Supporting Information

The synthesis of fluorescent benzofuro[2,3-*c*]pyridines via palladium-catalyzed heteroaromatic C−H addition and sequential tandem cyclization

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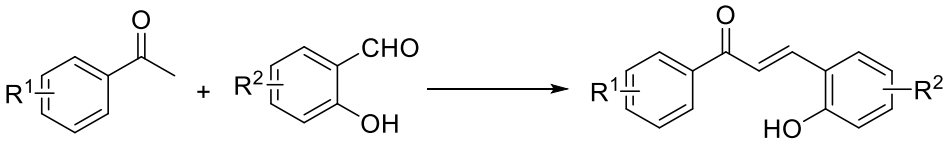
1. General Information

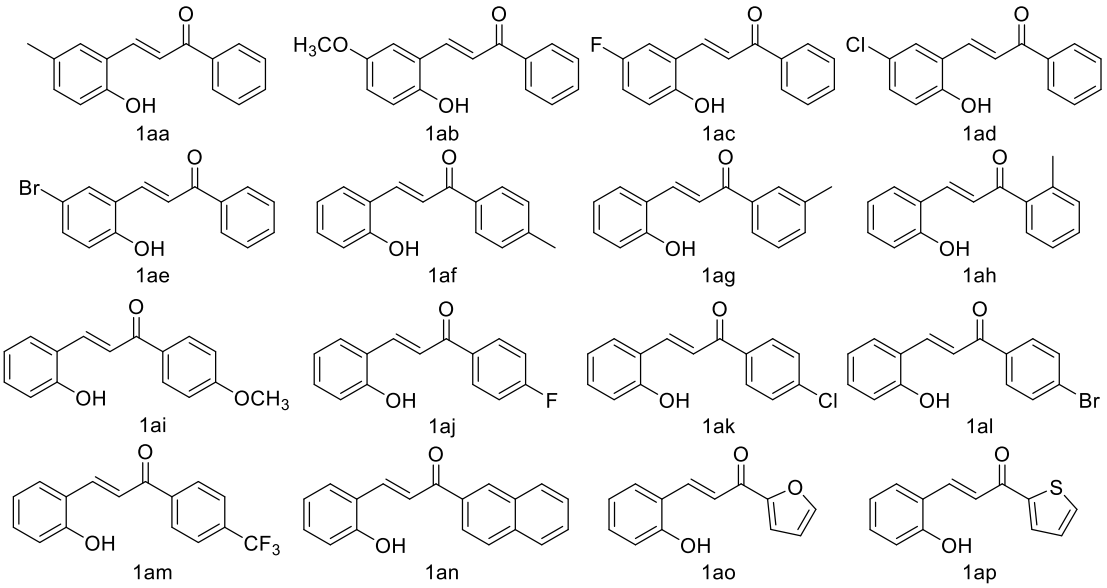
Chemicals were received from commercial sources without further purification or prepared by literature methods. Melting points are uncorrected and recorded on Digital Melting Point Apparatus WRS-1B. ^{1}H NMR and ^{13}C NMR spectra were measured on a 400 or 500 MHz Bruker spectrometer, using $CDCl_3$ as the solvent with tetramethylsilane (TMS) as the internal standard at room temperature. Chemical shifts are given in δ relative to TMS, the coupling constants J are given in Hz. High-resolution mass spectrometry (HRMS) was performed with a TOF MS instrument with an EI or ESI source. X-ray crystallographic analysis was done at the X-ray crystallography facility, Shanghai Institute of Organic Chemistry (SIOC), Chinese Academy of Sciences (CAS).

2. Experimental Section

2.1 General procedure for the synthesis of 1aa–1ap[1]

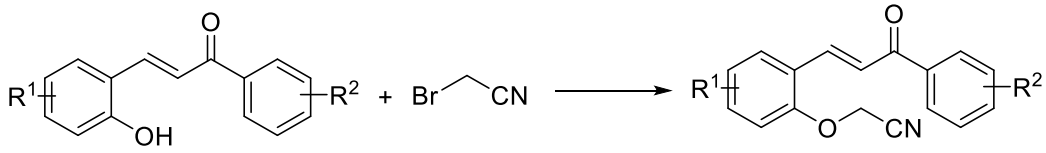


Substituted salicylaldehyde (10 mmol) and acetone or substituted acetophenone (10 mmol) were dissolved in 15 mL MeOH and cooled to 0 ℃. Then, 40% aqueous NaOH (4 mL) was added dropwise to the reaction mixture. After completion of addition, the reaction mixture was allowed to come to room temperature and stirred for overnight. The solvent was evaporated, and 1M aqueous HCl (20 mL) was added to it.The aqueous layer was extracted with EtOAc (3 x 30 mL). The combined organic layers were dried (Na_2SO_4), Evaporation of the solvent gave an solid which was further purified by flash chromatograph on silica gel eluting with the corresponding eluent to give **1aa–1ap** in 82% to 98% yields.

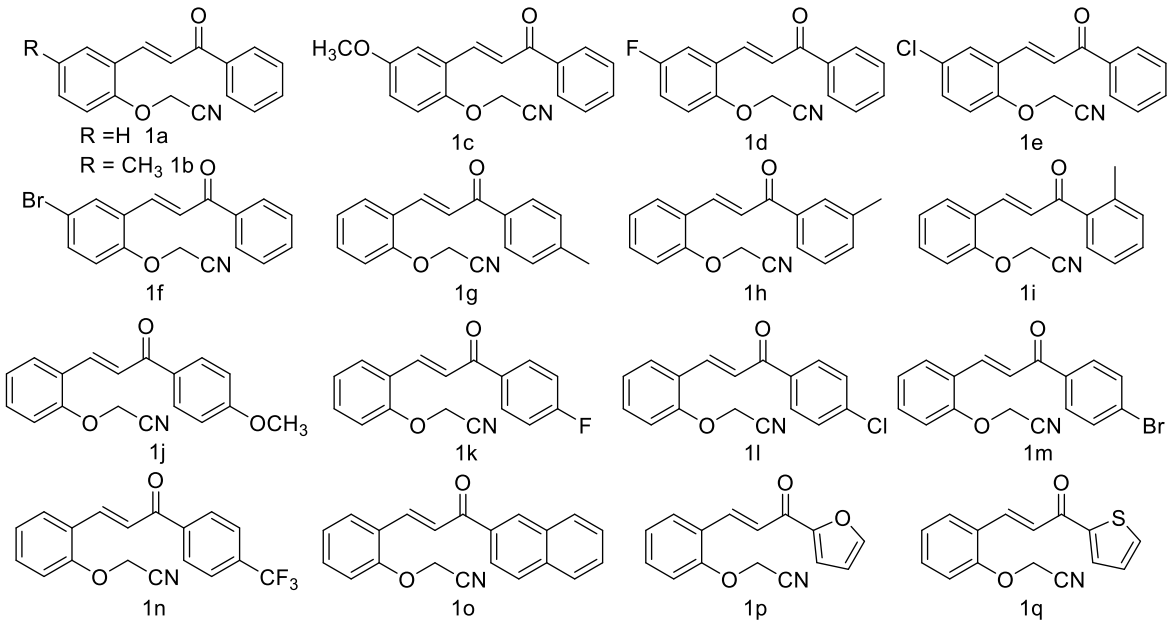


[1] P. Saha, A. Biswas, N. Molleti and V. K. Singh, Enantioselective synthesis of highly substituted chromans via the oxa-Michael-Michael cascade reaction with a bifunctional organocatalyst, *J. Org. Chem.*, 2015, **80**, 11115−11122.

2.2 General procedure for the synthesis of 1a-1q[2]



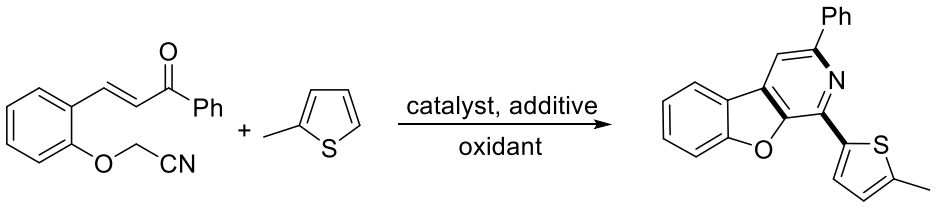
Substituted chalcone (10 mmol) and bromoacetonitrile (1.5 equiv) and K_2CO_3 (2.0 equiv) were dissolved in 15 mL DMF. The resulting reaction mixture was allowed to come to 50 ^oC and stirred for 12h. After the reaction mixture was cooled to room temperature, washed with saturated aq. 1M HCl, and extracted with ethylacetate (3 × 10 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and vaporated under a vacuum. The residue was purified by flash column chromatography with petroleum ether/ethyl acetate (4:1) to afford desired product **1a-1q** in 85% to 97% yields.



[2] K. Shibuya, B. Staels and J. C. Fruchart, Design and synthesis of highly potent and selective human peroxisome proliferator-activated receptor α agonists, *Bioorg. Med. Chem. Lett.*, 2007, **17**, 4689-4693.

2.3 Optimization of reaction conditions

Table S1 Optimization of the reaction conditions[a]

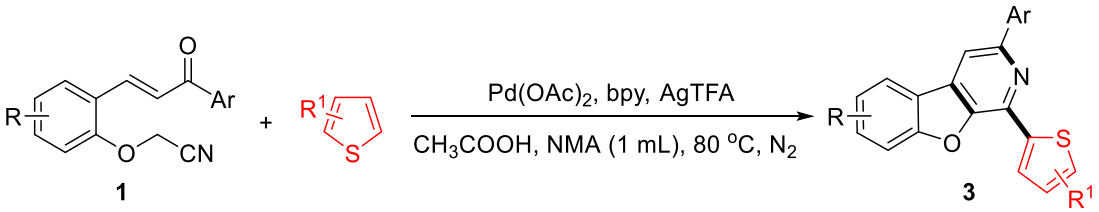


1a **2a** **3a**

Entry	Pd catalyst	Temperature (^{o}C)	Oxidant	Solvent	Yield (%)[b]
1	$Pd(OAc)_2$	80	Ag_2CO_3	DMA	46
2	$Pd(OAc)_2$	80	Ag_2CO_3	DMF	39
3	$Pd(OAc)_2$	80	Ag_2CO_3	THF	25
4	$Pd(OAc)_2$	80	Ag_2CO_3	toluene	10
5	$Pd(OAc)_2$	80	$AgCF_3CO_2$	NMA	72[c]
6	$Pd(OAc)_2$	80	$AgCF_3CO_2$	NMA	63[d]
7	$Pd(OAc)_2$	60	$AgCF_3CO_2$	NMA	56
8	$Pd(OAc)_2$	100	$AgCF_3CO_2$	NMA	84

[a]Conditions: **1a** (0.4 mmol), **2a** (0.2 mmol), Pd catalyst (10 mol %), bpy (20 mol %), CH_3CO_2H (0.8 mmol), oxidant (0.4 mmol), solvent (1 mL), 80 ^{o}C, 48 h, N_2. bIsolated yield. [c]CH_3CO_2H (0.4 mmol). [d]CH_3CO_2H (1.6 mmol).

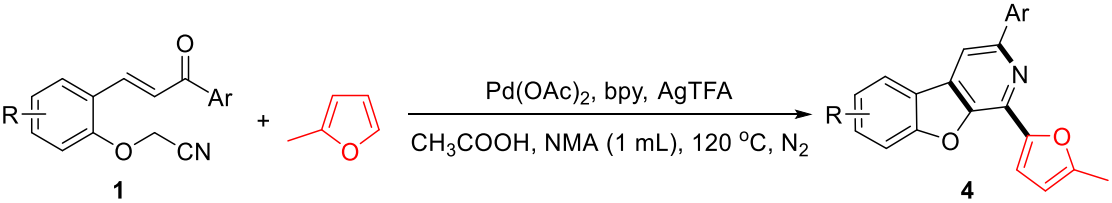
2.4 General procedure for the synthesis of 3



1 3

2-(Cyanomethoxy)chalcones (0.4 mmol, 2 equiv), thiophene (1 equiv), $Pd(OAc)_2$ (10 mmol%), bpy (20 mol%), AgTFA (2 equiv), N-methylacetamide (NMA) (1 mL) and CH_3COOH (0.8 mmol) were successively added to a Schlenk reaction tube. The reaction mixture was stirred vigorously at 80 ℃ for 48 hours. After the reaction mixture was cooled to room temperature, washed with saturated $NaHCO_3$, and extracted with ethylacetate (3 × 8 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and evaporated under a vacuum. The residue was purified by flash column chromatography with petroleum ether/ethyl acetate (20:1) to afford desired product.

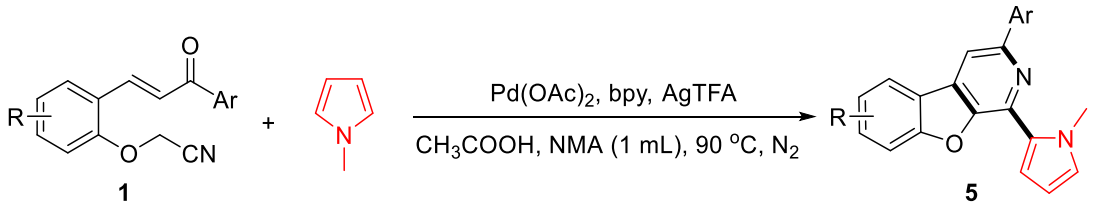
2.5 General procedure for the synthesis of 4



1 4

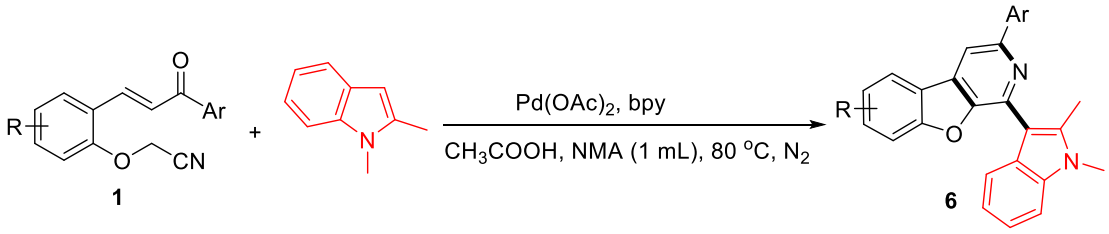
2-(Cyanomethoxy)chalcones (0.4 mmol, 2 equiv), 2-methylfuran (1 equiv), $Pd(OAc)_2$ (10 mmol%), bpy (20 mol%), AgTFA (2 equiv), N-methylacetamide (NMA) (1 mL) and CH_3COOH (0.8 mmol) were successively added to a Schlenk reaction tube. The reaction mixture was stirred vigorously at 120 ℃ for 48 hours. After the reaction mixture was cooled to room temperature, washed with saturated $NaHCO_3$, and extracted with ethylacetate (3 × 8 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and evaporated under a vacuum. The residue was purified by flash column chromatography with petroleum ether/ethyl acetate (20:1) to afford desired product.

2.6 General procedure for the synthesis of 5



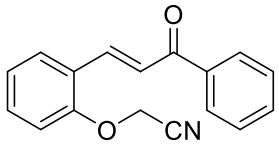
2-(Cyanomethoxy)chalcones (0.4 mmol, 2 equiv), N-methylpyrrole (1 equiv), $Pd(OAc)_2$ (10 mmol%), bpy (20 mol%), AgTFA (2 equiv), N-methylacetamide (NMA) (1 mL) and CH_3COOH (0.8 mmol) were successively added to a Schlenk reaction tube. The reaction mixture was stirred vigorously at 90 ℃ for 48 hours. After the reaction mixture was cooled to room temperature, washed with saturated $NaHCO_3$, and extracted with ethylacetate (3 × 8 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and evaporated under a vacuum. The residue was purified by flash column chromatography with petroleum ether/ethyl acetate (20:1) to afford desired product.

2.7 General procedure for the synthesis of 6

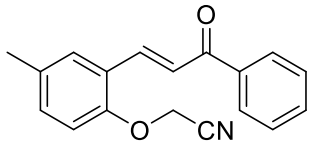


2-(Cyanomethoxy)chalcones (0.2 mmol, 1 equiv), 1,2-dimethylindole (2 equiv), $Pd(OAc)_2$ (10 mmol%), bpy (20 mol%), N-methylacetamide (NMA) (1 mL) and CH_3COOH (0.8 mmol) were successively added to a Schlenk reaction tube. The reaction mixture was stirred vigorously at 80 ℃ for 48 hours. After the reaction mixture was cooled to room temperature, washed with saturated $NaHCO_3$, and extracted with ethylacetate (3 × 8 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and evaporated under a vacuum. The residue was purified by flash column chromatography with petroleum ether/ethyl acetate (6:1) to afford desired product.

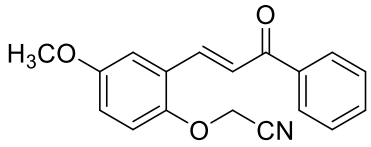
3. Analytical data for reactant



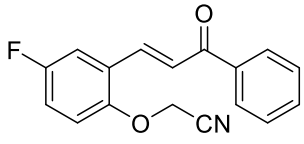
(E)-2-(2-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)acetonitrile ***(1a)***: White solid (2.4985 g, 95%), mp 110-101 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08-8.02 (m, 3H), 7.73-7.71 (m, 1H), 7.61-7.58 (m, 2H), 7.53-7.50 (m, 2H), 7.46-7.43 (m, 1H), 7.17-7.14 (m, 1H), 7.04 (d, J = 8.3 Hz, 1H), 4.88 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 190.6, 155.3, 138.6, 138.2, 132.8, 131.7, 129.2, 128.6, 128.55, 125.1, 124.0, 123.4, 114.7, 112.7, 53.9. HRMS calcd for $C_{17}H_{14}NO_2$ $[M + H]^+$: 264.1019, found 264.1020.



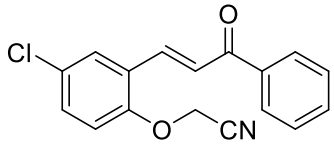
(E)-2-(4-methyl-2-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)acetonitrile ***(1b)****:* White solid (2.5761 g, 93%), mp 90-91 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05-8.02 (m, 3H), 7.60-7.56 (m, 2H), 7.53-7.50 (m, 3H), 7.23 (d, J = 8.2 Hz, 1H), 6.94 (d, J = 8.4 Hz, 1H), 4.84 (s, 2H), 2.36 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 190.6, 153.5, 138.7, 138.2, 132.9, 132.8, 132.3, 129.6, 128.6, 128.5, 124.9, 123.7, 114.8, 112.9, 54.1, 20.5. HRMS calcd for $C_{18}H_{16}NO_2$ $[M + H]^+$: 278.1176, found 278.1190.



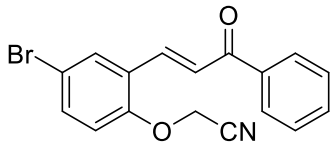
(E)-2-(4-methoxy-2-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)acetonitrile (***1c***): Yellow solid (2.6370 g, 90%), mp 116-117 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03-7.99 (m, 3H), 7.61-7.49 (m, 4H), 7.22 (d, J = 2.9 Hz, 1H), 7.02-6.95 (m, 2H), 4.80 (s, 2H), 3.84 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 190.5, 155.5, 149.7, 138.4, 138.1, 132.8, 128.6, 128.5, 126.3, 124.2, 116.8, 115.2, 119.4, 113.8, 55.8, 55.1. HRMS calcd for $C_{18}H_{16}NO_3$ $[M + H]^+$: 294.1125, found 294.1120.



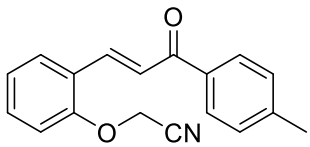
(E)-2-(4-fluoro-2-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)acetonitrile (***1d***): White solid (2.6976 g, 96%), mp 115-116 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03-7.98 (m, 3H), 7.63-7.50 (m, 4H), 7.44-7.41 (m, 1H), 7.16-7.11 (m, 1H), 7.04-7.00 (m, 1H), 4.85 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 190.1, 158.4 (d, J_{C-F} = 241.3 Hz), 151.5, 137.9, 137.1, 133.0, 128.7, 128.6, 127.0 (d, J_{C-F} = 7.5 Hz), 124.8, 118.0 (d, J_{C-F} = 22.5 Hz), 115.0 (d, J_{C-F} = 23.8 Hz), 114.8 (d, J_{C-F} = 8.8 Hz), 114.6, 54.8. HRMS calcd for $C_{17}H_{13}FNO_2$ $[M + H]^+$: 282.0925, found 282.0917.



(E)-2-(4-chloro-2-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)acetonitrile (***1e***): White solid (2.8809 g, 97%), mp 114-115 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03-7.96 (m, 3H), 7.65 (d, J = 8.4 Hz, 1H), 7.62-7.55 (m, 2H), 7.53-7.49 (m, 2H), 7.16-7.13 (m, 1H), 7.02 (d, J = 1.8 Hz, 1H), 4.88 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 190.2, 155.5, 137.9, 137.3, 137.1, 132.9, 130.0, 128.6, 128.5, 124.0, 123.7, 123.6, 114.2, 113.3, 53.9. HRMS calcd for $C_{17}H_{13}ClNO_2$ $[M + H]^+$: 298.0629 and 300.0600, found 298.0643 and 300.0605.

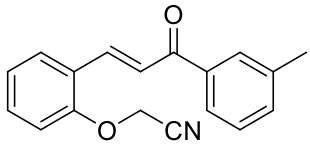


(E)-2-(4-bromo-2-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)acetonitrile (***1f***): White solid (3.2736 g, 96%), mp 113-114 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03-8.01 (m, 2H), 7.97 (d, J = 15.6 Hz, 1H), 7.82 (d, 2.4 Hz, 1H), 7.62-7.49 (m, 5H), 6.92 (d, J = 8.8 Hz, 1H), 4.86 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 190.0, 154.2, 137.8, 136.7, 134.0, 133.0, 131.4, 128.7, 128.5, 127.1, 124.2, 116.0, 114.4, 114.35, 54.0. HRMS calcd for $C_{17}H_{13}BrNO_2$ $[M + H]^+$: 342.0124 and 344.0104 found 342.0130 and 344.0110.

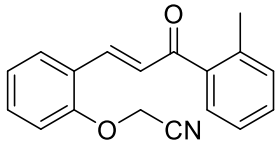


(E)-2-(2-(3-oxo-3-(p-tolyl)prop-1-en-1-yl)phenoxy)acetonitrile (***1g***): White solid

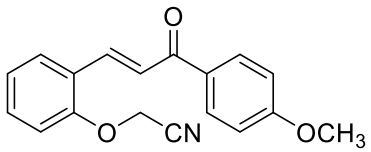
(2.5207 g, 91%), mp 104-105 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, J = 15.9 Hz, 1H), 7.94 (d, J = 8.2 Hz, 2H), 7.73-7.71 (m, 1H), 7.59 (d, J = 15.9 Hz, 1H), 7.45-7.41 (m, 1H), 7.31 (d, J = 7.9 Hz, 2H), 7.17-7.13 (m, 1H), 7.03 (d, J = 8.3 Hz, 1H), 4.88 (s, 2H), 2.44 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 190.1, 152.3, 143.7, 138.1, 135.6, 131.6, 129.3, 129.2, 128.7, 125.2, 124.0, 123.3, 114.7, 112.7, 53.9, 21.6. HRMS calcd for $C_{18}H_{16}NO_2$ $[M + H]^+$: 278.1176, found 278.1175.



(E)-2-(2-(3-oxo-3-(m-tolyl)prop-1-en-1-yl)phenoxy)acetonitrile (***1h***): White solid (2.4653 g, 89%), mp 106-107 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, J = 15.9 Hz, 1H), 7.84-7.81 (m, 2H), 7.74-7.71 (m, 1H), 7.58 (d, J = 15.9 Hz, 1H), 7.46-7.37 (m, 3H), 7.17-7.14 (m, 1H), 7.03 (d, J = 8.3 Hz, 1H), 4.88 (s, 2H), 2.44 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 190.8, 155.3, 138.5, 138.4, 138.2, 133.6, 131.6, 129.2, 129.1, 128.5, 125.7, 125.2, 124.1, 123.3, 114.7, 112.6, 55.9, 21.4. HRMS calcd for $C_{18}H_{16}NO_2$ $[M + H]^+$: 278.1176, found 278.1178.

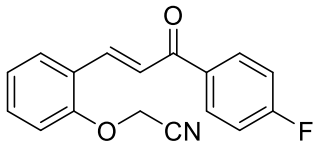


(E)-2-(2-(3-oxo-3-(o-tolyl)prop-1-en-1-yl)phenoxy)acetonitrile (***1i***): White solid (2.3545 g, 85%), mp 73-74 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, J = 16.2 Hz, 1H), 7.66 (d, J = 7.0 Hz, 1H), 7.53-7.51 (m, 1H), 7.45-7.37 (m, 2H), 7.30-7.29 (m, 2H), 7.19 (d, J = 16.4 Hz, 1H), 7.15-7.12 (m, 1H), 7.01 (d, J = 8.3 Hz, 1H), 4.83 (s, 2H), 2.46 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 196.3, 155.1, 139.3, 138.9, 137.1, 131.8, 131.3, 130.5, 129.0, 128.2, 128.16, 125.5, 124.8, 123.3, 114.6, 112.5, 53.7, 20.3. HRMS calcd for $C_{18}H_{16}NO_2$ $[M + H]^+$: 278.1176, found 278.1175.

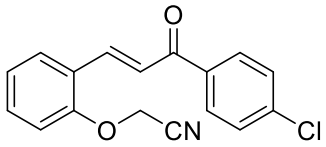


(E)-2-(2-(3-(4-methoxyphenyl)-3-oxoprop-1-en-1-yl)phenoxy)acetonitrile (***1j***): Yellow solid (2.6956 g, 92%), mp 106-107 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05-8.02 (m,

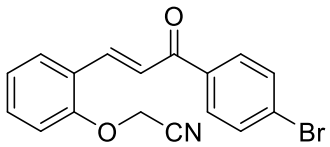
3H), 7.72-7.70 (m, 1H), 7.60 (d, J = 15.8 Hz, 1H), 7.44-7.41 (m, 1H), 7.16-7.13 (m, 1H), 7.03 (d, J = 8.3 Hz, 1H), 6.99 (d, J = 8.8 Hz, 2H), 4.88 (s, 2H), 3.89 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 188.8, 163.5, 155.3, 137.7, 131.5, 131.1, 130.9, 129.2, 125.3, 123.9, 123.3, 114.8, 113.9, 112.7, 55.5, 53.9. HRMS calcd for $C_{18}H_{16}NO_3$ $[M + H]^+$: 294.1125, found 294.1128.



(E)-2-(2-(3-(4-fluorophenyl)-3-oxoprop-1-en-1-yl)phenoxy)acetonitrile (***1k***): White solid (2.5852 g, 92%), mp 117-119 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08-8.04 (m, 3H), 7.72-7.70 (m, 1H), 7.56 (d, J = 15.8 Hz, 1H), 7.46-7.42 (m, 1H), 7.20-7.13 (m, 3H), 7.03 (d, J = 8.3 Hz, 1H), 4.89 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 188.9, 165.6 (d, J_{C-F} = 253.8 Hz), 155.3, 138.8, 134.5, 131.8, 131.1 (d, J_{C-F} = 8.8 Hz), 129.3, 125.0, 123.5, 123.3, 115.7 (d, J_{C-F} = 21.3 Hz), 114.7, 112.6, 53.8. HRMS calcd for $C_{17}H_{13}FNO_2$ $[M + H]^+$: 282.0925, found 282.0936.

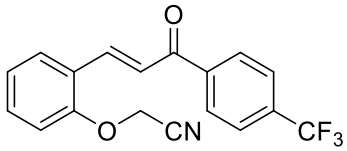


(E)-2-(2-(3-(4-chlorophenyl)-3-oxoprop-1-en-1-yl)phenoxy)acetonitrile (***1l***): White solid (2.7621 g, 93%), mp 122-123 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, J = 15.9 Hz, 1H), 7.96 (d, J = 8.4 Hz, 2H), 7.71 (d, J = 7.6 Hz, 1H), 7.54 (d, J = 15.9 Hz, 1H), 7.49-7.43 (m, 3H), 7.17-7.14 (m, 1H), 7.03 (d, J = 8.3 Hz, 1H), 4.88 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 189.3, 155.4, 139.3, 139.1, 136.5, 131.9, 129.9, 129.5, 129.4, 128.9, 124.9, 123.4, 114.7, 112.6, 53.8. HRMS calcd for $C_{17}H_{13}ClNO_2$ $[M + H]^+$: 298.0629 and 300.0600, found 298.0636 and 300.0598.

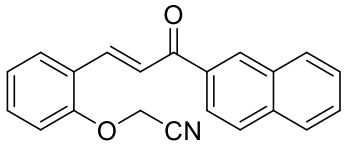


(E)-2-(2-(3-(4-bromophenyl)-3-oxoprop-1-en-1-yl)phenoxy)acetonitrile (***1m***): White solid (3.1713 g, 93%), mp 133-134 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, J = 15.9 Hz, 1H), 7.91-7.87 (m, 2H), 7.72-7.70 (m, 1H), 7.67-7.32 (m, 2H), 7.54 (d, J =

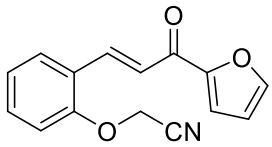
15.9 Hz, 1H), 7.48-7.43 (m, 1H), 7.18-7.14 (m, 1H), 7.03 (d, J = 8.3 Hz, 1H), 4.89 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 189.5, 155.4, 139.2, 136.9, 132.0, 130.1, 129.4, 127.9, 124.9, 123.4, 114.7, 112.6, 53.8. HRMS calcd for $C_{17}H_{13}BrNO_2$ $[M + H]^+$: 342.0124 and 344.0104, found 342.0121 and 344.0106.



(E)-2-(2-(3-oxo-3-(4-(trifluoromethyl)phenyl)prop-1-en-1-yl)phenoxy)acetonitrile (***1n***): White solid (3.2107 g, 97%), mp 122-123 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12-8.07 (m, 3H), 7.78 (d, J = 8.2 Hz, 2H), 7.74-7.71 (m, 1H), 7.56 (d, J = 15.9 Hz, 1H)), 7.49-7.45 (m, 1H), 7.19-7.15 (m, 1H), 7.04 (d, J = 8.3 Hz, 1H), 4.90 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 189.8, 155.5, 141.0, 139.9, 134.1 (d, J_{C-F} = 32.5 Hz), 132.2, 129.5, 128.8, 125.7 (d, J_{C-F} = 3.8 Hz), 124.7, 123.44, 123.7 (d, J_{C-F} = 273.8 Hz), 123.4, 114.6, 112.6, 53.8. HRMS calcd for $C_{18}H_{13}F_3NO_2$ $[M + H]^+$: 332.0893, found 332.0890.

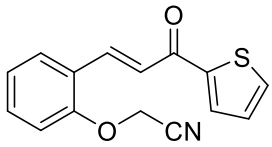


(E)-2-(2-(3-(naphthalen-2-yl)-3-oxoprop-1-en-1-yl)phenoxy)acetonitrile (***1o***): White solid (2.8483 g, 91%), mp 118-119 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.55 (s, 1H), 8.14-8.10 (m, 2H), 8.01 (d, J = 8.0 Hz, 1H), 7.94 (d, J = 8.6 Hz, 1H), 7.91 (d, J = 8.7 Hz, 1H), 7.79-7.75 (m, 2H), 7.63-7.56 (m, 2H), 7.46-7.43 (m, 1H), 7.19-7.16 (m, 1H), 7.03 (d, J = 8.3 Hz, 1H), 4.89 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 190.3, 155.4, 138.5, 135.5, 135.47, 132.6, 131.7, 130.0, 129.6, 129.4, 128.6, 128.4, 127.8, 126.8, 125.2, 124.5, 124.0, 123.3, 114.7, 112.6, 53.9. HRMS calcd for $C_{21}H_{16}NO_2$ $[M + H]^+$: 314.1176, found 314.1189.



(E)-2-(2-(3-(furan-2-yl)-3-oxoprop-1-en-1-yl)phenoxy)acetonitrile (***1p***): White solid (2.2011 g, 87%), mp 119-120 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, J = 16.0 Hz,

1H), 7.72-7.70 (m, 1H), 7.65 (s, 1H), 7.50 (d, J = 15.9 Hz, 1H), 7.45-7.40 (m, 1H), 7.33 (d, J = 3.6 Hz, 1H), 7.15-7.12 (m, 1H), 7.02 (d, J = 8.3 Hz, 1H), 6.60-6.59 (m, 1H), 4.89 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 178.0, 155.4, 153.7, 146.6, 137.7, 131.8, 129.3, 124.9, 123.3, 123.0, 117.6, 114.7, 112.6, 112.5, 53.8. HRMS calcd for $C_{15}H_{12}NO_3$ $[M + H]^+$: 254.0812, found 254.0810.



(E)-2-(2-(3-oxo-3-(thiophen-2-yl)prop-1-en-1-yl)phenoxy)acetonitrile (***1q***): White solid (2.3941 g, 89%), mp 136-137 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.09 (d, J = 15.8 Hz, 1H), 7.88-7.87 (m, 1H), 7.72-7.69 (m, 2H), 7.50 (d, J = 15.8 Hz, 1H), 7.46-7.43 (m, 1H), 7.20-7.15 (m, 2H), 7.04 (d, J = 8.3 Hz, 1H), 4.89 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 182.2, 155.4, 145.5, 138.0, 133.9, 131.9, 131.8, 129.5, 128.3, 125.0, 123.6, 123.4, 114.7, 112.6, 53.9. HRMS calcd for $C_{15}H_{12}NO_2S$ $[M + H]^+$: 270.0583, found 270.0578.

4. Spectroscopic study of 3a

The stock solution of different metal ions was prepared from metal nitrate salts of Hg^{2+}, Ag^{+}, Cu^{+}, Cu^{2+}, Pb^{2+}, Co^{2+}, Ni^{2+}, Zn^{2+}, Cd^{2+}, Mn^{2+}, Fe^{2+}, Fe^{3+}, Al^{3+} in acetonitrile. All spectroscopic study of **3a** was carried out in test solution of **3a** (10 μM) in 3 mL CH_3CN. The UV-vis and fluorescent titration of **3a** with Hg^{2+} was carried out by adding Hg^{2+} into the test solution of **3a**, and the total concentration of Hg^{2+} ranged from 0 to 15 μM. The UV-vis and fluorescence spectra were recorded 10s after each addition at ambient temperature. The fluorescence spectra were recorded by excitation wavelength of 340 nm with 5 nm slit widths for both excitation and emission. The sensing behavior was investigated by calculating the emission ratio F457/F398 based on the recorded spectra.

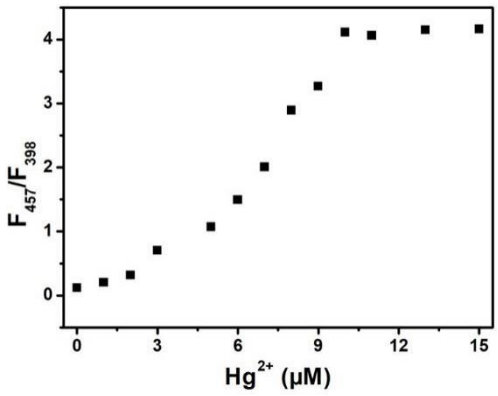


Figure S1 Emission ratio F457/F398 of 3a (10 μM) recorded upon titration with Hg^{2+} from 0 to 15 μM in CH_3CN.

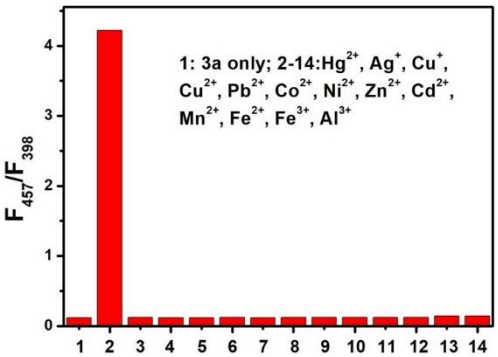


Figure S2 Emission ratio F457/F398 of **3a** (10 μM) in CH_3CN in the presence of different analytes (10 μM).

Table S2. Absorptions (λ_{abs}) and emissions (λ_{em}) data in CH_3CN.

Sample	λ_{abs} (nm)	λ_{em} (nm)	Sample	λ_{abs} (nm)	λ_{em} (nm)	Sample	λ_{abs} (nm)	λ_{em} (nm)
3a	351	398	**4a**	354	402	**5k**	359	417
3b	346	391	**4b**	352	404	**5l**	355	418
3c	354	408	**4c**	349	400	**5m**	355	419
3d	364	427	**4d**	343	417	**5n**	354	415
3e	363	434	**4e**	361	396	**5o**	353	405
3f	362	423	**4f**	351	428	**6a**	350	442
3g	365	432	**4g**	349	403	**6b**	353	447
3h	341	395	**4h**	357	399	**6c**	352	450
3i	348	429	**4i**	349	398	**6d**	348	461
3j	380	447	**4j**	352	404	**6e**	356	442
3k	356	402	**4k**	359	437	**6f**	353	446
3l	353	405	**4l**	355	410	**6g**	353	448
3m	345	397	**4m**	339	384	**6h**	360	467
3n	359	398	**4n**	349	405	**6i**	352	444
3o	353	397	**4o**	355	415	**6j**	356	449
3p	353	415	**4p**	357	408	**6k**	362	443
3q	353	402	**5a**	352	418	**6l**	356	442
3r	349	399	**5b**	357	413	**6m**	355	444
3s	361	405	**5c**	355	418	**6n**	355	447
3t	361	418	**5d**	347	426	**6o**	361	465
3u	360	413	**5e**	359	441	**6p**	360	462
3v	352	401	**5f**	359	430	**6q**	359	462
3w	356	405	**5g**	355	425			
3x	357	409	**5h**	353	418			
3y	356	409	**5i**	357	416			
3z	358	417	**5j**	361	425			

Table S3. Fluorescence quantum yield ($\mathbf{\Phi_F}$) in CH_3CN at 10 μM determined with an integrating sphere system.

Sample	**3a**	**3b**	**3n**	**3o**	**4e**	**4i**	**5a**	**5h**	**6a**	**6e**
$\mathbf{\Phi_F}$	0.43	0.42	0.26	0.55	0.61	0.78	0.93	0.95	0.90	0.94

Table **S4** A comparison of 3a with some other fluorescent chemosensors for Hg^{2+}.

Probe	Selectivity	Measurement	Enhancement	Reference
Coumarin based	Hg^{2+}	Turn-on	~50 fold	18a
Rhodamine based	Hg^{2+}	Turn-on	26 fold	18b
Coumarin based	Hg^{2+},Cu^{2+}	Turn-on	9 fold	18c
Julolidine based	Hg^{2+}, Mn^{2+}	Turn-off	~10 fold	17
Schiff base	Hg^{2+}	Ratiometric	3 fold	18d
Tetraphenylethene based	Hg^{2+}	Ratiometric	~2 fold	18e
Benzofuro[2,3-c]pyridine based	Hg^{2+}	Ratiometric	34 fold	this work

5. NMR Spectra for reactant

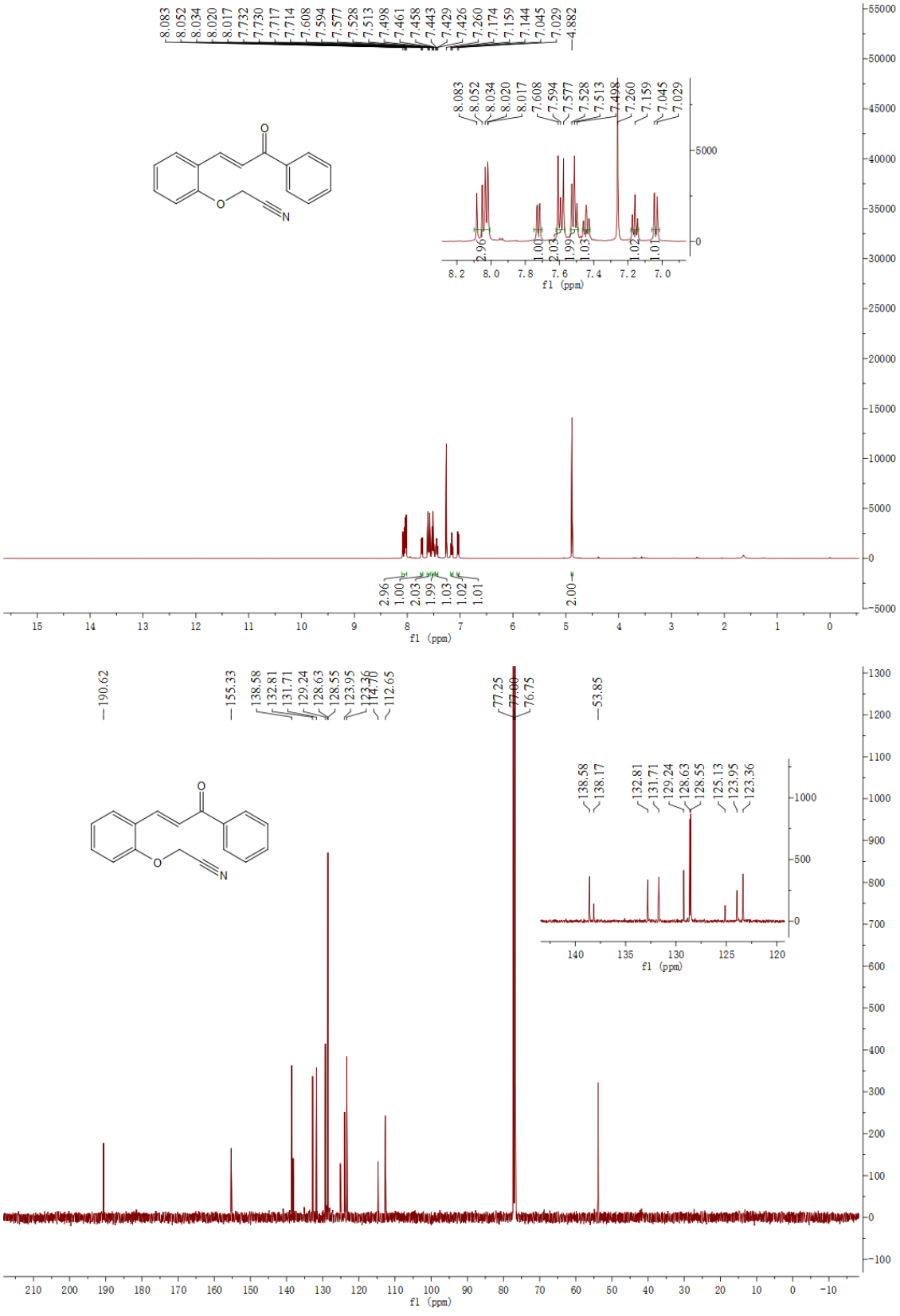


Figure S3. ^{1}H NMR of **1a** (500 MHz, $CDCl_3$) and ^{13}C NMR of **1a** (125 MHz, $CDCl_3$)

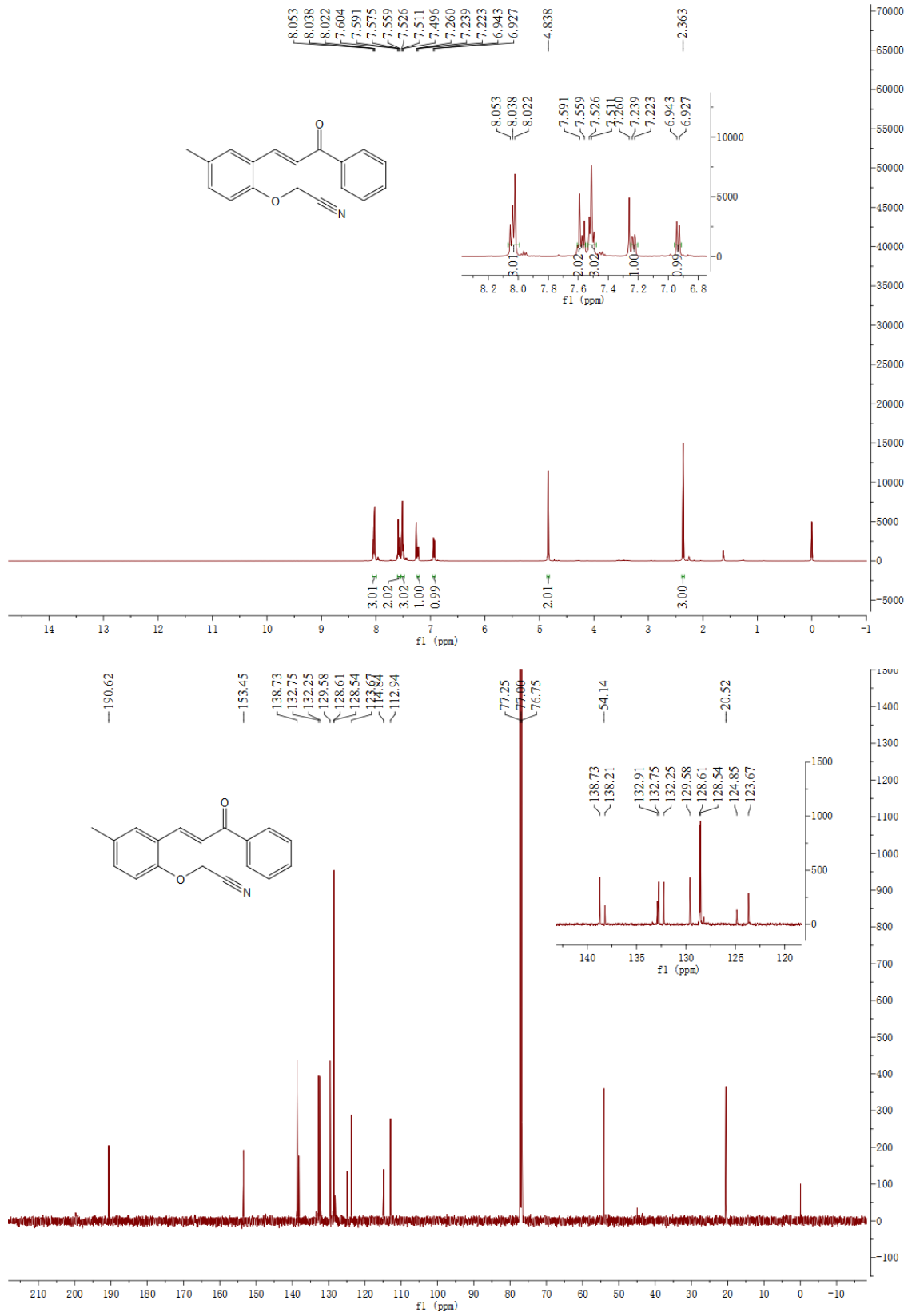


Figure S4. ^{1}H NMR of **1b** (500 MHz, $CDCl_3$) and ^{13}C NMR of **1b** (125 MHz, $CDCl_3$)

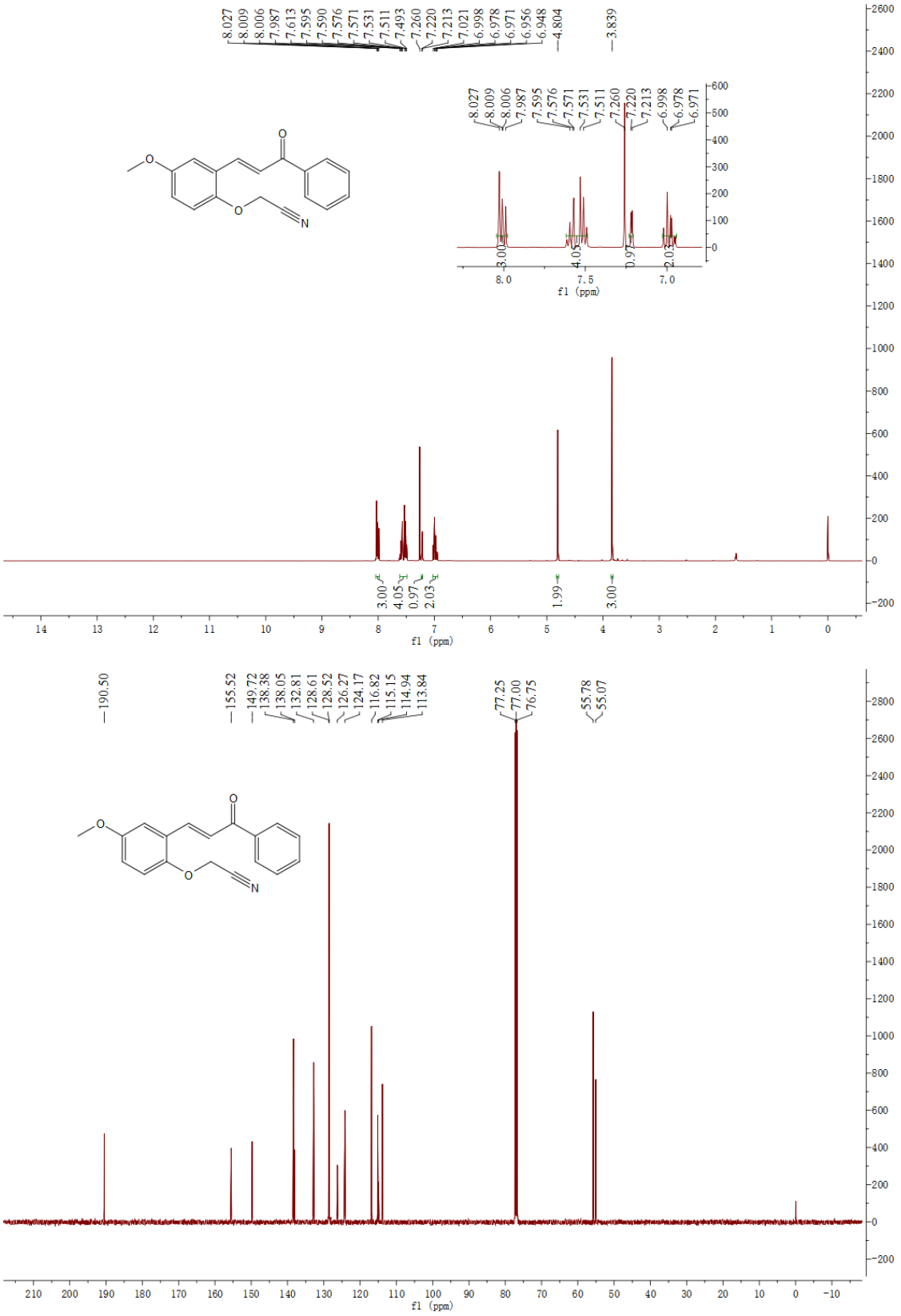


Figure S5. ^{1}H NMR of **1c** (400 MHz, $CDCl_3$) and ^{13}C NMR of **1c** (125 MHz, $CDCl_3$)

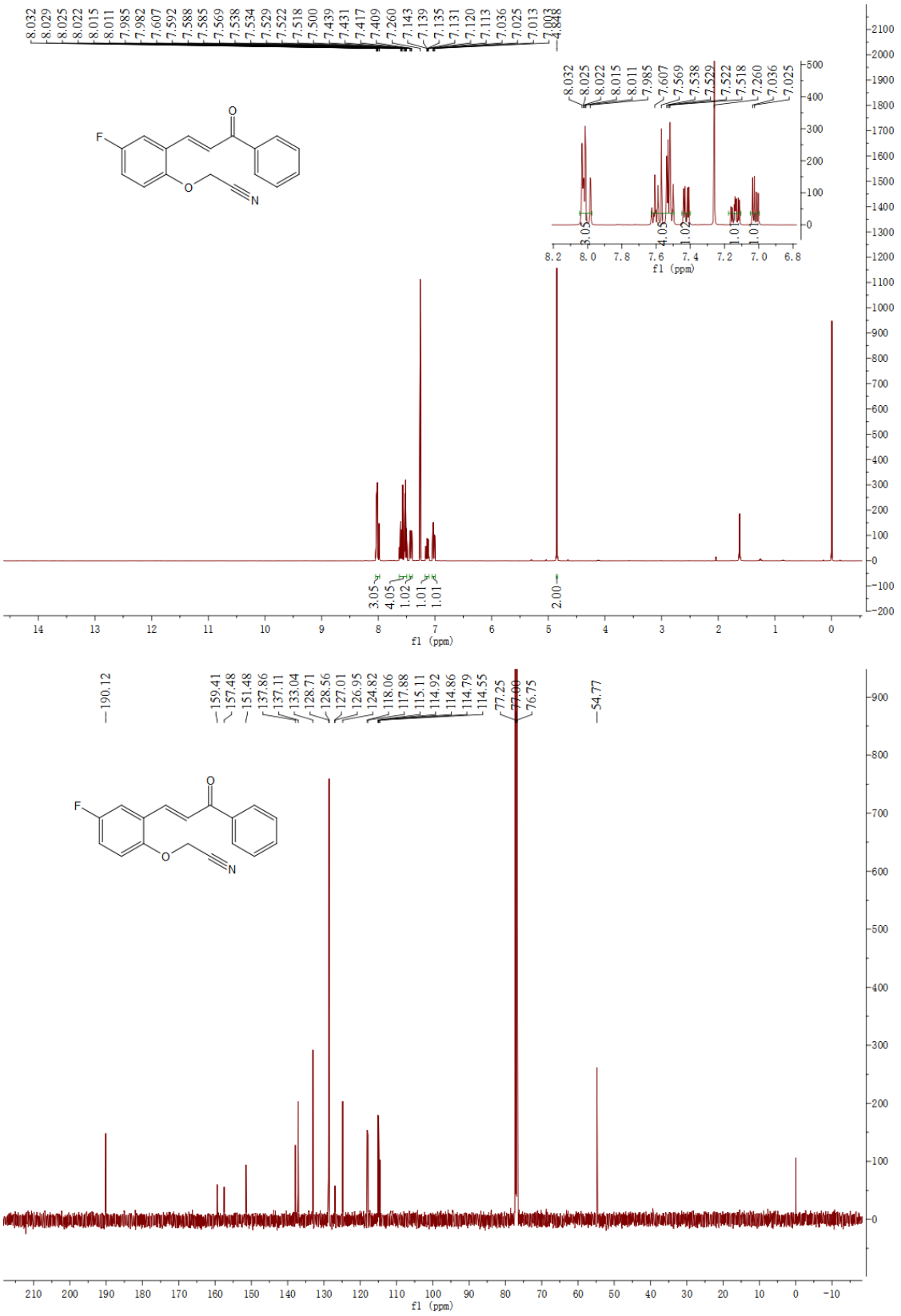


Figure S6. ^{1}H NMR of **1d** (400 MHz, $CDCl_3$) and ^{13}C NMR of **1d** (125 MHz, $CDCl_3$)

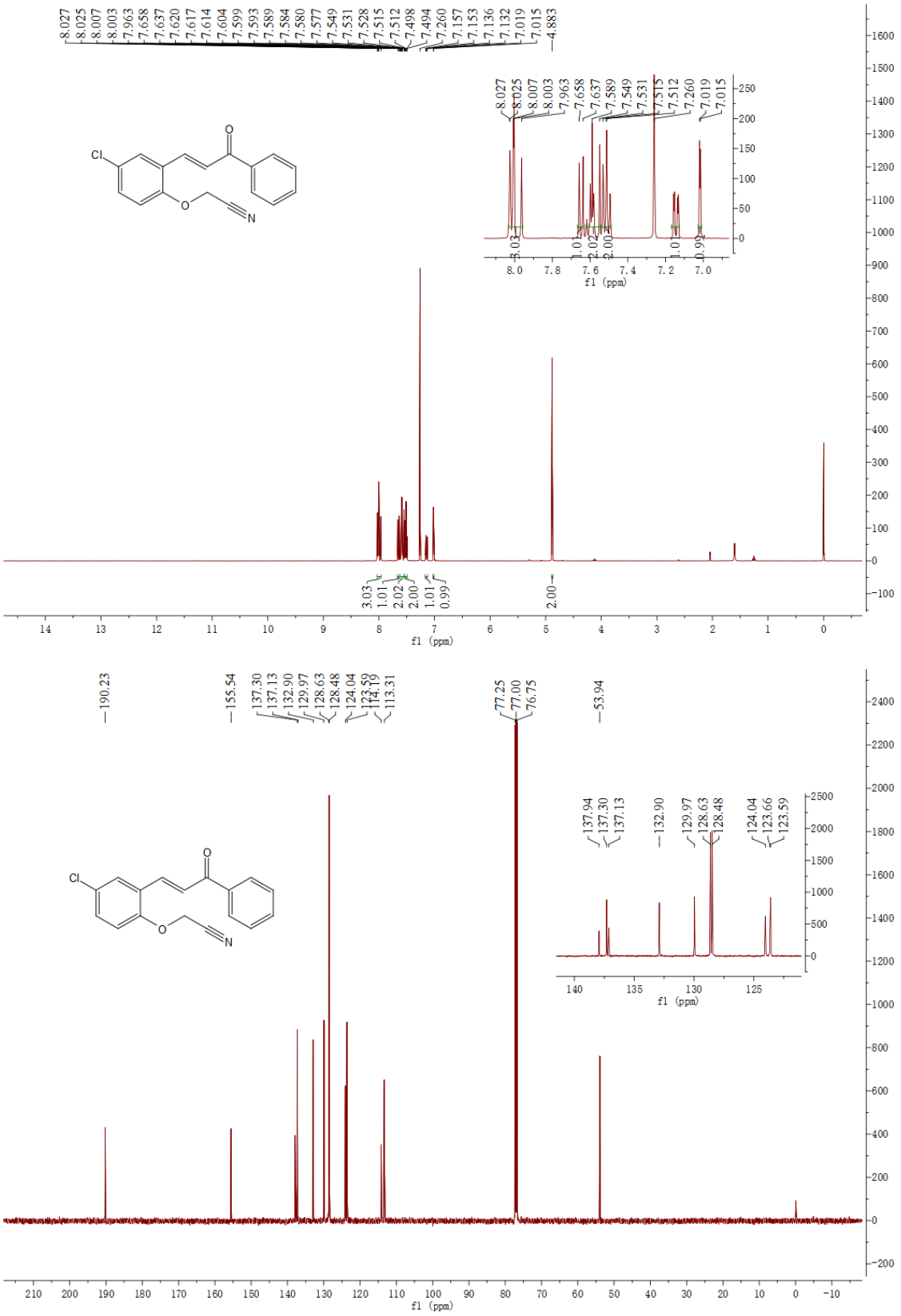


Figure S7. ^{1}H NMR of **1e** (400 MHz, $CDCl_3$) and ^{13}C NMR of **1e** (125 MHz, $CDCl_3$)

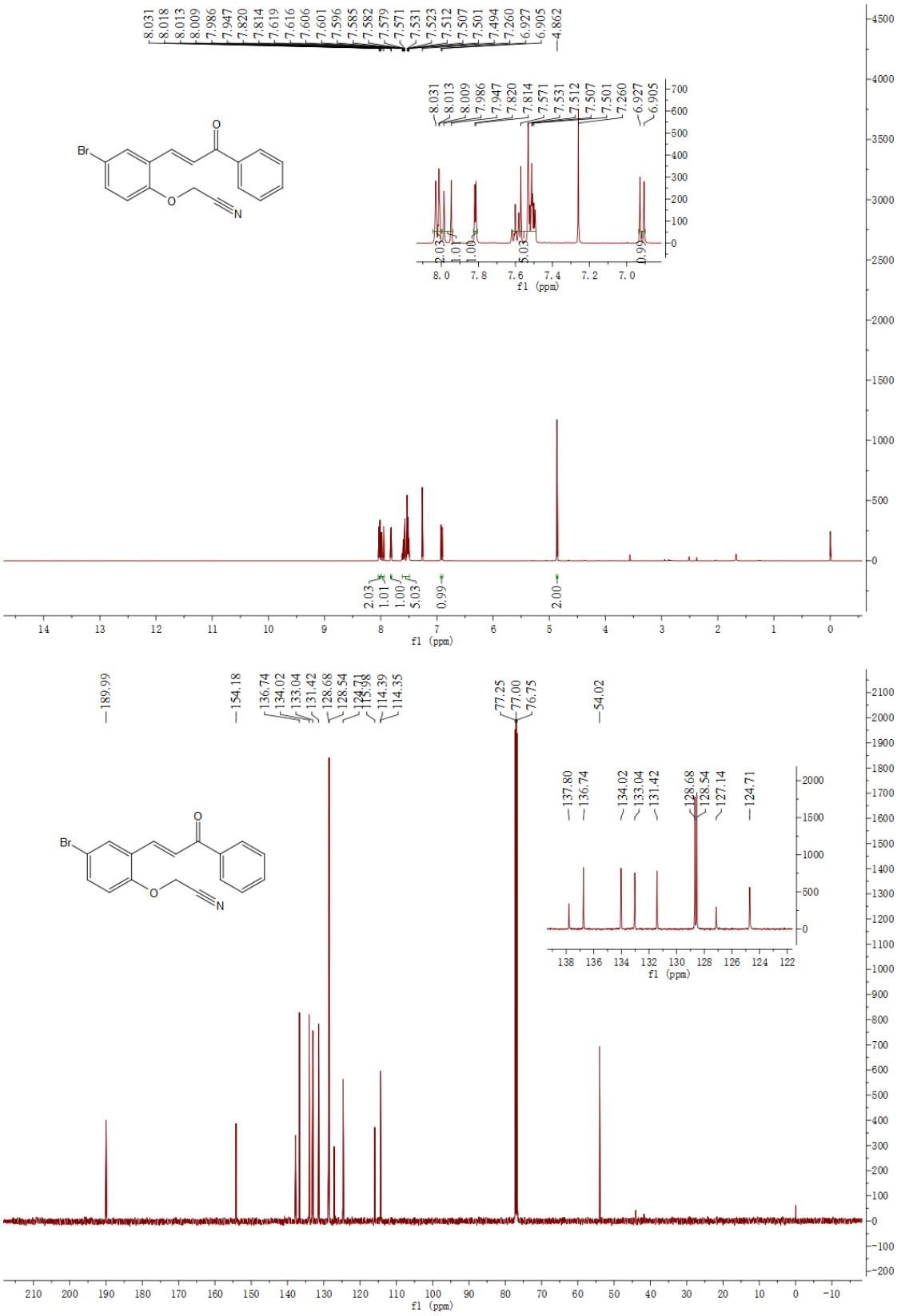


Figure S8. ^{1}H NMR of **1f** (400 MHz, $CDCl_3$) and ^{13}C NMR of **1f** (125 MHz, $CDCl_3$)

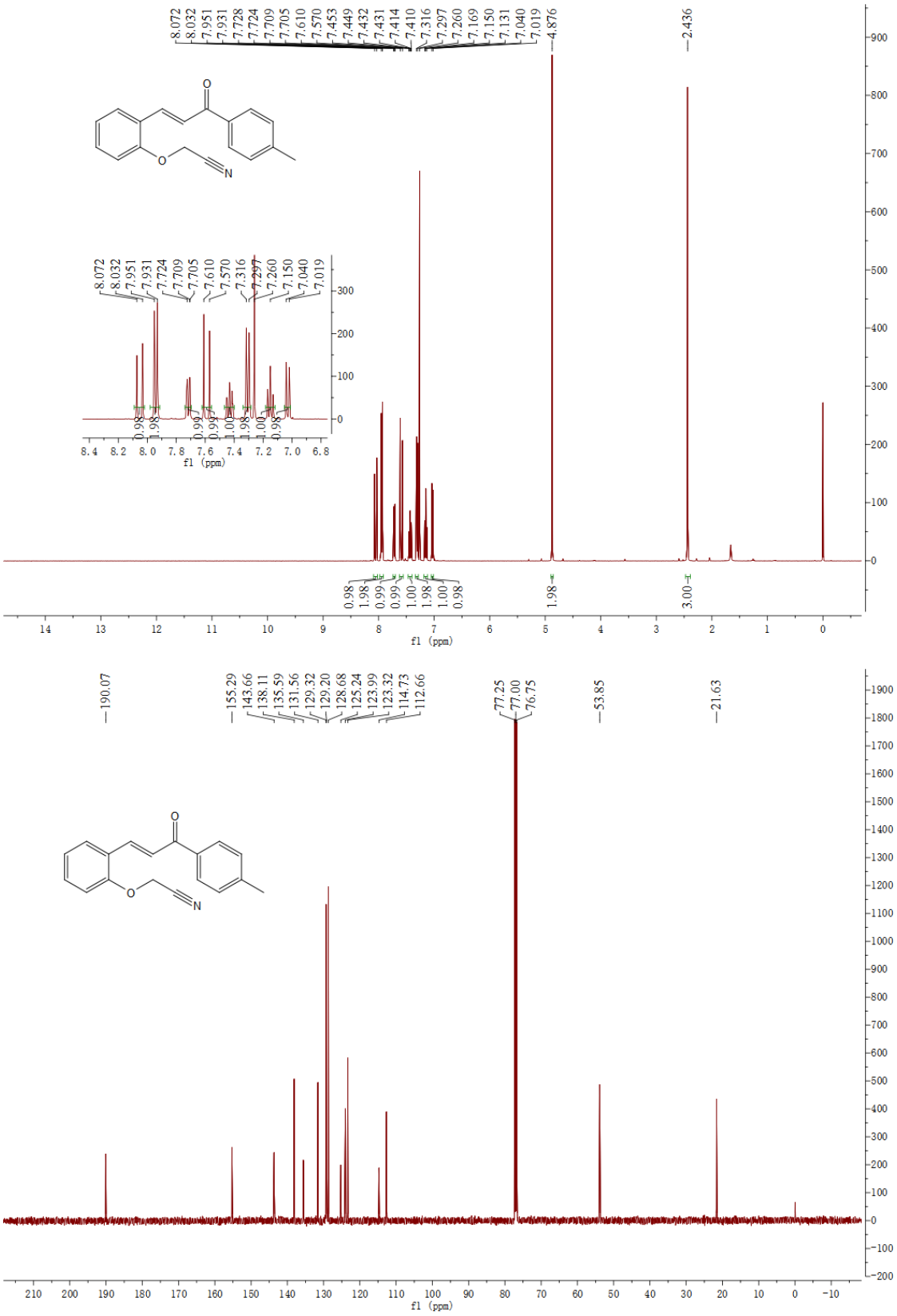


Figure S9. ^{1}H NMR of **1g** (400 MHz, $CDCl_3$) and ^{13}C NMR of **1g** (125 MHz, $CDCl_3$)

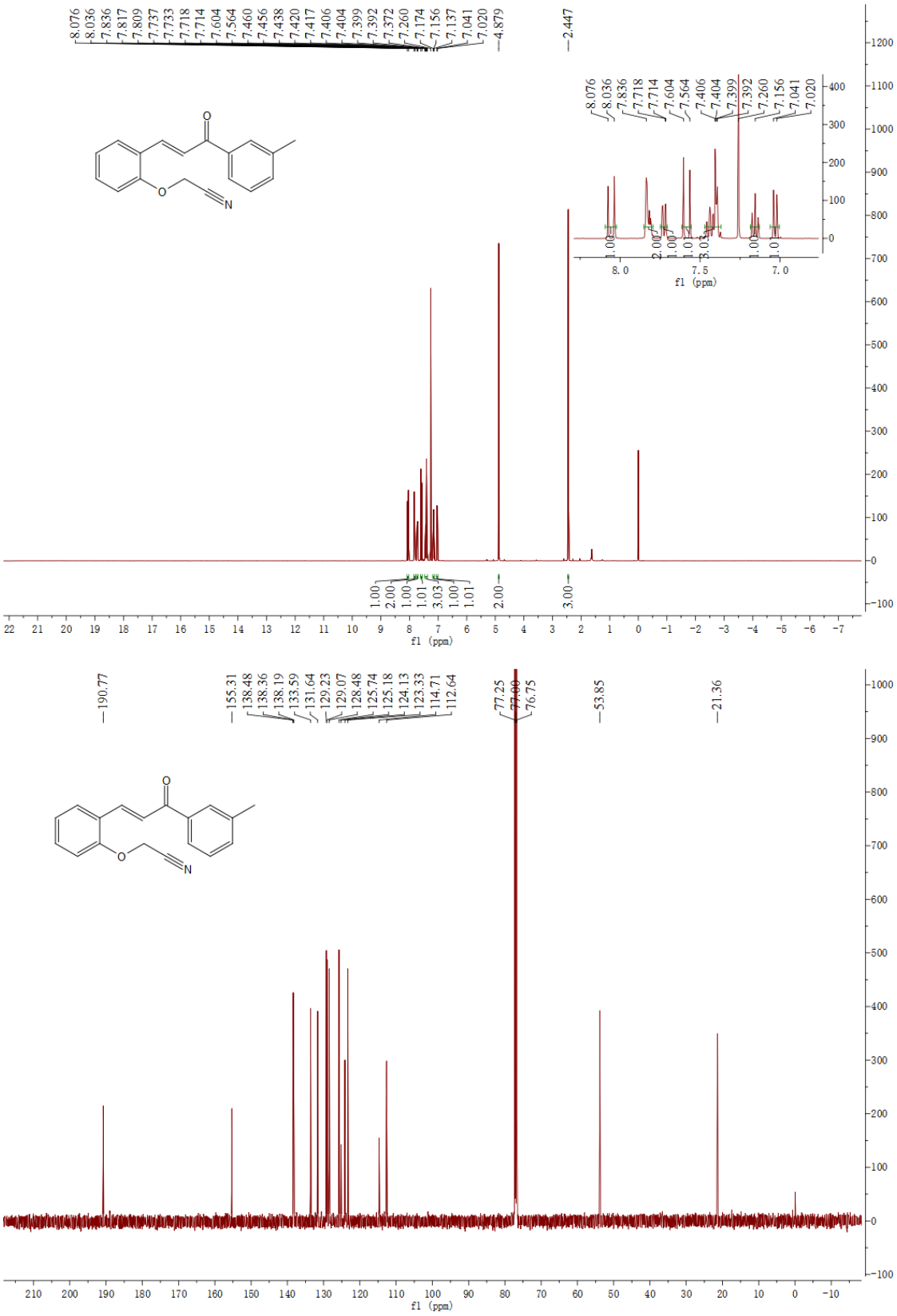


Figure S10. ^{1}H NMR of **1h** (400 MHz, $CDCl_3$) and ^{13}C NMR of **1h** (125 MHz, $CDCl_3$)

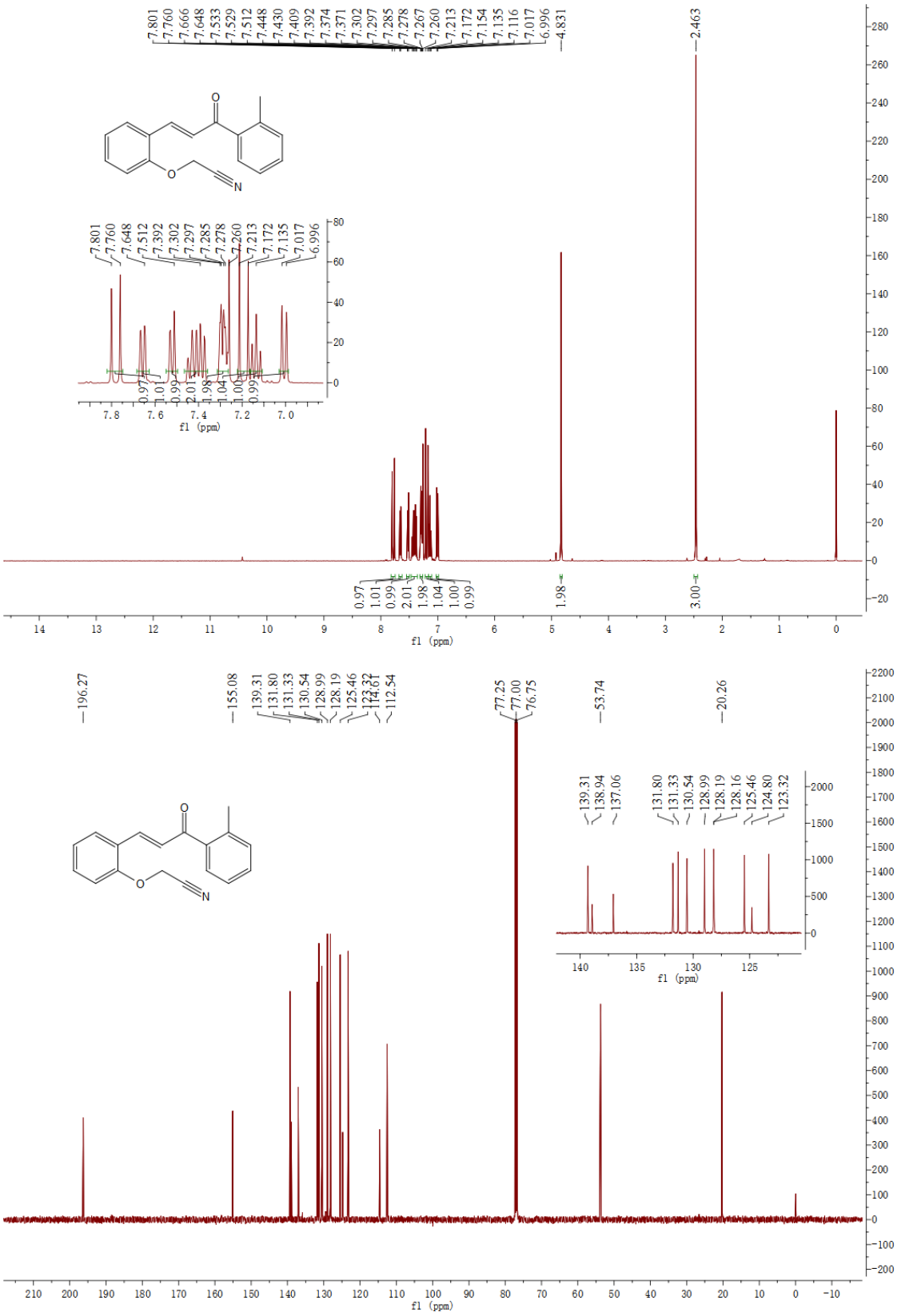


Figure S11. ^{1}H NMR of **1i** (400 MHz, $CDCl_3$) and ^{13}C NMR of **1i** (125 MHz, $CDCl_3$)

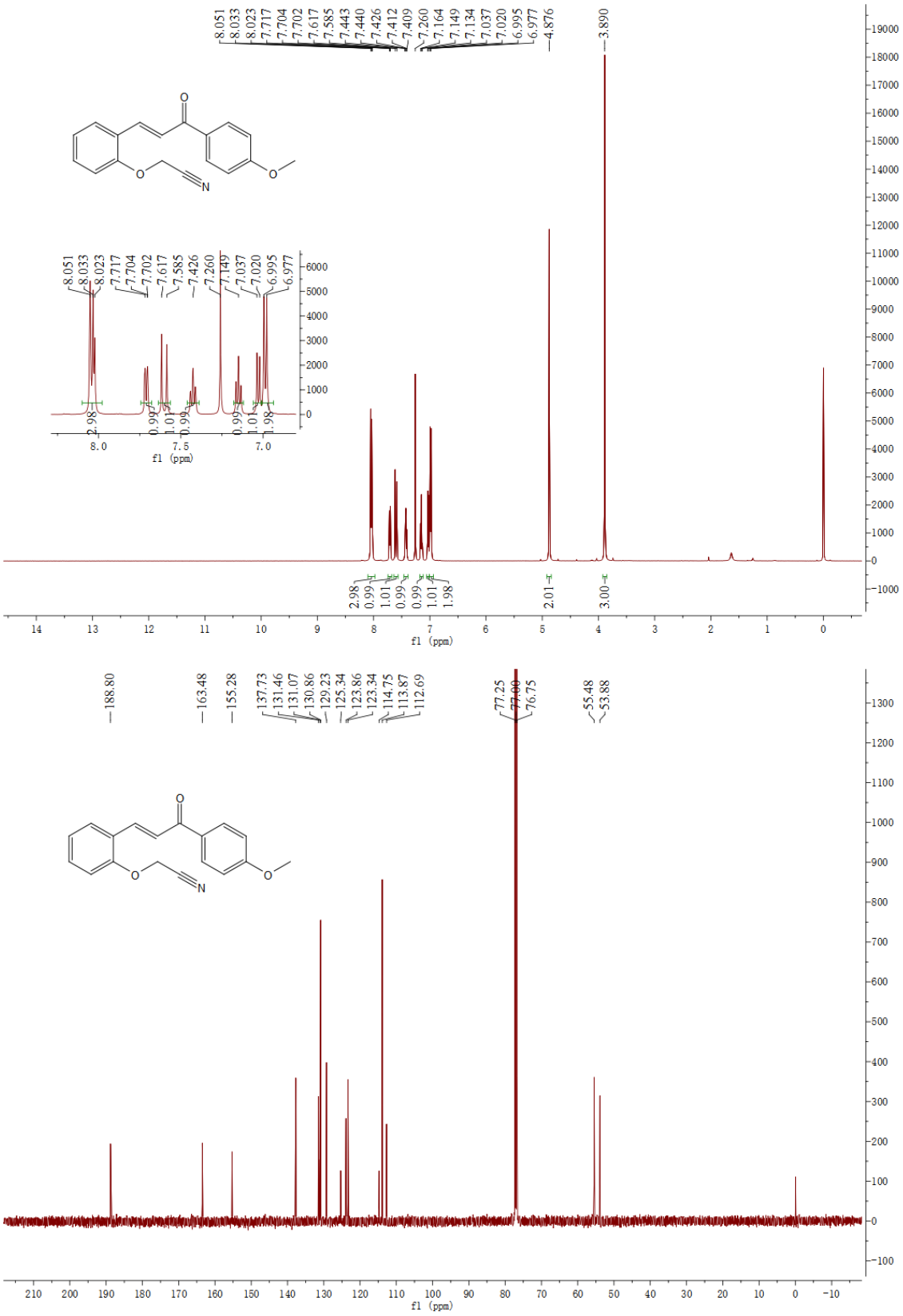


Figure S12. ^{1}H NMR of **1j** (500 MHz, $CDCl_3$) and ^{13}C NMR of **1j** (125 MHz, $CDCl_3$)

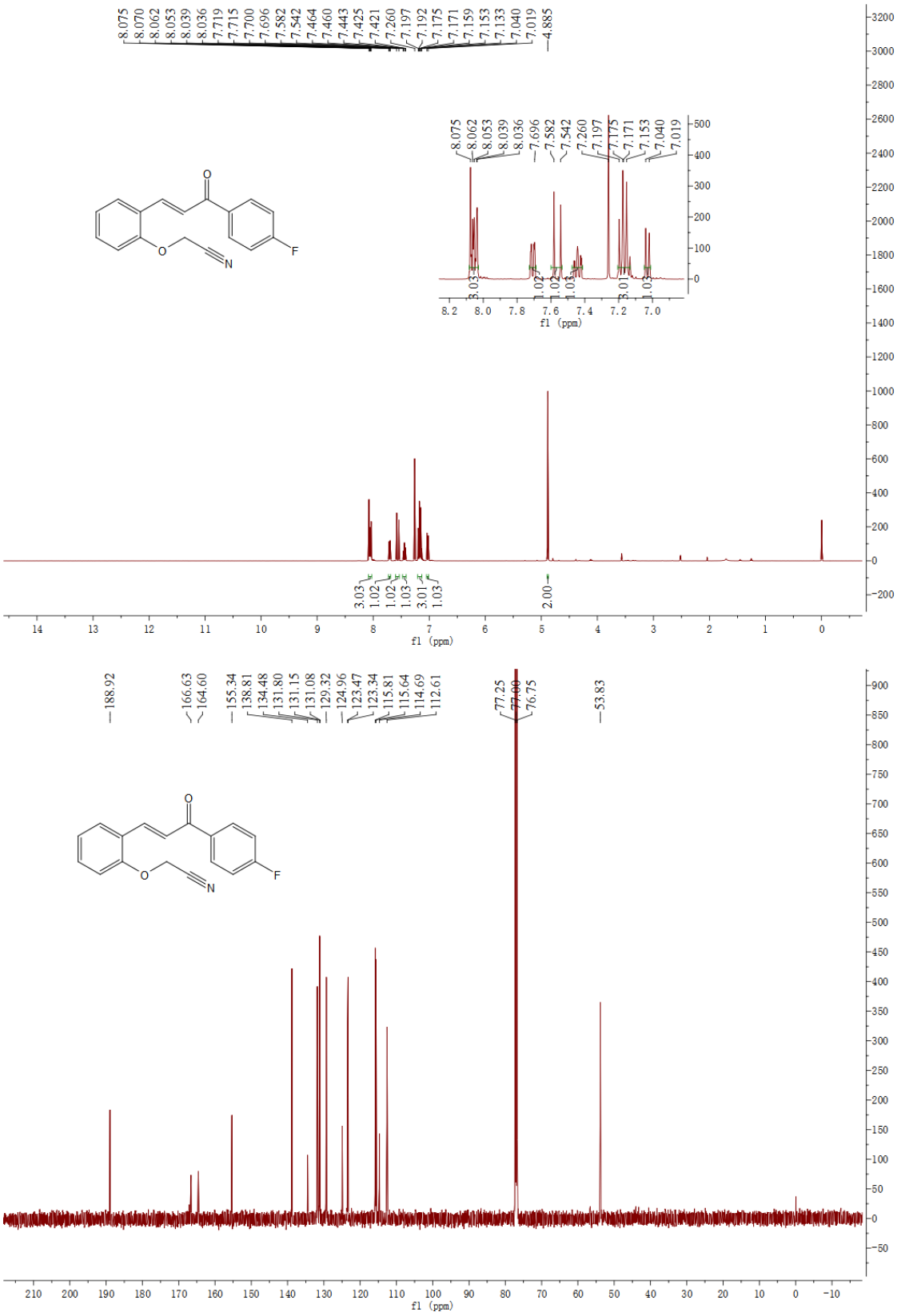


Figure S13. ^{1}H NMR of **1k** (400 MHz, $CDCl_3$) and ^{13}C NMR of **1k** (125 MHz, $CDCl_3$)

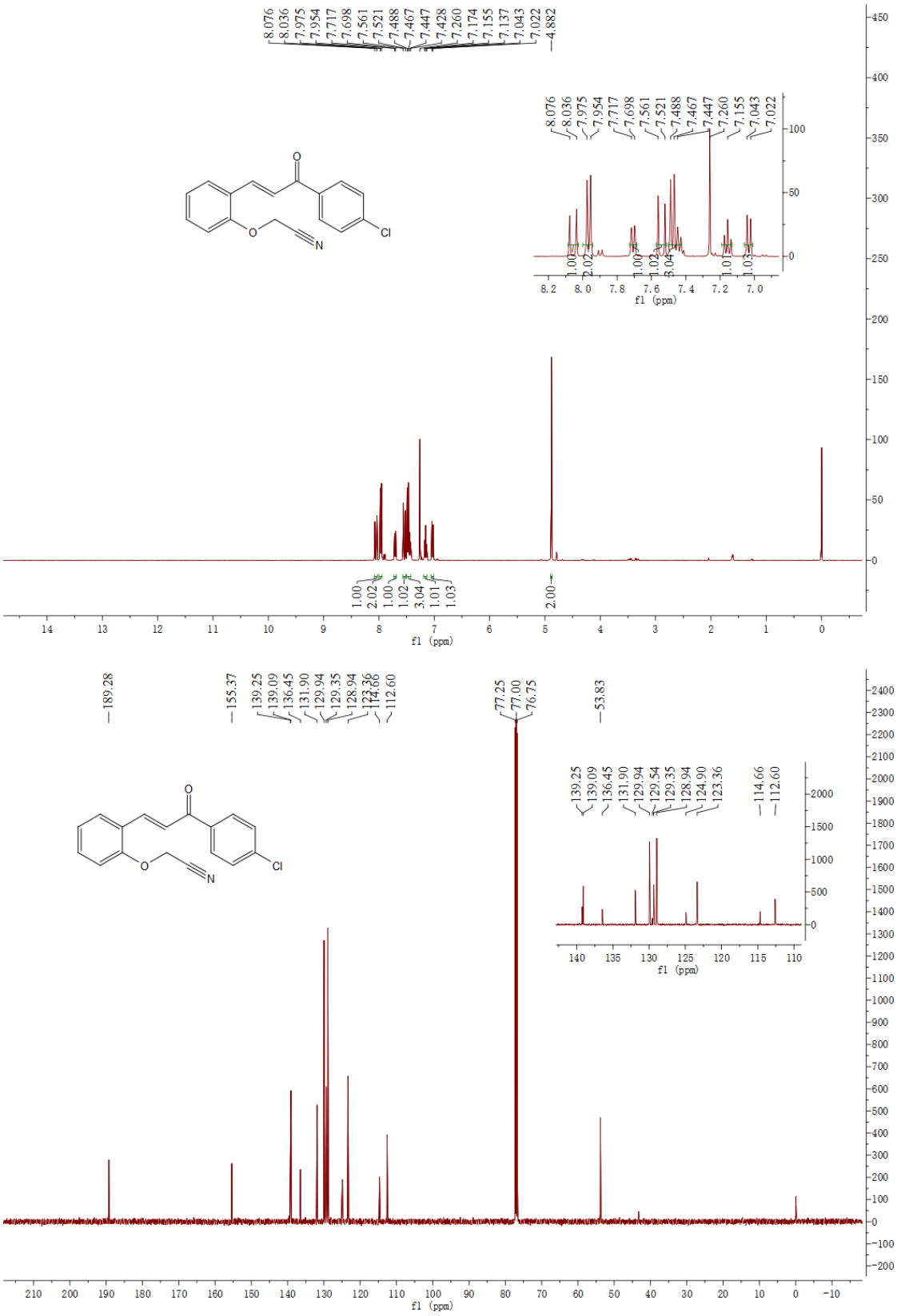


Figure S14. ^{1}H NMR of **1l** (400 MHz, $CDCl_3$) and ^{13}C NMR of **1l** (125 MHz, $CDCl_3$)

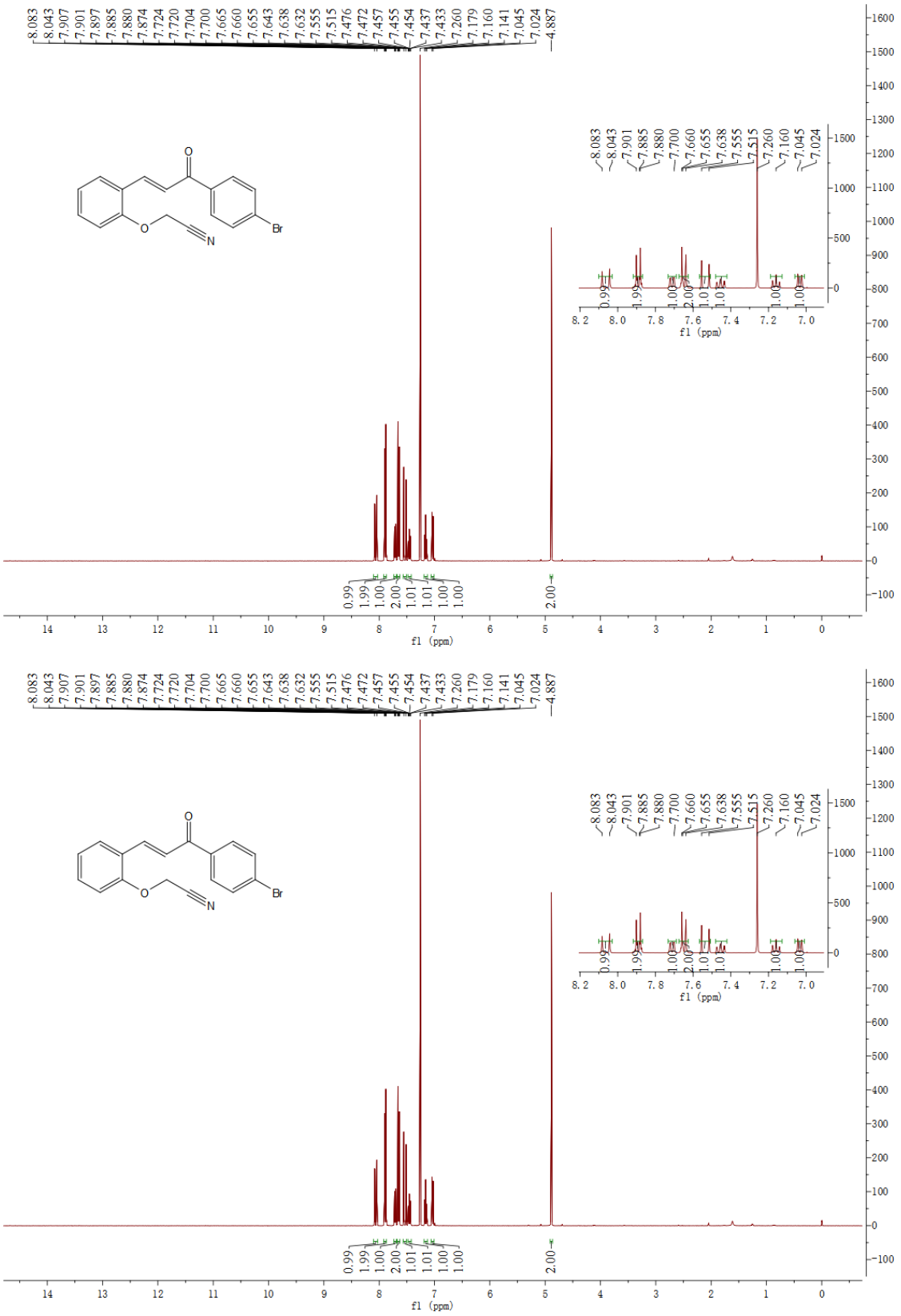


Figure S15. ^{1}H NMR of **1m** (400 MHz, $CDCl_3$) and ^{13}C NMR of **1m** (125 MHz, $CDCl_3$)

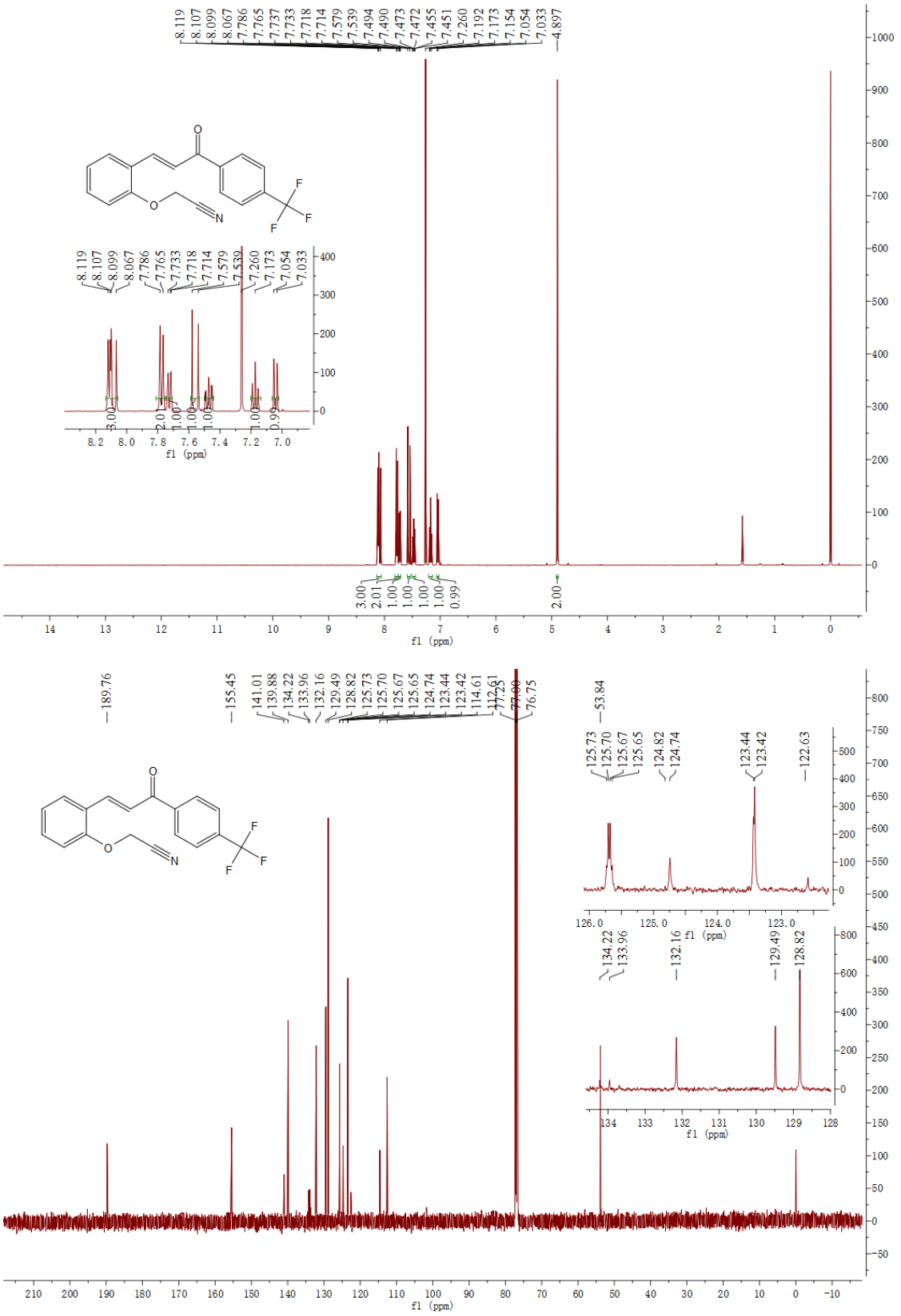


Figure S16. ^{1}H NMR of **1n** (400 MHz, $CDCl_3$) and ^{13}C NMR of **1n** (125 MHz, $CDCl_3$)

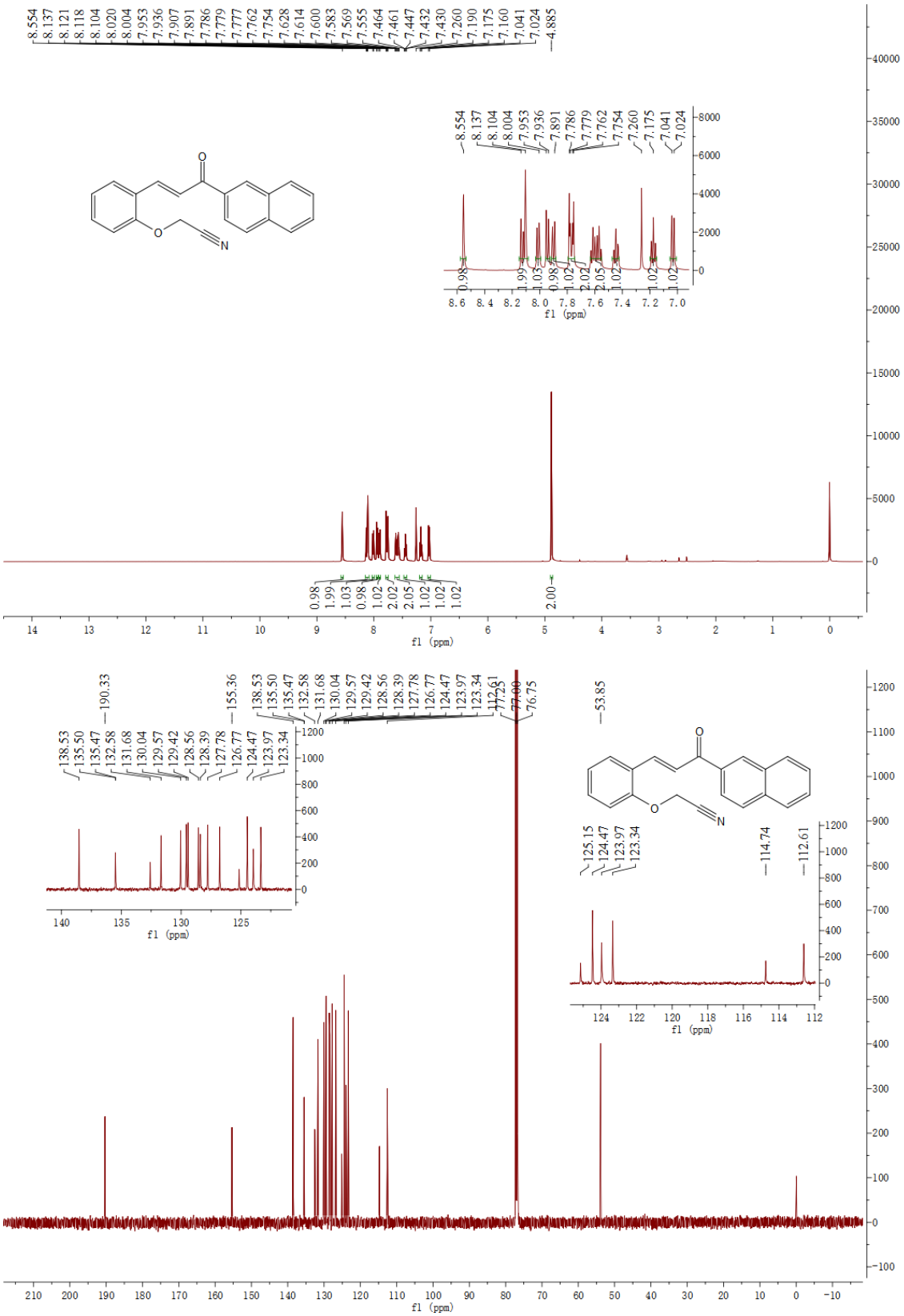


Figure S17. ^{1}H NMR of **1o** (500 MHz, $CDCl_3$) and ^{13}C NMR of **1o** (125 MHz, $CDCl_3$)

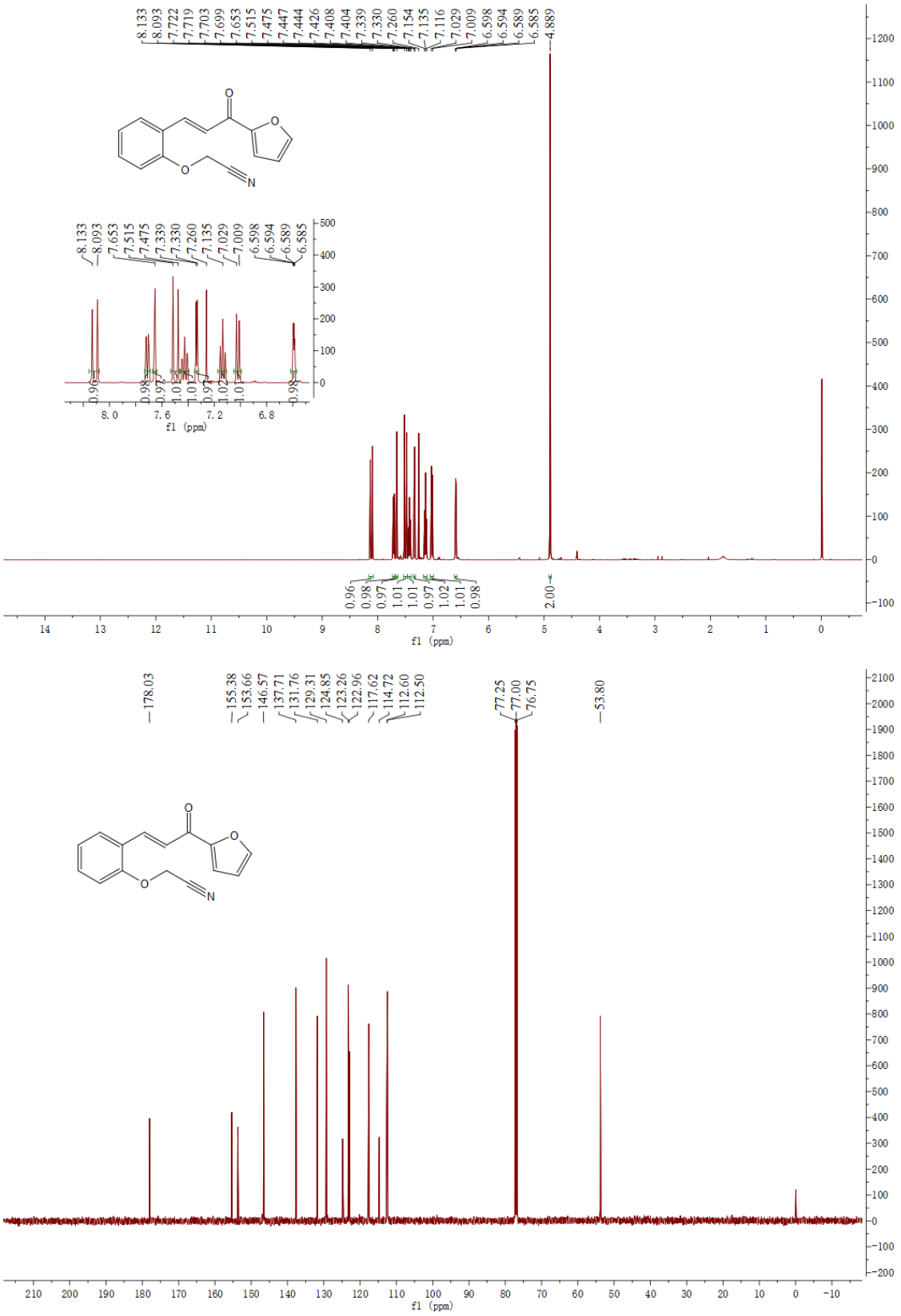


Figure S18. ^{1}H NMR of **1p** (400 MHz, $CDCl_3$) and ^{13}C NMR of **1p** (125 MHz, $CDCl_3$)

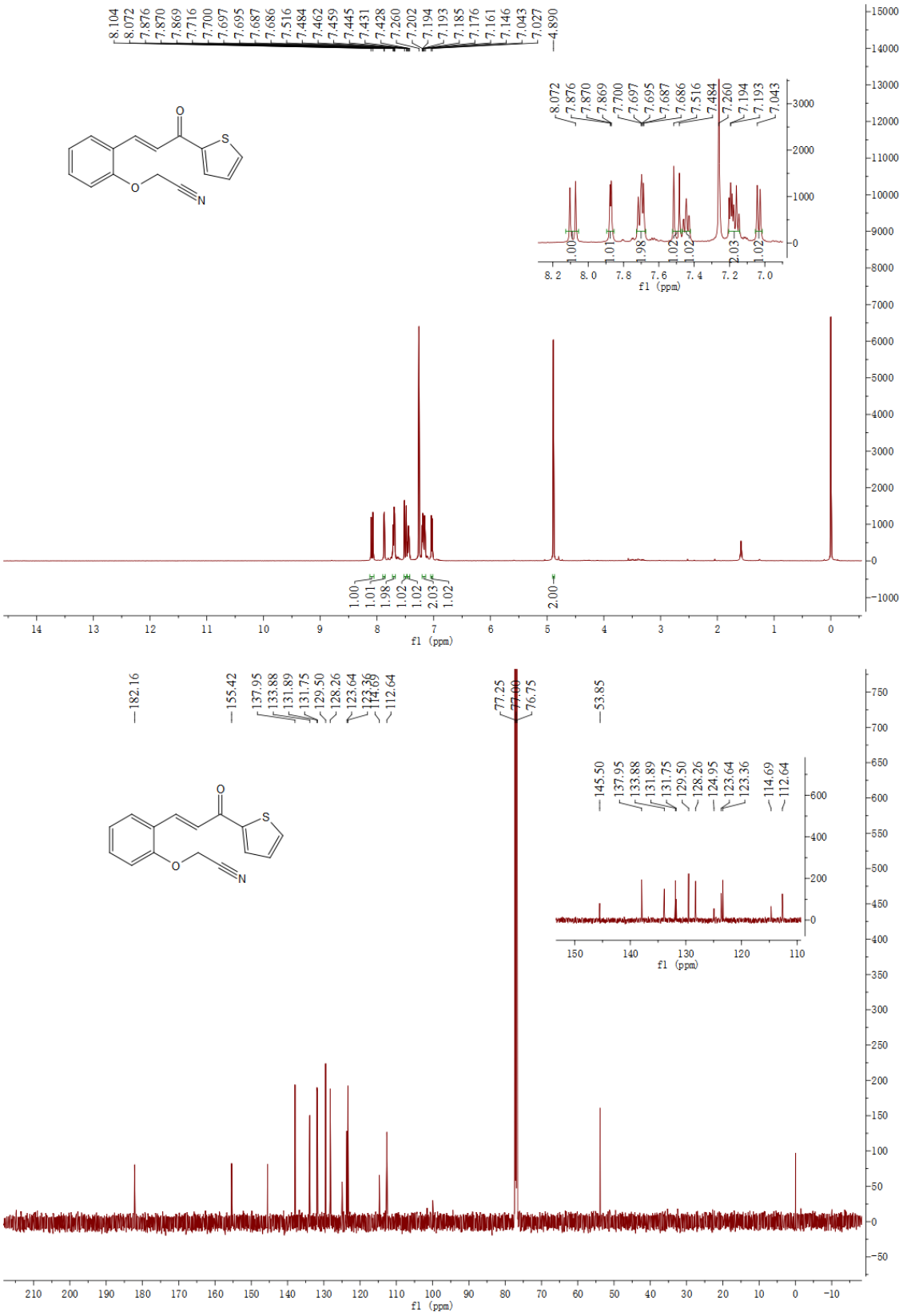
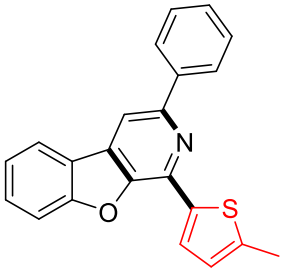
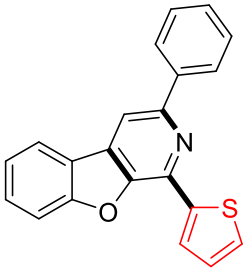


Figure S19. ^{1}H NMR of **1q** (500 MHz, $CDCl_3$) and ^{13}C NMR of **1q** (125 MHz, $CDCl_3$)

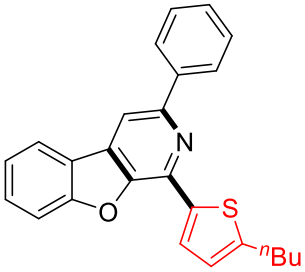
6. Analytical data for all products



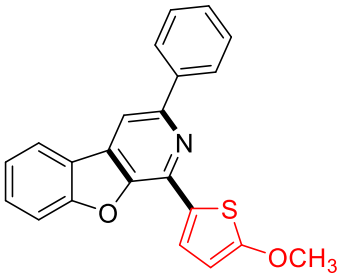
*1-(5-Methylthiophen-2-yl)-3-phenylbenzofuro[2,3-c]pyridine (**3a**)*: Pale-yellow solid (58.0 mg, 85%), mp 153-154 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.19 (d, J = 7.6 Hz, 2H), 8.11-8.09 (m, 2H), 8.03-8.01 (m, 1H), 7.70-7.67 (m, 1H), 7.62-7.59 (m, 1H), 7.54-7.51 (m, 2H), 7.44-7.40 (m, 2H), 6.93 (s, 1H), 2.61 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.1, 150.4, 147.6, 143.2, 139.3, 139.1, 137.5, 132.6, 129.7, 128.7, 128.65, 128.4, 127.0, 126.7, 123.4, 122.7, 121.9, 112.5, 109.4, 15.6. HRMS calcd for $C_{22}H_{16}NOS$ $[M + H]^+$: 342.0947, found 342.0950. Elemental analysis calcd (%) for $C_{22}H_{15}NOS$: C, 77.39; H, 4.43; N, 4.10. Found: C, 77.11; H, 4.45; N, 4.08.



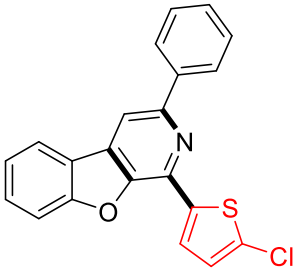
3-*Phenyl-1-(thiophen-2-yl)benzofuro[2,3-c]pyridine (**3b**)*: White solid (42.5 mg, 65%), mp 153-154 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36-8.36 (m, 1H), 8.23-8.20 (m, 2H), 8.18 (s, 1H), 8.07 (d, J = 7.7 Hz, 1H), 7.73 (d, J = 8.3 Hz, 1H), 7.66-7.62 (m, 1H), 7.55-7.52 (m, 3H), 7.47-7.43 (m, 2H), 7.29-7.27 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.2, 150.7, 147.8, 141.6, 139.3, 137.3, 132.9, 129.9, 128.7, 128.5, 128.3, 128.2, 128.1, 127.0, 123.6, 122.7, 122.0, 112.6, 110.0. HRMS calcd for $C_{21}H_{14}NOS$ $[M + H]^+$: 328.0791, found 328.0783. Elemental analysis calcd (%) for $C_{21}H_{13}NOS$: C, 77.04; H, 4.00; N, 4.28. Found: C, 77.21; H, 3.98; N, 4.27.



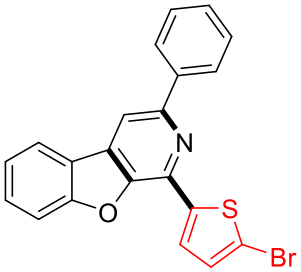
1-*(5-Butylthiophen-2-yl)-3-phenylbenzofuro[2,3-c]pyridine* (***3c***): Pale-yellow solid (61.3 mg, 80%), mp 134-135 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.20 (d, J = 7.7 Hz, 2H), 8.14 (d, J = 3.6 Hz, 1H), 8.10 (s, 1H), 8.03 (d, J = 7.7 Hz, 1H), 7.69 (d, J = 8.3 Hz, 1H), 7.62-7.59 (m, 1H), 7.54-7.51 (m, 2H), 7.44-7.40 (m, 2H), 6.94 (d, J = 3.5 Hz, 1H), 2.93 (t, J = 7.6 Hz, 2H), 1.82-1.76 (m, 2H), 1.51-1.44 (m, 2H), 0.99 (t, J = 7.6 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.1, 150.5, 149.4, 147.7, 139.3, 138.7, 137.6, 132.7, 129.7, 128.7, 128.5, 128.4, 127.0, 125.5, 123.4, 122.7, 121.9, 112.5, 109.4, 33.8, 30.2, 22.2, 13.8. HRMS calcd for $C_{25}H_{22}NOS$ $[M + H]^+$: 384.1417, found 384.1417. Elemental analysis calcd (%) for $C_{25}H_{21}NOS$: C, 78.30; H, 5.52; N, 3.65. Found: C, 78.51; H, 5.51; N, 3.63.



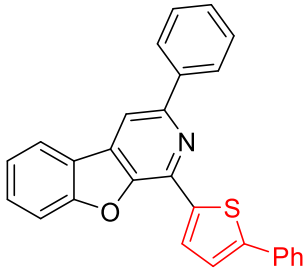
1-(5-Methoxythiophen-2-yl)-3-phenylbenzofuro[2,3-c]pyridine (***3d***): White solid (58.6 mg, 82%), mp 190-191 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, J = 7.6 Hz, 2H), 8.08 (s, 1H), 8.05 (d, J = 7.7 Hz, 1H), 8.01 (d, J = 4.1 Hz, 1H), 7.70 (d, J = 8.3 Hz, 1H), 7.64-7.60 (m, 1H), 7.54-7.50 (m, 2H), 7.45-7.40 (m, 2H), 6.37 (d, J = 4.1 Hz, 1H), 4.02 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 169.6, 157.1, 150.5, 147.8, 139.4, 137.9, 132.4, 129.6, 128.7, 128.4, 127.4, 127.0, 123.5, 122.8, 121.9, 112.6, 108.8, 105.6, 60.2. HRMS calcd for $C_{22}H_{16}NO_2S$ $[M + H]^+$: 358.0896, found 358.0900. Elemental analysis calcd (%) for $C_{22}H_{15}NO_2S$: C, 73.93; H, 4.23; N, 3.92. Found: C, 74.21; H, 4.21; N, 3.98.



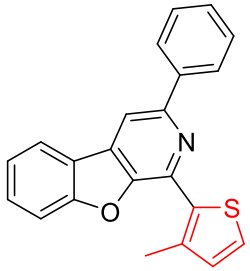
1-*(5-Chlorothiophen-2-yl)-3-phenylbenzofuro[2,3-c]pyridine* (***3e***): White solid (43.3 mg, 60%), mp 157-158 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17-8.13 (m, 3H), 8.05-8.03 (m, 2H), 7.68 (d, J = 8.2 Hz, 1H), 7.64-7.60 (m, 1H), 7.54-7.50 (m, 2H), 7.46-7.42 (m, 2H), 7.05 (d, J = 4.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.2, 150.6, 147.6, 140.5, 139.0, 136.4, 133.4, 133.0, 130.0, 128.7, 128.6, 127.6, 127.5, 126.9, 123.7, 122.5, 122.0, 122.6, 110.1. HRMS calcd for $C_{21}H_{13}ClNOS$ $[M + H]^+$: 362.0401 and 364.0371, found 362.0405 and 364.0378. Elemental analysis calcd (%) for $C_{21}H_{12}ClNOS$: C, 69.71; H, 3.34; N, 3.87. Found: C, 69.52; H, 3.36; N, 3.86.



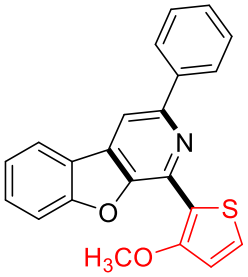
1-(5-Bromothiophen-2-yl)-3-phenylbenzofuro[2,3-c]pyridine (***3f***): yellow solid (43.7 mg, 54%), mp 180-181 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, J = 8.6 Hz, 3H), 8.05 (d, J = 7.6 Hz, 1H), 8.01 (d, J = 3.9 Hz, 1H), 7.70 (d, J = 8.3 Hz, 1H), 7.65-7.61 (m, 1H), 7.54-7.50 (m, 2H), 7.46-7.42 (m, 2H), 7.20 (d, J = 3.9 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.2, 150.7, 147.5, 143.4, 139.0, 136.4, 133.1, 131.2, 130.0, 128.8, 128.6, 128.4, 127.0, 123.7, 122.5, 122.0, 116.2, 112.6, 110.2. HRMS calcd for $C_{21}H_{13}BrNOS$ $[M + H]^+$: 405.9896 and 307.9875, found 405.9906 and 307.9879. Elemental analysis calcd (%) for $C_{21}H_{12}BrNOS$: C, 62.88; H, 2.98; N, 3.45. Found: C, 63.12; H, 2.96; N, 3.44.



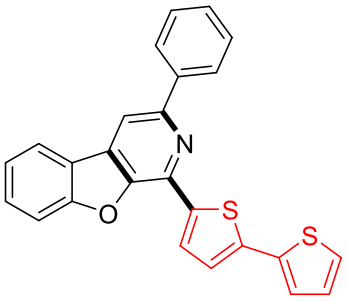
*3-Phenyl-1-(5-phenylthiophen-2-yl)benzofuro[2,3-c]pyridine (**3g**)*: yellow solid (56.4 mg, 70%), mp 180-181 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.28 (d, J = 3.8 Hz, 1H), 8.22 (d, J = 7.9 Hz, 2H), 8.15 (s, 1H), 8.06 (d, J = 7.7 Hz, 1H), 7.77 (d, J = 7.9 Hz, 2H), 7.72 (d, J = 8.3 Hz, 1H), 7.65-7.62 (m, 1H), 7.56-7.53 (m, 2H), 7.48-7.42 (m, 5H), 7.35-7.32 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.2, 150.7, 147.9, 146.7, 140.9, 139.3, 137.2, 134.5, 132.8, 129.8, 129.3, 128.9, 128.7, 128.5, 127.8, 127.0, 126.0, 124.3, 123.6, 122.7, 122.0, 112.6, 109.9. HRMS calcd for $C_{27}H_{18}NOS$ $[M + H]^+$: 404.1104, found 404.1117. Elemental analysis calcd (%) for $C_{27}H_{17}NOS$: C, 80.37; H, 4.25; N, 3.47. Found: C, 80.09; H, 4.27; N, 3.49.



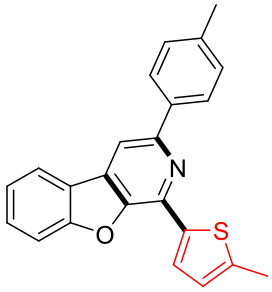
*1-(3-Methylthiophen-2-yl)-3-phenylbenzofuro[2,3-c]pyridine (**3h**)*: yellow solid (33.4 mg, 49%), mp 140-141 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22-8.19 (m, 3H), 8.07 (d, J = 7.7 Hz, 1H), 7.68 (d, J = 8.3 Hz, 1H), 7.63-7.59 (m, 1H), 7.55-7.51 (m, 2H), 7.49 (d, J = 5.0, 1H), 7.45-7.41 (m, 2H), 7.08 (d, J = 5.0 Hz, 1H), 2.71 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.0, 150.9, 148.9, 139.7, 138.5, 138.4, 132.8, 132.4, 131.4, 129.8, 128.7, 128.4, 127.1, 126.7, 123.1, 122.9, 121.9, 112.6, 110.1, 16.6. HRMS calcd for $C_{22}H_{16}NOS$ $[M + H]^+$: 342.0947, found 342.0950. Elemental analysis calcd (%) for $C_{22}H_{15}NOS$: C, 77.39; H, 4.43; N, 4.10. Found: C, 77.57; H, 4.42; N, 4.09.



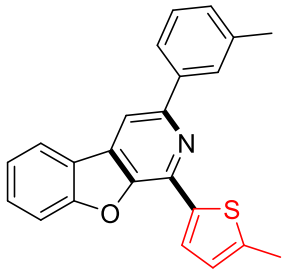
1-*(3-Methoxythiophen-2-yl)-3-phenylbenzofuro[2,3-c]pyridine* (***3i***): Yellow oil (45.7 mg, 64%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.20 (d, J = 9.9 Hz, 3H), 8.05 (d, J = 7.7 Hz, 1H), 7.67 (d, J = 8.3 Hz, 1H), 7.61-7.58 (m, 1H), 7.54-7.51 (m, 2H), 7.47 (d, J = 5.5 Hz, 1H), 7.44-7.39 (m, 2H), 7.05 (d, J = 5.5 Hz, 1H), 4.06 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.0, 156.3, 150.6, 148.7, 139.5, 136.8, 132.8, 129.7, 128.6, 128.3, 127.2, 127.0, 123.2, 122.8, 121.8, 117.8, 117.6, 112.5, 109.8, 59.2. HRMS calcd for $C_{22}H_{16}NO_2S$ $[M + H]^+$: 358.0896, found 358.0903. Elemental analysis calcd (%) for $C_{22}H_{15}NO_2S$: C, 73.93; H, 4.23; N, 3.92. Found: C, 73.72; H, 4.21; N, 3.91.



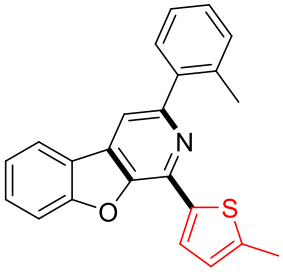
1-*([2,2'-Bithiophen]-5-yl)-3-phenylbenzofuro[2,3-c]pyridine* (***3j***): Yellow solid (44.2 mg, 52%), mp 179-180 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20-8.16 (m, 3H), 8.10 (s, 1H), 8.02 (d, J = 7.7 Hz, 1H), 7.69 (d, J = 8.3 Hz, 1H), 7.63-7.59 (m, 1H), 7.56-7.52 (m, 2H), 7.46-7.40 (m, 2H), 7.35 (d, J = 3.5 Hz, 1H), 7.31-7.28 (m, 2H), 7.09-7.07 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.1, 150.6, 147.8, 140.3, 139.8, 139.2, 137.7, 137.0, 132.8, 129.8, 129.0, 128.7, 128.5, 128.0, 127.0, 124.8, 124.2, 123.5, 122.6, 121.9, 112.6, 109.9. HRMS calcd for $C_{25}H_{16}NOS_2$ $[M + H]^+$: 410.0668, found 410.0661. Elemental analysis calcd (%) for $C_{25}H_{15}NOS_2$: C, 73.32; H, 3.69; N, 3.42. Found: C, 73.53; H, 3.68; N, 3.40.



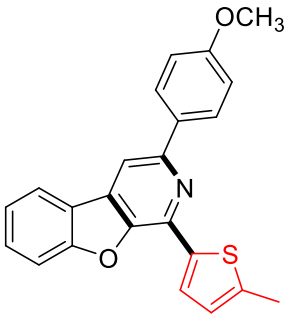
*1-(5-Methylthiophen-2-yl)-3-(p-tolyl)benzofuro[2,3-c]pyridine (**3k**)*: White solid (42.6 mg, 60%), mp 183-184 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11-8.10 (m, 4H), 8.04 (d, J = 10.6 Hz, 1H), 7.69 (d, J = 8.2 Hz, 1H), 7.62-7.58 (m, 1H), 7.43-7.40 (m, 1H), 7.32 (d, J = 7.7 Hz, 1H), 6.92 (d, J = 2.6 Hz, 2H), 2.61 (s, 3H), 2.44 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.1, 150.6, 147.5, 143.1, 139.2, 138.3, 137.4, 136.6, 132.6, 129.6, 129.4, 128.6, 126.9, 126.7, 123.4, 122.8, 121.9, 112.5, 109.1, 21.2, 15.6. HRMS calcd for $C_{23}H_{18}NOS$ $[M + H]^+$: 356.1104, found 356.1106. Elemental analysis calcd (%) for $C_{23}H_{17}NOS$: C, 77.72; H, 4.82; N, 3.94. Found: C, 77.49; H, 4.84; N, 3.93.



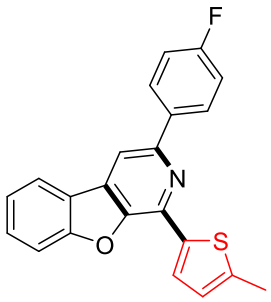
*1-(5-Methylthiophen-2-yl)-3-(m-tolyl)benzofuro[2,3-c]pyridine (**3l**)*: White solid (35.5 mg, 50%), mp 152-151 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11-8.09 (m, 2H), 8.04-7.98 (m, 3H), 7.68 (d, J = 8.3 Hz, 1H), 7.62-7.58 (m, 1H), 7.43-7.39 (m, 2H), 7.25-7.24 (m, 1H), 6.92 (d, J = 2.8 Hz, 1H), 2.61 (s, 3H), 2.51 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.1, 150.6, 147.6, 143.0, 139.3, 139.2, 138.2, 137.5, 132.6, 129.6, 129.2, 128.6, 127.7, 126.6, 124.2, 123.4, 122.7, 121.9, 112.5, 109.4, 21.7, 15.6. HRMS calcd for $C_{23}H_{18}NOS$ $[M + H]^+$: 356.1104, found 356.1099.Elemental analysis calcd (%) for $C_{23}H_{17}NOS$: C, 77.72; H, 4.82; N, 3.94. Found: C, 77.98; H, 4.81; N, 3.93.



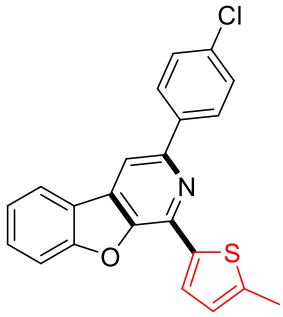
*1-(5-Methylthiophen-2-yl)-3-(o-tolyl)benzofuro[2,3-c]pyridine (**3m**)*: yellow oil (27.0 mg, 38%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, J = 3.6 Hz, 1H), 8.01 (d, J = 7.7 Hz, 1H), 7.81 (s, 1H), 7.72 (d, J = 8.3 Hz, 1H), 7.63-7.58 (m, 2H), 7.43-7.40 (m, 1H), 7.35-7.33 (m, 3H), 6.93-6.92 (m, 1H), 2.59 (s, 3H), 2.58 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.0, 153.3, 147.1, 143.0, 140.3, 139.1, 137.1, 136.6, 132.2, 130.9, 130.0, 129.6, 128.5, 128.0, 126.6, 125.8, 123.4, 122.7, 121.9, 113.2, 112.5, 20.9, 15.6. HRMS calcd for $C_{23}H_{18}NOS$ $[M + H]^+$: 356.1104, found 356.1109. Elemental analysis calcd (%) for $C_{23}H_{17}NOS$: C, 77.72; H, 4.82; N, 3.94. Found: C, 78.01; H, 4.80; N, 3.92.



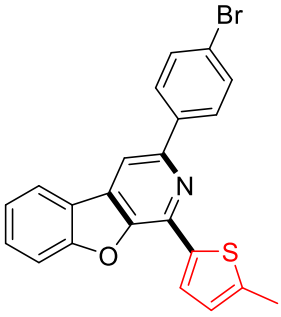
*3-(4-Methoxyphenyl)-1-(5-methylthiophen-2-yl)benzofuro[2,3-c]pyridine (**3n**)*: White solid (60.8 mg, 82%), mp 182-183 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, J = 8.6 Hz, 2H), 8.09 (d, J = 3.5 Hz, 1H), 8.03 (d, J = 7.3 Hz, 2H), 7.68 (d, J = 8.2 Hz, 1H), 7.62-7.58 (m, 1H), 7.43-7.39 (m, 1H), 7.04 (d, J = 8.5 Hz, 2H), 6.91 (d, J = 2.6 Hz, 1H), 3.89 (s, 3H), 2.60 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.1, 157.1, 150.3, 147.3, 143.0, 139.4, 137.4, 132.7, 132.2, 129.6, 128.5, 128.2, 126.7, 123.4, 122.8, 121.9, 114.1, 112.5, 108.5, 53.4, 15.6. HRMS calcd for $C_{23}H_{18}NO_2S$ $[M + H]^+$: 372.1053, found 372.1053. Elemental analysis calcd (%) for $C_{23}H_{17}NO_2S$: C, 74.37; H, 4.61; N, 3.77. Found: C, 74.60; H, 4.59; N, 3.76.



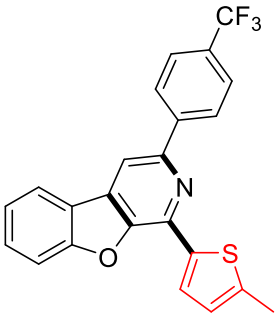
3-(4-Fluorophenyl)-1-(5-methylthiophen-2-yl)benzofuro[2,3-c]pyridine (***3o***): White solid (43.1 mg, 60%), mp 197-198 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.17-8.14 (m, 2H), 8.09 (d, J = 3.5 Hz, 1H), 8.03 (d, J = 9.8 Hz, 2H), 7.69 (d, J = 8.3 Hz, 1H), 7.63-7.60 (m, 1H), 7.44-7.41 (m, 1H), 7.20-7.17 (m, 2H), 6.92-6.91 (m, 1H), 2.60 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.3 (d, J_{C-F} = 246.3 Hz), 157.1, 149.5, 147.5, 143.2, 139.0, 137.6, 135.5, 132.7, 129.8, 128.8, 128.7 (d, J_{C-F} = 7.5 Hz), 126.7, 123.5, 122.6, 121.9, 115.5 (d, J_{C-F} = 21.3 Hz), 112.6, 109.0, 15.6. HRMS calcd for $C_{22}H_{15}FNOS$ $[M + H]^+$: 360.0853, found 360.0857. Elemental analysis calcd (%) for $C_{22}H_{14}FNOS$: C, 73.52; H, 3.93; N, 3.90. Found: C, 73.27; H, 3.95; N, 3.91.



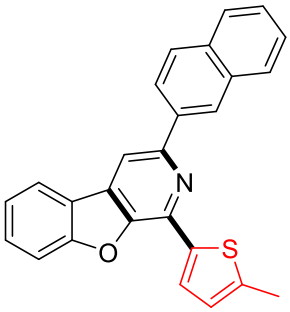
3-(4-Chlorophenyl)-1-(5-methylthiophen-2-yl)benzofuro[2,3-c]pyridine (***3p***): White solid (41.3 mg, 55%), mp 205-206 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.10-8.07 (m, 3H), 8.02 (s, 1H), 7.99 (d, J = 7.7 Hz, 2H), 7.67 (d, J = 8.3 Hz, 1H), 7.61-7.58 (m, 1H), 7.44 (d, J = 8.5 Hz, 1H), 7.42-7.39 (m, 1H), 6.90-6.89 (m, 1H), 2.59 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.1, 149.1, 147.7, 143.3, 138.9, 137.8, 137.7, 134.5, 132.7, 129.8, 128.8, 128.2, 126.7, 123.5, 122.6, 121.9, 112.6, 109.1, 15.6. HRMS calcd for $C_{22}H_{15}ClNOS$ $[M + H]^+$: 376.0557 and 378.0528, found 376.0549 and 378.0520. Elemental analysis calcd (%) for $C_{22}H_{14}ClNOS$: C, 70.30; H, 3.75; N, 3.73. Found: C, 70.51; H, 3.73; N, 3.72.



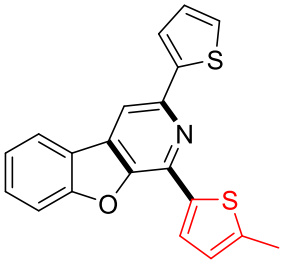
3-(4-Bromophenyl)-1-(5-methylthiophen-2-yl)benzofuro[2,3-c]pyridine ***(3q)***: White solid (40.2mg, 48%), mp 212-213 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, J = 3.6 Hz, 1H), 8.06-8.01 (m, 4H), 7.70 (d, J = 8.3 Hz, 1H), 7.64-7.60 (m, 3H), 7.45-7.41 (m, 1H), 6.92-6.91 (m, 1H), 2.60 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.2, 149.2, 147.7, 143.3, 138.9, 138.3, 137.7, 132.7, 131.8, 129.8, 128.8, 128.5, 126.7, 123.6, 122.8, 122.6, 121.9, 112.6, 109.1, 15.6. HRMS calcd for $C_{22}H_{15}BrNOS$ $[M + H]^+$: 420.0052 and 422.0032, found 420.0045 and 422.0028. Elemental analysis calcd (%) for $C_{22}H_{14}BrNOS$: C, 62.87; H, 3.36; N, 3.33. Found: C, 62.59; H, 3.38; N, 3.34.



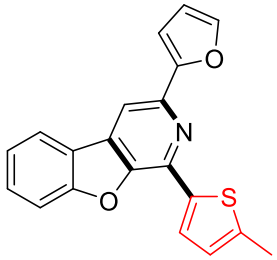
1-*(5-Methylthiophen-2-yl)-3-(4-(trifluoromethyl)phenyl)benzofuro[2,3-c]pyridine* ***(3r)***: White solid (47.4mg, 58%), mp 189-190 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (d, J = 8.1 Hz, 2H), 8.03 (d, J = 3.6 Hz, 1H), 8.01 (s, 1H), 7.96 (d, J = 7.7 Hz, 1H), 7.71 (d, J = 8.2 Hz, 2H), 7.65-7.57 (m, 2H), 7.41-7.38 (m, 1H), 6.89-6.88 (m, 1H), 2.58 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.1, 148.6, 147.9, 143.4, 142.6, 138.8, 137.8, 132.6, 130.2 (d, J_{C-F} = 31.3 Hz), 129.8, 128.9, 127.1, 126.8, 125.5 (q, J_{C-F} = 3.8 Hz), 124.4 (d, J_{C-F} = 270.0 Hz), 123.6, 122.5, 121.8, 112.6, 109.7, 15.6. HRMS calcd for $C_{23}H_{15}F_3NOS$ $[M + H]^+$: 410.0821, found 410.0826. Elemental analysis calcd (%) for $C_{23}H_{14}F_3NOS$: C, 67.47; H, 3.45; N, 3.42. Found: C, 67.66; H, 3.44; N, 3.41.



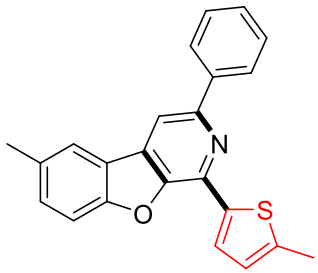
1-(5-Methylthiophen-2-yl)-3-(naphthalen-2-yl)benzofuro[2,3-c]pyridine (***3s***): White solid (57.1mg, 73%), mp 220-221 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.61 (s, 1H), 8.36 (d, J = 8.5 Hz, 1H), 8.23 (s, 1H), 8.13 (d, J = 3.6 Hz, 1H), 8.06 (d, J = 7.6 Hz, 1H), 8.01-7.96 (m, 2H), 7.90-7.88 (m, 1H), 7.69 (d, J = 8.3 Hz, 1H), 7.63-7.59 (m, 1H), 7.53-7.51 (m, 2H), 7.45-7.41 (m, 1H), 6.93 (d, J = 3.6 Hz, 1H), 2.62 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.2, 150.3, 147.7, 143.2, 139.1, 137.6, 136.7, 133.6, 133.5, 132.7, 129.7, 128.73, 128.7, 128.3, 127.7, 126.7, 126.2, 126.1, 126.0, 125.0, 123.5, 122.7, 121.9, 112.6, 109.7, 15.7. HRMS calcd for $C_{26}H_{18}NOS$ $[M + H]^+$: 392.1104, found 392.1107. Elemental analysis calcd (%) for $C_{26}H_{17}NOS$: C, 79.77; H, 4.38; N, 3.58. Found: C, 78.00; H, 4.46; N, 3.57.



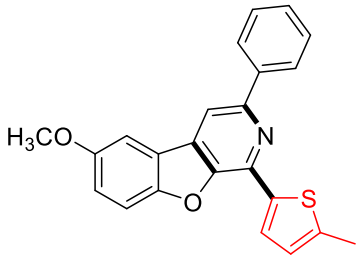
1-(5-Methylthiophen-2-yl)-3-(thiophen-2-yl)benzofuro[2,3-c]pyridine (***3t***): yellow solid (29.8 mg, 43%), mp 150-151 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, J = 3.6 Hz, 1H), 8.03 (d, J = 7.5 Hz, 1H), 7.99 (s, 1H), 7.69-7.67 (m, 2H), 7.63-7.59 (m, 1H), 7.44-7.38 (m, 2H), 7.15-7.13 (m, 1H), 6.92-6.91 (m, 1H), 2.61 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.2, 147.3, 146.1, 145.3, 143.5, 138.6, 137.5, 132.6, 129.8, 128.8, 127.9, 126.9, 126.7, 123.7, 123.5, 122.5, 122.0, 112.6, 107.8, 15.6. HRMS calcd for $C_{20}H_{14}NOS_2$ $[M + H]^+$: 348.0511, found 348.0516. Elemental analysis calcd (%) for $C_{20}H_{13}NOS_2$: C, 69.14; H, 3.77; N, 4.03. Found: C, 68.92; H, 3.89; N, 4.04.



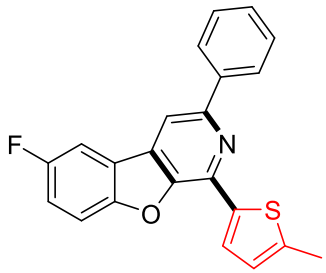
3-(Furan-2-yl)-1-(5-methylthiophen-2-yl)benzofuro[2,3-c]pyridine (***3u***): yellow solid (39.7 mg, 43%), mp 145-146 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10-8.08 (m, 2H), 8.03 (d, J = 7.7 Hz, 1H), 7.69 (d, J = 8.3 Hz, 1H), 7.63-7.59 (m, 1H), 7.55 (s, 1H), 7.44-7.40 (m, 1H), 7.16 (d, J = 3.2 Hz, 1H), 6.92-6.91 (m, 1H), 6.58-6.56 (m, 1H), 2.60 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.1, 154.2, 147.2, 143.3, 143.1, 142.6, 138.6, 137.8, 132.3, 129.7, 128.8, 126.7, 123.5, 122.7, 122.0, 112.5, 112.1, 108.0, 107.7, 15.6. HRMS calcd for $C_{20}H_{14}NO_2S$ $[M + H]^+$: 332.0740, found 332.0736. Elemental analysis calcd (%) for $C_{20}H_{13}NO_2S$: C, 72.49; H, 3.95; N, 4.23. Found: C, 72.67; H,3.94; N, 4.21.



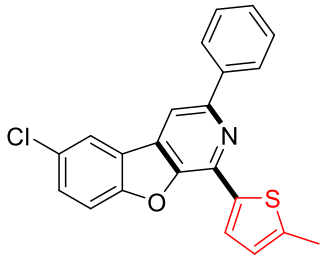
6-Methyl-1-(5-methylthiophen-2-yl)-3-phenylbenzofuro[2,3-c]pyridine (***3v***): White solid (60.4 mg, 85%), mp 140-141 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, J = 7.2 Hz, 2H), 8.08 (d, J = 3.6 Hz, 1H), 8.05 (s, 1H), 7.81 (s, 1H), 7.55-7.50 (m, 3H), 7.44-7.37 (m, 2H), 6.91 (d, J = 3.2 Hz, 1H), 2.61 (s, 3H), 2.52 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.5, 150.2, 147.9, 143.0, 139.4, 139.2, 137.4, 133.1, 132.6, 130.8, 128.6, 128.55, 128.3, 126.9, 126.6, 122.6, 121.7, 112.0, 109.3, 21.3, 15.6. HRMS calcd for $C_{23}H_{18}NOS$ $[M + H]^+$: 356.1104, found 356.1095. Elemental analysis calcd (%) for $C_{23}H_{17}NOS$: C, 77.72; H, 4.82; N, 3.94. Found: C, 77.91; H, 4.81; N, 4.92.



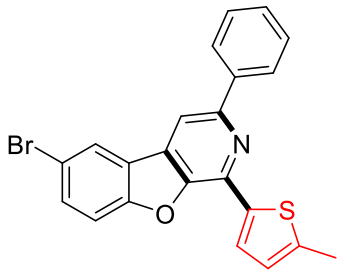
6-Methoxy-1-(5-methylthiophen-2-yl)-3-phenylbenzofuro[2,3-c]pyridine ***(3w)***: White solid (49.0 mg, 66%), mp 151-152 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.19 (d, J = 7.5 Hz, 2H), 8.07 (d, J = 3.5 Hz, 1H), 8.05 (s, 1H), 7.56 (d, J = 9.0 Hz, 1H), 7.53-7.50 (m, 2H), 7.43-7.40 (m, 2H), 7.19-7.17 (m, 1H), 6.91 (d, J = 2.7 Hz, 1H), 3.91 (s, 3H), 2.60 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.3, 151.9, 150.1, 148.3, 143.1, 139.3, 139.1, 137.6, 132.8, 128.7, 128.6, 128.4, 127.0, 126.7, 123.1, 118.3, 113.1, 109.3, 104.2, 56.0, 15.6. HRMS calcd for $C_{23}H_{18}NO_2S$ $[M + H]^+$: 372.1053, found 372.1050. Elemental analysis calcd (%) for $C_{23}H_{17}NO_2S$: C, 74.37; H, 4.61; N, 3.77. Found: C, 74.56; H, 4.60; N, 3.75.



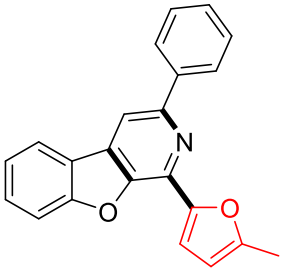
6-Fluoro-1-(5-methylthiophen-2-yl)-3-phenylbenzofuro[2,3-c]pyridine ***(3x)***: White solid (44.5 mg, 62%), mp 178-179 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, J = 7.2 Hz, 2H), 8.04 (d, J = 3.6 Hz, 1H), 8.01 (s, 1H), 7.66-7.64 (m, 1H), 7.61-7.58 (m, 1H), 7.53-7.49 (m, 2H), 7.44-7.41 (m, 1H), 7.33-7.28 (m, 1H), 6.90 (d, J = 2.4 Hz, 1H), 2.60 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.2 (d, J_{C-F} = 240.0 Hz), 153.1, 150.5, 148.5, 143.4, 139.1, 138.9, 137.8, 132.2 (d, J_{C-F} = 3.8 Hz), 128.7, 128.68, 128.5, 126.9, 126.7, 123.6 (d, J_{C-F} = 10.0 Hz), 117.3 (d, J_{C-F} = 26.3 Hz), 113.4 (d, J_{C-F} = 8.8 Hz), 109.2, 107.8 (d, J_{C-F} = 25.0 Hz), 15.6. HRMS calcd for $C_{22}H_{15}FNOS$ $[M + H]^+$: 360.0853, found 360.0847. Elemental analysis calcd (%) for $C_{22}H_{14}FNOS$: C, 73.52; H, 3.93; N, 3.90. Found: C, 73.41; H, 3.94; N, 3.92.



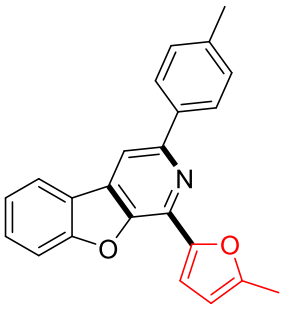
6-*Chloro-1-(5-methylthiophen-2-yl)-3-phenylbenzofuro[2,3-c]pyridine* (***3y***): White solid (55.5 mg, 74%), mp 182-183 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, J = 7.3 Hz, 2H), 8.01-7.99 (m, 2H), 7.94 (d, J = 1.8 Hz, 1H), 7.57-7.49 (m, 4H), 7.44-7.40 (m, 1H), 6.89 (d, J = 2.7 Hz, 1H), 2.59 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.3, 150.7, 148.1, 143.4, 139.1, 138.9, 137.8, 131.7, 129.7, 129.1, 128.74, 128.7, 128.6, 126.9, 126.7, 124.2, 121.7, 113.6, 109.2, 15.6. HRMS calcd for $C_{22}H_{15}ClNOS$ $[M + H]^+$: 376.0557 and 378.0528, found 376.0542 and 378.05231. Elemental analysis calcd (%) for $C_{22}H_{14}ClNOS$: C, 70.30; H, 3.75; N, 3.73. Found: C, 70.52; H, 3.73; N, 3.72.



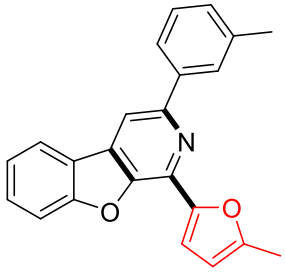
6-Bromo-1-(5-methylthiophen-2-yl)-3-phenylbenzofuro[2,3-c]pyridine (***3z***): White solid (56.8 mg, 68%), mp 201-202 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14-8.10 (m, 3H), 8.00-7.98 (m, 2H), 7.66-7.64 (m, 1H), 7.52-7.49 (m, 3H), 7.44-7.40 (m, 1H), 6.89 (d, J = 2.8 Hz, 1H), 2.59 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.8, 150.8, 147.9, 143.5, 139.1, 138.9, 137.8, 132.5, 131.5, 128.8, 128.7, 128.6, 127.0, 126.7, 124.8, 116.4, 114.1, 109.2, 15.6. HRMS calcd for $C_{22}H_{15}BrNOS$ $[M + H]^+$: 420.0052 and 422.0032, found 420.0045 and 422.0030. Elemental analysis calcd (%) for $C_{22}H_{14}BrNOS$: C, 62.87; H, 3.36; N, 3.33. Found: C, 62.59; H, 43.38; N, 3.32.



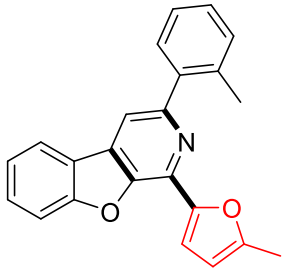
1-(5-Methylfuran-2-yl)-3-phenylbenzofuro[2,3-c]pyridine (***4a***): White solid (42.3 mg, 65%), mp 146-147 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.18 (d, J = 7.5 Hz, 2H), 8.11 (s, 1H), 8.03 (d, J = 7.6 Hz, 1H), 7.69 (d, J = 8.3 Hz, 1H), 7.62-7.59 (m, 1H), 7.54-7.49 (m, 3H), 7.44-7.40 (m, 2H), 6.28 (s, 1H), 2.55 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.1, 154.5, 151.1, 148.3, 147.4, 139.7, 134.2, 132.6, 129.7, 128.7, 128.4, 127.3, 123.4, 122.7, 121.9, 114.5, 112.6, 109.8, 108.5, 14.0. HRMS calcd for $C_{22}H_{16}NO_2$ [M + H]$^{+}$: 326.1176, found 326.1180. Elemental analysis calcd (%) for $C_{22}H_{15}NO_2$: C, 81.21; H, 4.65; N, 4.30. Found: C, 81.43; H, 4.63; N, 4.29.



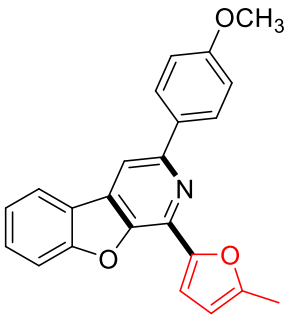
1-(5-Methylfuran-2-yl)-3-(p-tolyl)benzofuro[2,3-c]pyridine (***4b***): White solid (39.3 mg, 58%), mp 163-165 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07 (d, J = 6.9 Hz, 3H), 8.02 (d, J = 7.7 Hz, 1H), 7.69 (d, J = 8.3 Hz, 1H), 7.61-7.58 (m, 1H), 7.48 (d, J = 3.2 Hz, 1H), 7.42-7.39 (m, 1H), 7.32 (d, J = 7.9 Hz, 2H), 6.28 (d, J = 2.7 Hz, 1H), 2.54 (s, 3H), 2.44 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.1, 154.4, 151.1, 148.4, 147.2, 138.2, 136.9, 134.0, 132.6, 129.6, 129.4, 127.1, 123.4, 122.7, 121.8, 114.3, 112.5, 109.4, 108.4, 21.2, 14.0. HRMS calcd for $C_{23}H_{18}NO_2$ [M + H]$^{+}$: 340.1332, found 340.1336. Elemental analysis calcd (%) for $C_{23}H_{17}NO_2$: C, 81.40; H, 5.05; N, 4.13. Found: C, 81.23; H, 5.06; N, 4.14.



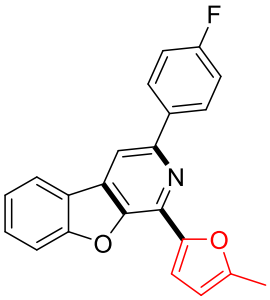
1-*(5-Methylfuran-2-yl)-3-(m-tolyl)benzofuro[2,3-c]pyridine* (***4c***): White solid (44.1 mg, 65%), mp 121-122 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (s, 1H), 8.05 (d, J = 7.2 Hz, 2H), 7.94 (d, J = 7.6 Hz, 1H), 7.70 (d, J = 8.3 Hz, 1H), 7.63-7.59 (m, 1H), 7.50 (d, J = 3.0 Hz, 1H), 7.44-7.39 (m, 2H), 7.25-7.23 (m, 1H), 6.30-6.29 (m, 1H), 2.55 (s, 3H), 2.50 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.1, 154.5, 151.4, 148.3, 147.4, 139.7, 138.3, 134.1, 132.6, 129.7, 129.2, 128.6, 128.0, 124.3, 123.4, 122.7, 121.9, 114.4, 112.6, 109.8, 108.4, 21.6, 14.0. HRMS calcd for $C_{23}H_{18}NO_2$ $[M + H]^+$: 340.1332, found 340.1330. Elemental analysis calcd (%) for $C_{23}H_{17}NO_2$: C, 81.40; H, 5.05; N, 4.13. Found: C, 81.25; H, 5.07; N, 4.12.



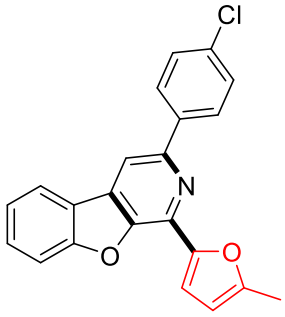
1-(5-Methylfuran-2-yl)-3-(o-tolyl)benzofuro[2,3-c]pyridine (***4d***): Yellow oil (33.9 mg, 50%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, J = 7.7 Hz, 1H), 7.81 (s, 1H), 7.73 (d, J = 8.3 Hz, 1H), 7.65-7.61 (m, 1H), 7.57-7.54 (m, 1H), 7.50 (d, J = 3.2 Hz, 1H), 7.45-7.41 (m, 1H), 7.33-7.29 (m, 3H), 6.28-6.27 (m, 1H), 2.50 (s, 3H), 2.496 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.1, 154.6, 153.5, 148.3, 146.9, 140.7, 136.4, 133.8, 132.1, 130.8, 130.1, 129.7, 128.1, 125.8, 123.5, 122.6, 121.9, 114.5, 113.3, 112.6, 108.4, 20.6, 14.1. HRMS calcd for $C_{23}H_{18}NO_2$ $[M + H]^+$: 340.1332, found 340.1342. Elemental analysis calcd (%) for $C_{23}H_{17}NO_2$: C, 81.40; H, 5.05; N, 4.13. Found: C, 81.58; H, 5.03; N, 4.12.



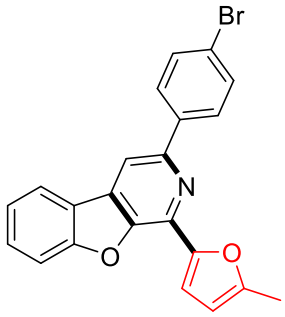
3-(4-Methoxyphenyl)-1-(5-methylfuran-2-yl)benzofuro[2,3-c]pyridine (***4e***): White solid (49.7 mg, 70%), mp 167-168 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.12 (d, J = 7.9 Hz, 2H), 8.01 (d, J = 8.3 Hz, 2H), 7.67 (d, J = 7.7 Hz, 1H), 7.60-7.57 (m, 1H), 7.46 (s, 1H), 7.41-7.38 (m, 1H), 7.04 (d, J = 7.9 Hz, 2H), 6.27 (s, 1H), 3.88 (s, 3H), 2.54 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.1, 157.1, 154.4, 150.8, 148.4, 147.0, 133.9, 132.6, 132.5, 129.6, 128.4, 123.3, 122.7, 121.8, 114.3, 114.1, 112.5, 108.9, 108.4, 55.3, 14.0. HRMS calcd for $C_{23}H_{18}NO_3$ $[M + H]^+$: 356.1281, found 356.1285. Elemental analysis calcd (%) for $C_{23}H_{17}NO_3$: C, 77.73; H, 4.82; N, 3.94. Found: C, 77.60; H, 4.44; N, 3.93.



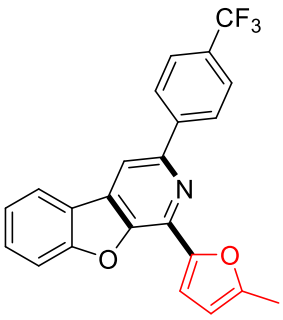
3-(4-Fluorophenyl)-1-(5-methylfuran-2-yl)benzofuro[2,3-c]pyridine (***4f***): White solid (43.9 mg, 64%), mp 160-161 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.15-8.12 (m, 2H), 8.00 (d, J = 9.6 Hz, 2H), 7.68 (d, J = 8.3 Hz, 1H), 7.61-7.58 (m, 1H), 7.46 (d, J = 3.2 Hz, 1H), 7.42-7.39 (m, 1H), 7.20-7.17 (m, 2H), 6.27 (d, J = 2.5 Hz, 1H), 2.53 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.3 (d, J_{C-F} = 246.3 Hz), 157.1, 154.5, 150.1, 148.2, 147.2, 136.0 (d, J_{C-F} = 2.5 Hz), 134.1, 132.6, 129.7, 128.9 (d, J_{C-F} = 7.5 Hz), 123.5, 122.6, 121.8, 115.5 (d, J_{C-F} = 21.3 Hz), 114.5, 112.6, 109.4, 108.5, 14.0. HRMS calcd for $C_{22}H_{15}FNO_2$ $[M + H]^+$: 344.1081, found 344.1081. Elemental analysis calcd (%) for $C_{22}H_{14}FNO_2$: C, 76.96; H, 4.11; N, 4.08. Found: C, 77.12; H, 4.10; N, 4.06.



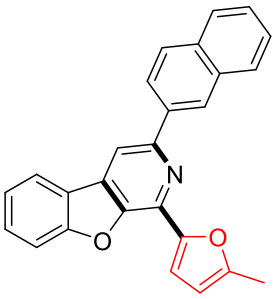
*3-(4-Chlorophenyl)-1-(5-methylfuran-2-yl)benzofuro[2,3-c]pyridine (**4g**)*: White solid (51.7 mg, 72%), mp 168-170 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07 (d, J = 8.4 Hz, 2H), 7.98-7.95 (m, 2H), 7.65 (d, J = 8.3 Hz, 1H), 7.59-756 (m, 1H), 7.46-7.43 (m, 3H), 7.40-7.37 (m, 1H), 6.26 (d, J = 2.1 Hz, 1H), 2.53 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.0, 154.5, 149.6, 148.1, 147.3, 138.1, 134.4, 134.2, 132.5, 129.7, 128.7, 128.4, 123.4, 122.5, 121.7, 114.6, 112.5, 109.4, 108.5, 14.0. HRMS calcd for $C_{22}H_{15}ClNO_2$ $[M + H]^+$: 360.0786 and 362.0756, found 360.0782 and 362.0758. Elemental analysis calcd (%) for $C_{22}H_{14}ClNO_2$: C, 73.44; H, 3.92; N, 3.89. Found: C, 73.26; H, 3.94; N, 4.88.



*3-(4-Bromophenyl)-1-(5-methylfuran-2-yl)benzofuro[2,3-c]pyridine (**4h**)*: White solid (56.4 mg, 70%), mp 163-164 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.01-7.95 (m, 4H), 7.65 (d, J = 8.3 Hz, 1H), 7.61-7.56 (m, 3H), 7.44 (d, J = 3.2 Hz, 1H), 7.40-7.37 (m, 1H), 6.27 (d, J = 2.5 Hz, 1H), 2.53 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.0, 154.5, 149.7, 148.1, 147.3, 138.6, 134.2, 132.5, 131.7, 129.7, 128.7, 123.5, 122.7, 122.5, 121.8, 114.6, 112.5, 109.4, 108.5, 14.0. HRMS calcd for $C_{22}H_{15}BrNO_2$ $[M + H]^+$: 404.0281 and 406.0260, found 404.0285 and 406.0259. Elemental analysis calcd (%) for $C_{22}H_{14}BrNO_2$: C, 65.36; H, 3.49; N, 3.46. Found: C, 65.23; H, 3.51; N, 3.47.

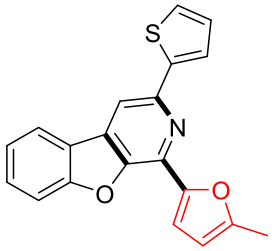


1-(5-Methylfuran-2-yl)-3-(4-(trifluoromethyl)phenyl)benzofuro[2,3-c]pyridine ***(4i)***: White solid (51.1 mg, 65%), mp 180-181 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.25 (d, J = 8.1 Hz, 2H), 8.07 (s, 1H), 8.00 (d, J = 7.7 Hz, 1H), 7.74 (d, J = 8.2 Hz, 2H), 7.68 (d, J = 8.3 Hz, 1H), 7.63-7.59 (m, 1H), 7.47 (d, J = 3.2 Hz, 1H), 7.43-740 (m, 1H), 6.28 (d, J = 3.2 Hz, 1H), 2.53 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.1, 154.7, 149.3, 148.1, 147.6, 143.0, 134.5, 132.6, 130.2 (d, J_{C-F} = 32.5 Hz), 129.9, 127.4, 125.6 (q, J_{C-F} = 3.8 Hz), 124.4 (d, J_{C-F} = 270.0 Hz), 123.6, 122.4, 121.8, 114.8, 112.6, 110.1, 108.5, 14.0. HRMS calcd for $C_{23}H_{15}F_3NO_2$ $[M + H]^+$: 394.1049, found 394.1050. Elemental analysis calcd (%) for $C_{23}H_{14}F_3NO_2$: C, 70.23; H, 3.59; N, 3.56. Found: C, 70.36; H, 3.57; N, 3.55.

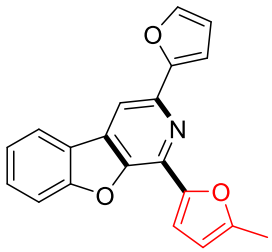


1-(5-Methylfuran-2-yl)-3-(naphthalen-2-yl)benzofuro[2,3-c]pyridine ***(4j)***: White solid (42.0 mg, 56%), mp 189-190 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (s, 1H), 8.35-8.33 (m, 1H), 8.25 (s, 1H), 8.07 (d, J = 7.7 Hz, 1H), 8.02-7.97 (m, 2H), 7.90-7.88 (m, 1H), 7.71 (d, J = 8.3 Hz, 1H), 7.64-7.60 (m, 1H), 7.55-7.49 (m, 3H), 7.56-7.42 (m, 1H), 6.31 (d, J = 3.1 Hz, 1H), 2.57 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.2, 154.6, 150.9, 148.3, 147.4, 137.1, 134.3, 133.7, 133.4, 132.7, 129.7, 128.7, 128.3, 127.7, 126.3, 126.2, 126.1, 125.2, 123.5, 122.7, 121.9, 114.6, 112.6, 110.1, 108.5, 14.1. HRMS calcd for $C_{26}H_{18}NO_2$ $[M + H]^+$: 376.1332, found 376.1337. Elemental analysis calcd (%) for $C_{26}H_{17}NO_2$: C, 83.18; H, 4.56; N, 3.73. Found: C,

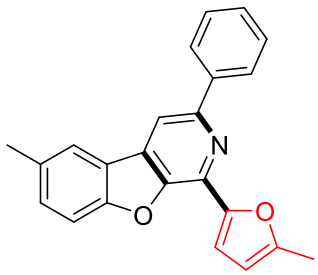
82.99; H, 4.54; N, 3.72.



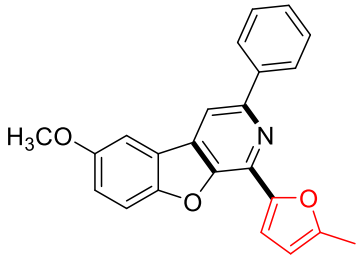
1-(5-Methylfuran-2-yl)-3-(thiophen-2-yl)benzofuro[2,3-c]pyridine (***4k***): Yellow solid (31.8 mg, 48%), mp 138-139 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02-8.00 (m, 2H), 7.70-7.66 (m, 2H), 7.62-7.58 (m, 1H), 7.46 (d, J = 3.2 Hz, 1H), 7.42-7.39 (m, 2H), 7.15-7.13 (m, 1H), 6.27 (d, J = 2.5 Hz, 1H), 2.54 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.2, 154.6, 148.0, 147.0, 146.4, 145.2, 134.1, 132.6, 129.8, 127.9, 126.8, 124.1, 123.5, 122.5, 121.9, 114.6, 112.6, 108.5, 108.1, 14.0. HRMS calcd for $C_{20}H_{14}NO_2S$ $[M + H]^+$: 332.0740, found 332.0746. Elemental analysis calcd (%) for $C_{20}H_{13}NO_2S$: C, 72.49; H, 3.95; N, 4.23. Found: C, 72.62; H, 3.94; N, 4.21.



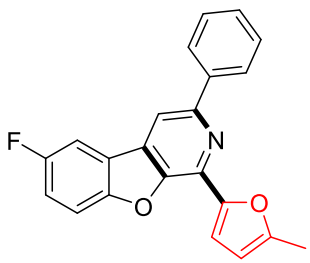
1-*(Furan-2-yl)-1-(5-methylfuran-2-yl)benzofuro[2,3-c]pyridine* (***4l***): Yellow solid (26.5 mg, 42%), mp 135-136 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11 (s, 1H), 8.03 (d, J = 7.7 Hz, 1H), 7.69 (d, J = 8.3 Hz, 1H), 7.63-7.64 (m, 1H), 7.56 (s, 1H), 7.48 (d, J = 3.2 Hz, 1H), 7.44-7.41 (m, 1H), 7.19 (d, J = 3.3 Hz, 1H), 6.58-6.57 (m, 1H), 6.27 (d, J = 3.0 Hz, 1H), 2.53 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.1, 154.7, 154.0, 147.8, 146.9, 143.4, 142.7, 134.3, 132.4, 129.8, 123.6, 122.6, 122.0, 114.8, 112.6, 112.0, 108.5, 108.1, 108.06, 14.0. HRMS calcd for $C_{20}H_{14}NO_3$ $[M + H]^+$: 316.0968, found 316.0970. Elemental analysis calcd (%) for $C_{20}H_{13}NO_3$: C, 76.18; H, 4.16; N, 4.44. Found: C, 76.02; H, 4.14; N, 4.43.



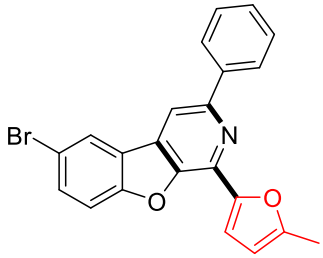
6-Methyl-1-(5-methylfuran-2-yl)-3-phenylbenzofuro[2,3-c]pyridine (***4m***): White solid (40.7 mg, 60%), mp 176-177 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17-8.15 (m, 2H), 8.08 (s, 1H), 7.83 (s, 1H), 7.59 (d, J = 8.4 Hz, 1H), 7.54-7.49 (m, 3H), 7.44-7.40 (m, 2H), 6.29-6.28 (m, 1H), 2.54 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.6, 154.5, 151.0, 148.3, 147.7, 139.8, 134.1, 133.2, 132.7, 131.0, 128.7, 128.4, 127.3, 122.7, 121.7, 114.5, 112.1, 109.8, 108.5, 21.3, 14.0. HRMS calcd for $C_{23}H_{18}NO_2$ $[M + H]^+$: 340.1332, found 340.1330. Elemental analysis calcd (%) for $C_{23}H_{17}NO_2$: C, 81.40; H, 5.05; N, 4.13. Found: C, 81.59; H, 5.03; N, 4.12.



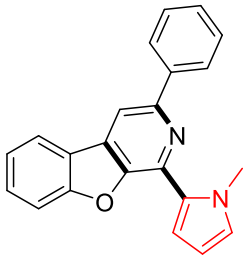
6-Methoxy-1-(5-methylfuran-2-yl)-3-phenylbenzofuro[2,3-c]pyridine (***4n***): White solid (41.2 mg, 58%), mp 121-122 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, J = 7.6 Hz, 2H), 8.05 (s, 1H), 7.57-7.49 (m, 3H), 7.48-7.40 (m, 1H), 7.19-7.16 (m, 1H), 6.27 (d, J = 3.2, 1H), 3.91 (s, 3H), 2.54 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.3, 154.4, 151.9, 150.7, 148.3, 148.0, 139.8, 134.2, 132.8, 128.7, 128.3, 127.2, 123.1, 118.4, 114.4, 113.1, 109.7, 108.4, 104.1, 56.0, 14.0. HRMS calcd for $C_{23}H_{18}NO_3$ $[M + H]^+$: 356.1281, found 356.1288. Elemental analysis calcd (%) for $C_{23}H_{17}NO_3$: C, 77.73; H, 4.82; N, 3.94. Found: C, 77.61; H, 4.84; N, 3.95.



6-Fluoro-1-(5-methylfuran-2-yl)-3-phenylbenzofuro[2,3-c]pyridine (***4o***): White solid (44.5 mg, 62%), mp 163-164 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16-8.14 (m, 2H), 8.03 (s, 1H), 7.69-7.66 (m, 1H), 7.64-7.61 (m, 1H), 7.54-750 (m, 2H), 7.45-7.41 (m, 2H), 7.34-7.29 (m, 1H), 6.28 (d, J = 2.6 Hz, 1H), 2.54 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.2 (d, J_{C-F} = 240.0 Hz), 154.7, 153.1, 151.2, 148.23, 148.2, 139.5, 134.5, 132.3 (d, J_{C-F} = 3.8 Hz), 128.7, 128.5, 127.2, 123.6 (d, J_{C-F} = 10 Hz), 117.3 (d, J_{C-F} = 25.0 Hz), 114.6, 113.4 (d, J_{C-F} = 8.8 Hz), 109.6, 108.5, 107.7 (d, J_{C-F} = 25.0 Hz), 14.0. HRMS calcd for $C_{22}H_{15}FNO_2$ $[M + H]^+$: 344.1081, found 344.1077. Elemental analysis calcd (%) for $C_{22}H_{14}FNO_2$: C, 76.96; H, 4.11; N, 4.08. Found: C, 77.09; H, 4.09; N, 4.07.

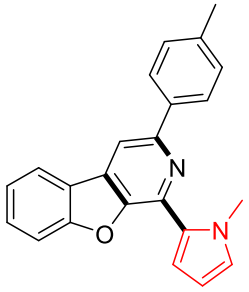


6-Bromo-1-(5-methylfuran-2-yl)-3-phenylbenzofuro[2,3-c]pyridine (***4p***): White solid (53.2 mg, 66%), mp 171-172 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14-8.12 (m, 3H), 8.00 (s, 1H), 7.68-7.65 (m, 1H), 7.55-7.49 (m, 3H), 7.44-7.41 (m, 2H), 6.27-6.26 (m, 1H), 2.53 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.7, 154.7, 151.4, 148.1, 147.6, 139.4, 134.4, 132.5, 131.5, 128.7, 128.5, 127.2, 124.7, 124.6, 116.3, 114.6, 114.1, 109.5, 108.5, 14.0. HRMS calcd for $C_{22}H_{15}BrNO_2$ $[M + H]^+$: 404.0281 and 406.0260, found 404.0285 and 406.0268. Elemental analysis calcd (%) for $C_{22}H_{14}BrNO_2$: C, 65.36; H, 3.49; N, 3.46. Found: C, 65.29; H, 3.50; N, 4.47.

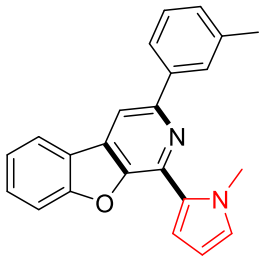


1-(1-Methyl-1H-pyrrol-2-yl)-3-phenylbenzofuro[2,3-c]pyridine (***5a***): Yellow oil (29.8 mg, 48%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.15-8.11 (m, 3H), 8.06 (d, J = 7.7 Hz, 1H),

7.71 (d, J = 8.3 Hz, 1H), 7.63-7.60 (m, 1H), 7.54-7.51 (m, 2H), 7.45-7.41 (m, 3H), 6.88 (s, 1H), 6.38 (d, J = 2.6 Hz, 1H), 4.27 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.0, 150.1, 148.6, 140.1, 137.5, 132.2, 129.5, 128.7, 128.3, 127.4, 127.1, 127.0, 123.3, 123.0, 121.7, 114.7, 112.6, 108.6, 108.0, 38.0. HRMS calcd for $C_{22}H_{17}N_2O$ $[M + H]^+$: 325.1335, found 325.1340. Elemental analysis calcd (%) for $C_{22}H_{16}N_2O$: C, 81.46; H, 4.97; N, 8.64. Found: C, 81.28; H, 4.98; N, 8.65.

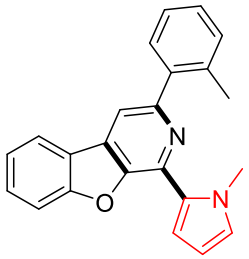


1-*(1-Methyl-1H-pyrrol-2-yl)-3-(p-tolyl)benzofuro[2,3-c]pyridine* (***5b***): White solid (40.6 mg, 60%), mp 131-132 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08-8.03 (m, 4H), 7.70 (d, J = 8.3 Hz, 1H), 7.62-7.59 (m, 1H), 7.44-7.40 (m, 2H), 7.33 (d, J = 7.9 Hz, 2H), 6.88-6.87 (m, 1H), 6.38-6.37 (m, 1H), 4.27 (s, 3H), 2.45 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.0, 150.1, 148.4, 138.1, 137.3, 137.2, 132.2, 129.43, 129.4, 127.4, 127.0, 126.8, 123.2, 123.0, 121.7, 114.6, 112.6, 108.2, 108.0, 38.0. 21.2. HRMS calcd for $C_{23}H_{19}N_2O$ $[M + H]^+$: 339.1492, found 339.1492. Elemental analysis calcd (%) for $C_{23}H_{18}N_2O$: C, 81.63; H, 5.36; N, 8.28. Found: C, 81.85; H, 5.34; N, 8.26.

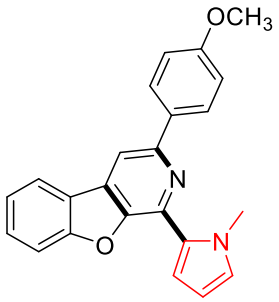


1-(1-Methyl-1H-pyrrol-2-yl)-3-(m-tolyl)benzofuro[2,3-c]pyridine (***5c***): White solid (39.2 mg, 58%), mp 111-112 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11 (s, 1H), 8.08 (d, J = 7.7 Hz, 1H), 7.96 (d, J = 9.4 Hz, 2H), 7.72 (d, J = 8.3 Hz, 1H), 7.64-7.61 (m, 1H), 7.46-7.42 (m, 3H), 7.28 (s, 1H), 6.91-6.90 (m, 1H), 6.40-6.39 (m, 1H), 4.28 (s, 3H), 2.51 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.0, 150.1, 148.5, 139.9, 138.2, 137.3, 132.2, 129.5, 129.0, 128.6, 127.7, 127.3, 127.1, 124.2, 123.3, 123.0, 121.7, 114.6,

112.6, 108.6, 108.0, 37.9, 21.7. HRMS calcd for $C_{23}H_{19}N_2O$ $[M + H]^+$: 339.1492, found 339.1495. Elemental analysis calcd (%) for $C_{23}H_{18}N_2O$: C, 81.63; H, 5.36; N, 8.28. Found: C, 81.46; H, 5.37; N, 8.29.

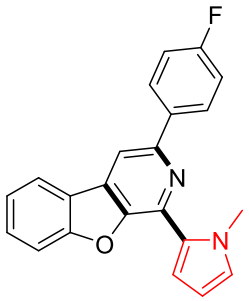


1-(1-Methyl-1H-pyrrol-2-yl)-3-(o-tolyl)benzofuro[2,3-c]pyridine ***(5d)***: Yellow oil (37.2 mg, 55%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.02 (d, J = 7.6 Hz, 1H), 7.76 (s, 1H), 7.72 (d, J = 8.4 Hz, 1H), 7.63-7.60 (m, 1H), 7.54 (d, J = 6.5 Hz, 1H), 7.44-7.40 (m, 2H), 7.35-7.32 (m, 3H), 6.84-6.83 (m, 1H), 6.37-6.35 (m, 1H), 4.14 (s, 3H), 2.46 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.9, 152.3, 148.0, 141.2, 137.2, 135.9, 131.6, 130.6, 130.0, 129.5, 127.8, 127.3, 127.0, 125.7, 123.3, 122.9, 121.8, 114.6, 112.6, 112.3, 107.9, 37.8, 20.6. HRMS calcd for $C_{23}H_{19}N_2O$ $[M + H]^+$: 339.1492, found 339.1500. Elemental analysis calcd (%) for $C_{23}H_{18}N_2O$: C, 81.63; H, 5.36; N, 8.28. Found: C, 81.41; H, 5.38; N, 8.29.

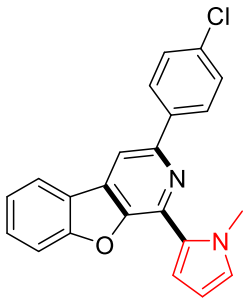


3-(4-Methoxyphenyl)-1-(1-methyl-1H-pyrrol-2-yl)benzofuro[2,3-c]pyridine ***(5e)***: White solid (48.1 mg, 68%), mp 157-158 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09-8.02 (m, 4H), 7.69 (d, J = 8.3 Hz, 1H), 7.62-7.58 (m, 1H), 7.43-7.39 (m, 2H), 7.04 (d, J = 8.5 Hz, 2H), 6.88-6.87 (m, 1H), 6.38-6.37 (m, 1H), 4.26 (s, 3H), 3.89 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.0, 157.0, 149.8, 148.2, 137.2, 132.7, 132.2, 129.4, 128.1, 127.4, 127.0, 123.2, 123.0, 121.7, 114.6, 114.1, 112.6, 108.0, 107.7, 55.4, 38.0. HRMS calcd for $C_{23}H_{19}N_2O_2$ $[M + H]^+$: 355.1441, found 355.1449. Elemental analysis calcd (%) for $C_{23}H_{18}N_2O_2$: C, 77.95; H, 5.12; N, 7.90. Found: C, 77.68; H,

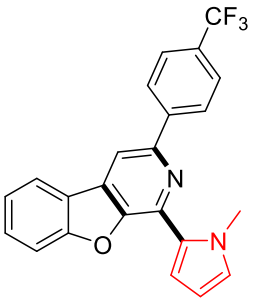
5.14; N, 7.91.



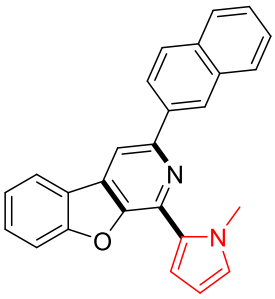
3-(4-Fluorophenyl)-1-(1-methyl-1H-pyrrol-2-yl)benzofuro[2,3-c]pyridine (***5f***): White solid (47.9 mg, 70%), mp 165-166 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.10-8.07 (m, 2H), 8.02 (d, J = 10.0 Hz, 2H), 7.69 (d, J = 8.3 Hz, 1H), 7.62-7.59 (m, 1H), 7.44-7.41 (m, 2H), 7.21-7.17 (m, 2H), 6.88 (s, 1H), 6.38-6.37 (m, 1H), 4.23 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.1 (d, J_{C-F} = 246.3 Hz), 156.9, 149.0, 148.4, 137.5, 136.2 (d, J_{C-F} = 2.5 Hz), 132.2, 129.5, 128.6 (d, J_{C-F} = 7.5 Hz), 127.2, 127.1, 123.3, 122.9, 121.7, 115.5 (d, J_{C-F} = 21.3 Hz), 114.8, 112.6, 108.2, 108.0, 38.0. HRMS calcd for $C_{22}H_{16}FN_2O$ $[M + H]^+$: 343.1241, found 343.1248. Elemental analysis calcd (%) for $C_{22}H_{15}FN_2O$: C, 77.18; H, 4.42; N, 8.18. Found: C, 77.01; H, 4.44; N, 8.19.



3-(4-Chlorophenyl)-1-(1-methyl-1H-pyrrol-2-yl)benzofuro[2,3-c]pyridine (***5g***): White solid (53.0 mg, 74%), mp 168-169 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05-8.01 (m, 4H), 7.68 (d, J = 8.3 Hz, 1H), 7.62-7.58 (m, 1H), 7.47-741 (m, 4H), 6.88 (s, 1H), 6.38-6.37 (m, 1H), 4.22 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.9, 148.7, 1485, 138.5, 137.6, 134.2, 132.1, 129.5, 128.8, 128.1, 127.2, 123.3, 122.8, 121.7, 114.8, 112.6, 108.3, 108.1, 38.0. HRMS calcd for $C_{22}H_{16}ClN_2O$ $[M + H]^+$: 359.0946 and 361.0916, found 359.0948 and 361.0922. Elemental analysis calcd (%) for $C_{22}H_{15}ClN_2O$: C, 73.64; H, 4.21; N, 7.81. Found: C, 73.82; H, 4.20; N, 7.79.

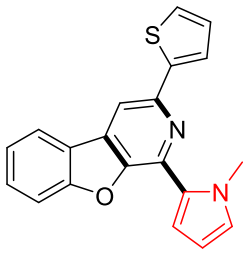


1-(1-Methyl-1H-pyrrol-2-yl)-3-(4-(trifluoromethyl)phenyl)benzofuro[2,3-c]pyridine ***(5h)***: White solid (59.6 mg, 76%), mp 173-174 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.20 (d, J = 8.1 Hz, 2H), 8.08 (s, 1H), 8.03 (d, J = 7.6 Hz, 1H), 7.75 (d, J = 8.2 Hz, 2H), 7.69 (d, J = 8.3 Hz, 1H), 7.63-7.59 (m, 1H), 7.44-7.42 (m, 2H), 6.89-6.88 (m, 1H), 6.39-6.37 (m, 1H), 4.22 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.9, 148.8, 148.3, 143.4, 137.8, 132.1, 130.0 (d, J_{C-F} = 32.5 Hz), 129.7, 127.4, 127.1, 125.6 (d, J_{C-F} = 3.8 Hz), 124.4 (d, J_{C-F} = 268.8 Hz), 123.4, 122.7, 121.7, 115.0, 112.6, 108.9, 108.1, 38.1. HRMS calcd for $C_{23}H_{16}F_3N_2O$ $[M + H]^+$: 393.1209, found 393.1212. Elemental analysis calcd (%) for $C_{23}H_{15}F_3N_2O$: C, 70.40; H, 3.85; N, 7.14. Found: C, 70.61 H, 3.83; N, 7.12.

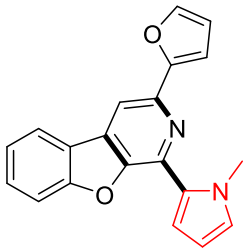


1-(1-Methyl-1H-pyrrol-2-yl)-3-(naphthalen-2-yl)benzofuro[2,3-c]pyridine ***(5i)***: White solid (54.6 mg, 73%), mp 191-192 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (s, 1H), 8.29 (d, J = 8.6 Hz, 1H), 8.22 (s, 1H), 8.08 (d, J = 7.6 Hz, 1H), 7.98 (d, J = 8.5 Hz, 2H), 7.90 (d, J = 7.0 Hz, 1H), 7.70 (d, J = 8.2 Hz, 1H), 7.63-7.59 (m, 1H), 7.56-7.52 (m, 2H), 7.46-7.42 (m, 2H), 6.91 (s, 1H), 6.41-6.40 (m, 1H), 4.30 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.0, 149.9, 148.6, 137.5, 137.4, 133.6, 133.3, 132.2, 129.5, 128.6, 128.3, 127.7, 127.4, 127.1, 126.22, 126.2, 126.0, 125.1, 123.3, 123.0, 121.7, 114.7, 112.6, 108.8, 108.0, 38.0. HRMS calcd for $C_{26}H_{19}N_2O$ $[M + H]^+$: 375.1492, found 375.1492. Elemental analysis calcd (%) for $C_{26}H_{18}N_2O$: C, 83.40; H, 4.85; N,

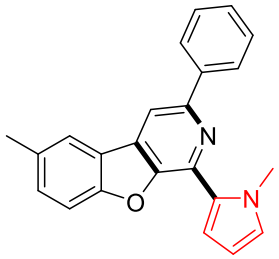
7.48. Found: C, 83.24; H, 4.86; N, 7.50.



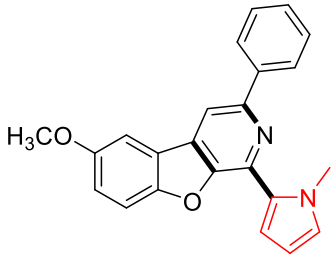
1-(1-Methyl-1H-pyrrol-2-yl)-3-(thiophen-2-yl)benzofuro[2,3-c]pyridine (***5j***): Yellow solid (33.0 mg, 50%), mp 136-138 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.03 (d, J = 7.7 Hz, 1H), 7.99 (s, 1H), 7.68 (d, J = 8.3 Hz, 1H), 7.64-7.58 (m, 2H), 7.44-7.40 (m, 2H), 7.37 (d, J = 5.0 Hz, 1H), 7.15-7.14 (m, 1H), 6.88 (s, 1H), 6.37-6.35 (m, 1H), 4.28 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.0, 148.1, 146.1, 145.2, 137.3, 132.0, 129.6, 127.9, 127.4, 126.9, 126.5, 123.3, 123.1, 122.8, 121.8, 114.9, 112.6, 108.0, 106.5, 38.3. HRMS calcd for $C_{20}H_{15}N_2OS$ $[M + H]^+$: 331.0900, found 331.0900. Elemental analysis calcd (%) for $C_{20}H_{14}N_2OS$: C, 72.70; H, 4.27; N, 8.48. Found: C, 72.89; H, 4.26; N, 8.46.



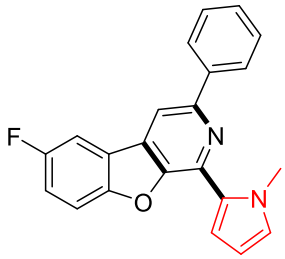
3-(Furan-2-yl)-1-(1-methyl-1H-pyrrol-2-yl)benzofuro[2,3-c]pyridine (***5k***): Yellow solid (26.4 mg, 42%), mp 129-130 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08-8.03 (m, 2H), 7.69 (d, J = 8.3 Hz, 1H), 7.62-7.56 (m, 2H), 7.44-7.39 (m, 2H), 7.04 (d, J = 3.2 Hz, 1H), 6.87 (s, 1H), 6.57-6.56 (m, 1H), 6.36-6.35 (m, 1H), 4.24 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.9, 154.6, 148.0, 142.5, 142.3, 137.6, 131.9, 129.5, 127.2, 127.0, 123.3, 122.9, 121.8, 114.8, 112.6, 112.0, 108.0, 107.4, 106.7, 37.8. HRMS calcd for $C_{20}H_{15}N_2O_2$ $[M + H]^+$: 315.1128, found 315.1138. Elemental analysis calcd (%) for $C_{20}H_{14}N_2O_2$: C, 76.42; H, 4.49; N, 8.91. Found: C, 76.58; H, 4.47; N, 8.89.



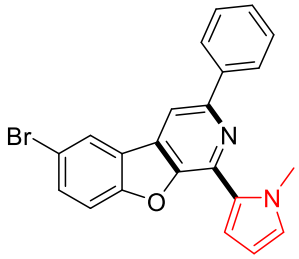
6-Methyl-1-(1-methyl-1H-pyrrol-2-yl)-3-phenylbenzofuro[2,3-c]pyridine ***(5l)***: White solid (27.0 mg, 40%), mp 148-149 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.13 (d, J = 7.8 Hz, 2H), 8.08 (s, 1H), 7.85 (s, 1H), 7.58 (d, J = 8.0 Hz, 1H), 7.53-7.50 (m, 2H), 7.44-7.39 (m, 3H), 6.88 (s, 1H), 6.36 (s, 1H), 4.26 (s, 3H), 2.55 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.5, 149.9, 148.9, 140.0, 137.4, 133.0, 132.3, 130.8, 128.7, 128.3, 127.3, 127.1, 127.0, 122.9, 121.6, 114.7, 112.1, 108.6, 108.0, 38.0, 21.3. HRMS calcd for $C_{23}H_{19}N_2O$ $[M + H]^+$: 339.1492, found 339.1499. Elemental analysis calcd (%) for $C_{23}H_{18}N_2O$: C, 81.63; H, 5.36; N, 8.28. Found: C, 81.45; H, 5.37; N, 8.30.



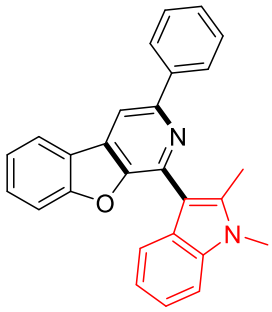
6-Methoxy-1-(1-methyl-1H-pyrrol-2-yl)-3-phenylbenzofuro[2,3-c]pyridine ***(5m)***: White solid (42.5 mg, 60%), mp 151-152 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 (d, J = 7.5 Hz, 2H), 8.07 (s, 1H), 7.58 (d, J = 9.0 Hz, 1H), 7.53-7.47 (m, 3H), 7.44-7.39 (m, 2H), 7.20-7.18 (m, 1H), 6.87 (s, 1H), 6.37-6.36 (m, 1H), 4.27 (s, 3H), 3.94 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.2, 151.7, 149.7, 149.2, 140.1, 137.5, 132.3, 128.7, 128.2, 127.4, 127.0, 126.9, 123.4, 118.1, 114.6, 113.1, 108.4, 108.0, 104.1, 56.1, 38.0. HRMS calcd for $C_{23}H_{19}N_2O_2$ $[M + H]^+$: 355.1441, found 355.1442. Elemental analysis calcd (%) for $C_{23}H_{18}N_2O_2$: C, 77.95; H, 5.12; N, 7.90. Found: C, 77.76; H, 5.13; N,7.92.



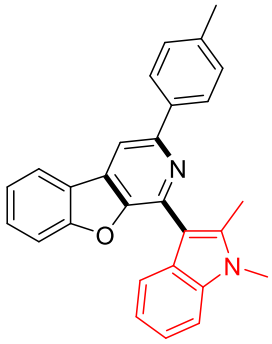
6-Fluoro-1-(1-methyl-1H-pyrrol-2-yl)-3-phenylbenzofuro[2,3-c]pyridine (***5n***): White solid (30.8 mg, 45%), mp 158-160 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.12 (d, J = 7.8 Hz, 2H), 8.04 (s, 1H), 7.71-7.69 (m, 1H), 7.65-7.62 (m, 1H), 7.53-7.50 (m, 2H), 7.44-7.39 (m, 2H), 7.34-7.32 (m, 1H), 6.88 (s, 1H), 6.37-6.36 (m, 1H), 4.26 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.2 (d, J_{C-F} = 238.8 Hz), 152.9, 150.1, 149.4, 139.9, 137.9, 131.8 (d, J_{C-F} = 3.8 Hz), 128.7, 128.3, 127.3, 127.2, 126.9, 123.9 (d, J_{C-F} = 10.0 Hz), 117.1 (d, J_{C-F} = 26.3 Hz), 114.8, 113.5 (d, J_{C-F} = 8.8 Hz), 108.4, 108.1, 107.6 (d, J_{C-F} = 25.0 Hz), 38.1. HRMS calcd for $C_{22}H_{16}FN_2O$ $[M + H]^+$: 343.1241, found 343.1239. Elemental analysis calcd (%) for $C_{22}H_{15}FN_2O$: C, 77.18; H, 4.42; N, 8.18. Found: C, 77.32; H, 4.41; N, 8.17.



6-Bromo-1-(1-methyl-1H-pyrrol-2-yl)-3-phenylbenzofuro[2,3-c]pyridine (***5o***): White solid (40.2 mg, 50%), mp 158-159 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 (d, J = 1.9 Hz, 1H), 8.09 (d, J = 7.5 Hz, 2H), 7.99 (s, 1H), 7.68-7.66 (m, 1H), 7.55-7.50 (m, 3H), 7.44-7.42 (m, 1H), 7.38-7.37 (m, 1H), 6.87 (d, J = 1.8 Hz, 1H), 6.37-6.36 (m, 1H), 4.24 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.5, 150.3, 148.7, 139.7, 137.7, 132.3, 131.0, 128.7, 128.4, 127.4, 127.0, 126.9, 125.0, 124.6, 116.2, 114.9, 114.1, 108.3, 108.1, 38.1. HRMS calcd for $C_{22}H_{16}BrN_2O$ $[M + H]^+$: 403.0441 and 405.0420, found 403.0443 and 405.0426. Elemental analysis calcd (%) for $C_{22}H_{15}BrN_2O$: C, 65.52; H, 3.75; N, 6.95. Found: C, 65.36; H, 3.74; N, 6.94.

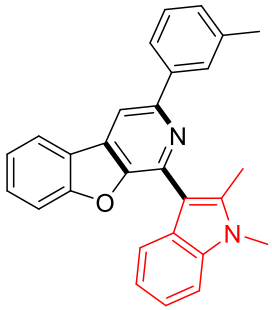


*1-(1,2-Dimethyl-1H-indol-3-yl)-3-phenylbenzofuro[2,3-c]pyridine (**6a**)*: White solid (66.7 mg, 86%), mp 227-228 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.25 (d, J = 10.2 Hz, 3H), 8.12 (d, J = 7.7 Hz, 1H), 7.90 (d, J = 7.9 Hz, 1H), 7.64-7.59 (m, 2H), 7.55-7.52 (m, 2H), 7.47-7.39 (m, 3H), 7.30-7.27 (m, 1H), 7.22-7.19 (m, 1H), 3.83 (s, 3H), 2.74 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.9, 150.9, 149.8, 140.3, 139.9, 137.5, 137.1, 132.3, 129.5, 128.6, 128.2, 127.1, 127.0, 123.2, 121.9, 121.4, 120.2, 120.16, 112.5, 109.2, 109.0, 108.9, 29.7, 21.1. HRMS calcd for $C_{27}H_{21}N_2O$ $[M + H]^+$: 389.1648, found 389.1652. Elemental analysis calcd (%) for $C_{27}H_{20}N_2O$: C, 83.48; H, 5.19; N, 7.21. Found: C, 83.59; H, 5.18; N, 7.20.

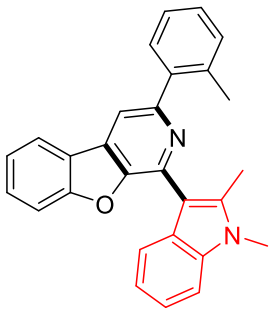


*1-(1,2-Dimethyl-1H-indol-3-yl)-3-(p-tolyl)benzofuro[2,3-c]pyridine (**6b**)*: White solid (64.3 mg, 80%), mp 219-220 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (s, 1H), 8.14-8.11 (m, 3H), 7.87 (d, J = 7.8 Hz, 1H), 7.63-7.58 (m, 2H), 7.46-7.42 (m, 1H), 7.39 (d, J = 8.4 Hz, 1H), 7.34 (d, J = 8.0 Hz, 2H), 7.29-7.28 (m, 1H), 7.21-7.17 (m, 1H), 3.83 (s, 3H), 2.73 (s, 3H), 2.44 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.8, 151.0, 149.7, 140.2, 138.0, 137.4, 137.3, 137.1, 132.2, 129.4, 129.35, 127.0, 126.9, 123.3, 123.1, 121.8, 121.3, 120.3, 120.1, 112.5, 109.4, 108.8, 108.5, 29.6, 21.2, 12.0. HRMS calcd for $C_{28}H_{23}N_2O$ $[M + H]^+$: 403.1805, found 403.1803. Elemental analysis calcd (%) for $C_{28}H_{22}N_2O$: C, 83.56; H, 5.51; N, 6.96. Found: C, 83.74; H, 5.49; N,

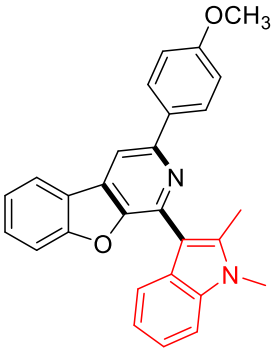
7.94.



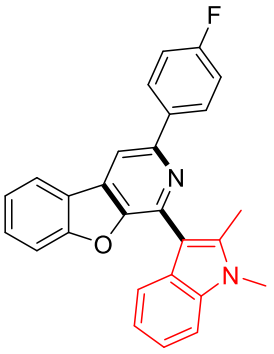
1-(1,2-Dimethyl-1H-indol-3-yl)-3-(m-tolyl)benzofuro[2,3-c]pyridine ***(6c)***: White solid (61.9 mg, 77%), mp 206-207 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (s, 1H), 8.14-8.05 (m, 3H), 7.92 (d, J = 7.8 Hz, 1H), 7.65-7.58 (m, 2H), 7.47-7.40 (m, 3H), 7.31-7.27 (m, 2H), 7.23-7.20 (m, 1H), 3.83 (s, 3H), 2.74 (s, 3H), 2.51 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.9, 151.2, 149.9, 140.3, 140.1, 138.2, 137.5, 137.2, 132.3, 129.5, 129.0, 128.6, 127.8, 127.1, 124.2, 123.3, 123.2, 121.9, 121.4, 120.4, 120.2, 112.6, 109.4, 109.1, 108.9, 29.7, 21.7, 12.1. HRMS calcd for $C_{28}H_{23}N_2O$ [M + H]$^{+}$: 403.1805, found 403.1798. Elemental analysis calcd (%) for $C_{28}H_{22}N_2O$: C, 83.56; H, 5.51; N, 6.96. Found: C, 83.69; H, 5.48; N, 7.95.



1-(1,2-Dimethyl-1H-indol-3-yl)-3-(o-tolyl)benzofuro[2,3-c]pyridine ***(6d)***: White solid (22.5 mg, 28%), mp 206-207 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, J = 7.86 Hz, 1H), 7.94 (s, 1H), 7.85 (d, J = 7.9 Hz, 1H), 7.68-7.60 (m, 3H), 7.48-7.44 (m, 1H), 7.42-7.36 (m, 4H), 7.32-7.28 (m, 1H), 7.24-7.20 (m, 1H), 3.81 (s, 3H), 2.70 (s, 3H), 2.59 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.8, 153.6, 149.5, 141.3, 140.0, 137.2, 137.0, 135.9, 131.5, 130.5, 130.2, 129.5, 127.8, 127.0, 125.7, 123.2, 123.1, 121.9, 121.2, 120.1, 120.0, 112.9, 112.5, 109.1, 108.8, 29.6, 20.8, 11.9. HRMS calcd for $C_{28}H_{23}N_2O$ [M + H]$^{+}$: 403.1805, found 403.1795. Elemental analysis calcd (%) for $C_{28}H_{22}N_2O$: C, 83.56; H, 5.51; N, 6.96. Found: C, 83.42; H, 5.52; N, 7.98.

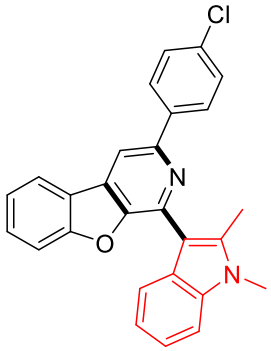


1-(1,2-Dimethyl-1H-indol-3-yl)-3-(4-methoxyphenyl)benzofuro[2,3-c]pyridine ***(6e)***: White solid (71.9 mg, 86%), mp 236-237 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20-8.18 (m, 3H), 8.10 (d, J = 7.7 Hz, 1H), 7.90 (d, J = 7.8 Hz, 1H), 7.62-7.56 (m, 2H), 7.45-7.38 (m, 2H), 7.29-7.27 (m, 1H), 7.21-7.17 (m, 1H), 7.07-7.04 (m, 2H), 3.89 (s, 3H), 3.83 (s, 3H), 2.72 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.0, 156.9, 150.7, 149.5, 140.1, 137.4, 137.1, 132.8, 132.3, 129.4, 128.2, 127.0, 123.3, 123.1, 121.9, 121.3, 120.3, 120.1, 114.1, 112.5, 109.4, 108.9, 108.1, 55.3, 29.7, 12.1. HRMS calcd for $C_{28}H_{23}N_2O_2$ $[M + H]^+$: 419.1754, found 419.1763. Elemental analysis calcd (%) for $C_{28}H_{22}N_2O_2$: C, 80.36; H, 5.30; N, 6.69. Found: C, 80.52; H, 5.28; N, 6.67.

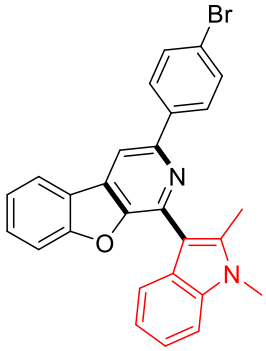


1-*(1,2-Dimethyl-1H-indol-3-yl)-3-(4-fluorophenyl)benzofuro[2,3-c]pyridine* ***(6f)***: White solid (51.2 mg, 63%), mp 219-197 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24-8.19 (m, 3H), 8.10 (d, J = 7.7 Hz, 1H), 7.91 (d, J = 7.8 Hz, 1H), 7.64-7.58 (m, 2H), 7.46-7.39 (m, 2H), 7.31-7.28 (m, 1H), 7.23-7.19 (m, 3H), 3.82 (s, 3H), 2.71 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.1 (d, J_{C-F} = 246.3 Hz), 156.9, 150.0, 149.8, 140.4, 137.4, 137.1, 136.2 (d, J_{C-F} = 2.5 Hz), 132.3, 129.6, 128.7 (d, J_{C-F} = 7.5 Hz), 127.0, 123.2, 123.1, 121.9, 121.4, 120.2, 120.16, 115.5 (d, J_{C-F} = 21.3 Hz), 112.5, 109.2, 108.9, 108.6, 29.7, 12.0. HRMS calcd for $C_{27}H_{20}FN_2O$ $[M + H]^+$: 407.1554, found 407.1562. Elemental analysis calcd (%) for $C_{27}H_{19}FN_2O$: C, 79.79; H, 4.71; N, 6.89.

Found: C, 79.92; H, 4.70; N, 6.88.

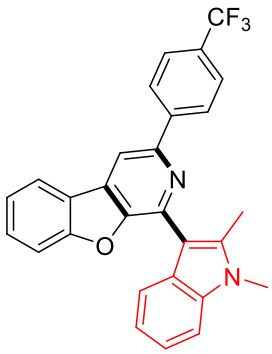


3-(4-Chlorophenyl)-1-(1,2-dimethyl-1H-indol-3-yl)benzofuro[2,3-c]pyridine ***(6g)***: White solid (54.0 mg, 64%), mp 244-245 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (S, 1H), 8.19-8.15 (m, 2H), 8.11 (d, J = 7.6 Hz, 1H), 7.85 (d, J = 7.8 Hz, 1H), 7.64-7.59 (m, 2H), 7.49-7.43 (m, 3H), 7.40 (d, J = 8.0 Hz, 1H), 7.29-7.27 (m, 1H), 7.21-7.17 (m, 1H), 3.84 (s, 3H), 2.71 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.9, 149.9, 149.7, 140.5, 138.5, 137.5, 137.1, 134.3, 132.3, 129.6, 128.8, 128.2, 127.0, 123.3, 123.1, 121.9, 121.4, 120.2, 120.17, 112.5, 109.2, 108.9, 108.8, 29.7, 12.1. HRMS calcd for $C_{27}H_{20}ClN_2O$ $[M + H]^+$: 423.1259 and 425.1229, found 423.1263 and 425.1225. Elemental analysis calcd (%) for $C_{27}H_{19}ClN_2O$: C, 76.68; H, 4.53; N, 6.62. Found: C, 76.53; H, 4.54; N, 6.64.

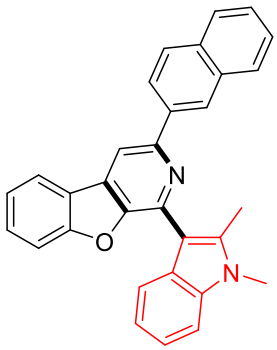


3-(4-Bromophenyl)-1-(1,2-dimethyl-1H-indol-3-yl)benzofuro[2,3-c]pyridin ***(6h)***: White solid (53.1 mg, 57%), mp 250-251 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (s, 1H), 8.13-8.10 (m, 3H), 7.86 (d, J = 7.9 Hz, 1H), 7.65-7.58 (m, 4H), 7.46-7.38 (m, 2H), 7.29-7.28 (m, 1H), 7.21-7.17 (m, 1H), 3.83 (s, 3H), 2.70 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.9, 149.9, 149.7, 140.5, 138.9, 137.5, 137.1, 132.3, 131.8, 129.6, 128.6, 127.0, 123.3, 123.1, 122.6, 121.9, 121.5, 120.2, 120.17, 112.6, 109.2, 108.9, 108.8, 29.7, 12.1. HRMS calcd for $C_{27}H_{20}BrN_2O$ $[M + H]^+$: 467.0754 and 469.0733,

found 467.0753 and 469.0728. Elemental analysis calcd (%) for $C_{27}H_{19}BrN_2O$: C, 69.39; H, 4.10; N, 5.99. Found: C, 69.52; H, 4.09; N, 5.98.

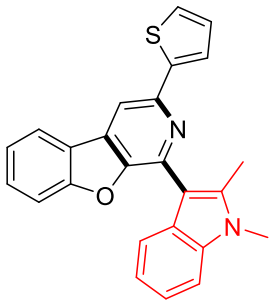


1-(1,2-Dimethyl-1H-indol-3-yl)-3-(4-(trifluoromethyl)phenyl)benzofuro[2,3-c]pyridine ***(6i)***: White solid (75.7 mg, 83%), mp 239-240 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (d, J = 8.1 Hz, 2H), 8.29 (s, 1H), 8.13 (d, J = 7.7 Hz, 1H), 7.86 (d, J = 7.8 Hz, 1H), 7.77 (d, J = 8.2 Hz, 2H), 7.65-7.60 (m, 2H), 7.49-7.45 (m, 1H), 7.40 (d, J = 8.0 Hz, 1H), 7.30-7.28 (m, 1H), 7.21-7.17 (m, 1H), 3.84 (s, 3H), 2.72 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.0, 150.2, 149.3, 143.2, 140.8, 137.7, 137.2, 132.5, 130.2 (d, J_{C-F} = 32.5 Hz), 129.8, 127.3, 126.9, 125.6 (d, J_{C-F} = 3.8 Hz), 124.4 (d, J_{C-F} = 270.0 Hz), 1235, 123.0, 122.0, 121.6, 120.4, 120.2, 112.6, 109.4, 109.1, 109.0, 29.8, 12.2. HRMS calcd for $C_{28}H_{20}F_3N_2O$ $[M + H]^+$: 457.1522, found 457.1514. Elemental analysis calcd (%) for $C_{28}H_{19}F_3N_2O$: C, 73.68; H, 4.20; N, 6.14. Found: C, 73.82; H, 4.19; N, 6.12.

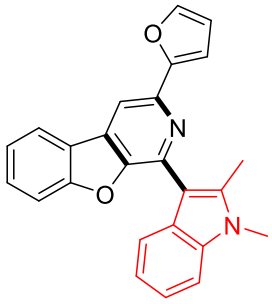


1-(1,2-Dimethyl-1H-indol-3-yl)-3-(naphthalen-2-yl)benzofuro[2,3-c]pyridine ***(6j)***: White solid (63.1 mg, 72%), mp 205-206 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.76 (s, 1H), 8.49-8.46 (m, 1H), 8.42 (s, 1H), 7.17 (d, J = 7.6 Hz, 1H), 8.05-8.01 (m, 3H), 7.95-7.92 (m, 1H), 7.68-7.60 (m, 2H), 7.57-7.54 (m, 2H), 7.50-7.43 (m, 2H), 7.36-7.33 (m, 1H), 7.30-7.26 (m, 1H), 3.84 (s, 3H), 2.78 (s, 3H); ^{13}C NMR (125 MHz,

$CDCl_3$) δ 156.9, 150.8, 149.9, 140.4, 137.44, 137.4, 137.1, 133.7, 133.4, 132.3, 129.5, 128.6, 128.2, 127.6, 127.1, 126.1, 126.06, 126.0, 125.1, 123.2, 123.19, 121.9, 121.4, 120.3, 120.2, 112.5, 109.4, 109.2, 108.9, 29.6, 12.1. HRMS calcd for $C_{31}H_{23}N_2O$ [M + H]$^+$: 439.1805, found 439.1804. Elemental analysis calcd (%) for $C_{31}H_{22}N_2O$: C, 84.91; H, 5.06; N, 6.39. Found: C, 84.68; H, 5.07; N, 6.41.

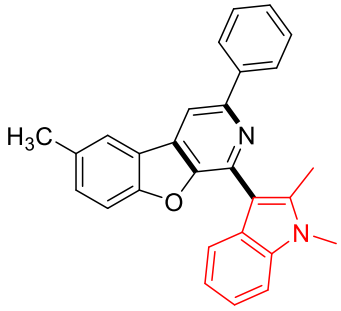


1-(1,2-Dimethyl-1H-indol-3-yl)-3-(thiophen-2-yl)benzofuro[2,3-c]pyridine ***(6k)***: White solid (49.6 mg, 63%), mp 206-207 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (s, 1H), 8.09 (d, J = 7.6 Hz, 1H), 7.94 (d, J = 7.8 Hz, 1H), 7.73 (d, J = 3.5 Hz, 1H), 7.62-7.57 (m, 2H), 7.45-7.38 (m, 3H), 7.30-7.28 (m, 1H), 7.22-7.15 (m, 2H), 3.82 (s, 3H), 2.73 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.9, 149.3, 146.4, 146.0, 140.3, 137.9, 137.1, 132.2, 129.6, 127.9, 126.9, 126.6, 123.4, 123.2, 123.1, 121.9, 121.4, 120.5, 120.2, 112.5, 108.9, 108.8, 107.1, 29.7, 12.1. HRMS calcd for $C_{25}H_{19}N_2OS$ [M + H]$^+$: 395.1213, found 395.1218. Elemental analysis calcd (%) for $C_{25}H_{18}N_2OS$: C, 76.12; H, 4.60; N, 7.10. Found: C, 76.32; H, 4.58; N, 7.08.

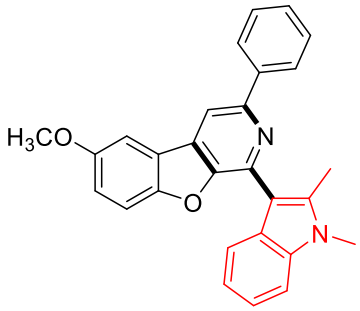


1-*(1,2-Dimethyl-1H-indol-3-yl)-3-(furan-2-yl)benzofuro[2,3-c]pyridine* ***(6l)***: White solid (53.7 mg, 71%), mp 201-202 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (s, 1H), 8.10 (d, J = 7.7 Hz, 1H), 7.88 (d, J = 7.9 Hz, 1H), 7.62-7.56 (m, 3H), 7.45-7.37 (m, 2H), 7.29-7.27 (m, 1H), 7.20-7.17 (m, 2H), 6.58-6.57 (m, 1H), 3.82 (s, 3H), 2.70 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.8, 154.7, 149.3, 143.5, 142.4, 140.6, 137.6,

137.1, 131.9, 129.5, 127.0, 123.3, 123.2, 122.0, 121.4, 120.3, 120.2, 112.5, 112.0, 109.0, 108.8, 107.6, 107.2, 29.7, 12.0. HRMS calcd for $C_{25}H_{19}N_2O_2$ [M + H]$^+$: 379.1441, found 379.1448. Elemental analysis calcd (%) for $C_{25}H_{18}N_2O_2$: C, 79.35; H, 4.79; N, 7.40. Found: C, 79.21; H, 4.80; N, 67.41.

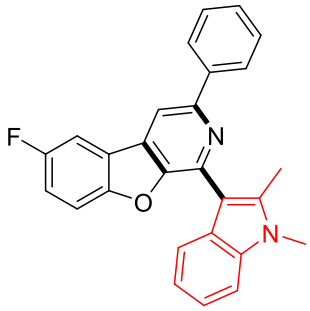


1-(1,2-Dimethyl-1H-indol-3-yl)-6-methyl-3-phenylbenzofuro[2,3-c]pyridine ***(6m)***: White solid (50.7 mg, 63%), mp 217-218 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26-8.23 (m, 3H), 7.90 (d, J = 8.2 Hz, 2H), 7.55-7.50 (m, 3H), 7.45-7.38 (m, 3H), 7.30-7.28 (m, 1H), 7.22-7.18 (m, 1H), 3.82 (s, 3H), 2.72 (s, 3H), 2.57 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.3, 150.8, 150.2, 140.2, 140.0, 137.4, 137.1, 132.9, 132.3, 130.7, 128.6, 128.2, 127.0, 123.2, 121.7, 121.3, 120.3, 120.1, 112.0, 109.3, 109.0, 108.8, 29.7, 21.3, 12.1. HRMS calcd for $C_{28}H_{23}N_2O$ [M + H]$^+$: 403.1805, found 403.1799. Elemental analysis calcd (%) for $C_{28}H_{22}N_2O$: C, 83.56; H, 5.51; N, 6.96. Found: C, 83.64; H, 5.50; N, 6.95.

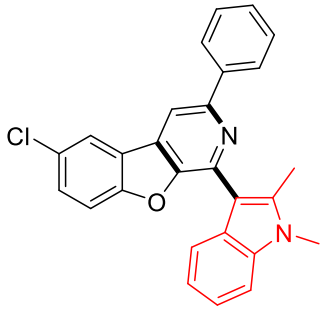


1-(1,2-Dimethyl-1H-indol-3-yl)-6-methoxy-3-phenylbenzofuro[2,3-c]pyridine ***(6n)***: White solid (67.7 mg, 81%), mp 187-188 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26-8.23 (m, 3H), 7.90 (d, J = 7.8 Hz, 1H), 7.56-7.51 (m, 4H), 7.44-7.38 (m, 2H), 7.30-7.28 (m, 1H), 7.22-7.19 (m, 2H), 3.96 (s, 3H), 3.82 (s, 3H), 2.72 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.2, 151.7, 150.6, 150.56, 140.4, 140.1, 137.4, 137.1, 132.4, 128.6, 128.1, 127.02, 127.0, 123.7, 121.3, 120.3, 120.1, 118.2, 113.1, 109.3, 108.8, 104.3, 56.1,

29.7, 12.1. HRMS calcd for $C_{28}H_{23}N_2O_2$ $[M + H]^+$: 419.1754, found 419.1761. Elemental analysis calcd (%) for $C_{28}H_{22}N_2O_2$: C, 80.36; H, 5.30; N, 6.69. Found: C, 80.25; H, 5.31; N, 6.70.

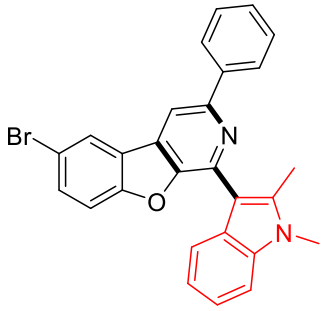


1-(1,2-Dimethyl-1H-indol-3-yl)-6-fluoro-3-phenylbenzofuro[2,3-c]pyridine ***(6o)***: White solid (62.5 mg, 77%), mp 242-243 ^oC. ^1H NMR (500 MHz, $CDCl_3$) δ 8.26 (d, J = 7.9 Hz, 2H), 8.20 (s, 1H), 7.92 (d, J = 7.9 Hz, 1H), 7.77-7.75 (m, 1H), 7.57-7.54 (m, 3H), 7.47-7.44 (m, 1H), 7.41 (d, J = 8.1 Hz, 1H), 7.33-7.29 (m, 2H), 7.25-7.22 (m, 1H), 3.81 (s, 3H), 2.72 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.0 (d, J_{C-F} = 238.8 Hz), 152.8, 150.9, 150.7, 140.6, 139.8, 137.5, 137.0, 131.9 (d, J_{C-F} = 3.8 Hz), 128.6, 128.3, 126.94, 126.9, 124.1 (d, J_{C-F} = 10 Hz), 121.4, 120.2, 120.15, 117.1 (d, J_{C-F} = 25.0 Hz), 113.3 (d, J_{C-F} = 8.8 Hz), 109.1, 108.9, 108.8, 107.7 (d, J_{C-F} = 25.0 Hz), 29.6, 12.0. HRMS calcd for $C_{27}H_{20}FN_2O$ $[M + H]^+$: 407.1554, found 407.1554. Elemental analysis calcd (%) for $C_{27}H_{19}FN_2O$: C, 79.79; H, 4.71; N, 6.89. Found: C, 79.68; H, 4.70; N, 6.88.

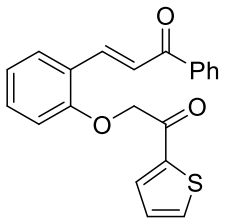


6-Chloro-1-(1,2-dimethyl-1H-indol-3-yl)-3-phenylbenzofuro[2,3-c]pyridine ***(6p)***: White solid (64.1 mg, 76%), mp 251-252 ^oC. ^1H NMR (400 MHz, $CDCl_3$) δ 8.23-8.19 (m, 3H), 8.08 (s, 1H), 7.87 (d, J = 7.8 Hz, 1H), 7.54-7.51 (m, 4H), 7.45-7.38 (m, 2H), 7.30-7.28 (m, 1H), 7.22-7.18 (m, 1H), 3.81 (s, 3H), 2.71 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.1, 151.2, 150.3, 140.7, 139.7, 137.6, 137.1, 131.3, 129.6, 128.8, 128.7,

128.4, 127.0, 126.9, 124.7, 121.7, 121.4, 120.2, 120.16, 113.6, 109.1, 108.9, 108.85, 29.7, 12.1. HRMS calcd for $C_{27}H_{20}ClN_2O$ $[M + H]^+$: 423.1259 and 425.1229, found 423.1268 and 425.1230. Elemental analysis calcd (%) for $C_{27}H_{19}ClN_2O$: C, 76.68; H, 4.53; N, 6.62. Found: C, 76.79; H, 4.52; N, 6.61.



6-Bromo-1-(1,2-dimethyl-1H-indol-3-yl)-3-phenylbenzofuro[2,3-c]pyridine (***6q***): White solid (67.0 mg, 74%), mp 260-261 ^oC. ^1H NMR (400 MHz, $CDCl_3$) δ 8.25-8.19 (m, 4H), 7.86 (d, J = 7.8 Hz, 1H), 7.69-7.66 (m, 1H), 7.54-7.48 (m, 3H), 7.45-7.38 (m, 2H), 7.30-7.28 (m, 1H), 7.21-7.17 (m, 1H), 3.82 (s, 3H), 2.71 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.5, 151.3, 150.2, 140.6, 139.7, 137.6, 137.1, 132.3, 131.2, 128.7, 128.4, 127.0, 126.9, 125.3, 124.8, 121.5, 120.3, 120.2, 116.1, 114.1, 109.1, 108.9, 108.85, 29.7, 12.1. HRMS calcd for $C_{27}H_{20}BrN_2O$ $[M + H]^+$: 467.0754 and 469.0733, found 467.0760 and 469.0741. Elemental analysis calcd (%) for $C_{27}H_{19}BrN_2O$: C, 69.39; H, 4.10; N, 5.99. Found: C, 69.52; H, 4.09; N, 5.97.



(E)-3-(2-(2-oxo-2-(Thiophen-2-yl)ethoxy)phenyl)-1-phenylprop-2-en-1-one (***8a***): ^1H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, J = 15.9 Hz, 1H), 8.07-8.05 (m, 2H), 7.94-7.93 (m, 1H), 7.87 (d, J = 15.8 Hz, 1H), 7.71-7.69 (m, 1H), 7.66-7.64 (m, 1H), 7.59-7.55 (m, 1H), 7.51-7.47 (m, 2H), 7.36-7.32 (m, 1H), 7.16-7.14 (m, 1H), 7.07-7.03 (m, 1H), 6.89 (d, J = 8.3 Hz, 1H), 5.22 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 191.0, 187.2, 157.1, 140.5, 140.1, 138.4, 134.7, 133.0, 132.6, 131.5, 130.4, 128.6, 128.5, 128.4, 124.5, 123.9, 121.9, 112.3, 71.5.

7. NMR spectra for all products

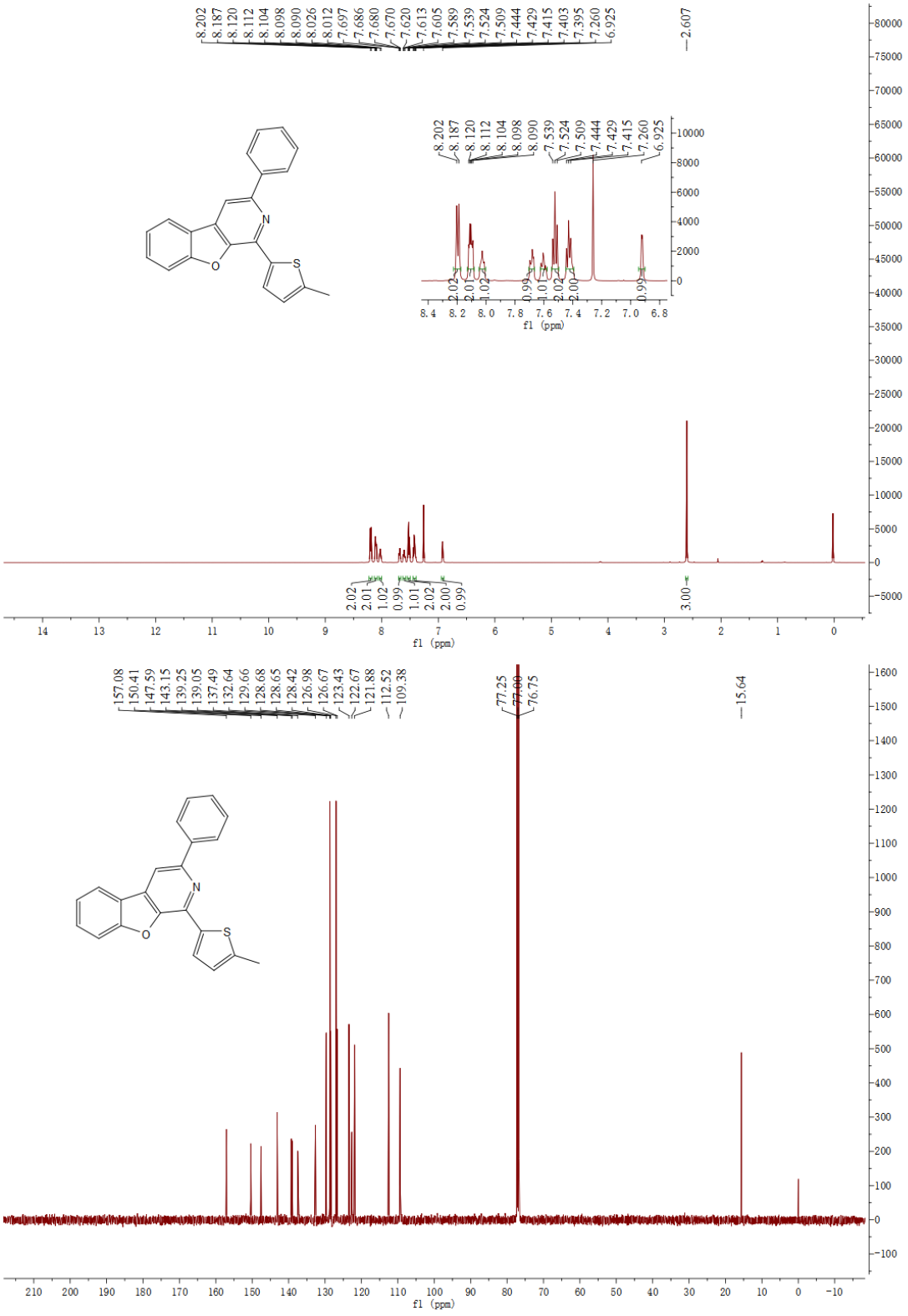


Figure S20. ^{1}H NMR of **3a** (500 MHz, $CDCl_3$) and ^{13}C NMR of **3a** (125 MHz, $CDCl_3$)

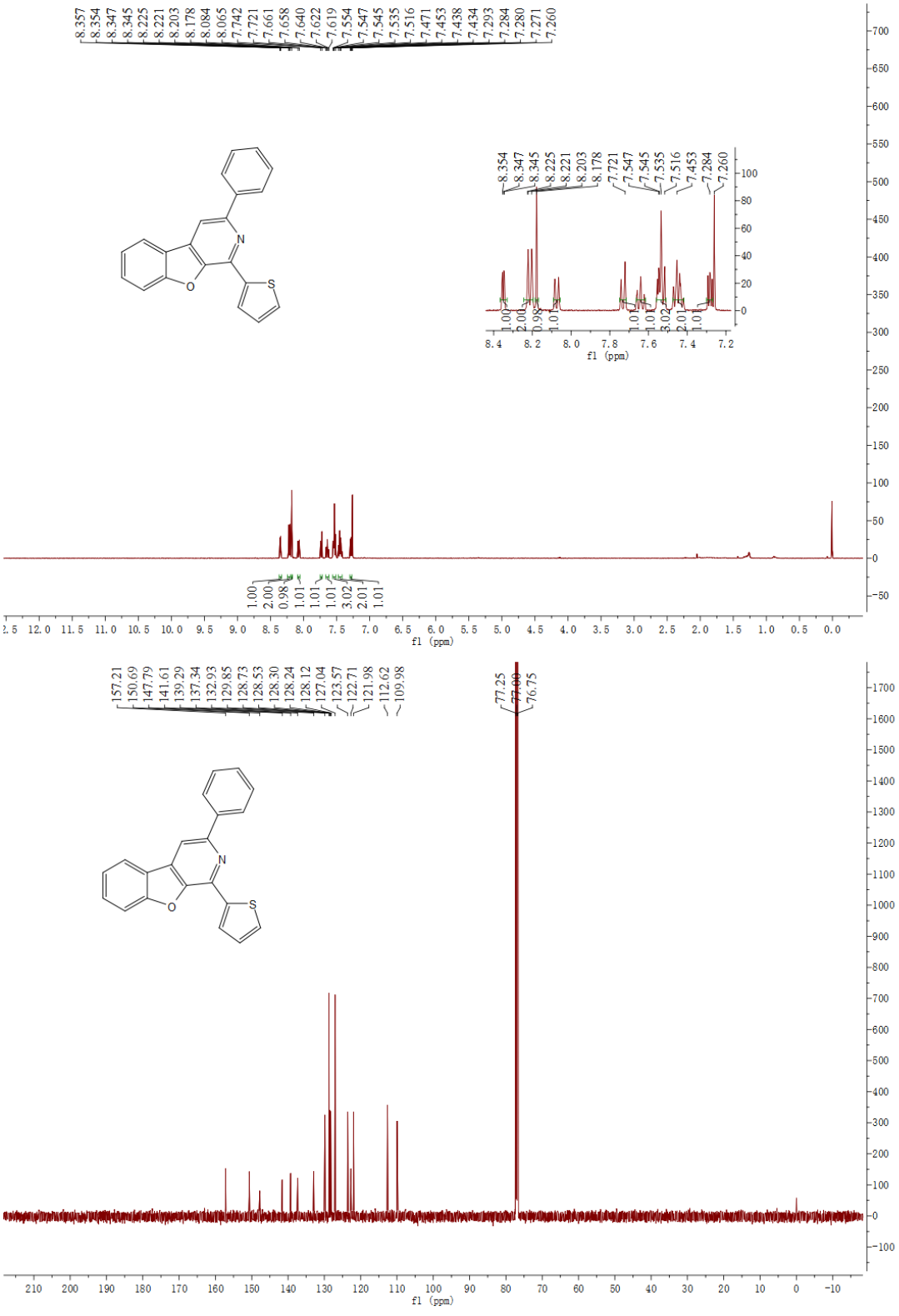


Figure S21. ^{1}H NMR of **3b** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3b** (125 MHz, $CDCl_3$)

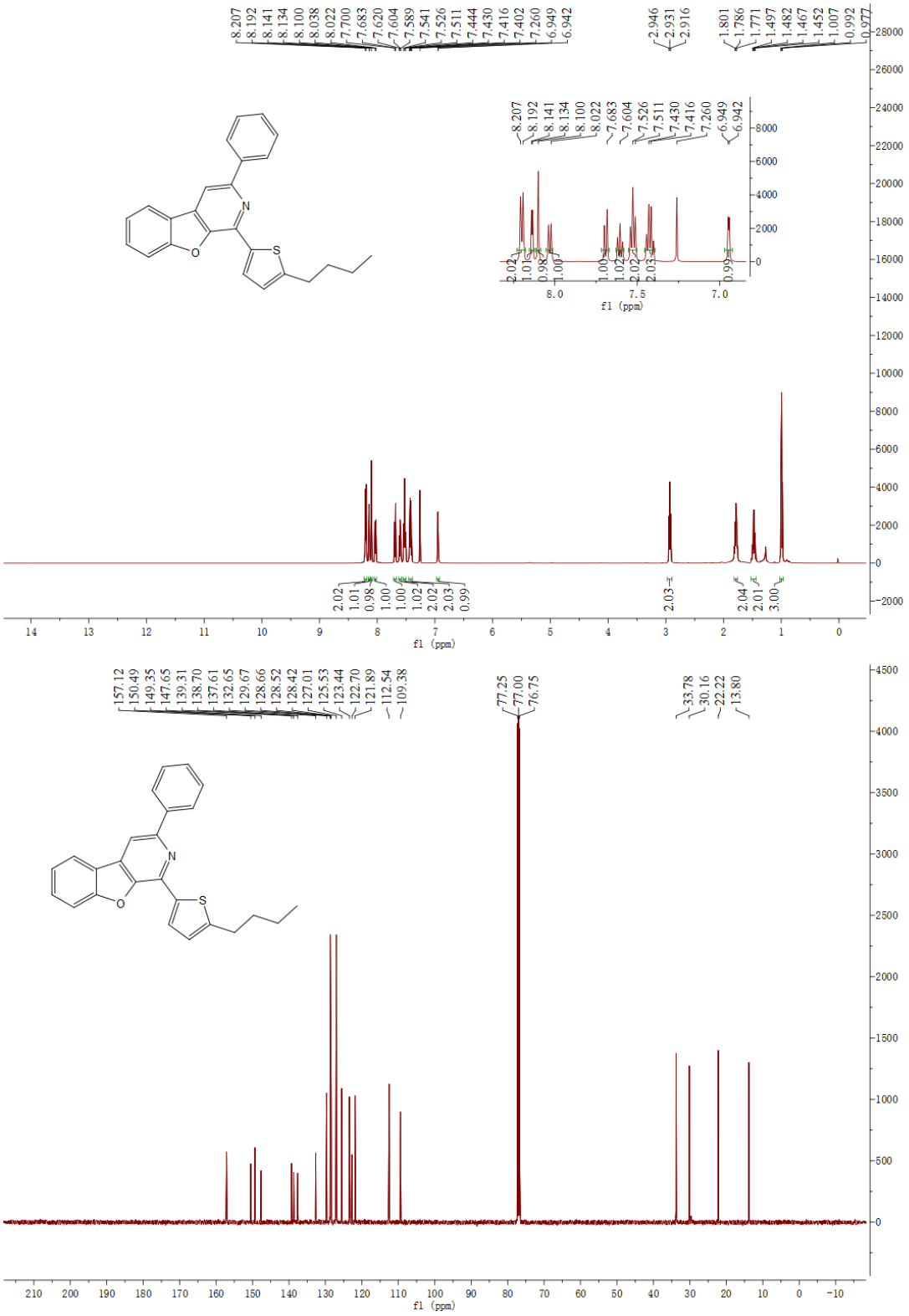


Figure S22. ^{1}H NMR of **3c** (500 MHz, $CDCl_3$) and ^{13}C NMR of **3c** (125 MHz, $CDCl_3$)

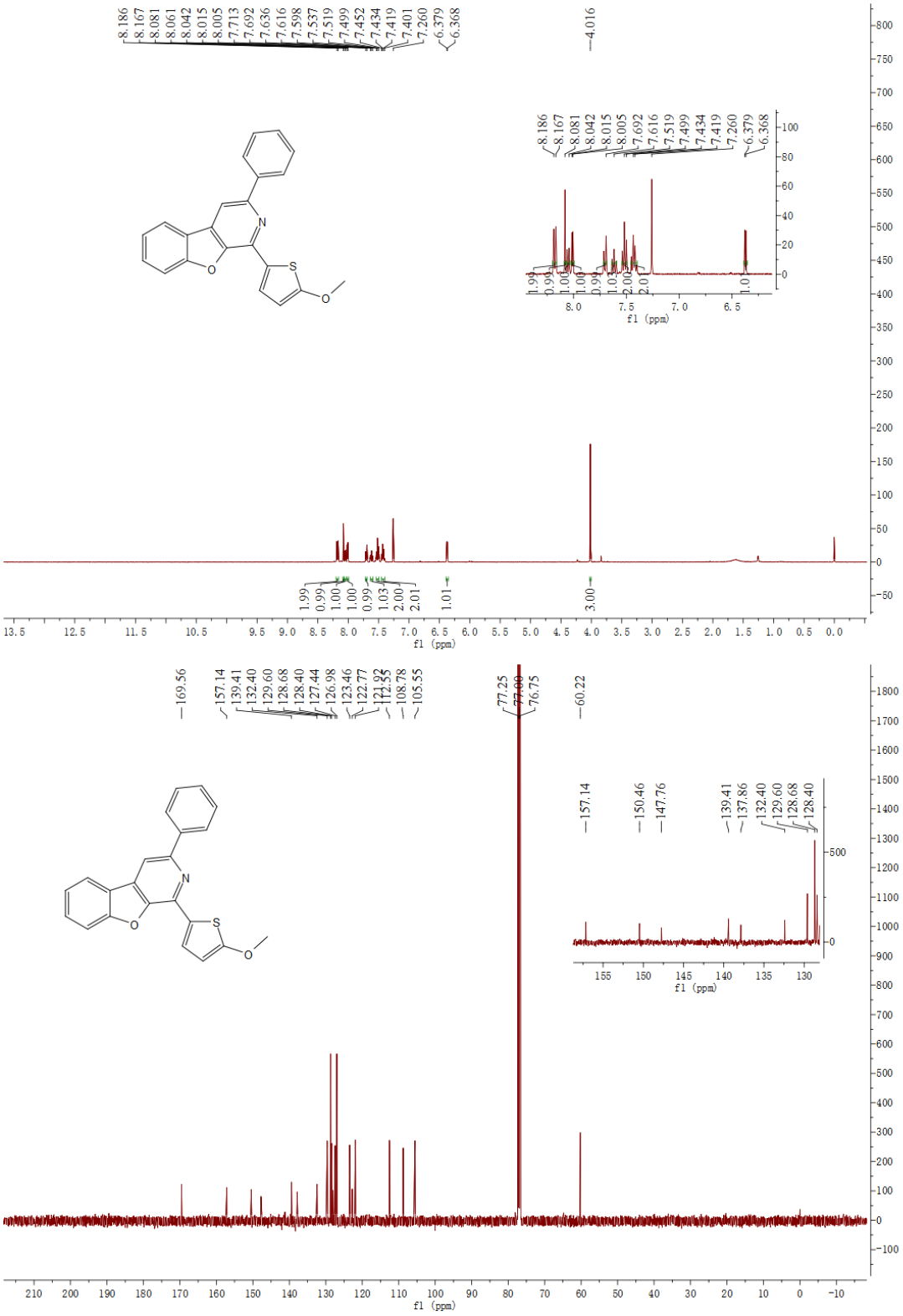


Figure S23. ^{1}H NMR of **3d** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3d** (125 MHz, $CDCl_3$)

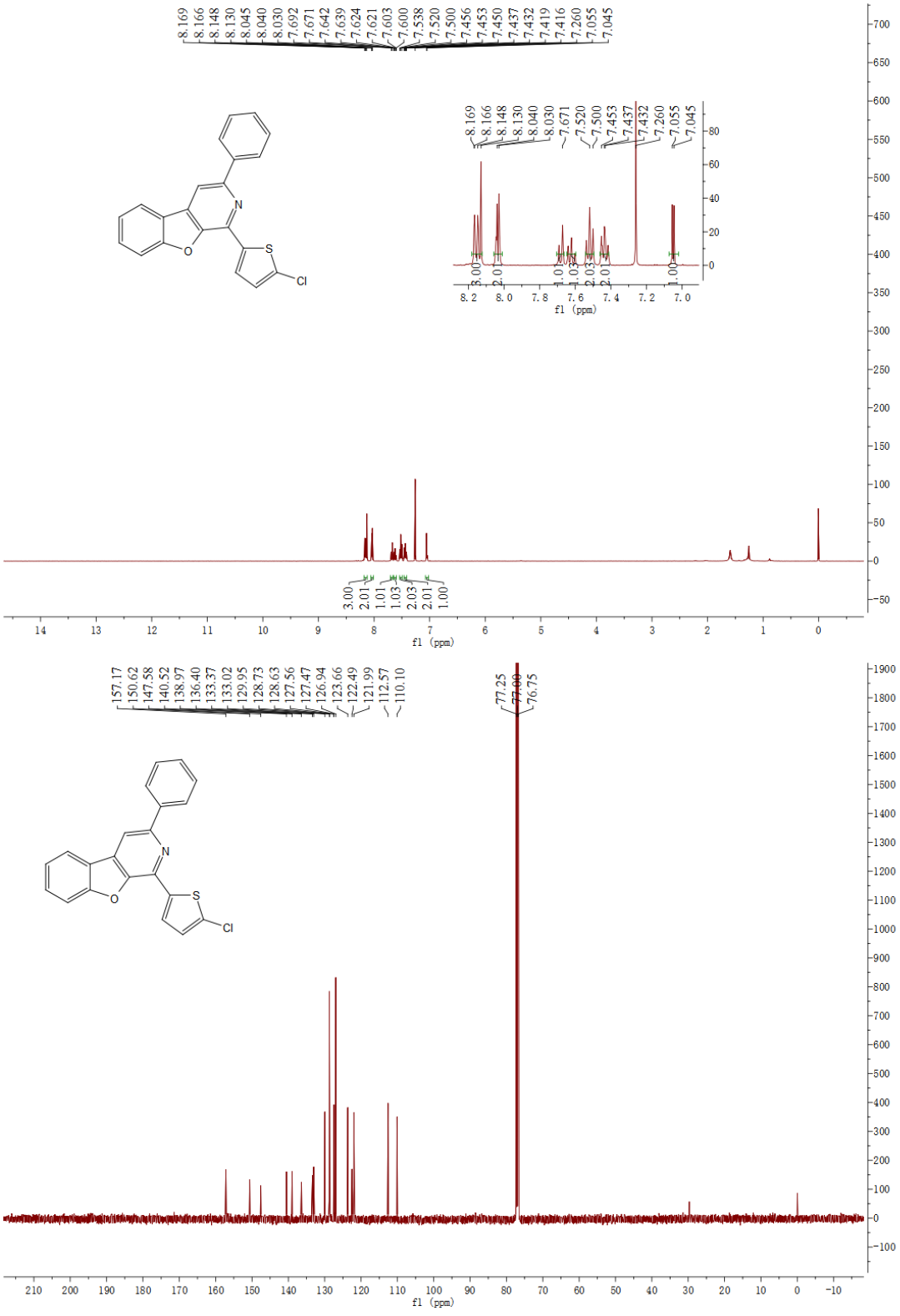


Figure S24. ^{1}H NMR of **3e** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3e** (125 MHz, $CDCl_3$)

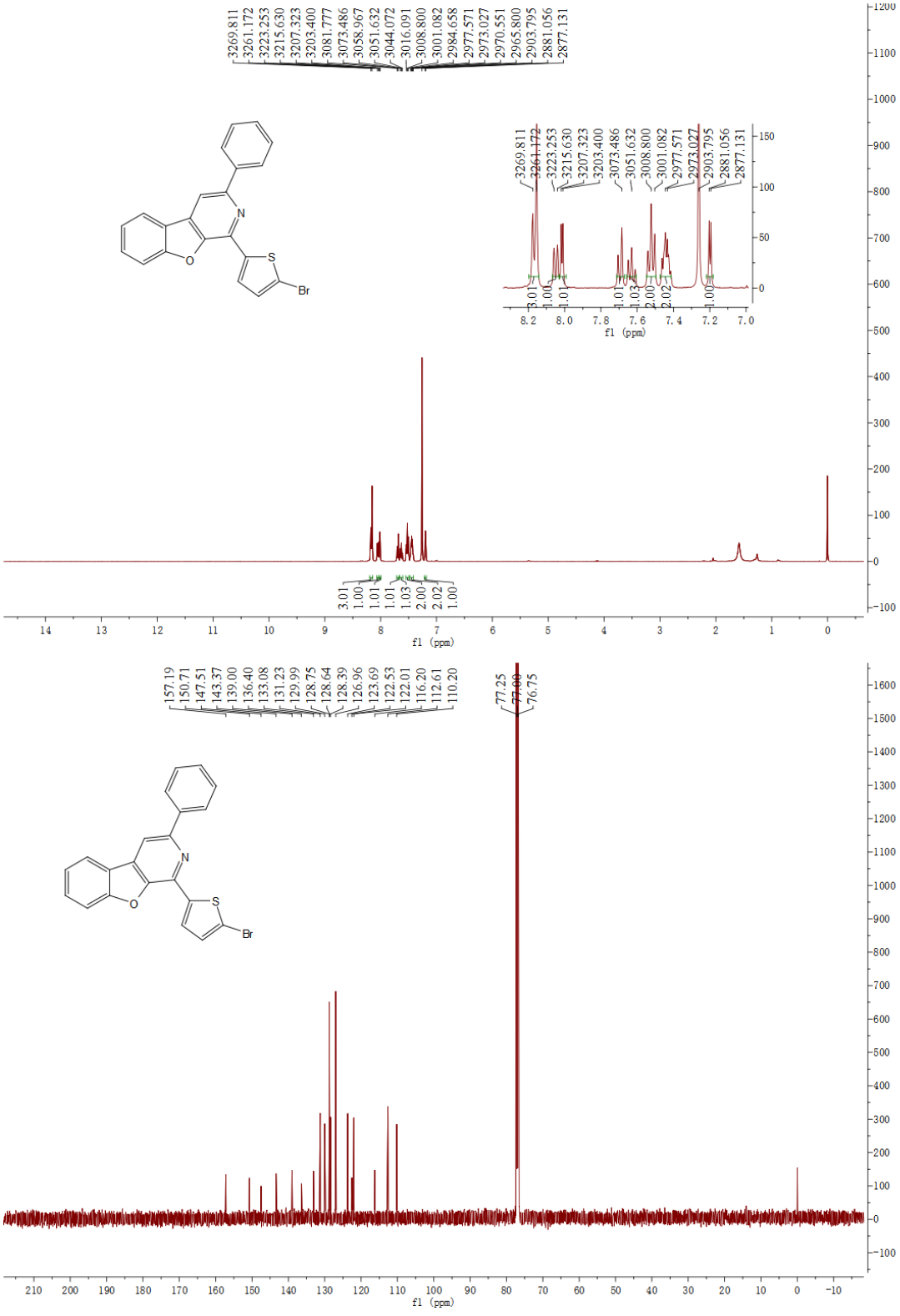


Figure S25. ^{1}H NMR of **3f** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3f** (125 MHz, $CDCl_3$)

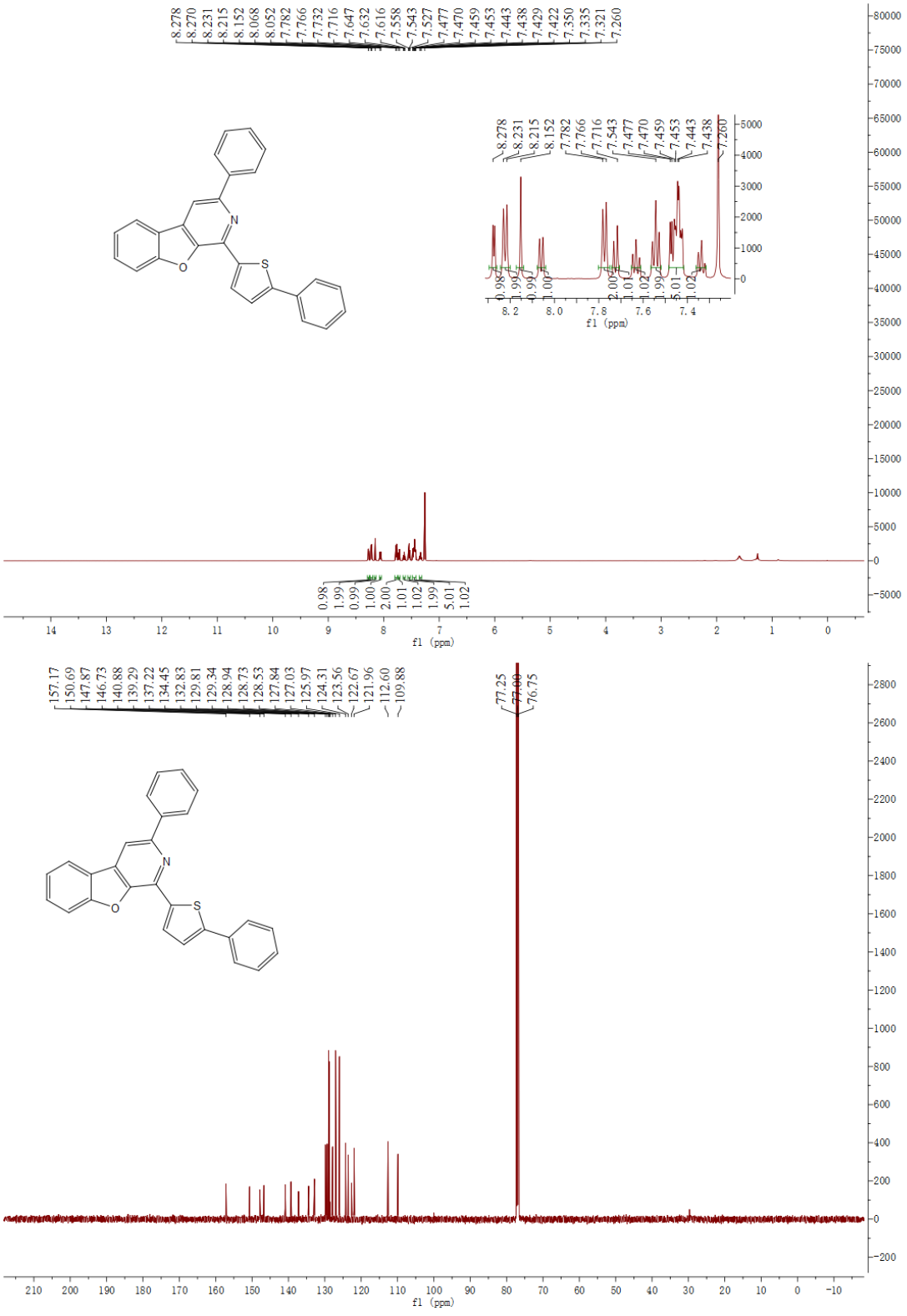


Figure S26. ^{1}H NMR of **3g** (500 MHz, $CDCl_3$) and ^{13}C NMR of **3g** (125 MHz, $CDCl_3$)

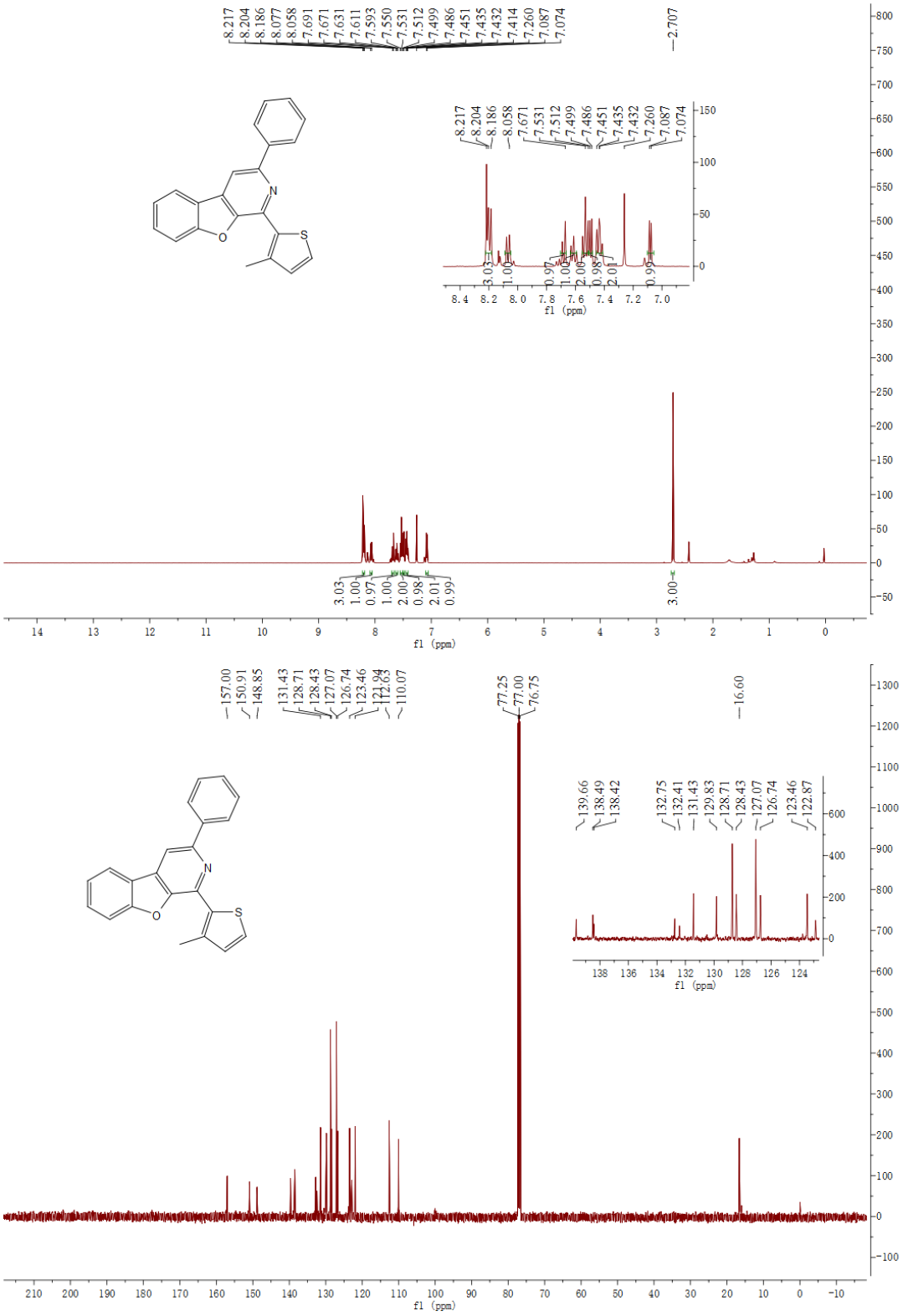


Figure S27. ^{1}H NMR of **3h** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3h** (125 MHz, $CDCl_3$)

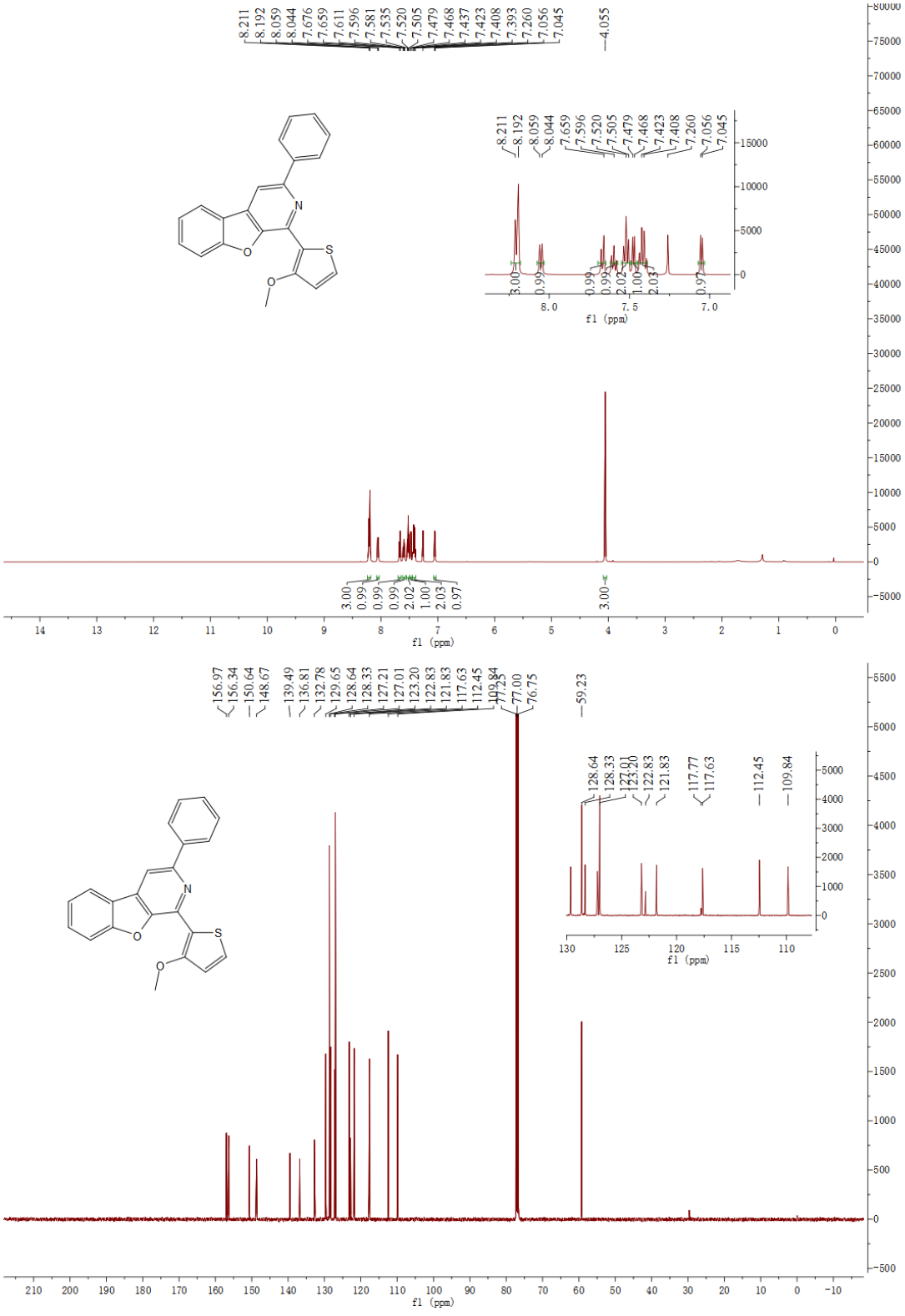


Figure S28. ^{1}H NMR of **3i** (500 MHz, $CDCl_3$) and ^{13}C NMR of **3i** (125 MHz, $CDCl_3$)

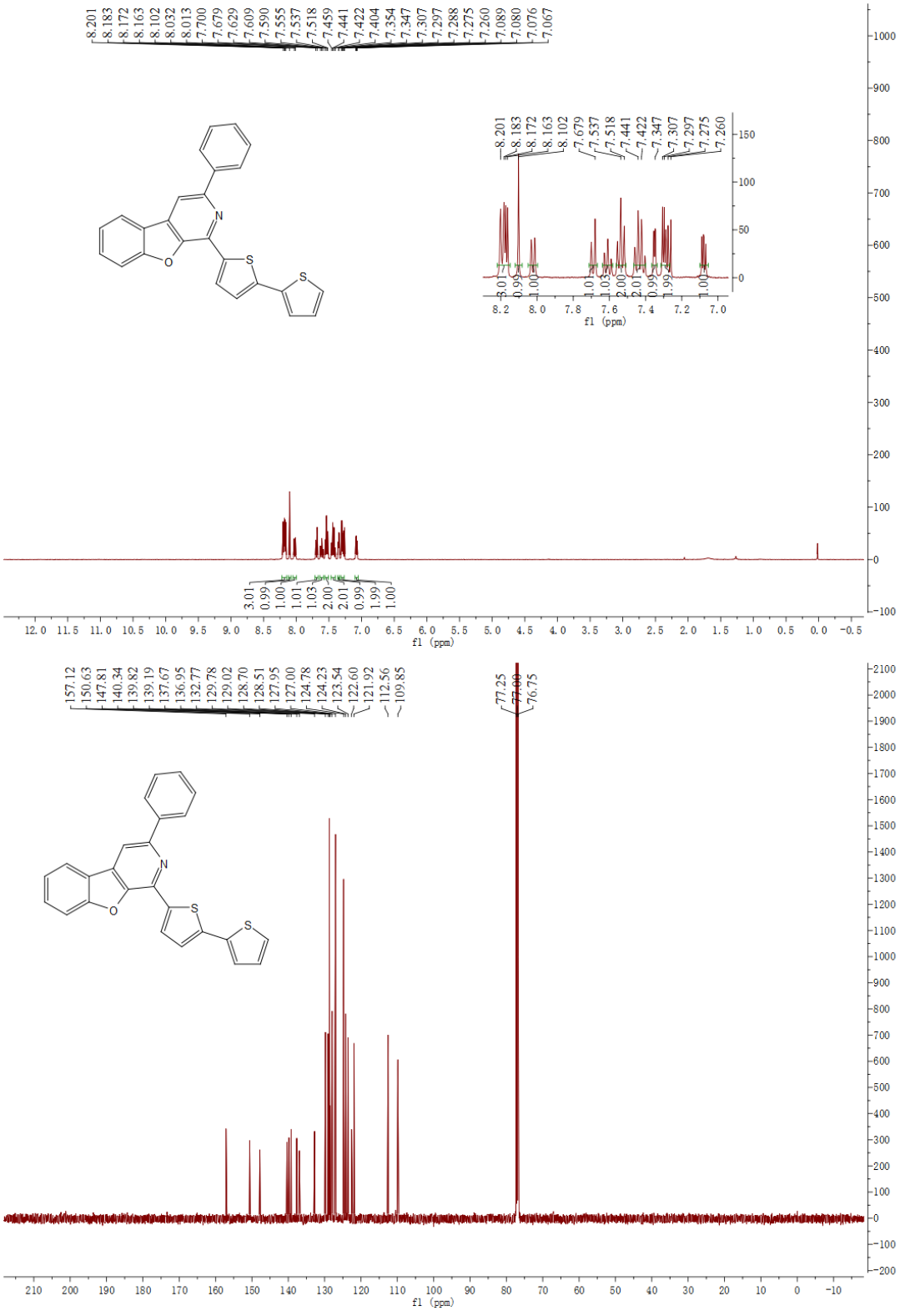


Figure S29. ^{1}H NMR of **3j** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3j** (125 MHz, $CDCl_3$)

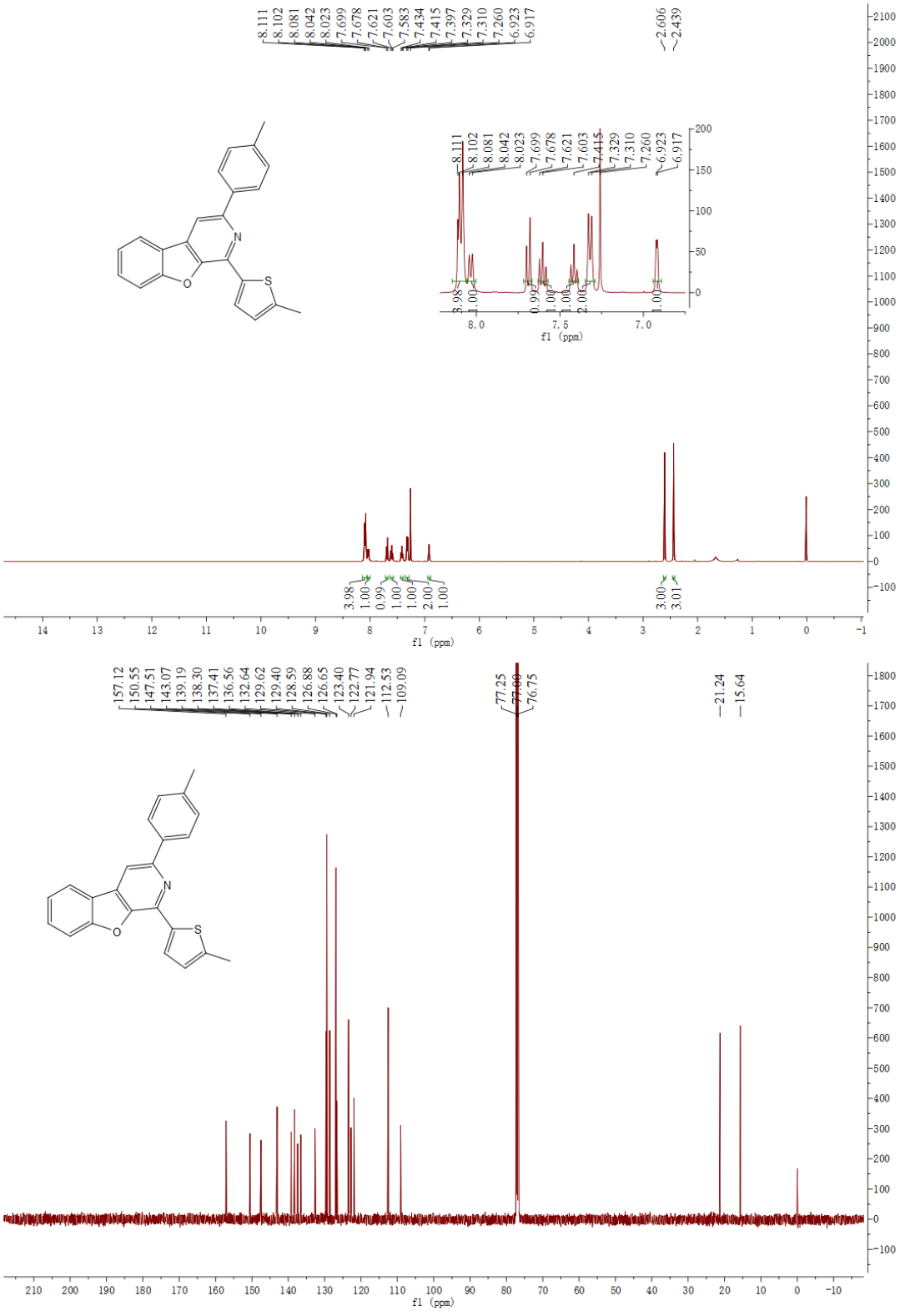


Figure S30. ^{1}H NMR of **3k** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3k** (125 MHz, $CDCl_3$)

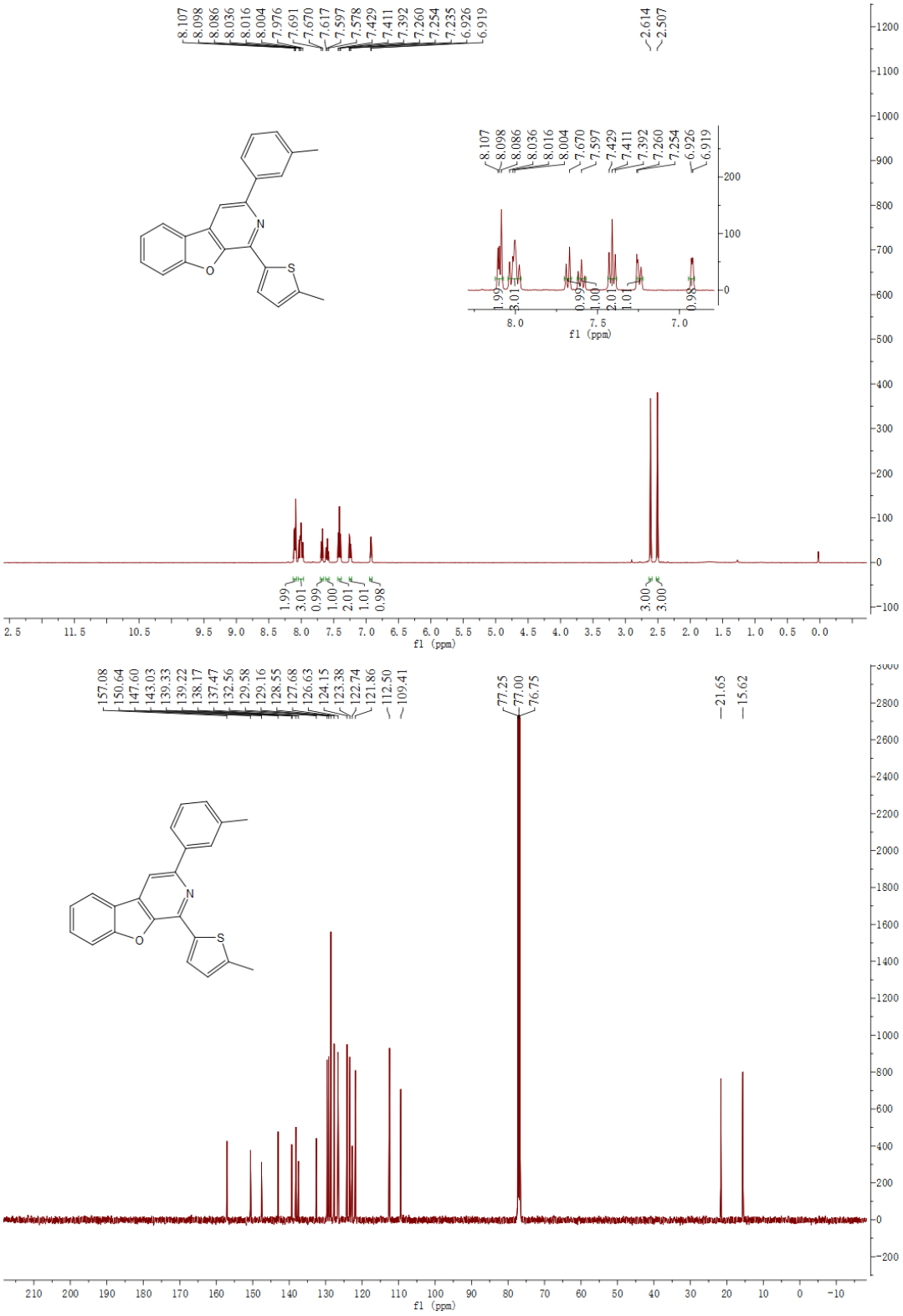


Figure S31. ^{1}H NMR of **3l** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3l** (125 MHz, $CDCl_3$)

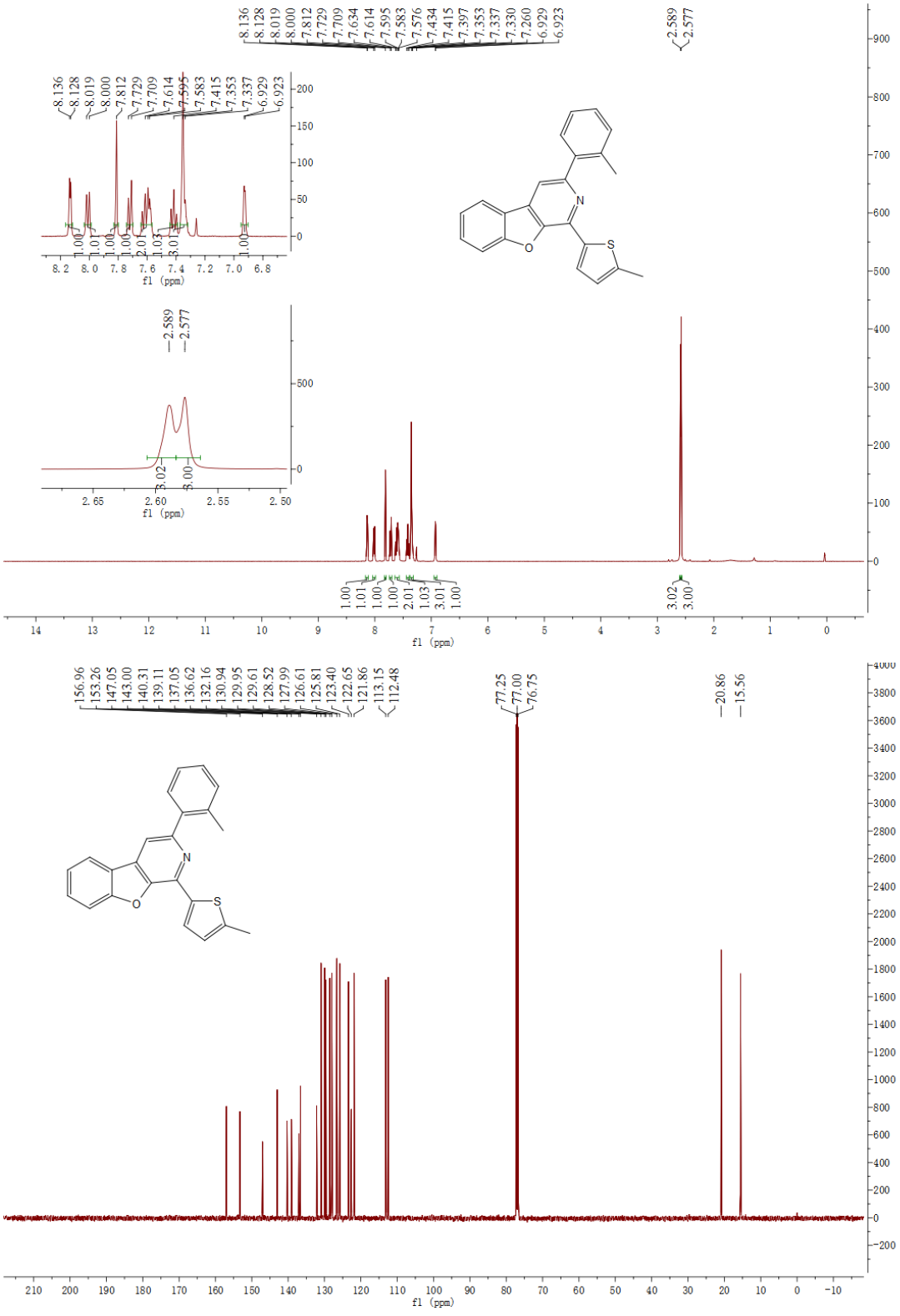


Figure S32. ^{1}H NMR of **3m** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3m** (125 MHz, $CDCl_3$)

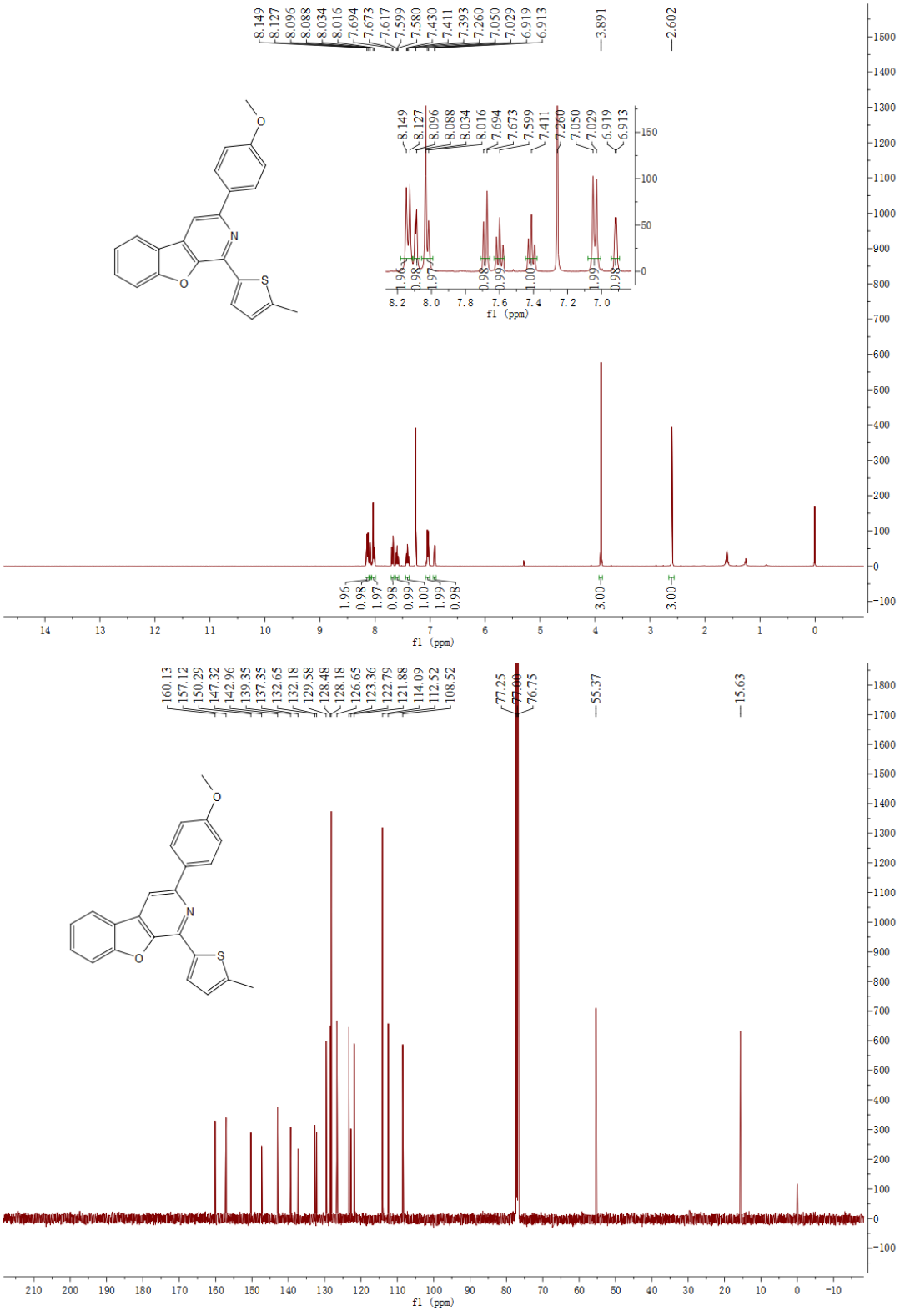


Figure S33. ^{1}H NMR of **3n** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3n** (125 MHz, $CDCl_3$)

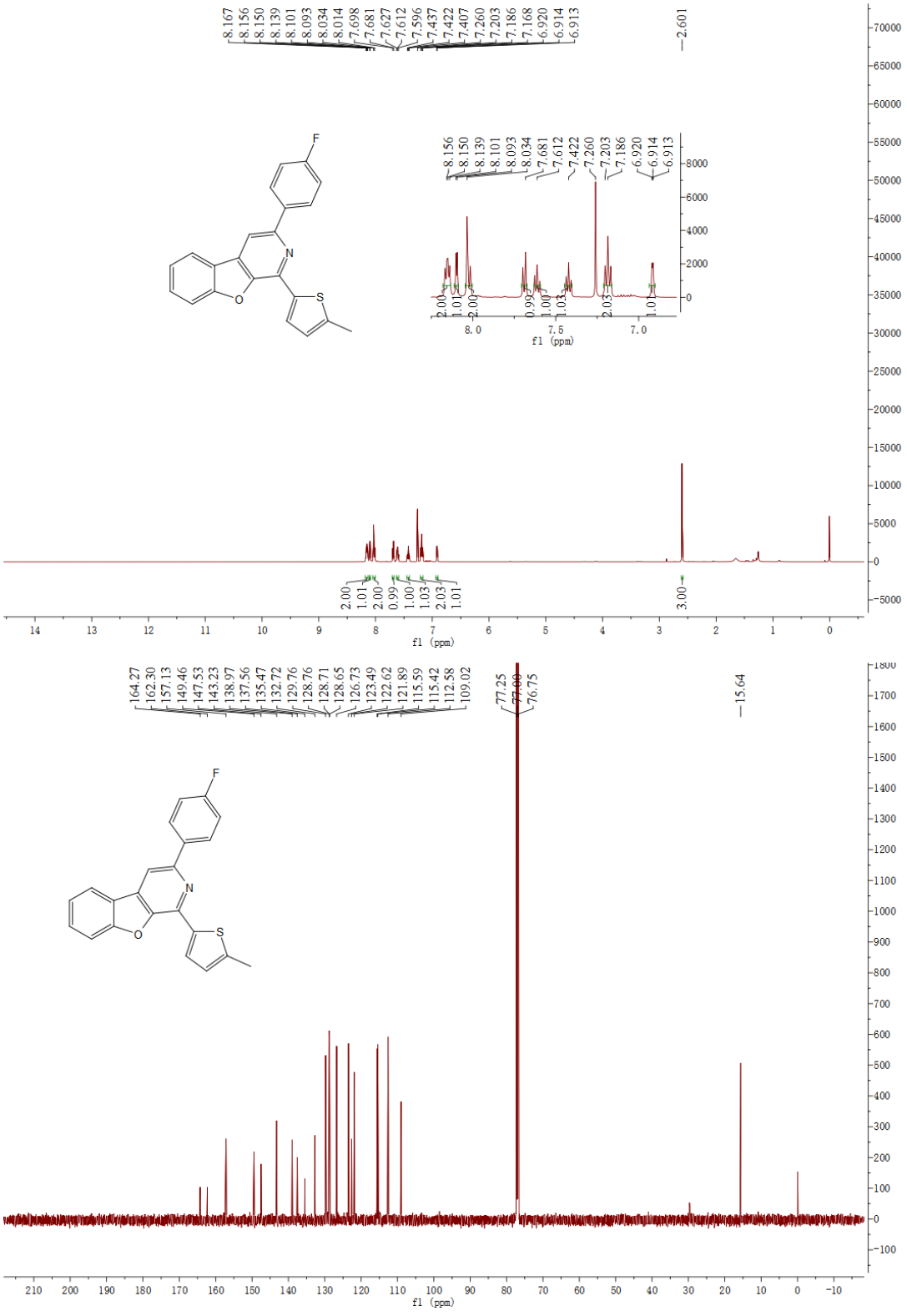


Figure S34. ^{1}H NMR of **3o** (500 MHz, $CDCl_3$) and ^{13}C NMR of **3o** (125 MHz, $CDCl_3$)

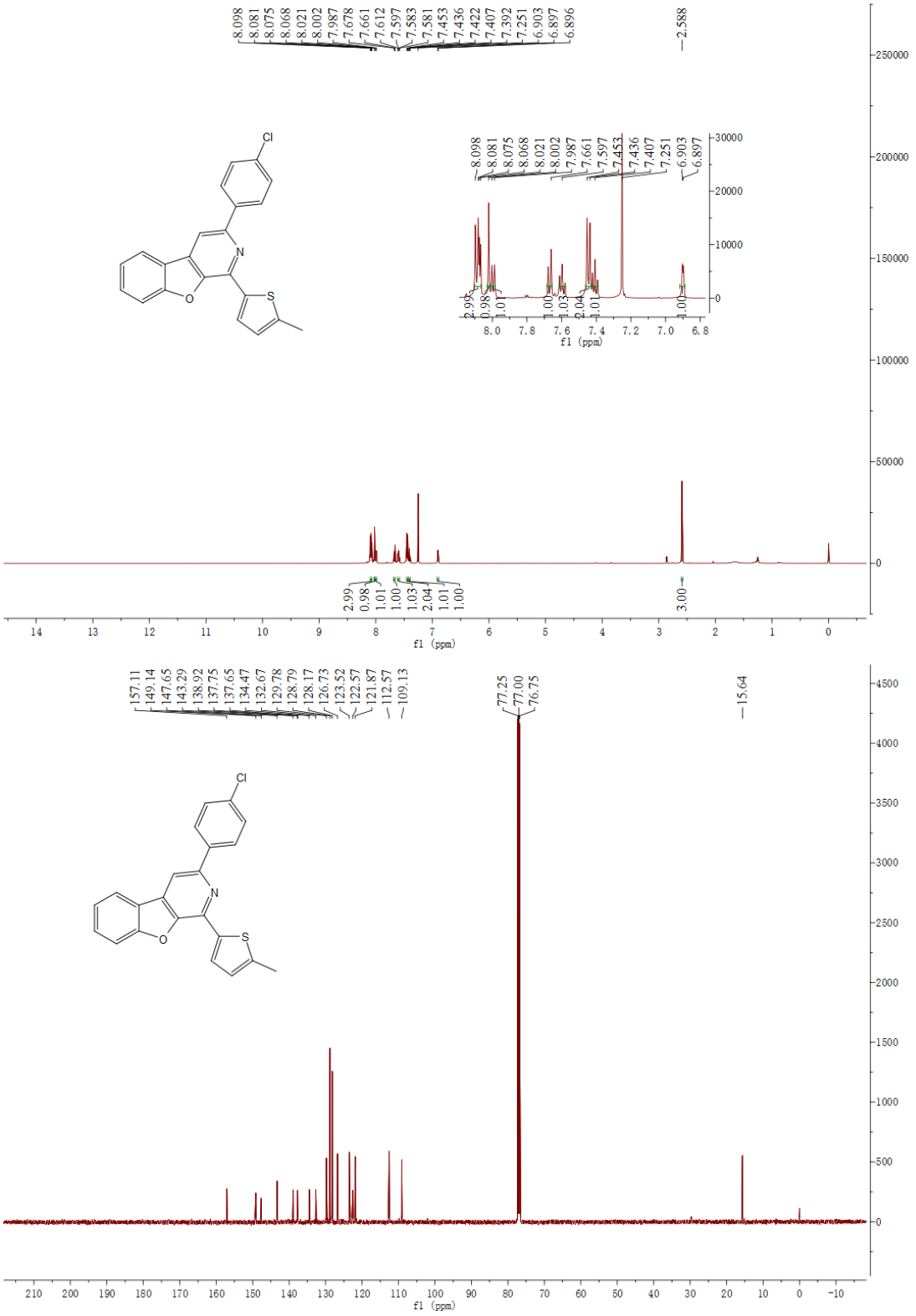


Figure S35. ^{1}H NMR of **3p** (500 MHz, $CDCl_3$) and ^{13}C NMR of **3p** (125 MHz, $CDCl_3$)

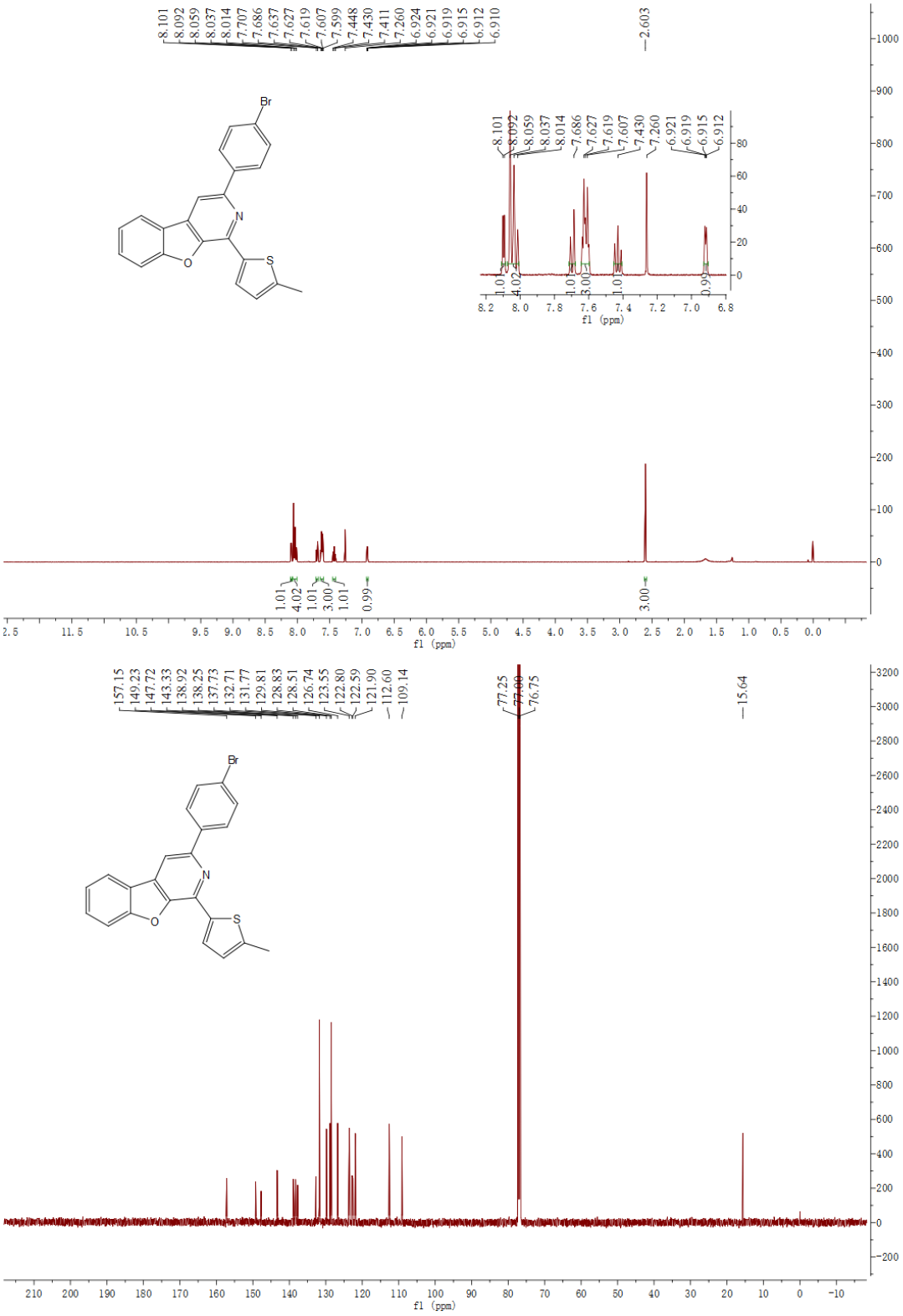


Figure S36. ^{1}H NMR of **3q** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3q** (125 MHz, $CDCl_3$)

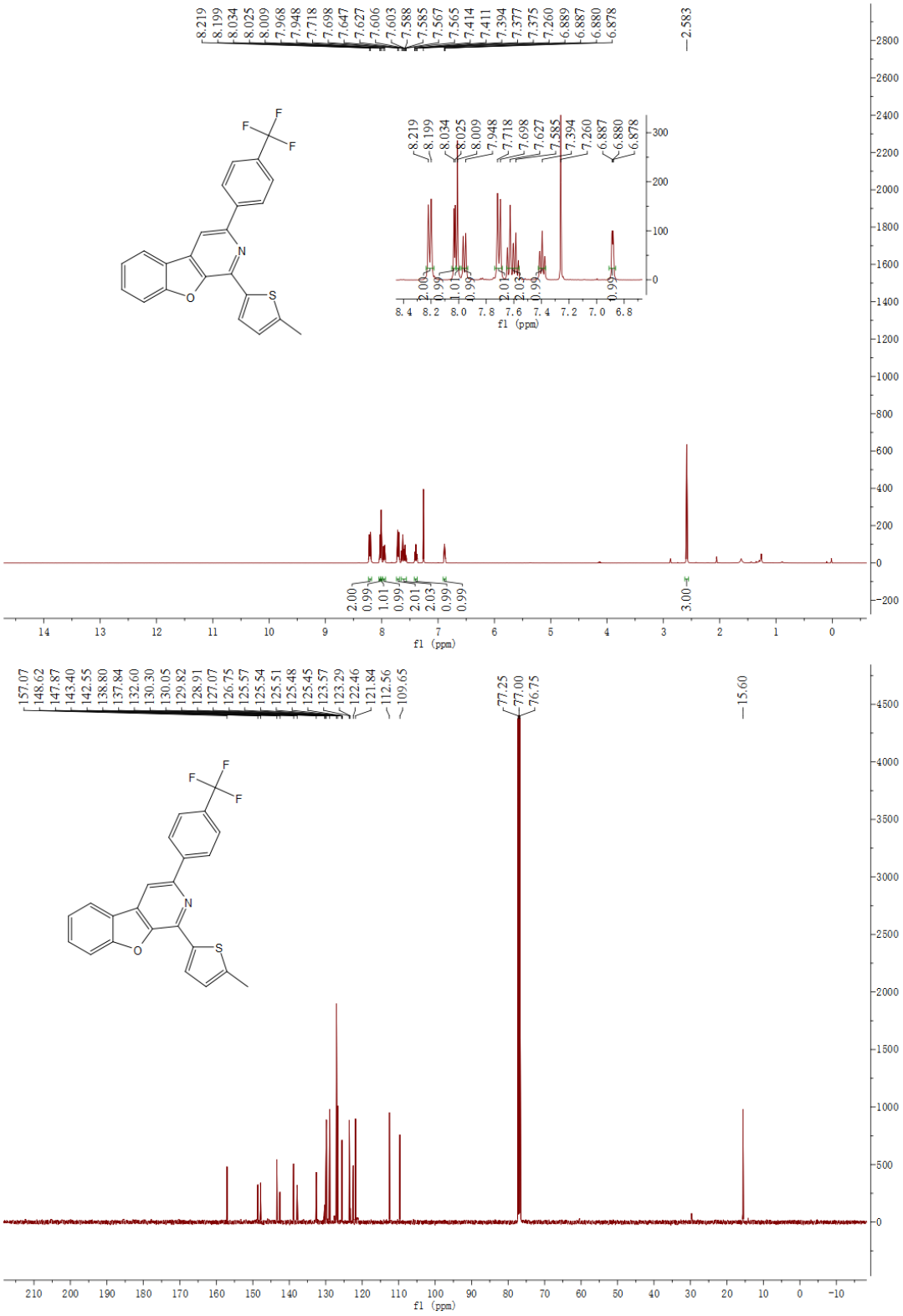


Figure S37. ^{1}H NMR of **3r** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3r** (125 MHz, $CDCl_3$)

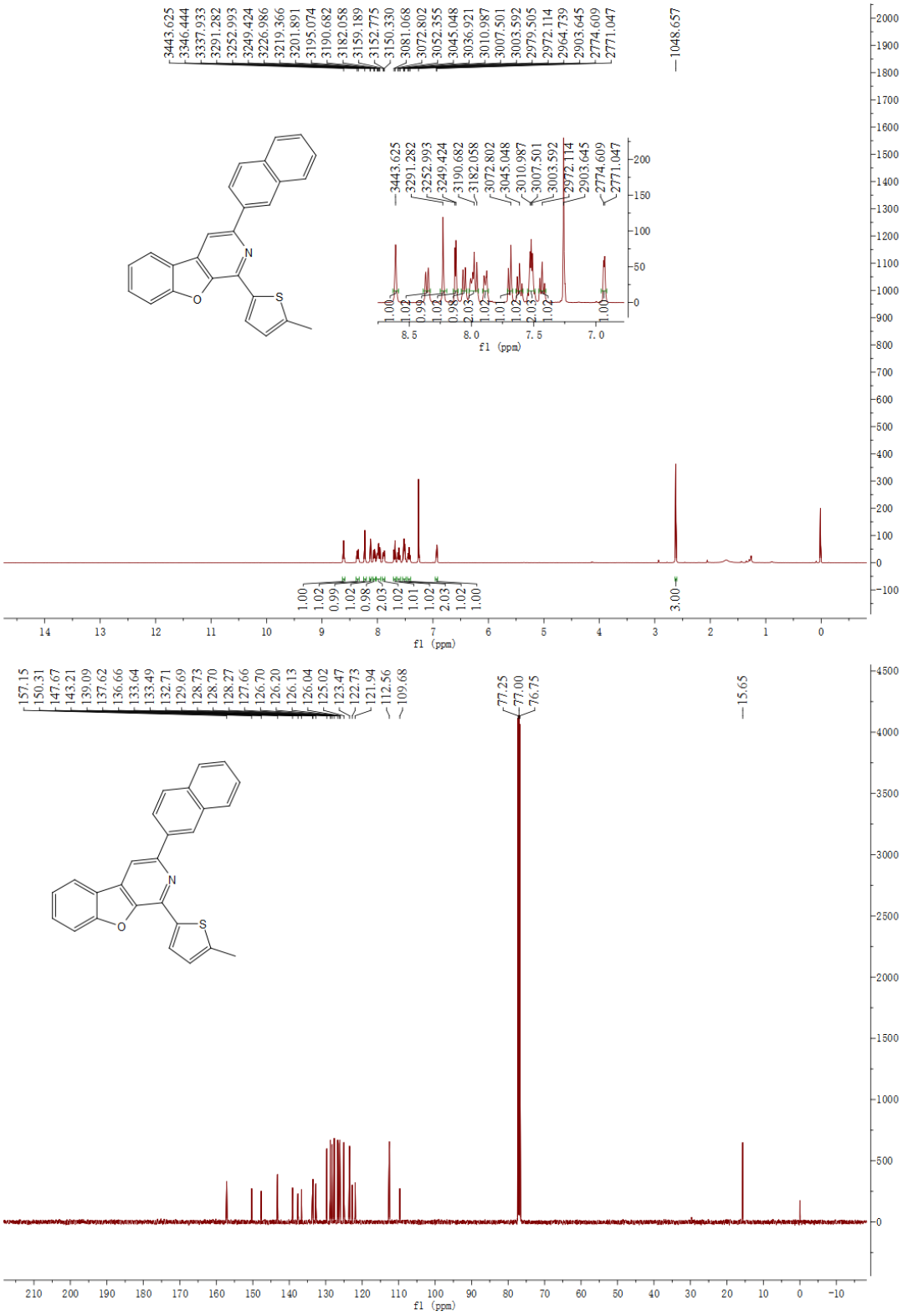


Figure S38. ^{1}H NMR of **3s** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3s** (125 MHz, $CDCl_3$)

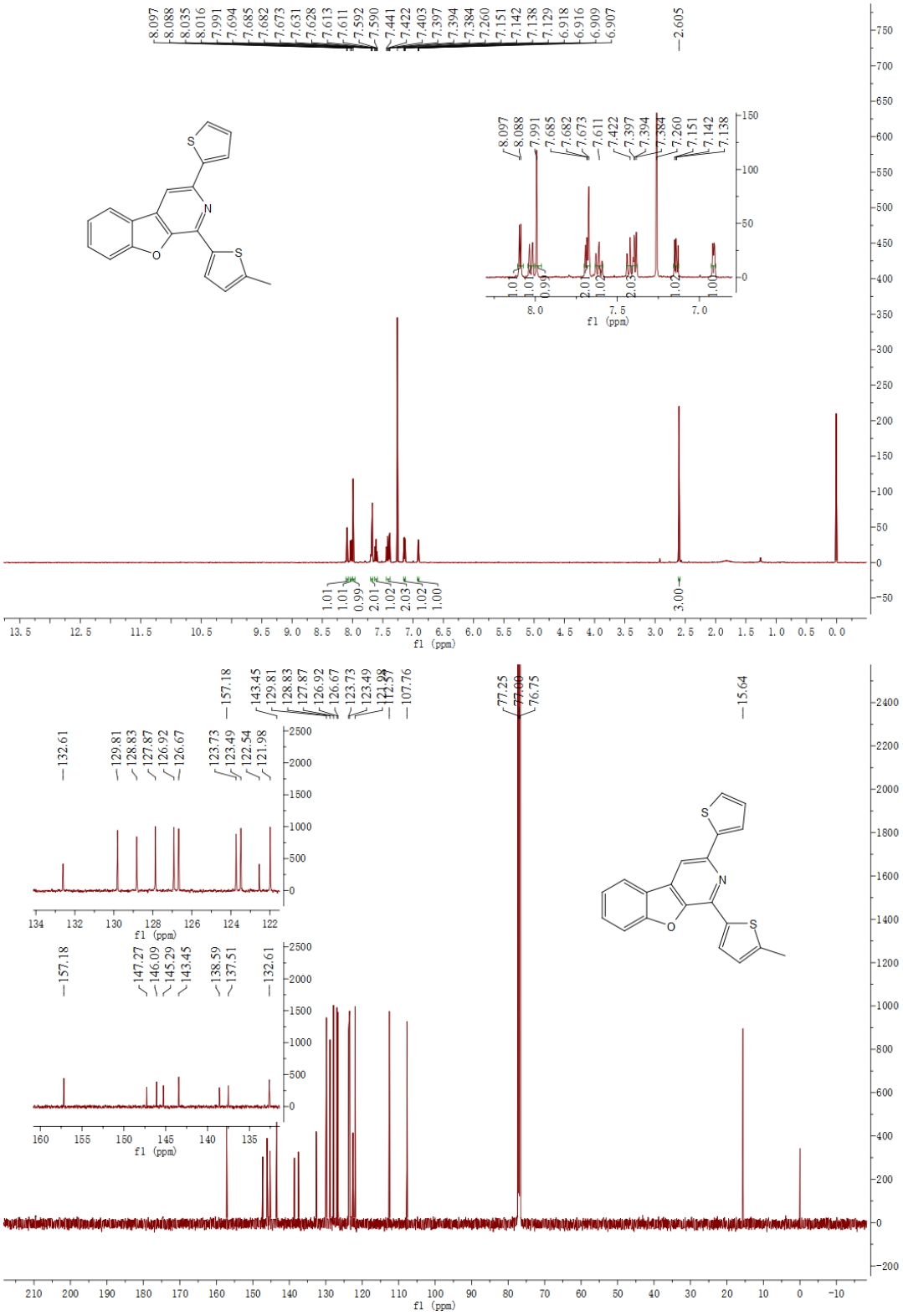


Figure S39. ^{1}H NMR of **3t** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3t** (125 MHz, $CDCl_3$)

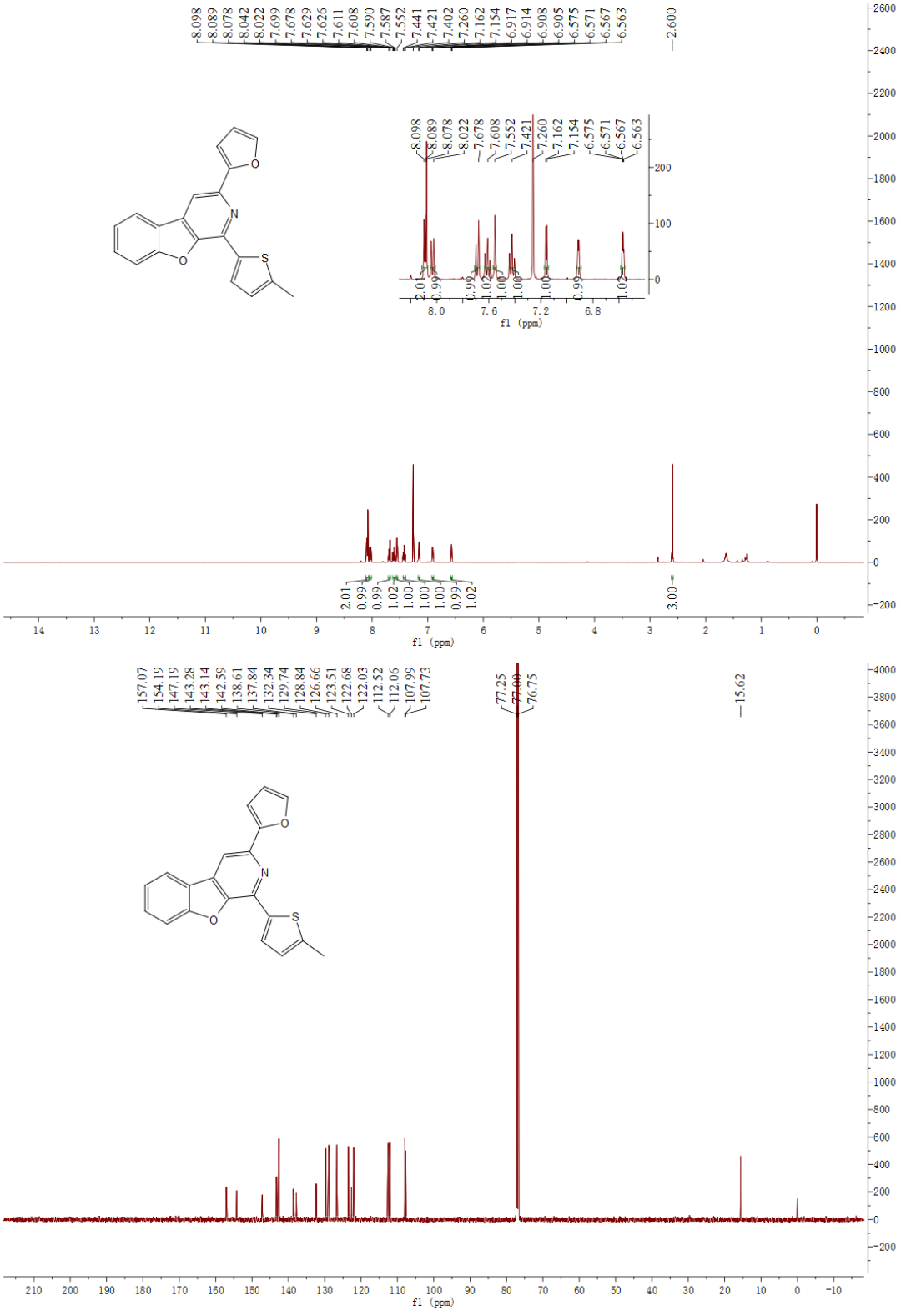


Figure S40. ^{1}H NMR of **3u** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3u** (125 MHz, $CDCl_3$)

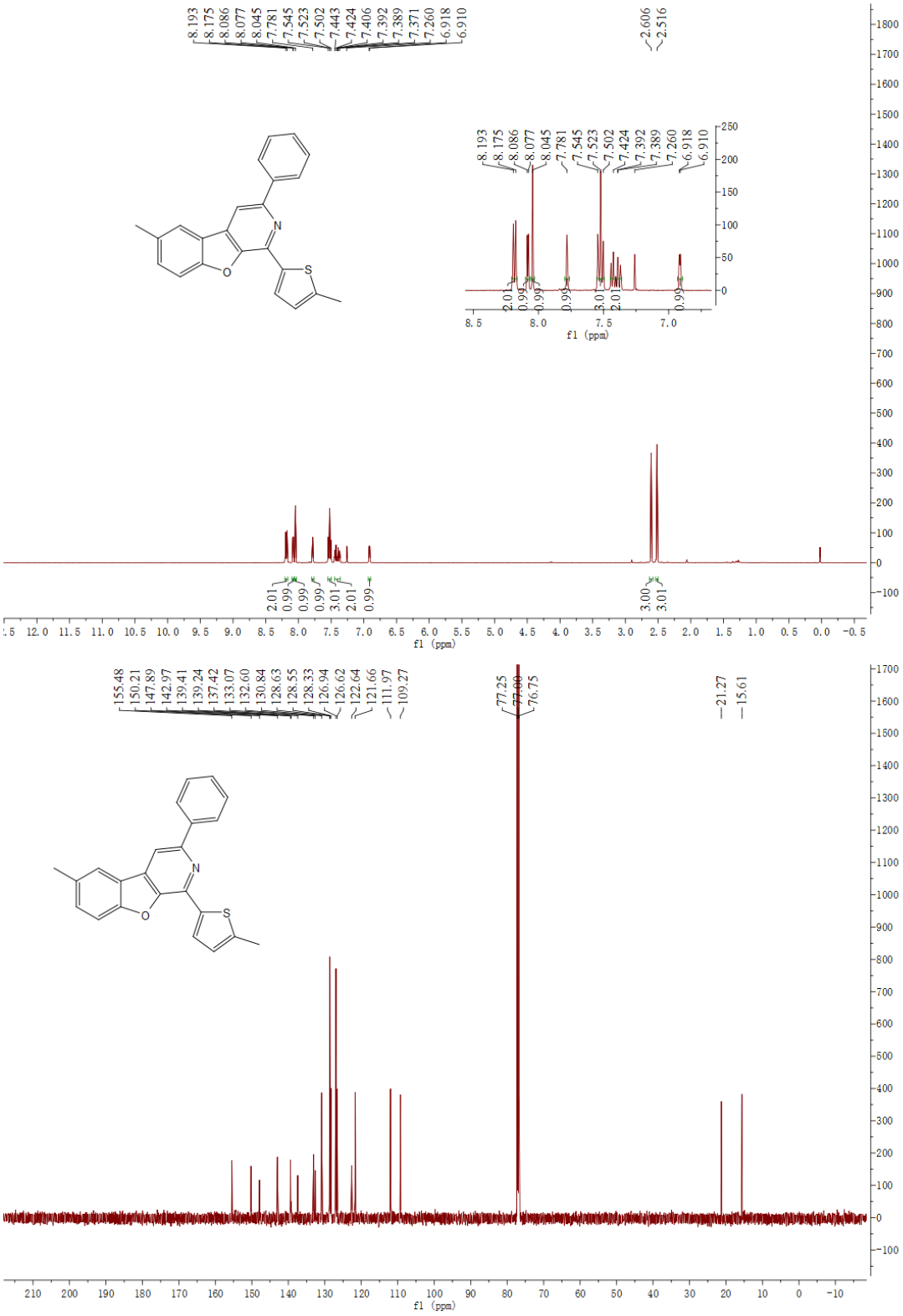


Figure S41. ^{1}H NMR of **3v** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3v** (125 MHz, $CDCl_3$)

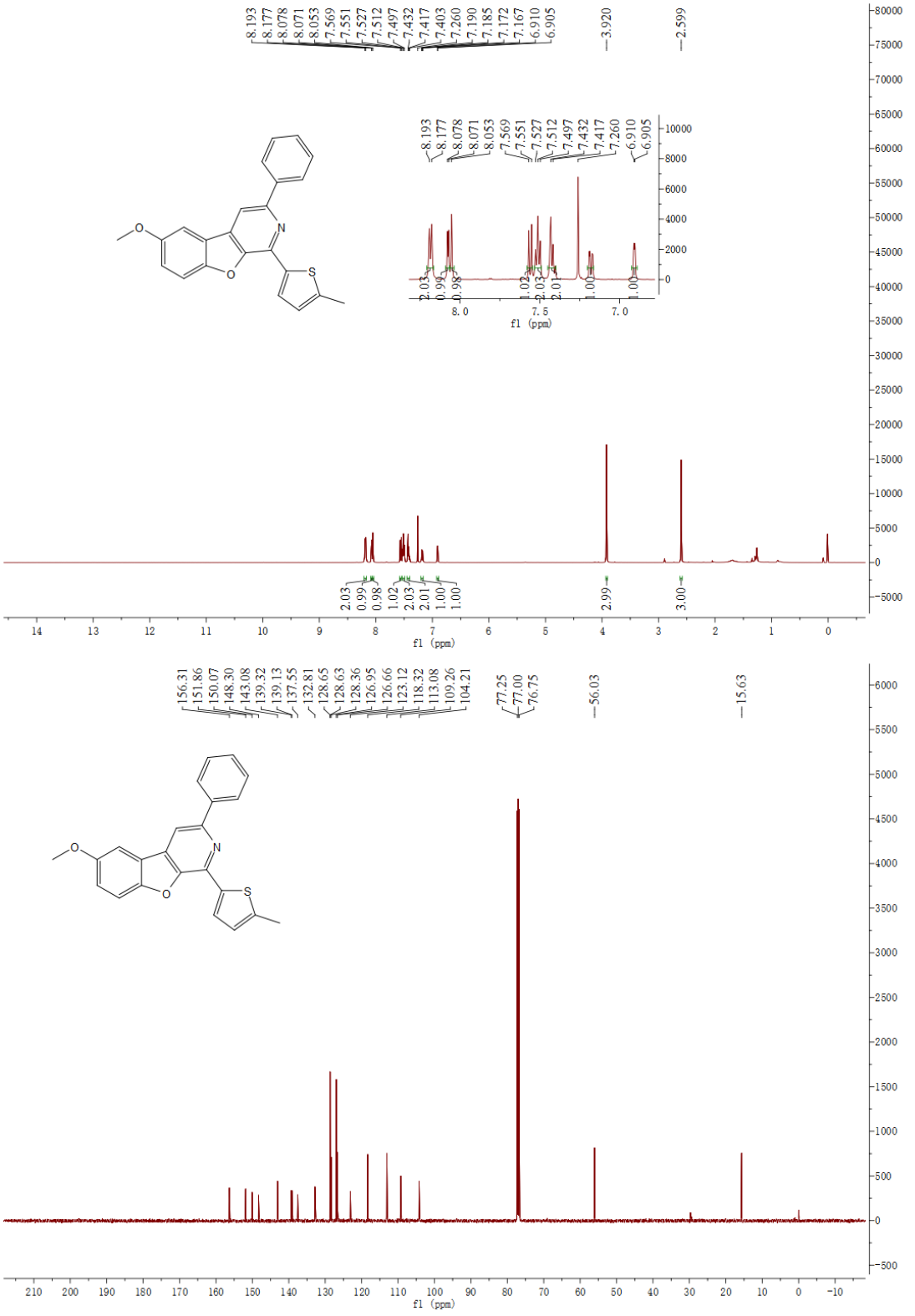


Figure S42. ^{1}H NMR of **3w** (500 MHz, $CDCl_3$) and ^{13}C NMR of **3w** (125 MHz, $CDCl_3$)

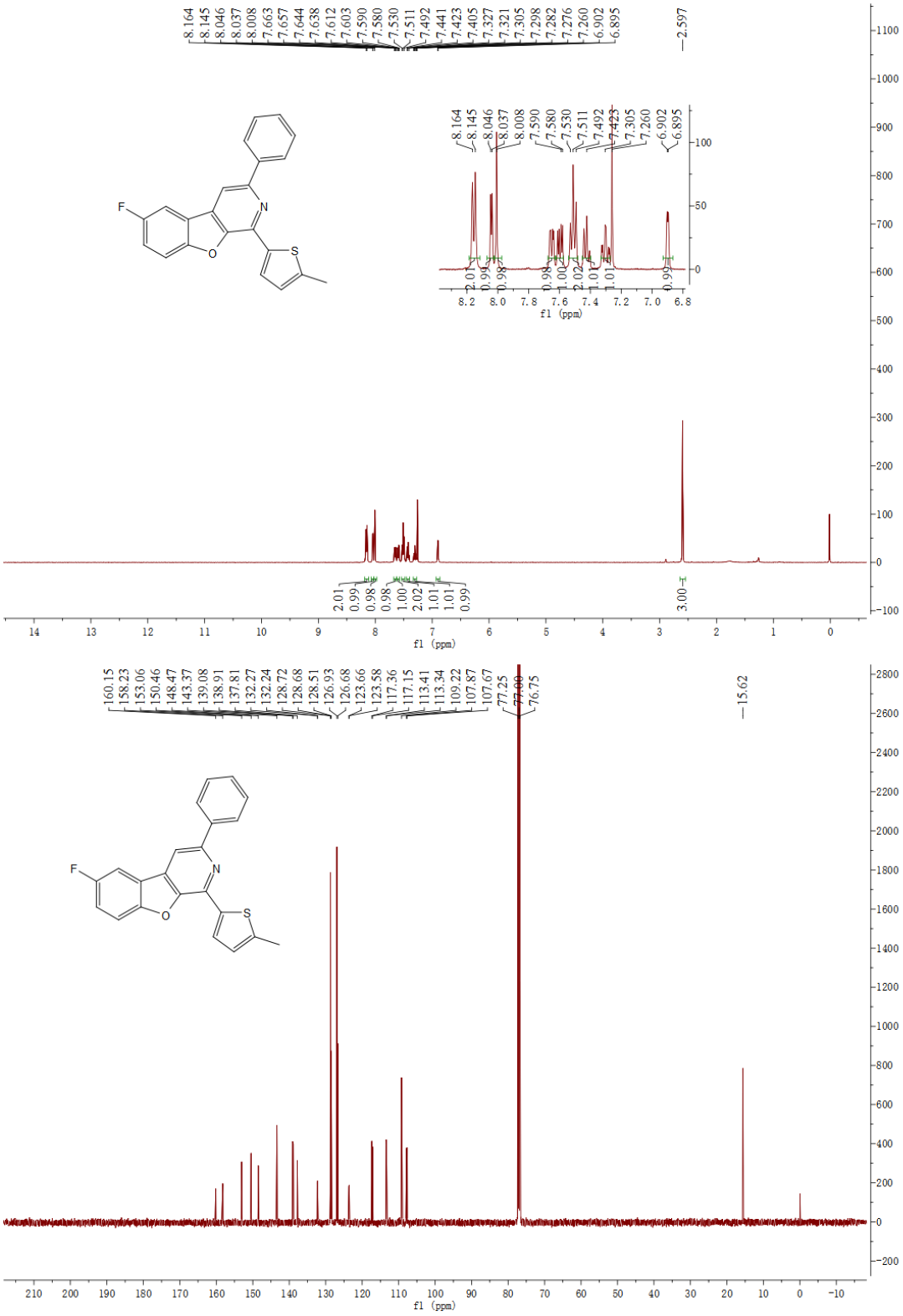


Figure S43. ^{1}H NMR of **3x** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3x** (125 MHz, $CDCl_3$)

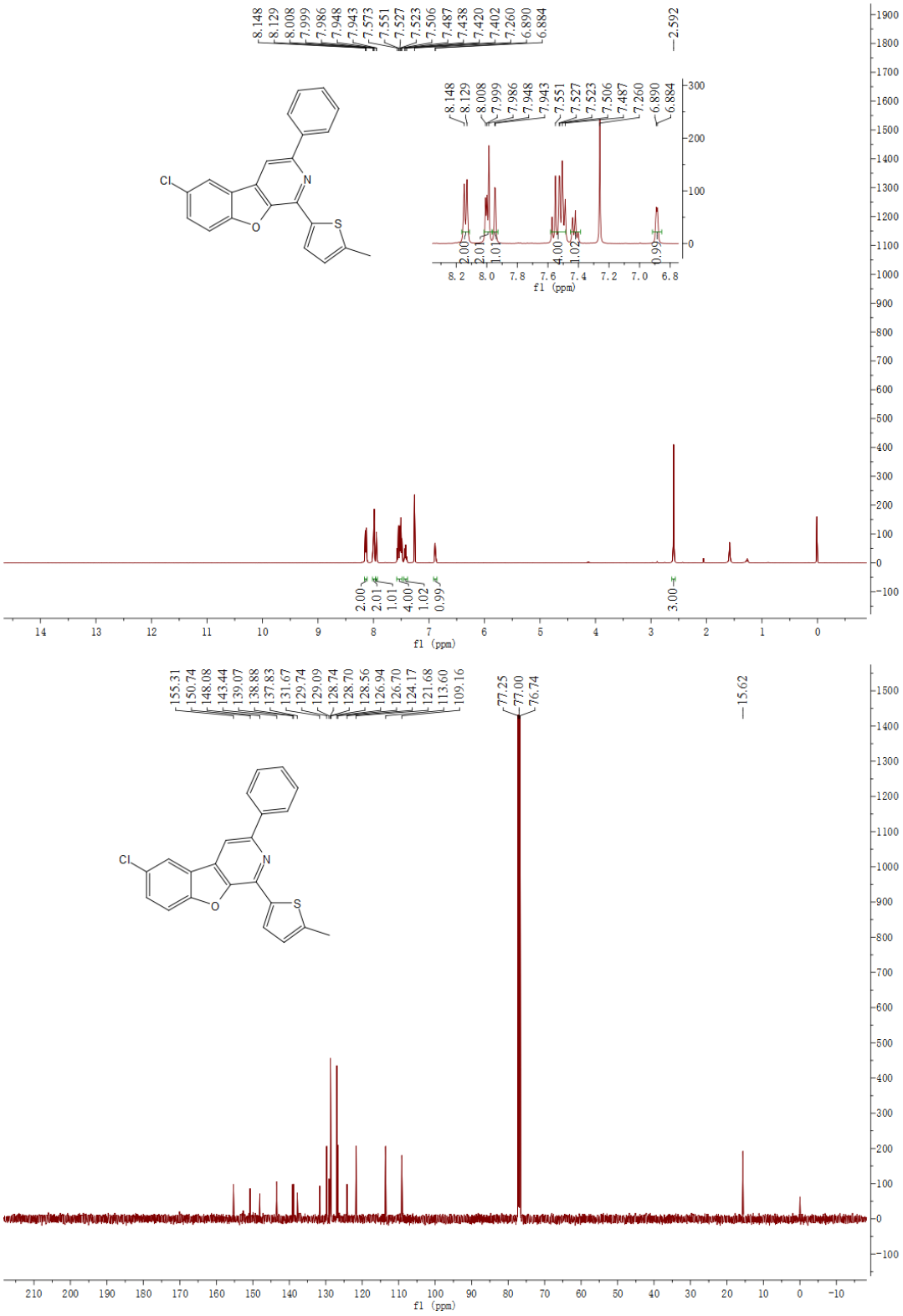


Figure S44. ^{1}H NMR of **3y** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3y** (125 MHz, $CDCl_3$)

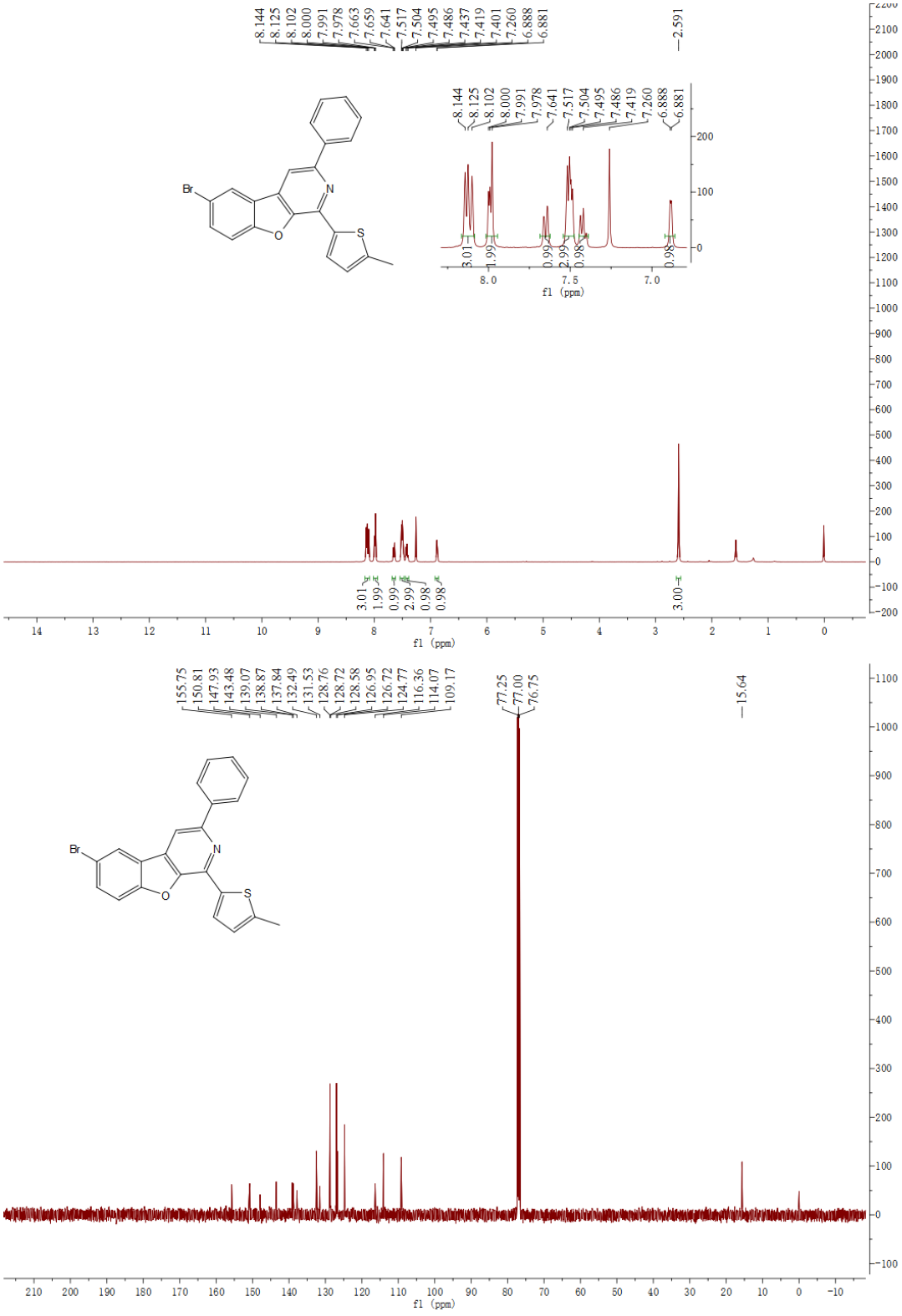


Figure S45. ^{1}H NMR of **3z** (400 MHz, $CDCl_3$) and ^{13}C NMR of **3z** (125 MHz, $CDCl_3$)

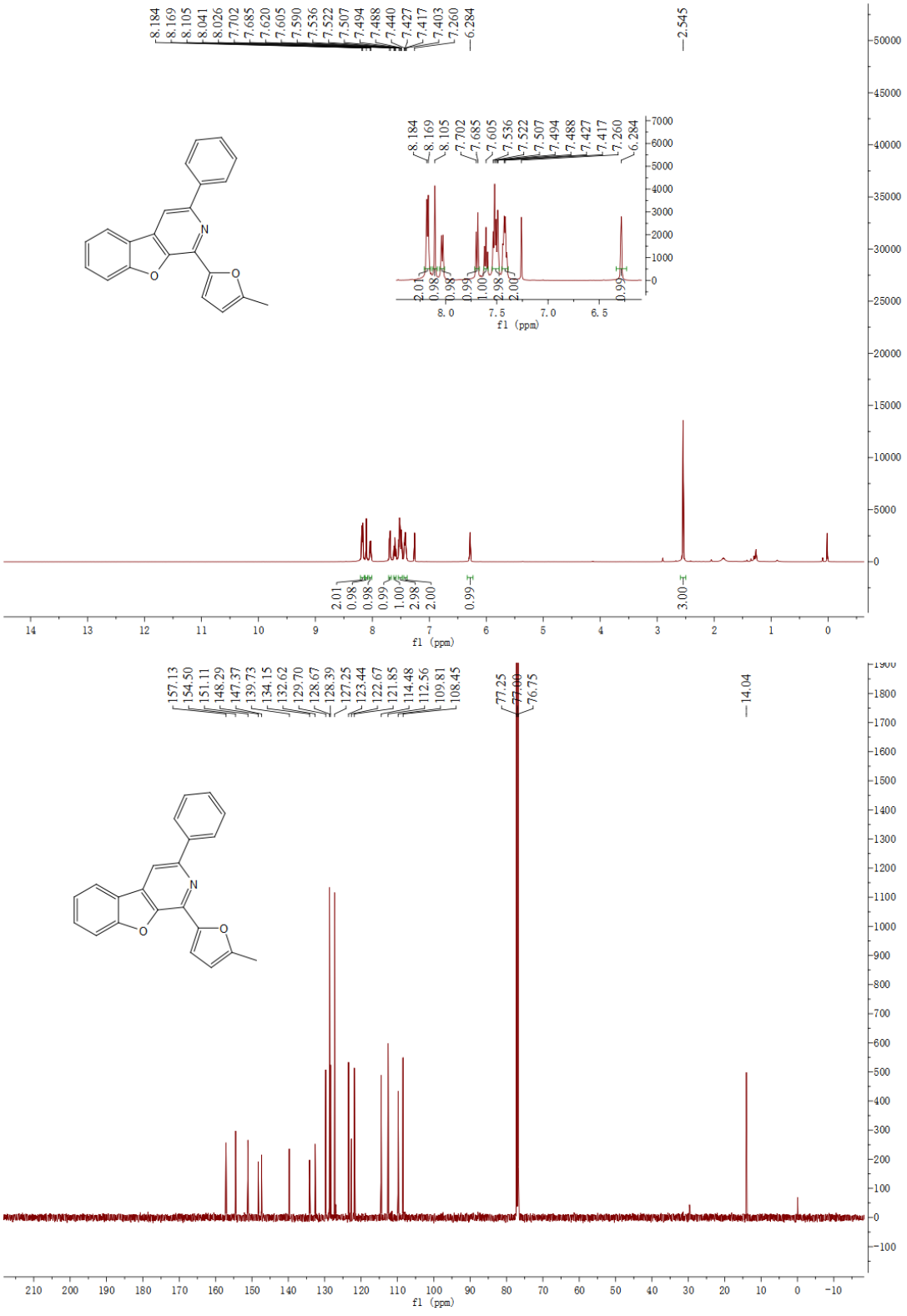


Figure S46. ^{1}H NMR of **4a** (500 MHz, $CDCl_3$) and ^{13}C NMR of **4a** (125 MHz, $CDCl_3$)

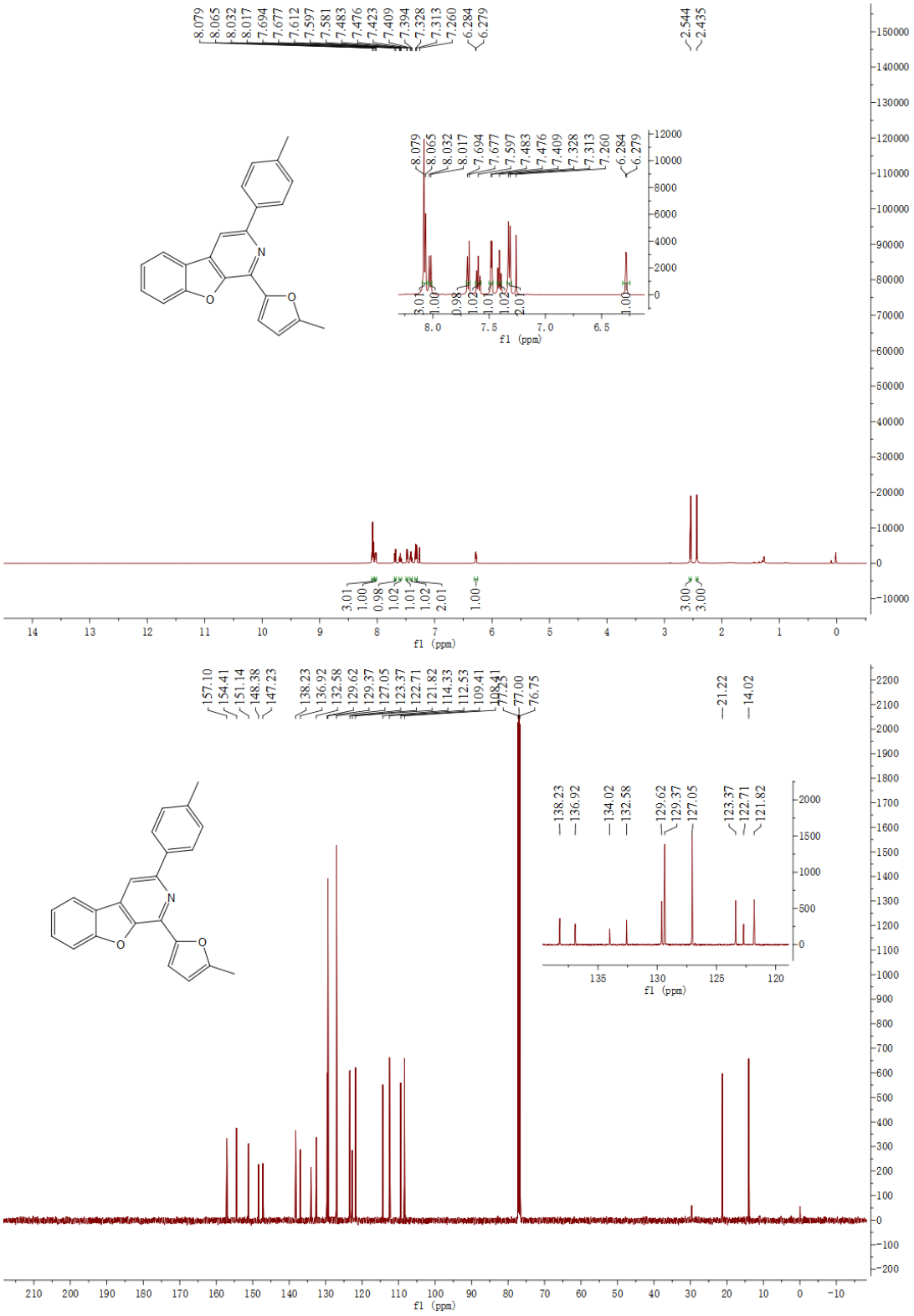


Figure S47. ^{1}H NMR of **4b** (500 MHz, $CDCl_3$) and ^{13}C NMR of **4b** (125 MHz, $CDCl_3$)

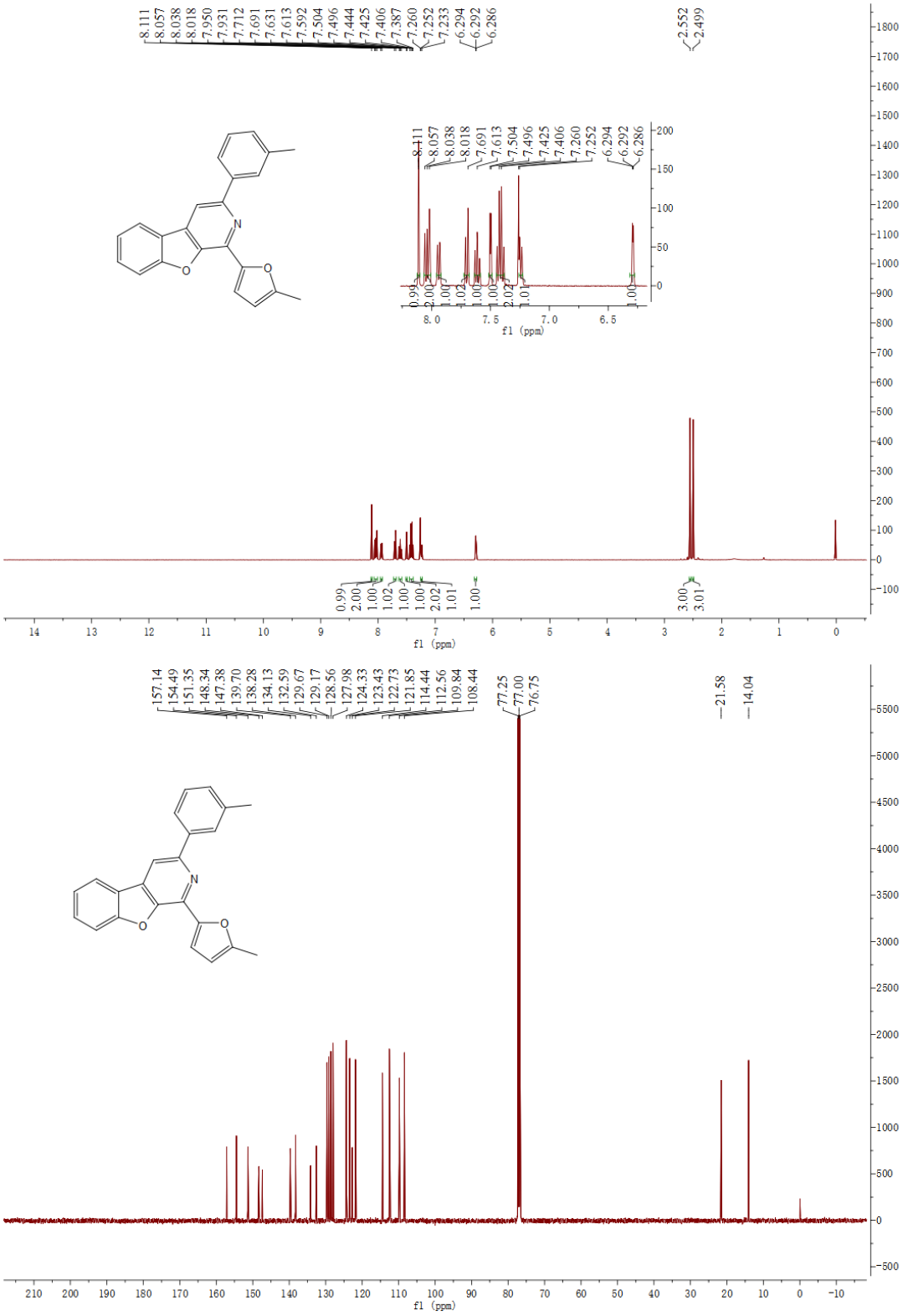


Figure S48. ^{1}H NMR of **4c** (400 MHz, $CDCl_3$) and ^{13}C NMR of **4c** (125 MHz, $CDCl_3$)

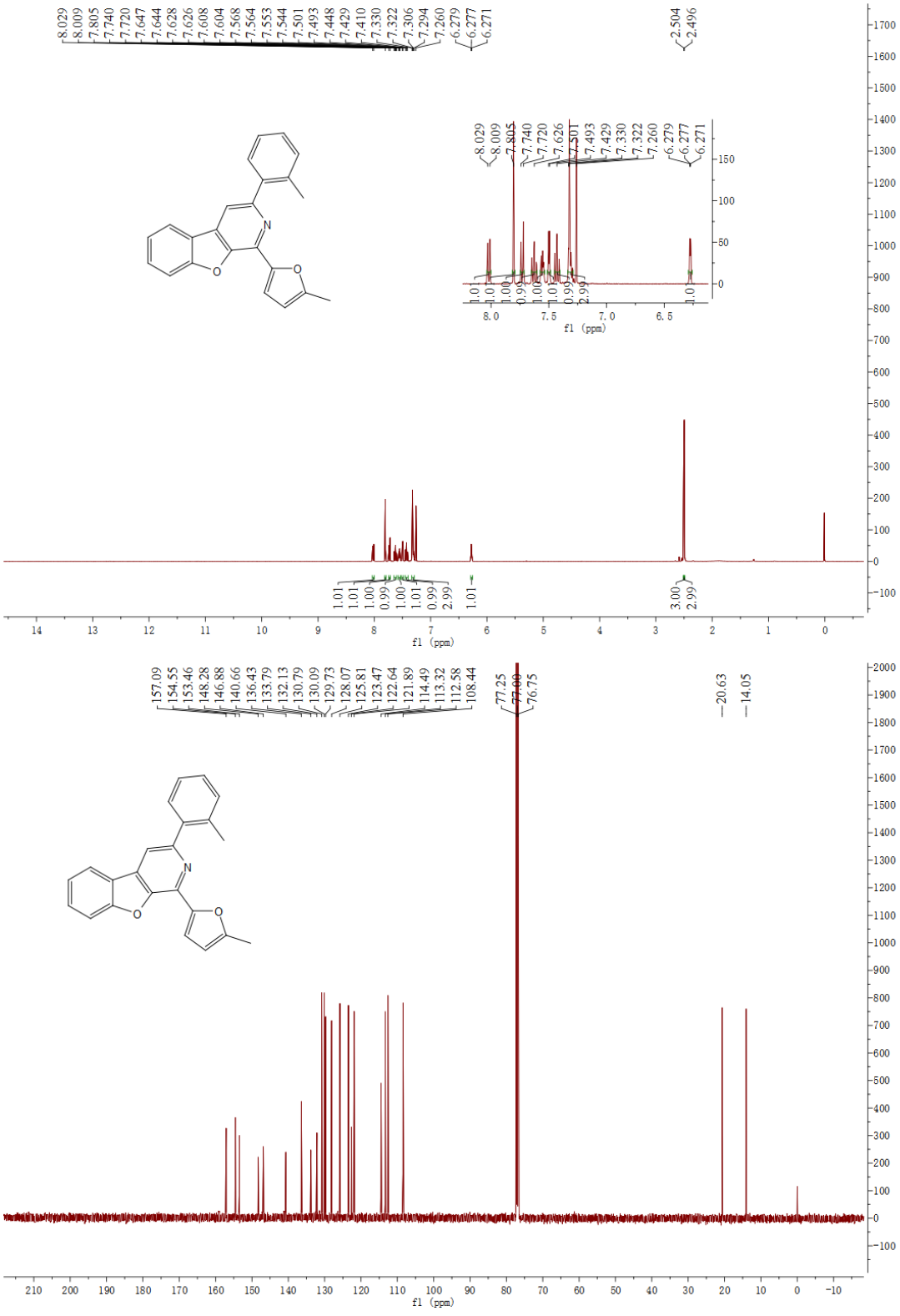


Figure S49. ^{1}H NMR of **4d** (400 MHz, $CDCl_3$) and ^{13}C NMR of **4d** (125 MHz, $CDCl_3$)

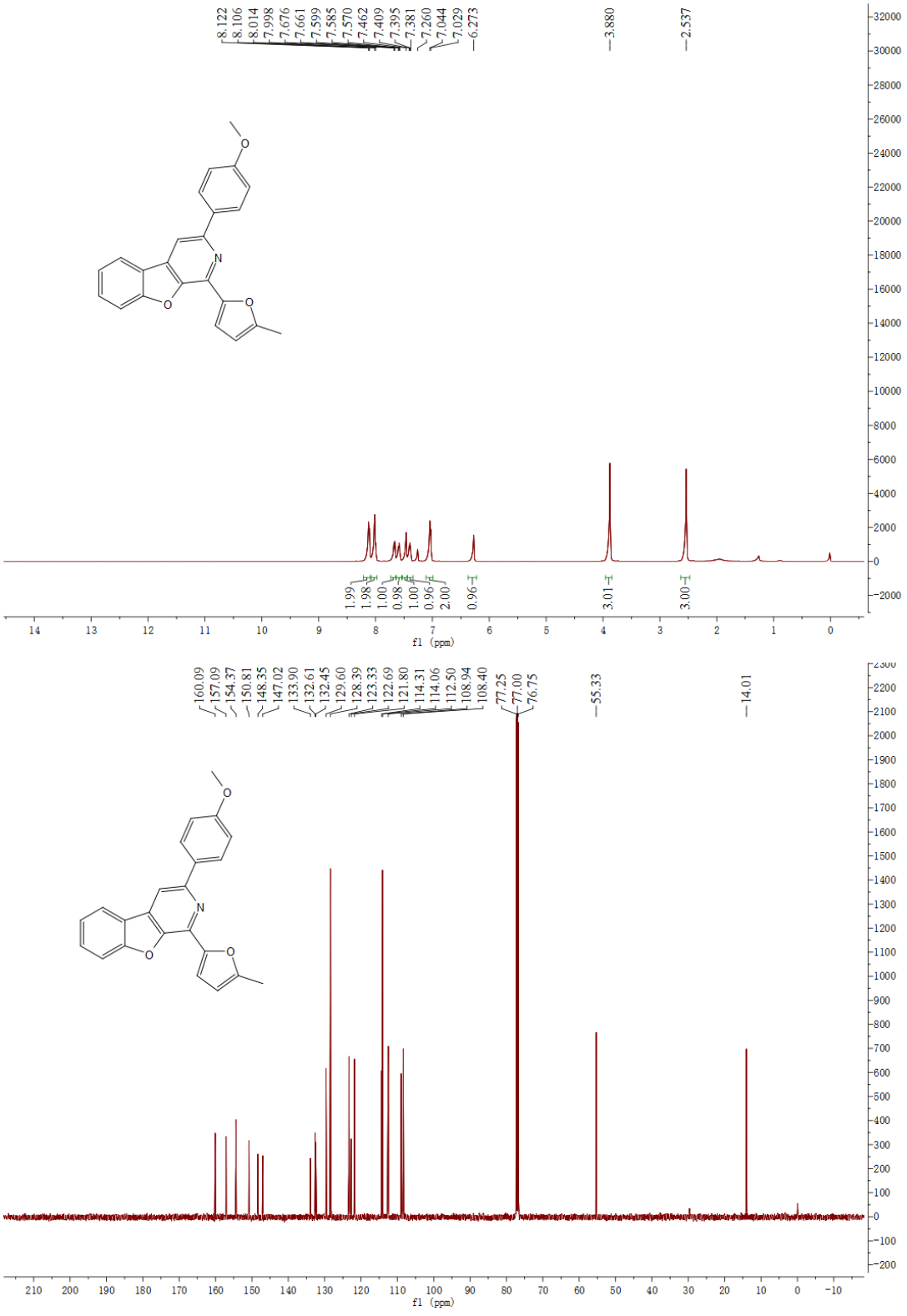


Figure S50. ^{1}H NMR of **4e** (500 MHz, $CDCl_3$) and ^{13}C NMR of **4e** (125 MHz, $CDCl_3$)

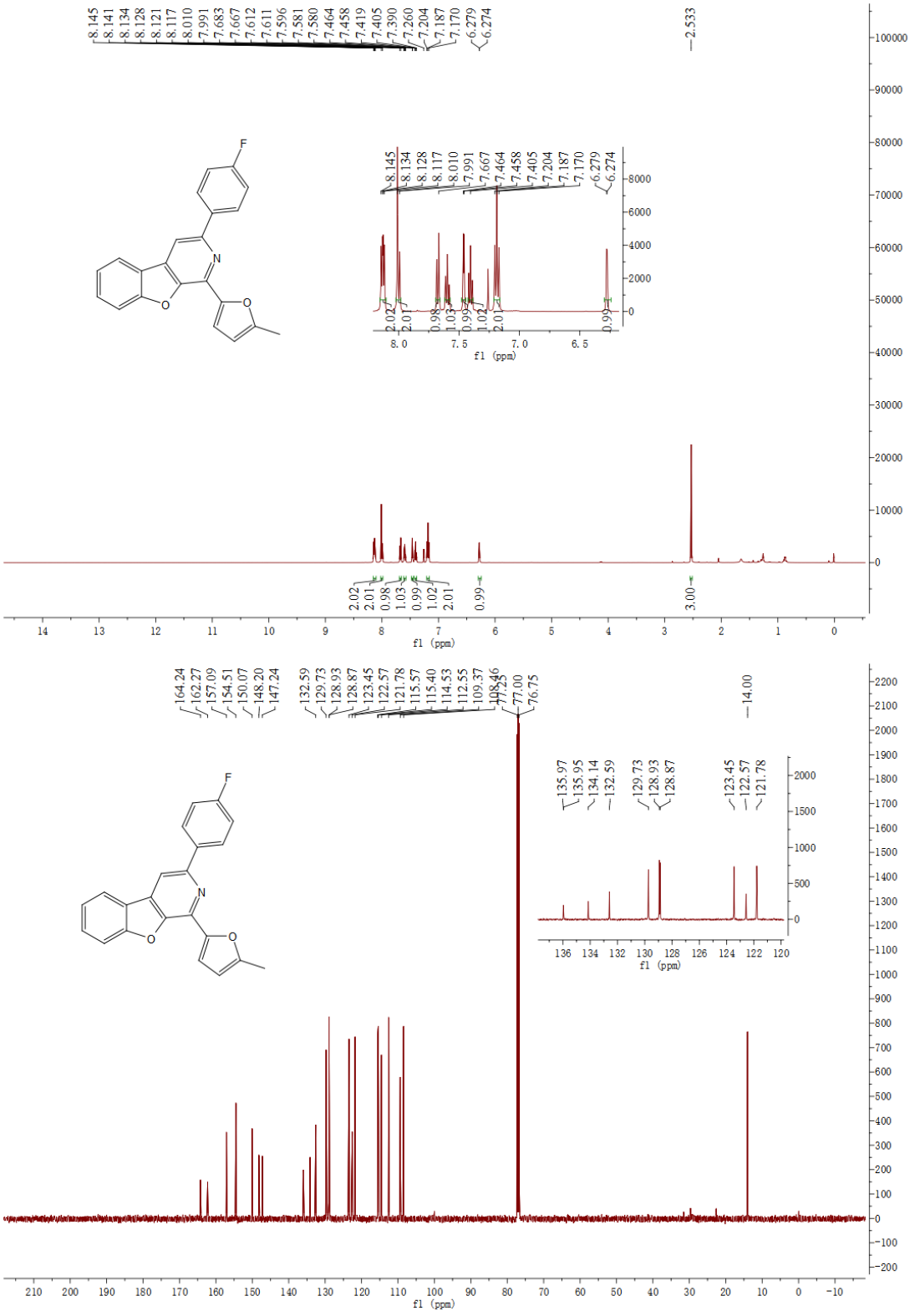


Figure S51. ^{1}H NMR of **4f** (500 MHz, $CDCl_3$) and ^{13}C NMR of **4f** (125 MHz, $CDCl_3$)

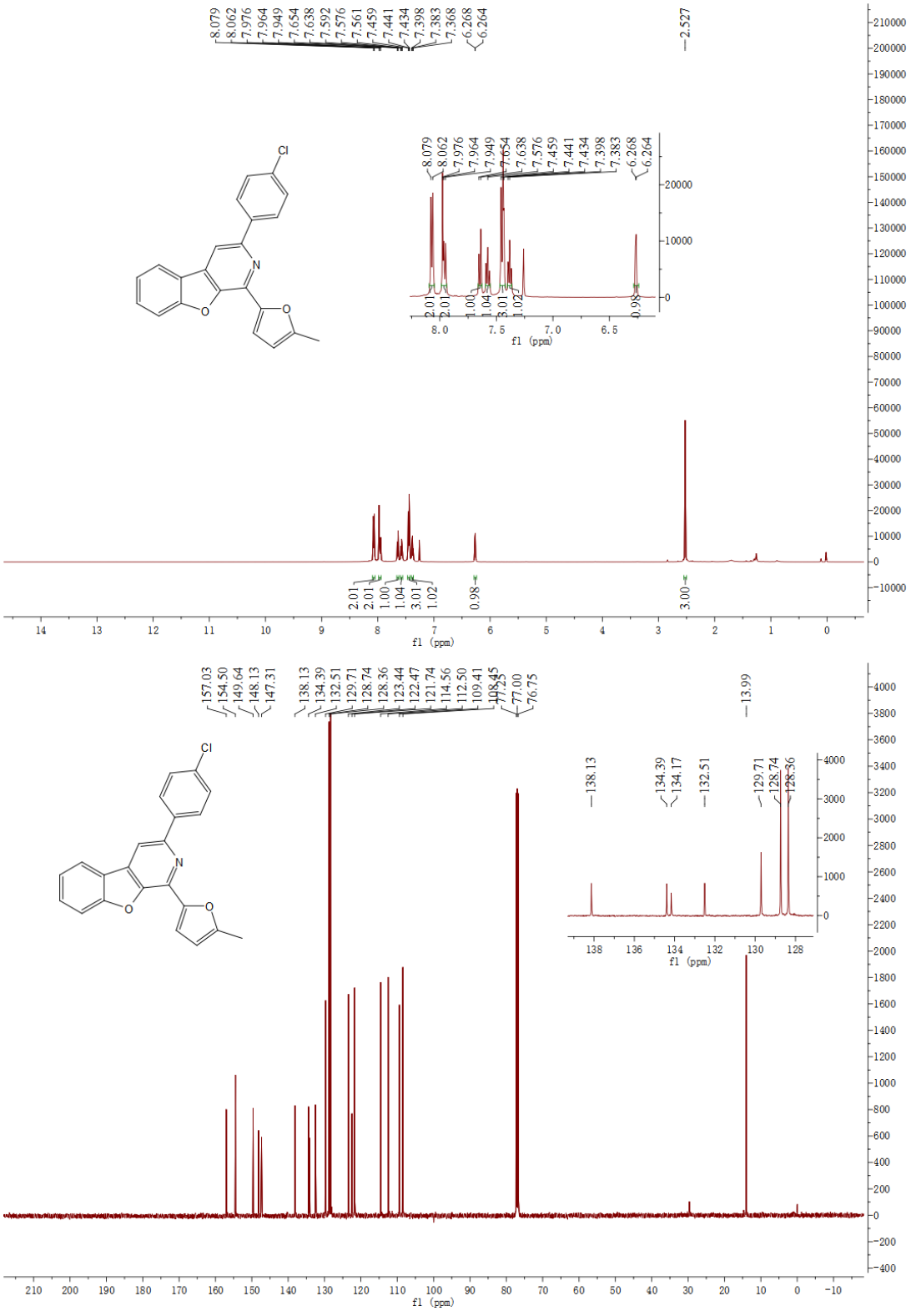


Figure S52. ^{1}H NMR of **4g** (500 MHz, $CDCl_3$) and ^{13}C NMR of **4g** (125 MHz, $CDCl_3$)

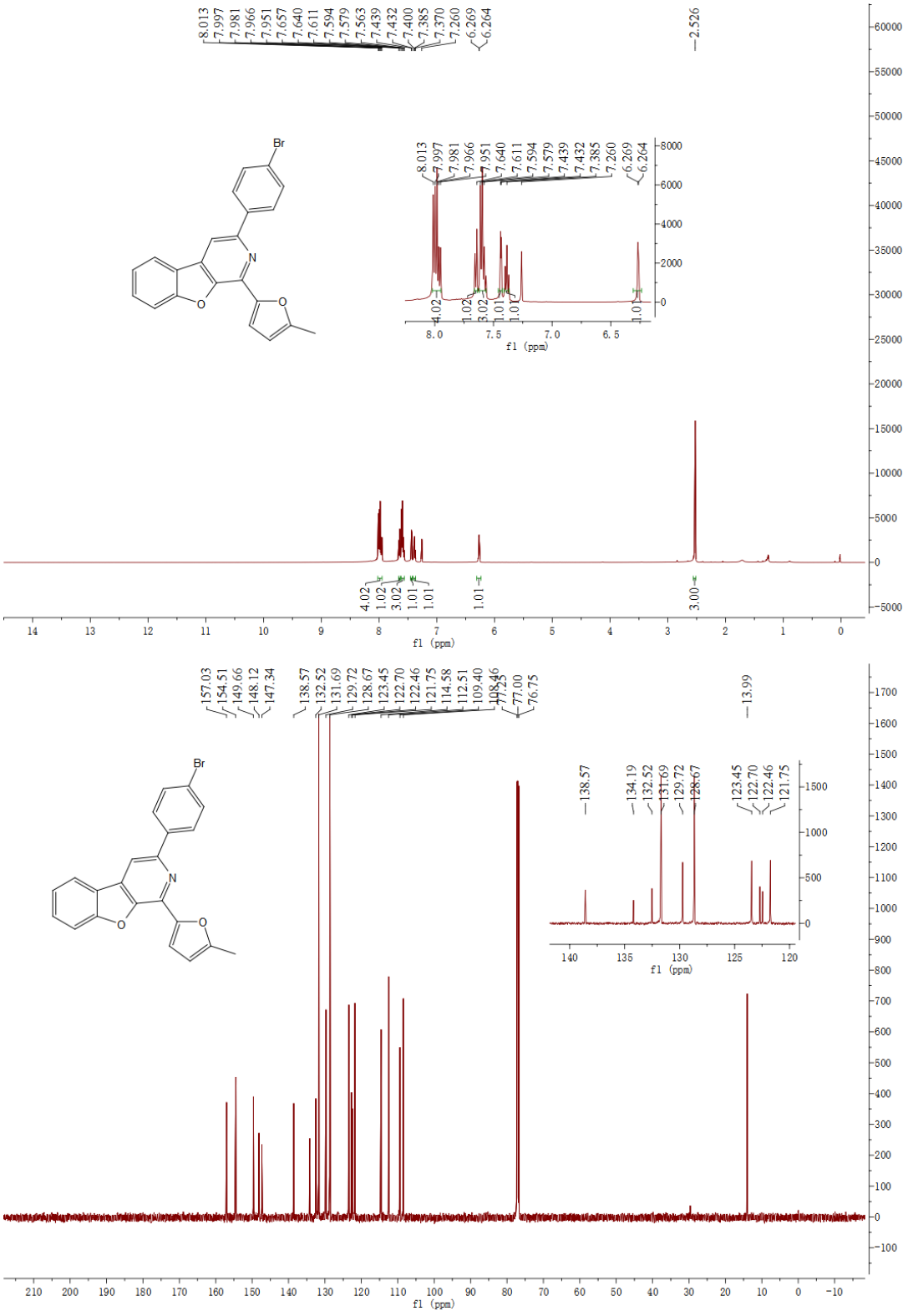


Figure S53. ^{1}H NMR of **4h** (500 MHz, $CDCl_3$) and ^{13}C NMR of **4h** (125 MHz, $CDCl_3$)

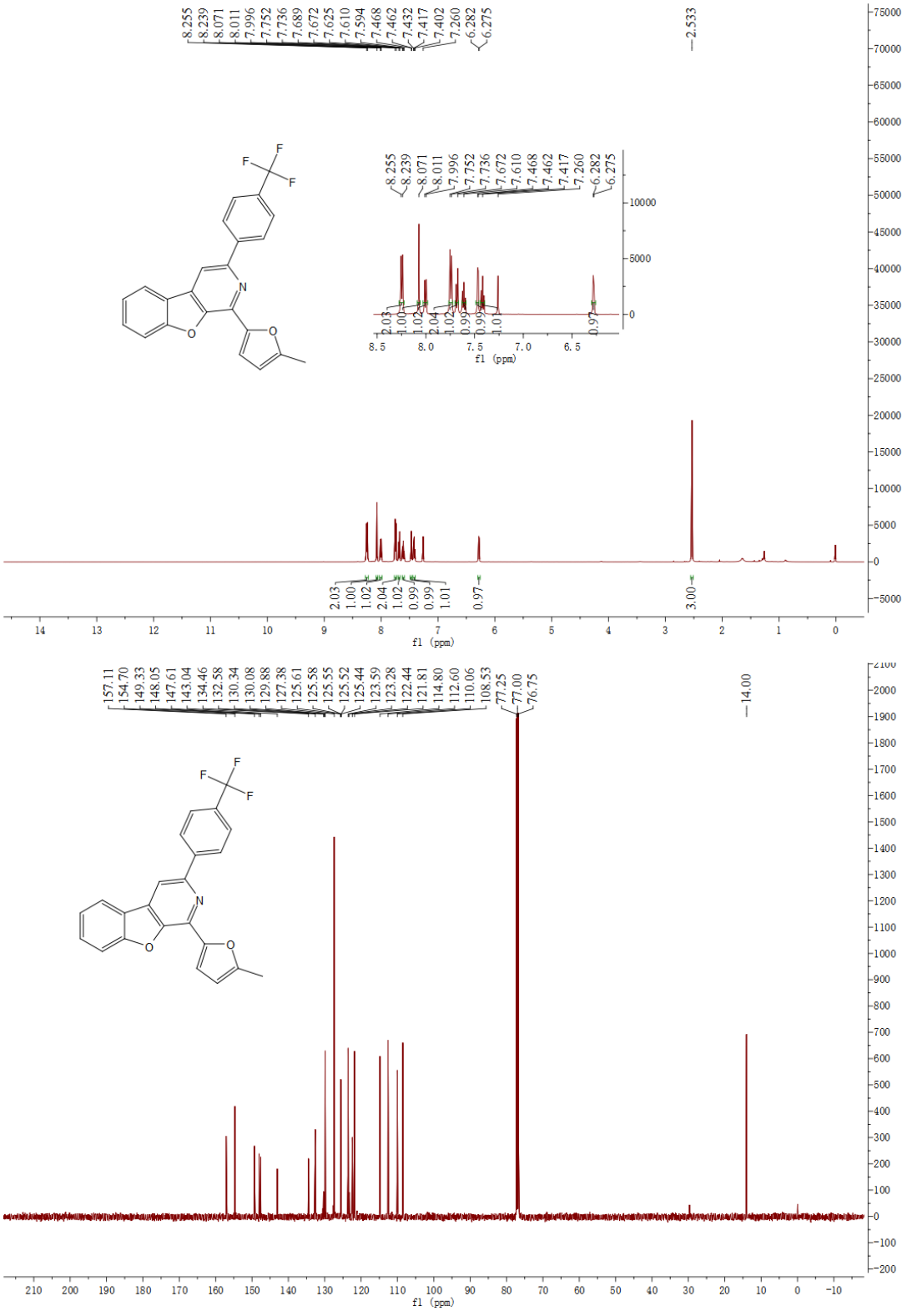


Figure S54. ^{1}H NMR of **4i** (500 MHz, $CDCl_3$) and ^{13}C NMR of **4i** (125 MHz, $CDCl_3$)

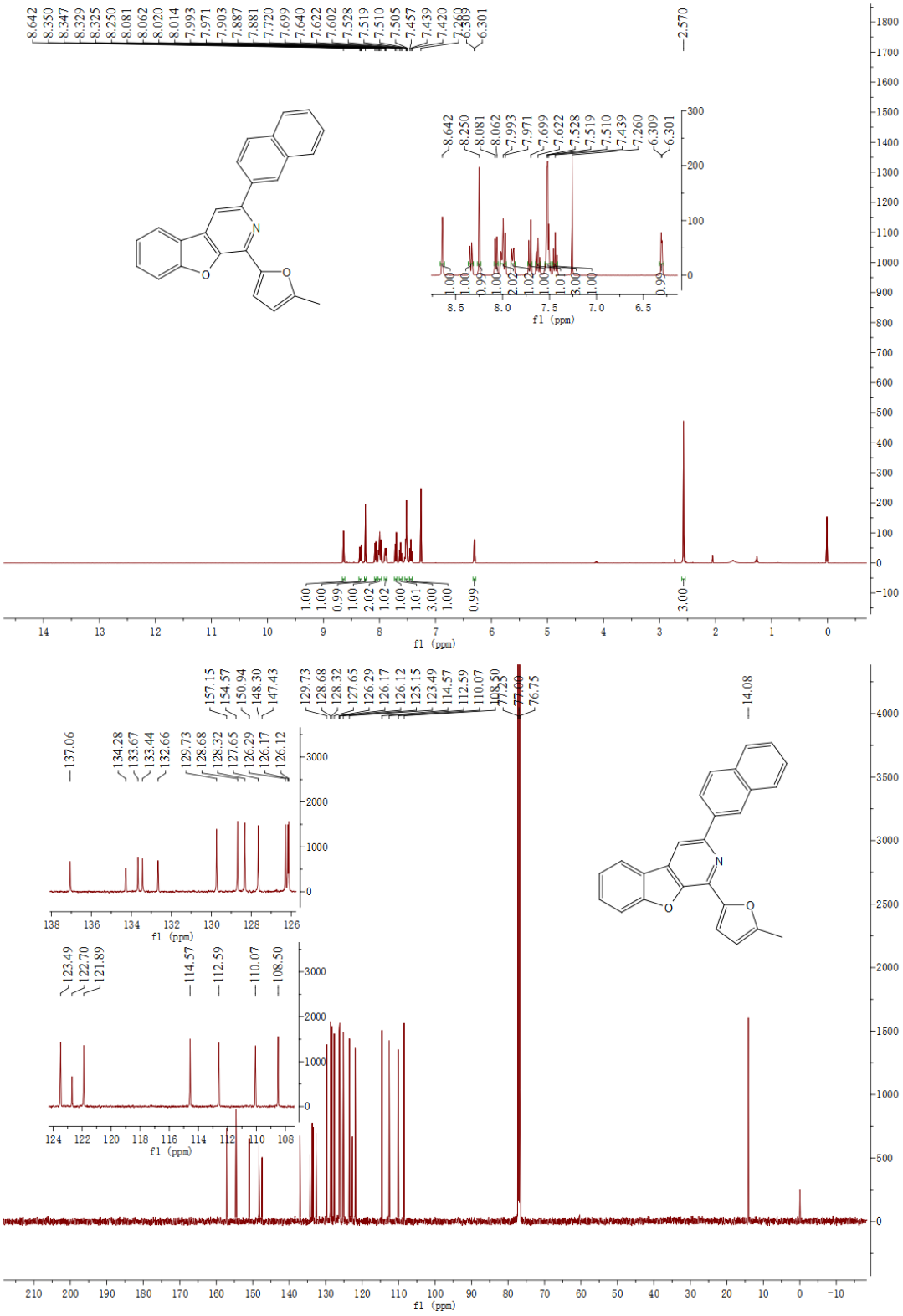


Figure S55. ^{1}H NMR of **4j** (400 MHz, $CDCl_3$) and ^{13}C NMR of **4j** (125 MHz, $CDCl_3$)

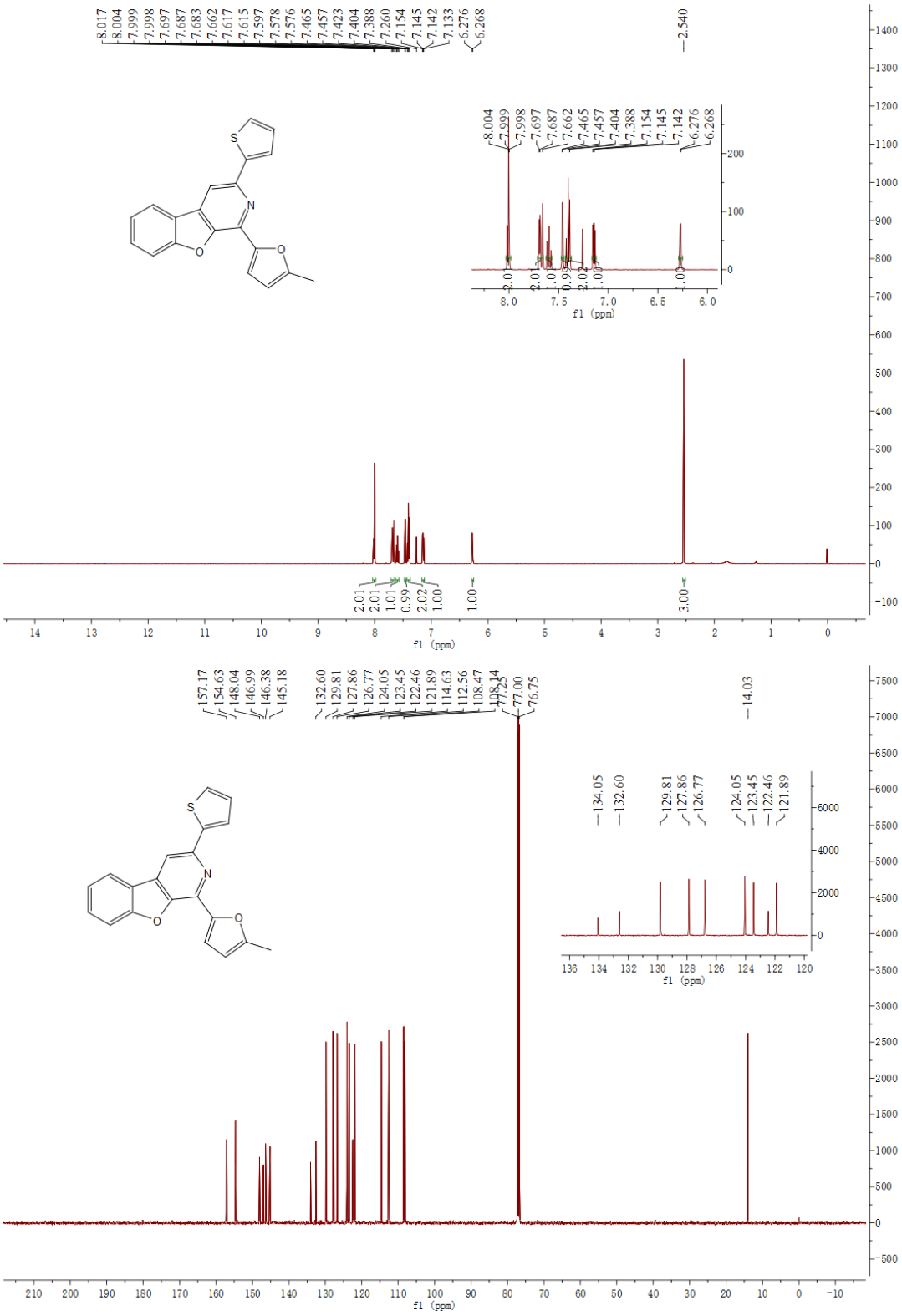


Figure S56. ^{1}H NMR of **4k** (400 MHz, $CDCl_3$) and ^{13}C NMR of **4k** (125 MHz, $CDCl_3$)

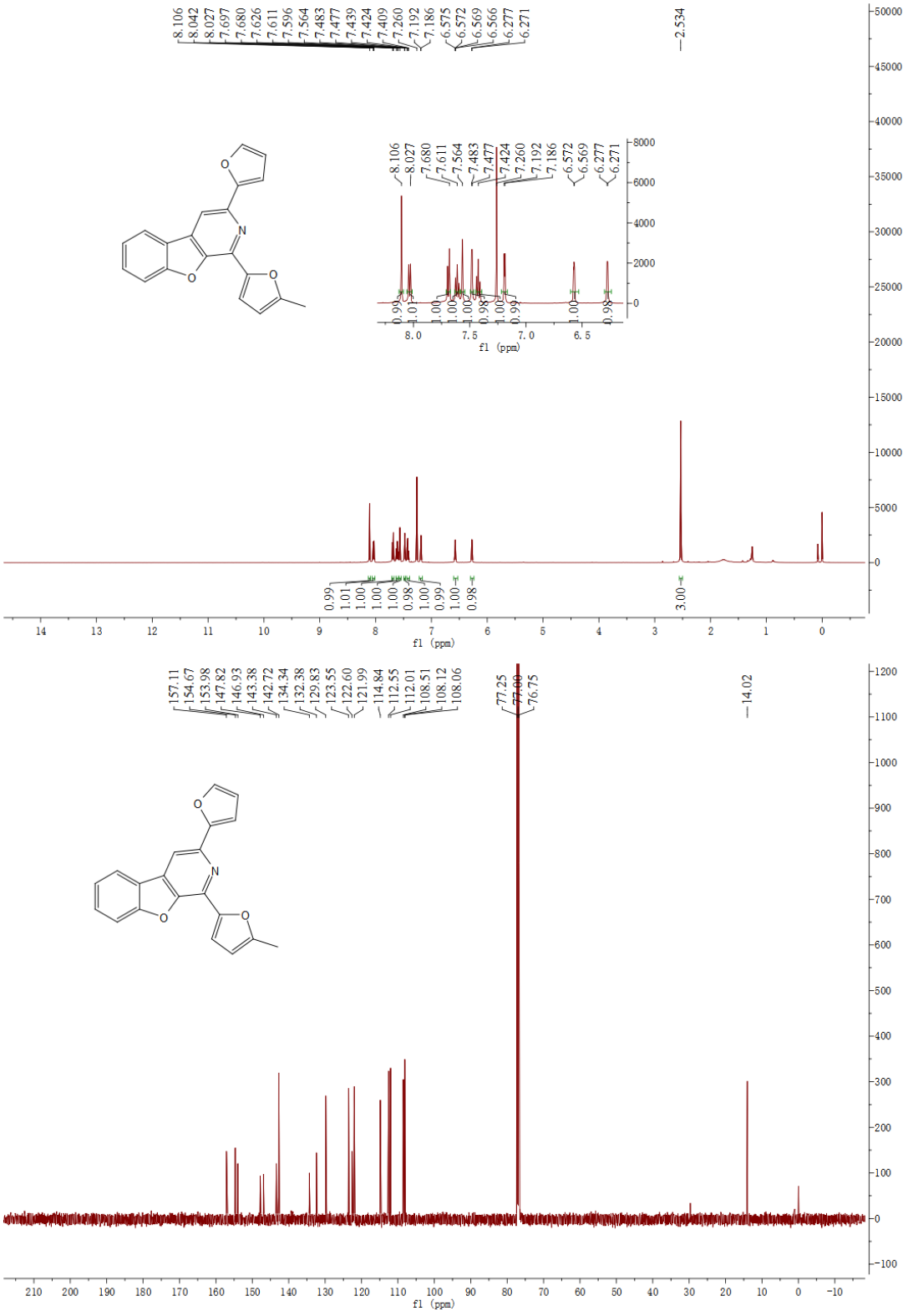


Figure S57. ^{1}H NMR of **4l** (500 MHz, $CDCl_3$) and ^{13}C NMR of **4l** (125 MHz, $CDCl_3$)

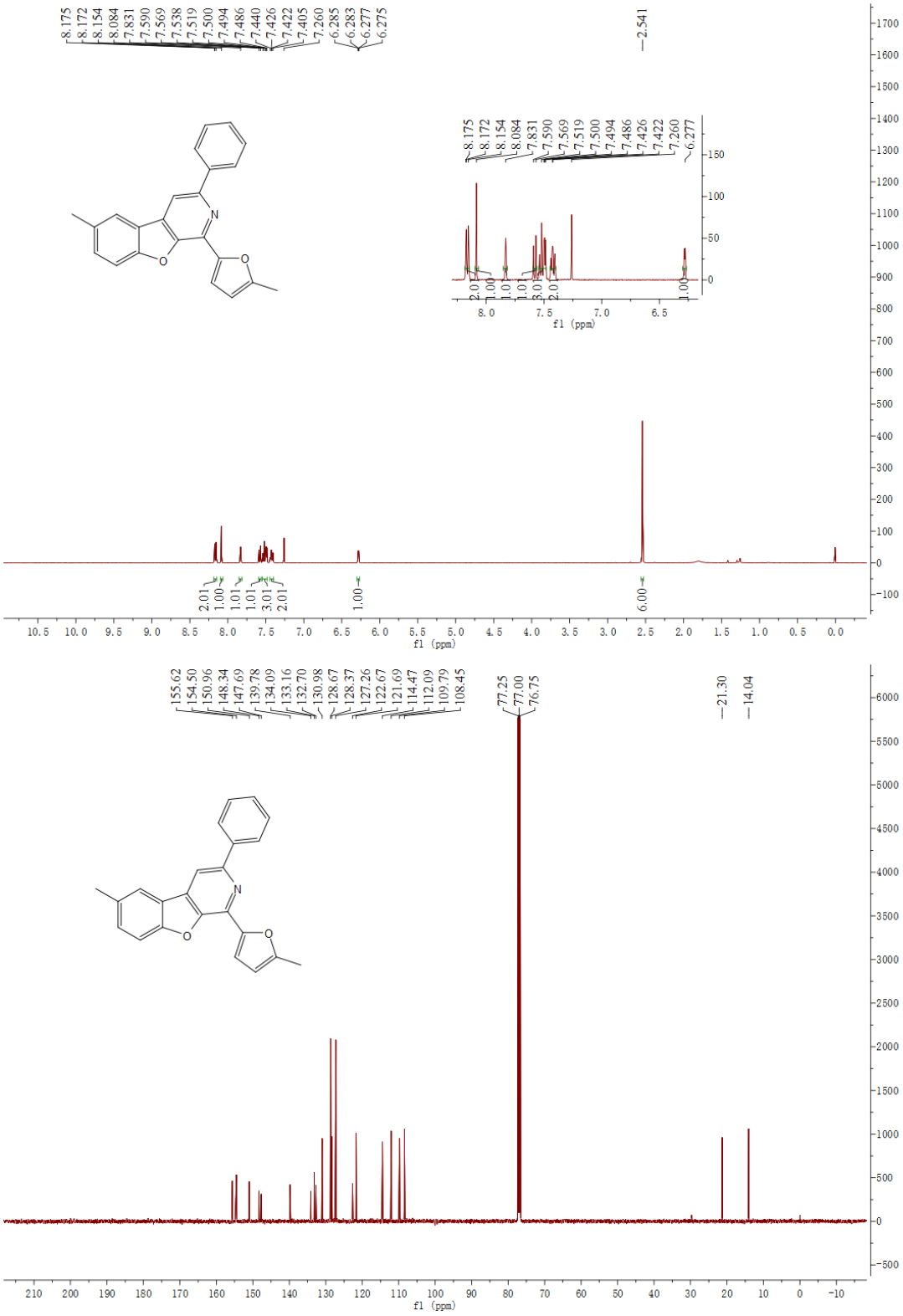


Figure S58. ^{1}H NMR of **4m** (400 MHz, $CDCl_3$) and ^{13}C NMR of **4m** (125 MHz, $CDCl_3$)

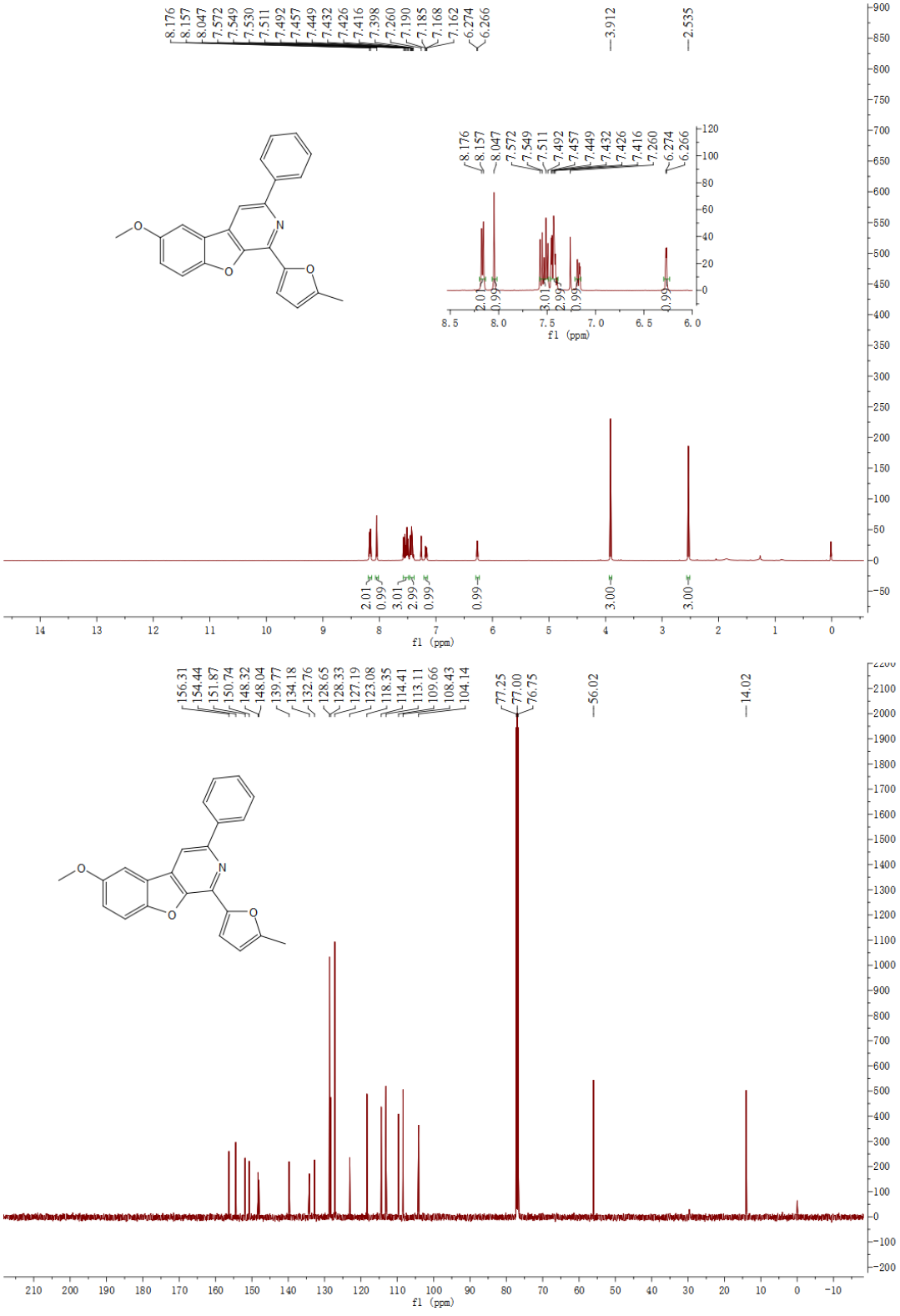


Figure S59. ^{1}H NMR of **4n** (400 MHz, $CDCl_3$) and ^{13}C NMR of **4n** (125 MHz, $CDCl_3$)

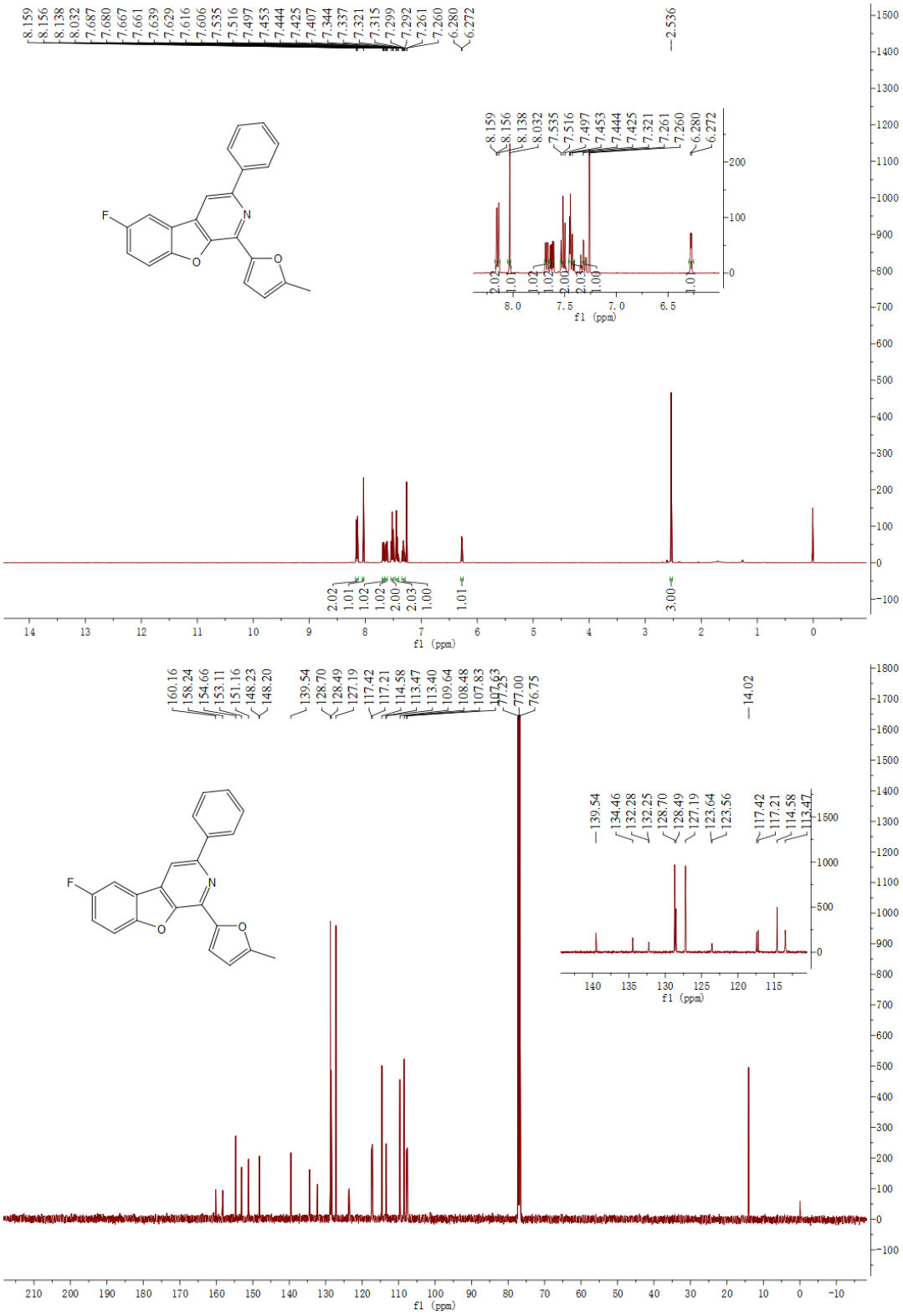


Figure S60. ^{1}H NMR of **4o** (400 MHz, $CDCl_3$) and ^{13}C NMR of **4o** (125 MHz, $CDCl_3$)

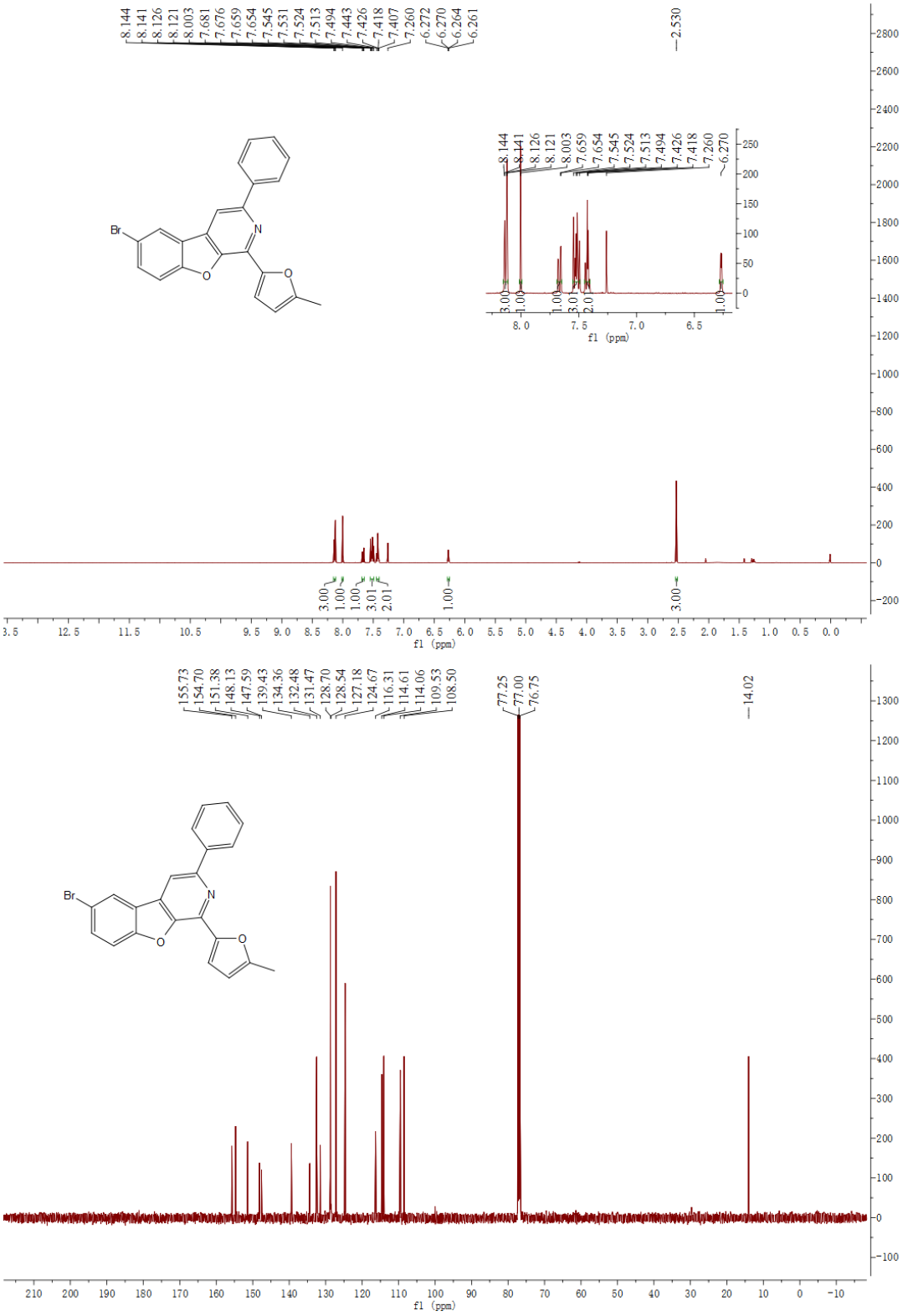


Figure S61. ^{1}H NMR of **4p** (400 MHz, $CDCl_3$) and ^{13}C NMR of **4p** (125 MHz, $CDCl_3$)

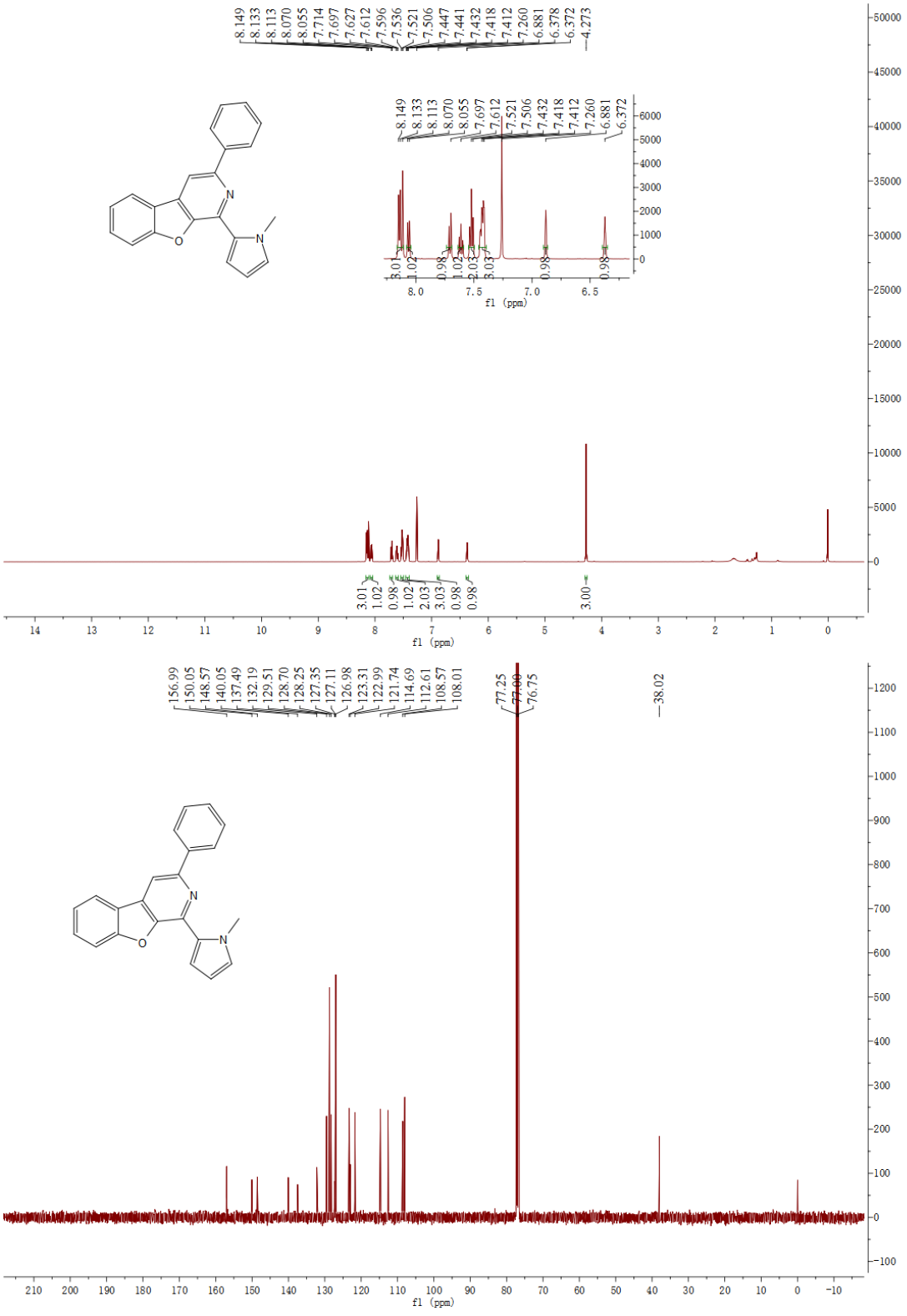


Figure S62. ^{1}H NMR of **5a** (500 MHz, $CDCl_3$) and ^{13}C NMR of **5a** (125 MHz, $CDCl_3$)

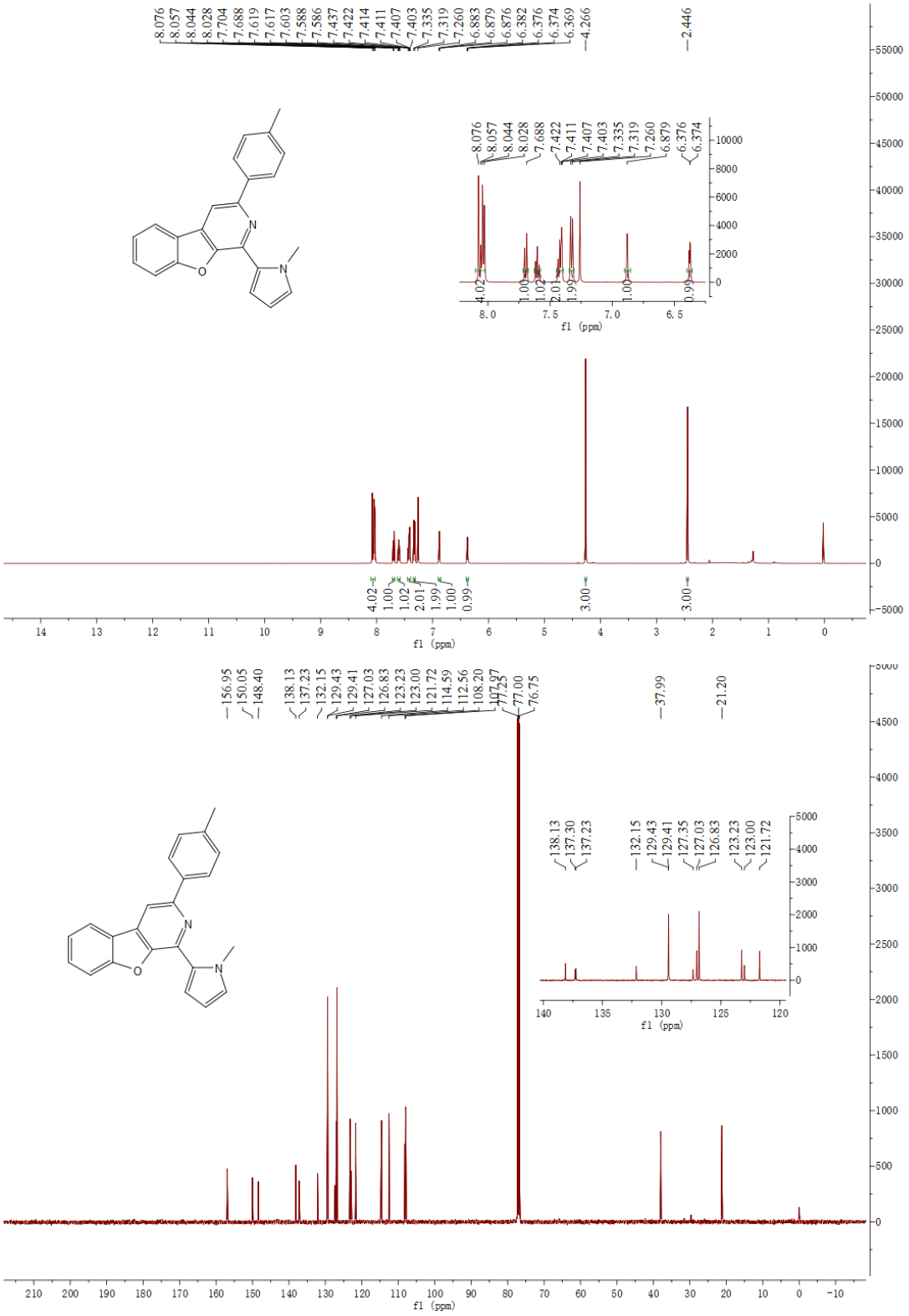


Figure S63. ^{1}H NMR of **5b** (500 MHz, $CDCl_3$) and ^{13}C NMR of **5b** (125 MHz, $CDCl_3$)

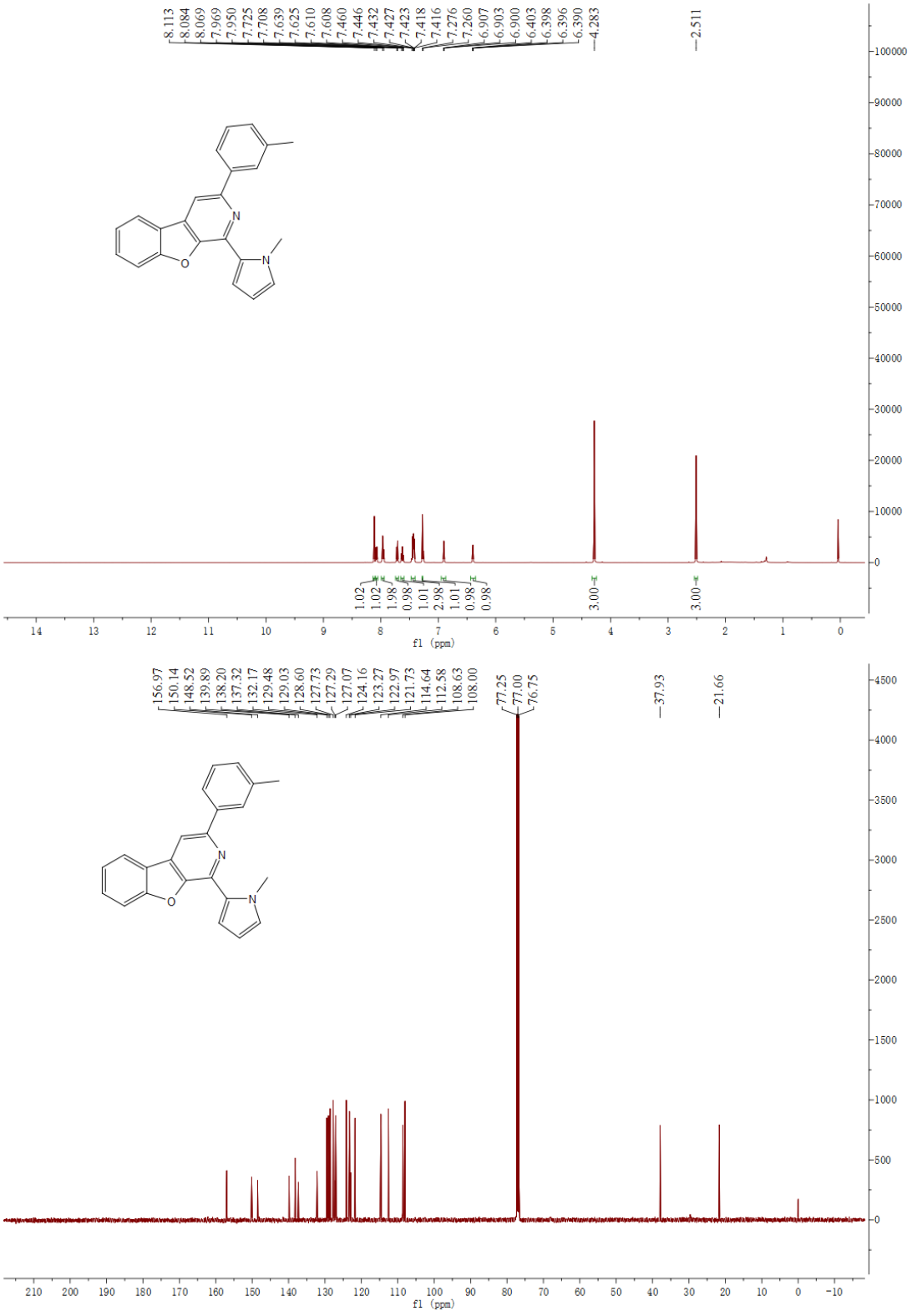


Figure S64. ^{1}H NMR of **5c** (500 MHz, $CDCl_3$) and ^{13}C NMR of **5c** (125 MHz, $CDCl_3$)

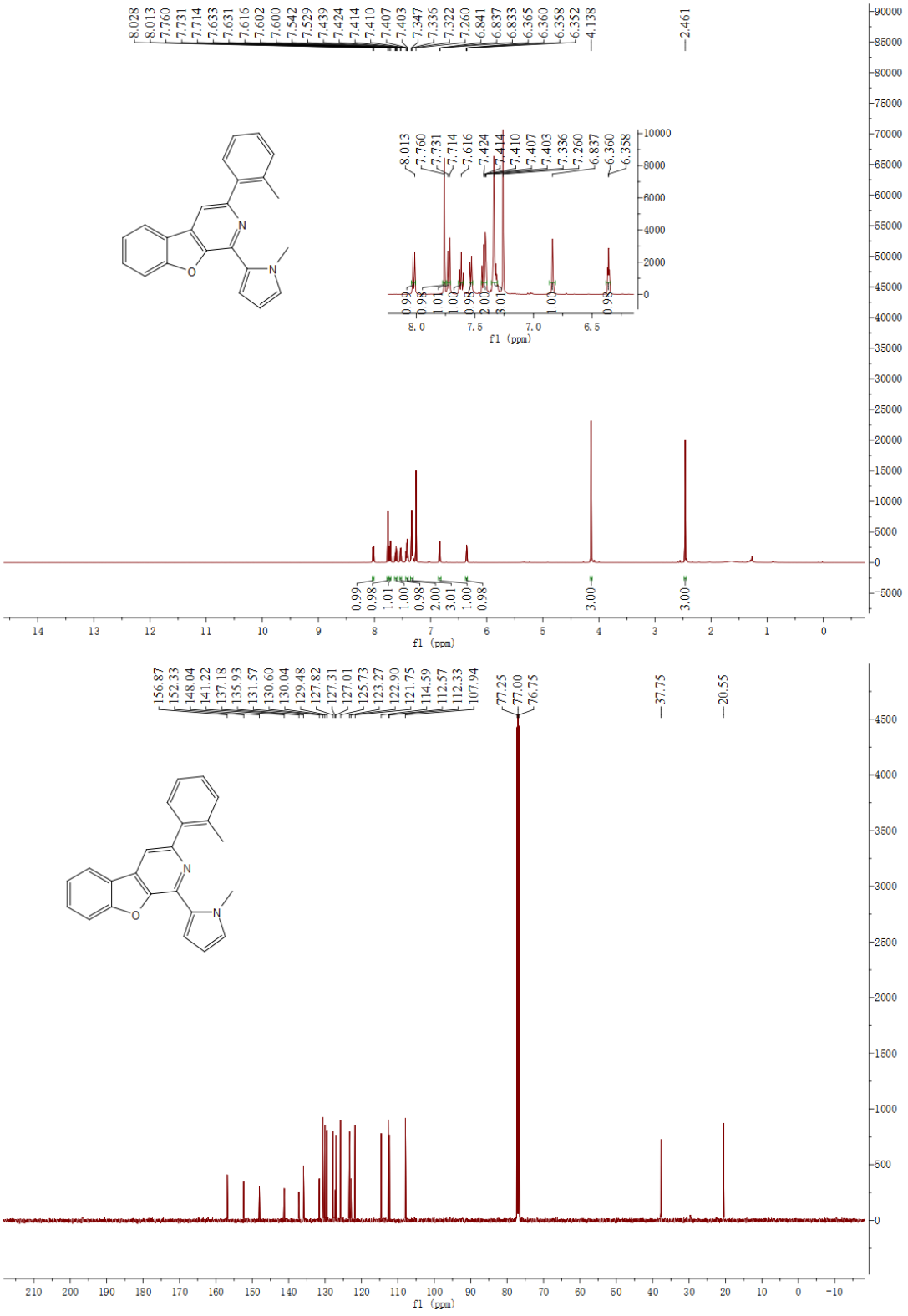


Figure S65. ^{1}H NMR of **5d** (500 MHz, $CDCl_3$) and ^{13}C NMR of **5d** (125 MHz, $CDCl_3$)

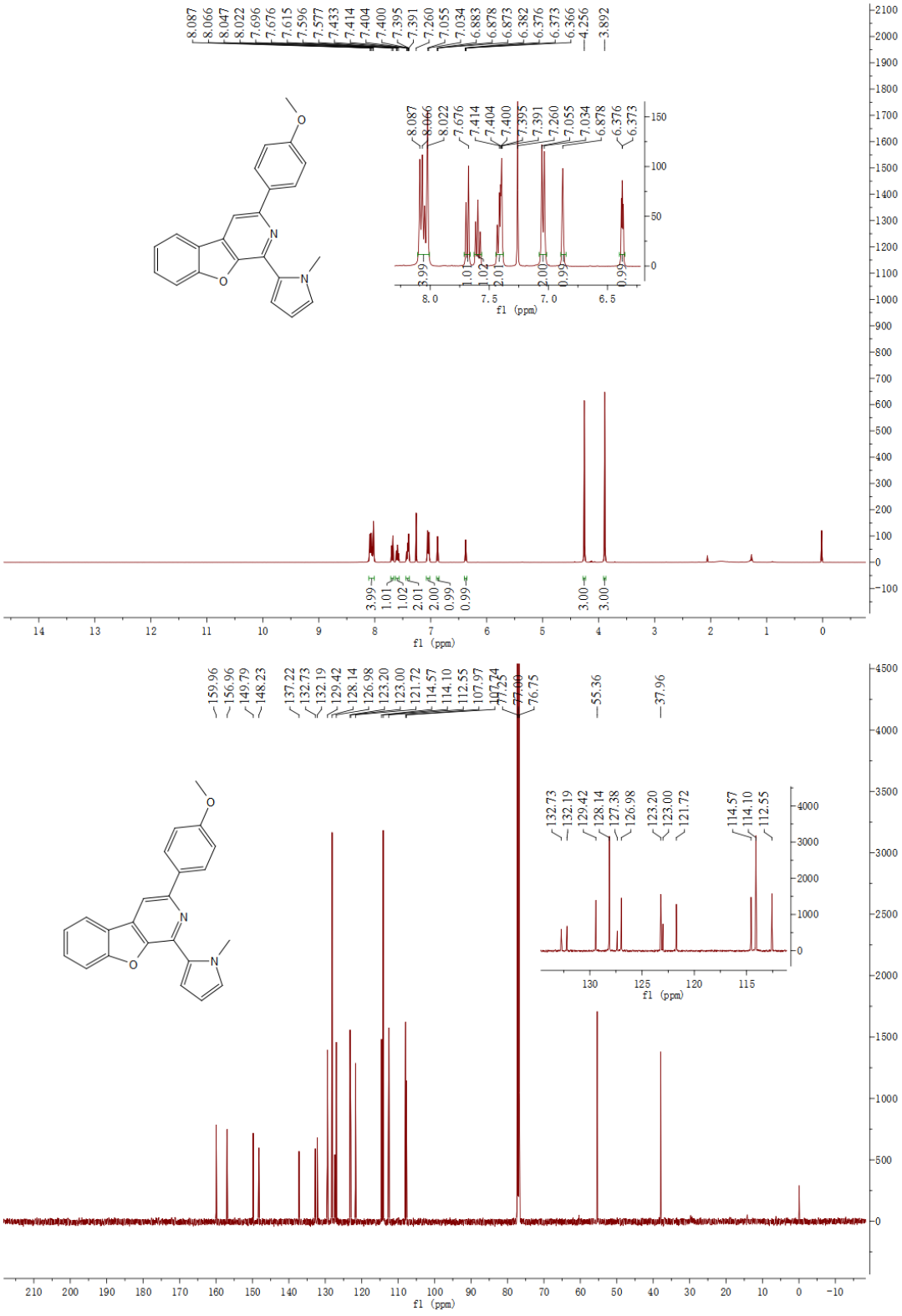


Figure S66. ^{1}H NMR of **5e** (400 MHz, $CDCl_3$) and ^{13}C NMR of **5e** (125 MHz, $CDCl_3$)

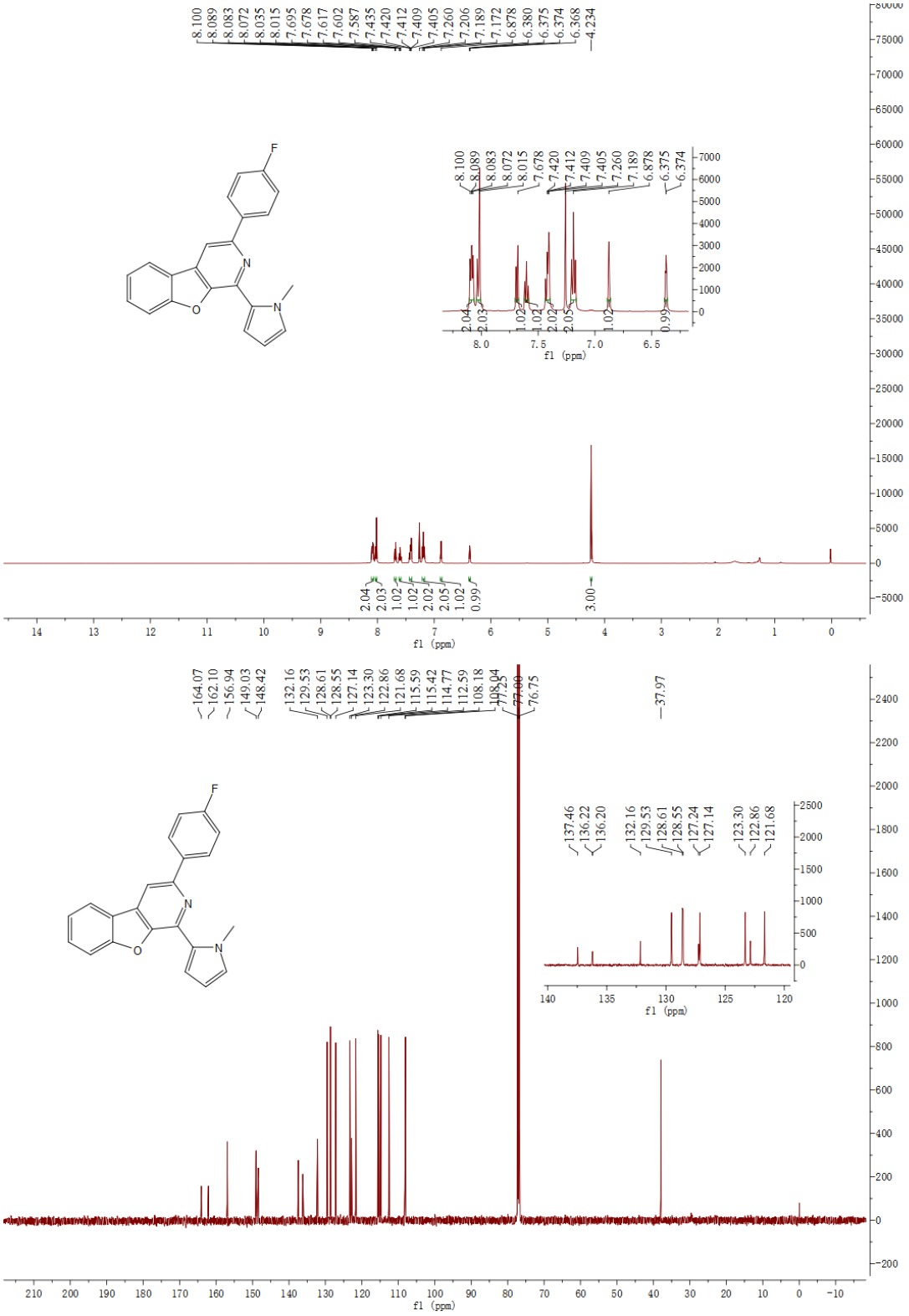


Figure S67. ^{1}H NMR of **5f** (500 MHz, $CDCl_3$) and ^{13}C NMR of **5f** (125 MHz, $CDCl_3$)

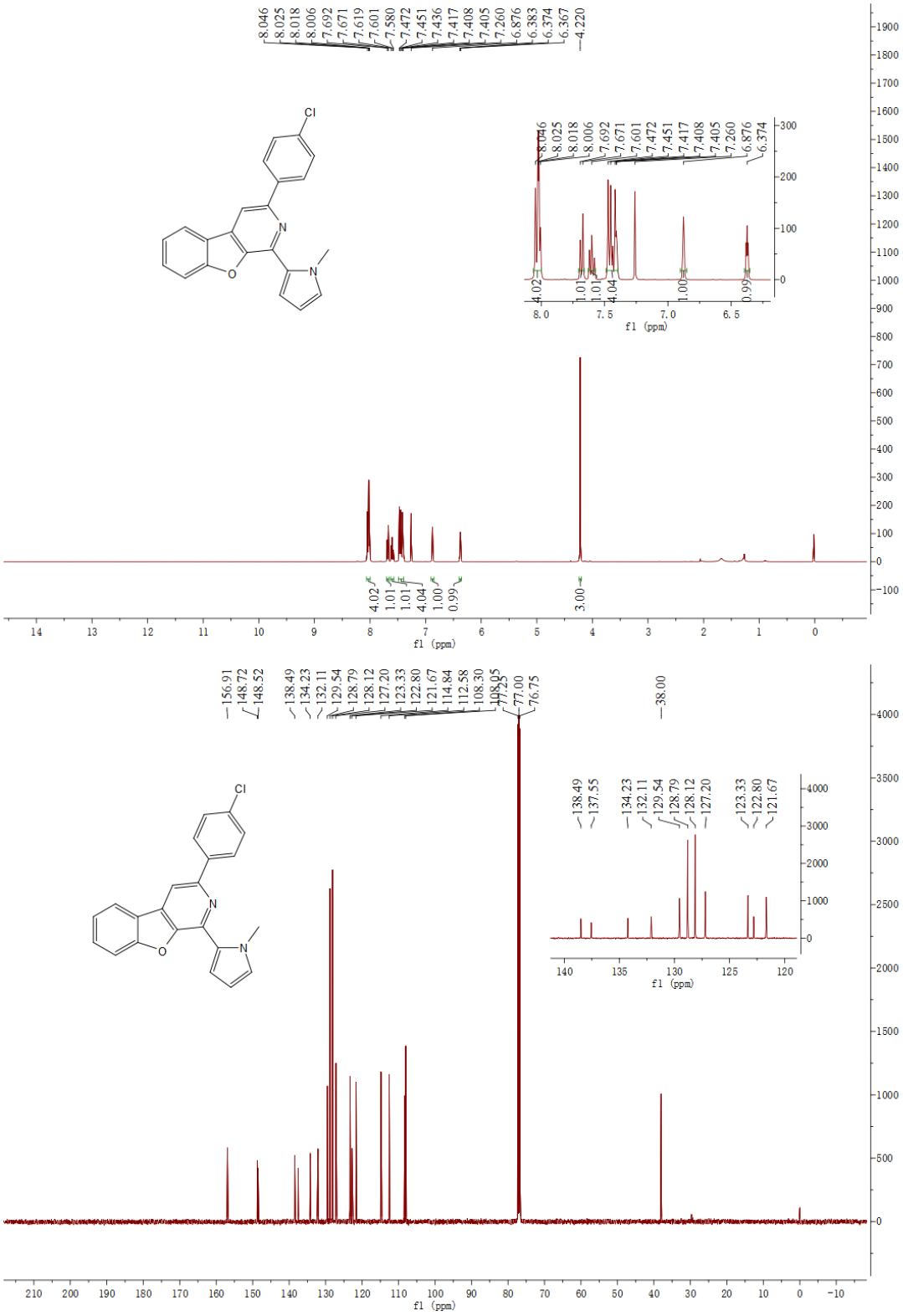


Figure S68. ^{1}H NMR of **5g** (400 MHz, $CDCl_3$) and ^{13}C NMR of **5g** (125 MHz, $CDCl_3$)

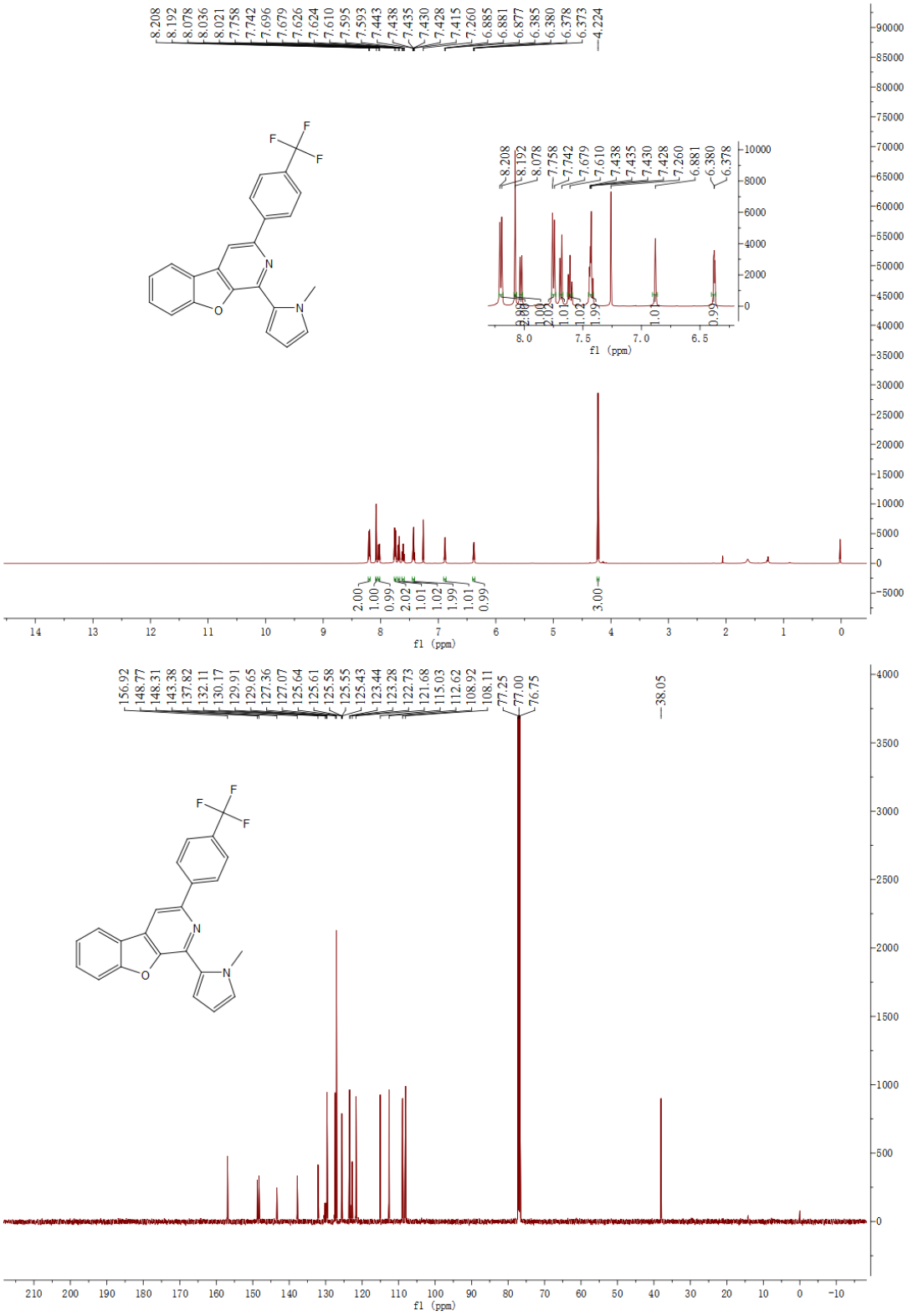


Figure S69. ^{1}H NMR of **5h** (500 MHz, $CDCl_3$) and ^{13}C NMR of **5h** (125 MHz, $CDCl_3$)

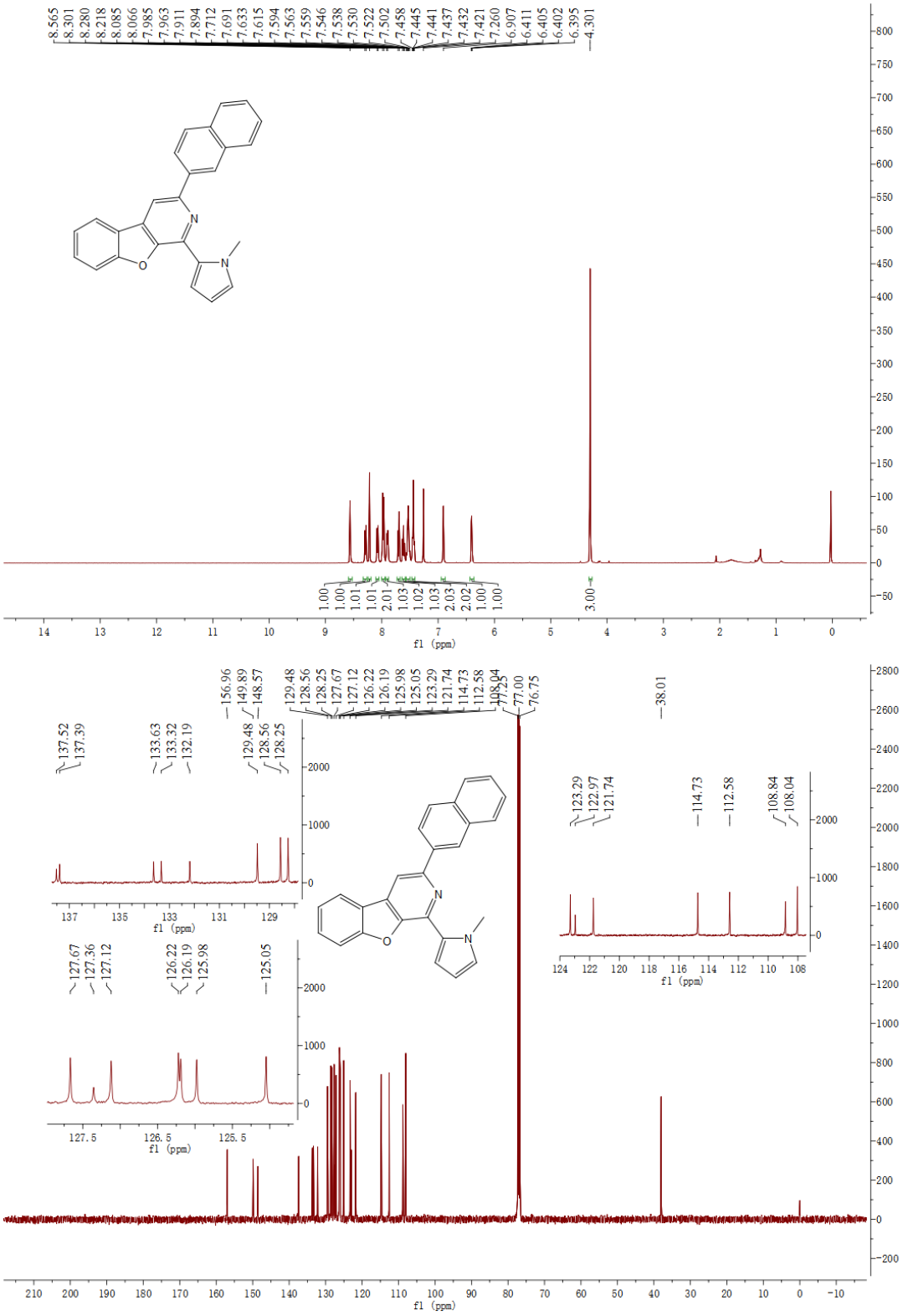


Figure S70. ^{1}H NMR of **5i** (400 MHz, $CDCl_3$) and ^{13}C NMR of **5i** (125 MHz, $CDCl_3$)

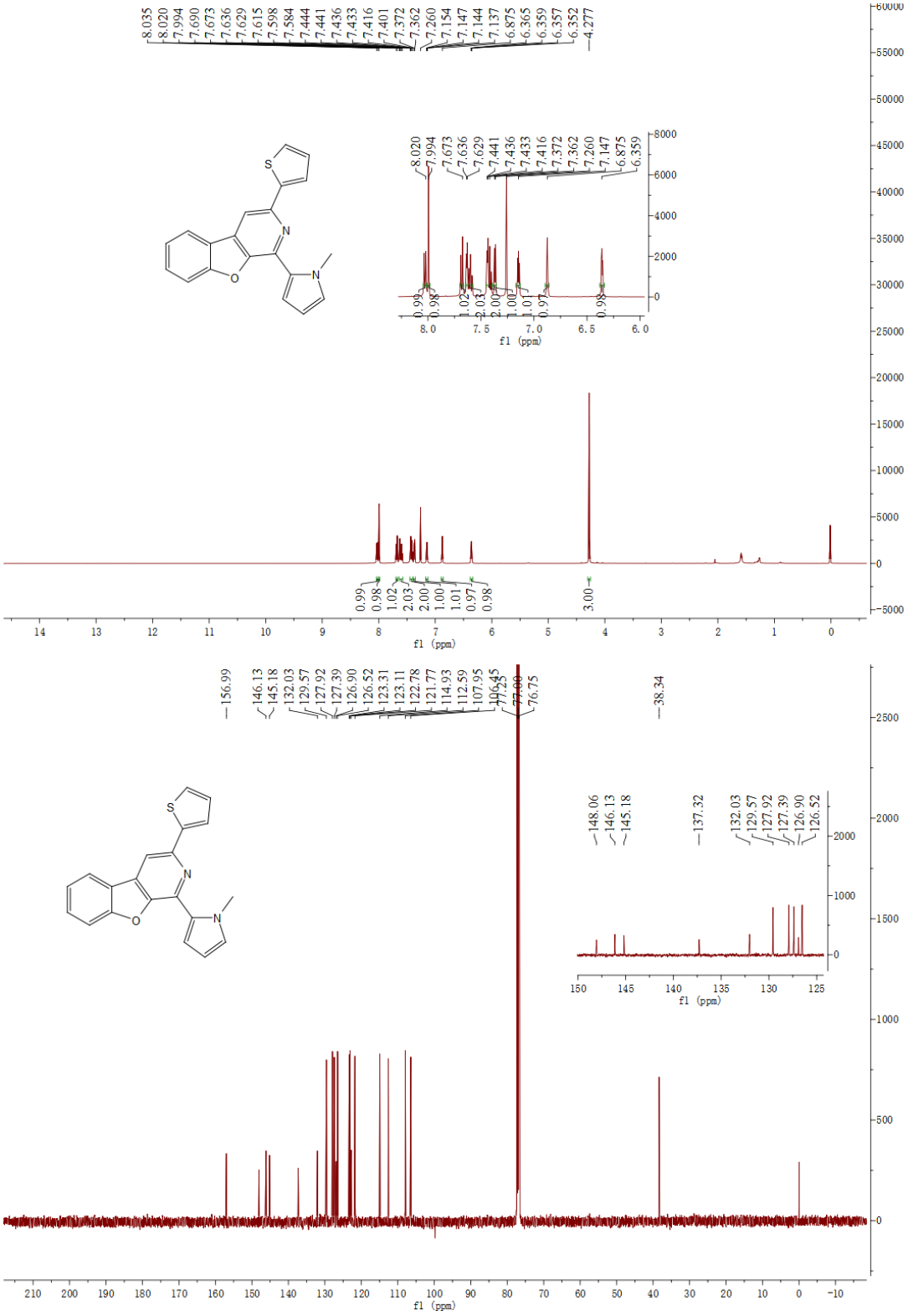


Figure S71. ^{1}H NMR of **5j** (500 MHz, $CDCl_3$) and ^{13}C NMR of **5j** (125 MHz, $CDCl_3$)

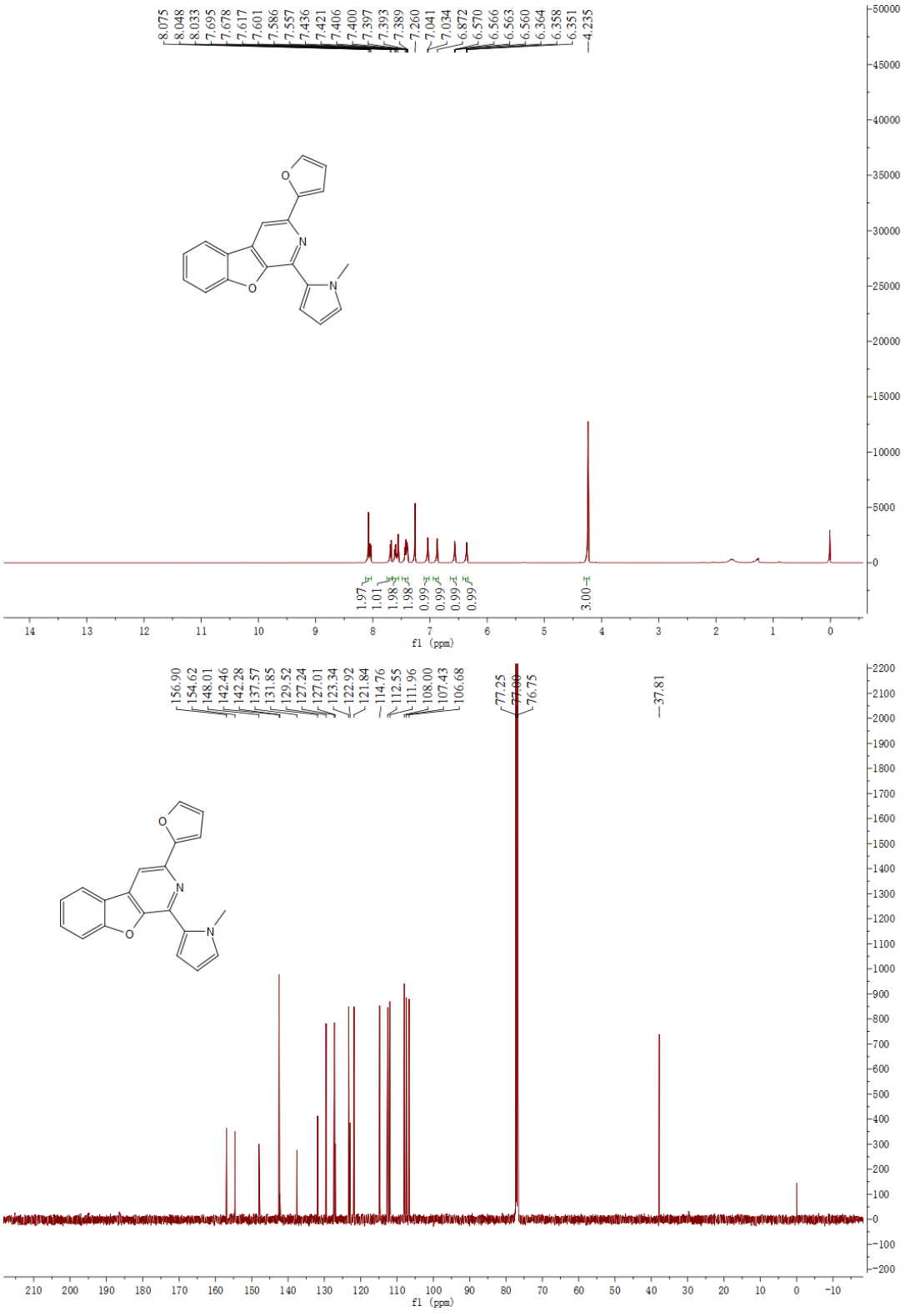


Figure S72. ^{1}H NMR of **5k** (500 MHz, $CDCl_3$) and ^{13}C NMR of **5k** (125 MHz, $CDCl_3$)

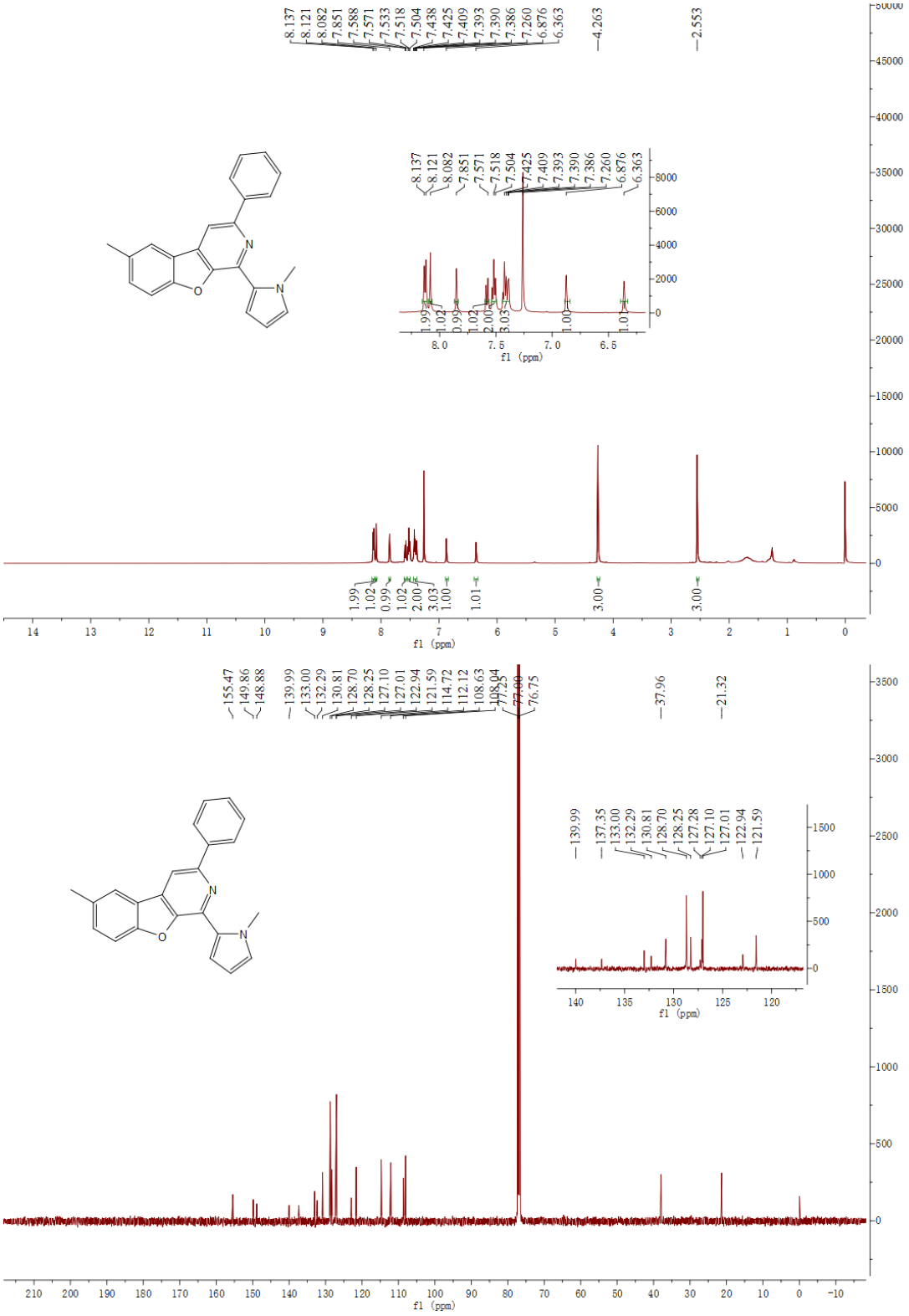


Figure S73. ^{1}H NMR of **5l** (500 MHz, $CDCl_3$) and ^{13}C NMR of **5l** (125 MHz, $CDCl_3$)

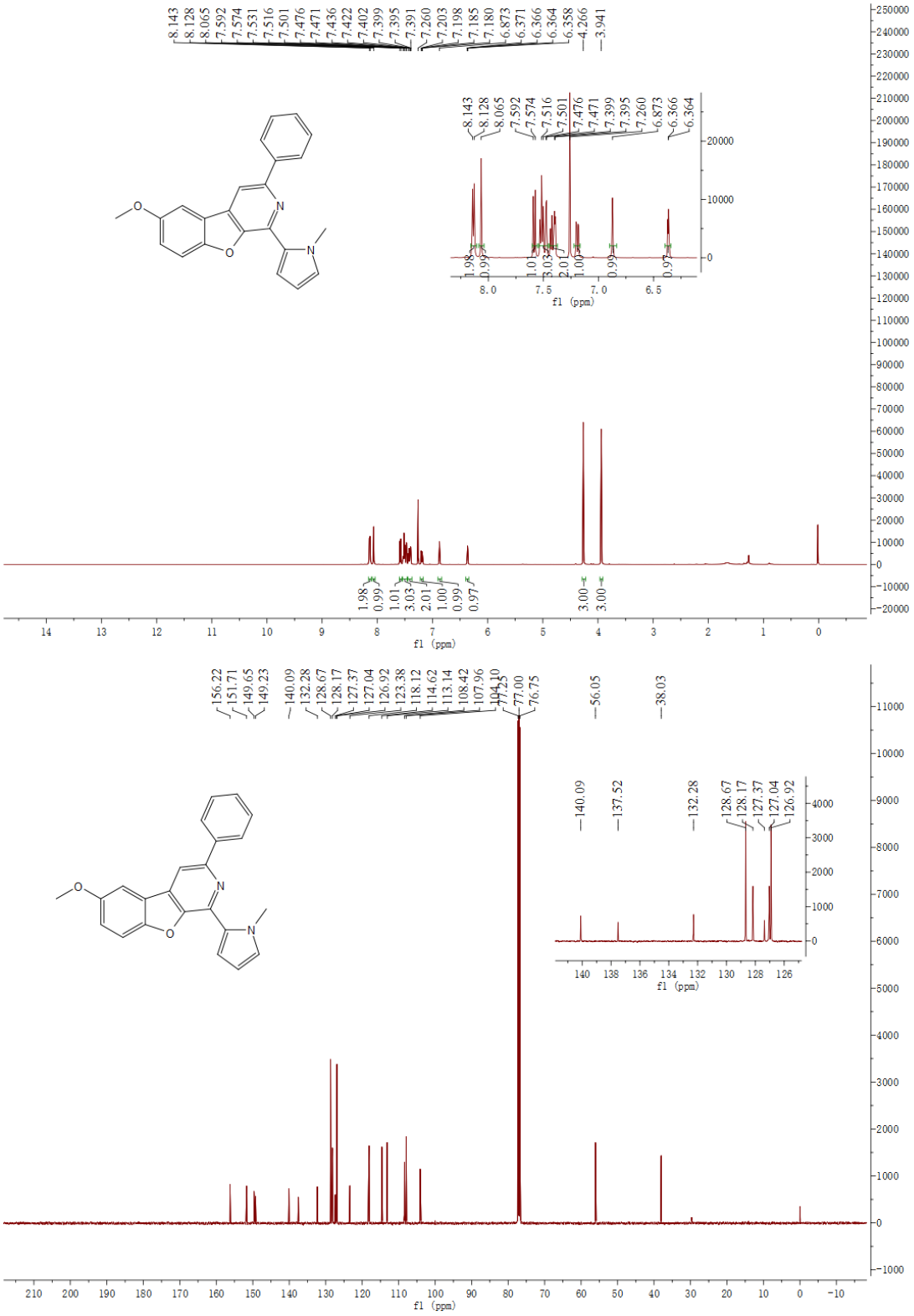


Figure S74. ^{1}H NMR of **5m** (500 MHz, $CDCl_3$) and ^{13}C NMR of **5m** (125 MHz, $CDCl_3$)

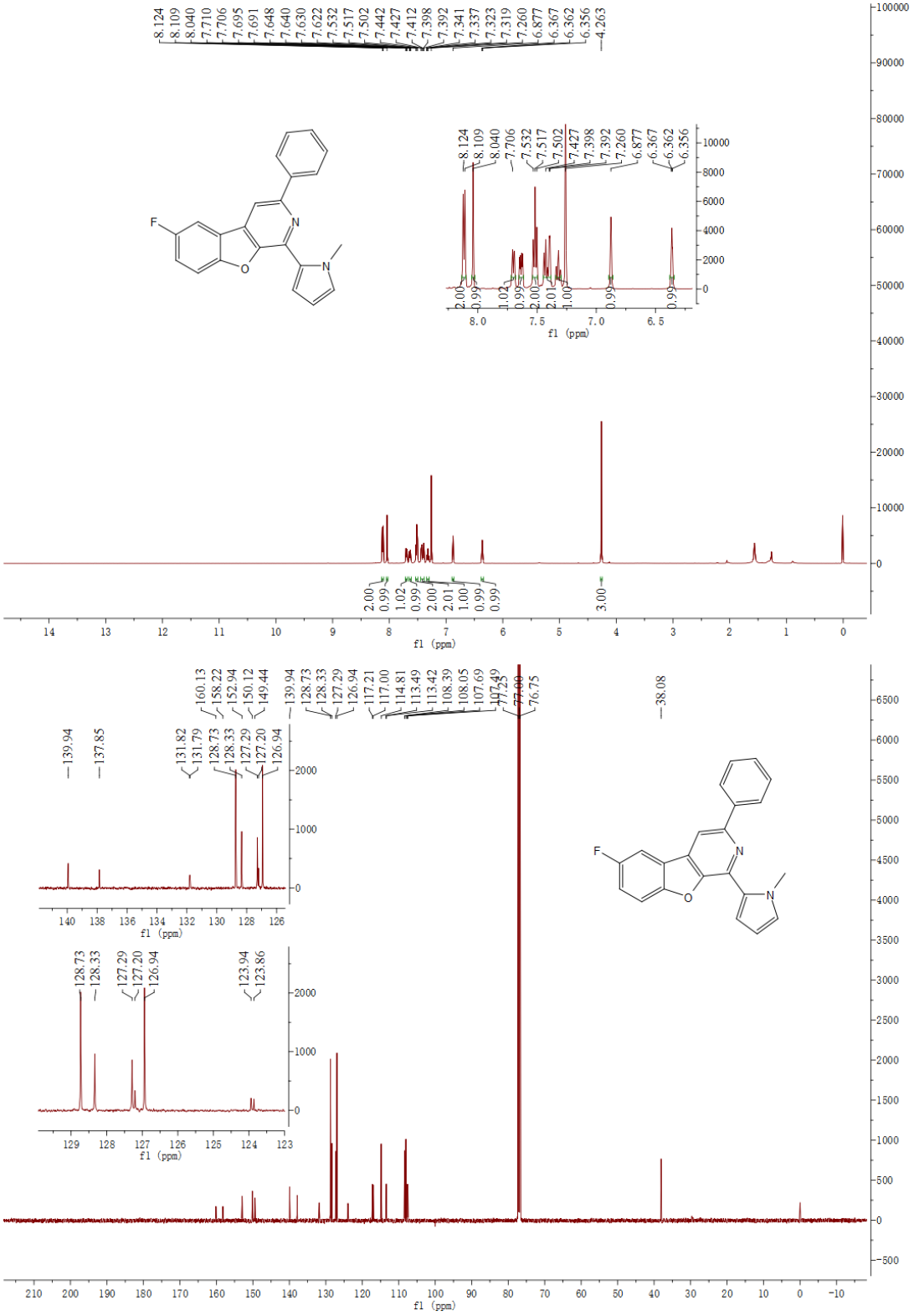


Figure S75. ^{1}H NMR of **5n** (500 MHz, $CDCl_3$) and ^{13}C NMR of **5n** (125 MHz, $CDCl_3$)

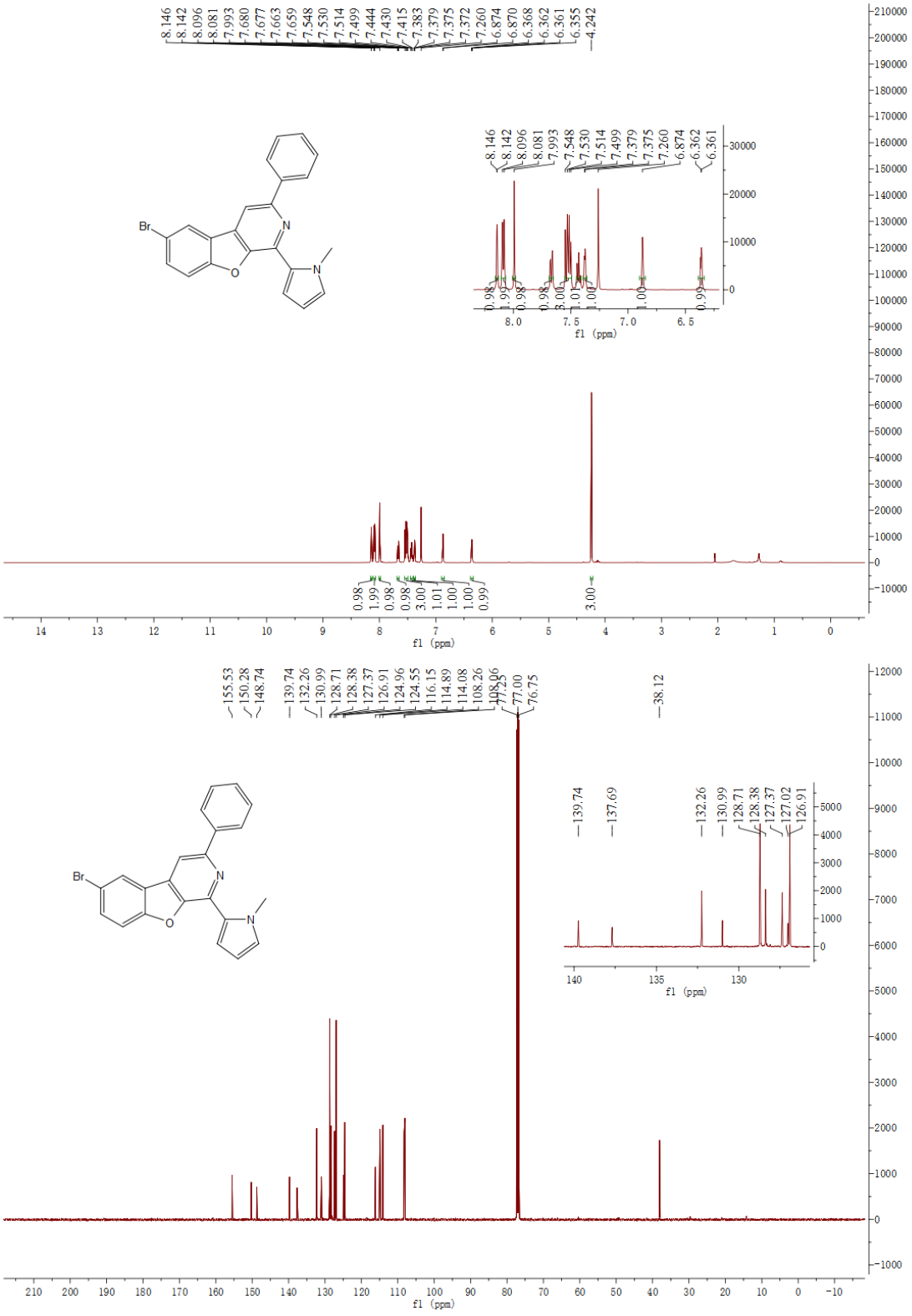


Figure S76. ^{1}H NMR of **5o** (500 MHz, $CDCl_3$) and ^{13}C NMR of **5o** (125 MHz, $CDCl_3$)

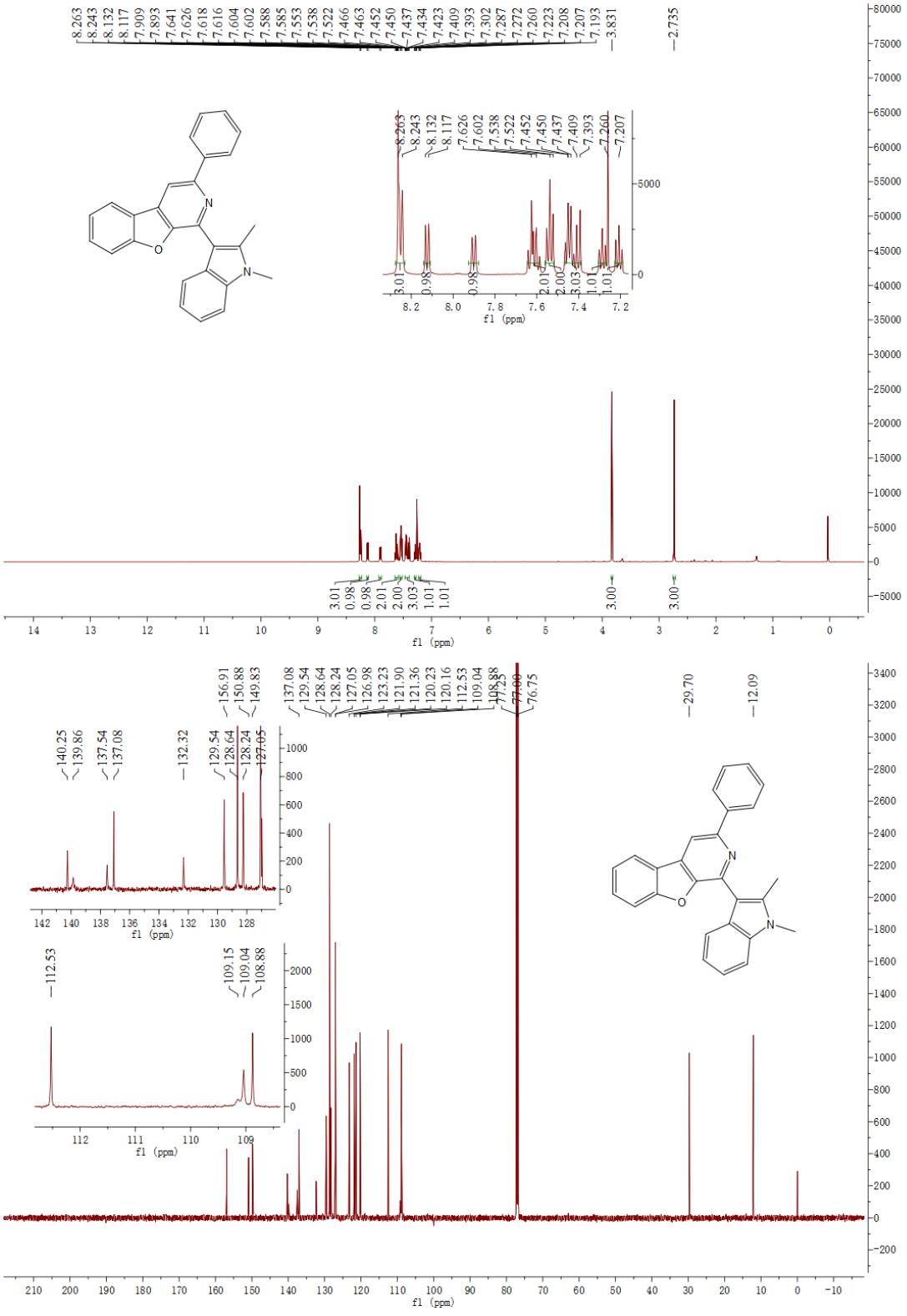


Figure S77. ^{1}H NMR of **6a** (500 MHz, $CDCl_3$) and ^{13}C NMR of **6a** (125 MHz, $CDCl_3$)

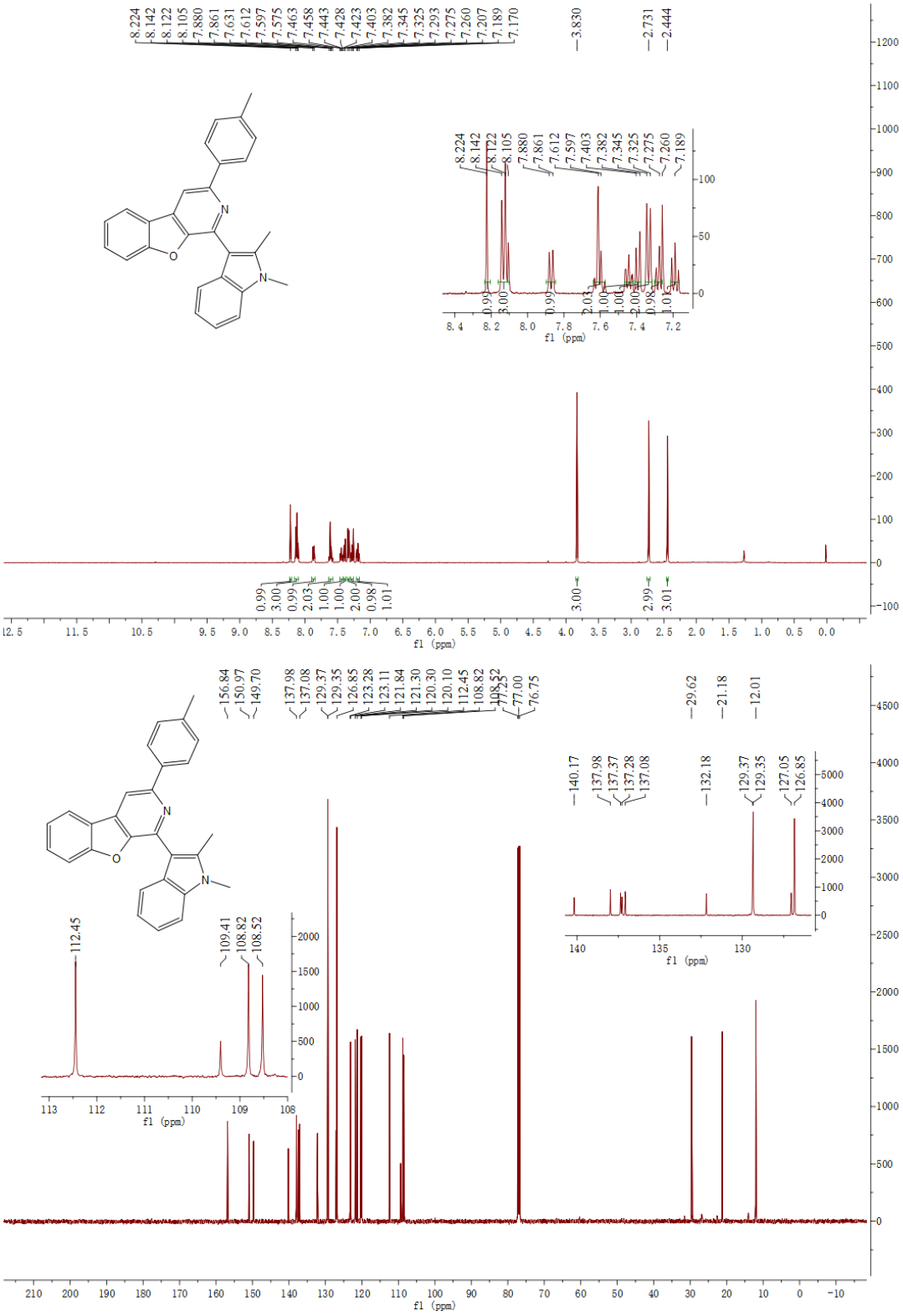


Figure S78. ^{1}H NMR of **6b** (400 MHz, $CDCl_3$) and ^{13}C NMR of **6b** (125 MHz, $CDCl_3$)

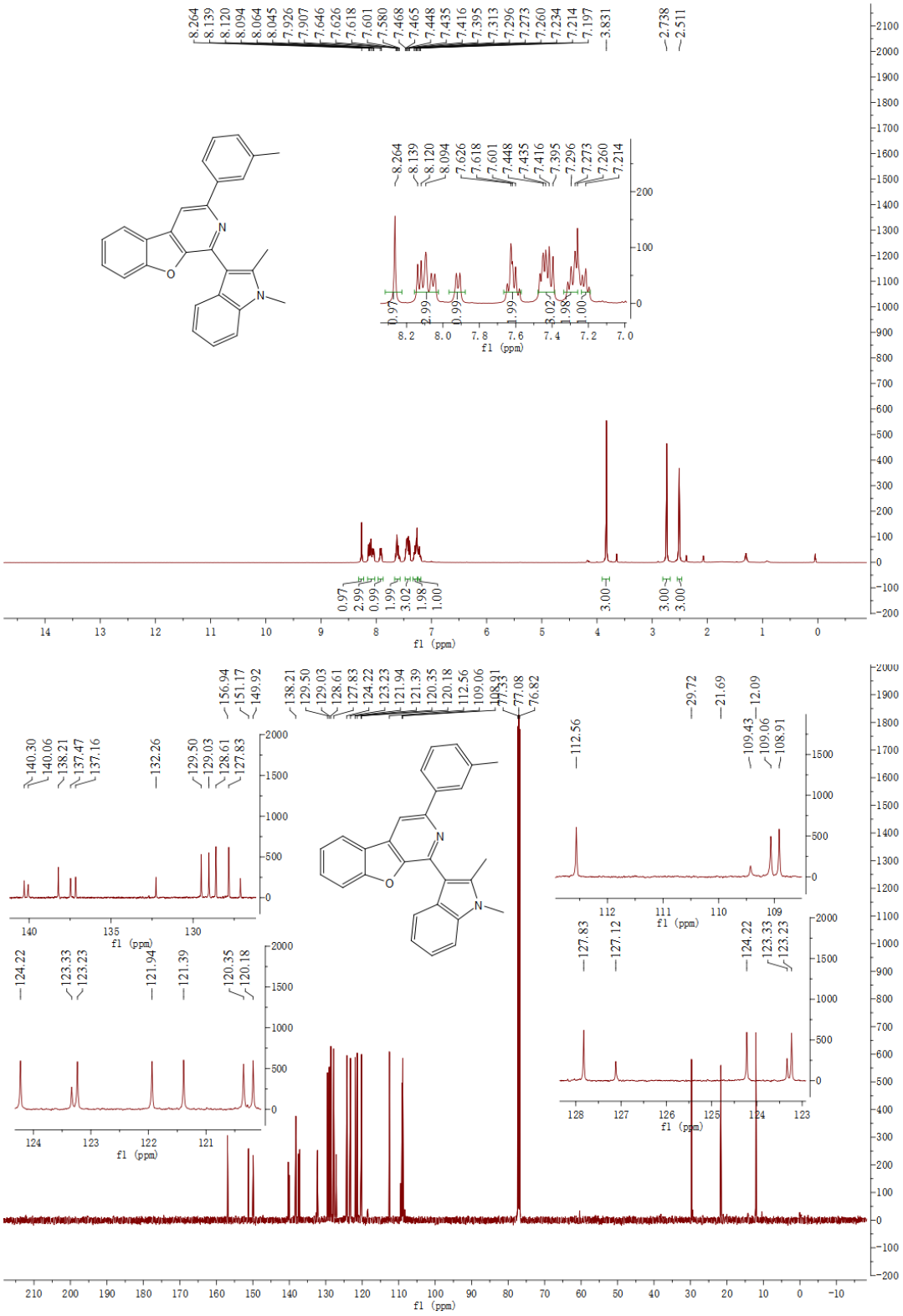


Figure S79. ^{1}H NMR of **6c** (400 MHz, $CDCl_3$) and ^{13}C NMR of **6c** (125 MHz, $CDCl_3$)

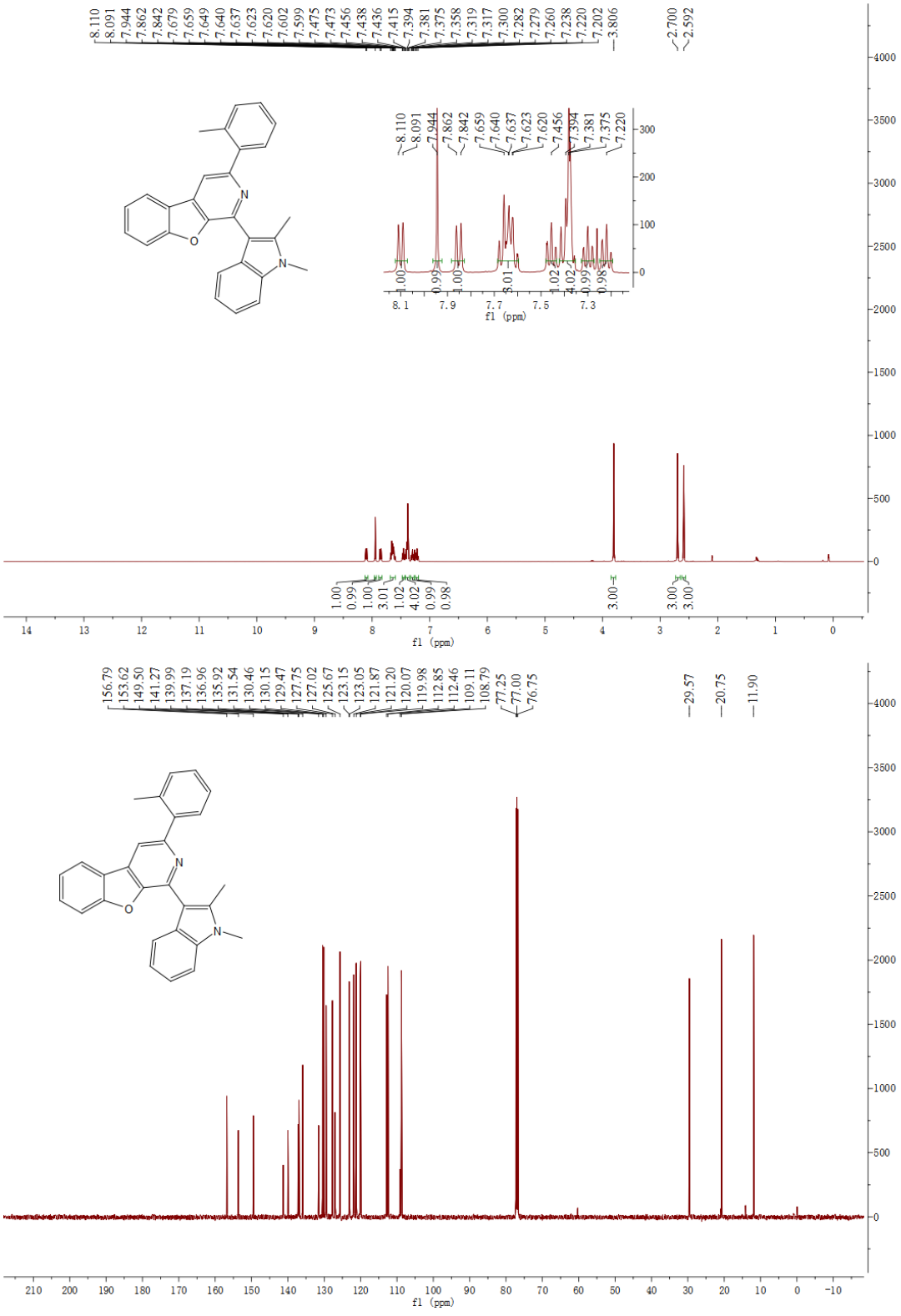


Figure S80. ^{1}H NMR of **6d** (400 MHz, $CDCl_3$) and ^{13}C NMR of **6d** (125 MHz, $CDCl_3$)

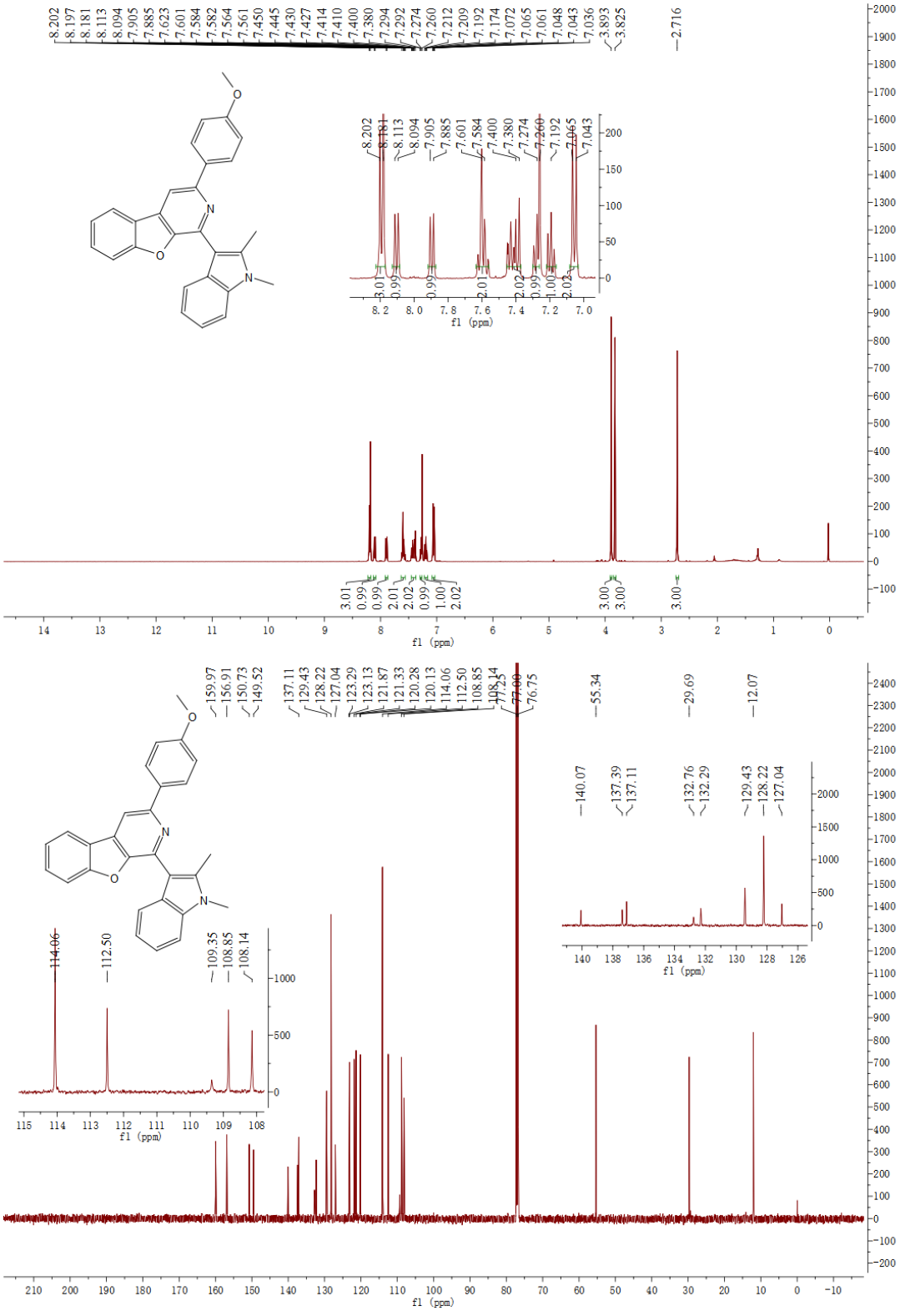


Figure S81. ^{1}H NMR of **6e** (400 MHz, $CDCl_3$) and ^{13}C NMR of **6e** (125 MHz, $CDCl_3$)

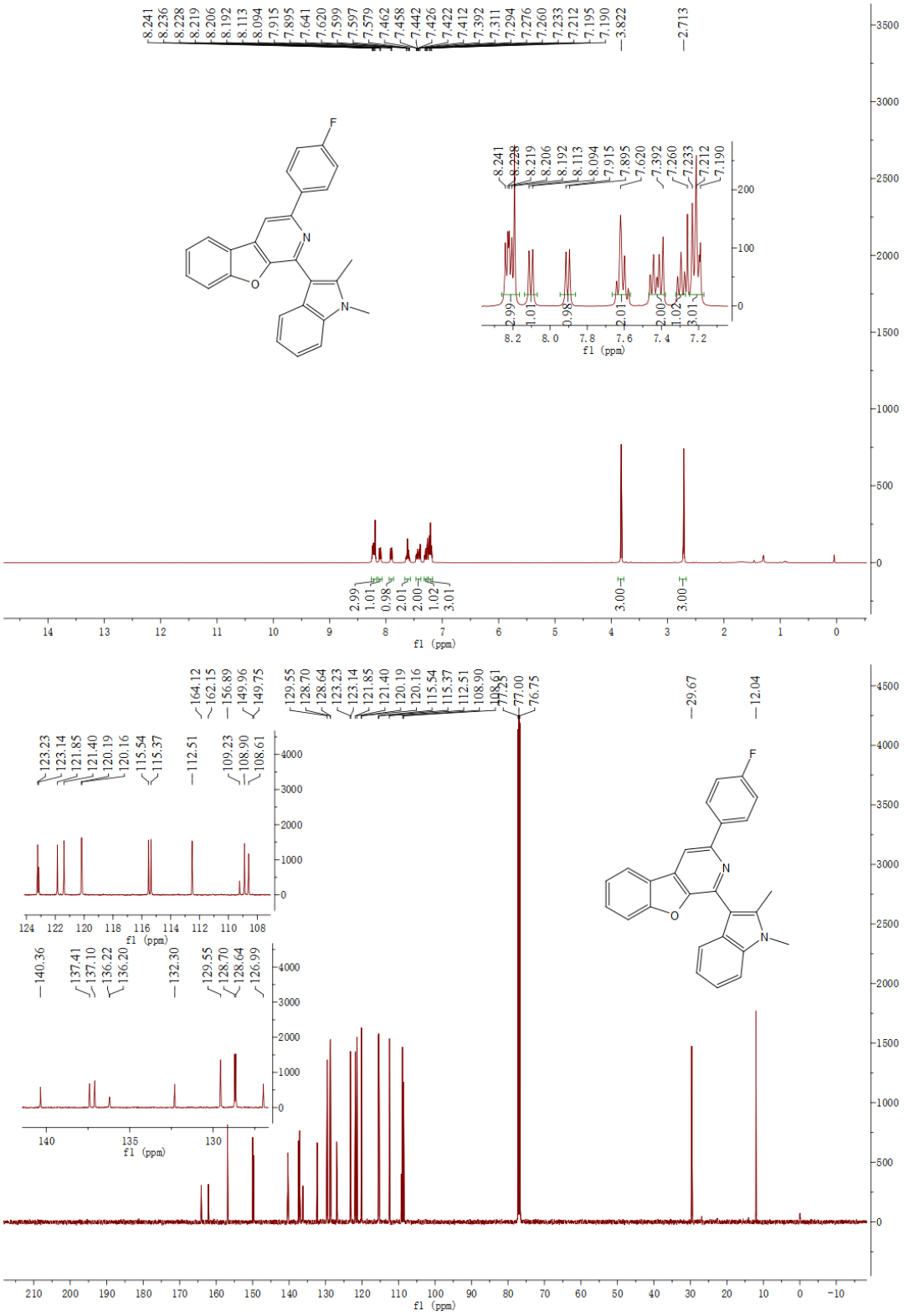


Figure S82. ^{1}H NMR of **6f** (400 MHz, $CDCl_3$) and ^{13}C NMR of **6f** (125 MHz, $CDCl_3$)

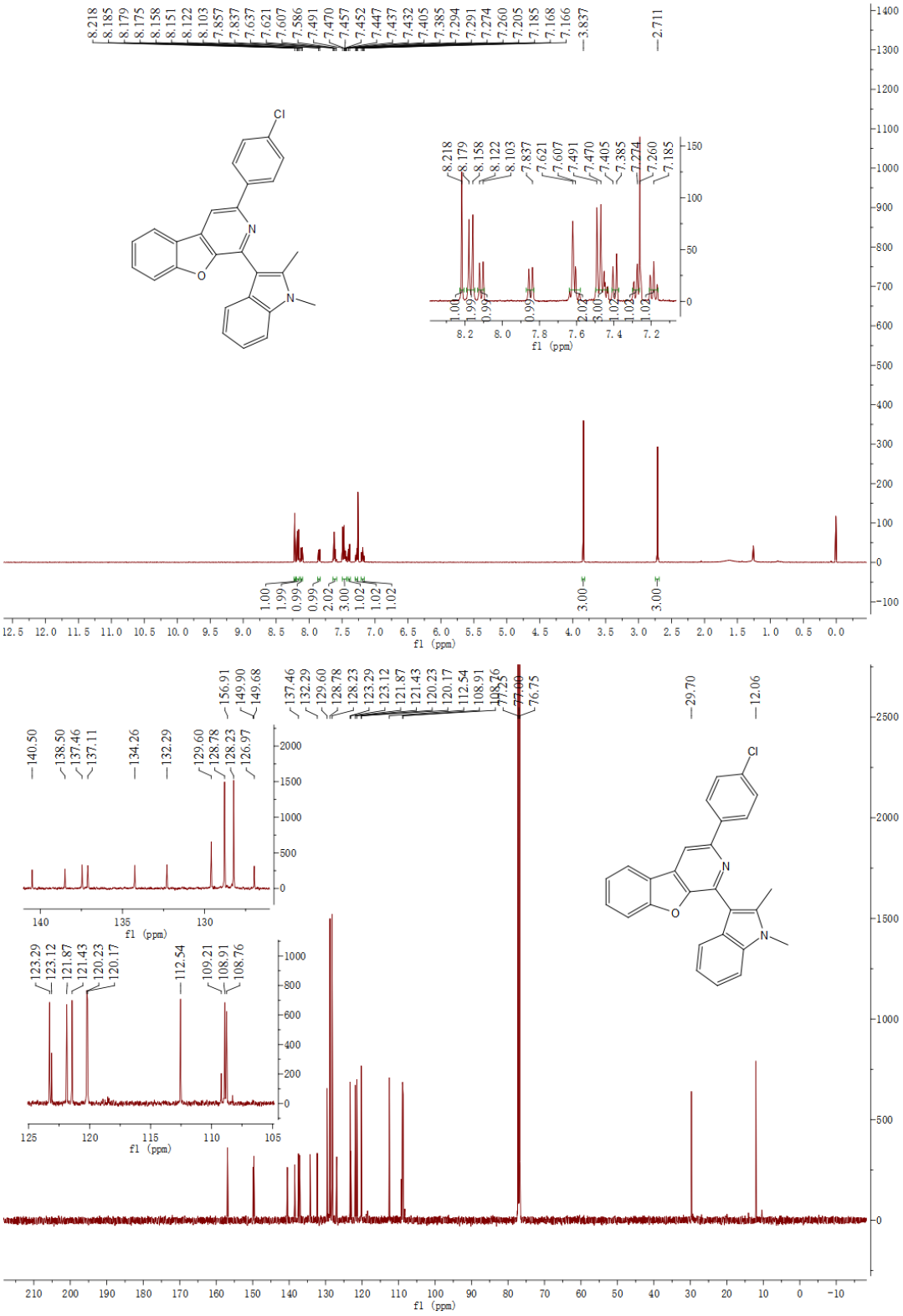


Figure S83. ^{1}H NMR of **6g** (400 MHz, $CDCl_3$) and ^{13}C NMR of **6g** (125 MHz, $CDCl_3$)

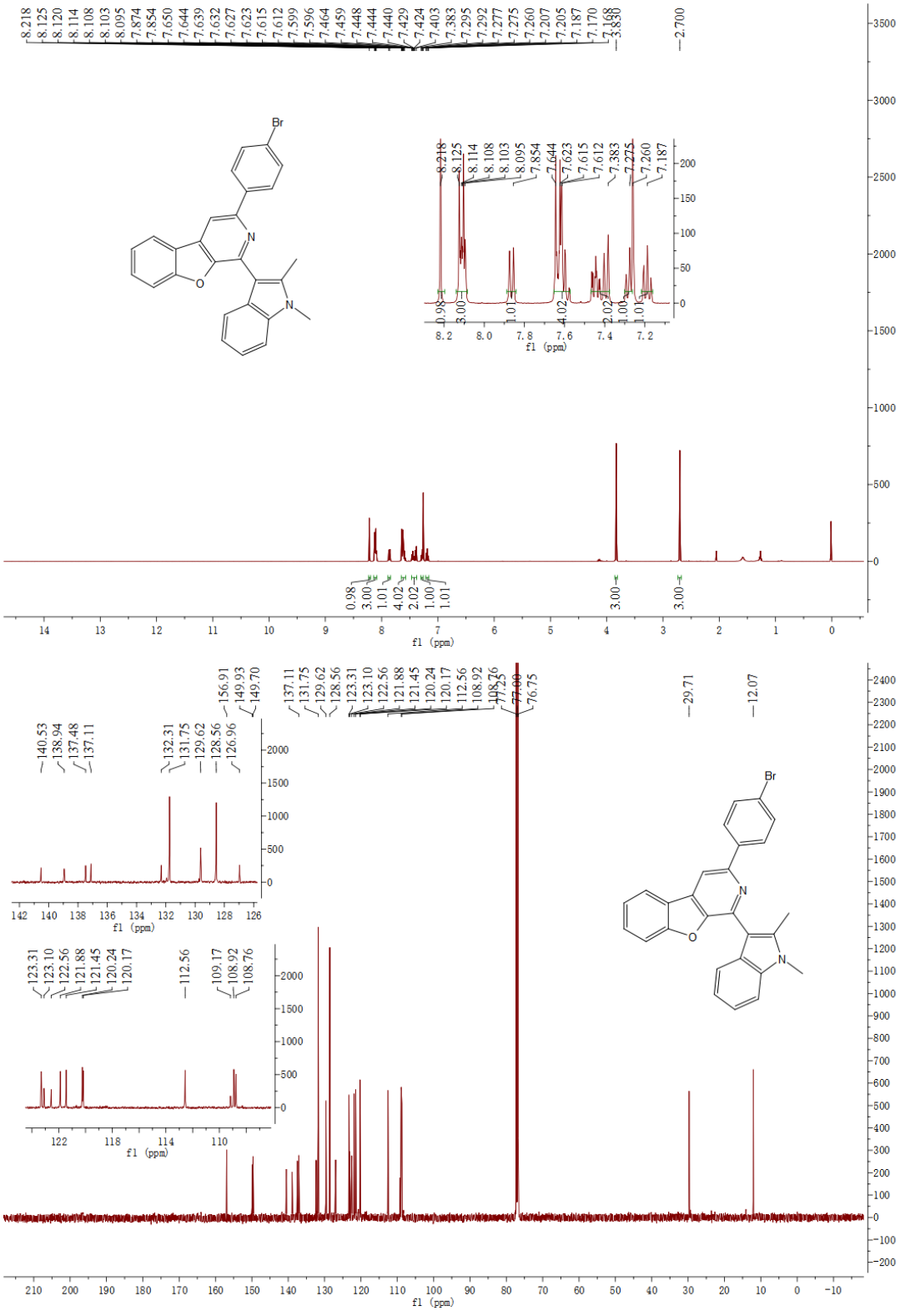


Figure S84. ^{1}H NMR of **6h** (400 MHz, $CDCl_3$) and ^{13}C NMR of **6h** (125 MHz, $CDCl_3$)

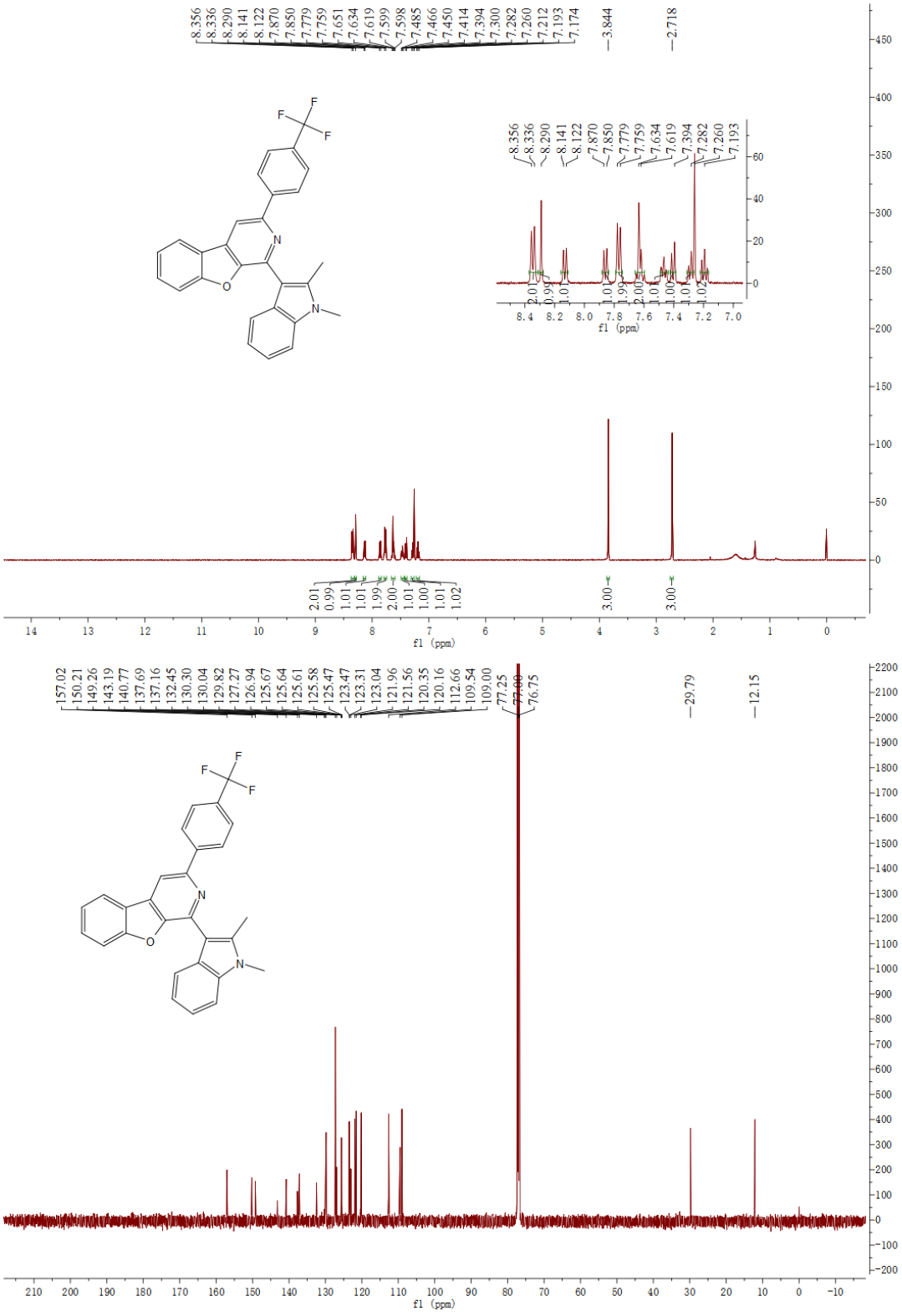


Figure S85. ^{1}H NMR of **6i** (400 MHz, $CDCl_3$) and ^{13}C NMR of **6i** (125 MHz, $CDCl_3$)

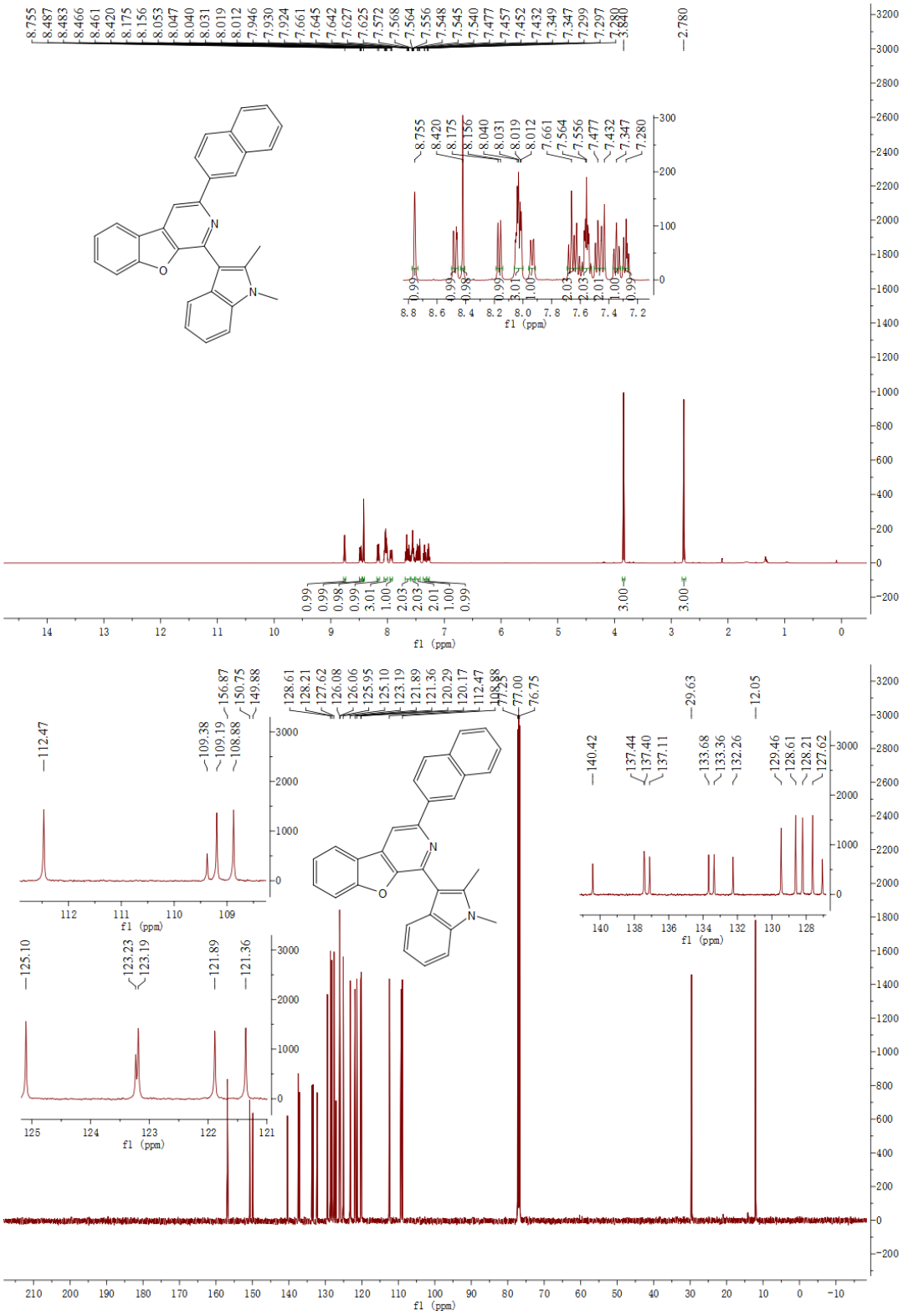


Figure S86. ^{1}H NMR of **6j** (400 MHz, $CDCl_3$) and ^{13}C NMR of **6j** (125 MHz, $CDCl_3$)

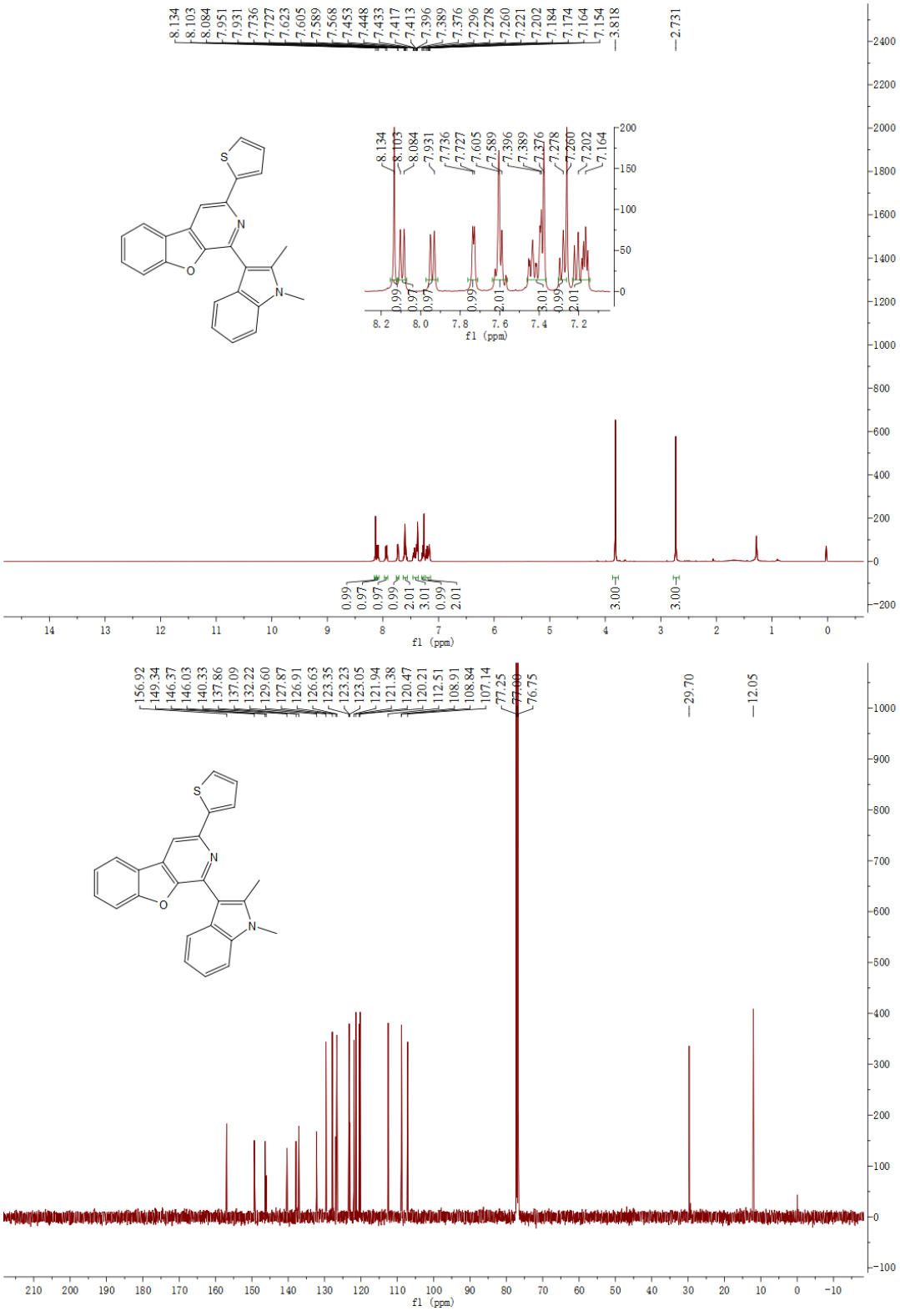


Figure S87. ^{1}H NMR of **6k** (400 MHz, $CDCl_3$) and ^{13}C NMR of **6k** (125 MHz, $CDCl_3$)

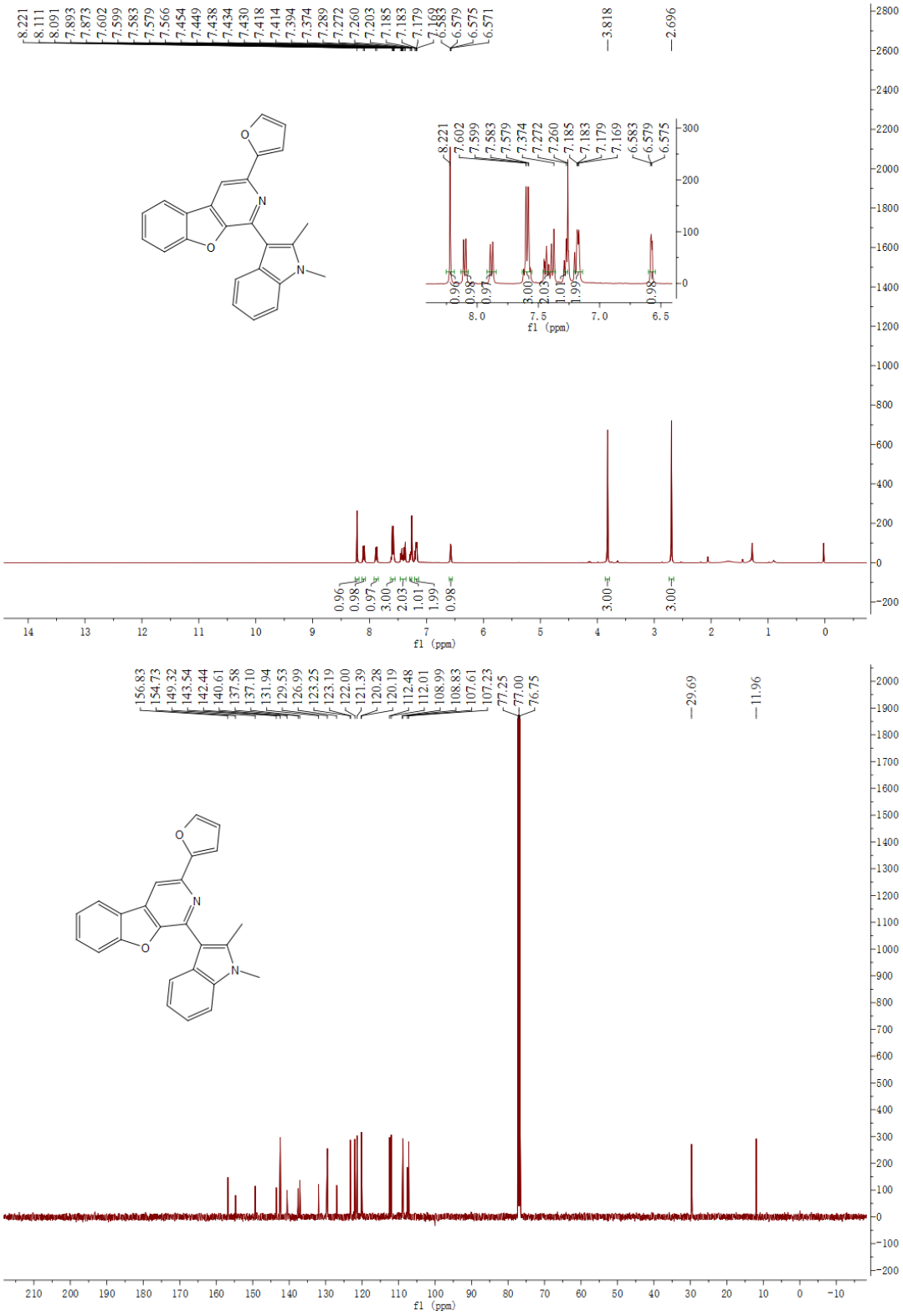


Figure S88. ^{1}H NMR of **6l** (400 MHz, $CDCl_3$) and ^{13}C NMR of **6l** (125 MHz, $CDCl_3$)

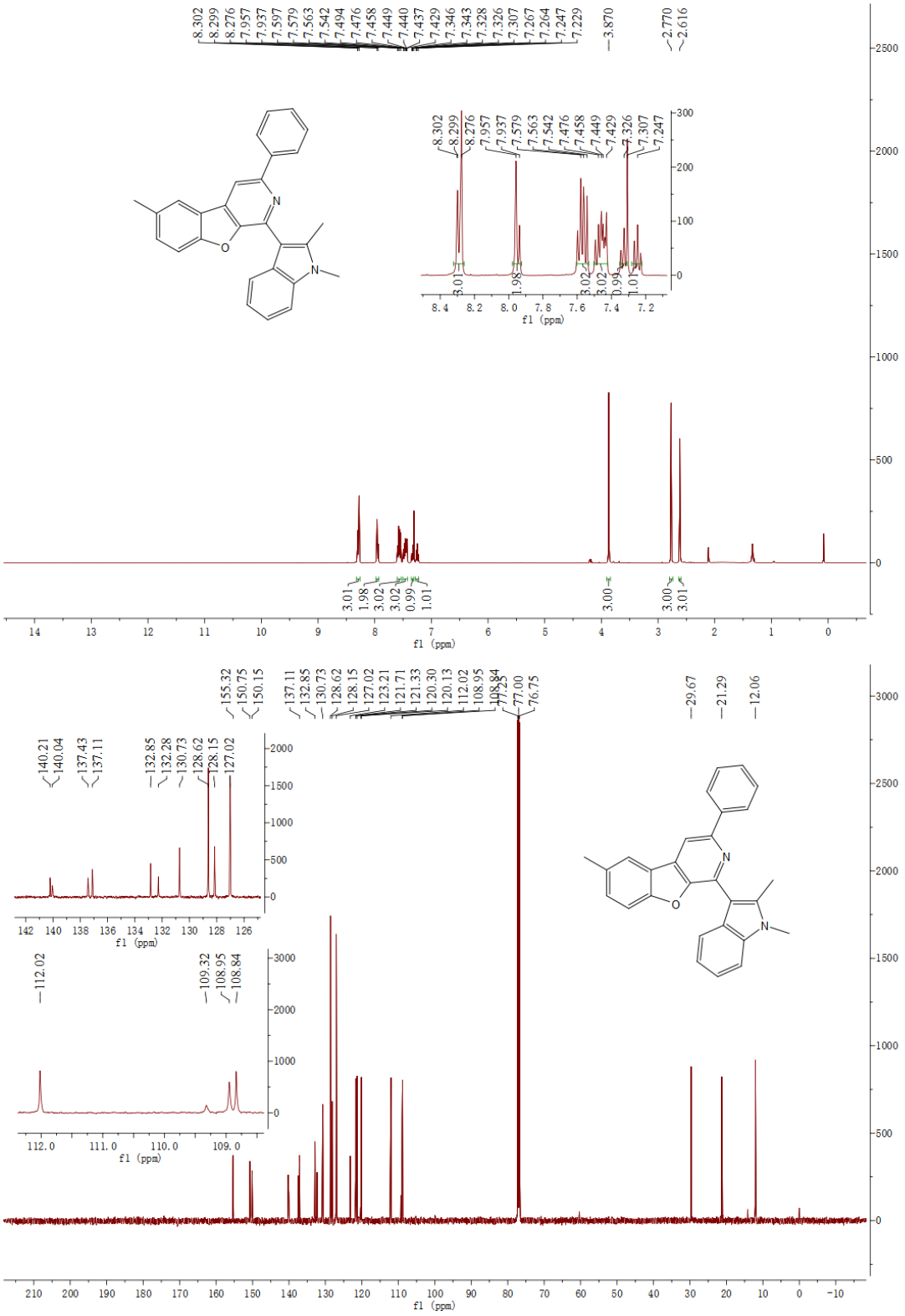


Figure S89. ^{1}H NMR of **6m** (400 MHz, $CDCl_3$) and ^{13}C NMR of **6m** (125 MHz, $CDCl_3$)

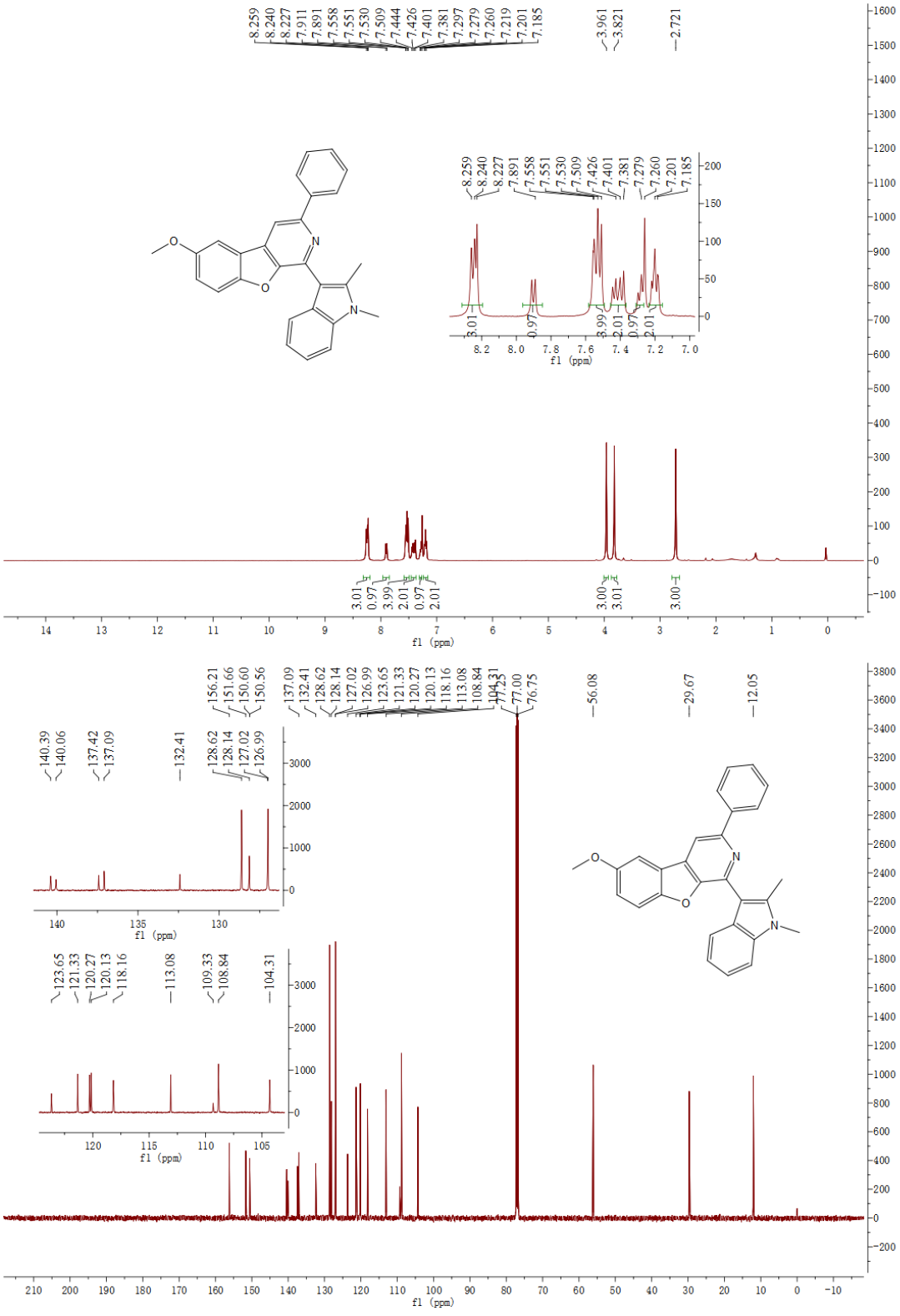


Figure S90. ^{1}H NMR of **6n** (400 MHz, $CDCl_3$) and ^{13}C NMR of **6n** (125 MHz, $CDCl_3$)

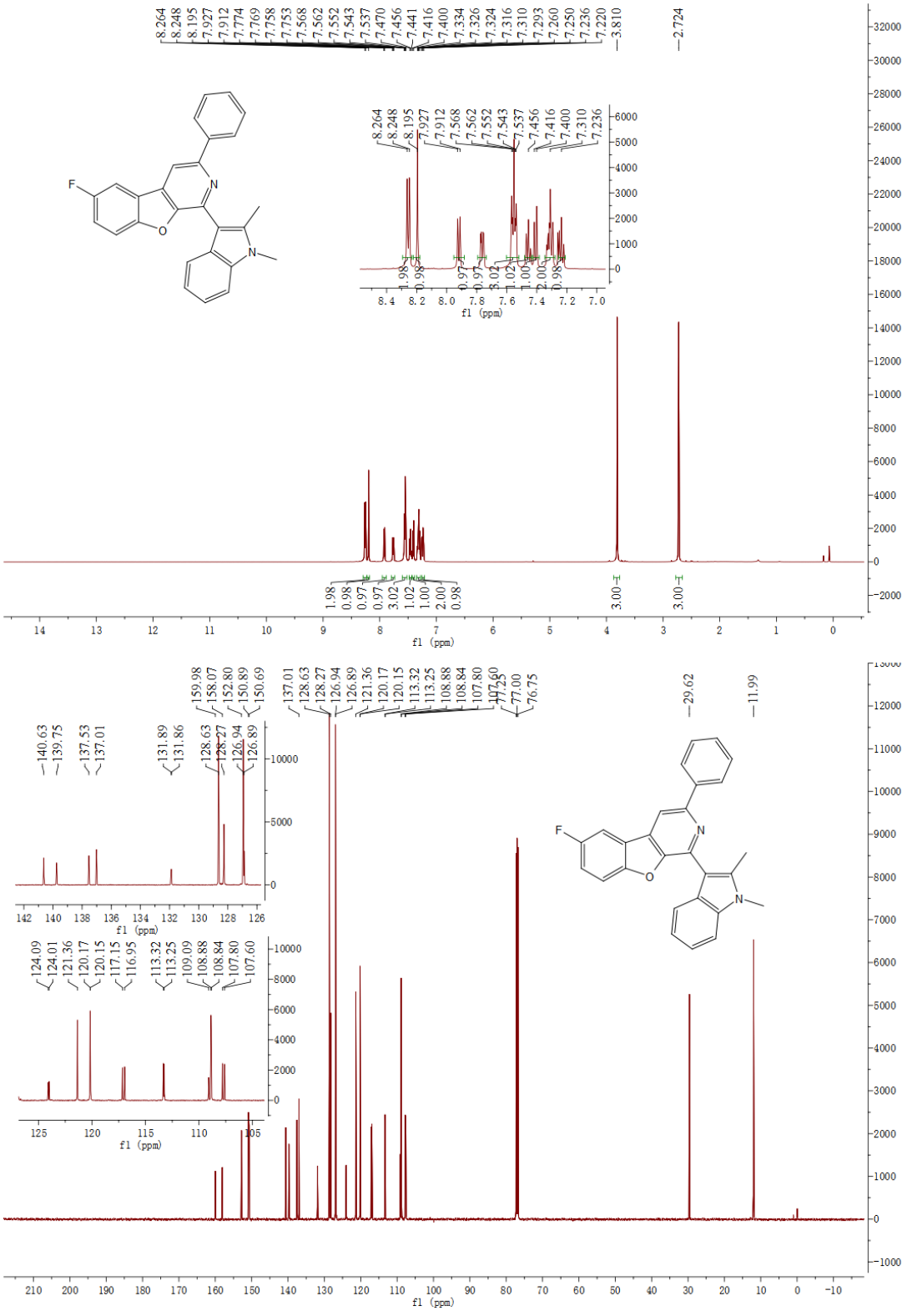


Figure S91. ^{1}H NMR of **6o** (500 MHz, $CDCl_3$) and ^{13}C NMR of **6o** (125 MHz, $CDCl_3$)

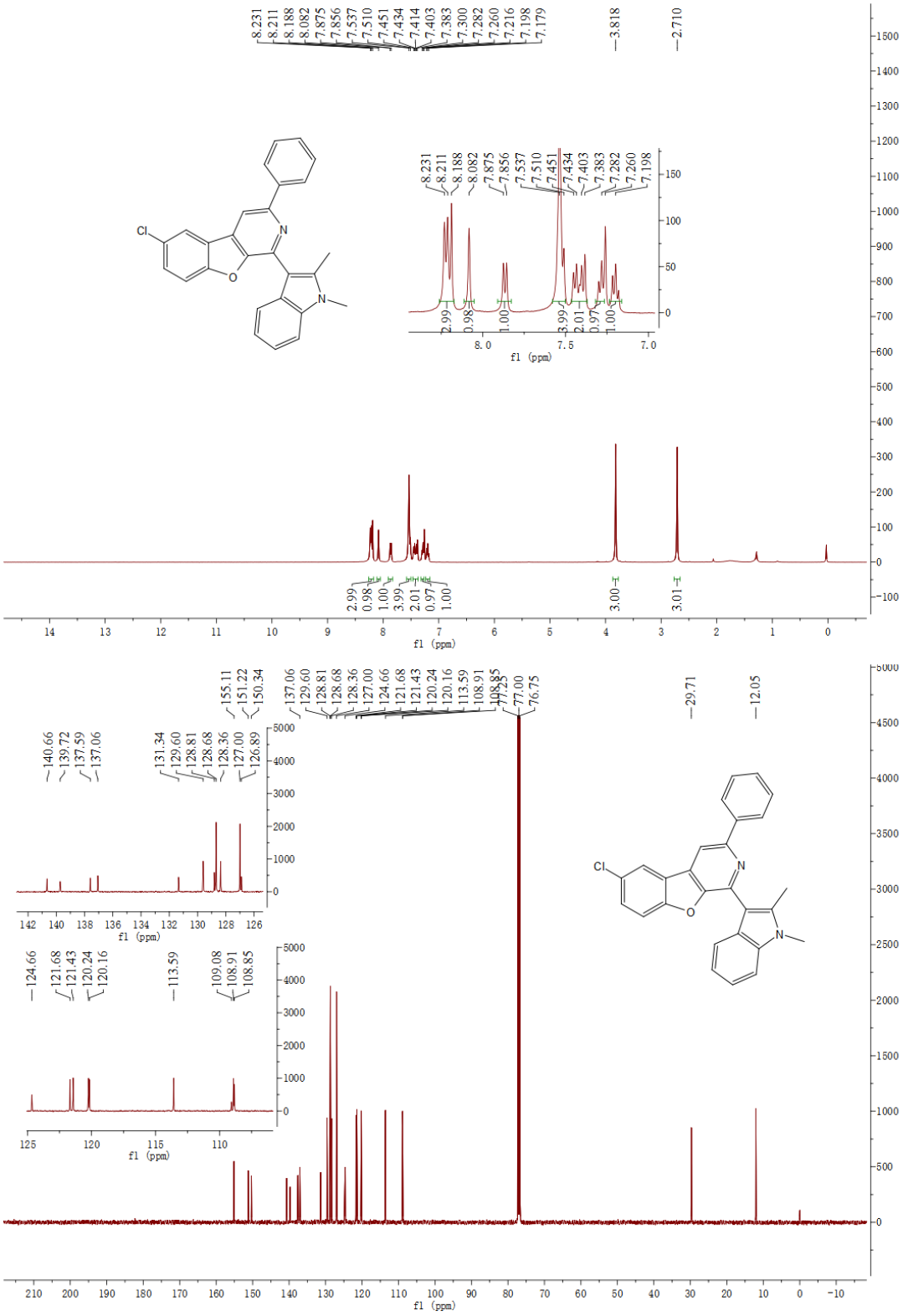


Figure S92. ^{1}H NMR of **6p** (400 MHz, $CDCl_3$) and ^{13}C NMR of **6p** (125 MHz, $CDCl_3$)

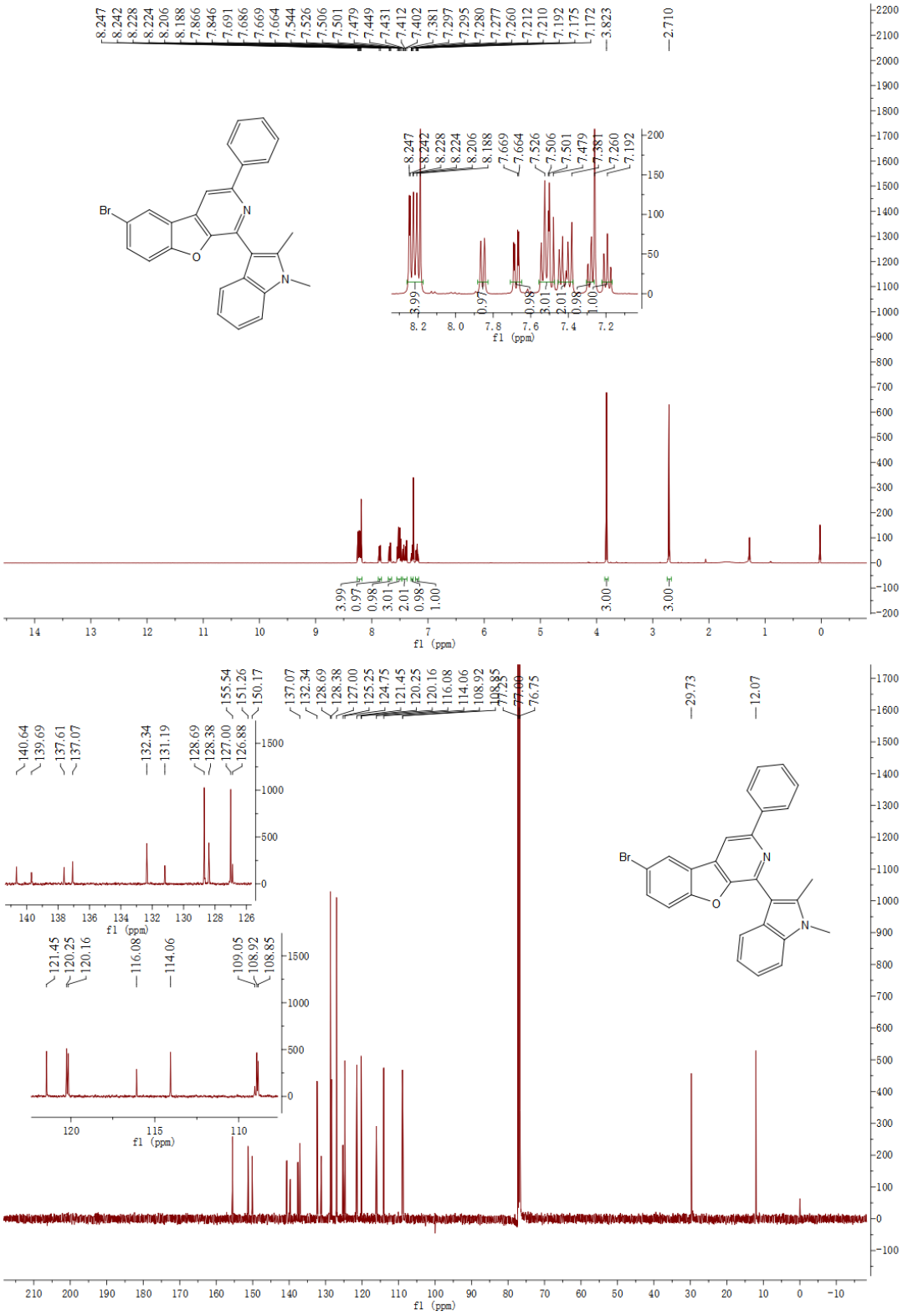


Figure S93. ^{1}H NMR of **6q** (400 MHz, $CDCl_3$) and ^{13}C NMR of **6q** (125 MHz, $CDCl_3$)

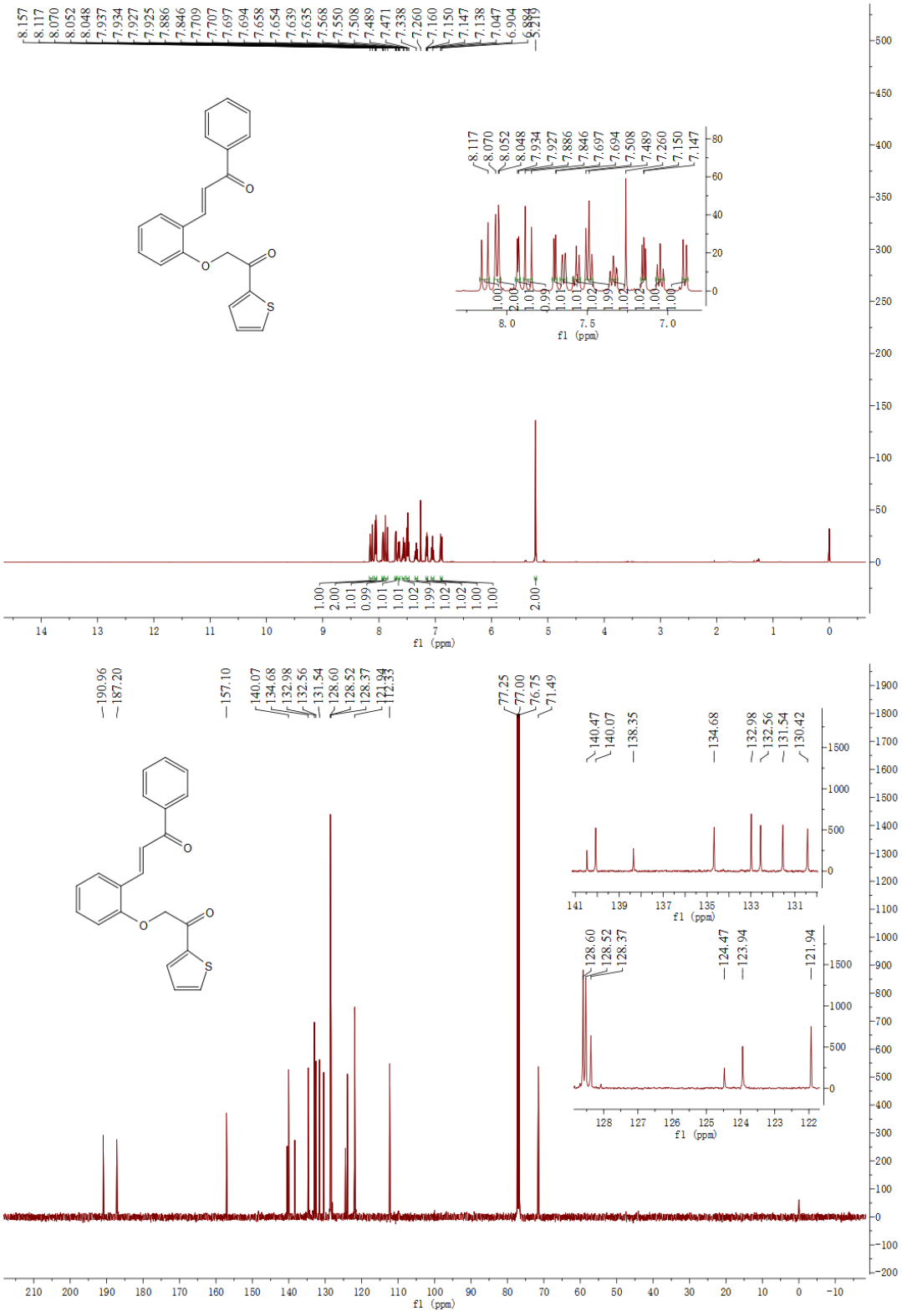


Figure S94. ^{1}H NMR of **8a** (400 MHz, $CDCl_3$) and ^{13}C NMR of **8a** (125 MHz, $CDCl_3$)

8. X-ray crystallographic data for product 3r, 4i, 5h, 6p

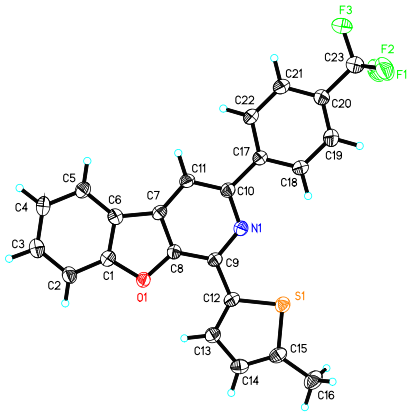


Figure S95 X-ray crystal structure **3r**

Table S5. Crystal data and structure refinement for **3r**.

Identification code	mo_dd19333_0m	
Empirical formula	C23 H14 F3 N O S	
Formula weight	409.41	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 5.1204(6) Å	a= 90 °.
	b = 15.2957(17) Å	b= 90.630(4) °.
	c = 11.7653(14) Å	g = 90 °.
Volume	921.40(18) Å^3	
Z	2	
Density (calculated)	1.476 Mg/m^3	
Absorption coefficient	0.220 mm^{-1}	
F(000)	420	
Crystal size	0.170 x 0.140 x 0.100 mm^3	
Theta range for data collection	2.663 to 25.990 °.	
Index ranges	-6<=h<=6, -18<=k<=18, -14<=l<=14	
Reflections collected	15773	
Independent reflections	3614 [R(int) = 0.0668]	
Completeness to theta = 25.242 °	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.5446	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3614 / 37 / 290	

Goodness-of-fit on F^2	1.052
Final R indices [I>2sigma(I)]	R1 = 0.0567, wR2 = 0.1453
R indices (all data)	R1 = 0.0630, wR2 = 0.1513
Absolute structure parameter	0.04(4)
Extinction coefficient	n/a
Largest diff. peak and hole	0.357 and -0.260 e.Å^{-3}

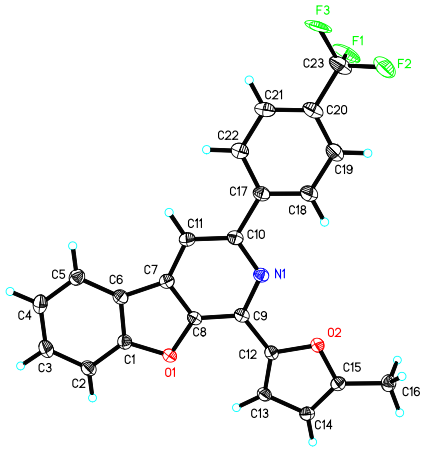


Figure S96 X-ray crystal structure **4i**

Table S6. Crystal data and structure refinement for **4i**.

Identification code	mo_dd19331_0m	
Empirical formula	C23 H14 F3 N O2	
Formula weight	393.35	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 19.5929(10) Å	a= 90 °.
	b = 4.9462(2) Å	b= 116.132(2) °.
	c = 20.1844(9) Å	g = 90 °.
Volume	1756.13(14) Å^3	
Z	4	
Density (calculated)	1.488 Mg/m^3	
Absorption coefficient	0.117 mm^{-1}	
F(000)	808	
Crystal size	0.180 x 0.150 x 0.120 mm^3	
Theta range for data collection	2.316 to 25.499 °.	
Index ranges	-23<=h<=23, -5<=k<=5, -24<=l<=24	
Reflections collected	19900	

Independent reflections	3241 [R(int) = 0.0615]
Completeness to theta = 25.242 °	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.6659
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3241 / 48 / 291
Goodness-of-fit on F^2	1.017
Final R indices [I>2sigma(I)]	R1 = 0.0644, wR2 = 0.1645
R indices (all data)	R1 = 0.0833, wR2 = 0.1831
Extinction coefficient	0.018(4)
Largest diff. peak and hole	0.790 and -0.615 e.Å^{-3}

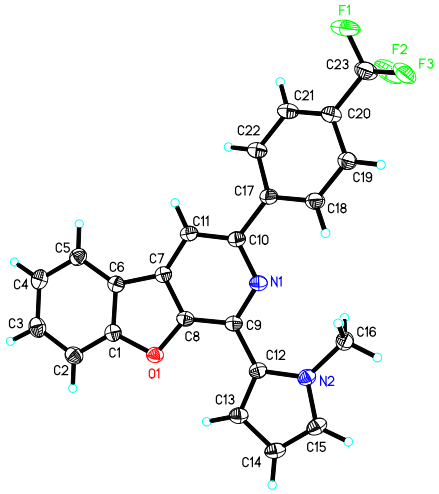


Figure S97 X-ray crystal structure **5h**

Table S7. Crystal data and structure refinement for **5h**.

Identification code	dd19330	
Empirical formula	C23 H15 F3 N2 O	
Formula weight	392.37	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 19.7618(6) Å	a= 90 °.
	b = 5.1518(2) Å	b= 114.9310(10) °.
	c = 19.2059(8) Å	g = 90 °.
Volume	1773.12(12) Å3	
Z	4	
Density (calculated)	1.470 Mg/m3	

Absorption coefficient	0.113 mm-1
F(000)	808
Crystal size	0.200 x 0.160 x 0.130 mm3
Theta range for data collection	2.273 to 25.495 °.
Index ranges	-23<=h<=23, -5<=k<=6, -21<=l<=23
Reflections collected	16683
Independent reflections	3278 [R(int) = 0.0666]
Completeness to theta = 25.242 °	99.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.3895
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	3278 / 108 / 327
Goodness-of-fit on F2	1.055
Final R indices [I>2sigma(I)]	R1 = 0.0474, wR2 = 0.1176
R indices (all data)	R1 = 0.0586, wR2 = 0.1282
Extinction coefficient	0.043(5)
Largest diff. peak and hole	0.272 and -0.295 e.Å-3

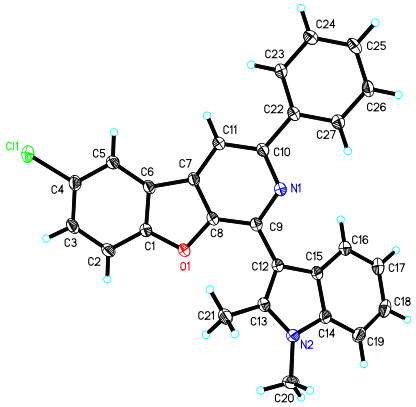


Figure S98 X-ray crystal structure **6p**

Table S8. Crystal data and structure refinement for **6p**.

Identification code	mo_dd19332_0m	
Empirical formula	C27 H19 Cl N2 O	
Formula weight	422.89	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 7.5249(7) Å	a= 109.203(3) °.

	b = 12.0711(12) Å	b= 106.952(3) °.
	c = 12.6412(13) Å	g = 98.580(3) °.
Volume	998.33(17) Å^3	
Z	2	
Density (calculated)	1.407 Mg/m^3	
Absorption coefficient	0.215 mm^{-1}	
F(000)	440	
Crystal size	0.180 x 0.160 x 0.130 mm^3	
Theta range for data collection	2.841 to 25.498 °.	
Index ranges	-9<=h<=8, -14<=k<=14, -14<=l<=15	
Reflections collected	13828	
Independent reflections	3697 [R(int) = 0.0484]	
Completeness to theta = 25.242 °	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.4982	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3697 / 0 / 283	
Goodness-of-fit on F^2	1.037	
Final R indices [I>2sigma(I)]	R1 = 0.0500, wR2 = 0.1362	
R indices (all data)	R1 = 0.0585, wR2 = 0.1463	
Extinction coefficient	0.038(8)	
Largest diff. peak and hole	0.337 and -0.328 e.Å^{-3}	