 116.4, 109.0, 56.8, 44.2, 42.6, 27.1, 25.9, 14.5; **HRMS (ESI-TOF)**: [M + H] $^+$ Calcd for $C_{27}H_{26}N_3^+$, 392.2121; found, 392.2113.
 **B25**	**1-(1-(3-(Tert-butyldimethylsilyl)propyl)-1H-indol-3-yl)-2-phenyl-1,2,3,4-tetrahydroisoquinoline (B25)** Compound **B25** was isolated in 67% yield (64 mg, colourless oil); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.53 (d, *J* = 7.9 Hz, 1H), 7.34 – 7.10 (m, 8H), 7.06 – 6.97 (m, 3H), 6.76 (t, *J* = 7.2 Hz, 1H), 6.53 (s, 1H), 6.17 (s, 1H), 4.11 (t, *J* = 6.7 Hz, 2H), 3.62 (dd, *J* = 7.6, 4.4 Hz, 2H), 3.54 – 3.37 (m, 2H), 3.06 (dt, *J* = 15.5, 7.6 Hz, 1H), 2.87 – 2.68 (m, 1H), 1.97 – 1.82 (m, 2H), 0.87 (s, 9H), -0.02 (d, *J* = 6.0 Hz, 6H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 149.8, 137.5, 136.6, 135.5, 129.2, 128.8, 128.2, 128.0, 127.0, 126.6, 125.7, 121.5, 120.2, 119.0, 118.0, 117.5, 115.8, 109.4, 59.4, 56.6, 42.5, 42.2, 32.8, 26.6, 25.9, 18.2, -5.4, -5.5; **HRMS (ESI-TOF)**: [M + H] $^+$ Calcd for $C_{32}H_{41}N_2OSi^+$, 497.2983; found, 497.2978.
 **B26**	**1-(1-(4-Bromobutyl)-1H-indol-3-yl)-2-phenyl-1,2,3,4-tetrahydroisoquinoline (B26)** Compound **B26** was isolated in 52% yield (48 mg, pale yellow solid); mp 121-123 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.54 (d, *J* = 7.9 Hz, 1H), 7.34 – 7.20 (m, 8H), 7.04 (m, 3H), 6.81 (t, *J* = 7.2 Hz, 1H), 6.56 (s, 1H), 6.21 (s, 1H), 4.11 – 3.90 (m, 2H), 3.72 – 3.59 (m, 2H), 3.45 (t, *J* = 6.4 Hz, 2H), 3.11 (m, 1H), 2.86 (m, 1H), 1.98 – 1.84 (m, 2H), 1.73 – 1.59 (m, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 149.8, 137.4, 136.5, 135.5, 129.1, 128.8, 128.0, 127.6, 127.1, 126.6, 125.7, 121.6, 120.33, 119.1, 118.1, 117.7, 116.0, 109.2, 56.7, 45.4, 44.3, 42.3, 29.7, 27.4, 26.8; **HRMS (ESI-TOF)**: [M + H] $^+$ Calcd for $C_{27}H_{28}BrN_2^+$, 459.1430; found, 459.1430.
 **B27**	**1-(1-(5-Bromopentyl)-1H-indol-3-yl)-2-phenyl-1,2,3,4-tetrahydroisoquinoline (B27)** Compound **B27** was isolated in 45% yield (43 mg, pale yellow solid); mp 93-95 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.56 (d, *J* = 8.0 Hz, 1H), 7.37 – 7.27 (m, 8H), 7.05 (m, 3H), 6.81 (t, *J* = 7.1 Hz, 1H), 6.57 (s, 1H), 6.21 (s, 1H), 4.01 (t, *J* = 7.0 Hz, 2H), 3.65 (m, 2H), 3.47 (t, *J* = 6.5 Hz, 2H), 3.11 (m, 1H), 2.86 (m, 1H), 1.85 – 1.72 (m, 3H), 1.47 – 1.23 (m, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 149.8, 137.5, 136.5, 135.5, 129.1, 128.8, 128.0, 127.8, 127.0, 126.6, 125.65, 121.5, 120.3, 119.1, 118.0, 117.5, 115.8, 109.2, 56.7, 45.9,

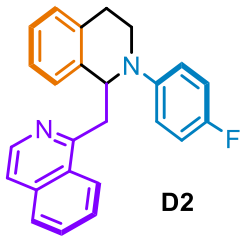
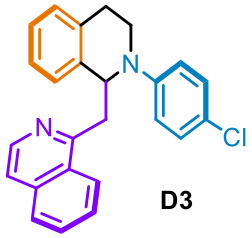
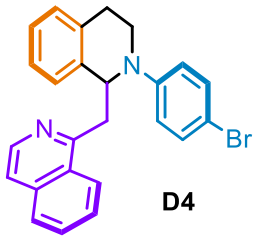
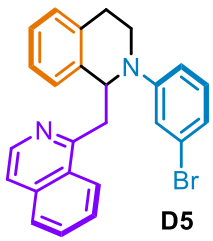
	44.6, 42.3, 32.0, 29.3, 26.7, 24.2; **HRMS (ESI-TOF)**: [M + H] $^{+}$ Calcd for $C_{28}H_{30}BrN_2^{+}$, 473.1587; found, 473.1588.
 **B28**	**6-(3-(2-Phenyl-1,2,3,4-tetrahydroisoquinolin-1-yl)-1H-indol-1-yl)hexan-2-one (B28)** Compound **B28** was isolated in 95% yield (80 mg, pale yellow solid); mp 99-101 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.55 (d, *J* = 7.9 Hz, 1H), 7.37 – 7.11 (m, 8H), 7.03 (m, 3H), 6.79 (t, *J* = 7.1 Hz, 1H), 6.55 (s, 1H), 6.20 (s, 1H), 3.99 (t, *J* = 7.0 Hz, 2H), 3.64 (d, *J* = 4.6 Hz, 2H), 3.20 – 2.95 (m, 1H), 2.85 (m, 1H), 2.36 (t, *J* = 7.2 Hz, 2H), 2.07 (s, 3H), 1.80 – 1.68 (m, 2H), 1.50 (m, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 208.1, 149.8, 137.5, 136.4, 135.5, 129.1, 128.7, 128.0, 127.7, 127.0, 126.5, 125.6, 121.5, 120.2, 119.0, 118.0, 117.5, 115.8, 109.2, 56.6, 46.0, 42.8, 42.2, 29.8, 29.4, 26.7, 20.9; **HRMS (ESI-TOF)**: [M + H] $^{+}$ Calcd for $C_{29}H_{31}N_2O^{+}$, 423.2431; found, 423.2427.
 **B29**	**Methyl-2-(3-(2-phenyl-1,2,3,4-tetrahydroisoquinolin-1-yl)-1H-indol-1-yl)acetate (B29)** Compound **B29** was isolated in 68% yield (54 mg, pale yellow solid); mp 105-107 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.63 (d, *J* = 8.0 Hz, 1H), 7.41 – 7.34 (m, 1H), 7.33 – 7.18 (m, 7H), 7.10 (t, *J* = 7.1 Hz, 3H), 6.84 (t, *J* = 7.2 Hz, 1H), 6.56 (s, 1H), 6.25 (s, 1H), 4.72 (s, 2H), 3.73 (s, 3H), 3.69 (dd, *J* = 7.9, 4.4 Hz, 2H), 3.12 (dt, *J* = 15.9, 7.6 Hz, 1H), 2.83 (dt, *J* = 16.2, 4.3 Hz, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 169.0, 149.7, 137.3, 137.2, 135.7, 129.3, 129.0, 128.6, 128.1, 127.2, 126.8, 125.8, 122.31, 120.6, 119.8, 119.1, 118.1, 115.8, 109.0, 56.5, 52.5, 47.6, 42.2, 26.4; **HRMS (ESI-TOF)**: [M + H] $^{+}$ Calcd for $C_{26}H_{25}N_2O_2^{+}$, 397.1911; found, 397.1903.
 **B30**	**Ethyl2-(3-(2-phenyl-1,2,3,4-tetrahydroisoquinolin-1-yl)-1H-indol-1-yl)propanoate (B30)** Compound **B30** was isolated in 70% yield (59 mg, pale yellow solid); mp 90-92 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.58 (dd, *J* = 26.9, 7.9 Hz, 1H), 7.44 – 7.14 (m, 8H), 7.07 (d, *J* = 8.0 Hz, 3H), 6.82 (t, *J* = 7.1 Hz, 1H), 6.71 (d, *J* = 11.5 Hz, 1H), 6.23 (s, 1H), 5.06 (q, *J* = 7.1 Hz, 1H), 4.19 – 4.10 (m, 2H), 3.67 (dd, *J* = 7.3, 3.3 Hz, 2H), 3.20 – 3.09 (m, 1H), 2.90 – 2.69 (m, 1H), 1.70 (t, *J* = 7.0 Hz, 3H), 1.20 (m, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 171.2, 149.9, 137.2, 135.6, 129.2, 128.9, 128.1, 127.4, 126.7, 125.7, 125.4, 122.0, 120.5, 119.7, 118.3, 116.3, 115.8, 109.6, 61.5, 57.4, 54.1, 42.4, 26.0, 17.5, 14.1; **HRMS (ESI-TOF)**: [M + H] $^{+}$ Calcd for $C_{28}H_{29}N_2O_2^{+}$, 425.2224; found, 425.2217.
2. Analytical data for α-(quinolin-2-ylmethyl)-*N*-aryl THIQs (C1-C16)	
 **C1**	**2-((2-Phenyl-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl)quinolone (C1)** [7] Compound **C1** was isolated in 87% yield (61 mg); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.16 (d, *J* = 8.5 Hz, 1H), 7.94 (d, *J* = 8.4 Hz, 1H), 7.80 – 7.68 (m, 2H), 7.50 (t, *J* = 7.5 Hz, 1H), 7.23 – 7.10 (m, 4H), 7.07 (d, *J* = 8.4 Hz, 1H), 7.05 – 6.91 (m, 3H), 6.89 (d, *J* = 7.5 Hz, 1H), 6.69 (t, *J* = 7.2 Hz, 1H), 5.50 (t, *J* = 7.0 Hz, 1H), 3.80 (ddd, *J* = 13.1, 8.7, 4.7 Hz, 1H), 3.74 – 3.62 (m, 2H), 3.35 (dd, *J* = 13.5, 7.0 Hz, 1H), 3.14 (ddd, *J* = 14.6, 11.5, 7.3 Hz, 1H), 2.94 (dt, *J* = 15.9, 5.0 Hz, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 159.8, 149.3, 148.0, 138.2, 135.8, 134.8, 129.3, 129.1, 129.1, 128.6, 127.5, 127.3, 126.9, 126.6, 125.8, 125.7, 122.8, 117.3, 114.0, 60.0, 45.5, 41.7, 27.2.

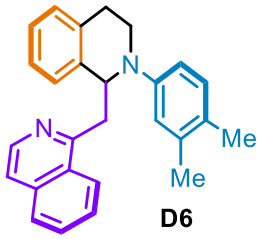
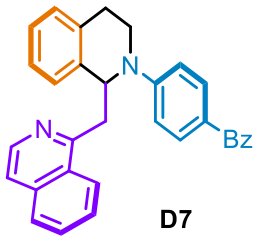
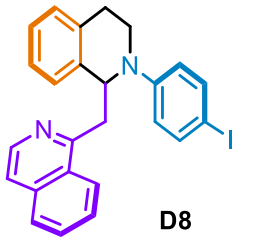
 **C2**	**2-((2-(p-Tolyl)-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl)quinoline (C2)** [7] Compound **C2** was isolated in 64% yield (47 mg); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.18 (dd, *J* = 15.7, 8.2 Hz, 1H), 8.00 – 7.93 (m, 1H), 7.83 – 7.72 (m, 2H), 7.59 – 7.46 (m, 1H), 7.22 – 7.09 (m, 3H), 7.06 – 6.93 (m, 4H), 6.93 – 6.83 (m, 2H), 5.50 – 5.41 (m, 1H), 3.89 – 3.59 (m, 3H), 3.39 (dt, *J* = 12.4, 6.5 Hz, 1H), 3.22 – 3.07 (m, 1H), 2.99 – 2.80 (m, 1H), 2.25 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 160.0, 148.0, 147.4, 138.3, 135.8, 134.8, 129.7, 129.3, 129.0, 128.7, 127.5, 127.4, 126.9, 126.6, 125.8, 125.7, 122.8, 114.8, 60.3, 45.4, 41.7, 27.0, 20.3, 20.0.
 **C3**	**2-((2-(4-(tert-Butyl)phenyl)-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl)quinoline (C3)** Compound **C3** was isolated in 67% yield (54 mg, pale yellow solid); mp 91-93 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.14 (d, *J* = 8.4 Hz, 1H), 7.94 (d, *J* = 8.4 Hz, 1H), 7.79 – 7.67 (m, 2H), 7.50 (dd, *J* = 8.0, 7.0 Hz, 1H), 7.20 – 7.14 (m, 4H), 7.08 (d, *J* = 8.3 Hz, 1H), 7.00 (t, *J* = 7.0 Hz, 1H), 6.91 – 6.85 (m, 3H), 5.44 (t, *J* = 6.9 Hz, 1H), 3.79 (ddd, *J* = 12.9, 8.8, 4.4 Hz, 1H), 3.67 (dt, *J* = 13.5, 6.3 Hz, 2H), 3.32 (dd, *J* = 13.5, 6.8 Hz, 1H), 3.19 – 3.07 (m, 1H), 2.90 (dt, *J* = 16.1, 4.8 Hz, 1H), 1.24 (s, 9H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 160.0, 148.0, 147.1, 140.0, 138.3, 135.7, 134.8, 129.2, 129.1, 128.6, 127.5, 127.3, 126.9, 126.5, 125.9, 125.7, 125.6, 122.8, 114.0, 60.3, 45.6, 41.6, 33.7, 31.5, 27.2; **HRMS (ESI-TOF)**: [M + H] $^+$ Calcd for $C_{29}H_{31}N_2^+$, 407.2482; found, 407.2485.
 **C4**	**2-((2-(4-Fluorophenyl)-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl)quinoline (C4)** [7] Compound **C4** was isolated in 88% yield (65 mg); **^{1}H NMR (600 MHz, $CDCl_3$)** δ 8.11 (d, J = 8.4 Hz, 1H), 7.95 (d, J = 8.3 Hz, 1H), 7.76 (d, J = 8.1 Hz, 1H), 7.73 – 7.68 (m, 1H), 7.55 – 7.47 (m, 1H), 7.19 – 7.11 (m, 2H), 7.06 (d, J = 8.3 Hz, 1H), 7.04 – 6.97 (m, 1H), 6.90 (d, J = 7.6 Hz, 1H), 6.88 – 6.77 (m, 4H), 5.36 (t, J = 7.1 Hz, 1H), 3.80 – 3.71 (m, 1H), 3.61 (ddd, J = 17.8, 12.0, 6.3 Hz, 2H), 3.32 (dd, J = 13.7, 6.7 Hz, 1H), 3.13 – 3.01 (m, 1H), 2.88 (dt, J = 16.1, 4.7 Hz, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 159.8, 155.9 (d, *J* = 236.6 Hz), 148.0, 146.1, 138.1, 135.8, 134.6, 129.4, 129.0, 128.7, 127.6, 127.3, 126.9, 126.7, 125.9 (d, *J* = 5.9 Hz), 122.7, 115.9 (d, *J* = 7.2 Hz), 115.4 (d, *J* = 22.0 Hz), 60.5, 45.5, 42.2, 27.0.
 **C5**	**2-((2-(4-Chlorophenyl)-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl)quinoline (C5)** [7] Compound **C5** was isolated in 85% yield (65 mg); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.12 (d, *J* = 8.4 Hz, 1H), 7.94 (d, *J* = 8.4 Hz, 1H), 7.73 (dd, *J* = 16.9, 8.2 Hz, 2H), 7.50 (t, *J* = 7.5 Hz, 1H), 7.16 (dt, *J* = 13.6, 8.3 Hz, 4H), 7.00 (dd, *J* = 8.3, 5.5 Hz, 2H), 6.87 (d, *J* = 7.6 Hz, 1H), 6.80 (d, *J* = 9.0 Hz, 2H), 5.42 (t, *J* = 7.0 Hz, 1H), 3.74 (ddd, *J* = 13.0, 8.5, 4.9 Hz, 1H), 3.65 – 3.56 (m, 2H), 3.31 (dd, *J* = 13.6, 6.9 Hz, 1H), 3.14 – 3.03 (m, 1H), 2.93 (dt, *J* = 16.0, 5.2 Hz, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 159.5, 147.8, 137.9, 135.9, 134.6, 129.4, 128.8, 128.57, 127.5, 127.3, 126.9, 126.8, 125.9, 125.9, 122.7, 122.0, 115.0, 60.0, 45.4, 41.9, 27.2.

 **C6**	**2-((2-(4-Bromophenyl)-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl)quinoline (C6)** [7] Compound **C6** was isolated in 82% yield (70 mg); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.12 (d, *J* = 8.4 Hz, 1H), 7.94 (d, *J* = 8.4 Hz, 1H), 7.73 (dd, *J* = 16.9, 8.2 Hz, 2H), 7.50 (t, *J* = 7.5 Hz, 1H), 7.16 (dt, *J* = 13.6, 8.3 Hz, 4H), 7.00 (dd, *J* = 8.3, 5.5 Hz, 2H), 6.87 (d, *J* = 7.6 Hz, 1H), 6.80 (d, *J* = 9.0 Hz, 2H), 5.42 (t, *J* = 7.0 Hz, 1H), 3.74 (ddd, *J* = 13.0, 8.5, 4.9 Hz, 1H), 3.65 – 3.56 (m, 2H), 3.31 (dd, *J* = 13.6, 6.9 Hz, 1H), 3.14 – 3.03 (m, 1H), 2.93 (dt, *J* = 16.0, 5.2 Hz, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 159.5, 148.2, 148.0, 137.9, 135.9, 134.6, 131.7, 129.41, 129.0, 128.6, 127.6, 127.2, 126.9, 126.8, 125.9, 125.9, 122.7, 115.4, 109.1, 60.0, 45.4, 41.8, 27.1.
 **C7**	**4-(1-(Quinolin-2-ylmethyl)-3,4-dihydroisoquinolin-2(1H)-yl)benzonitrile (C7)** Compound **C7** was isolated in 80% yield (60 mg, pale yellow solid); mp 95-97 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.15 (d, *J* = 8.5 Hz, 1H), 7.93 (d, *J* = 8.3 Hz, 1H), 7.75 (t, *J* = 7.8 Hz, 2H), 7.56 – 7.50 (m, 1H), 7.38 (d, *J* = 9.0 Hz, 2H), 7.23 – 7.13 (m, 2H), 7.06 – 6.99 (m, 1H), 6.95 (dd, *J* = 8.6, 6.9 Hz, 3H), 6.82 (d, *J* = 7.6 Hz, 1H), 5.58 (t, *J* = 7.0 Hz, 1H), 3.80 (dt, *J* = 12.1, 5.9 Hz, 1H), 3.70 – 3.58 (m, 2H), 3.30 (dd, *J* = 13.7, 7.7 Hz, 1H), 3.09 (t, *J* = 6.1 Hz, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 158.7, 151.4, 148.0, 137.3, 136.1, 134.3, 133.4, 129.6, 129.0, 128.4, 127.6, 127.2, 127.2, 126.9, 126.2, 126.1, 122.6, 120.6, 112.3, 97.9, 59.2, 45.2, 42.2, 27.6; **HRMS (ESI-TOF)**: [M + H] $^+$ Calcd for $C_{26}H_{22}N_3^+$, 376.1808; found, 376.1807.
 **C8**	**2-((2-([1,1'-Biphenyl]-4-yl)-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl)quinolone (C8)** Compound **C8** was isolated in 85% yield (73 mg, pale yellow solid); mp 115-117 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.18 (d, *J* = 8.4 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 1H), 7.79 – 7.71 (m, 2H), 7.54 – 7.47 (m, 3H), 7.45 – 7.34 (m, 4H), 7.28 – 7.23 (m, 1H), 7.20 – 7.13 (m, 2H), 7.11 – 6.98 (m, 4H), 6.92 (d, *J* = 7.6 Hz, 1H), 5.56 (t, *J* = 7.0 Hz, 1H), 3.87 – 3.80 (m, 1H), 3.72 (ddd, *J* = 20.7, 12.4, 6.3 Hz, 2H), 3.38 (dd, *J* = 13.6, 6.9 Hz, 1H), 3.21 – 3.13 (m, 1H), 2.97 (dt, *J* = 15.9, 5.0 Hz, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 159.7, 148.6, 148.0, 141.1, 138.1, 135.9, 134.8, 129.9, 129.3, 129.1, 128.6, 127.7, 127.6, 127.3, 126.9, 126.7, 126.3, 126.0, 125.9, 125.8, 122.8, 114.0, 60.0, 45.5, 41.7, 27.3; **HRMS (ESI-TOF)**: [M + H] $^+$ Calcd for $C_{31}H_{27}N_2^+$, 427.2169; found, 427.2169.
 **C9**	**2-((2-(3-Bromophenyl)-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl)quinoline (C9)** Compound **C9** was isolated in 78% yield (67 mg, pale yellow oil); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.19 (d, *J* = 8.3 Hz, 1H), 7.96 (d, *J* = 8.3 Hz, 1H), 7.74 (dd, *J* = 15.6, 8.0 Hz, 2H), 7.51 (t, *J* = 7.3 Hz, 1H), 7.19 (t, *J* = 10.0 Hz, 3H), 7.08 – 6.93 (m, 3H), 6.92 – 6.79 (m, 2H), 6.75 (d, *J* = 7.7 Hz, 1H), 5.47 (t, *J* = 6.7 Hz, 1H), 3.79 – 3.70 (m, 1H), 3.67 – 3.57 (m, 2H), 3.33 (dd, *J* = 13.5, 6.9 Hz, 1H), 3.16 – 3.06 (m, 1H), 2.96 (dt, *J* = 10.4, 5.0 Hz, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 159.3, 150.3, 137.9, 136.1, 134.6, 130.2, 129.8, 129.47, 128.7, 128.5, 127.5, 127.2, 126.9, 126.8, 126.0, 123.4, 122.6, 122.3, 119.8, 116.5, 112.0, 59.9, 45.4, 41.7, 27.3; **HRMS (ESI-TOF)**: [M + H] $^+$ Calcd for $C_{25}H_{22}BrN_2^+$, 429.0961; found, 429.0961.

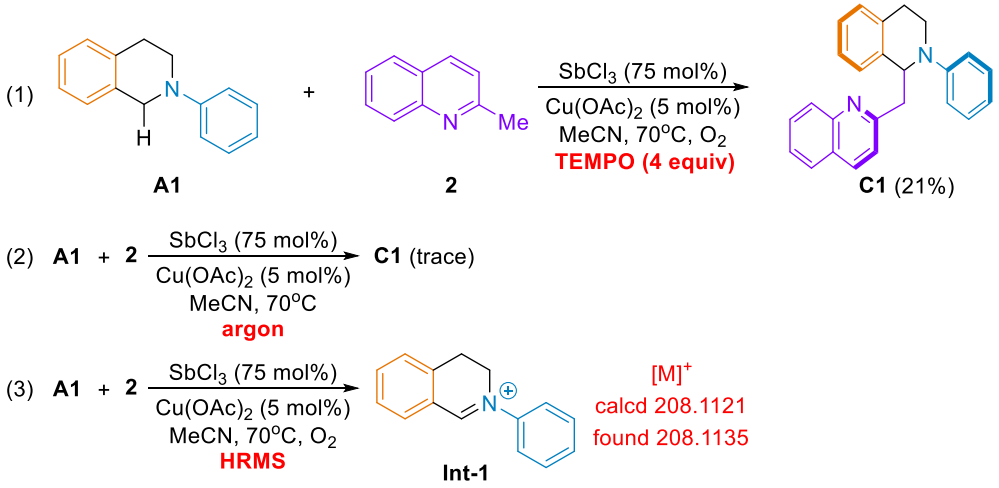
 **C10**	**2-((2-(3,4-Dimethylphenyl)-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl)quinoline (C10)** Compound **C10** was isolated in 60% yield (45 mg, pale yellow solid); mp 88-90 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.12 (d, *J* = 8.5 Hz, 1H), 7.92 (d, *J* = 8.3 Hz, 1H), 7.76 – 7.66 (m, 2H), 7.48 – 7.45 (m, 1H), 7.13 – 7.11 (m, 2H), 7.08 (d, *J* = 8.3 Hz, 1H), 7.02 – 7.00 (m, 1H), 6.93 (d, *J* = 7.7 Hz, 1H), 6.87 (d, *J* = 8.2 Hz, 1H), 6.68 (d, *J* = 2.7 Hz, 1H), 6.64 (dd, *J* = 8.3, 2.7 Hz, 1H), 5.39 (t, *J* = 7.0 Hz, 1H), 3.77 – 3.70 (m, 1H), 3.71 – 3.65 (m, 1H), 3.59 (dd, *J* = 13.6, 7.7 Hz, 1H), 3.37 – 3.29 (m, 1H), 3.15 – 3.08 (m, 1H), 2.84 (dt, *J* = 16.0, 4.5 Hz, 1H), 2.07 (s, 6H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 160.2, 148.1, 147.8, 138.5, 137.0, 135.7, 134.9, 130.1, 129.2, 129.1, 128.7, 127.5, 127.4, 126.9, 126.5, 125.8, 125.7, 122.8, 116.5, 112.1, 60.4, 45.5, 41.6, 27.1, 20.2, 18.5; **HRMS (ESI-TOF)**: $[M + H]^+$ Calcd for $C_{27}H_{27}N_2^+$, 379.2169; found, 379.2171.
 **C11**	**2-((2-(Naphthalen-1-yl)-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl)quinoline (C11)** Compound **C11** was isolated in 42% yield (34 mg, pale yellow solid); mp 110-112 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.98 (s, 1H), 7.87 (dd, *J* = 18.7, 7.8 Hz, 2H), 7.75 – 7.59 (m,3H), 7.43 (dd, *J* = 15.4, 7.9 Hz, 2H), 7.33 (t, *J* = 7.5 Hz, 1H), 7.30 – 7.10 (m, 7H), 6.90 (d, *J* = 7.4 Hz, 1H), 5.16 (s, 1H), 4.08 – 3.88 (m, 1H), 3.68 (d, *J* = 9.4 Hz, 1H), 3.50 (dd, *J* = 13.4, 4.8 Hz, 2H), 2.85 (s, 1H), 2.66 (s, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 160.4, 148.2, 138.8, 135.7, 135.0, 134.6, 129.3, 129.1, 128.8, 128.1, 127.4, 127.1, 126.8, 126.5, 126.0, 125.6, 125.5, 125.5, 125.0, 124.0, 123.3, 122.2, 118.4, 61.9, 44.7; **HRMS (ESI-TOF)**: $[M + H]^+$ Calcd for $C_{29}H_{25}N_2^+$, 401.2012; found, 401.2013.
 **C12**	**2-((2-(Naphthalen-2-yl)-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl)quinoline (C12)** Compound **C12** was isolated in 48% yield (38 mg, pale yellow solid); mp 108-110 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.27 (d, *J* = 8.5 Hz, 1H), 7.94 (d, *J* = 8.4 Hz, 1H), 7.76 – 7.67 (m, 2H), 7.58 – 7.44 (m, 4H), 7.30 – 7.25 (m, 1H), 7.21 (dd, *J* = 9.1, 2.6 Hz, 1H), 7.18 – 7.02 (m, 7H), 5.64 (dd, *J* = 7.8, 6.2 Hz, 1H), 3.94 – 3.81 (m, 2H), 3.71 (dd, *J* = 13.6, 7.9 Hz, 1H), 3.49 (dd, *J* = 13.6, 6.3 Hz, 1H), 3.16 (ddd, *J* = 15.6, 8.7, 6.4 Hz, 1H), 2.93 (dt, *J* = 16.1, 4.5 Hz, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 159.6, 147.126, 137.9, 136.8, 134.7, 134.6, 129.95, 128.7, 128.7, 128.1, 127.5, 127.5, 127.3, 127.2, 126.9, 126.7, 126.3, 126.3, 126.0, 125.9, 122.8, 122.3, 117.8, 108.5, 60.0, 44.9, 41.7, 27.1; **HRMS (ESI-TOF)**: $[M + H]^+$ Calcd for $C_{29}H_{25}N_2^+$, 401.2012; found, 401.2014.
 **C13**	**Phenyl(4-(1-(quinolin-2-ylmethyl)-3,4-dihydroisoquinolin-2(1H)-yl)phenyl)methanone (C13)** Compound **C13** was isolated in 37% yield (34 mg, pale yellow solid); mp 136-138 °C; **^{1}H NMR (600 MHz, $CDCl_3$)** δ 8.13 (d, *J* = 8.4 Hz, 1H), 7.92 (d, *J* = 8.3 Hz, 1H), 7.73 (dd, *J* = 18.5, 8.8 Hz, 4H), 7.65 (d, *J* = 7.1 Hz, 2H), 7.50 (t, *J* = 7.4 Hz, 2H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.21 – 7.15 (m, 2H), 7.01 (t, *J* = 7.3 Hz, 1H), 6.97 (dd, *J* = 8.7, 2.4 Hz, 3H), 6.85 (d, *J* = 7.6 Hz, 1H), 5.64 (t, *J* = 7.0 Hz, 1H), 3.85 (dt, *J* = 12.2, 6.0 Hz, 1H), 3.74 – 3.64 (m, 2H), 3.33 (dd, *J* = 13.6, 7.5 Hz, 1H), 3.15 – 3.05 (m, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 195.0, 158.9, 152.1, 148.0, 139.2, 137.5, 136.1, 134.5, 132.7, 131.1, 129.51, 129.5, 129.0, 128.4, 128.0, 127.6, 127.2, 127.1, 126.9, 126.1, 126.0, 125.3, 122.6, 111.4, 59.3, 45.3, 42.2, 27.7; **HRMS (ESI-TOF)**: $[M + H]^+$ Calcd for $C_{32}H_{27}N_2O^+$, 455.2118; found, 455.2119.

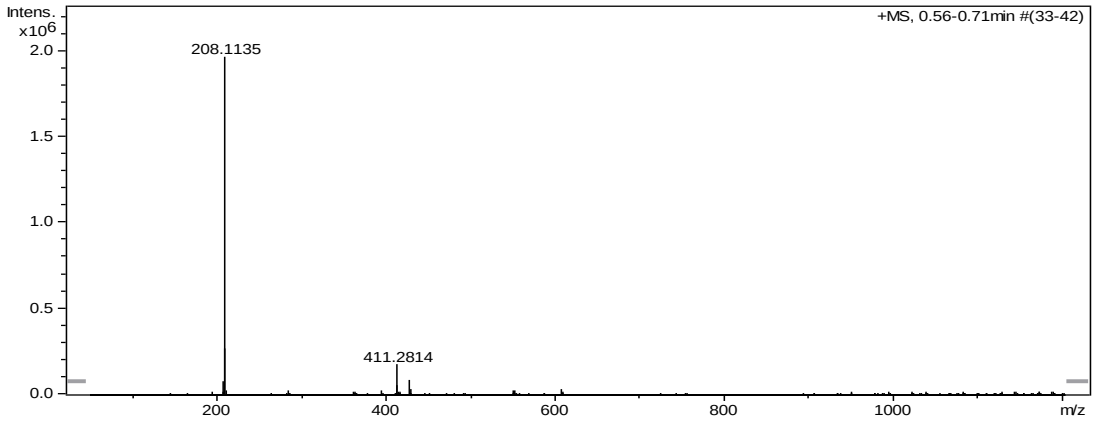
 C14	**2-((2-(4-Iodophenyl)-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl)quinoline (C14)** Compound **C14** was isolated in 80% yield (76 mg, pale yellow solid); mp 151-153 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.12 (d, *J* = 8.4 Hz, 1H), 7.94 (d, *J* = 8.4 Hz, 1H), 7.73 (dt, *J* = 8.3, 4.9 Hz, 2H), 7.56 – 7.46 (m, 1H), 7.36 (t, *J* = 6.1 Hz, 2H), 7.17 – 7.12 (m, 2H), 7.05 – 6.97 (m, 2H), 6.87 (d, *J* = 7.6 Hz, 1H), 6.71 (d, *J* = 9.0 Hz, 2H), 5.42 (t, *J* = 7.0 Hz, 1H), 3.74 (ddd, *J* = 13.0, 8.4, 4.9 Hz, 1H), 3.69 – 3.55 (m, 2H), 3.31 (dd, *J* = 13.6, 7.0 Hz, 1H), 3.16 – 3.03 (m, 1H), 2.94 (dt, *J* = 15.9, 5.3 Hz, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 159.4, 148.7, 148.0, 137.9, 137.6, 135.9, 134.6, 129.4, 129.0, 128.5, 127.6, 127.2, 126.9, 126.8, 125.9, 125.9, 122.6, 116.0, 78.2, 59.8, 45.4, 41.6, 27.2; **HRMS (ESI-TOF)**: [M + H] $^+$ Calcd for $C_{25}H_{22}IN_2^+$, 477.0822; found, 477.0822.
 C15	**7-Fluoro-2-((2-phenyl-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl)quinoline (C15)** Compound **C15** was isolated in 64% yield (47 mg, pale yellow oil); **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.93 (d, *J* = 8.4 Hz, 1H), 7.82 (dd, *J* = 10.4, 2.2 Hz, 1H), 7.73 (dd, *J* = 8.9, 6.2 Hz, 1H), 7.30 (td, *J* = 8.7, 2.5 Hz, 1H), 7.24 – 7.14 (m, 4H), 7.08 – 7.01 (m, 2H), 6.98 (d, *J* = 8.2 Hz, 2H), 6.91 (d, *J* = 7.6 Hz, 1H), 6.72 (t, *J* = 7.2 Hz, 1H), 5.51 (t, *J* = 7.0 Hz, 1H), 3.81 (ddd, *J* = 13.2, 8.7, 4.8 Hz, 1H), 3.75 – 3.64 (m, 2H), 3.36 (dd, *J* = 13.5, 6.9 Hz, 1H), 3.15 (ddd, *J* = 14.3, 8.6, 5.5 Hz, 1H), 2.95 (dt, *J* = 16.0, 5.1 Hz, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 163.1 (d, *J* = 249.1 Hz), 161.0, 149.3, 149.0 (d, *J* = 12.7 Hz), 138.1, 135.7, 134.9, 129.5 (d, *J* = 10.1 Hz), 129.2, 128.6, 127.3, 126.7, 125.8, 123.9, 122.1 (d, *J* = 2.5 Hz), 117.5, 116.3 (d, *J* = 25.0 Hz), 114.0, 112.7 (d, *J* = 17.4 Hz), 59.9, 45.5, 41.7, 27.2; **HRMS (ESI-TOF)**: [M + H] $^+$ Calcd for $C_{25}H_{22}FN_2^+$, 369.1762; found, 369.1761.
 C16	**7-Chloro-2-((2-phenyl-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl)quinolone (C16)** Compound **C16** was isolated in 39% yield (30 mg, pale yellow oil); **^{1}H NMR (600 MHz, $CDCl_3$)** δ 8.23 – 8.16 (m, 1H), 7.92 (d, *J* = 8.2 Hz, 1H), 7.69 (d, *J* = 8.5 Hz, 1H), 7.49 – 7.44 (m, 1H), 7.25 – 7.15 (m, 4H), 7.08 – 7.02 (m, 2H), 6.97 (d, *J* = 8.4 Hz, 2H), 6.91 (d, *J* = 7.8 Hz, 1H), 6.72 (dd, *J* = 14.9, 7.6 Hz, 1H), 5.49 (dd, *J* = 14.5, 7.3 Hz, 1H), 3.79 (dd, *J* = 8.3, 4.6 Hz, 1H), 3.68 (ddd, *J* = 21.3, 13.6, 7.4 Hz, 2H), 3.35 (dd, *J* = 13.5, 7.1 Hz, 1H), 3.13 (dd, *J* = 8.2, 5.7 Hz, 1H), 2.96 (dt, *J* = 15.9, 5.1 Hz, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 161.1, 149.2, 148.4, 138.1, 135.6, 135.1, 134.9, 129.2, 128.8, 128.6, 128.1, 127.3, 126.9, 126.7, 125.8, 125.2, 123.0, 117.5, 114.0, 59.9, 45.4, 41.8, 27.3; **HRMS (ESI-TOF)**: [M + H] $^+$ Calcd for $C_{25}H_{22}ClN_2^+$, 385.1466; found, 385.1468.
3. Analytical data for α-(isoquinolin-1-ylmethyl)-*N*-aryl THIQs (D1-D8)	
 D1	**1-((2-Phenyl-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl)isoquinoline (D1)** Compound **D1** was isolated in 91% yield (64 mg, pale yellow oil); **^{1}H NMR (600 MHz, $CDCl_3$)** δ 8.58 (d, *J* = 5.6 Hz, 1H), 7.87 (d, *J* = 8.5 Hz, 1H), 7.76 (d, *J* = 8.1 Hz, 1H), 7.59 (t, *J* = 7.5 Hz, 1H), 7.53 (d, *J* = 5.5 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 1H), 7.26 – 7.16 (m, 3H), 7.12 (t, *J* = 7.3 Hz, 1H), 6.93 (dd, *J* = 16.5, 7.9 Hz, 3H), 6.78 – 6.67 (m, 2H), 5.63 (t, *J* = 6.8 Hz, 1H), 3.98 (dd, *J* = 13.7, 6.5 Hz, 1H), 3.92 – 3.85 (m, 1H), 3.70 (ddd, *J* = 17.9, 12.7, 6.4 Hz, 2H), 3.22 – 3.12 (m, 1H), 3.06 (dt, *J* = 11.3, 5.1 Hz, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 159.3, 149.2, 141.9, 138.1, 136.2, 134.8, 129.6, 129.15, 128.5, 128.0, 127.2, 126.8, 126.7, 125.7, 125.0, 119.5,

	119.5, 117.3, 113.9, 60.0, 42.0, 40.8, 27.6; **HRMS (ESI-TOF)**: [M + H] $^{+}$ Calcd for $C_{25}H_{23}N_2^{+}$, 351.1856; found, 351.1855.
 **D2**	**1-((2-(4-Fluorophenyl)-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl)isoquinoline (D2)** Compound **D2** was isolated in 57% yield (42 mg, pale yellow oil); **^{1}H NMR (600 MHz, $CDCl_3$)** δ 8.49 (s, 1H), 7.83 (s, 1H), 7.73 (s, 1H), 7.57 (d, *J* = 5.4 Hz, 1H), 7.48 (s, 1H), 7.42 (s, 1H), 7.14 (s, 1H), 7.09 (d, *J* = 5.1 Hz, 1H), 6.90 (d, *J* = 4.6 Hz, 1H), 6.77 (dd, *J* = 26.5, 13.9 Hz, 5H), 5.47 (d, *J* = 4.6 Hz, 1H), 3.92 – 3.83 (m, 1H), 3.80 (s, 1H), 3.69 – 3.62 (m, 1H), 3.56 (d, *J* = 6.3 Hz, 1H), 3.17 – 3.03 (m, 1H), 2.97 (d, *J* = 15.1 Hz, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 159.3, δ 155.8 (d, *J* = 236.5 Hz), 145.9, 141.9, 138.1, 136.2, 134.5, 129.7, 128.6, 127.9, 127.3, 127.2, 126.8, 126.7, 125.7, 125.0, 119.5, 115.7 (d, *J* = 7.2 Hz), 115.3 (d, *J* = 22.0 Hz), 60.6, 42.3, 40.8, 27.4; **HRMS (ESI-TOF)**: [M + H] $^{+}$ Calcd for $C_{25}H_{22}FN_2^{+}$, 369.1762; found, 369.1761.
 **D3**	**1-((2-(4-Chlorophenyl)-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl)isoquinoline (D3)** Compound **D3** was isolated in 78% yield (60 mg, pale yellow oil); **^{1}H NMR (600 MHz, $CDCl_3$)** δ 8.53 (d, *J* = 5.7 Hz, 1H), 7.82 (d, *J* = 8.5 Hz, 1H), 7.75 (d, *J* = 8.2 Hz, 1H), 7.58 (t, *J* = 7.5 Hz, 1H), 7.51 (d, *J* = 5.7 Hz, 1H), 7.42 (t, *J* = 7.7 Hz, 1H), 7.17 (d, *J* = 7.5 Hz, 1H), 7.11 (t, *J* = 7.4 Hz, 1H), 7.05 (d, *J* = 8.9 Hz, 2H), 6.92 (t, *J* = 7.4 Hz, 1H), 6.77 (t, *J* = 7.5 Hz, 3H), 5.52 (t, *J* = 6.9 Hz, 1H), 3.89 (dd, *J* = 13.9, 6.9 Hz, 1H), 3.81 (ddd, *J* = 12.6, 7.9, 5.2 Hz, 1H), 3.68 (dd, *J* = 13.9, 7.0 Hz, 1H), 3.61 – 3.53 (m, 1H), 3.16 – 2.99 (m, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 159.0, 147.6, 141.9, 137.9, 136.1, 134.5, 129.7, 128.8, 128.5, 127.9, 127.3, 127.1, 126.9, 126.8, 125.8, 124.9, 121.8, 119.6, 114.8, 60.0, 42.1, 40.7, 27.5; **HRMS (ESI-TOF)**: [M + H] $^{+}$ Calcd for $C_{25}H_{22}ClN_2^{+}$, 385.1466; found, 385.1464.
 **D4**	**1-((2-(4-Bromophenyl)-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl)isoquinoline (D4)** Compound **D4** was isolated in 80% yield (69 mg, pale yellow solid); m p: 83-85 °C; **^{1}H NMR (600 MHz, $CDCl_3$)** δ 8.53 (d, *J* = 5.6 Hz, 1H), 7.82 (d, *J* = 8.5 Hz, 1H), 7.74 (dd, *J* = 8.0, 2.6 Hz, 1H), 7.60 – 7.55 (m, 1H), 7.51 (dd, *J* = 5.4, 2.6 Hz, 1H), 7.45 – 7.39 (m, 1H), 7.18 (dd, *J* = 11.3, 3.8 Hz, 3H), 7.11 (t, *J* = 7.3 Hz, 1H), 6.92 (t, *J* = 7.2 Hz, 1H), 6.79 (d, *J* = 7.5 Hz, 1H), 6.76 – 6.65 (m, 2H), 5.53 (t, *J* = 6.7 Hz, 1H), 3.89 (ddd, *J* = 13.7, 6.8, 2.5 Hz, 1H), 3.80 (ddd, *J* = 12.5, 7.9, 4.9 Hz, 1H), 3.72 – 3.64 (m, 1H), 3.56 (ddd, *J* = 8.6, 7.2, 4.0 Hz, 1H), 3.09 (tt, *J* = 22.0, 11.8 Hz, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 159.0, 148.0, 141.9, 137.8, 136.1, 134.5, 131.7, 129.7, 128.5, 127.9, 127.3, 127.1, 126.9, 126.8, 125.9, 124.8, 119.6, 115.2, 109.0, 59.9, 42.0, 40.7, 27.5; **HRMS (ESI-TOF)**: [M + Na] $^{+}$ Calcd for $C_{25}H_{21}BrN_2Na^{+}$, 451.0780; found, 451.0781.
 **D5**	**1-((2-(3-Bromophenyl)-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl)isoquinoline (D5)** Compound **D5** was isolated in 24% yield (21 mg, pale yellow oil); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.56 (d, *J* = 4.4 Hz, 1H), 7.88 (d, *J* = 8.1 Hz, 1H), 7.76 (d, *J* = 7.9 Hz, 1H), 7.60 (t, *J* = 6.7 Hz, 1H), 7.57 – 7.42 (m, 2H), 7.15 (dd, *J* = 15.0, 8.0 Hz, 2H), 6.94 (s, 3H), 6.85 (d, *J* = 7.4 Hz, 1H), 6.76 (dd, *J* = 17.4, 7.9 Hz, 2H), 5.57 (d, *J* = 6.3 Hz, 1H), 3.92 (dd, *J* = 13.3, 6.7 Hz, 1H), 3.81 (d, *J* = 5.9 Hz, 1H), 3.71 (dd, *J* = 13.4, 6.3 Hz, 1H), 3.65 – 3.54 (m, 1H), 3.08 (d, *J* = 17.1 Hz, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 158.8, 150.2, 141.9, 137.8, 136.2, 134.5, 130.2, 129.7, 128.5, 127.9, 127.3, 127.1,

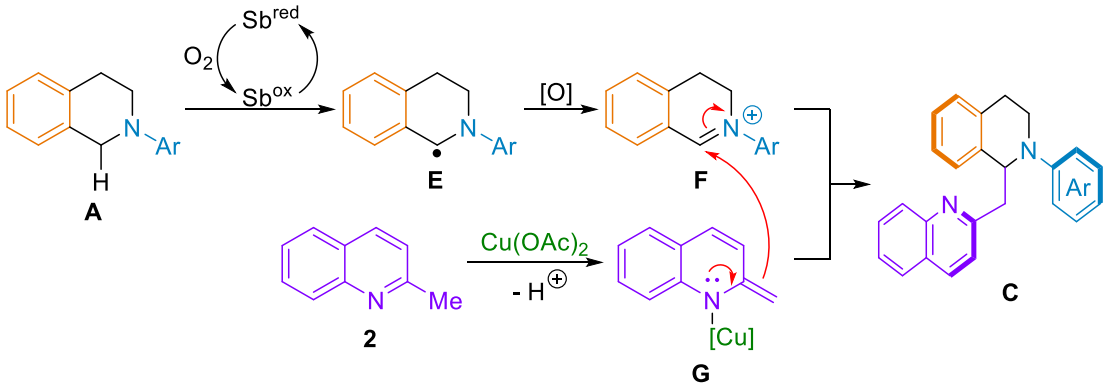
	127.0, 126.9, 125.9, 124.8, 123.3, 119.7, 116.3, 11.0, 59.8, 41.9, 40.9, 27.6; **HRMS (ESI-TOF)**: [M + H] $^{+}$ Calcd for $C_{25}H_{22}BrN_2^{+}$, 429.0961; found, 429.0963.
 **D6**	**1-((2-(3,4-Dimethylphenyl)-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl)isoquinoline (D6)** Compound **D6** was isolated in 75% yield (57 mg, pale yellow oil); **^{1}H NMR (600 MHz, $CDCl_3$)** δ 8.51 (d, *J* = 5.7 Hz, 1H), 7.94 (d, *J* = 8.5 Hz, 1H), 7.76 (d, *J* = 8.2 Hz, 1H), 7.60 (t, *J* = 7.5 Hz, 1H), 7.55 – 7.36 (m, 2H), 7.22 – 7.04 (m, 2H), 6.91 (dd, *J* = 14.2, 7.9 Hz, 2H), 6.74 (d, *J* = 7.6 Hz, 1H), 6.64 (s, 2H), 5.53 (t, *J* = 6.8 Hz, 1H), 3.95 (dd, *J* = 13.6, 7.0 Hz, 1H), 3.89 – 3.77 (m, 1H), 3.74 – 3.54 (m, 2H), 3.20 – 3.08 (m, 1H), 2.96 (dt, *J* = 15.9, 4.4 Hz, 1H), 2.12 (d, *J* = 11.7 Hz, 6H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 159.5, 147.6, 141.9, 138.2, 136.9, 136.2, 134.7, 130.1, 129.6, 128.6, 127.9, 127.3, 127.2, 126.8, 126.5, 125.6, 125.5, 125.2, 119.4, 116.5, 112.2, 60.4, 41.6, 40.8, 27.4, 20.3, 18.6; **HRMS (ESI-TOF)**: [M + H] $^{+}$ Calcd for $C_{27}H_{27}N_2^{+}$, 379.2169; found, 379.2170.
 **D7**	**(4-(1-(Isoquinolin-1-ylmethyl)-3,4-dihydroisoquinolin-2(1H)-yl)phenyl)(phenyl)methanone (D7)** Compound **E7** was isolated in 50% yield (45 mg, pale yellow solid); m p: 137-139 °C; **^{1}H NMR (600 MHz, $CDCl_3$)** δ 8.54 (d, *J* = 5.7 Hz, 1H), 7.76 (dd, *J* = 16.3, 8.4 Hz, 2H), 7.69 (dd, *J* = 7.9, 4.2 Hz, 4H), 7.58 (t, *J* = 7.5 Hz, 1H), 7.51 (t, *J* = 5.9 Hz, 2H), 7.43 (dd, *J* = 14.5, 7.2 Hz, 3H), 7.20 (d, *J* = 7.5 Hz, 1H), 7.12 (t, *J* = 7.4 Hz, 1H), 6.92 (d, *J* = 7.3 Hz, 1H), 6.83 (dd, *J* = 13.7, 8.3 Hz, 3H), 5.72 (t, *J* = 6.9 Hz, 1H), 3.92 (dt, *J* = 8.8, 6.6 Hz, 2H), 3.73 (ddd, *J* = 18.6, 13.1, 6.6 Hz, 2H), 3.16 (dd, *J* = 10.4, 5.4 Hz, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 195.0, 158.4, 152.0, 141.9, 139.2, 137.5, 136.1, 134.4, 132.7, 131.1, 129.7, 129.5, 128.2, 128.0, 127.9, 127.3, 127.1, 127.0, 126.1, 125.2, 124.6, 119.71, 111.2, 59.2, 42.4, 40.7, 27.9; **HRMS (ESI-TOF)**: [M + H] $^{+}$ Calcd for $C_{32}H_{27}N_2O^{+}$, 455.2118; found, 455.2116.
 **D8**	**1-((2-(4-Iodophenyl)-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl)isoquinoline (D8)** Compound **D8** was isolated in 56% yield (21 mg, pale yellow solid); mp: 152-154 °C; **^{1}H NMR (600 MHz, $CDCl_3$)** δ 8.52 (d, *J* = 5.7 Hz, 1H), 7.81 (d, *J* = 8.5 Hz, 1H), 7.75 (d, *J* = 8.2 Hz, 1H), 7.58 (t, *J* = 7.3 Hz, 1H), 7.51 (d, *J* = 5.7 Hz, 1H), 7.42 (t, *J* = 7.7 Hz, 1H), 7.35 (t, *J* = 9.8 Hz, 2H), 7.19 – 7.07 (m, 2H), 6.92 (t, *J* = 7.3 Hz, 1H), 6.78 (d, *J* = 7.6 Hz, 1H), 6.61 (d, *J* = 9.0 Hz, 2H), 5.52 (t, *J* = 6.9 Hz, 1H), 3.93 – 3.84 (m, 1H), 3.79 (ddd, *J* = 12.7, 7.8, 5.1 Hz, 1H), 3.67 (dd, *J* = 13.9, 7.0 Hz, 1H), 3.60 – 3.52 (m, 1H), 3.15 – 2.99 (m, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 158.9, 148.5, 141.9, 137.8, 137.5, 136.1, 134.5, 129.68, 128.4, 127.9, 127.3, 127.1, 126.9, 126.8, 125.9, 124.8, 119.6, 115.8, 78.1, 59.7, 41.9, 40.7, 27.5; **HRMS (ESI-TOF)**: [M + H] $^{+}$ Calcd for $C_{25}H_{22}IN_2^{+}$, 477.0822; found, 477.0822

Control experiments and the proposed mechanism





To elucidate the mechanism of the direct C–H functionalization of tetrahydroisoquinoline derivatives mediated by antimony trichloride, a series of control experiments were conducted using the model reaction between *N*-phenyltetrahydroisoquinoline **A1** and 2-methylquinoline (**2**). When the radical inhibitor TEMPO (4.0 equiv) was introduced under standard reaction conditions, the yield of the target product **C1** was significantly suppressed to 21% (eq 1), suggesting the potential involvement of radical intermediates. Furthermore, carrying out the reaction under an argon atmosphere resulted in only trace amounts of **C1** (eq 2), which aligns with our previous findings [8] that molecular oxygen, in conjunction with $SbCl_3$, is essential for generating a high-valent antimony species responsible for initiating the α-C-H functionalization. Supporting evidence was obtained through high-resolution mass spectrometry (HRMS) analysis of the reaction mixture (eq 3), which successfully detected the signal corresponding to the key intermediate **Int-1**. This observation indicates that **A1** is first oxidized to an iminium ion intermediate by the high-valent antimony species, which subsequently undergoes nucleophilic addition by 2-methylquinoline **2** to afford the α-substituted tetrahydroisoquinoline derivative **C1**.

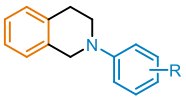


Based on the control experiments and previous findings, [8] a reaction mechanism involving radical intermediates is proposed. Initially, molecular oxygen activates antimony trichloride to generate a high-valent antimony species, which oxidizes tetrahydroisoquinoline **A** to the radical intermediate **E**. This radical is further oxidized under oxidative conditions (by oxygen or copper acetate) to form the iminium ion **F**. Concurrently, copper acetate acts as a Lewis acid to activate 2-methylquinoline, promoting its deprotonation and conversion into the enamine intermediate **G**. This enamine then undergoes nucleophilic attack on the iminium ion **F**. Subsequent elimination of the copper acetate catalyst affords the final product **C**. An analogous mechanistic pathway is envisaged for reactions involving indole derivatives (**1**) or 1-methylisoquinoline (**4**) with tetrahydroisoquinolines **A**, wherein the nucleophile attacking the iminium ion **F** is replaced by the corresponding indoles **1** or 1-methylisoquinoline **4**.

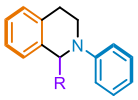
UV spectra of the THIQ derivatives

Table S1. Chemical structures and UV spectra of THIQs

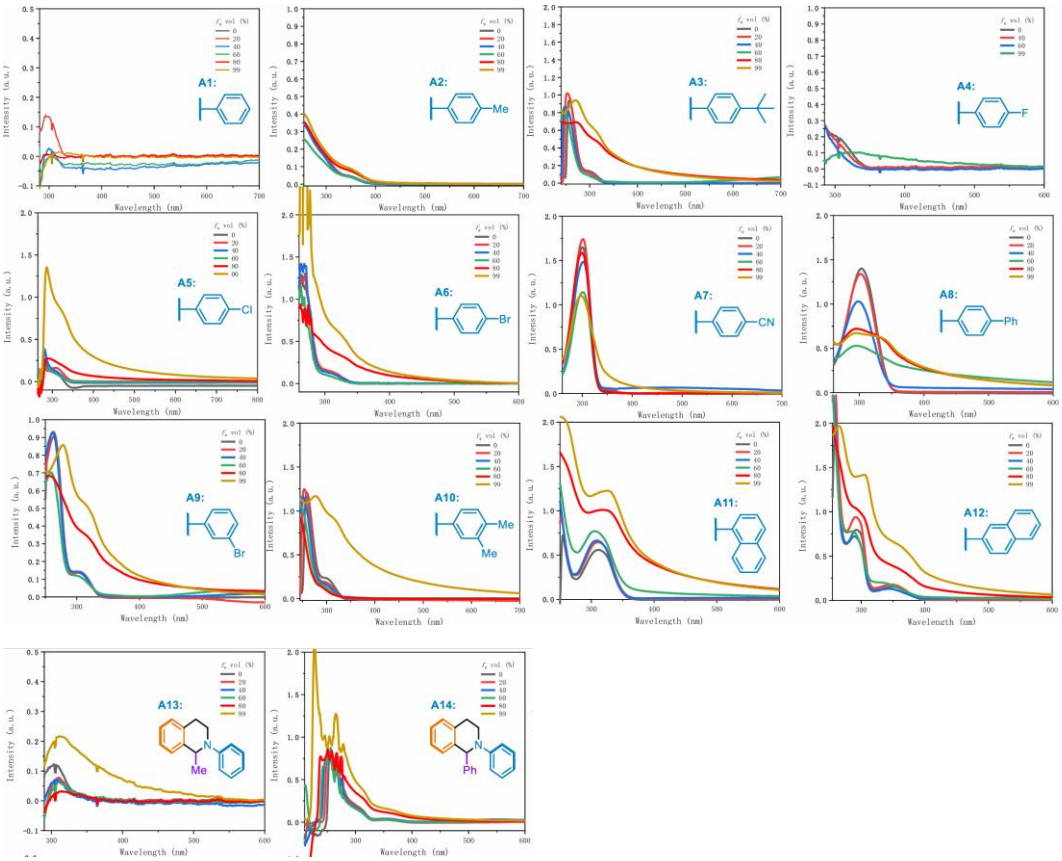
A series:



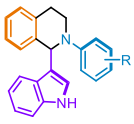
A1: R = H
A2: R = 4-Me
A3: R = 4-*t*-Bu
A4: R = 4-F
A5: R = 4-Cl
A6: R = 4-Br
A7: R = 4-CN
A8: R = 4-Ph
A9: R = 3-Br
A10: R = 3,4-Me
A11: R = 1-Np
A12: R = 2-Np



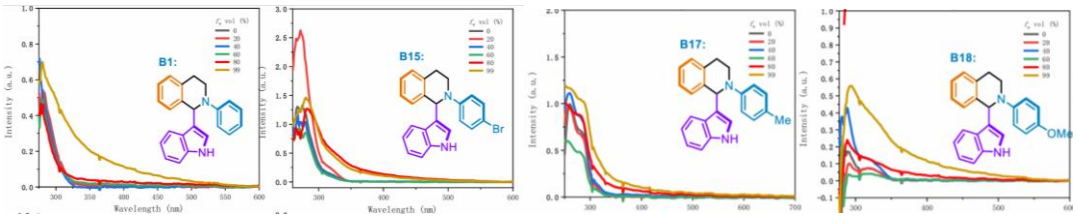
A13: R = Me
A14: R = Ph



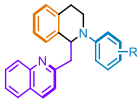
B series:



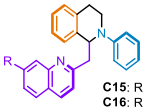
B1: R = H
B15: R = 4-bR
B17: R = 4-Me
B18: R = 4-OMe



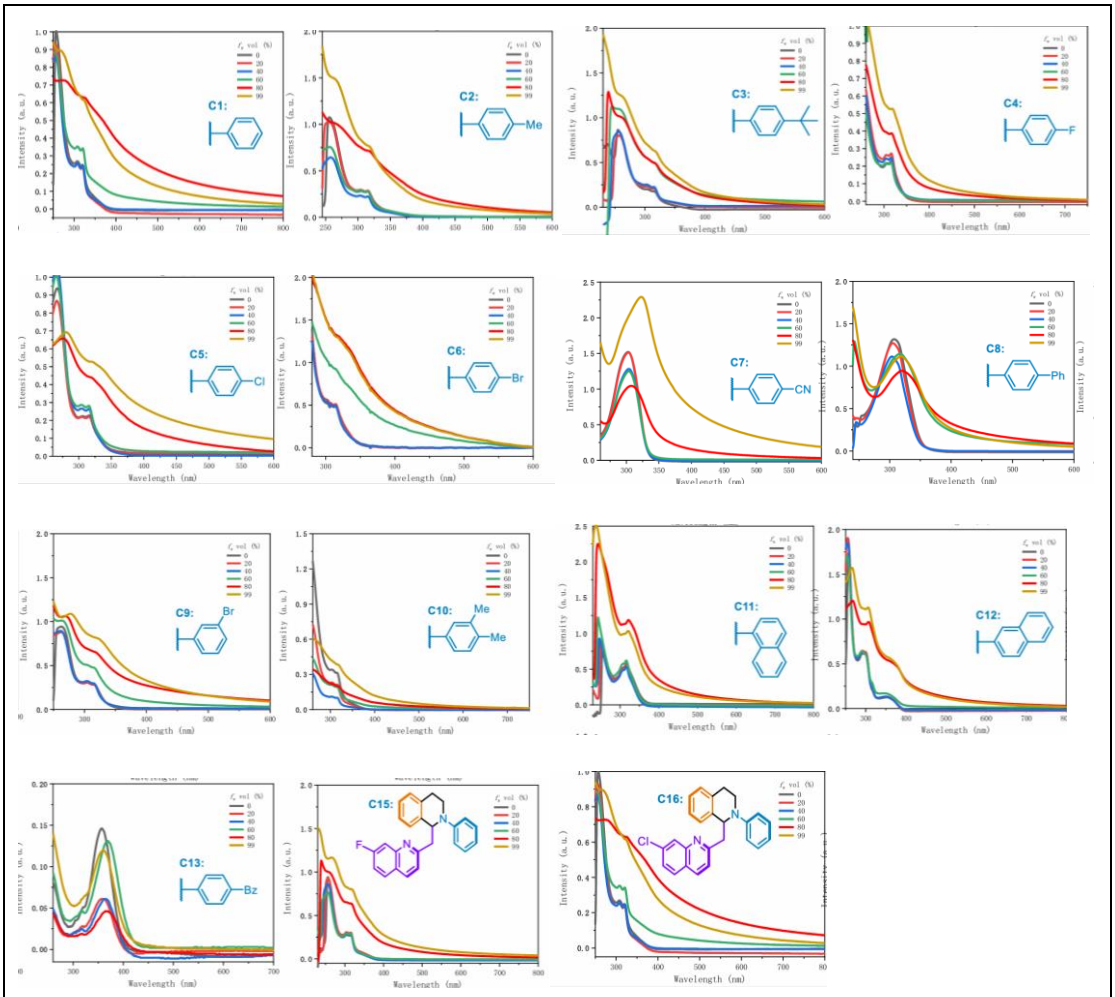
C series:



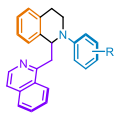
C1, R = H
C2, R = 4-Me
C3, R = 4-*t*-Bu
C4, R = 4-F
C5, R = 4-Cl
C6, R = 4-Br
C7, R = 4-CN
C8, R = 4-Ph
C9, R = 3-Br
C10, R = 3,4-Me
C11, R = 1-Np
C12, R = 2-Np
C13, R = 4-Bz



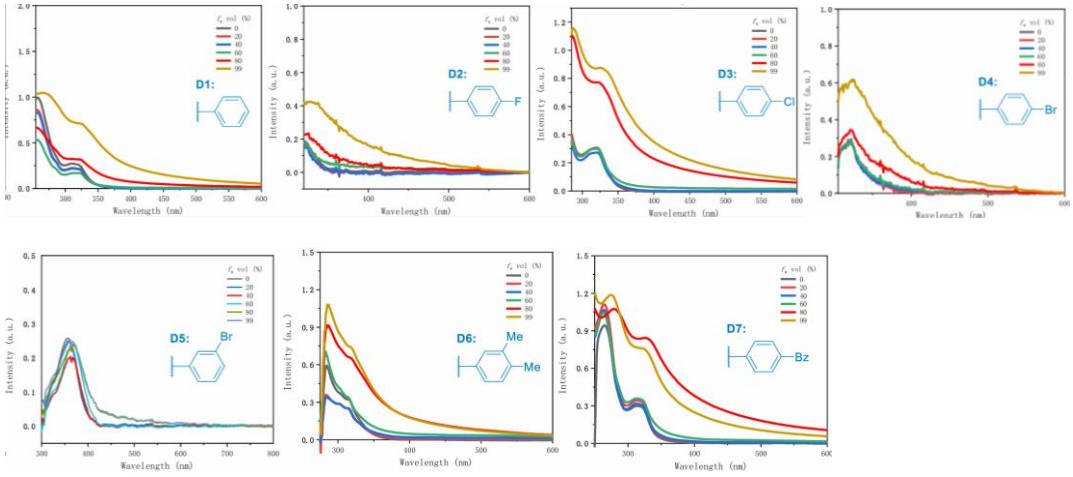
C15: R = F
C16: R = Cl



D series:



D1: R = H, 91%;
D2: R = 4-F, 57%;
D3: R = 4-Cl, 78%;
D4: R = 4-Br, 80%;
D5: R = 3-Br, 24%;
D6: R = 3,4-Me, 75%;
D7: R = 4-Bz, 50%;
D8: R = 4-I, 56%.

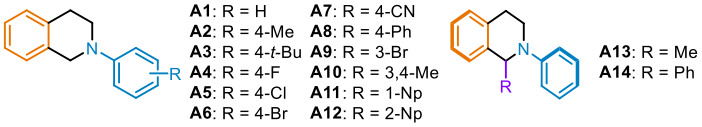


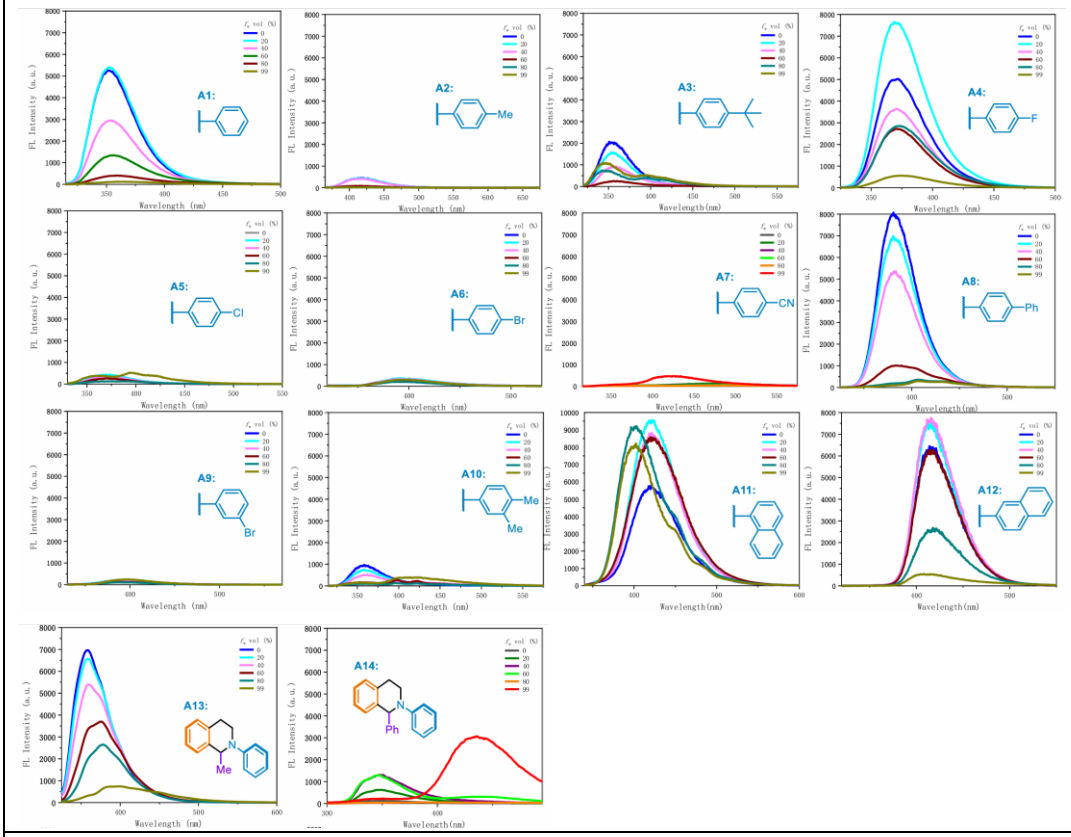
Fluorescent spectra of the THIQ derivatives

The compounds were dissolved in DMSO to prepare 2 mM stock solution. Testing solutions were prepared by diluting 10 μL of stock solution into 2mL DMSO/H_2O mixed solution, the proportions of H_2O are as follows by 0%, 20%, 40%, 60%, 80%, 99%.

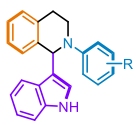
Table S2. Chemical structures and Fluorescent spectra of THIQs

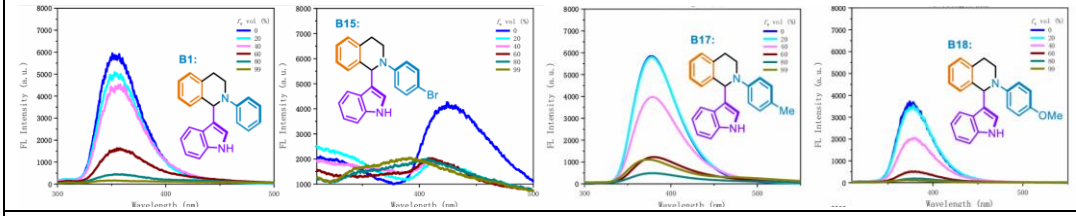
A series:



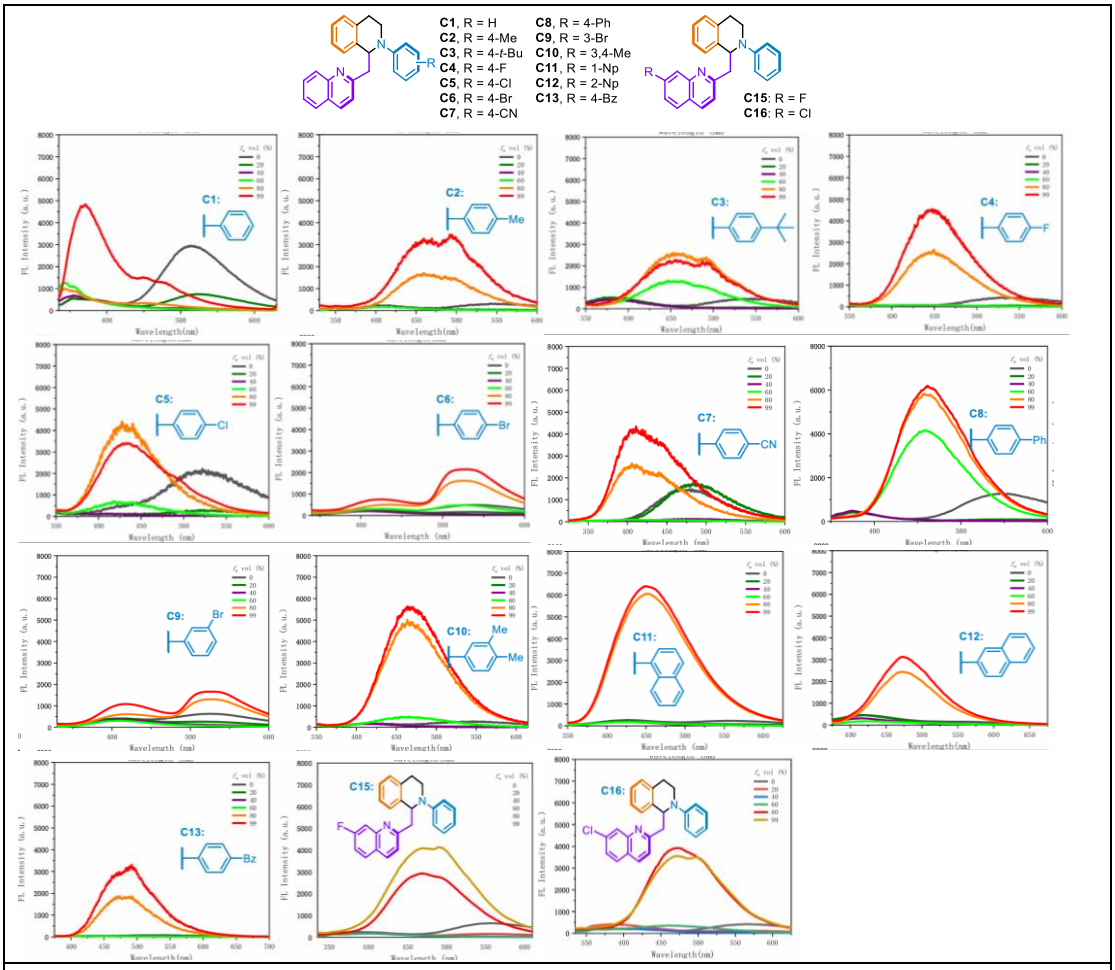


B series:

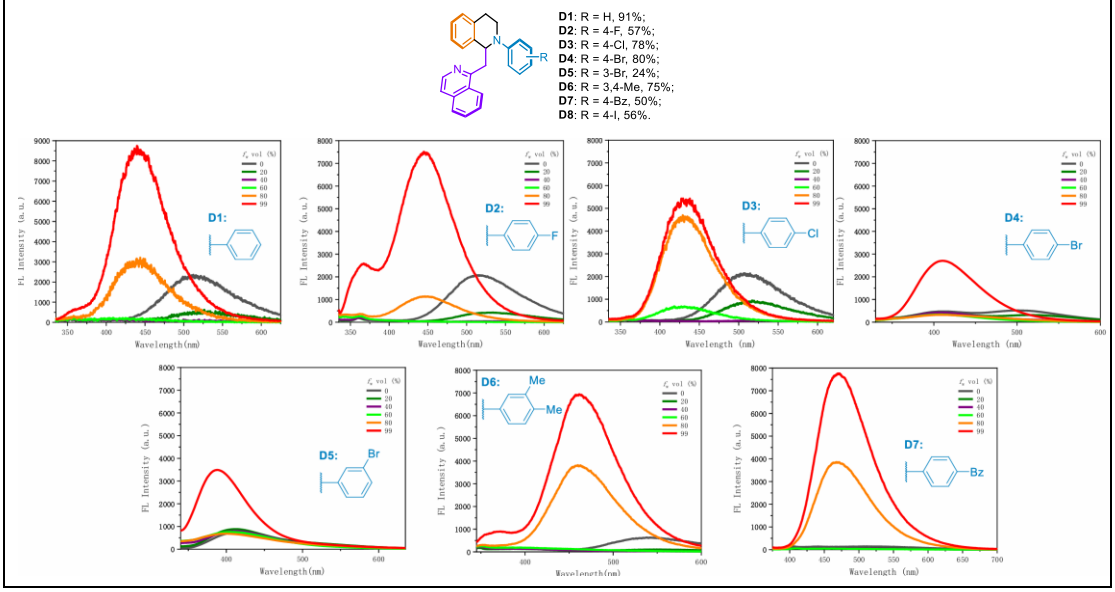




C series:


C1, R = H
C2, R = 4-Me
C3, R = 4-t-Bu
C4, R = 4-F
C5, R = 4-Cl
C6, R = 4-Br
C7, R = 4-CN
C8, R = 4-Ph
C9, R = 3-Br
C10, R = 3,4-Me
C11, R = 1-Np
C12, R = 2-Np
C13, R = 4-Bz
C15: R = F
C16: R = Cl
C1:
C2:
C3:
C4:
C5:
C6:
C7:
C8:
C9:
C10:
C11:
C12:
C13:
C15:
C16:
FL Intensity (a.u.)
Wavelength (nm)

D series:


D1: R = H, 91%;
D2: R = 4-F, 57%;
D3: R = 4-Cl, 78%;
D4: R = 4-Br, 80%;
D5: R = 3-Br, 24%;
D6: R = 3,4-Me, 75%;
D7: R = 4-Bz, 50%;
D8: R = 4-I, 56%.
D1:
D2:
D3:
D4:
D5:
D6:
D7:
FL Intensity (a.u.)
Wavelength (nm)

Fluorescence quantum yields

Relative fluorescence quantum yields.

Quinine sulfate dihydrate in H_2O was used as the reference standard (Φ_s = 54%). The fluorescence quantum yield (Φ_x) was calculated using the following formula:

$$\Phi_x = \Phi_s \times \frac{F_x}{F_s} \times \frac{A_s}{A} \times \frac{\eta_x^2}{\eta_s^2}$$

where the subscripts "x" and "s" represent the sample and the quinine sulfate standard, respectively. *F* is the integrated fluorescence peak area, *A* is the absorbance at the excitation wavelength, and η is the refractive index of the solvent. The quantum yields obtained from this calculation are listed below.

$\Phi_{\mathbf{C13}}$ = 1.78%, $\Phi_{\mathbf{D7}}$ = 12.95%

Absolute fluorescence quantum yields.

The absolute fluorescence quantum yields (Φ'_{FL}) of **C13** and **E7** were measured using an integrating sphere coupled to an absolute PL quantum yield spectrometer (Hitachi F-7000). The quantum yield is defined as the ratio of emitted photons (N_{em}) to absorbed photons (N_{abs}), and was calculated using the following equation:

$$\Phi'_{FL} = \frac{N_{em}}{N_{abs}} = \frac{\alpha \int \frac{\lambda}{hc} I_{em}(\lambda) d\lambda}{\alpha \int \frac{\lambda}{hc} [I_{ex}(\lambda) - I'_{ex}(\lambda)] d\lambda}$$

Here, λ is the wavelength, h is Planck's constant, c is the speed of light, and I_{em} (λ) is the emission spectrum. I_{ex} (λ) and I'_{ex} (λ) represent the spectra of the excitation beam measured without and with the sample in place, respectively. This absolute method ensures that the measured Φ_{FL} values are independent of the sample's shape, thickness, and the excitation laser power. The measured absolute fluorescence quantum yields were determined to be:

$\Phi'_{\mathbf{C13}}$ = 1.97%, $\Phi'_{\mathbf{D7}}$ = 13.50%

References

[1] W. Luo, J. Yang, J. Cheng, *iScience* 2020, **23**, 100851.

[2] O. Basl é, C. Li, *Org. Lett.* 2008, **10**, 3661.

[3] J. Wu, J. Zhong, Q. Meng, T. Lei, X. Gao, C. Tung. *Org. Lett*. 2015, **17**, 884.

[4] C. Huo, C. Wang, M. Wu, X. Jia, X. Wang, Y. Yuan. *Org. Biomol. Chem*. 2014, **12**, 3123.

[5] J. Zhong, Q. Meng, B. Liu, X. Li, X. Gao, T. Lei. *Org. Lett*. 2014, **16**, 1988.

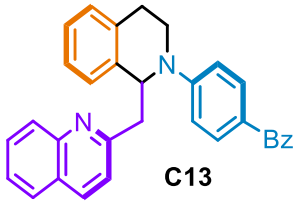
[6] P. Jha, S. Husen, R. Kumar, *Green Chem*. 2021, **23**, 2950.

[7] F. Wang, C. Luo, G. Deng, L. Yang, *Green Chem*. 2014, **16**, 2428.

[8] (a) J. Mao, Y. Hu, S. He, S. Zhang, Q. Ma, Y. Yuan, X. Jia *Org. Lett.* 2024, **26**, 11201; (b) Y. Su, S. Zhang, Y. Yuan, Q. Ma, Z. Sun, Y. Yuan, X. Jia *Chem. Commun.*, 2021, **57**, 9878–9881; (c) Q. Ma, S. Zhang, Y. Li, H. Ding, Z. Sun, Y. Yuan, X. Jia *Synthesis* 2023, **55**, 1593; (d) Y. Li, S. Zhang, Q. Ma, H. Ding, Z. Sun, Y. Yuan, X. Jia *Chem Asian J.* 2022, e202200656.

X-ray structure analysis of C13

The solid was crystallized by slow vapor diffusion of ethyl acetate and hexane layered on top at room temperature. CCDC 2498695 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre (CCDC).



C13

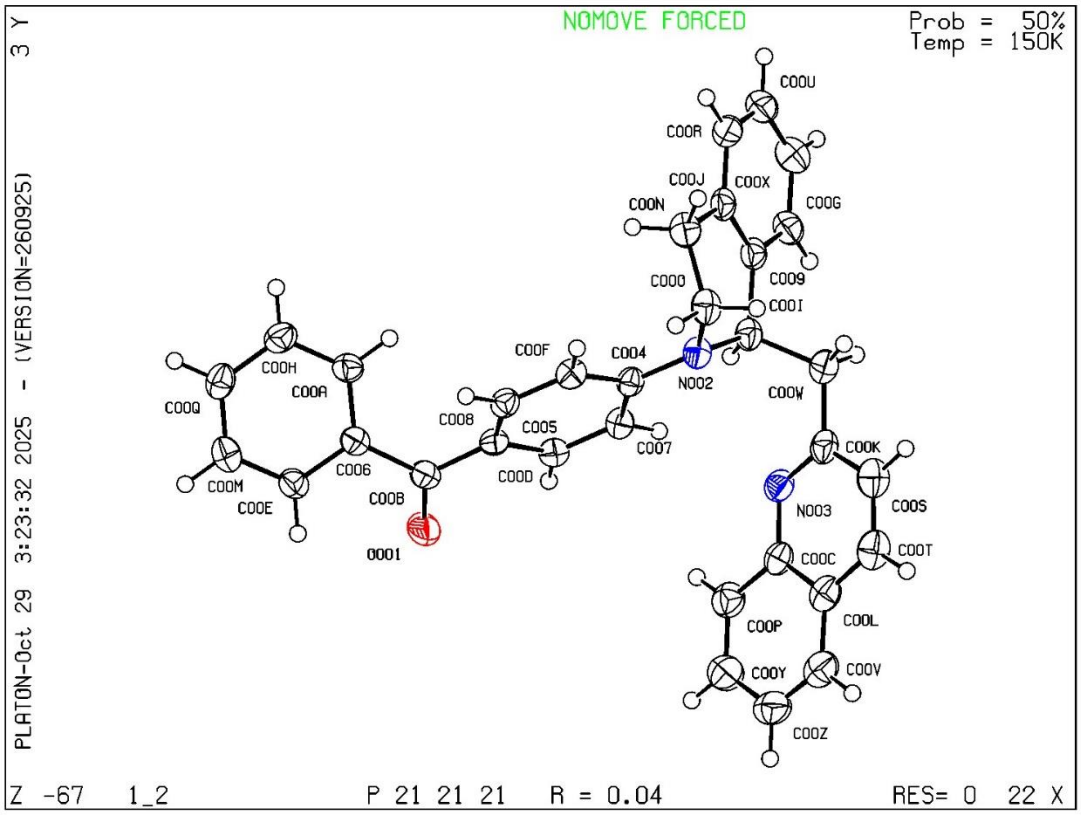


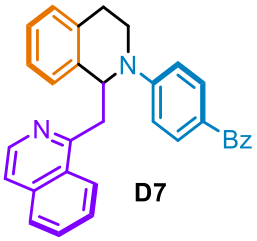
Figure S1. ORTEP drawing of **C13** with 50% probability displacement ellipsoids.

Table Crystal data and structure refinement for C13

CCDC number	**2498695**
Empirical formula	$C_{32}H_{26}N_2O$
Formula weight	454.55
Temperature [K]	150.00
Crystal system	orthorhombic
Space group (number)	$P2_12_12_1$ (19)
a [Å]	11.6092(9)
b [Å]	12.2172(10)
c [Å]	16.4574(13)
α [°]	90
β [°]	90
γ [°]	90
Volume [Å^3]	2334.2(3)
Z	4
ρ_{calc} [gcm^{-3}]	1.293
μ [mm^{-1}]	0.387
F(000)	960
Crystal size [mm^3]	0.03×0.03×0.03
Crystal colour	metallic light yellow
Crystal shape	block
Radiation	GaK_α (λ=1.34139 Å)
2θ range [°]	7.84 to 105.94 (0.84 Å)
Index ranges	−13 ≤ h ≤ 13; −14 ≤ k ≤ 14; 19 ≤ l ≤ 19
Reflections collected	30689
Independent reflections	4113; R_{int} = 0.0849; R_{sigma} = 0.0490
Completeness to θ = 52.972°	100.0 %
Data / Restraints / Parameters	4113 / 0 / 317
Absorption correction T_{min}/T_{max} (method)	0.5421 / 0.7519 (none)
Goodness-of-fit on F^2	1.092
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0388 wR_2 = 0.0940
Final *R* indexes [all data]	R_1 = 0.0450 wR_2 = 0.0972
Largest peak/hole [eÅ^{-3}]	0.23/−0.21
Extinction coefficient	0.0040(7)
Flack X parameter	-0.1(3)

X-ray structure analysis of D7

The solid was crystallized by slow vapor diffusion of ethyl acetate and hexane layered on top at room temperature. CCDC 2401143 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre (CCDC).



D7

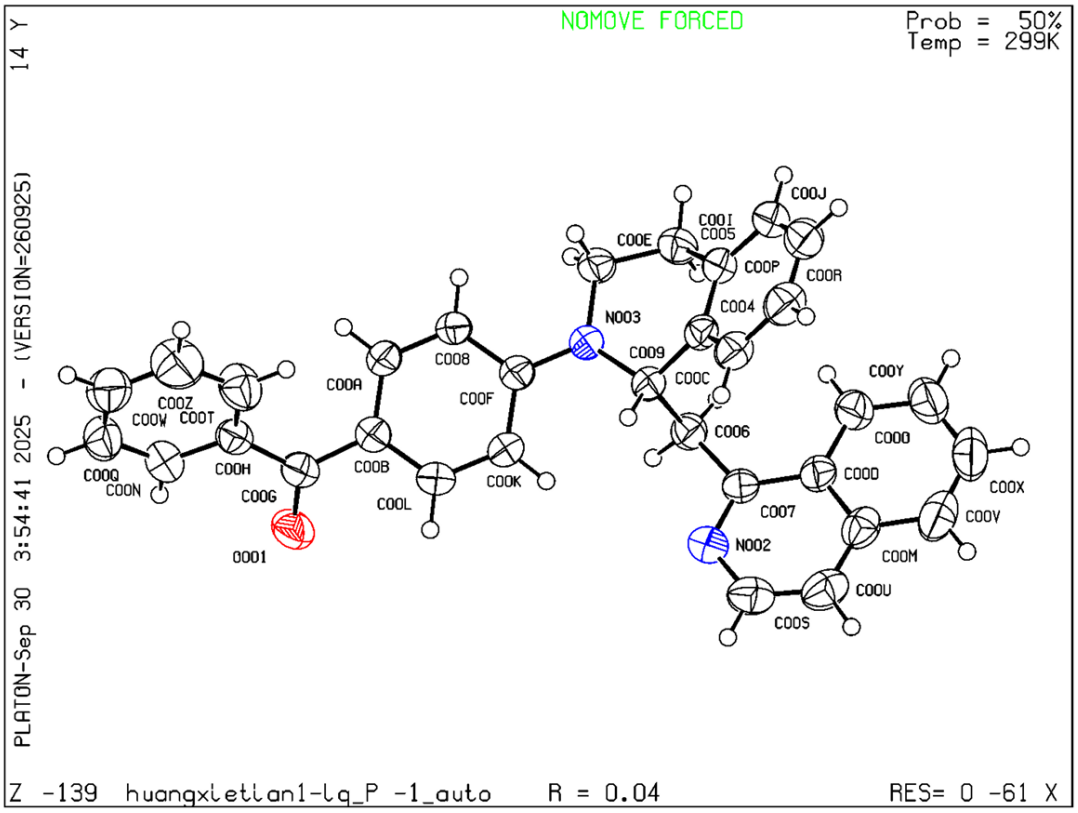
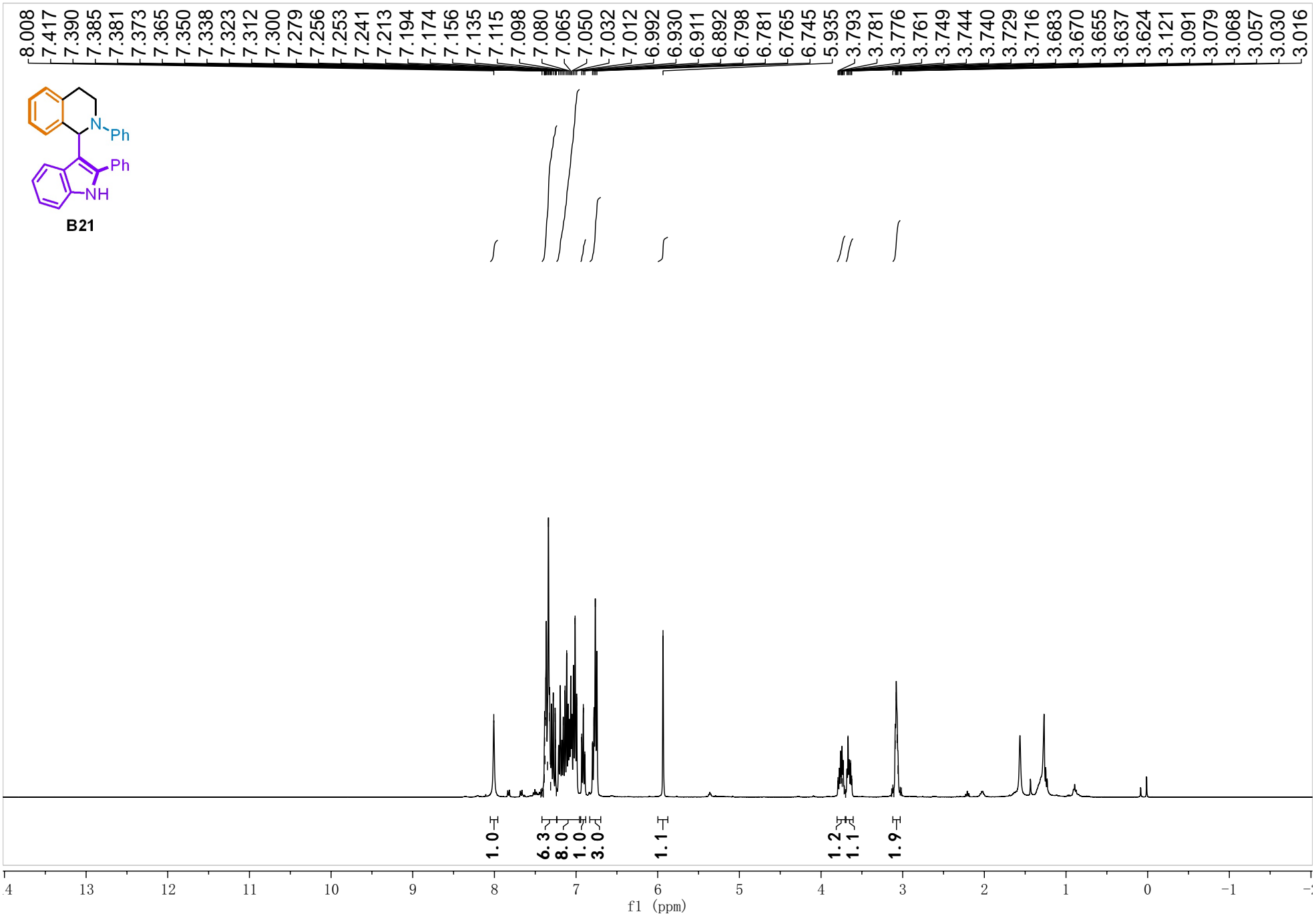


Figure S2. ORTEP drawing of **D7** with 50% probability displacement ellipsoids.

Table Crystal data and structure refinement for D7

CCDC number	**2401143**
Empirical formula	$C_{32}H_{26}N_2O$
Formula weight	454.55
Temperature [K]	299.13 (10)
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	8.8121 (2)
b [Å]	10.1918 (2)
c [Å]	13.9891 (4)
α [°]	99.490 (2)
β [°]	97.145 (2)
γ [°]	103.344 (2)
Volume [Å^3]	1188.33 (5)
Z	2
ρ_{calc} [gcm^{-3}]	1.270
μ [mm^{-1}]	0.596
F(000)	480
Crystal size [mm^3]	0.12×0.15×0.18
Crystal colour	clear light colourless
Crystal shape	block
Radiation	Cu K_α (λ=1.54184 Å)
2θ range [°]	6.50 to 133.20 (0.84 Å)
Index ranges	$-8 \le h \le 10$; $12 \le k \le 12$; $16 \le l \le 16$
Reflections collected	12784
Independent reflections	4178; R_{int} = 0.0234; R_{sigma} = 0.0228
Completeness to θ = 66.599°	99.8 %
Data / Restraints / Parameters	4178 / 0 / 317
Absorption correction T_{min}/T_{max} (method)	0.9251 / 1.0000 (multi-scan)
Goodness-of-fit on F^2	1.051
Final *R* indexes [$I \ge 2\sigma(I)$]	R_1 = 0.0366; wR_2 = 0.0968
Final *R* indexes [all data]	R_1 = 0.0419; wR_2 = 0.1006
Largest peak/hole [eÅ^{-3}]	0.15/−0.14
Extinction coefficient	0.0114 (11)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Ph
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1.2
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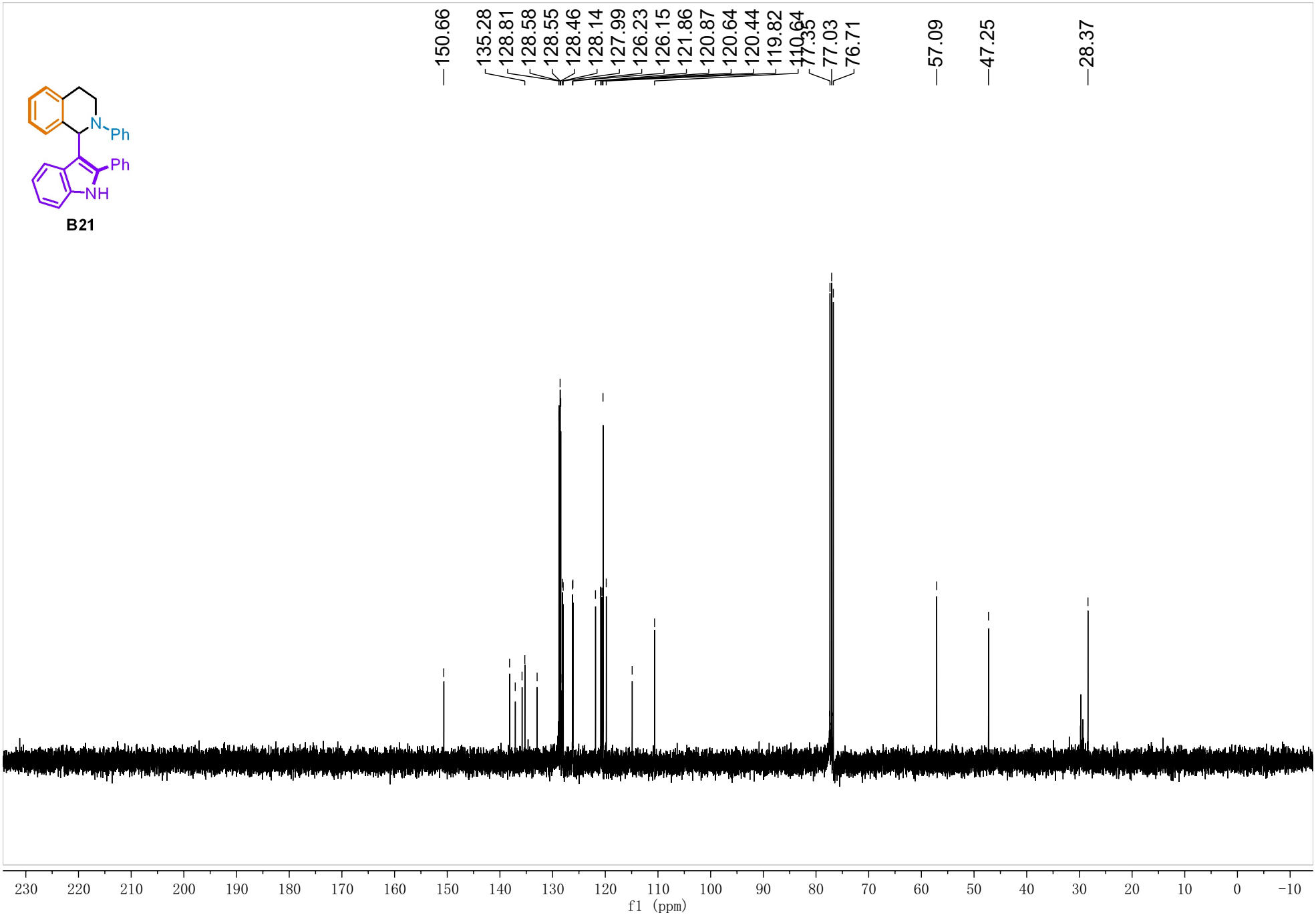
f1 (ppm)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76.71
57.09
47.25
28.37
N
Ph
Ph
NH
B21
230
220
210
200
190
180
170
160
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140
130
120
110
100
90
80
70
60
50
40
30
20
10
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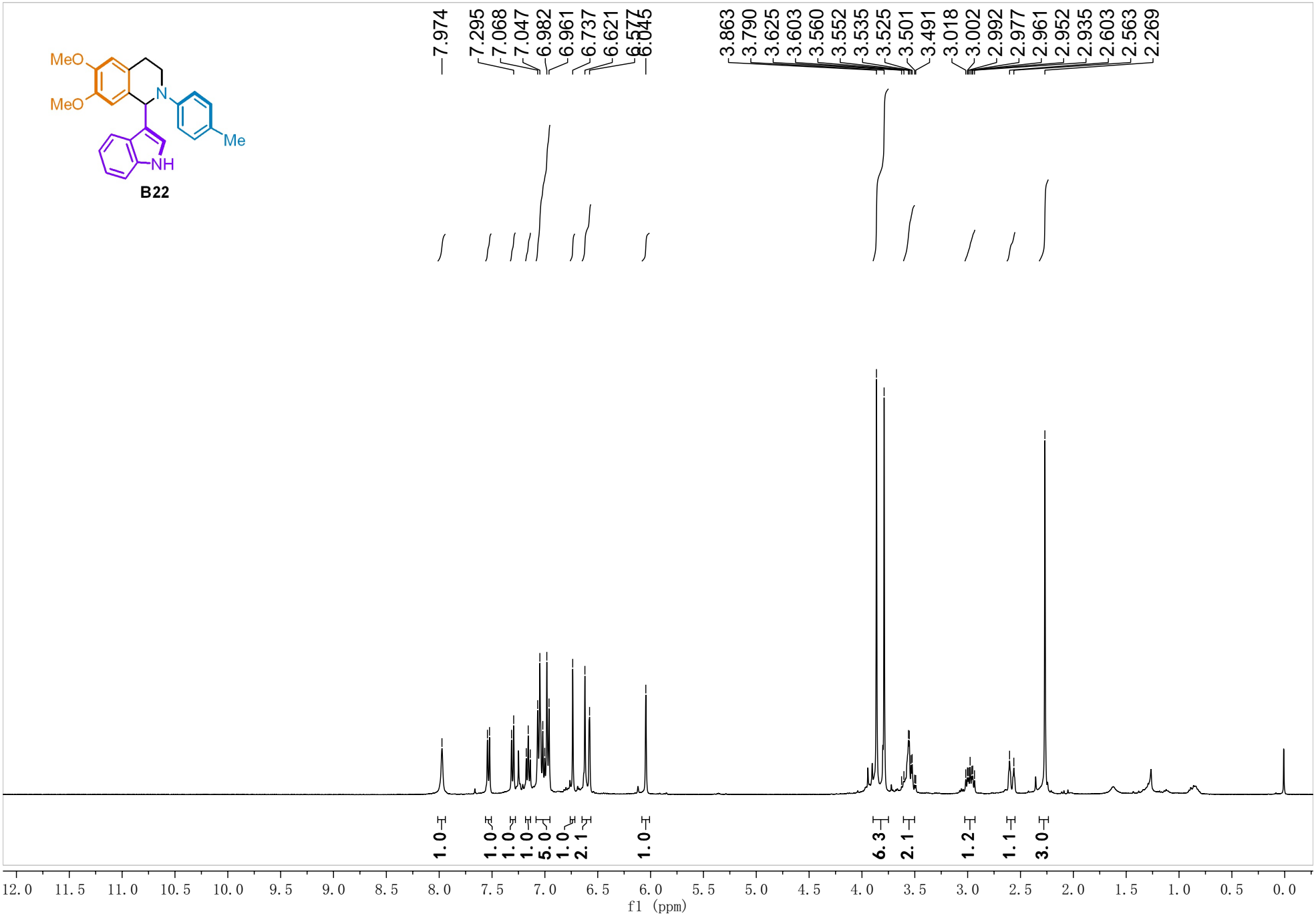
−10
f1 (ppm)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MeO
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Me
NH
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6.621
6.577
6.545
3.863
3.790
3.625
3.603
3.560
3.552
3.535
3.525
3.501
3.491
3.018
3.002
2.992
2.977
2.961
2.952
2.935
2.603
2.563
2.269
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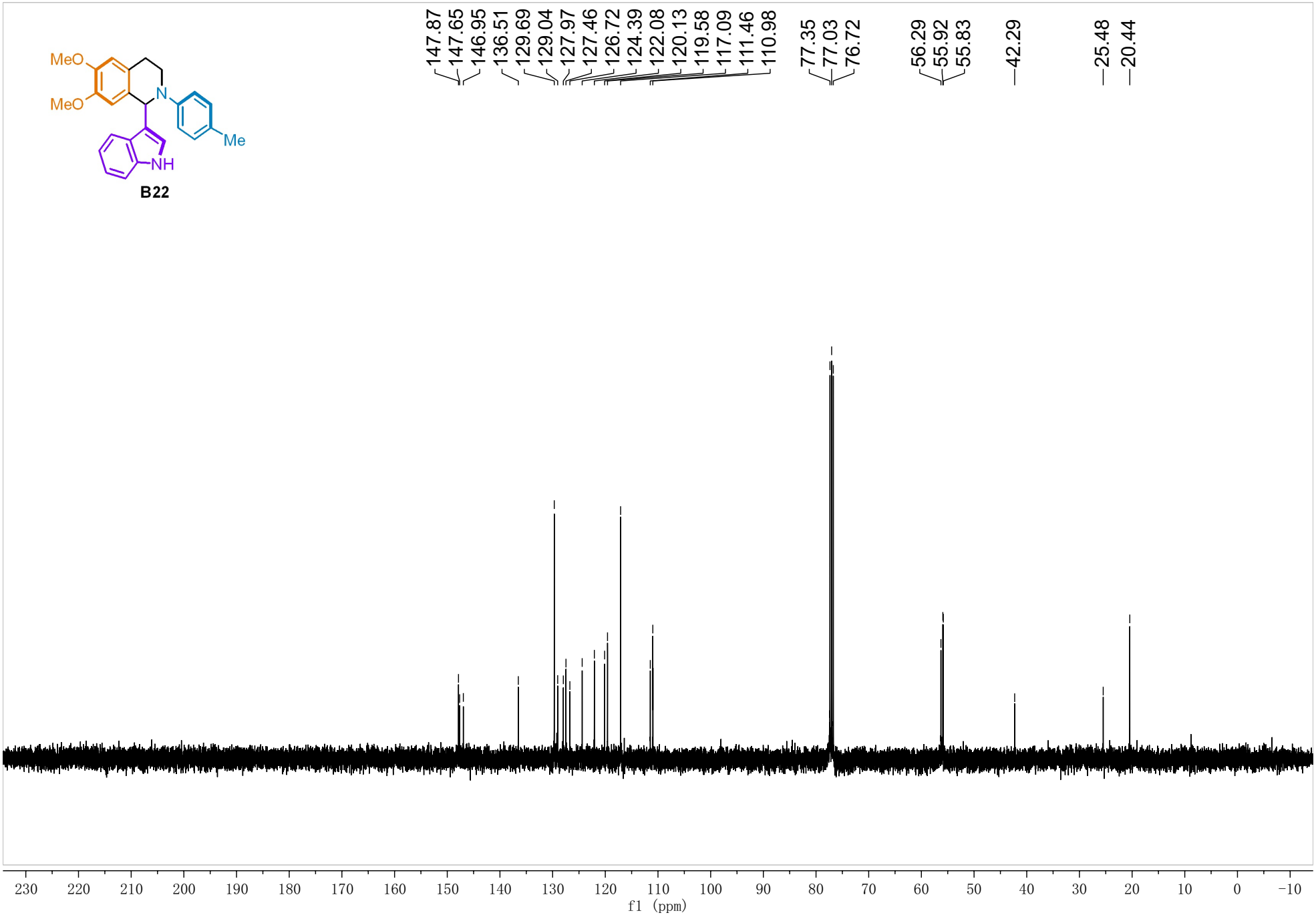
1.0
1.0
1.0
5.0
1.0
2.1
1.0
6.3
2.1
1.2
1.1
3.0
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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MeO
N
Me
NH
B22
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136.51
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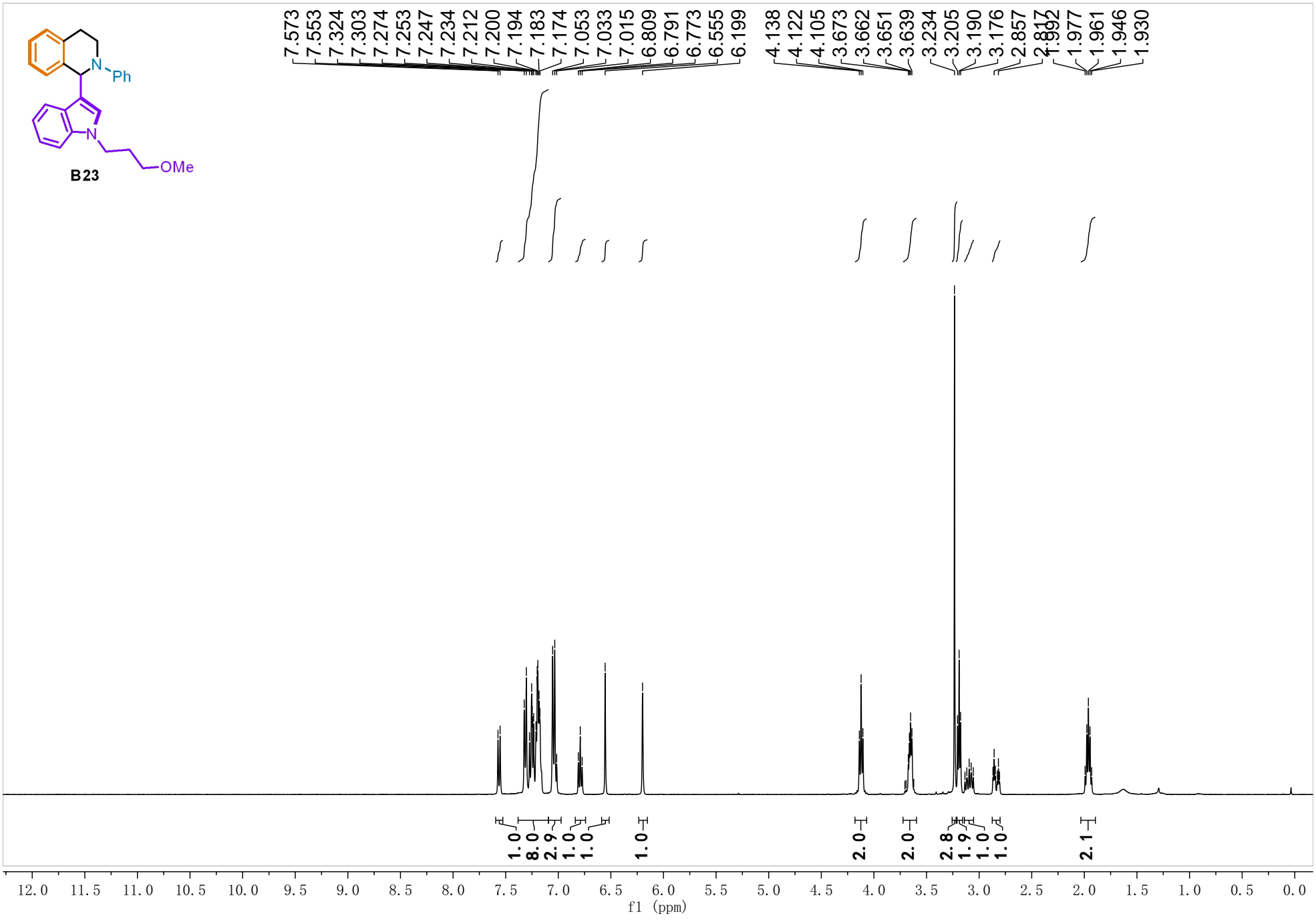
129.04
127.97
127.46
126.72
124.39
122.08
120.13
119.58
117.09
111.46
110.98
77.35
77.03
76.72
56.29
55.92
55.83
42.29
25.48
20.44
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)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7.253
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7.234
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7.200
7.194
7.183
7.174
7.053
7.033
7.015
6.809
6.791
6.773
6.555
6.199
4.138
4.122
4.105
3.673
3.662
3.651
3.639
3.234
3.205
3.190
3.176
2.857
2.817
1.992
1.977
1.961
1.946
1.930
N
Ph
N
OMe
B23
1.0
8.0
2.9
1.0
1.0
1.0
2.0
2.0
2.8
1.9
1.0
1.0
2.1
12.0
11.5
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9.5
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7.5
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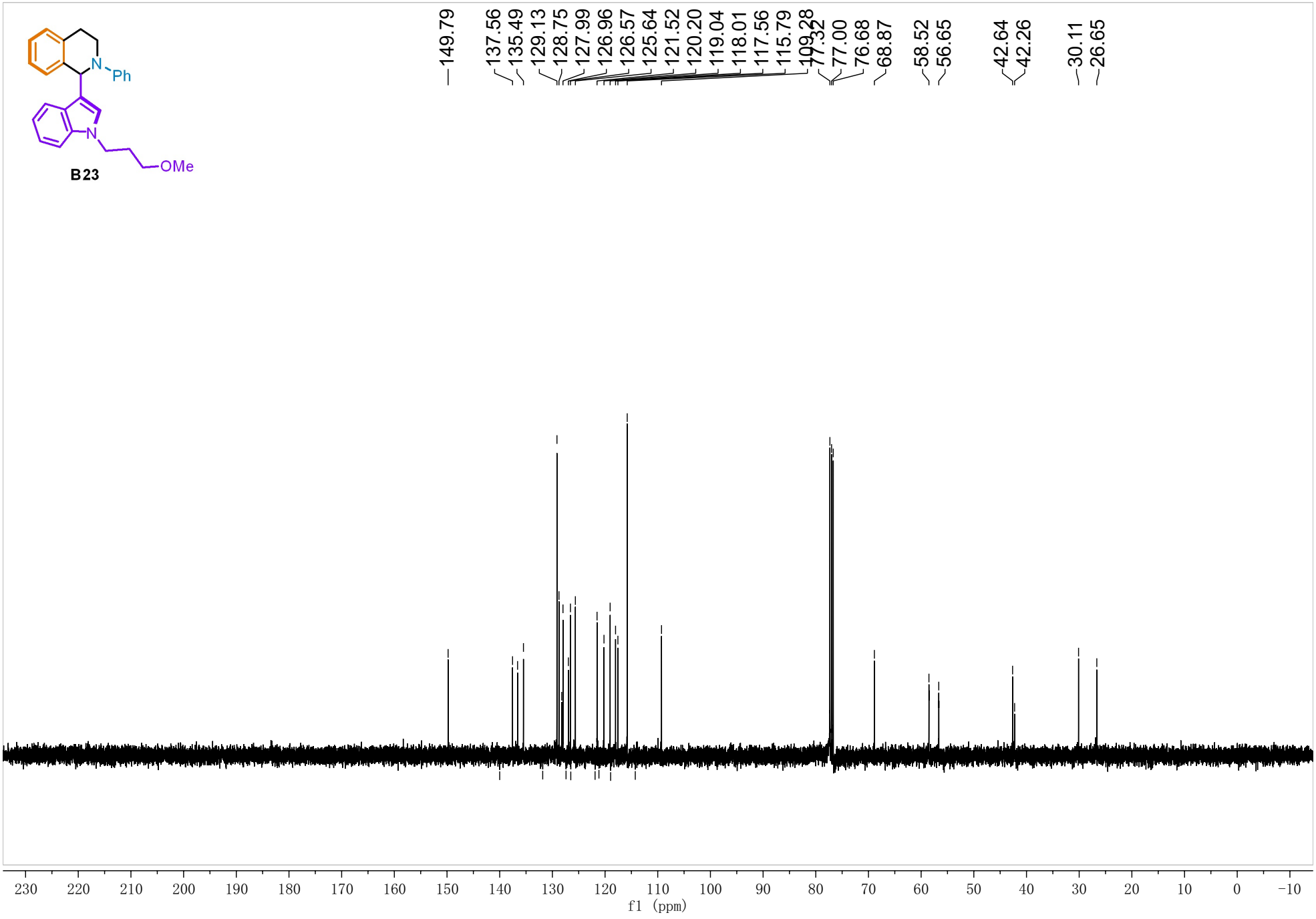
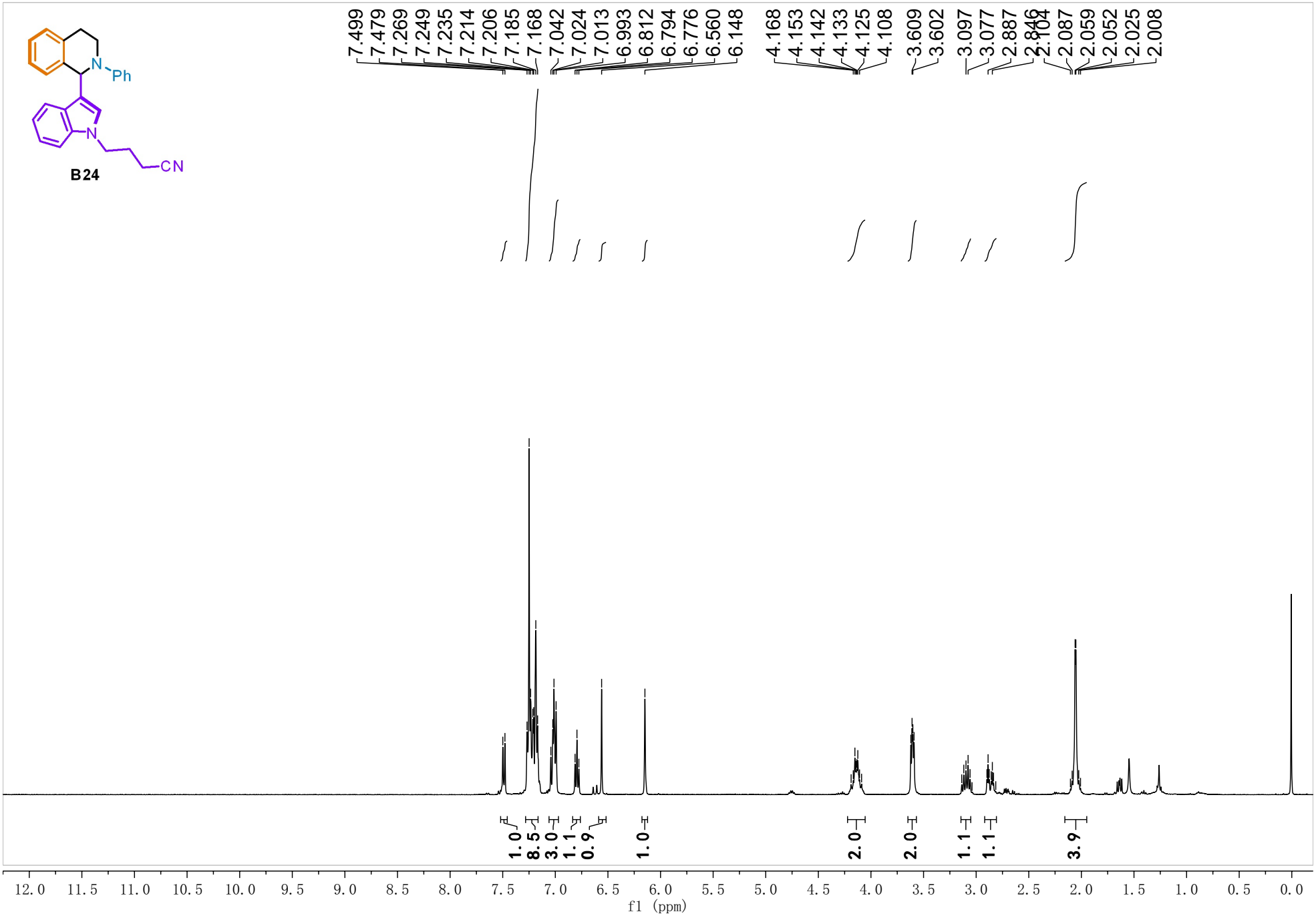
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


N
Ph
N
OMe
B23
149.79
137.56
135.49
129.13
128.75
127.99
126.96
126.57
125.64
121.52
120.20
119.04
118.01
117.56
115.79
109.28
77.32
77.00
76.68
68.87
58.52
56.65
42.64
42.26
30.11
26.65
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)


B24
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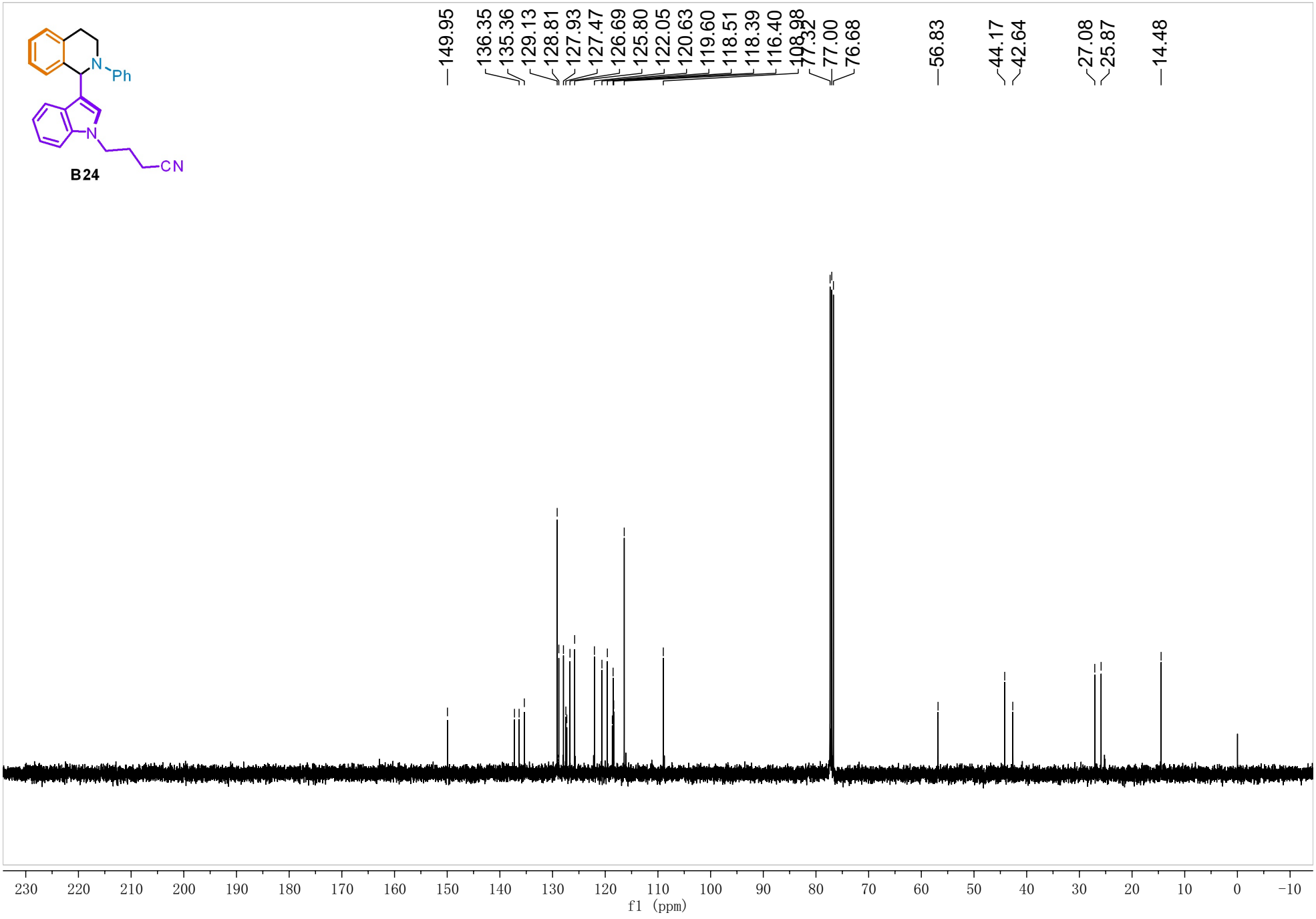
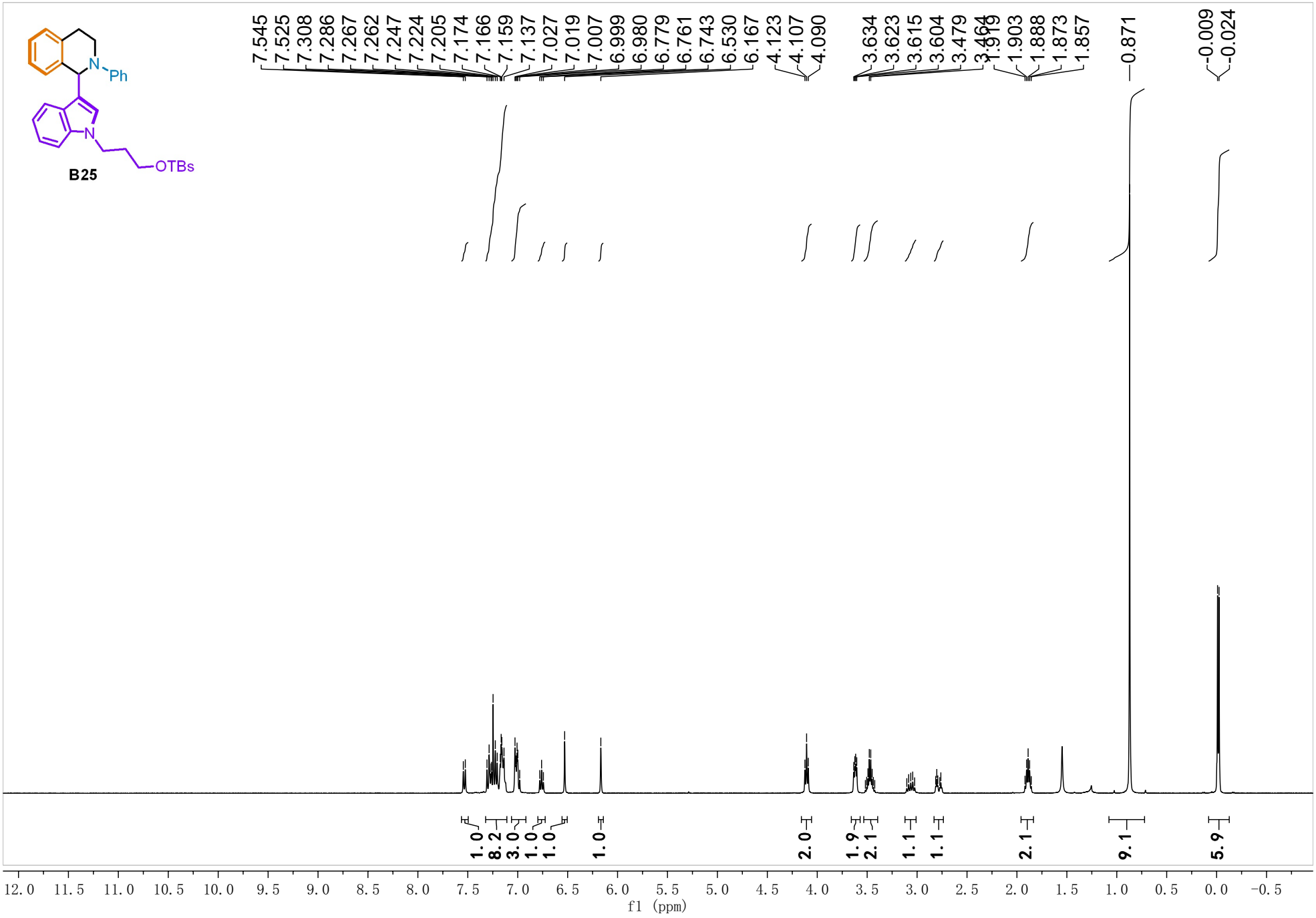
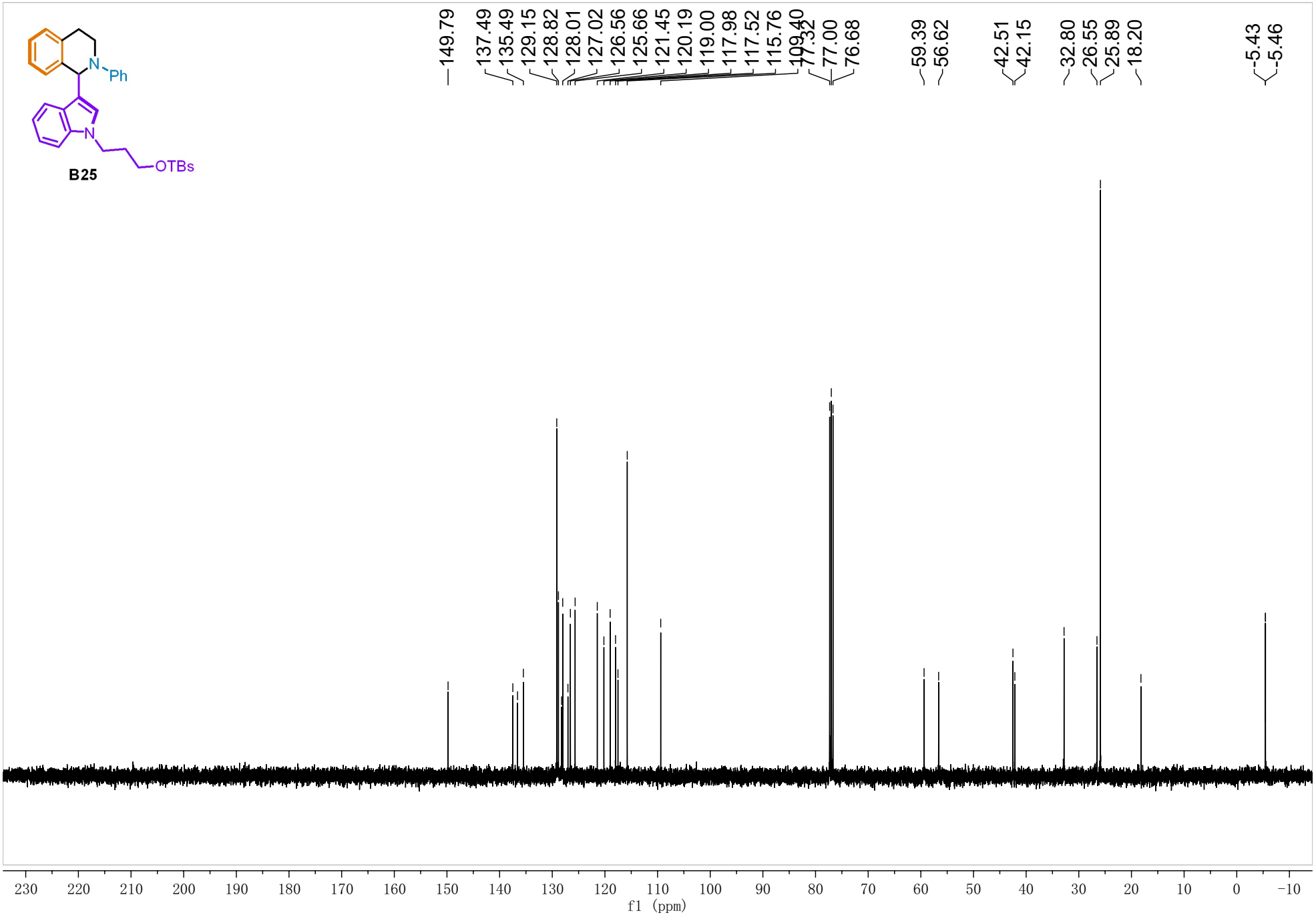
7.479
7.269
7.249
7.235
7.214
7.206
7.185
7.168
7.042
7.024
7.013
6.993
6.812
6.794
6.776
6.560
6.148
4.168
4.153
4.142
4.133
4.125
4.108
3.609
3.602
3.097
3.077
2.887
2.846
2.104
2.087
2.059
2.052
2.025
2.008
1.0
8.5
3.0
1.1
0.9
1.0
2.0
2.0
1.1
1.1
3.9
f1 (ppm)


149.95
136.35
135.36
129.13
128.81
127.93
127.47
126.69
125.80
122.05
120.63
119.60
118.51
118.39
116.40
108.98
77.32
77.00
76.68
56.83
44.17
42.64
27.08
25.87
14.48
N
Ph
N
CN
B24
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)


N
Ph
N
OTBs
B25
7.545
7.525
7.308
7.286
7.267
7.262
7.247
7.224
7.205
7.174
7.166
7.159
7.137
7.027
7.019
7.007
6.999
6.980
6.779
6.761
6.743
6.530
6.167
4.123
4.107
4.090
3.634
3.623
3.615
3.604
3.479
3.464
3.919
1.903
1.888
1.873
1.857
0.871
-0.009
-0.024
1.0
8.2
3.0
1.0
1.0
1.0
2.0
1.9
2.1
1.1
1.1
2.1
9.1
5.9
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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137.49
135.49
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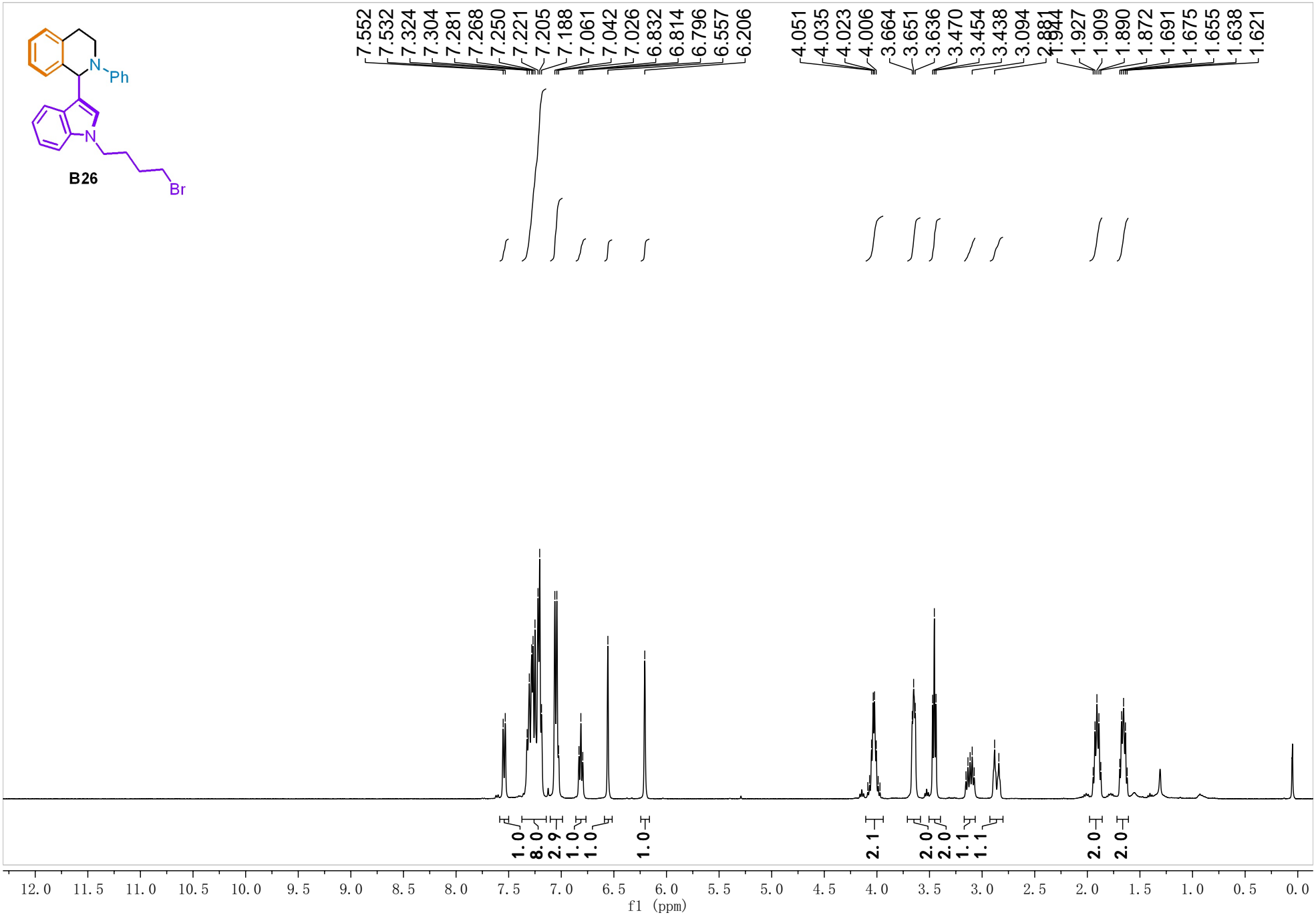
128.01
127.02
126.56
125.66
121.45
120.19
119.00
117.98
117.52
115.76
109.40
77.32
77.00
76.68
59.39
56.62
42.51
42.15
32.80
26.55
25.89
18.20
-5.43
-5.46
N
Ph
N
OTBs
B25
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


N
Ph
N
Br
B26
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7.532
7.324
7.304
7.281
7.268
7.250
7.221
7.205
7.188
7.061
7.042
7.026
6.832
6.814
6.796
6.557
6.206
4.051
4.035
4.023
4.006
3.664
3.651
3.636
3.470
3.454
3.438
3.094
1.927
1.909
1.890
1.872
1.691
1.675
1.655
1.638
1.621
1.0
8.0
2.9
1.0
1.0
1.0
2.1
2.0
2.0
1.1
1.1
2.0
2.0
12.0
11.5
11.0
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10.0
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9.0
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7.5
7.0
6.5
6.0
5.5
5.0
4.5
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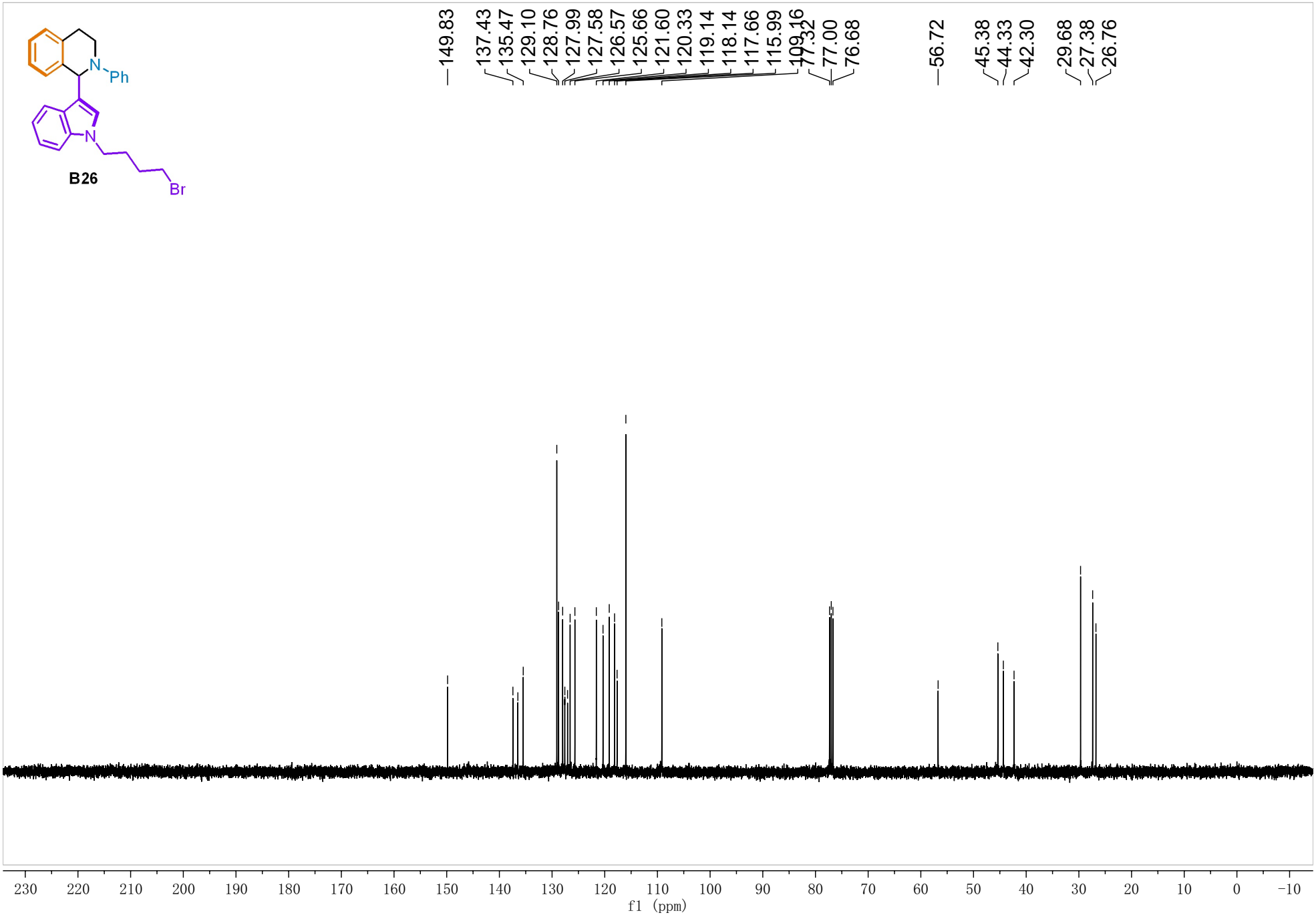
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


N
Ph
N
Br
B26
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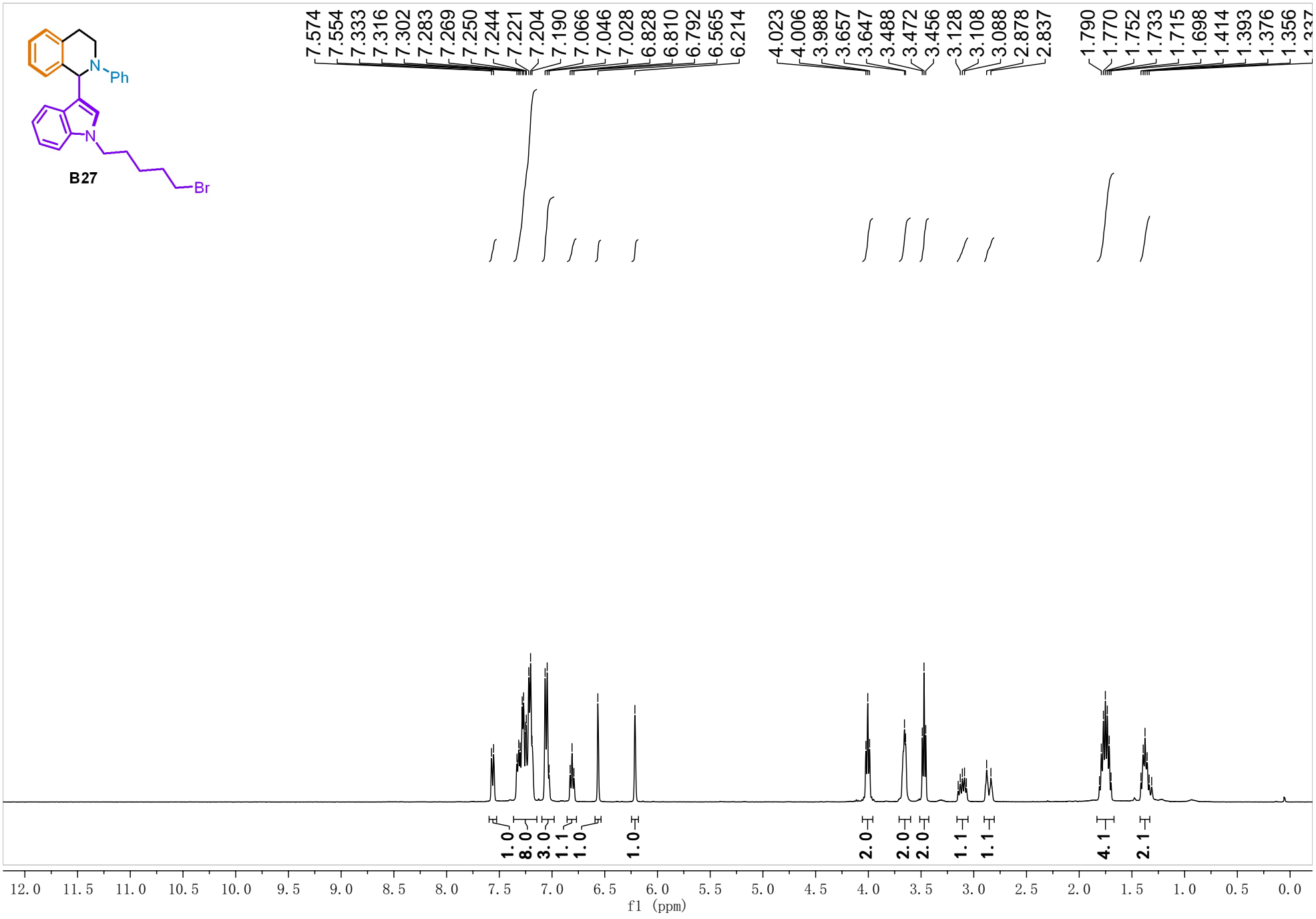
137.43
135.47
129.10
128.76
127.99
127.58
126.57
125.66
121.60
120.33
119.14
118.14
117.66
115.99
109.16
77.32
77.00
76.68
56.72
45.38
44.33
42.30
29.68
27.38
26.76
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)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N
Ph
N
Br
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7.302
7.283
7.269
7.250
7.244
7.221
7.204
7.190
7.066
7.046
7.028
6.828
6.810
6.792
6.565
6.214
4.023
4.006
3.988
3.657
3.647
3.488
3.472
3.456
3.128
3.108
3.088
2.878
2.837
1.790
1.770
1.752
1.733
1.715
1.698
1.414
1.393
1.376
1.356
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3.0
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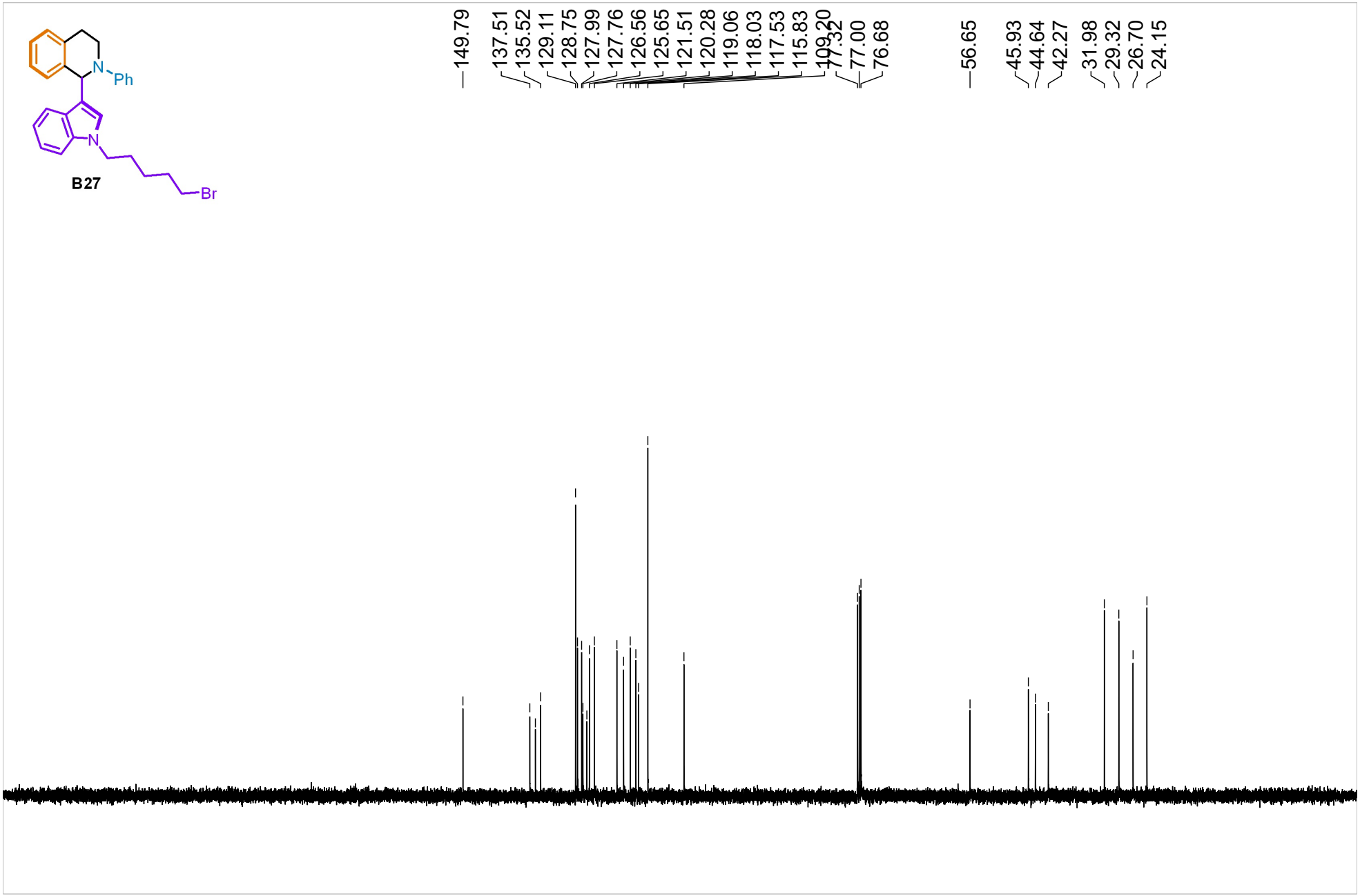
1.0
2.0
2.0
2.0
1.1
1.1
4.1
2.1
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


N
Ph
N
Br
B27
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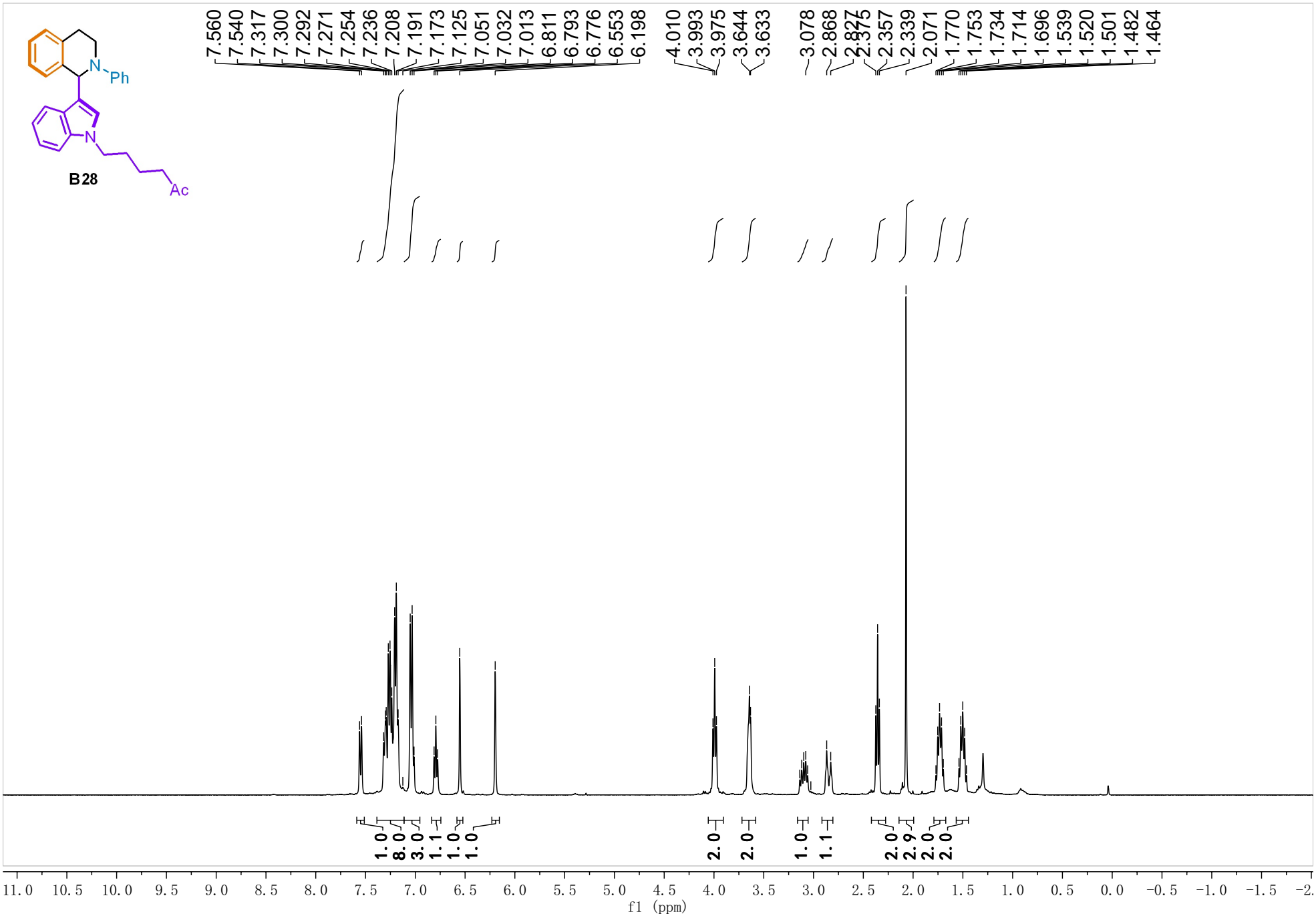
128.75
127.99
127.76
126.56
125.65
121.51
120.28
119.06
118.03
117.53
115.83
109.20
77.32
77.00
76.68
56.65
45.93
44.64
42.27
31.98
29.32
26.70
24.15
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


B28
Ac
Ph
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N
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7.254
7.236
7.208
7.191
7.173
7.125
7.051
7.032
7.013
6.811
6.793
6.776
6.553
6.198
4.010
3.993
3.975
3.644
3.633
3.078
2.868
2.827
2.375
2.357
2.339
2.071
1.770
1.753
1.734
1.714
1.696
1.539
1.520
1.501
1.482
1.464
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8.0
3.0
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1.0
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2.0
1.0
1.1
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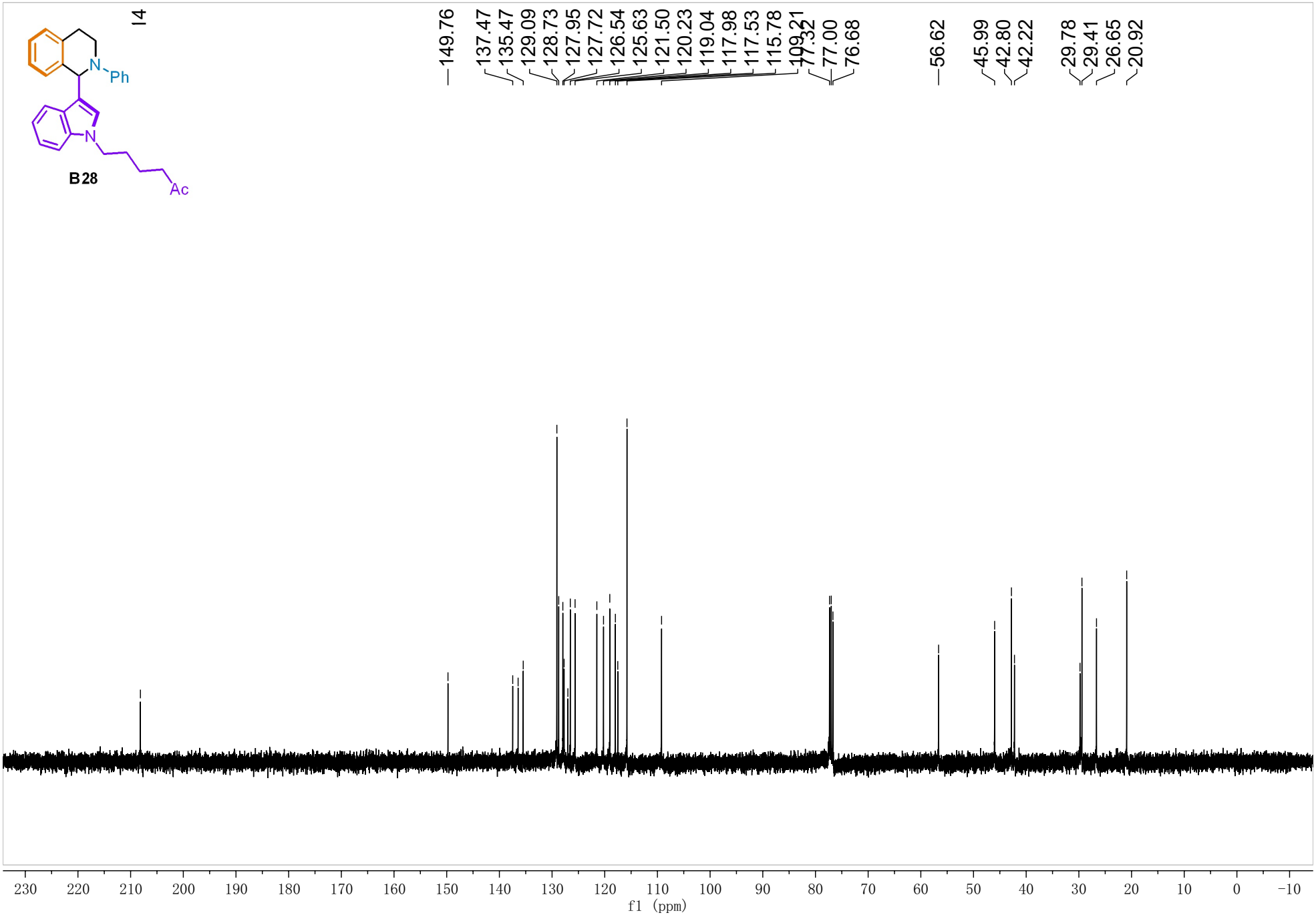
2.0
f1 (ppm)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Ph
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Ac
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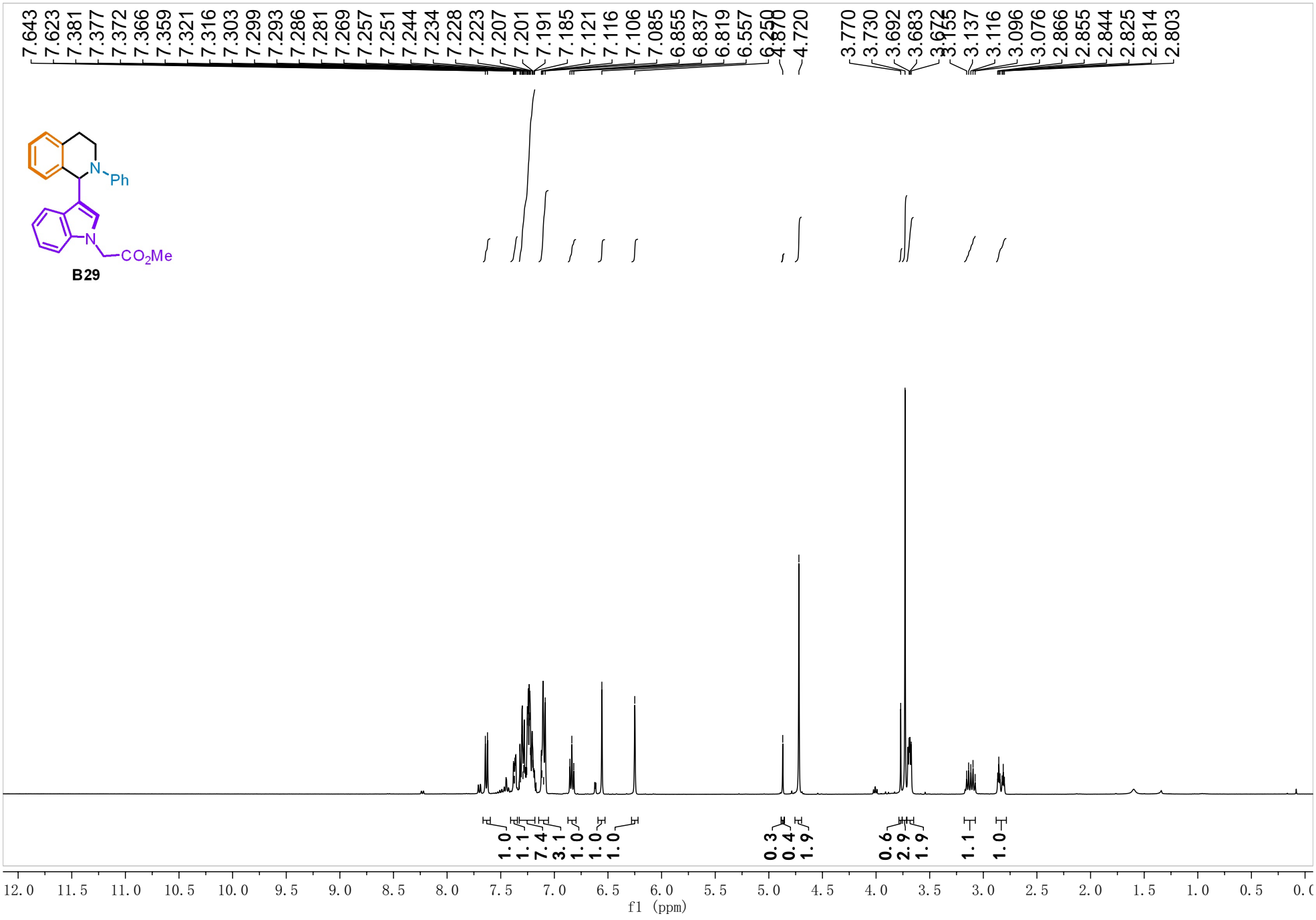
127.72
126.54
125.63
121.50
120.23
119.04
117.98
117.53
115.78
109.21
77.32
77.00
76.68
56.62
45.99
42.80
42.22
29.78
29.41
26.65
20.92
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)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7.286
7.281
7.269
7.257
7.251
7.244
7.234
7.228
7.223
7.207
7.201
7.191
7.185
7.121
7.116
7.106
7.085
6.855
6.837
6.819
6.557
6.250
4.870
4.720
3.770
3.730
3.692
3.683
3.672
3.155
3.137
3.116
3.096
3.076
2.866
2.855
2.844
2.825
2.814
2.803
N
Ph
N
CO2Me
B29
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1.1
7.4
3.1
1.0
1.0
1.0
0.3
0.4
1.9
0.6
2.9
1.9
1.1
1.0
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
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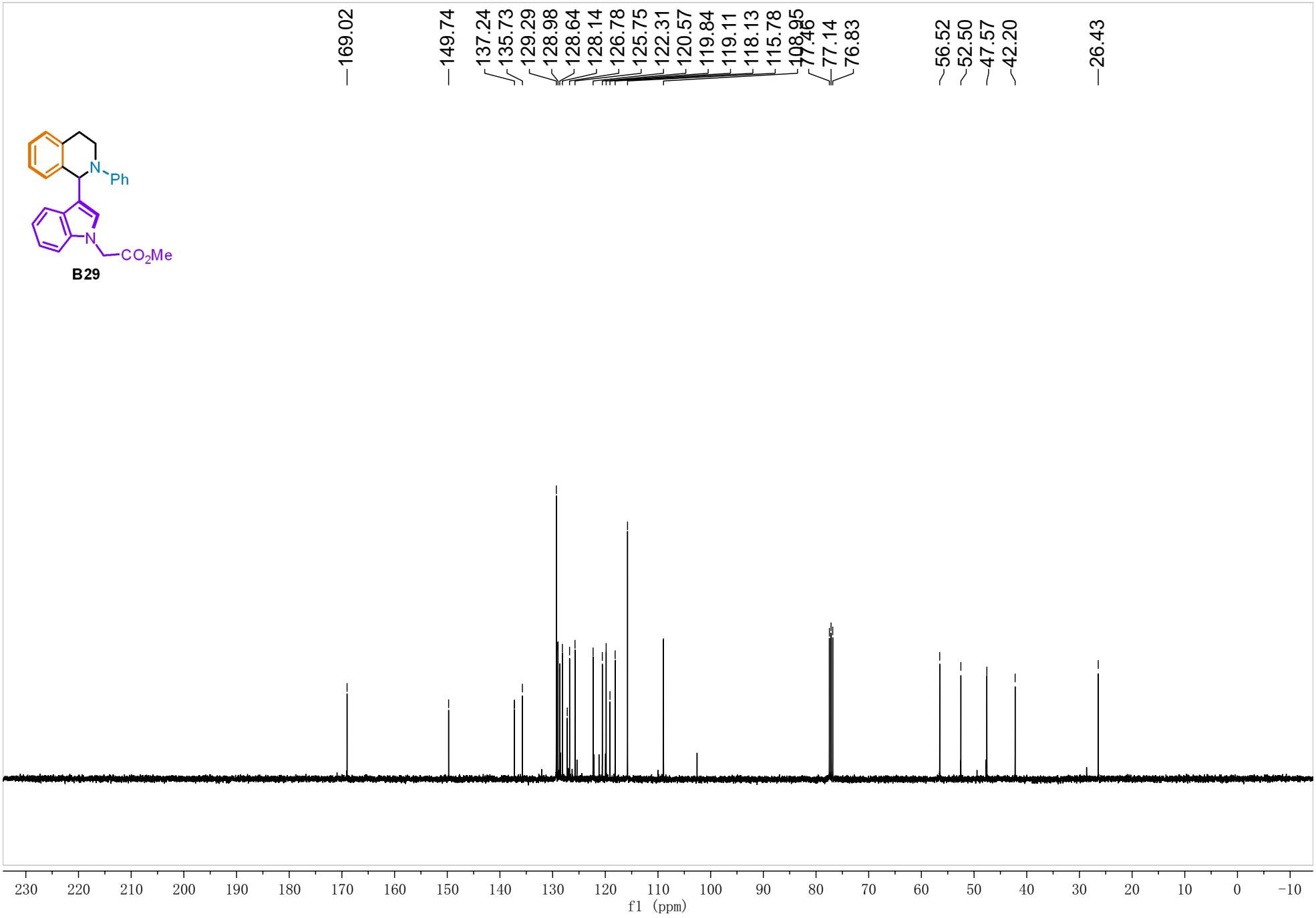
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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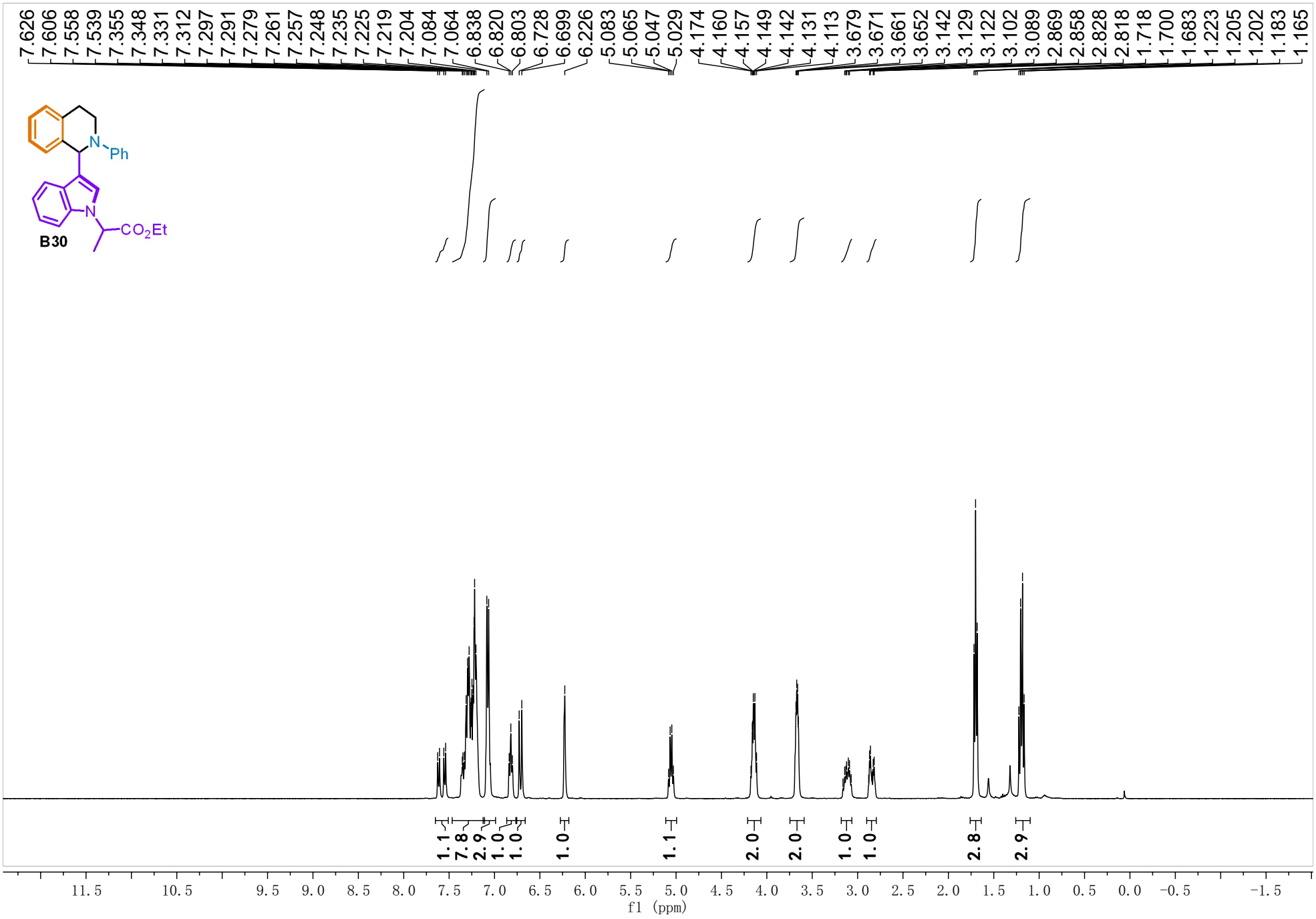
128.64
128.14
126.78
125.75
122.31
120.57
119.84
119.11
118.13
115.78
108.95
77.46
77.14
76.83
56.52
52.50
47.57
42.20
26.43
N
Ph
N
CO2Me
B29
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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7.331
7.312
7.297
7.291
7.279
7.261
7.257
7.248
7.235
7.225
7.219
7.204
7.084
7.064
6.838
6.820
6.803
6.728
6.699
6.226
5.083
5.065
5.047
5.029
4.174
4.160
4.157
4.149
4.142
4.131
4.113
3.679
3.671
3.661
3.652
3.142
3.129
3.122
3.102
3.089
2.869
2.858
2.828
2.818
1.718
1.700
1.683
1.223
1.205
1.202
1.183
1.165
N
Ph
N
CO2Et
B30
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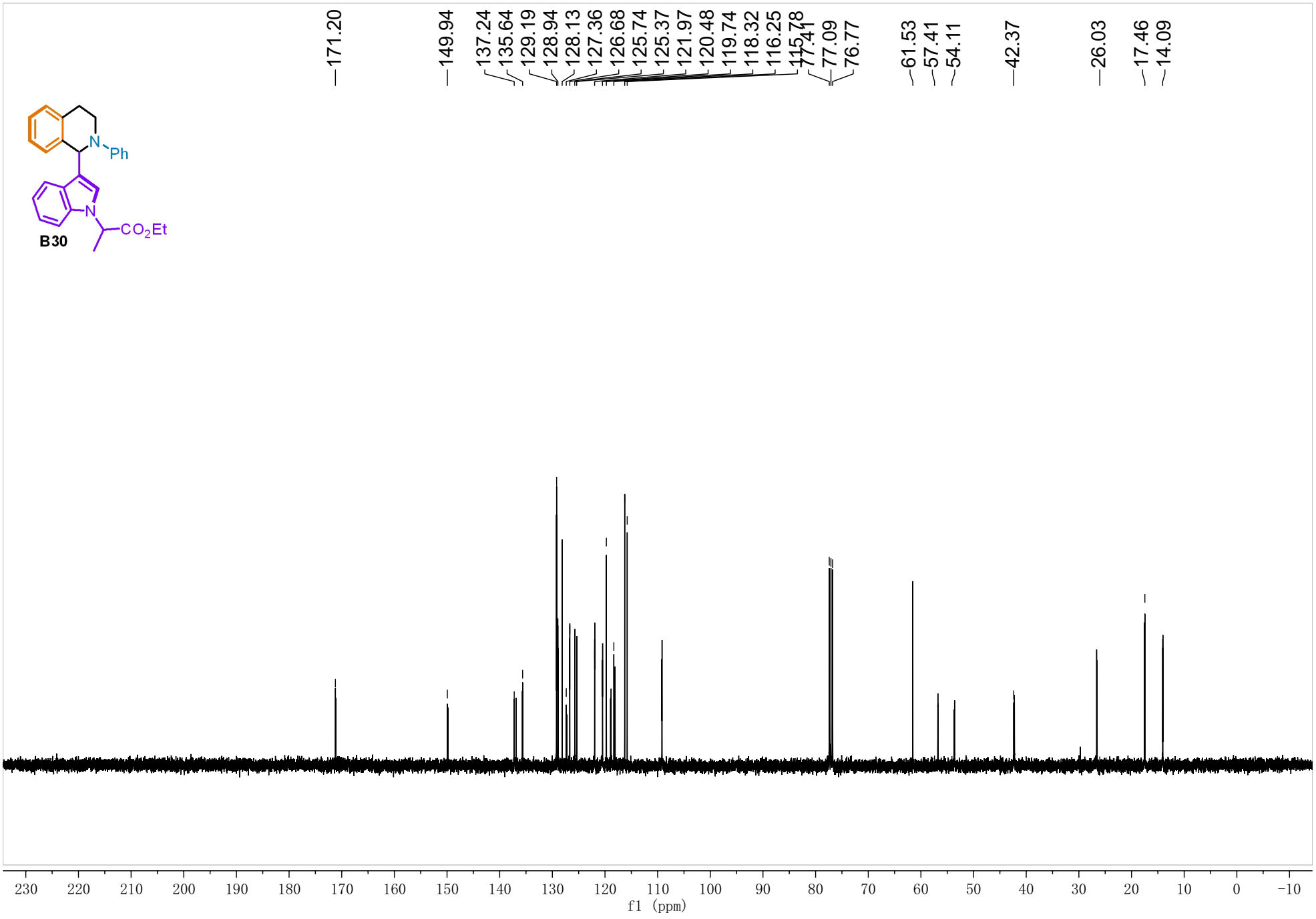
7.8
2.9
1.0
1.0
1.0
1.1
2.0
2.0
1.0
1.0
2.8
2.9
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.5
f1 (ppm)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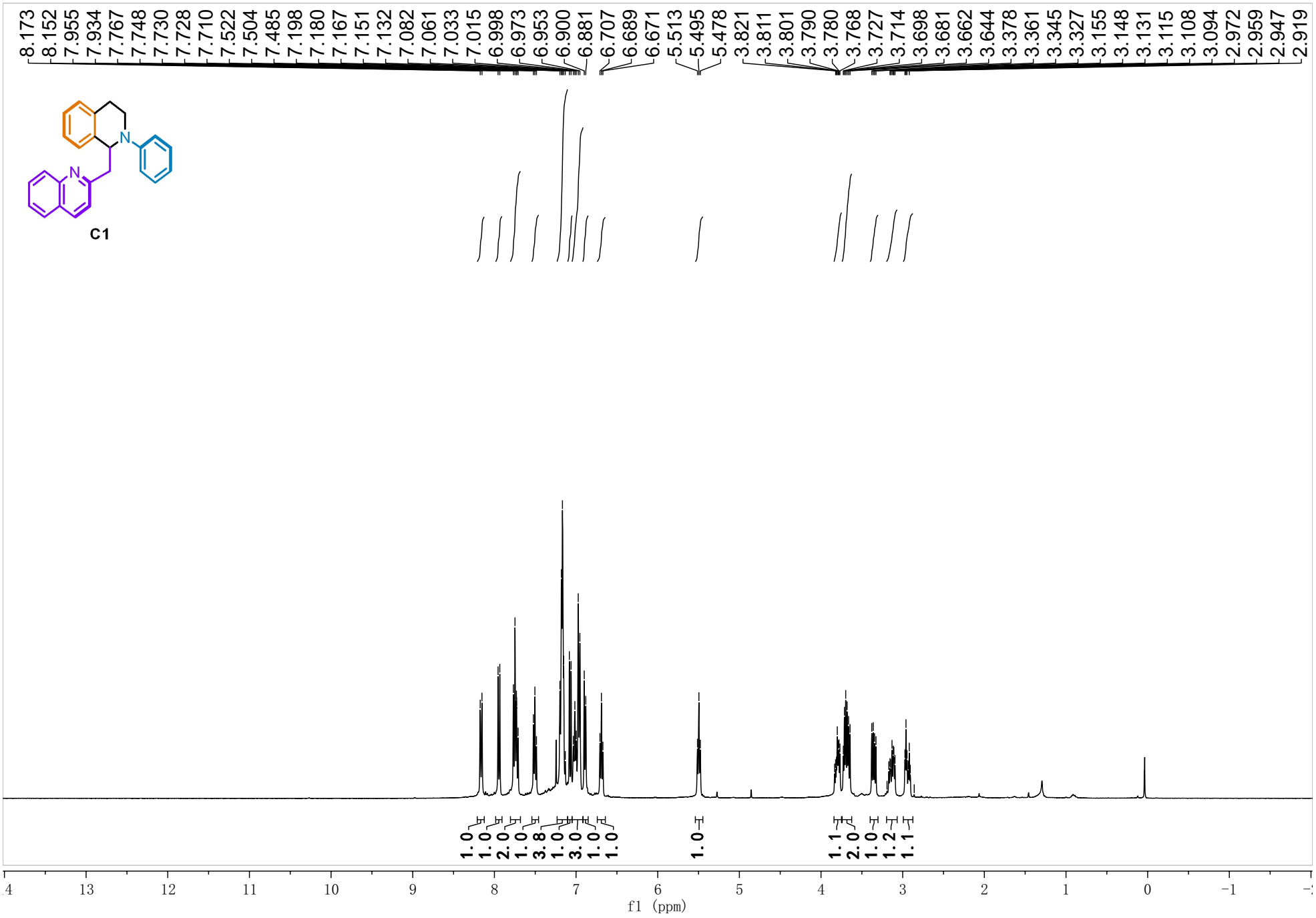
128.94
128.13
127.36
126.68
125.74
125.37
121.97
120.48
119.74
118.32
116.25
115.78
77.41
77.09
76.77
61.53
57.41
54.11
42.37
26.03
17.46
14.09
N
Ph
N
CO2Et
B30
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)


8.173
8.152
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7.728
7.710
7.522
7.504
7.485
7.198
7.180
7.167
7.151
7.132
7.082
7.061
7.033
7.015
6.998
6.973
6.953
6.900
6.881
6.707
6.689
6.671
5.513
5.495
5.478
3.821
3.811
3.801
3.790
3.780
3.768
3.727
3.714
3.698
3.681
3.662
3.644
3.378
3.361
3.345
3.327
3.155
3.148
3.131
3.115
3.108
3.094
2.972
2.959
2.947
2.919
N
N
C1
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1.0
2.0
1.0
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1.0
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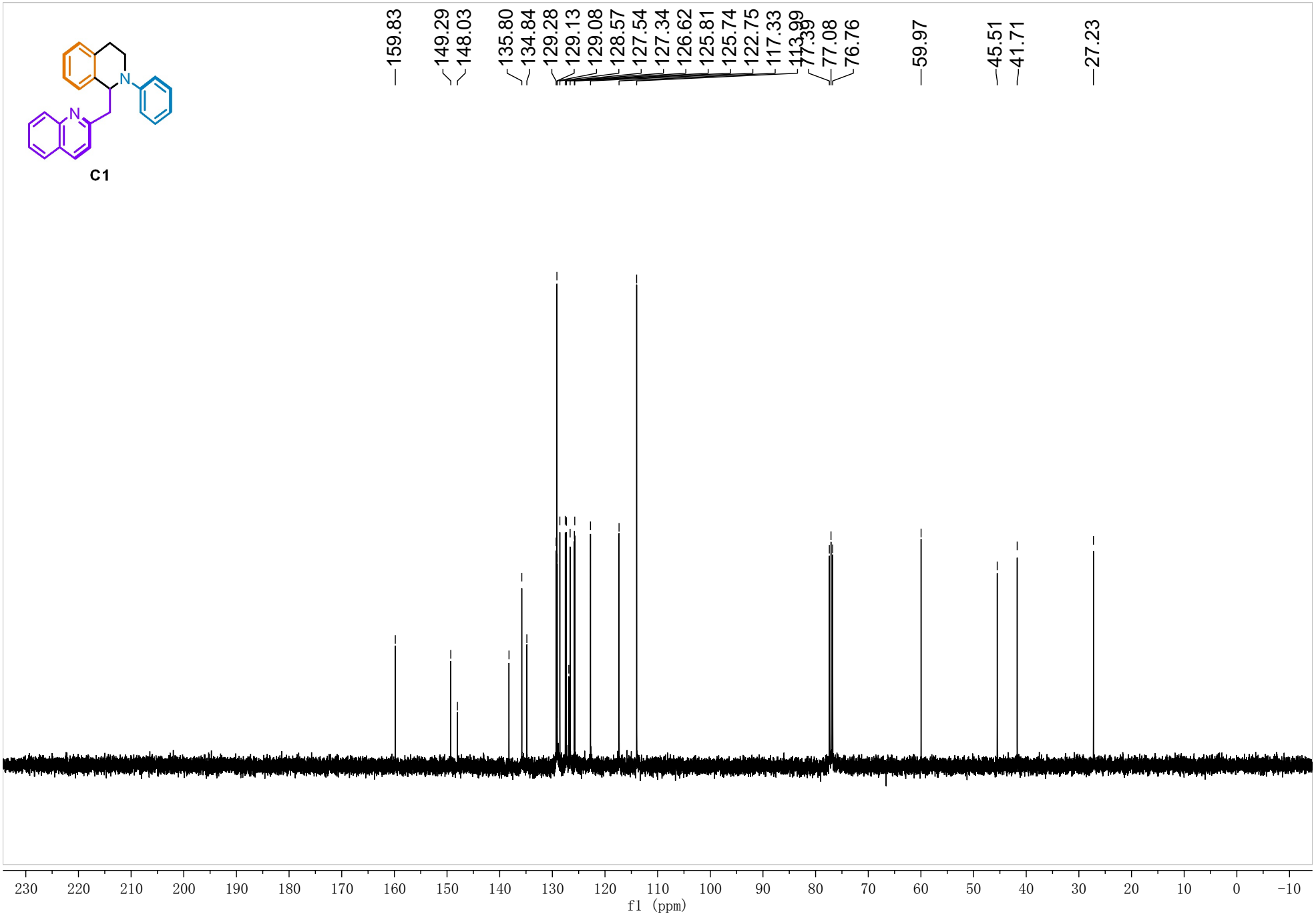
f1 (ppm)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125.74
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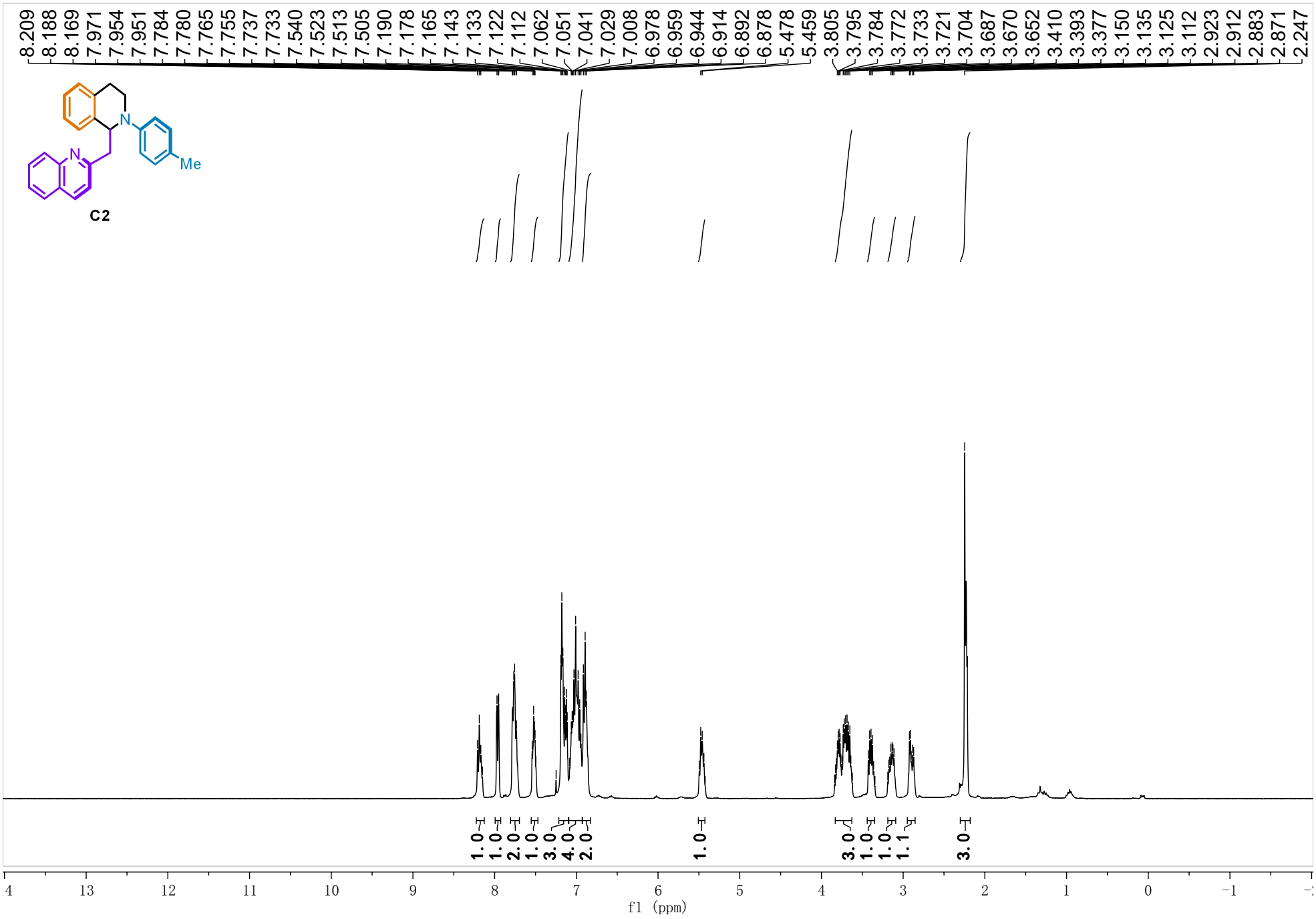
77.08
76.76
59.97
45.51
41.71
27.23
C1
f1 (ppm)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7.737
7.733
7.540
7.523
7.513
7.505
7.190
7.178
7.165
7.143
7.133
7.122
7.112
7.062
7.051
7.041
7.029
7.008
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6.959
6.944
6.914
6.892
6.878
5.478
5.459
3.805
3.795
3.784
3.772
3.733
3.721
3.704
3.687
3.670
3.652
3.410
3.393
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3.125
3.112
2.923
2.912
2.883
2.871
2.247
N
N
Me
C2
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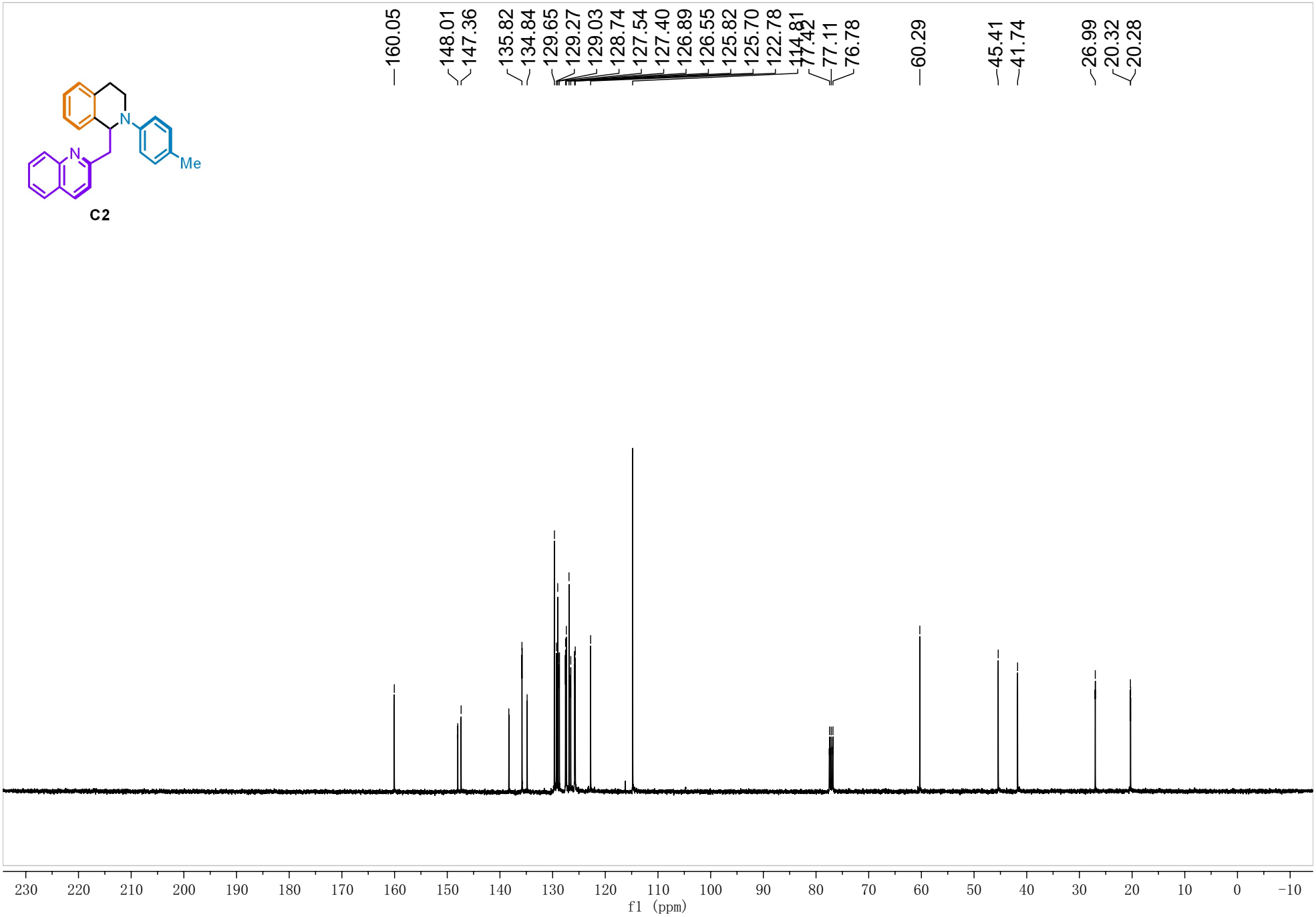
3.0
f1 (ppm)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76.78
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45.41
41.74
26.99
20.32
20.28
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N
Me
C2
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180
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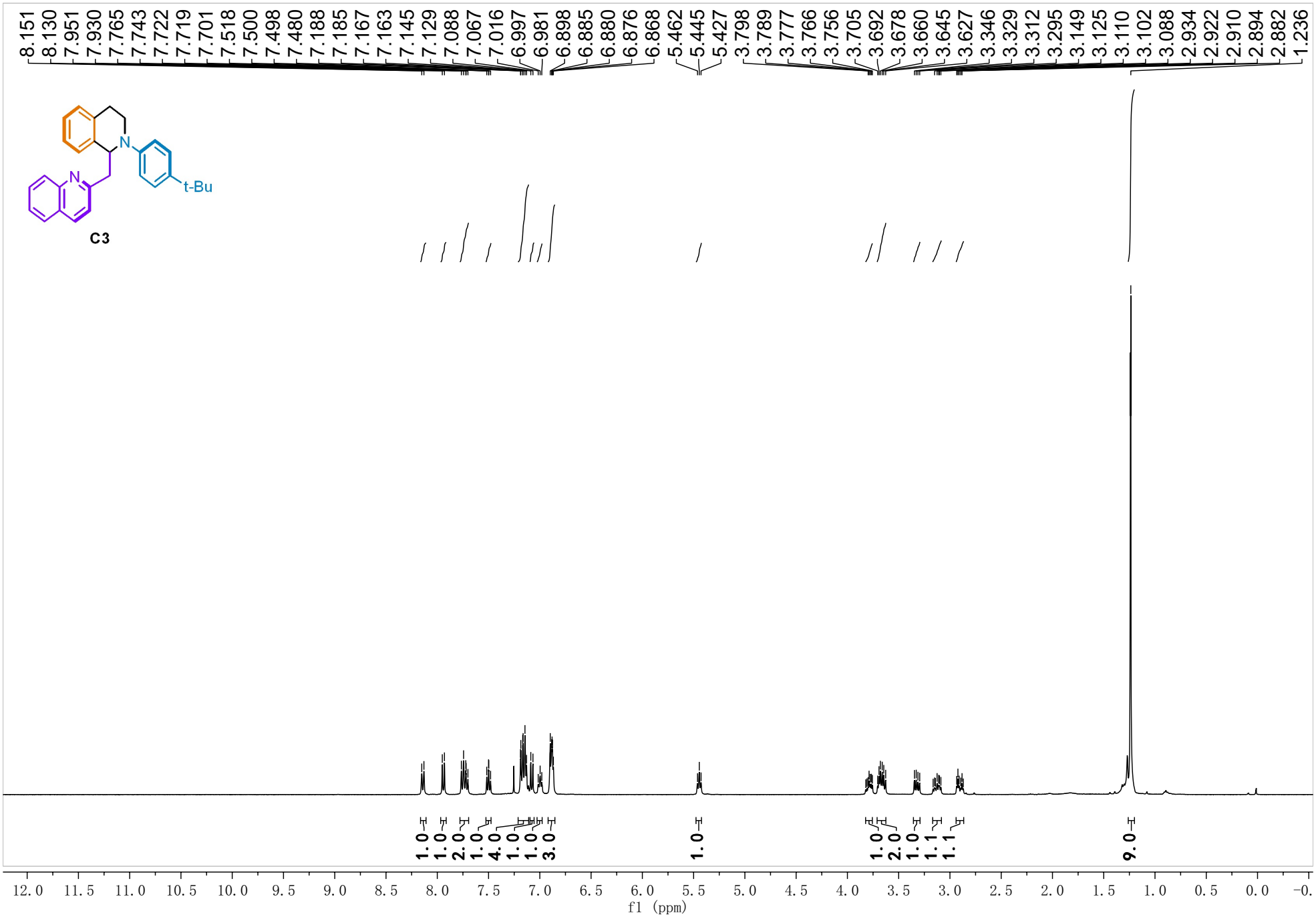
f1 (ppm)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7.518
7.500
7.498
7.480
7.188
7.185
7.167
7.163
7.145
7.129
7.088
7.067
7.016
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6.898
6.885
6.880
6.876
6.868
5.462
5.445
5.427
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3.692
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3.645
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3.346
3.329
3.312
3.295
3.149
3.125
3.110
3.102
3.088
2.934
2.922
2.910
2.894
2.882
1.236
N
N
t-Bu
C3
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6.5
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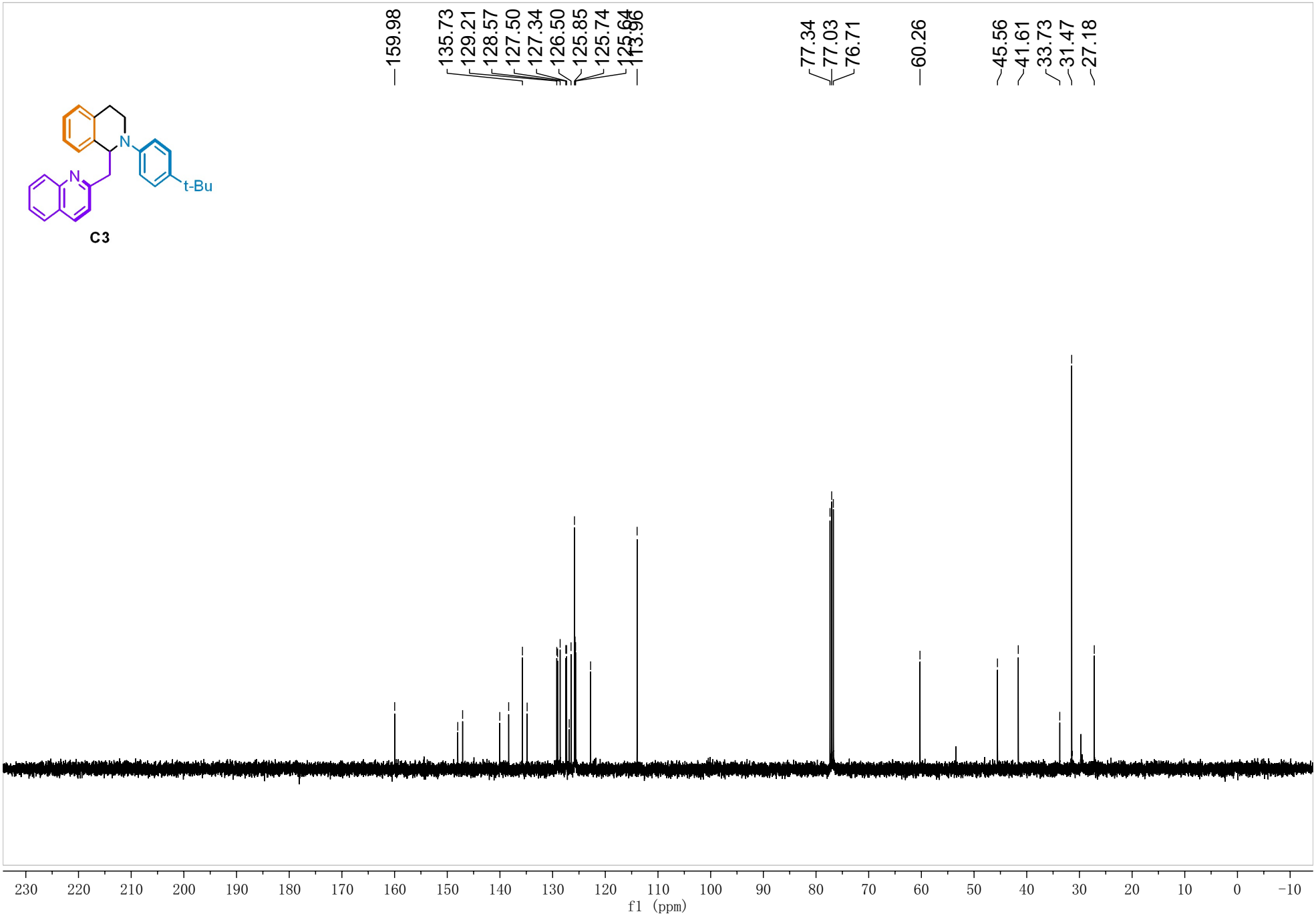
f1 (ppm)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76.71
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45.56
41.61
33.73
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N
t-Bu
C3
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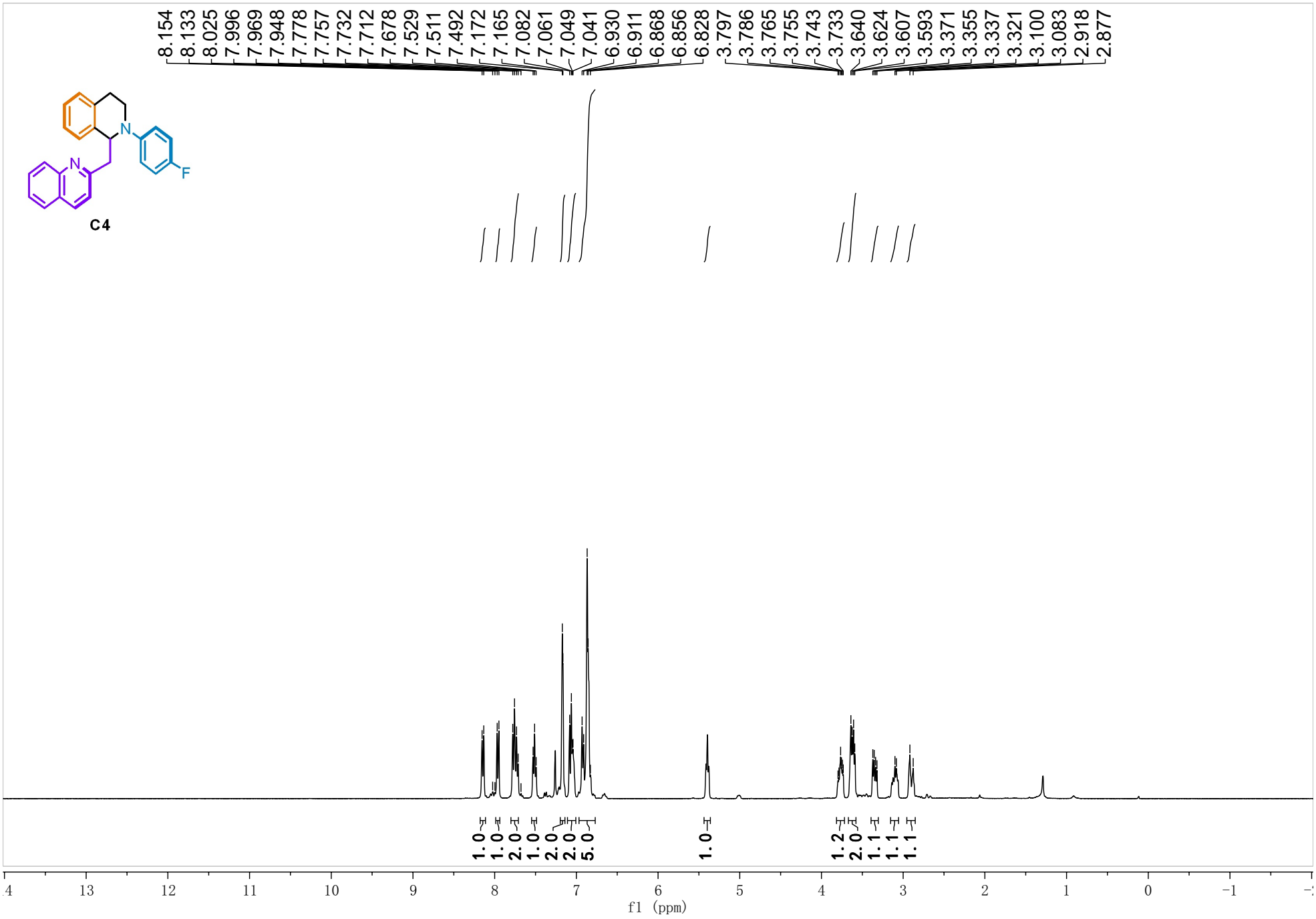
f1 (ppm)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7.757
7.732
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7.678
7.529
7.511
7.492
7.172
7.165
7.082
7.061
7.049
7.041
6.930
6.911
6.868
6.856
6.828
3.797
3.786
3.765
3.755
3.743
3.733
3.640
3.624
3.607
3.593
3.371
3.355
3.337
3.321
3.100
3.083
2.918
2.877
N
N
F
C4
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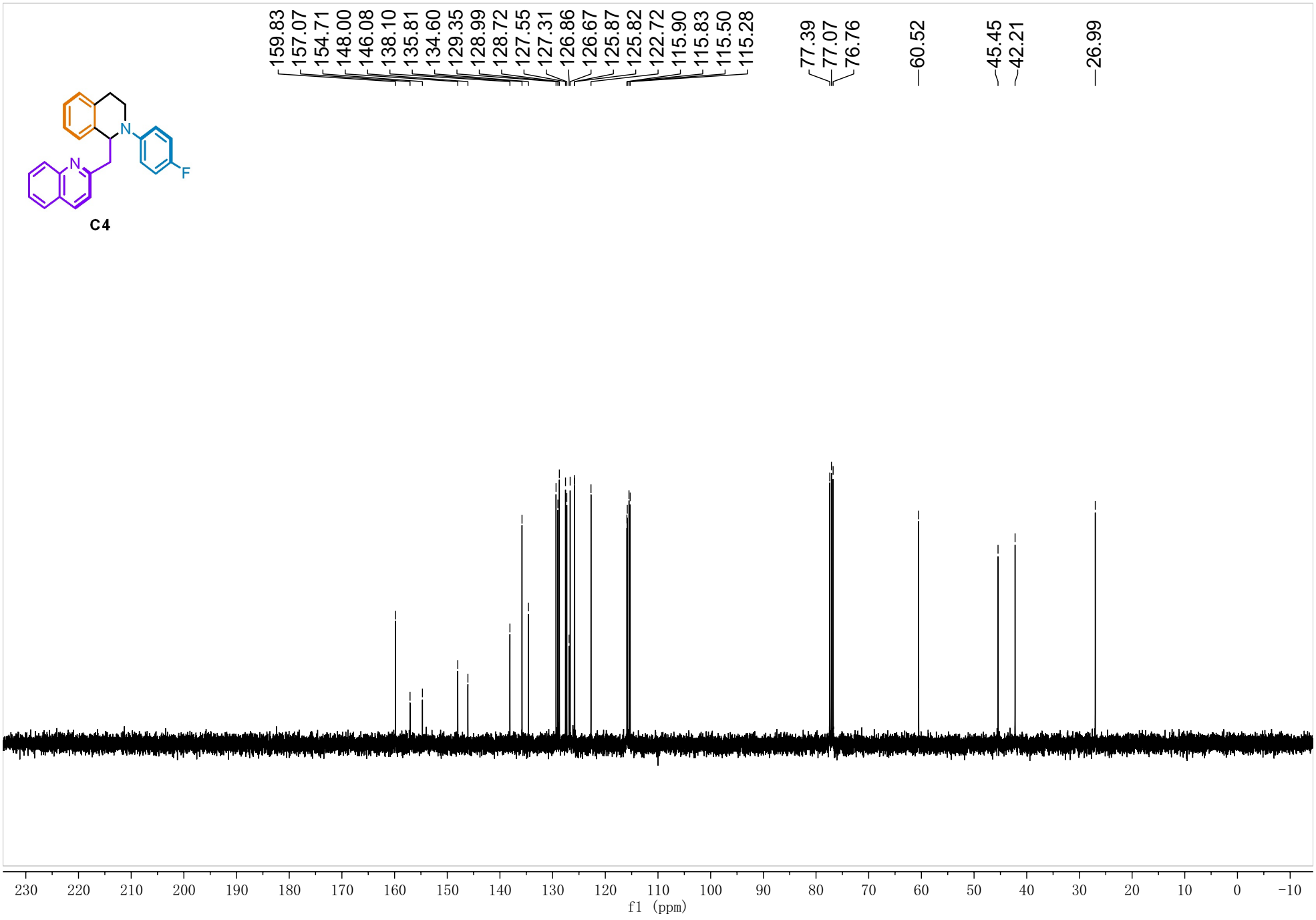
1.1
1.1
f1 (ppm)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134.60
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127.55
127.31
126.86
126.67
125.87
125.82
122.72
115.90
115.83
115.50
115.28
77.39
77.07
76.76
60.52
45.45
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N
F
C4
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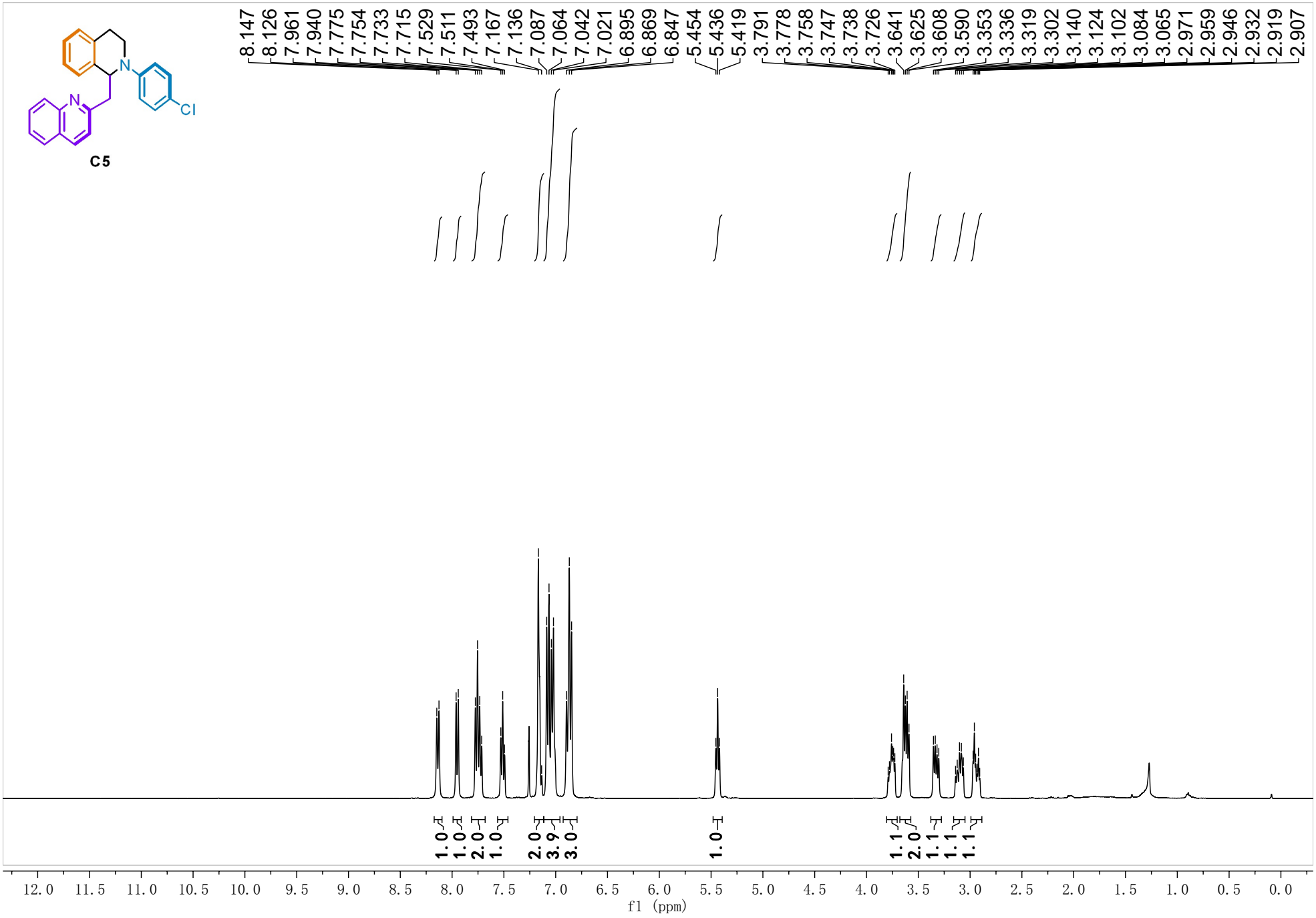
f1 (ppm)


C5
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7.493
7.167
7.136
7.087
7.064
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7.021
6.895
6.869
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3.778
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3.747
3.738
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3.641
3.625
3.608
3.590
3.353
3.336
3.319
3.302
3.140
3.124
3.102
3.084
3.065
2.971
2.959
2.946
2.932
2.919
2.907
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2.0
1.0
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3.9
3.0
1.0
1.1
2.0
1.1
1.1
1.1
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
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3.0
2.5
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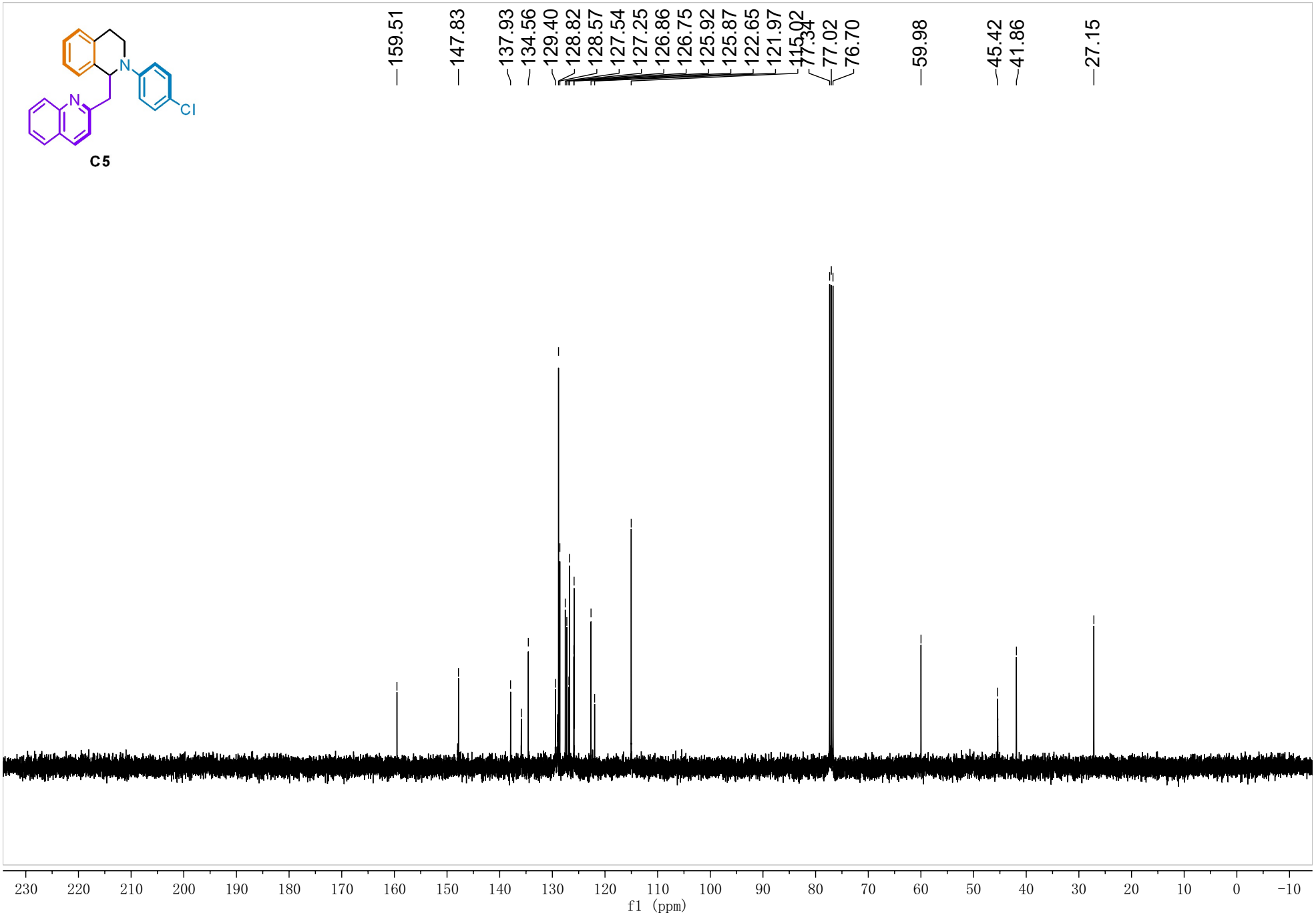
0.0
f1 (ppm)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125.87
122.65
121.97
115.02
77.34
77.02
76.70
59.98
45.42
41.86
27.15
N
N
Cl
C5
230
220
210
200
190
180
170
160
150
140
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120
110
100
90
80
70
60
50
40
30
20
10
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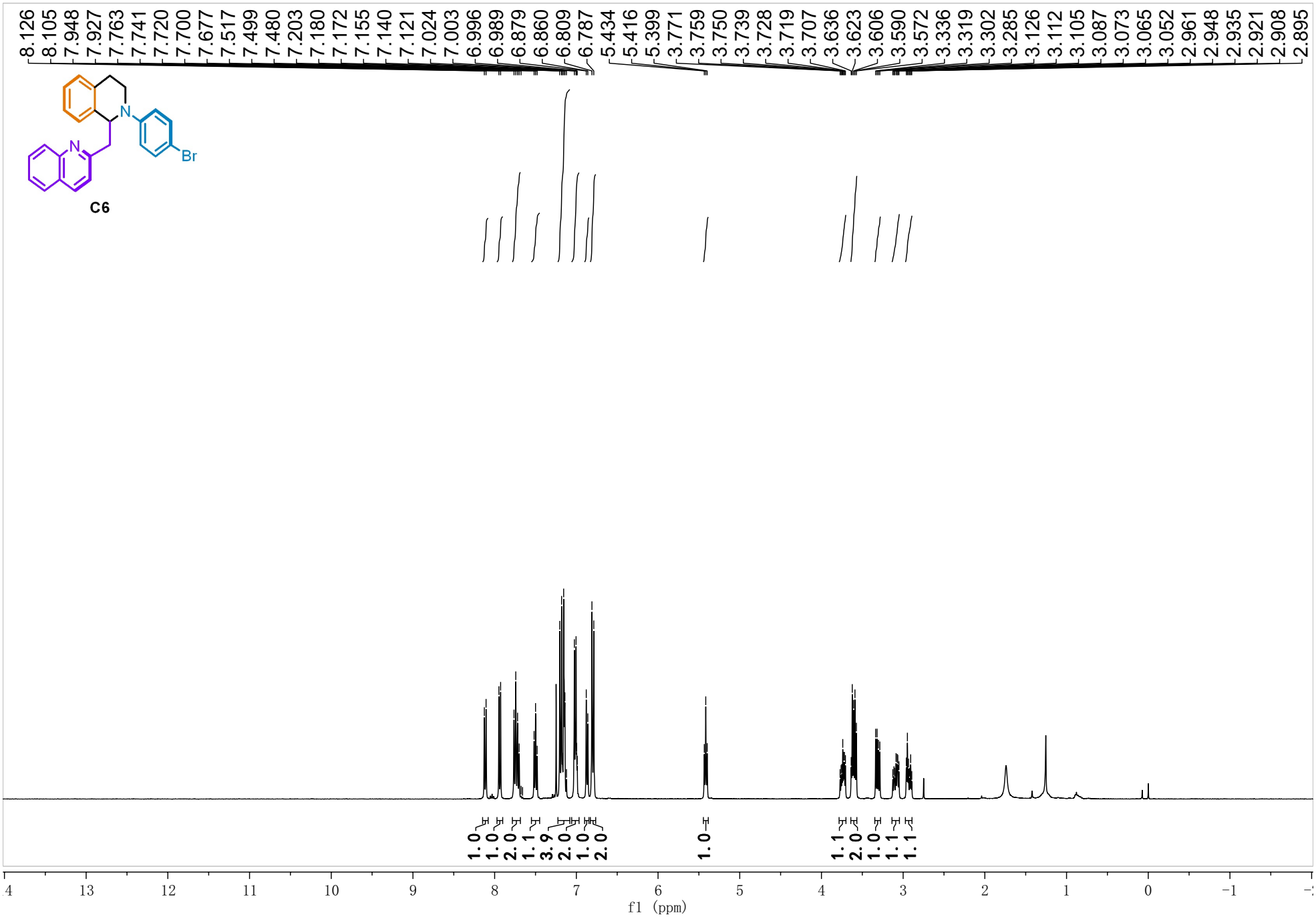
−10
f1 (ppm)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7.480
7.203
7.180
7.172
7.155
7.140
7.121
7.024
7.003
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6.989
6.879
6.860
6.809
6.787
5.434
5.416
5.399
3.771
3.759
3.750
3.739
3.728
3.719
3.707
3.636
3.623
3.606
3.590
3.572
3.336
3.319
3.302
3.285
3.126
3.112
3.105
3.087
3.073
3.065
3.052
2.961
2.948
2.935
2.921
2.908
2.895
N
N
Br
C6
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1.0
2.0
1.1
3.9
2.0
1.0
2.0
1.0
1.1
2.0
1.0
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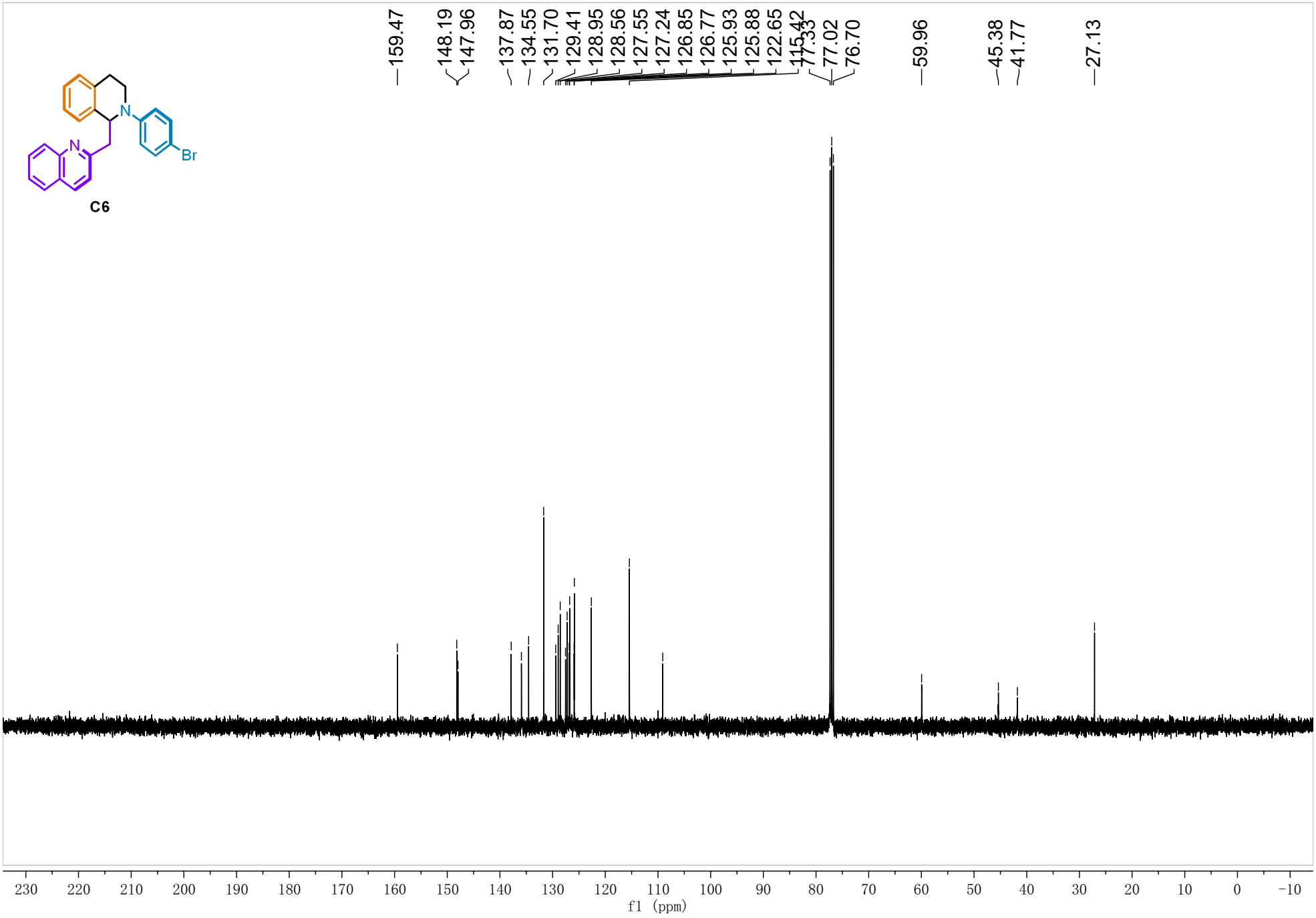
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
f1 (ppm)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127.55
127.24
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125.88
122.65
115.42
77.33
77.02
76.70
59.96
45.38
41.77
27.13
N
N
Br
C6
230
220
210
200
190
180
170
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100
90
80
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50
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30
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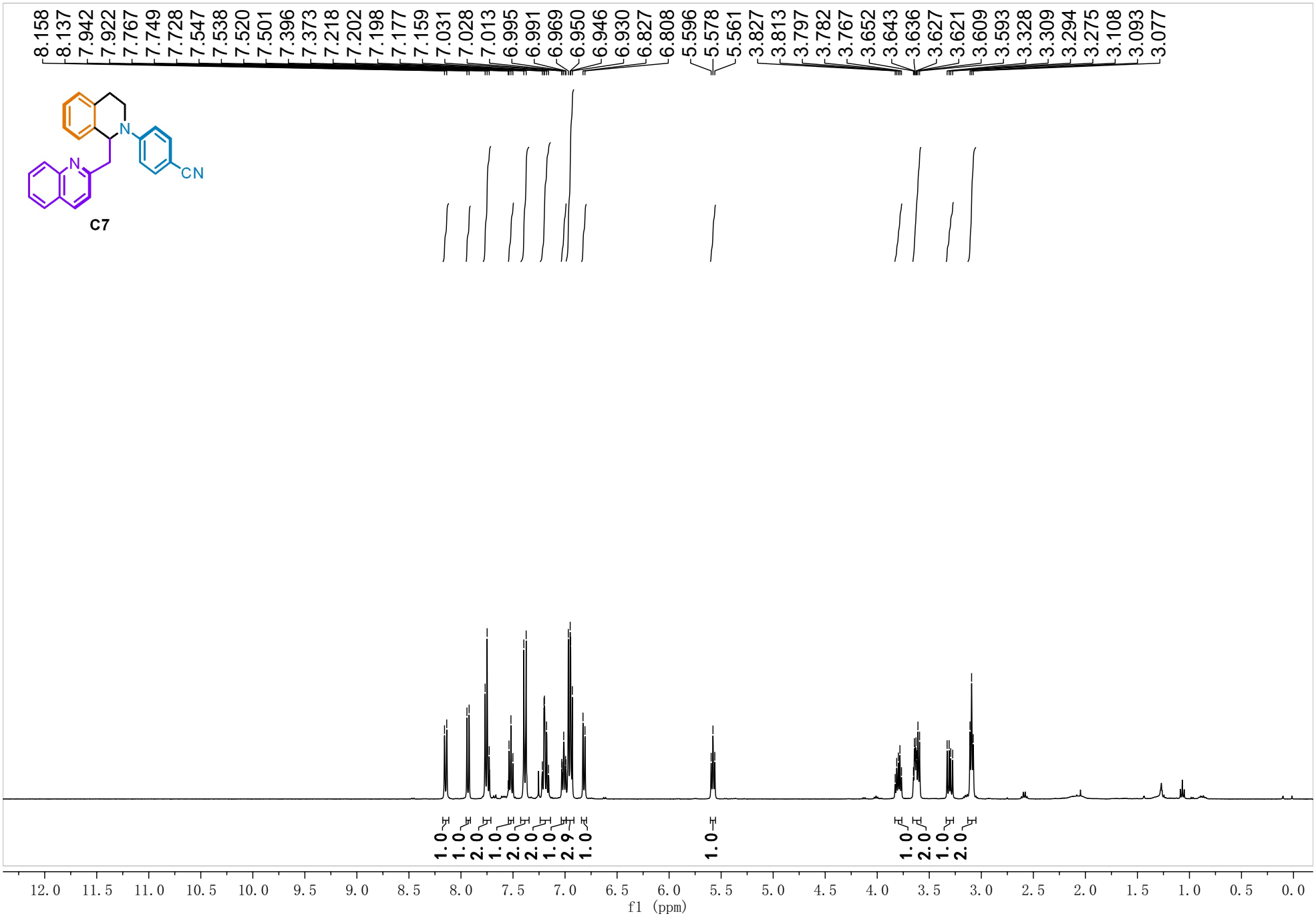
−10
f1 (ppm)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7.202
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7.013
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3.636
3.627
3.621
3.609
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N
CN
C7
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6.5
6.0
5.5
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3.0
2.5
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1.0
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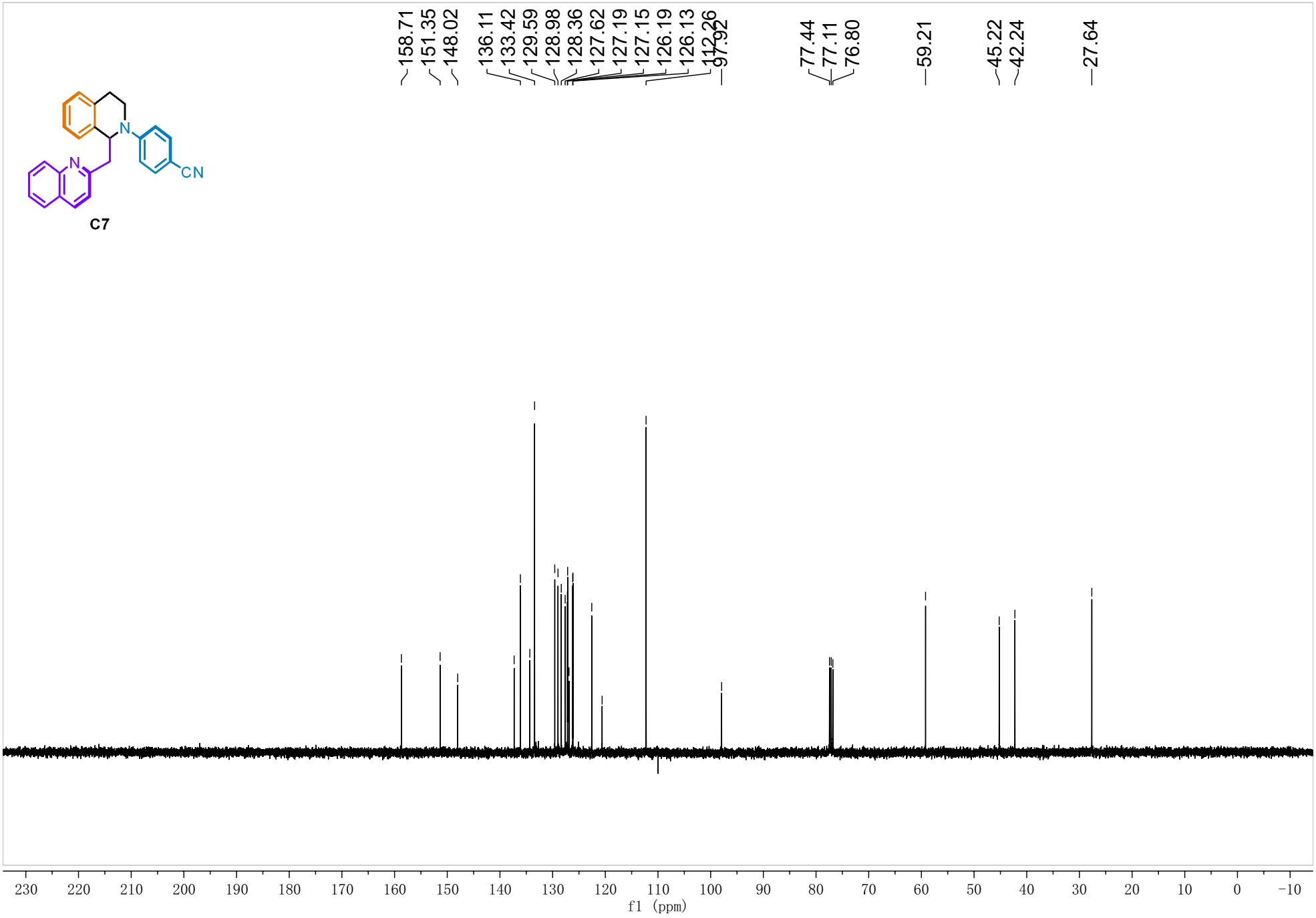
f1 (ppm)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126.13
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97.92
77.44
77.11
76.80
59.21
45.22
42.24
27.64
N
N
CN
C7
230
220
210
200
190
180
170
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100
90
80
70
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50
40
30
20
10
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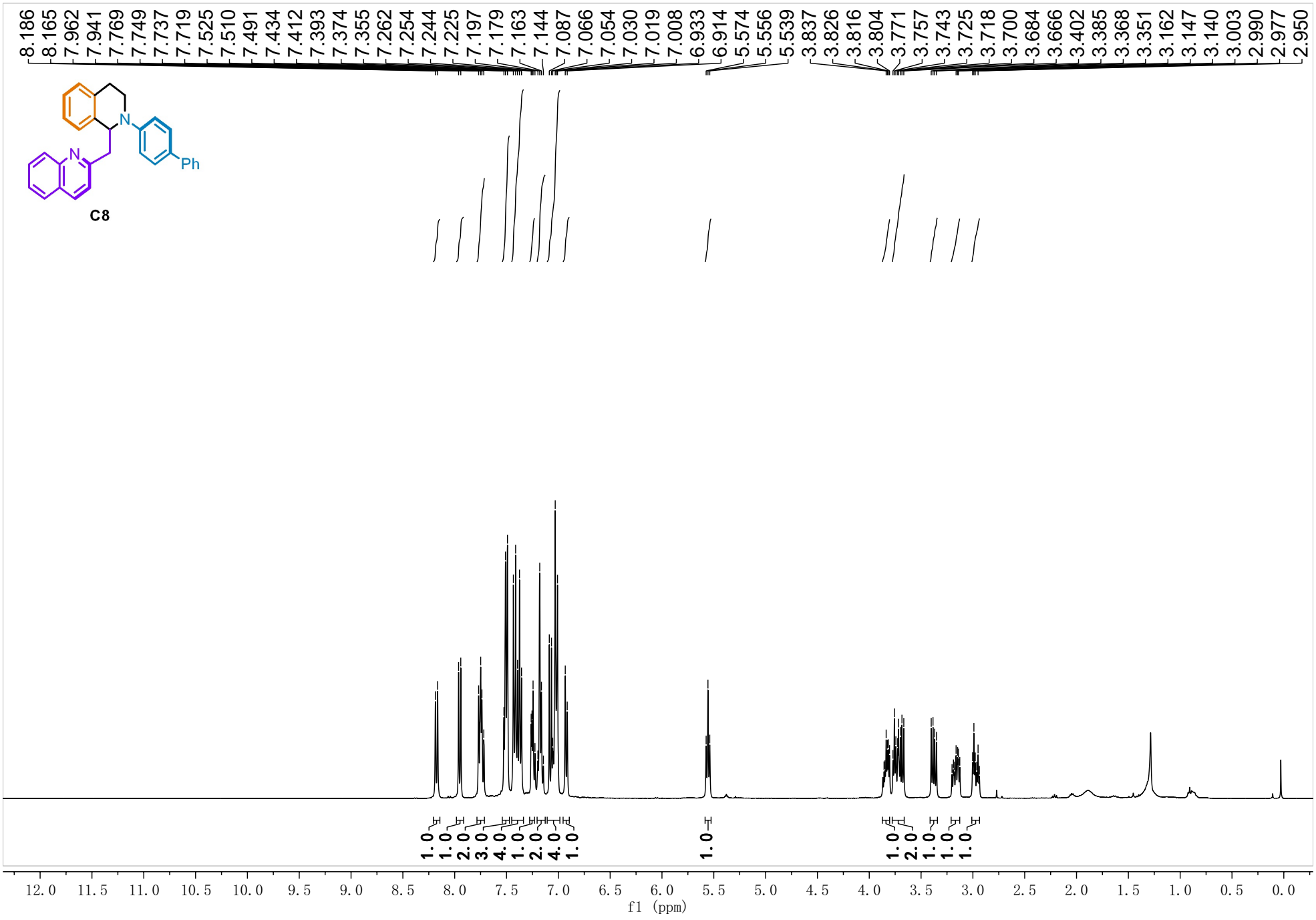
−10
f1 (ppm)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7.225
7.197
7.179
7.163
7.144
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7.066
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3.147
3.140
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2.977
2.950
N
N
Ph
C8
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3.0
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1.0
2.0
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6.0
5.5
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2.5
2.0
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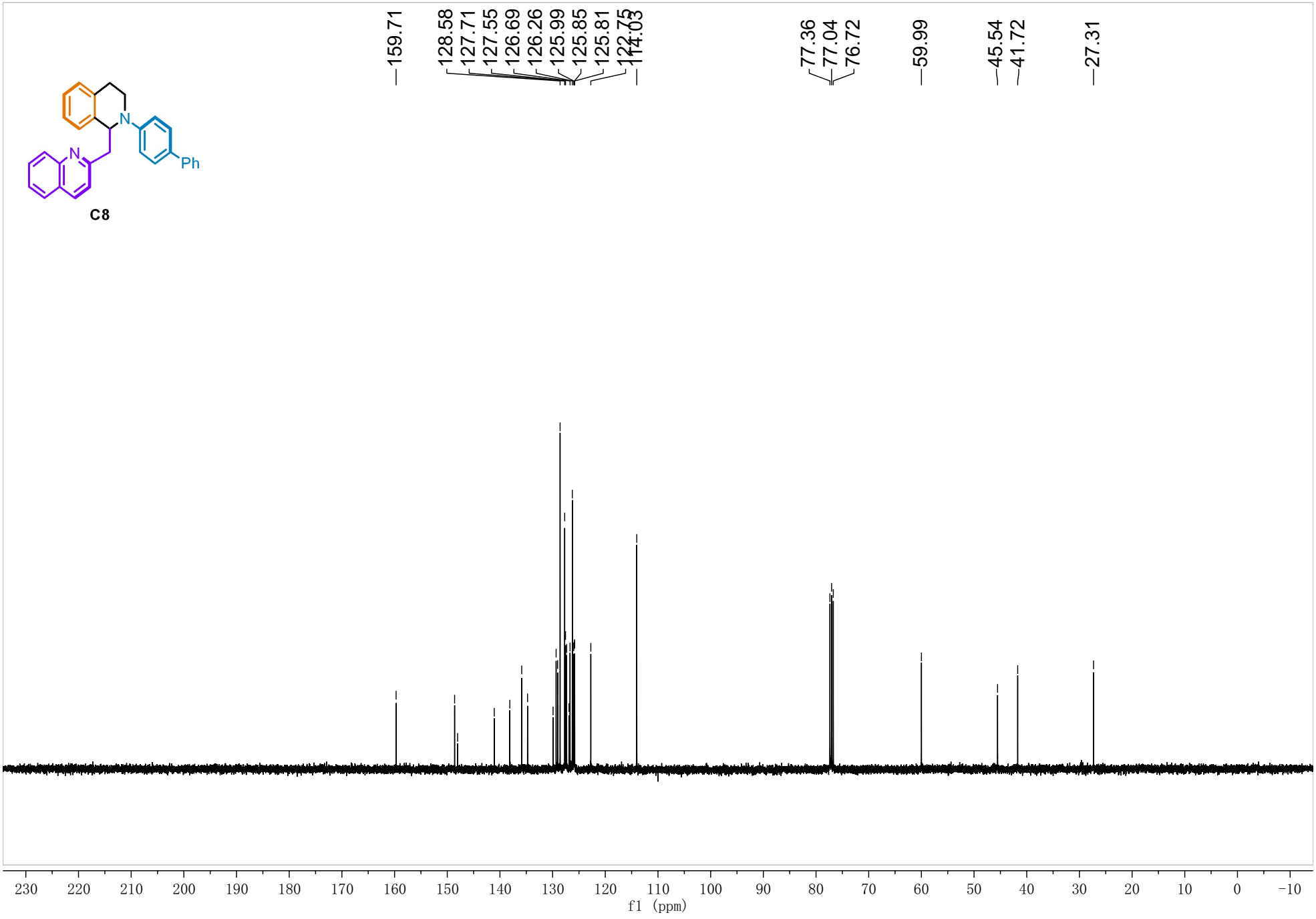
0.0
f1 (ppm)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45.54
41.72
27.31
N
N
Ph
C8
230
220
210
200
190
180
170
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100
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80
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30
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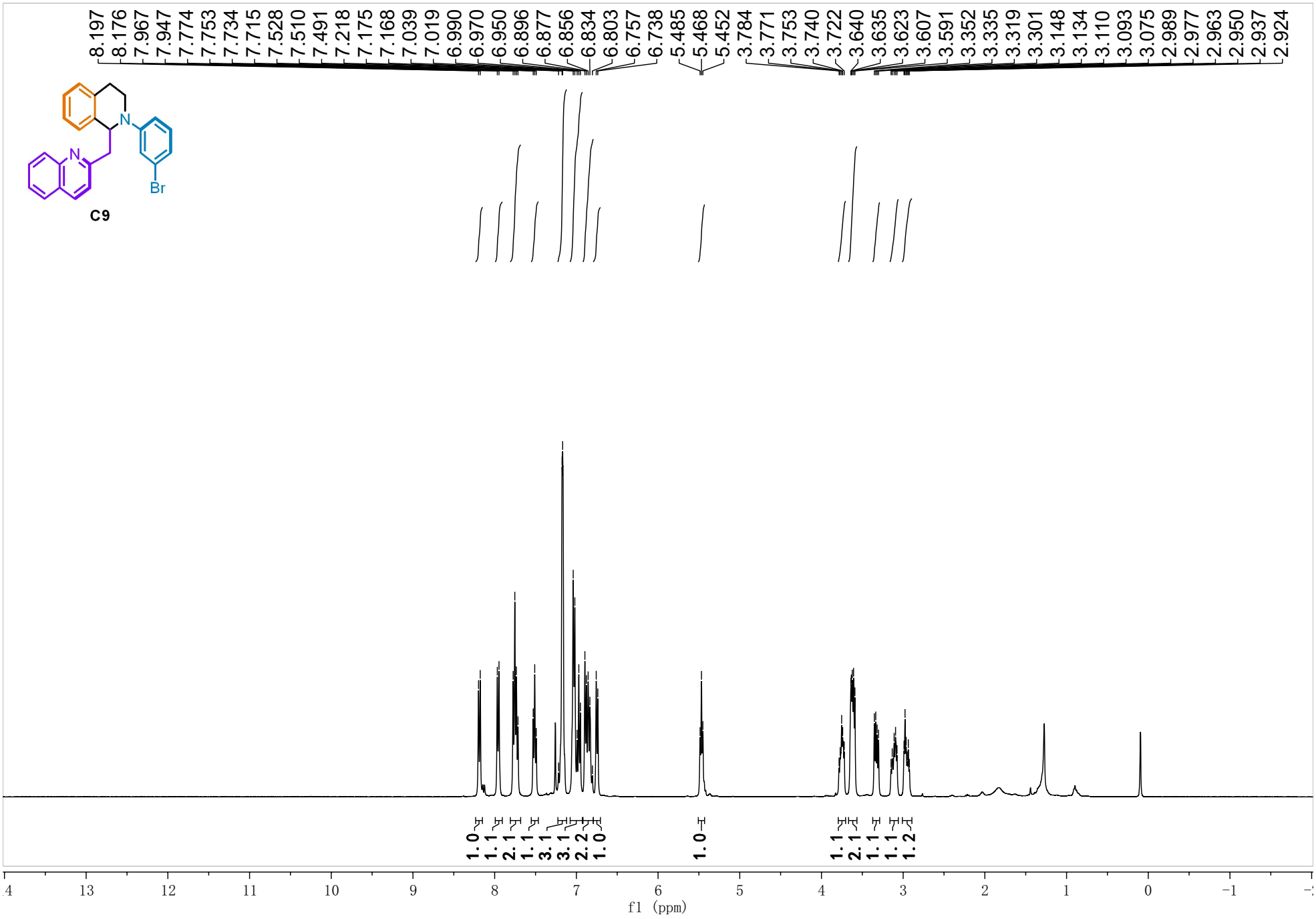
f1 (ppm)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Br
C9
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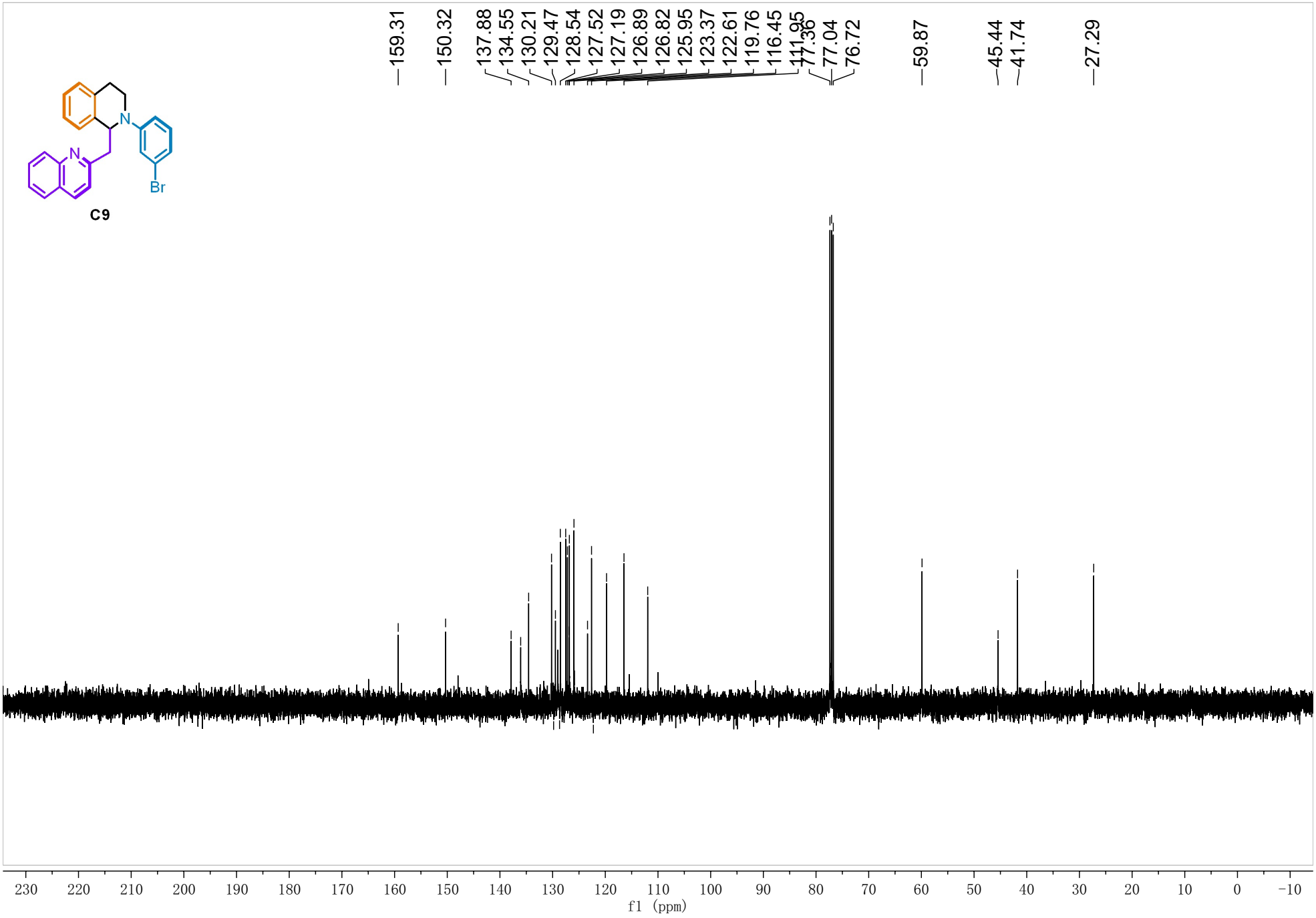
f1 (ppm)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122.61
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111.95
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77.04
76.72
59.87
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41.74
27.29
N
N
Br
C9
230
220
210
200
190
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170
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80
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40
30
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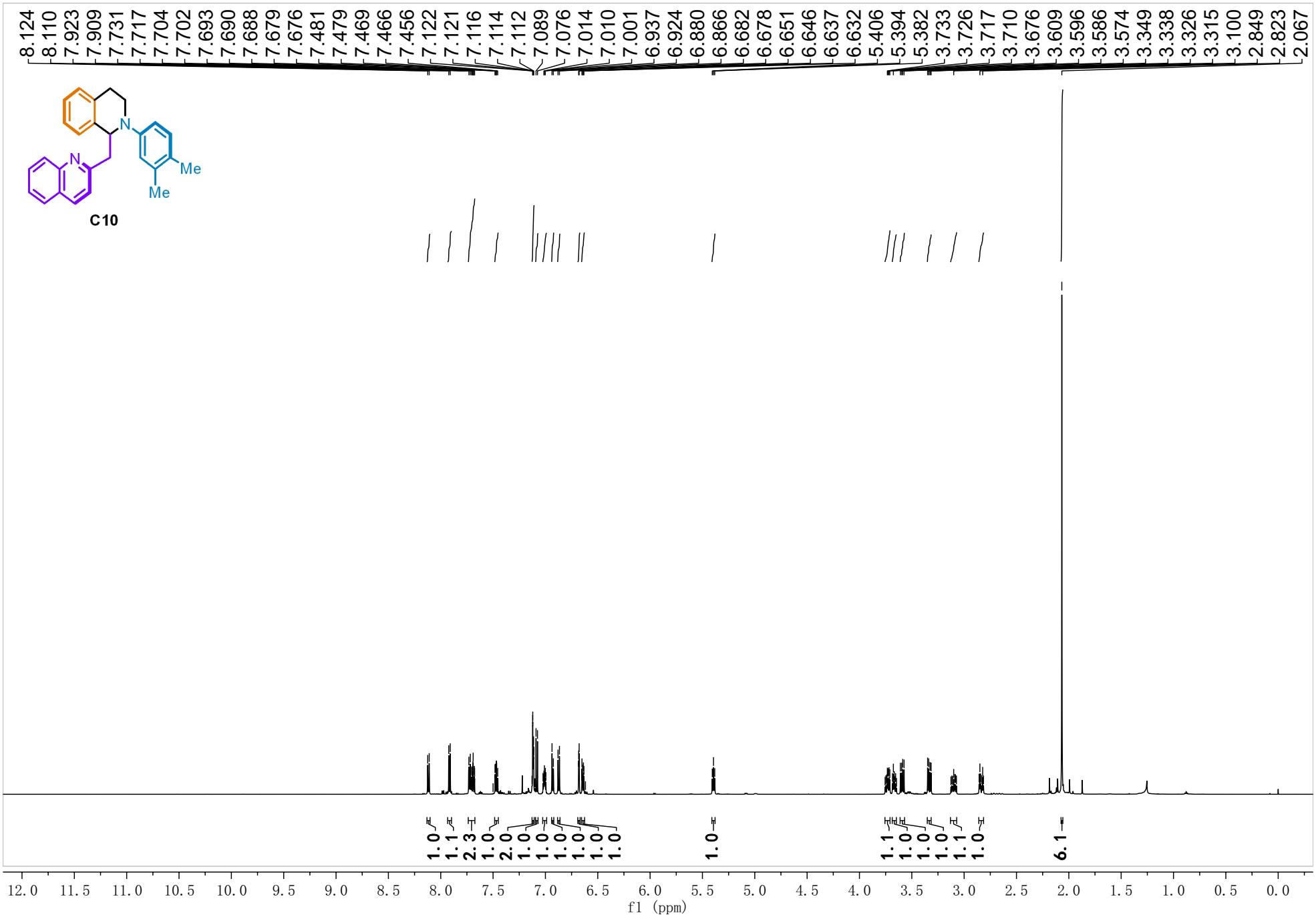
−10
f1 (ppm)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N
Me
Me
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6.5
6.0
5.5
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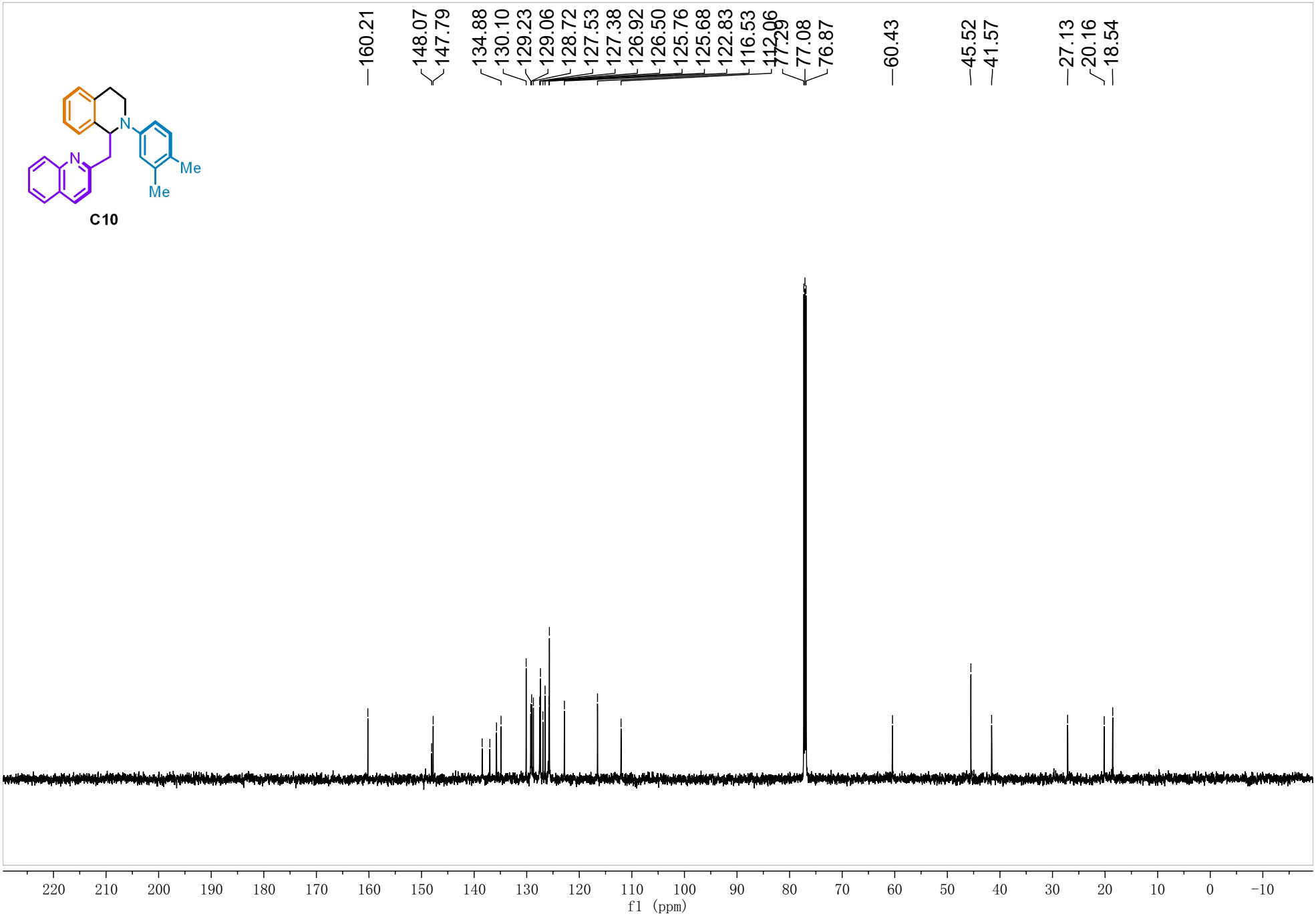
f1 (ppm)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125.68
122.83
116.53
112.06
77.29
77.08
76.87
60.43
45.52
41.57
27.13
20.16
18.54
N
N
Me
Me
C10
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200
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180
170
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80
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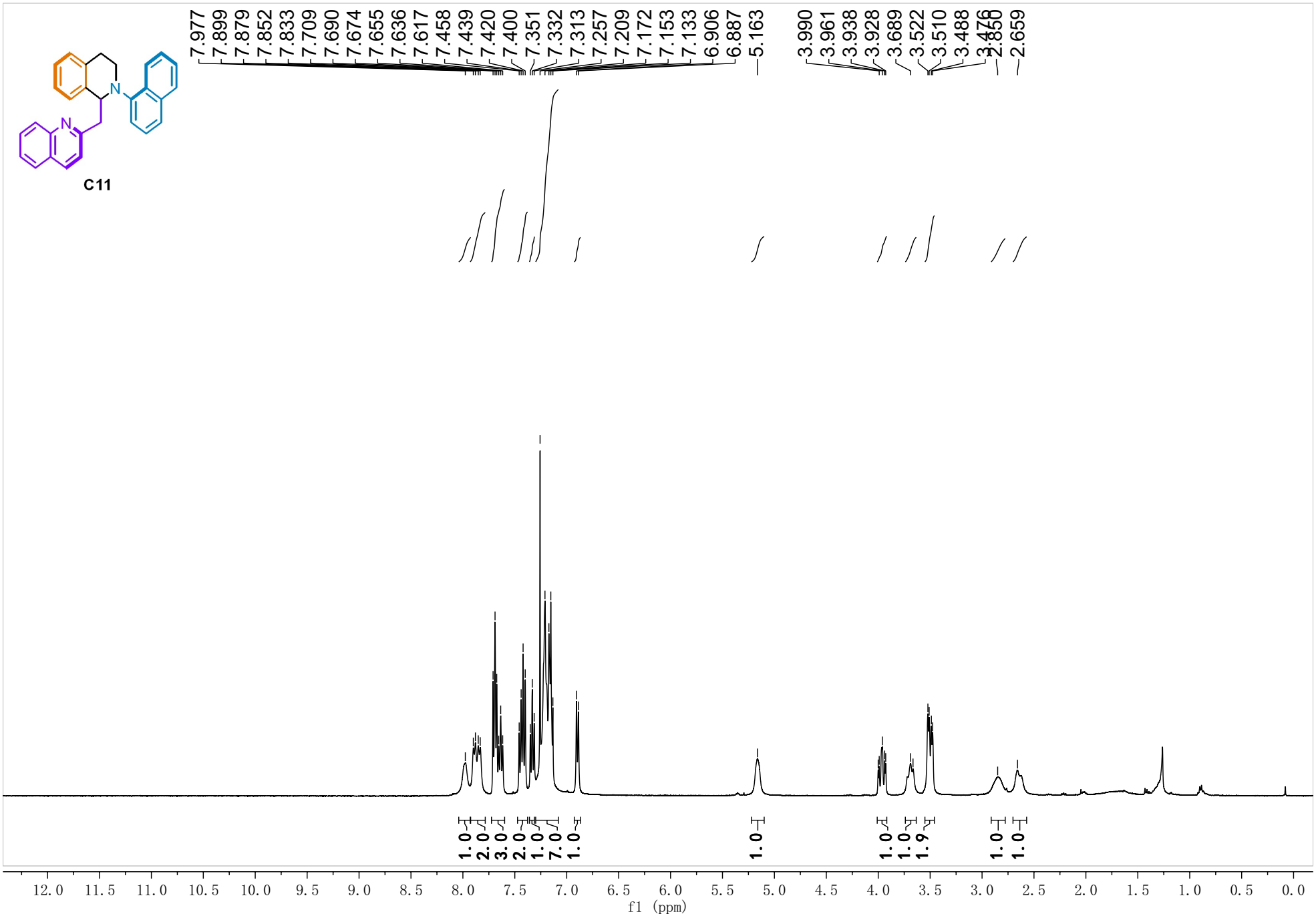
−10
f1 (ppm)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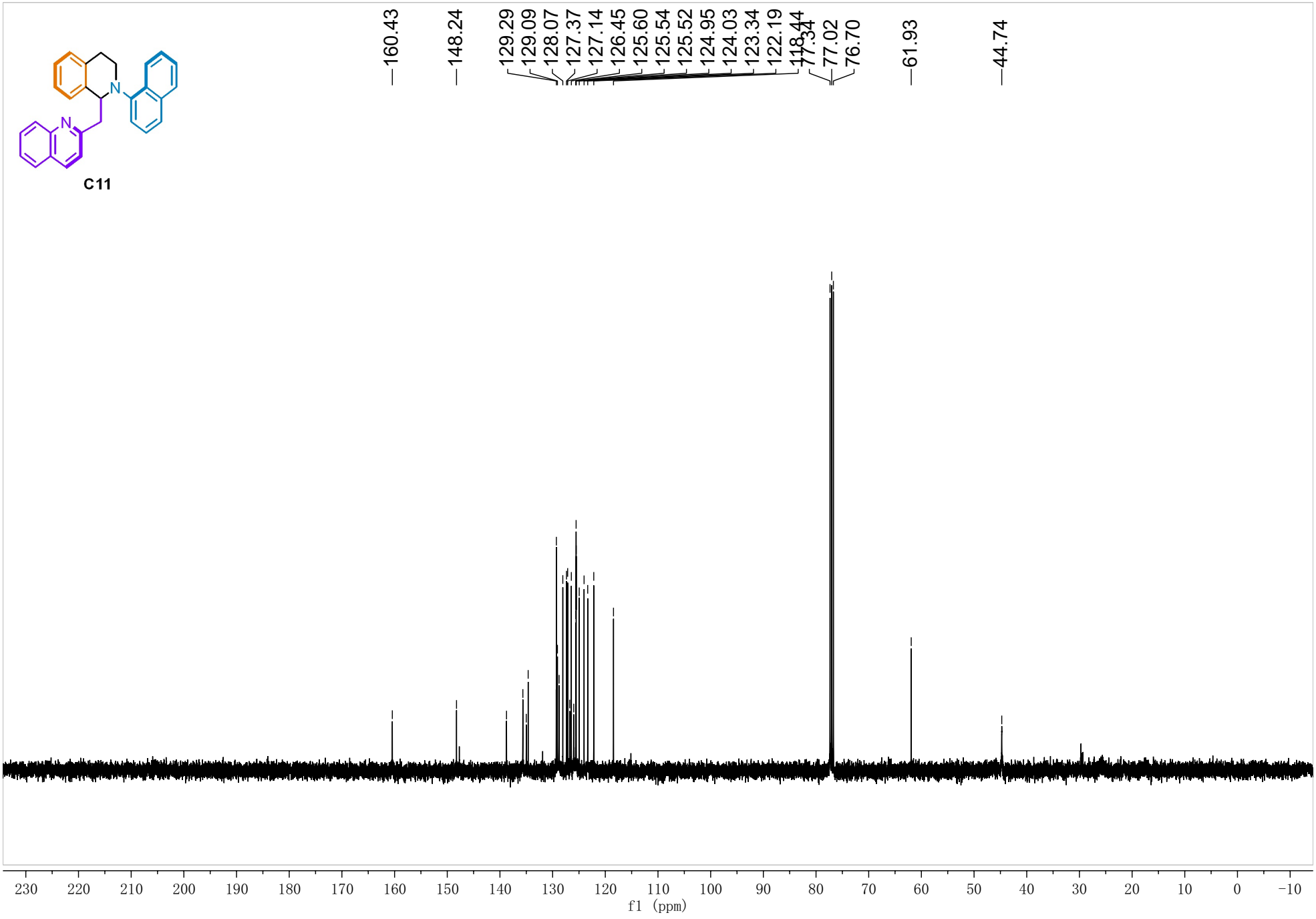
7.439
7.420
7.400
7.351
7.332
7.313
7.257
7.209
7.172
7.153
7.133
6.906
6.887
5.163
3.990
3.961
3.938
3.928
3.689
3.522
3.510
3.488
3.476
2.850
2.659
C11
1.0
2.0
3.0
2.0
1.0
7.0
1.0
1.0
1.0
1.0
1.9
1.0
1.0
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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125.52
124.95
124.03
123.34
122.19
118.44
77.34
77.02
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61.93
44.74
C11
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220
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180
170
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100
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80
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30
20
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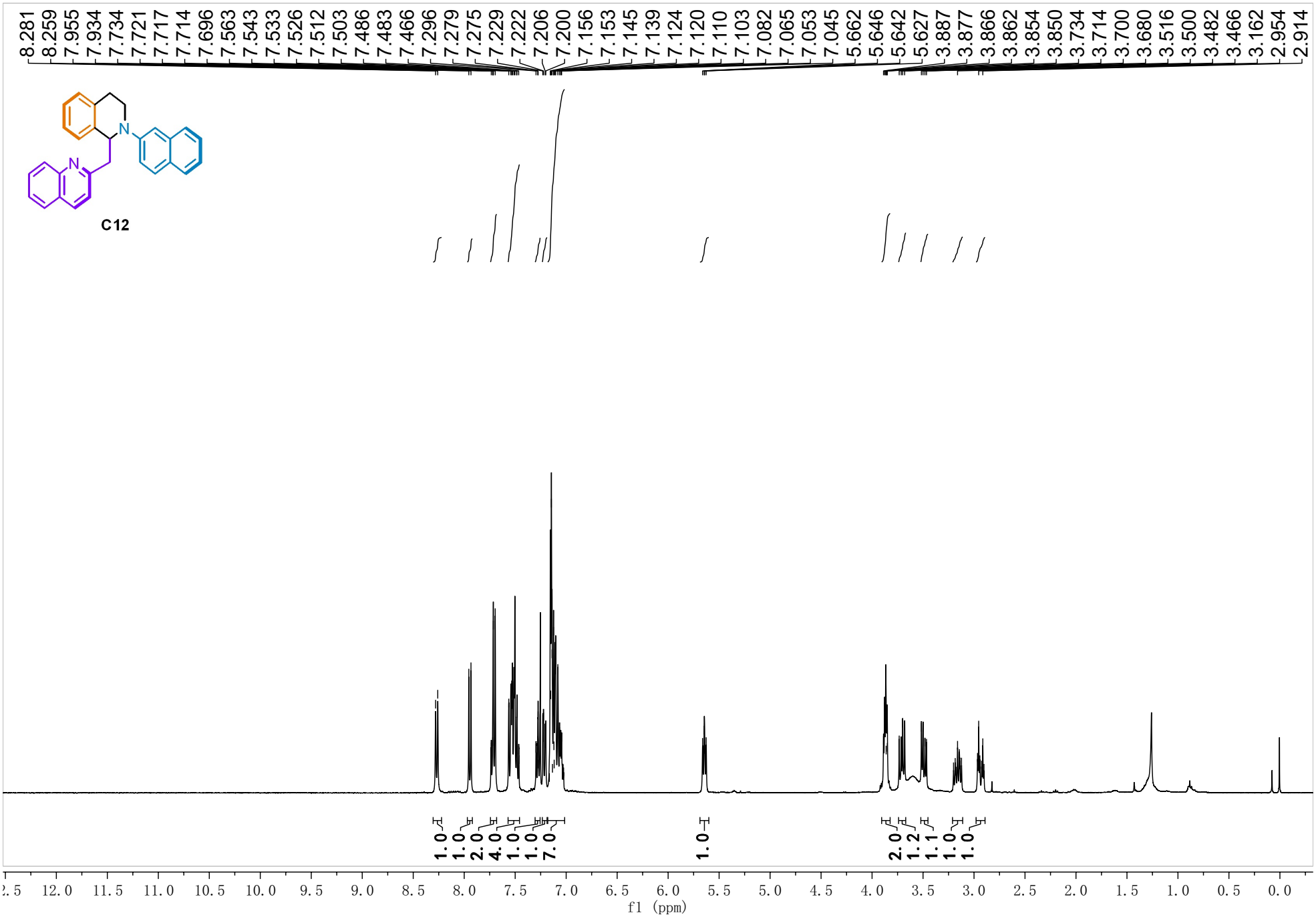
−10
f1 (ppm)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7.526
7.512
7.503
7.486
7.483
7.466
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7.279
7.275
7.229
7.222
7.206
7.200
7.156
7.153
7.145
7.139
7.124
7.120
7.110
7.103
7.082
7.065
7.053
7.045
5.662
5.646
5.642
5.627
3.887
3.877
3.866
3.862
3.854
3.850
3.734
3.714
3.700
3.680
3.516
3.500
3.482
3.466
3.162
2.954
2.914
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N
C12
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1.0
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1.0
7.0
1.0
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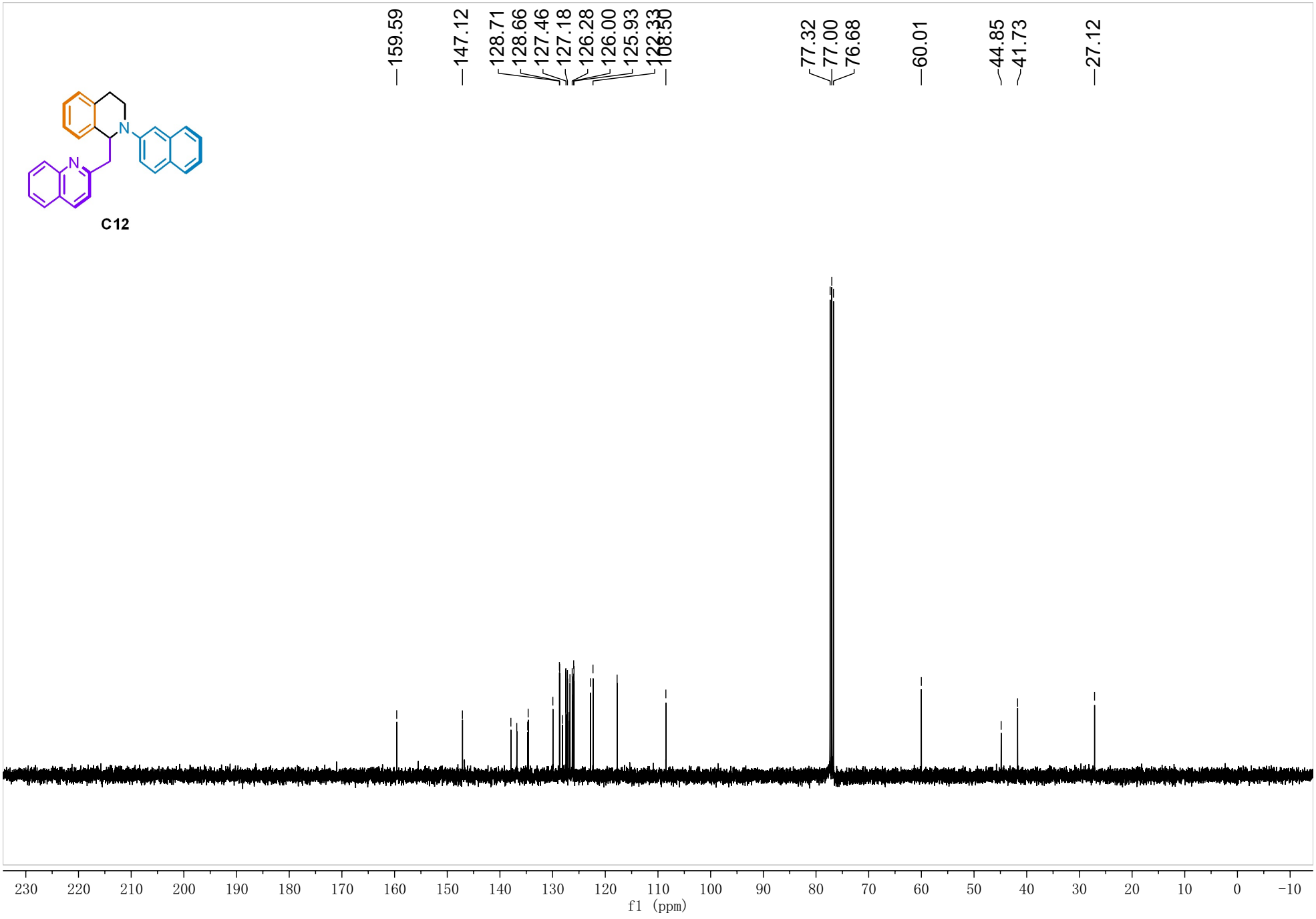
1.0
f1 (ppm)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77.32
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41.73
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N
C12
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210
200
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180
170
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30
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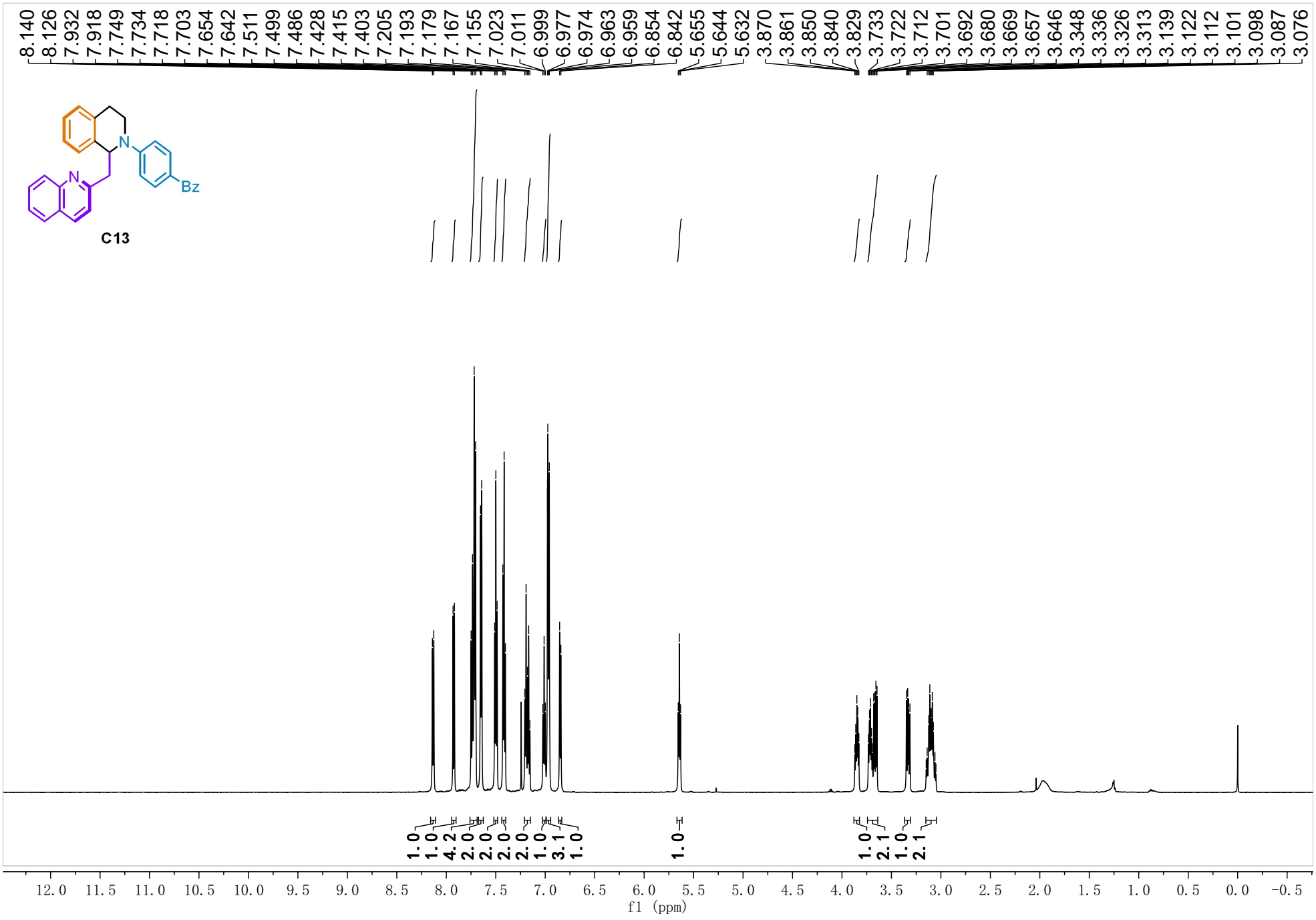
f1 (ppm)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7.734
7.718
7.703
7.654
7.642
7.511
7.499
7.486
7.428
7.415
7.403
7.205
7.193
7.179
7.167
7.155
7.023
7.011
6.999
6.977
6.974
6.963
6.959
6.854
6.842
5.655
5.644
5.632
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3.861
3.850
3.840
3.829
3.733
3.722
3.712
3.701
3.692
3.680
3.669
3.657
3.646
3.348
3.336
3.326
3.313
3.139
3.122
3.112
3.101
3.098
3.087
3.076
N
N
Bz
C13
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1.0
4.2
2.0
2.0
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1.0
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1.0
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1.0
2.1
1.0
2.1
12.0
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6.5
6.0
5.5
5.0
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3.0
2.5
2.0
1.5
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0.5
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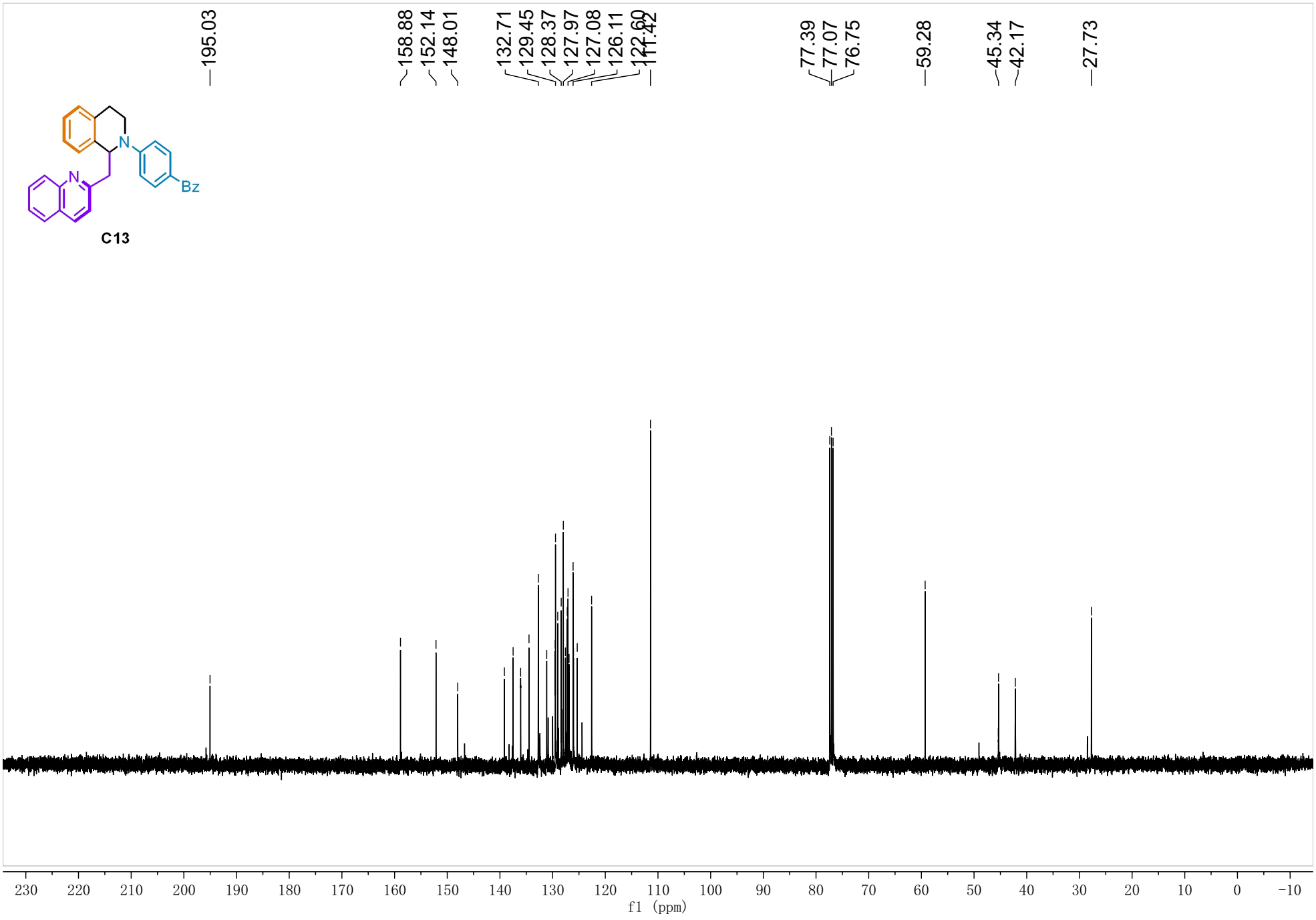
f1 (ppm)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127.97
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126.11
122.60
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77.39
77.07
76.75
59.28
45.34
42.17
27.73
N
N
Bz
C13
230
220
210
200
190
180
170
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100
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80
70
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40
30
20
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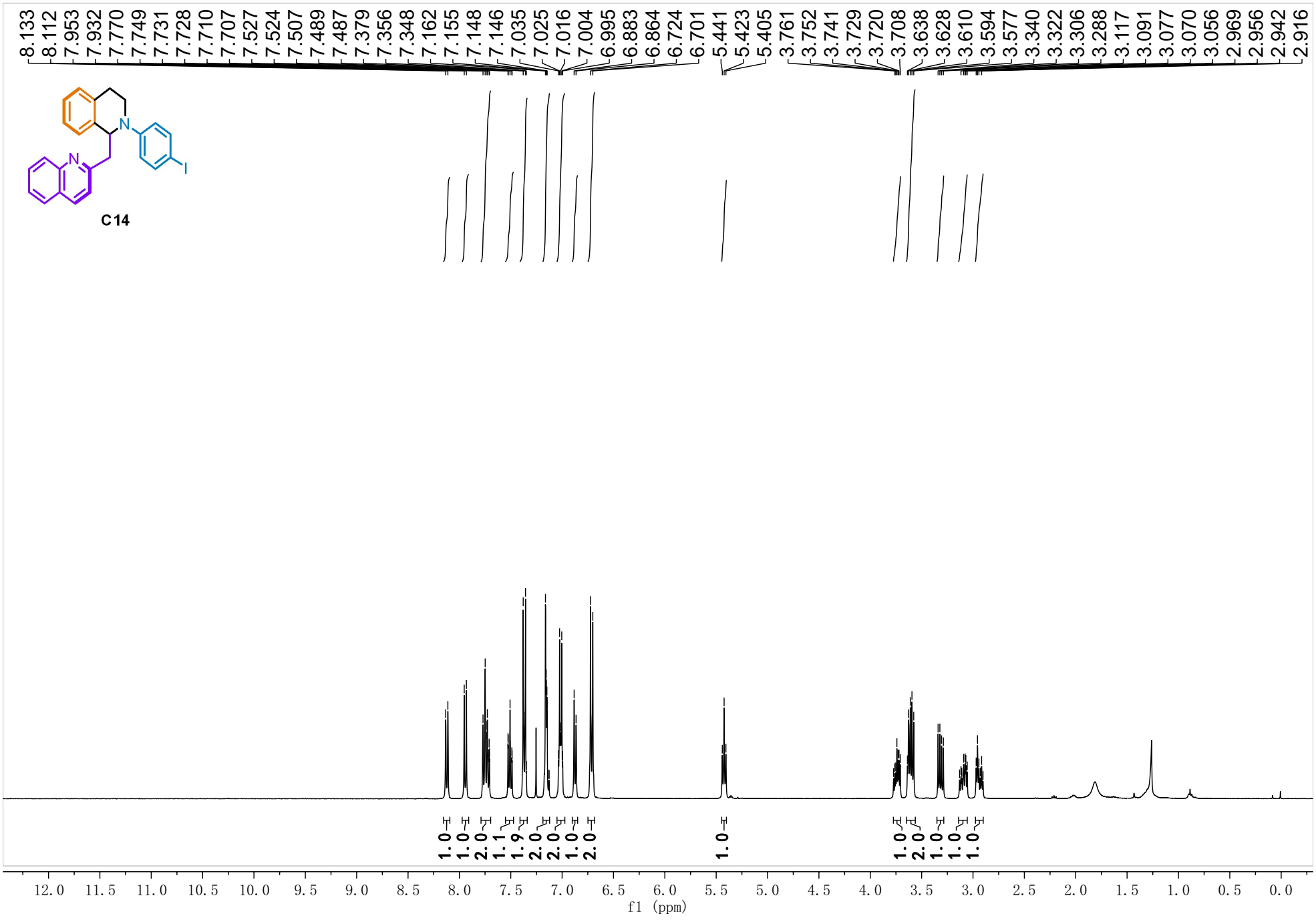
−10
f1 (ppm)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7.728
7.710
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7.524
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7.489
7.487
7.379
7.356
7.348
7.162
7.155
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7.146
7.035
7.025
7.016
7.004
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6.883
6.864
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5.423
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3.752
3.741
3.729
3.720
3.708
3.638
3.628
3.610
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3.340
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3.056
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2.916
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N
I
C14
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1.0
2.0
1.1
1.9
2.0
2.0
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2.0
1.0
1.0
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1.0
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6.5
6.0
5.5
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2.5
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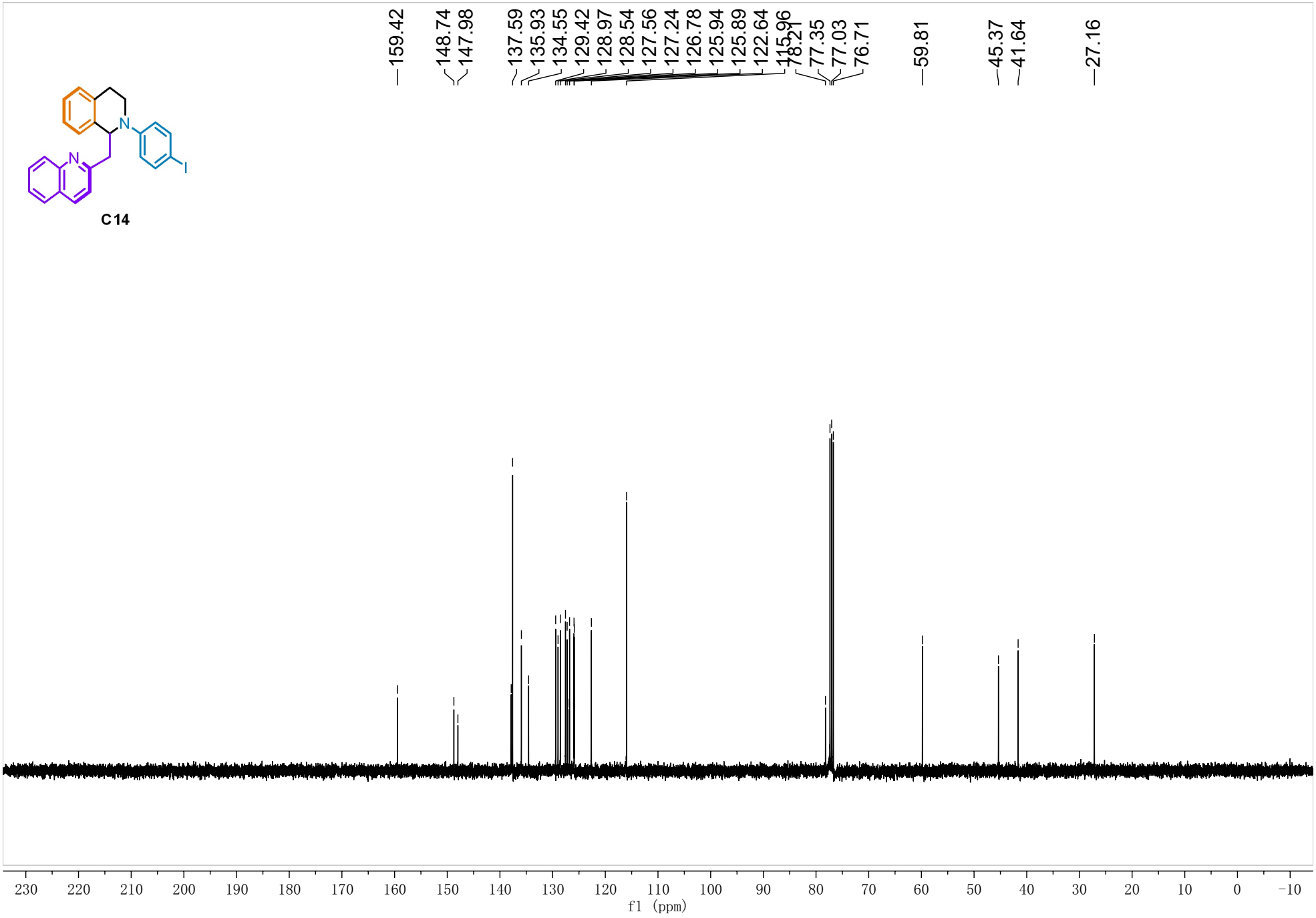
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125.94
125.89
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115.96
78.21
77.35
77.03
76.71
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45.37
41.64
27.16
N
N
I
C14
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210
200
190
180
170
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80
70
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30
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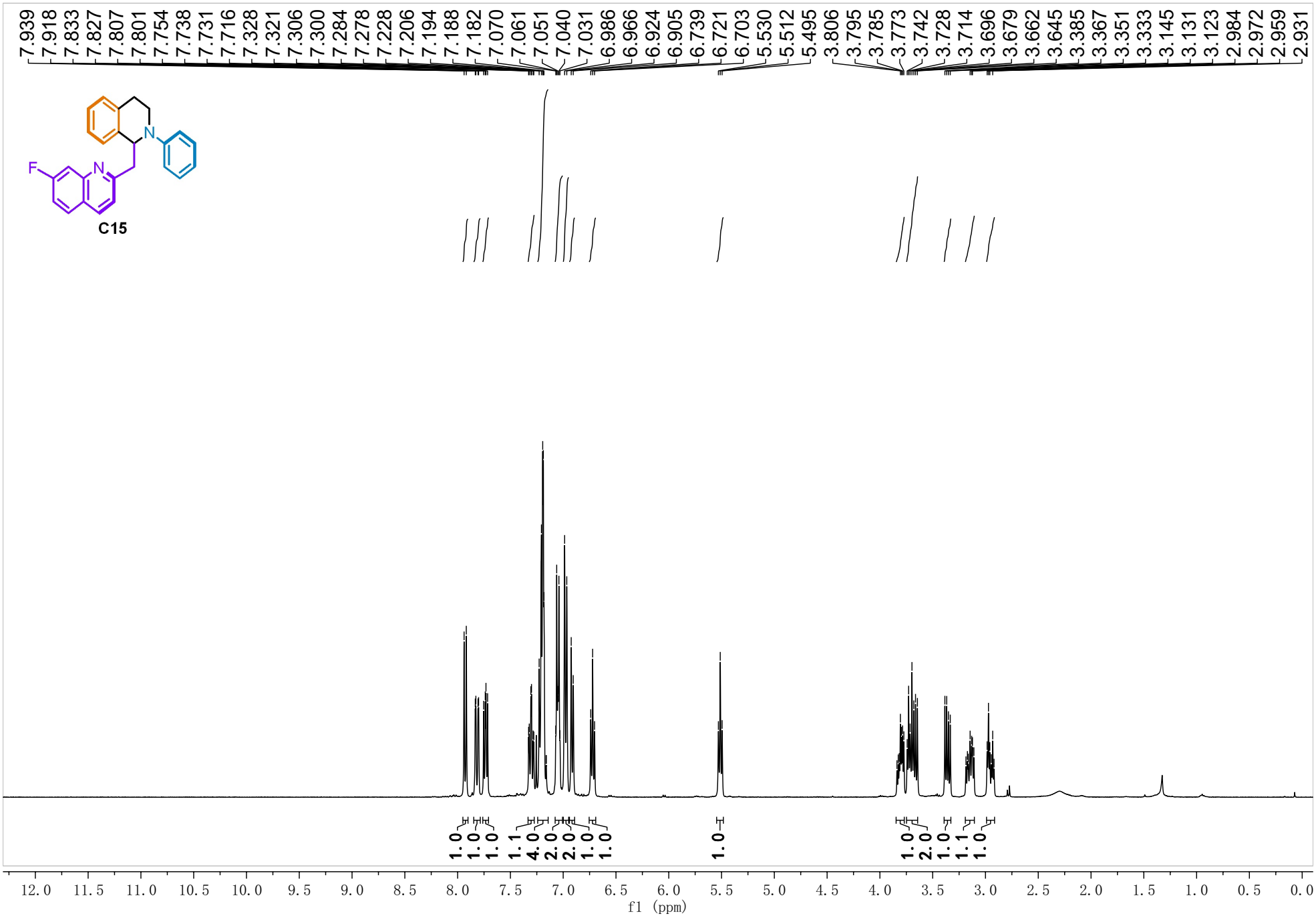
f1 (ppm)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7.300
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7.206
7.194
7.188
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3.333
3.145
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3.123
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2.972
2.959
2.931
F
N
N
C15
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1.0
1.0
1.1
4.0
2.0
2.0
1.0
1.0
1.0
1.0
2.0
1.0
1.1
1.0
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6.5
6.0
5.5
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2.5
2.0
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1.0
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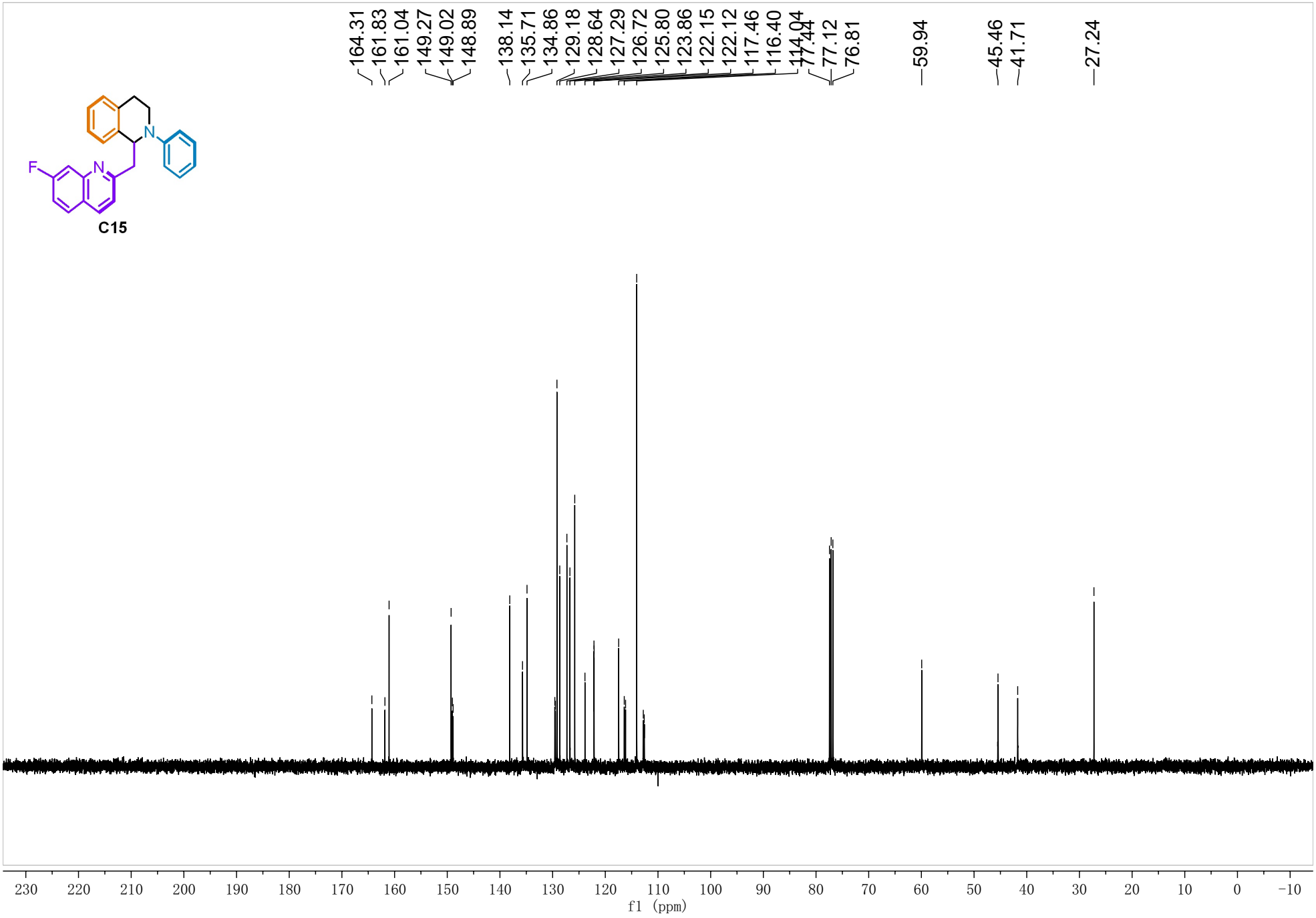
0.0
f1 (ppm)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125.80
123.86
122.15
122.12
117.46
116.40
114.04
77.44
77.12
76.81
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45.46
41.71
27.24
F
N
N
C15
230
220
210
200
190
180
170
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140
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120
110
100
90
80
70
60
50
40
30
20
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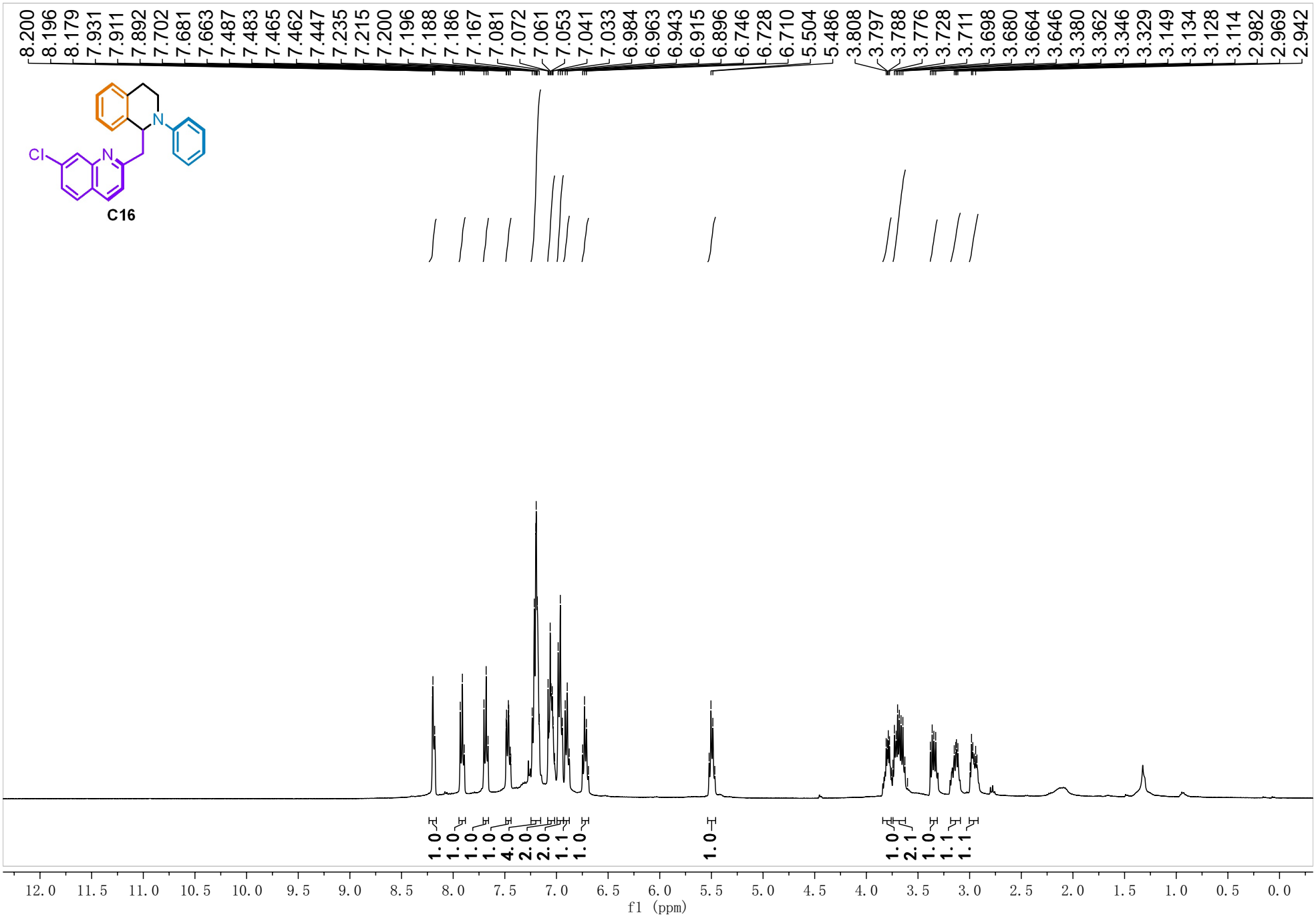
−10
f1 (ppm)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7.053
7.041
7.033
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N
C16
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7.0
6.5
6.0
5.5
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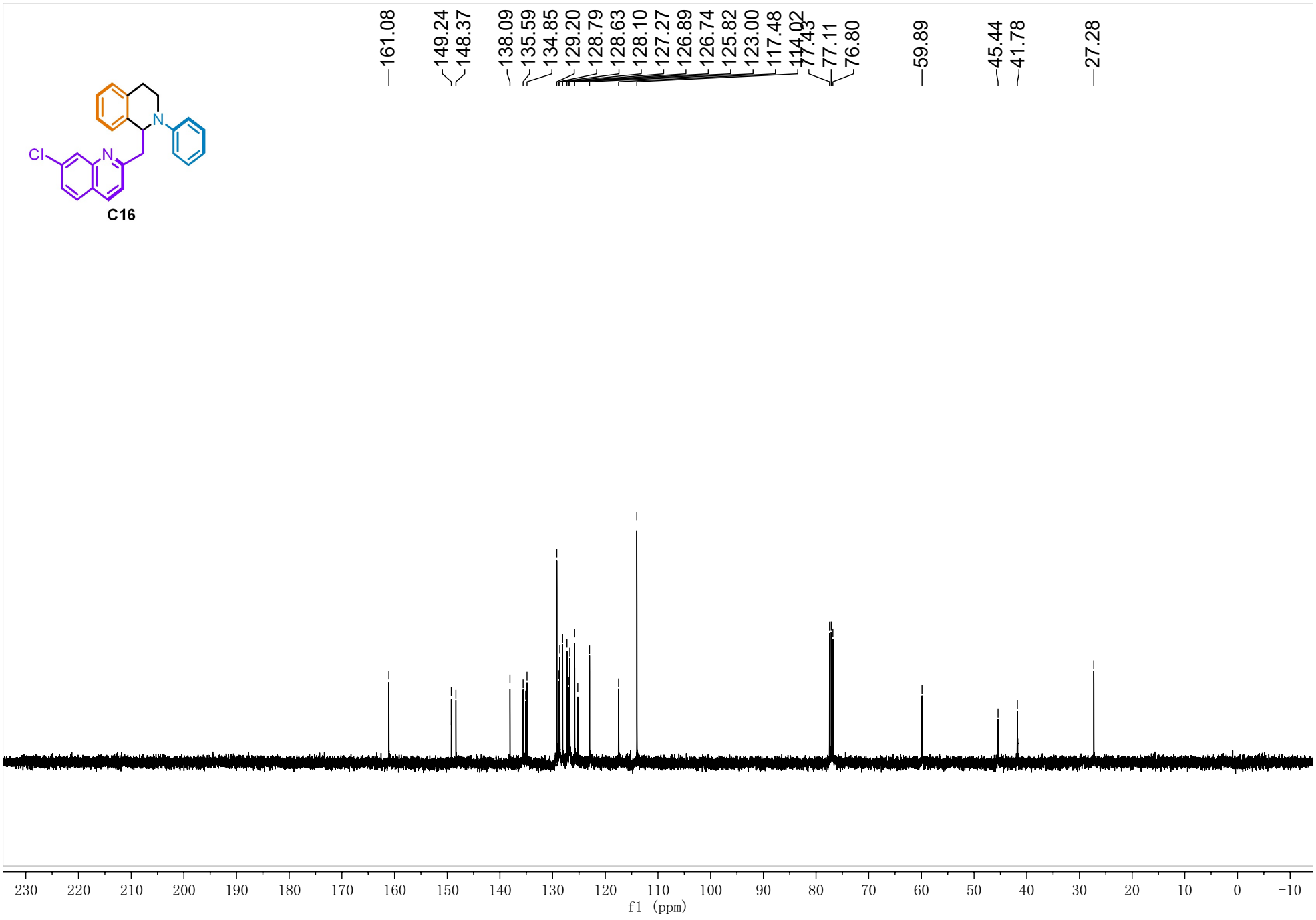
1.0
0.5
0.0
f1 (ppm)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127.27
126.89
126.74
125.82
123.00
117.48
114.02
77.43
77.11
76.80
59.89
45.44
41.78
27.28
Cl
N
N
C16
230
220
210
200
190
180
170
160
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140
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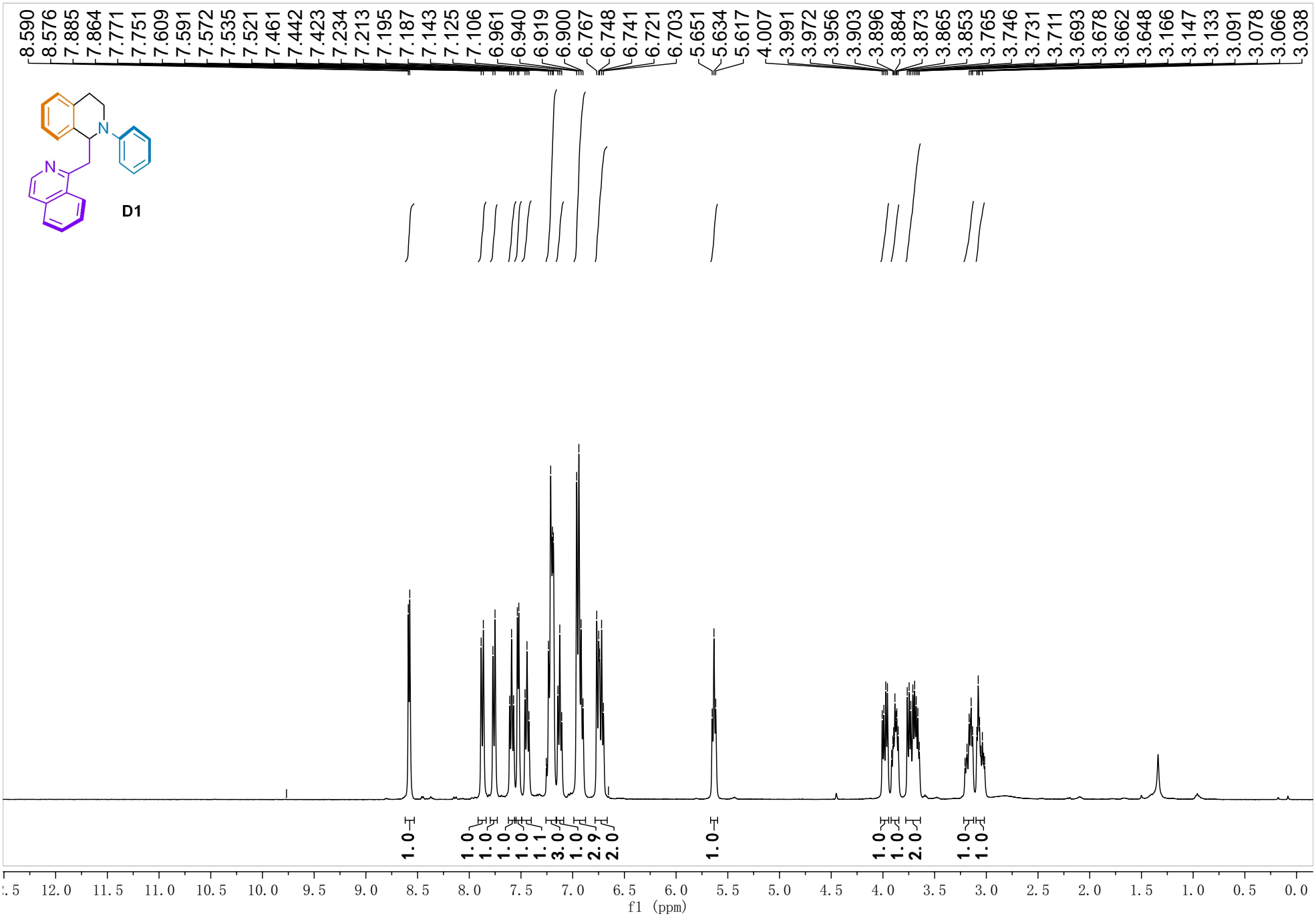
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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7.213
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7.143
7.125
7.106
6.961
6.940
6.919
6.900
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3.765
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3.731
3.711
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3.678
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3.648
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3.066
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N
D1
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1.0
1.0
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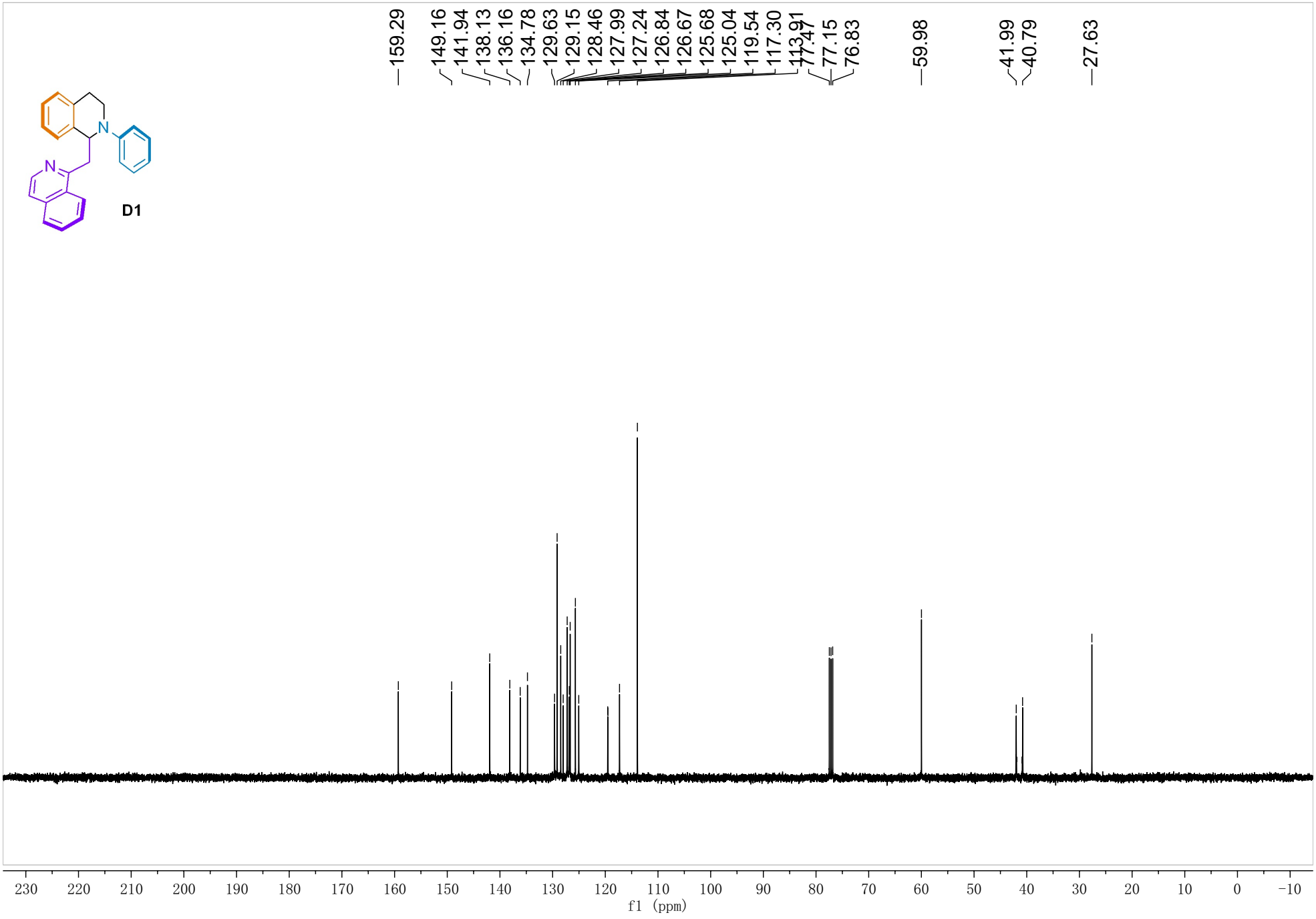
1.0
f1 (ppm)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125.68
125.04
119.54
117.30
113.91
77.47
77.15
76.83
59.98
41.99
40.79
27.63
N
N
D1
230
220
210
200
190
180
170
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140
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120
110
100
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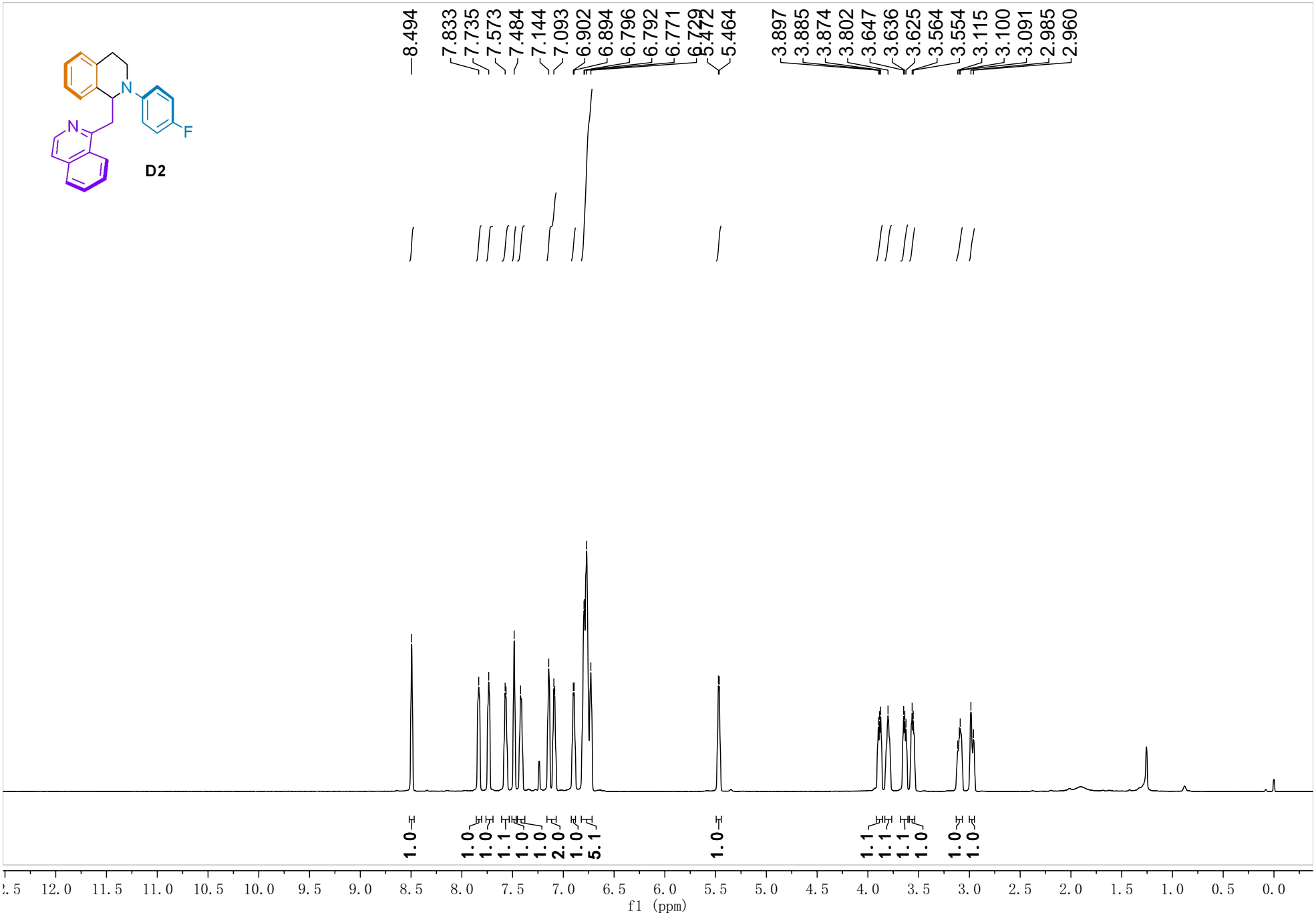
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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6.722
5.472
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3.897
3.885
3.874
3.802
3.647
3.636
3.625
3.564
3.554
3.115
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2.985
2.960
N
N
F
D2
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1.0
1.0
1.1
1.0
1.0
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1.0
1.1
1.1
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1.0
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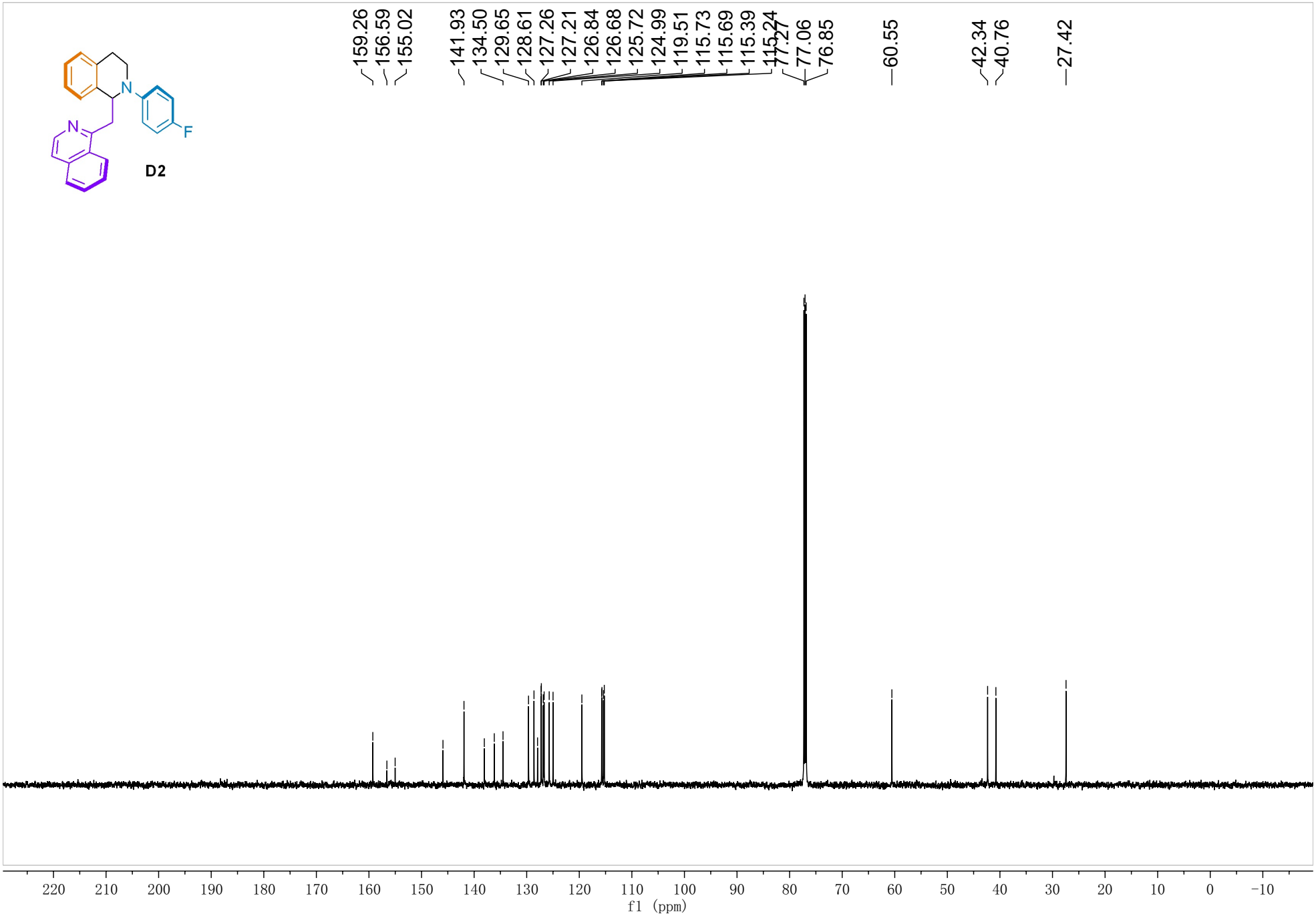
1.0
f1 (ppm)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119.51
115.73
115.69
115.39
115.24
77.27
77.06
76.85
60.55
42.34
40.76
27.42
N
N
F
D2
220
210
200
190
180
170
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80
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30
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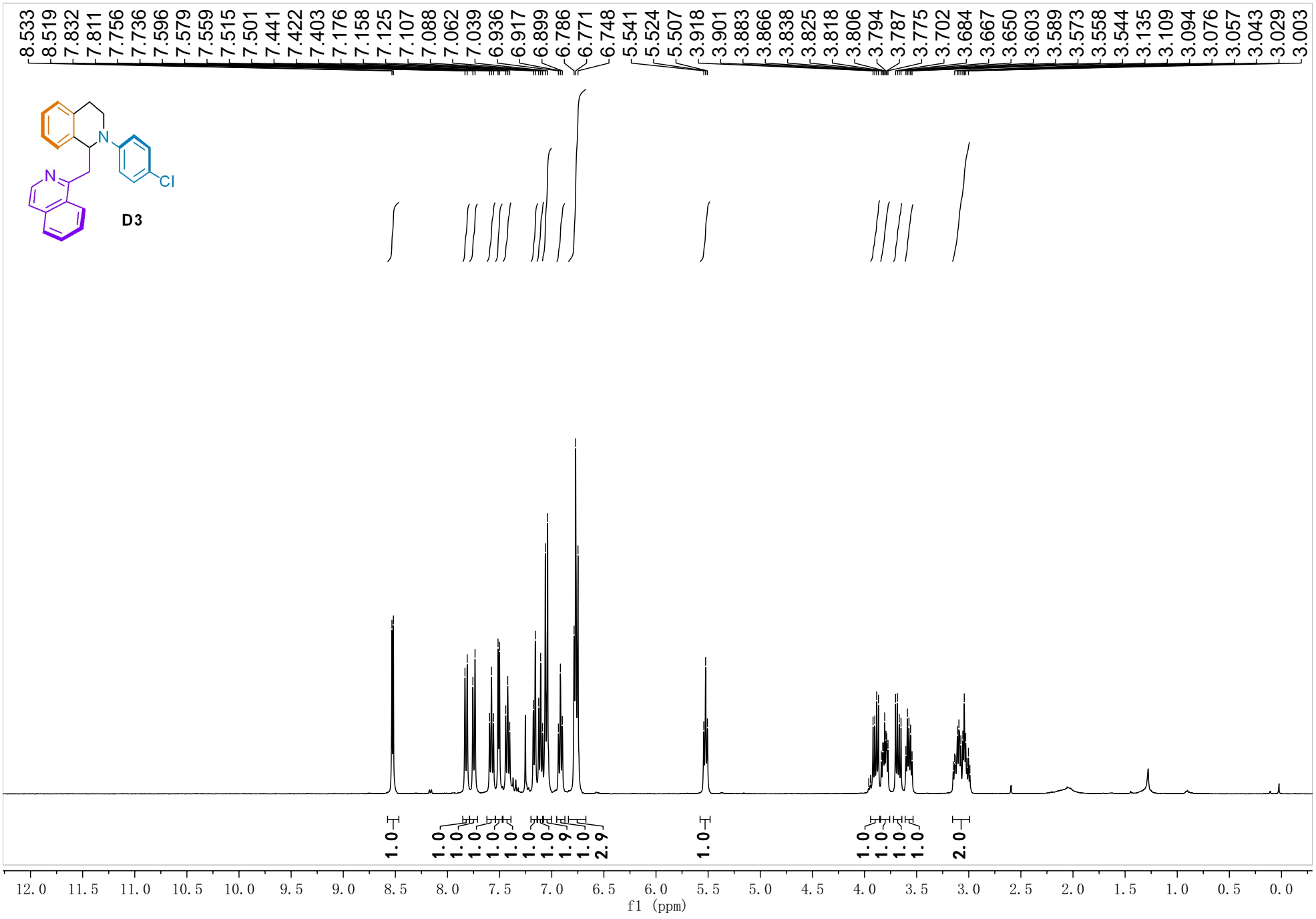
−10
f1 (ppm)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7.422
7.403
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7.088
7.062
7.039
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3.043
3.029
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Cl
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1.0
1.0
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1.0
1.0
1.0
1.0
2.0
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
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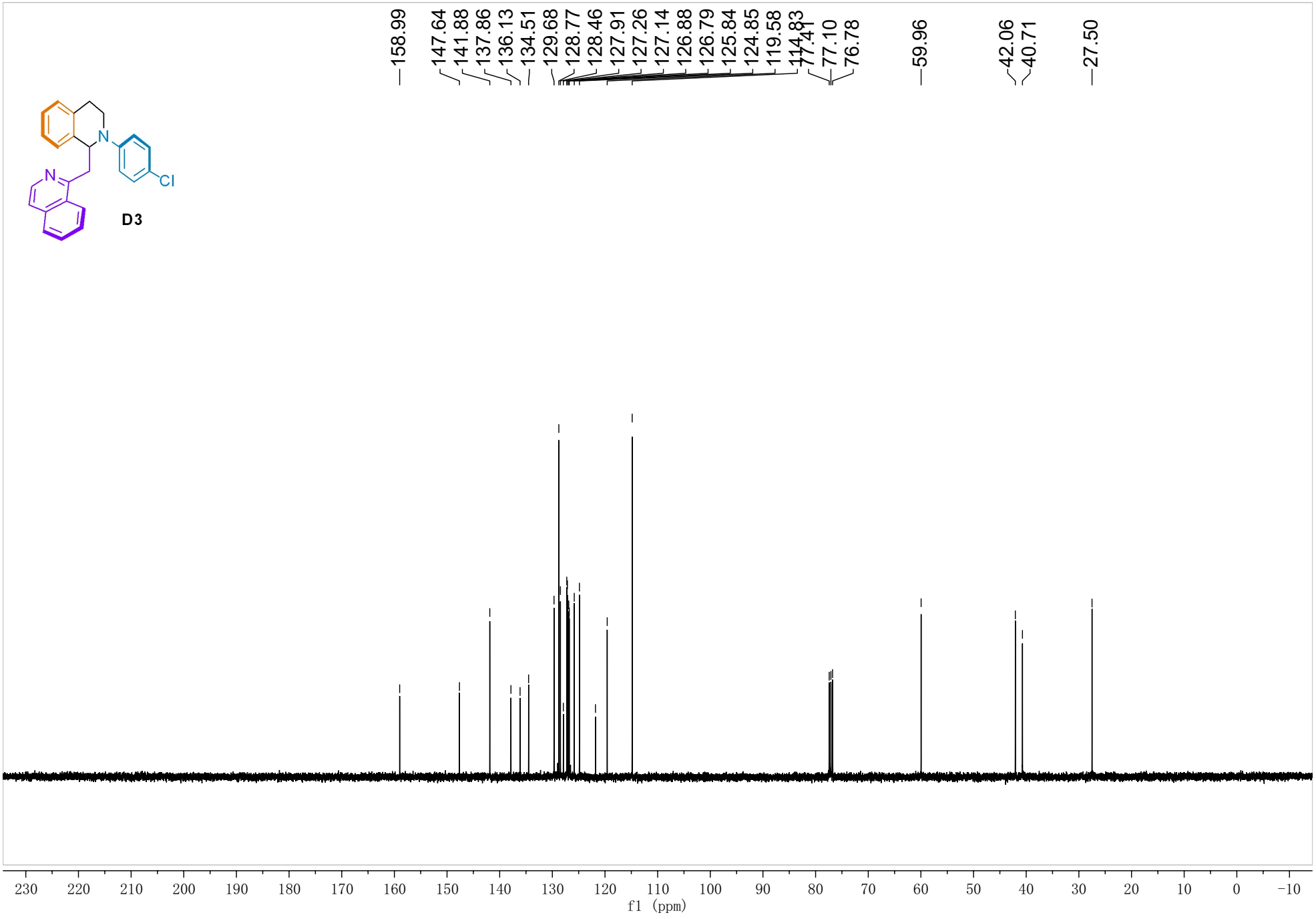
f1 (ppm)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136.13
134.51
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128.77
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127.91
127.26
127.14
126.88
126.79
125.84
124.85
119.58
114.83
77.41
77.10
76.78
59.96
42.06
40.71
27.50
N
N
Cl
D3
230
220
210
200
190
180
170
160
150
140
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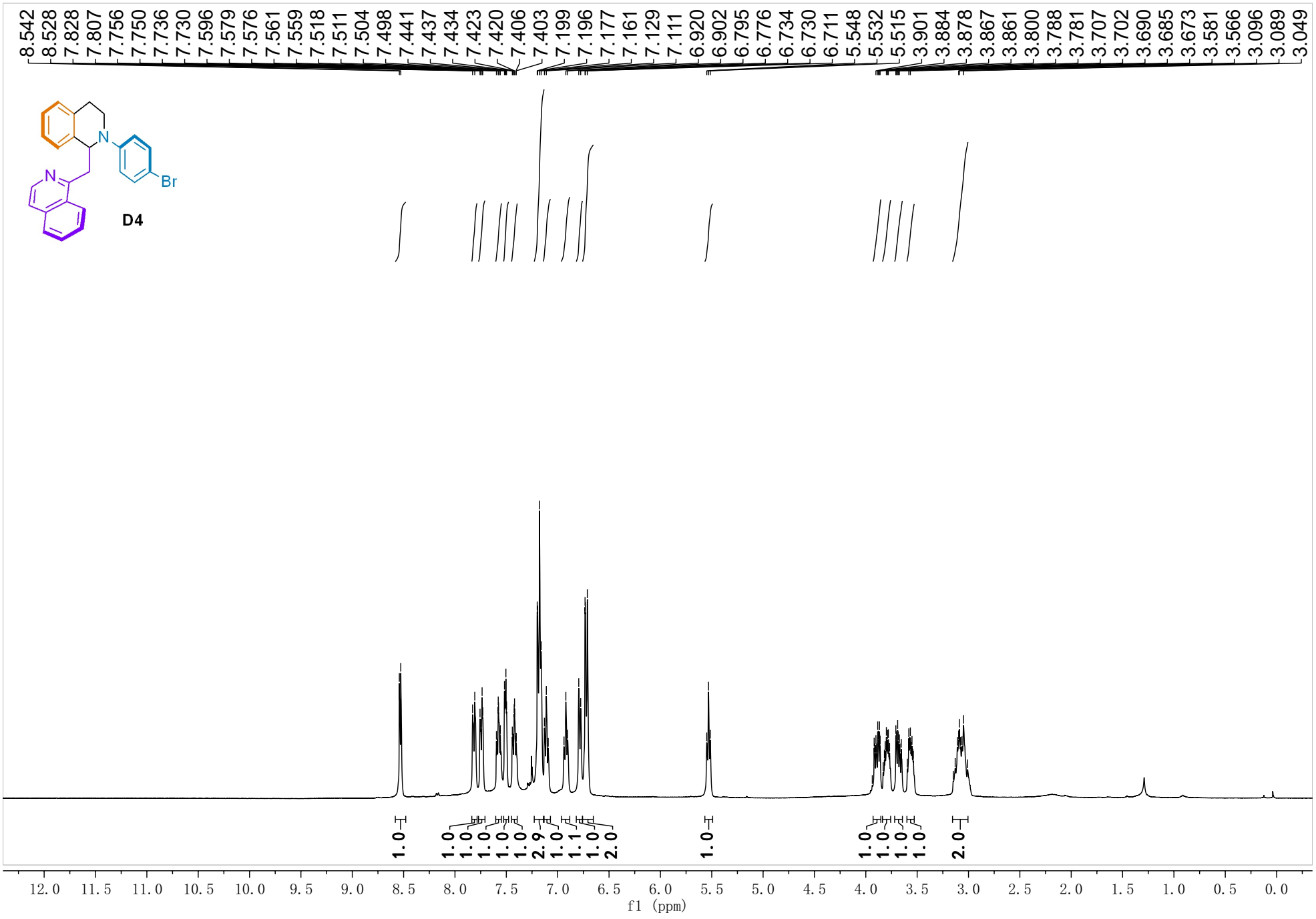
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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7.756
7.750
7.736
7.730
7.596
7.579
7.576
7.561
7.559
7.518
7.511
7.504
7.498
7.441
7.437
7.434
7.423
7.420
7.406
7.403
7.199
7.196
7.177
7.161
7.129
7.111
6.920
6.902
6.795
6.776
6.734
6.730
6.711
5.548
5.532
5.515
3.901
3.884
3.878
3.867
3.861
3.800
3.788
3.781
3.707
3.702
3.690
3.685
3.673
3.581
3.566
3.096
3.089
3.049
N
N
Br
D4
1.0
1.0
1.0
1.0
1.0
2.9
1.0
1.1
1.0
2.0
1.0
1.0
1.0
1.0
1.0
2.0
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
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3.5
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2.5
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1.0
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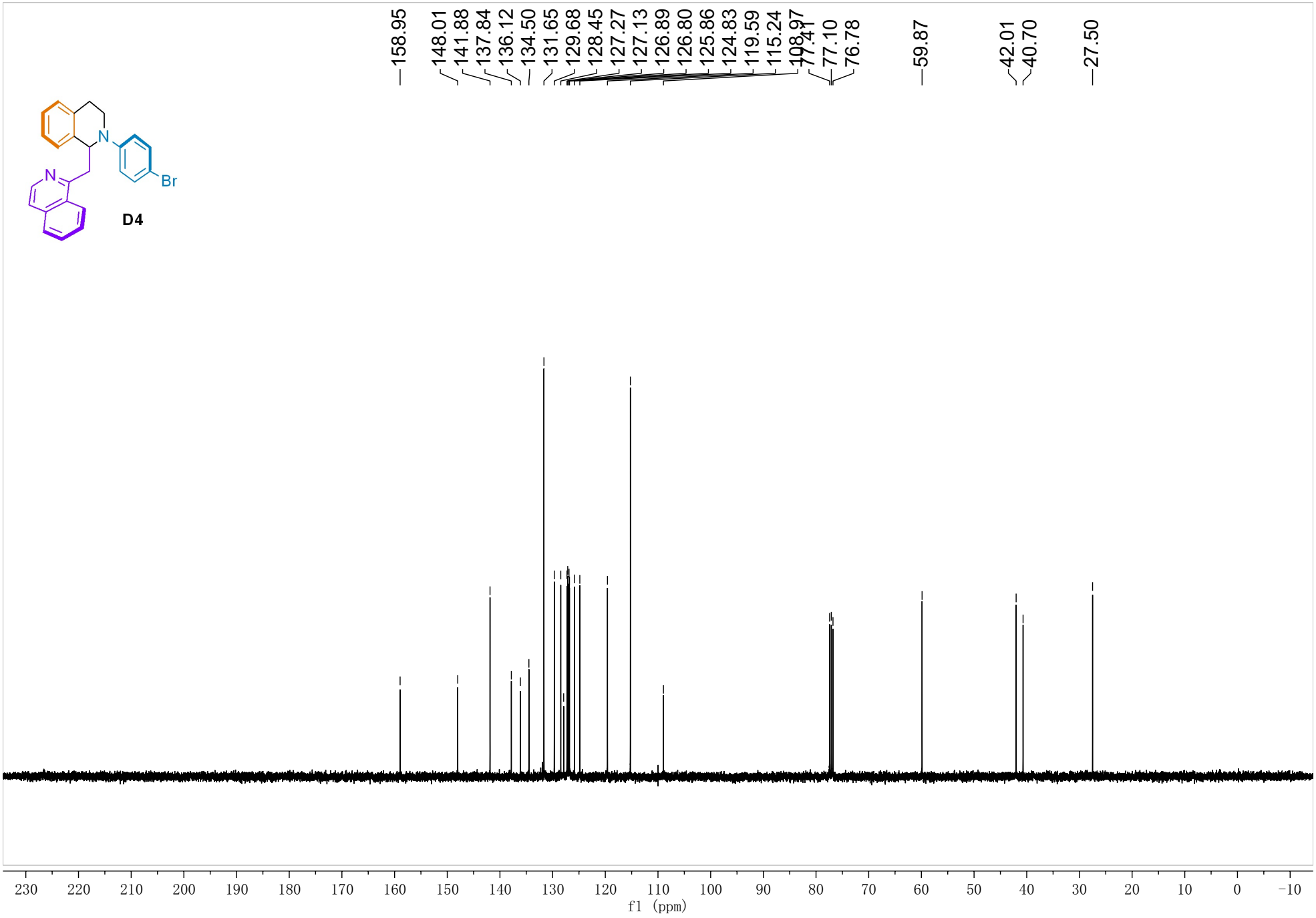
0.0
f1 (ppm)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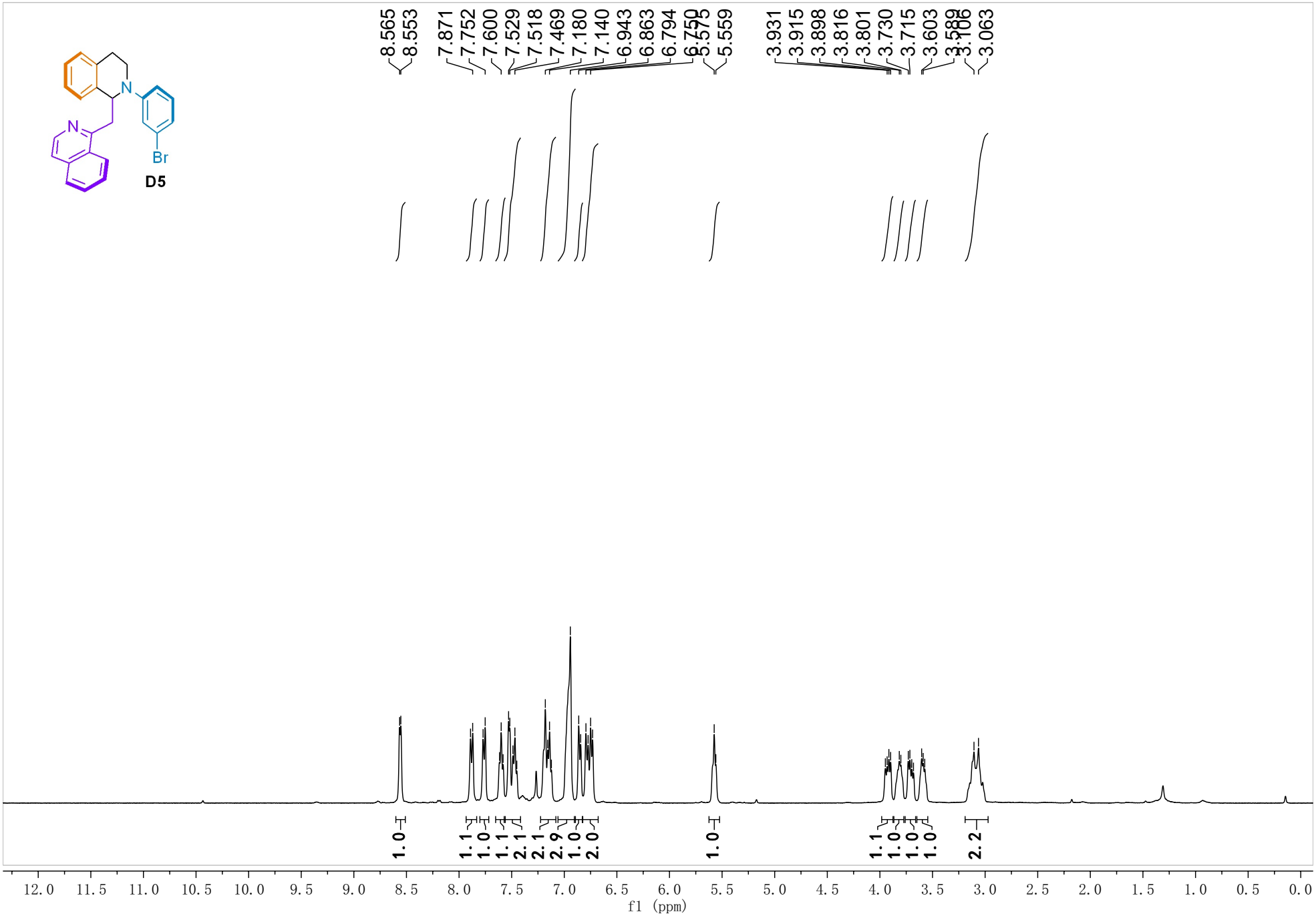
127.13
126.89
126.80
125.86
124.83
119.59
115.24
108.97
77.41
77.10
76.78
59.87
42.01
40.70
27.50
N
N
Br
D4
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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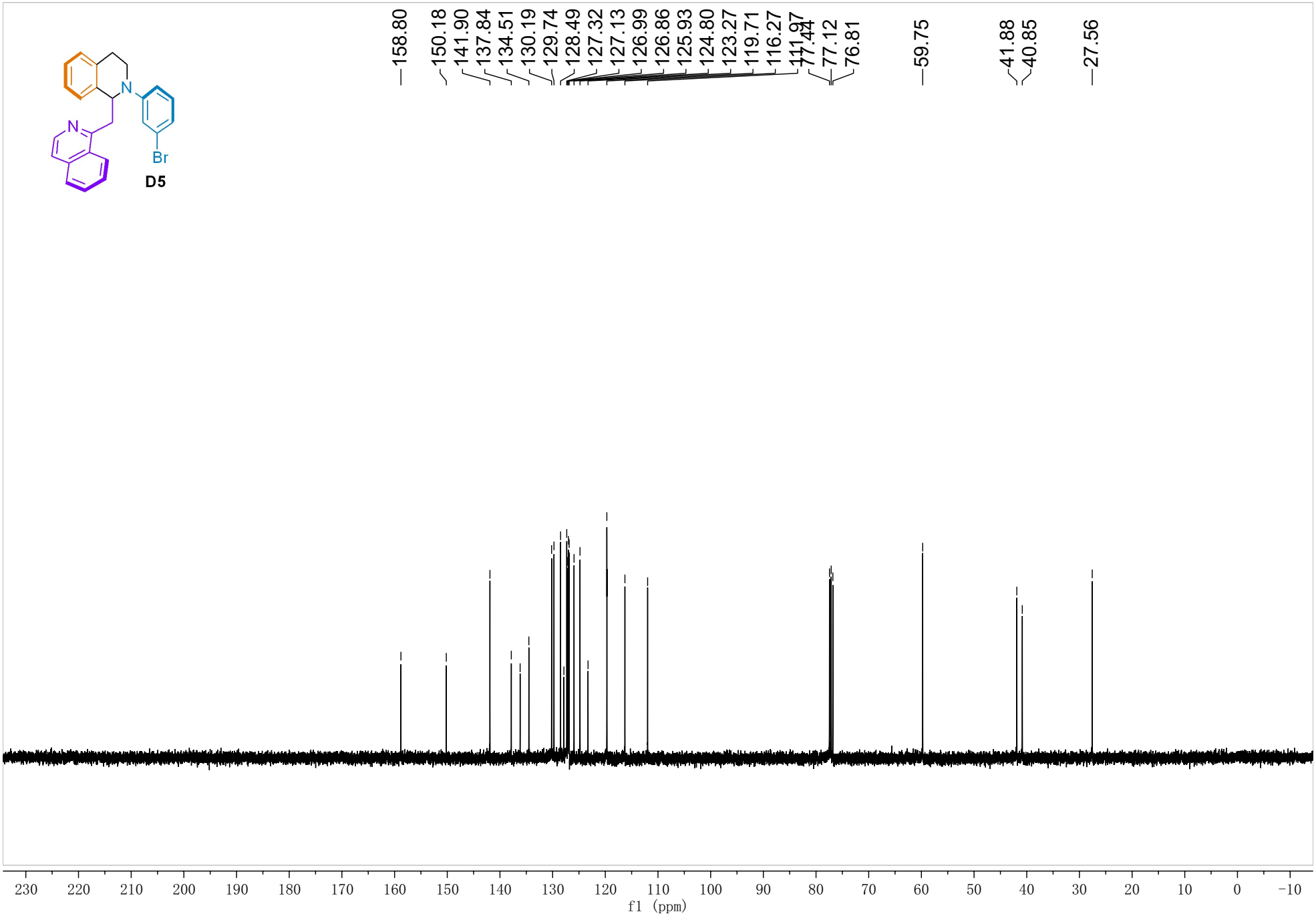
7.529
7.518
7.469
7.180
7.140
6.943
6.863
6.794
6.750
5.575
5.559
3.931
3.915
3.898
3.816
3.801
3.730
3.715
3.603
3.589
3.106
3.063
N
N
Br
D5
1.0
1.1
1.0
1.1
2.1
2.1
2.9
1.0
2.0
1.0
1.1
1.0
1.0
1.0
2.2
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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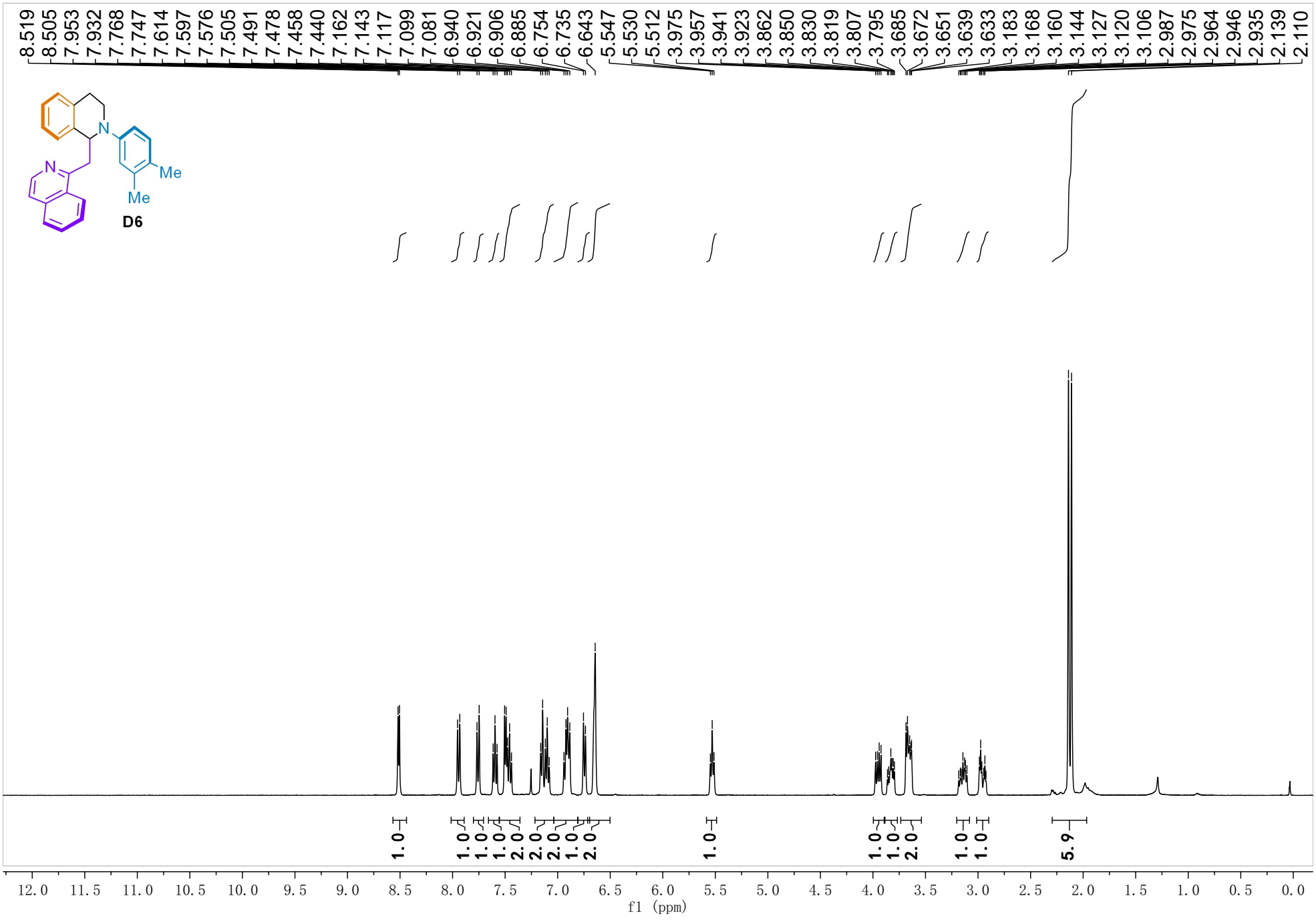
134.51
130.19
129.74
128.49
127.32
127.13
126.99
126.86
125.93
124.80
123.27
119.71
116.27
111.97
77.44
77.12
76.81
59.75
41.88
40.85
27.56
N
N
Br
D5
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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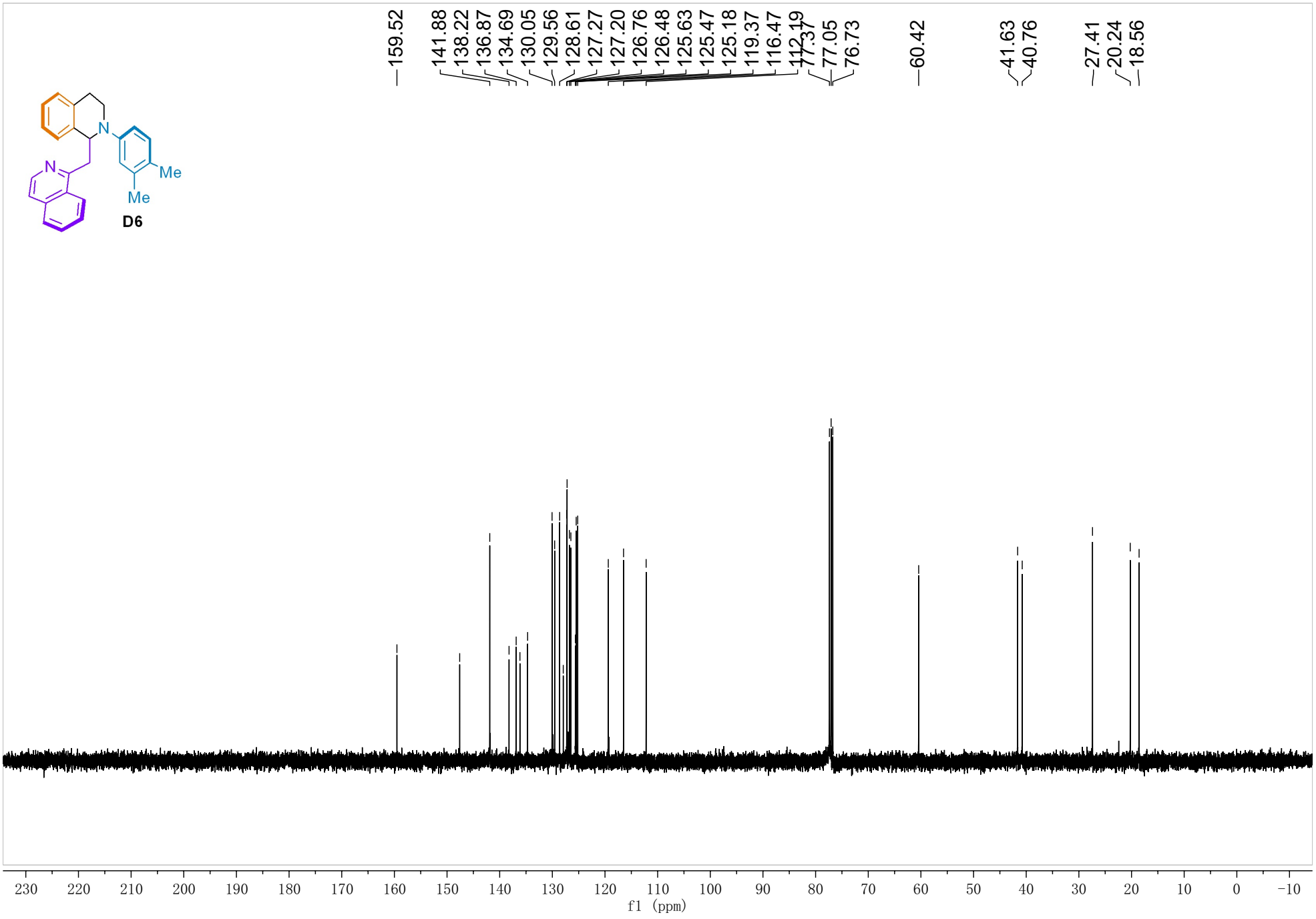
8.505
7.953
7.932
7.768
7.747
7.614
7.597
7.576
7.505
7.491
7.478
7.458
7.440
7.162
7.143
7.117
7.099
7.081
6.940
6.921
6.906
6.885
6.754
6.735
6.643
5.547
5.530
5.512
3.975
3.957
3.941
3.923
3.862
3.850
3.830
3.819
3.807
3.795
3.685
3.672
3.651
3.639
3.633
3.183
3.168
3.160
3.144
3.127
3.120
3.106
2.987
2.975
2.964
2.946
2.935
2.139
2.110
N
N
Me
Me
D6
1.0
1.0
1.0
1.0
2.0
2.0
2.0
1.0
2.0
1.0
1.0
2.0
1.0
1.0
5.9
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)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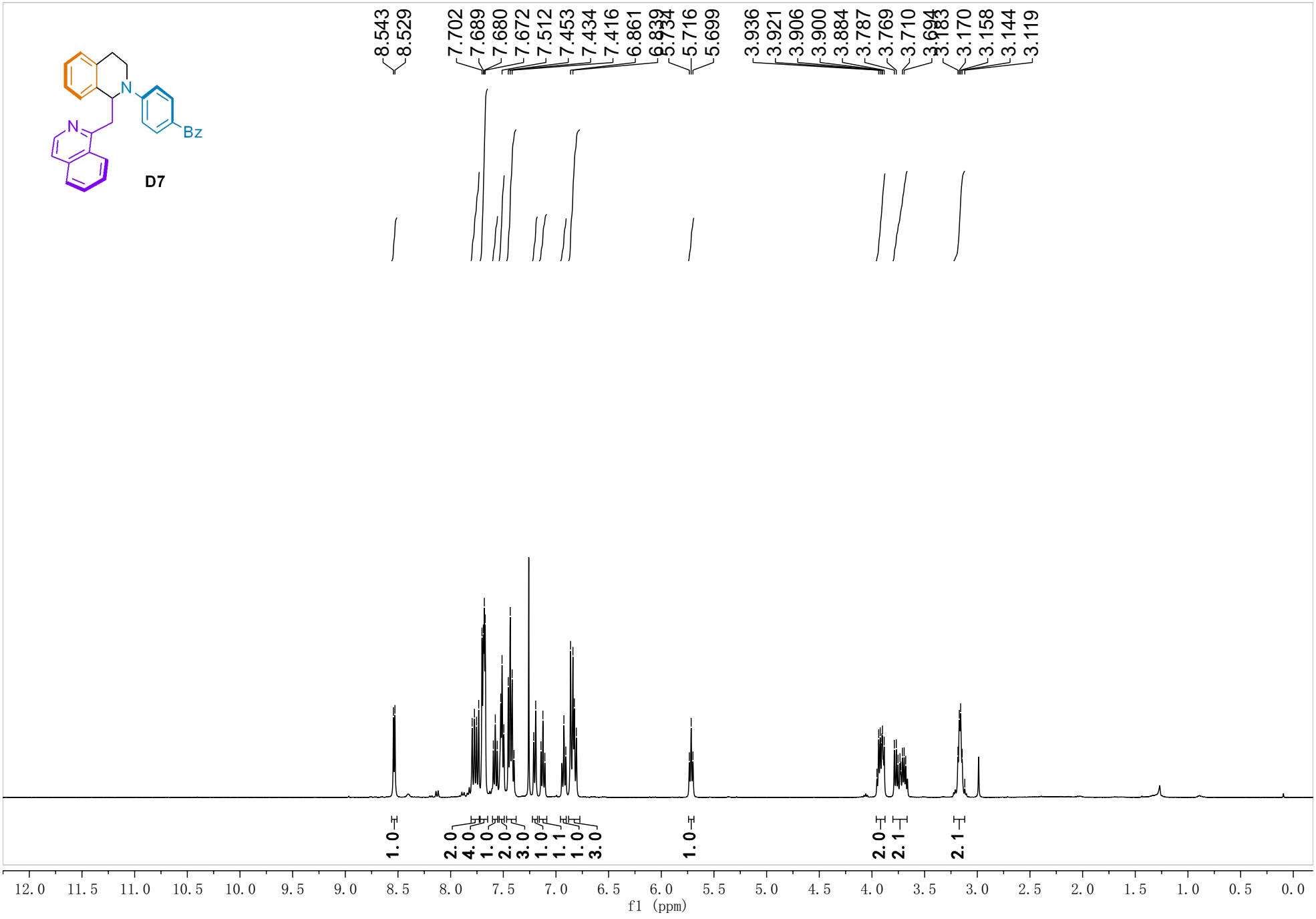
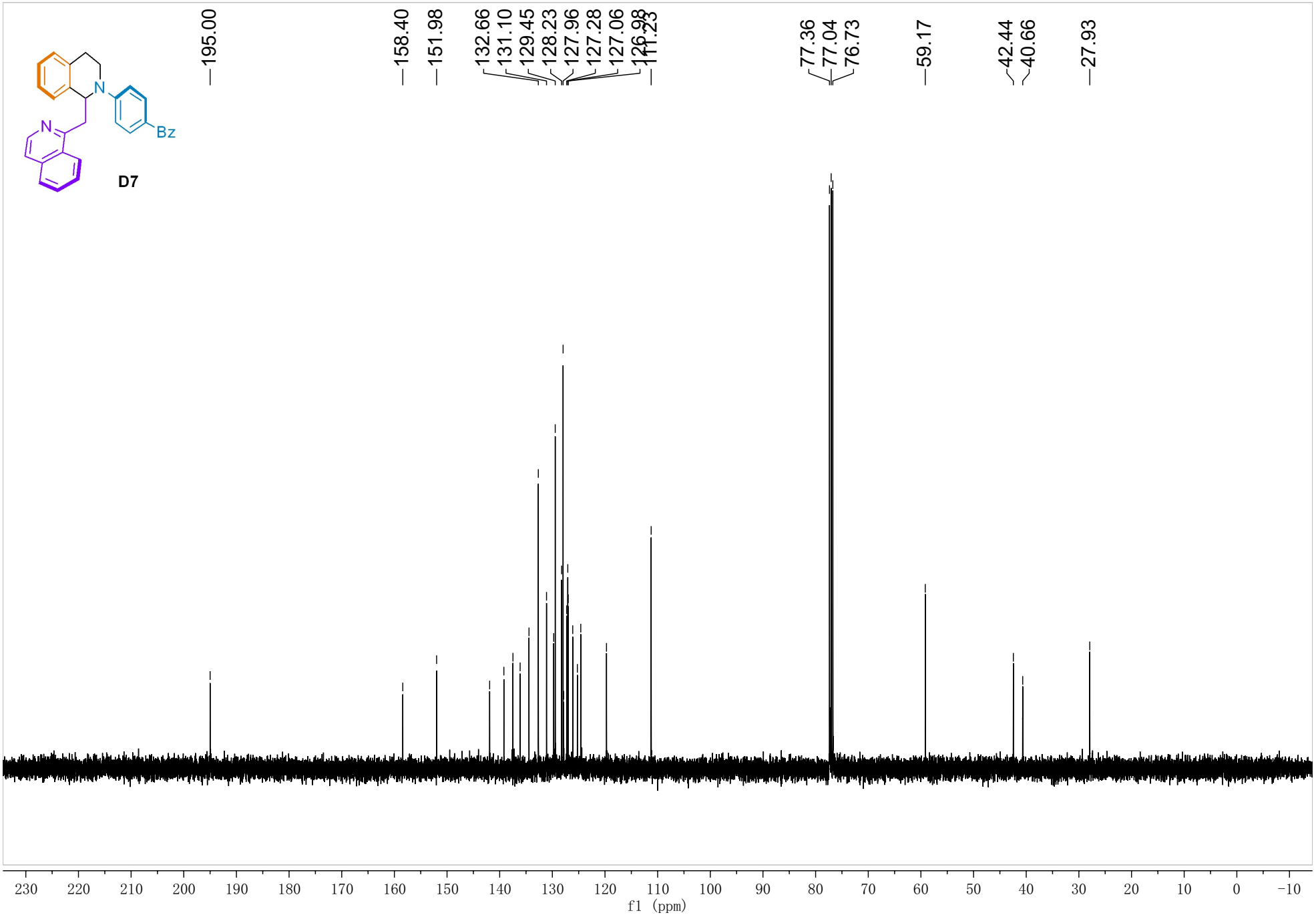
138.22
136.87
134.69
130.05
129.56
128.61
127.27
127.20
126.76
126.48
125.63
125.47
125.18
119.37
116.47
112.19
77.37
77.05
76.73
60.42
41.63
40.76
27.41
20.24
18.56
N
N
Me
Me
D6
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)


8.543
8.529
7.702
7.689
7.680
7.672
7.512
7.453
7.434
7.416
6.861
5.734
5.716
5.699
3.936
3.921
3.906
3.900
3.884
3.787
3.769
3.710
3.170
3.158
3.144
3.119
N
N
Bz
D7
1.0
2.0
4.0
1.0
2.0
3.0
1.0
1.1
1.0
3.0
1.0
2.0
2.1
2.1
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)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132.66
131.10
129.45
128.23
127.96
127.28
127.06
126.98
111.23
77.36
77.04
76.73
59.17
42.44
40.66
27.93
N
N
Bz
D7
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)