Supporting Information

Copper(I) Catalyzed C(sp^2)-N bond formation: Synthesis of Pyrrolo[3,2-*c*]quinolinone Derivatives

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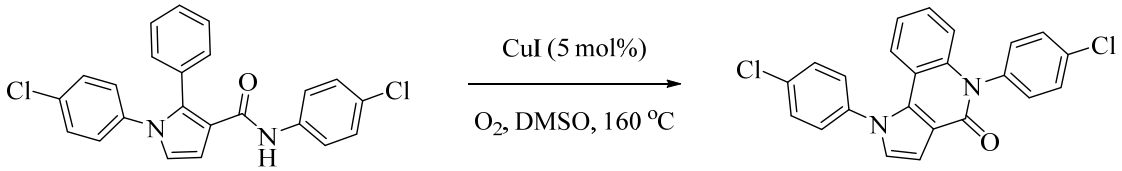
I. General remarks:

All reagents were purchased from commercial sources and used without further treatment. DMSO was distilled under reduced pressure from CaH_2 and stored over molecular sieves. All reactions were carried out under O_2 atmosphere. Petroleum ether (PE) used refers to the 60–90 ^oC boiling point fraction of petroleum. ^1H NMR and ^{13}C NMR spectra were recorded on a 400 MHz NMR spectrometer (^1H, 400 MHz; ^{13}C, 100 MHz at 25 °C). Coupling constants are reported in Hz. All high-resolution mass spectra (HRMS) were measured on a mass spectrometer (ESI-oa-TOF). Melting points were measured on a melting point apparatus equipped with a thermometer and are uncorrected. All reactions were monitored by TLC with GF254 silica gel coated plates. Flash chromatography was carried out on SiO_2 (silica gel 200−300 mesh).

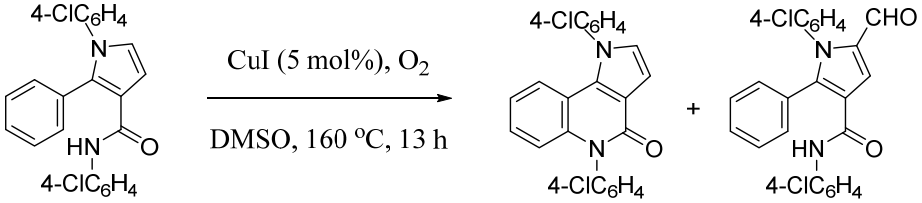
II. Typical experimental procedure for the synthesis of **2** (**2a** as an example):



1a **2a**

To an oven-dried round-bottom flask (25 mL) equipped with an oxygen balloon was added *N*,1-bis(4-chlorophenyl)-2-phenyl-1*H*-pyrrole-3-carboxamide **1a** (81.4 mg, 0.2 mmol), CuI (1.9 mg, 0.01 mmol), the mixture was well stirred for 9 h in DMSO (1.5 mL) at 160 ^oC (the whole process was closely monitored by TLC). After cooling, the mixture was added water (5.0 mL), and the aqueous phase was extracted with EtOAc (10 mL×3). The combined organic layer was dried over sodium sulfate. The solvent was evaporated, and the residue was purified by a short flash silica gel column chromatography (Eluent: EtOAc/PE = 1/3) to give 1,5-bis(4-chlorophenyl)-1*H*-pyrrolo[3,2-*c*]quinolin-4(5*H*)-one **2a** as a white solid (69%, the yield is an average of four times).

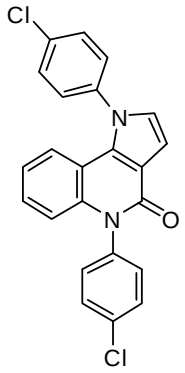
III. Mechanism probing experiments.



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

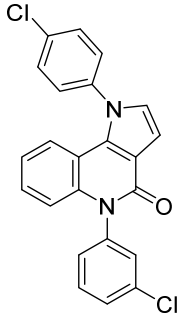
Radical trapping agents (1.0 equiv)	Yield of **2a**	Yield of **3a**
---	69%	≤10%
1,4-Dinitrobenzene	34%	27%
Diallyl ether	25%	35%
Hydroquinone	16%	24%

IV. Analytical data of compounds **2**



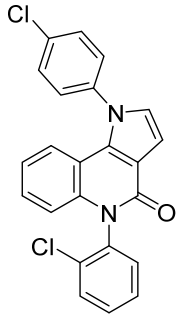
1,5-Bis(4-chlorophenyl)-1*H*-pyrrolo[3,2-*c*]quinolin-4(5*H*)-one (2a)

The product was isolated by flash chromatography (Eluent: EtOAc/PE = 1/3) as a white solid (65 mg, 69%). mp 187-190 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.75 (d, J = 8.4 Hz, 2H), 7.68 (t, J = 8.4 Hz, 4H), 7.38 (d, J = 8.4 Hz, 3H), 7.24-7.20 (m, 1H), 6.99 (d, J = 3.6 Hz, 2H), 6.88 (d, J = 2.4 Hz, 1H), 6.60 (d, J = 8.8 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.5, 138.6, 137.4, 134.1, 133.2, 132.7, 131.6, 130.1, 129.8, 129.3, 127.5, 121.7, 120.7, 116.8, 116.2, 113.4, 106.4. (Two carbons are not observed). HRMS (ESI), *m/z* calcd. for $C_{23}H_{15}Cl_2N_2O$ ($[M+H]^+$) 405.0556, found: 405.0562.



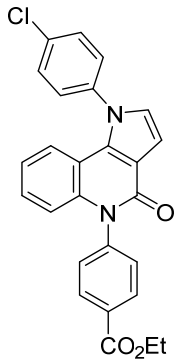
5-(3-Chlorophenyl)-1-(4-chlorophenyl)-1*H*-pyrrolo[3,2-*c*]quinolin-4(5*H*)-one (2b)

The product was isolated by flash chromatography (Eluent: EtOAc/PE = 1/3) as a white solid (49 mg, 61%). mp 173-175 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.76 (d, J = 9.2 Hz, 2H), 7.69-7.64 (m, 4H), 7.53 (s, 1H), 7.39 (d, J = 3.2 Hz, 1H), 7.35-7.33 (m, 1H), 7.25-7.22 (m, 1H), 7.03-6.98 (m, 2H), 6.88 (d, J = 3.2 Hz, 1H), 6.58 (d, J = 8.4 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.4, 139.9, 138.6, 138.5, 134.08, 134.05, 132.6, 131.7, 130.1, 129.8, 129.2, 128.8, 128.6, 127.5, 121.7, 120.68, 116.75, 116.20, 113.34, 106.32. (One carbon is not observed). HRMS (ESI), *m/z* calcd. for $C_{23}H_{15}Cl_2N_2O$ ($[M+H]^+$) 405.0556, found: 405.0548.



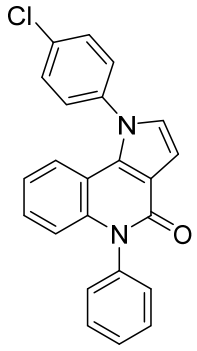
5-(2-Chlorophenyl)-1-(4-chlorophenyl)-1*H*-pyrrolo[3,2-*c*]quinolin-4(5*H*)-one (2c)

The product was isolated by flash chromatography (Eluent: EtOAc/PE = 1/3) as a white solid (49 mg, 60%). mp 147-150 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.80-7.75 (m, 4H), 7.68-7.60 (m, 3H), 7.51 (dd, J = 6.0, 3.6 Hz, 1H), 7.39 (d, J = 3.2 Hz, 1H), 7.26-7.22 (m, 1H), 7.01 (d, J = 4.0 Hz, 2H), 6.90 (d, J = 2.8 Hz, 1H), 6.46 (d, J = 8.4 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.0, 138.6, 137.7, 135.8, 134.1, 132.7, 131.7, 130.7, 130.6, 130.1, 129.9, 129.4, 129.0, 127.7, 121.9, 120.9, 116.1, 116.0, 113.4, 106.4. (One carbon is not observed). HRMS (ESI), *m/z* calcd. for $C_{23}H_{15}Cl_2N_2O$ ($[M+H]^+$) 405.0556, found: 405.0557.



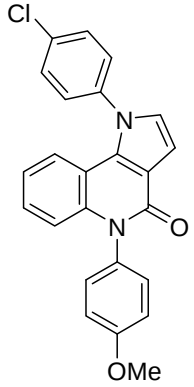
Ethyl 4-(1-(4-chlorophenyl)-4-oxo-1*H*-pyrrolo[3,2-*c*]quinolin-5(4*H*)-yl)benzoate (2d)

The product was isolated by flash chromatography (Eluent: EtOAc/PE = 1/3) as a white solid (56 mg, 63%). mp 213-217 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.20 (d, J = 8.4 Hz, 2H), 7.76-7.74 (m, 2H), 7.69-7.67 (m, 2H), 7.51 (d, J = 8.4 Hz, 2H), 7.38 (d, J = 3.2 Hz, 1H), 7.23-7.19 (m, 1H), 7.00 (d, J = 4.0 Hz, 2H), 6.88 (d, J =2.8 Hz, 1H), 6.55 (d, J = 8.8 Hz, 1H), 4.39 (q, J = 7.2 Hz, 2H), 1.37 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 165.2, 158.4, 142.9, 138.6, 138.4, 134.1, 132.7, 130.9, 130.3, 130.12, 130.09, 129.9, 129.3, 127.5, 121.8, 120.8, 116.8, 116.2, 113.4, 106.3, 61.1, 14.2. HRMS (ESI), *m/z* calcd. for $C_{26}H_{19}ClN_2O_3$ ($[M+H]^+$) 443.1157, found: 415.1214.



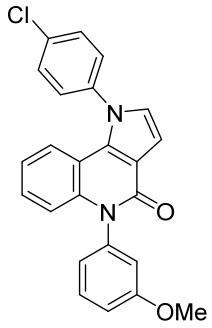
1-(4-Chlorophenyl)-5-phenyl-1*H*-pyrrolo[3,2-*c*]quinolin-4(5*H*)-one (2e)

The product was isolated by flash chromatography (Eluent: EtOAc/PE = 1/3) as a white solid (34 mg, 46%). mp 212-215 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.75 (d, J = 8.4 Hz, 2H), 7.69-7.62 (m, 4H), 7.56 (t, J = 7.2 Hz, 1H), 7.37 (d, J = 2.8 Hz, 1H), 7.32 (d, J = 7.2 Hz, 2H), 7.20 (t, J = 6.4 Hz, 1H), 7.00-6.95 (m, 2H), 6.87 (d, J = 2.8 Hz, 1H), 6.55 (d, J = 8.4 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.6, 138.9, 138.7, 138.5, 134.1, 132.6, 130.1, 130.0, 129.8, 129.6, 129.3, 128.6, 127.4, 121.5, 120.7, 116.9, 116.4, 113.3, 106.3. HRMS (ESI), *m/z* calcd. for $C_{23}H_{16}ClN_2O$ ($[M+H]^+$) 371.0946, found: 371.0955.



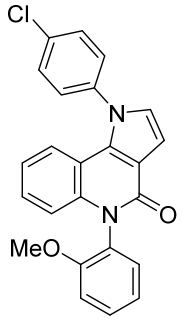
1-(4-Chlorophenyl)-5-(4-methoxyphenyl)-1*H*-pyrrolo[3,2-*c*]quinolin-4(5*H*)-one (2f)

The product was isolated by flash chromatography (Eluent: EtOAc/PE = 1/3) as a white solid (56 mg, 70%). mp 231-235 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.75 (d, J = 8.8 Hz, 2H), 7.68 (m, J = 8.8 Hz, 2H), 7.37 (d, J = 2.8 Hz, 1H), 7.24-7.15 (m, 5H), 6.98 (m, J = 4.0 Hz, 2H), 6.86 (d, J = 3.2 Hz, 1H), 6.61 (d, J = 8.4 Hz, 1H), 3.86 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 159.0, 158.8, 139.2, 138.7, 134.0, 132.5, 130.8, 130.5, 130.1, 129.7, 129.3, 127.3, 121.4, 120.6, 117.0, 116.4, 115.2, 113.3, 106.3, 55.4. HRMS (ESI), *m/z* calcd. for $C_{24}H_{18}ClN_2O_2$ ($[M+H]^+$) 401.1051, found: 401.1064.



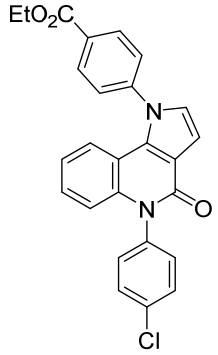
1-(4-Chlorophenyl)-5-(3-methoxyphenyl)-1*H*-pyrrolo[3,2-*c*]quinolin-4(5*H*)-one (2g)

The product was isolated by flash chromatography (Eluent: EtOAc/PE = 1/3) as a white solid (52 mg, 65%). mp 149-153 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.76-7.68 (m, 4H), 7.54 (t, J = 8.0 Hz, 1H), 7.38 (d, J = 3.2 Hz, 1H), 7.24-7.20 (m, 1H), 7.14-7.12 (m, 1H), 6.99-6.97 (m, 2H), 6.90-6.87(m, 3H), 6.60 (d, J = 8.4 Hz, 1H), 3.79 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 160.6, 158.4, 139.6, 138.8, 138.7, 134.1, 132.6, 130.7, 130.1, 129.7, 129.3, 127.4, 121.53, 121.49, 120.6, 117.0, 116.4, 115.1, 114.3, 113.3, 106.3, 55.4. HRMS (ESI), *m/z* calcd. for $C_{24}H_{18}ClN_2O_2$ ($[M+H]^+$) 401.1051, found: 401.1061.



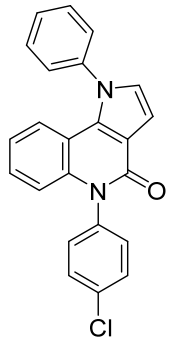
1-(4-Chlorophenyl)-5-(2-methoxyphenyl)-1*H*-pyrrolo[3,2-*c*]quinolin-4(5*H*)-one (2h)

The product was isolated by flash chromatography (Eluent: EtOAc/PE = 1/3) as a white solid (42 mg, 53%). mp 194-197 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.74-7.68 (m, 4H), 7.56-7.52 (m, 1H), 7.35 (d, J = 3.2 Hz, 1H), 7.30 (d, J = 8.0 Hz, 1H), 7.25-7.15 (m, 3H), 6.99-6.94 (m, 2H), 6.86 (d, J = 3.2 Hz, 1H), 6.55 (d, J = 8.4 Hz, 1H), 3.66 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.3, 155.5, 138.7, 138.4, 134.1, 132.6, 130.7, 130.3, 130.1, 129.6, 129.4, 127.5, 126.4, 121.44, 121.36, 120.6, 116.5, 116.3, 113.4, 112.8, 106.3, 55.6. HRMS (ESI), *m/z* calcd. for $C_{24}H_{18}ClN_2O_2$ ($[M+H]^+$) 401.1051, found: 401.1065.



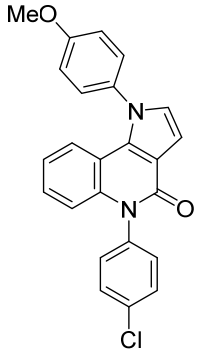
Ethyl 4-(5-(4-chlorophenyl)-4-oxo-4,5-dihydro-1*H*-pyrrolo[3,2-*c*]quinolin-1-yl)benzoate (2k)

The product was isolated by flash chromatography (Eluent: EtOAc/PE = 1/3) as a White solid (65 mg, 73%). mp 224-228 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.23 (d, J = 8.4 Hz, 2H), 7.79 (d, J = 8.4 Hz, 2H), 7.71-7.69 (m, 2H), 7.43 (d, J = 3.2 Hz, 1H), 7.42-7.38 (m, 2H), 7.25-7.21 (m, 1H), 6.70-6.95 (m, 2H), 6.91 (d, J = 2.8 Hz, 1H), 6.60 (d, J = 8.4 Hz, 1H), 4.40 (q, J = 7.2 Hz, 2H), 1.38 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 165.0, 158.5, 143.6, 138.7, 137.4, 133.2, 132.5, 131.6, 130.9, 130.6, 130.1, 129.7, 127.7, 127.6, 121.7, 120.9, 116.8, 116.6, 106.6, 61.3, 14.2. (One carbon is not observed). HRMS (ESI), *m/z* calcd. for $C_{26}H_{20}ClN_2O_3$ ($[M+H]^+$) 443.1157, found: 443.1162.



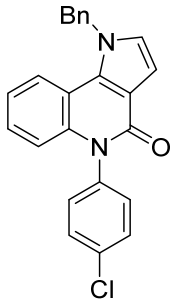
5-(4-Chlorophenyl)-1-phenyl-1*H*-pyrrolo[3,2-*c*]quinolin-4(5*H*)-one (2l)

The product was isolated by flash chromatography (Eluent: EtOAc/PE = 1/3) as a white solid (38 mg, 52%). mp: 241-245 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.70-7.67 (m, 5H), 7.63-7.61 (m, 2H), 7.41-7.37 (m, 3H), 7.22-7.18 (m, 1H), 6.93-6.91 (m, 2H), 6.87 (d, J = 3.2 Hz, 1H), 6.58 (d, J = 8.8 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.6, 139.7, 138.6, 137.4, 133.1, 132.6, 131.6, 130.12, 130.09, 129.7, 129.6, 127.4, 121.5, 120.7, 116.8, 116.0, 113.5, 106.1. (One carbon is not observed). HRMS (ESI), *m/z* calcd. for $C_{23}H_{16}ClN_2O$ ($[M+H]^+$) 371.0946, found: 371.0965.



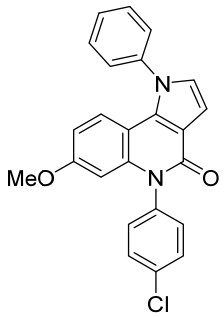
5-(4-Chlorophenyl)-1-(4-methoxyphenyl)-1*H*-pyrrolo[3,2-*c*]quinolin-4(5*H*)-one (2m)

The product was isolated by flash chromatography (Eluent: EtOAc/PE = 1/3) as a white solid (58 mg, 73%). mp 198-200 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.69 (d, J = 8.0 Hz, 2H), 7.53 (d, J = 8.4 Hz, 2H), 7.38 (d, J = 8.0 Hz, 2H), 7.31 (d, J = 2.4 Hz, 1H), 7.20 (d, J = 8.0 Hz, 3H), 7.00-6.93 (m, 2H), 6.84 (s, 1H), 6.57 (d, J = 8.4 Hz, 1H), 3.89 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 159.8, 158.6, 138.6, 137.5, 133.1, 132.8, 132.4, 131.6, 130.1, 130.0, 128.6, 127.3, 121.5, 120.7, 116.7, 115.8, 115.1, 113.6, 105.8, 55.6. HRMS (ESI), m/z calcd. for $C_{24}H_{18}ClN_2O_2$ ($[M+H]^+$) 401.1051, found: 401.1068.



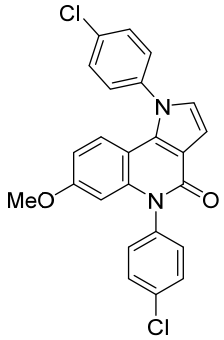
1-Benzyl-5-(4-chlorophenyl)-1*H*-pyrrolo[3,2-*c*]quinolin-4(5*H*)-one (2n)

The product was isolated by flash chromatography (Eluent: EtOAc/PE = 1/3) as a white solid (38 mg, 50%). mp 226-228 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.91 (d, J = 8.0 Hz, 1H), 7.67 (d, J = 8.8 Hz, 2H), 7.49 (d, J = 3.2 Hz, 1H), 7.38-7.34 (m, 4H), 7.26 (t, J = 7.6 Hz, 1H), 7.20 (t, J = 7.6 Hz, 1H), 7.11-7.06 (m, 3H), 6.81 (d, J = 2.8 Hz, 1H), 6.56 (d, J = 8.4 Hz, 1H), 5.89 (s, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.5, 138.3, 137.53, 137.51, 133.0, 131.9, 131.6, 130.1, 130.0, 128.9, 127.4, 127.0, 125.8, 121.8, 121.7, 116.53, 116.48, 113.7, 105.2, 52.3. HRMS (ESI), *m/z* calcd. for $C_{24}H_{18}ClN_2O$ ($[M+H]^+$) 385.1102, found: 385.1120.



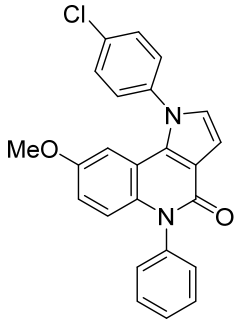
5-(4-Chlorophenyl)-7-methoxy-1-phenyl-1*H*-pyrrolo[3,2-*c*]quinolin-4(5*H*)-one (2p)

The product was isolated by flash chromatography (Eluent: EtOAc/PE = 1/3) as a white solid (52 mg, 65%). mp 210-213 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.71-7.67 (m, 5H), 7.62-7.59 (m, 2H), 7.38 (d, J = 8.4 Hz, 2H), 7.29 (d, J = 2.8 Hz, 1H), 6.85 (d, J = 9.2, 1H), 6.81 (d, J = 2.8, 1H), 6.63 (dd, J_1 = 9.2 Hz, J_2 = 2.4 Hz, 1H), 5.97 (d, J = 2.0 Hz, 1H), 3.56 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.9, 158.3, 140.3, 139.7, 137.4, 133.2, 133.1, 131.6, 130.14, 130.12, 129.6, 128.8, 127.4, 122.2, 114.2, 108.0, 107.5, 105.9, 102.0, 55.2. HRMS (ESI), *m/z* calcd. for $C_{24}H_{18}ClN_2O_2$ ($[M+H]^+$) 401.1051, found: 401.1059.



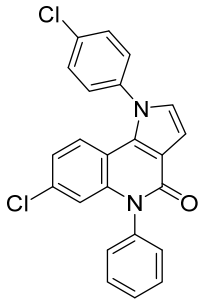
1,5-Bis(4-chlorophenyl)-8-methoxy-1,5-dihydro-4*H*-pyrrolo[3,2-*c*]quinolin-4-one (2q)

The product was isolated by flash chromatography (Eluent: EtOAc/PE = 1/3) as a White solid (62 mg, 71%). mp 234-238 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.75-7.65 (m, 6H), 7.37 (d, J = 8.0 Hz, 2H), 7.29 (d, J = 2.0 Hz, 1H), 6.91 (d, J = 8.4 Hz, 1H), 6.82 (d, J = 2.0 Hz, 1H), 6.72 (d, J = 8.4 Hz, 1H), 5.98 (s, 1H), 3.57 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.8, 158.3, 140.3, 138.6, 137.3, 134.0, 133.2, 131.5, 130.1, 129.3, 128.8, 122.2, 114.4, 108.2, 107.4, 106.2, 102.1, 55.2. (Two carbons are not observed). HRMS (ESI), *m/z* calcd. for $C_{24}H_{16}Cl_2N_2O_2$ ($[M+H]^+$) 435.0662, found: 435.0668.



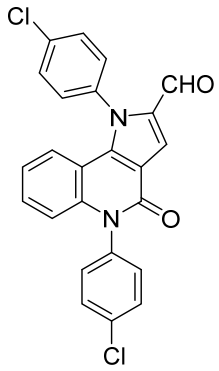
1-(4-Chlorophenyl)-6-methoxy-5-phenyl-1*H*-pyrrolo[3,2-*c*]quinolin-4(5*H*)-one (2r)

The product was isolated by flash chromatography (Eluent: EtOAc/PE = 1/3) as a White solid (18 mg, 23%). mp 92-96 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.81-7.76 (m, 2H), 7.71 (d, J = 8.8 Hz, 2H), 7.63 (t, J = 7.2 Hz, 2H), 7.55 (t, J = 7.2 Hz, 1H), 7.40 (d, J = 3.2 Hz, 1H), 7.30 (d, J = 7.6 Hz, 2H), 6.89-6.86 (m, 1H), 6.47 (d, J = 9.2 Hz, 1H), 6.41 (d, J = 2.8 Hz, 1H), 3.41 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.2, 153.4, 138.6, 138.5, 134.1, 133.3, 132.2, 130.0, 129.64, 129.60, 128.5, 118.1, 116.7, 114.7, 113.8, 106.4, 104.2, 54.7. (Two carbons are not observed). HRMS (ESI), *m/z* calcd. for $C_{24}H_{18}ClN_2O_2$ ($[M+H]^+$) 401.1051, found: 401.1054.



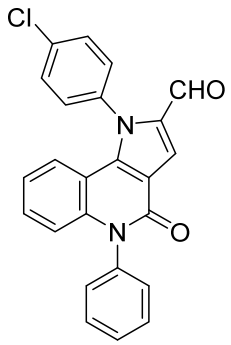
7-Chloro-1-(4-chlorophenyl)-5-phenyl-1*H*-pyrrolo[3,2-*c*]quinolin-4(5*H*)-one (2t)

The product was isolated by flash chromatography (Eluent: EtOAc/PE = 1/3) as a White solid (54 mg, 67%). mp 228-230 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.75 (d, J = 8.4 Hz, 2H), 7.69-7.64 (m, 4H), 7.59 (t, J = 7.2 Hz, 1H), 7.42 (d, J = 2.8 Hz, 1H), 7.36 (d, J = 7.2 Hz, 2H), 7.10 (d, J = 8.4 Hz, 1H), 6.99 (d, J = 8.8 Hz, 1H), 6.89 (d, J = 3.2 Hz, 1H), 6.46 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.5, 139.9, 138.3, 137.9, 134.2, 131.9, 131.6, 130.3, 130.2, 129.5, 129.2, 129.0, 122.3, 121.6, 116.5, 116.0, 112.3, 106.5. (One carbon is not observed). HRMS (ESI), *m/z* calcd. for $C_{23}H_{15}Cl_2N_2O$ ($[M+H]^+$) 405.0556, found: 405.0565.



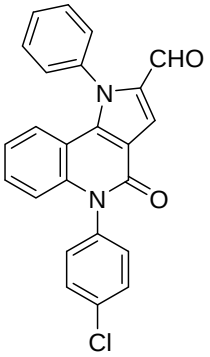
1,5-Bis(4-Chlorophenyl)-4-oxo-4,5-dihydro-1*H*-pyrrolo[3,2-*c*]quinoline-2-carbaldehyde (4a)

The product was isolated by flash chromatography (Eluent: EtOAc/PE = 1/3) as a White solid (30 mg, 35%). mp 212-216 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.65 (s, 1H), 7.83 (s, 1H), 7.77-7.68 (m, 6H), 7.41 (d, J = 8.4 Hz, 2H), 7.33 (t, J = 8.0 Hz, 1H), 7.00 (t, J = 7.6 Hz, 1H), 6.77 (d, J = 8.0 Hz, 1H), 6.62 (d, J = 8.4 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 180.6, 158.1, 140.5, 137.9, 137.0, 136.8, 136.0, 134.7, 133.4, 131.5, 130.2, 130.1, 129.7, 122.1, 122.0, 119.4, 117.3, 115.8, 112.7. (One carbon is not observed) HRMS (ESI), *m/z* calcd. for $C_{24}H_{14}Cl_2N_2O_2$ ([M+Na]$^+$) 455.0325, found: 455.0330.



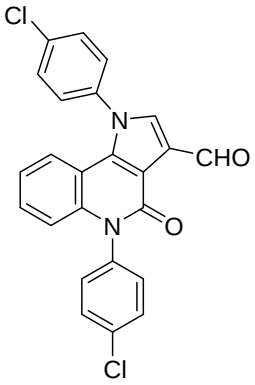
1-(4-Chlorophenyl)-4-oxo-5-phenyl-4,5-dihydro-1*H*-pyrrolo[3,2-*c*]quinoline-2-carbaldehyde (4e)

The product was isolated by flash chromatography (Eluent: EtOAc/PE = 1/3) as a White solid (25 mg, 31%). mp 111-113 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.66 (s, 1H), 7.83 (s, 1H), 7.77-7.69 (m, 4H), 7.65 (t, J = 7.2 Hz, 2H), 7.58 (t, J = 7.6 Hz, 1H), 7.36-7.29 (m, 3H), 6.99 (t, J = 8.0 Hz, 1H), 6.78 (d, J = 7.2 Hz, 1H), 6.58 (d, J = 8.4 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 180.5, 158.1, 140.7, 137.90, 137.87, 137.8, 137.0, 136.0, 134.6, 130.11, 130.09, 130.07, 129.5, 129.4, 128.7, 121.9, 119.3, 117.2, 116.0, 112.6. HRMS (ESI), *m/z* calcd. for $C_{24}H_{15}ClN_2O_2$ ([M+H]$^+$) 399.0894, found: 399.0911.



5-(4-Chlorophenyl)-4-oxo-1-phenyl-4,5-dihydro-1*H*-pyrrolo[3,2-*c*]quinoline-2-carbaldehyde (4l)

The product was isolated by flash chromatography (Eluent: EtOAc/PE = 1/3) as a White solid (25 mg, 32%). mp 261-264 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.62 (s, 1H), 7.80 (s, 1H), 7.73-7.63 (m, 6H), 7.42 (d, J = 8.8 Hz, 2H), 7.30 (t, J = 7.6 Hz, 1H), 6.91 (t, J = 7.6 Hz, 1H), 6.67 (d, J = 7.2 Hz, 1H), 6.60 (d, J = 8.4 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 180.5, 158.2, 140.5, 137.8, 137.7, 136.9, 136.1, 133.4, 131.5, 130.21, 130.15, 129.7, 129.5, 128.2, 122.0, 121.9, 118.4, 117.2, 115.7, 112.8. HRMS (ESI), *m/z* calcd. for $C_{24}H_{15}ClN_2O_2$ ([M+Na]$^+$) 421.0714, found: 421.0731.

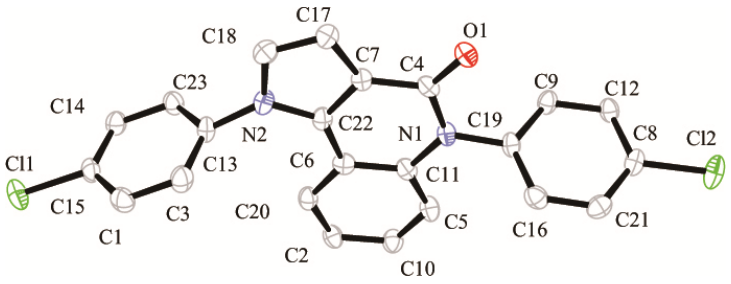


1,5-Bis(4-chlorophenyl)-4-oxo-4,5-dihydro-1*H*-pyrrolo[3,2-*c*]quinoline-3-carbaldehyde (4a')

The product was isolated by flash chromatography (Eluent: EtOAc/PE = 1/4) as a White solid (24 mg, 28%). mp 185-189 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.60 (s, 1H), 8.13 (s, 1H), 7.80-7.71 (m, 6H), 7.44 (d, J = 8.4 Hz, 2H), 7.32 (t, J = 7.6 Hz, 1H), 7.05 (t, J = 7.6 Hz, 1H), 6.93 (d, J = 8.0 Hz, 1H), 6.66 (d, J = 8.4 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 186.9, 158.3, 138.8, 137.7, 136.8, 134.9, 134.5, 133.4, 132.6, 131.5, 130.22, 130.16, 129.3, 128.5, 122.3, 122.1, 121.0, 117.0, 113.9, 112.8. HRMS (ESI), *m/z* calcd. for $C_{24}H_{14}Cl_2N_2O_2$ ([M+Na]$^+$) 455.0325, found: 455.0331

V. X-ray single crystal diffraction data.

2a:



Note: Ortep drawing of **2a** with thermal ellipsoids set at 50% probability

Table 1. Crystal data and structure refinement for **2a**

Identification code	**2a**
Empirical formula	$C_{23}H_{14}Cl_2N_2O$
Formula weight	405.26
Temperature	100.01(10) K
Wavelength	1.54184 A
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 8.9936(3) A alpha = 90 deg.
	b = 20.9137(5) A beta = 112.585(4) deg.
	c=10.6975(4) A gamma = 90 deg.
Volume	1857.79(10) A^3
Z, Calculated density	4, 1.449 Mg/m^3
Absorption coefficient	3.274 mm^-1
F(000)	832
Theta range for data collection	4.23 to 70.08 deg.
Limiting indices	-10<=h<=10, -23<=k<=25, -13<=l<=12
Reflections collected / unique	3092 / 3521 [R(int) = 0.0417]
Completeness to theta = 25.00	99.9%
Absorption correction	Empirical
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2014 / 0 / 253
Goodness-of-fit on F^2	1.031
Final R indices [I>2sigma(I)]	R1 = 0.0417, ωR2 = 0.0991
R indices (all data)	R1 = 0.0479, ωR2 = 0.1029

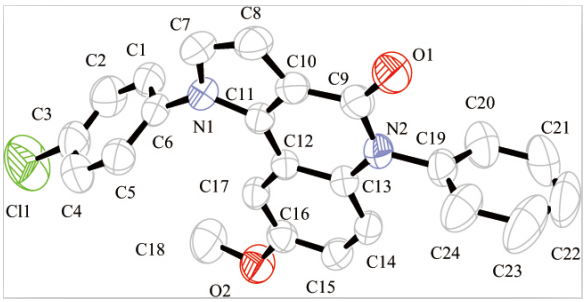
Largest diff. peak and hole	0.834 and -0.473 e·Å^{-3}

Table 2. Bond lengths [A] and angles [deg] for **2a**

C(2)- C(10) 1.393(3)	C(8)-C(12) 1.384(3)
C(2)- C(20) 1.382(3)	C(8)-C(21) 1.379(3)
N(3)- C(4) 1.391(3)	C(9)-C(12) 1.384(3)
N(3)-C(11) 1.415(3)	C(9)-C(19) 1.380(3)
N(3)-C(19) 1.443(3)	C(10)-C(24) 1.377(3)
C(4)-C(7) 1.453(3)	C(11)-C(24) 1.396(3)
N(5)-C(13) 1.447(3)	C(13)-C(23) 1.389(3)
N(5)-C(18) 1.382(3)	C(13)-C(25) 1.389(3)
N(5)-C(22) 1.370(3)	C(14)-C(15) 1.385(3)
C(6)-C(11) 1.414(3)	C(14)-C(23) 1.392(3)
C(6)-C(20) 1.410(3)	C(15)-C(26) 1.385(3)
C(6)-C(22) 1.445(3)	C(16)-C(19) 1.384(3)
C(7)-C(17) 1.410(3)	C(16)-C(21) 1.384(3)
C(7)-C(22) 1.382(3)	C(17)-C(18) 1.375(3)
	C(25)-C(26) 1.389(3)
C(20)-C(2)-C(10) 119.0 (2)	C(19)-C(9)-C(12) 120.12 (19)
C(4)-N(3)-C(11) 124.12 (17)	C(24)-C(10)-C(2) 121.5 (2)
C(4)-N(3)-C(19) 115.43 (17)	C(6)-C(11)-N(3) 121.28 (19)
C(11)-N(3)-C(19) 120.45 (18)	C(24)-C(11)-N(3) 119.45 (19)
O(1)- C(4)- N(3) 121.94 (19)	C(24)-C(11)-C(6) 119.27 (19)
O(1)-C(4)-C(7) 123.56 (19)	C(8)-C(12)-C(9) 118.5 (2)
N(3)-C(4)-C(7) 114.44 (17)	C(23)-C(13)-N(5) 119.31 (19)
C(18)-N(5)-C(13) 120.31 (18)	C(25)-C(13)-N(5) 119.70 (19)
C(22)-N(5)-C(13) 130.27 (19)	C(25)-C(13)-C(23) 120.7 (2)
C(22)-N(5)-C(18) 109.28 (18)	C(15)-C(14)-C(23) 119.18 (19)
C(11)-C(6)-C(22) 115.20 (19)	C(14)-C(15)-Cl(1) 119.44 (17)
C(20)-C(6)-C(11) 119.13 (19)	C(26)-C(15)-Cl(1) 118.99 (17)
C(20)-C(6)-C(22) 125.63 (19)	C(26)-C(15)-C(14) 121.6 (2)
C(17)-C(7)-C(4) 128.01 (19)	C(19)-C(16)-C(21) 119.6 (2)
C(22)-C(7)-C(4) 122.16 (19)	C(18)-C(17)-C(7) 105.63 (19)
C(22)-C(7)-C(17) 109.62 (18)	C(17)-C(18)-N(5) 109.00 (19)

C(12)-C(8)-Cl(2) 118.88 (17)	C(9)-C(19)-N(3) 119.56 (19)
C(21)-C(8)-Cl(2) 119.20 (17)	C(9)-C(19)-C(16) 120.73 (19)
C(21)-C(8)-C(12) 121.89 (19)	C(16)-C(19)-N(3) 119.64 (19)
C(2)-C(20)-C(6) 120.8 (2)	C(13)-C(23)-C(14) 119.6 (2)
C(8)-C(21)-C(16) 119.0 (2)	C(10)-C(24)-C(11) 120.2 (2)
N(5)-C(22)-C(6) 131.15 (19)	C(13)-C(25)-C(26) 119.8 (2)
N(5)-C(22)-C(7) 106.46 (18)	C(15)-C(26)-C(25) 119.1 (2)
C(7)-C(22)-C(6) 122.35 (19)	

2r:



Note: Ortep drawing of **2r** with thermal ellipsoids set at 50% probability

Table 1. Crystal data and structure refinement for **2r**

Identification code	**2r**
Empirical formula	$C_{24}H_{17}ClN_2O_2$
Formula weight	400.85
Temperature	291(2) K
Wavelength	1.54184 A
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 8.0462 (5) A alpha = 90 deg.
	b = 9.2337 (6) A beta = 90 deg.
	c = 26.6656 (13) A gamma = 90 deg.
Volume	1981.1 (2) A^3
Z, Calculated density	4, 1.344 Mg/m^3
Absorption coefficient	1.890 mm^-1
F(000)	832
Theta range for data collection	3.31 to 72.47 deg.

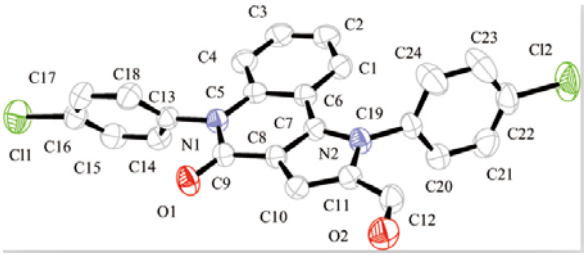
Limiting indices	-8<=h<=9, -11<=k<=11, -17<=l<=32
Reflections collected / unique	3048 / 3843 [R(int) = 0.0399]
Completeness to theta = 25.00	99.9%
Absorption correction	Empirical
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2014 / 0 / 264
Goodness-of-fit on F^2	1.041
Final R indices [I>2sigma(I)]	R1 = 0.0399, ωR2 = 0.1013
R indices (all data)	R1 = 0.0529, ωR2 = 0.1123
Largest diff. peak and hole	0.120 and -0.156 e·Å^{-3}

Table 2. Bond lengths [A] and angles [deg] for **2r**

Cl(1)-C(3) 1.735 (3)	C(16)-O(2)-C(18) 117.1 (2)
O(1)-C(9) 1.228 (3)	C(7)-N(1)-C(6) 124.03 (19)
O(2)-C(16) 1.379 (3)	C(11)-N(1)-C(6) 127.5 (2)
O(2)-C(18) 1.410 (3)	C(11)-N(1)-C(7) 108.52 (19)
N(1)-C(6) 1.441 (3)	C(9)-N(2)-C(13) 124.39 (18)
N(1)-C(7) 1.382 (3)	C(9)-N(2)-C(19) 116.89 (18)
N(1)-C(11) 1.376 (3)	C(13)-N(2)-C(19) 118.58 (19)
N(2)-C(9) 1.391 (3)	C(6)-C(1)-C(2) 119.8 (3)
N(2)-C(13) 1.407 (3)	C(3)-C(2)-C(1) 119.0 (3)
N(2)-C(19) 1.444 (3)	C(2)-C(3)-Cl(1) 119.2 (2)
C(1)-C(2) 1.379 (3)	C(2)-C(3)-C(4) 121.6(2)
C(1)-C(6) 1.376 (3)	C(4)-C(3)-Cl(1) 119.2(2)
C(2)-C(3) 1.370 (5)	C(5)-C(4)-C(3) 118.9(3)
C(3)-C(4) 1.383 (4)	C(4)-C(5)-C(6) 119.8(2)
C(4)-C(5) 1.373 (3)	C(1)-C(6)-N(1) 119.7(2)
C(5)-C(6) 1.376 (3)	C(5)-C(6)-N(1) 119.4 (2)
C(7)-C(8) 1.353 (3)	C(5)-C(6)-C(1) 120.8 (2)
C(8)-C(10) 1.415 (3)	C(8)-C(7)-N(1) 109.4 (2)
C(9)-C(10) 1.442 (3)	C(7)-C(8)-C(10) 106.6 (2)
C(10)-C(11) 1.379 (3)	O(1)-C(9)-N(2) 121.3 (2)
C(11)-C(12) 1.439 (3)	O(1)- C(9)-C(10) 124.3 (2)
C(12)-C(13) 1.414 (3)	N(2)-C(9)-C(10) 114.43 (18)

C(12)-C(17) 1.397 (3)	C(8)-C(10)-C(9) 129.5 (2)
C(13)-C(14) 1.398 (3)	C(11)-C(10)-C(8) 108.5(2)
C(14)-C(15) 1.369 (3)	C(11)-C(10)-C(9) 121.95 (19)
C(15)-C(16) 1.383 (3)	N(1)-C(11)-C(10) 107.04 (19)
C(16)-C(17) 1.369 (3)	N(1)-C(11)-C(12) 130.15 (19)
C(19)-C(20) 1.358 (5)	C(10)-C(11)-C(12) 122.81 (18)
C(19)-C(24) 1.362 (4)	C(13)-C(12)-C(11) 115.05 (18)
C(20)-C(21) 1.385 (5)	C(17)-C(12)-C(11) 125.65 (19)
C(21)-C(22) 1.370 (7)	C(17)-C(12)-C(13) 119.28 (18)
C(22)-C(23) 1.338 (7)	N(2)-C(13)-C(12) 121.07(18)
C(23)-C(24) 1.396 (4)	C(14)-C(13)-N(2) 120.77 (18)
C(16)-C(17)-C(12) 120.66 (18)	C(14)-C(13)-C(12) 118.15 (18)
C(20)-C(19)-N(2) 118.9 (3)	C(15)-C(14)-C(13) 121.6 (2)
C(20)-C(19)-C(24) 121.2 (3)	C(14)-C(15)-C(16) 119.8 (2)
C(24)-C(19)-N(2) 119.9 (3)	O(2)- C(16)-C(15) 115.6 (2)
C(19)-C(20)-C(21) 119.4 (4)	C(17)-C(16)-O(2) 123.9(2)
C(22)-C(21)-C(20) 120.0 (5)	C(17)-C(16)-C(15) 120.5 (2)
C(23)-C(22)-C(21) 119.9 (4)	C(22)-C(23)-C(24) 121.1 (4)
C(19)-C(24)-C(23) 118.4(4)	

4a:



Note: Ortep drawing of **4a** with thermal ellipsoids set at 50% probability

Table 1. Crystal data and structure refinement for **4a**

Identification code	**4a**
Empirical formula	$C_{24}H_{14}Cl_2N_2O_2$
Formula weight	433.27
Temperature	291(2) K
Wavelength	1.54184 A

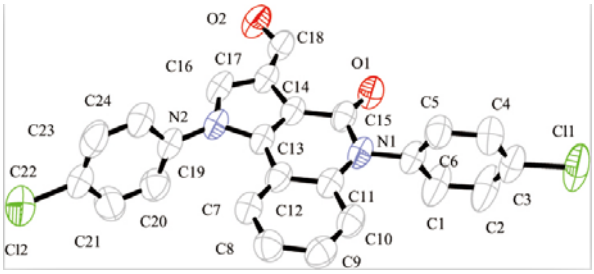
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 6.3775 (5) A alpha = 80.819 (6) deg.
	b = 12.1686 (10) A beta = 88.955(5) deg.
	c = 13.4121 (8) A gamma = 75.537 (7) deg.
Volume	994.69(12) A^3
Z, Calculated density	2, 1.447 Mg/m^3
Absorption coefficient	3.137 mm^-1
F(000)	444
Theta range for data collection	3.796 to 72.174 deg.
Limiting indices	-7<=h<=6, -14<=k<=14, -16<=l<=11
Reflections collected / unique	2754 / 3554 [R(int) = 0.0475]
Completeness to theta = 25.00	100%
Absorption correction	Empirical
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2014 / 0 / 271
Goodness-of-fit on F^2	1.046
Final R indices [I>2sigma(I)]	R1 = 0.0475, ωR2 = 0.1165
R indices (all data)	R1 = 0.0623, ωR2 = 0.1292
Largest diff. peak and hole	0.272 and -0.349 e·Å^{-3}

Table 2. Bond lengths [A] and angles [deg] for **4a**

Cl(1)-C(16) 1.744 (2)	C(5)-N(1)-C(13) 120.00 (18)
Cl(2)-C(22) 1.736 (2)	C(9)-N(1)-C(5) 124.15 (18)
O(1)-C(9) 1.219 (3)	C(9)-N(1)-C(13) 115.81 (18)
O(2)-C(12) 1.208 (3)	C(7)-N(2)-C(11) 108.06 (18)
N(1)-C(5) 1.411 (3)	C(7)-N(2)-C(19) 128.32 (19)
N(1)-C(9) 1.396 (3)	C(11)-N(2)-C(19) 123.34 (19)
N(1)-C(13) 1.445 (3)	C(2)-C(1)-C(6) 121.1 (2)
N(2)-C(7) 1.369 (3)	C(3)-C(2)-C(1) 120.0 (2)
N(2)-C(11) 1.401 (3)	C(2)-C(3)-C(4) 120.6 (2)
N(2)-C(19) 1.440 (3)	C(3)-C(4)-C(5) 120.7 (2)
C(1)-C(2) 1.381 (3)	N(1)-C(5)-C(6) 120.95 (19)
C(1)-C(6) 1.403 (3)	C(4)-C(5)-N(1) 119.9 (2)
C(2)-C(3) 1.376 (4)	C(4)-C(5)-C(6) 119.1 (2)

C(3)-C(4) 1.376 (3)	C(1)-C(6)-C(5) 118.5 (2)
C(4)-C(5) 1.402 (3)	C(1)-C(6)-C(7) 125.6 (2)
C(5)-C(6) 1.417 (3)	C(5)-C(6)-C(7) 115.88 (19)
C(6)-C(7) 1.442 (3)	N(2)-C(7)-C(6) 130.6 (2)
C(7)-C(8) 1.386 (3)	N(2)-C(7)-C(8) 107.53 (19)
C(8)-C(9) 1.445 (3)	C(8)-C(7)-C(6) 121.8 (2)
C(8)-C(10) 1.408 (3)	C(7)-C(8)-C(9) 122.5 (2)
C(10)-C(11) 1.360 (3)	C(7)-C(8)-C(10) 108.63 (19)
C(11)-C(12) 1.451 (3)	C(10)-C(8)-C(9) 128.8 (2)
C(13)-C(14) 1.380 (3)	O(1)-C(9)-N(1) 121.2 (2)
C(13)-C(18) 1.379 (3)	O(1)-C(9)-C(8) 124.2 (2)
C(14)-C(15) 1.382 (3)	N(1)-C(9)-C(8) 114.57 (18)
C(15)-C(16) 1.380 (4)	C(11)-C(10)-C(8) 106.73 (19)
C(16)-C(17) 1.369 (4)	N(2)-C(11)-C(12) 122.7 (2)
C(17)-C(18) 1.388 (4)	C(10)-C(11)-N(2) 109.06 (19)
C(19)-C(20) 1.368 (3)	C(10)-C(11)-C(12) 128.3 (2)
C(19)-C(24) 1.375 (4)	O(2)-C(12)-C(11) 123.2 (2)
C(20)-C(21) 1.380 (4)	C(14)-C(13)-N(1) 120.2 (2)
C(21)-C(22) 1.375 (4)	C(18)-C(13)-N(1) 119.2 (2)
C(22)-C(23) 1.365 (5)	C(18)-C(13)-C(14) 120.5 (2)
C(23)-C(24) 1.384 (4)	C(13)-C(14)-C(15) 120.2 (2)
C(16)-C(15)-C(14) 118.6 (2)	C(20)-C(19)-C(24) 120.5 (2)
C(15)-C(16)-Cl(1) 119.6 (2)	C(24)-C(19)-N(2) 120.0 (2)
C(17)-C(16)-Cl(1) 118.4 (2)	C(19)-C(20)-C(21) 120.0 (3)
C(17)-C(16)-C(15) 122.0 (2)	C(22)-C(21)-C(20) 119.3 (3)
C(16)-C(17)-C(18) 119.1 (3)	C(21)-C(22)-Cl(2) 120.4 (2)
C(13)-C(18)-C(17) 119.7 (2)	C(23)-C(22)-Cl(2) 118.5 (2)
C(20)-C(19)-N(2) 119.5 (2)	C(23)-C(22)-C(21) 121.1 (3)
C(22)-C(23)-C(24) 119.4 (3)	C(19)-C(24)-C(23) 119.7 (3)

4a':



Note: Ortep drawing of **4a'** with thermal ellipsoids set at 50% probability

Table 1. Crystal data and structure refinement for **4a'**

Identification code	**4a'**
Empirical formula	$C_{24}H_{14}Cl_2N_2O_2$
Formula weight	433.27
Temperature	291(2) K
Wavelength	1.54184 A
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 5.2005 (5) A alpha = 73.584 (12) deg.
	b = 13.556 (3) A beta = 85.490 (8) deg.
	c = 15.6215 (13) A gamma = 87.120 (12) deg.
Volume	1052.6 (2) A^3
Z, Calculated density	2, 1.367 Mg/m^3
Absorption coefficient	2.964 mm^-1
F(000)	444
Theta range for data collection	2.96 to 67.12 deg.
Limiting indices	-4<=h<=6, -16<=k<=14, -18<=l<=18
Reflections collected / unique	2071 / 3774 [R(int) = 0.0698]
Completeness to theta = 25.00	99.8%
Absorption correction	Empirical
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2014 / 0 / 272
Goodness-of-fit on F^2	1.026
Final R indices [I>2sigma(I)]	R1 = 0.0698, ωR2 = 0.1908
R indices (all data)	R1 = 0.1141, ωR2 = 0.2294
Largest diff. peak and hole	0.347 and -0.214 e·$Å^{-3}$

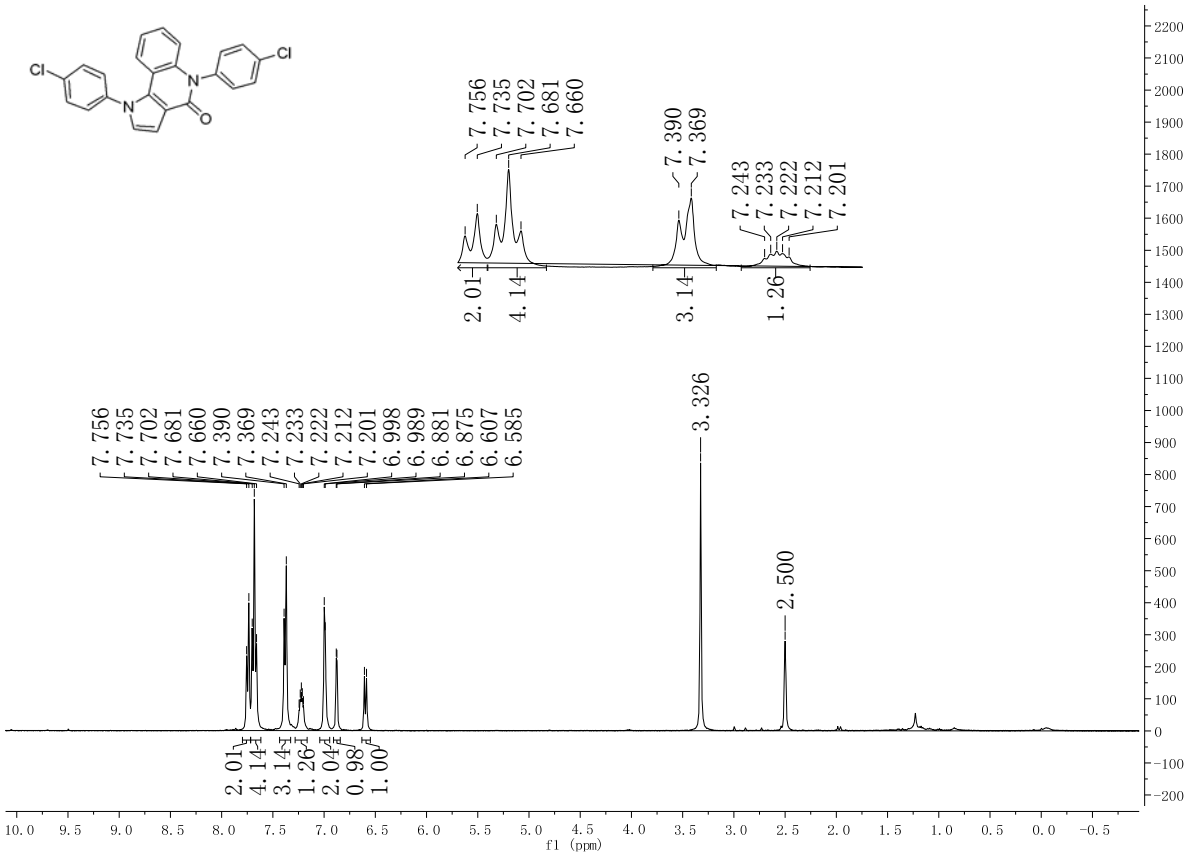
Table 2. Bond lengths [A] and angles [deg] for **4a'**

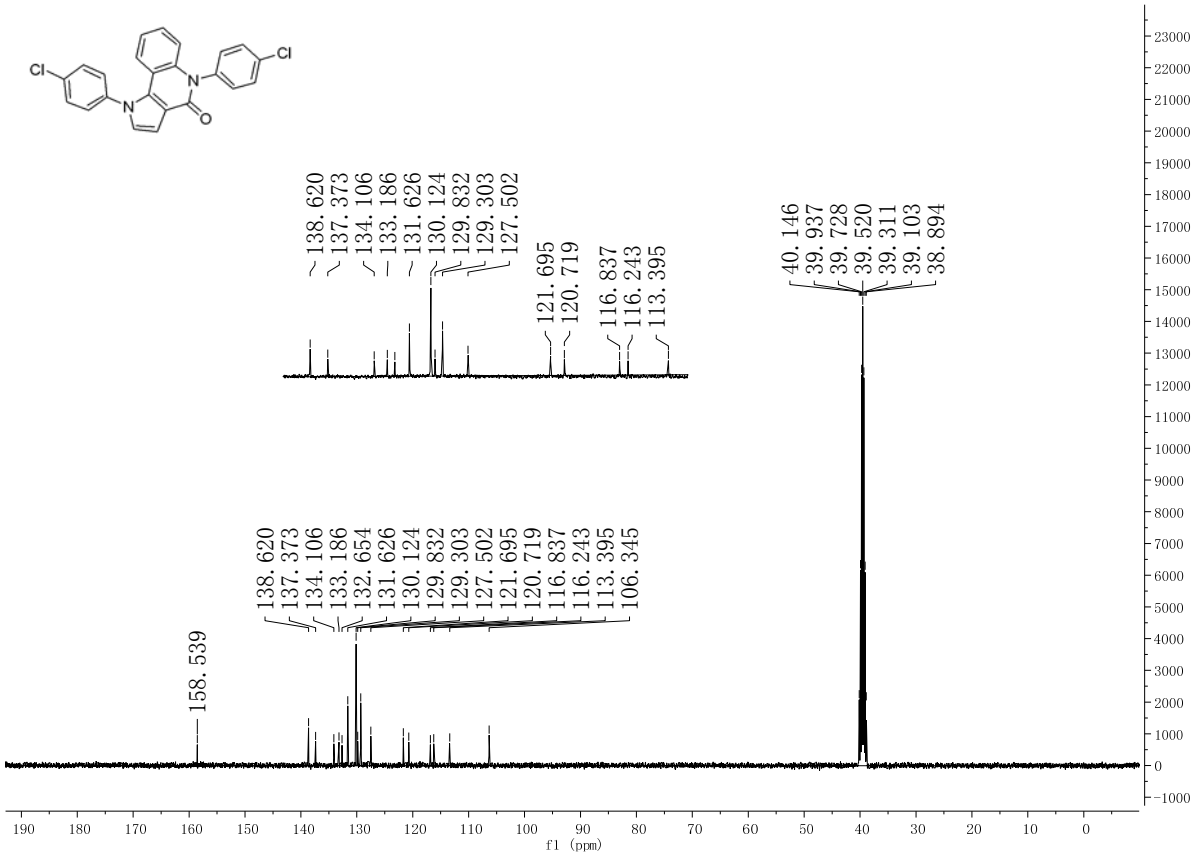
Cl(1)-C(3) 1.747 (4)	C(11)-N(1)-C(6) 119.3 (3)
Cl(2)-C(22) 1.751 (5)	C(15)-N(1)-C(6) 116.4 (4)
O(1)-C(15) 1.227 (5)	C(15)-N(1)-C(11) 124.1 (3)
O(2)-C(18) 1.208 (5)	C(13)-N(2)-C(19) 129.6 (4)
N(1)-C(6) 1.454 (5)	C(16)-N(2)-C(13) 108.0 (4)
N(1)-C(11) 1.403 (5)	C(16)-N(2)-C(19) 122.4 (3)
N(1)-C(15) 1.396 (5)	C(6)-C(1)-C(2) 119.9 (5)
N(2)-C(13) 1.390 (4)	C(3)-C(2)-C(1) 119.7 (5)
N(2)-C(16) 1.368 (5)	C(2)-C(3)-Cl(1) 120.0 (4)
N(2)-C(19) 1.430 (5)	C(2)-C(3)-C(4) 121.4 (4)
C(1)-C(2) 1.378 (6)	C(4)-C(3)-Cl(1) 118.5 (4)
C(1)-C(6) 1.359 (6)	C(3)-C(4)-C(5) 118.8 (5)
C(2)-C(3) 1.356 (8)	C(6)-C(5)-C(4) 120.1 (4)
C(3)-C(4) 1.357 (7)	C(1)-C(6)-N(1) 120.8 (4)
C(4)-C(5) 1.388 (6)	C(1)-C(6)-C(5) 120.0 (4)
C(5)-C(6) 1.370 (6)	C(5)-C(6)-N(1) 119.2 (4)
C(7)-C(8) 1.387 (6)	C(8)-C(7)-C(12) 121.4 (4)
C(7)-C(12) 1.397 (6)	C(9)-C(8)-C(7) 119.3 (4)
C(8)-C(9) 1.379 (6)	C(10)-C(9)-C(8) 120.7 (4)
C(9)-C(10) 1.374 (6)	C(9)-C(10)-C(11) 121.0 (4)
C(10)-C(11) 1.403 (6)	N(1)-C(11)-C(12) 121.3 (3)
C(11)-C(12) 1.413 (5)	C(10)-C(11)-N(1) 120.0 (4)
C(12)-C(13) 1.439 (5)	C(10)-C(11)-C(12) 118.7 (4)
C(13)-C(14) 1.374 (6)	C(7)-C(12)-C(11) 118.8 (4)
C(14)-C(15) 1.444 (5)	C(7)-C(12)-C(13) 125.8 (4)
C(14)-C(17) 1.428 (5)	C(11)-C(12)-C(13) 115.3 (4)
C(16)-C(17) 1.372 (6)	N(2)-C(13)-C(12) 130.1 (4)
C(19)-C(20) 1.366 (6)	C(14)-C(13)-N(2) 107.3 (3)
C(19)-C(24) 1.375 (6)	C(14)-C(13)-C(12) 122.6 (3)
C(21)-C(22) 1.357 (7)	C(13)-C(14)-C(15) 122.2 (4)
C(22)-C(23) 1.361 (7)	C(13)-C(14)- C(17) 109.0 (3)
C(23)-C(24) 1.369 (6)	C(17)-C(14)-C(15) 128.8 (4)
O(1)-C(15)-N(1) 121.1 (3)	O(2)-C(18)-C(17) 125.4 (4)

O(1)-C(15)-C(14) 124.4 (4)	C(20)-C(19)-N(2) 119.9 (4)
N(1)-C(15)-C(14) 114.5 (4)	C(20)-C(19)-C(24) 120.1 (4)
N(2)-C(16)-C(17) 110.7 (4)	C(24)-C(19)-N(2) 119.9 (4)
C(14)-C(17)-C(18) 129.9 (4)	C(19)-C(20)-C(21) 120.2 (5)
C(16)-C(17)-C(14) 105.0 (4)	C(22)-C(21)-C(20) 118.7 (5)
C(16)-C(17)-C(18) 125.1 (4)	C(21)-C(22)-Cl(2) 118.8 (5)
C(21)-C(22)-C(23) 121.4 (5)	C(23)-C(22)-Cl(2) 119.8 (4)
C(22)-C(23)-C(24) 120.1 (5)	C(23)-C(24)-C(19) 119.4 (5)

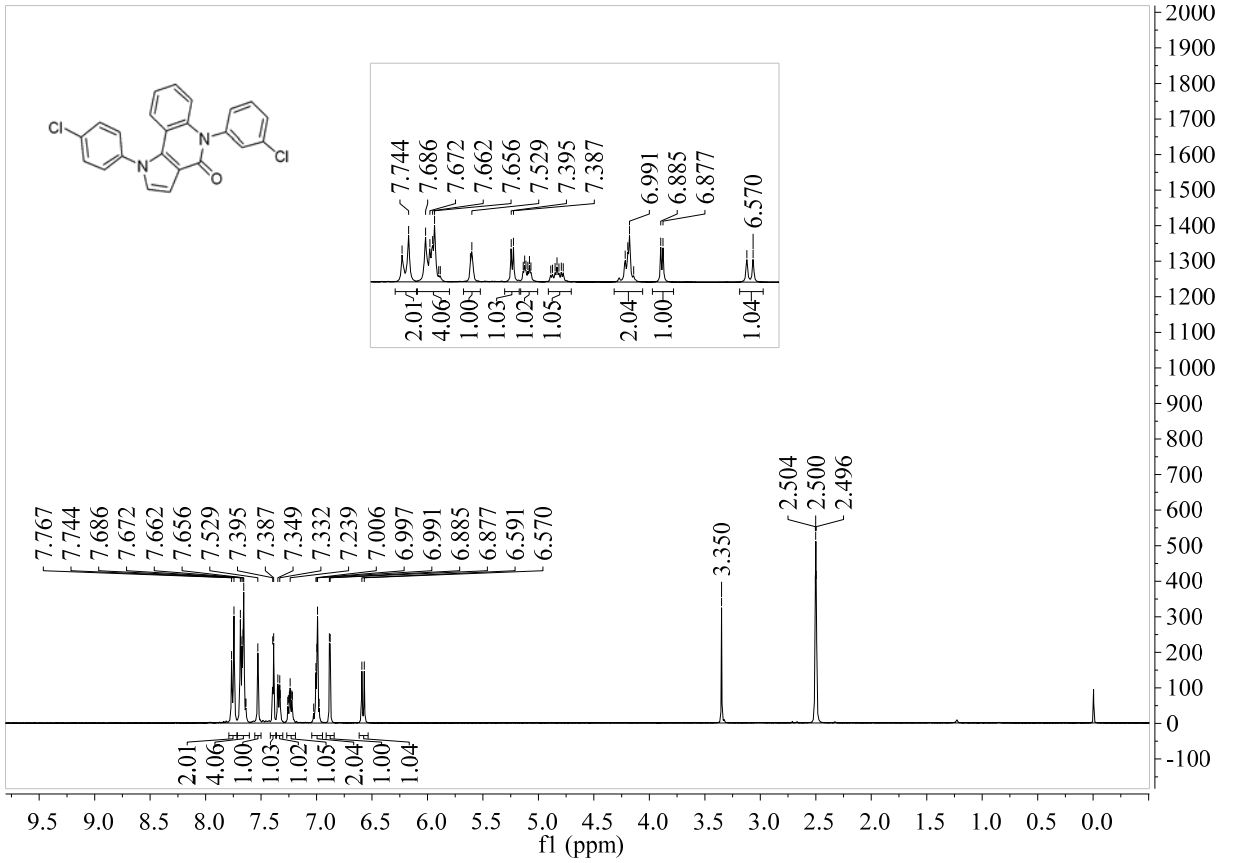
VI. ^{1}H NMR and ^{13}C NMR spectra copies.

Compound **2a**





Compound **2b**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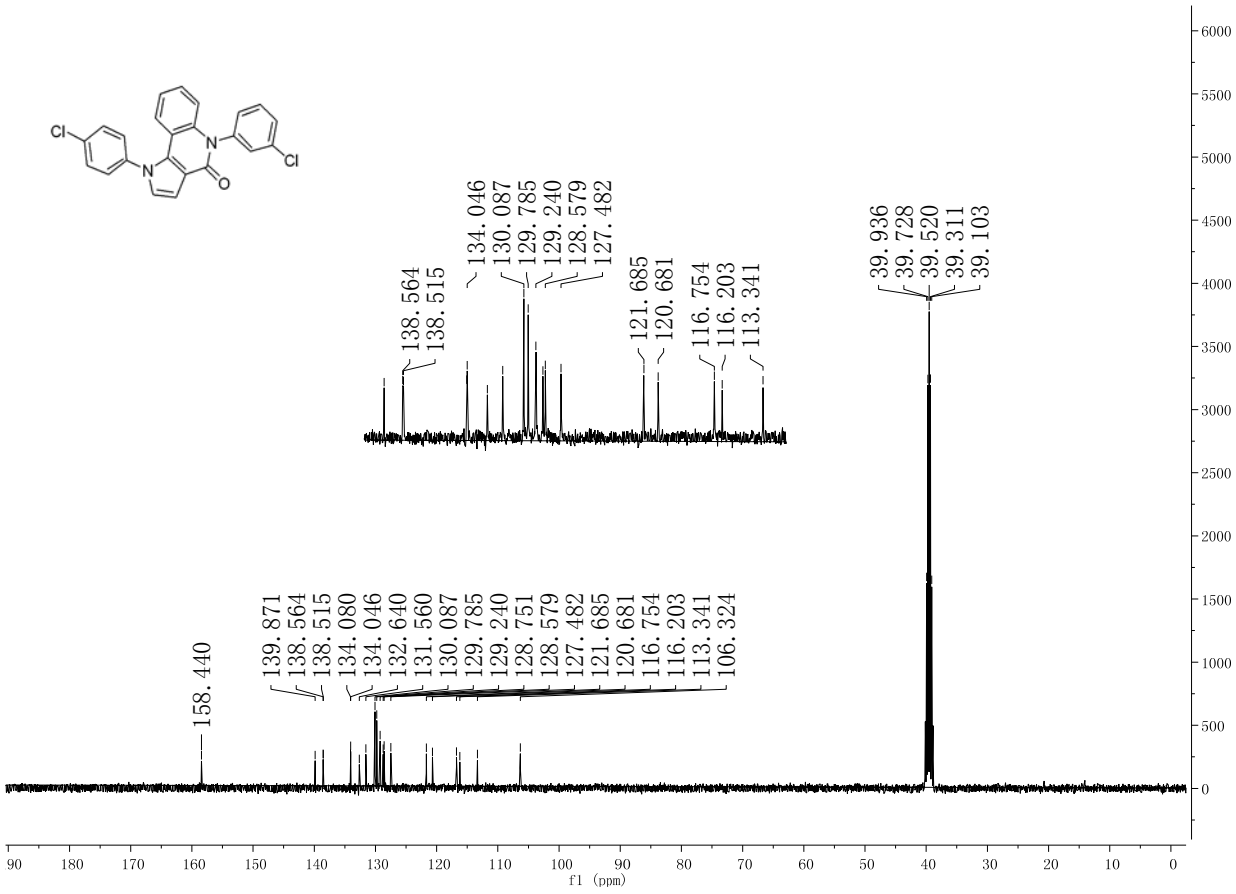
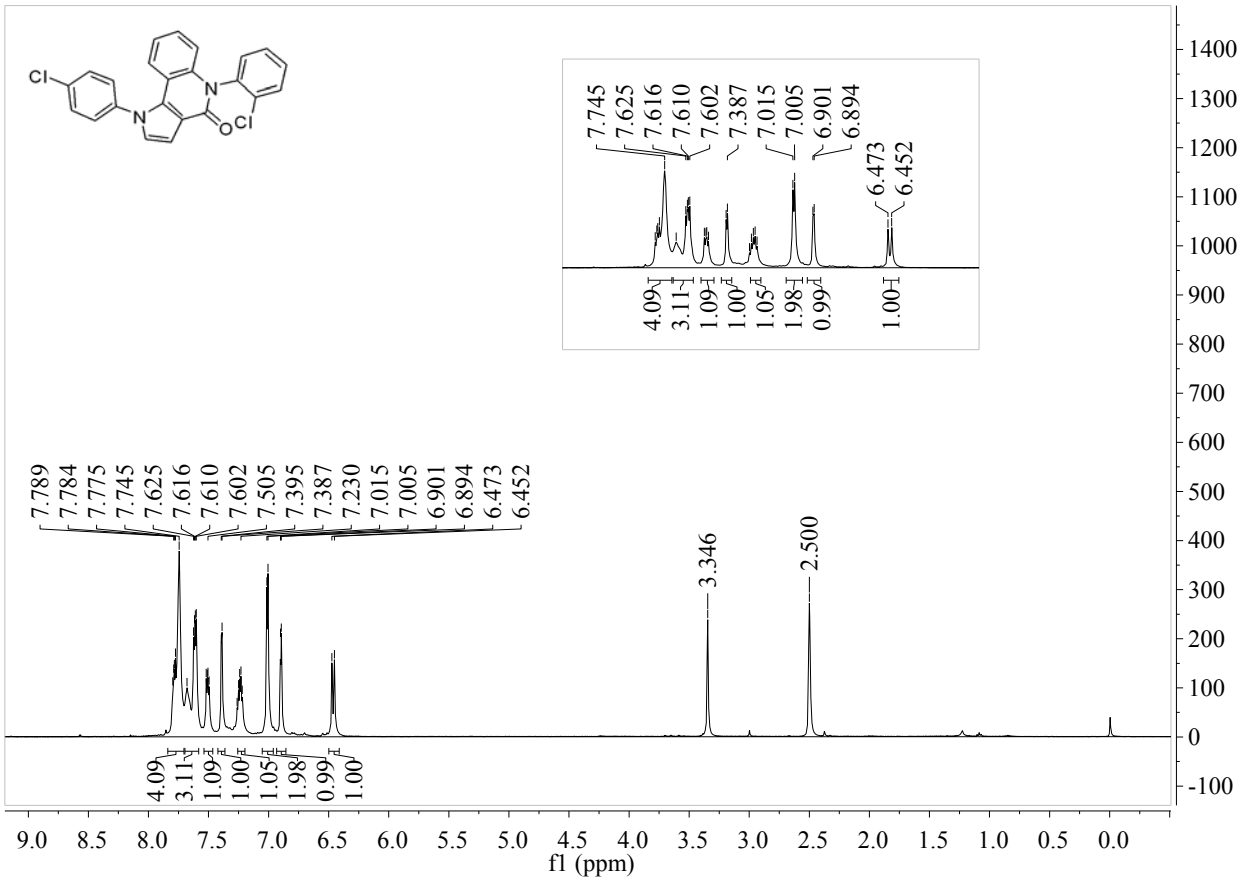
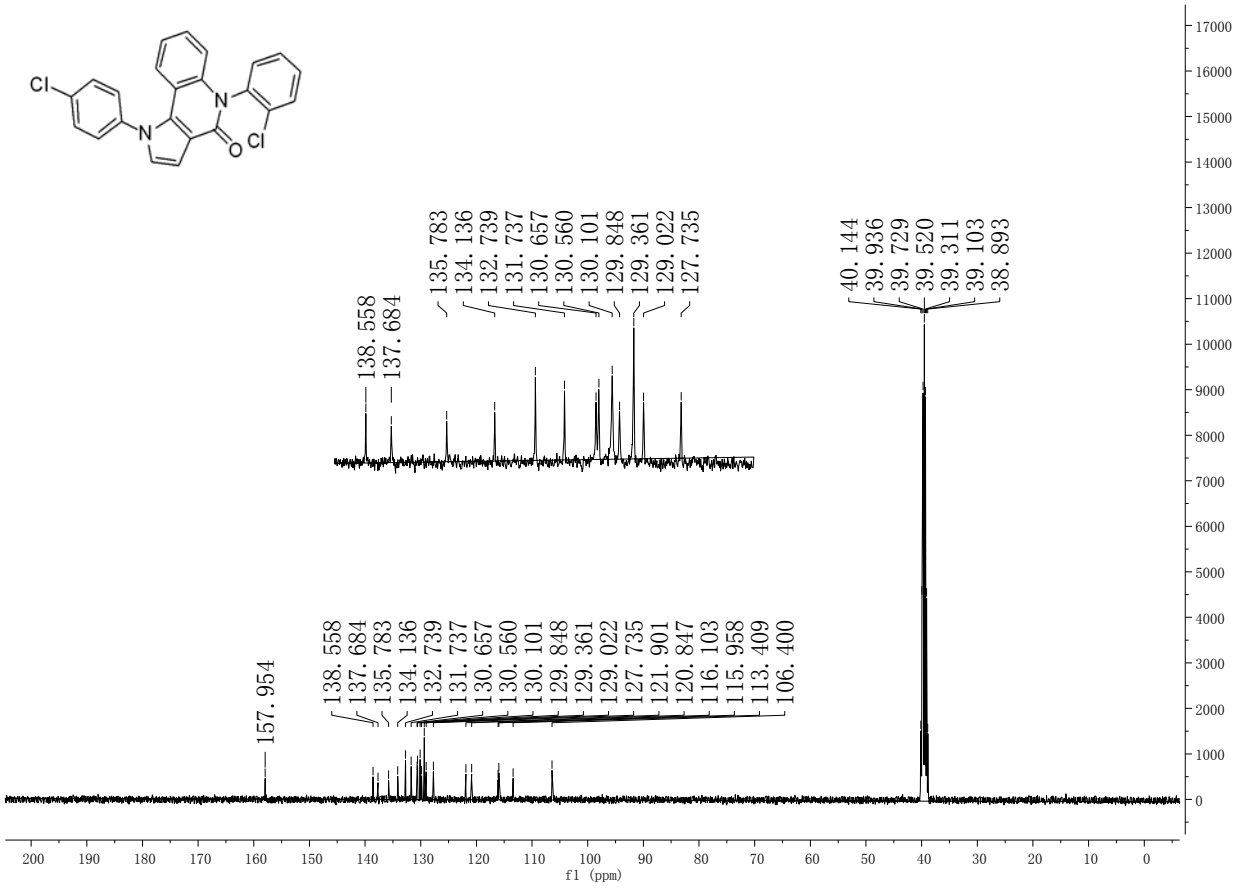
7.744
7.686
7.672
7.662
7.656
7.529
7.395
7.387
7.349
7.332
7.239
7.006
6.997
6.991
6.885
6.877
6.591
6.570
3.350
2.504
2.500
2.496
2.01
4.06
1.00
1.03
1.02
1.05
2.04
1.00
1.04
f1 (ppm)

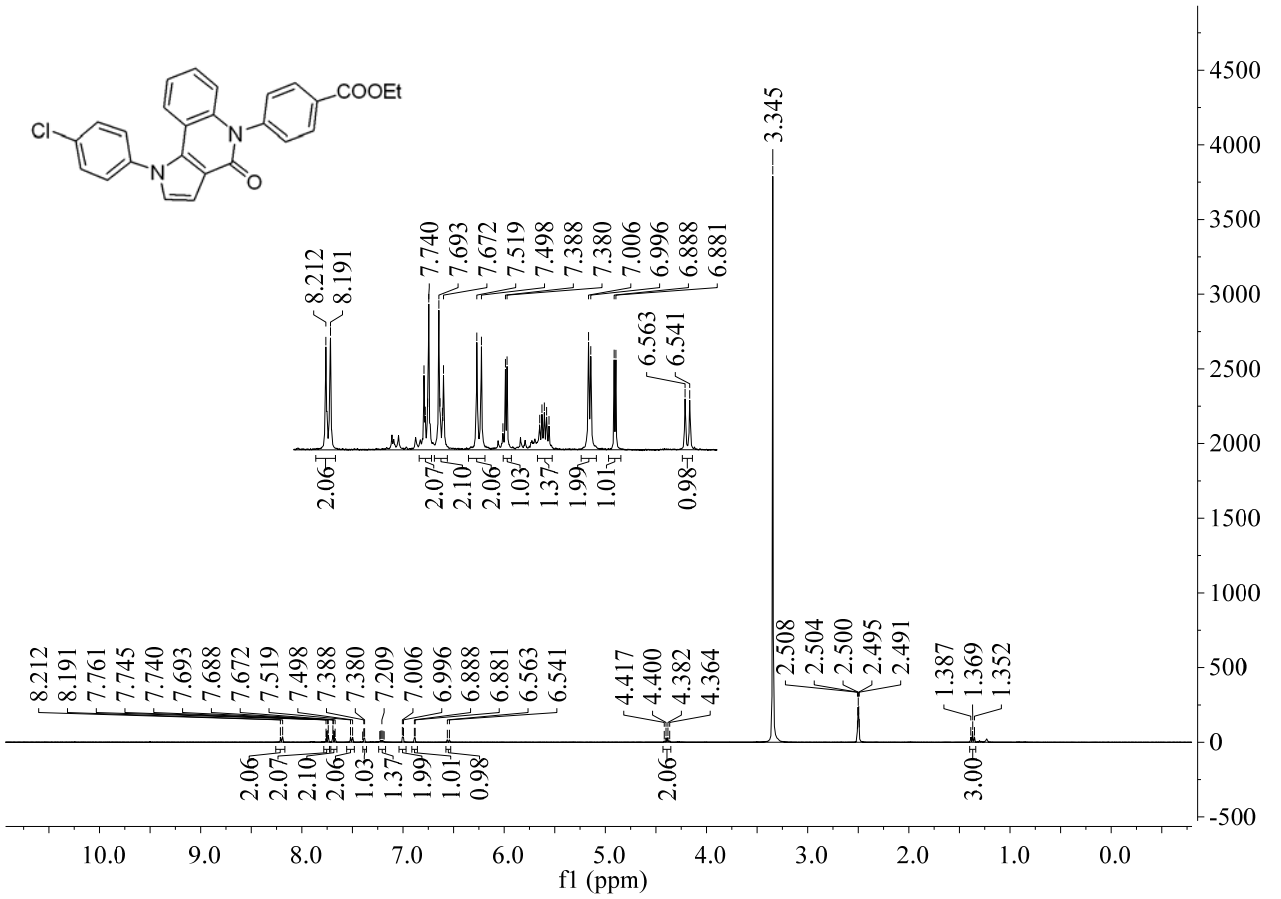

158.440
139.871
138.564
138.515
134.080
134.046
132.640
131.560
130.087
129.785
129.240
128.751
128.579
127.482
121.685
120.681
116.754
116.203
113.341
106.324
39.936
39.728
39.520
39.311
39.103
f1 (ppm)

Compound **2c**


7.789
7.784
7.775
7.745
7.625
7.616
7.610
7.602
7.505
7.395
7.387
7.230
7.015
7.005
6.901
6.894
6.473
6.452
3.346
2.500
4.09
3.11
1.09
1.00
1.05
1.98
0.99
1.00
f1 (ppm)


138.558
137.684
135.783
134.136
132.739
131.737
130.657
130.560
130.101
129.848
129.361
129.022
127.735
40.144
39.936
39.729
39.520
39.311
39.103
38.893
157.954
121.901
120.847
116.103
115.958
113.409
106.400
f1 (ppm)

Compound **2d**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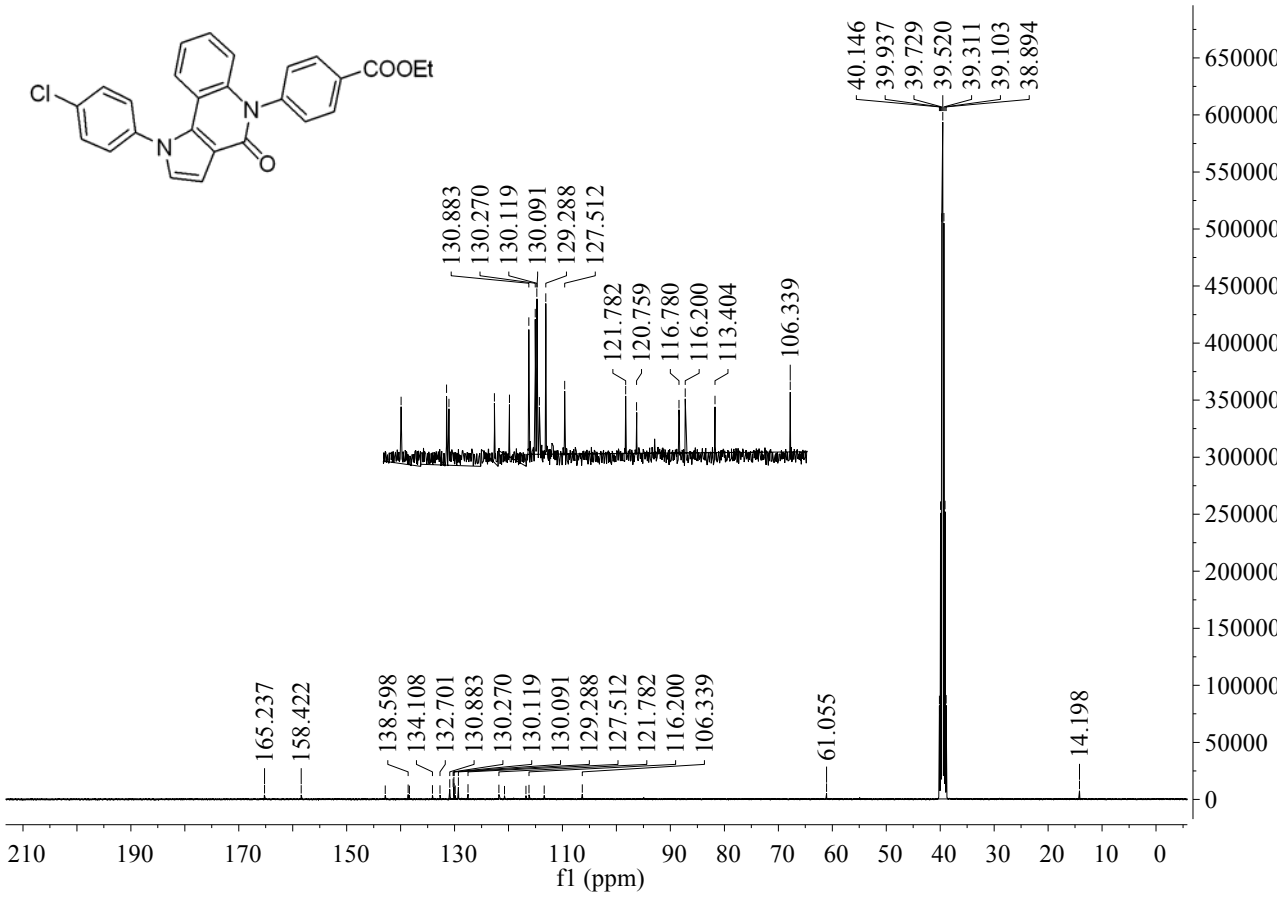
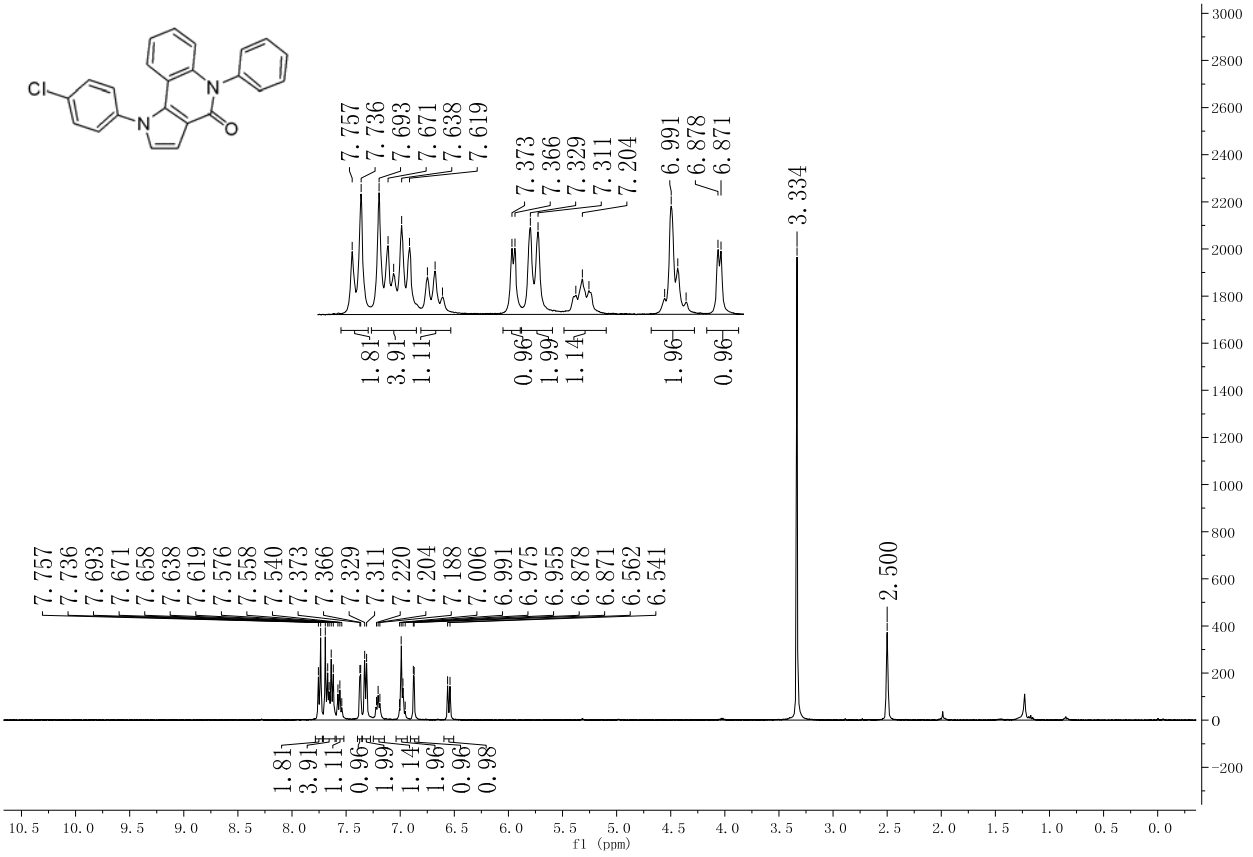
N
N
O
COOEt
8.212
8.191
7.761
7.745
7.740
7.693
7.688
7.672
7.519
7.498
7.388
7.380
7.209
7.006
6.996
6.888
6.881
6.563
6.541
4.417
4.400
4.382
4.364
3.345
2.508
2.504
2.500
2.495
2.491
1.387
1.369
1.352
f1 (ppm)


Cl
N
N
O
COOEt
165.237
158.422
138.598
134.108
132.701
130.883
130.270
130.119
130.091
129.288
127.512
121.782
120.759
116.780
116.200
113.404
106.339
61.055
40.146
39.937
39.729
39.520
39.311
39.103
38.894
14.198
f1 (ppm)

Compound **2e**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N
O
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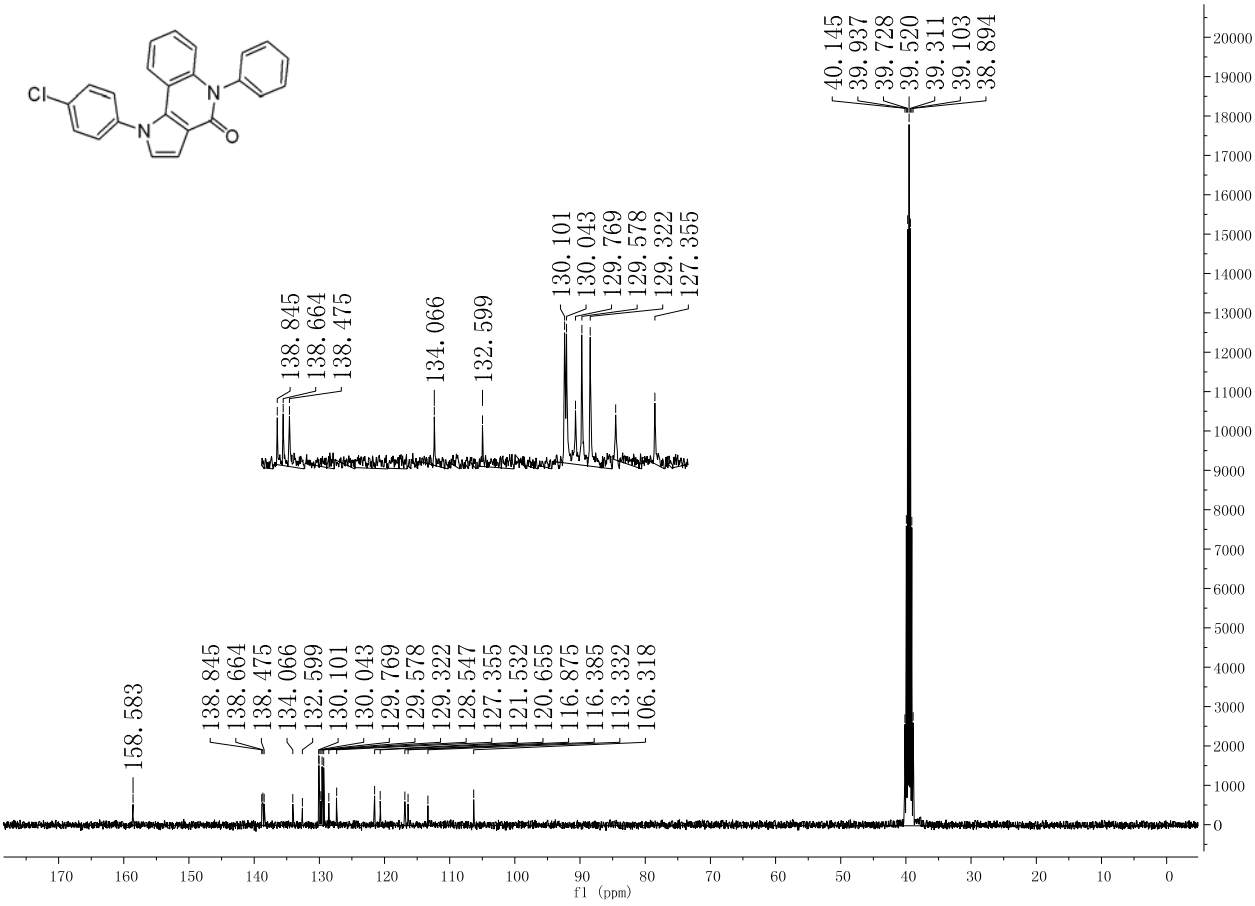
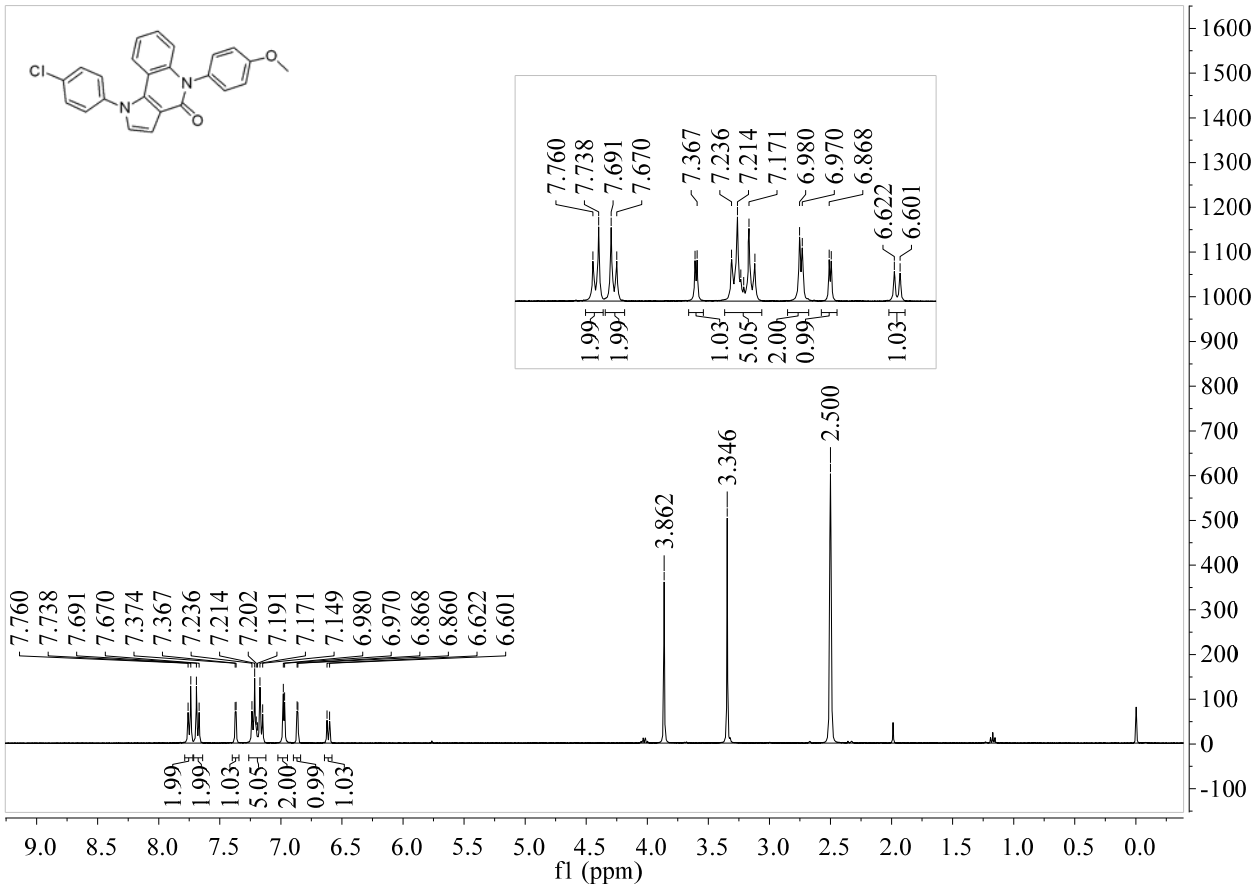
7.736
7.693
7.671
7.658
7.638
7.619
7.576
7.558
7.540
7.373
7.366
7.329
7.311
7.220
7.204
7.188
7.006
6.991
6.975
6.955
6.878
6.871
6.562
6.541
3.334
2.500
1.81
3.91
1.11
0.96
1.99
1.14
1.96
0.96
0.98
f1 (ppm)


Cl
N
O
40.145
39.937
39.728
39.520
39.311
39.103
38.894
138.845
138.664
138.475
134.066
132.599
130.101
130.043
129.769
129.578
129.322
127.355
158.583
138.845
138.664
138.475
134.066
132.599
130.101
130.043
129.769
129.578
129.322
128.547
127.355
121.532
120.655
116.875
116.385
113.332
106.318
f1 (ppm)

Compound **2f**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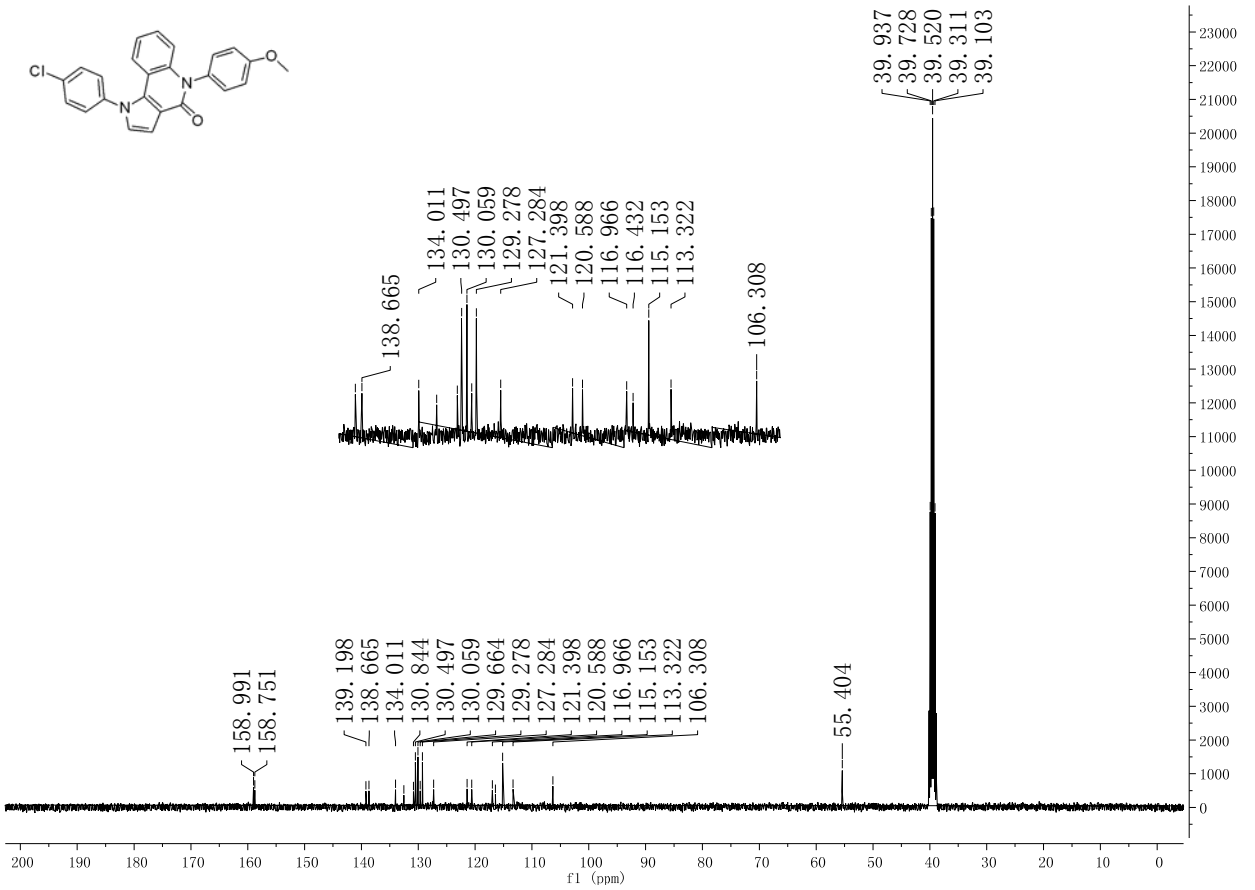
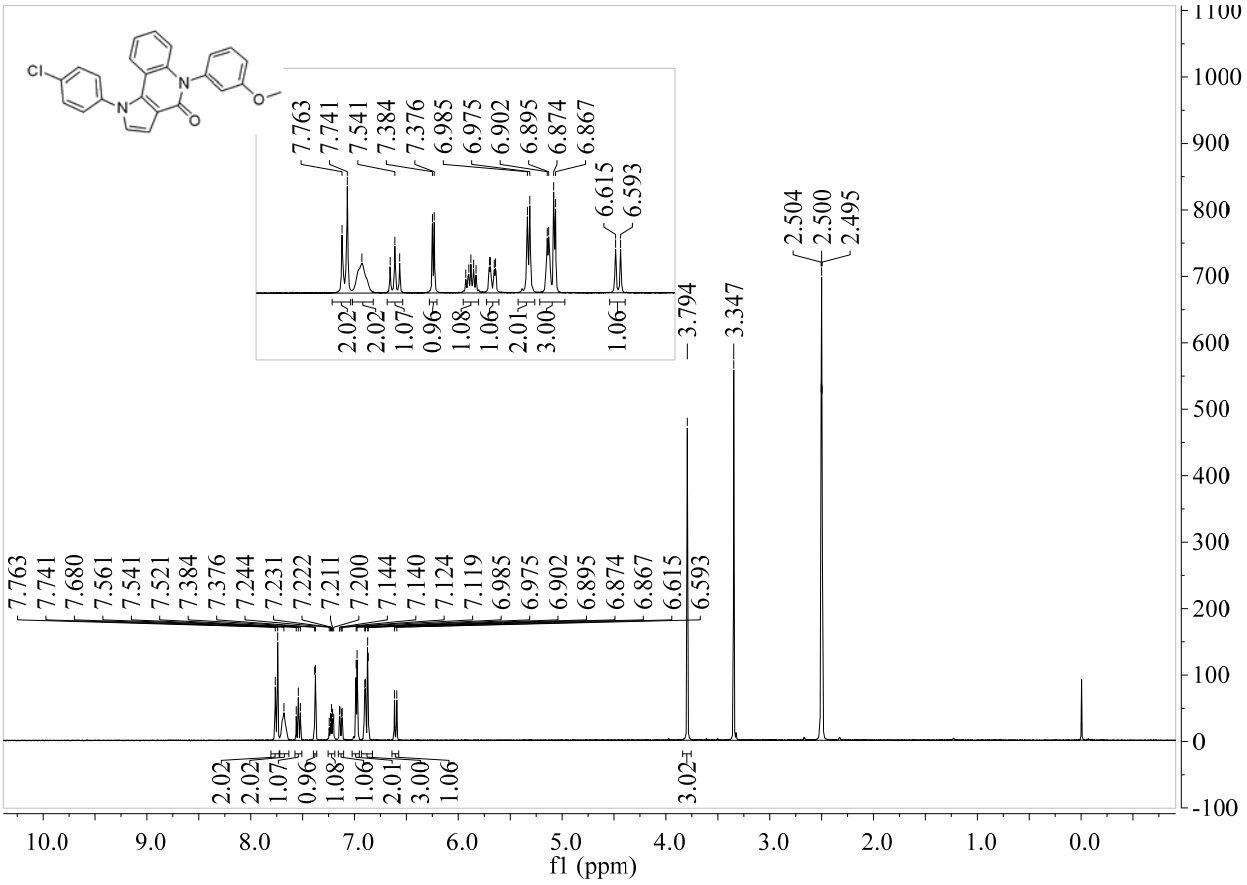
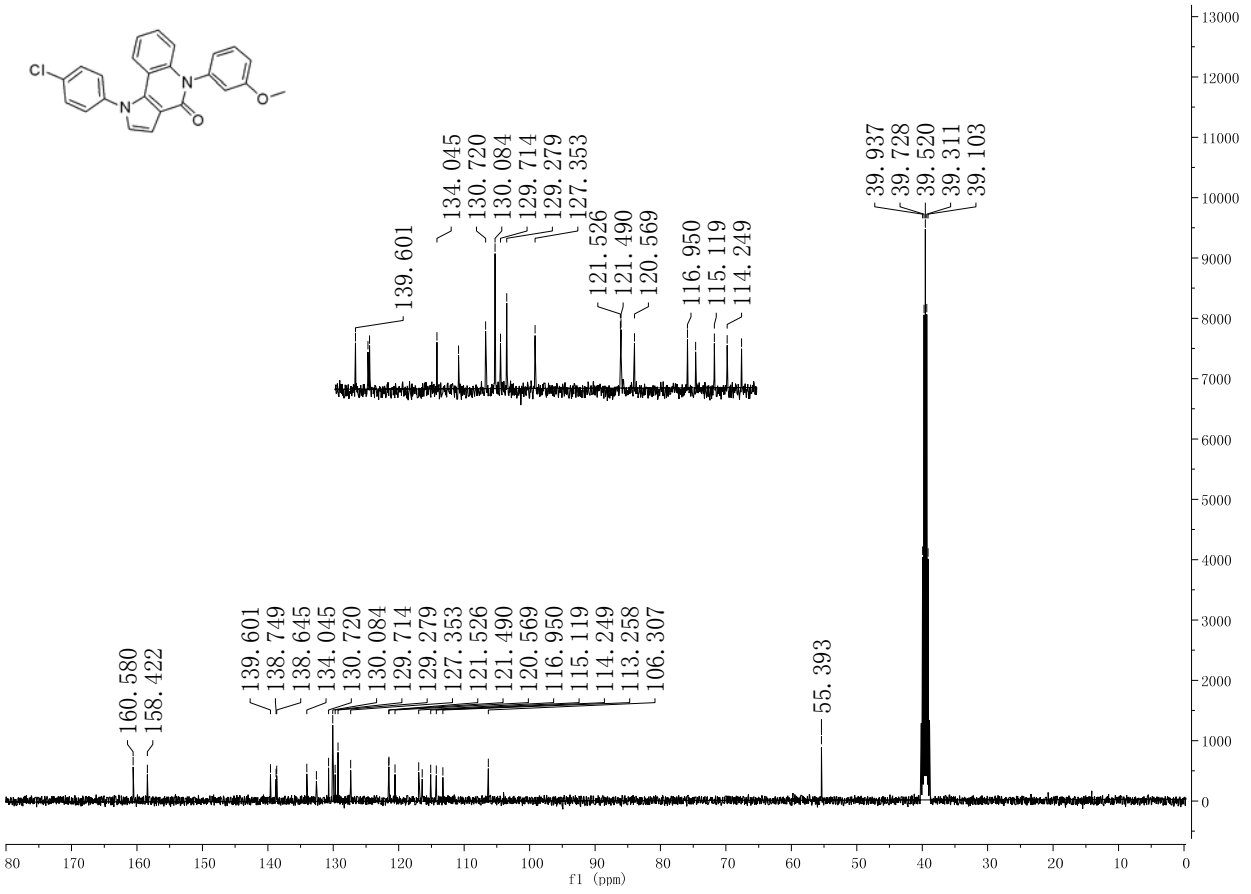
7.738
7.691
7.670
7.374
7.367
7.236
7.214
7.202
7.191
7.171
7.149
6.980
6.970
6.868
6.860
6.622
6.601
3.862
3.346
2.500
1.99
1.99
1.03
5.05
2.00
0.99
1.03
f1 (ppm)


39.937
39.728
39.520
39.311
39.103
138.665
134.011
130.497
130.059
129.278
127.284
121.398
120.588
116.966
116.432
115.153
113.322
106.308
158.991
158.751
139.198
138.665
134.011
130.844
130.497
130.059
129.664
129.278
127.284
121.398
120.588
116.966
115.153
113.322
106.308
55.404
f1 (ppm)

Compound **2g**


7.763
7.741
7.680
7.561
7.541
7.521
7.384
7.376
7.244
7.231
7.222
7.211
7.200
7.144
7.140
7.124
7.119
6.985
6.975
6.902
6.895
6.874
6.867
6.615
6.593
3.794
3.347
2.504
2.500
2.495
f1 (ppm)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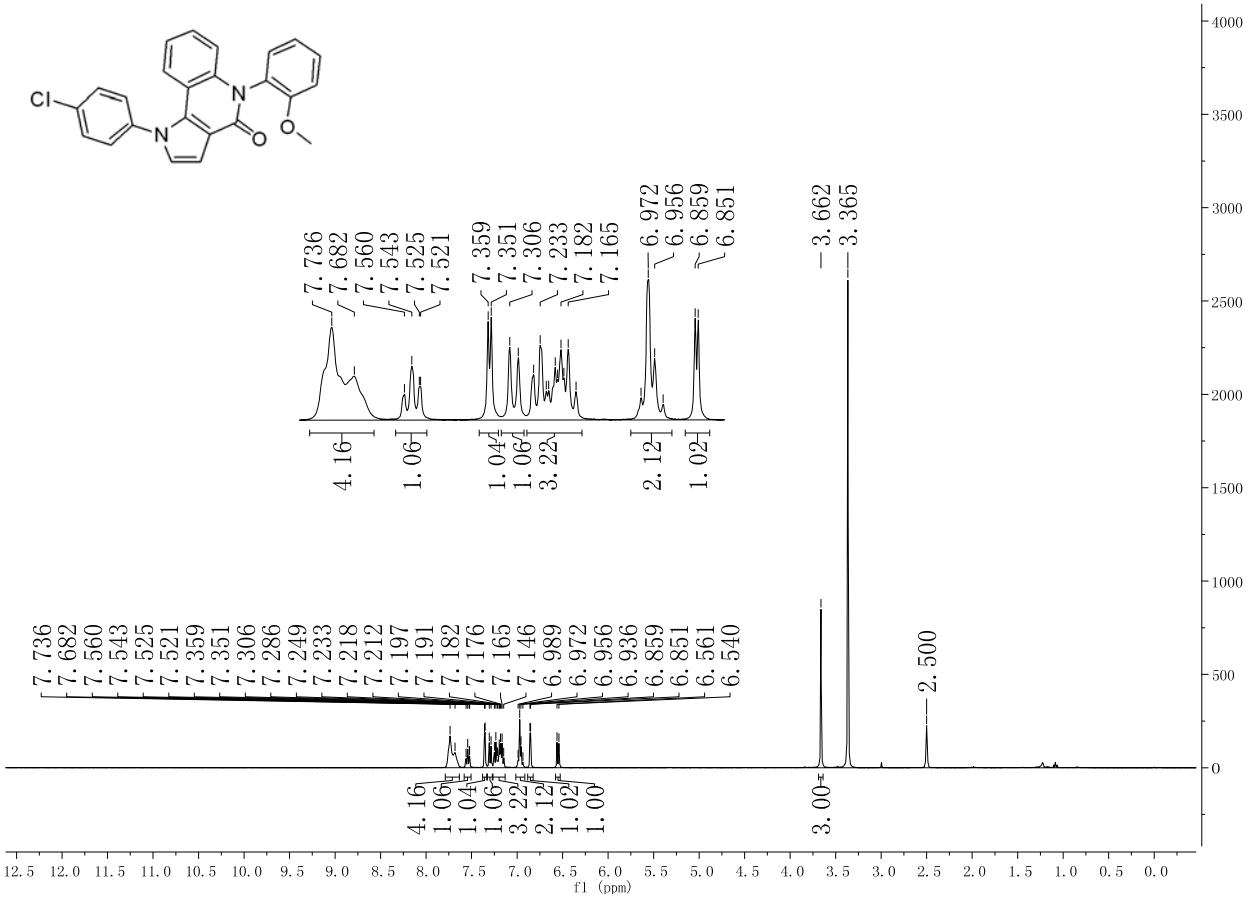
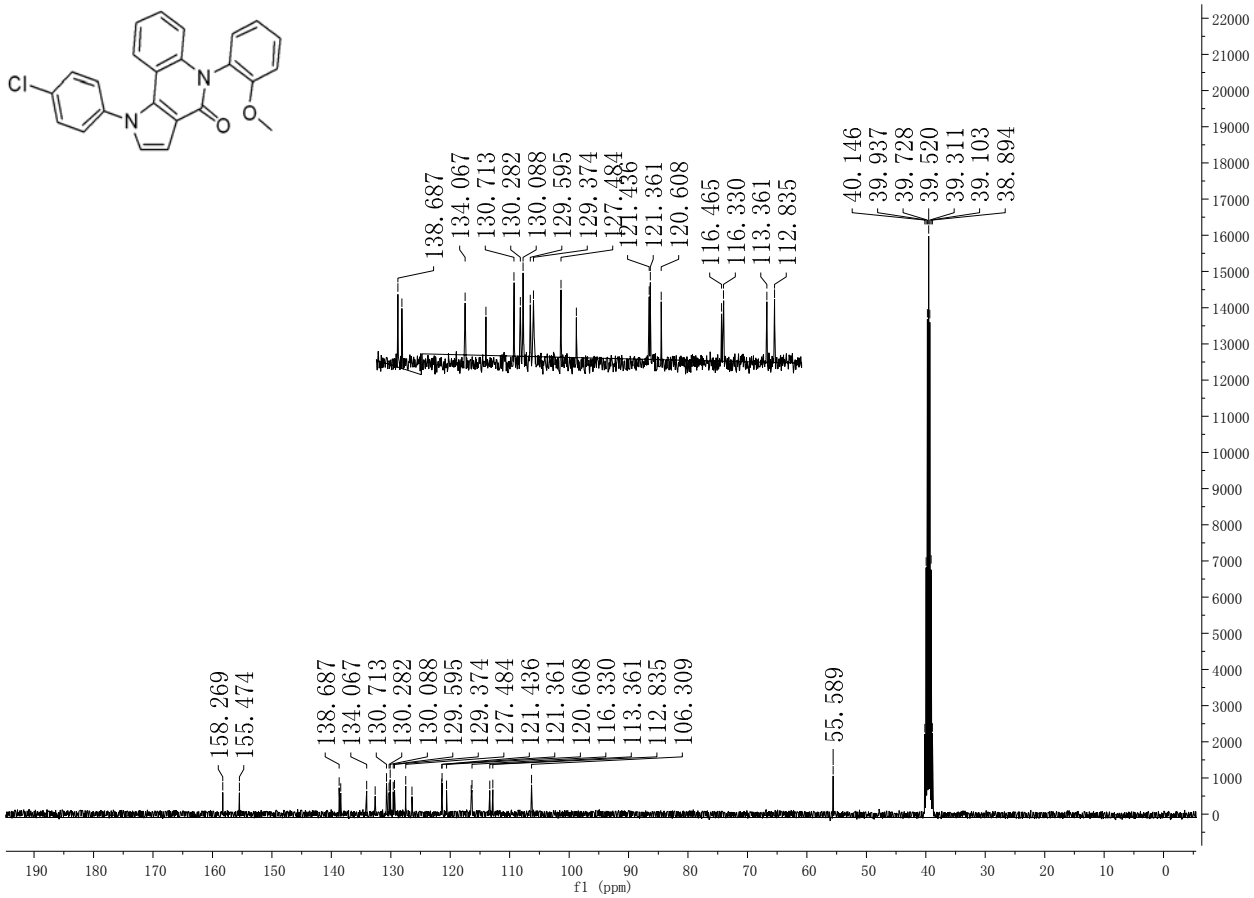
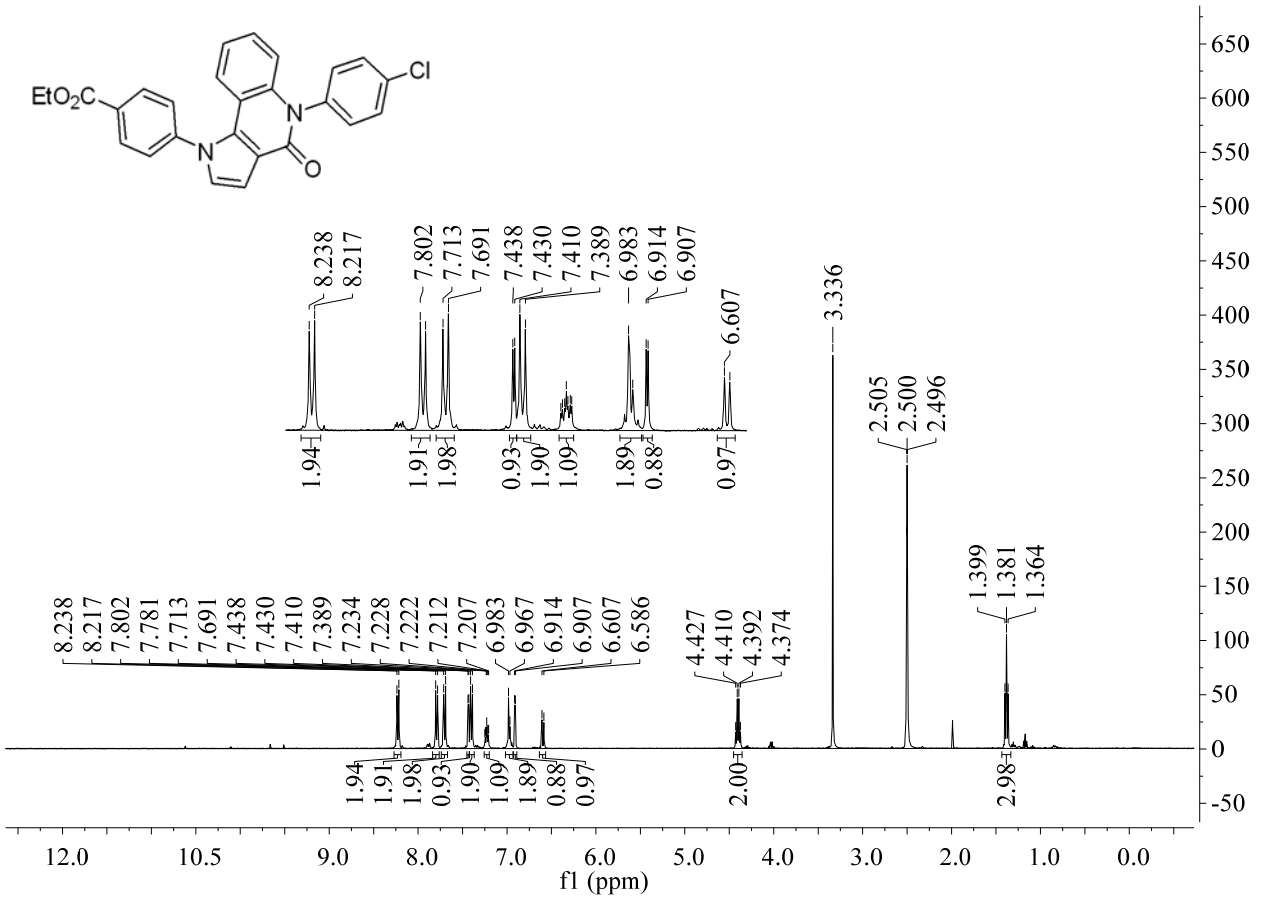
138.749
138.645
134.045
130.720
130.084
129.714
129.279
127.353
121.526
121.490
120.569
116.950
115.119
114.249
113.258
106.307
160.580
158.422
55.393
39.937
39.728
39.520
39.311
39.103
f1 (ppm)

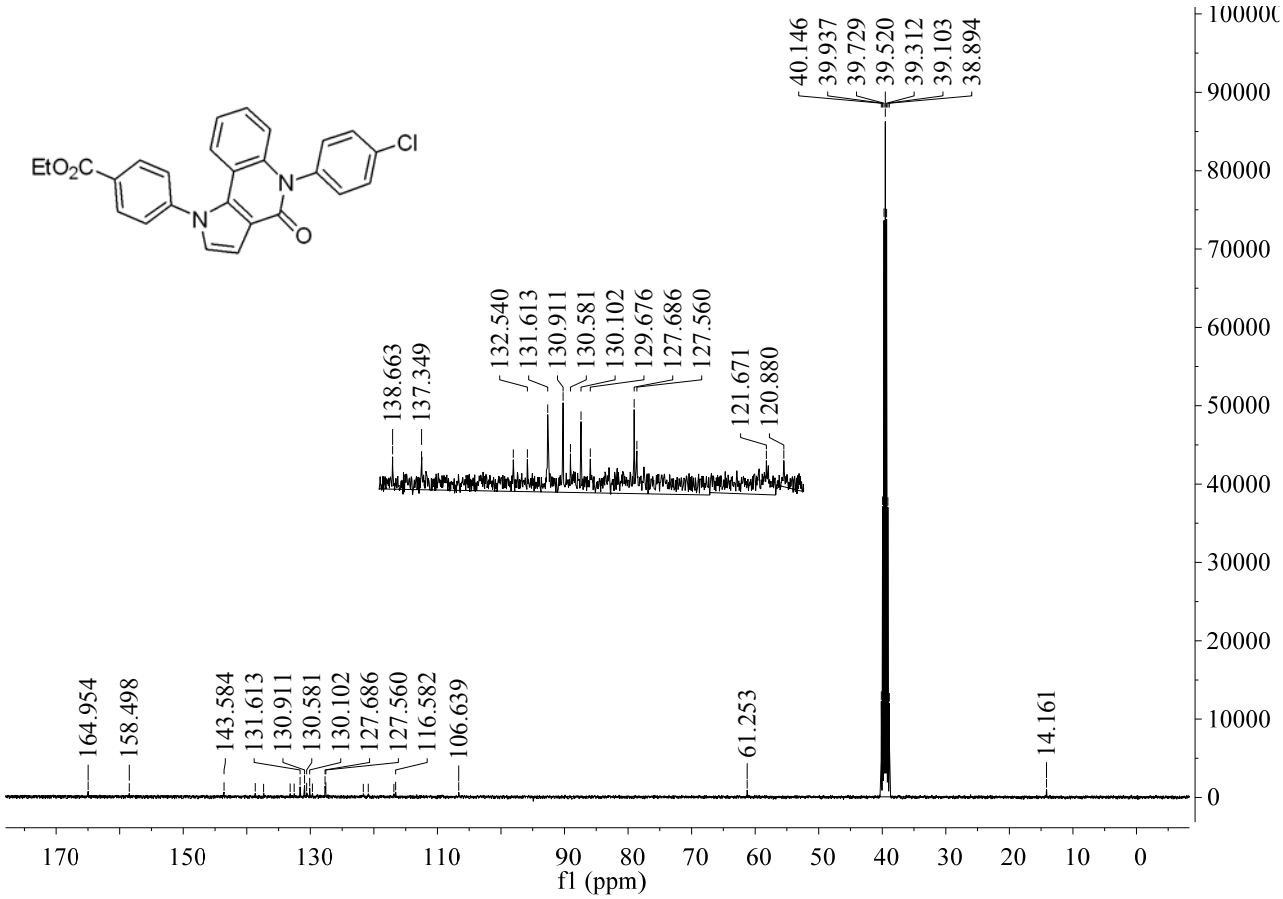
Compound **2h**


Cl
N
O
7.736
7.682
7.560
7.543
7.525
7.521
7.359
7.351
7.306
7.233
7.182
7.165
6.972
6.956
6.859
6.851
3.662
3.365
4.16
1.06
1.04
1.06
3.22
2.12
1.02
7.736
7.682
7.560
7.543
7.525
7.521
7.359
7.351
7.306
7.286
7.249
7.233
7.218
7.212
7.197
7.191
7.182
7.176
7.165
7.146
6.989
6.972
6.956
6.936
6.859
6.851
6.561
6.540
2.500
4.16
1.06
1.04
1.06
3.22
2.12
1.02
1.00
3.00
f1 (ppm)

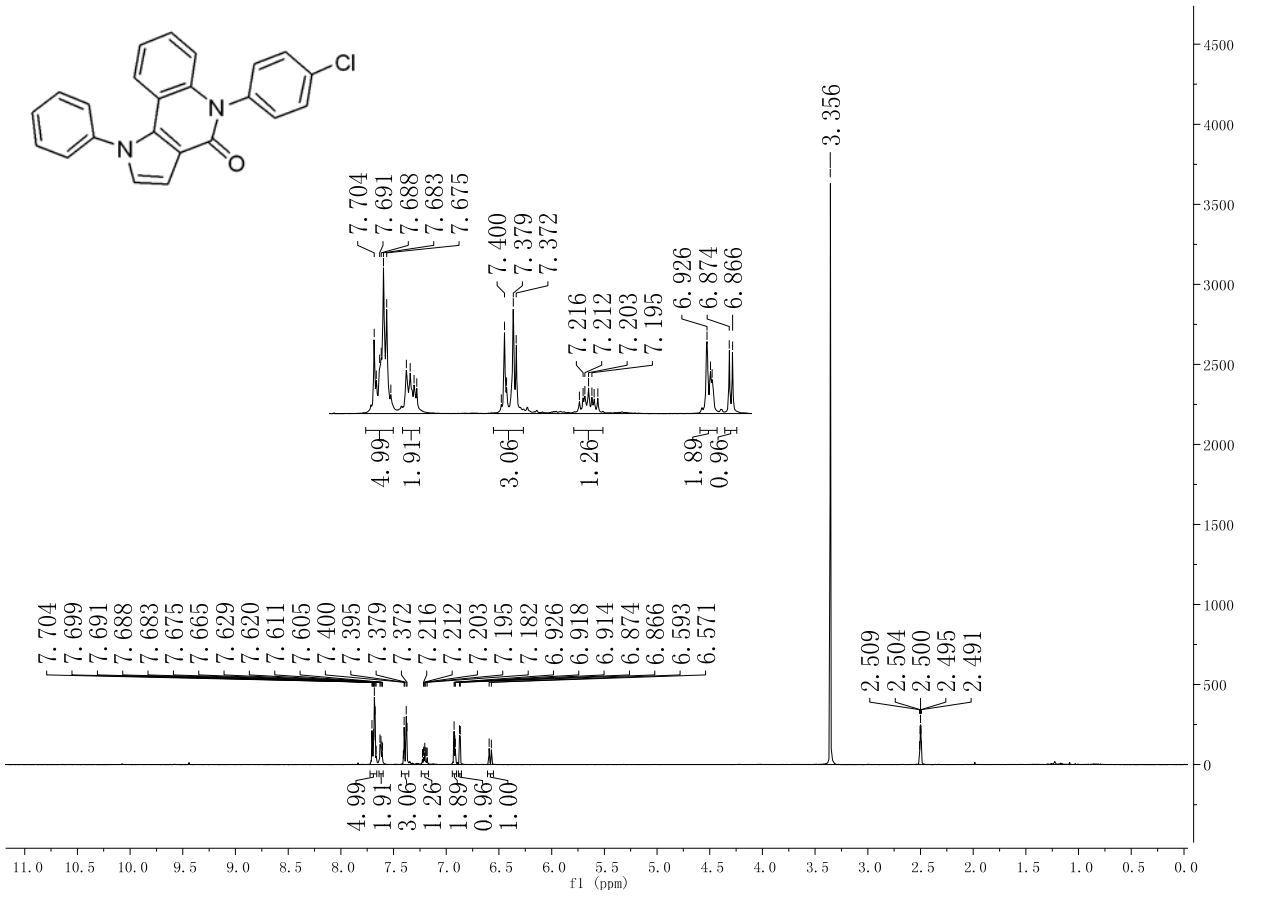

Cl
N
O
138.687
134.067
130.713
130.282
130.088
129.595
129.374
127.484
121.436
121.361
120.608
116.465
116.330
113.361
112.835
40.146
39.937
39.728
39.520
39.311
39.103
38.894
158.269
155.474
138.687
134.067
130.713
130.282
130.088
129.595
129.374
127.484
121.436
121.361
120.608
116.330
113.361
112.835
106.309
55.589
f1 (ppm)

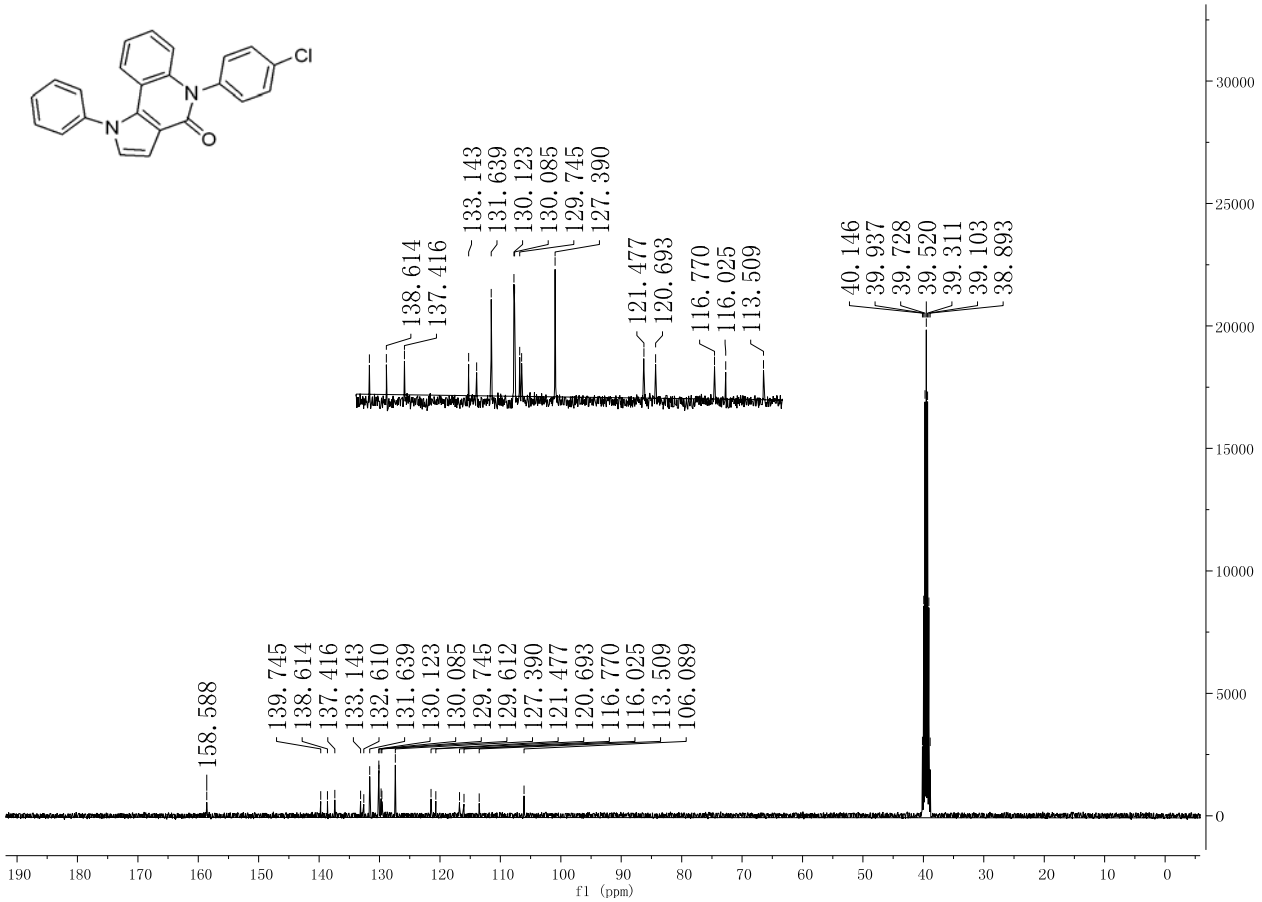
Compound **2k**


EtO2C
Cl
N
O
8.238
8.217
7.802
7.781
7.713
7.691
7.438
7.430
7.410
7.389
7.234
7.228
7.222
7.212
7.207
6.983
6.967
6.914
6.907
6.607
6.586
4.427
4.410
4.392
4.374
3.336
2.505
2.500
2.496
1.399
1.381
1.364
1.94
1.91
1.98
0.93
1.90
1.09
1.89
0.88
0.97
2.00
2.98
f1 (ppm)

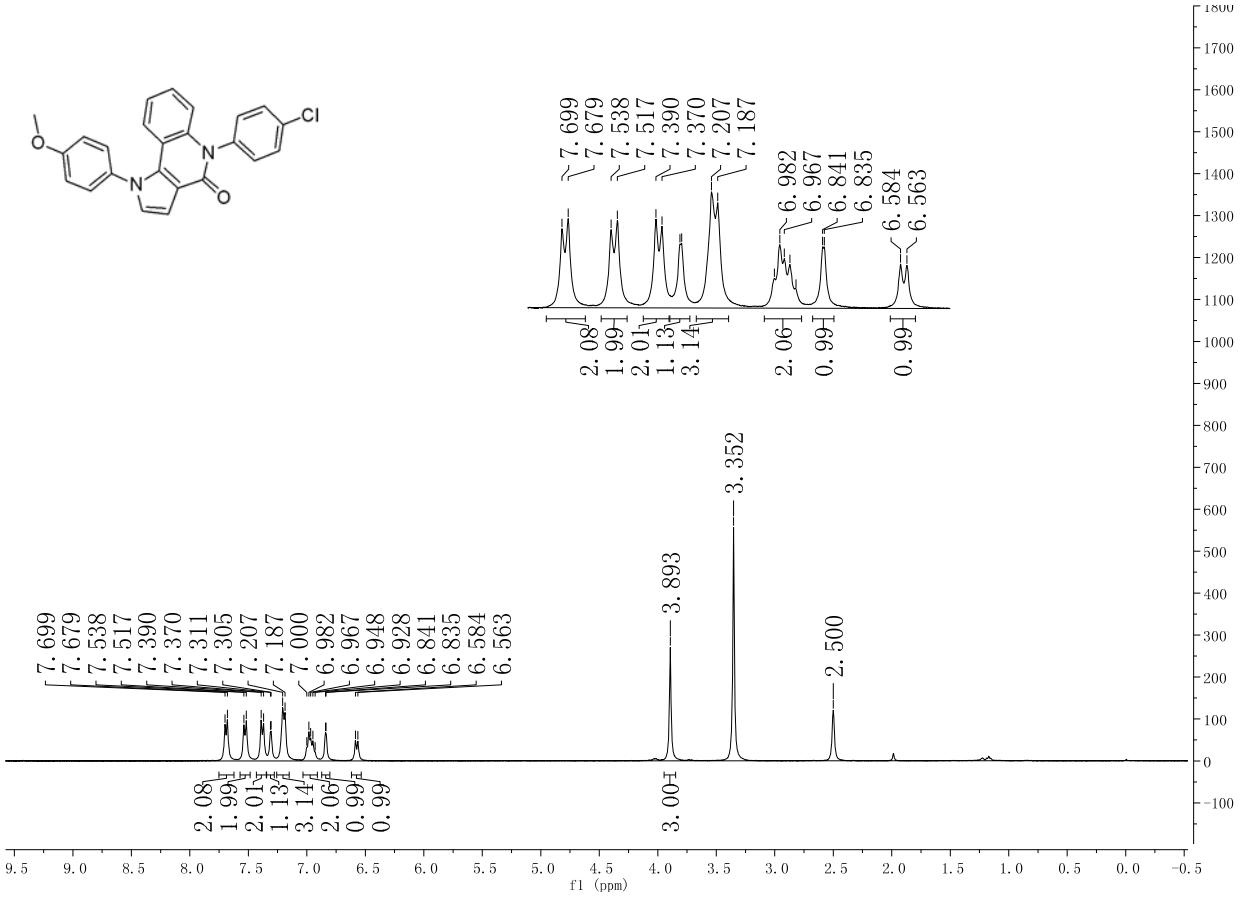

EtO2C
Cl
N
O
40.146
39.937
39.729
39.520
39.312
39.103
38.894
138.663
137.349
132.540
131.613
130.911
130.581
130.102
129.676
127.686
127.560
121.671
120.880
164.954
158.498
143.584
131.613
130.911
130.581
130.102
127.686
127.560
116.582
106.639
61.253
14.161
f1 (ppm)

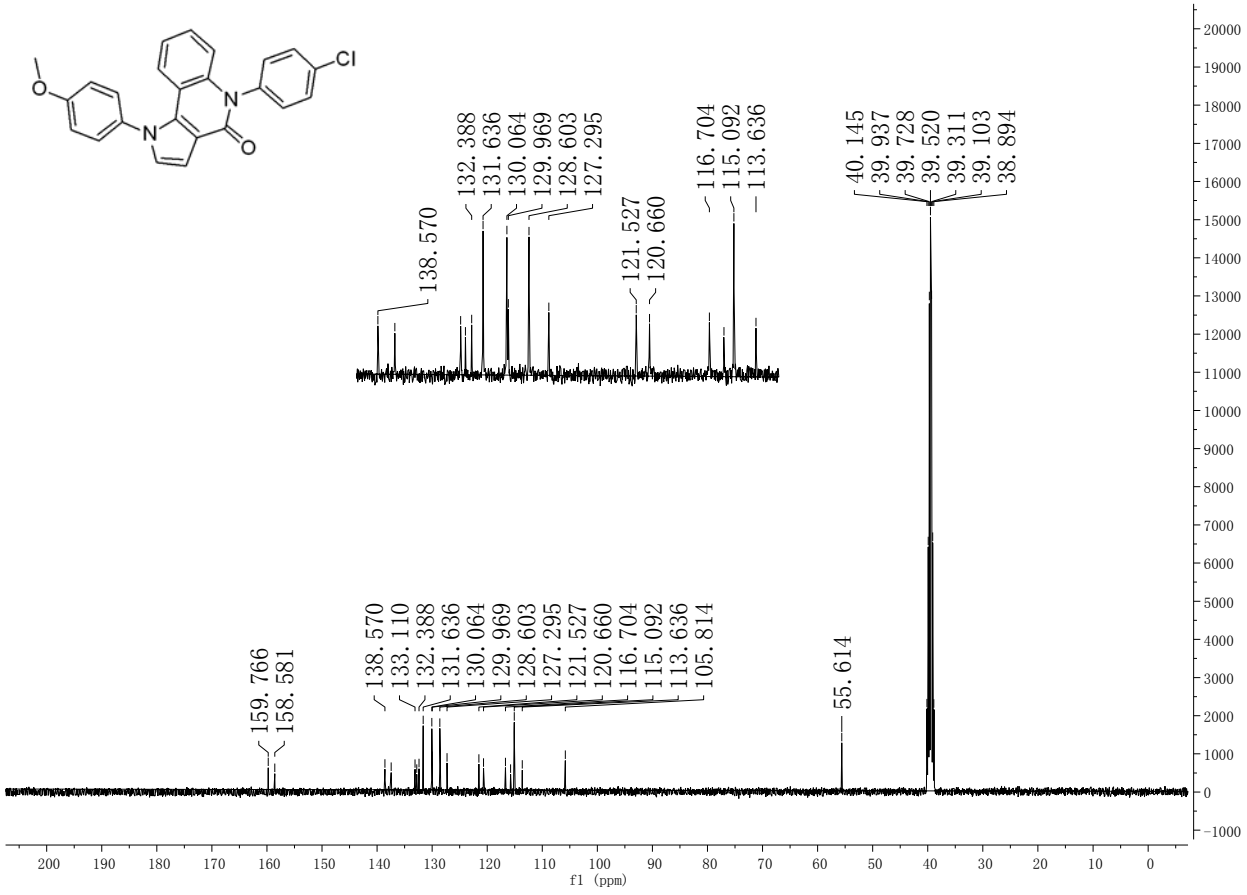
Compound **2l**


Cl
N
O
7.704
7.691
7.688
7.683
7.675
7.400
7.379
7.372
7.216
7.212
7.203
7.195
6.926
6.874
6.866
3.356
2.509
2.504
2.500
2.495
2.491
4.99
1.91
3.06
1.26
1.89
0.96
f1 (ppm)

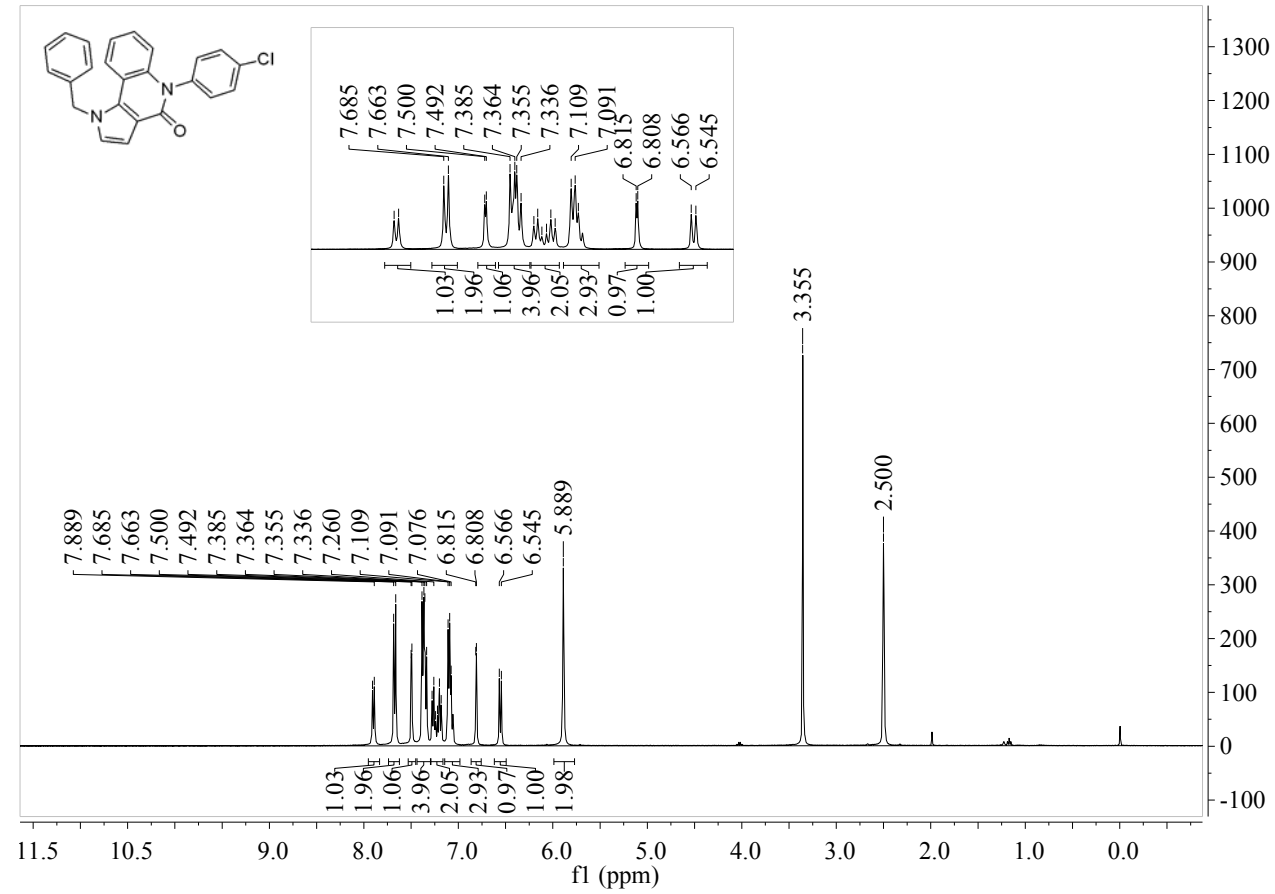

Cl
N
O
133.143
131.639
130.123
130.085
129.745
127.390
138.614
137.416
121.477
120.693
116.770
116.025
113.509
40.146
39.937
39.728
39.520
39.311
39.103
38.893
158.588
139.745
138.614
137.416
133.143
132.610
131.639
130.123
130.085
129.745
129.612
127.390
121.477
120.693
116.770
116.025
113.509
106.089
f1 (ppm)

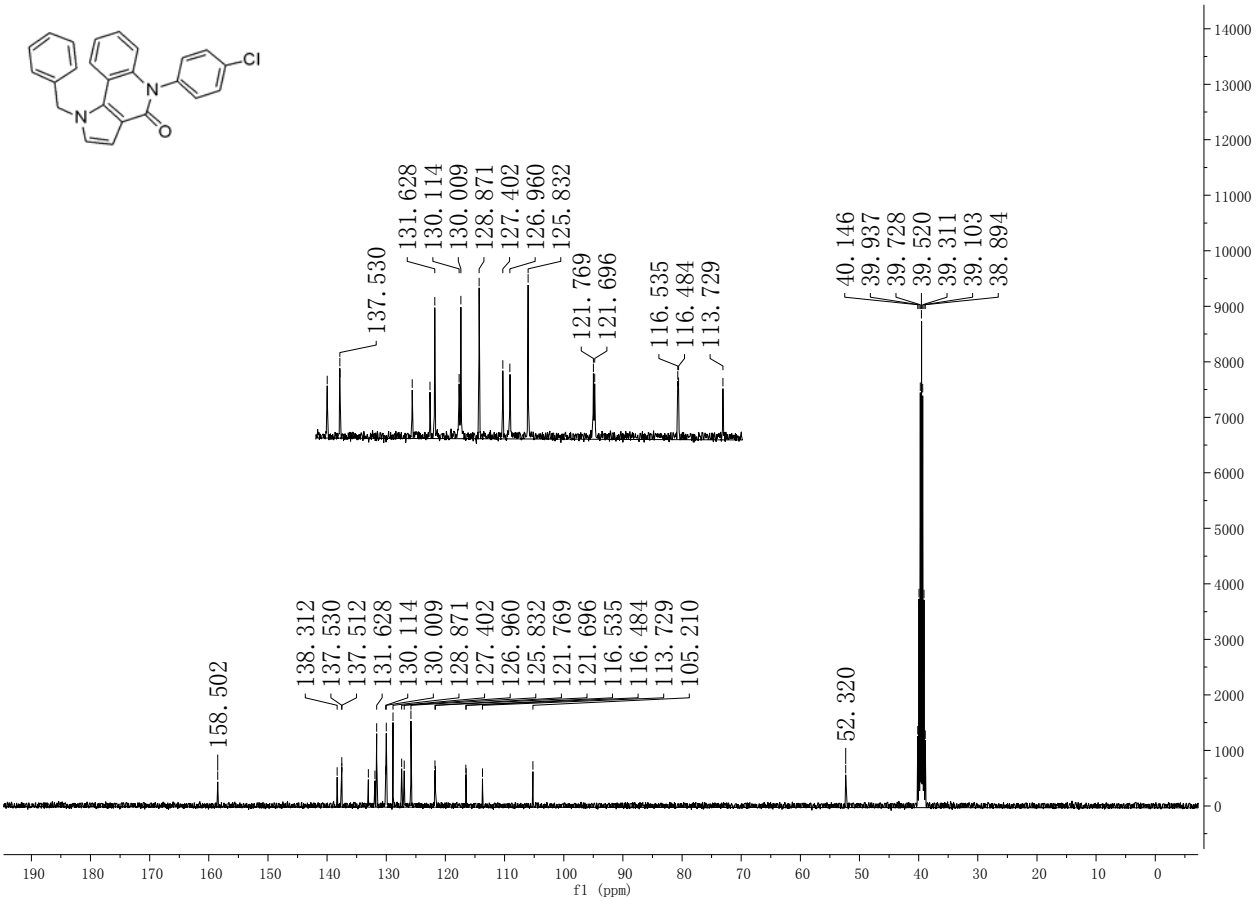
Compound **2m**


Cl
O
N
O
7.699
7.679
7.538
7.517
7.390
7.370
7.311
7.305
7.207
7.187
7.000
6.982
6.967
6.948
6.928
6.841
6.835
6.584
6.563
3.893
3.352
2.500
2.08
1.99
2.01
1.13
3.14
2.06
0.99
0.99
3.00
f1 (ppm)

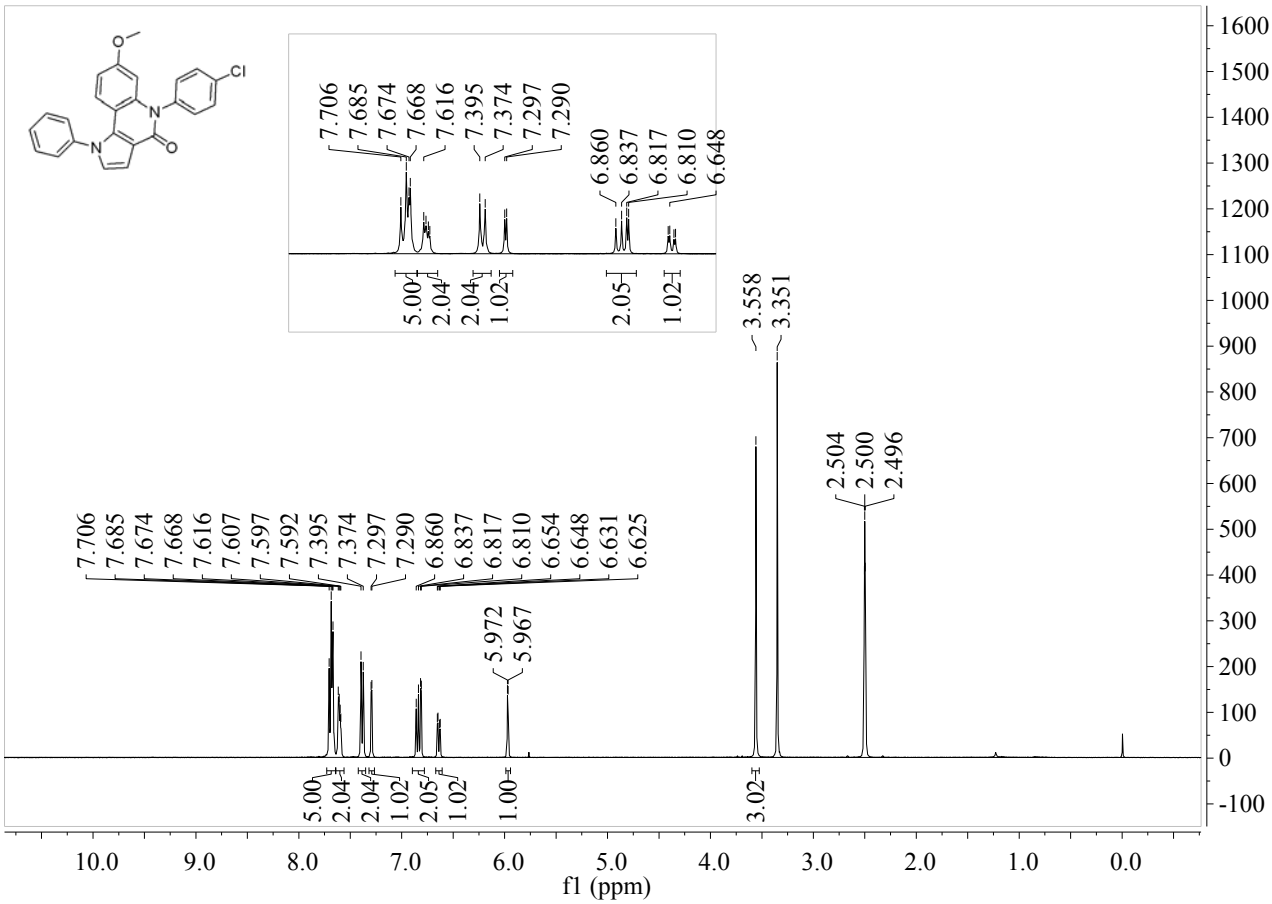

Cl
O
N
O
138.570
132.388
131.636
130.064
129.969
128.603
127.295
121.527
120.660
116.704
115.092
113.636
40.145
39.937
39.728
39.520
39.311
39.103
38.894
159.766
158.581
138.570
133.110
132.388
131.636
130.064
129.969
128.603
127.295
121.527
120.660
116.704
115.092
113.636
105.814
55.614
f1 (ppm)

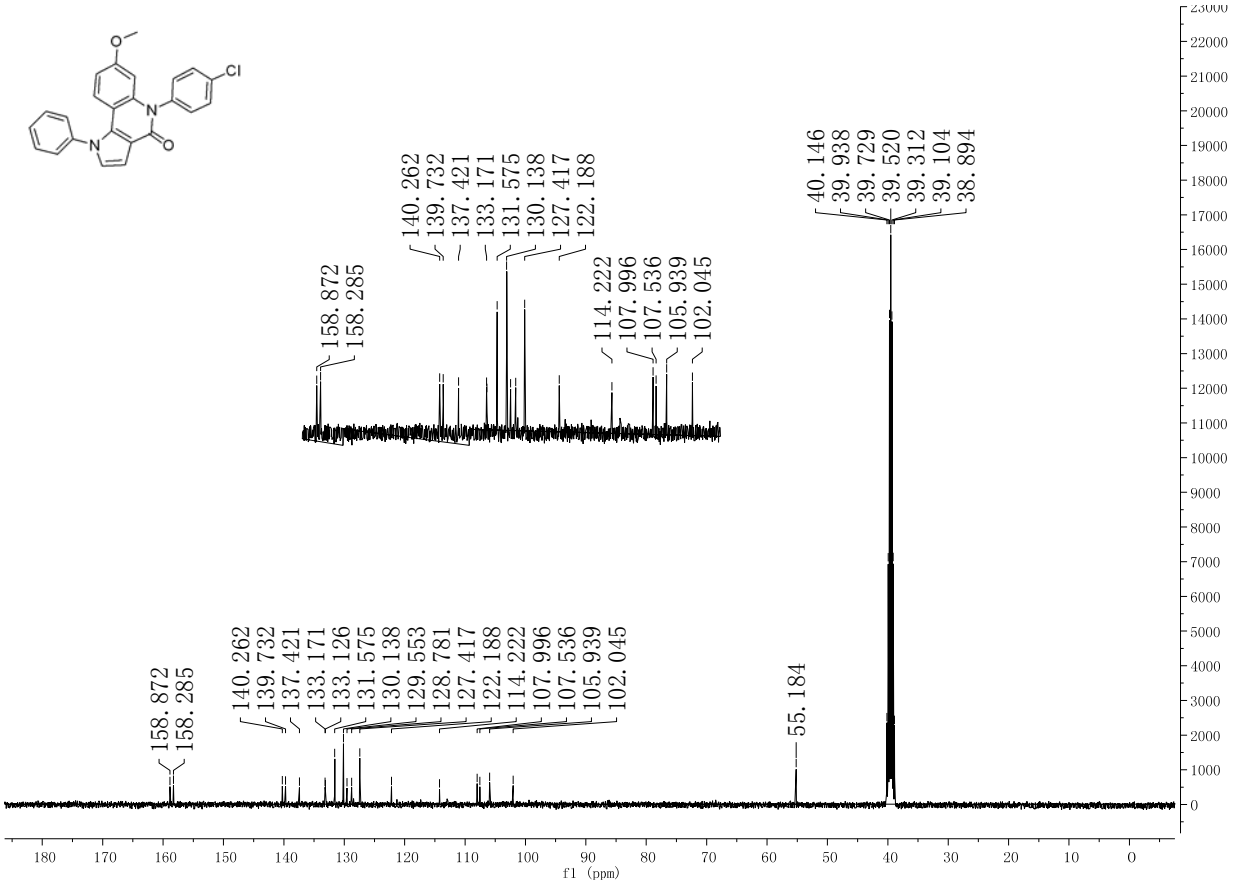
Compound **2n**


Cl
N
O
7.685
7.663
7.500
7.492
7.385
7.364
7.355
7.336
7.109
7.091
6.815
6.808
6.566
6.545
1.03
1.96
1.06
3.96
2.05
2.93
0.97
1.00
3.355
2.500
7.889
7.685
7.663
7.500
7.492
7.385
7.364
7.355
7.336
7.260
7.109
7.091
7.076
6.815
6.808
6.566
6.545
5.889
1.03
1.96
1.06
3.96
2.05
2.93
0.97
1.00
1.98
f1 (ppm)

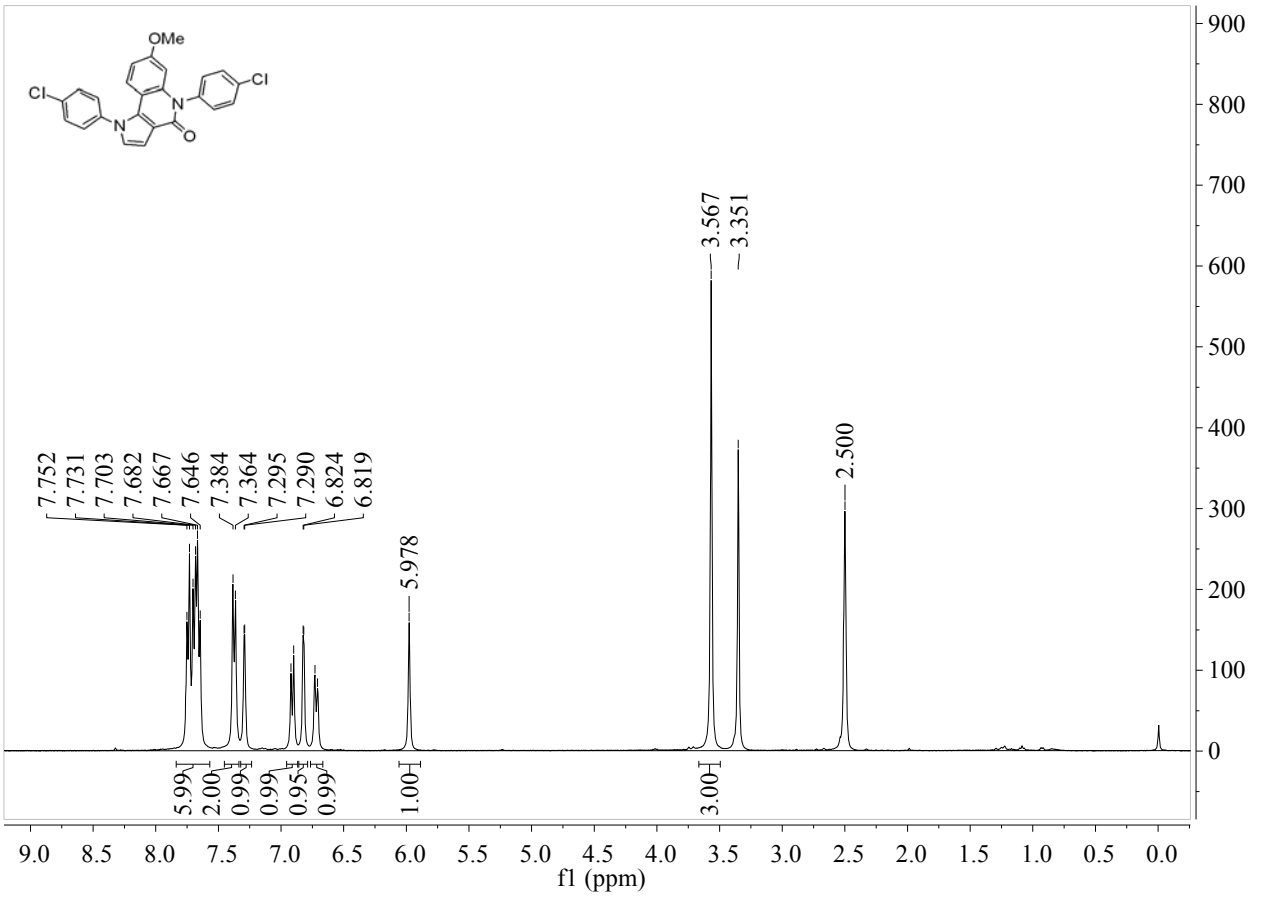

Cl
N
O
137.530
131.628
130.114
130.009
128.871
127.402
126.960
125.832
121.769
121.696
116.535
116.484
113.729
40.146
39.937
39.728
39.520
39.311
39.103
38.894
158.502
138.312
137.530
137.512
131.628
130.114
130.009
128.871
127.402
126.960
125.832
121.769
121.696
116.535
116.484
113.729
105.210
52.320
f1 (ppm)

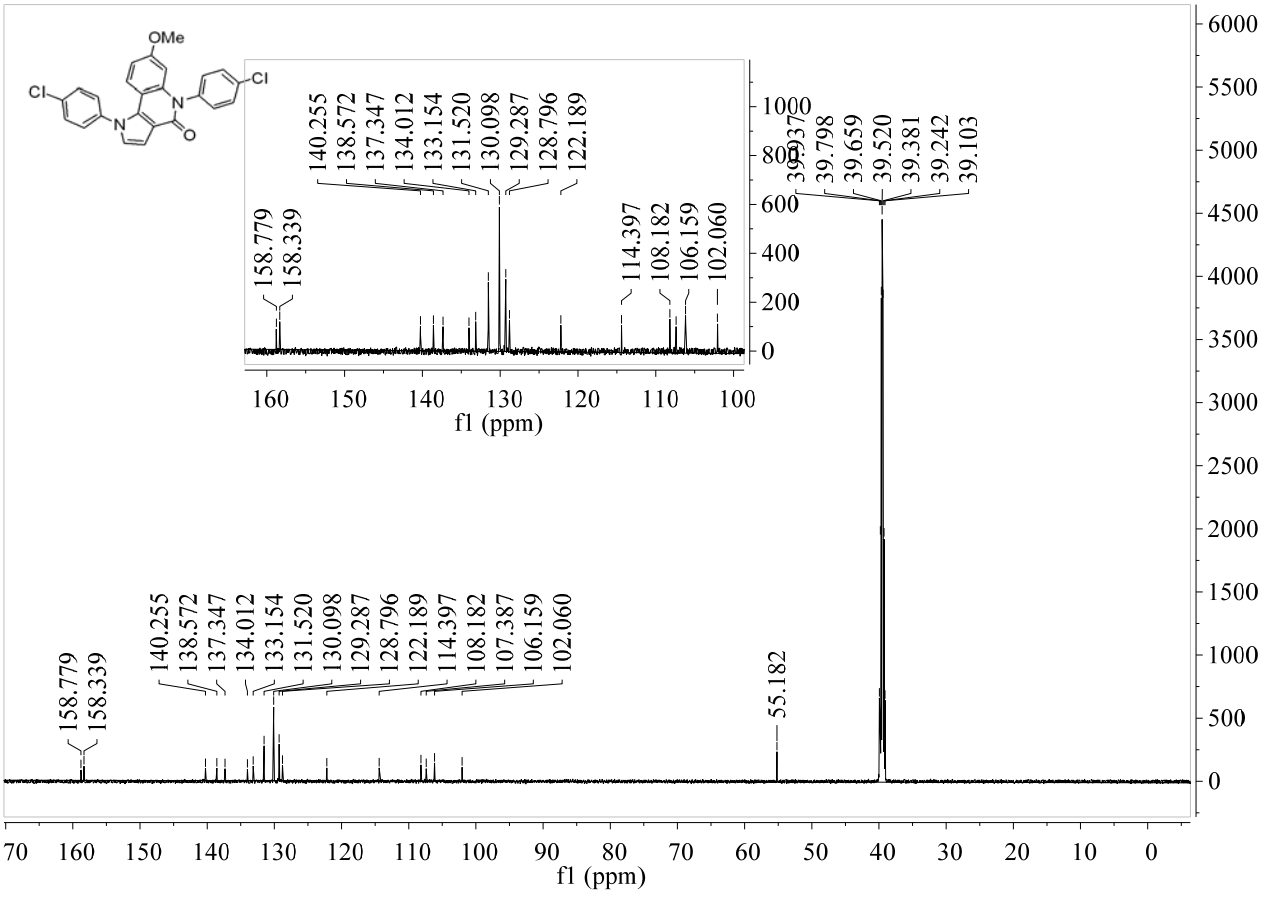
Compound **2p**


7.706
7.685
7.674
7.668
7.616
7.607
7.597
7.592
7.395
7.374
7.297
7.290
6.860
6.837
6.817
6.810
6.654
6.648
6.631
6.625
5.972
5.967
3.558
3.351
2.504
2.500
2.496
f1 (ppm)

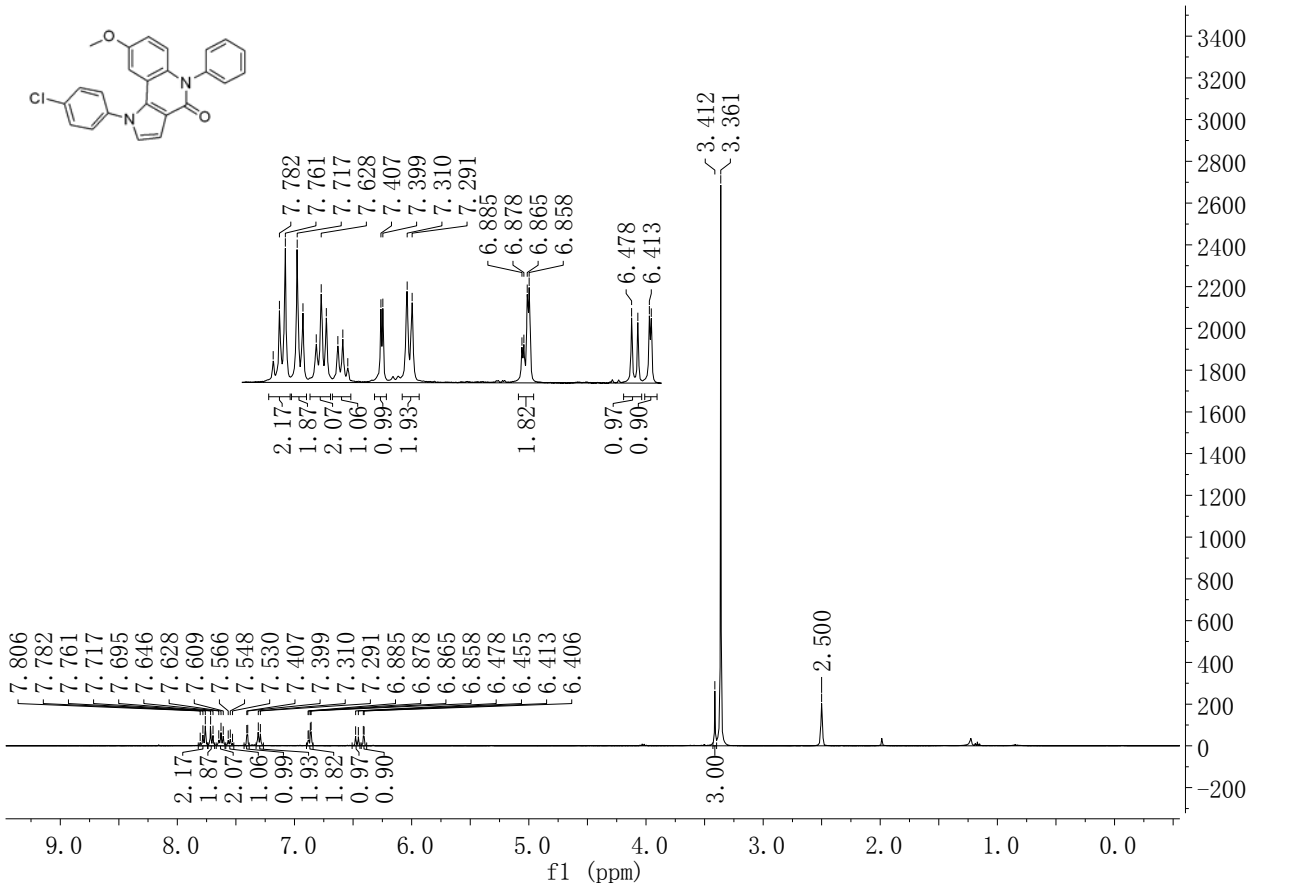

158.872
158.285
140.262
139.732
137.421
133.171
131.575
130.138
129.553
128.781
127.417
122.188
114.222
107.996
107.536
105.939
102.045
55.184
40.146
39.938
39.729
39.520
39.312
39.104
38.894
f1 (ppm)

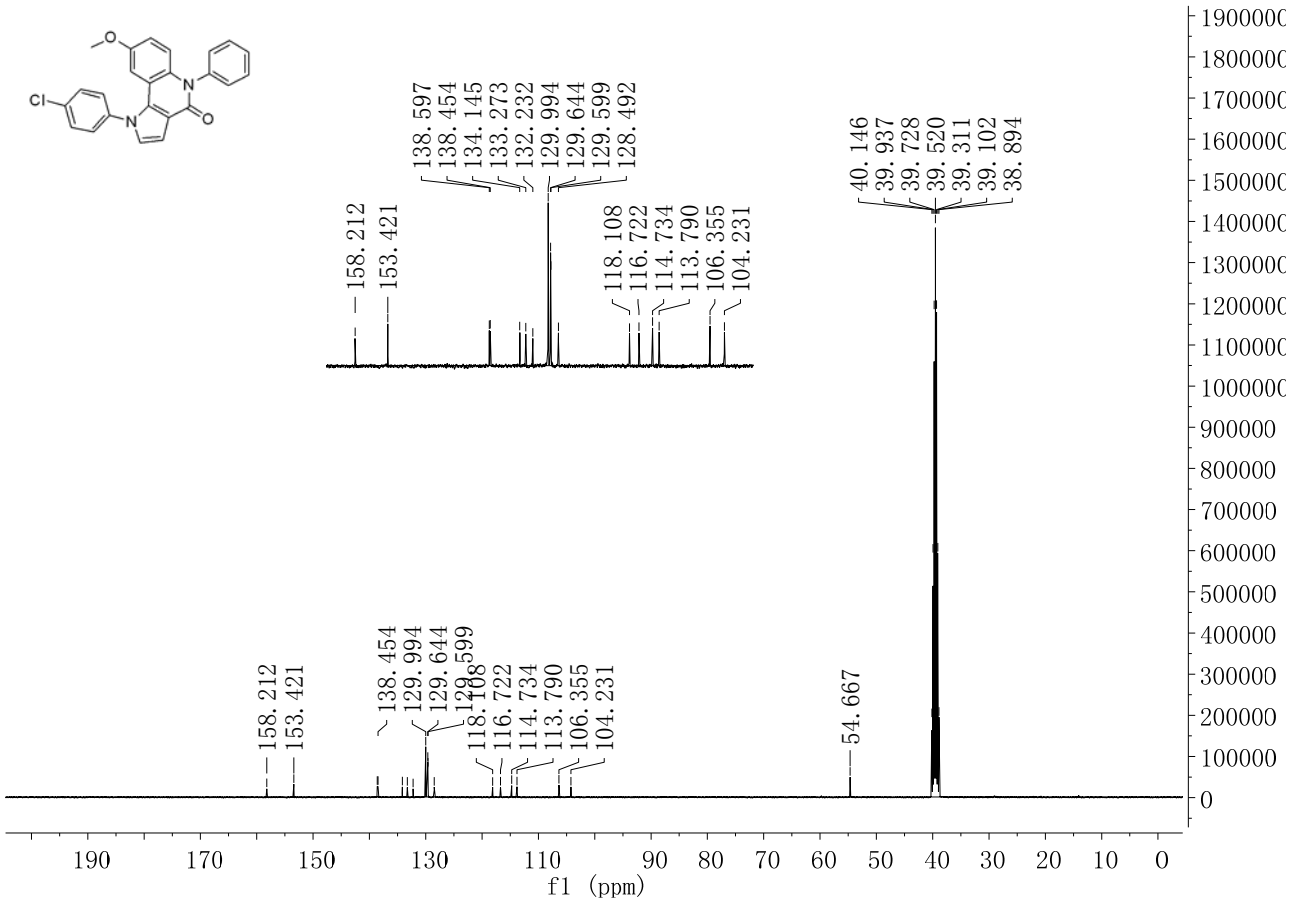
Compound **2q**


OMe
Cl
Cl
N
O
7.752
7.731
7.703
7.682
7.667
7.646
7.384
7.364
7.295
7.290
6.824
6.819
5.978
3.567
3.351
2.500
5.99
2.00
0.99
0.99
0.95
0.99
1.00
3.00
f1 (ppm)

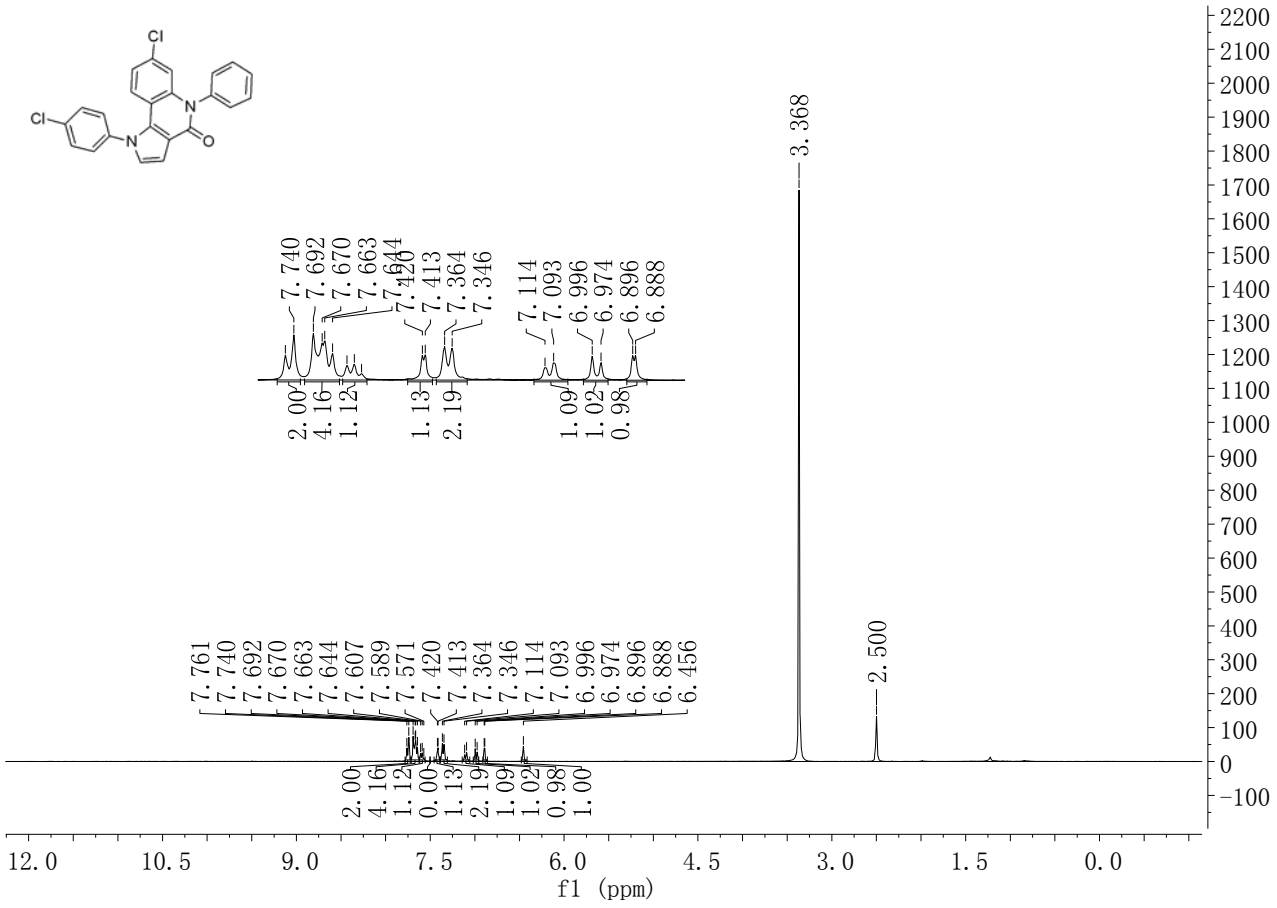

OMe
Cl
Cl
N
O
140.255
138.572
137.347
134.012
133.154
131.520
130.098
129.287
128.796
122.189
158.779
158.339
114.397
108.182
106.159
102.060
39.937
39.798
39.659
39.520
39.381
39.242
39.103
55.182
f1 (ppm)

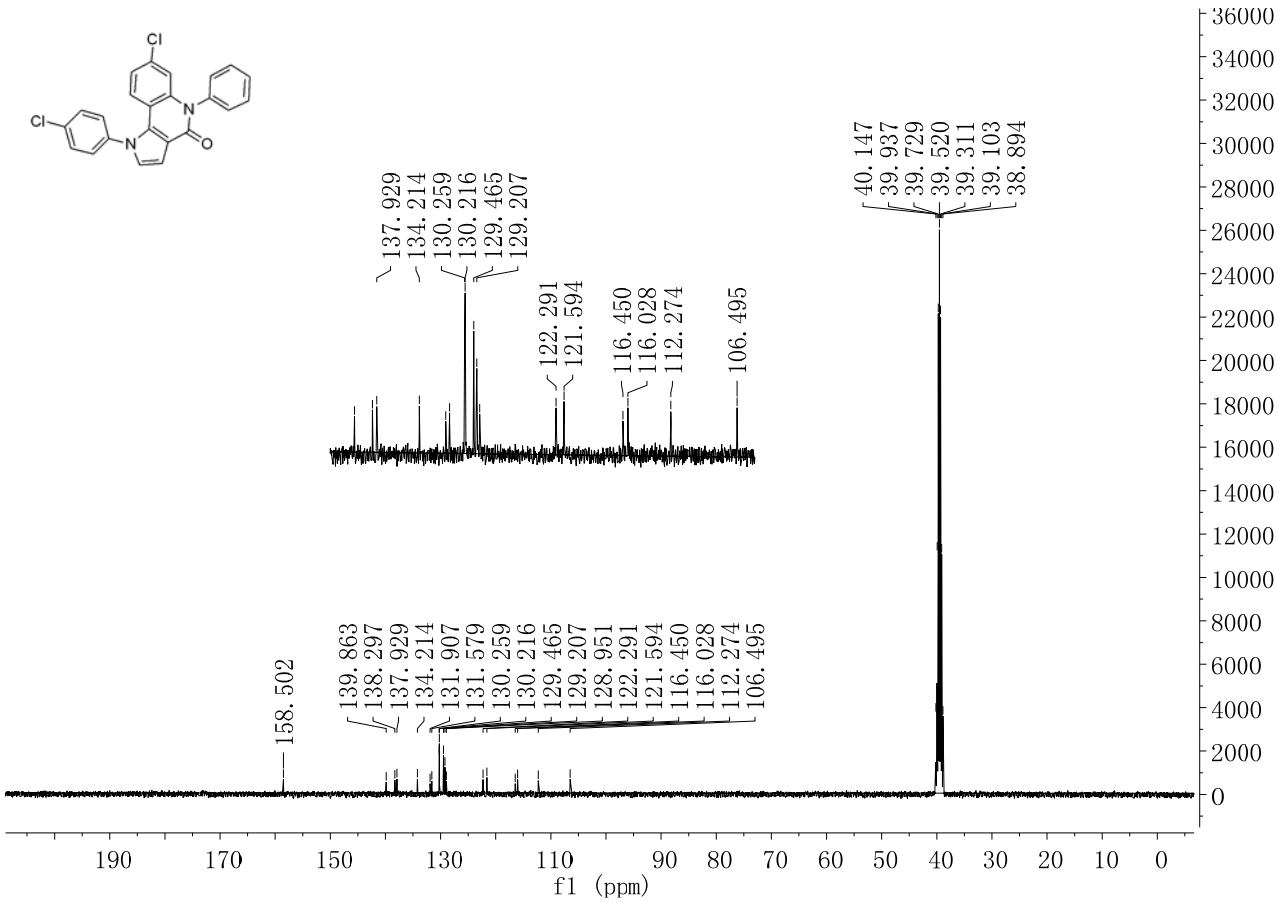
Compound **2r**


7.806
7.782
7.761
7.717
7.695
7.646
7.628
7.609
7.566
7.548
7.530
7.407
7.399
7.310
7.291
6.885
6.878
6.865
6.858
6.478
6.455
6.413
6.406
3.412
3.361
2.500
f1 (ppm)

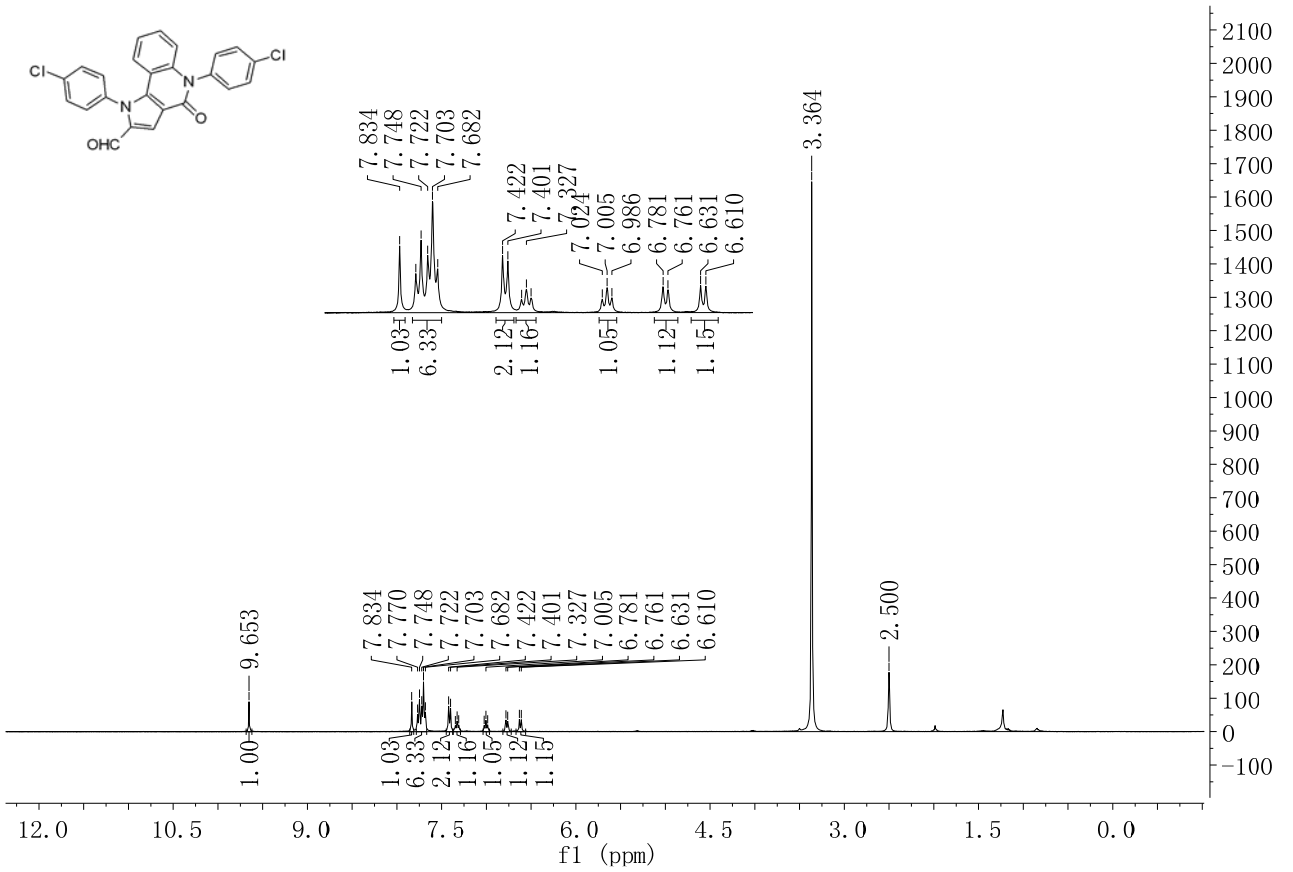

158.212
153.421
138.597
138.454
134.145
133.273
132.232
129.994
129.644
129.599
128.492
118.108
116.722
114.734
113.790
106.355
104.231
40.146
39.937
39.728
39.520
39.311
39.102
38.894
54.667
f1 (ppm)

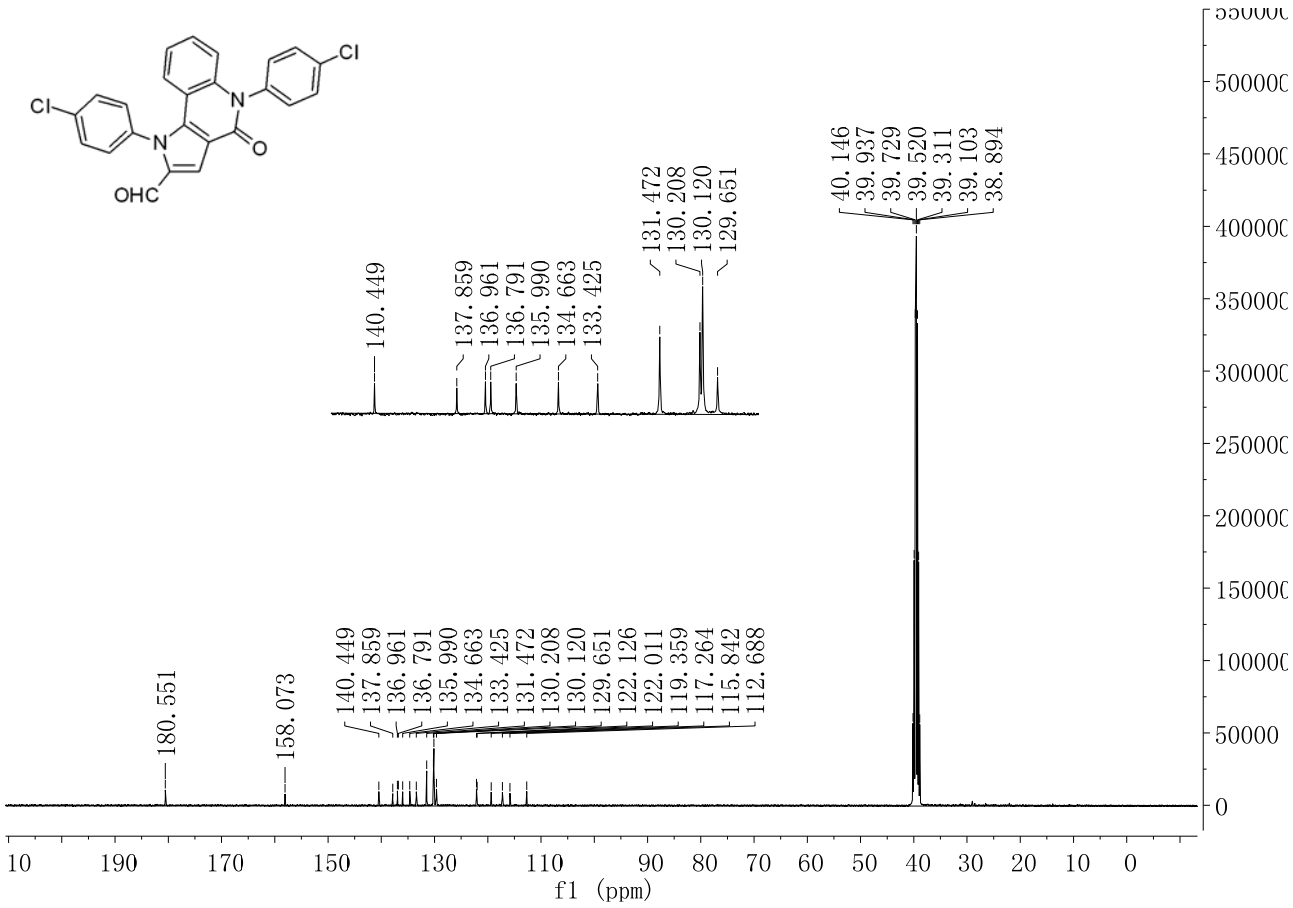
Compound **2t**


Cl
Cl
N
O
7.761
7.740
7.692
7.670
7.663
7.644
7.607
7.589
7.571
7.420
7.413
7.364
7.346
7.114
7.093
6.996
6.974
6.896
6.888
6.456
3.368
2.500
2.00
4.16
1.12
0.00
1.13
2.19
1.09
1.02
0.98
1.00
f1 (ppm)

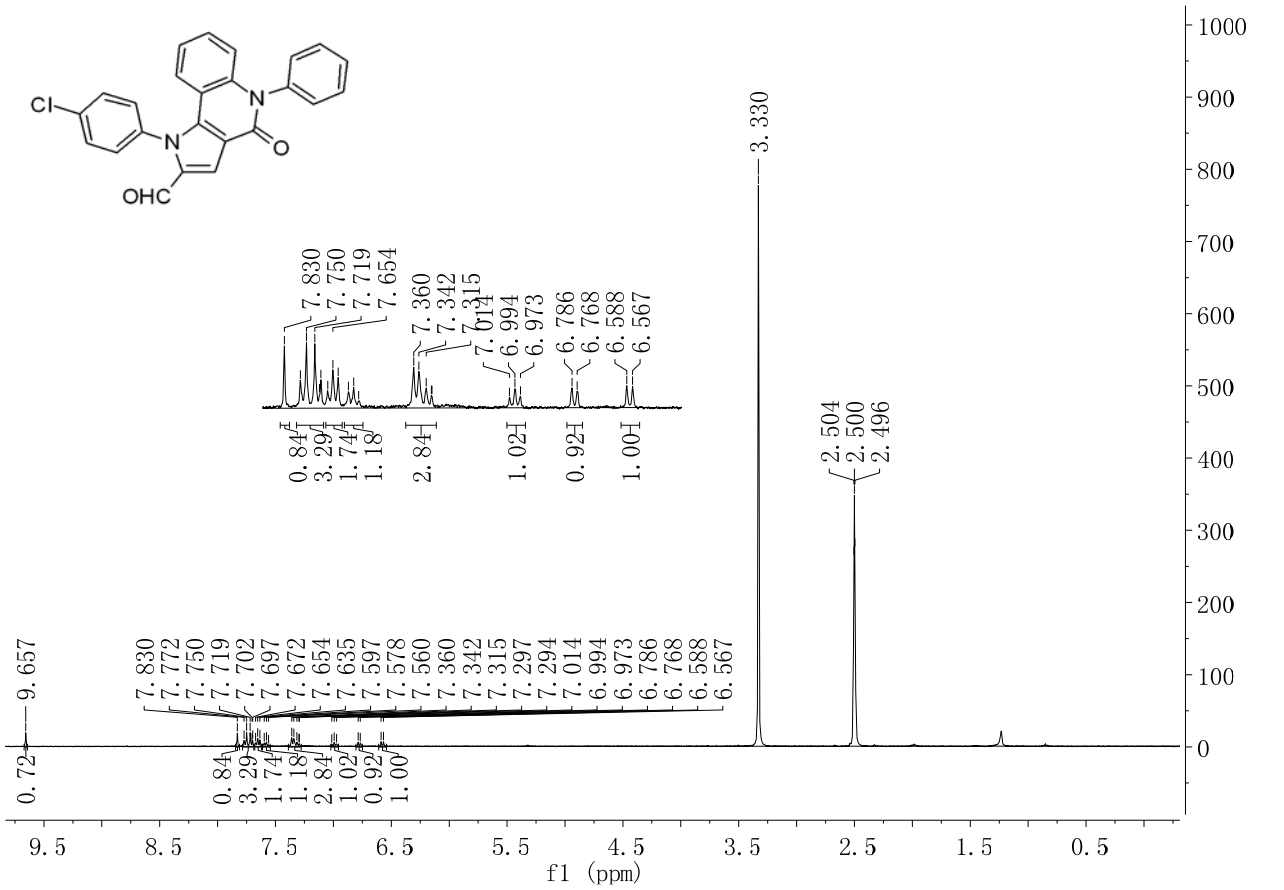

Cl
Cl
N
O
158.502
139.863
138.297
137.929
134.214
131.907
131.579
130.259
130.216
129.465
129.207
128.951
122.291
121.594
116.450
116.028
112.274
106.495
40.147
39.937
39.729
39.520
39.311
39.103
38.894
f1 (ppm)

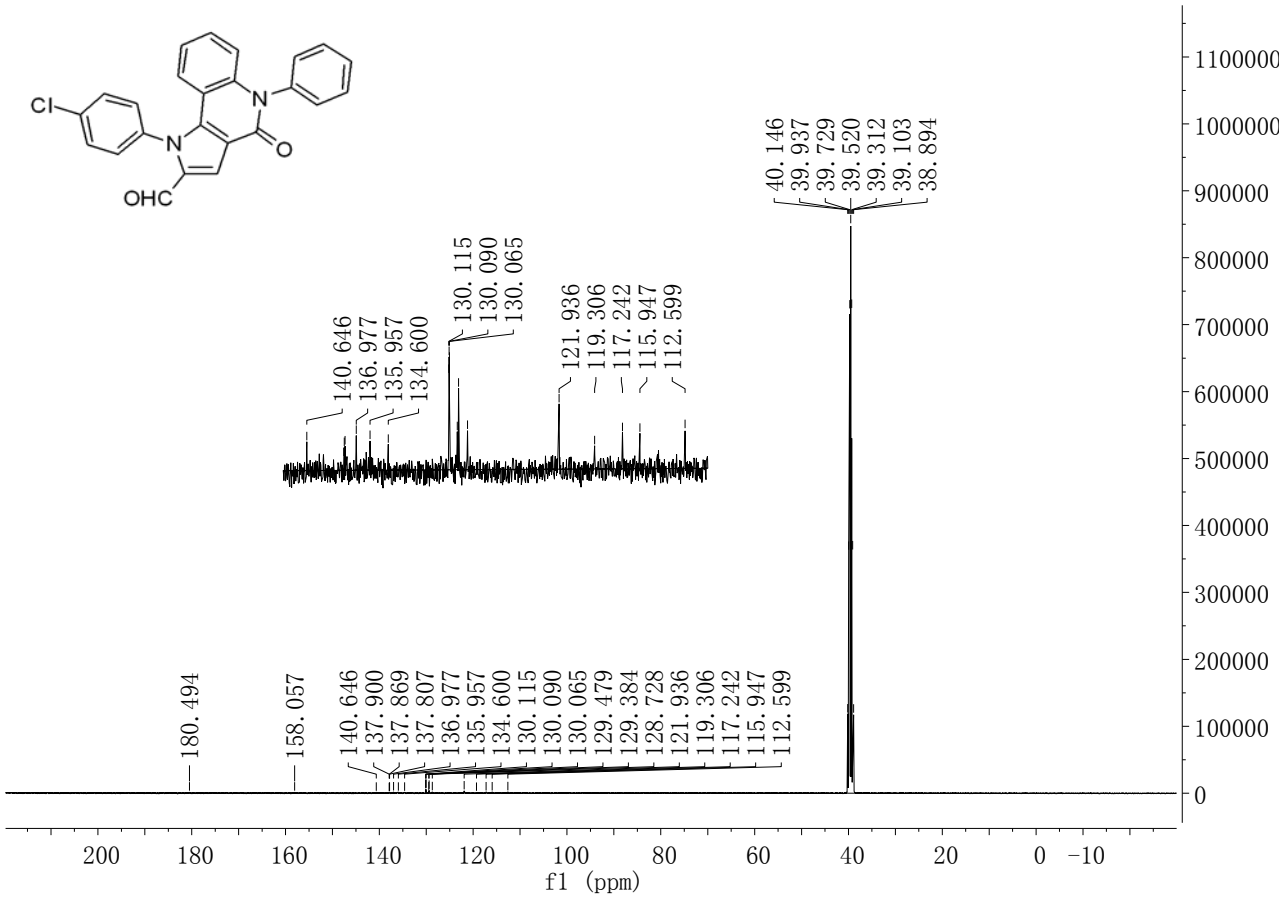
Compound **4a**


Cl
Cl
N
N
O
OHC
7.834
7.748
7.722
7.703
7.682
7.422
7.401
7.327
7.024
7.005
6.986
6.781
6.761
6.631
6.610
3.364
1.03
6.33
2.12
1.16
1.05
1.12
1.15
9.653
7.834
7.770
7.748
7.722
7.703
7.682
7.422
7.401
7.327
7.005
6.781
6.761
6.631
6.610
2.500
1.00
1.03
6.33
2.12
1.16
1.05
1.12
1.15
12.0
10.5
9.0
7.5
6.0
4.5
3.0
1.5
0.0
f1 (ppm)

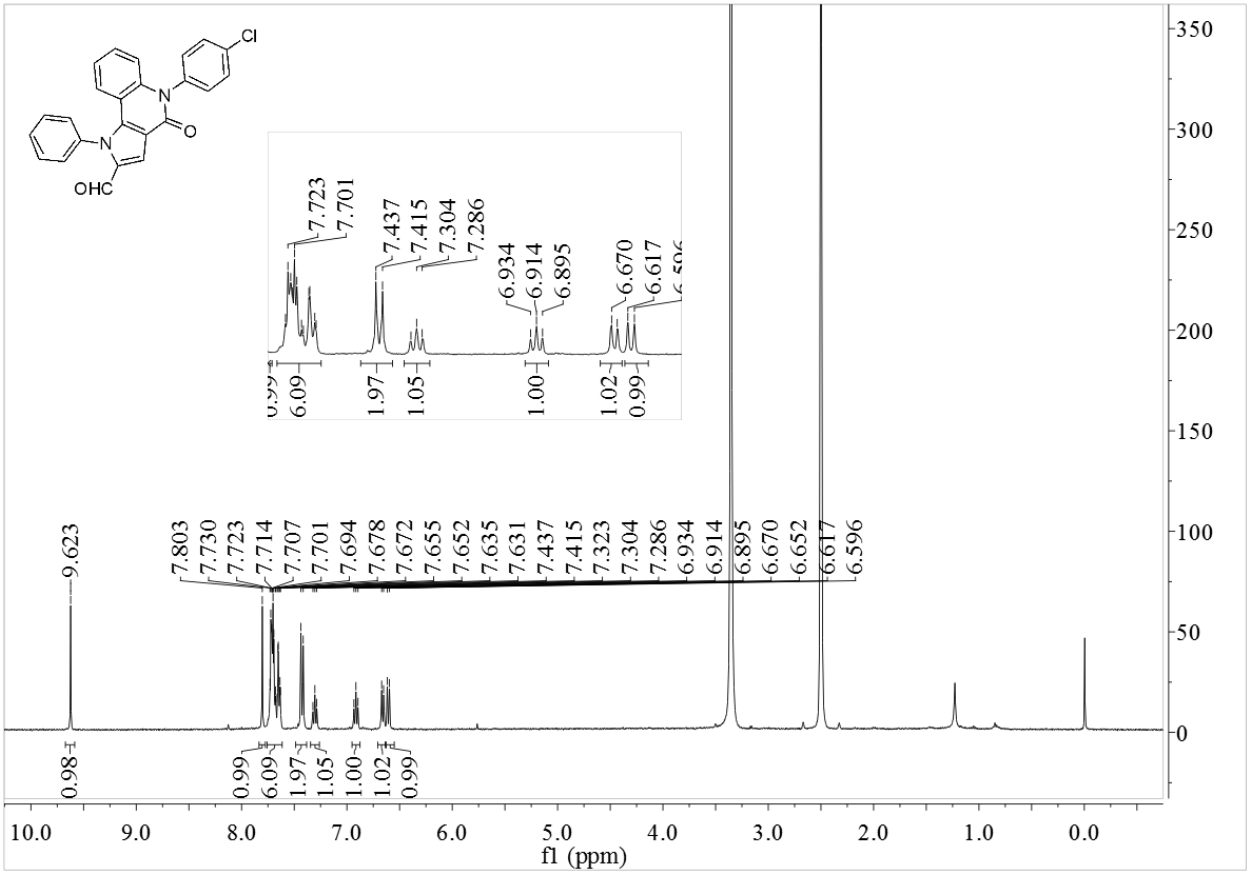

Cl
Cl
N
N
O
OHC
140.449
137.859
136.961
136.791
135.990
134.663
133.425
131.472
130.208
130.120
129.651
40.146
39.937
39.729
39.520
39.311
39.103
38.894
180.551
158.073
140.449
137.859
136.961
136.791
135.990
134.663
133.425
131.472
130.208
130.120
129.651
122.126
122.011
119.359
117.264
115.842
112.688
10
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

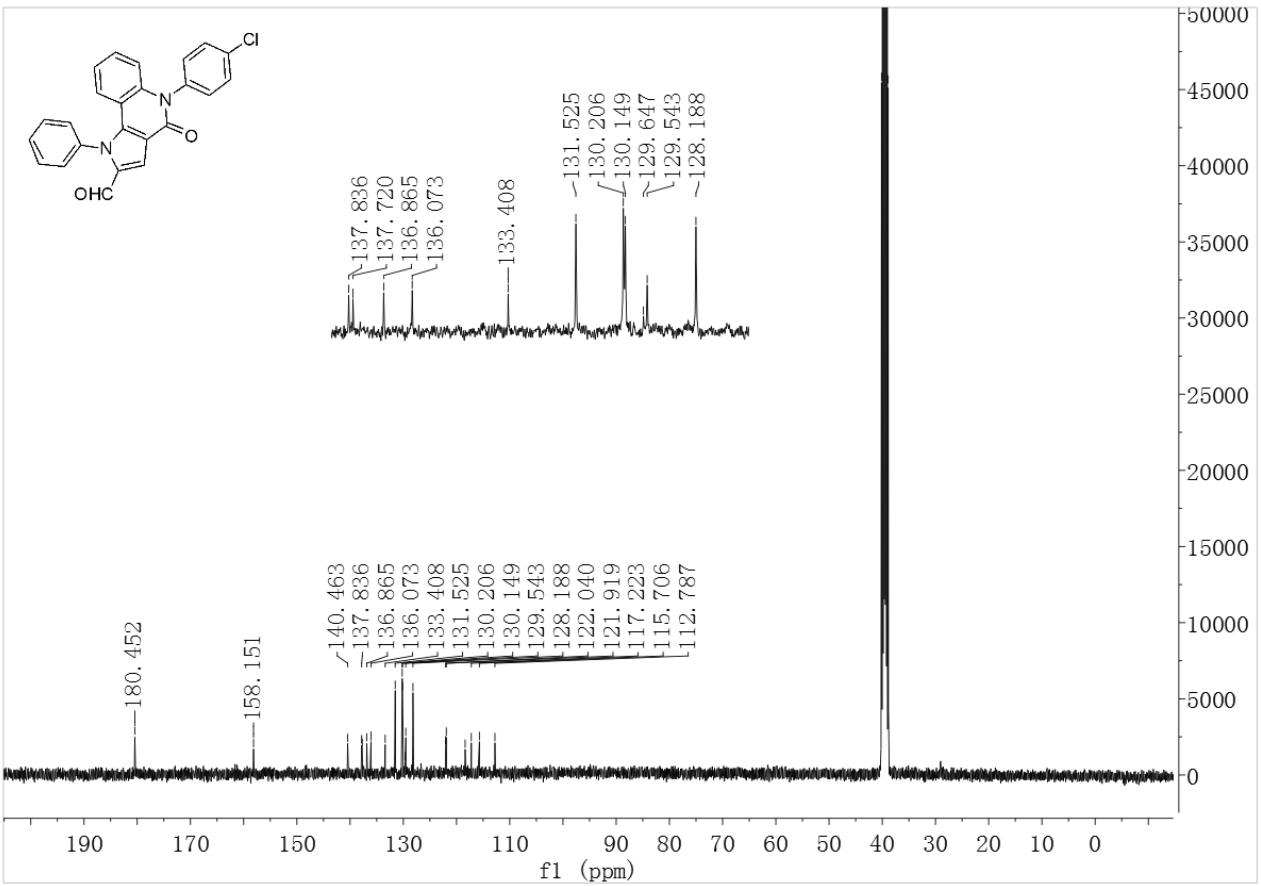
Compound **4e**


Cl
N
O
OHC
9.657
7.830
7.772
7.750
7.719
7.702
7.697
7.672
7.654
7.635
7.597
7.578
7.560
7.360
7.342
7.315
7.297
7.294
7.014
6.994
6.973
6.786
6.768
6.588
6.567
3.330
2.504
2.500
2.496
0.72
0.84
3.29
1.74
1.18
2.84
1.02
0.92
1.00
f1 (ppm)

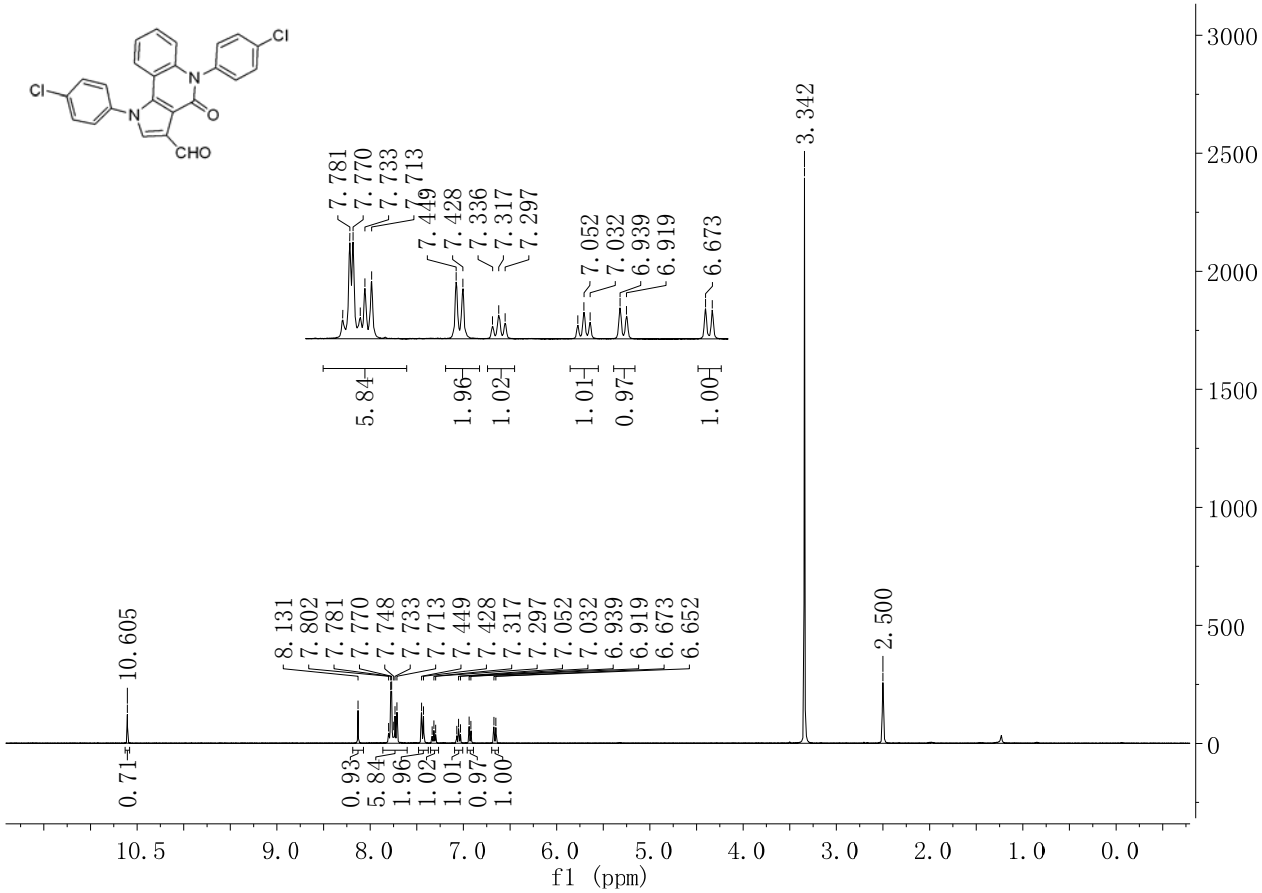

Cl
N
O
OHC
180.494
158.057
140.646
137.900
137.869
137.807
136.977
135.957
134.600
130.115
130.090
130.065
129.479
129.384
128.728
121.936
119.306
117.242
115.947
112.599
40.146
39.937
39.729
39.520
39.312
39.103
38.894
f1 (ppm)

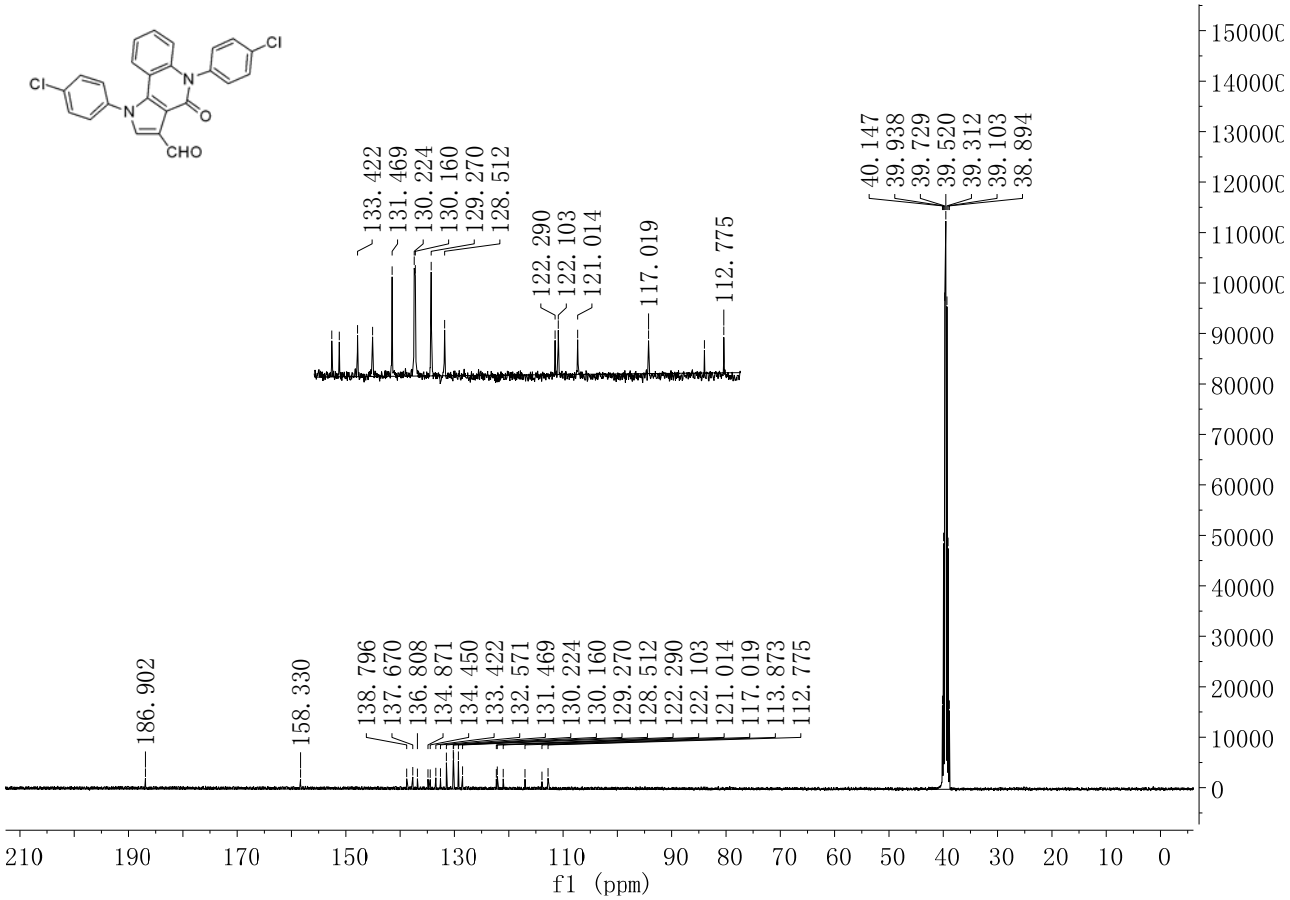
Compound **4l**


Cl
N
O
OHC
9.623
7.803
7.730
7.723
7.714
7.707
7.701
7.694
7.678
7.672
7.655
7.652
7.635
7.631
7.437
7.415
7.323
7.304
7.286
6.934
6.914
6.895
6.670
6.652
6.617
6.596
0.98
0.99
6.09
1.97
1.05
1.00
1.02
0.99
f1 (ppm)


Cl
N
O
OHC
137.836
137.720
136.865
136.073
133.408
131.525
130.206
130.149
129.647
129.543
128.188
180.452
158.151
140.463
137.836
136.865
136.073
133.408
131.525
130.206
130.149
129.543
128.188
122.040
121.919
117.223
115.706
112.787
f1 (ppm)

Compound **4a'**


Cl
Cl
N
O
CHO
7.781
7.770
7.733
7.713
7.449
7.428
7.336
7.317
7.297
7.052
7.032
6.939
6.919
6.673
3.342
2.500
10.605
8.131
7.802
7.781
7.770
7.748
7.733
7.713
7.449
7.428
7.317
7.297
7.052
7.032
6.939
6.919
6.673
6.652
5.84
1.96
1.02
1.01
0.97
1.00
0.71
0.93
f1 (ppm)


Cl
Cl
N
O
CHO
133.422
131.469
130.224
130.160
129.270
128.512
122.290
122.103
121.014
117.019
112.775
40.147
39.938
39.729
39.520
39.312
39.103
38.894
186.902
158.330
138.796
137.670
136.808
134.871
134.450
133.422
132.571
131.469
130.224
130.160
129.270
128.512
122.290
122.103
121.014
117.019
113.873
112.775
f1 (ppm)