Supporting Information

Synthesis of fused quinazolinones via visible light induced cyclization of 2-aminobenzaldehydes with tetrahydroisoquinolines

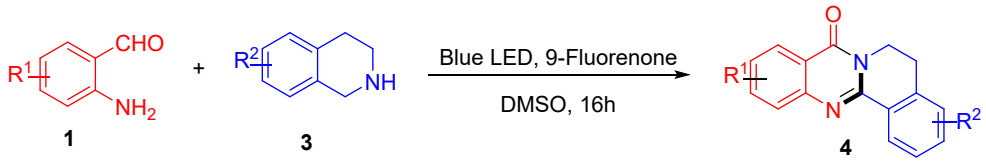
Table of Contents

Contents

1. General information

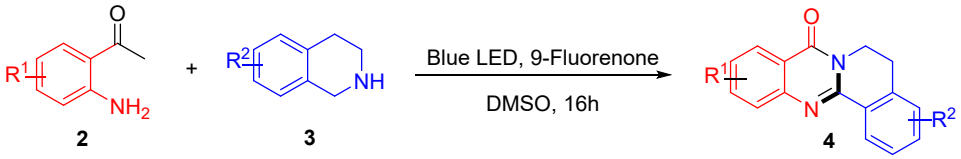
All reactions were carried out under an atmosphere of air unless otherwise noted. Column chromatography was performed using silica gel (200-300 mesh). ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker-AV (500 and 126 MHz, respectively) instrument using $CDCl_3$ as solvent and TMS as an internal standard. The structures of known compounds were further corroborated by comparing their ^{1}H NMR, ^{13}C NMR data and with those of literature. Most reagents were obtained from commercial suppliers and used without further purification.

2. General procedure



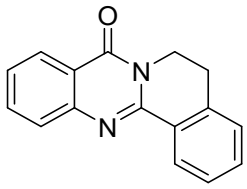
Add 2-aminobenzaldehyde (0.2 mmol, 1.0 equiv.), tetrahydroisoquinoline (0.6 mmol, 3.0 equiv.), 9-fluorenone (4 mol%, 0.04 equiv.) and 2 mL DMSO to 10 ml glass test tube. The reaction mixture was then stirred at room temperature and the test tube was illuminated with an 18W blue LED (λ=460~462 nm) for 16 hours. At the end of the reaction, the reactants were extracted by ethyl acetate for 3 times, the organic phase was collected, and the solvent was vacuum concentrated and purified by

silica gel fast chromatography to obtain the required product.

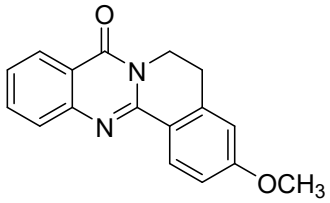


2-aminoacetophenone (0.2 mmol, 1.0 eq), tetrahydroisoquinoline (0.6 mmol, 3.0 equiv.), 9-fluorenone (4 mol%, 0.04 equiv.) and 2 mL DMSO were added to 10 ml glass test tubes. The reaction mixture was then stirred at 40℃ and the tube was illuminated with an 18w blue LED for 16 hours. At the end of the reaction, the reactants were extracted by ethyl acetate for 3 times, the organic phase was collected, the solvent vacuum concentrated, and the silica gel was purified by rapid chromatography to obtain the required products

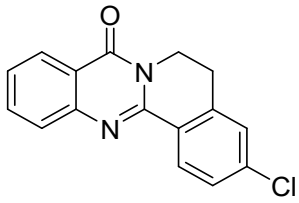
3. Analytical data for the compounds prepared



5,6-dihydro-8H-isoquinolino[1,2-b] quinazolin-8-one (4a): Yield 90%; white solid, m.p. 155.9~157.4 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.48 (d, *J* = 7.6 Hz, 1H), 8.31 (d, *J* = 7.8 Hz, 1H), 7.80 – 7.72 (m, 2H), 7.45 (tt, *J* = 13.6, 6.8 Hz, 3H), 7.28 (d, *J* = 7.3 Hz, 1H), 4.43 – 4.39 (m, 2H), 3.10 (t, *J* = 6.5 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.7, 149.5, 147.7, 137.1, 134.3, 131.8, 129.5, 128.1, 127.7, 127.6, 127.6, 126.9, 126.6, 120.7, 39.6, 27.5. This compound is known.[1]

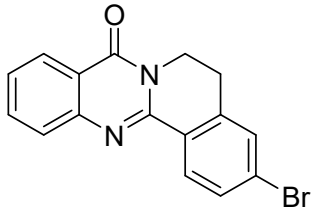


3-methoxy-5,6-dihydro-8H-isoquinolino[1,2-b] quinazolin-8-one (4b): Yield 90%; white solid, m.p. 188.9~190.2 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.41 (d, *J* = 8.8 Hz, 1H), 8.28 (d, *J* = 7.9 Hz, 1H), 7.72 (d, *J* = 3.7 Hz, 2H), 7.42 (dt, *J* = 8.1, 4.1 Hz, 1H), 6.94 (dd, *J* = 8.8, 2.5 Hz, 1H), 6.75 (d, *J* = 2.2 Hz, 1H), 4.42 – 4.38 (m, 2H), 3.87 (s, 3H), 3.06 (t, *J* = 6.5 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.4, 161.8, 149.4, 148.0, 139.0, 134.2, 130.0, 127.3, 126.8, 126.0, 122.1, 120.4, 113.7, 112.1, 55.5, 39.5, 27.7. This compound is known.[2]



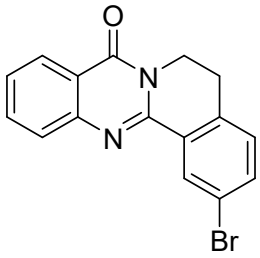
3-chloro-5,6-dihydro-8H-isoquinolino[1,2-b] quinazolin-8-one(4c):

Yield 51%; white solid, m.p. 194.8~196.2 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.41 (d, *J* = 8.4 Hz, 1H), 8.29 (d, *J* = 7.9 Hz, 1H), 7.75 (d, *J* = 5.3 Hz, 2H), 7.46 (td, *J* = 6.8, 5.8, 2.2 Hz, 1H), 7.42 – 7.36 (m, 1H), 7.28 (s, 1H), 4.40 (t, *J* = 6.4 Hz, 2H), 3.08 (t, *J* = 6.4 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.5, 148.5, 147.6, 138.6, 137.8, 134.4, 129.6, 128.0, 128.0, 127.6, 127.5, 126.9, 126.7, 120.7, 39.4, 27.3. This compound is known.[3]



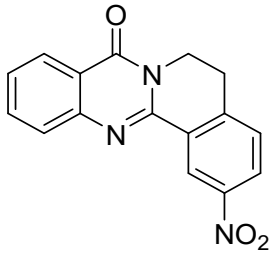
3-bromo-5,6-dihydro-8H-isoquinolino[1,2-b] quinazolin-8-one(4d):

Yield 80%; white solid, m.p. 151.3~152.1 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (d, *J* = 7.9 Hz, 1H), 8.32 (d, *J* = 7.9 Hz, 1H), 7.76 (d, *J* = 3.6 Hz, 2H), 7.73 (dd, *J* = 8.0, 1.1 Hz, 1H), 7.48 (dp, *J* = 8.7, 4.6 Hz, 1H), 7.31 (t, *J* = 7.9 Hz, 1H), 4.44 – 4.38 (m, 2H), 3.22 (t, *J* = 6.5 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.5, 148.5, 147.7, 136.8, 135.5, 134.4, 131.7, 128.7, 127.7, 127.4, 126.9, 126.9, 123.3, 120.8, 39.0, 27.4. This compound is known. [4]



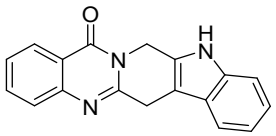
2-bromo-5,6-dihydro-8H-isoquinolino[1,2-b] quinazolin-8-one(4e):

Yield 89%; white solid, m.p. 208.2~210.1 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, *J* = 8.5 Hz, 1H), 8.30 (dt, *J* = 8.0, 1.1 Hz, 1H), 7.78 – 7.72 (m, 2H), 7.56 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.49 – 7.43 (m, 2H), 4.43 – 4.37 (m, 2H), 3.08 (t, *J* = 6.5 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.5, 148.6, 147.6, 138.8, 134.4, 131.0, 130.5, 129.7, 128.6, 127.6, 126.9, 126.8, 126.4, 120.8, 39.4, 27.2. This compound is known. [4]

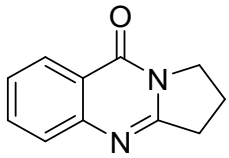


2-nitro-5,6-dihydro-8H-isoquinolino[1,2-b] quinazolin-8-one(4f):

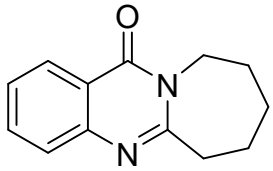
Yield 27%; yellow solid, m.p. 243.1~244.7 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.37 – 9.27 (m, 1H), 8.30 (d, *J* = 8.0 Hz, 2H), 7.80 (q, *J* = 8.0, 6.5 Hz, 2H), 7.56 – 7.44 (m, 2H), 4.46 (t, *J* = 6.3 Hz, 2H), 3.23 (t, *J* = 6.2 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.3, 147.8, 147.3, 147.2, 143.4, 134.6, 131.1, 128.9, 127.9, 127.4, 127.0, 125.8, 123.4, 120.9, 39.0, 27.6. This compound is known. [5]



6,14-dihydroindolo [3',2':4,5] pyrido[2,1-b] quinazolin-8(5H)-one(4g): Yield 65%; white solid, m.p. 259.3~261.2 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.03 (s, 1H), 8.33 (d, *J* = 7.8 Hz, 1H), 7.70 – 7.59 (m, 3H), 7.42 (t, *J* = 7.2 Hz, 1H), 7.26 (d, *J* = 3.6 Hz, 2H), 7.15 (dt, *J* = 7.5, 3.6 Hz, 1H), 4.59 (t, *J* = 6.8 Hz, 2H), 3.23 (t, *J* = 6.8 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.6, 147.3, 145.2, 138.4, 134.5, 127.3, 127.0, 126.4, 126.3, 125.6, 125.6, 121.1, 120.6, 120.1, 118.6, 112.2, 77.1, 41.2, 19.7. This compound is known. [5]

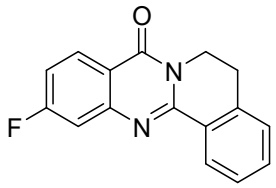


2,3-dihydropyrrolo[2,1-b] quinazolin-9(1H)-one(4h): Yield 48%; Viscous liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.28 (d, *J* = 7.9 Hz, 1H), 7.76 – 7.70 (m, 1H), 7.64 (d, *J* = 8.1 Hz, 1H), 7.45 (t, *J* = 7.5 Hz, 1H), 4.25 – 4.16 (m, 2H), 3.18 (t, *J* = 8.0 Hz, 2H), 2.29 (p, *J* = 7.8 Hz, 2H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 156.3, 154.7, 144.4, 129.4, 122.0, 121.6, 121.5, 115.7, 41.8, 27.8, 14.8. This compound is known. [6]



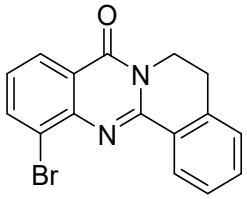
7,8,9,10-tetrahydroazepino[2,1-b] quinazolin-12(6H)-one(4i): Yield 42%; Viscous liquid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.10 (d, *J* = 7.7

Hz, 1H), 7.78 (t, *J* = 7.1 Hz, 1H), 7.58 (d, *J* = 8.1 Hz, 1H), 7.48 (t, *J* = 7.5 Hz, 1H), 4.39 – 4.29 (m, 2H), 3.08 – 3.02 (m, 2H), 1.80 – 1.73 (m, 4H), 1.72 – 1.67 (m, 2H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.4, 160.6, 147.7, 134.7, 127.1, 126.9, 126.7, 120.2, 42.5, 37.1, 29.3, 28.0, 25.4. This compound is known. [6]



11-fluoro-5,6-dihydro-8H-isoquinolino[1,2-b] quinazolin-8-one(4j):

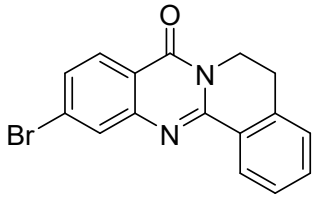
Yield 45%; white solid, m.p. 169.6~171.6 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.46 (d, *J* = 7.6 Hz, 1H), 8.38 – 8.24 (m, 1H), 7.46 (ddd, *J* = 31.0, 15.1, 8.4 Hz, 3H), 7.30 (d, *J* = 7.3 Hz, 1H), 7.17 (t, *J* = 8.4 Hz, 1H), 4.40 (t, *J* = 6.3 Hz, 2H), 3.11 (t, *J* = 6.2 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.5, 165.5, 161.1, 150.6, 150.0, 149.9, 137.2, 132.1, 129.7, 129.6, 129.2, 128.2, 127.7, 127.6, 117.5, 115.5, 115.3, 112.8, 112.6, 39.6, 27.4. This compound is known. [7]



12-bromo-5,6-dihydro-8H-isoquinolino[1,2-b] quinazolin-8-one(4k):

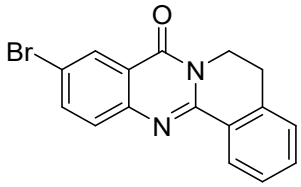
Yield 39%; white solid, m.p. 231.2~233.5 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.60 (d, *J* = 5.9 Hz, 1H), 8.26 (d, *J* = 6.9 Hz, 1H), 8.02 (d, *J* = 6.6 Hz, 1H), 7.56 – 7.40 (m, 2H), 7.29 (dd, *J* = 15.7, 7.1 Hz, 2H), 4.50 –

4.28 (m, 2H), 3.21 – 3.00 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.3, 150.0, 145.5, 137.9, 137.0, 132.2, 129.3, 128.6, 127.9, 127.5, 126.9, 126.5, 122.9, 122.2, 39.8, 27.3. This compound is known. [2]



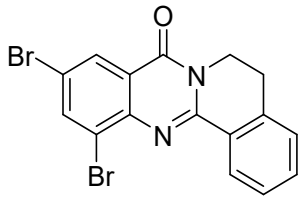
11-bromo-5,6-dihydro-8H-isoquinolino[1,2-b] quinazolin-8-one(4l):

Yield 68%; white solid, m.p. 174.7~176.5 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.37 (d, *J* = 7.4 Hz, 1H), 8.06 (d, *J* = 8.4 Hz, 1H), 7.87 (s, 1H), 7.51 – 7.32 (m, 3H), 7.24 – 7.16 (m, 1H), 4.41 – 4.21 (m, 2H), 3.09 – 2.94 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.3, 150.5, 148.8, 137.1, 132.1, 130.3, 129.8, 129.2, 128.9, 128.4, 128.2, 127.7, 127.6, 119.5, 39.7, 27.3. This compound is known. [7]

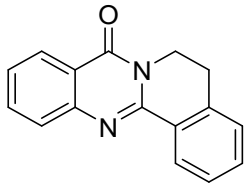


10-bromo-5,6-dihydro-8H-isoquinolino[1,2-b] quinazolin-8-one(4m):

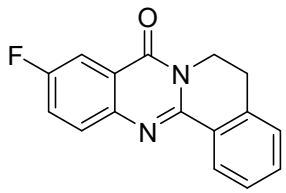
Yield 70%; white solid, m.p. 190.6~191.2 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.47 – 8.37 (m, 2H), 7.79 (dd, *J* = 8.7, 2.3 Hz, 1H), 7.61 (d, *J* = 8.7 Hz, 1H), 7.45 (dt, *J* = 28.5, 7.4 Hz, 2H), 7.27 (d, *J* = 7.2 Hz, 1H), 4.42 – 4.35 (m, 2H), 3.09 (t, *J* = 6.4 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.6, 149.8, 146.6, 137.4, 137.1, 132.0, 129.4, 129.2, 128.1, 127.7, 127.6, 122.0, 120.0, 39.8, 27.3. This compound is known. [2]



10,12-dibromo-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(4n): Yield 30%; white solid, m.p. 200.6~202.2 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 – 8.38 (m, 2H), 7.80 (dd, *J* = 8.7, 2.2 Hz, 1H), 7.62 (d, *J* = 8.7 Hz, 1H), 7.46 (dt, *J* = 23.4, 7.3 Hz, 2H), 4.39 (t, *J* = 6.5 Hz, 2H), 3.10 (t, *J* = 6.4 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.6, 149.8, 146.7, 137.4, 137.0, 132.0, 129.4, 129.3, 128.1, 127.7, 127.6, 122.1, 119.9, 39.8, 27.4. ESI-HRMS calcd for [$C_{16}H_{10}Br_2N_2O$ + H] 404.9233, found 404.92298.

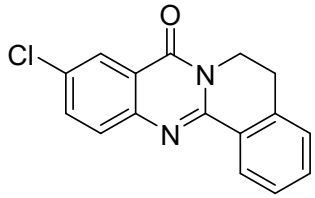


5,6-dihydro-8H-isoquinolino[1,2-b] quinazolin-8-one (4a-from 2-aminophenone**):** Yield 50%; white solid, m.p. 153.9~156.4 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (dd, *J* = 7.7, 1.2 Hz, 1H), 8.32 (d, *J* = 8.3 Hz, 1H), 7.76 (dd, *J* = 6.4, 1.4 Hz, 2H), 7.51 – 7.42 (m, 3H), 7.29 (d, *J* = 7.2 Hz, 1H), 4.46 – 4.39 (m, 2H), 3.11 (t, *J* = 6.5 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.8, 149.4, 147.8, 137.1, 134.3, 131.7, 129.6, 128.1, 127.7, 127.6, 127.5, 126.9, 126.6, 120.8, 39.6, 27.5. This compound is known. [1]



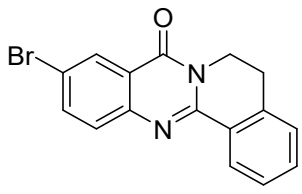
10-fluoro-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(4o):

Yield 51%; white solid, m.p. 204.8~205.1 ℃;[1]H NMR (500 MHz, $CDCl_3$) δ 8.44 (d, J = 7.0 Hz, 1H), 7.92 (d, J = 5.5 Hz, 1H), 7.82 – 7.72 (m, 1H), 7.45 (dd, J = 17.2, 6.3 Hz, 3H), 7.28 (d, J = 6.6 Hz, 1H), 4.44 – 4.37 (m, 2H), 3.15 – 3.06 (m, 2H); [13]C NMR (126 MHz, $CDCl_3$) δ161.1, 160.8 (J_{C-F}=248.2 Hz), 148.8, 144.5, 136.9, 131.8, 130.8 (J_{C-F}=7.6 Hz) 129.3, 127.9, 127.7, 127.6, 122.9 (J_{C-F}=25.2Hz), 121.9 (J_{C-F}=10.1Hz), 111.7 (J_{C-F}=23.9Hz), 39.8, 27.4. This compound is known. [2]



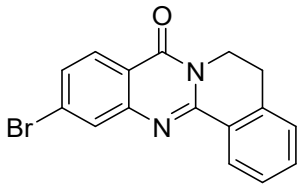
10-chloro-5,6-dihydro-8H-isoquinolino[1,2-b] quinazolin-8-one(4p):

Yield 70%; white solid, m.p. 178.6~180.2℃; [1]H NMR (400 MHz, $CDCl_3$) δ 8.36 (d, *J* = 7.7 Hz, 1H), 8.21 – 8.12 (m, 1H), 7.64 – 7.54 (m, 2H), 7.37 (dt, *J* = 22.0, 7.3 Hz, 2H), 7.20 (d, *J* = 8.3 Hz, 1H), 4.31 (t, *J* = 6.5 Hz, 2H), 3.02 (t, *J* = 6.4 Hz, 2H); [13]C NMR (101 MHz, $CDCl_3$) δ 160.6, 149.8, 146.7, 137.4, 137.0, 132.0, 129.4, 129.3, 128.1, 127.7, 127.6, 122.1, 120.0, 39.8, 27.4. This compound is known. [2]

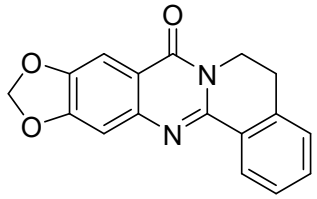


10-bromo-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(4m-from 2-aminophenone**):** Yield 55%; white solid, m.p. 194.7~196.4 ℃; [1]H

NMR (400 MHz, $CDCl_3$) δ 8.46 – 8.39 (m, 2H), 7.80 (dd, *J* = 8.7, 2.3 Hz, 1H), 7.60 (s, 1H), 7.51 – 7.39 (m, 2H), 7.27 (d, *J* = 8.1 Hz, 1H), 4.42 – 4.36 (m, 2H), 3.09 (t, *J* = 6.5 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.6, 149.8, 146.7, 137.4, 137.0, 132.0, 129.4, 129.3, 128.1, 127.7, 127.6, 122.1, 120.0, 39.8, 27.4. This compound is known. [2]

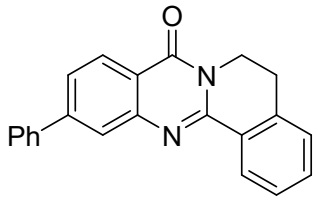


11-bromo-5,6-dihydro-8H-isoquinolino[1,2-b] quinazolin-8-one(4l- from 2-aminophenone**):** Yield 55%; white solid, m.p. 176.7~179.2 ℃; Yield 70%; white solid, m.p. 174.7~176.5 ℃; ^1H NMR (500 MHz, $CDCl_3$) δ 8.37 (d, *J* = 7.4 Hz, 1H), 8.06 (d, *J* = 8.4 Hz, 1H), 7.87 (s, 1H), 7.51 – 7.32 (m, 3H), 7.24 – 7.16 (m, 1H), 4.41 – 4.21 (m, 2H), 3.09 – 2.94 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.3, 150.5, 148.8, 137.1, 132.1, 130.3, 129.8, 129.2, 128.9, 128.4, 128.2, 127.7, 127.6, 119.5, 39.7, 27.3. This compound is known. [7]

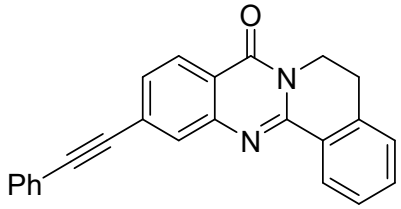


5,6-dihydro-8H- [1,3] dioxolo[4,5-g] isoquinolino[1,2-b] quinazolin-8-one(4q): Yield 21%; white solid, m.p. 200.9~203.1 ℃; ^1H NMR (400 MHz, $CDCl_3$) δ 8.42 (d, *J* = 7.4 Hz, 1H), 7.62 (s, 1H), 7.44 (p, *J* = 6.9 Hz, 2H), 7.26 (s, 1H), 7.12 (s, 1H), 6.10 (s, 2H), 4.39 (t, *J* = 6.4 Hz, 2H), 3.09

(t, *J* = 6.3 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.0, 148.2, 147.4, 145.8, 136.8, 131.5, 129.6, 127.7, 127.6, 127.5, 115.8, 105.8, 102.1, 39.6, 27.5. This compound is known. [1]

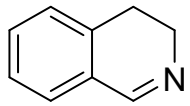


11-phenyl-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(5a): Yield 81%; light yellow solid, m.p.188.5-189.7^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.51 (d, J = 7.5 Hz, 1H), 8.36 (d, J = 8.3 Hz, 1H), 8.01 (s, 1H), 7.77 – 7.68 (m, 3H), 7.53 – 7.40 (m, 5H), 7.30 (d, J = 7.2 Hz, 1H), 4.43 (t, J = 6.5 Hz, 2H), 3.12 (t, J = 6.4 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.6, 148.1, 147.1, 139.8, 137.2, 131.9, 129.5, 129.0, 128.4, 128.1, 127.7, 127.6, 127.5, 127.4, 125.8, 125.6, 39.6, 27.5. This compound is known. [4]



11-(phenylethynyl)-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one(5b): Yield 78%; light yellow solid, m.p.196.5-197.7^{o}C;^{1}H NMR (500 MHz, $CDCl_3$) δ 8.48 (d, J = 7.1 Hz, 1H), 8.26 (d, J = 8.2 Hz, 1H), 7.93 (s, 1H), 7.61 – 7.54 (m, 3H), 7.51 – 7.42 (m, 3H), 7.41 – 7.36 (m, 3H), 7.30 – 7.27 (m, 1H), 4.43 – 4.39 (m, 2H), 3.10 (t, J = 6.4 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.3, 150.0, 147.7, 132.0, 131.9, 130.5,

129.3, 128.5, 128.2, 127.7, 127.6, 127.0, 126.6, 92.6, 88.6, 39.7, 27.4. This compound is known. [4]



3,4-dihydroisoquinoline (6): Yield 90%; light yellow liquid;^{1}H NMR (500 MHz, $CDCl_3$) δ 8.35 (s, 1H), 7.36 (t, J = 7.2 Hz, 1H), 7.29 (q, J = 7.6 Hz, 2H), 7.16 (d, J = 7.3 Hz, 1H), 3.77 (t, J = 6.8 Hz, 2H), 2.78 – 2.73 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.5, 136.6, 131.2, 128.5, 127.5, 127.3, 127.1, 47.3, 25.0. This compound is known. [7]

4. Reference

[1] Nam T S. Copper-catalyzed synthesis of pyrido-fused quinazolinones from 2-aminoarylmethanols and isoquinolines or tetrahydroisoquinolines[J]. Organic & Biomolecular Chemistry, 2021, 19(21): 4726-4732.

[2] Wang D, Xiao F, Zhang F, et al. Copper‐Catalyzed Aerobic Oxidative Ring Expansion of Isatins: A Facile Entry to Isoquinolino‐Fused Quinazolinones[J]. Chinese Journal of Chemistry, 2021, 39(1): 87-92.

[3] Li J, Wang Z B, Xu Y, et al. Catalyst-free cyclization of anthranils and cyclic amines: one-step synthesis of rutaecarpine[J]. Chemical Communications, 2019, 55(80): 12072-12075.

[4] Jia F C, Chen T Z, Hu X Q. TFA/TBHP-promoted oxidative cyclisation for the construction of tetracyclic quinazolinones and rutaecarpine[J]. Organic Chemistry Frontiers, 2020, 7(13): 1635-1639.

[5] Xie L, Lu C, Jing D, et al. Metal‐free synthesis of polycyclic quinazolinones enabled by a $(NH4)_2S_2O_8$‐promoted intramolecular oxidative cyclization[J].

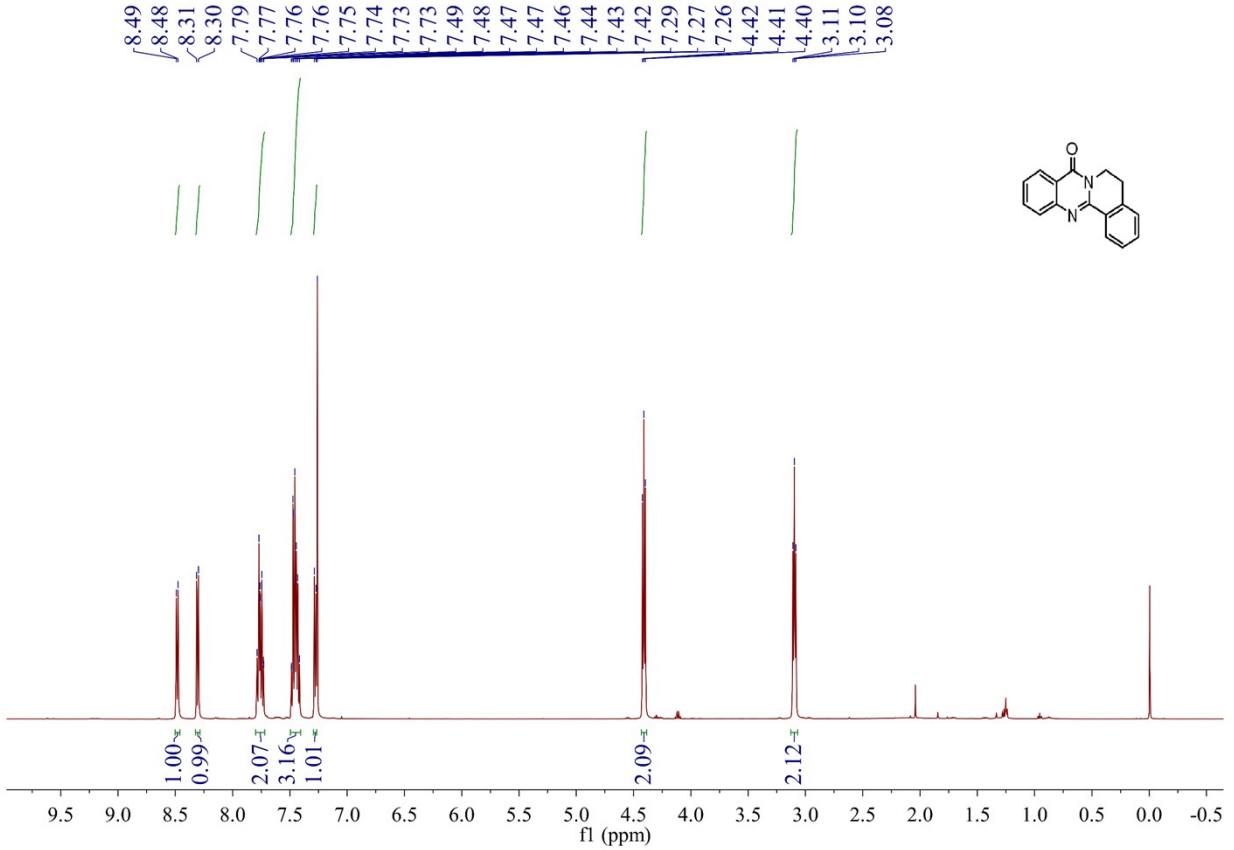
European Journal of Organic Chemistry, 2019, 2019(22): 3649-3653.

[6] Gil C, Bräse S. Efficient Solid‐Phase Synthesis of Highly Functionalized 1, 4‐Benzodiazepin‐5‐one Derivatives and Related Compounds by Intramolecular Aza–Wittig Reactions[J]. Chemistry–A European Journal, 2005, 11(9): 2680-2688.

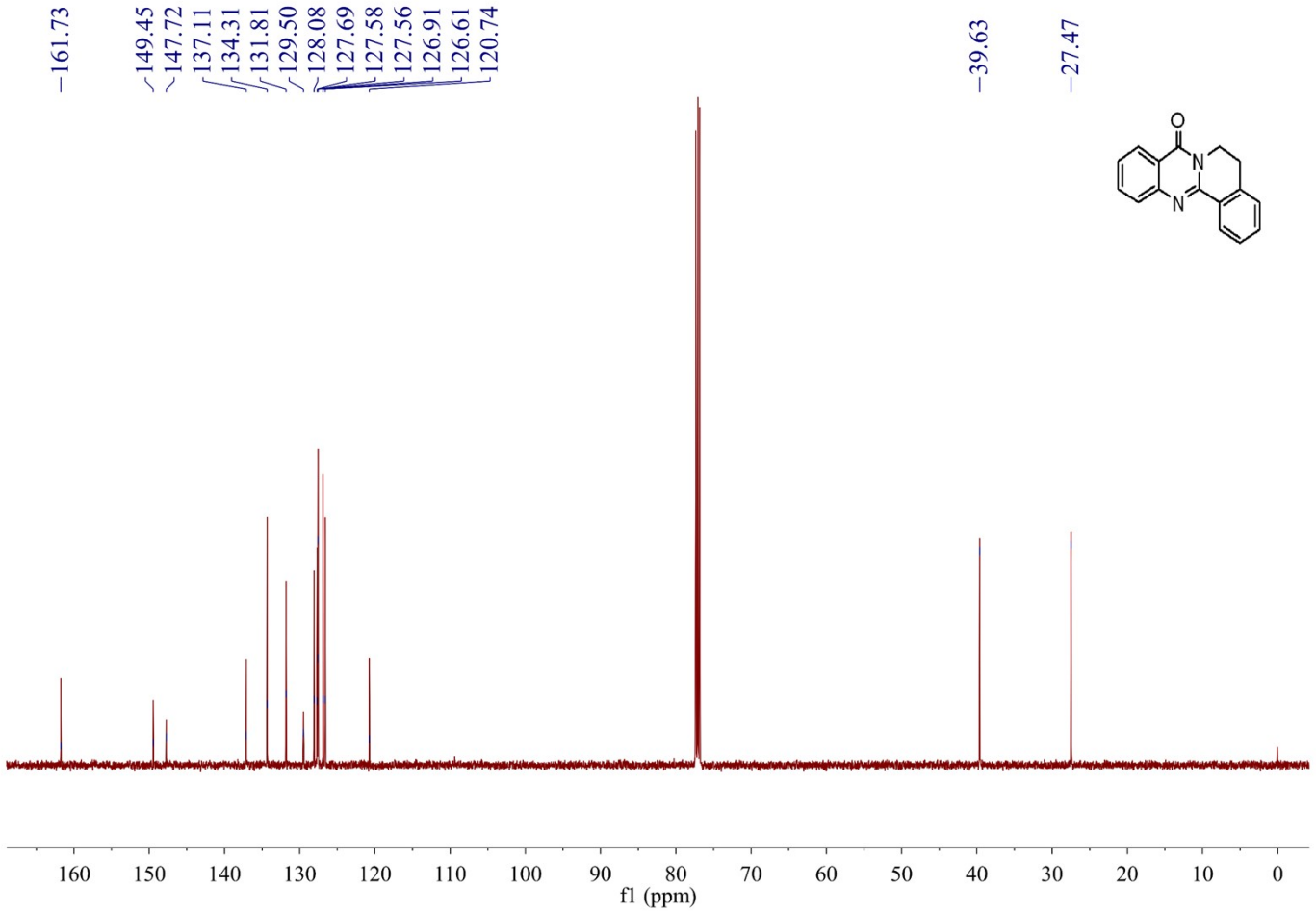
[7] Chen X, Xia F, Zhao Y, et al. TBHP‐Mediated Oxidative Decarboxylative Cyclization in Water: Direct and Sustainable Access to Anti‐malarial Polycyclic Fused Quinazolinones and Rutaecarpine[J]. Chinese Journal of Chemistry, 2020, 38(11): 1239-1244.

5. Spectral data for the compounds prepared

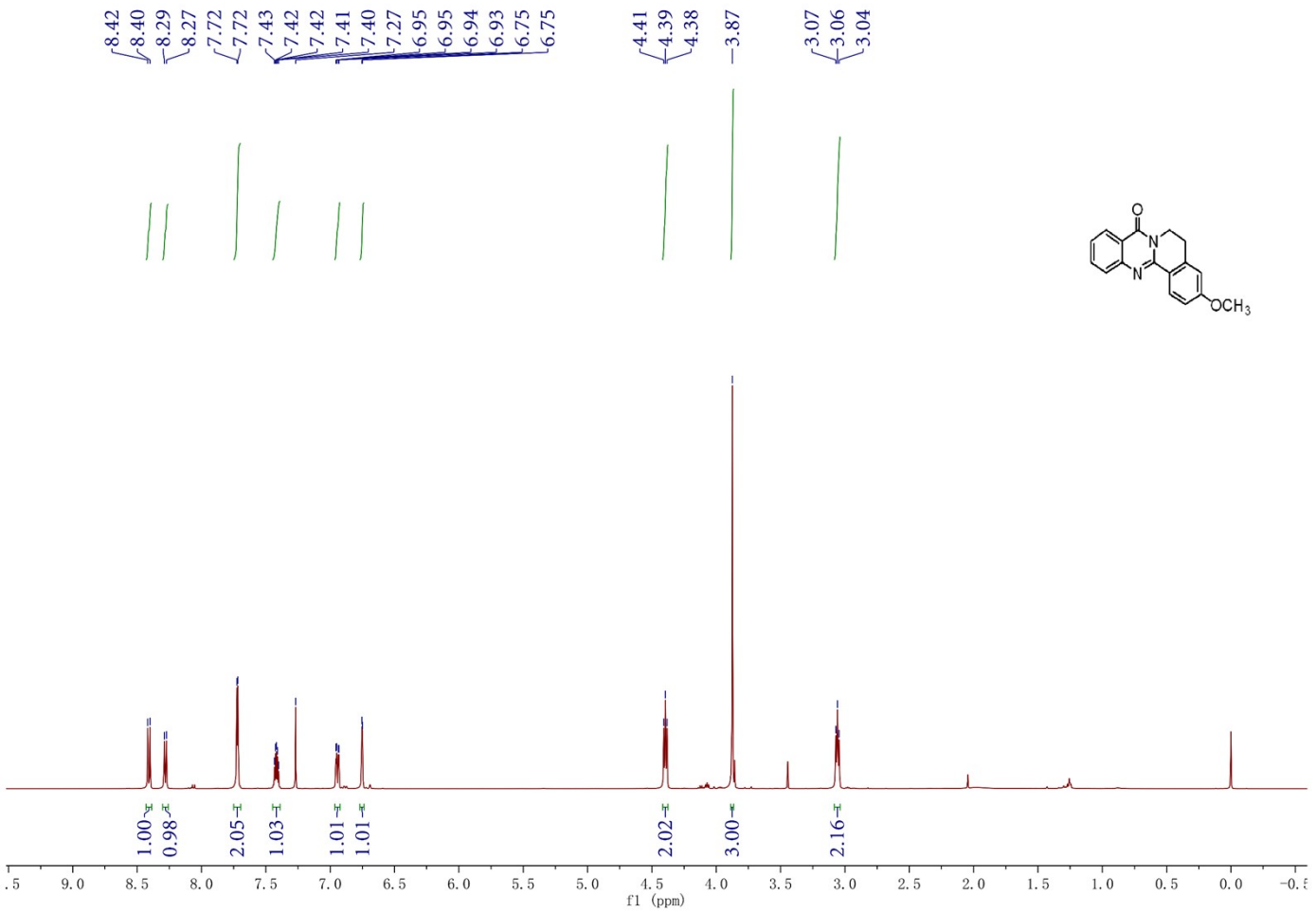
^{1}H NMR ($CDCl_3$, 500 MHz) spectra of **4a**



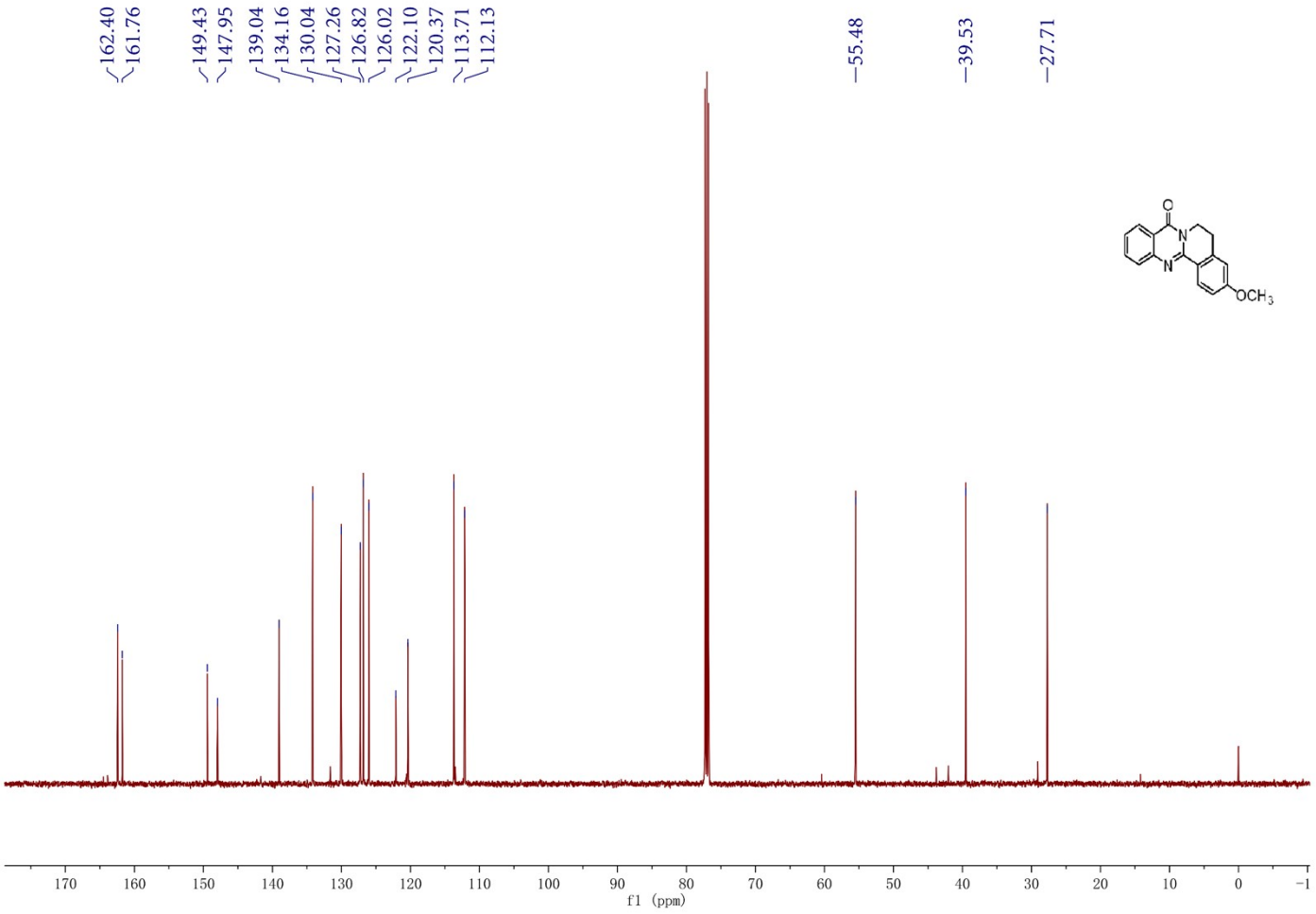
^{13}C NMR ($CDCl_3$, 126 MHz) spectra of **4a**



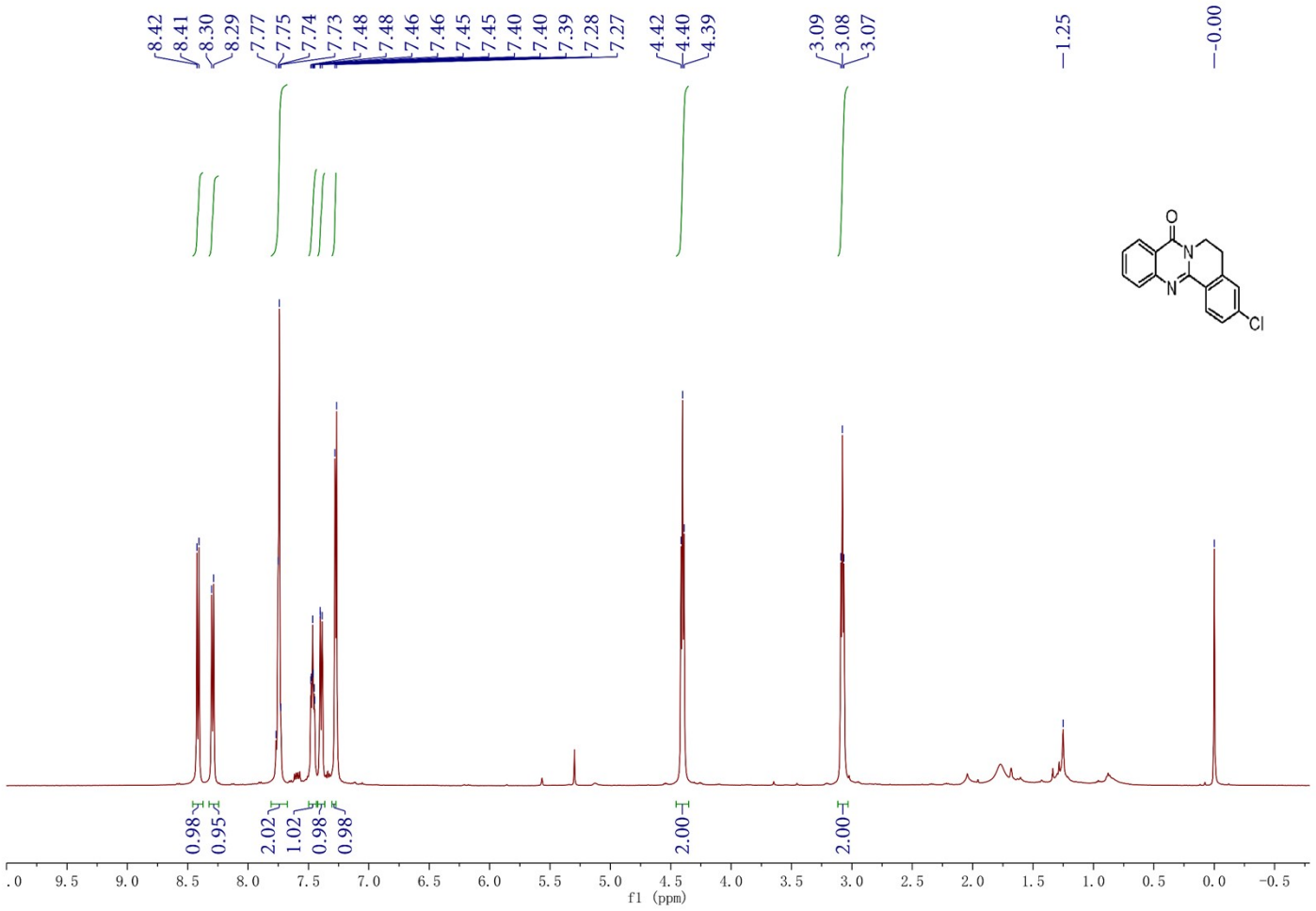
^{1}H NMR ($CDCl_3$, 500 MHz) spectra of **4b**



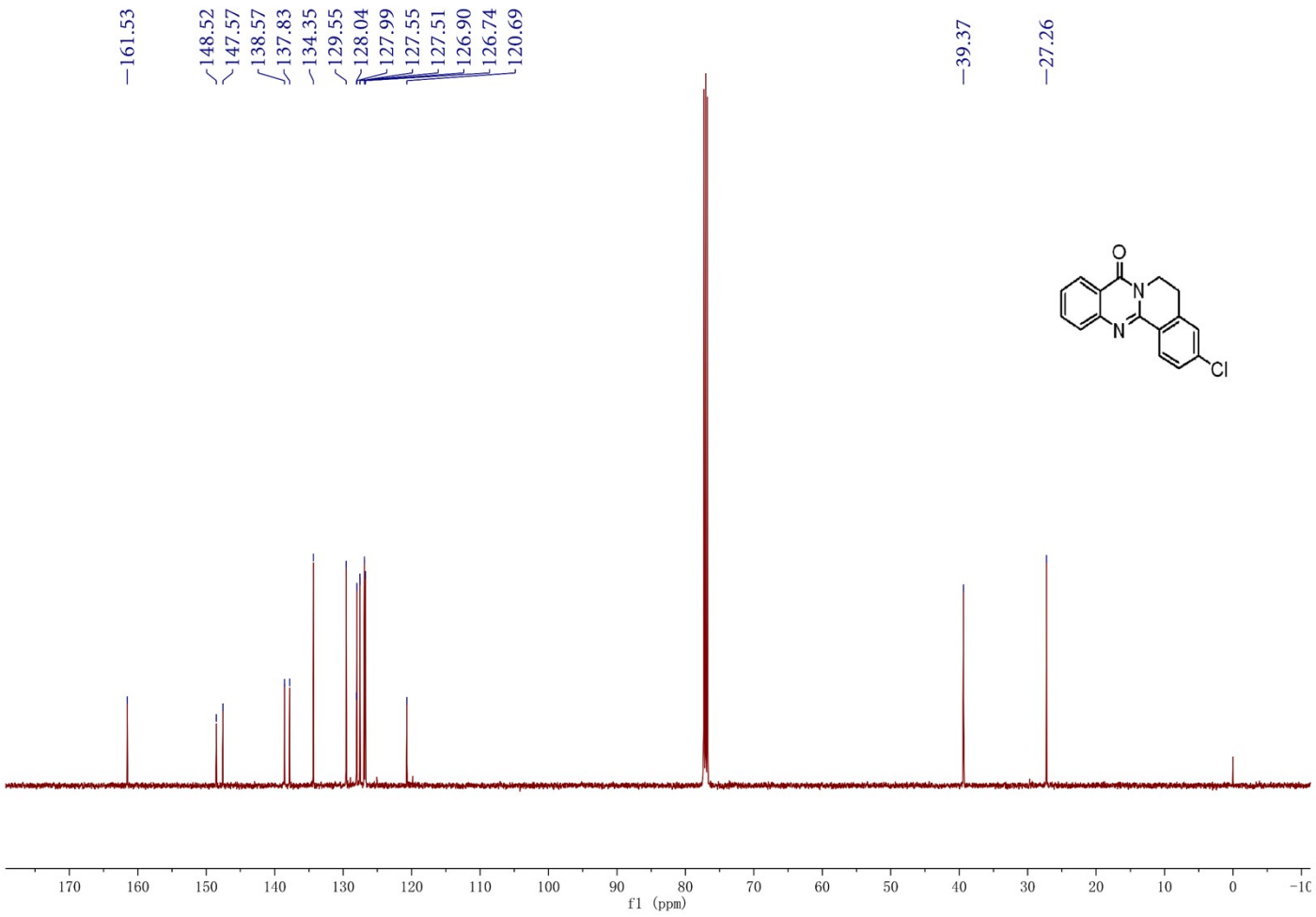
^{13}C NMR ($CDCl_3$, 126 MHz) spectra of **4b**



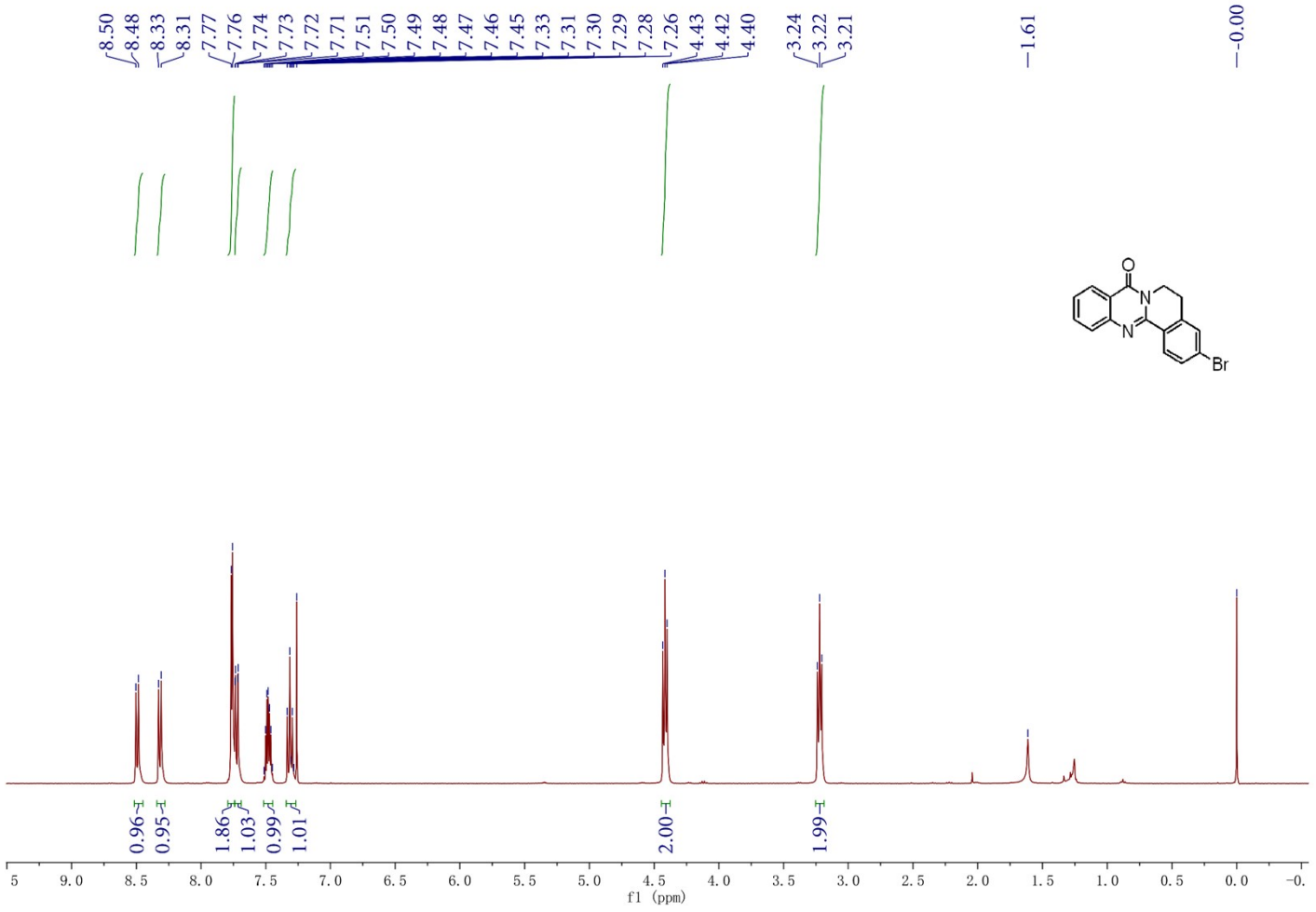
^{1}H NMR ($CDCl_3$, 500 MHz) spectra of **4c**



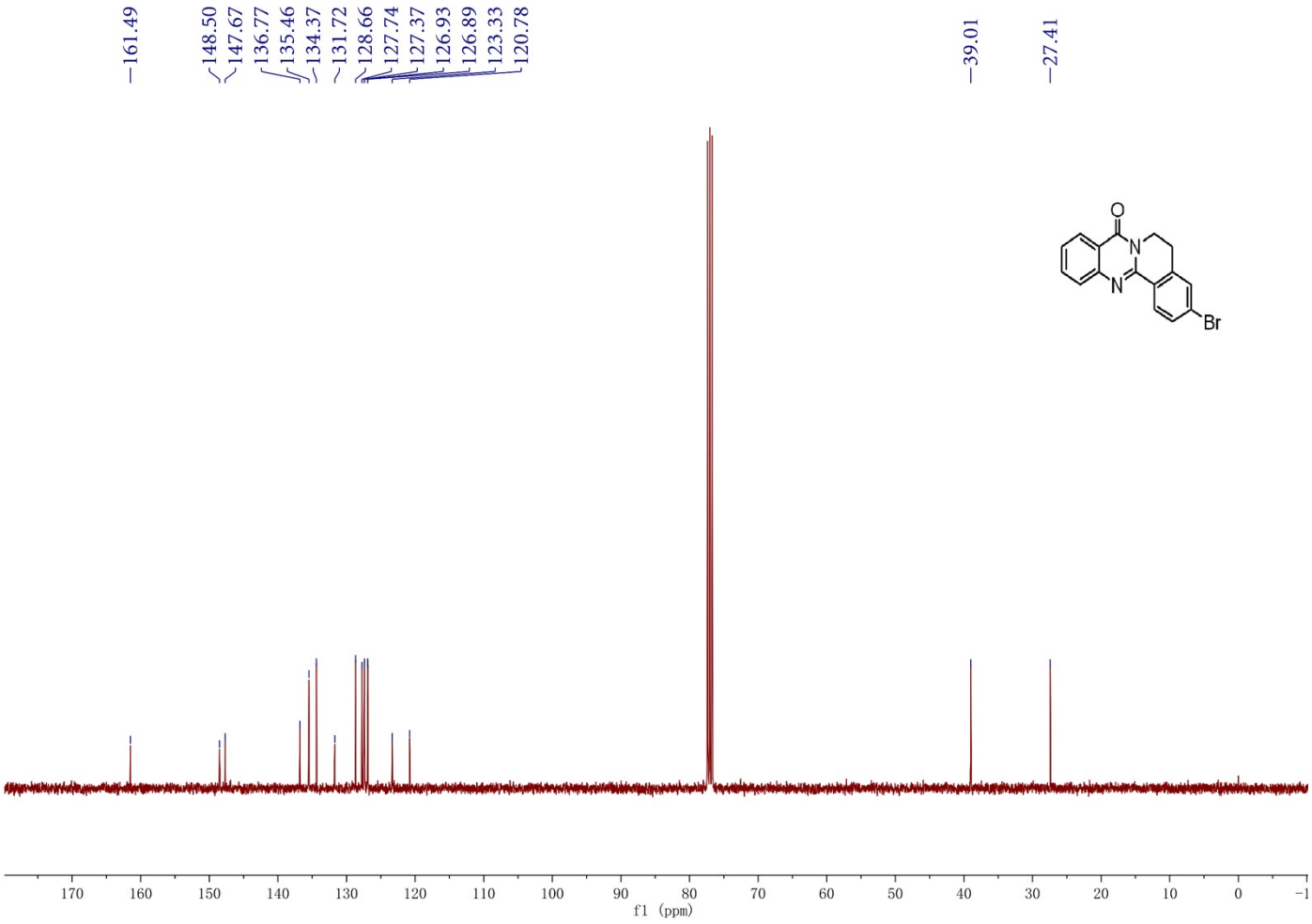
^{13}C NMR ($CDCl_3$, 126 MHz) spectra of **4c**



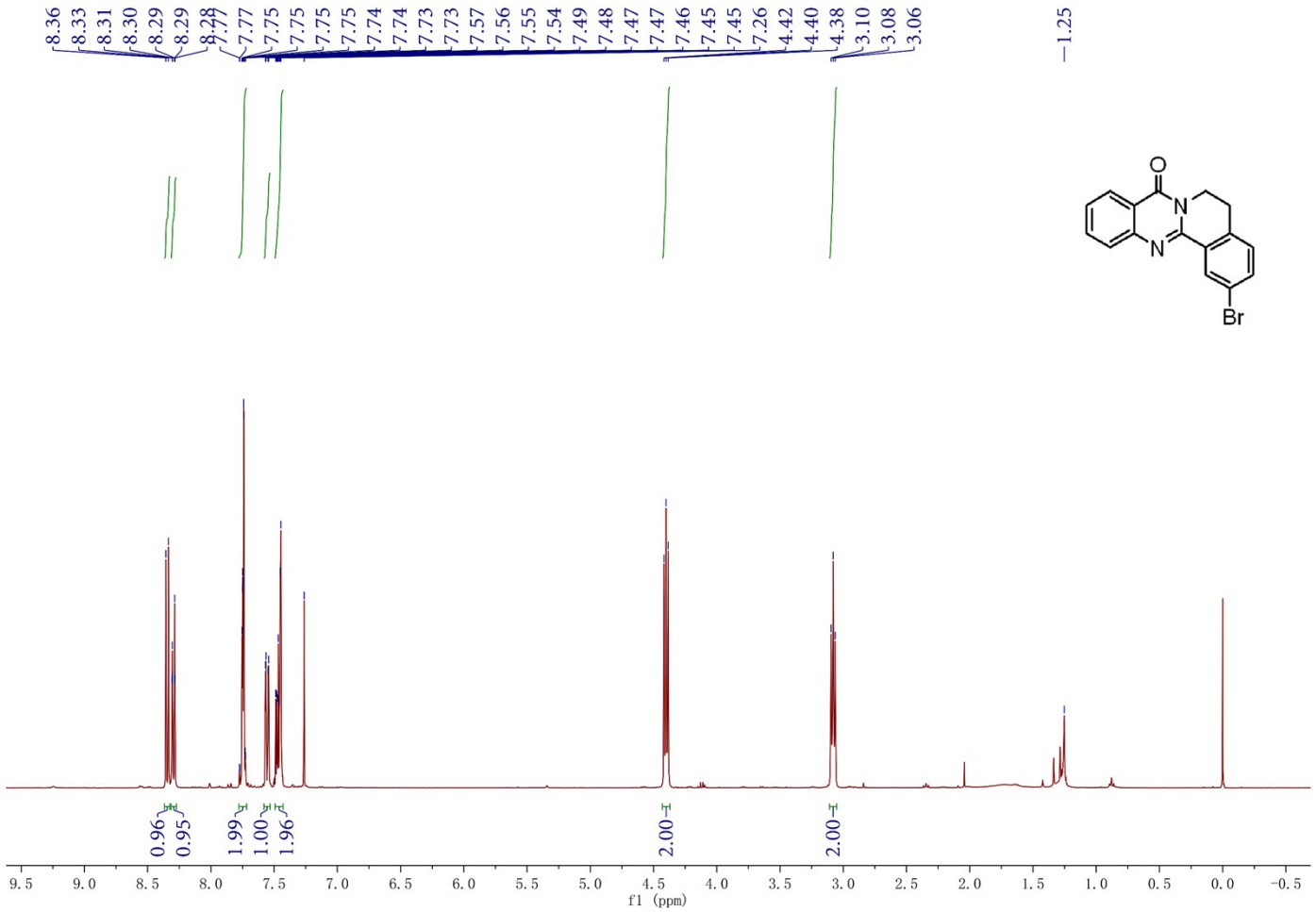
^{1}H NMR ($CDCl_3$, 500 MHz) spectra of **4d**



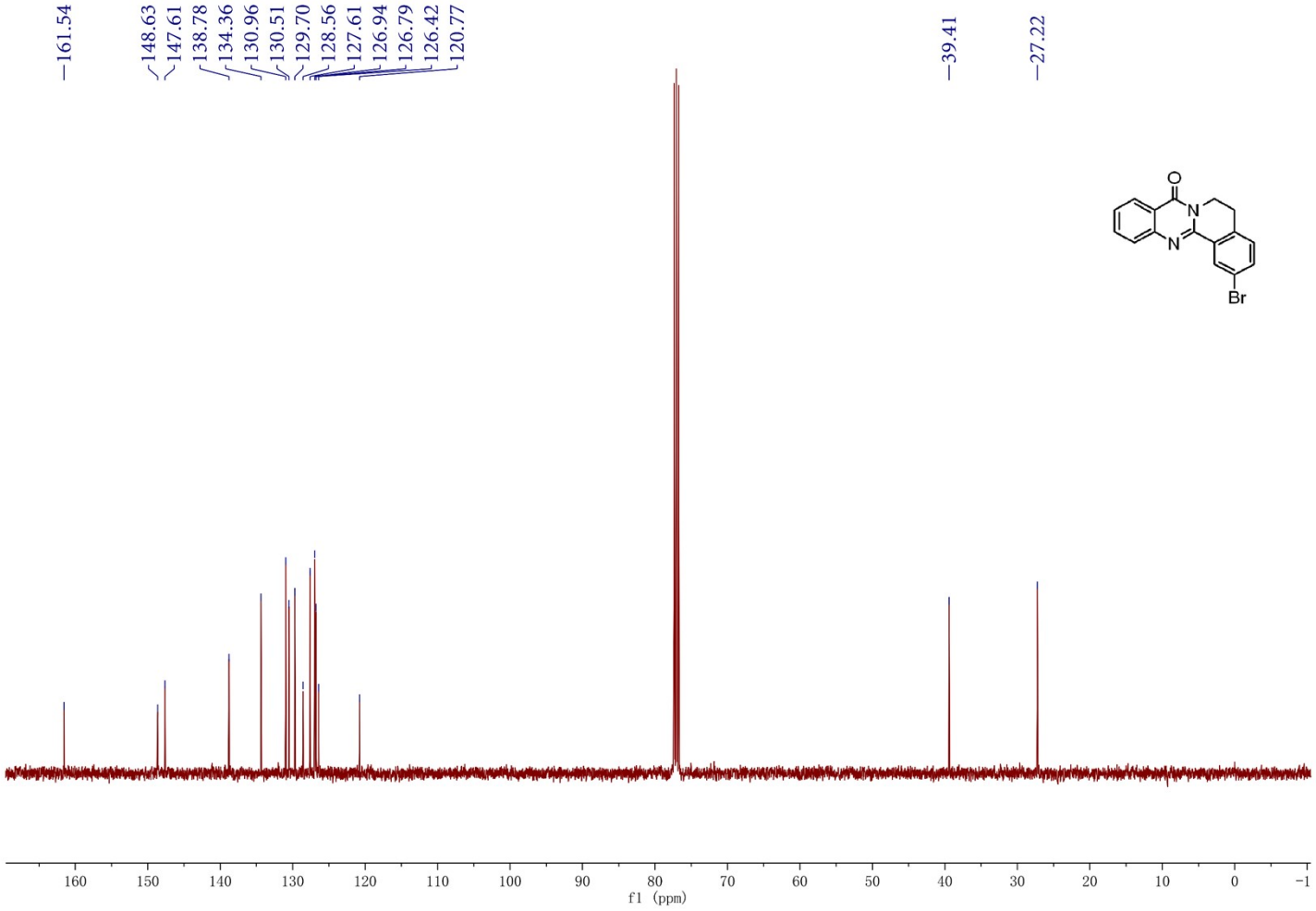
^{13}C NMR ($CDCl_3$, 126 MHz) spectra of **4d**



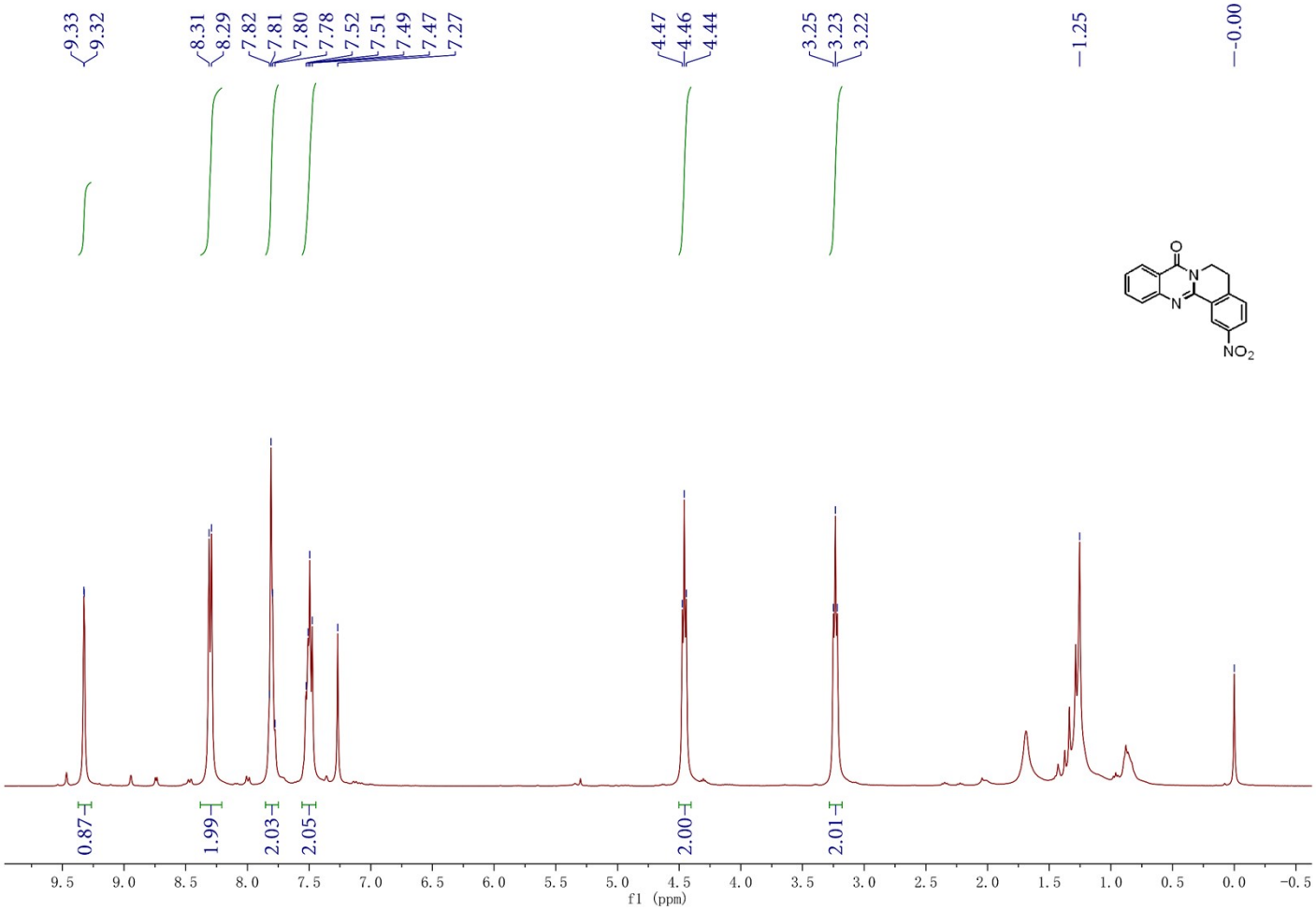
^{1}H NMR ($CDCl_3$, 500 MHz) spectra of **4e**



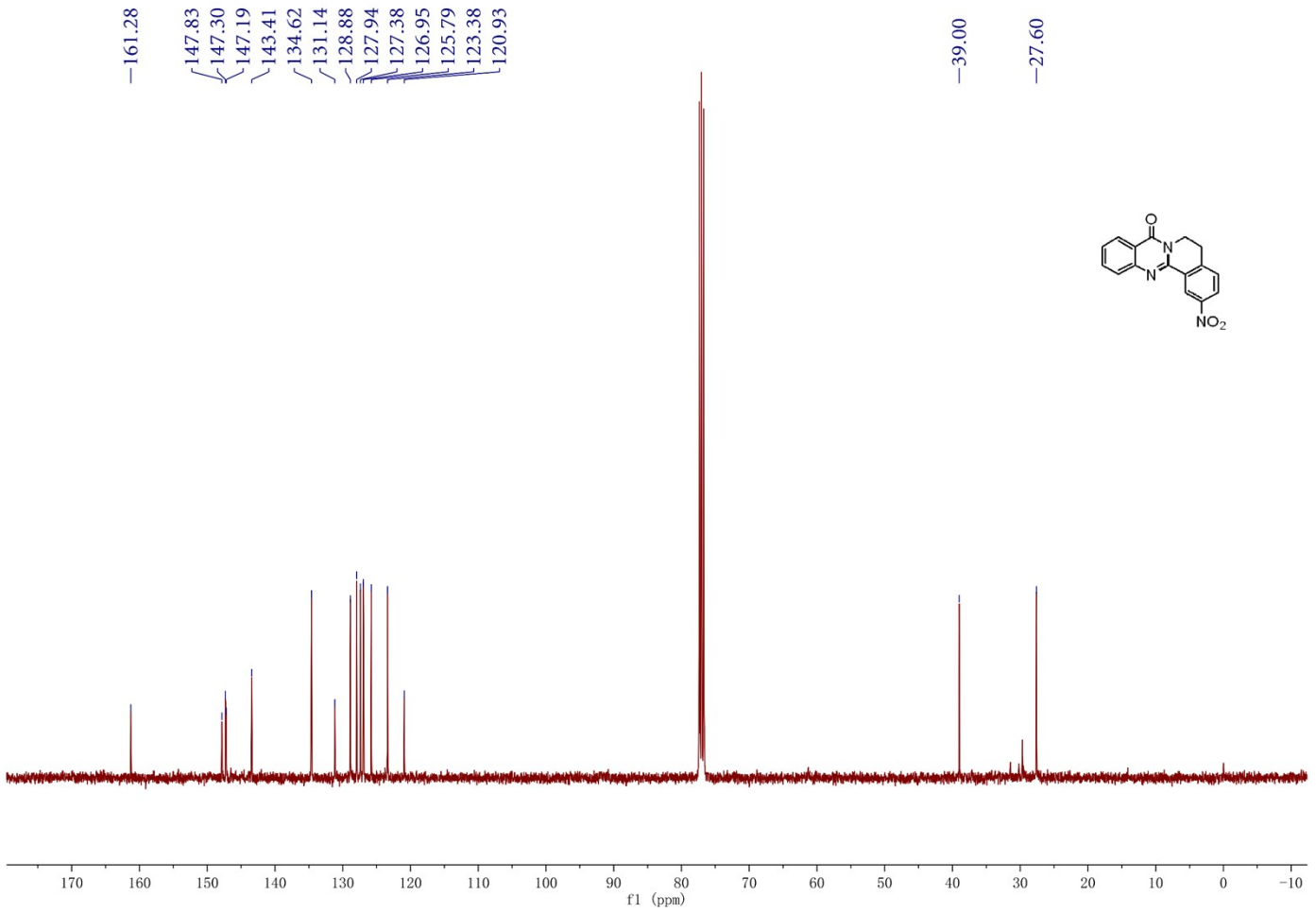
^{13}C NMR ($CDCl_3$, 126 MHz) spectra of **4e**



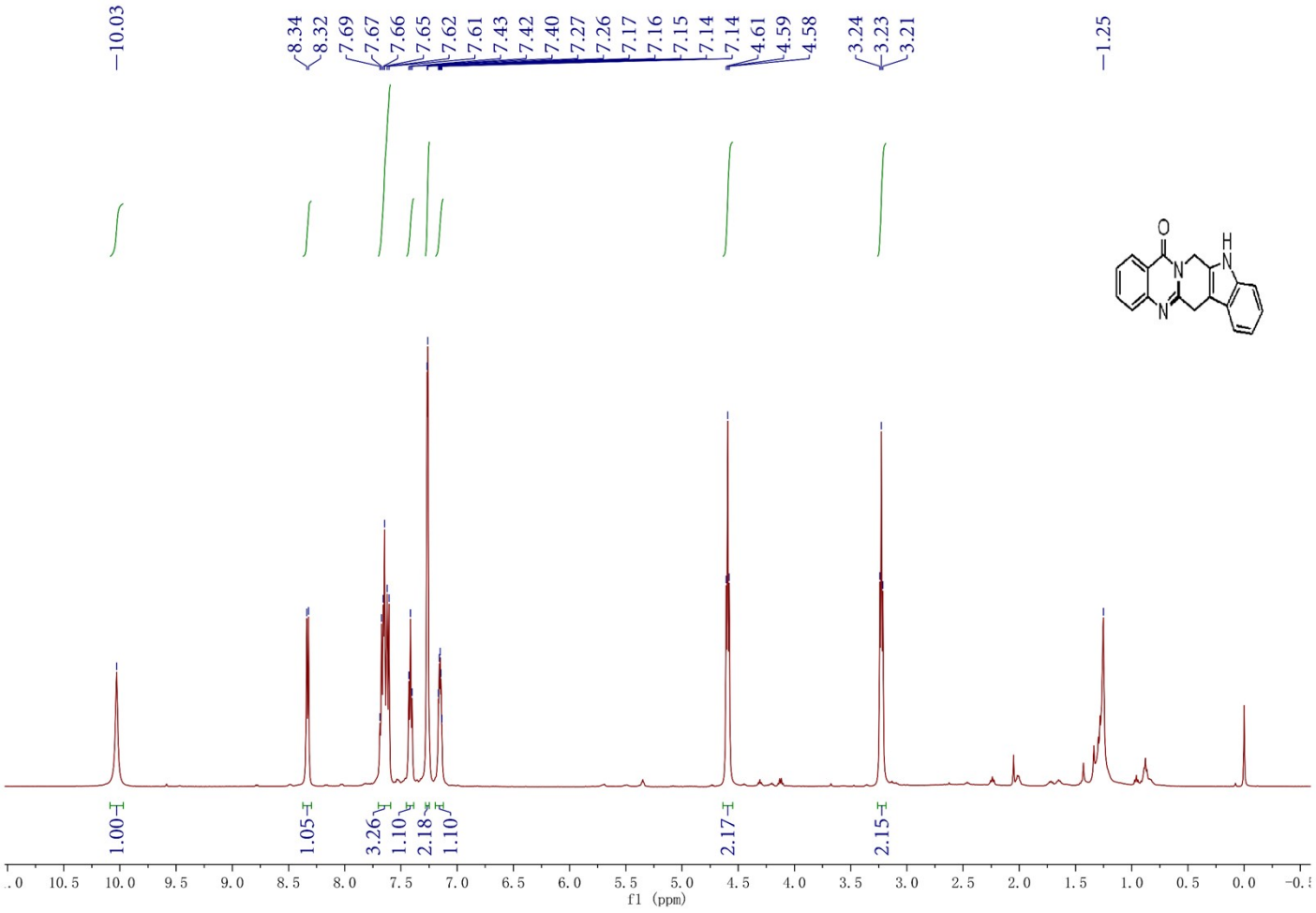
^{1}H NMR ($CDCl_3$, 500 MHz) spectra of **4f**



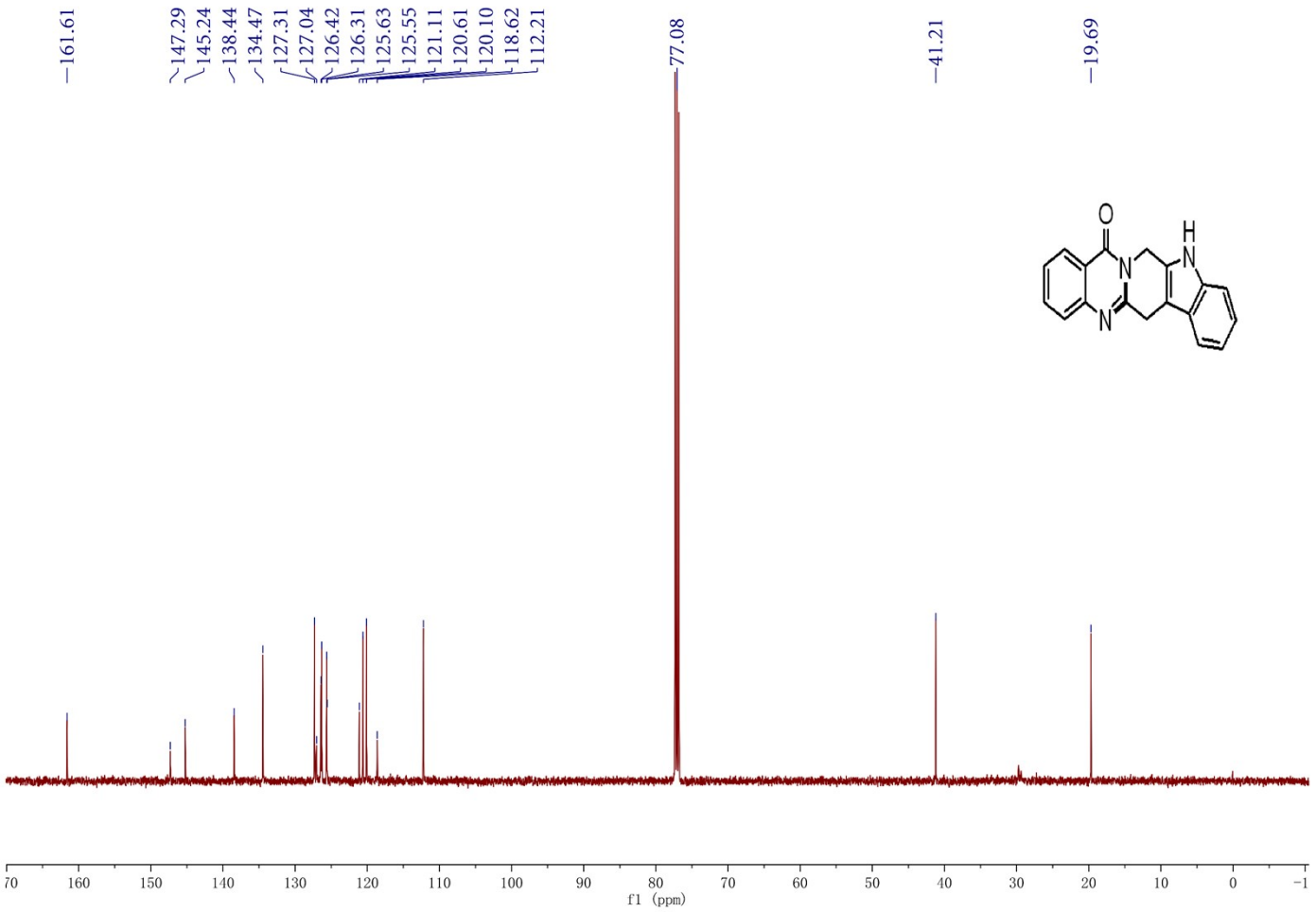
^{13}C NMR ($CDCl_3$, 126 MHz) spectra of **4f**



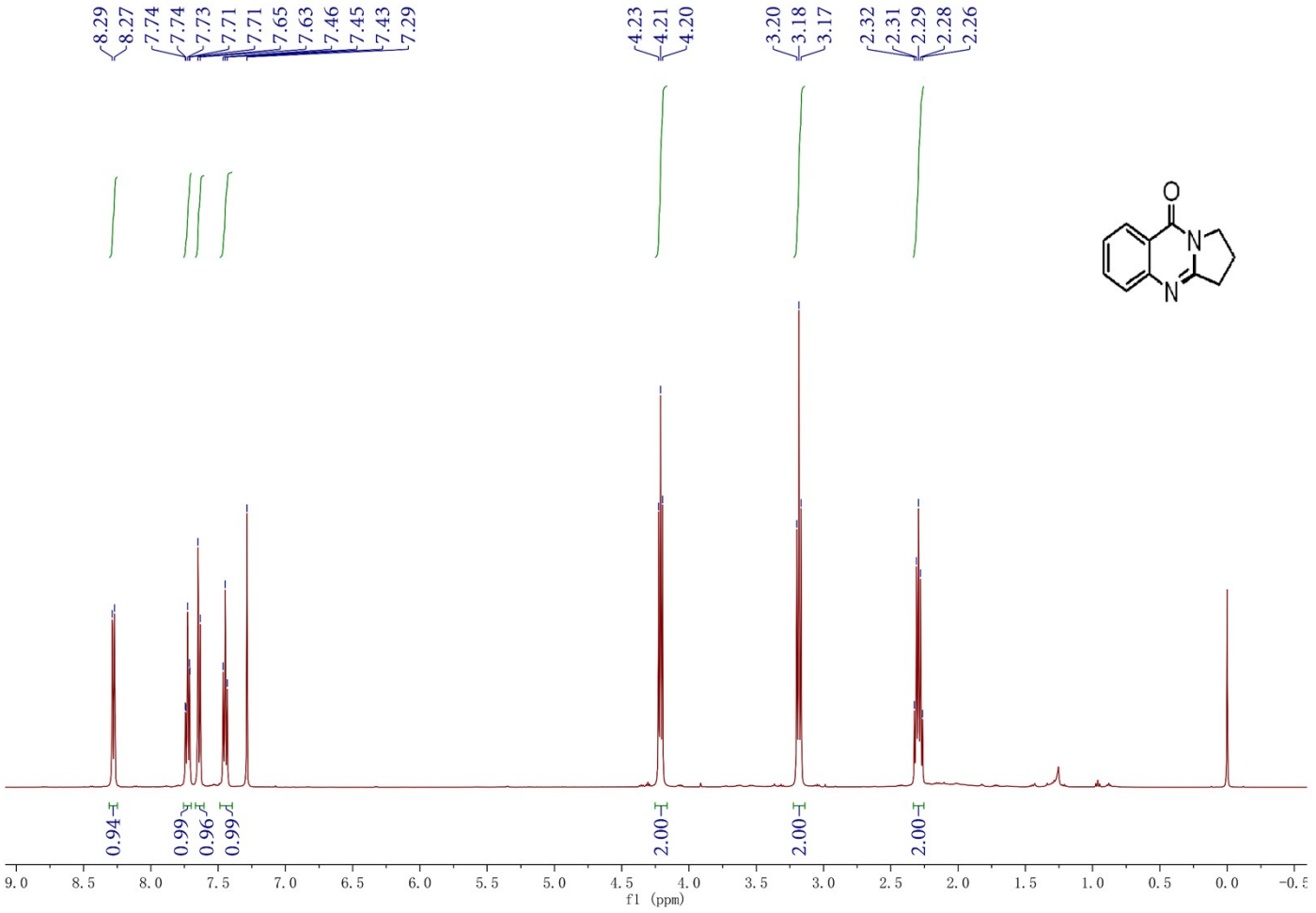
^{1}H NMR ($CDCl_3$, 500 MHz) spectra of **4g**



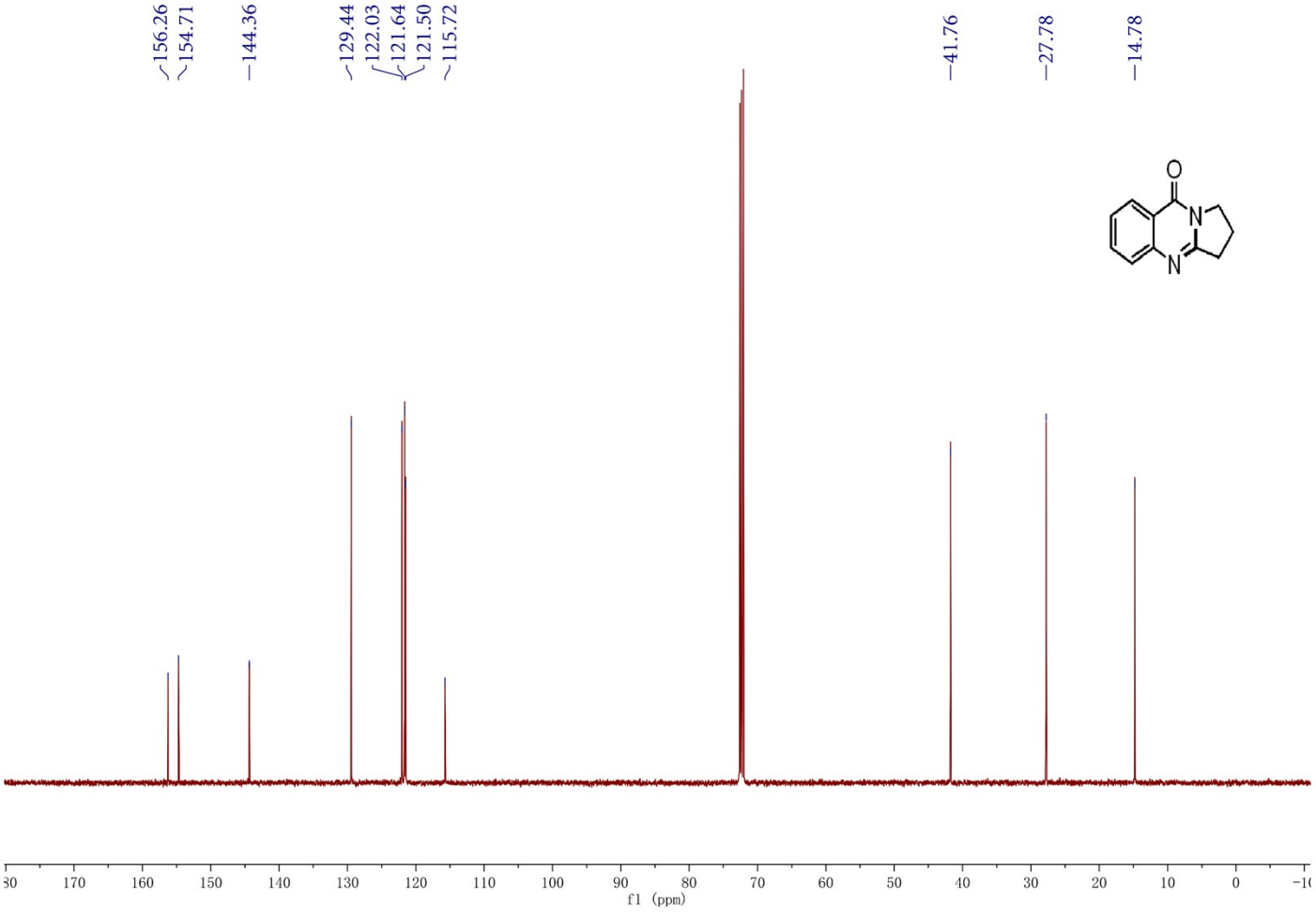
^{13}C NMR ($CDCl_3$, 126 MHz) spectra of **4g**



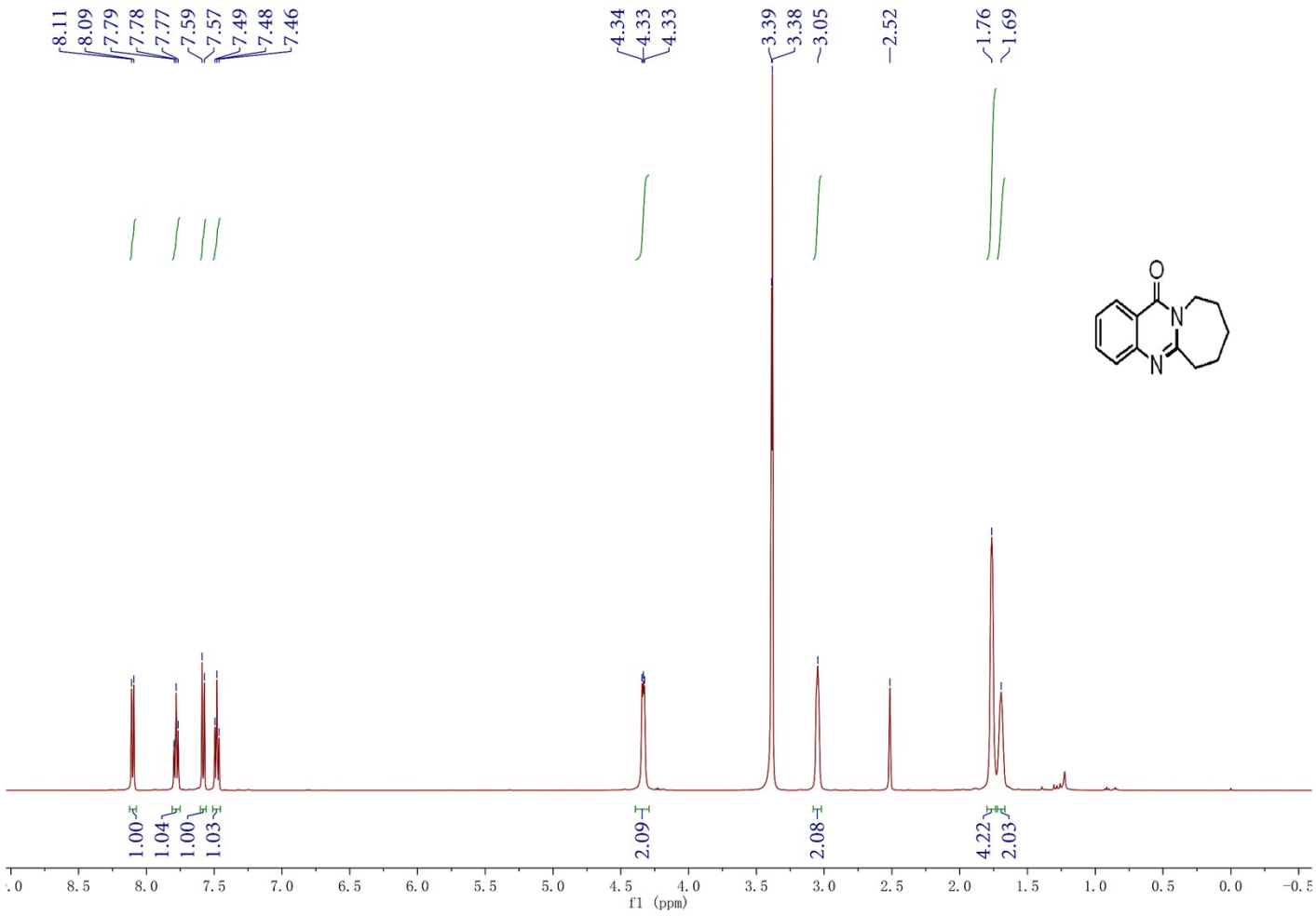
^{1}H NMR ($CDCl_3$, 500 MHz) spectra of **4h**



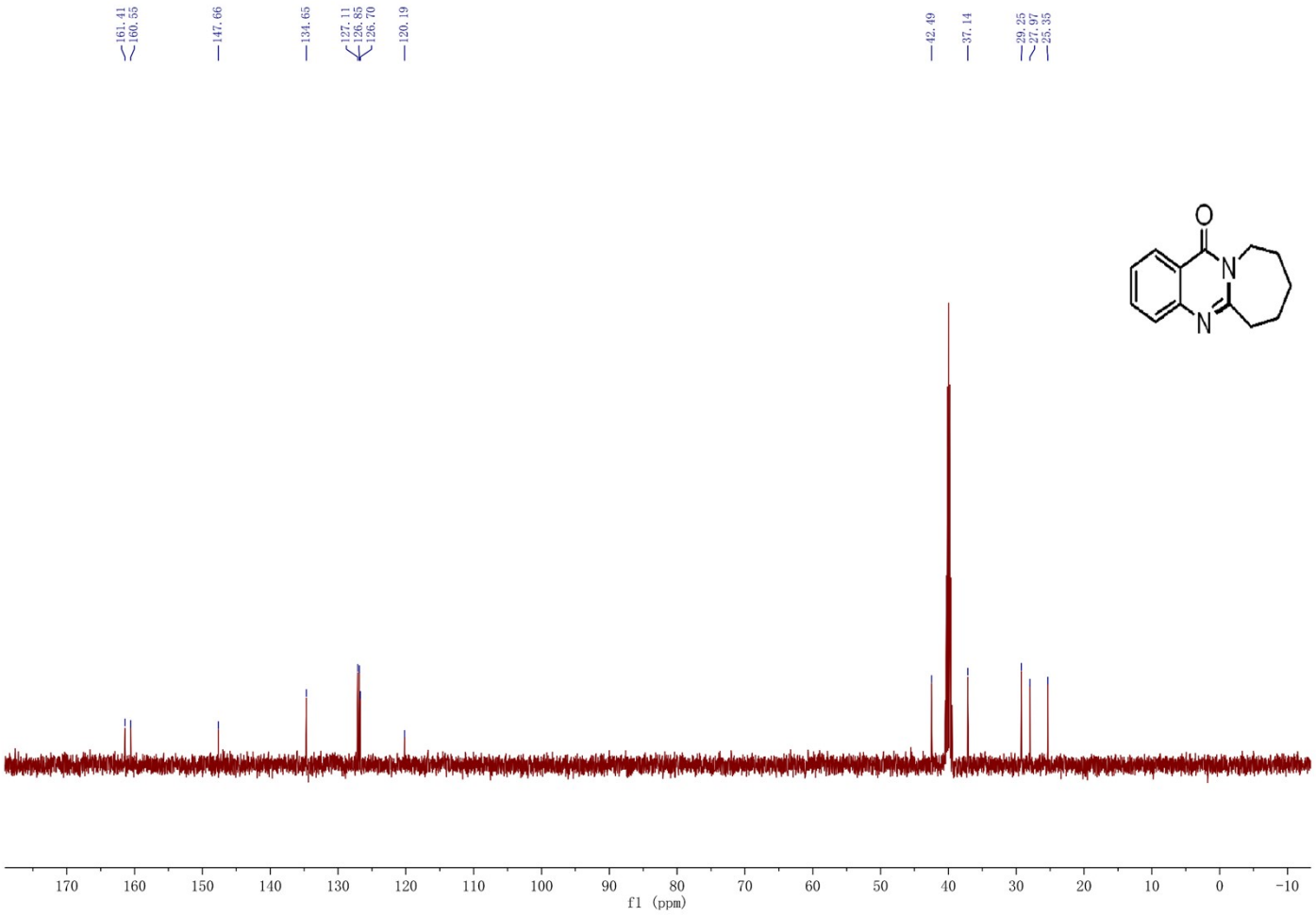
^{13}C NMR ($CDCl_3$, 126 MHz) spectra of **4h**



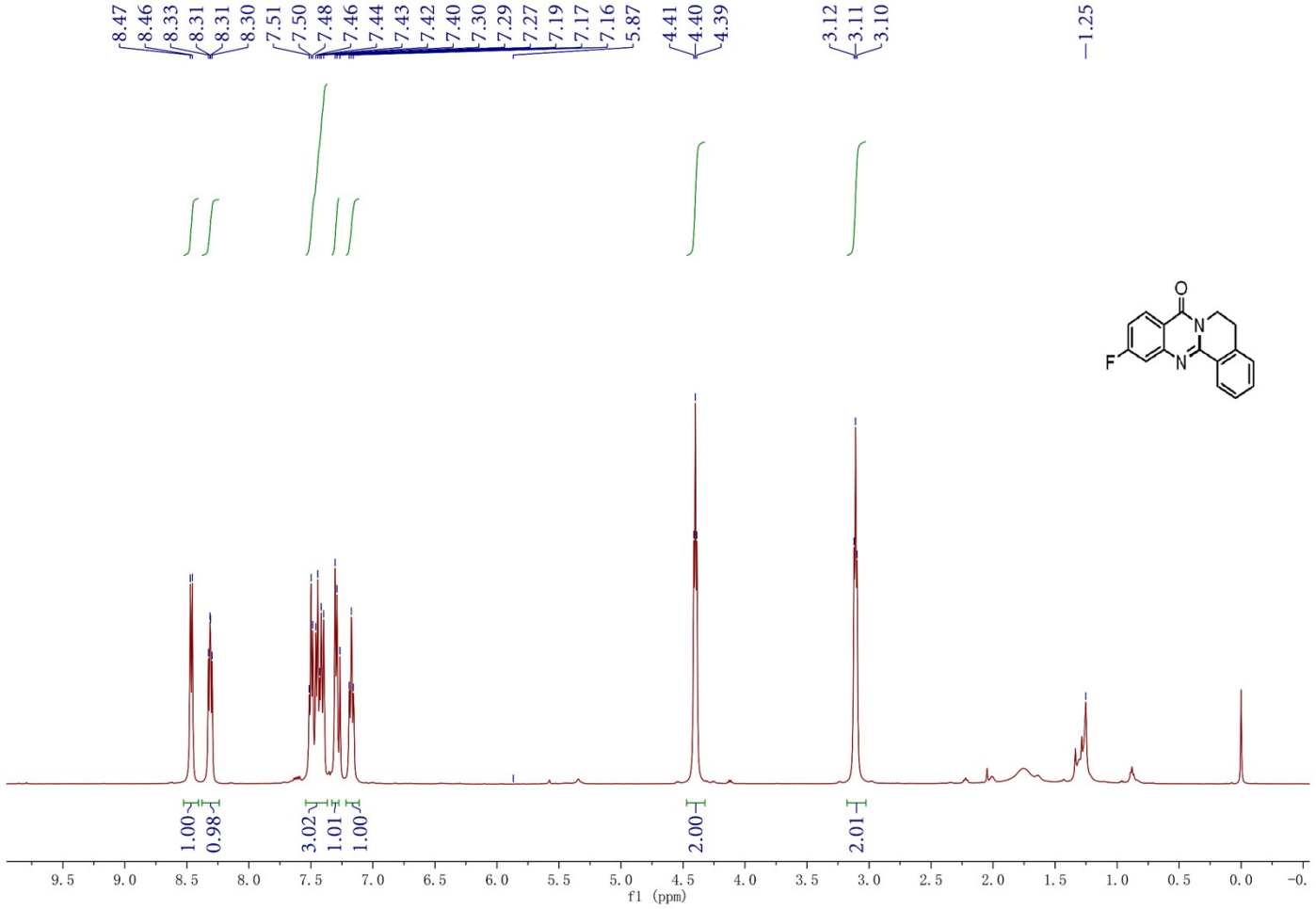
^{1}H NMR ($CDCl_3$, 500 MHz) spectra of **4i**



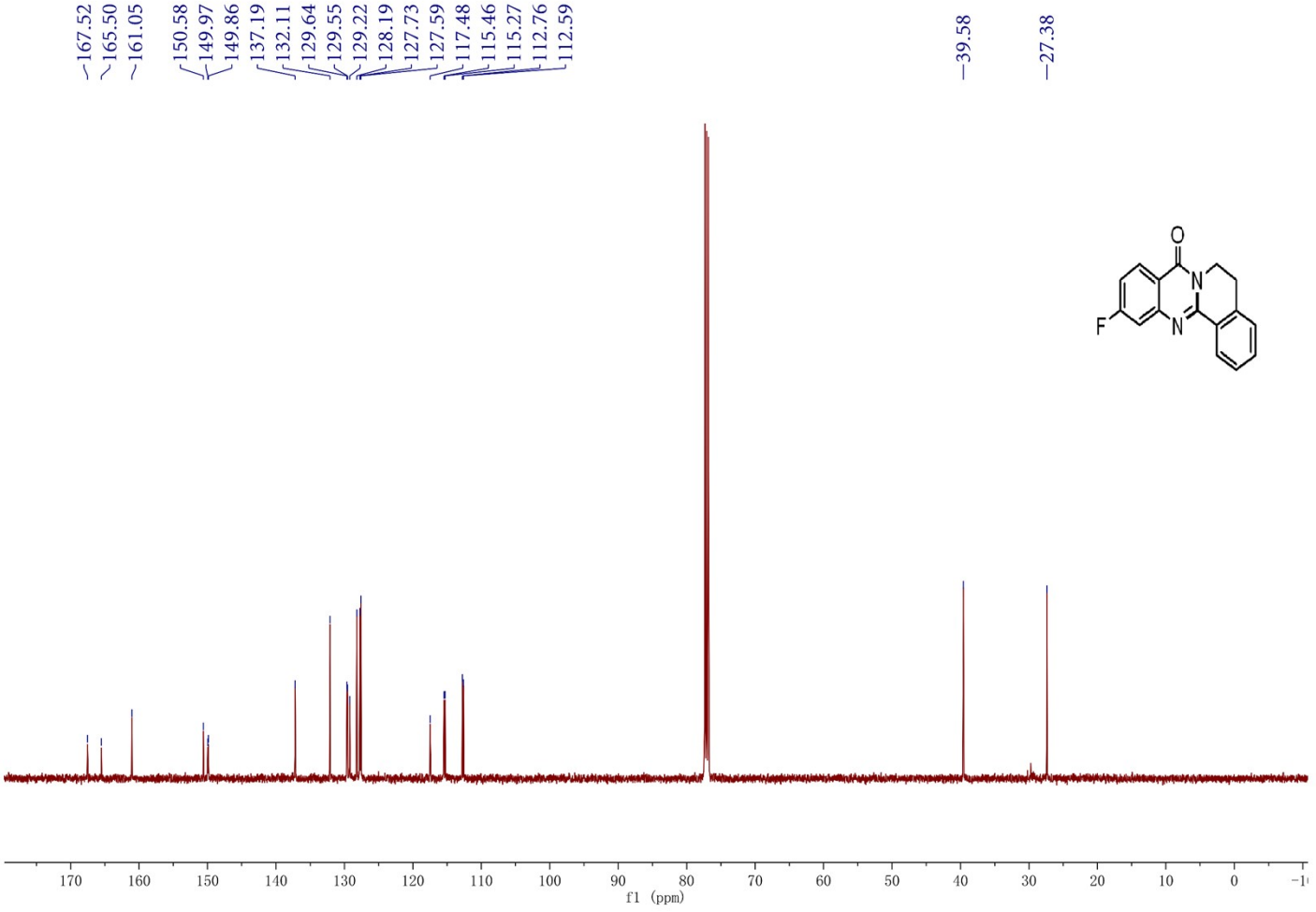
^{13}C NMR ($CDCl_3$, 126 MHz) spectra of **4i**



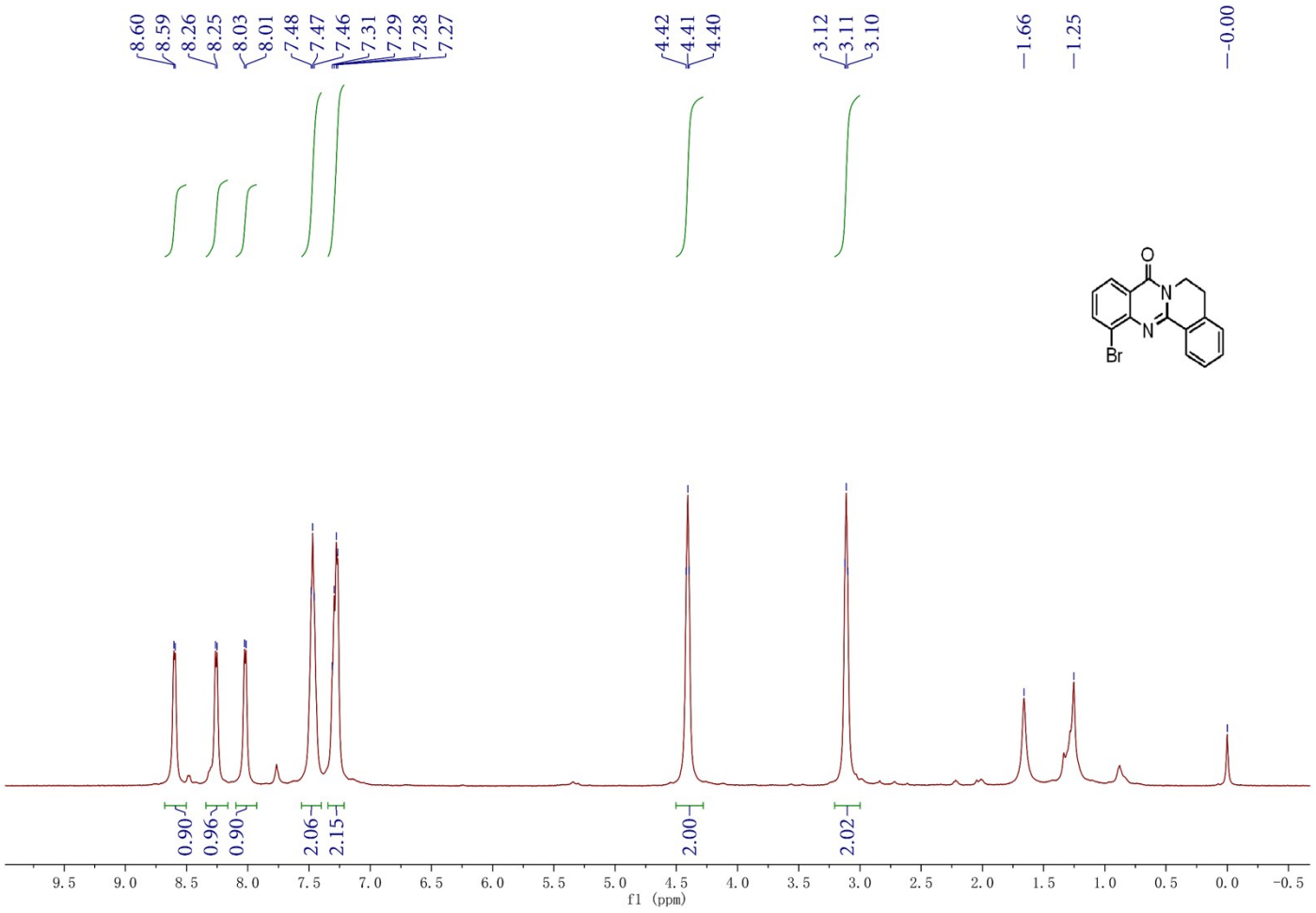
^{1}H NMR ($CDCl_3$, 500 MHz) spectra of **4j**



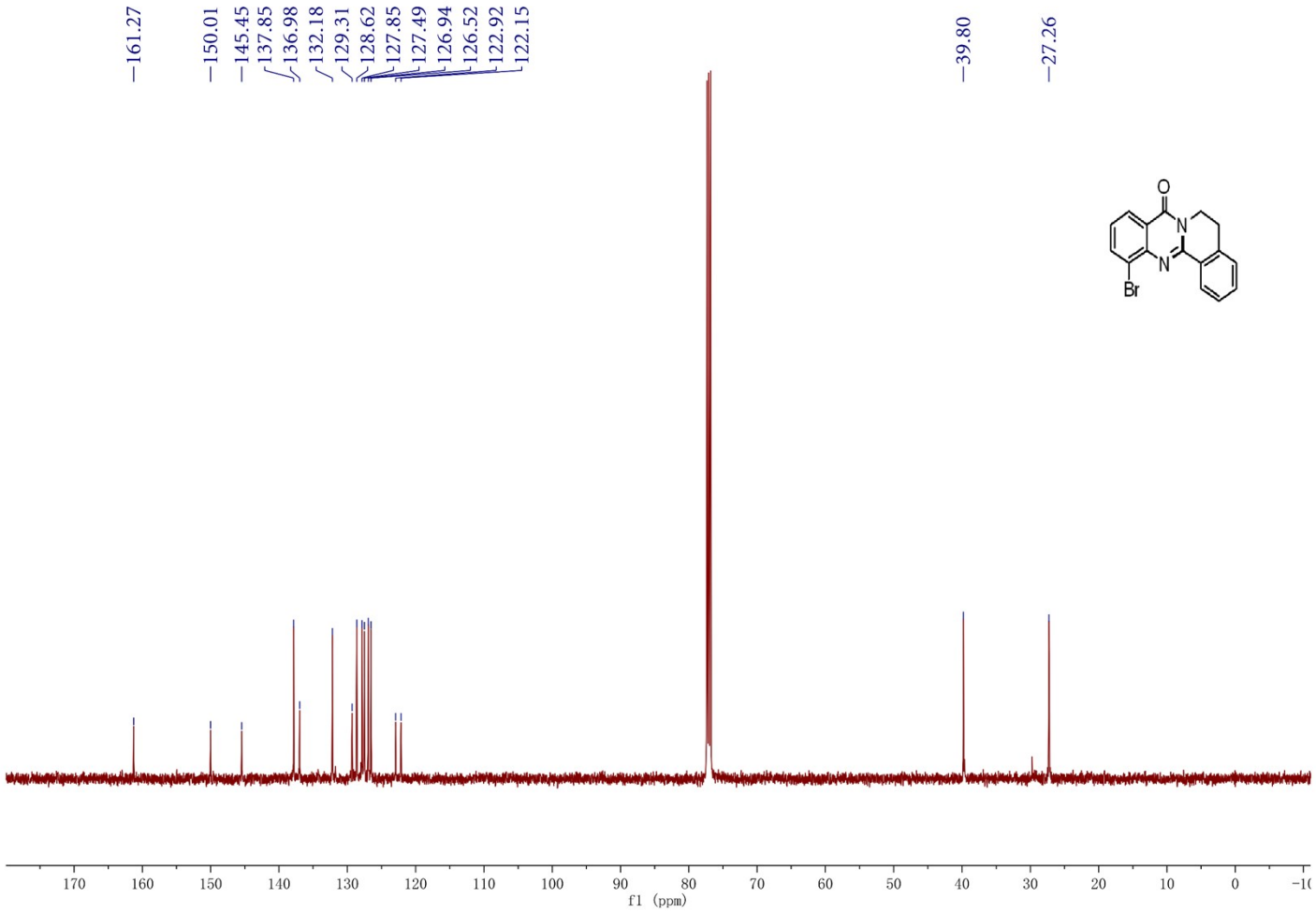
^{13}C NMR ($CDCl_3$, 126 MHz) spectra of **4j**



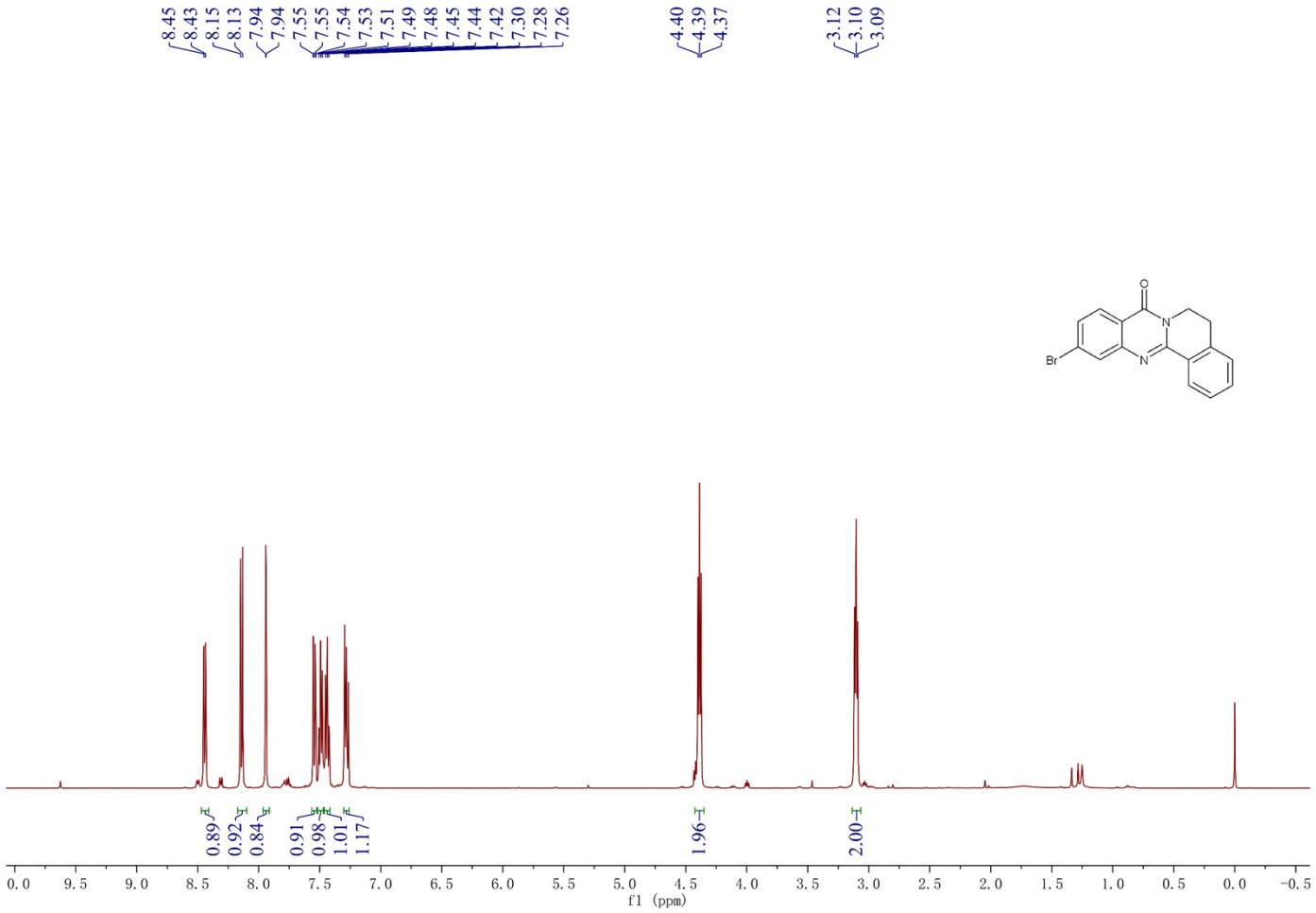
^{1}H NMR ($CDCl_3$, 500 MHz) spectra of **4k**



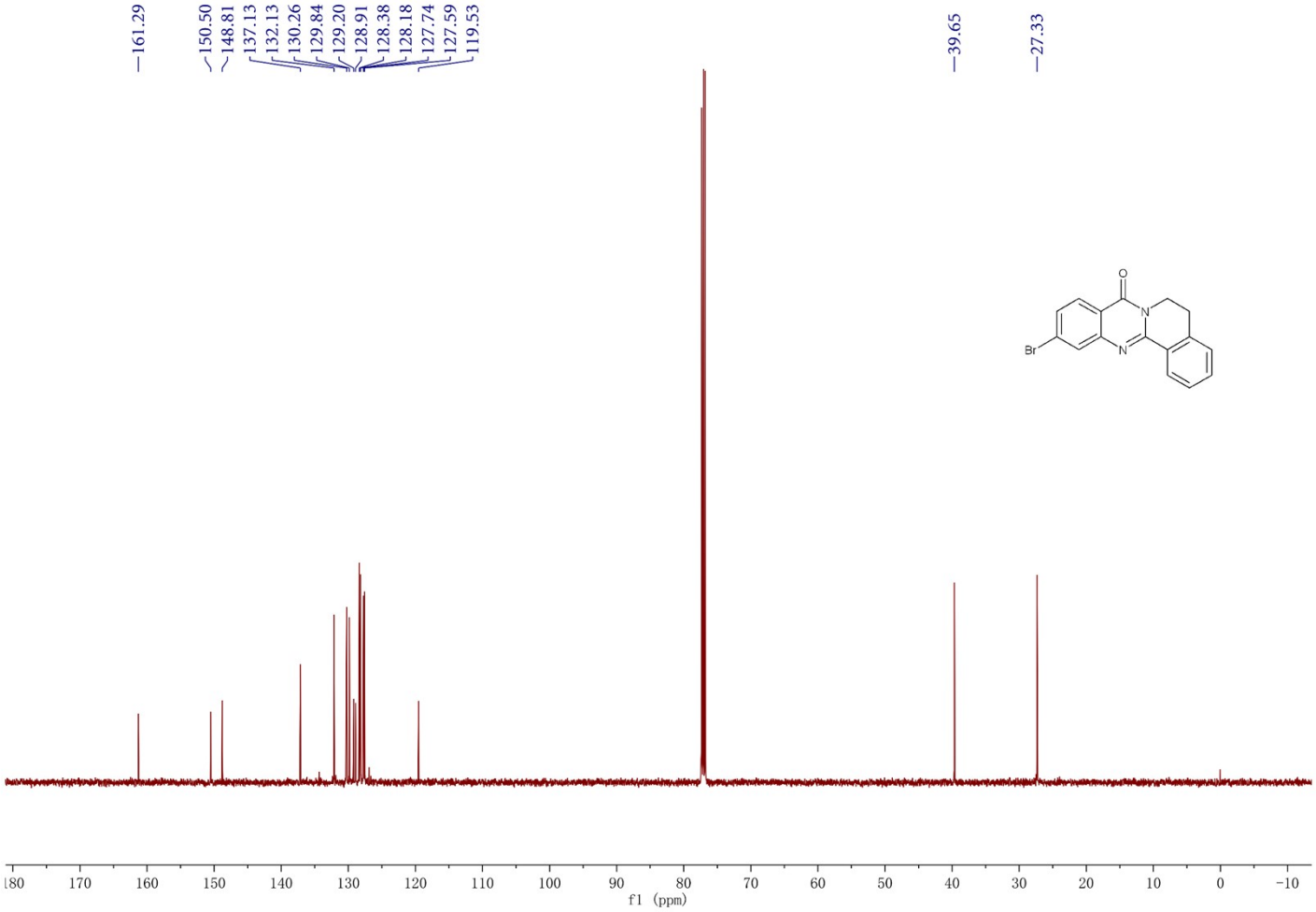
^{13}C NMR ($CDCl_3$, 126 MHz) spectra of **4k**



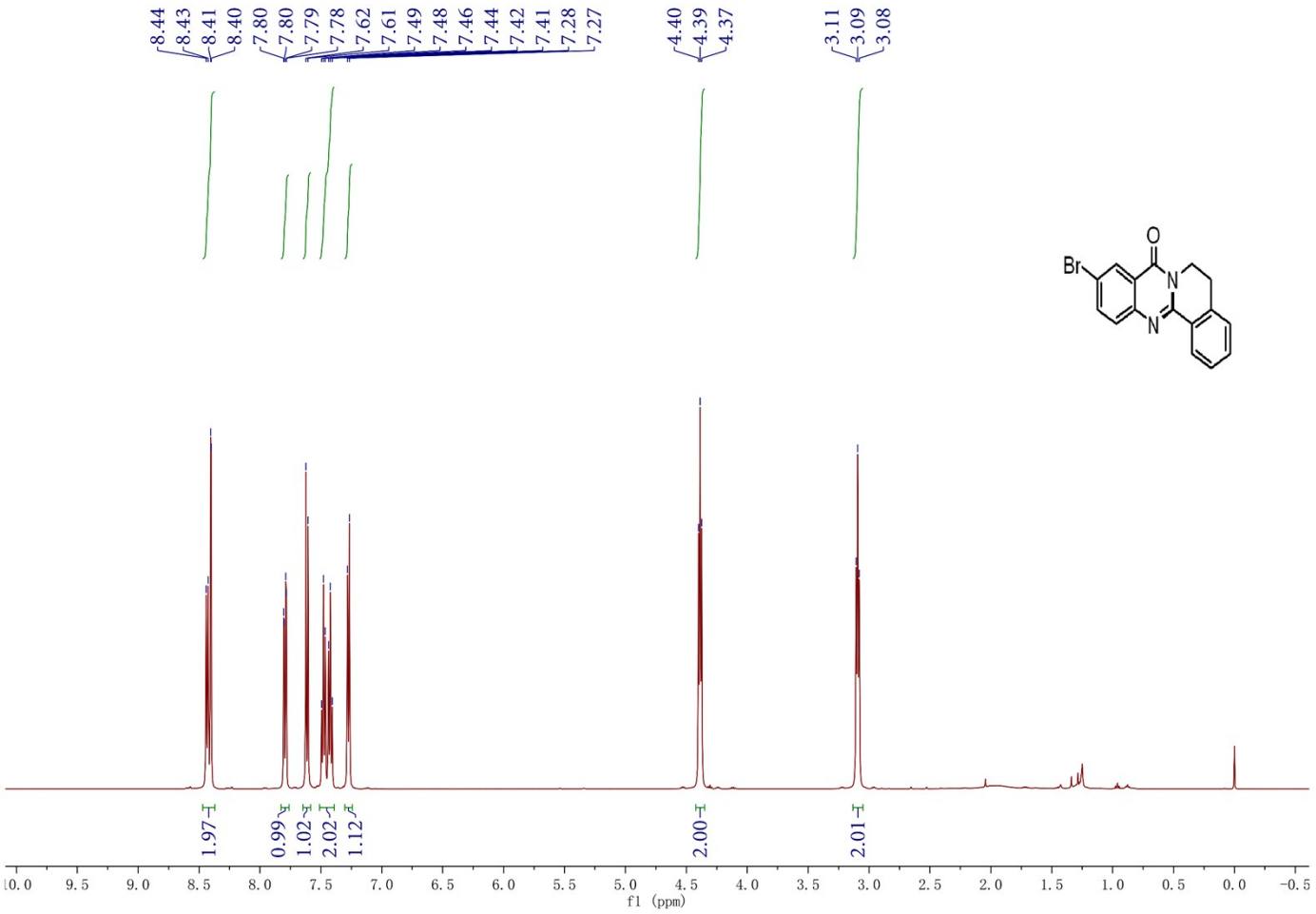
^{1}H NMR ($CDCl_3$, 500 MHz) spectra of **4l**



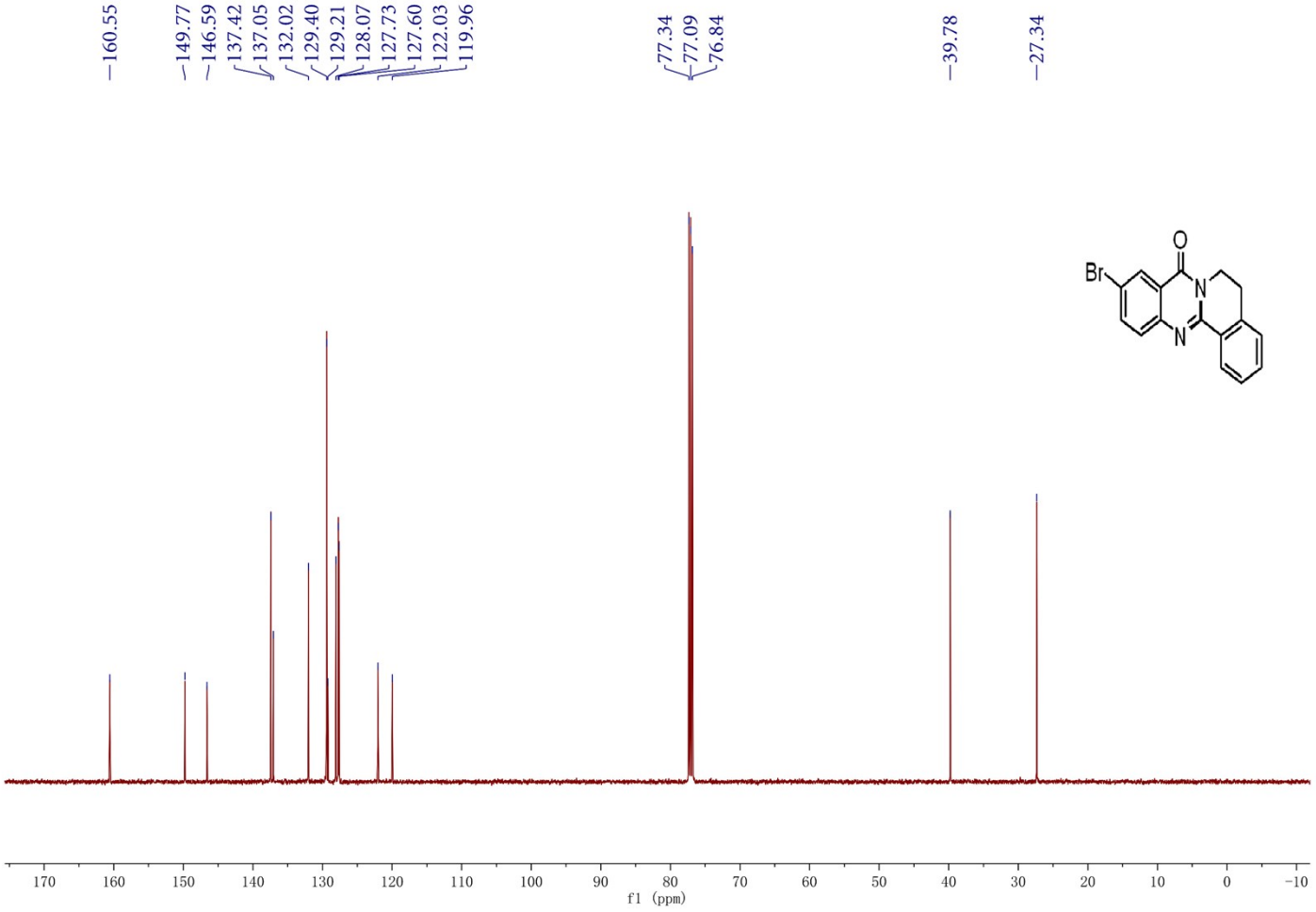
^{13}C NMR ($CDCl_3$, 126 MHz) spectra of **4l**



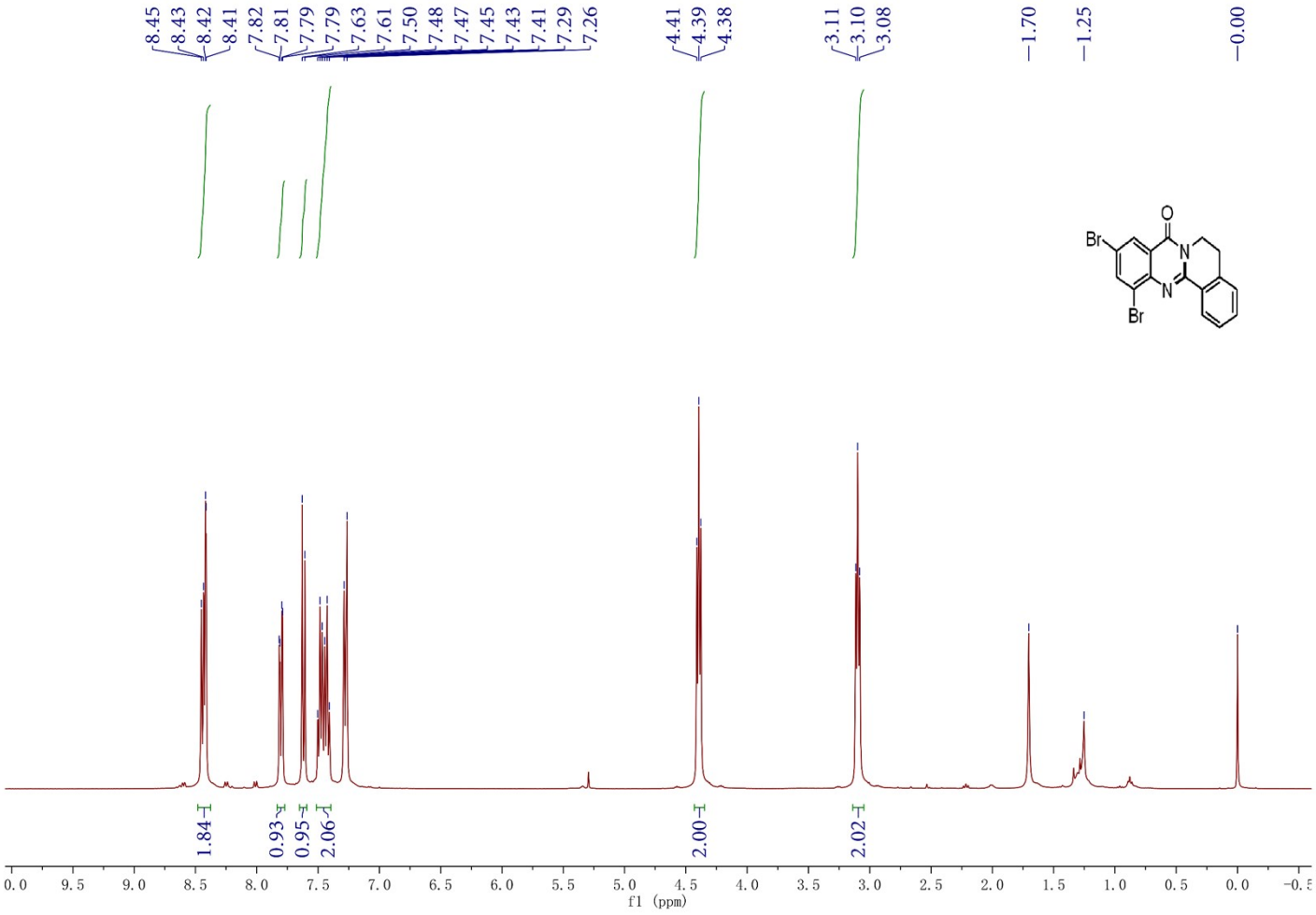
^{1}H NMR ($CDCl_3$, 500 MHz) spectra of **4m**



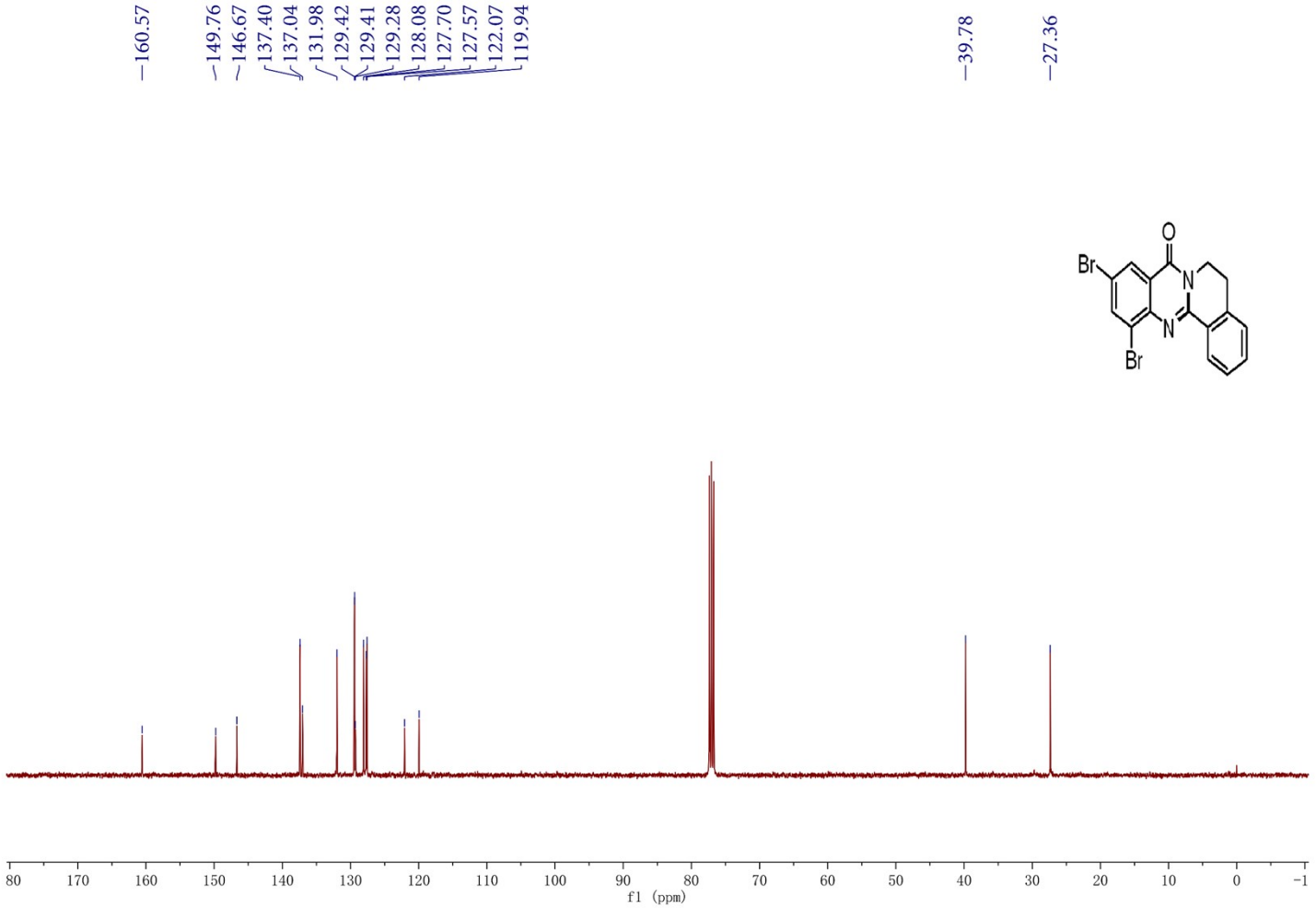
^{13}C NMR ($CDCl_3$, 126 MHz) spectra of **4m**



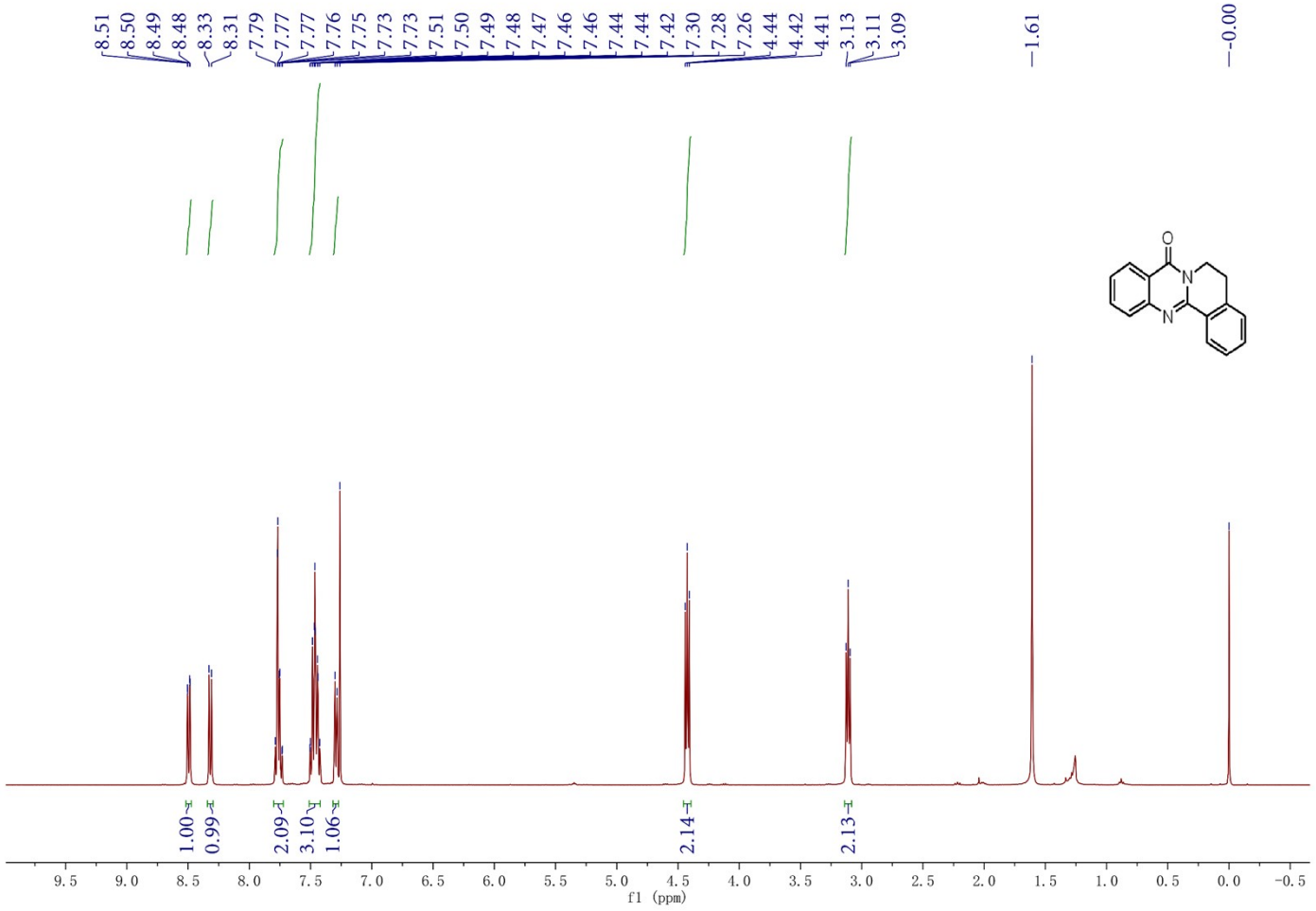
^{1}H NMR ($CDCl_3$, 500 MHz) spectra of **4n**



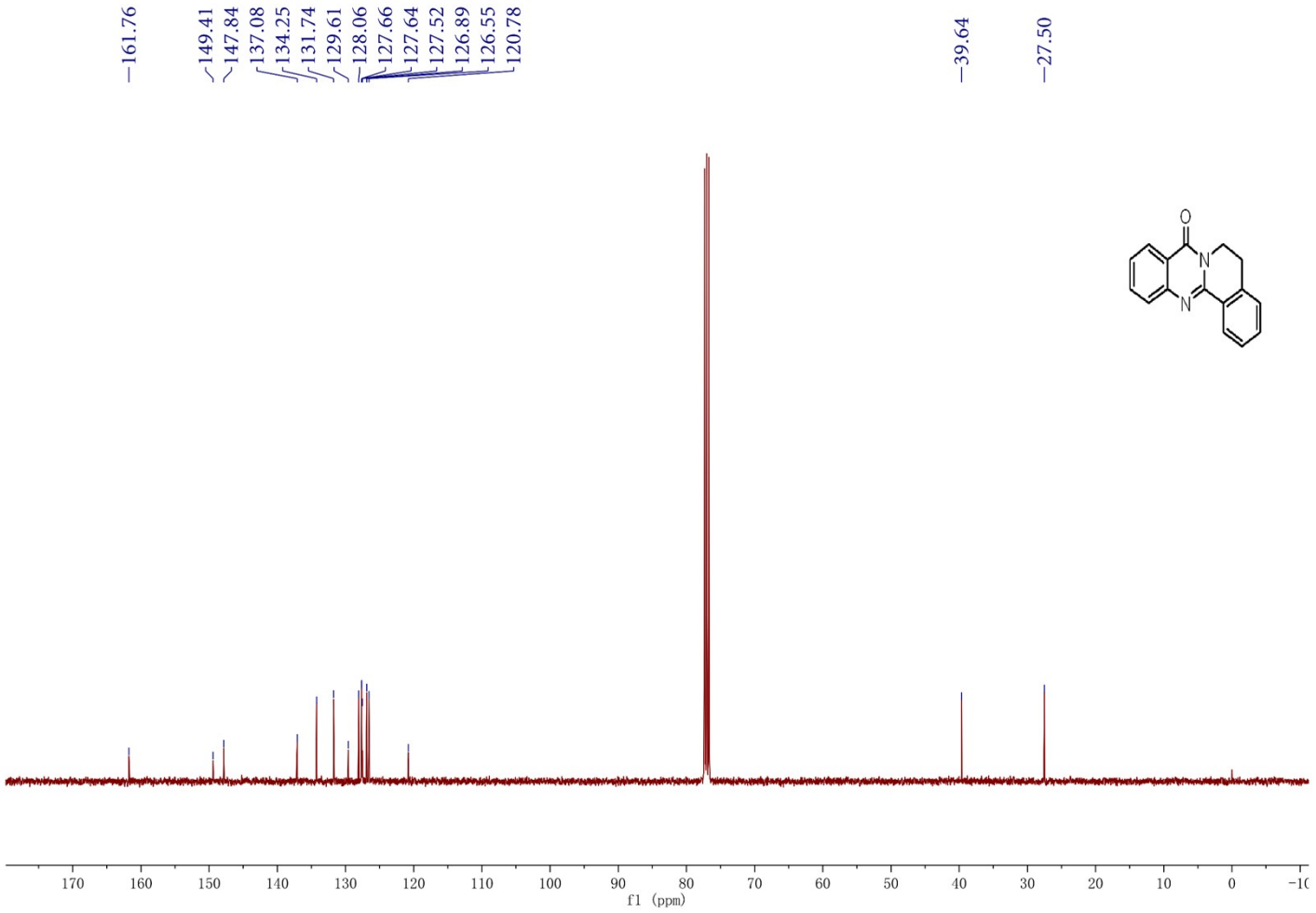
^{13}C NMR ($CDCl_3$, 126 MHz) spectra of **4n**



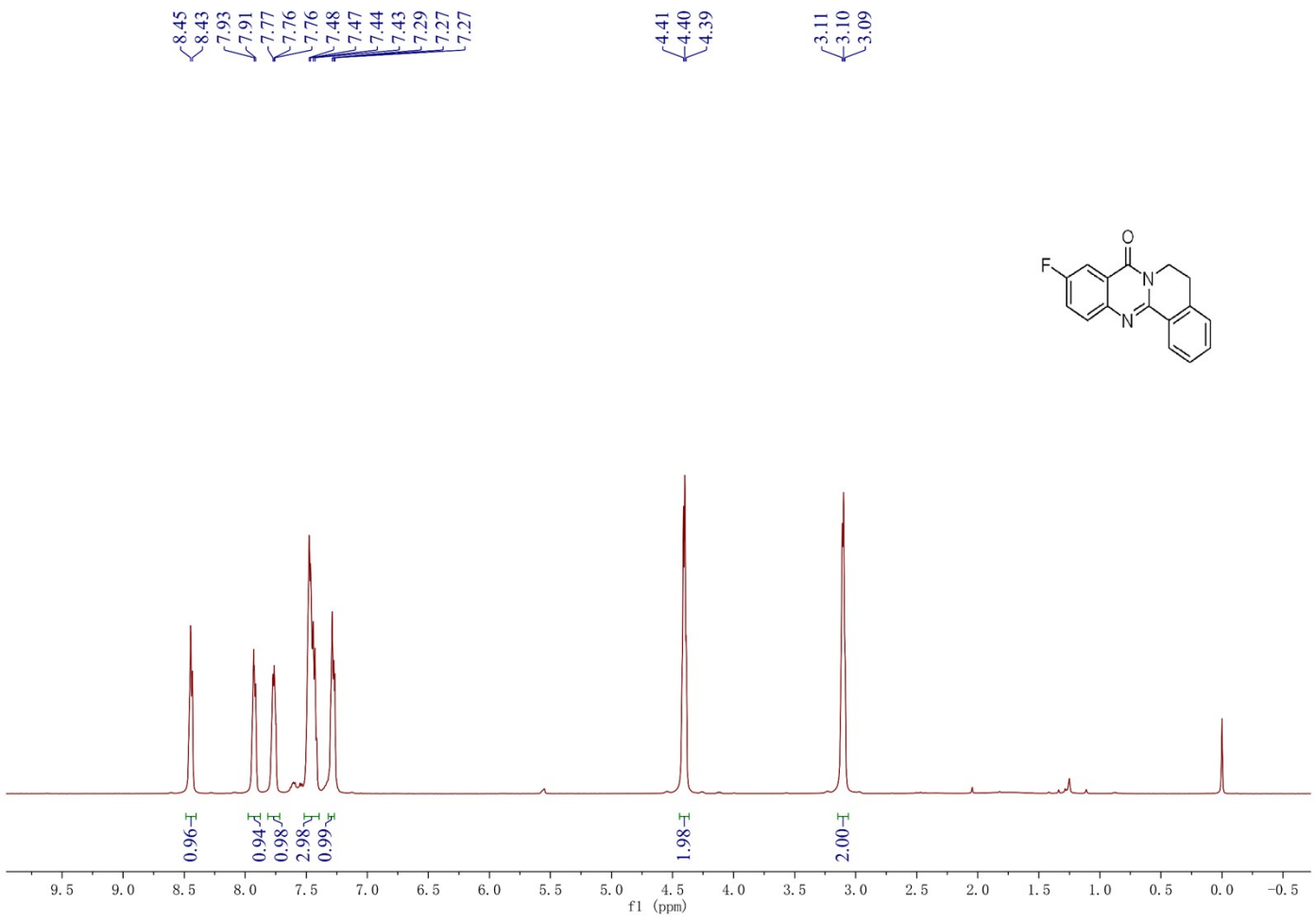
^{1}H NMR ($CDCl_3$, 500 MHz) spectra of **4a** (from 2-aminophenone)



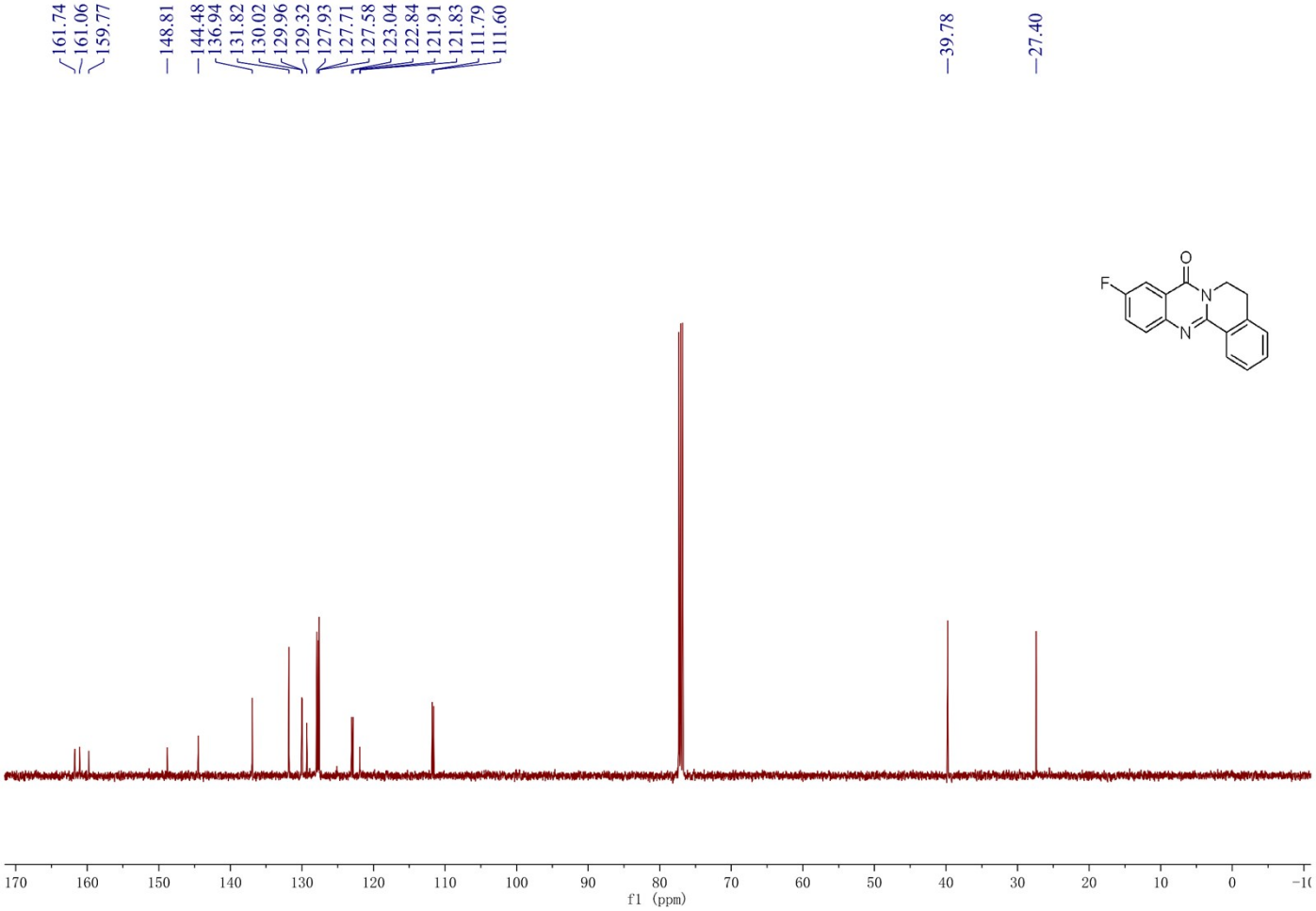
^{13}C NMR ($CDCl_3$, 126 MHz) spectra of **4a**(from 2-aminophenone)



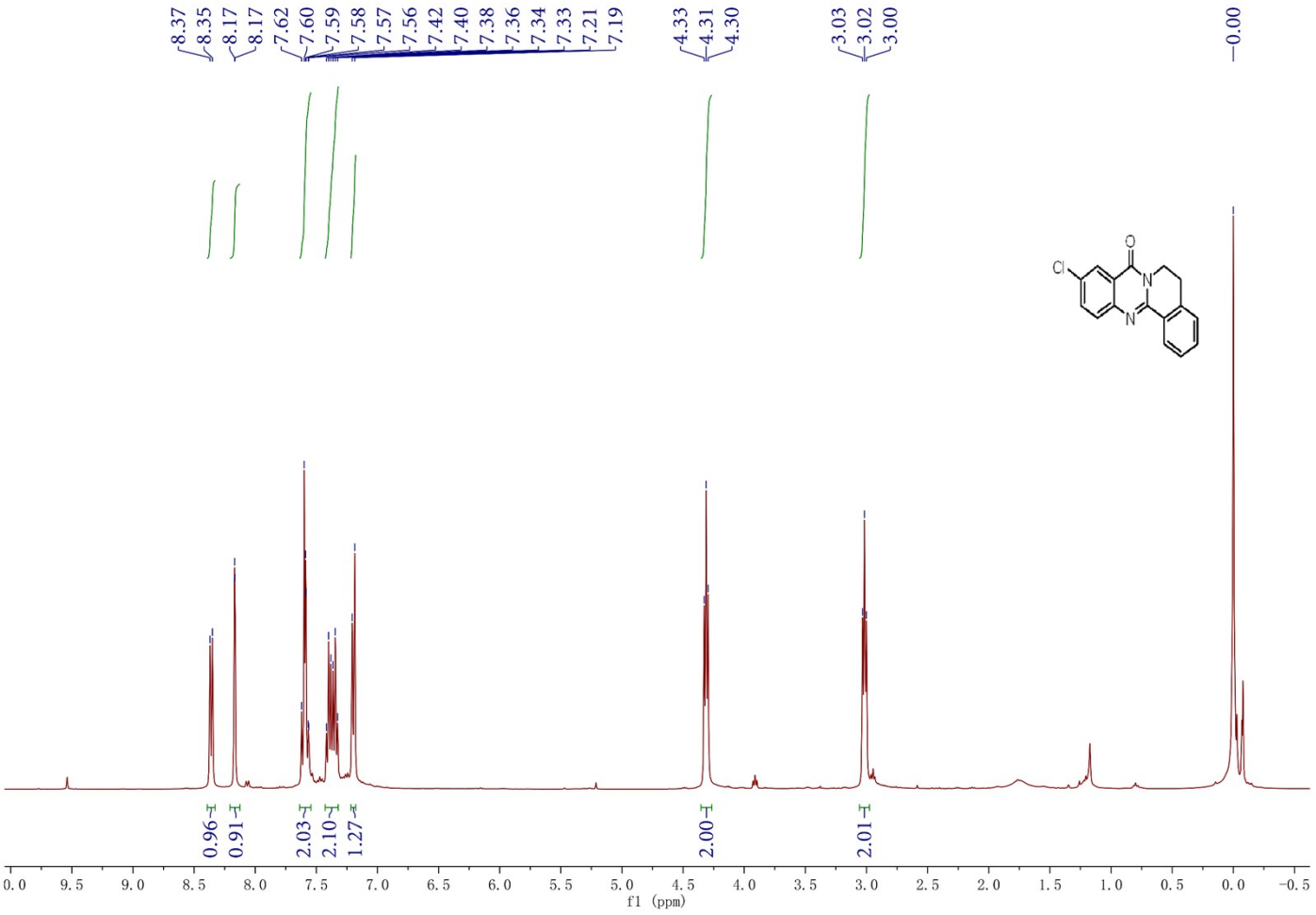
^{1}H NMR ($CDCl_3$, 500 MHz) spectra of **4o**



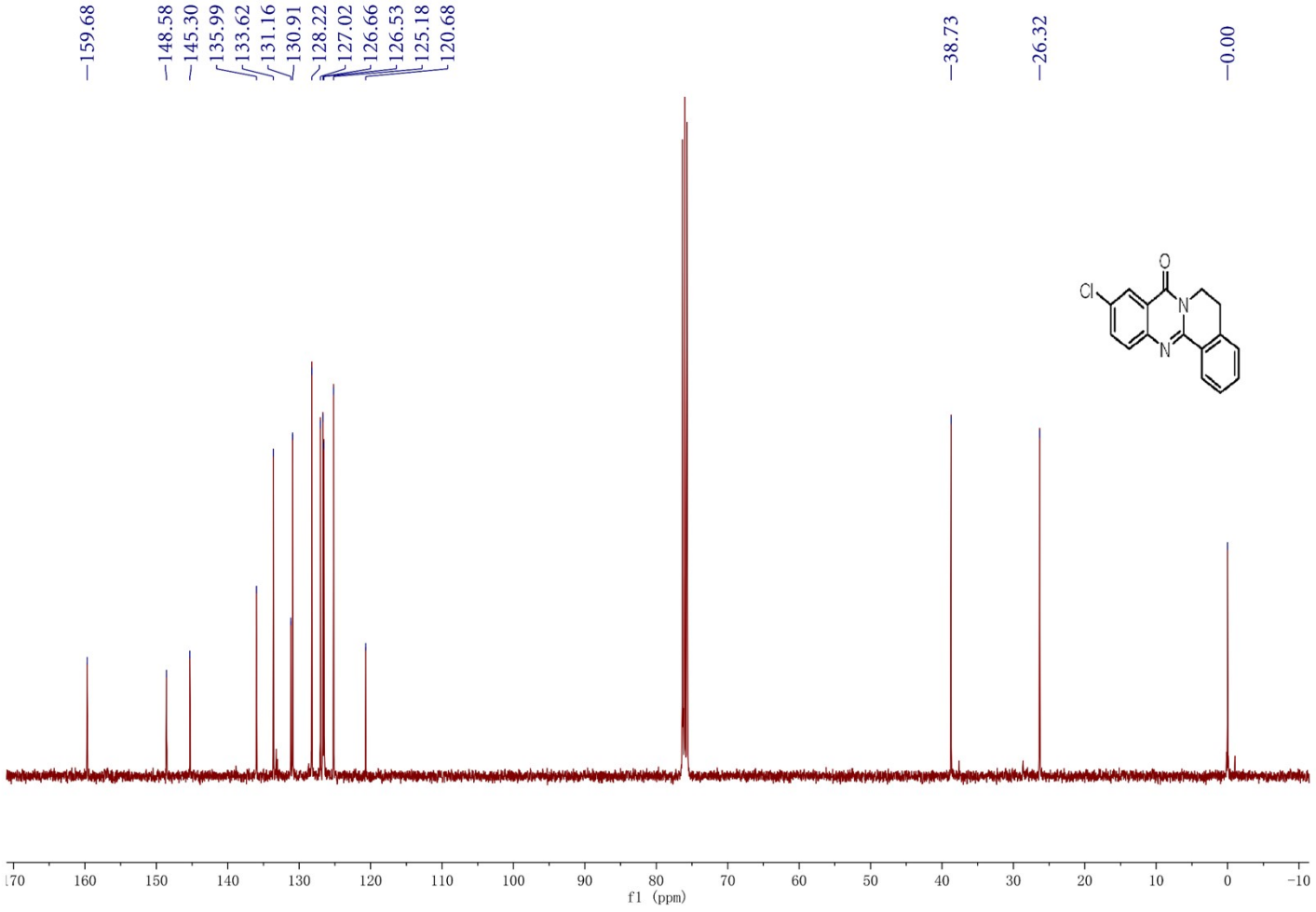
^{13}C NMR ($CDCl_3$, 126 MHz) spectra of **4o**



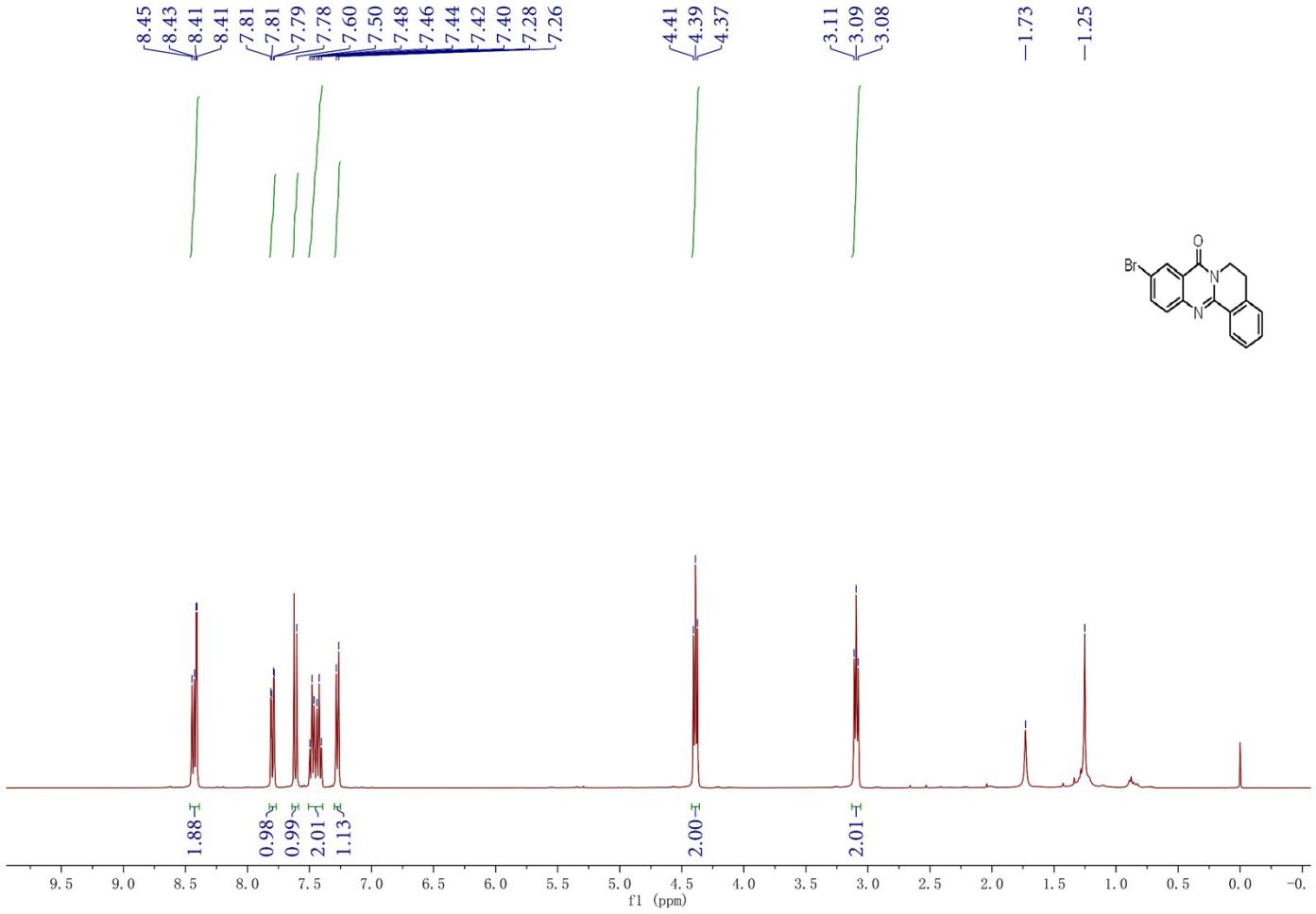
^{1}H NMR ($CDCl_3$, 500 MHz) spectra of **4p**



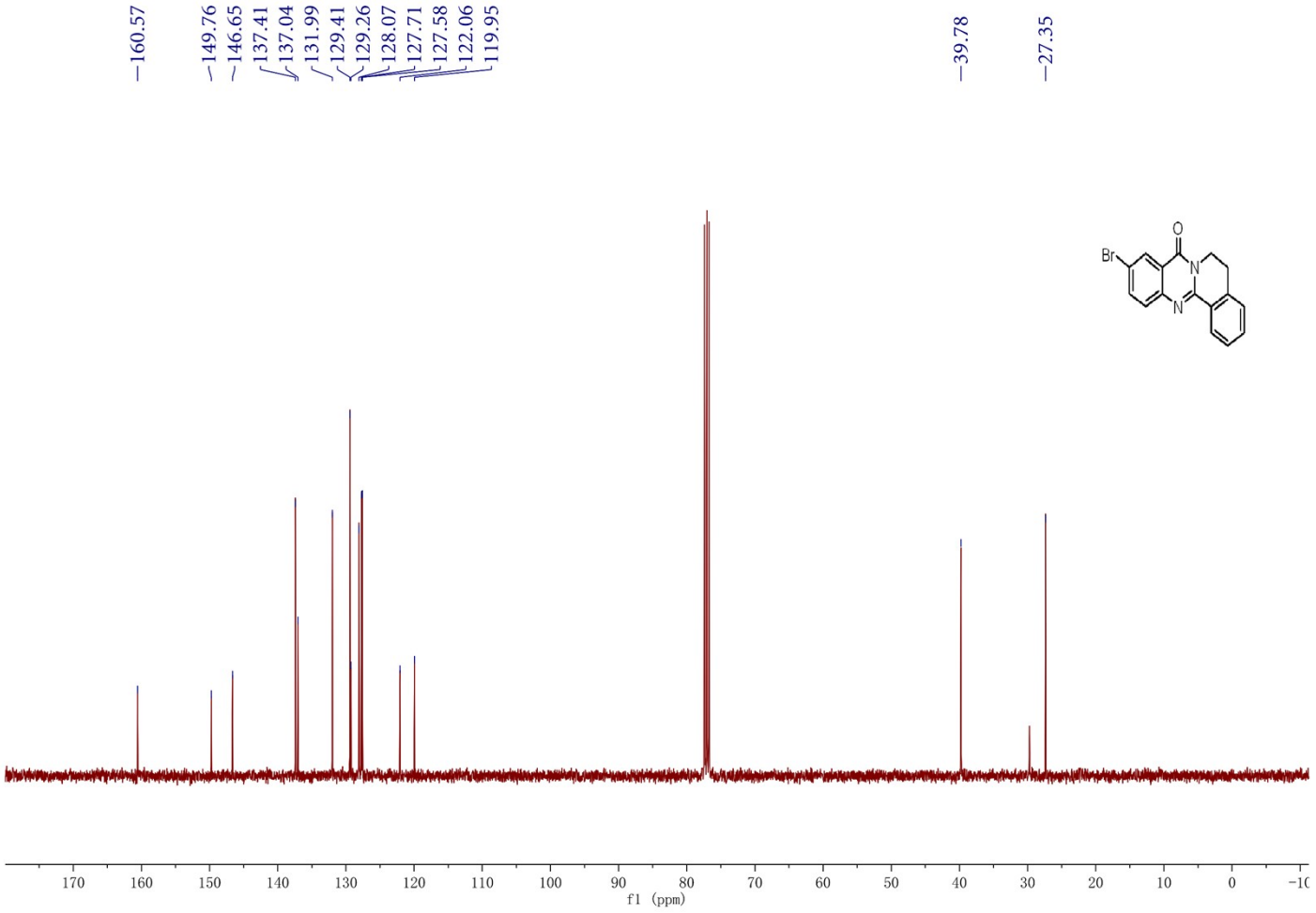
^{13}C NMR ($CDCl_3$, 126 MHz) spectra of **4p**



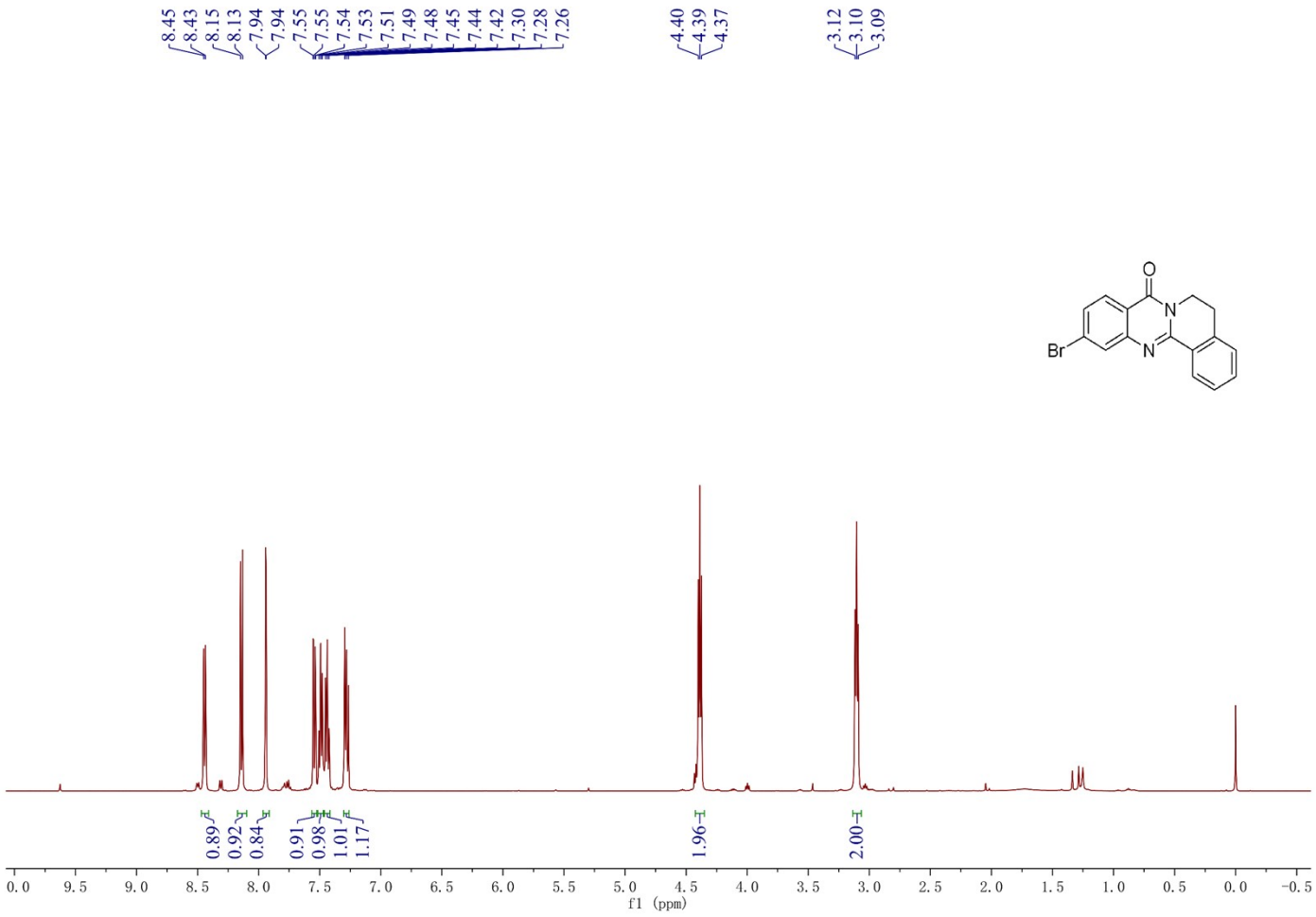
^{1}H NMR ($CDCl_3$, 500 MHz) spectra of **4m**(from 2-aminophenone)



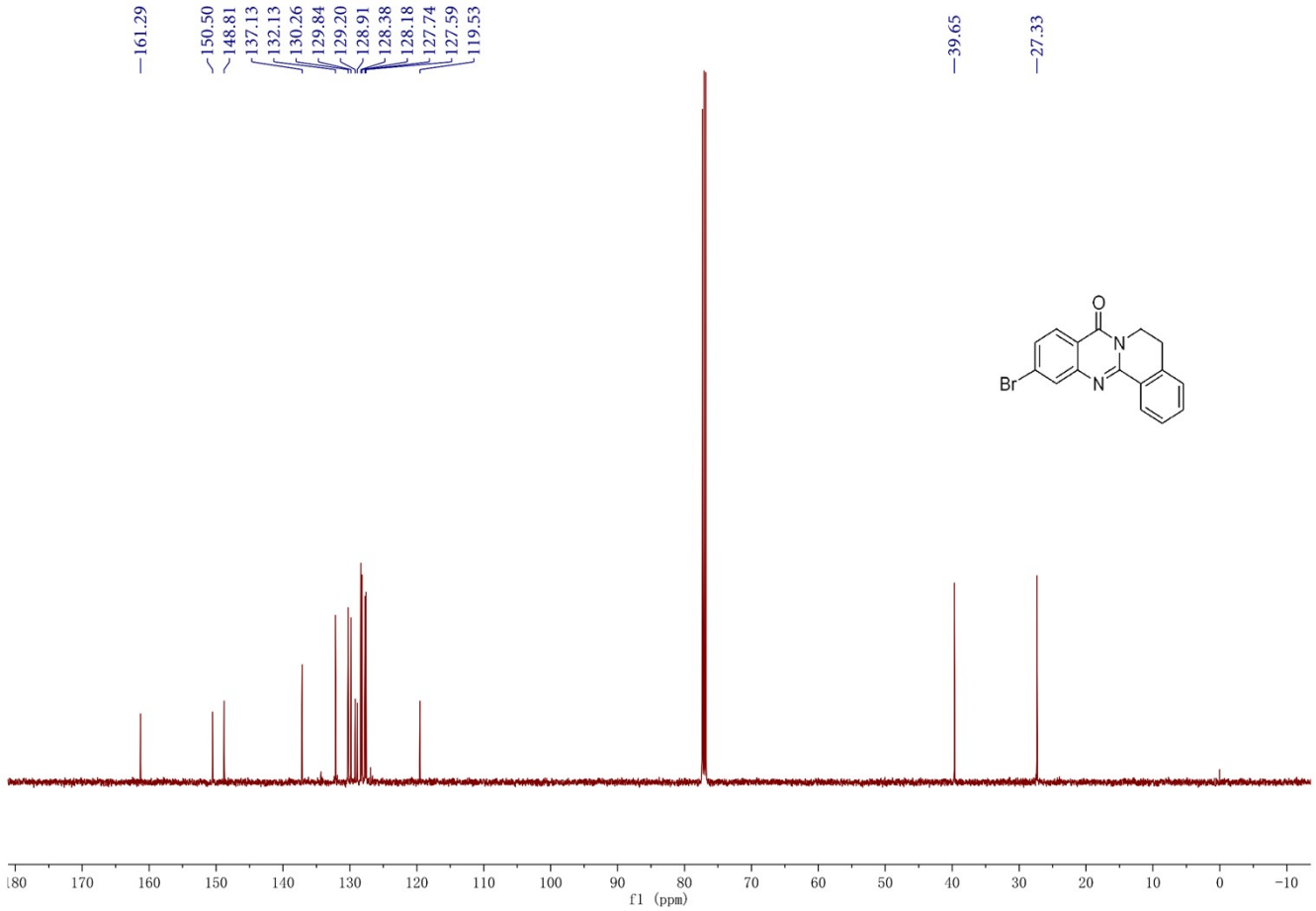
^{13}C NMR ($CDCl_3$, 126 MHz) spectra of **4m**(from 2-aminophenone)



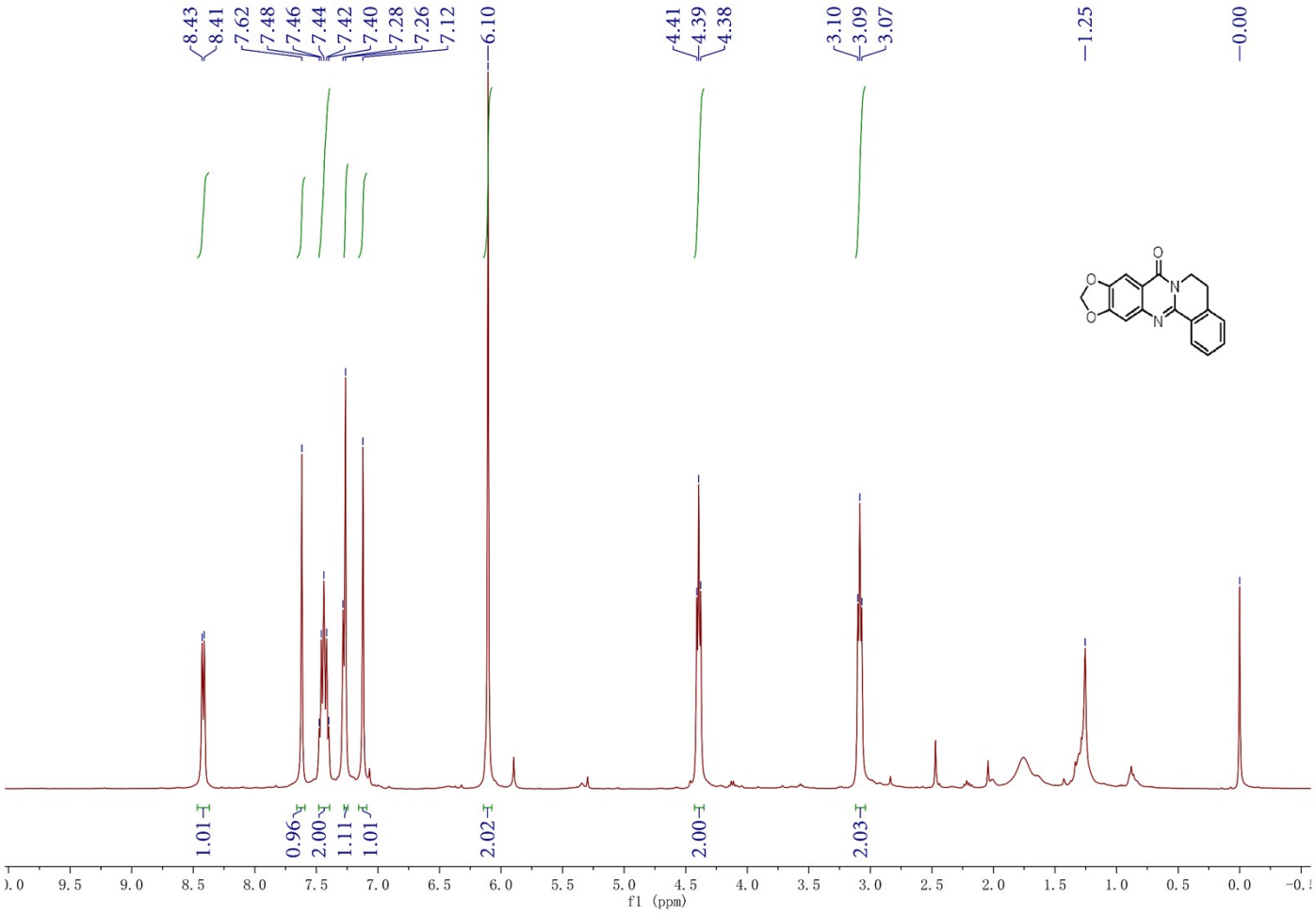
^{1}H NMR ($CDCl_3$, 500 MHz) spectra of **4l**(from 2-aminophenone)



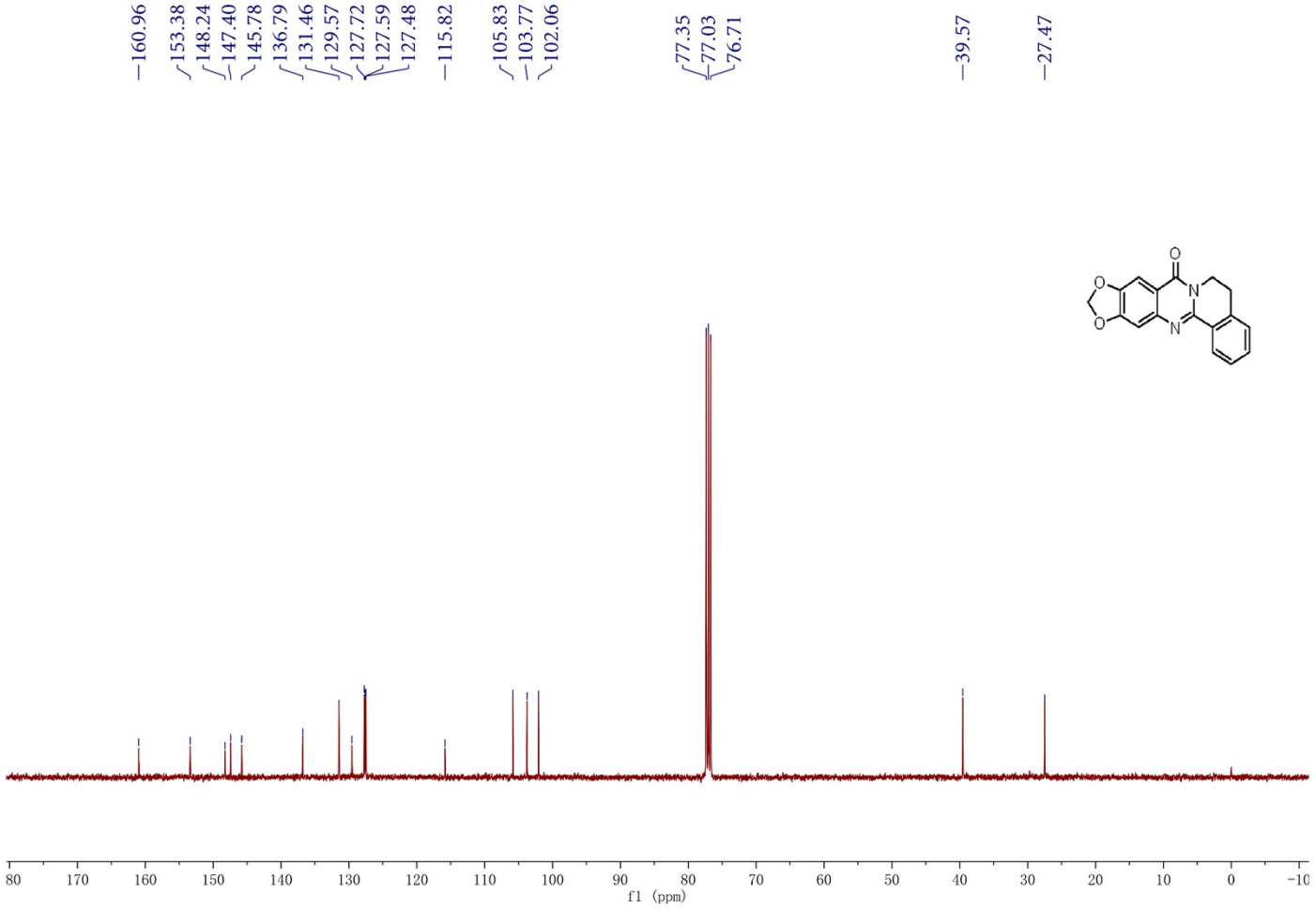
^{13}C NMR ($CDCl_3$, 126 MHz) spectra of **4l**(from 2-aminophenone)



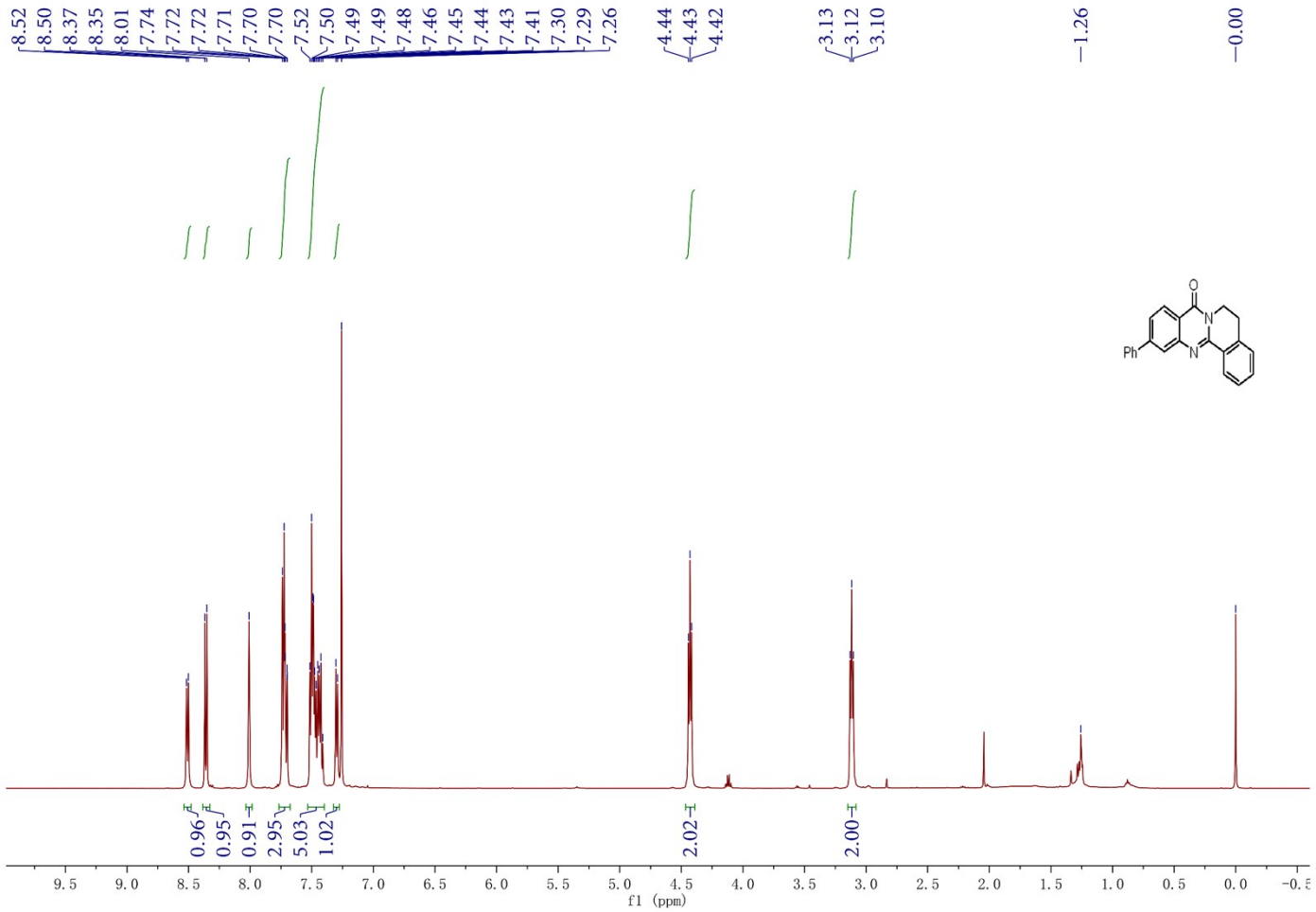
^{1}H NMR ($CDCl_3$, 500 MHz) spectra of **4q**



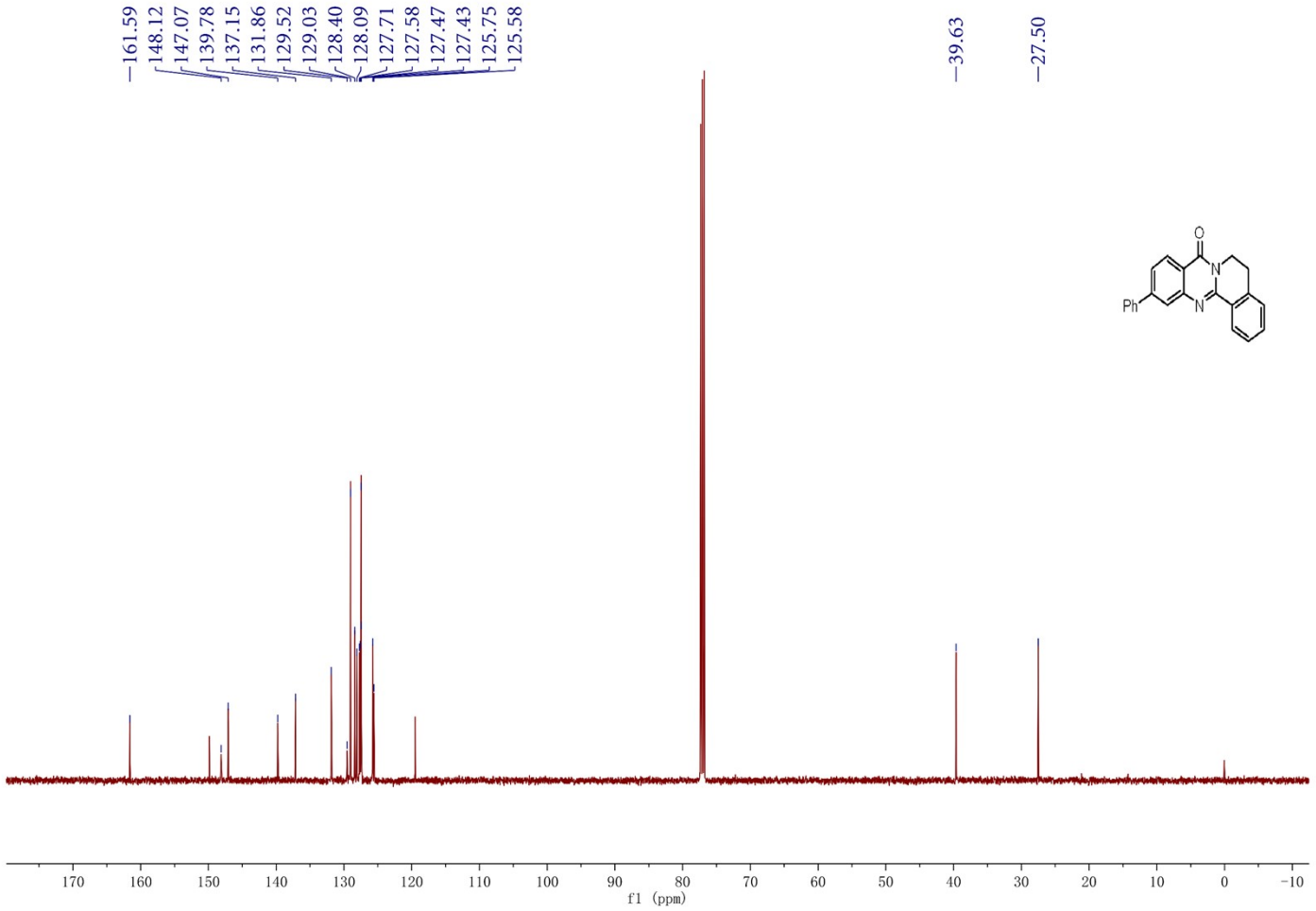
^{13}C NMR ($CDCl_3$, 126 MHz) spectra of **4q**



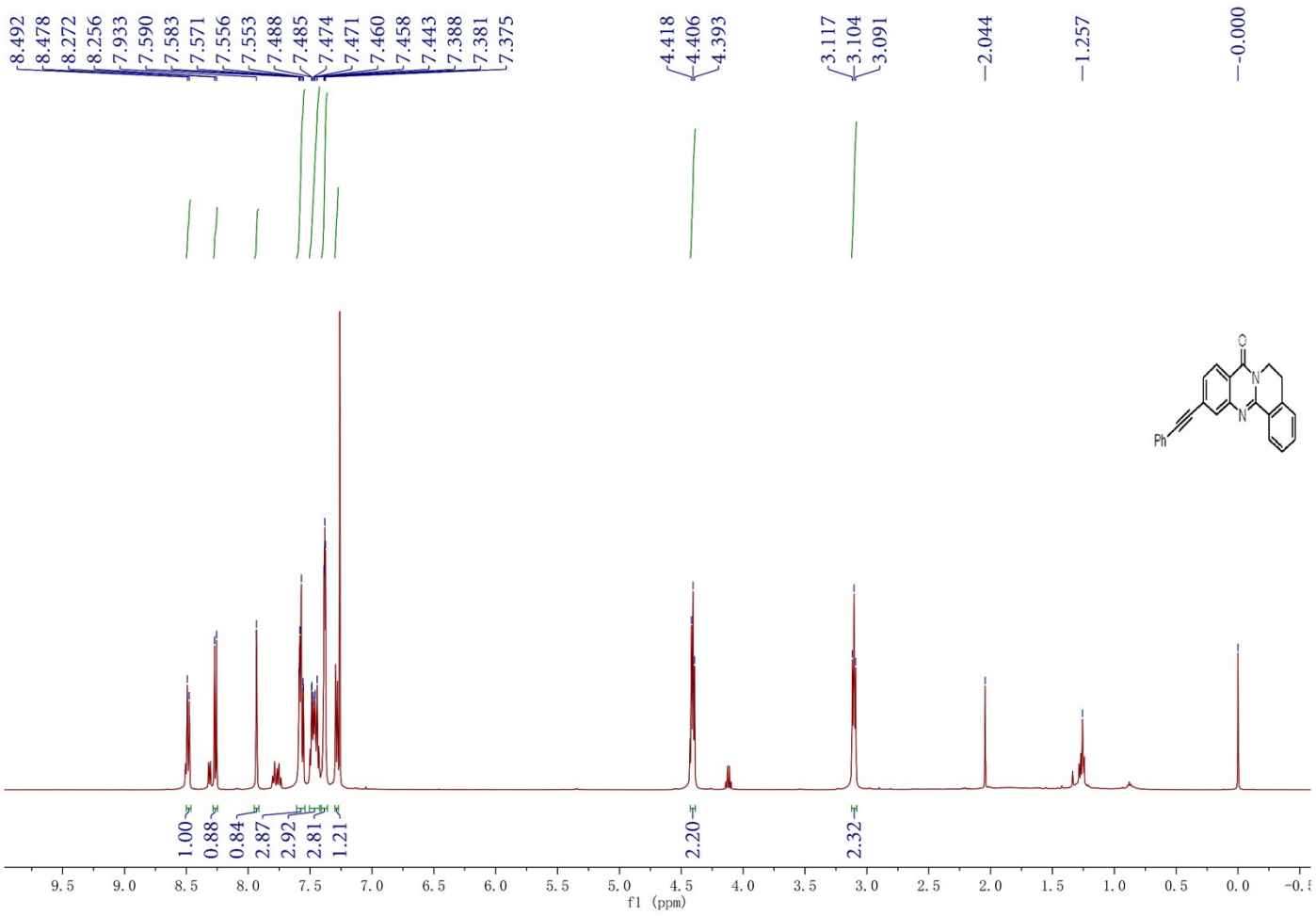
^{1}H NMR ($CDCl_3$, 500 MHz) spectra of **5a**



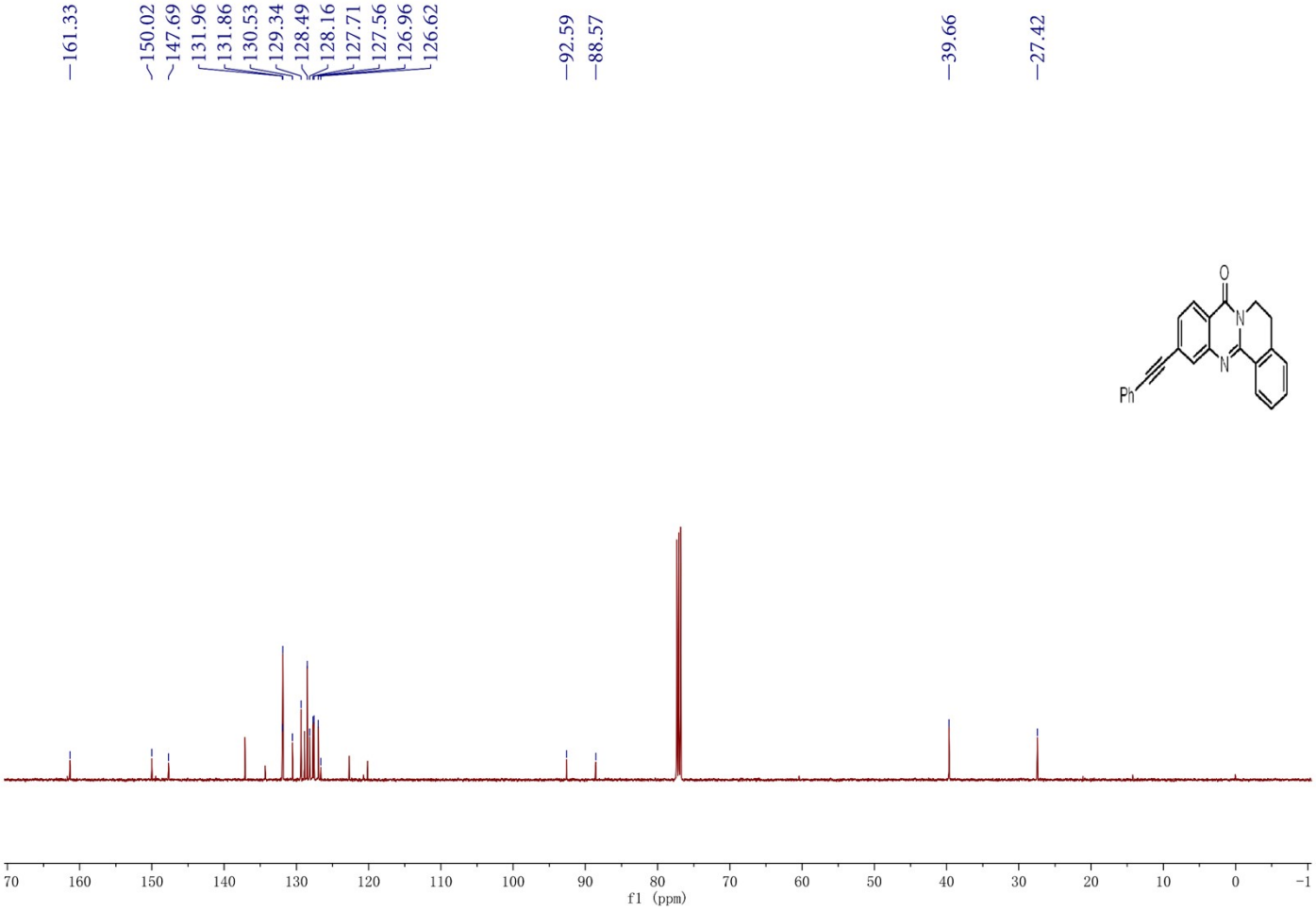
^{13}C NMR ($CDCl_3$, 126 MHz) spectra of **5a**



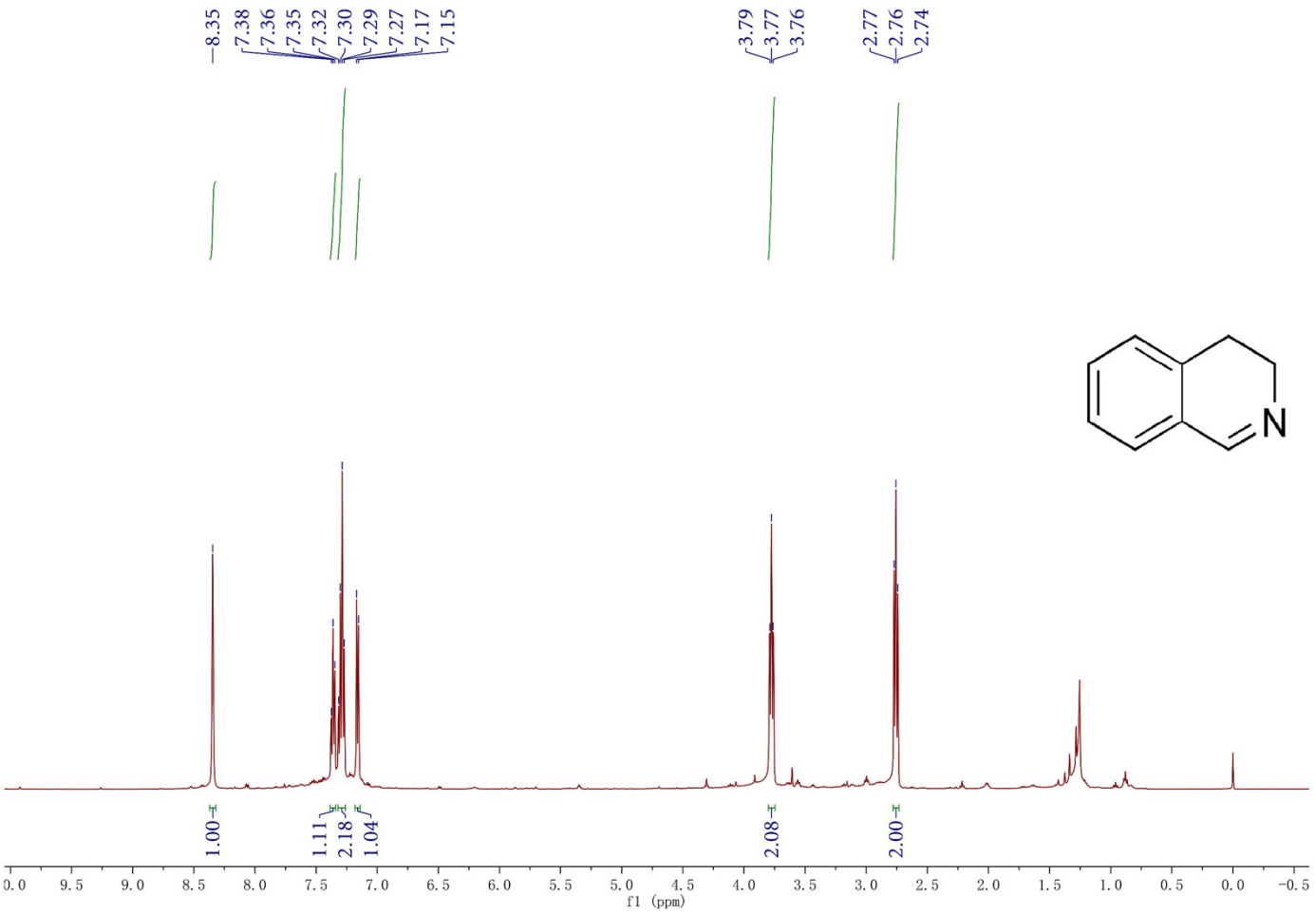
^{1}H NMR ($CDCl_3$, 500 MHz) and spectra of **5b**



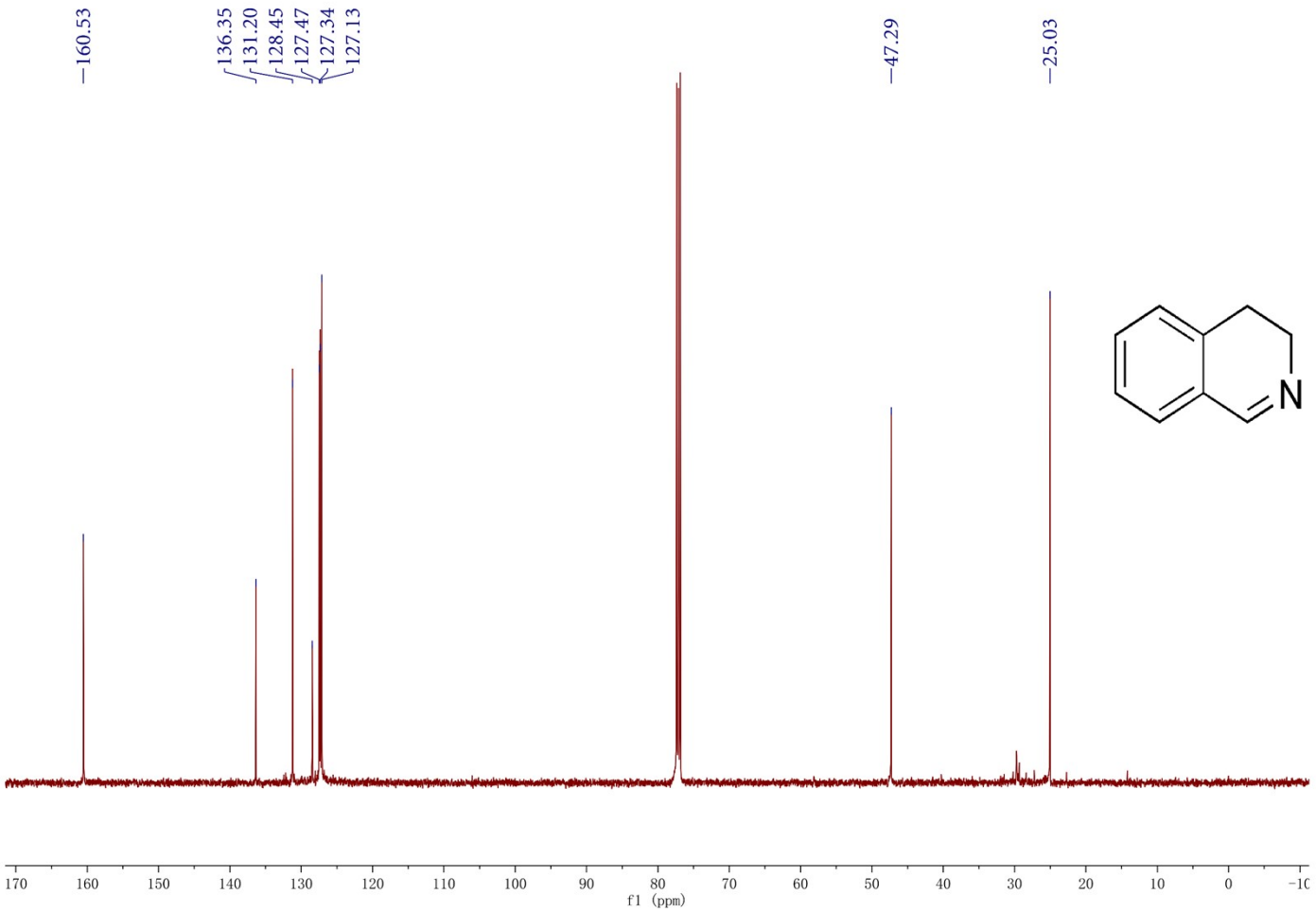
^{13}C NMR ($CDCl_3$, 126 MHz) spectra of **5b**



^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) spectra of **6**



^{13}C NMR ($CDCl_3$, 126 MHz) spectra of **6**



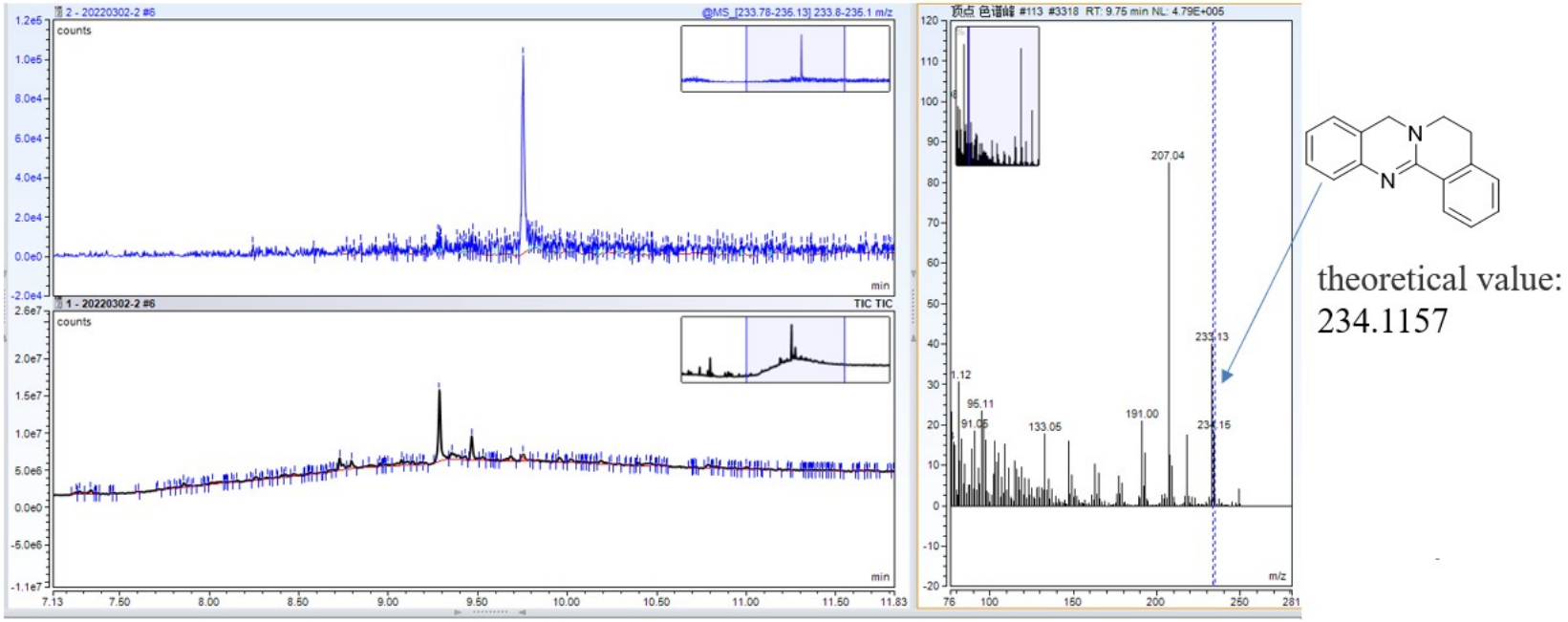


Figure 1 J GC-MS detection

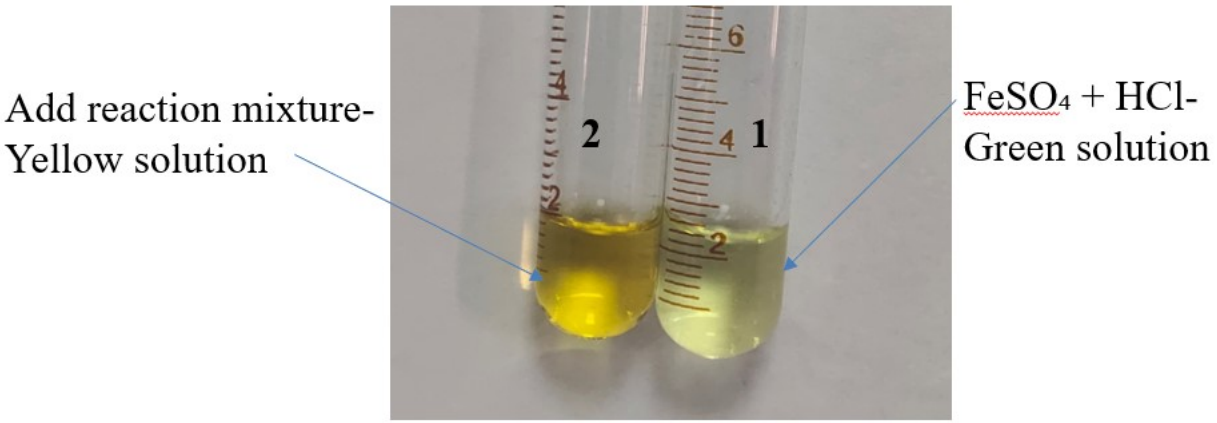


Figure 2 Detection of H_2O_2