

Supporting Informations

Copper and electrocatalytic synergy for the construction of fused quinazolinones with 2-Aminobenzaldehydes and cyclic amines

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1. General information

All glassware was oven dried at 110 °C for several hours and cooled down under vacuum. Unless otherwise noted, materials were obtained from commercial suppliers and used without further purification. **The instrument for electrolysis** was dual display potentiostat (DJS-292B) (made in China). Anode electrode is carbon rod and cathodic electrode is aluminum rod.

Thin-layer chromatography was performed with EMD silica gel 60 F254 plates eluting with solvents indicated, visualized by a 254 nm UV lamp and stained with phosphomolybdic acid (PMA). Flash chromatography columns were packed with 200- 300 mesh silica gel in petroleum (bp. 60-90 °C). **¹H NMR, ¹³C NMR** and spectra were obtained on Bruker Advance III (400 MHz). Chemical shifts were denoted in ppm (δ), and calibrated by using residual undeuterated solvent CDCl₃ (7.26 ppm), tetramethylsilane (0.00 ppm) as internal reference for ¹H NMR and the deuterated solvent CDCl₃ (77.00 ppm) tetramethylsilane (0.00 ppm) as internal standard for ¹³C NMR, multiplicities are as indicated: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. **High-resolution mass spectral analysis (HRMS) data** was measured on a Waters Acquity UPLC I-Class plus Xevo G2-XS (Q-TOF) mass spectrum by means of the ESI technique.

2 Typical experimental procedure

A 15-mL oven-dried undivided three-necked bottle was equipped with a aluminum rod cathode and a carbon rod anode which were connected to a DC regulated power supply (Figure S1). 2-aminobenzaldehyde **1a** (0.2 mmol) or 2-aminoacetophenone **2a** (0.2 mmol), tetrahydroisoquinoline **3a** (0.3 mmol), NH₄I (0.5 mmol), Cu(CH₃COO)₂ (0.003 mmol) and ⁿBu₄NBF₄ (0.5 mmol) dissolved in 10 mL CH₃OH, 30 °C, under O₂ atmosphere were added to the cell and electrolyzed at a constant current of 5 mA. The electrolysis was terminated when the starting materials were consumed as determined by TLC. After electrolysis, the reaction mixture was diluted in 40 mL ethyl acetate, washed with a saturated solution of brine (3 × 15 mL), dried (Na₂SO₄) and concentrated in vacuum, and the resulting residue was purified by silica gel column chromatography (petroleum/ethyl acetate) to afford the products desired product **4a**.



Figure S1 Electrolysis setup



Figure S2 Gram-scale amplification Electrolysis setup

3 Antibacterial Activity Experiments

Table S1 Summary of antibacterial activity of test samples and fluconazole against *Candida albicans*^a

Compound	MIC ₅₀ (ug/mL)		FICI	
	Candida albicans fluconazole sensitive strain (SC5314)	Fluconazole resistant strains of Candida albicans (ATCC 14053)	Candida albicans fluconazole sensitive strain (SC5314)	Fluconazole resistant strains of Candida albicans (ATCC 14053)
FLC	1.53	>200	--	--
4a	>200	>200	--	--
4r	>200	>200	--	--
4t	>200	>200	--	--
4o	>200	>200	--	--
4v	>200	>200	--	--
4i	>200	>200	--	--
4b	>200	>200	--	--
4f	>200	>200	--	--
4j	>200	>200	--	--
4k	>200	>200	--	--
4c	>200	>200	--	--
4h	>200	>200	--	--
4l	>200	>200	--	--
4n	>200	>200	--	--
4e	>200	>200	--	--
4m	>200	>200	--	--
4d	>200	>200	--	--
4y	>200	>200	--	--
4g	>200	>200	--	--
4a+FLC	1.81	12.11	1.19	0.061
4r+FLC	1.31	2.54	0.86	0.013
4t+FLC	1.06	1.41	0.70	0.007
4o+FLC	2.16	11.02	1.42	0.055
4v+FLC	1.56	73.49	1.03	0.367
4i+FLC	1.99	28.28	1.30	0.049
4b+FLC	1.26	38.92	0.83	0.062
4f+FLC	1.40	4.14	0.92	0.021
4j+FLC	1.61	72.53	1.06	0.363
4k+FLC	1.37	21.23	0.90	0.106
4c+FLC	1.03	1.37	0.67	0.007
4h+FLC	1.61	14.48	1.05	0.072
4l+FLC	0.79	1.39	0.52	0.007
4n+FLC	1.40	>200	0.92	--
4e+FLC	1.75	1.81	1.15	0.009
4m+FLC	2.63	3.25	1.73	0.016

4d+FLC	1.56	14.47	1.02	0.072
4y+FLC	1.20	2.82	0.79	0.014
4g+FLC	1.33	12.15	0.87	0.061

^a Take a 96 well culture plate, dilute the sample and fluconazole to an initial concentration of 200 μ g/mL, with 100 μ L per well, and perform 5-fold dilution. There are 6 concentration gradients, with 3 replicate wells for each concentration gradient. After activating the strain twice, prepare a fungal suspension. Add 100 μ L of fungal suspension to each well of a 96 well plate to achieve a final concentration of 1×10^5 CFU/mL. Incubate in a 37 $^{\circ}$ C constant temperature incubator for 24 hours. Measure the OD value at 625nm using an enzyme-linked immunosorbent assay (ELISA) reader. Simultaneously set up blank control of culture medium, bacterial solution control, and fluconazole positive drug control in the experiment.

4 Cyclic voltammetry experiments

Cyclic voltammetry was performed in a three-electrode cell connected to a schlenk line under nitrogen at room temperature. The working electrode was a steady glassy carbon disk electrode ($\approx 5.0 \text{ mm}^2$), the counter electrode a platinum wire. The reference was an Ag/AgNO₃ electrode submerged in 0.1 M nBu₄NClO₄ and 0.01 M AgNO₃ in CH₃CN. 10 mL of CH₃OH were poured into the electrochemical cell in all experiments. The redox potential of ferrocene/ferrocenium (Fc/Fc⁺) was measured (same experimental conditions) and used to provide an internal reference. The potential values were then adjusted relative to Fc/Fc⁺. The scan rate is 0.1 V/s, ranging from -0.2 V to 1.0 V.

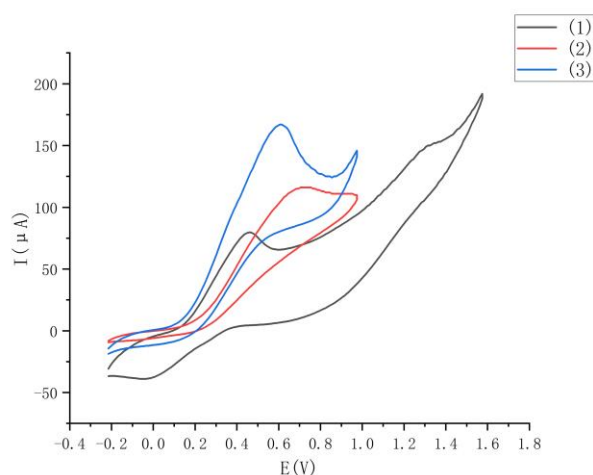
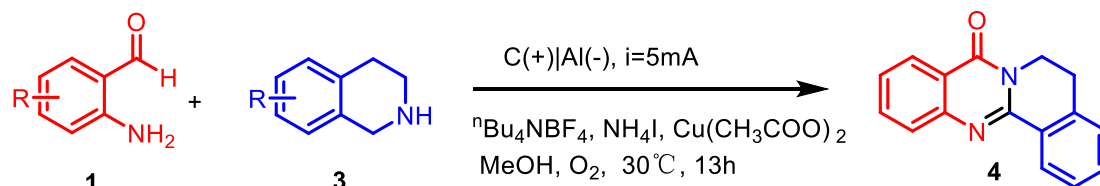


Figure S3 CV plotting convention (IUPAC)

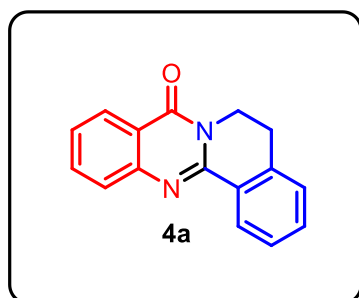
In the Figure S3, cyclic voltammograms of in 10 mL of CH₃OH solution containing different compounds: (1) nBu₄NBF₄ (0.05 mmol), NH₄I (0.05 mmol); (2) nBu₄NBF₄ (0.05 mmol), NH₄I (0.05 mmol), tetrahydroisoquinoline (0.03 mmol); (3)

$n\text{Bu}_4\text{NBF}_4$ (0.05 mmol), NH_4I (0.05 mmol), 2-aminobenzaldehyde (0.02 mmol); with a GC disk working electrode ($\approx 5.0 \text{ mm}^2$), Pt counter electrode, and Ag/AgNO₃ reference electrode (internal solution, 0.1 M $n\text{Bu}_4\text{NClO}_4$ and 0.01 M AgNO₃ in CH₃CN) at 0.1 V/s scan rate.

5 Analytical data



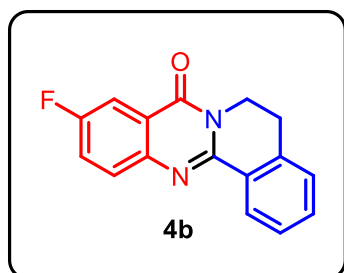
General procedure for the preparation of **4a**: A 10-mL oven-dried undivided three-necked bottle was equipped with a aluminum rod cathode and a carbon rod anode, constant current = 5 mA, **1a** (0.2mmol), **3a** (0.3 mmol), $n\text{Bu}_4\text{NBF}_4$ (0.5 mmol), NH_4I (0.5 mmol), $\text{Cu}(\text{CH}_3\text{COO})_2$ (0.003 mmol), CH₃OH (10 mL), 30°C, under O₂ atmosphere, undivided cell. Then stirred for 13 h. The resulting brown mixture was concentrated under a vacuum, the crude product was purified by flash column chromatography using petroleum ether/ethyl acetate (30:1) to give the title compounds **4a**.



5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one (4a): According to the general procedure, **4a** was obtained using 2-aminobenzaldehyde **1** (24.2 mg, 0.2 mmol) and tetrahydroisoquinoline **3** (40.0 mg, 0.3 mmol) in 94% yield (46.6 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 15:1).

¹H NMR (400 MHz, DMSO-*d*₆) δ 8.37 (d, $J = 6.4 \text{ Hz}$, 1H), 8.18 – 8.15 (m, 1H), 7.85 – 7.81 (m, 1H), 7.74 (d, $J = 6.8 \text{ Hz}$, 1H), 7.57 – 7.50 (m, 2H), 7.47 (t, $J = 3.6 \text{ Hz}$, 1H), 7.41 (d, $J = 7.6 \text{ Hz}$, 1H), 4.31 – 4.28 (t, 2H), 3.13 – 3.10 (t, 2H).

¹³C NMR (100 MHz, DMSO-*d*₆) δ 160.6, 149.3, 147.3, 137.7, 134.4, 131.8, 129.1, 127.8, 127.4, 127.3, 127.2, 126.5, 126.3, 120.4, 39.2, 26.4.



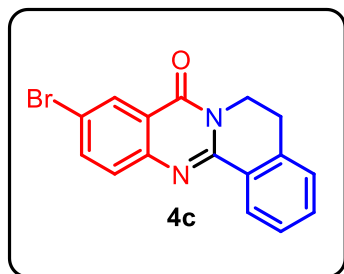
10-fluoro-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(4b): According to the general procedure, **4b** was obtained using 2-Amino-5-fluorobenzaldehyde (27.8 mg, 0.2 mmol) and

tetrahydroisoquinoline **3** (40.0 mg, 0.3 mmol) in 69% yield (36.7 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 30:1).

$^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6$) δ 8.33 (d, $J = 7.6$ Hz, 1H), 7.83 – 7.79 (m, 2H), 7.74 – 7.69 (m, 1H), 7.54 (t, $J = 7.6$ Hz, 1H), 7.45 (t, $J = 8.0$ Hz, 1H), 7.40 (d, $J = 7.6$ Hz, 1H), 4.30 – 4.27 (t, 2H), 3.13 – 3.09 (t, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 160.8, 160.5 (d, $J = 244.0$ Hz), 148.6, 144.3, 136.8, 131.6, 129.9, 129.1, 127.7, 127.4, 122.7 (d, $J = 24.0$ Hz), 121.7, 111.4 (d, $J = 23.0$ Hz), 39.6, 27.2.

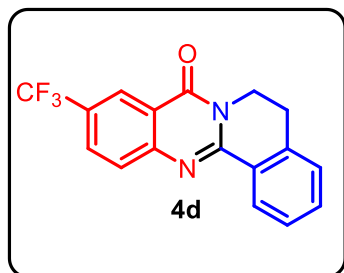
$^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -113.2.



10-bromo-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(4c): According to the general procedure, **4c** was obtained using 2-Amino-5-bromobenzaldehyde (40.0 mg, 0.2 mmol) and tetrahydroisoquinoline **3** (40.0 mg, 0.3 mmol) in 81% yield (52.8 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 25:1).

$^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6$) δ 8.35 (d, $J = 7.6$ Hz, 1H), 8.23 (d, $J = 2.4$ Hz, 1H), 7.98 – 7.96 (m, 1H), 7.69 (d, $J = 8.4$ Hz, 1H), 7.58 – 7.54 (m, 1H), 7.48 – 7.40 (m, 2H), 4.29 – 4.27 (t, 2H), 3.13 – 3.10 (t, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 160.7, 149.8, 146.7, 137.5, 137.1, 132.1, 129.5, 129.5, 129.3, 128.1, 127.8, 127.7, 122.1, 120.0, 39.9, 27.4.

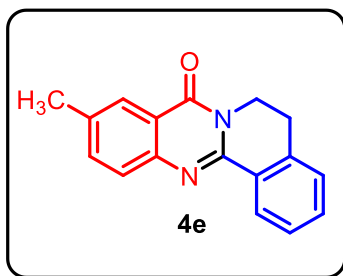


10-trifluoromethyl-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(4d): According to the general procedure, **4d** was obtained using 2-Amino-5-trifluoromethylbenzaldehyde (37.8 mg, 0.2 mmol) and tetrahydroisoquinoline **3** (40.0 mg, 0.3 mmol) in 70% yield (44.3 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 25:1).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.46 (d, $J = 6.4$ Hz, 1H), 7.70 – 7.64 (m, 1H), 7.56 (d, $J = 8.4$ Hz, 1H), 7.52 – 7.48 (m, 1H), 7.44 (t, $J = 7.6$ Hz, 1H), 7.30 (d, $J = 7.6$ Hz, 1H), 7.12 – 7.07 (m, 1H), 4.40 – 4.37 (t, 2H), 3.12 – 3.09 (t, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 161.5 (d, $J = 264.0$ Hz), 159.0 (d, $J = 4.0$ Hz), 150.4 (d, $J = 1.0$ Hz), 150.0, 137.4, 134.6 (d, $J = 10.0$ Hz), 132.2, 129.2, 128.3, 127.8, 127.7, 123.7 (d, $J = 4.0$ Hz), 113.1 (d, $J = 21.0$ Hz), 110.6 (d, $J = 7.0$ Hz), 39.4, 27.5.

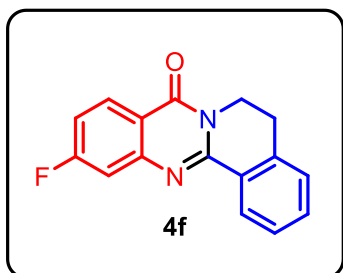
$^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -111.8.



10-methyl-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(4e): According to the general procedure, **4e** was obtained using 2-Amino-5-methylbenzaldehyde (27.0 mg, 0.2 mmol) and tetrahydroisoquinoline **3** (40.0 mg, 0.3 mmol) in 85% yield (44.6 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 30:1).

¹H NMR (400 MHz, CDCl₃) δ 8.55 – 8.52 (m, 1H), 8.16 (d, *J* = 8.0 Hz, 1H), 7.60 (d, *J* = 7.2 Hz, 1H), 7.49 – 7.41 (m, 2H), 7.34 (t, *J* = 7.6 Hz, 1H), 7.28 (d, *J* = 5.6 Hz, 1H), 4.43 – 4.40 (t, 2H), 3.12 – 3.08 (t, 2H), 2.71 (s, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 162.2, 148.1, 146.4, 137.1, 136.3, 134.9, 131.7, 130.1, 128.2, 127.7, 127.6, 126.3, 124.7, 120.8, 39.7, 27.6, 17.4.

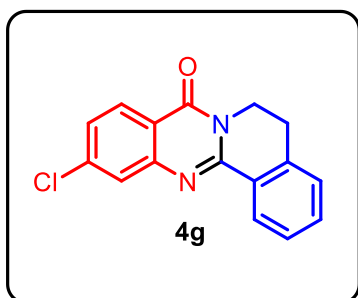


11-fluoro-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(4f): According to the general procedure, **4f** was obtained using 2-Amino-4-fluorobenzaldehyde (27.8 mg, 0.2 mmol) and tetrahydroisoquinoline **3** (40.0 mg, 0.3 mmol) in 71% yield (37.8 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 30:1).

¹H NMR (400 MHz, CDCl₃) δ 8.46 (d, *J* = 8.0 Hz, 1H), 8.32 – 8.29 (m, 1H), 7.51 – 7.43 (m, 2H), 7.41 – 7.38 (m, 1H), 7.29 (d, *J* = 7.6 Hz, 1H), 7.19 – 7.14 (m, 1H), 4.41 – 4.38 (t, 2H), 3.12 – 3.08 (t, 2H).

¹³C NMR (100 MHz, CDCl₃) δ 166.6 (d, *J* = 252.0 Hz), 161.2, 150.7, 150.1 (d, *J* = 13.0 Hz), 137.3, 132.2, 129.7 (d, *J* = 11.0 Hz), 129.4, 128.3, 127.8, 127.7, 117.6 (d, *J* = 2.0 Hz), 115.4 (d, *J* = 23.0 Hz), 112.8 (d, *J* = 22.0 Hz), 39.7, 27.5.

¹⁹F NMR (376 MHz, CDCl₃) δ -103.9.

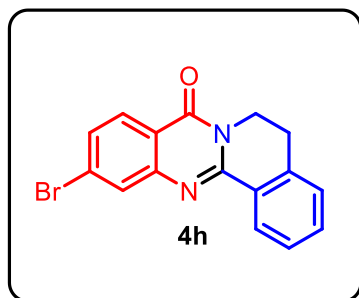


11-chloro-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(4g): According to the general

l procedure, **4g** was obtained using 2-Amino-4-chlorobenzaldehyde (31.1 mg, 0.2 mmol) and tetrahydroisoquinoline **3** (40.0 mg, 0.3 mmol) in 95% yield (53.6 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 30:1).

¹H NMR (400 MHz, CDCl₃) δ 8.46 – 8.43 (m, 1H), 8.22 (d, *J* = 8.4 Hz, 1H), 7.75 (d, *J* = 2.0 Hz, 1H), 7.51 – 7.43 (m, 2H), 7.40 – 7.38 (m, 1H), 7.29 (d, *J* = 7.6 Hz, 1H), 4.40 – 4.37 (t, 2H), 3.12 – 3.08 (t, 2H).

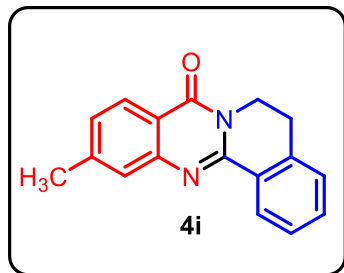
¹³C NMR (100 MHz, CDCl₃) δ 160.3, 150.7, 148.9, 140.5, 137.2, 132.2, 129.3, 128.5, 128.3, 127.8, 127.7, 127.2, 127.2, 119.3, 39.7, 27.5.



11-bromo-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(4h): According to the general procedure, **4h** was obtained using 2-Amino-4-bromobenzaldehyde (40.0 mg, 0.2 mmol) and tetrahydroisoquinoline **3** (40.0 mg, 0.3 mmol) in 90% yield (58.7 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 25:1).

¹H NMR (400 MHz, CDCl₃) δ 8.36 – 8.34 (m, 1H), 8.05 (d, *J* = 8.8 Hz, 1H), 7.84 (d, *J* = 2.0 Hz, 1H), 7.46 – 7.32 (m, 3H), 7.20 (d, *J* = 8.0 Hz, 1H), 4.31 – 4.28 (t, 2H), 3.03 – 3.00 (t, 2H).

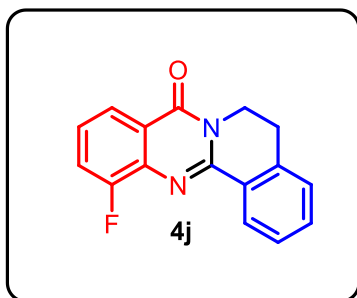
¹³C NMR (100 MHz, CDCl₃) δ 161.4, 150.6, 148.9, 137.2, 132.2, 130.3, 129.9, 129.3, 129.0, 128.4, 128.3, 127.8, 127.7, 119.6, 39.7, 27.4.



11-methyl-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(4i): According to the general procedure, **4i** was obtained using 2-Amino-4-methylbenzaldehyde (27.0 mg, 0.2 mmol) and tetrahydroisoquinoline **3** (40.0 mg, 0.3 mmol) in 87% yield (45.6 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 30:1).

¹H NMR (400 MHz, CDCl₃) δ 8.48 – 8.46 (m, 1H), 8.19 (d, *J* = 8.0 Hz, 1H), 7.57 (s, 1H), 7.49 – 7.40 (m, 2H), 7.28 (d, *J* = 6.8 Hz, 2H), 4.41 – 4.38 (t, 2H), 3.11 – 3.07 (t, 2H), 2.51 (s, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 161.8, 149.6, 148.0, 145.3, 137.2, 131.8, 129.8, 128.3, 128.1, 127.7, 127.6, 127.4, 126.8, 118.5, 39.6, 27.6, 22.0.

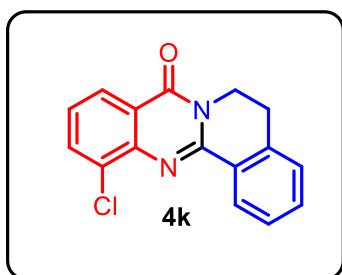


12-fluoro-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(4j): According to the general procedure, **4j** was obtained using 2-Amino-3-fluorobenzaldehyde (27.8 mg, 0.2 mmol) and tetrahydroisoquinoline **3** (40.0 mg, 0.3 mmol) in 67% yield (35.7 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 30:1).

¹H NMR (400 MHz, CDCl₃) δ 8.56 – 8.53 (m, 1H), 8.10 – 8.08 (m, 1H), 7.51 – 7.44 (m, 3H), 7.41 – 7.36 (m, 1H), 7.29 (d, *J* = 7.2 Hz, 1H), 4.44 – 4.41 (t, 2H), 3.13 – 3.10 (t, 2H).

¹³C NMR (100 MHz, CDCl₃) δ 161.0 (d, *J* = 3.0 Hz), 157.4 (d, *J* = 255.0 Hz), 150.0, 137.6 (d, *J* = 12.0 Hz), 137.1, 132.2, 129.5, 128.6, 127.9, 127.6, 126.5 (d, *J* = 8.0 Hz), 122.8 (d, *J* = 1.0 Hz), 122.5 (d, *J* = 4.0 Hz), 119.7 (d, *J* = 19.0 Hz), 39.9, 27.5 .

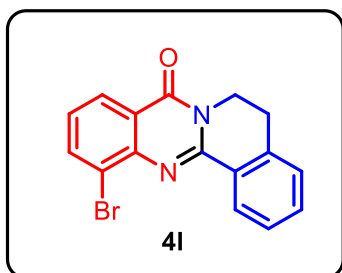
¹⁹F NMR (376 MHz, CDCl₃) δ -125.6.



12-chloro-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(4k): According to the general procedure, **4k** was obtained using 2-Amino-3-chlorobenzaldehyde (31.1 mg, 0.2 mmol) and tetrahydroisoquinoline **3** (40.0 mg, 0.3 mmol) in 81% yield (45.7 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 30:1).

¹H NMR (400 MHz, CDCl₃) δ 8.44 (d, *J* = 4.0 Hz, 1H), 8.25 (d, *J* = 2.4 Hz, 1H), 7.70 – 7.64 (m, 2H), 7.50 – 7.40 (m, 2H), 7.28 (d, *J* = 7.2 Hz, 1H), 4.41 – 4.38 (t, 2H), 3.11 – 3.08 (t, 2H).

¹³C NMR (100 MHz, CDCl₃) δ 160.9, 149.7, 146.5, 137.1, 134.8, 132.3, 132.1, 129.4, 128.2, 127.8, 127.7, 126.3, 121.8, 39.9, 27.5.

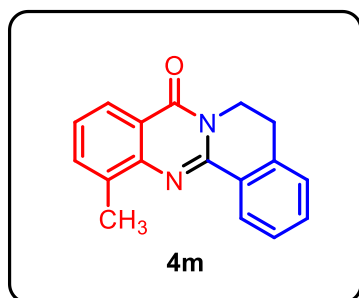


12-bromo-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(4l): According to the general procedure, **4l** was obtained using 2-Amino-3-bromobenzaldehyde (40.0 mg, 0.2 mmol) and

tetrahydroisoquinoline **3** (40.0 mg, 0.3 mmol) in 77% yield (50.2 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 25:1).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.34 – 8.32 (m, 1H), 8.30 (d, $J = 2.4$ Hz, 1H), 7.71 – 7.68 (m, 1H), 7.50 (d, $J = 8.8$ Hz, 1H), 7.40 – 7.36 (m, 1H), 7.34 – 7.30 (m, 1H), 7.17 (d, $J = 7.2$ Hz, 1H), 4.30 – 4.27 (t, 2H), 3.01 – 2.98 (t, 2H).

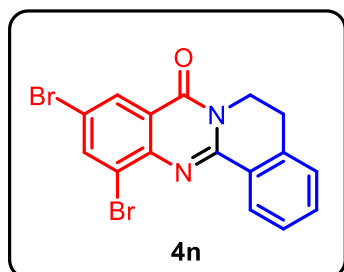
$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 160.6, 149.8, 146.7, 137.4, 137.1, 132.0, 129.5, 129.5, 129.3, 128.1, 127.8, 127.6, 122.1, 120.0, 39.8, 27.4.



12-methyl-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(4m): According to the general procedure, **4m** was obtained using 2-Amino-3-methylbenzaldehyde (27.0 mg, 0.2 mmol) and tetrahydroisoquinoline **3** (40.0 mg, 0.3 mmol) in 91% yield (47.7 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 30:1).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.41 – 8.39 (m, 1H), 8.03 (d, $J = 8.0$ Hz, 1H), 7.46 (d, $J = 6.8$ Hz, 1H), 7.35 – 7.28 (m, 2H), 7.21 (t, $J = 7.6$ Hz, 1H), 7.14 (t, $J = 5.6$ Hz, 1H), 4.29 – 4.26 (t, 2H), 2.98 – 2.95 (t, 2H), 2.59 (s, 3H).

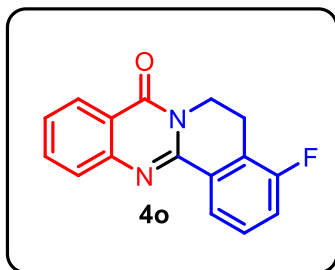
$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 162.1, 148.0, 146.3, 137.0, 136.1, 134.7, 131.6, 130.0, 128.1, 127.6, 127.5, 126.1, 124.6, 120.7, 39.6, 27.5, 17.4.



10,12-dibromo-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(4n): According to the general procedure, **4n** was obtained using 2-Amino-3,5-Dibromobenzaldehyde (55.8 mg, 0.2 mmol) and tetrahydroisoquinoline **3** (40.0 mg, 0.3 mmol) in 63% yield (50.9 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 20:1).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.60 – 8.57 (m, 1H), 8.39 (d, $J = 2.0$ Hz, 1H), 8.13 (d, $J = 2.0$ Hz, 1H), 7.54 – 7.49 (m, 1H), 7.49 – 7.44 (m, 1H), 7.29 (d, $J = 8.0$ Hz, 1H), 4.42 – 4.38 (t, 2H), 3.13 – 3.10 (t, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 160.3, 150.5, 144.7, 140.4, 137.1, 132.6, 129.6, 129.2, 128.8, 128.1, 127.7, 124.1, 123.0, 119.6, 40.1, 27.3.

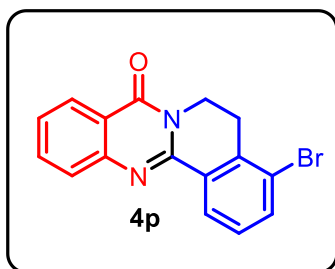


4-fluoro-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(4o): According to the general procedure, **4o** was obtained using 2-aminobenzaldehyde **1** (24.2 mg, 0.2 mmol) and 5-Fluoro-1,2,3,4-tetrahydroisoquinoline hydrochloride (56.3 mg, 0.3 mmol) in 53% yield (28.2 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 30:1).

¹H NMR (400 MHz, CDCl₃) δ 8.53 – 8.49 (m, 1H), 8.31 (d, *J* = 8.0 Hz, 1H), 8.76 – 8.74 (m, 2H), 7.48 – 7.44 (m, 1H), 7.15 – 7.10 (m, 1H), 7.01 – 6.98 (m, 1H), 4.44 – 4.41 (t, 2H), 3.12 – 3.08 (t, 2H).

¹³C NMR (100 MHz, CDCl₃) δ 164.9 (d, *J* = 252.0 Hz), 161.8, 148.8, 147.9, 139.8 (d, *J* = 9.0 Hz), 134.5, 130.9 (d, *J* = 10.0 Hz), 127.7, 127.1, 126.7, 126.0 (dd, *J* = 8.0, 5.0 Hz), 120.8, 115.3 (d, *J* = 21.0 Hz), 114.4 (d, *J* = 22.0 Hz), 39.6, 27.7.

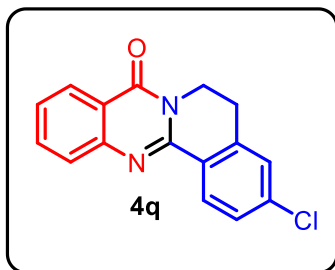
¹⁹F NMR (376 MHz, CDCl₃) δ -107.6.



4-bromo-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(4p): According to the general procedure, **4p** was obtained using 2-aminobenzaldehyde **1** (24.2 mg, 0.2 mmol) and 5-bromo-1,2,3,4-tetrahydroisoquinoline hydrochloride (74.6 mg, 0.3 mmol) in 51% yield (33.3 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 30:1).

¹H NMR (400 MHz, CDCl₃) δ 8.51 (d, *J* = 8.0 Hz, 1H), 8.32 (d, *J* = 8.0 Hz, 1H), 7.80 – 7.72 (m, 3H), 7.51 – 7.47 (m, 1H), 7.32 (t, *J* = 8.0 Hz, 1H), 4.44 – 4.40 (t, 2H), 3.24 – 3.21 (t, 2H).

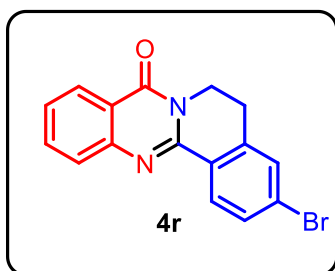
¹³C NMR (100 MHz, CDCl₃) δ 161.7, 147.8, 136.9, 136.6, 134.5, 131.9, 128.2, 127.9, 127.5, 127.1, 127.1, 123.5, 120.9, 39.2, 27.6.



3-chloro-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(4q): According to the general procedure, **4q** was obtained using 2-aminobenzaldehyde **1** (24.2 mg, 0.2 mmol) and 6-Chloro-1,2,3,4-tetrahydroisoquinoline hydrochloride (61.2 mg, 0.3 mmol) in 50% yield (28.2 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 25:1).

¹H NMR (400 MHz, DMSO-*d*₆) δ 8.35 (d, *J* = 8.4 Hz, 1H), 8.18 – 8.15 (m, 1H), 7.86 – 7.82 (m, 1H), 7.74 (d, *J* = 8.4 Hz, 1H), 7.55 – 7.51(m, 3H), 4.31 – 4.28 (t, 2H), 3.14 – 3.11 (t, 2H).

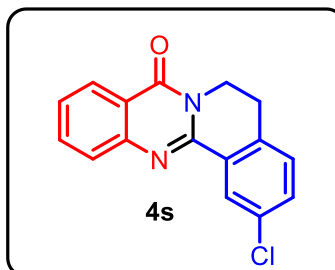
¹³C NMR (100 MHz, CDCl₃) δ 161.7, 148.7, 147.7, 138.7, 138.0, 134.5, 129.7, 128.2, 128.1, 127.7, 127.7, 127.1, 126.9, 120.8, 39.5, 27.4.



3-bromo-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(4r): According to the general procedure, **4r** was obtained using 2-aminobenzaldehyde **1** (24.2 mg, 0.2 mmol) and 6-bromo-1,2,3,4-tetrahydroisoquinoline hydrochloride (74.6 mg, 0.3 mmol) in 51% yield (33.3 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 30:1).

¹H NMR (400 MHz, CDCl₃) δ 8.36 (d, *J* = 8.4 Hz, 1H), 8.30 (d, *J* = 8.0 Hz, 1H), 7.76 – 7.75 (m, 2H), 7.58 – 7.55 (m, 1H), 7.49 – 7.45 (m, 2H), 4.42 – 4.39 (t, 2H), 3.10 – 3.07 (t, 2H).

¹³C NMR (100 MHz, CDCl₃) δ 161.7, 148.8, 147.8, 138.9, 134.5, 131.1, 130.7, 129.9, 128.7, 127.8, 127.1, 126.9, 126.6, 120.9, 39.6, 27.4.

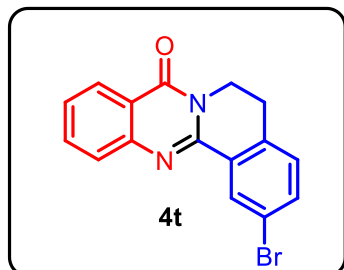


2-chloro-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(4s): According to the general procedure, **4s** was obtained using 2-aminobenzaldehyde **1** (24.2 mg, 0.2 mmol) and 7-Chloro-1,2,3,4-tetrahydroisoquinoline hydrochloride (61.2 mg, 0.3 mmol) in 52% yield (29.3 mg)

and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 25:1).

$^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6$) δ 8.31 (d, $J = 2.4$ Hz, 1H), 8.18 – 8.15 (m, 1H), 7.87 – 7.83 (m, 1H), 7.78 (d, $J = 8.0$ Hz, 1H), 7.62 – 7.59 (m, 1H), 7.56 – 7.52 (m, 1H), 7.46 (d, $J = 8.0$ Hz, 1H), 4.30 – 4.27 (t, 2H), 3.13 – 3.10 (t, 2H).

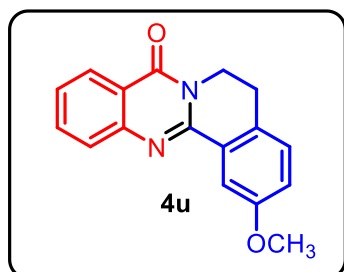
$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 161.7, 148.3, 147.6, 135.4, 134.5, 133.8, 131.8, 131.2, 129.1, 128.0, 127.8, 127.1, 127.0, 121.0, 39.6, 27.1.



2-bromo-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(4t): According to the general procedure, **4t** was obtained using 2-aminobenzaldehyde **1** (24.2 mg, 0.2 mmol) and 7-bromo-o-1,2,3,4-tetrahydroisoquinoline hydrochloride (74.6 mg, 0.3 mmol) in 86% yield (56.1 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 30:1).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.63 (d, $J = 2.0$ Hz, 1H), 8.31 (d, $J = 8.0$ Hz, 1H), 7.78 – 7.77 (d, 2H), 7.60 – 7.57 (m, 1H), 7.50 – 7.46 (m, 1H), 7.18 (d, $J = 8.0$ Hz, 1H), 4.42 – 4.39 (t, 2H), 3.08 – 3.05 (t, 2H).

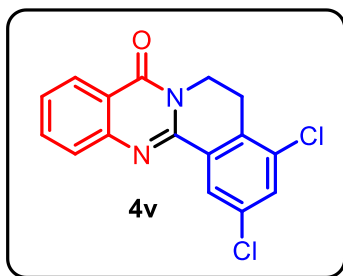
$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 161.7, 148.1, 147.7, 135.9, 134.7, 134.6, 131.5, 130.9, 129.3, 127.9, 127.1, 127.1, 121.6, 121.0, 39.6, 27.2.



2-methoxy-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(4u): According to the general procedure, **4u** was obtained using 2-aminobenzaldehyde **1** (24.2 mg, 0.2 mmol) and 7-methoxy-1,2,3,4-tetrahydroisoquinoline hydrochloride (48.9 mg, 0.3 mmol) in 57% yield (31.7 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 15:1).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.32 (d, $J = 7.6$ Hz, 1H), 8.01 (d, $J = 2.8$ Hz, 1H), 7.80 – 7.74 (m, 2H), 7.47 (t, $J = 1.6$ Hz, 1H), 7.20 (d, $J = 8.4$ Hz, 1H), 7.06 – 7.04 (m, 1H), 4.42 – 4.38 (t, 2H), 3.94 (s, 3H), 3.06 – 3.02 (t, 2H).

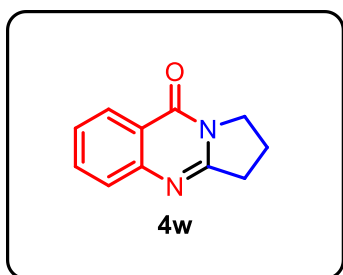
$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 161.9, 159.2, 149.5, 147.8, 134.4, 130.6, 129.6, 128.8, 127.7, 127.0, 126.7, 120.9, 119.4, 111.4, 55.8, 30.0, 26.8.



2,4-dichloro-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(4v): According to the general procedure, **4v** was obtained using 2-aminobenzaldehyde **1** (24.2 mg, 0.2 mmol) and 5,7-Chloro-1,2,3,4-tetrahydroisoquinoline hydrochloride (60.3 mg, 0.3 mmol) in 43% yield (31.0 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 20:1).

¹H NMR (400 MHz, CDCl₃) δ 8.46 (d, *J* = 2.0 Hz, 1H), 8.33 – 8.31 (m, 1H), 7.79 – 7.78 (m, 2H), 7.78 (d, *J* = 8.0 Hz, 1H), 7.53 – 7.49 (m, 1H), 4.41 – 4.40 (t, 2H), 3.20 – 3.17 (t, 2H).

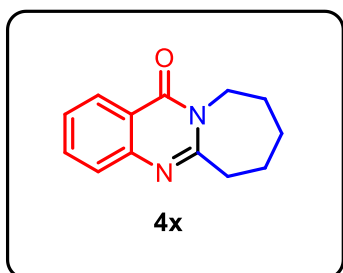
¹³C NMR (100 MHz, CDCl₃) δ 160.4, 146.3, 133.5, 132.8, 132.7, 132.4, 131.5, 130.7, 126.8, 126.3, 125.9, 125.6, 119.8, 37.8, 23.2.



2,3-dihydropyrrolo[2,1-b]quinazolin-9(1H)-one(4w): According to the general procedure, **4w** was obtained using 2-aminobenzaldehyde **1** (24.2 mg, 0.2 mmol) and Pyrrolidine (21.3 mg, 0.3 mmol) in 26% yield (9.7 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 10:1).

¹H NMR (400 MHz, CDCl₃) δ 7.67 – 7.65 (m, 1H), 7.54 – 7.47 (m, 2H), 7.32 – 7.28 (m, 1H), 1.33 – 1.25 (t, 6H).

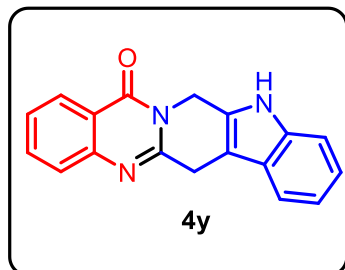
¹³C NMR (100 MHz, CDCl₃) δ 144.6, 134.9, 134.3, 129.2, 124.5, 120.5, 31.6, 30.3, 29.9.



7,8,9,10-tetrahydroazepino[2,1-b]quinazolin-12(6H)-one(4x): According to the general procedure, **4x** was obtained using 2-aminobenzaldehyde **1** (24.2 mg, 0.2 mmol) and Hexamethyleneimine (29.8 mg, 0.3 mmol) in 35% yield (15.0 mg) and as a yellow oil (silica gel flash chromatography: petroleum ether/ethyl acetate = 10:1).

¹H NMR (400 MHz, CDCl₃) δ 8.27 – 8.24 (m, 1H), 7.73 – 7.69 (m, 1H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.46 – 7.42 (m, 1H), 4.41– 4.38 (t, 2H), 3.09 – 3.06 (t, 2H), 1.89 – 1.81 (m, 6H),.

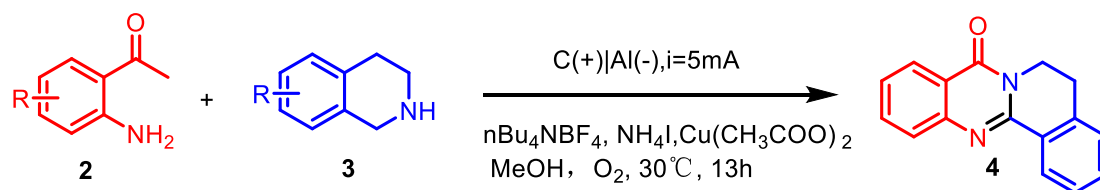
¹³C NMR (100 MHz, CDCl₃) δ 162.1, 160.0, 134.4, 127.2, 126.8, 126.6, 120.3, 43.1, 37.8, 29.7, 28.2, 25.6.



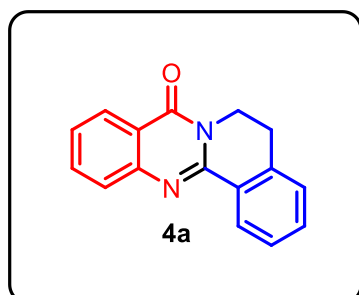
6,14-dihydroindolo [3',2':4,5] pyrido[2,1-b] quinazolin-8(5H)-one(4y): According to the general procedure, **4y** was obtained using 2-aminobenzaldehyde **1** (24.2 mg, 0.2 mmol) and 1,2,3,4-Tetrahydro-9H-Pyrido [3,4-B] Indole (51.7 mg, 0.3 mmol) in 22% yield (12.6 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 10:1).

¹H NMR (400 MHz, CDCl₃) δ 9.59 (s, 1H), 8.34 – 8.31 (m, 1H), 7.72 – 7.68 (m, 1H), 7.65 – 7.62 (t, 2H), 7.44 – 7.40 (m, 1H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.31 (t, *J* = 8.0 Hz, 1H), 7.17 (t, *J* = 7.6 Hz, 1H), 4.61– 4.57 (t, 2H), 3.25 – 3.22 (t, 2H).

¹³C NMR (100 MHz, CDCl₃) δ 161.7, 147.5, 145.3, 138.5, 134.5, 127.4, 127.2, 126.6, 126.4, 125.7, 125.7, 121.3, 120.7, 120.2, 118.6, 112.3, 41.3, 19.8.



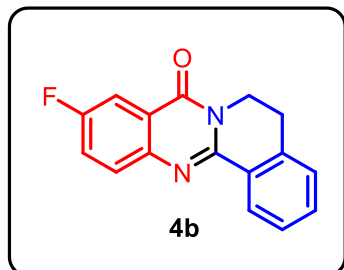
General procedure for the preparation of **4a**: A 10-mL oven-dried undivided three-necked bottle was equipped with a aluminum rod cathode and a carbon rod anode, constant current = 5 mA, **2a** (0.2mmol), **3a** (0.3 mmol), ⁿBu₄NBF₄ (0.5 mmol), NH₄I (0.5 mmol), Cu(CH₃COO)₂ (0.003 mmol), CH₃OH (10 mL), 30°C, under O₂ atmosphere, undivided cell. Then stirred for 15 h. The resulting brown mixture was concentrated under a vacuum, the crude product was purified by flash column chromatography using petroleum ether/ethyl acetate (30:1) to give the title compounds **4a**.



5,6-dihydro-8H-isoquinolino[1,2-b] quinazolin-8-one (4a): According to the general procedure, **4a** was obtained using 2-Aminoacetophenone **2** (27.0 mg, 0.2 mmol) and tetrahydroisquinoline **3** (40.0 mg, 0.3 mmol) in 60% yield (29.8 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 30:1).

¹H NMR (400 MHz, CDCl₃) δ 8.38 (d, *J* = 7.6 Hz, 1H), 8.21 (d, *J* = 7.6 Hz, 1H), 7.67 – 7.64 (m, 2H), 7.38 – 7.33 (m, 3H), 7.19 – 7.17 (m, 1H), 4.33 – 4.29 (t, 2H), 3.01 – 2.98 (t, 2H).

¹³C NMR (100 MHz, CDCl₃) δ 160.6, 149.3, 146.7, 136.0, 133.2, 130.7, 128.5, 126.9, 126.6, 126.5, 126.5, 125.8, 125.5, 119.7, 39.2, 26.4.

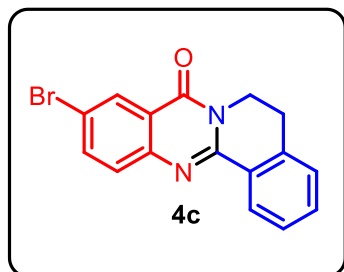


10-fluoro-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(4b): According to the general procedure, **4b** was obtained using 1-(2-Amino-5-fluorophenyl)ethanone (30.6 mg, 0.2 mmol) and tetrahydroisoquinoline **3** (40.0 mg, 0.3 mmol) in 49% yield (26.1 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 30:1).

¹H NMR (400 MHz, CDCl₃) δ 8.35 (d, *J* = 7.6 Hz, 1H), 7.83 (d, *J* = 8.4 Hz, 1H), 7.66 (s, 1H), 7.39 – 7.34 (m, 3H), 7.19 (d, *J* = 6.8 Hz, 1H), 4.33 – 4.29 (t, 2H), 3.03 – 2.99 (t, 2H).

¹³C NMR (100 MHz, CDCl₃) δ 161.1 (d, *J* = 4.0 Hz), 160.8 (d, *J* = 247.0 Hz), 148.9, 144.6, 137.0, 131.9, 130.1 (d, *J* = 8.0 Hz), 129.4, 128.0, 127.8, 127.6, 123.0 (d, *J* = 24.0 Hz), 122.0 (d, *J* = 8.0 Hz), 111.7 (d, *J* = 23.0 Hz), 39.9, 27.5.

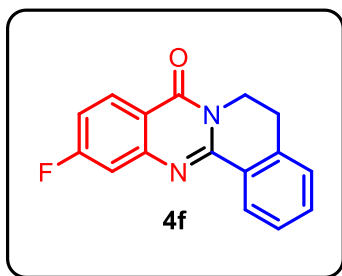
¹⁹F NMR (376 MHz, CDCl₃) δ -113.0.



10-bromo-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(4c): According to the general procedure, **4c** was obtained using 1-(2-Amino-5-bromophenyl)ethanone (42.8 mg, 0.2 mmol) and tetrahydroisoquinoline **3** (40.0 mg, 0.3 mmol) in 70.6% yield (46.0 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 25:1).

¹H NMR (400 MHz, CDCl₃) δ 8.47 – 8.44 (m, 2H), 7.84 – 7.81 (m, 1H), 7.64 (d, *J* = 8.8 Hz, 1H), 7.50 (d, *J* = 7.2 Hz, 1H), 7.44 (d, *J* = 7.6 Hz, 1H), 7.30 (d, *J* = 7.2 Hz, 1H), 4.43 – 4.39 (t, 2H), 3.13 – 3.09 (t, 2H).

¹³C NMR (100 MHz, CDCl₃) δ 160.8, 149.9, 146.8, 137.6, 137.2, 132.2, 129.6, 129.4, 128.2, 127.9, 127.7, 122.2, 120.1, 39.9, 27.5.

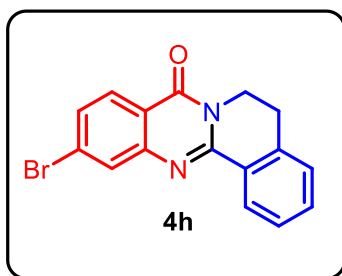


11-fluoro-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(4f): According to the general procedure, **4f** was obtained using 1-(2-Amino-4-fluorophenyl)ethanone (30.6 mg, 0.2 mmol) and tetrahydroisoquinoline **3** (40.0 mg, 0.3 mmol) in 40% yield (21.3 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 30:1).

¹H NMR (400 MHz, CDCl₃) δ 8.47– 8.44 (m, 1H), 8.32– 8.29 (m, 1H), 7.51 – 7.43 (m, 2H), 7.41 – 7.38 (m, 1H), 7.29 (d, *J* = 7.6 Hz, 1H), 7.19 – 7.14 (m, 1H), 4.41 – 4.38 (t, 2H), 3.12 – 3.08 (t, 2H).

¹³C NMR (100 MHz, CDCl₃) δ 166.6 (d, *J* = 252.0 Hz), 161.2, 150.7, 150.1 (d, *J* = 14.0 Hz), 137.3, 132.2, 129.7 (d, *J* = 11.0 Hz), 129.4, 128.3, 127.8, 127.7, 117.6 (d, *J* = 2.0 Hz), 115.4 (d, *J* = 23.0 Hz), 112.8 (d, *J* = 21.0 Hz), 39.7, 27.5.

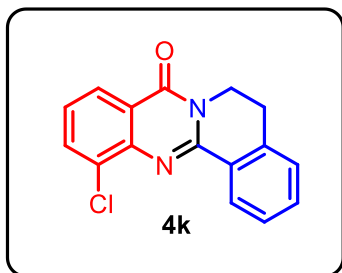
¹⁹F NMR (376 MHz, CDCl₃) δ -103.9.



11-bromo-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(4h): According to the general procedure, **4h** was obtained using 1-(2-Amino-4-bromophenyl)ethanone (42.8 mg, 0.2 mmol) and tetrahydroisoquinoline **3** (40.0 mg, 0.3 mmol) in 78% yield (50.9 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 25:1).

¹H NMR (400 MHz, CDCl₃) δ 8.46 – 8.44 (m, 1H), 8.15 (d, *J* = 8.8 Hz, 1H), 7.95 (d, *J* = 2.0 Hz, 1H), 7.56 – 7.54 (m, 1H), 7.52 – 7.48 (m, 1H), 7.46 – 7.42 (m, 1H), 7.29 (d, *J* = 7.2 Hz, 1H), 4.41 – 4.38 (t, 2H), 3.12 – 3.09 (t, 2H).

¹³C NMR (100 MHz, CDCl₃) δ 161.4, 150.6, 149.0, 137.3, 132.2, 130.4, 130.0, 129.4, 129.0, 128.5, 128.3, 127.9, 127.7, 119.7, 39.8, 27.5.

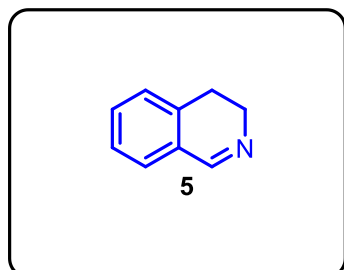


12-chloro-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(4k): According to the general procedure, **4k** was obtained using 1-(2-Amino-3-chlorophenyl)ethanone (33.9 mg, 0.2 mmol) and tetrahydroisoquinoline **3** (40.0 mg, 0.3 mmol) in 59% yield (33.9 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 30:1).

ellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 30:1).

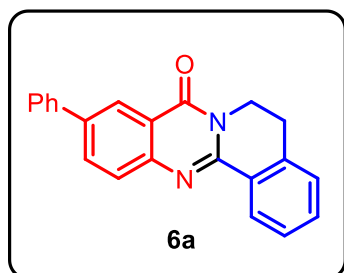
¹H NMR (400 MHz, CDCl₃) δ 8.45 (d, *J* = 7.6 Hz, 1H), 8.26 (d, *J* = 2.4 Hz, 1H), 7.71 – 7.65 (m, 2H), 7.51 – 7.41 (m, 2H), 7.29 (d, *J* = 11.2 Hz, 1H), 4.42 – 4.39 (t, 2H), 3.12 – 3.09 (t, 2H).

¹³C NMR (100 MHz, CDCl₃) δ 161.4, 150.1, 144.6, 137.1, 134.6, 132.3, 132.2, 129.5, 128.7, 128.0, 127.6, 126.6, 125.9, 122.4, 39.9, 27.4.



3,4-dihydroisoquinoline(5): 48% yield (12.6 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 30:1).

¹H NMR (400 MHz, CDCl₃) δ 8.25 (s, 1H), 7.30 – 7.26 (m, 1H), 7.24 – 7.18 (m, 2H), 7.08 (d, *J* = 7.6 Hz, 1H), 4.71 – 4.67 (m, 2H), 2.69 – 2.65 (t, 2H).



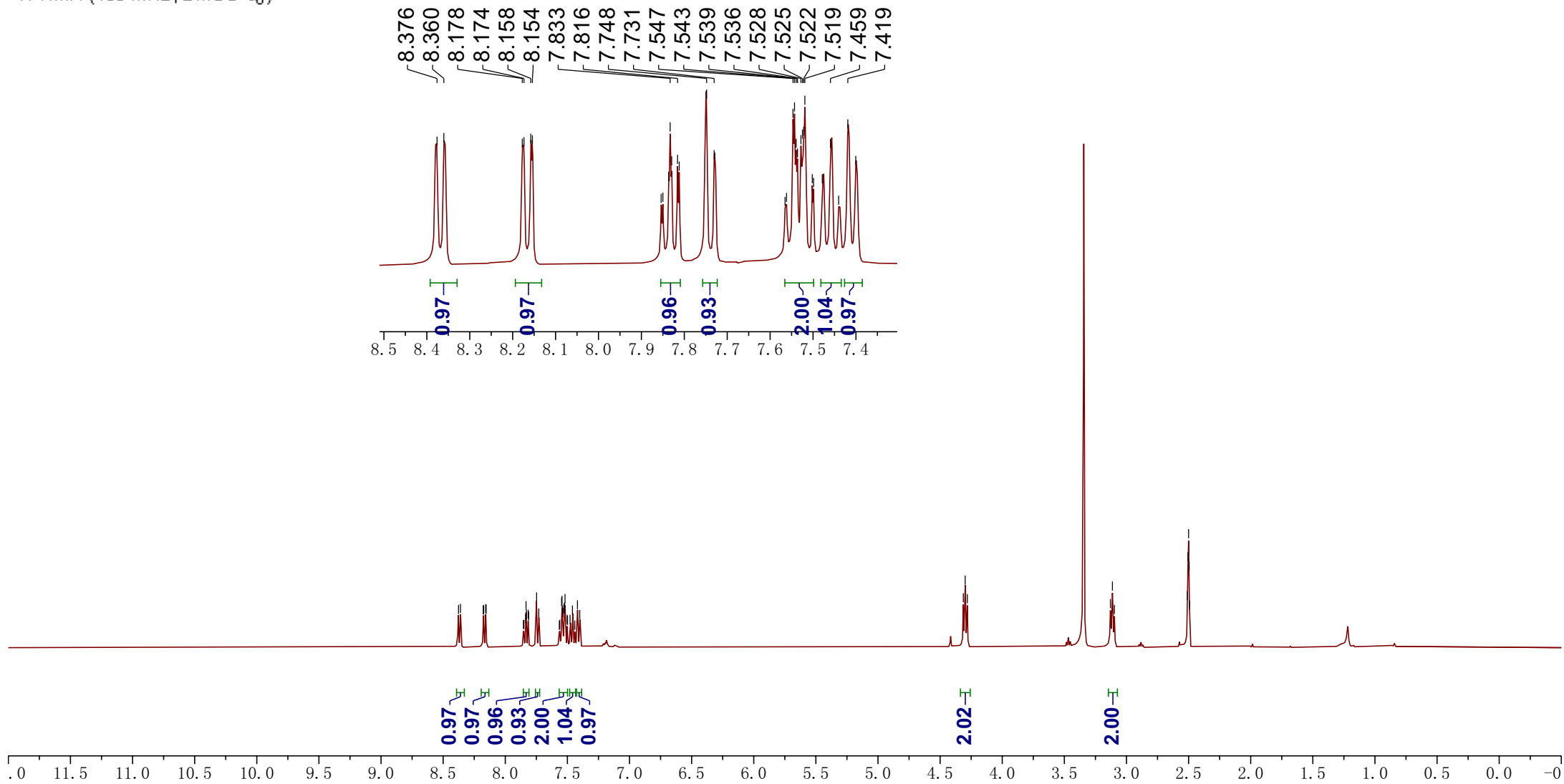
10-phenyl-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(6a): 80% yield (13.0 mg) and as a yellow solid (silica gel flash chromatography: petroleum ether/ethyl acetate = 30:1).

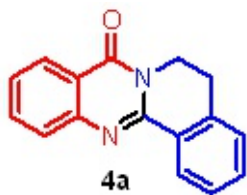
¹H NMR (400 MHz, CDCl₃) δ 8.57 (s, 1H), 8.51 (d, *J* = 7.6 Hz, 1H), 8.02 (d, *J* = 8.8 Hz, 1H), 7.85 (d, *J* = 7.2 Hz, 1H), 7.74 – 7.72 (d, 2H), 7.51 – 7.45 (m, 4H), 7.44 – 7.37 (m, 1H), 7.31 (d, *J* = 7.2 Hz, 1H), 4.47 – 4.44 (t, 2H), 3.15 – 3.11 (t, 2H).

¹³C NMR (100 MHz, CDCl₃) δ 162.0, 149.5, 147.2, 139.9, 139.5, 137.2, 133.3, 131.9, 129.8, 129.1, 128.3, 128.2, 127.9, 127.8, 127.7, 127.3, 124.9, 121.1, 39.9, 27.6.



^1H NMR (400 MHz, $\text{DMSO-}d_6$)

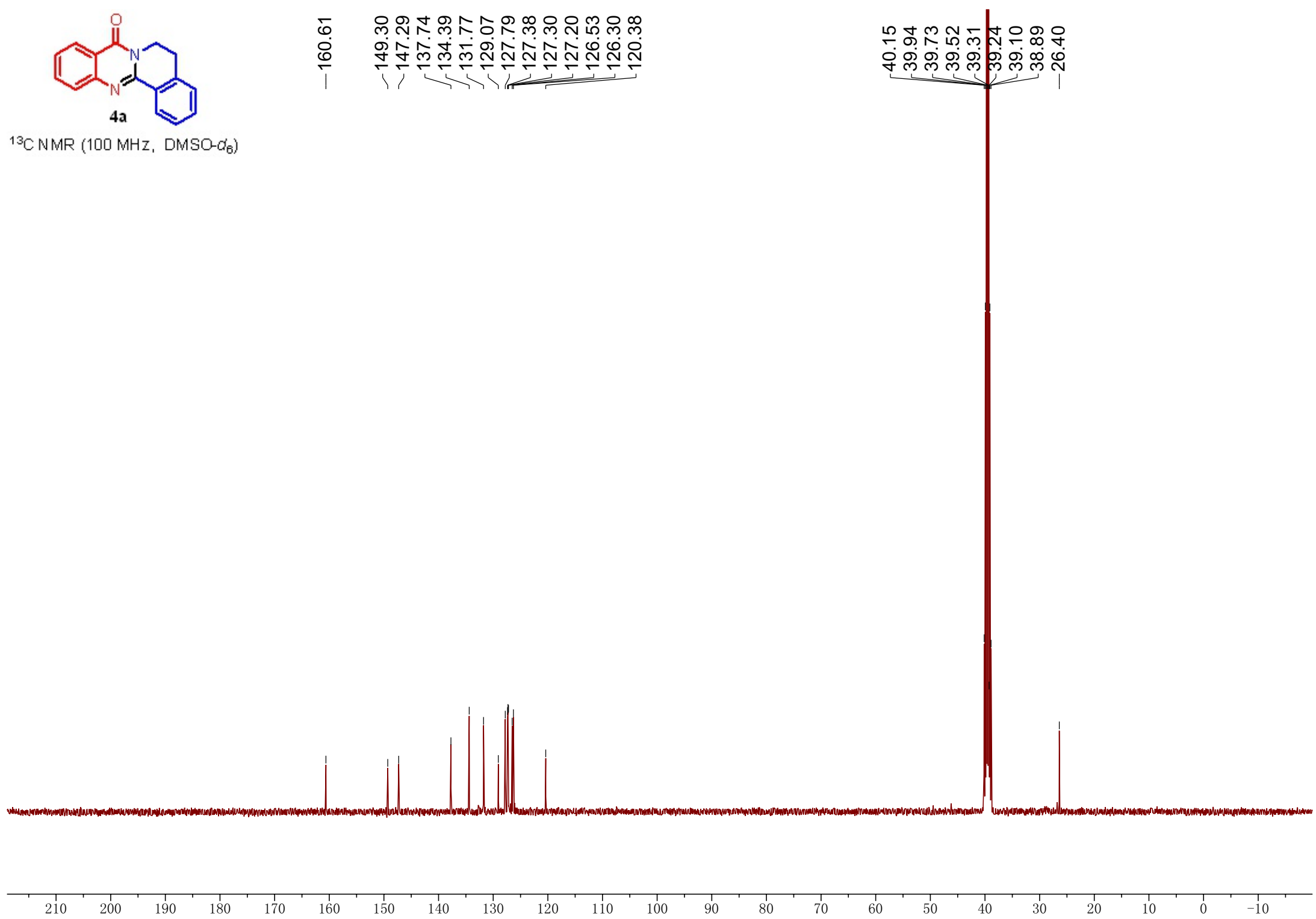




^{13}C NMR (100 MHz, $\text{DMSO-}d_6$)

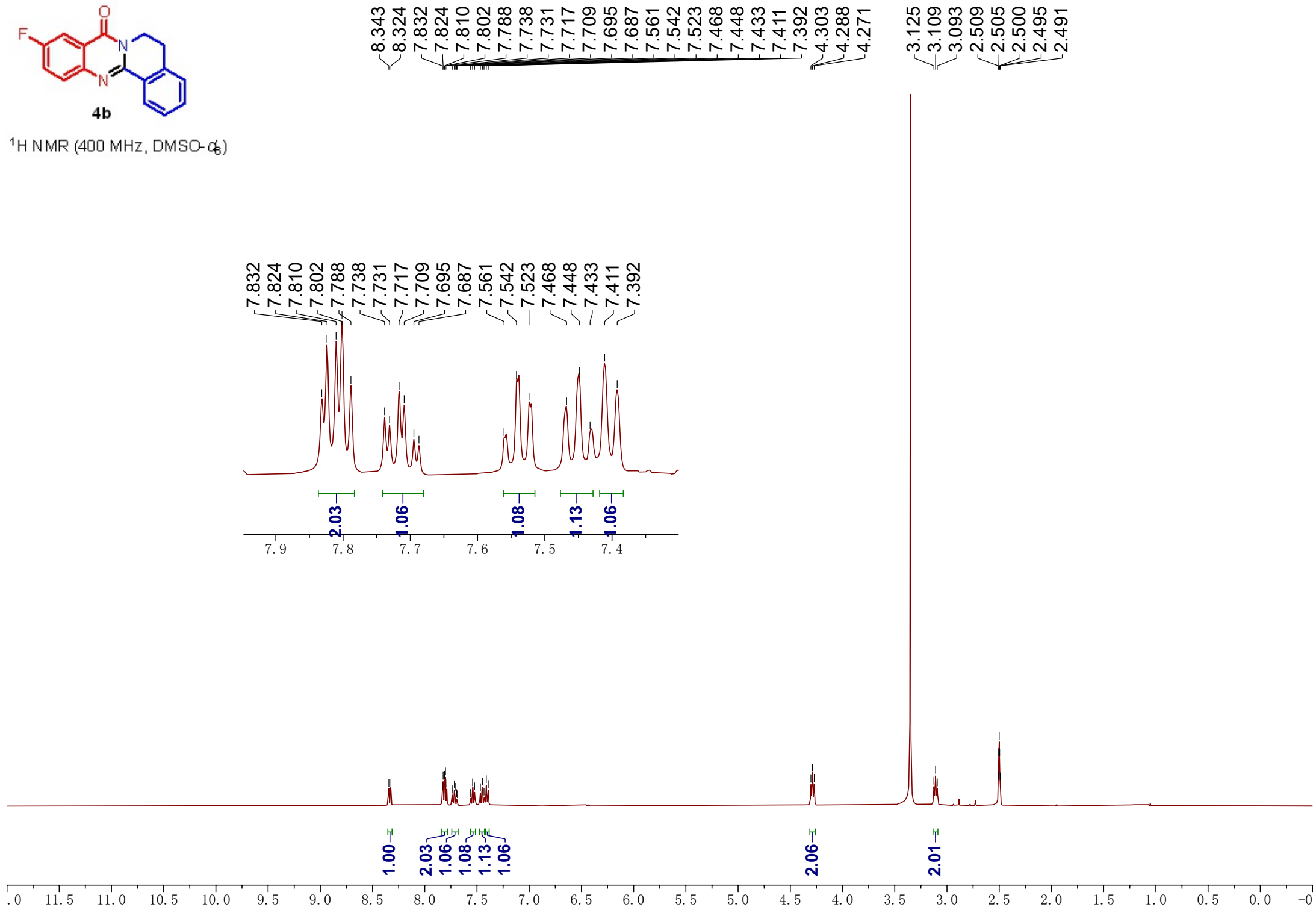
- 160.61
- 149.30
- 147.29
- 137.74
- 134.39
- 131.77
- 129.07
- 127.79
- 127.38
- 127.30
- 127.20
- 126.53
- 126.30
- 120.38

- 40.15
- 39.94
- 39.73
- 39.52
- 39.31
- 39.24
- 39.10
- 38.89
- 26.40





¹H NMR (400 MHz, DMSO-*d*₆)





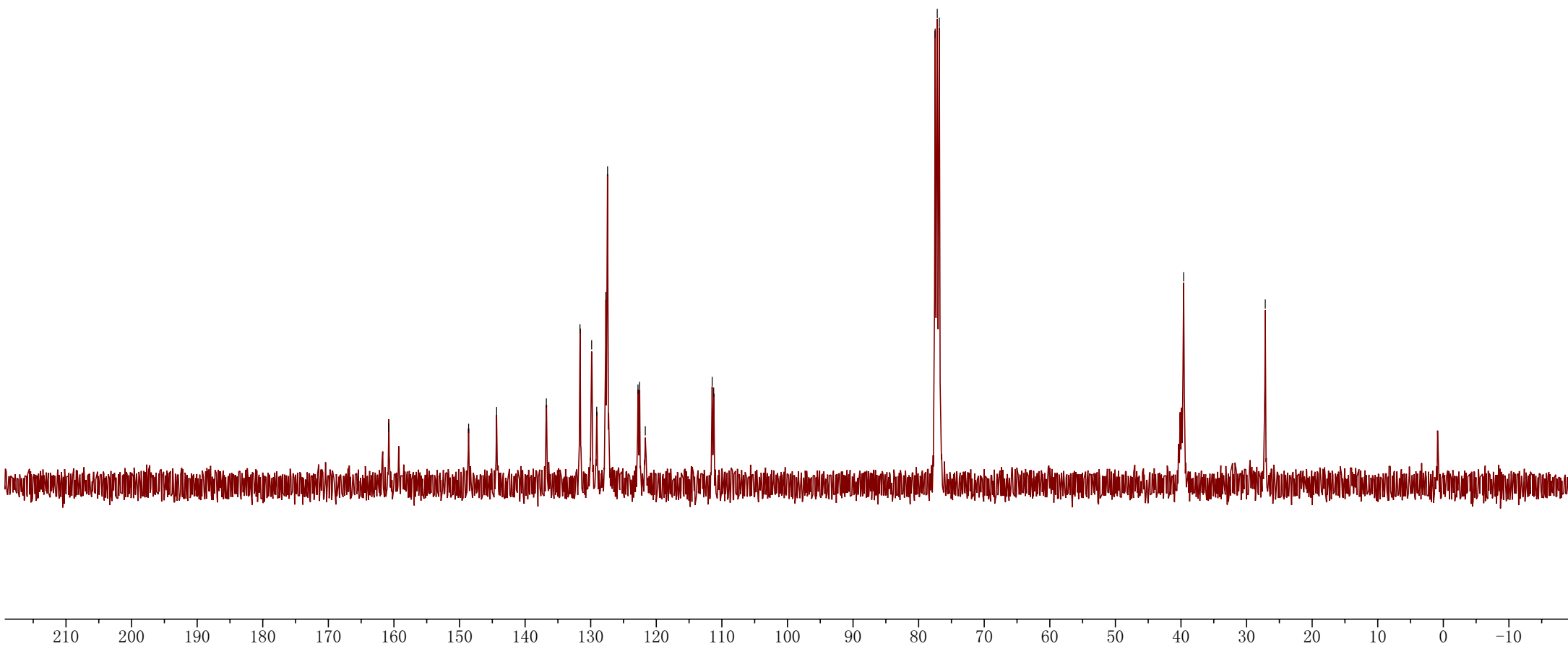
^{13}C NMR (100 MHz, CDCl_3)

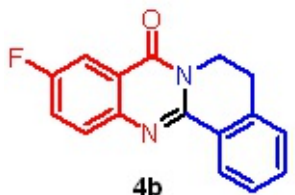
160.80
148.61
144.34
136.76
131.63
129.85
129.09
127.68
127.43
122.79
122.55
121.68
111.48
111.25

77.48
77.16
76.84

39.60

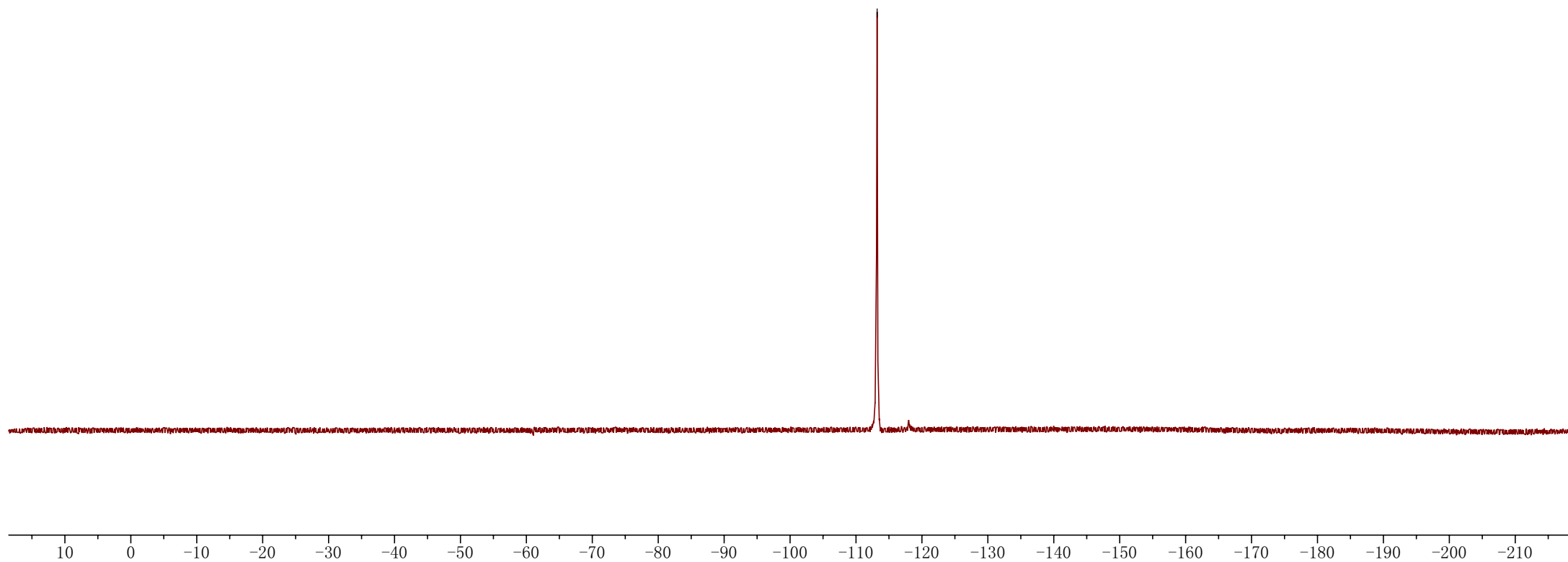
27.15

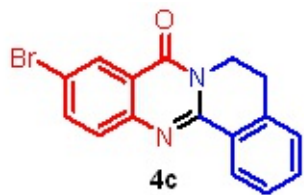




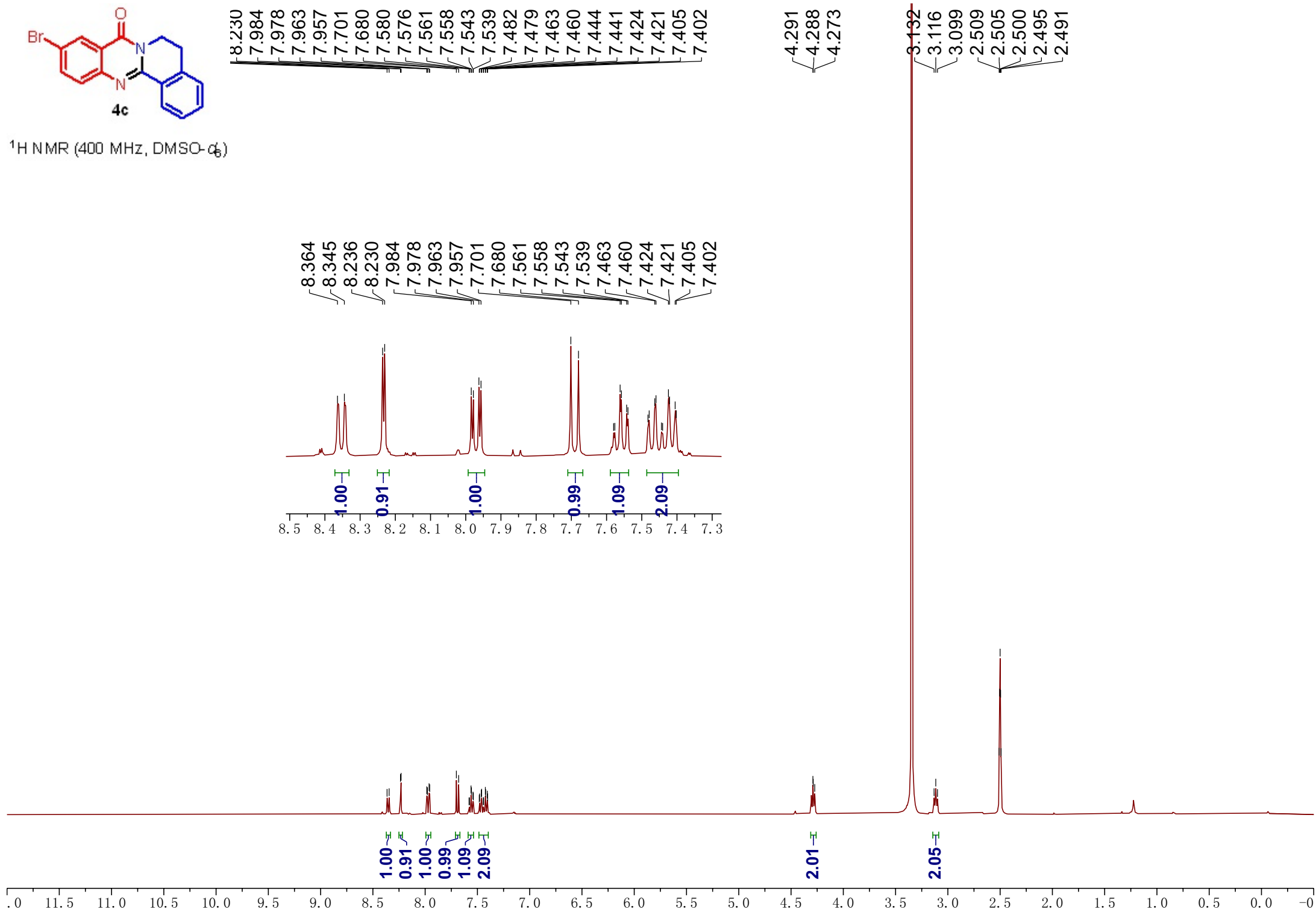
^{19}F NMR (376 MHz, CDCl_3)

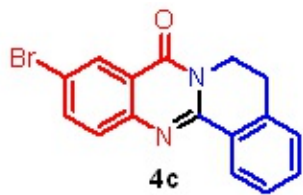
—113.21





¹H NMR (400 MHz, DMSO-*d*₆)





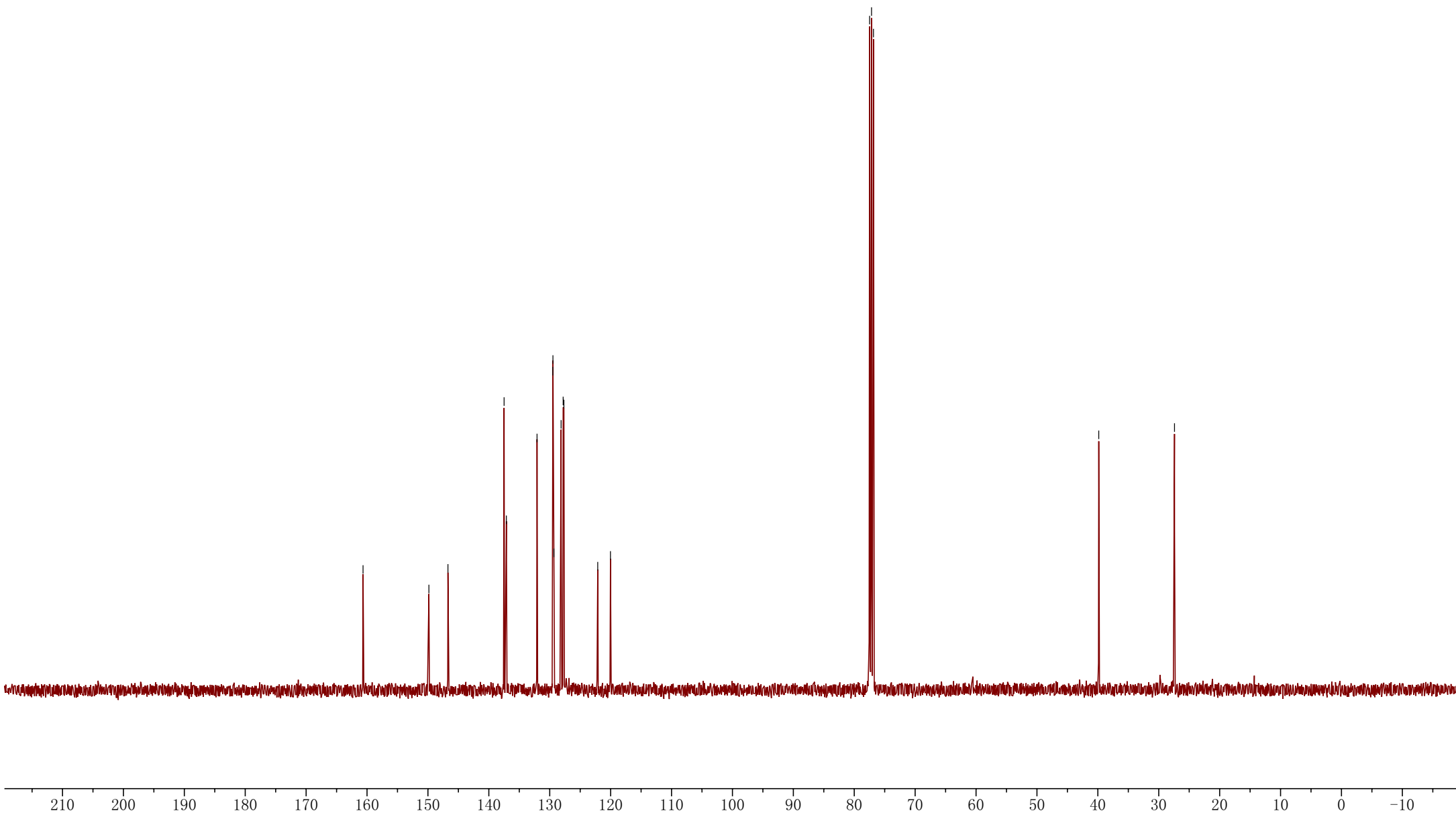
^{13}C NMR (100 MHz, CDCl_3)

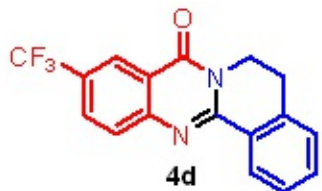
— 160.66
— 149.84
— 146.71
— 137.49
— 137.12
— 132.08
— 129.50
— 129.47
— 129.32
— 128.13
— 127.80
— 127.67
— 122.12
— 120.03

{ 77.48
— 77.16
— 76.84

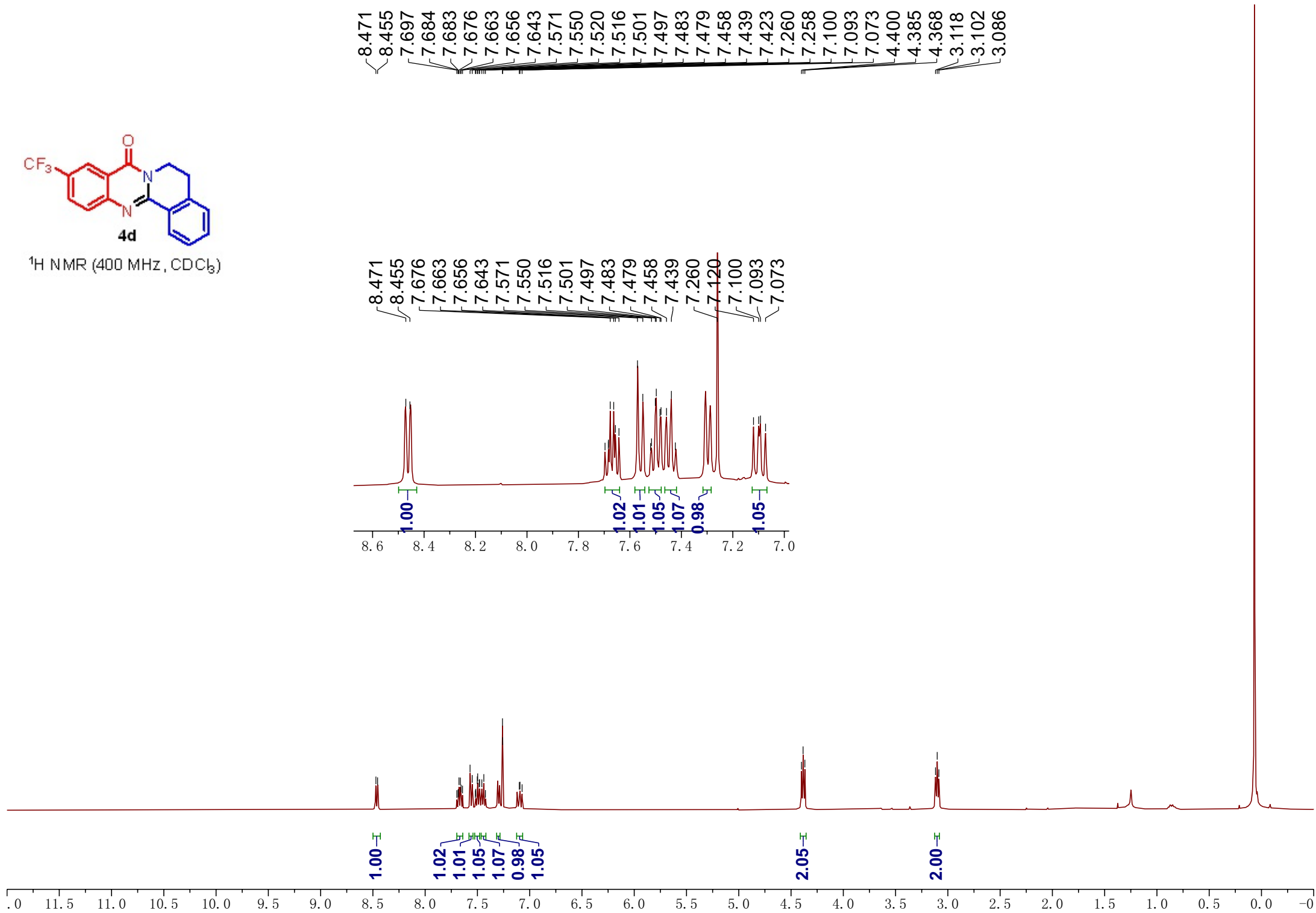
— 39.85

— 27.42





¹H NMR (400 MHz, CDCl₃)





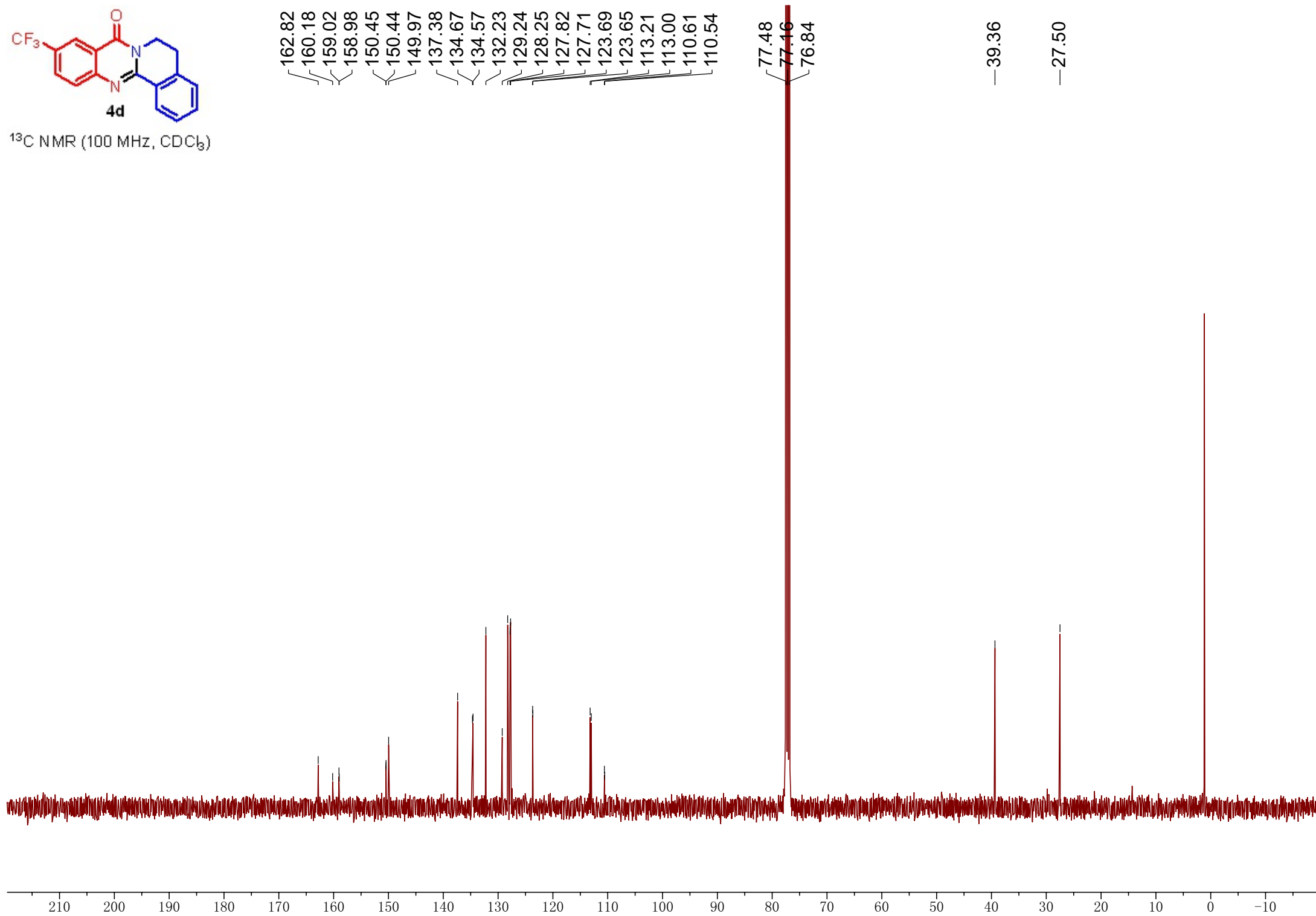
^{13}C NMR (100 MHz, CDCl_3)

162.82
160.18
159.02
158.98
150.45
150.44
149.97
137.38
134.67
134.57
132.23
129.24
128.25
127.82
127.71
123.69
123.65
113.21
113.00
110.61
110.54

77.48
77.16
76.84

—39.36

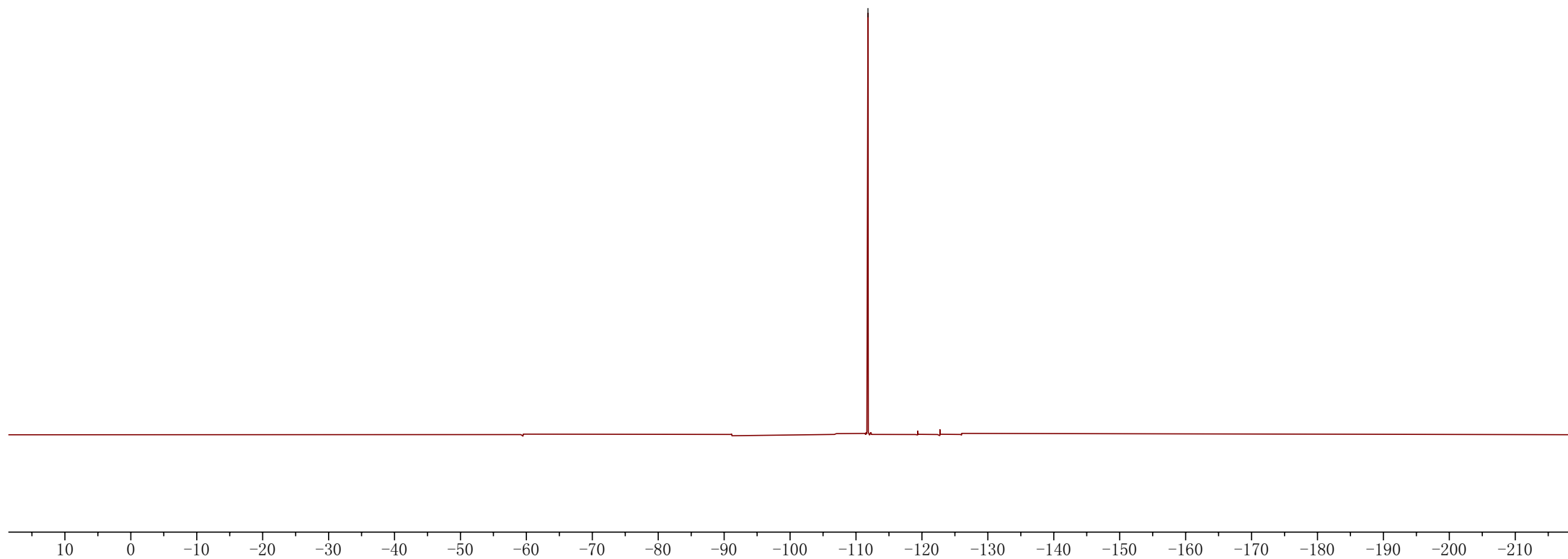
—27.50





^{19}F NMR (376 MHz, CDCl_3)

---111.813

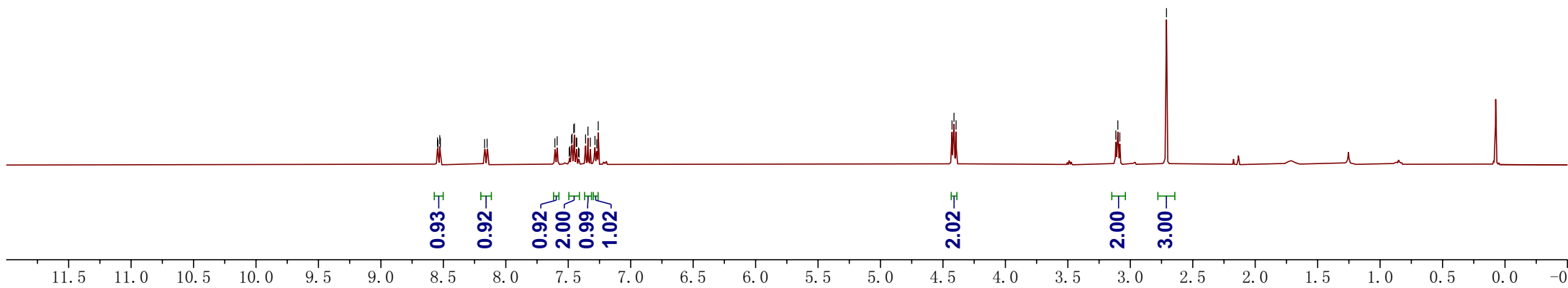
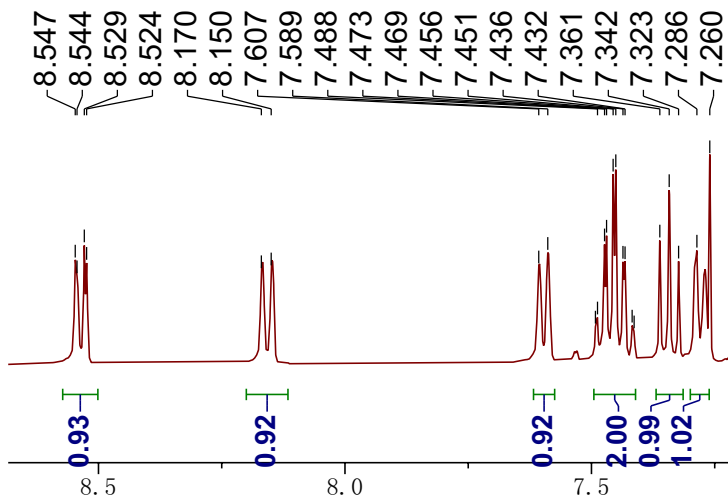




¹H NMR (400 MHz, CDCl₃)

8.547
8.544
8.529
8.524
8.170
8.150
7.607
7.589
7.492
7.488
7.473
7.469
7.456
7.451
7.436
7.432
7.418
7.413
7.361
7.342
7.323
7.286
7.272
7.260
4.427
4.412
4.395

3.116
3.100
3.084
2.710





^{13}C NMR (100 MHz, CDCl_3)

— 162.23

— 148.14

— 146.41

— 137.08

— 136.25

— 134.86

— 131.68

— 130.10

— 128.18

— 127.69

— 127.61

— 126.27

— 124.66

— 120.81

— 77.48

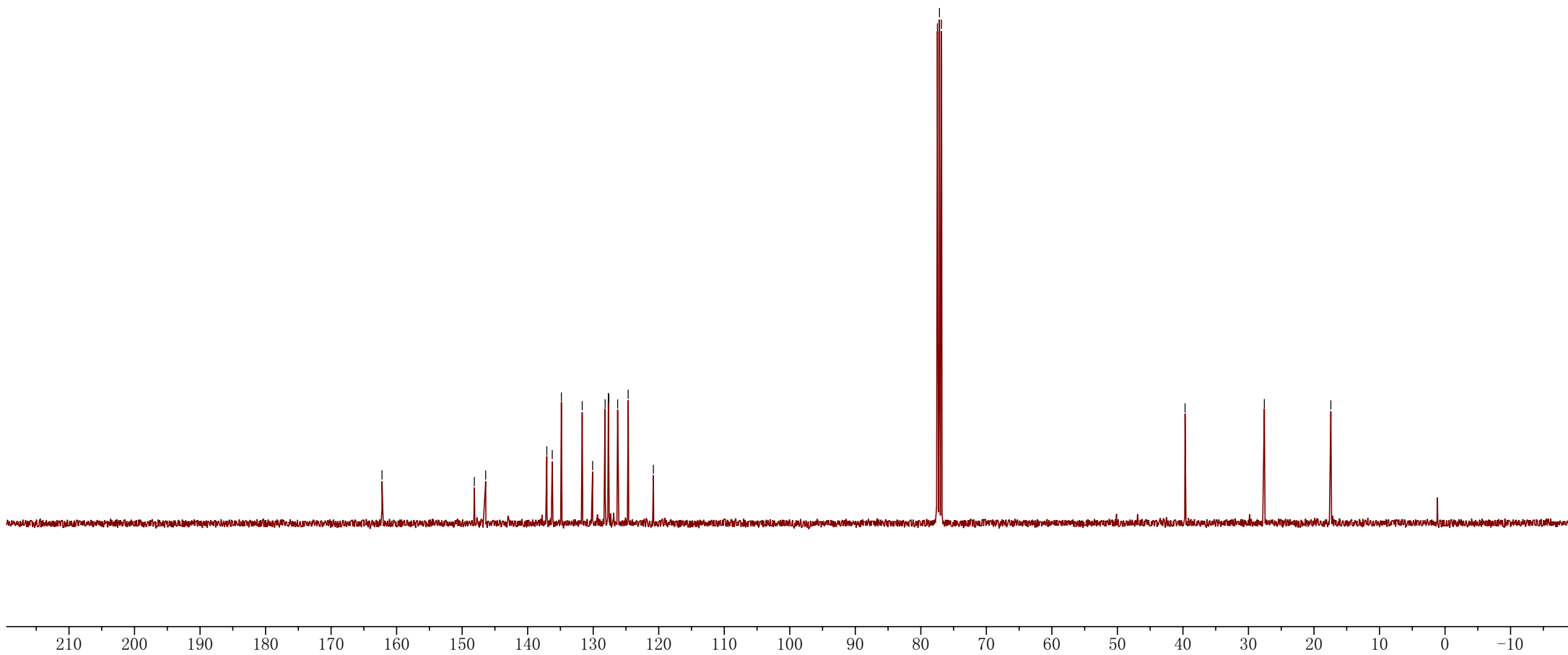
— 77.16

— 76.84

— 39.68

— 27.58

— 17.43

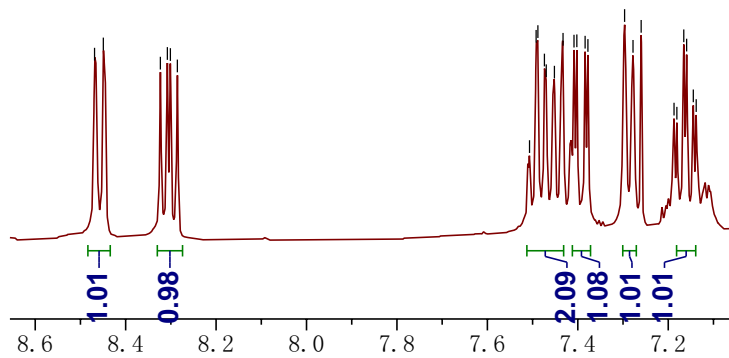




¹H NMR (400 MHz, CDCl₃)

8.469
8.449
8.323
8.308
8.301
8.286
7.507
7.492
7.488
7.474
7.470
7.452
7.433
7.408
7.402
7.384
7.378
7.297
7.278
7.260
7.187
7.181
7.166
7.159
7.145
7.138
4.409
4.393
4.376
3.116
3.100
3.084

8.469
8.449
8.323
8.308
8.301
8.286
7.492
7.488
7.474
7.470
7.433
7.408
7.402
7.384
7.378
7.297
7.278
7.260
7.166
7.159



1.01
0.98
2.09
1.08
1.01
1.01
2.01
2.00

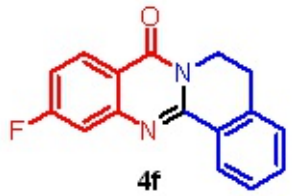
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

167.89
165.37
161.16
150.69
150.15
150.02
137.29
132.19
129.75
129.64
129.38
128.30
127.82
127.68
117.62
117.60
115.56
115.33
112.91
112.69

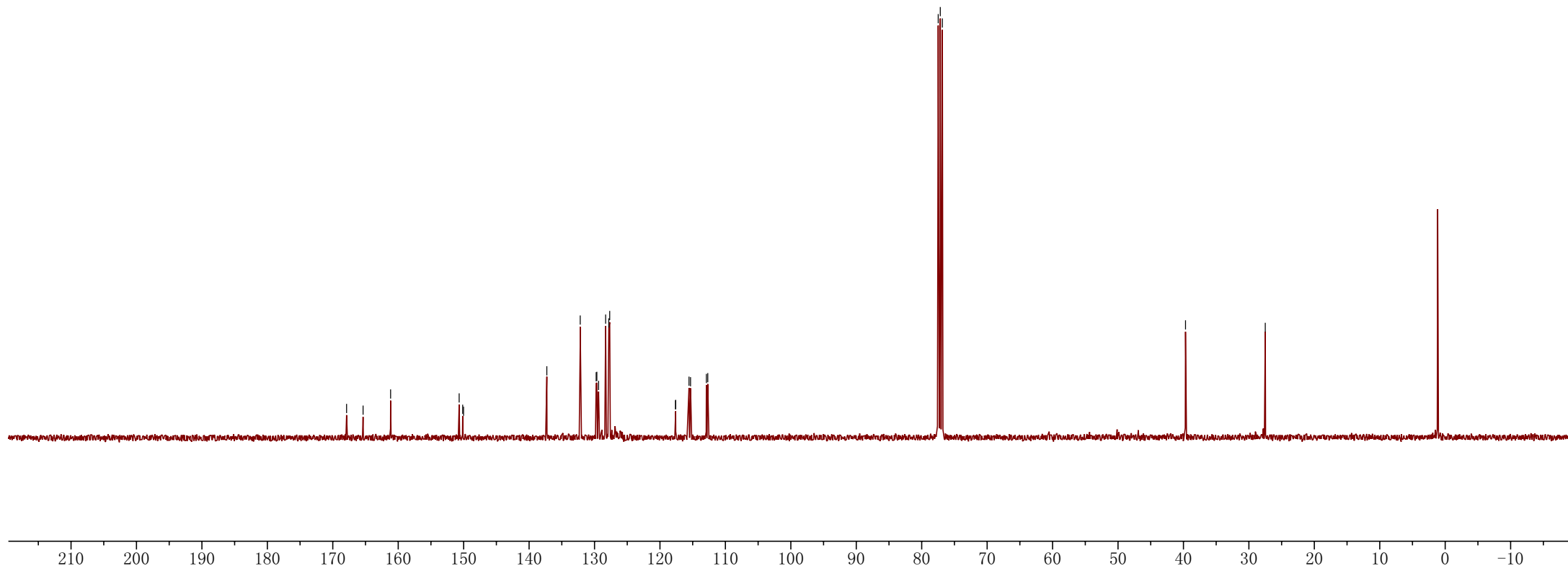
77.48
77.16
76.84

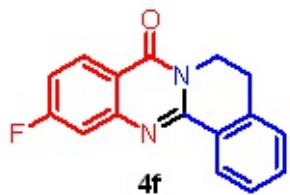
39.68

27.50



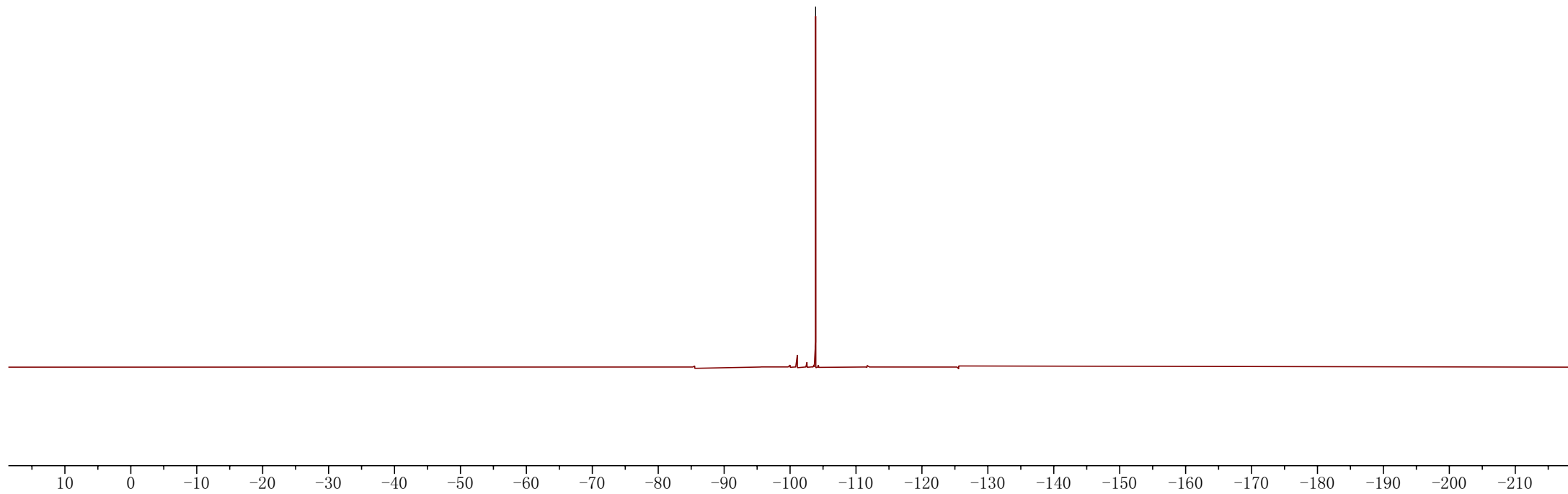
¹³C NMR (100 MHz, CDCl₃)

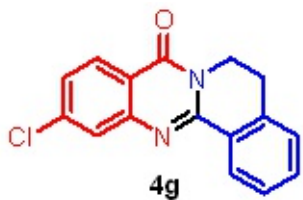




^{19}F NMR (376 MHz, CDCl_3)

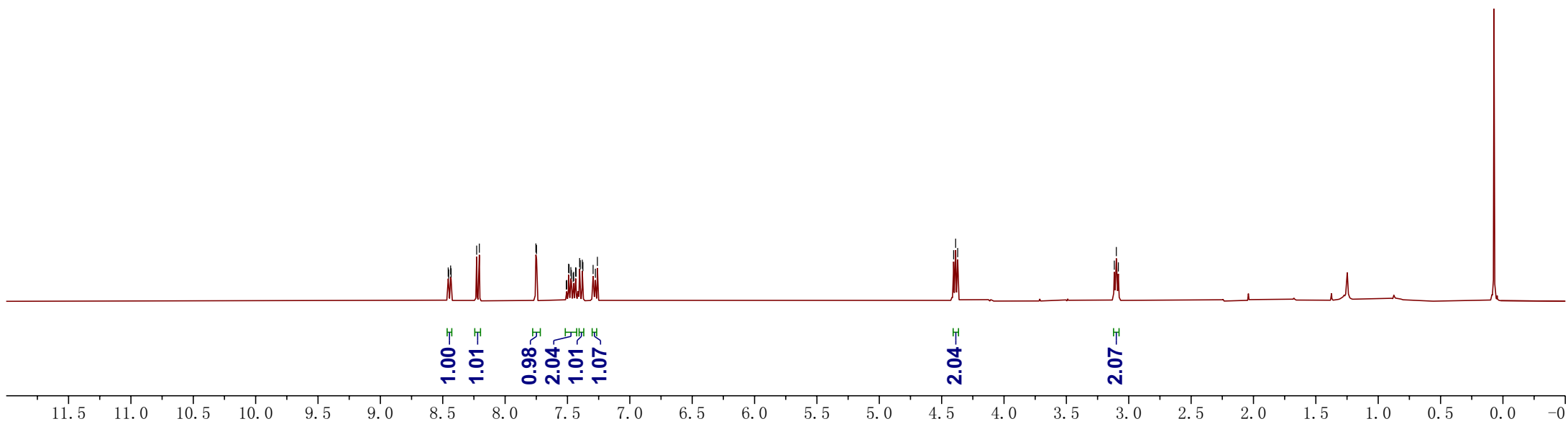
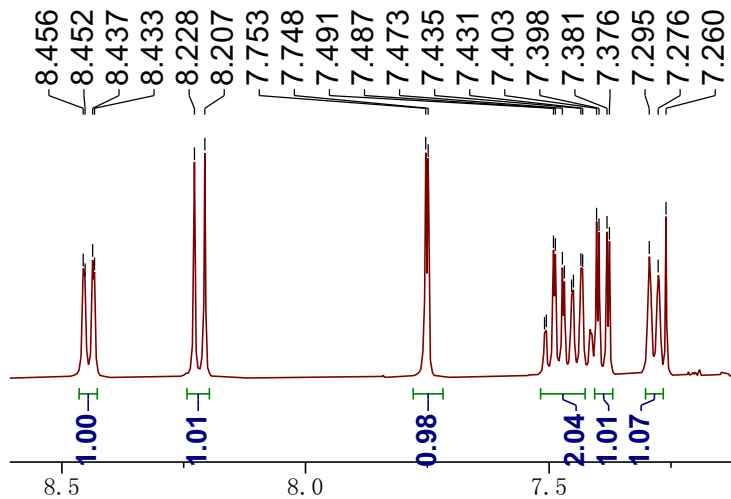
---103.88





¹H NMR (400 MHz, CDCl₃)

8.456
8.452
8.437
8.433
8.228
8.207
7.753
7.748
7.509
7.506
7.491
7.487
7.473
7.435
7.431
7.403
7.398
7.381
7.376
7.295
7.276
7.260
4.404
4.388
4.371
3.116
3.099
3.083





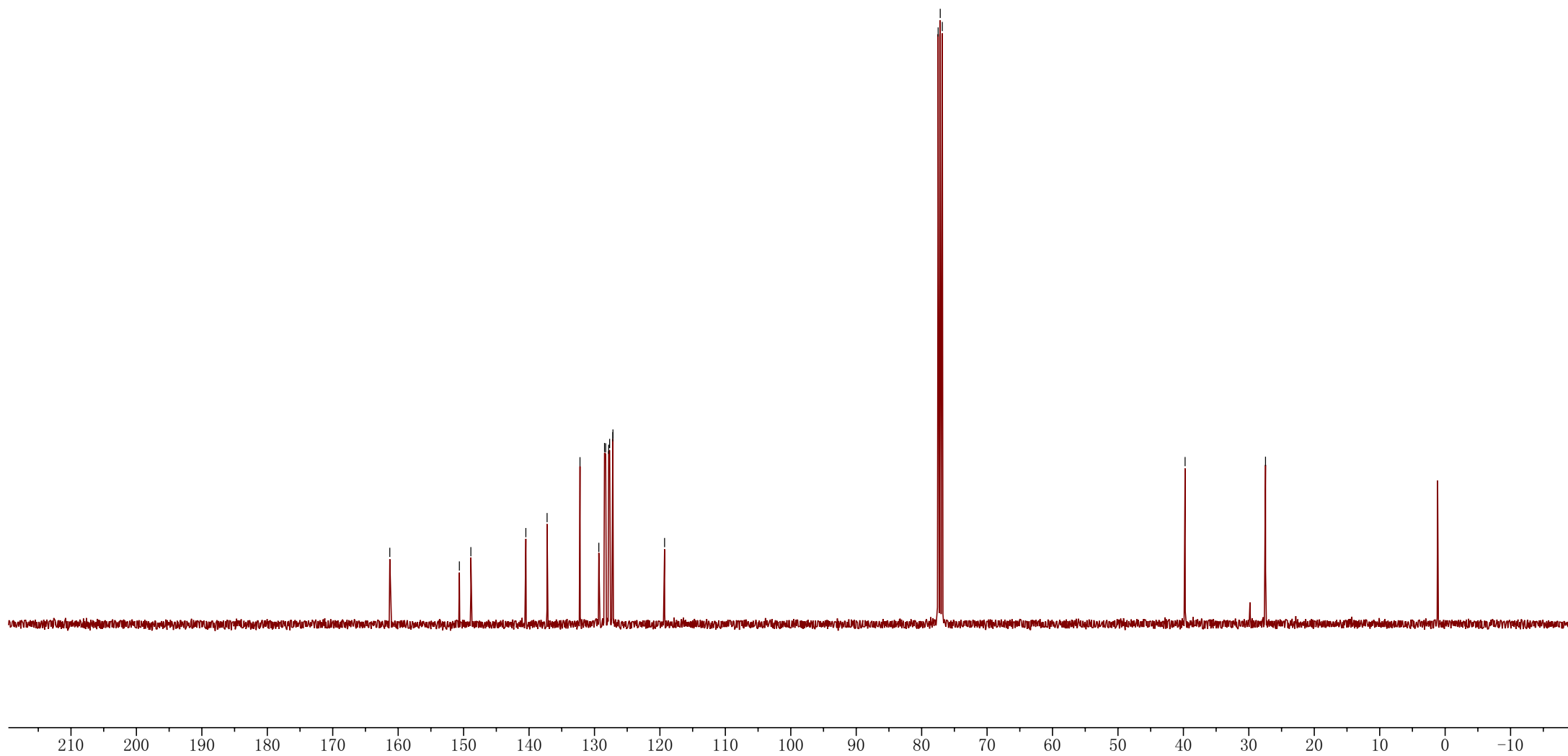
^{13}C NMR (100 MHz, CDCl_3)

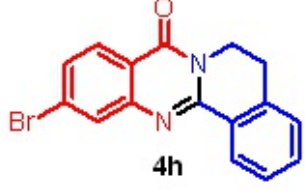
— 161.28
— 150.65
— 148.89
— 140.49
— 137.24
— 132.21
— 129.33
— 128.47
— 128.29
— 127.83
— 127.68
— 127.20
— 127.18
— 119.29

— 77.48
— 77.16
— 76.84

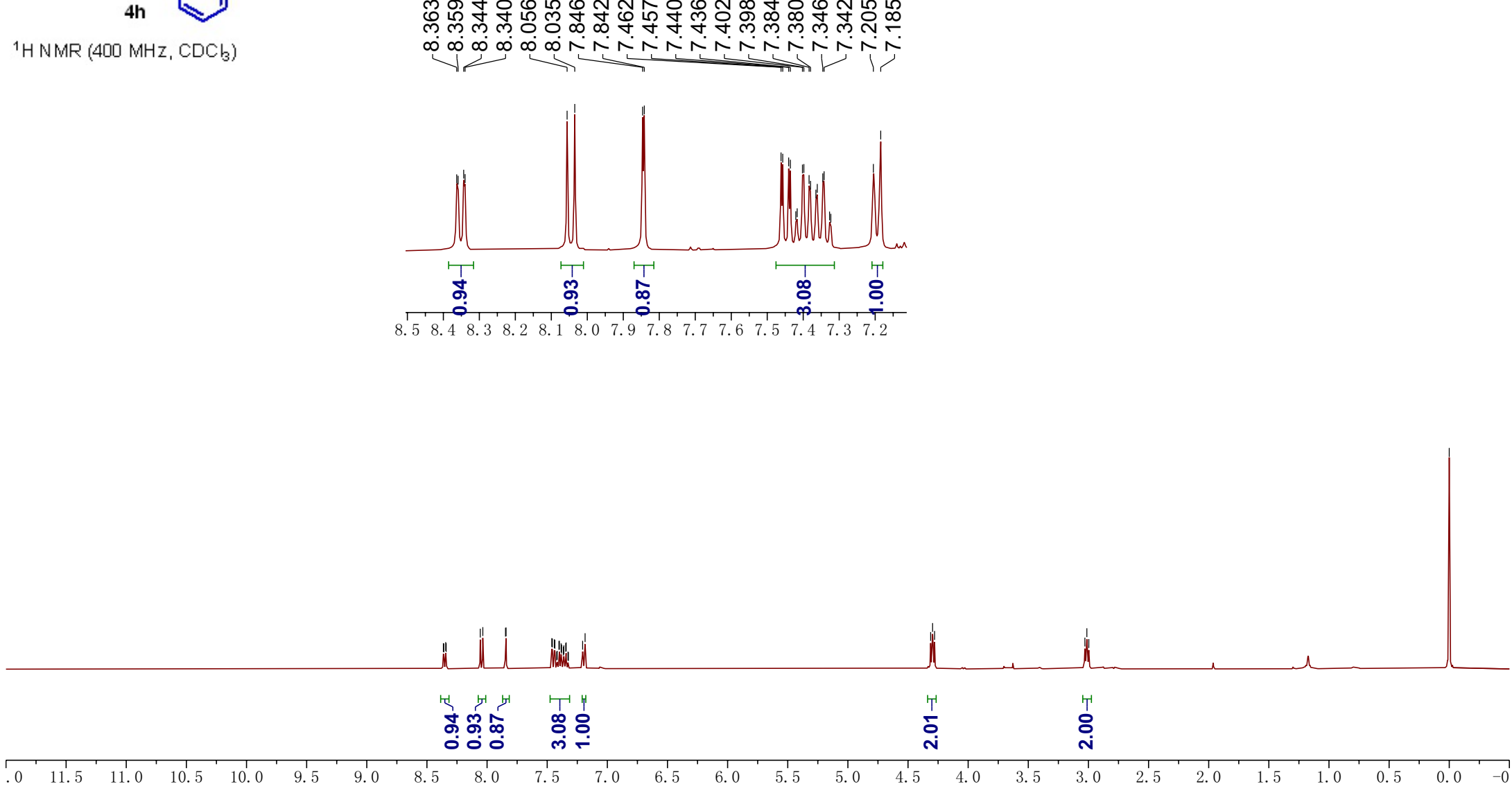
— 39.74

— 27.45





¹H NMR (400 MHz, CDCl₃)





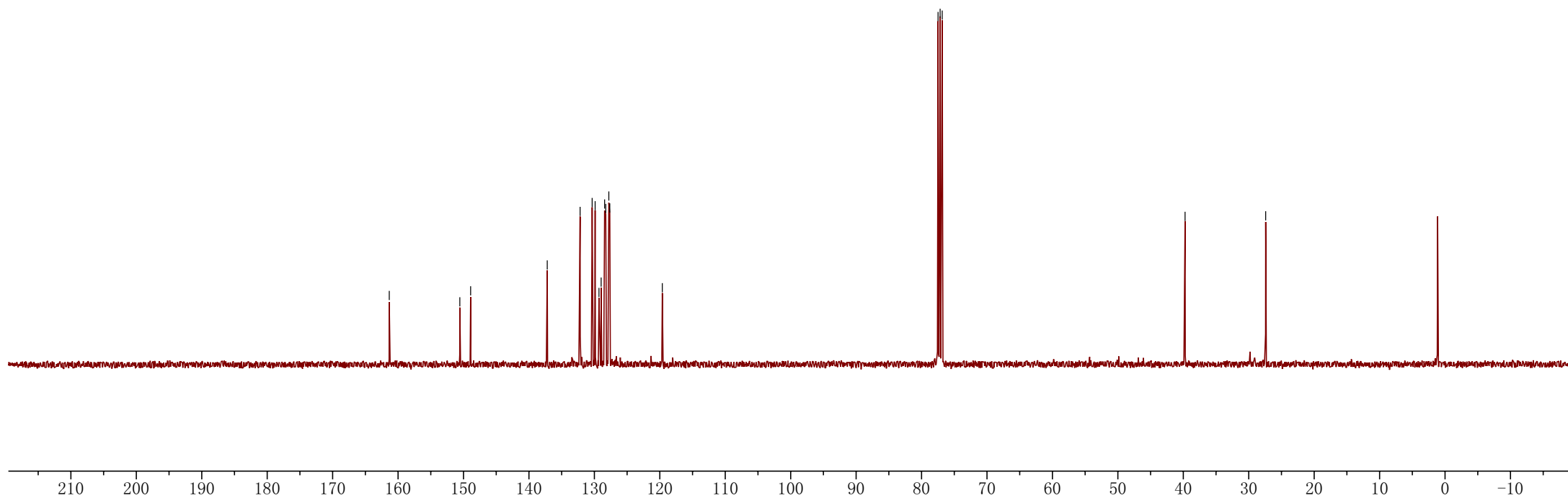
^{13}C NMR (100 MHz, CDCl_3)

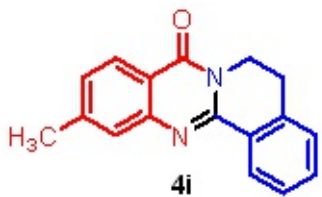
— 161.35
— 150.56
— 148.91
— 137.20
— 132.18
— 130.34
— 129.88
— 129.30
— 128.96
— 128.44
— 128.26
— 127.79
— 127.65
— 119.62

— 77.48
— 77.16
— 76.84

— 39.73

— 27.41



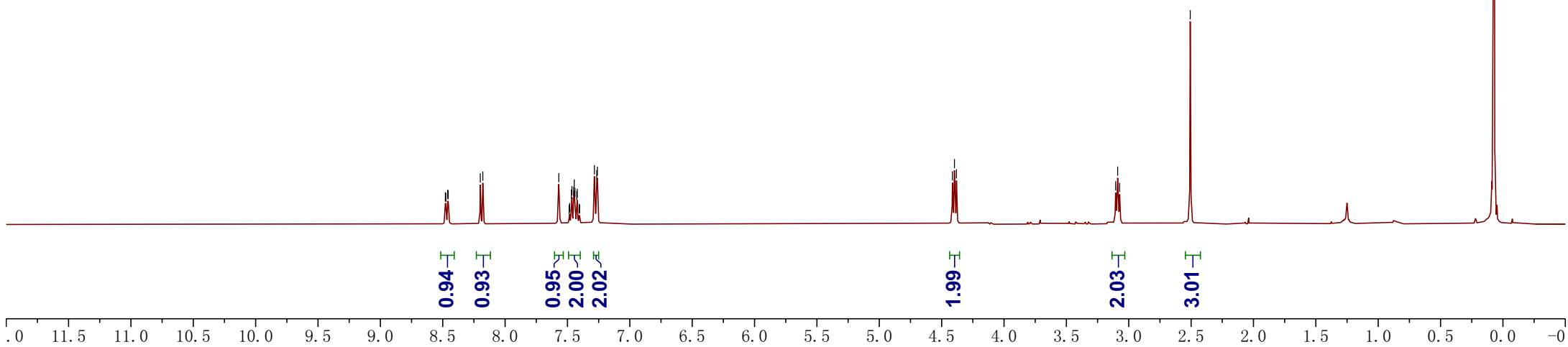
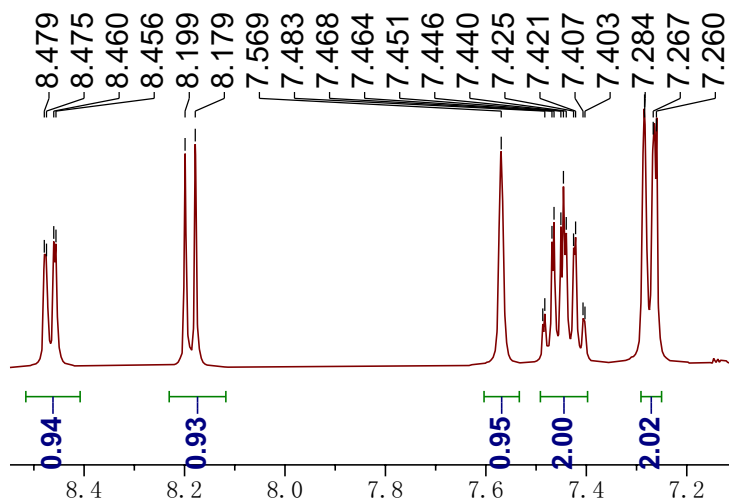


¹H NMR (400 MHz, CDCl₃)

8.479
8.475
8.460
8.456
8.199
8.179
7.569
7.487
7.483
7.468
7.464
7.451
7.446
7.440
7.425
7.421
7.407
7.403
7.284
7.266
7.260
4.414
4.397
4.381

3.105
3.089
3.073

—2.507





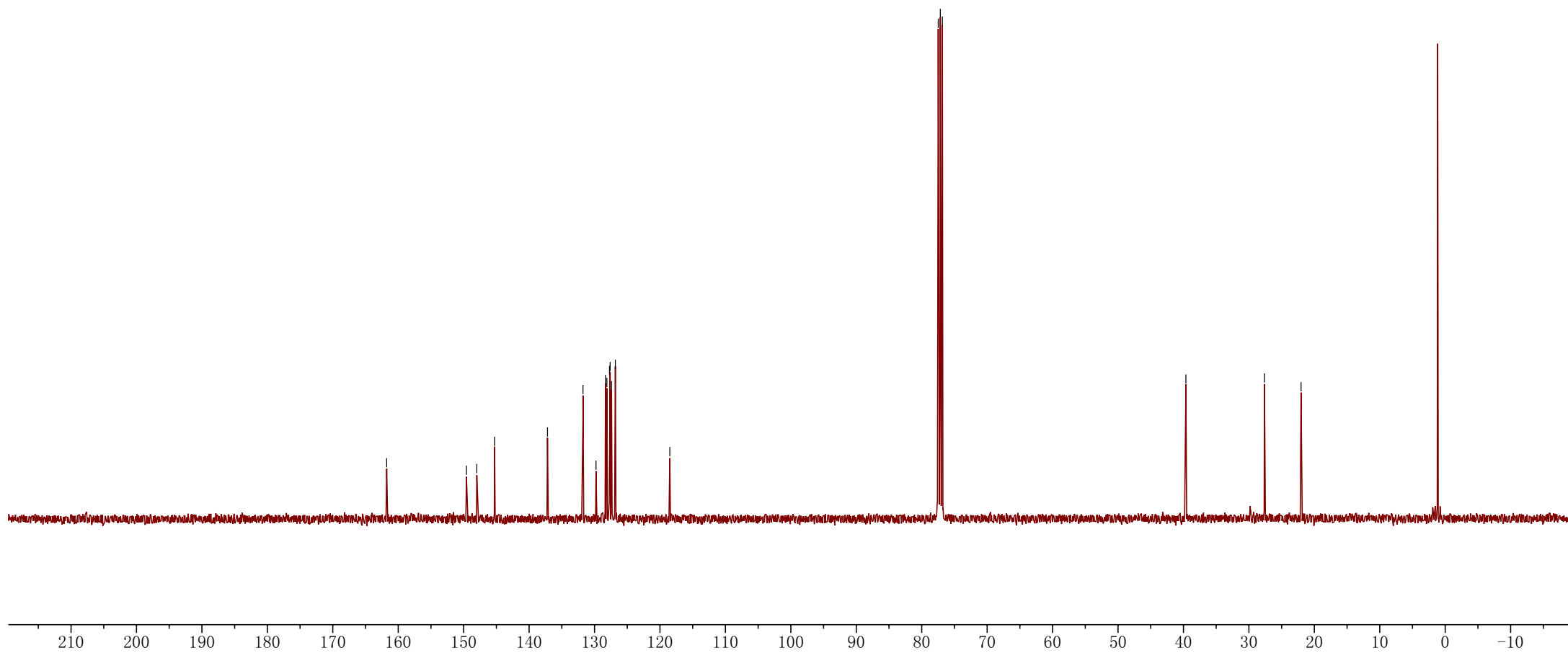
^{13}C NMR (100 MHz, CDCl_3)

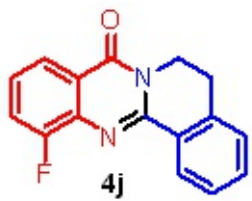
— 161.76
— 149.58
— 147.99
— 145.28
— 137.19
— 131.76
— 129.77
— 128.33
— 128.11
— 127.72
— 127.61
— 127.41
— 126.82
— 118.50

— 77.48
— 77.16
— 76.84

— 39.63

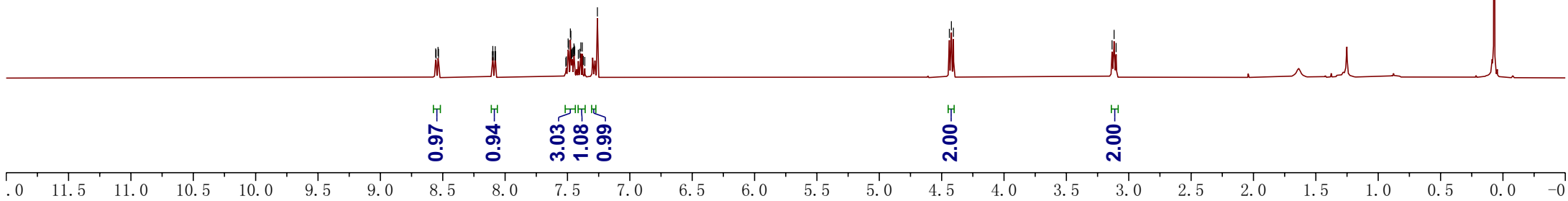
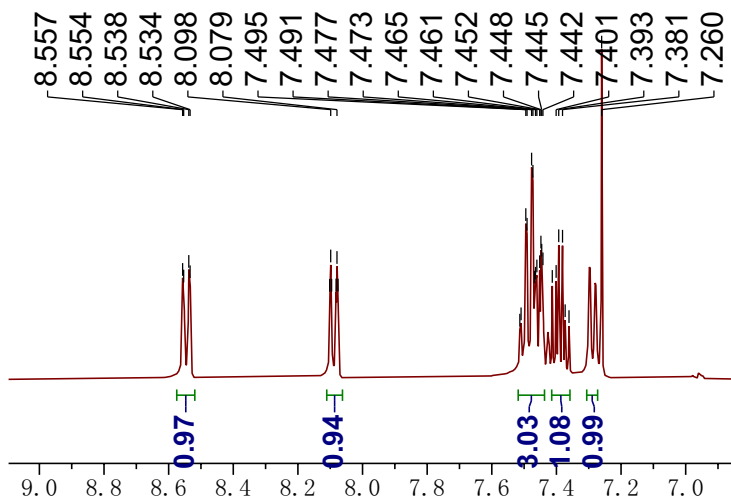
— 27.63
— 22.03





¹H NMR (400 MHz, CDCl₃)

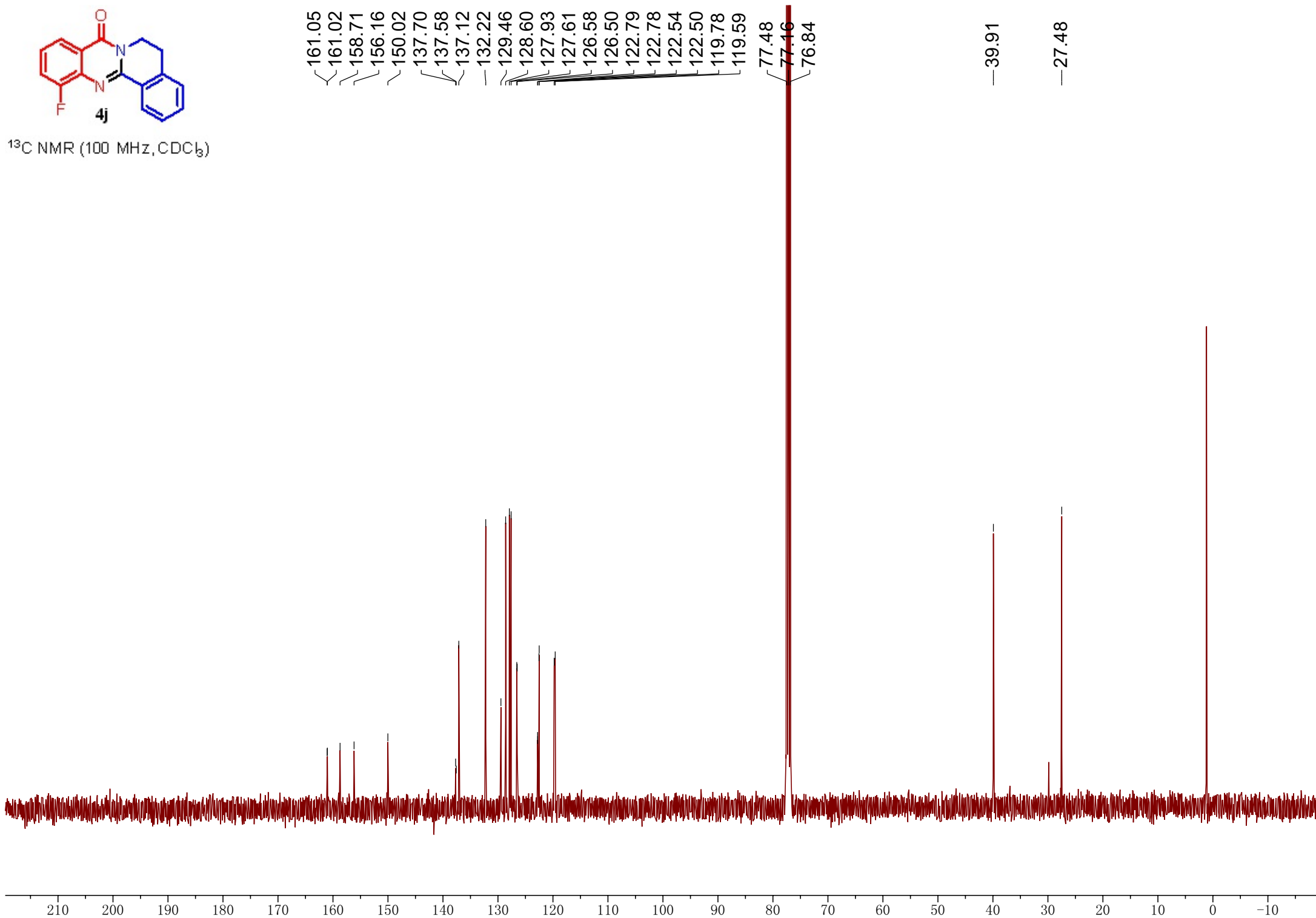
8.557
8.554
8.538
8.534
8.102
8.098
8.096
8.082
8.079
8.076
7.513
7.509
7.495
7.491
7.477
7.473
7.468
7.465
7.461
7.452
7.448
7.445
7.442
7.442
7.413
7.401
7.393
7.381
7.373
7.361
7.260
4.438
4.422
4.406
3.134
3.118
3.101





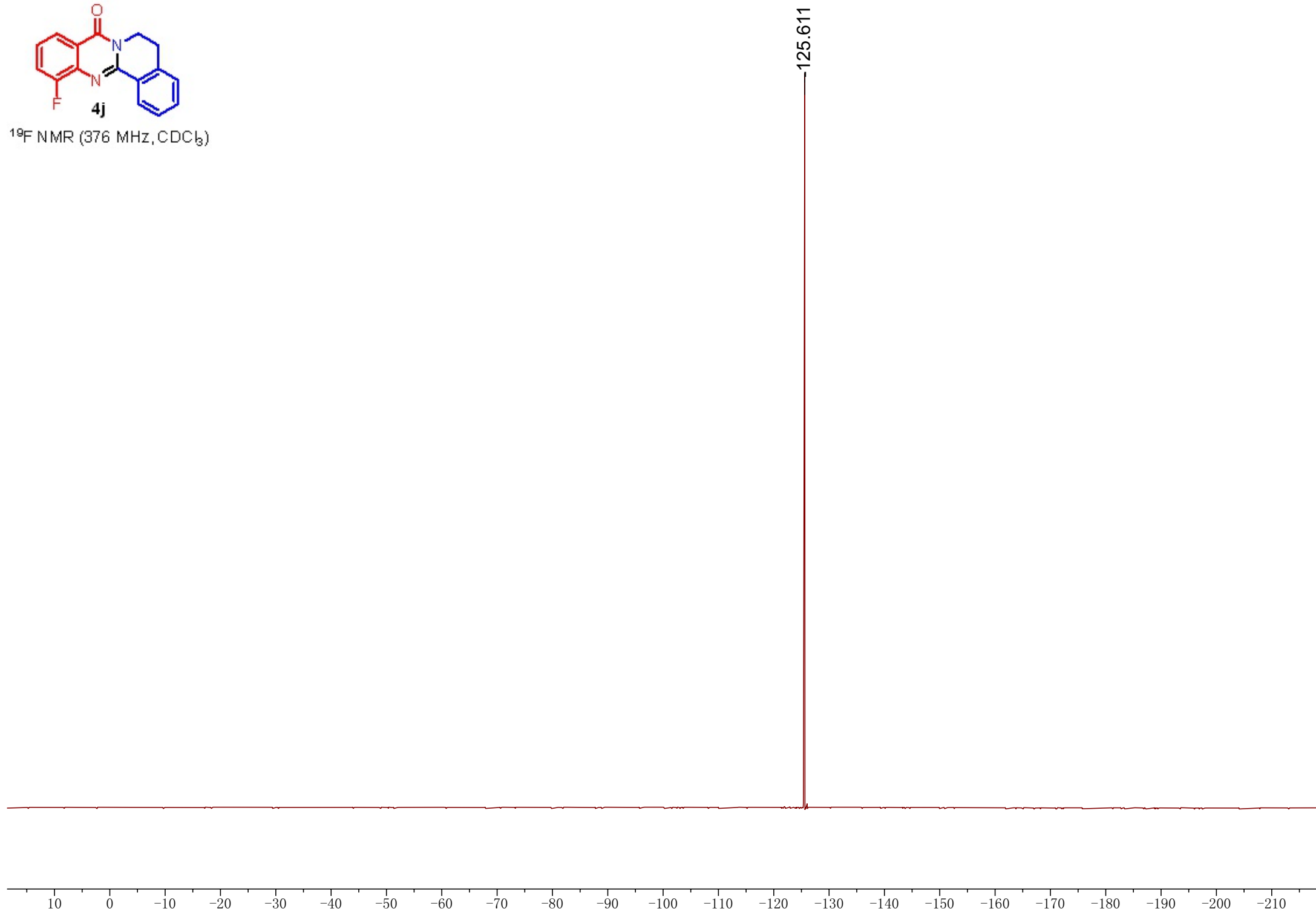
^{13}C NMR (100 MHz, CDCl_3)

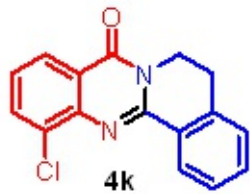
161.05
161.02
158.71
156.16
150.02
137.70
137.58
137.12
132.22
129.46
128.60
127.93
127.61
126.58
126.50
122.79
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122.54
122.50
119.78
119.59
77.48
77.16
76.84
-39.91
-27.48





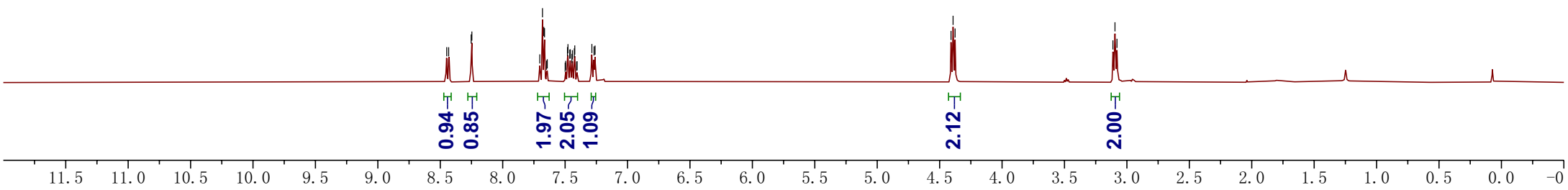
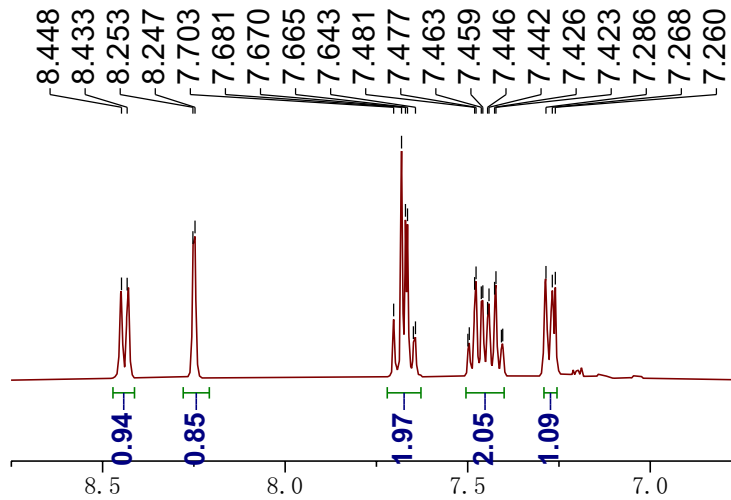
^{19}F NMR (376 MHz, CDCl_3)

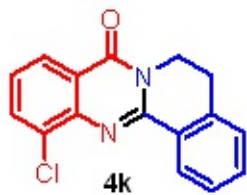




¹H NMR (400 MHz, CDCl₃)

8.448
8.433
8.253
8.247
7.703
7.681
7.670
7.665
7.649
7.643
7.499
7.496
7.481
7.477
7.463
7.459
7.446
7.442
7.426
7.423
7.408
7.404
7.286
7.268
7.260
4.409
4.392
4.376
3.112
3.096
3.079





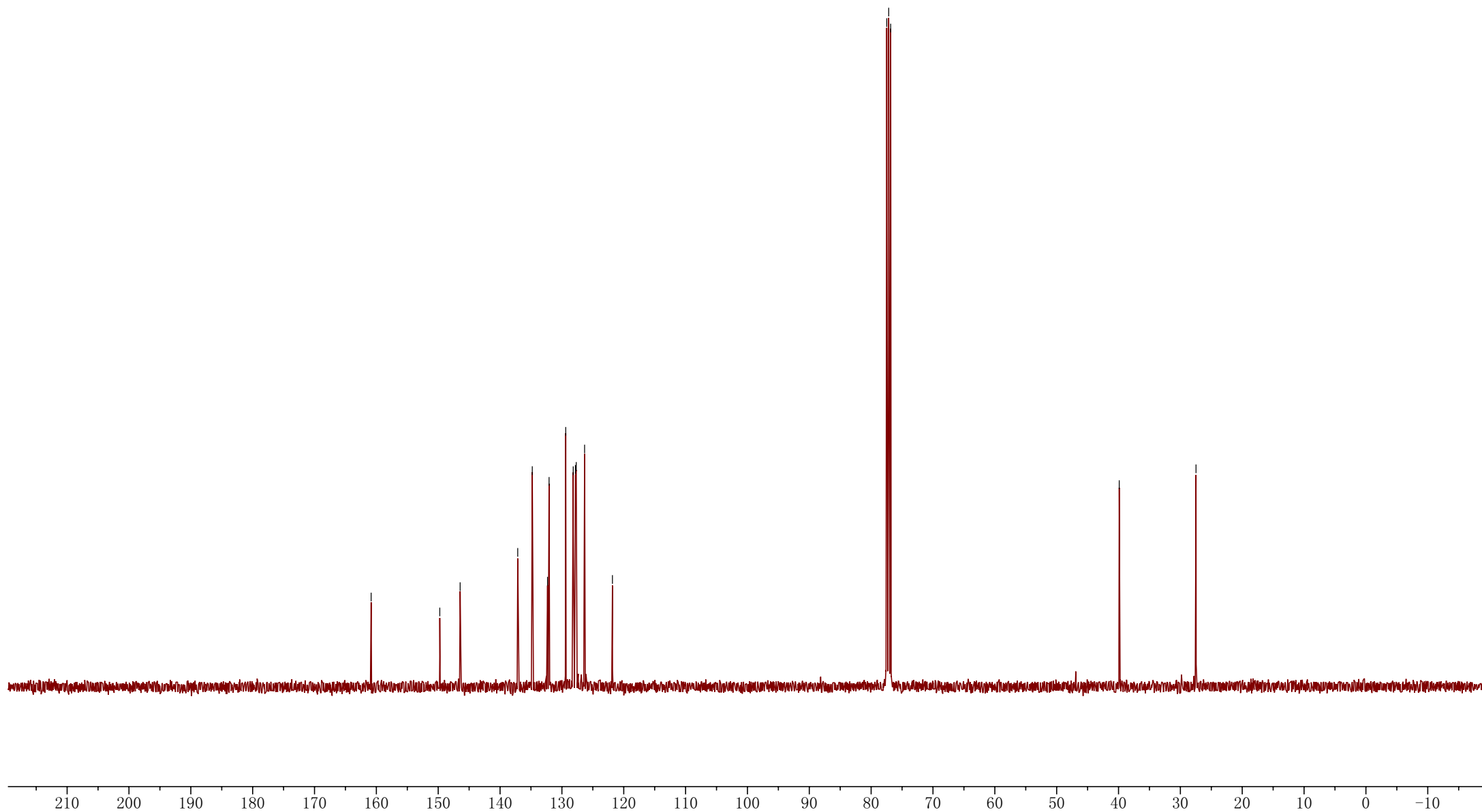
¹³C NMR (100 MHz, CDCl₃)

— 160.85
— 149.74
— 146.45
137.14
134.79
132.32
132.07
129.38
128.17
127.82
127.69
126.33
121.83

77.48
77.16
76.84

— 39.89

— 27.47

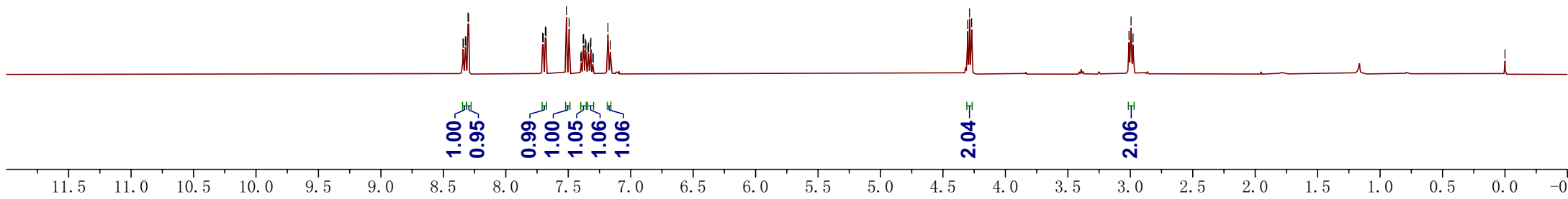
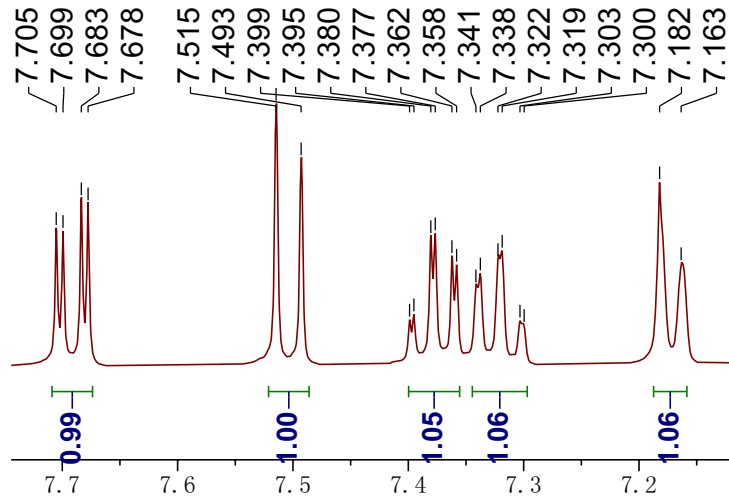




4I

^1H NMR (400 MHz, CDCl_3)

8.343
8.339
8.323
8.319
8.303
8.297
7.705
7.700
7.684
7.678
7.515
7.493
7.399
7.395
7.380
7.381
7.377
7.362
7.358
7.342
7.338
7.322
7.319
7.303
7.300
7.182
7.164
4.303
4.287
4.270
3.010
2.994
2.978





4I

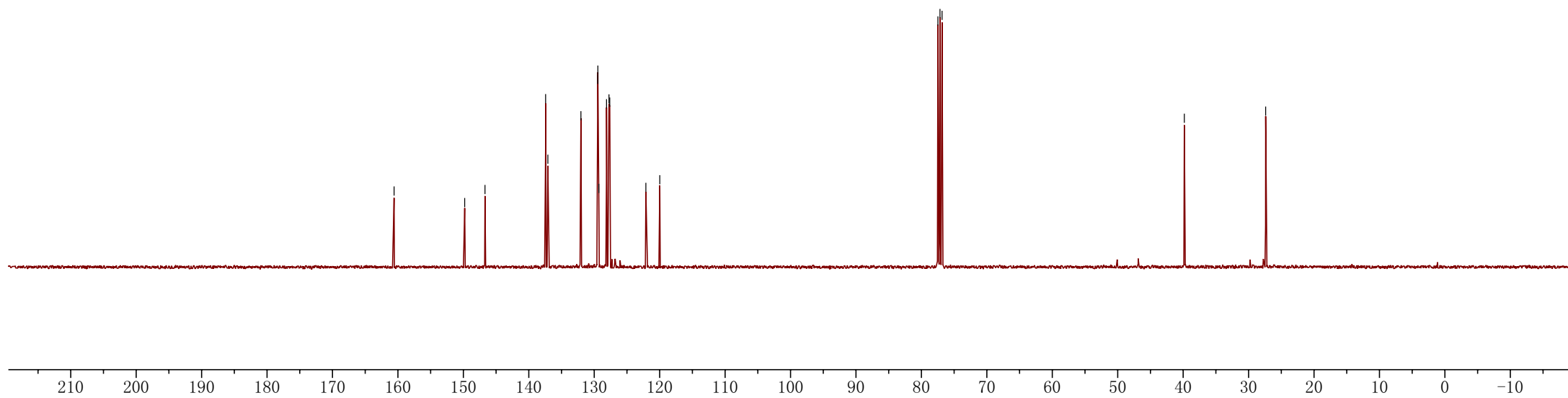
^{13}C NMR (100 MHz, CDCl_3)

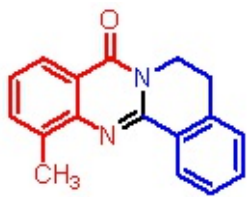
— 160.59
— 149.80
— 146.69
137.43
137.09
132.04
129.46
129.45
129.30
128.12
127.75
127.63
122.11
119.98

77.48
77.16
76.84

— 39.82

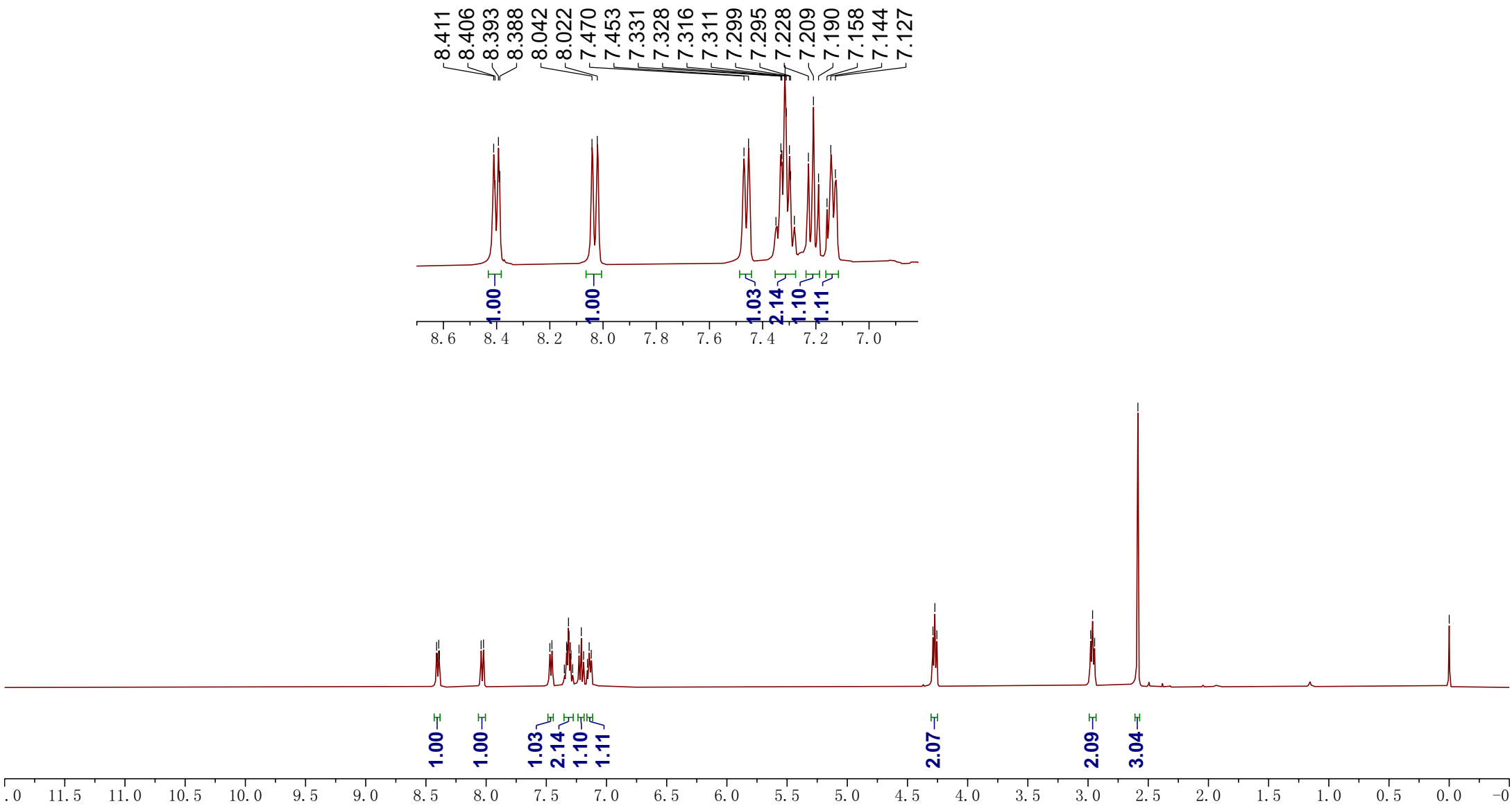
— 27.39

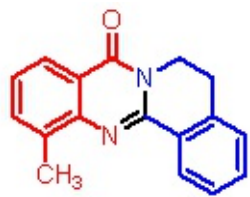




4m

¹H NMR (400 MHz, CDCl₃)





4m

^{13}C NMR (100 MHz, CDCl_3)

—162.07

—148.01

—146.29

—136.97

—136.13

—134.73

—131.55

—129.97

—128.07

—127.56

—127.50

—126.14

—124.56

—120.71

—77.48

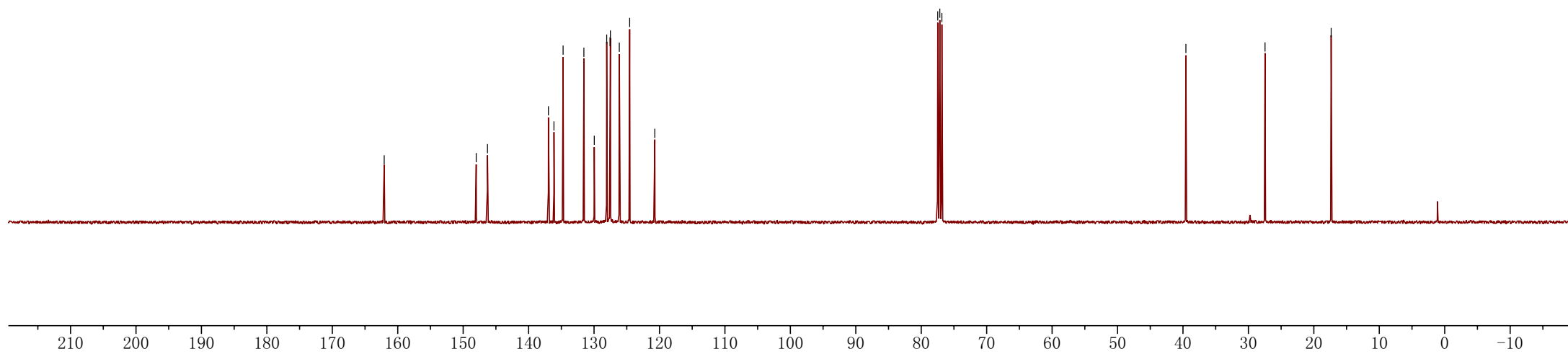
—77.16

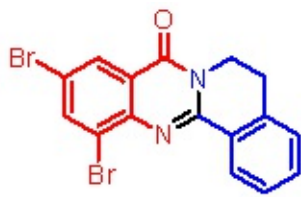
—76.84

—39.55

—27.46

—17.35



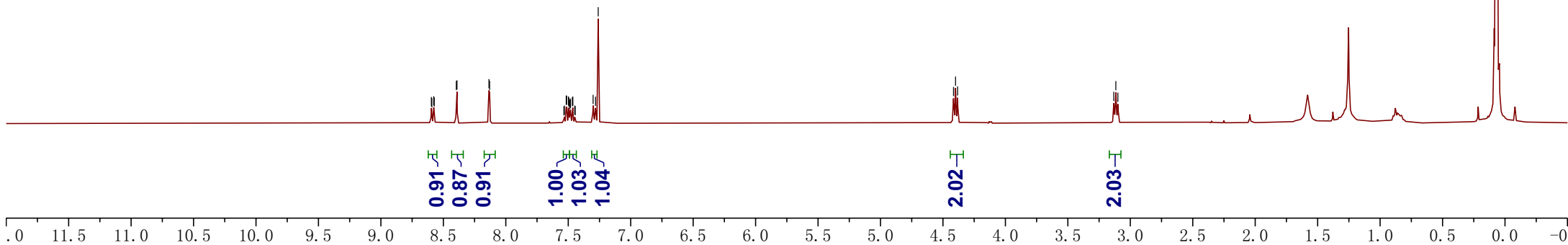
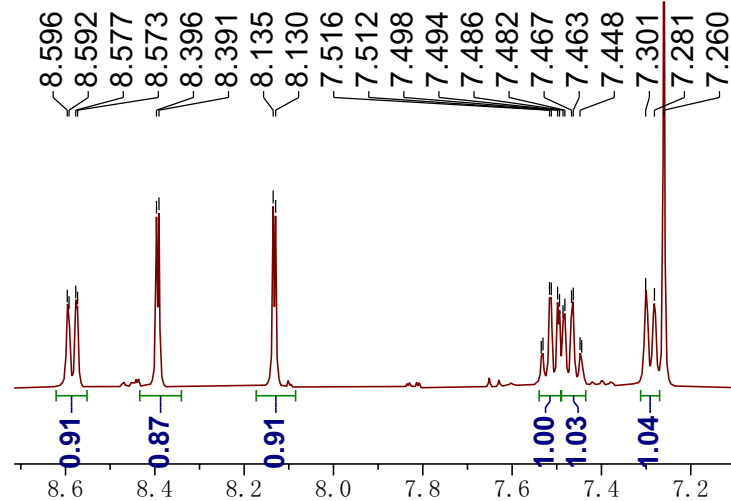


4n

$^1\text{H NMR}$ (400 MHz, CDCl_3)

8.596
8.592
8.577
8.573
8.396
8.391
8.135
8.130
7.535
7.531
7.516
7.512
7.498
7.494
7.486
7.482
7.467
7.463
7.448
7.444
7.301
7.281
7.260
4.415
4.399
4.383

3.132
3.116
3.100





4n

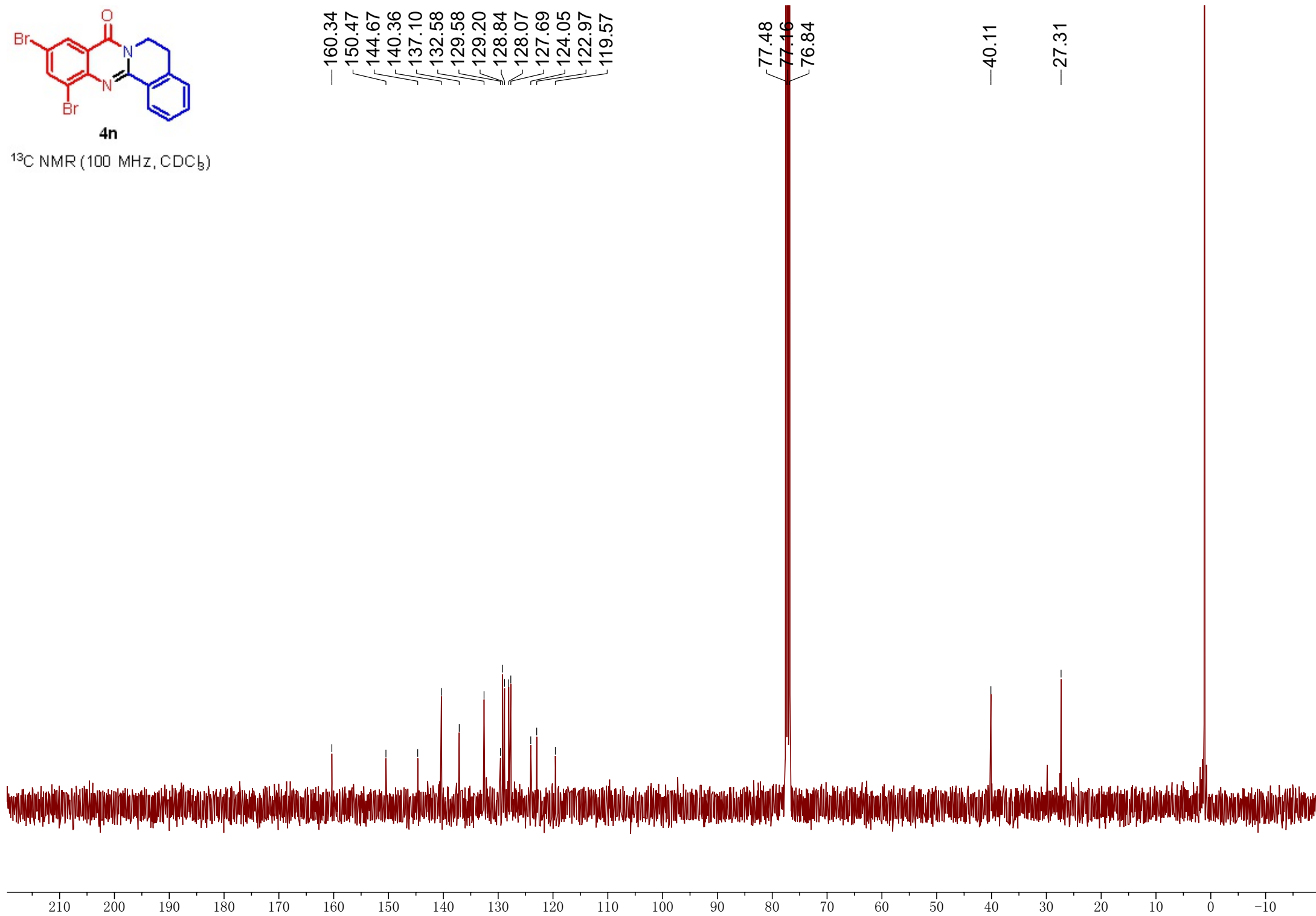
^{13}C NMR (100 MHz, CDCl_3)

160.34
150.47
144.67
140.36
137.10
132.58
129.58
129.20
128.84
128.07
127.69
124.05
122.97
119.57

77.48
77.16
76.84

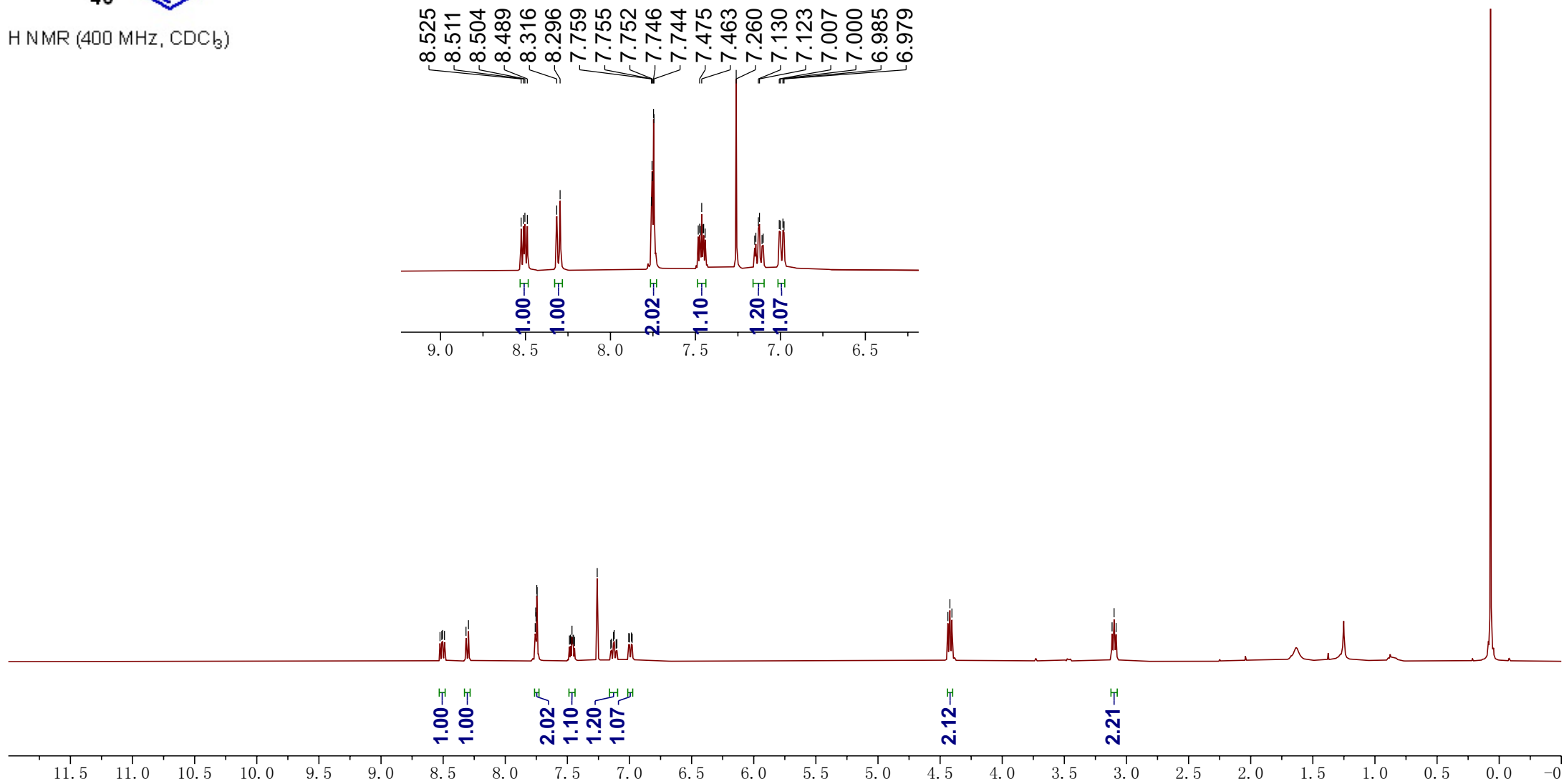
40.11

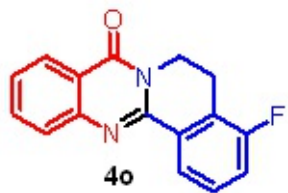
27.31





¹H NMR (400 MHz, CDCl₃)





^{13}C NMR (100 MHz, CDCl_3)

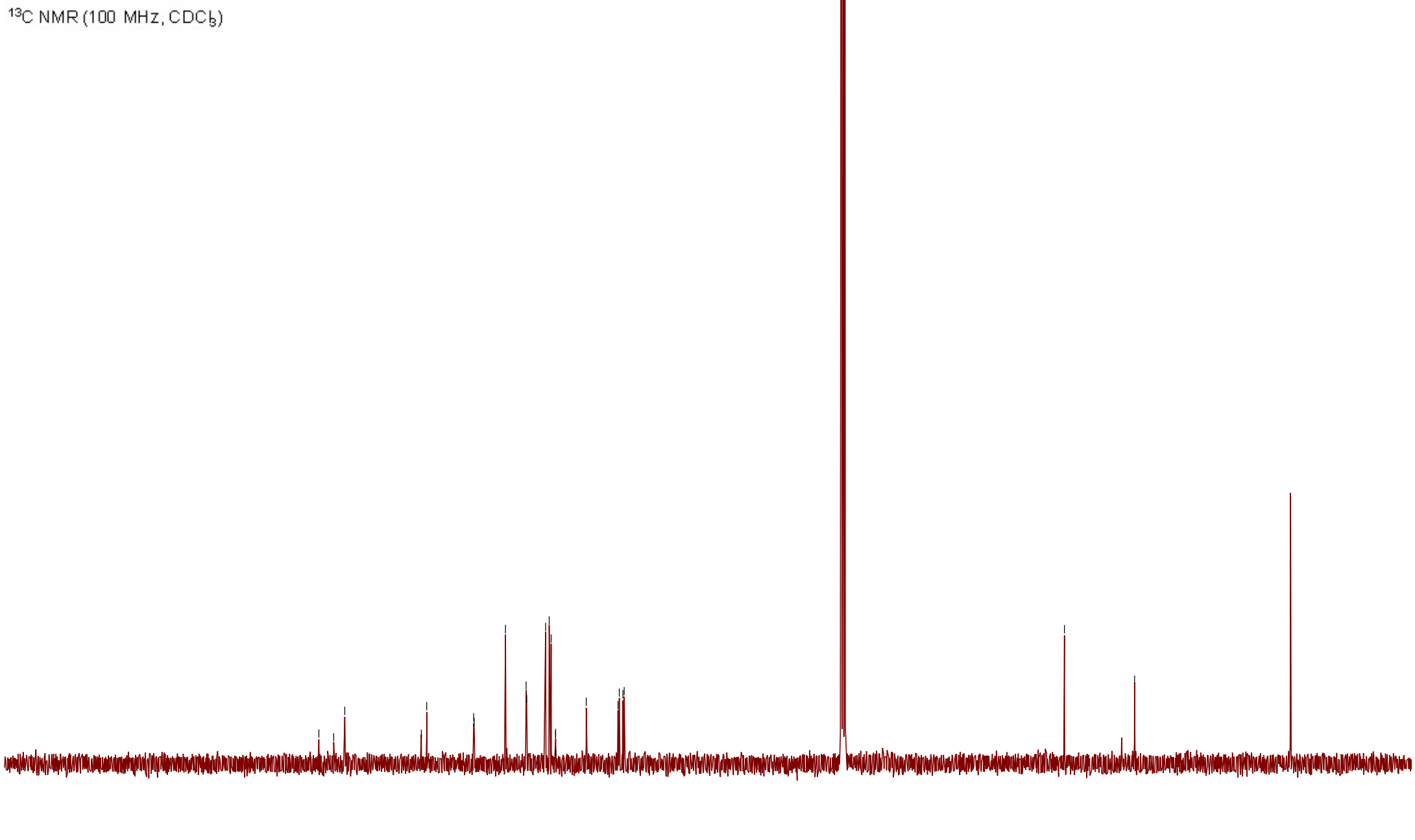
166.17
163.65
161.77

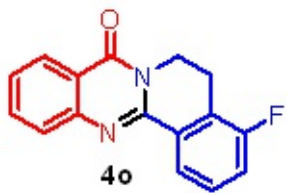
148.77
147.85
139.89
139.80
134.48
130.98
130.88
127.67
127.06
126.73
126.04
125.99
125.96
125.92
120.77
115.37
115.16
114.54
114.32

77.48
77.16
76.84

39.56

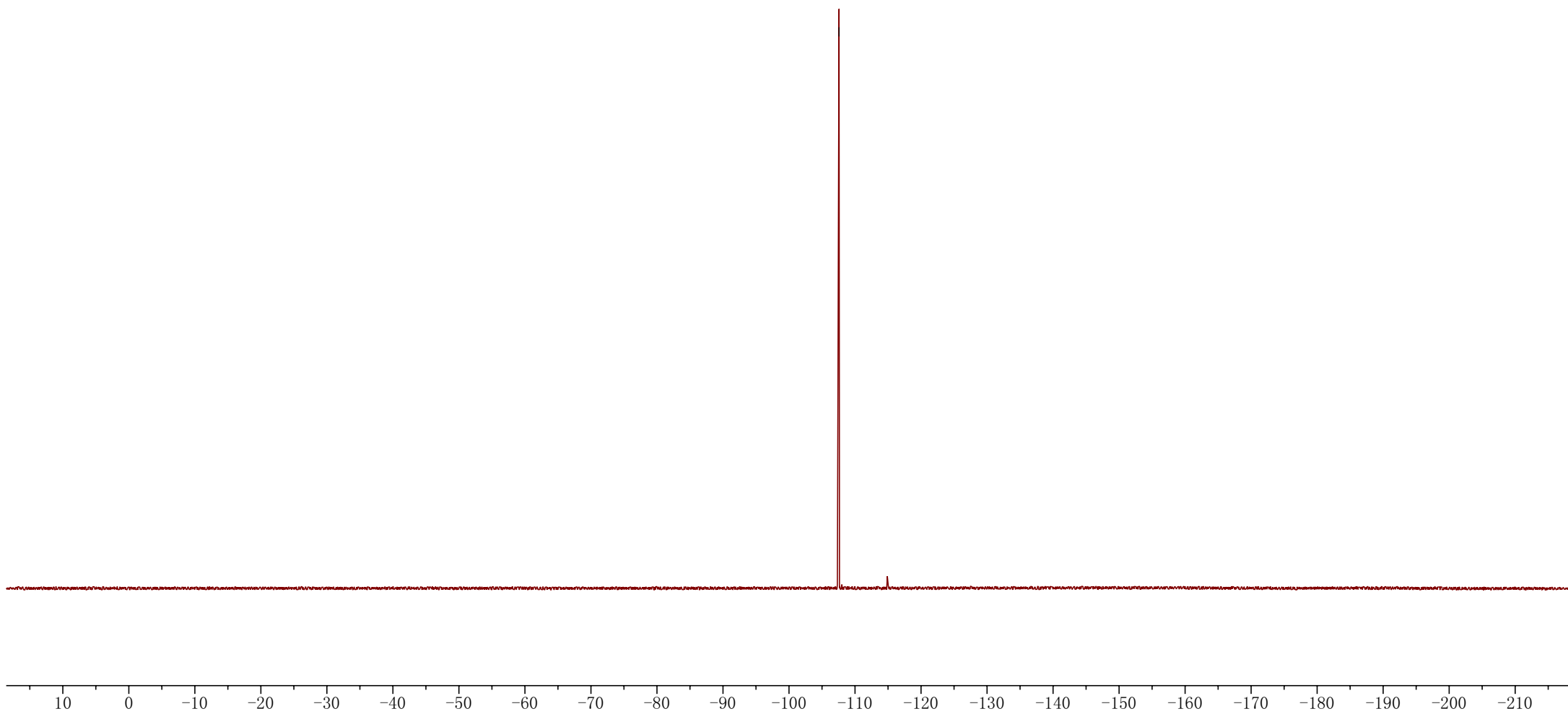
27.65

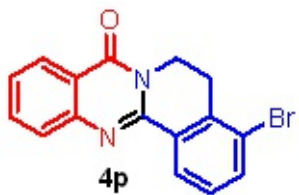




^{19}F NMR (376 MHz, CDCl_3)

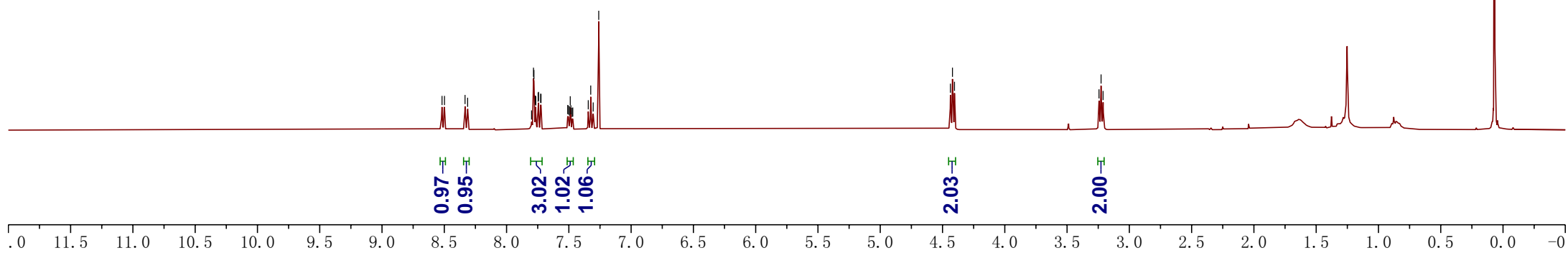
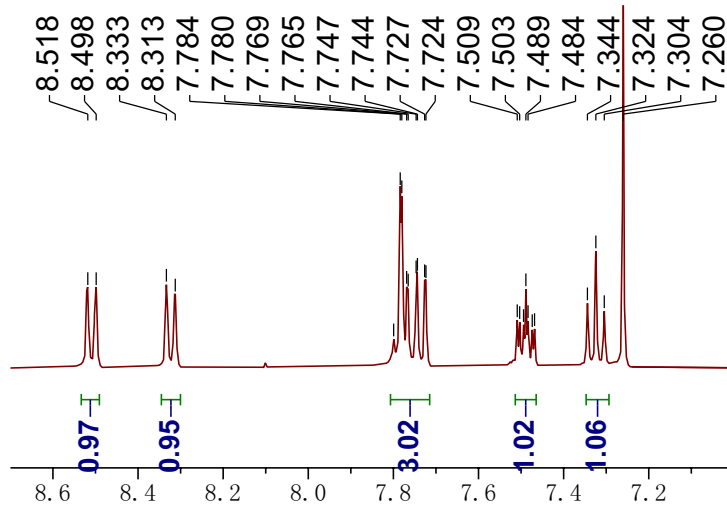
---107.579

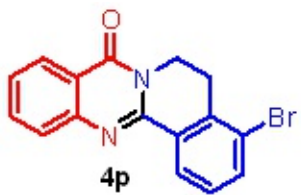




¹H NMR (400 MHz, CDCl₃)

8.518
8.498
8.333
8.313
7.799
7.784
7.780
7.769
7.765
7.747
7.744
7.727
7.724
7.509
7.503
7.494
7.489
7.484
7.484
7.474
7.468
7.344
7.324
7.304
7.260
4.436
4.420
4.404
3.244
3.227
3.211





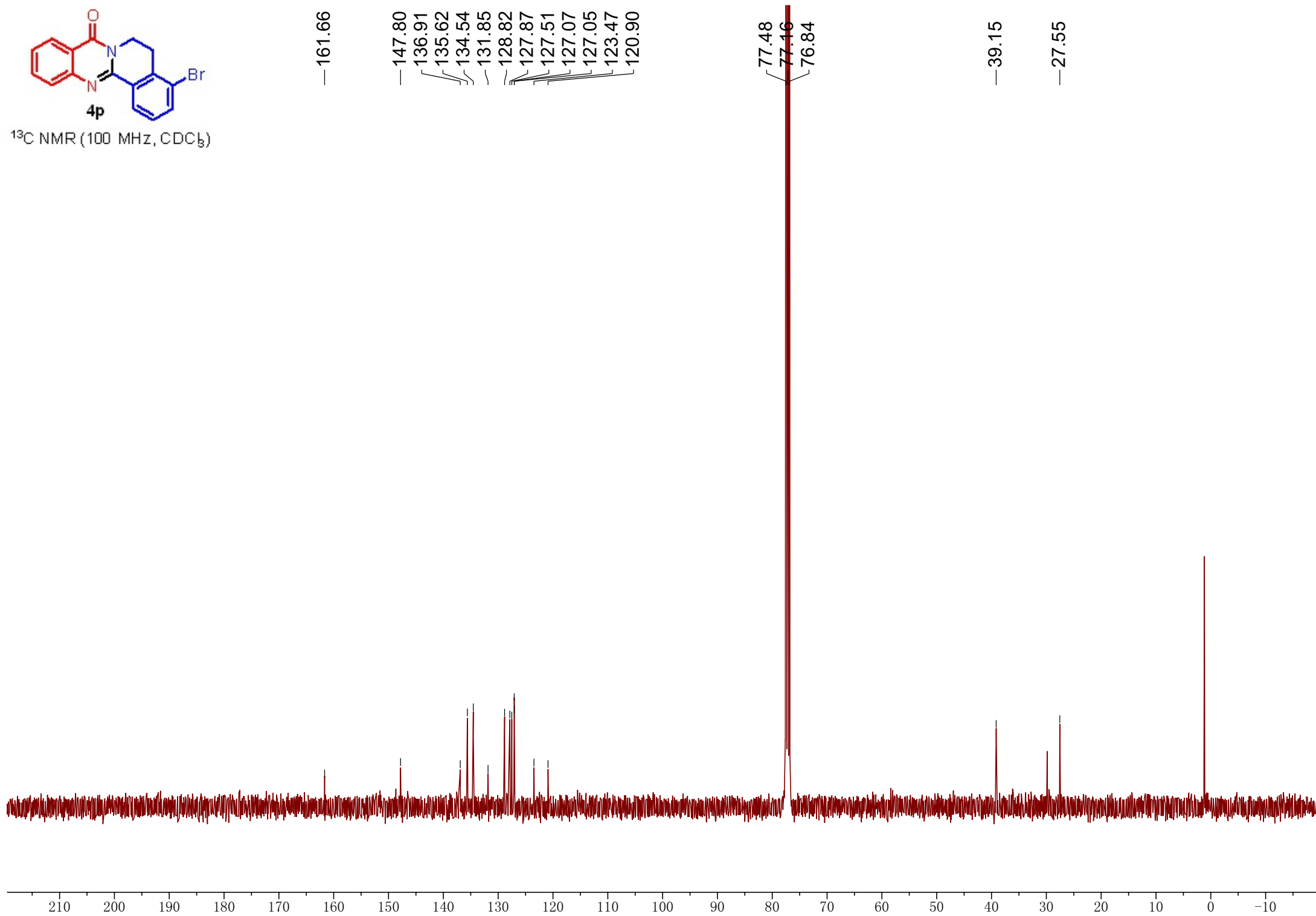
^{13}C NMR (100 MHz, CDCl_3)

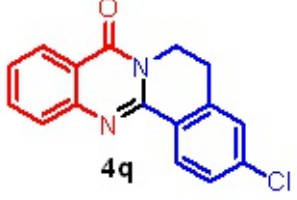
—161.66
—147.80
—136.91
—135.62
—134.54
—131.85
—128.82
—127.87
—127.51
—127.07
—127.05
—123.47
—120.90

77.48
77.16
76.84

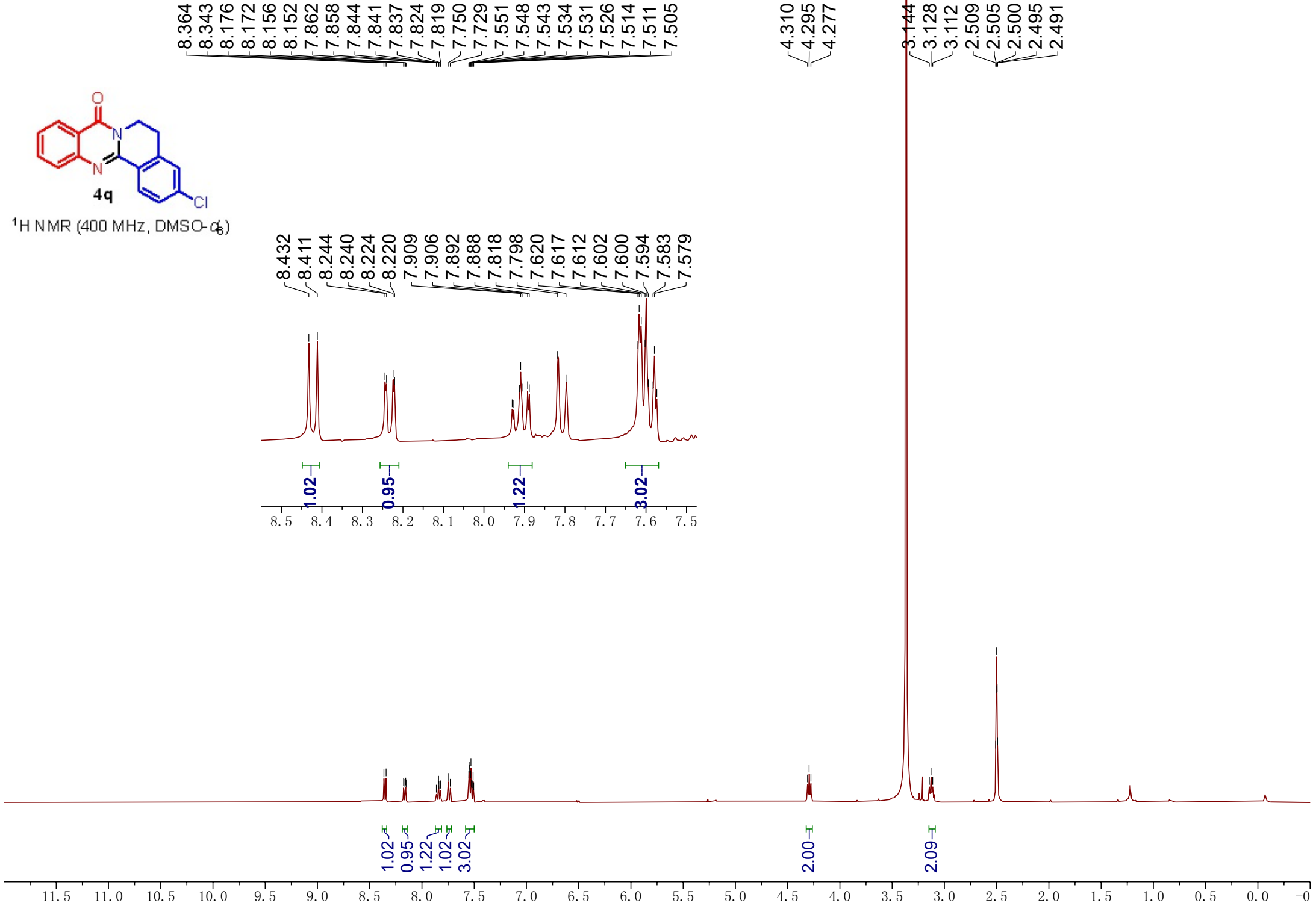
—39.15

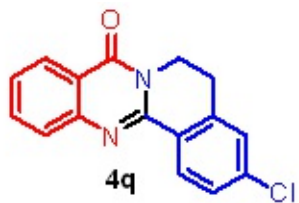
—27.55





¹H NMR (400 MHz, DMSO-d₆)





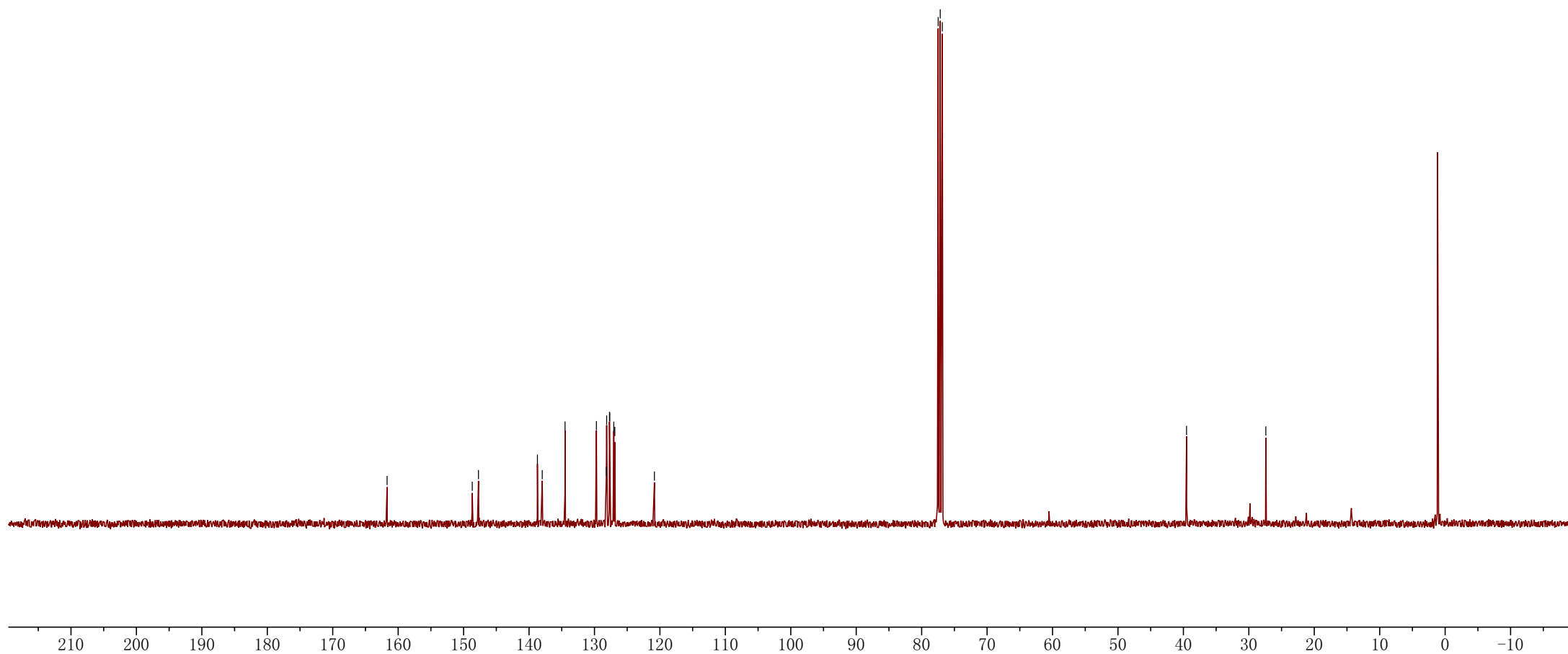
^{13}C NMR (100 MHz, CDCl_3)

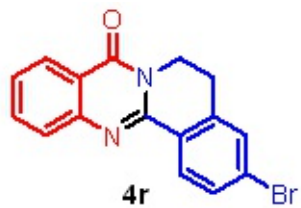
— 161.69
— 148.68
— 147.73
— 138.72
— 137.98
— 134.50
— 129.71
— 128.20
— 128.14
— 127.71
— 127.66
— 127.05
— 126.89
— 120.84

— 77.48
— 77.16
— 76.84

— 39.52

— 27.40

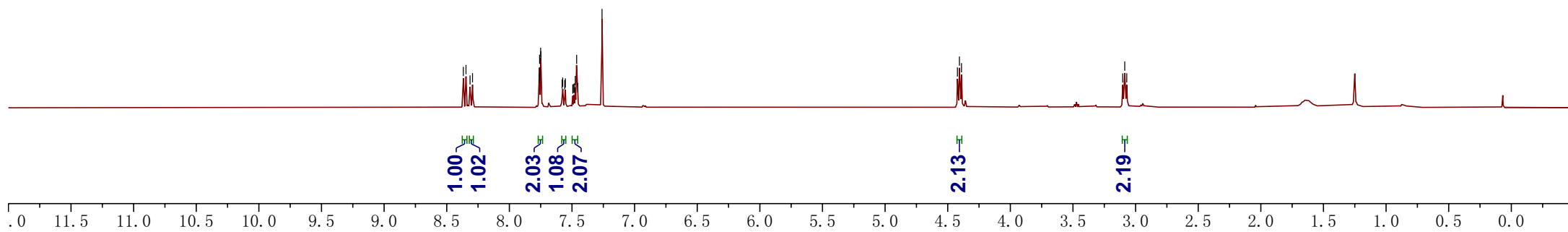
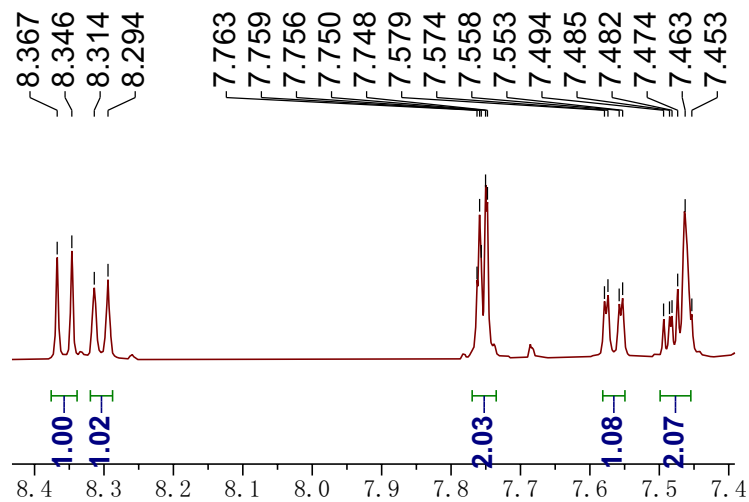


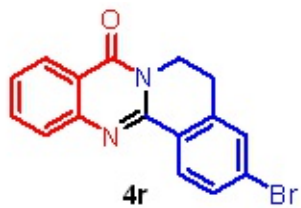


¹H NMR (400 MHz, CDCl₃)

8.367
8.346
8.314
8.294
7.763
7.759
7.756
7.750
7.748
7.579
7.574
7.558
7.553
7.494
7.485
7.482
7.474
7.463
7.453
7.260
4.422
4.407
4.390

3.103
3.087
3.070





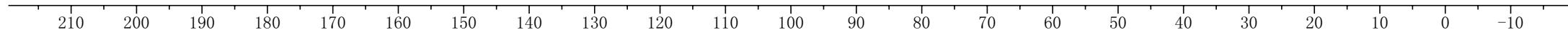
^{13}C NMR (100 MHz, CDCl_3)

—161.70
148.78
147.76
138.92
134.51
131.10
130.65
129.85
128.70
127.76
127.08
126.93
126.56
120.91

77.48
77.16
76.84

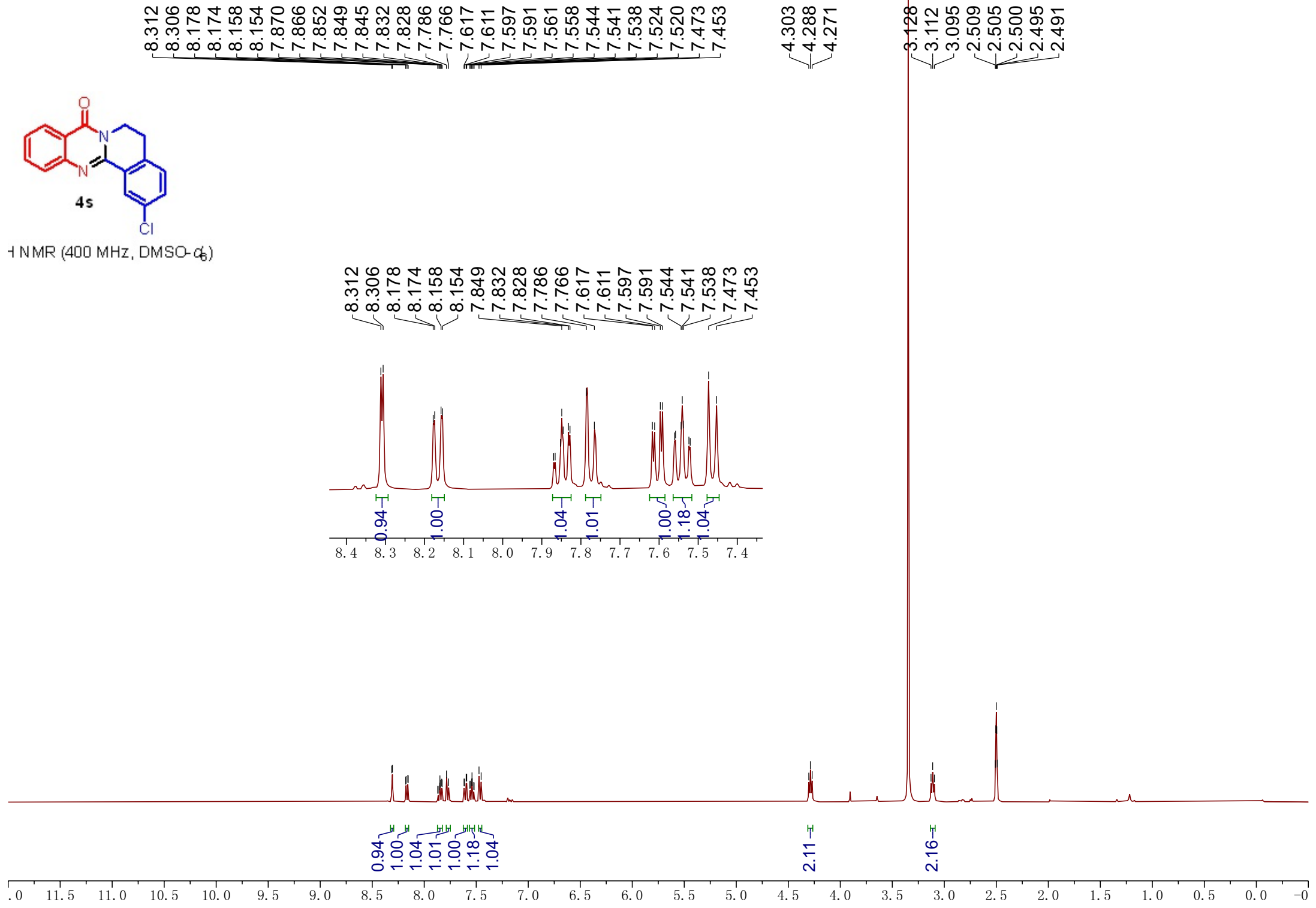
—39.55

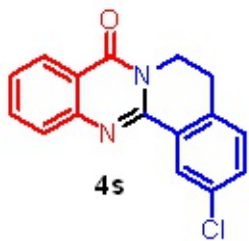
—27.36



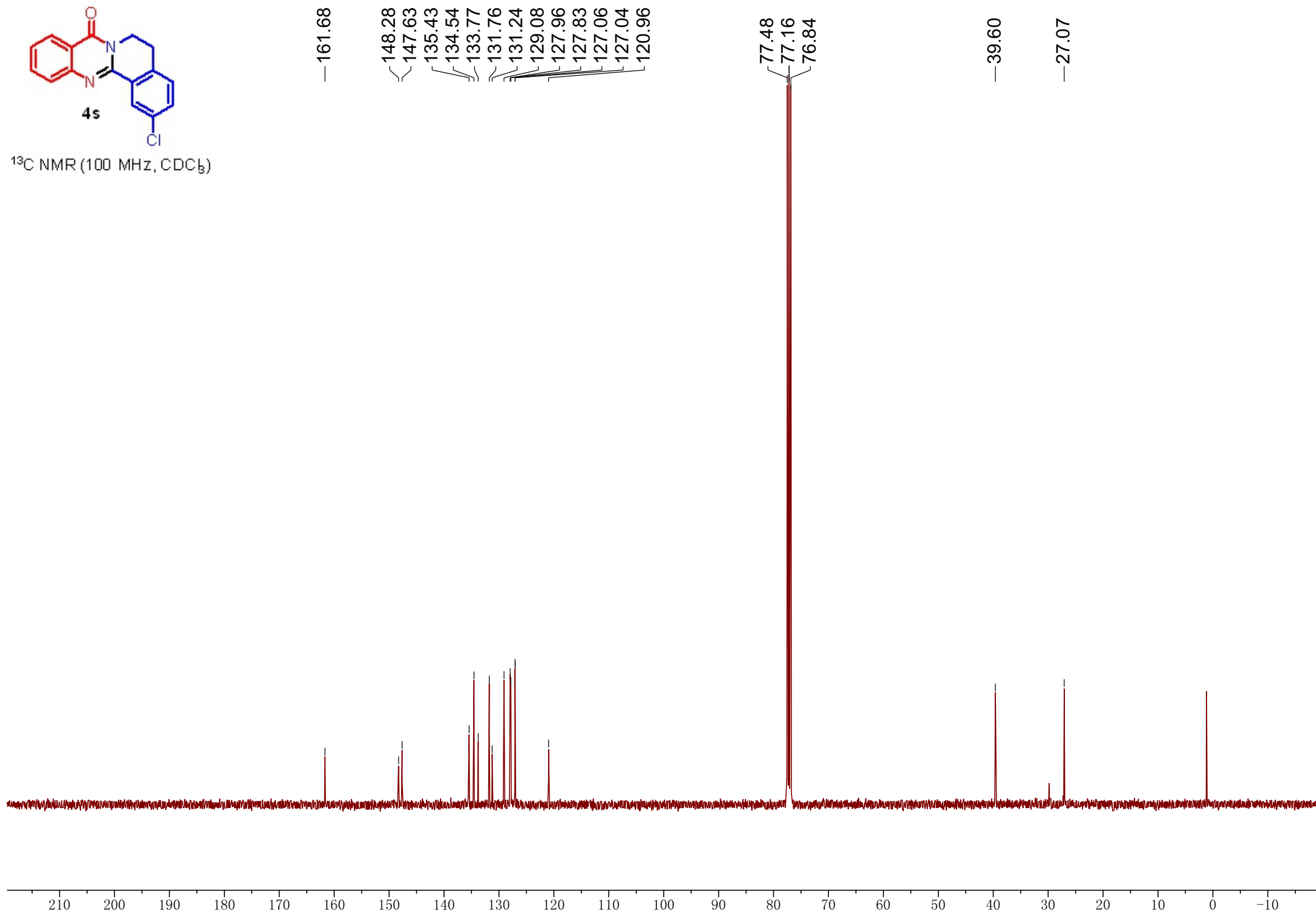


¹H NMR (400 MHz, DMSO-d₆)





^{13}C NMR (100 MHz, CDCl_3)

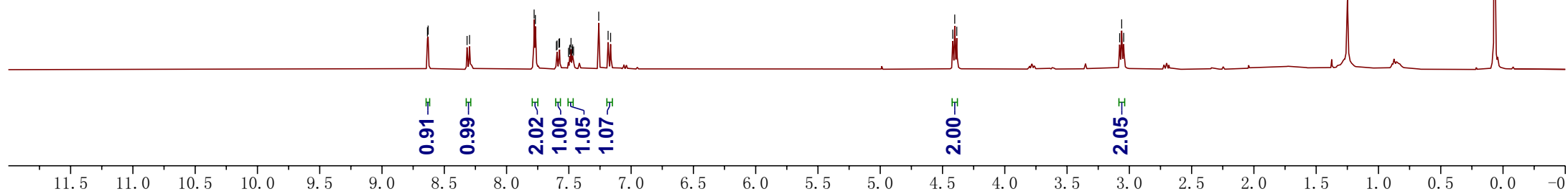
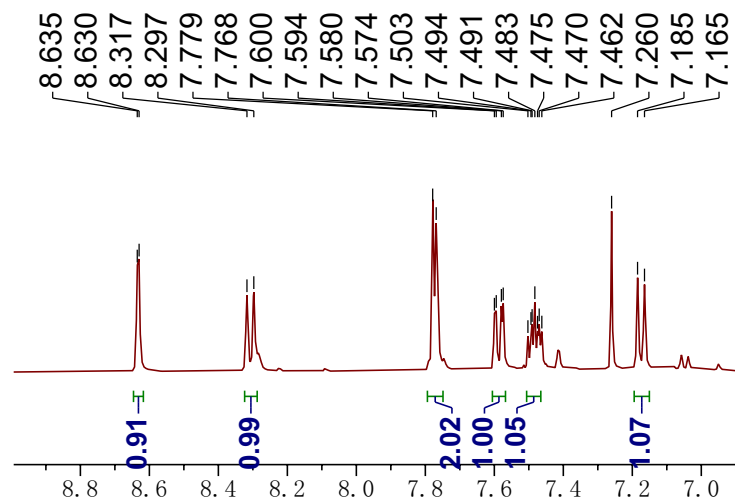




¹H NMR (400 MHz, CDCl₃)

8.635
8.630
8.317
8.297
7.779
7.768
7.600
7.594
7.580
7.574
7.503
7.494
7.491
7.483
7.475
7.470
7.462
7.260
7.185
7.165
4.418
4.402
4.386

3.078
3.062
3.045





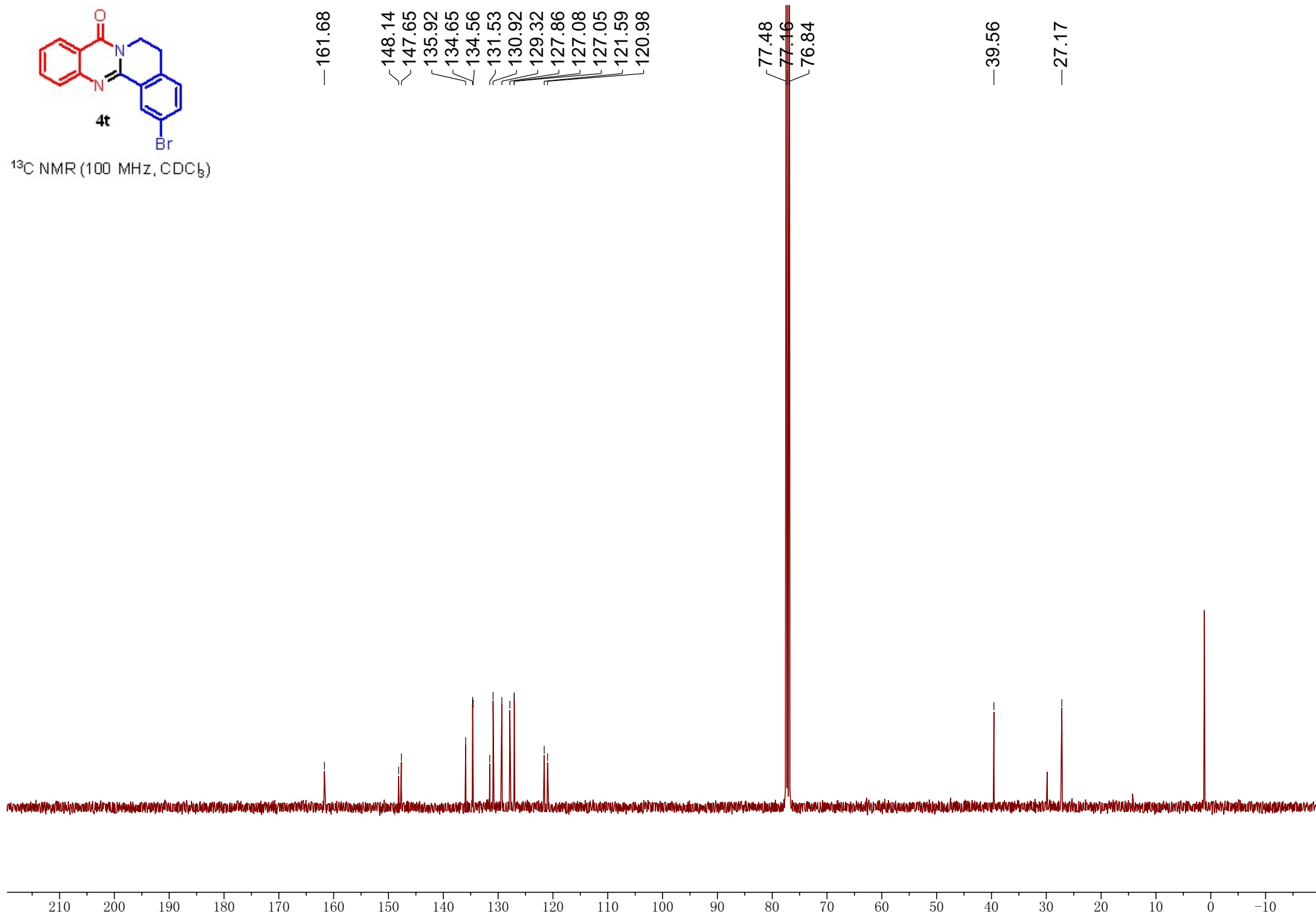
^{13}C NMR (100 MHz, CDCl_3)

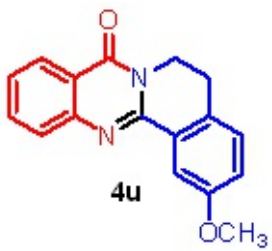
—161.68
148.14
147.65
135.92
134.65
134.56
131.53
130.92
129.32
127.86
127.08
127.05
121.59
120.98

77.48
77.16
76.84

—39.56

—27.17



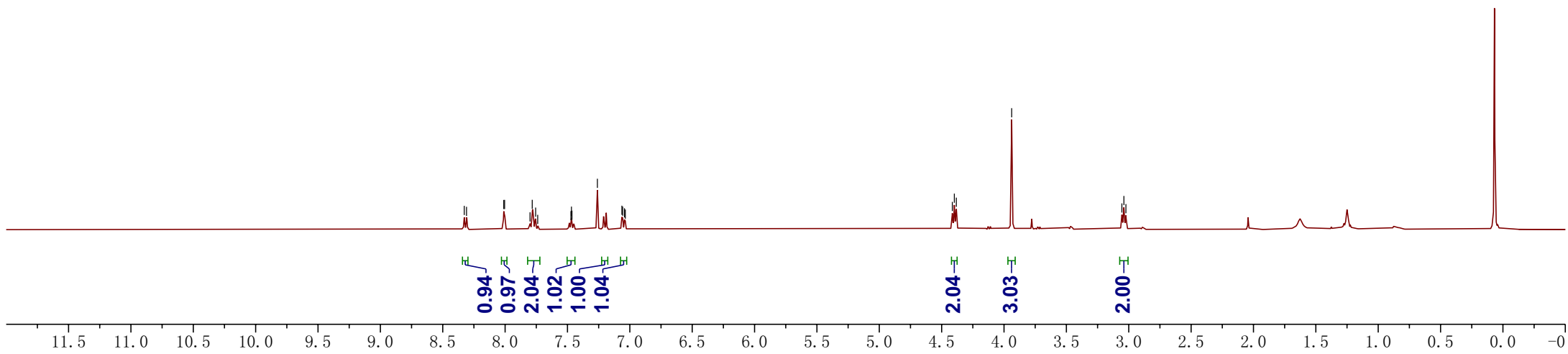
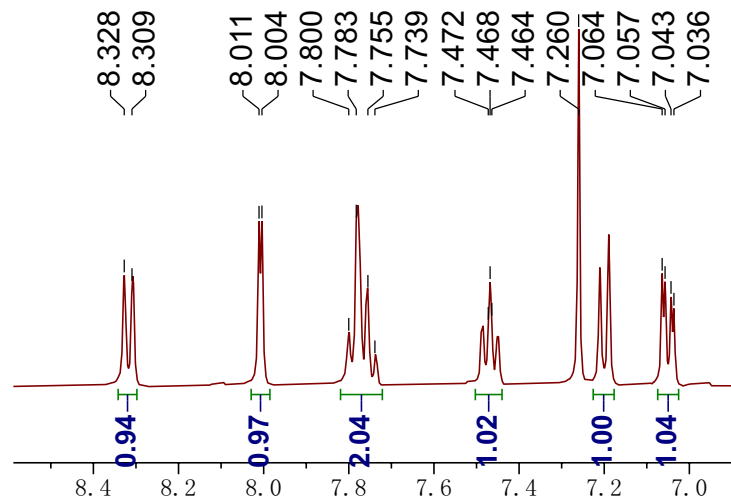


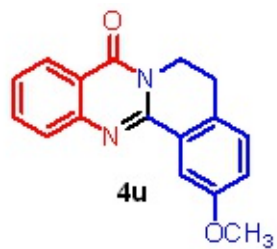
¹H NMR (400 MHz, CDCl₃)

8.328
8.309
8.011
8.004
7.800
7.783
7.755
7.739
7.472
7.468
7.464
7.260
7.064
7.057
7.043
7.036

4.415
4.398
4.382
—
3.939

3.055
3.039
3.023





^{13}C NMR (100 MHz, CDCl_3)

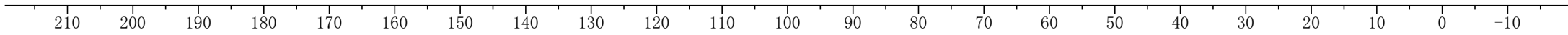
161.91
159.20
149.46
147.83
134.37
130.57
129.60
128.78
127.72
127.02
126.72
120.92
119.42
111.40

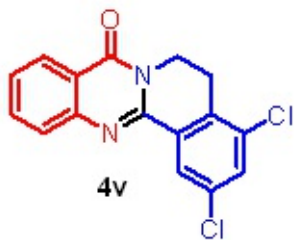
77.48
77.16
76.84

55.78

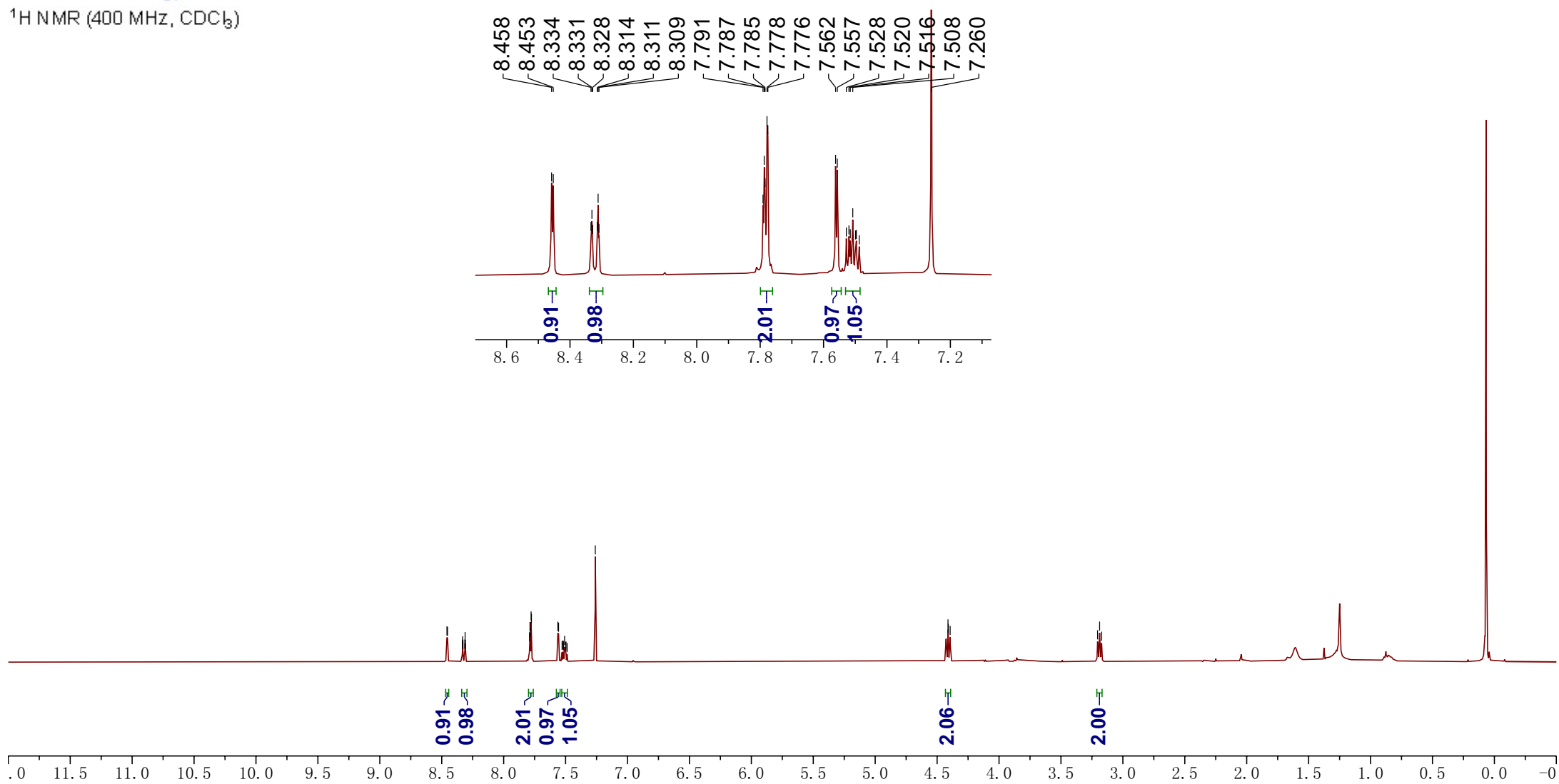
40.04

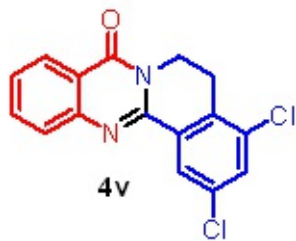
26.76



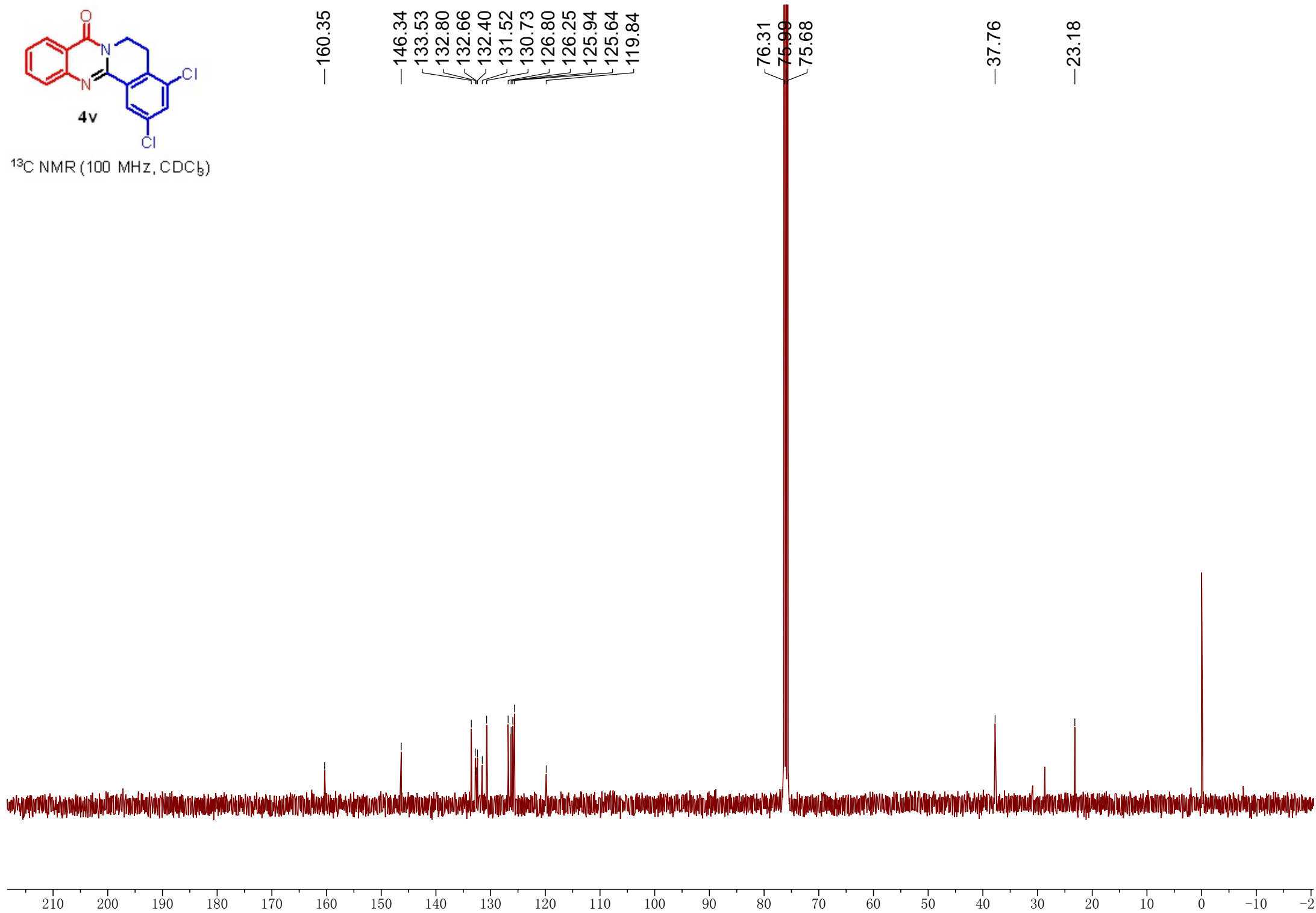


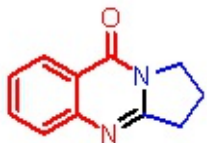
¹H NMR (400 MHz, CDCl₃)





^{13}C NMR (100 MHz, CDCl_3)



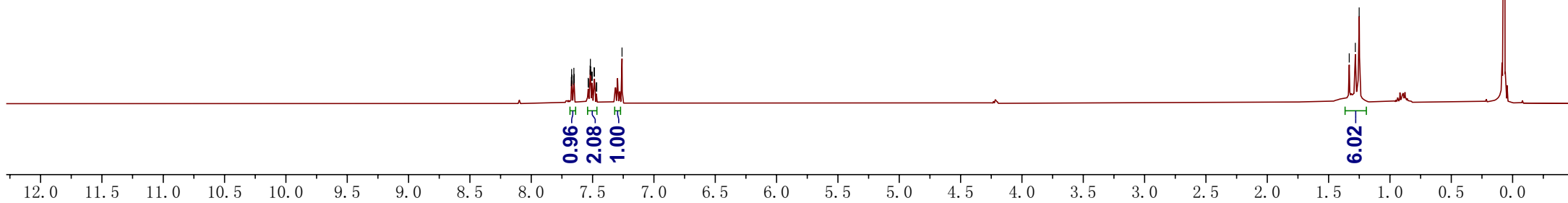
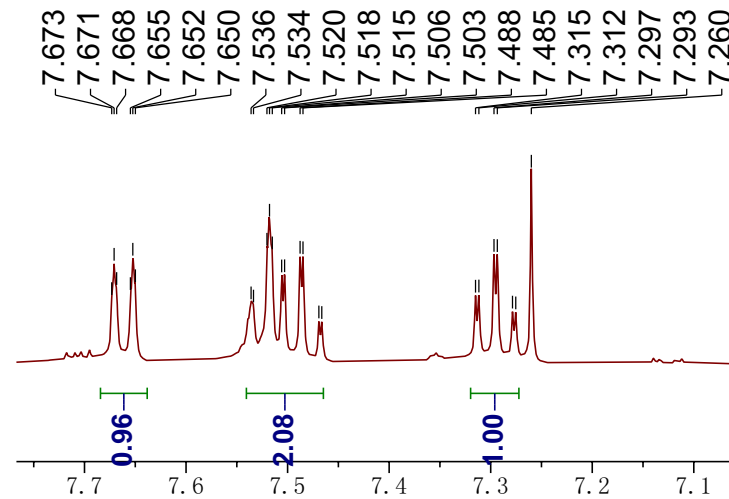


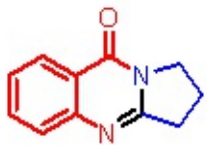
4w

^1H NMR (400 MHz, CDCl_3)

7.673
7.671
7.668
7.655
7.652
7.650
7.536
7.534
7.520
7.518
7.515
7.506
7.503
7.488
7.485
7.469
7.466
7.260

1.332
1.282
1.251





4w

^{13}C NMR (100 MHz, CDCl_3)

— 144.59

— 134.85

— 134.31

— 129.24

— 124.49

— 120.46

— 77.48

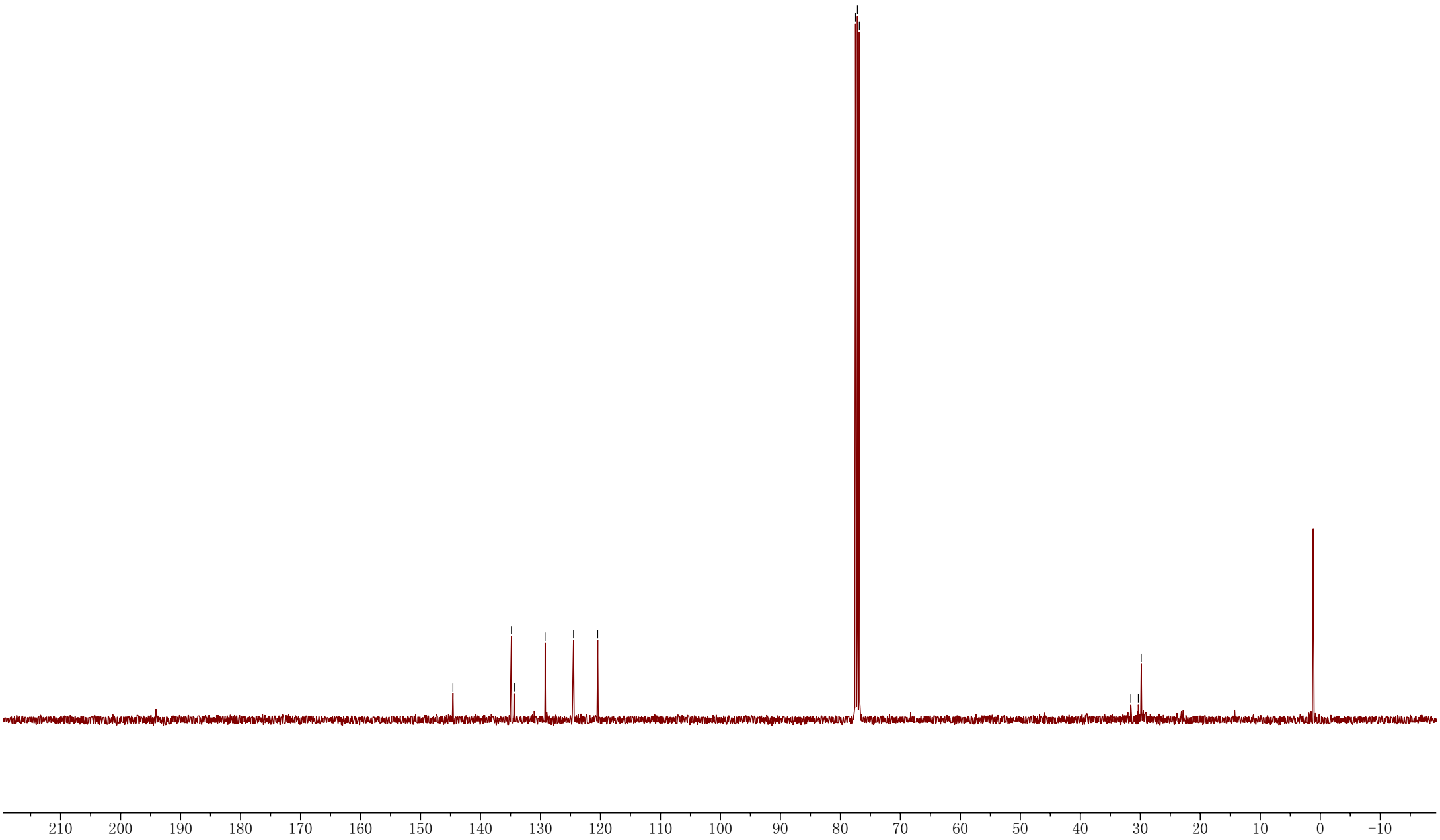
— 77.16

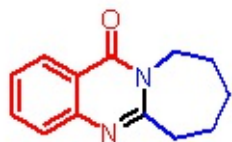
— 76.84

— 31.58

— 30.33

— 29.85





4x

¹H NMR (400 MHz, CDCl₃)

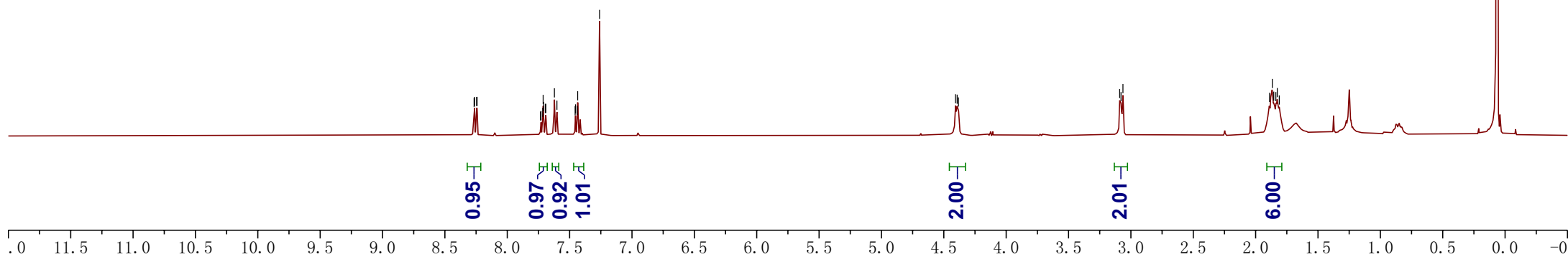
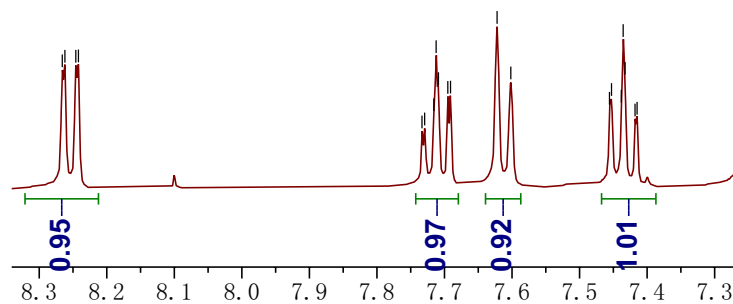
8.266
8.262
8.246
8.242
7.733
7.729
7.716
7.712
7.709
7.695
7.691
7.622
7.602
7.456
7.453
7.438
7.435
7.260

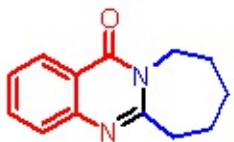
4.406
4.393
4.383

3.090
3.079
3.064

1.888
1.866
1.855
1.838
1.827
1.810

8.266
8.262
8.246
8.242
7.733
7.729
7.716
7.712
7.709
7.695
7.691
7.622
7.602
7.456
7.453
7.438
7.435
7.433
7.418
7.415





4x

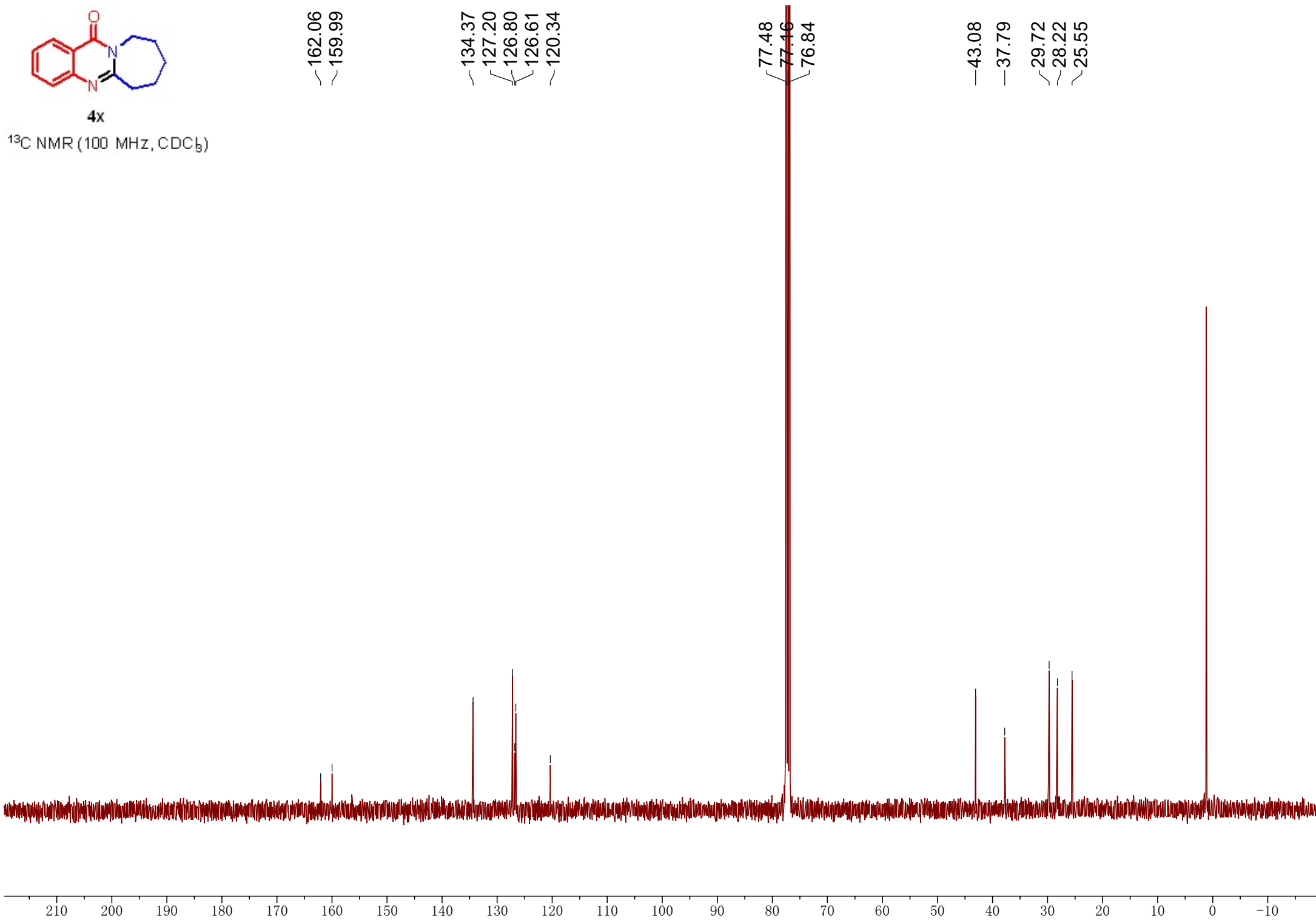
^{13}C NMR (100 MHz, CDCl_3)

~162.06
~159.99

~134.37
~127.20
~126.80
~126.61
~120.34

77.48
77.16
76.84

~43.08
~37.79
~29.72
~28.22
~25.55



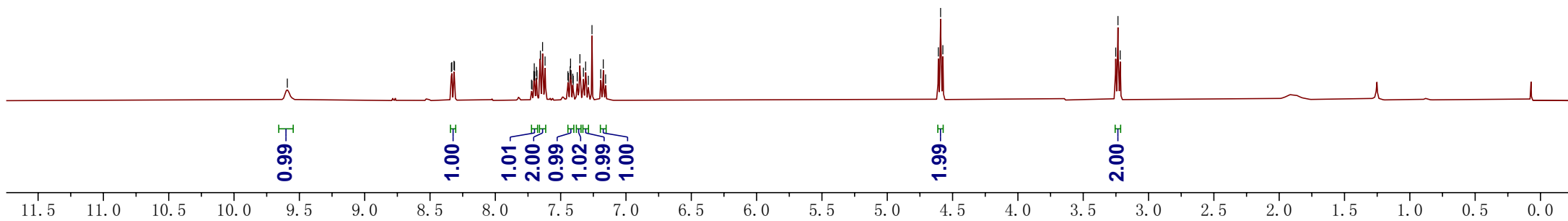
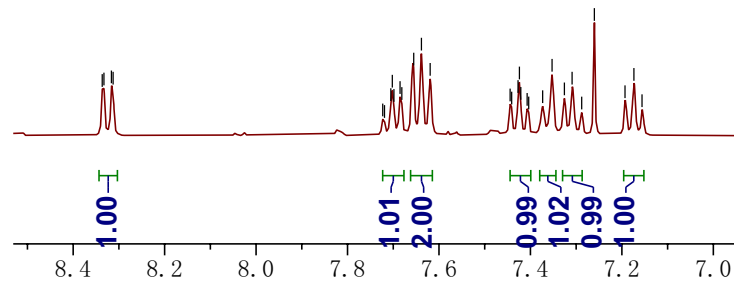


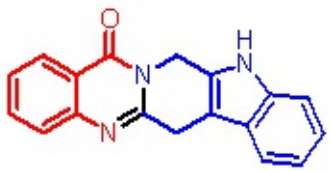
—9.592

¹H NMR (400 MHz, CDCl₃)

8.336
8.333
8.316
8.313
7.723
7.719
7.705
7.702
7.699
7.685
7.681
7.655
7.638
7.619
7.444
7.441
7.427
7.424
7.421
7.407
7.404
7.373
7.353
7.326
7.309
7.288
7.260
7.193
7.174
7.156
4.609
4.592
4.574
3.251
3.234
3.217

8.336
8.333
8.316
8.313
7.705
7.702
7.685
7.681
7.655
7.638
7.619
7.427
7.424
7.421
7.353
7.326
7.309
7.260
7.193
7.174





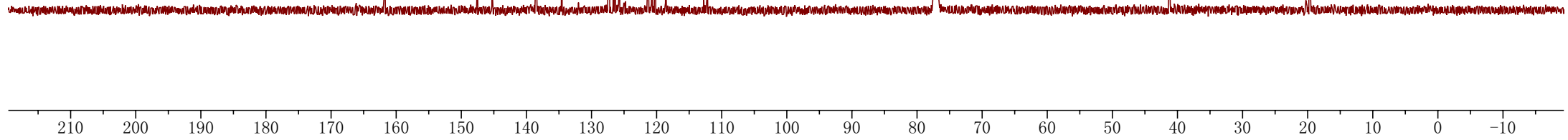
^{13}C NMR (100 MHz, CDCl_3)

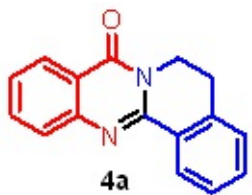
161.74
147.53
145.28
138.49
134.53
127.40
127.23
126.62
126.38
125.71
125.69
121.26
120.72
120.20
118.61
112.27

77.48
77.16
76.84

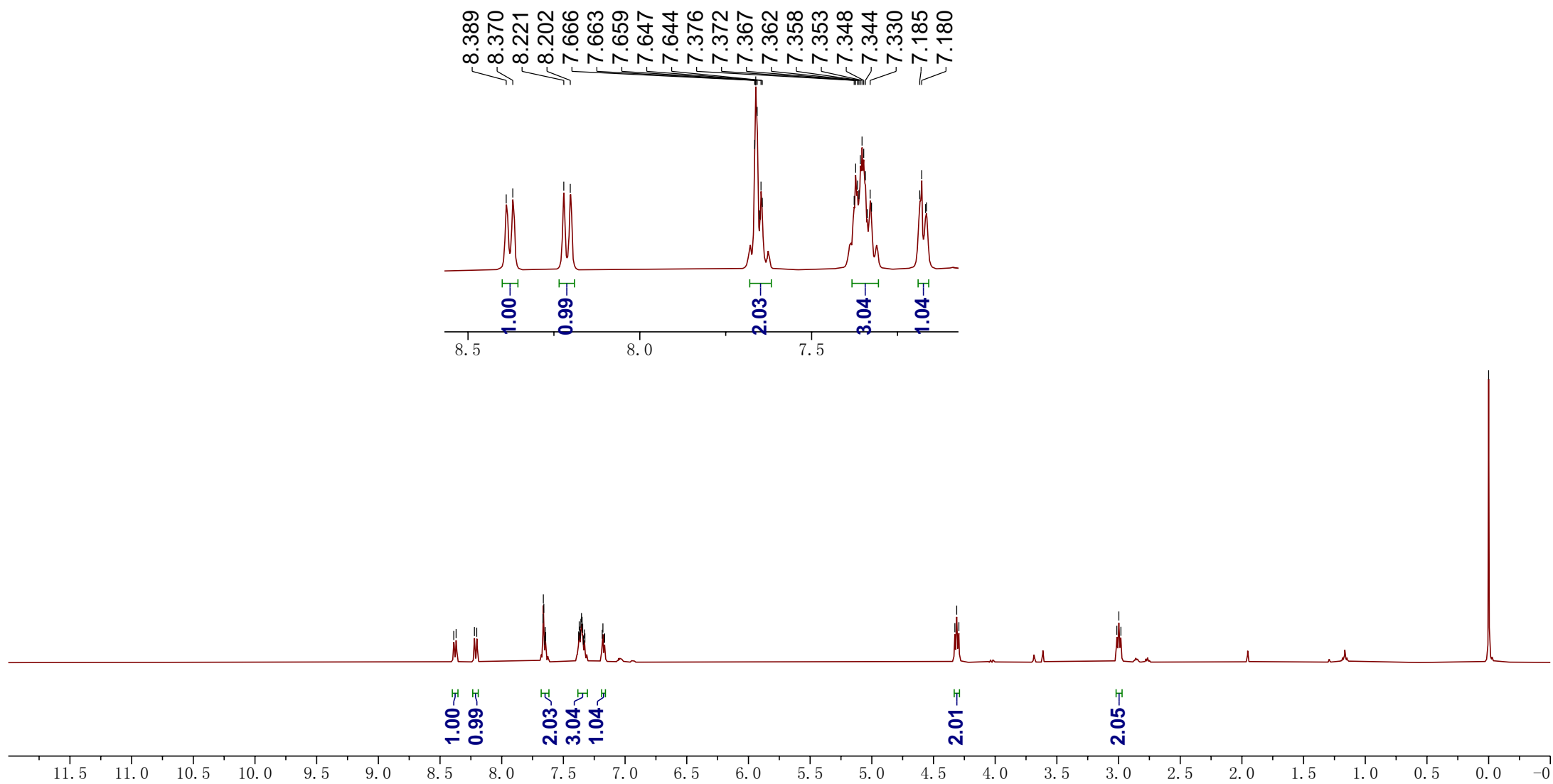
41.29

19.79





¹H NMR (400 MHz, CDCl₃)





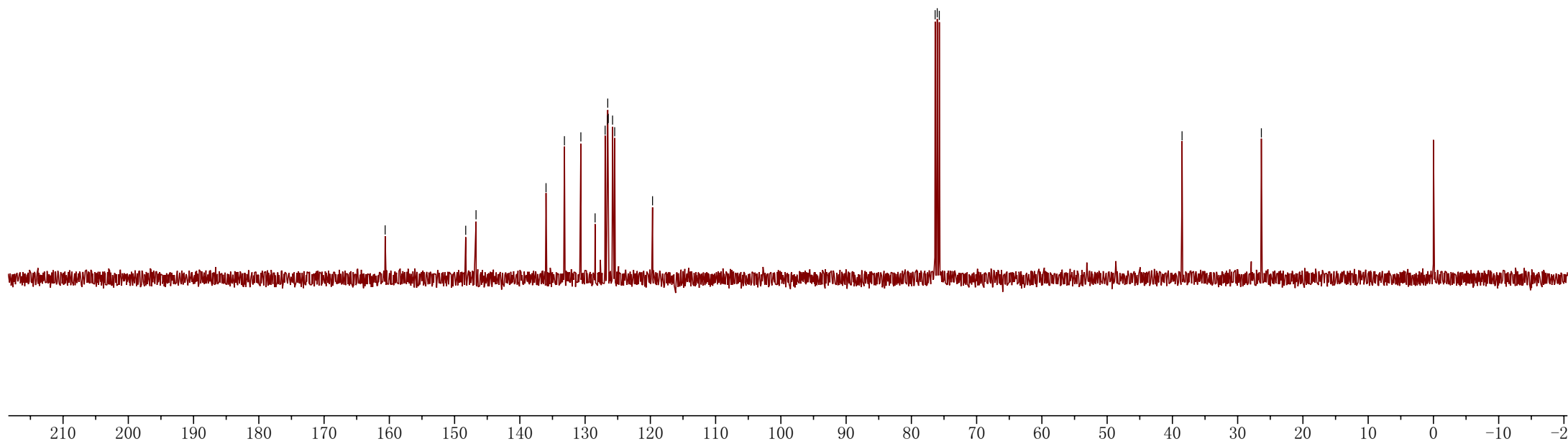
^{13}C NMR (100 MHz, CDCl_3)

—160.64
—148.29
—146.71
—135.99
—133.17
—130.65
—128.47
—126.93
—126.56
—126.53
—126.45
—125.79
—125.47
—119.66

—76.36
—76.04
—75.72

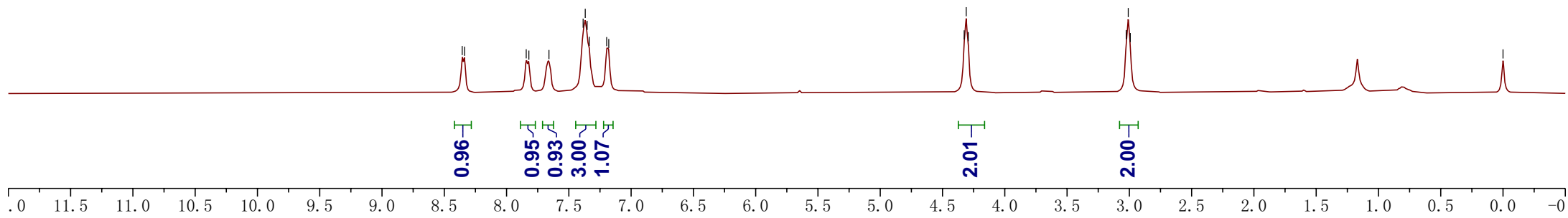
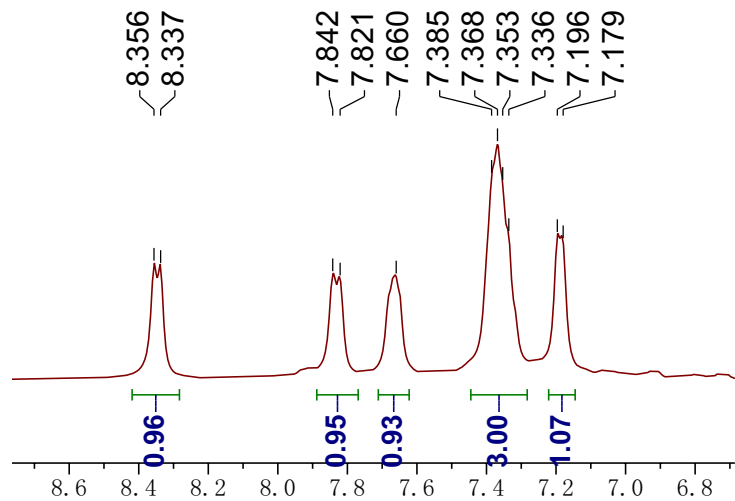
—38.52

—26.37





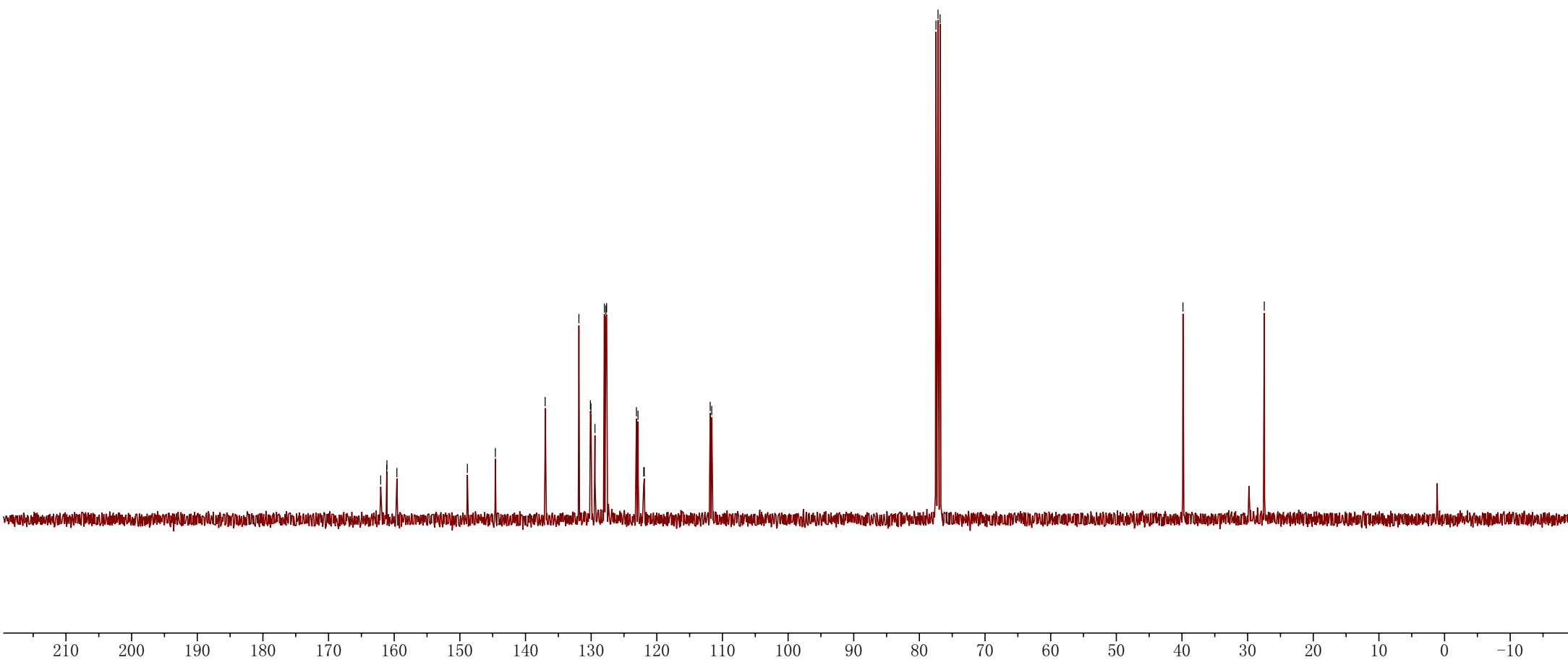
¹H NMR (400 MHz, CDCl₃)





4b

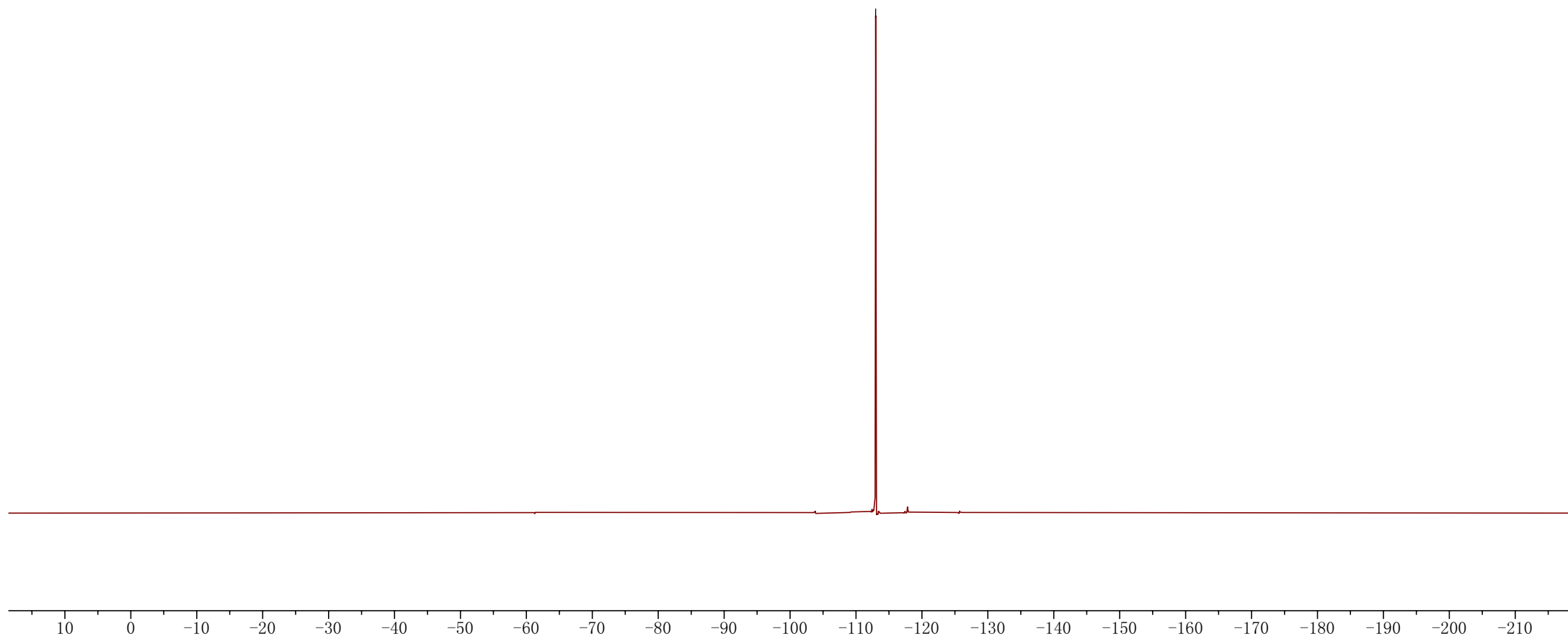
^{13}C NMR (100 MHz, CDCl_3)

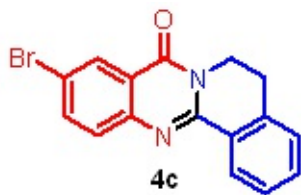




^{19}F NMR (376 MHz, CDCl_3)

---112.98



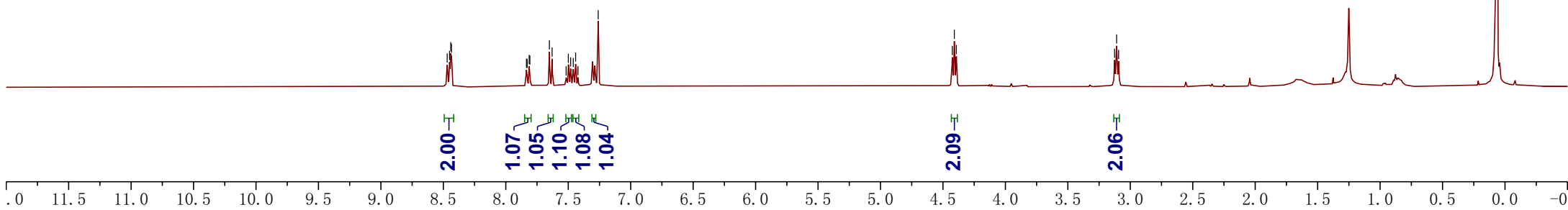
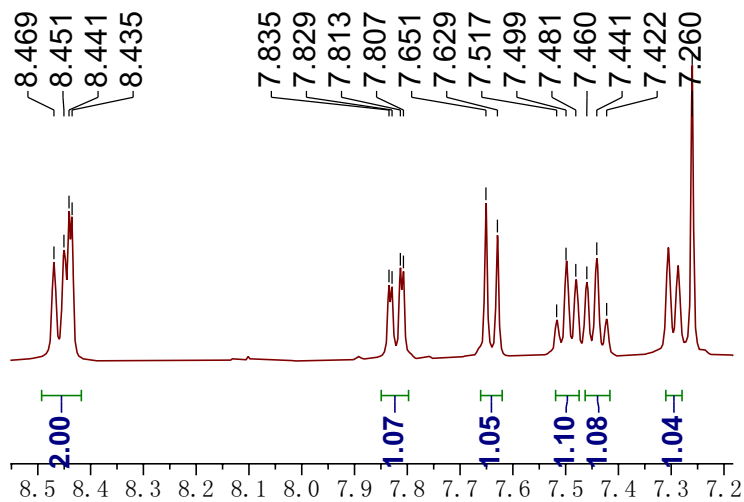


¹H NMR (400 MHz, CDCl₃)

8.469
8.451
8.441
8.435
7.835
7.829
7.813
7.807
7.651
7.629
7.517
7.499
7.481
7.460
7.441
7.422
7.260

4.425
4.409
4.393

3.126
3.110
3.093





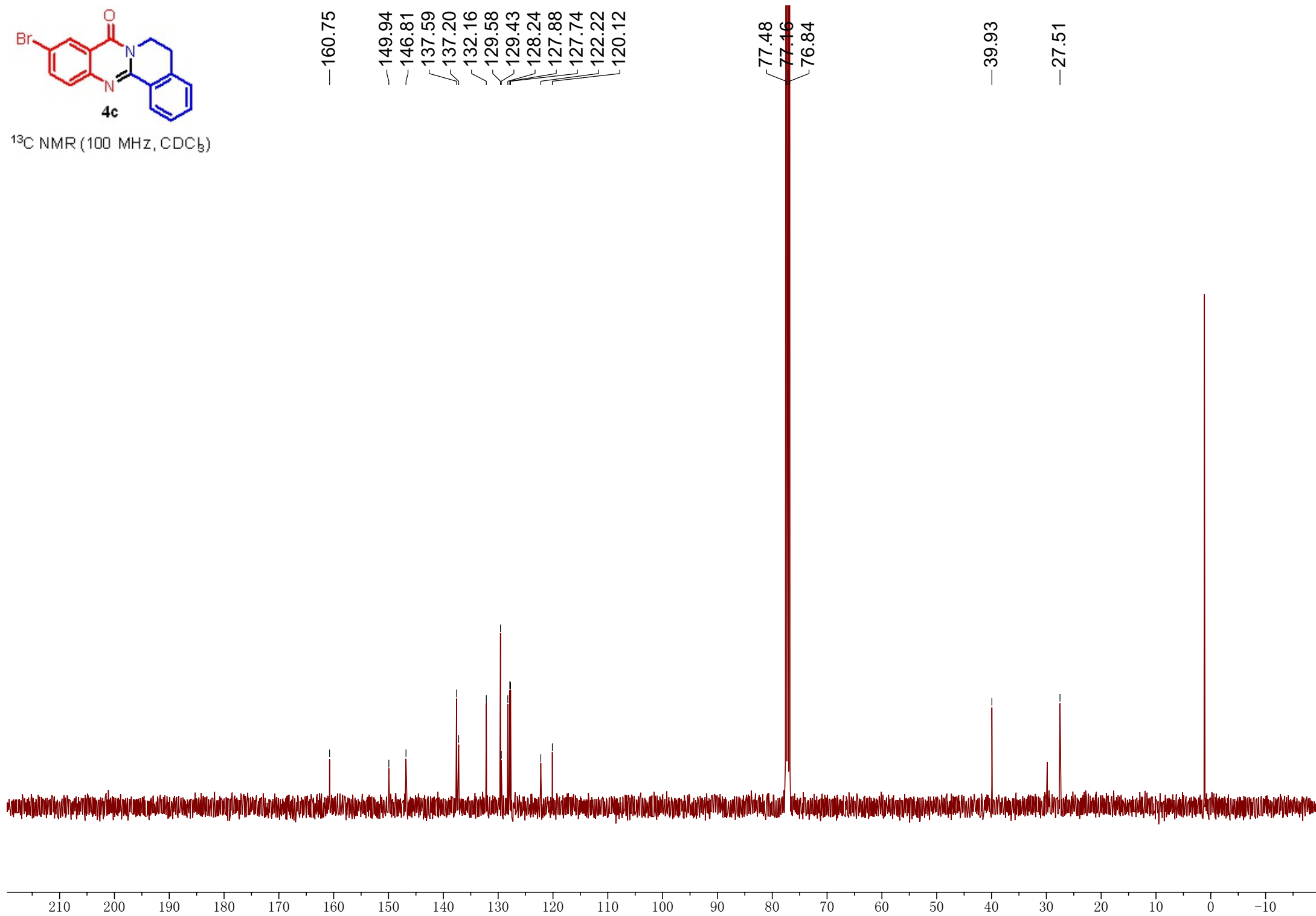
^{13}C NMR (100 MHz, CDCl_3)

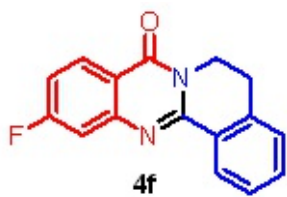
— 160.75
— 149.94
— 146.81
137.59
137.20
132.16
129.58
129.43
128.24
127.88
127.74
122.22
120.12

77.48
77.16
76.84

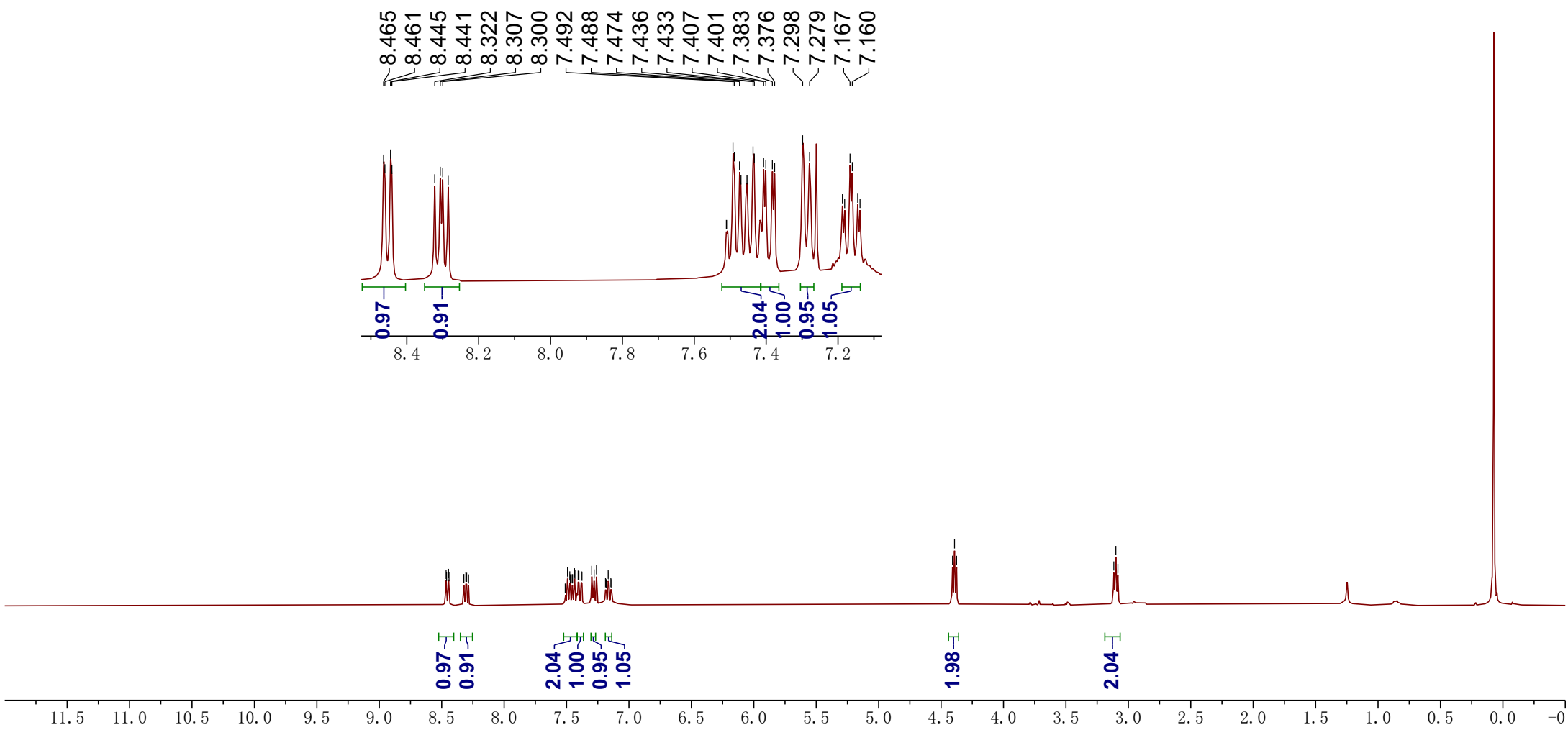
— 39.93

— 27.51





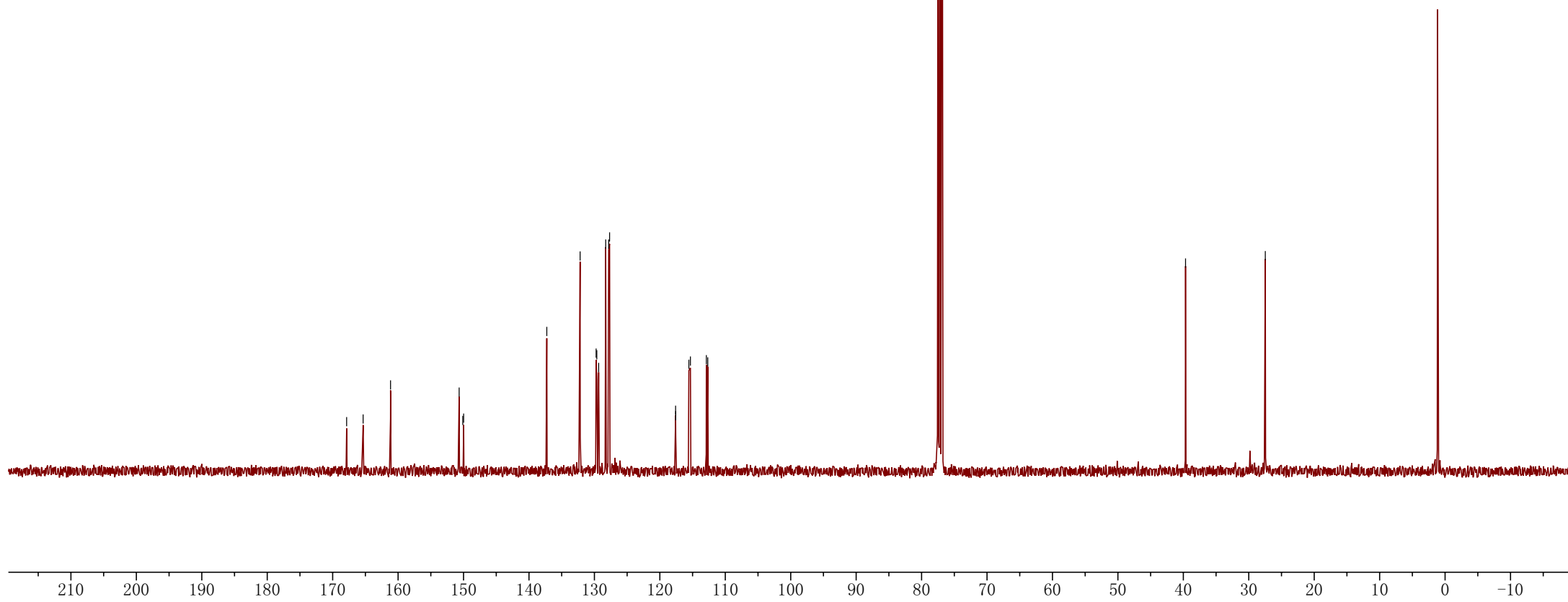
¹H NMR (400 MHz, CDCl₃)





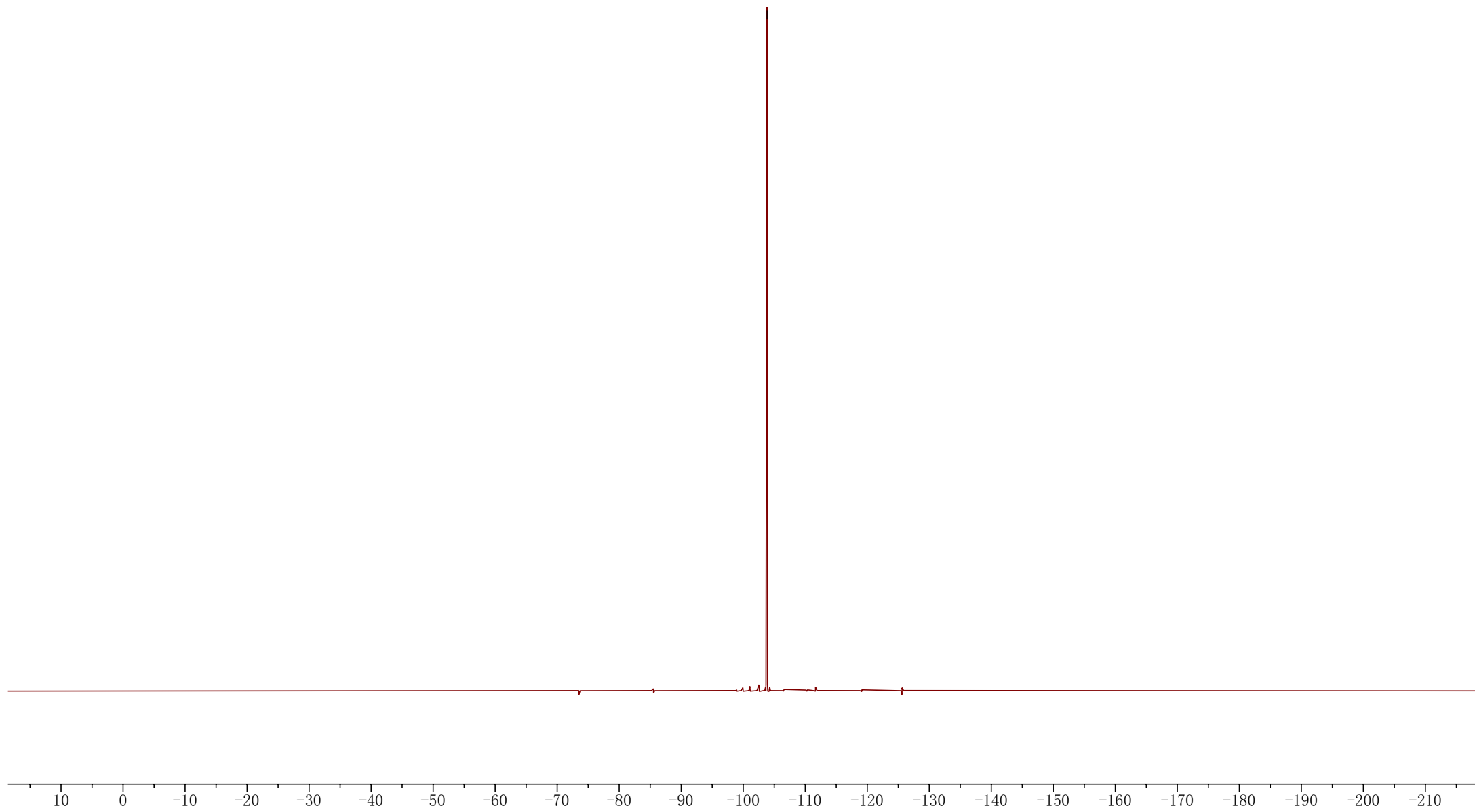
^{13}C NMR (100 MHz, CDCl_3)

- 167.87
- 165.35
- 161.16
- 150.67
- 150.12
- 149.98
- 137.28
- 132.19
- 129.74
- 129.63
- 129.35
- 128.27
- 127.82
- 127.68
- 117.59
- 117.57
- 115.56
- 115.33
- 112.89
- 112.68
- 77.48
- 77.16
- 76.84
- 39.66
- 27.47



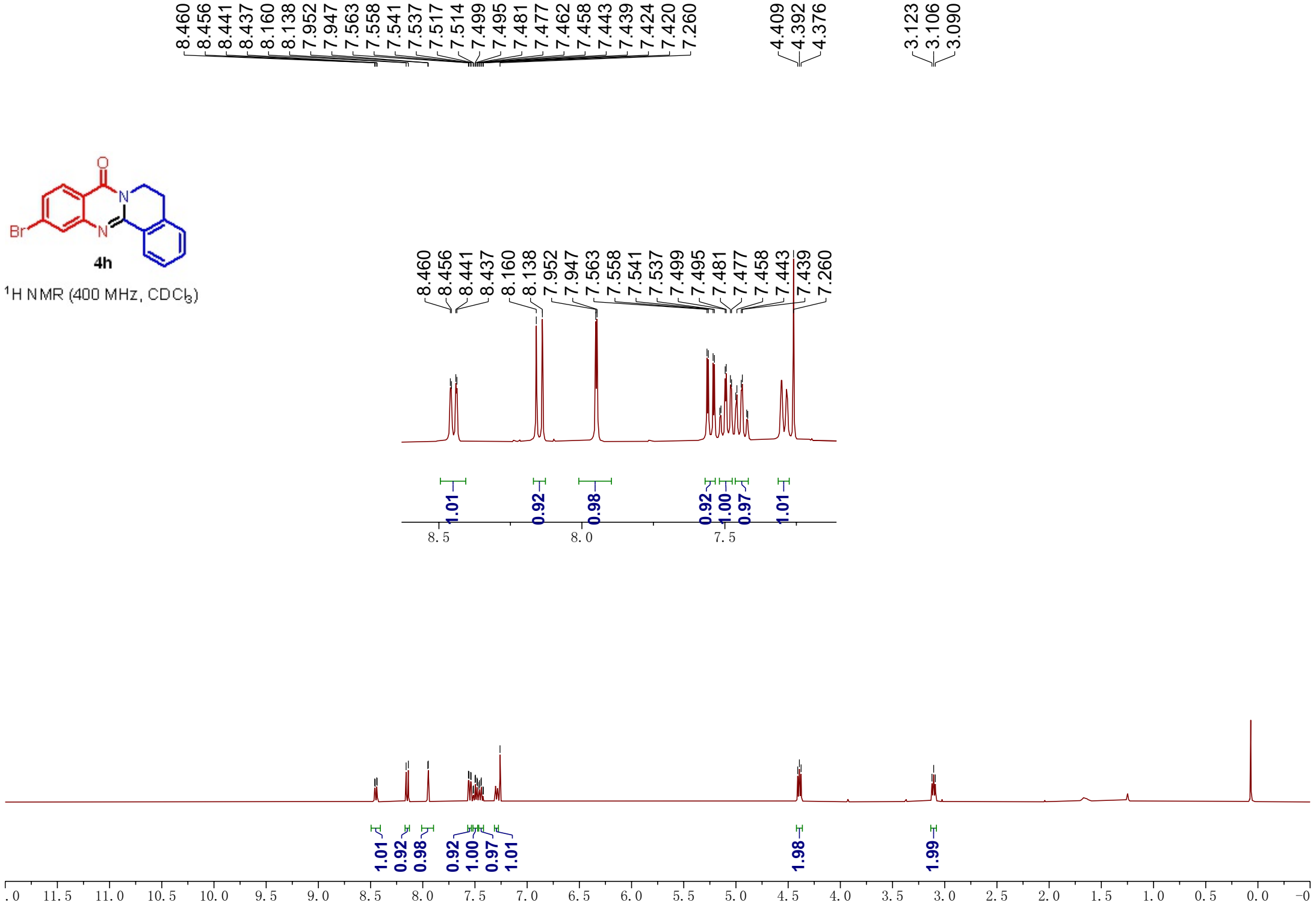


^{19}F NMR (376 MHz, CDCl_3)





¹H NMR (400 MHz, CDCl₃)





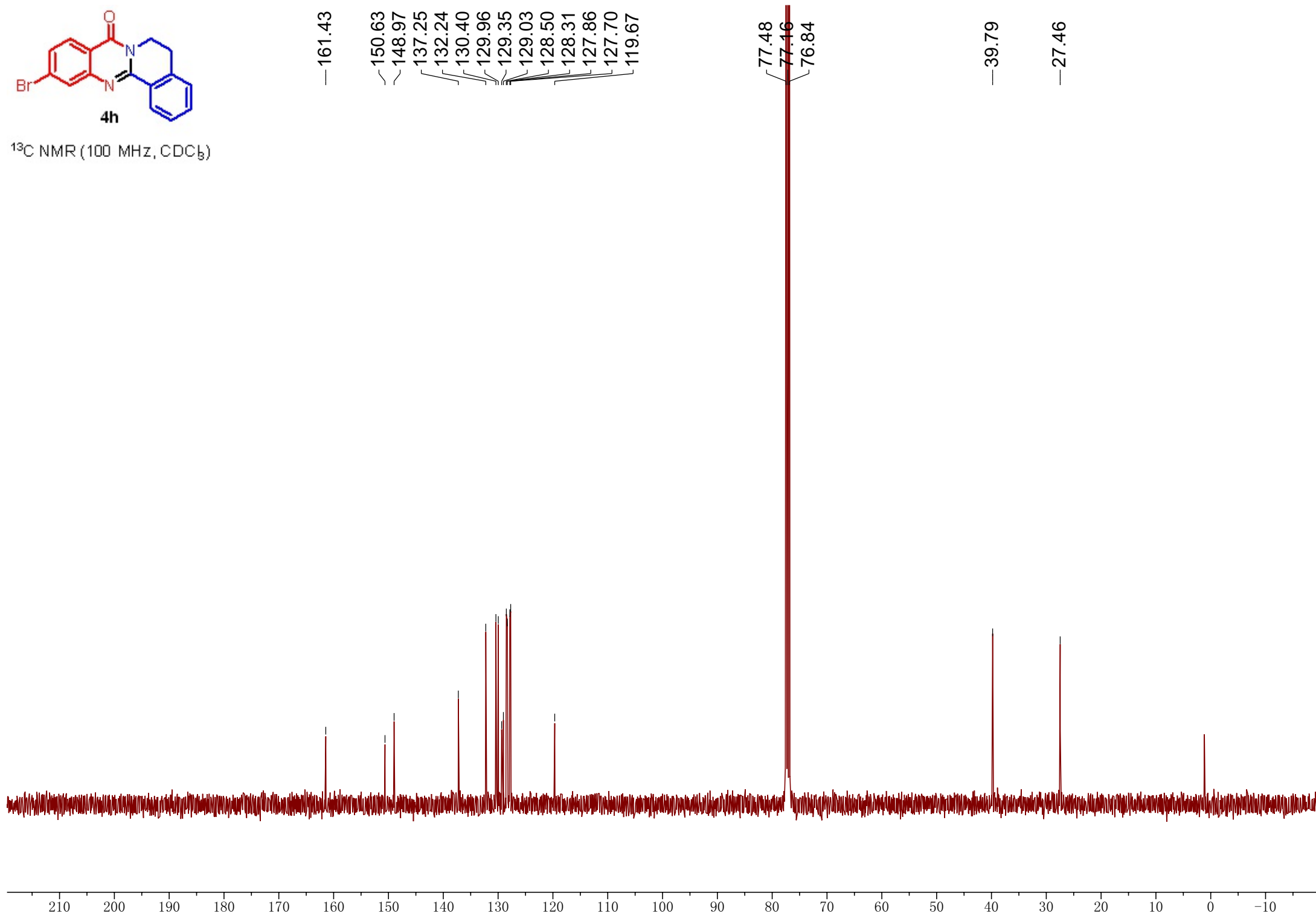
^{13}C NMR (100 MHz, CDCl_3)

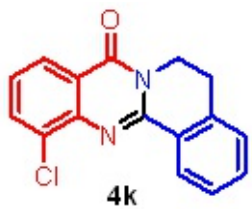
161.43
150.63
148.97
137.25
132.24
130.40
129.96
129.35
129.03
128.50
128.31
127.86
127.70
119.67

77.48
77.16
76.84

39.79

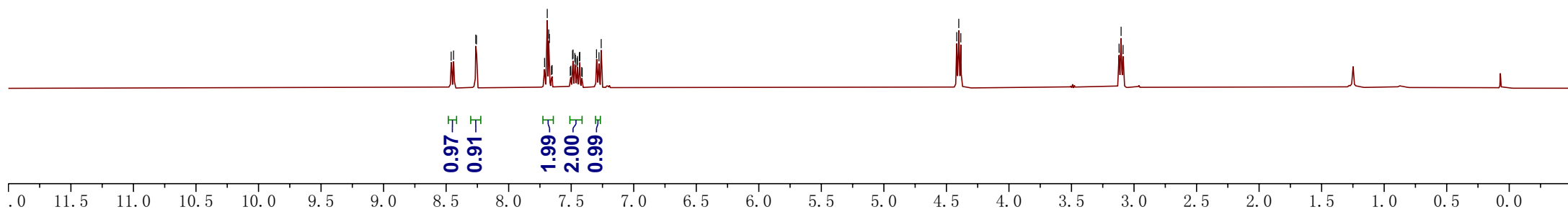
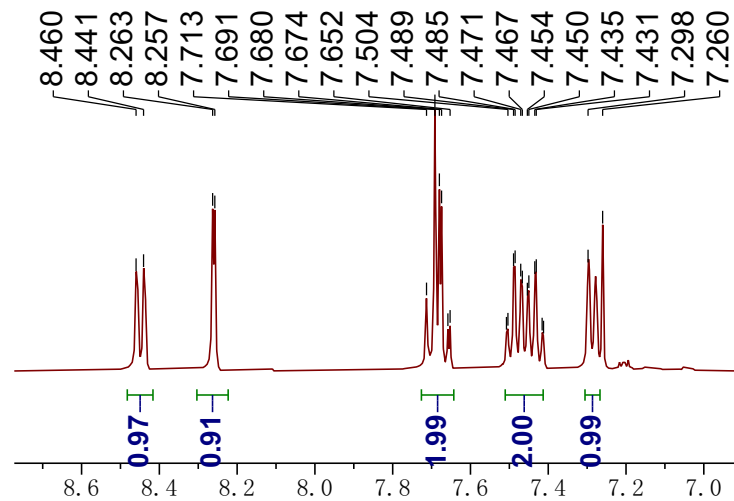
27.46

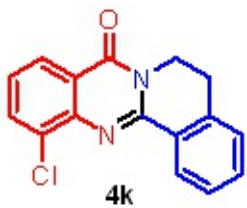




¹H NMR (400 MHz, CDCl₃)

8.460
8.441
8.263
8.257
7.713
7.691
7.680
7.674
7.658
7.652
7.507
7.504
7.489
7.485
7.471
7.467
7.454
7.450
7.435
7.431
7.416
7.412
7.298
7.278
7.260
4.417
4.401
4.385
3.120
3.103
3.087





4k

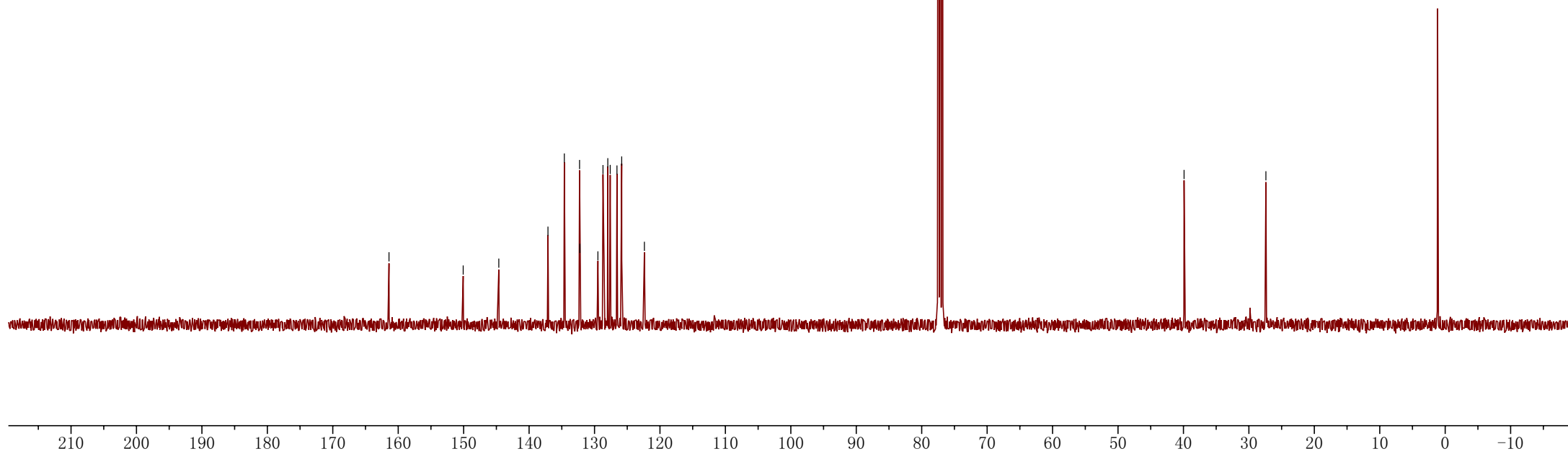
^{13}C NMR (100 MHz, CDCl_3)

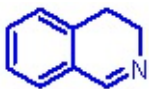
161.41
150.07
144.63
137.12
134.61
132.29
132.24
129.48
128.71
127.97
127.60
126.57
125.85
122.38

77.48
77.16
76.84

39.90

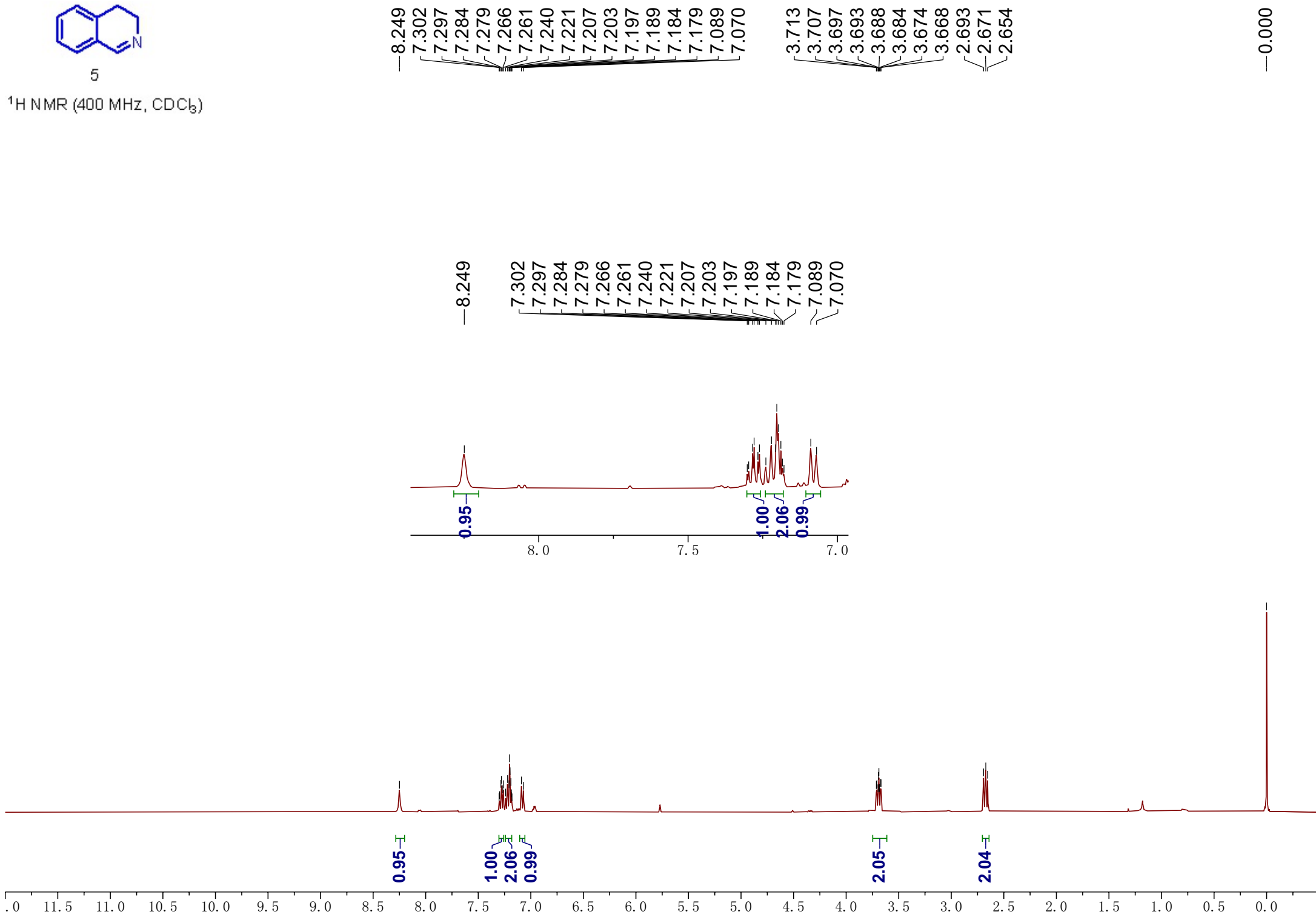
27.40

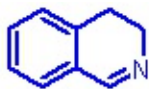




5

¹H NMR (400 MHz, CDCl₃)





5

^{13}C NMR (100 MHz, CDCl_3)

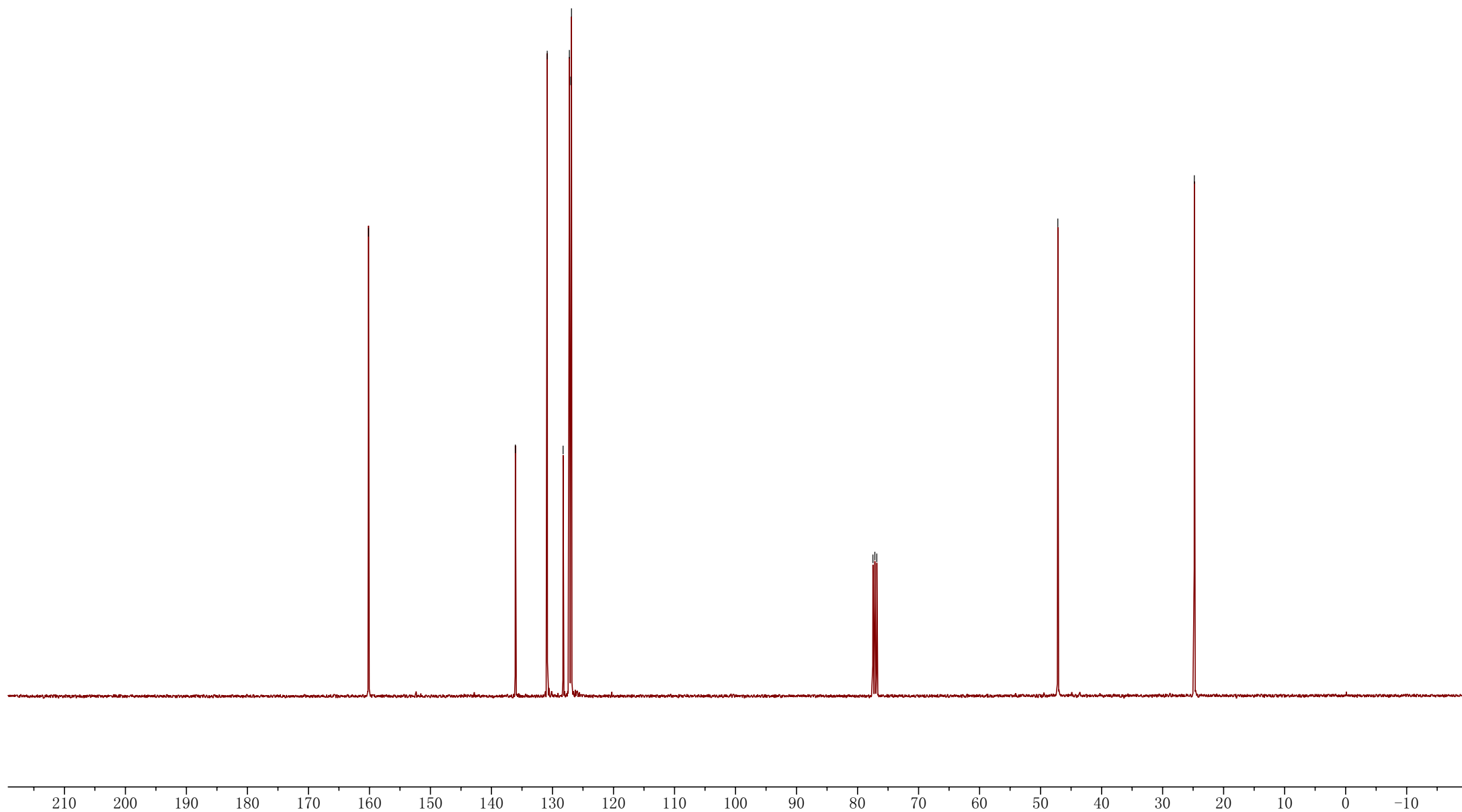
—160.14

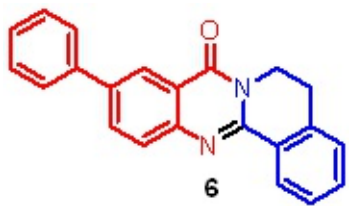
136.09
130.86
128.26
127.23
127.00
126.88

77.48
77.16
76.84

—47.17

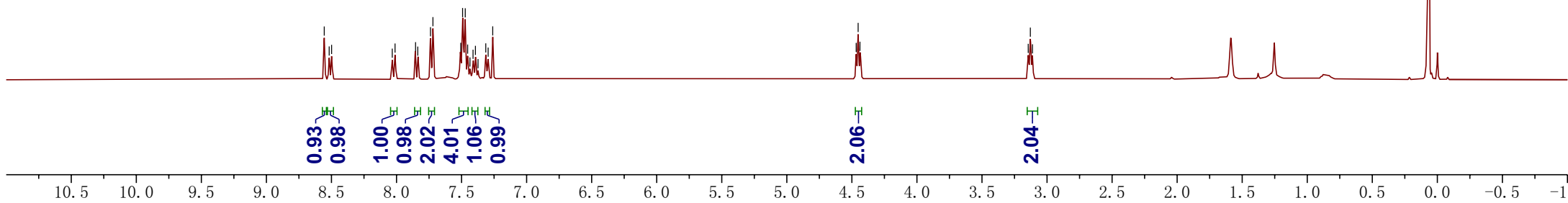
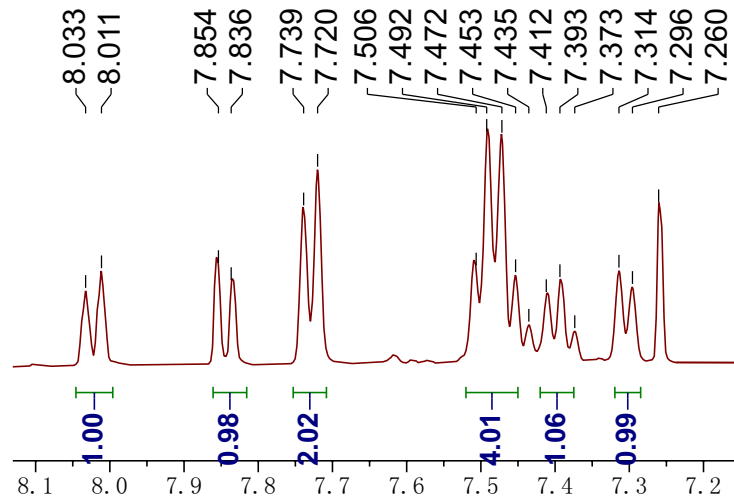
—24.80

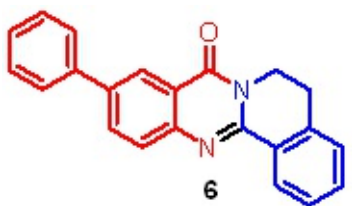




¹H NMR (400 MHz, CDCl₃)

8.556
8.518
8.499
8.033
8.011
7.854
7.836
7.739
7.720
7.506
7.492
7.472
7.453
7.435
7.412
7.393
7.373
7.314
7.296
7.260
4.467
4.452
4.438
3.145
3.128
3.112





^{13}C NMR (100 MHz, CDCl_3)

