

Electronic Supplementary Information (ESI)

Palladium-catalyzed tandem reaction of epoxynitriles with arylboronic acids in aqueous medium: divergent synthesis of furans and pyrroles

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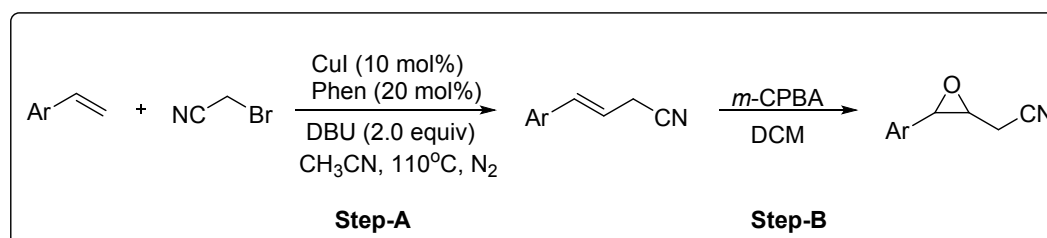
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1. General information.

^1H NMR and ^{13}C NMR spectra were measured on a 500 MHz Bruker spectrometer, using $\text{DMSO-}d_6$ or CDCl_3 as the solvent with tetramethylsilane (TMS) as the internal standard at room temperature. Chemical shifts are given δ relative to tetramethylsilane, and the coupling constants J are given in hertz. High-resolution mass spectra (HRMS) were recorded on an electrospray ionization (ESI) quadrupole time-of-flight mass spectrometer. Substrates of epoxide were synthesized according to the related literature.¹⁻² Unless otherwise noted, materials were obtained commercially and used without further purification. Flash column chromatography was performed over silica gel (300–400 mesh).

2. Experimental section.

2.1. General procedure for the synthesis of 2-(3-aryloxiran-2-yl)acetonitriles (1a-e).¹⁻²

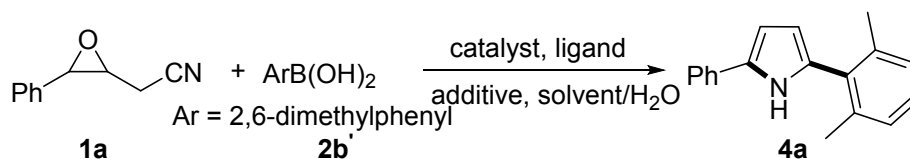


Step-A¹: To a solution of the styrene (350 μL , 3 mmol) in CH_3CN (10 ml) was added the 2-bromoacetonitrile (380 μL , 6 mmol), 1,10-phenanthroline (108 mg, 0.6 mmol), CuI (57 mg, 0.3 mmol), and DBU (910 μL , 6 mmol) under N_2 in a round-bottomed flask. The reaction mixture was stirred at 110 $^\circ\text{C}$ for 5 h. After the reaction finished, the reaction mixture was cooled to room temperature and quenched by water. The mixture was extracted with EtOAc (3.0 mL \times 3), the combined organic phases were dried over anhydrous Na_2SO_4 and the solvent was evaporated under vacuum. The residue was purified by column chromatography (petroleum ether /ethyl acetate = 40:1) to give the corresponding (*E*)-4-arylbut-3-enitriles.

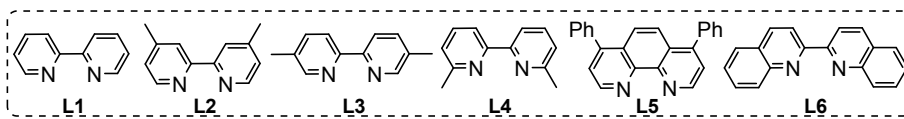
Step-B²: To a solution of *m*-CPBA (0.52 g, 3 mmol), in dichloromethane (2.0 mL) was added (*E*)-4-arylbut-3-enitriles (2 mmol) at 0 $^\circ\text{C}$. After being stirred at r.t. for

2.3. Optimization of reaction conditions for the synthesis of pyrrole^a

Table S2. Optimization of the reaction conditions for the synthesis of **4a**^a

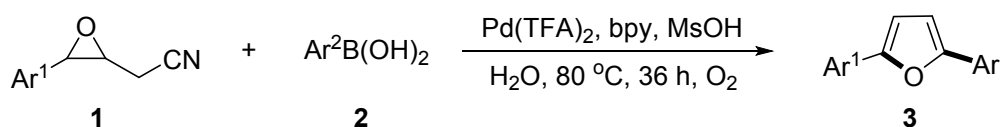


Entry	Pd catalyst	Ligand	Additive	Solvent	Yield (%) ^b
1	Pd(OAc) ₂	L1	TsOH•H ₂ O	MeOH/H ₂ O	54
2	Pd(OAc) ₂	L1	TsOH•H ₂ O	EtOH/H ₂ O	65
3	Pd(OAc) ₂	L1	TsOH•H ₂ O	ⁿ PrOH/H ₂ O	67
4	Pd(OAc) ₂	L1	TsOH•H ₂ O	HFIP/H ₂ O	33
5	Pd(OAc) ₂	L1	TsOH•H ₂ O	ⁱ PrOH/H ₂ O	78
6	Pd(OAc) ₂	L1	MsOH	ⁱ PrOH/H ₂ O	67
7	Pd(OAc) ₂	L1	TfOH	ⁱ PrOH/H ₂ O	52
8	Pd(OAc) ₂	L1	TFA	ⁱ PrOH/H ₂ O	55
9	Pd(OAc) ₂	L1	AcOH	ⁱ PrOH/H ₂ O	49
10	Pd(OAc) ₂	L1	D-CSA	ⁱ PrOH/H ₂ O	65
11	Pd(TFA) ₂	L1	TsOH•H ₂ O	ⁱ PrOH/H ₂ O	74
12	Pd(acac) ₂	L1	TsOH•H ₂ O	ⁱ PrOH/H ₂ O	66
13	PdCl ₂	L1	TsOH•H ₂ O	ⁱ PrOH/H ₂ O	45
14	Pd(MeCN) ₂ Cl ₂	L1	TsOH•H ₂ O	ⁱ PrOH/H ₂ O	trace
15	Pd ₂ (dba) ₃	L1	TsOH•H ₂ O	ⁱ PrOH/H ₂ O	51
16	Pd(PhP ₃) ₂ Cl ₂	L1	TsOH•H ₂ O	ⁱ PrOH/H ₂ O	trace
17	---	L1	TsOH•H ₂ O	ⁱ PrOH/H ₂ O	0
18	Pd(OAc) ₂	L2	TsOH•H ₂ O	ⁱ PrOH/H ₂ O	59
19	Pd(OAc) ₂	L3	TsOH•H ₂ O	ⁱ PrOH/H ₂ O	68
20	Pd(OAc) ₂	L4	TsOH•H ₂ O	ⁱ PrOH/H ₂ O	35
21	Pd(OAc) ₂	L5	TsOH•H ₂ O	ⁱ PrOH/H ₂ O	49
22	Pd(OAc) ₂	L6	TsOH•H ₂ O	ⁱ PrOH/H ₂ O	15
23	Pd(OAc) ₂	---	TsOH•H ₂ O	ⁱ PrOH/H ₂ O	0
24	Pd(OAc) ₂	L1	---	ⁱ PrOH/H ₂ O	0



^aConditions: **1a** (0.3 mmol), **2a** (0.6 mmol), Pd catalyst (5 mol %), ligand (10 mol %), additive (2 equiv), solvent/H₂O (0.5: 2.5 mL), 100 °C, 24 h, N₂. ^bIsolated yield.

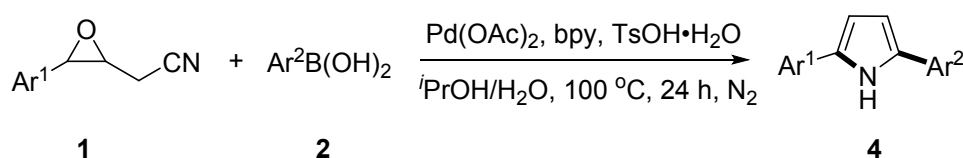
2.4. General procedure for the synthesis of furans.



2-(3-aryloxiran-2-yl)acetonitriles **1** (0.3 mmol, 1.0 equiv), arylboronic acid **2** (0.6

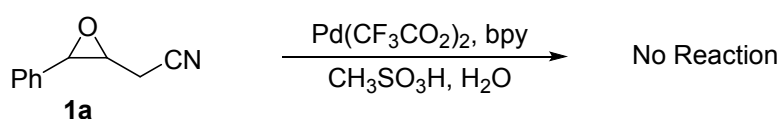
mmol, 2.0 equiv), Pd(TFA)₂ (0.015 mmol, 5 mol%), 2,2'-bipyridyl (**L1**) (0.03 mmol, 10 mol%), MsOH (3 mmol, 10 equiv) and H₂O (4.0 mL) were successively added into a Schlenk reaction tube under O₂ atmosphere. The reaction mixture was stirred vigorously at 80 °C in an oil bath for 36 h. After the reaction equilibrium, the mixture was poured into ethyl acetate, which was washed with saturated NaHCO₃ (2 × 10 mL) and then brine (10 mL). After the aqueous layer was extracted with ethyl acetate, the combined organic layers were dried over anhydrous Na₂SO₄ and evaporated under a vacuum. The residue was purified by flash column chromatography with hexane to afford the desired furans **3**.

2.5. General procedure for the synthesis of pyrroles.



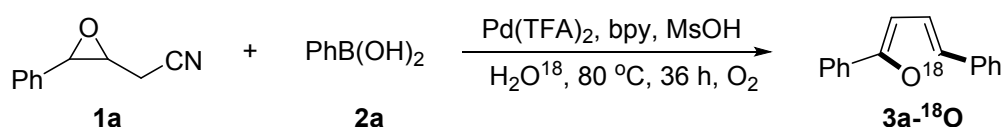
2-(3-aryloxiran-2-yl)acetonitriles **1** (0.3 mmol, 1.0 equiv.), arylboronic acid **2** (0.6 mmol, 2.0 equiv), Pd(OAc)₂ (0.015 mmol, 5 mol%) and 2,2'-bipyridyl (**L1**) (0.03 mmol, 10 mol%), TsOH·H₂O (0.6 mmol, 2.0 equiv) and *i*PrOH/H₂O (0.5 mL: 2.5 mL) were successively added into a Schlenk reaction tube under N₂ atmosphere. The reaction mixture was stirred vigorously at 100 °C in an oil bath for 24 h. After the reaction equilibrium, the mixture was poured into ethyl acetate, which was washed with saturated NaHCO₃ (2 × 10 mL) and then brine (10 mL). After the aqueous layer was extracted with ethyl acetate, the combined organic layers were dried over anhydrous Na₂SO₄ and evaporated under a vacuum. The residue was purified by flash column chromatography with petroleum ether/ethyl acetate (16:1) to afford the desired products pyrroles **4**.

3. Control experiments.

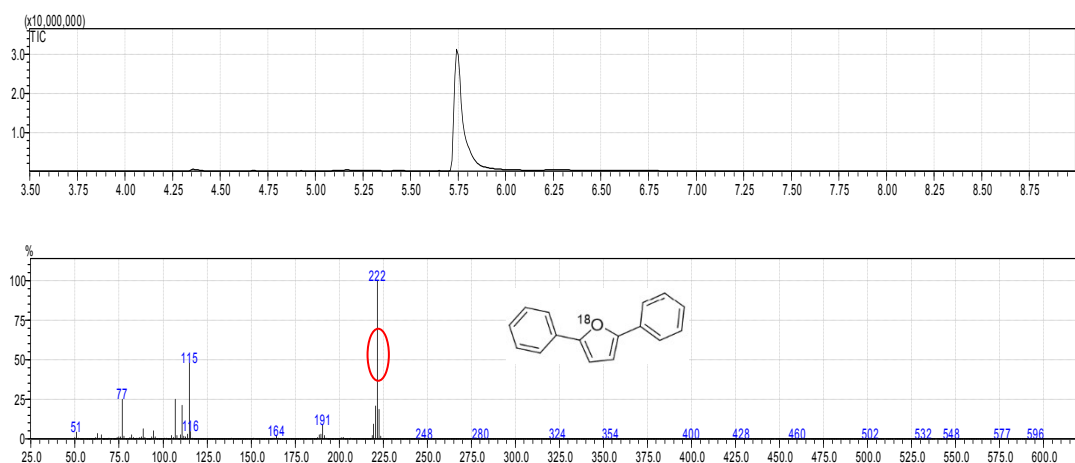


2-(3-phenyloxiran-2-yl)acetonitrile **1a** (0.3 mmol, 1.0 equiv), Pd(TFA)₂ (0.015 mmol,

5 mol%), 2,2'-bipyridyl (**L1**) (0.03 mmol, 10 mol%), MsOH (3 mmol, 10 equiv) and H₂O (4 mL) were successively added into a Schlenk reaction tube under O₂ atmosphere. The reaction mixture was stirred vigorously at 80 °C in an oil bath for 36 h. After the reaction equilibrium, the solution was detected by TLC analysis, no target furan product was found.



2-(3-phenyloxiran-2-yl)acetonitrile **1a** (0.3 mmol, 1.0 equiv), phenylboronic acid **2a** (0.6 mmol, 2.0 equiv), Pd(TFA)₂ (0.015 mmol, 5 mol%), 2,2'-bipyridyl (**L1**) (0.03 mmol, 10 mol%), MsOH (3 mmol, 10 equiv) and H₂O¹⁸ (20 equiv) were successively added into a Schlenk reaction tube under O₂ atmosphere. The reaction mixture was stirred vigorously at 80 °C in an oil bath for 36 h. After the reaction equilibrium, the mixture was poured into ethyl acetate, which was washed with saturated NaHCO₃ (2 × 10 mL) and then brine (10 mL). After the aqueous layer was extracted with ethyl acetate, the combined organic layers were dried over anhydrous Na₂SO₄ and evaporated under a vacuum. The residue was purified by flash column chromatography with hexane to afford furans **3a-¹⁸O** in 75% yield.

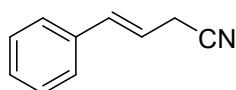


The ¹⁸O-labeled Furan Product Determined by GC-MS Analysis.

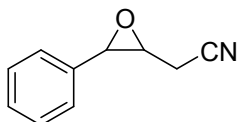
4. Reference.

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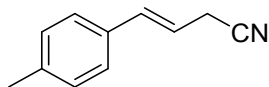
5. Analytical data for reactants.



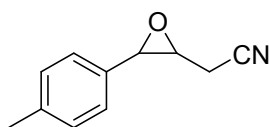
(*E*)-4-phenylbut-3-enenitrile (**1a'**): Colorless oil. Petroleum ether/ethyl acetate = 40/1 as eluent for column chromatography. $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 7.46 (d, J = 7.5 Hz, 2H), 7.35 (t, J = 7.5 Hz, 2H), 7.28 (t, J = 7.5 Hz, 1H), 6.67 (d, J = 16.0 Hz, 1H), 6.28–6.24 (m, 1H), 3.54 (d, J = 6.0 Hz, 2H); $^{13}\text{C NMR}$ (125 MHz, $\text{DMSO-}d_6$) δ 135.8, 133.0, 128.7, 127.9, 126.3, 119.0, 118.5, 19.8. Spectroscopic data for the title compound were consistent with those reported in the literature.¹



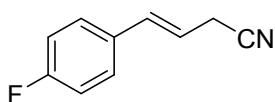
2-(3-phenyloxiran-2-yl)acetonitrile (**1a**): Colorless oil. Petroleum ether/ethyl acetate = 7/1 as eluent for column chromatography. $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 7.39-7.31 (m, 5H), 3.95 (s, 1H), 3.45 (d, $J = 3.5$ Hz, 1H), 3.25-3.21 (m, 1H), 3.05-3.00 (m, 1H); $^{13}\text{C NMR}$ (125 MHz, $\text{DMSO-}d_6$) δ 136.0, 128.5, 128.4, 126.0, 117.2, 57.0, 56.0, 20.2. **HRMS** calcd for $\text{C}_{10}\text{H}_{10}\text{NO}^+$ $[\text{M}+\text{H}]^+$: 160.0757, found: 160.0757.



(*E*)-4-(*p*-tolyl)but-3-enenitrile (**1b'**): Colorless oil. Petroleum ether/ethyl acetate = 40/1 as eluent for column chromatography. $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.28 (d, $J = 8.0$ Hz, 2H), 7.16 (d, $J = 8.0$ Hz, 2H), 6.70 (d, $J = 16.0$ Hz, 1H), 6.02-5.97 (m, 1H), 3.26-3.25 (m, 2H), 2.36 (s, 3H); $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 138.2, 134.5, 133.0, 129.4, 126.4, 117.5, 115.7, 21.2, 20.7. Spectroscopic data for the title compound were consistent with those reported in the literature.¹

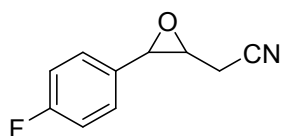


2-(3-(*p*-tolyl)oxiran-2-yl)acetonitrile (**1b**): Colorless oil. Petroleum ether/ethyl acetate = 7/1 as eluent for column chromatography. $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.19-7.15 (m, 4H), 3.85-3.84 (m, 1H), 3.25-3.22 (m, 1H), 2.90-2.78 (m, 2H), 2.36 (s, 3H). $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 138.7, 132.2, 129.3, 125.7, 115.7, 57.8, 56.0, 21.2, 20.9. **HRMS** calcd for $\text{C}_{11}\text{H}_{12}\text{NO}^+$ $[\text{M}+\text{H}]^+$: 174.0914, found: 174.0913.

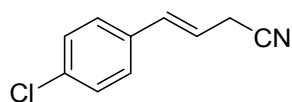


(*E*)-4-(4-fluorophenyl)but-3-enenitrile (**1c'**): Colorless oil. Petroleum ether/ethyl acetate = 40/1 as eluent for column chromatography. $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.33-7.30 (m, 2H), 7.01 (t, $J = 8.5$ Hz, 2H), 6.67 (d, $J = 16.0$ Hz, 1H), 5.98-5.93 (m, 1H), 3.26 (d, $J = 5.5$ Hz, 2H); $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 163.7, 161.7, 133.4,

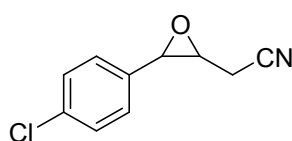
132.0, 131.9, 128.2, 128.1, 117.3, 116.7, 116.6, 115.8, 115.6, 20.7. Spectroscopic data for the title compound were consistent with those reported in the literature.¹



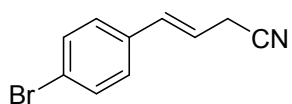
2-(3-(4-fluorophenyl)oxiran-2-yl)acetonitrile (**1c**): Colorless oil. Petroleum ether/ethyl acetate = 7/1 as eluent for column chromatography. ¹H NMR (500 MHz, CDCl₃) δ 7.17-7.14 (m, 2H), 6.98-6.94 (m, 2H), 3.79 (s, 1H), 3.13-3.12 (m, 1H), 2.79-2.78 (m, 2H). ¹³C NMR (125 MHz, CDCl₃) δ 164.2, 162.2, 131.1 (2C), 127.6 (2C), 116.0, 115.8, 115.5, 57.4, 56.2, 21.1. HRMS calcd for C₁₀H₉FNO⁺ [M+H]⁺: 178.0663, found: 178.0662.



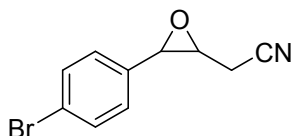
(*E*)-4-(4-chlorophenyl)but-3-enenitrile (**1d'**): Colorless oil. Petroleum ether/ethyl acetate = 40/1 as eluent for column chromatography. ¹H NMR (500 MHz, CDCl₃) δ 7.23-7.19 (m, 4H), 6.61 (d, *J* = 16.0 Hz, 1H), 5.98-5.92 (m, 1H), 3.21-3.20 (m, 2H); ¹³C NMR (125 MHz, CDCl₃) δ 134.2, 134.0, 133.4, 128.9, 127.7, 117.6, 117.2, 20.8. Spectroscopic data for the title compound were consistent with those reported in the literature.¹



2-(3-(4-chlorophenyl)oxiran-2-yl)acetonitrile (**1d**): Colorless oil. Petroleum ether/ethyl acetate = 7/1 as eluent for column chromatography. ¹H NMR (500 MHz, CDCl₃) δ 7.34 (d, *J* = 8.5 Hz, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 3.87 (s, 1H), 3.23-3.19 (m, 1H), 2.89-2.88 (m, 2H). ¹³C NMR (125 MHz, CDCl₃) δ 134.8, 133.8, 128.9, 127.1, 115.2, 57.2, 56.2, 21.0. HRMS calcd for C₁₀H₉ClNO⁺ [M+H]⁺: 194.0367, found: 194.0364.

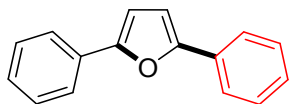


(*E*)-4-(4-bromophenyl)but-3-enenitrile (**1e'**): White solid. Petroleum ether/ethyl acetate = 40/1 as eluent for column chromatography. $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.46-7.44 (m, 2H), 7.23-7.22 (m, 2H), 6.67 (d, $J = 16.0$ Hz, 1H), 6.07-6.02 (m, 1H), 3.28-3.27 (m, 2H); $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 134.7, 133.6, 132.0, 128.1, 122.3, 117.7, 117.1, 20.9. Spectroscopic data for the title compound were consistent with those reported in the literature.¹

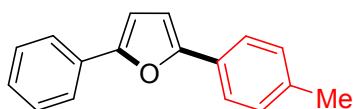


2-(3-(4-bromophenyl)oxiran-2-yl)acetonitrile (**1e**): Colorless oil. Petroleum ether/ethyl acetate = 7/1 as eluent for column chromatography. $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.49 (d, $J = 8.5$ Hz, 2H), 7.14 (d, $J = 8.5$ Hz, 2H), 3.86 (d, $J = 1.5$ Hz, 1H), 3.22-3.20 (m, 1H), 2.89-2.88 (m, 2H). $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 134.4, 131.8, 127.4, 122.7, 115.4, 57.2, 56.1, 20.9. **HRMS** calcd for $\text{C}_{10}\text{H}_9\text{BrNO}^+$ $[\text{M}+\text{H}]^+$: 237.9862, found: 237.9864.

6. Analytical data for all products.

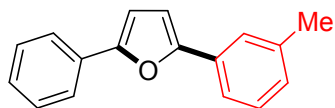


2,5-diphenylfuran (**3a**): White solid (56.8 mg, 86%), Hexane as eluent for column chromatography. $^1\text{H NMR}$ (500 MHz, $\text{DMSO}-d_6$) δ 7.82 (d, $J = 7.5$ Hz, 4H), 7.45 (t, $J = 7.5$ Hz, 4H), 7.29 (t, $J = 8.0$ Hz, 2H), 7.00 (s, 2H); $^{13}\text{C NMR}$ (125 MHz, $\text{DMSO}-d_6$) δ 152.6, 130.1, 128.9, 127.5, 123.4, 108.1. Spectroscopic data for the title compound were consistent with those reported in the literature.³

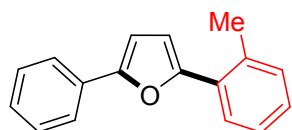


2-phenyl-5-(*p*-tolyl)furan (**3b**): Pale yellow solid (59.7 mg, 85%), Hexane as eluent for column chromatography. $^1\text{H NMR}$ (500 MHz, $\text{DMSO}-d_6$) δ 7.81-7.79 (m, 2H), 7.71 (d, $J = 8.0$ Hz, 2H), 7.44 (t, $J = 8.0$ Hz, 2H), 7.30 (t, $J = 7.5$ Hz, 1H), 7.26 (d, $J = 7.5$ Hz, 2H), 7.06-7.05 (m, 1H), 7.00-6.99 (m, 1H), 2.33 (s, 3H); $^{13}\text{C NMR}$ (125 MHz,

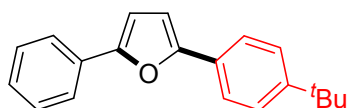
DMSO- d_6) δ 152.8, 152.2, 137.0, 130.2, 129.4, 128.9, 127.5, 127.4, 123.4, 123.3, 108.1, 107.4, 20.8. Spectroscopic data for the title compound were consistent with those reported in the literature.³



2-phenyl-5-(*m*-tolyl)furan (**3c**): Pale yellow solid (59.0 mg, 84%), Hexane as eluent for column chromatography. $^1\text{H NMR}$ (500 MHz, DMSO- d_6) δ 7.82 (d, $J = 7.5$ Hz, 2H), 7.65 (s, 1H), 7.61 (d, $J = 8.0$ Hz, 1H), 7.45 (t, $J = 7.5$ Hz, 2H), 7.35-7.29 (m, 2H), 7.12 (d, $J = 7.5$ Hz, 1H), 7.07 (d, $J = 3.5$ Hz, 1H), 7.05 (d, $J = 3.5$ Hz, 1H), 2.37 (s, 3H); $^{13}\text{C NMR}$ (125 MHz, DMSO- d_6) δ 152.8, 152.5, 138.1, 130.1, 130.0, 128.9, 128.8, 128.3, 127.5, 123.9, 123.4, 120.7, 108.1, 108.0, 21.0. Spectroscopic data for the title compound were consistent with those reported in the literature.³

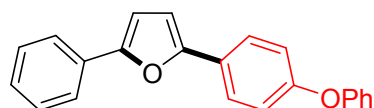


2-phenyl-5-(*o*-tolyl)furan (**3d**): Yellow oil (56.9 mg, 81%), Hexane as eluent for column chromatography. $^1\text{H NMR}$ (500 MHz, DMSO- d_6) δ 7.81-7.79 (m, 3H), 7.45 (t, $J = 7.5$ Hz, 2H), 7.32-7.29 (m, 3H), 7.25-7.22 (m, 1H), 7.08 (d, $J = 3.5$ Hz, 1H), 6.86 (d, $J = 3.5$ Hz, 1H), 2.52 (s, 3H); $^{13}\text{C NMR}$ (125 MHz, DMSO- d_6) δ 152.4, 152.3, 133.8, 131.3, 130.1, 129.3, 128.9, 127.6, 127.5, 126.4, 126.2, 123.4, 111.2, 107.8, 21.7. Spectroscopic data for the title compound were consistent with those reported in the literature.³

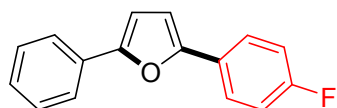


2-(4-(*tert*-butyl)phenyl)-5-phenylfuran (**3e**): White solid (53.9 mg, 65%), Hexane as eluent for column chromatography. $^1\text{H NMR}$ (500 MHz, DMSO- d_6) δ 7.80 (d, $J = 7.0$ Hz, 2H), 7.73 (d, $J = 8.5$ Hz, 2H), 7.47-7.44 (m, 4H), 7.30 (t, $J = 7.5$ Hz, 1H), 7.06 (d, $J = 3.0$ Hz, 1H), 7.00 (d, $J = 3.0$ Hz, 1H), 1.30 (s, 9H); $^{13}\text{C NMR}$ (125 MHz, DMSO- d_6) δ 152.8, 152.3, 150.2, 130.2, 129.0, 127.5, 127.4, 125.6, 123.4, 123.3, 108.1, 107.5, 34.4, 31.0. Spectroscopic data for the title compound were consistent with

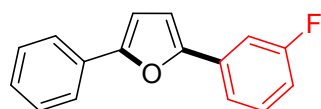
those reported in the literature.³



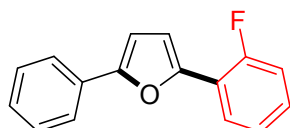
2-(4-phenoxyphenyl)-5-phenylfuran (**3f**): Yellowish solid (82.5 mg, 88%), Hexane as eluent for column chromatography. ¹H NMR (500 MHz, DMSO-*d*₆) δ 7.84-7.79 (m, 4H), 7.46-7.39 (m, 4H), 7.30 (t, *J* = 7.5 Hz, 1H), 7.17 (t, *J* = 8.0 Hz, 1H), 7.08-7.02 (m, 5H), 6.98 (d, *J* = 3.5 Hz, 1H); ¹³C NMR (125 MHz, DMSO-*d*₆) δ 156.4, 156.1, 152.4, 152.3, 130.1, 130.0, 128.8, 127.3, 124.6, 124.3, 123.5, 123.0, 118.0, 117.7, 108.2, 107.5. Spectroscopic data for the title compound were consistent with those reported in the literature.³



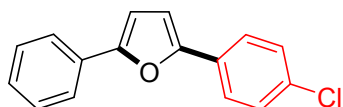
2-(4-fluorophenyl)-5-phenylfuran (**3g**): White solid (56.5 mg, 79%), Hexane as eluent for column chromatography. ¹H NMR (500 MHz, DMSO-*d*₆) δ 7.88-7.85 (m, 2H), 7.81 (d, *J* = 7.5 Hz, 2H), 7.41 (t, *J* = 8.0 Hz, 2H), 7.29-7.18 (m, 3H), 7.01-6.98 (m, 2H); ¹³C NMR (125 MHz, DMSO-*d*₆) δ 162.5, 160.6, 152.6, 151.8, 130.0, 128.9, 127.1, 126.1, 124.8, 124.1, 123.1, 116.0, 113.8, 108.1, 107.0. Spectroscopic data for the title compound were consistent with those reported in the literature.³



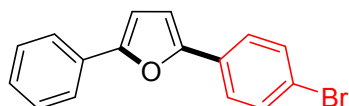
2-(3-fluorophenyl)-5-phenylfuran (**3h**): White solid (35.0 mg, 49%), Hexane as eluent for column chromatography. ¹H NMR (500 MHz, CDCl₃) δ 7.74 (d, *J* = 8.0 Hz, 2H), 7.49 (d, *J* = 7.5 Hz, 1H), 7.42-7.39 (m, 3H), 7.39-7.34 (m, 1H), 7.30 (t, *J* = 7.5 Hz, 1H), 6.98-6.95 (m, 1H), 6.77-6.75 (m, 2H); ¹³C NMR (125 MHz, CDCl₃) δ 164.2, 162.3, 153.9, 152.1, 132.9, 132.8, 130.4, 130.1, 129.5, 128.8, 126.5, 123.4, 119.5, 119.3, 114.2, 114.1, 109.7, 109.2, 108.8, 107.1. Spectroscopic data for the title compound were consistent with those reported in the literature.³



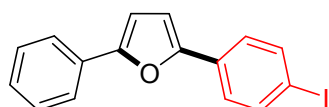
2-(2-fluorophenyl)-5-phenylfuran (**3i**): Yellow oil (32.9 mg, 46%), Hexane as eluent for column chromatography. $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.95-7.92 (m, 1H), 7.76-7.74 (m, 2H), 7.40 (t, $J = 8.0$ Hz, 2H), 7.29-7.28 (m, 1H), 7.23-7.19 (m, 2H), 7.14-7.10 (m, 1H), 6.93 (t, $J = 3.5$ Hz, 1H), 6.77 (d, $J = 3.5$ Hz, 1H); $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 159.8, 157.8, 153.3, 147.6, 147.5, 130.6, 128.7, 128.2, 128.1, 126.5, 126.0, 124.6, 124.1, 123.5, 123.1, 119.1, 118.8, 116.0, 115.5, 113.5, 112.5, 106.6, 106.5. Spectroscopic data for the title compound were consistent with those reported in the literature.³



2-(4-chlorophenyl)-5-phenylfuran (**3j**): White solid (51.2 mg, 67%), Hexane as eluent for column chromatography. $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 7.81 (d, $J = 8.0$ Hz, 2H), 7.76 (d, $J = 8.5$ Hz, 2H), 7.62 (d, $J = 7.0$ Hz, 2H), 7.33 (t, $J = 7.5$ Hz, 2H), 7.21 (t, $J = 8.0$ Hz, 1H), 7.13 (d, $J = 3.0$ Hz, 1H), 7.08 (d, $J = 3.0$ Hz, 1H); $^{13}\text{C NMR}$ (125 MHz, $\text{DMSO-}d_6$) δ 153.0, 151.5, 131.8, 129.9, 129.3, 129.0, 127.7, 125.4, 123.5, 120.4, 109.0, 108.3. Spectroscopic data for the title compound were consistent with those reported in the literature.³

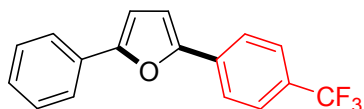


2-(4-bromophenyl)-5-phenylfuran (**3k**): White solid (47.6 mg, 53%), Hexane as eluent for column chromatography. $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 7.84-7.81 (m, 4H), 7.50 (d, $J = 8.5$ Hz, 2H), 7.45 (t, $J = 7.5$ Hz, 2H), 7.32 (t, $J = 7.5$ Hz, 1H), 7.14 (d, $J = 3.5$ Hz, 1H), 7.08 (d, $J = 3.0$ Hz, 1H); $^{13}\text{C NMR}$ (125 MHz, $\text{DMSO-}d_6$) δ 153.0, 151.5, 131.8, 129.9, 129.0, 128.9, 127.6, 125.0, 122.7, 107.3, 106.8. Spectroscopic data for the title compound were consistent with those reported in the literature.³

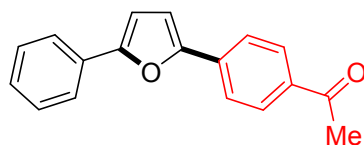


2-(4-iodophenyl)-5-phenylfuran (**3l**): White solid (50.9 mg, 49%), Hexane as eluent for column chromatography. $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 7.82-7.79 (m, 4H),

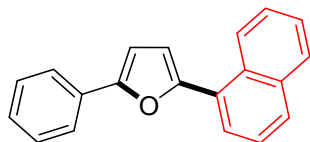
7.62 (d, $J = 8.0$ Hz, 2H), 7.45 (t, $J = 7.5$ Hz, 2H), 7.22 (t, $J = 8.0$ Hz, 1H), 7.12 (d, $J = 3.0$ Hz, 1H), 6.95 (d, $J = 3.0$ Hz, 1H); ^{13}C NMR (125 MHz, DMSO- d_6) δ 153.0, 151.7, 137.6, 129.9, 129.6, 128.9, 127.6, 124.8, 123.8, 108.7, 108.2, 93.5. HRMS calcd for $\text{C}_{16}\text{H}_{12}\text{IO}^+$ $[\text{M}+\text{H}]^+$: 346.9928, found: 346.9925.



2-phenyl-5-(4-(trifluoromethyl)phenyl)furan (**3m**): Light yellow solid (31.1 mg, 36%), Hexane as eluent for column chromatography. ^1H NMR (500 MHz, CDCl_3) δ 7.83 (d, $J = 8.5$ Hz, 2H), 7.77-7.76 (m, 2H), 7.65 (d, $J = 8.5$ Hz, 2H), 7.43 (t, $J = 8.0$ Hz, 2H), 7.31 (t, $J = 8.0$ Hz, 1H), 6.86 (d, $J = 3.5$ Hz, 1H), 6.78 (d, $J = 3.5$ Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 154.5, 151.8, 133.9, 130.4, 129.0, 128.8, 127.9, 125.8, 125.7, 125.3, 124.0, 123.6, 123.1, 109.3, 107.4. Spectroscopic data for the title compound were consistent with those reported in the literature.³

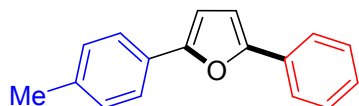


1-(4-(5-phenylfuran-2-yl)phenyl)ethan-1-one (**3n**): Pale yellow solid (32.3 mg, 41%), Hexane as eluent for column chromatography. ^1H NMR (500 MHz, DMSO- d_6) δ 8.02 (d, $J = 8.5$ Hz, 2H), 7.95 (d, $J = 8.5$ Hz, 2H), 7.86 (d, $J = 7.5$ Hz, 2H), 7.47 (t, $J = 7.5$ Hz, 2H), 7.35 (t, $J = 7.5$ Hz, 1H), 7.31 (d, $J = 3.5$ Hz, 1H), 7.16 (d, $J = 3.5$ Hz, 1H), 7.26 (s, 3H); ^{13}C NMR (125 MHz, DMSO- d_6) δ 197.0, 153.8, 151.6, 135.3, 133.9, 130.0, 129.0, 128.9, 128.0, 123.7, 123.3, 110.9, 108.6, 26.6. HRMS calcd for $\text{C}_{18}\text{H}_{15}\text{O}_2^+$ $[\text{M}+\text{H}]^+$: 263.1067, found: 263.1067.

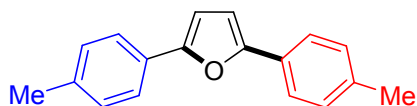


2-(naphthalen-1-yl)-5-phenylfuran (**3o**): Yellow oil (53.5 mg, 66%), Hexane as eluent for column chromatography. ^1H NMR (500 MHz, DMSO- d_6) δ 8.50 (d, $J = 8.5$ Hz, 1H), 8.01 (d, $J = 8.0$ Hz, 1H), 7.96 (d, $J = 8.0$ Hz, 1H), 7.90 (d, $J = 7.5$ Hz, 1H), 7.84 (d, $J = 8.0$ Hz, 2H), 7.66-7.57 (m, 3H), 7.47 (t, $J = 8.0$ Hz, 2H), 7.32 (t, $J = 7.5$ Hz,

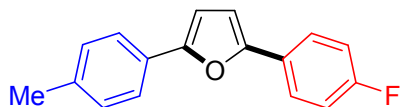
1H), 7.19 (d, $J = 3.5$ Hz, 1H), 7.07 (d, $J = 3.5$ Hz, 1H); ^{13}C NMR (125 MHz, DMSO- d_6) δ 153.1, 152.2, 133.7, 130.1, 129.3, 129.0, 128.7, 128.6, 127.6, 127.4, 127.1, 126.1, 125.8, 125.6, 124.9, 123.5, 112.0, 108.0. Spectroscopic data for the title compound were consistent with those reported in the literature.³



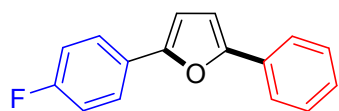
2-phenyl-5-(*p*-tolyl)furan (**3p**): Pale yellow solid (45.7 mg, 65%), Hexane as eluent for column chromatography. ^1H NMR (500 MHz, DMSO- d_6) δ 7.81-7.79 (m, 2H), 7.71 (d, $J = 8.0$ Hz, 2H), 7.44 (t, $J = 8.0$ Hz, 2H), 7.30 (t, $J = 7.5$ Hz, 1H), 7.26 (d, $J = 7.5$ Hz, 2H), 7.06-7.05 (m, 1H), 7.00-6.99 (m, 1H), 2.33 (s, 3H); ^{13}C NMR (125 MHz, DMSO- d_6) δ 152.8, 152.2, 137.0, 130.2, 129.4, 128.9, 127.5, 127.4, 123.4, 123.3, 108.1, 107.4, 20.8. Spectroscopic data for the title compound were consistent with those reported in the literature.³



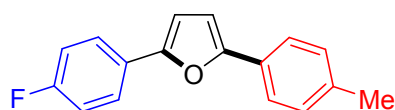
2,5-di-*p*-tolylfuran (**3q**): White solid (54.4 mg, 73%), Hexane as eluent for column chromatography. ^1H NMR (500 MHz, DMSO- d_6) δ 7.69 (d, $J = 7.5$ Hz, 4H), 7.25 (d, $J = 7.5$ Hz, 4H), 6.97 (s, 2H), 2.33 (s, 6H); ^{13}C NMR (125 MHz, DMSO- d_6) δ 152.4, 136.8, 129.4, 127.6, 123.3, 107.3, 20.8. Spectroscopic data for the title compound were consistent with those reported in the literature.⁴



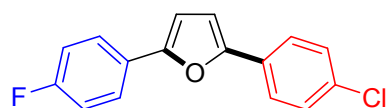
2-(4-fluorophenyl)-5-(*p*-tolyl)furan (**3r**): White solid (50.0 mg, 66%), Hexane as eluent for column chromatography. ^1H NMR (500 MHz, DMSO- d_6) δ 7.84 (t, $J = 7.5$ Hz, 2H), 7.70 (d, $J = 7.5$ Hz, 2H), 7.30-7.25 (m, 4H), 7.03 (d, $J = 3.0$ Hz, 1H), 6.99 (d, $J = 3.0$ Hz, 1H), 2.33 (s, 3H); ^{13}C NMR (125 MHz, DMSO- d_6) δ 152.9, 151.4, 137.0, 129.4, 127.4, 125.5, 125.4, 123.4, 116.0, 115.8, 107.9, 107.4, 20.8. Spectroscopic data for the title compound were consistent with those reported in the literature.⁵



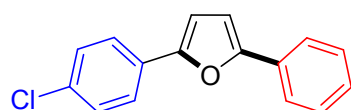
2-(4-fluorophenyl)-5-phenylfuran (**3s**): White solid (60.8 mg, 85%), Hexane as eluent for column chromatography. $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 7.88-7.85 (m, 2H), 7.81 (d, $J = 7.5$ Hz, 2H), 7.45 (t, $J = 7.5$ Hz, 2H), 7.33-7.28 (m, 3H), 7.08-7.06 (m, 2H); $^{13}\text{C NMR}$ (125 MHz, $\text{DMSO-}d_6$) δ 162.5, 160.6, 152.6, 151.8, 130.0, 128.9, 127.5, 126.8, 125.6, 125.5, 123.4, 116.0, 115.8, 108.2, 108.0. Spectroscopic data for the title compound were consistent with those reported in the literature.³



2-(4-fluorophenyl)-5-(*p*-tolyl)furan (**3t**): White solid (56.0 mg, 74%), Hexane as eluent for column chromatography. $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 7.84 (t, $J = 7.5$ Hz, 2H), 7.70 (d, $J = 7.5$ Hz, 2H), 7.30-7.25 (m, 4H), 7.03 (d, $J = 3.0$ Hz, 1H), 6.99 (d, $J = 3.0$ Hz, 1H), 2.33 (s, 3H); $^{13}\text{C NMR}$ (125 MHz, $\text{DMSO-}d_6$) δ 152.9, 151.4, 137.0, 129.4, 127.4, 125.5, 125.4, 123.4, 116.0, 115.8, 107.9, 107.4, 20.8. Spectroscopic data for the title compound were consistent with those reported in the literature.⁵

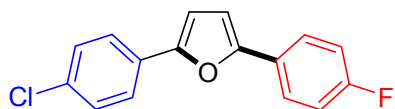


2-(4-chlorophenyl)-5-(4-fluorophenyl)furan (**3u**): White solid (61.4 mg, 75%), Hexane as eluent for column chromatography. $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 7.88-7.82 (m, 4H), 7.50 (d, $J = 8.5$ Hz, 2H), 7.29 (t, $J = 8.5$ Hz, 2H), 7.13 (d, $J = 3.5$ Hz, 1H), 7.07 (d, $J = 3.5$ Hz, 1H); $^{13}\text{C NMR}$ (125 MHz, $\text{DMSO-}d_6$) δ 162.6, 160.6, 152.1, 151.5, 131.9, 128.9, 128.8, 126.6, 125.7, 125.6, 125.1, 116.0, 115.8, 109.0, 108.1. Spectroscopic data for the title compound were consistent with those reported in the literature.⁶

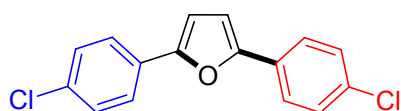


2-(4-chlorophenyl)-5-phenylfuran (**3v**): White solid (54.3 mg, 71%), Hexane as eluent for column chromatography. $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 7.81 (d, $J = 8.0$ Hz, 2H), 7.76 (d, $J = 8.5$ Hz, 2H), 7.63 (d, $J = 8.5$ Hz, 2H), 7.45 (t, $J = 8.0$ Hz, 2H), 7.32

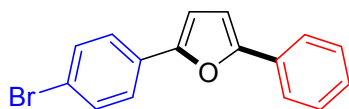
(t, $J = 7.5$ Hz, 1H), 7.13 (d, $J = 3.0$ Hz, 1H), 7.08 (d, $J = 3.0$ Hz, 1H); ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) δ 153.0, 151.5, 131.8, 129.9, 129.3, 129.0, 127.7, 125.4, 123.5, 120.4, 109.0, 108.3. Spectroscopic data for the title compound were consistent with those reported in the literature.³



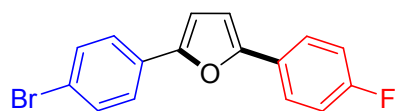
2-(4-chlorophenyl)-5-(4-fluorophenyl)furan (**3w**): White solid (61.4 mg, 75%), Hexane as eluent for column chromatography. ^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ 7.88-7.82 (m, 4H), 7.50 (d, $J = 8.5$ Hz, 2H), 7.29 (t, $J = 8.5$ Hz, 2H), 7.13 (d, $J = 3.5$ Hz, 1H), 7.07 (d, $J = 3.5$ Hz, 1H); ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) δ 162.6, 160.6, 152.1, 151.5, 131.9, 128.9, 128.8, 126.6, 125.7, 125.6, 125.1, 116.0, 115.8, 109.0, 108.1. Spectroscopic data for the title compound were consistent with those reported in the literature.⁶



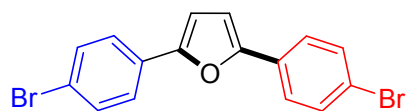
2,5-bis(4-chlorophenyl)furan (**3x**): White solid (59.0 mg, 68%), Hexane as eluent for column chromatography. ^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ 7.84 (d, $J = 8.5$ Hz, 4H), 7.50 (d, $J = 8.5$ Hz, 4H), 7.15 (s, 2H); ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) δ 151.8, 132.0, 128.9, 128.8, 125.2, 109.0. Spectroscopic data for the title compound were consistent with those reported in the literature.⁶



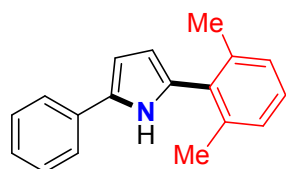
2-(4-bromophenyl)-5-phenylfuran (**3y**): White solid (35.9 mg, 40%), Hexane as eluent for column chromatography. ^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ 7.84-7.81 (m, 4H), 7.50 (d, $J = 8.5$ Hz, 2H), 7.45 (t, $J = 7.5$ Hz, 2H), 7.32 (t, $J = 7.5$ Hz, 1H), 7.14 (d, $J = 3.5$ Hz, 1H), 7.05 (d, $J = 3.5$ Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 153.0, 151.5, 131.8, 129.9, 129.0, 128.9, 127.7, 125.1, 123.5, 108.9, 108.3. Spectroscopic data for the title compound were consistent with those reported in the literature.³



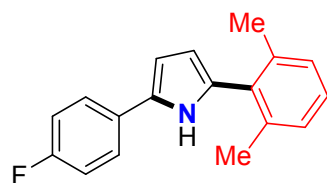
2-(4-bromophenyl)-5-(4-fluorophenyl)furan (**3z**): White solid (64.7 mg, 68%), Hexane as eluent for column chromatography. $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 7.87 (t, $J = 7.5$ Hz, 2H), 7.77 (d, $J = 8.0$ Hz, 2H), 7.63 (d, $J = 7.5$ Hz, 2H), 7.22 (t, $J = 9.0$ Hz, 2H), 7.09 (d, $J = 2.5$ Hz, 1H), 7.01 (d, $J = 2.5$ Hz, 1H); $^{13}\text{C NMR}$ (125 MHz, $\text{DMSO-}d_6$) δ 162.6, 160.6, 152.2, 151.5, 131.8, 129.2, 126.6, 125.7, 125.6, 125.4, 120.4, 116.0, 115.8, 109.0, 108.1. **HRMS** calcd for $\text{C}_{16}\text{H}_{11}\text{BrFO}^+$ $[\text{M}+\text{H}]^+$: 316.9972, found: 316.9972.



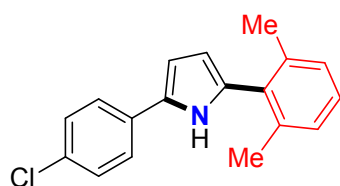
2,5-bis(4-bromophenyl)furan (**3aa**): White solid (53.3 mg, 47%), Hexane as eluent for column chromatography. $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 7.78 (d, $J = 8.5$ Hz, 4H), 7.64 (d, $J = 8.5$ Hz, 4H), 7.17 (s, 2H); $^{13}\text{C NMR}$ (125 MHz, $\text{DMSO-}d_6$) δ 151.9, 131.9, 129.1, 125.5, 120.6, 109.2. Spectroscopic data for the title compound were consistent with those reported in the literature.⁴



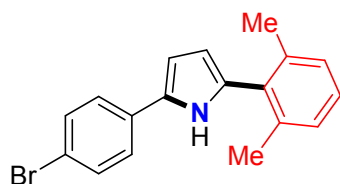
2-(2,6-dimethylphenyl)-5-phenyl-1H-pyrrole (**4a**): White solid (57.9 mg, 78%), Petroleum ether/ethyl acetate = 16/1 as eluent for column chromatography. $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 11.19 (s, 1H), 7.67 (d, $J = 7.5$ Hz, 2H), 7.31 (t, $J = 7.5$ Hz, 2H), 7.19-7.16 (m, 1H), 7.11 (t, $J = 7.0$ Hz, 3H), 7.61-7.60 (m, 1H), 5.99-5.97 (m, 1H), 2.16 (s, 6H); $^{13}\text{C NMR}$ (125 MHz, $\text{DMSO-}d_6$) δ 137.8, 133.8, 133.0, 130.8, 130.6, 128.6, 127.5, 127.1, 125.1, 123.1, 109.0, 106.0, 20.5. **HRMS** calcd for $\text{C}_{18}\text{H}_{18}\text{N}^+$ $[\text{M}+\text{H}]^+$: 248.1434, found: 248.1431.



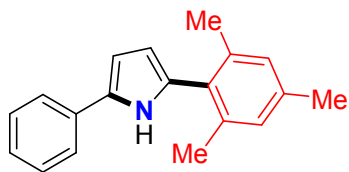
2-(2,6-dimethylphenyl)-5-(4-fluorophenyl)-1*H*-pyrrole (**4b**): White solid (66.9 mg, 84%), Petroleum ether/ethyl acetate = 16/1 as eluent for column chromatography. ¹H NMR (500 MHz, CDCl₃) δ 8.26 (s, 1H), 7.52-7.49 (m, 2H), 7.31 (t, *J* = 8.0 Hz, 1H), 7.23 (d, *J* = 7.5 Hz, 2H), 7.16-7.11 (m, 2H), 6.65-6.64 (m, 1H), 6.24-6.22 (m, 1H), 2.34 (s, 6H); ¹³C NMR (125 MHz, CDCl₃) δ 162.4, 160.4, 138.7, 133.4, 131.0, 130.7, 129.5, 129.4, 128.2, 127.6, 125.2, 125.1, 116.0, 115.8, 110.3, 106.4, 20.8. HRMS calcd for C₁₈H₁₇FN⁺ [M+H]⁺: 266.134, found: 266.1341.



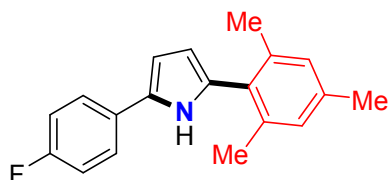
2-(4-chlorophenyl)-5-(2,6-dimethylphenyl)-1*H*-pyrrole (**4c**): White solid (68.5 mg, 81%), Petroleum ether/ethyl acetate = 16/1 as eluent for column chromatography. ¹H NMR (500 MHz, CDCl₃) δ 8.18 (s, 1H), 7.33 (d, *J* = 8.5 Hz, 2H), 7.26 (d, *J* = 8.5 Hz, 2H), 7.18-7.15 (m, 1H), 7.08 (d, *J* = 7.5 Hz, 2H), 6.56-6.54 (m, 1H), 6.10-6.09 (m, 1H), 2.19 (s, 6H); ¹³C NMR (125 MHz, CDCl₃) δ 138.6, 133.2, 131.5, 131.4, 131.3, 130.4, 129.1, 128.2, 127.5, 124.6, 110.5, 107.0, 20.8. HRMS calcd for C₁₈H₁₇ClN⁺ [M+H]⁺: 282.1044, found: 282.1042.



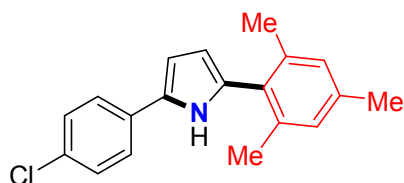
2-(4-bromophenyl)-5-(2,6-dimethylphenyl)-1*H*-pyrrole (**4d**): White solid (69.5 mg, 71%), Petroleum ether/ethyl acetate = 16/1 as eluent for column chromatography. ¹H NMR (500 MHz, CDCl₃) δ 8.20 (s, 1H), 7.44 (d, *J* = 8.5 Hz, 2H), 7.30 (d, *J* = 8.5 Hz, 2H), 7.21-7.16 (m, 1H), 7.10 (d, *J* = 7.5 Hz, 2H), 6.58-6.57 (m, 1H), 6.11-6.10 (m, 1H), 2.20 (s, 6H); ¹³C NMR (125 MHz, CDCl₃) δ 138.6, 133.2, 132.0, 131.8, 131.4, 130.3, 128.2, 127.5, 124.9, 119.3, 110.4, 107.0, 20.8. HRMS calcd for C₁₈H₁₇BrN⁺ [M+H]⁺: 326.0539, found: 326.0536.



2-mesityl-5-phenyl-1*H*-pyrrole (**4e**): Yellow solid (51.8 mg, 66%), Petroleum ether/ethyl acetate = 16/1 as eluent for column chromatography. **¹H NMR** (500 MHz, DMSO-*d*₆) δ 11.12 (s, 1H), 7.66 (d, *J* = 7.5 Hz, 2H), 7.31 (t, *J* = 7.5 Hz, 2H), 7.11 (t, *J* = 7.0 Hz, 1H), 6.94 (s, 2H), 6.59 (s, 1H), 5.94 (s, 1H), 2.27 (s, 3H), 2.12 (s, 6H); **¹³C NMR** (125 MHz, DMSO-*d*₆) δ 137.5, 136.5, 133.1, 130.9, 130.7, 130.6, 128.6, 127.7, 125.0, 123.1, 109.1, 105.9, 20.6, 20.4. **HRMS** calcd for C₁₉H₂₀N⁺ [M+H]⁺: 262.1590, found: 262.1588.

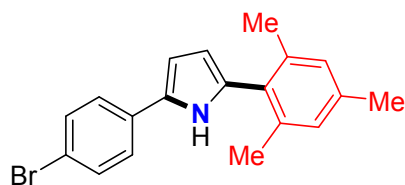


2-(4-fluorophenyl)-5-mesityl-1*H*-pyrrole (**4f**): White solid (46.9 mg, 56%), Petroleum ether/ethyl acetate = 16/1 as eluent for column chromatography. **¹H NMR** (500 MHz, CDCl₃) δ 8.22 (s, 1H), 7.50-7.47 (m, 2H), 7.14-7.10 (m, 2H), 7.05 (s, 2H), 6.62-6.61 (m, 1H), 6.20-6.19 (m, 1H), 2.43 (s, 3H), 2.29 (s, 6H); **¹³C NMR** (125 MHz, CDCl₃) δ 162.3, 160.4, 138.5, 137.9, 131.0, 130.5, 130.4, 129.5, 129.4, 128.3, 125.1, 125.0, 116.0, 115.8, 110.4, 106.3, 21.2, 20.7. **HRMS** calcd for C₁₉H₁₉FN⁺ [M+H]⁺: 280.1496, found: 280.1496.

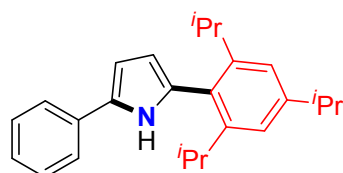


2-(4-chlorophenyl)-5-mesityl-1*H*-pyrrole (**4g**): Yellow solid (41.7 mg, 47%), Petroleum ether/ethyl acetate = 16/1 as eluent for column chromatography. **¹H NMR** (500 MHz, CDCl₃) δ 8.26 (s, 1H), 7.44 (d, *J* = 8.5 Hz, 2H), 7.38 (d, *J* = 8.5 Hz, 2H), 7.04 (s, 2H), 6.67-6.66 (m, 1H), 6.20-6.19 (m, 1H), 2.43 (s, 3H), 2.28 (m, 6H); **¹³C NMR** (125 MHz, CDCl₃) δ 138.5, 138.0, 131.5, 131.4, 131.3, 130.3, 130.2, 129.1, 128.3, 124.6, 110.6, 107.0, 21.2, 20.7. **HRMS** calcd for C₁₉H₁₉ClN⁺ [M+H]⁺:

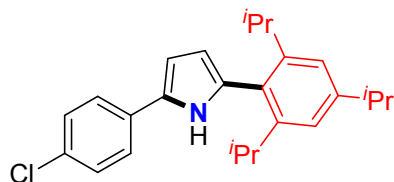
296.1201, found: 296.1203.



2-(4-bromophenyl)-5-mesityl-1*H*-pyrrole (**4h**): White solid (38.9 mg, 38%), Petroleum ether/ethyl acetate = 16/1 as eluent for column chromatography. $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.18 (s, 1H), 7.50 (d, $J = 8.0$ Hz, 2H), 7.34 (d, $J = 8.0$ Hz, 2H), 7.00 (s, 2H), 6.63 (d, $J = 2.0$ Hz, 1H), 6.16 (d, $J = 2.0$ Hz, 1H), 2.38 (s, 3H), 2.23 (s, 6H); $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 138.4, 138.0, 132.0, 131.9, 131.4, 130.2, 130.1, 128.3, 124.9, 119.2, 110.5, 107.0, 21.1, 20.7. **HRMS** calcd for $\text{C}_{19}\text{H}_{19}\text{BrN}^+$ $[\text{M}+\text{H}]^+$: 340.0696, found: 340.0693.

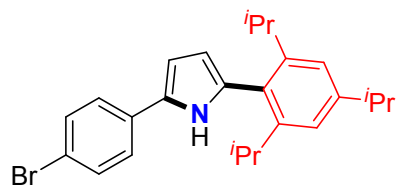


2-phenyl-5-(2,4,6-triisopropylphenyl)-1*H*-pyrrole (**4i**): Yellow solid (43.5 mg, 42%), Petroleum ether/ethyl acetate = 16/1 as eluent for column chromatography. $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.72 (s, 1H), 7.52 (d, $J = 8.0$ Hz, 2H), 7.37 (t, $J = 7.5$ Hz, 2H), 7.18 (t, $J = 7.5$ Hz, 1H), 7.11 (s, 2H), 6.64-6.62 (m, 1H), 6.16-6.15 (m, 1H), 3.02-2.95 (m, 1H), 2.93-2.85 (m, 2H), 1.33 (d, $J = 8.5$ Hz, 6H), 1.16 (s, 12H); $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 149.6, 149.4, 133.0, 131.0, 130.5, 128.9, 128.8, 125.7, 123.3, 120.6, 110.9, 106.1, 34.5, 30.7, 24.1. **HRMS** calcd for $\text{C}_{25}\text{H}_{32}\text{N}^+$ $[\text{M}+\text{H}]^+$: 346.2529, found: 346.2527.



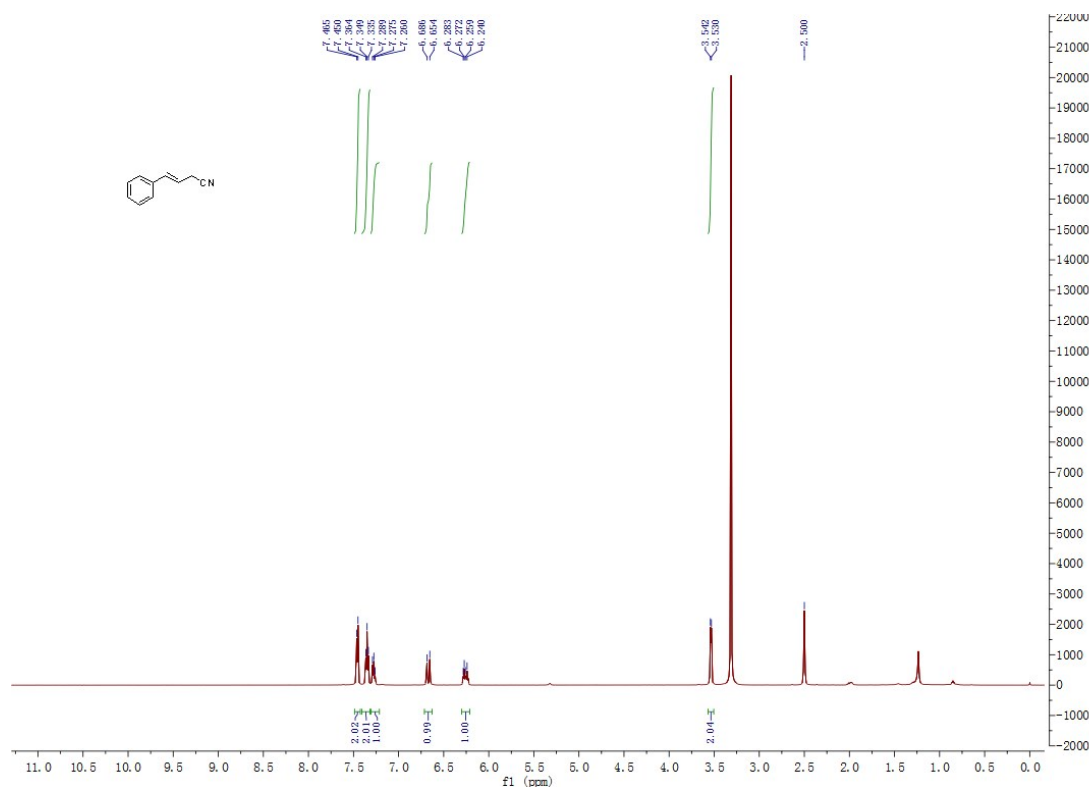
2-(4-chlorophenyl)-5-(2,4,6-triisopropylphenyl)-1*H*-pyrrole (**4j**): Yellow solid (44.4 mg, 39%), Petroleum ether/ethyl acetate = 16/1 as eluent for column chromatography. $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.23 (s, 1H), 7.39-7.36 (m, 2H), 7.31 (d, $J = 8.5$ Hz, 2H), 7.10 (s, 2H), 6.61-6.60 (m, 1H), 6.17-6.16 (m, 1H), 3.00-2.94 (m, 1H), 2.87-2.82

(m, 2H), 1.33-1.31 (m, 6H), 1.18 (s, 12H); ^{13}C NMR (125 MHz, CDCl_3) δ 149.6, 149.5, 131.5, 131.2, 131.0, 130.0, 129.0, 128.3, 128.2, 124.5, 120.7, 111.2, 106.7, 34.5, 30.7, 24.1. **HRMS** calcd for $\text{C}_{25}\text{H}_{31}\text{ClN}^+$ $[\text{M}+\text{H}]^+$: 380.2140, found: 380.2140.

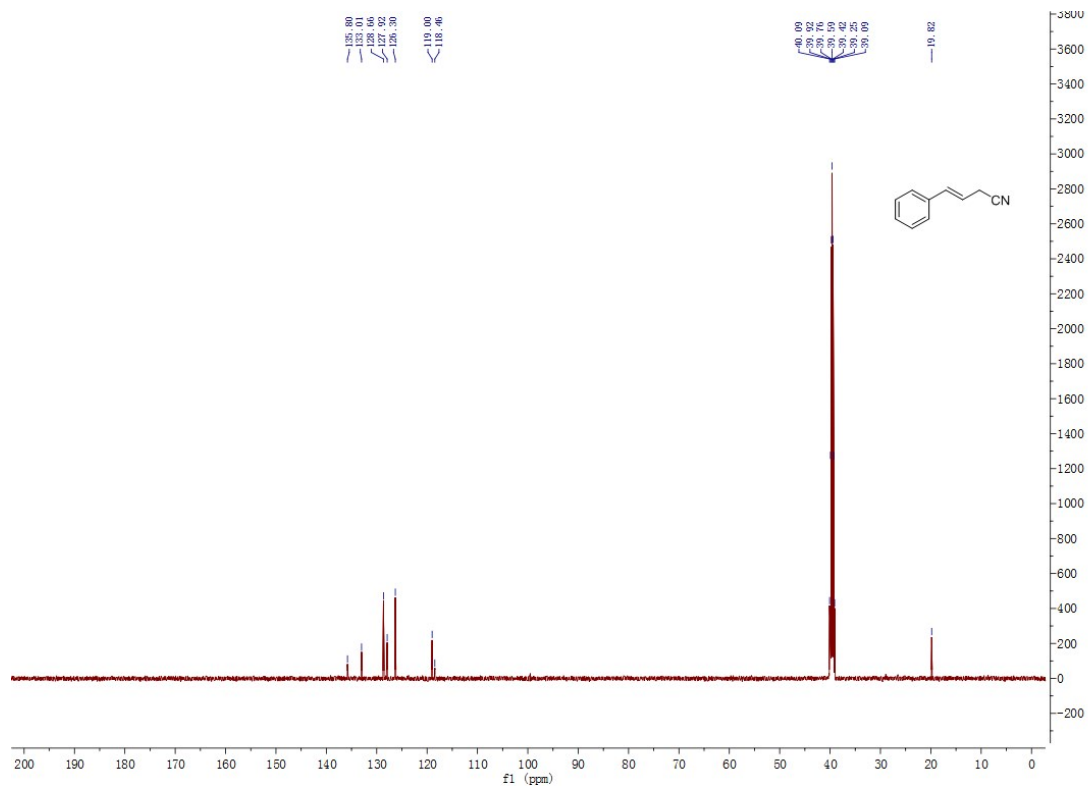


2-(4-bromophenyl)-5-(2,4,6-triisopropylphenyl)-1*H*-pyrrole (**4k**): Yellow solid (35.7 mg, 28%), Petroleum ether/ethyl acetate = 16/1 as eluent for column chromatography. ^1H NMR (500 MHz, CDCl_3) δ 8.18 (s, 1H), 7.49 (d, $J = 8.5$ Hz, 2H), 7.33 (d, $J = 8.5$ Hz, 2H), 7.10 (s, 2H), 6.62-6.61 (m, 1H), 6.18-6.16 (m, 1H), 3.01-2.93 (m, 1H), 2.90-2.80 (m, 2H), 1.33 (d, $J = 7.0$ Hz, 6H), 1.18 (d, $J = 5.5$ Hz, 12H); ^{13}C NMR (125 MHz, CDCl_3) δ 149.6, 149.5, 132.0, 131.9, 131.1, 129.9, 128.2, 124.8, 120.7, 119.2, 111.3, 106.8, 34.5, 30.7, 24.5, 24.0. **HRMS** calcd for $\text{C}_{25}\text{H}_{31}\text{BrN}^+$ $[\text{M}+\text{H}]^+$: 424.1635, found: 424.1636.

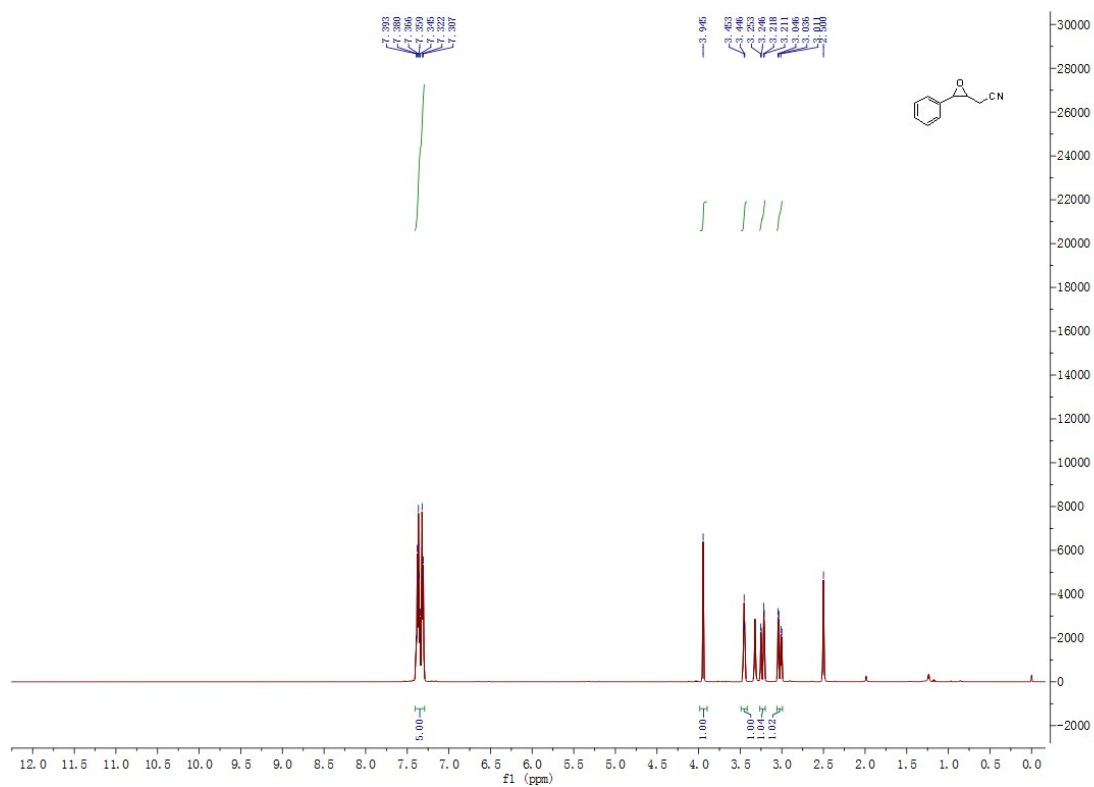
7. NMR spectra for reactants.



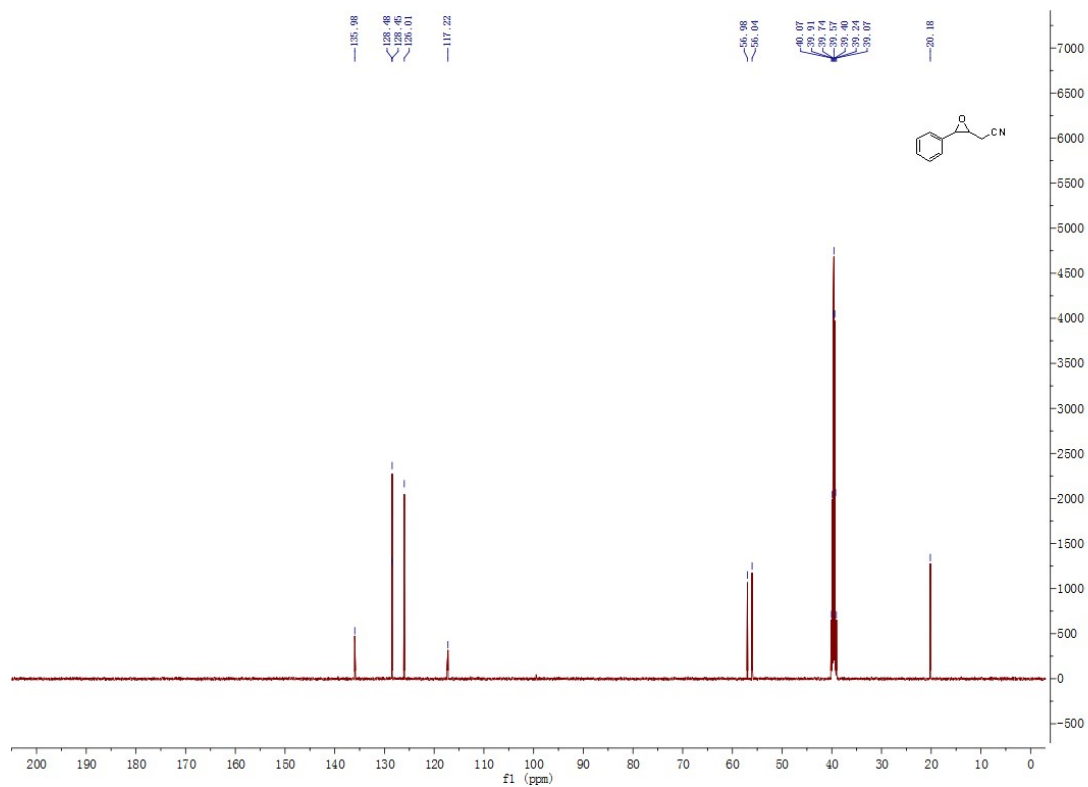
^1H NMR (500 MHz, $\text{DMSO}-d_6$) of compound **1a'**



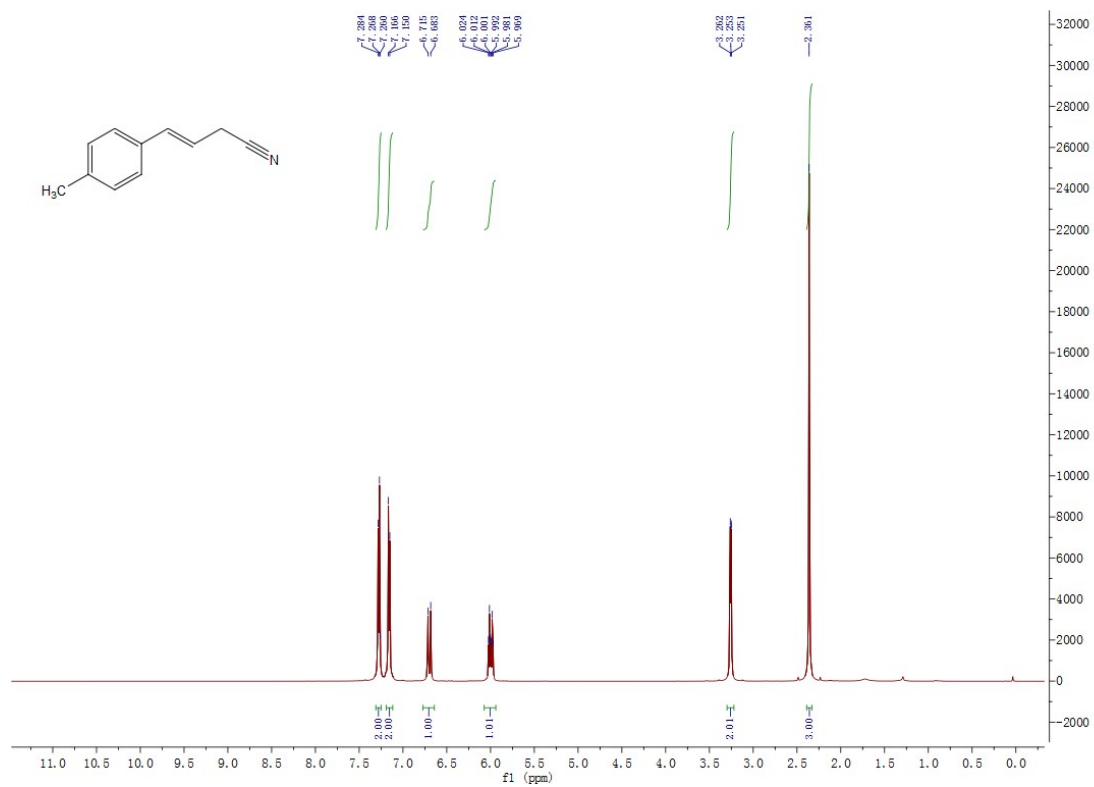
^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) of compound **1a'**



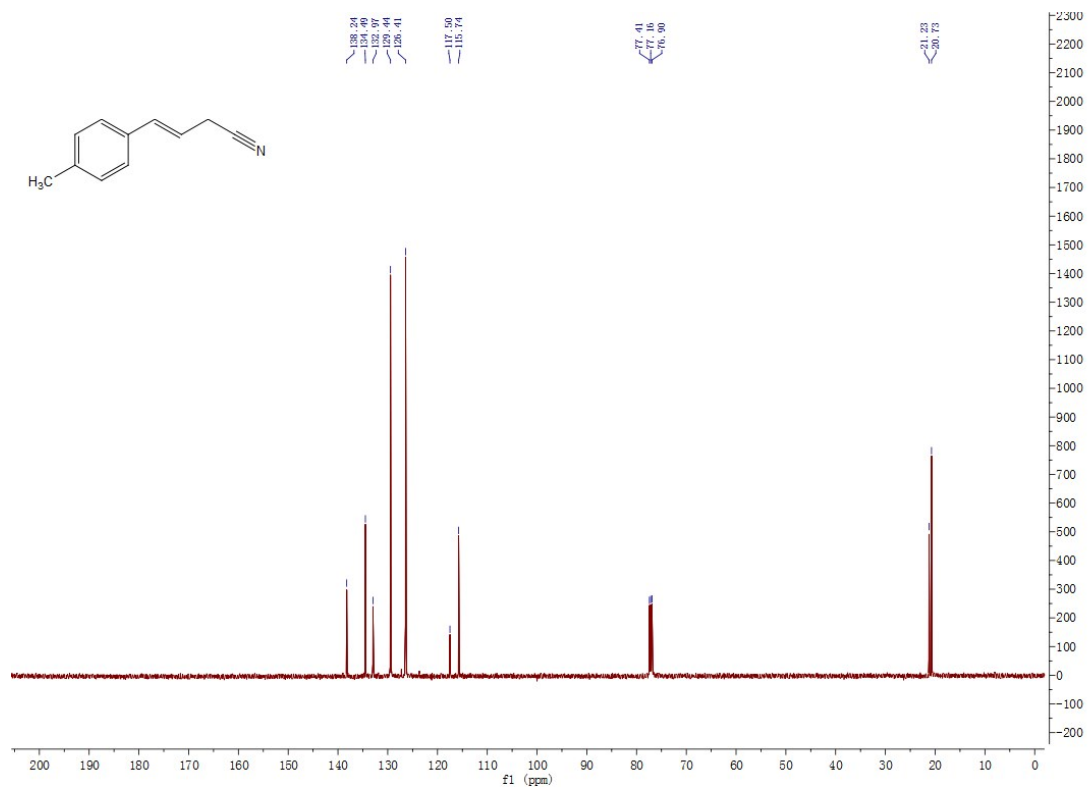
^1H NMR (500 MHz, $\text{DMSO-}d_6$) of compound **1a**



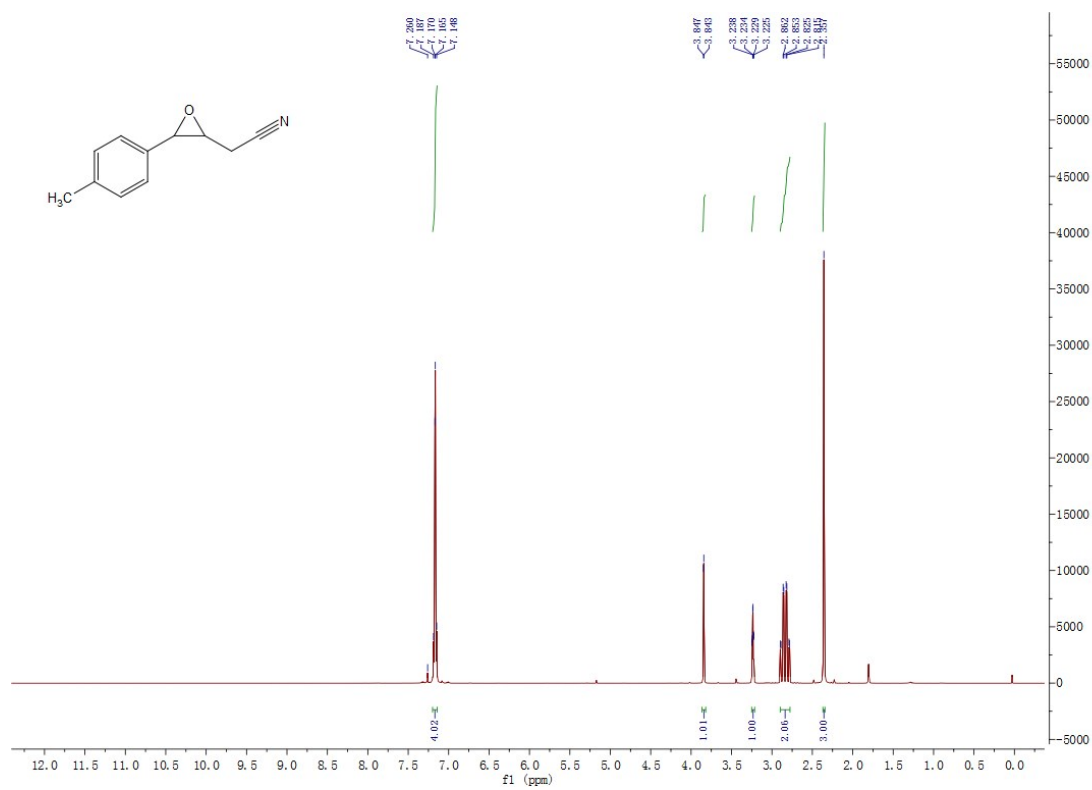
^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) of compound **1a**



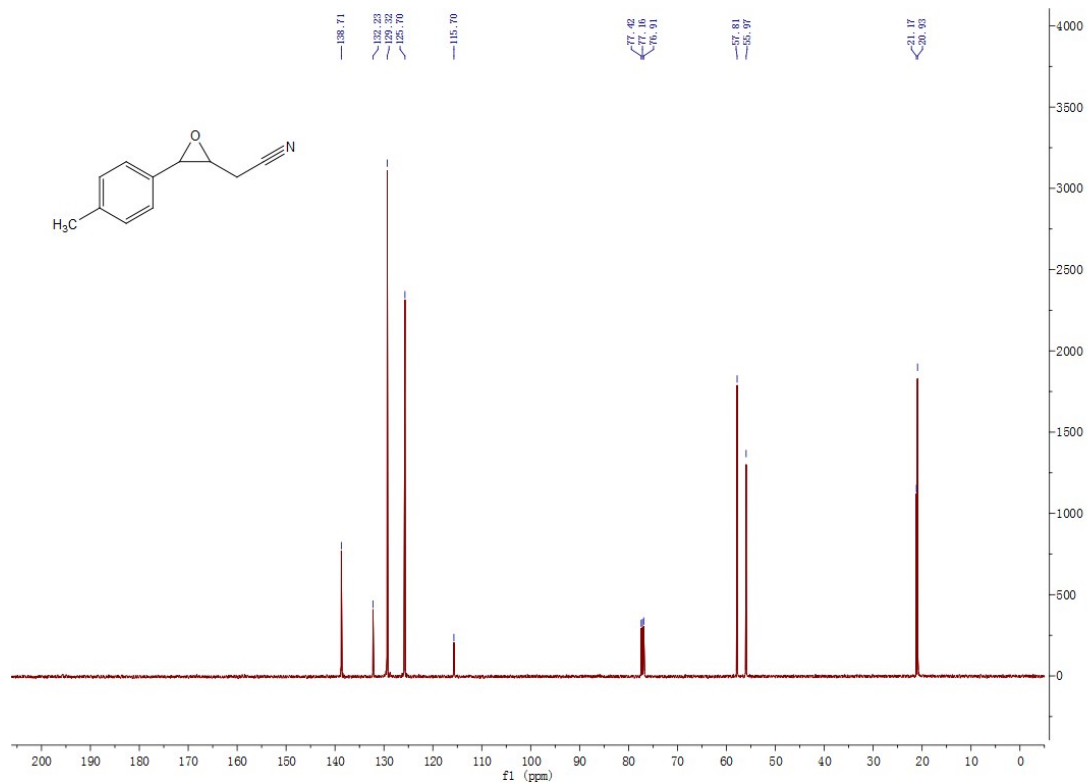
^1H NMR (500 MHz, CDCl_3) of compound **1b'**



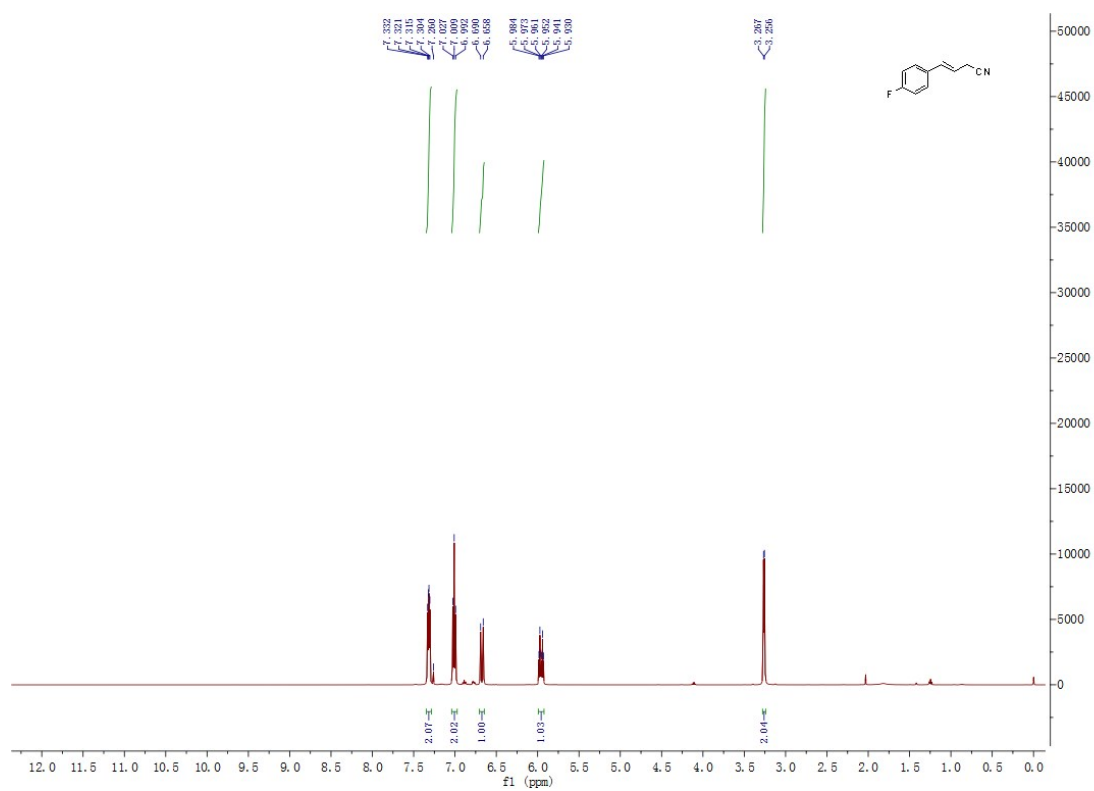
^{13}C NMR (125 MHz, CDCl_3) of compound **1b'**



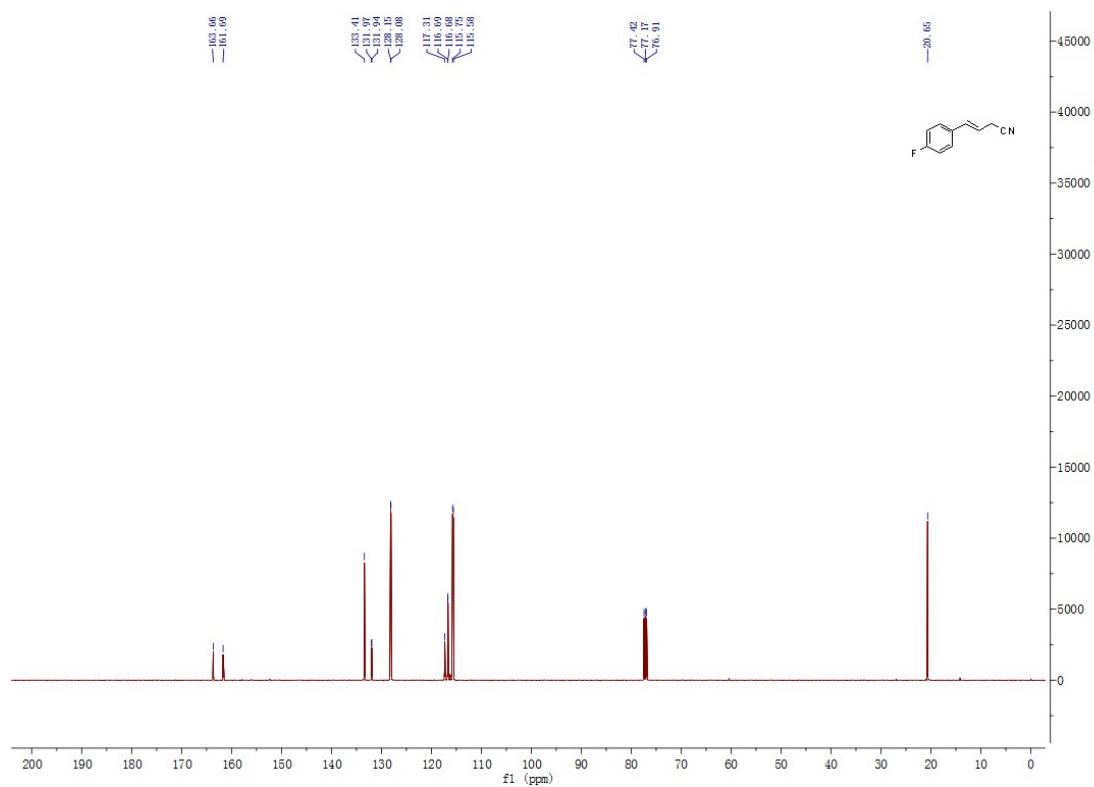
^1H NMR (500 MHz, CDCl_3) of compound **1b**



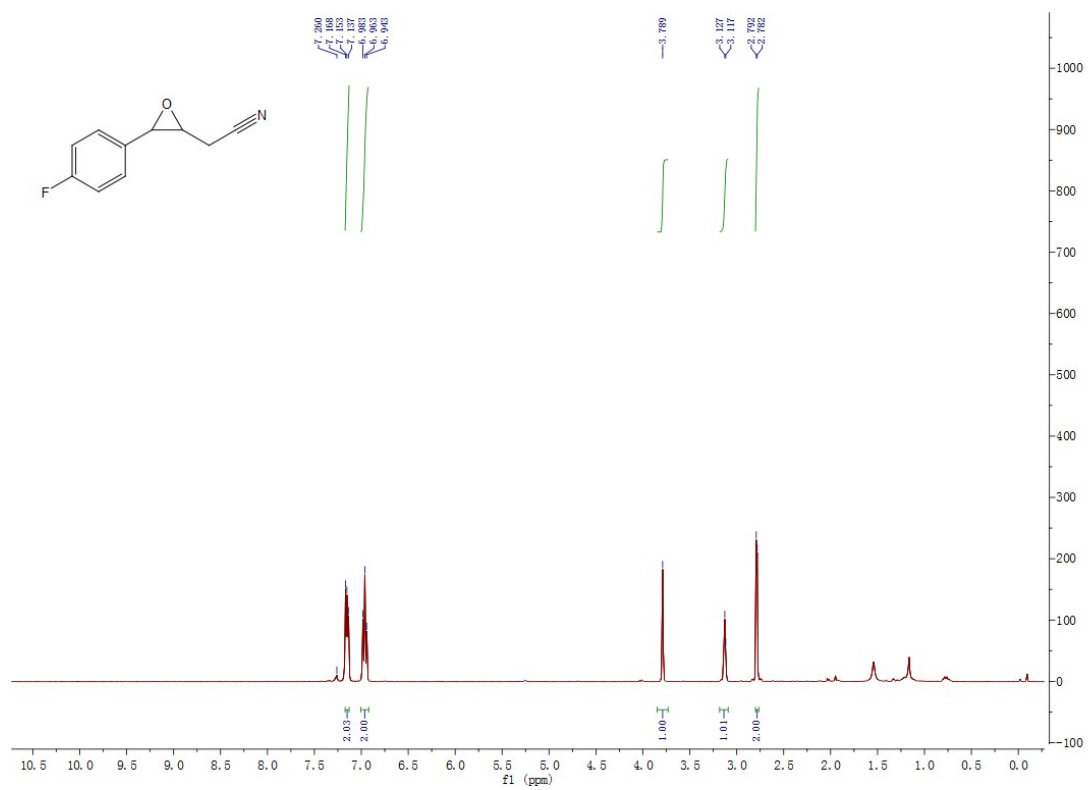
^{13}C NMR (125 MHz, CDCl_3) of compound **1b**



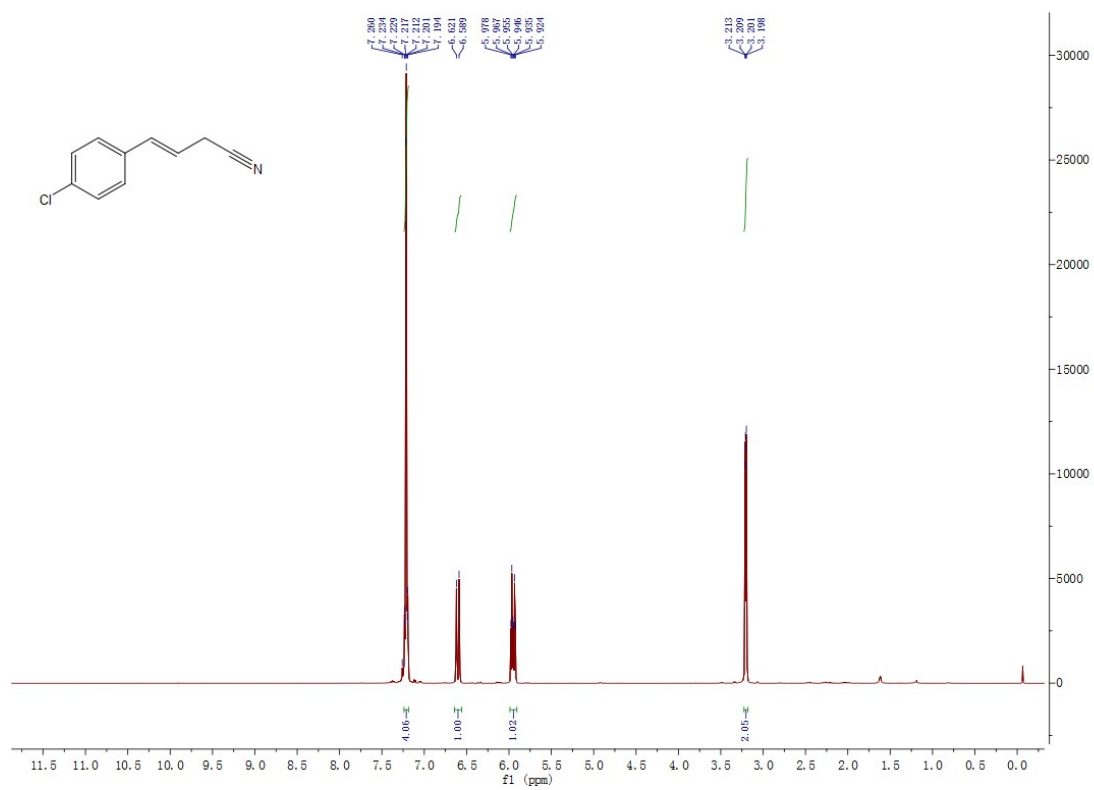
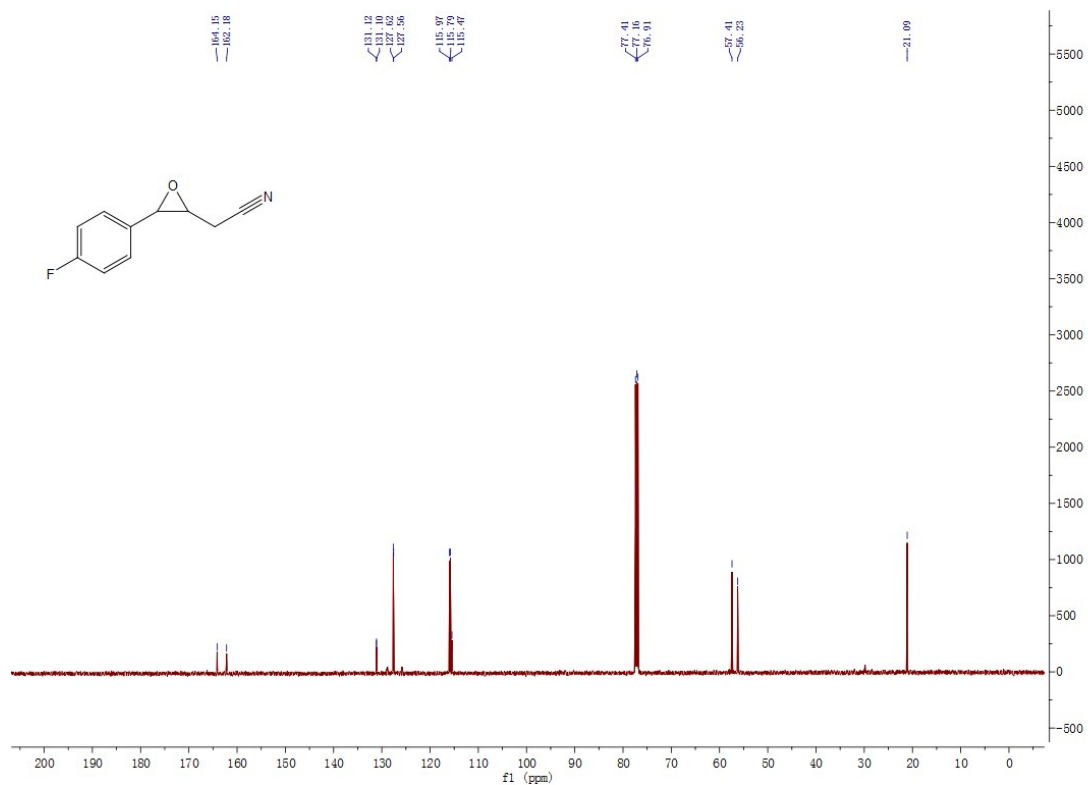
^1H NMR (500 MHz, CDCl_3) of compound **1c'**

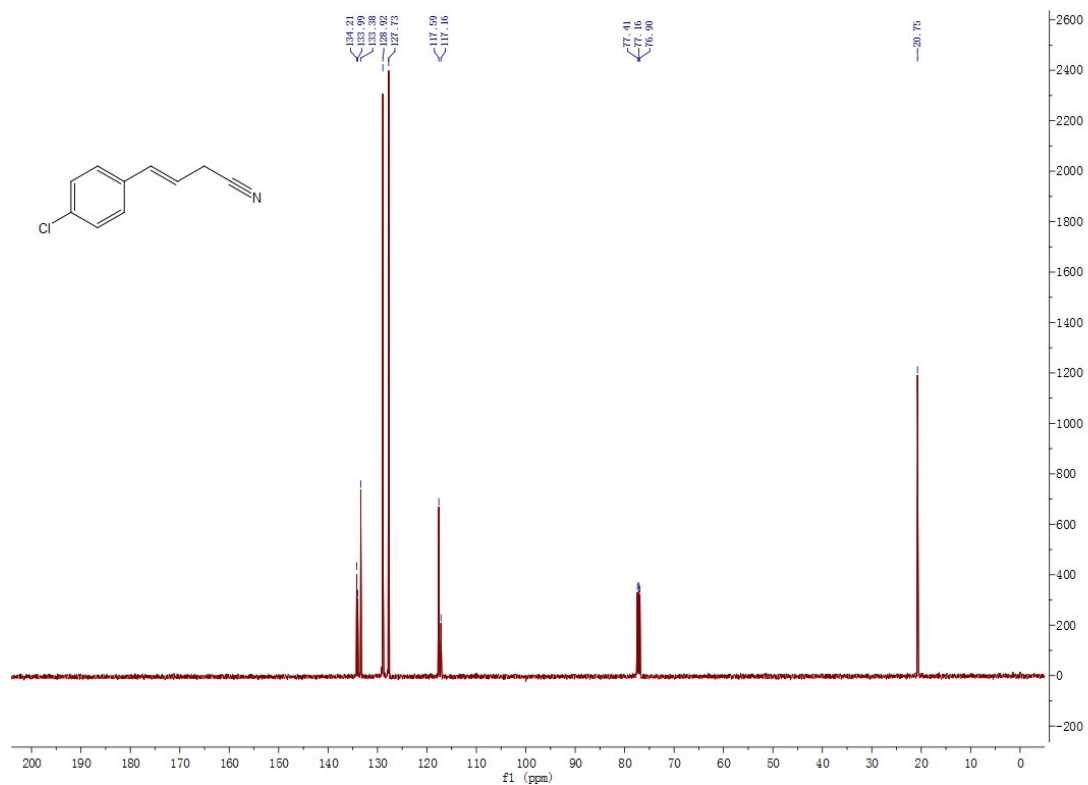


^{13}C NMR (125 MHz, CDCl_3) of compound **1c'**

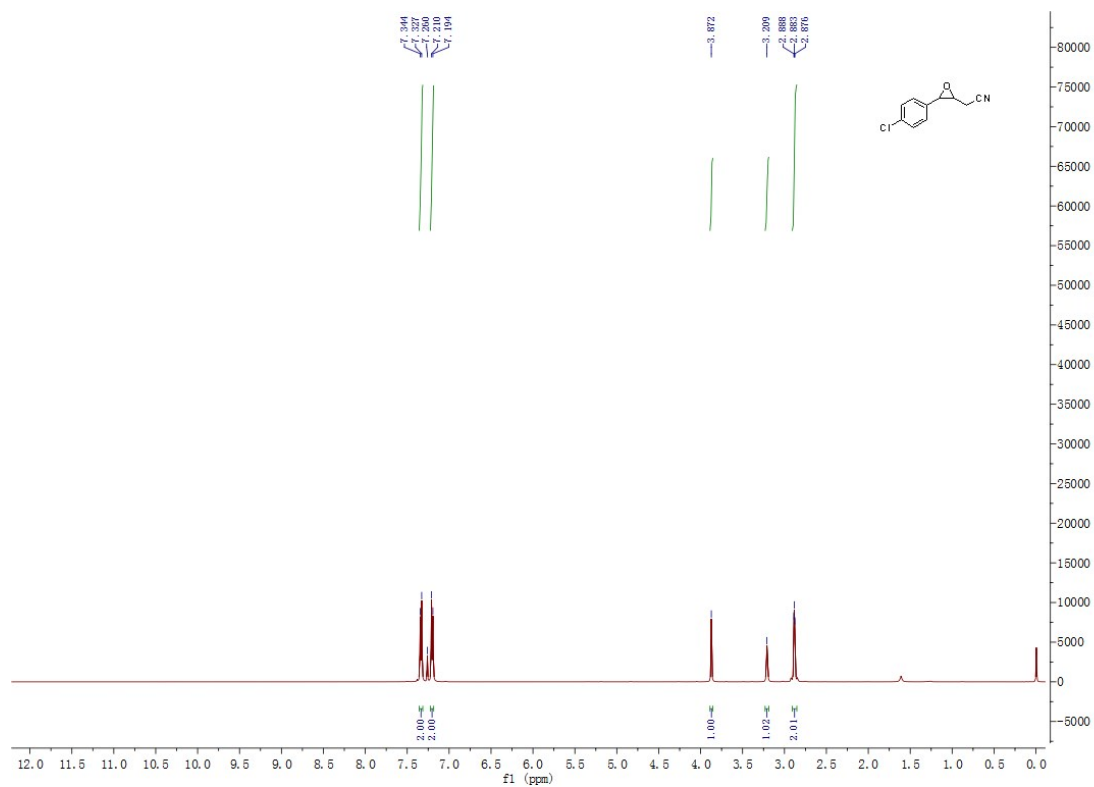


^1H NMR (500 MHz, CDCl_3) of compound **1c**

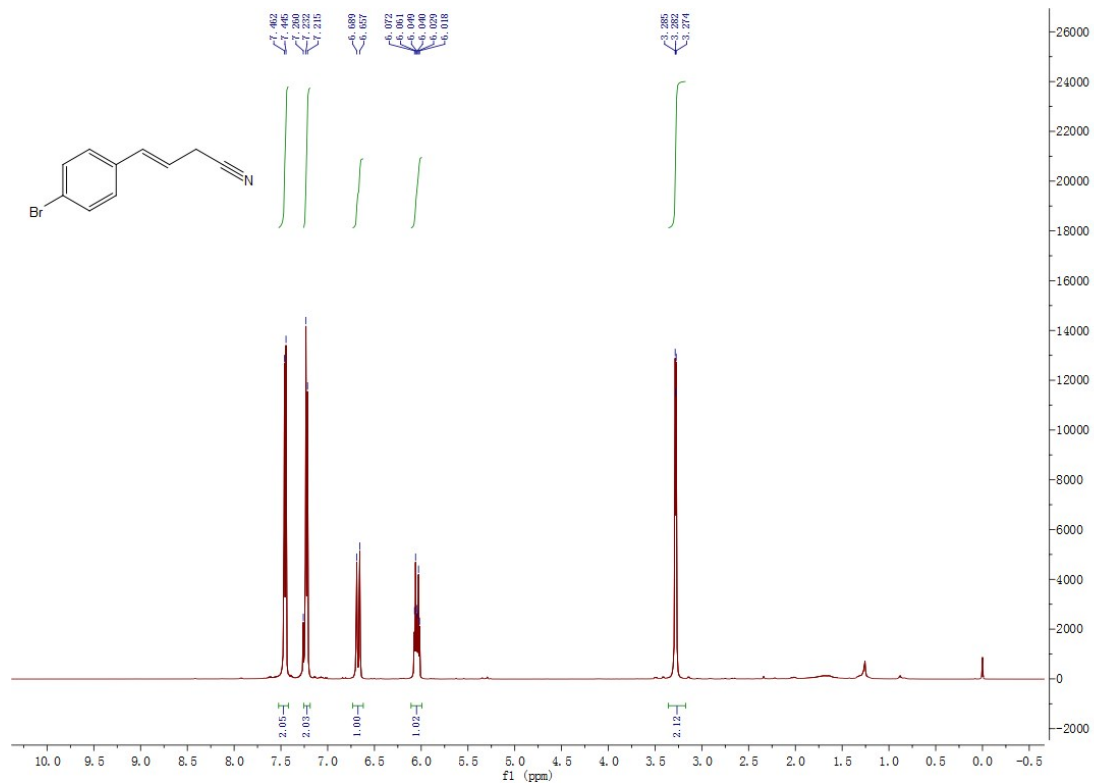
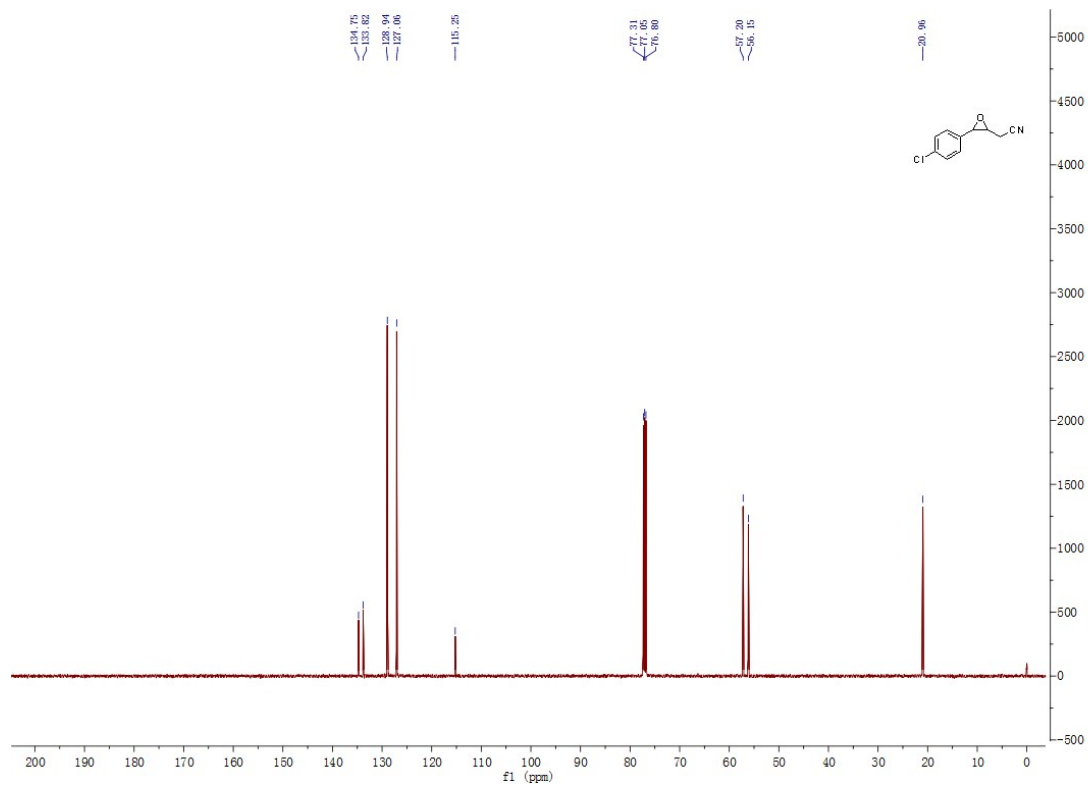


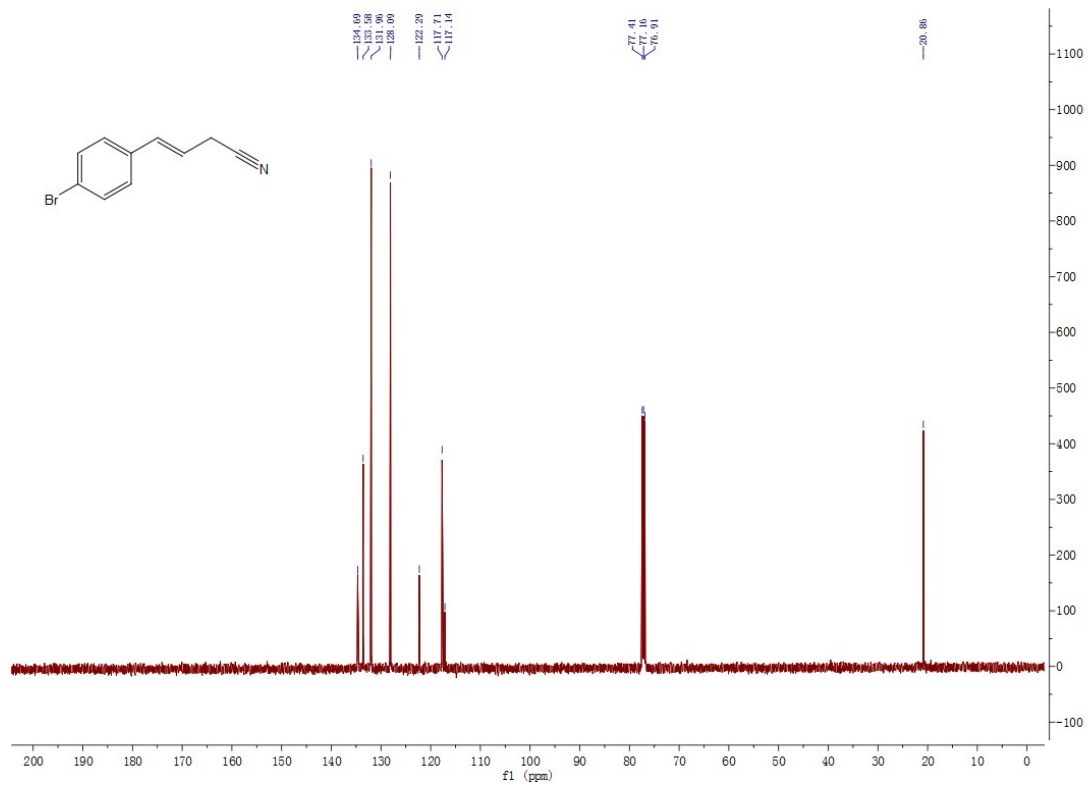


^{13}C NMR (125 MHz, CDCl_3) of compound **1d'**

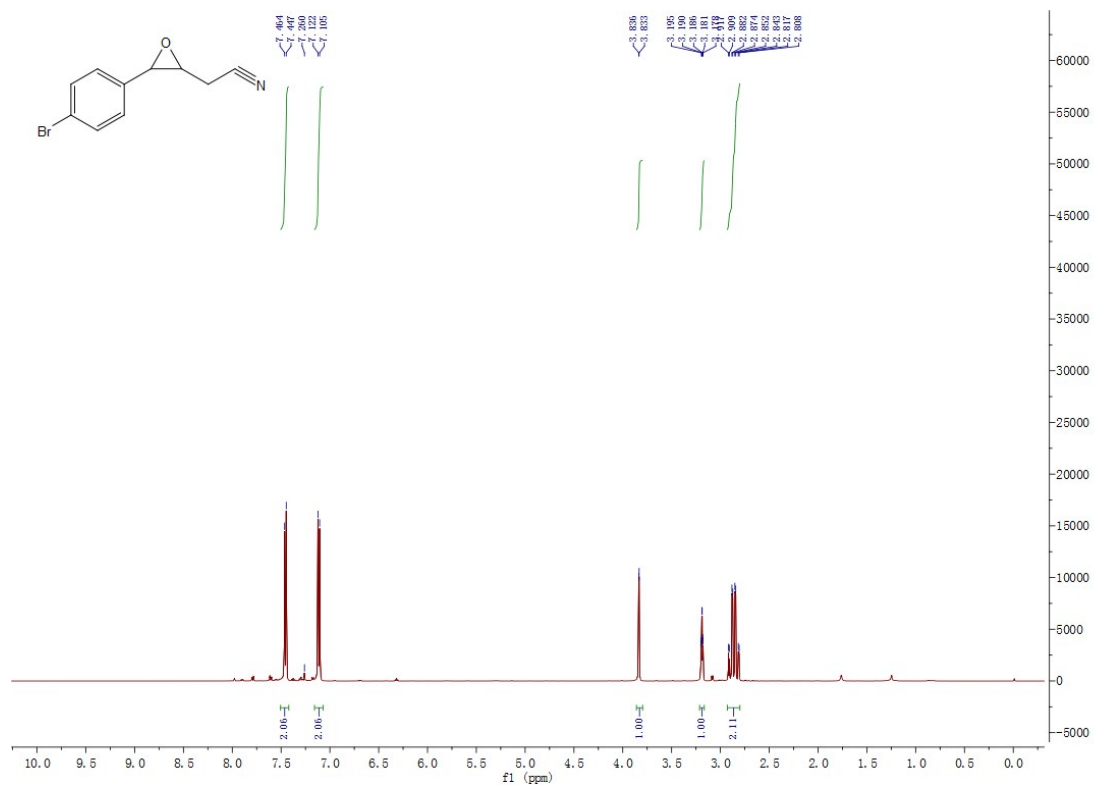


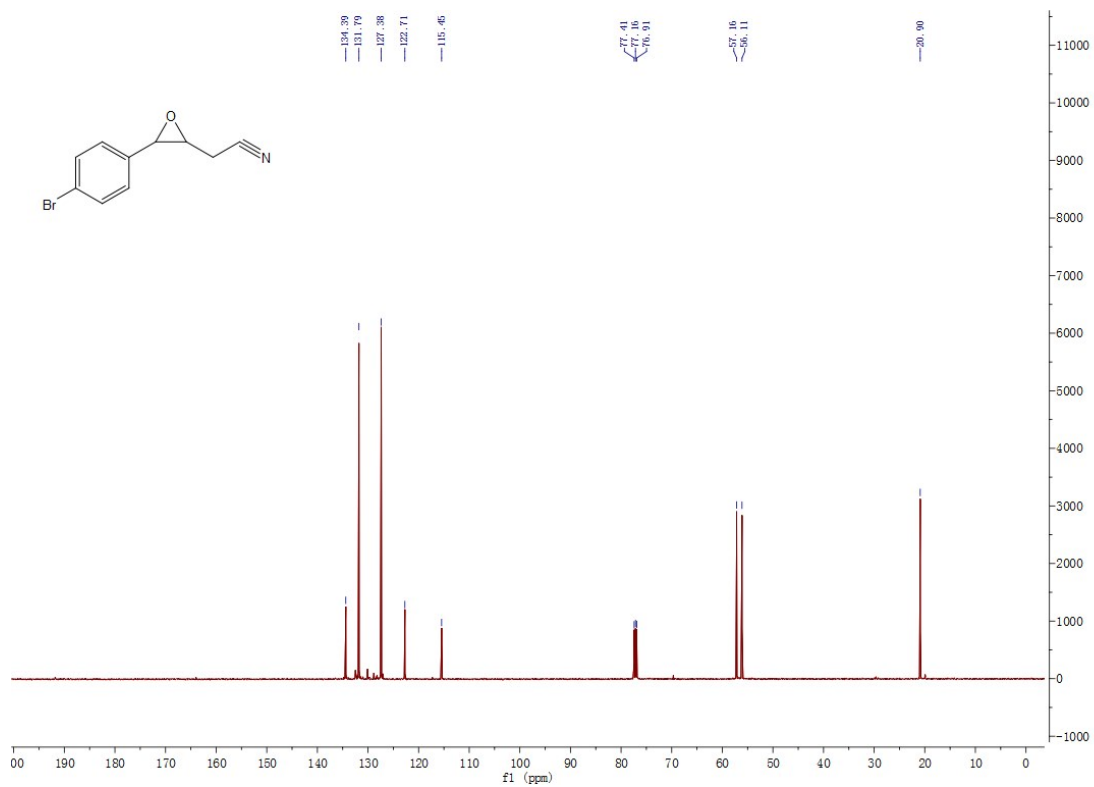
^1H NMR (500 MHz, CDCl_3) of compound **1d**



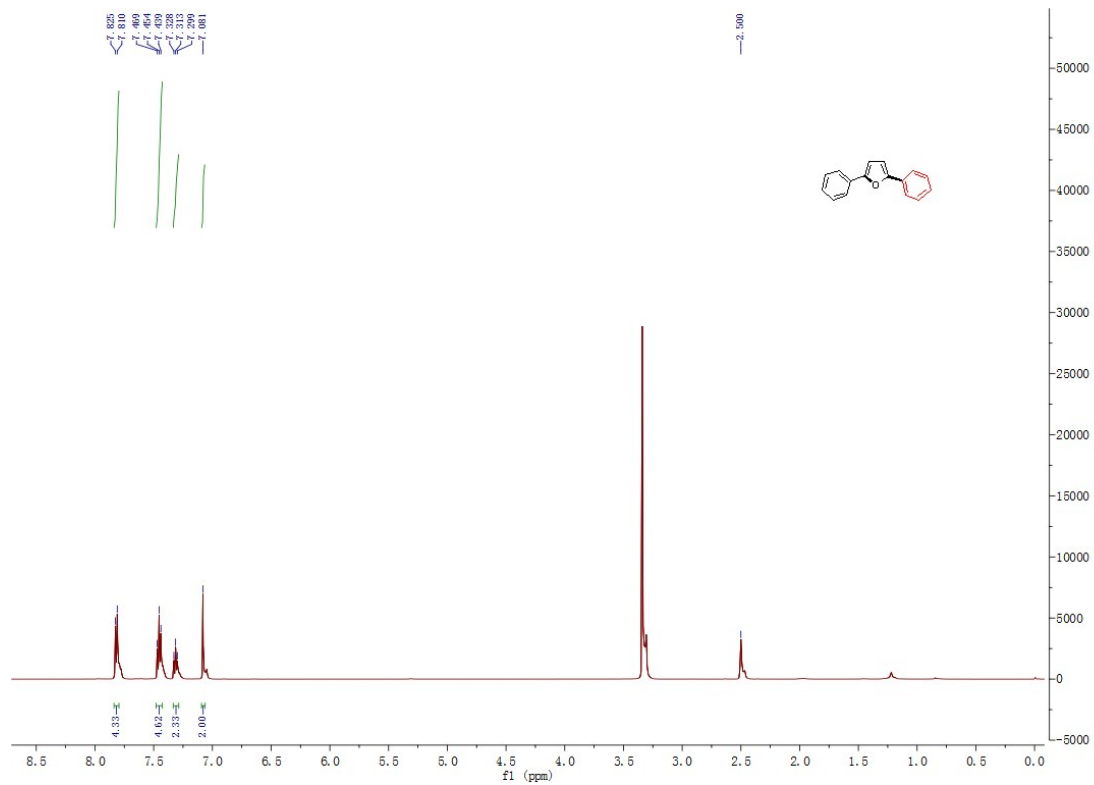


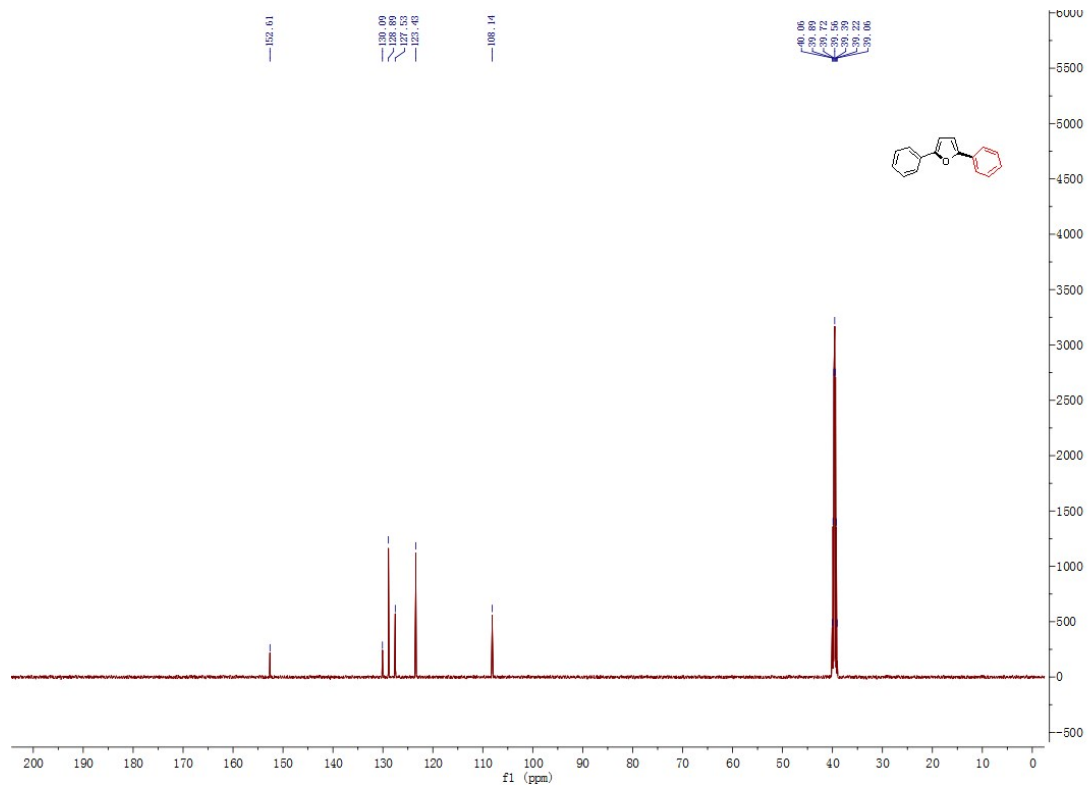
¹³C NMR (125 MHz, CDCl₃) of compound **1e'**



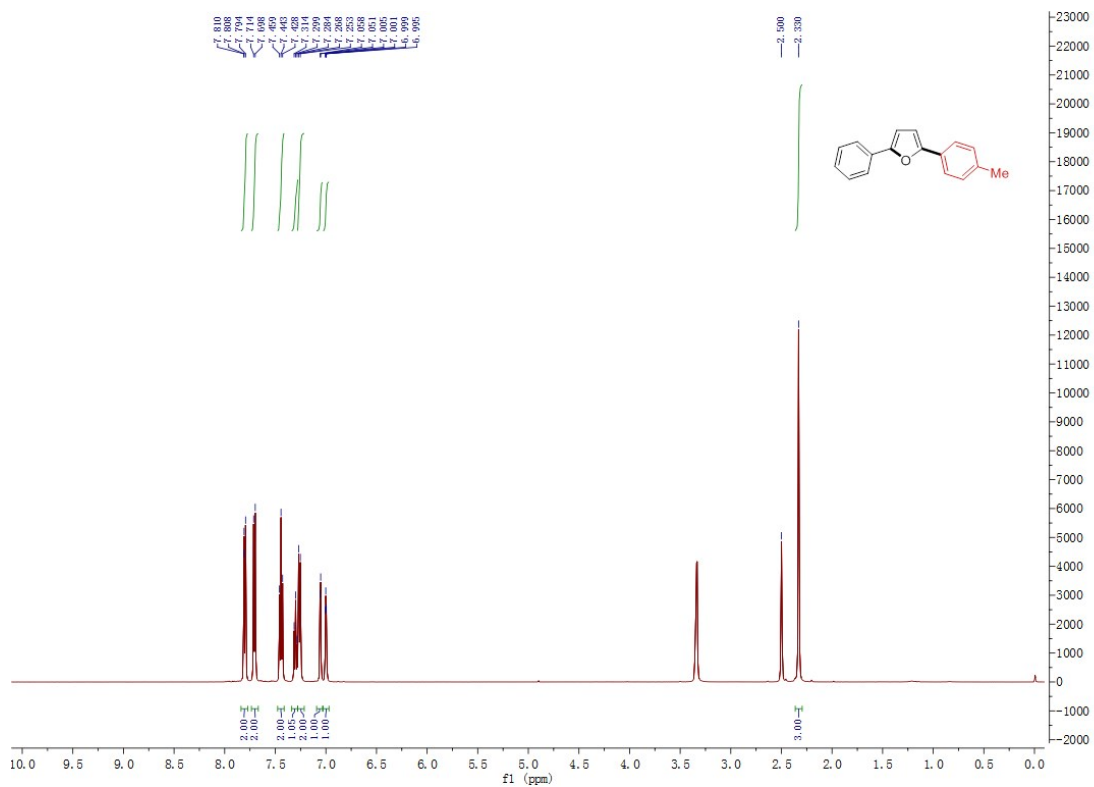


8. NMR spectra for all products

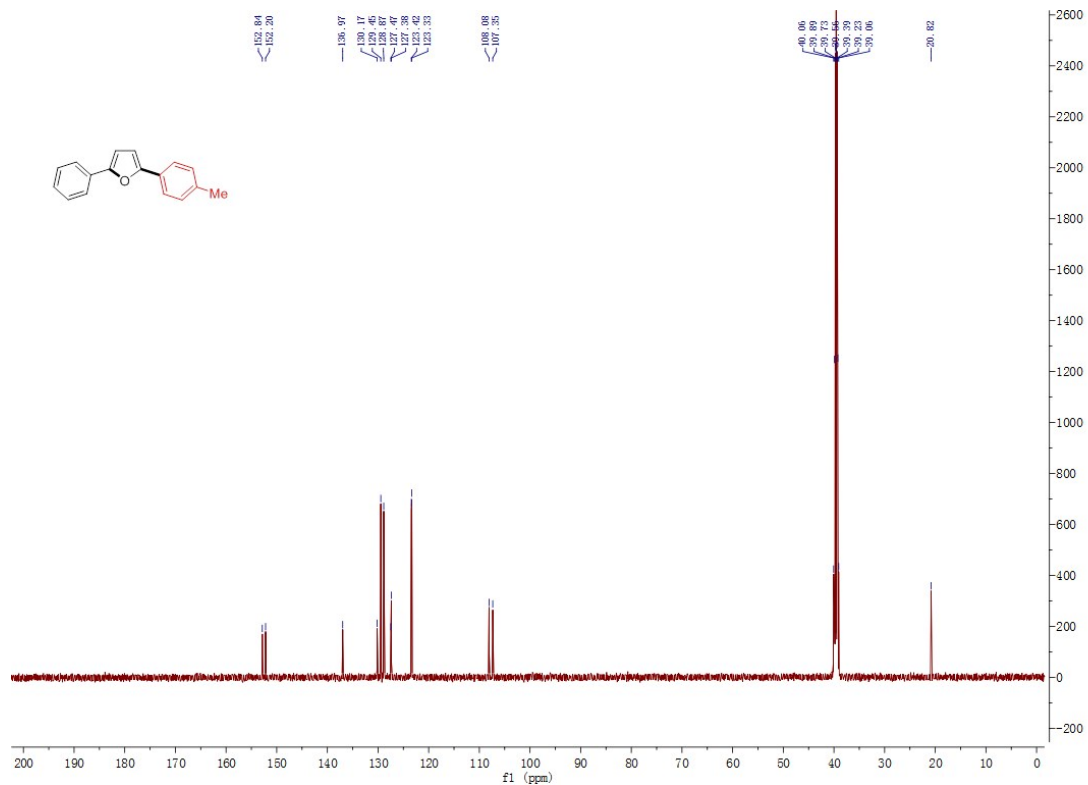




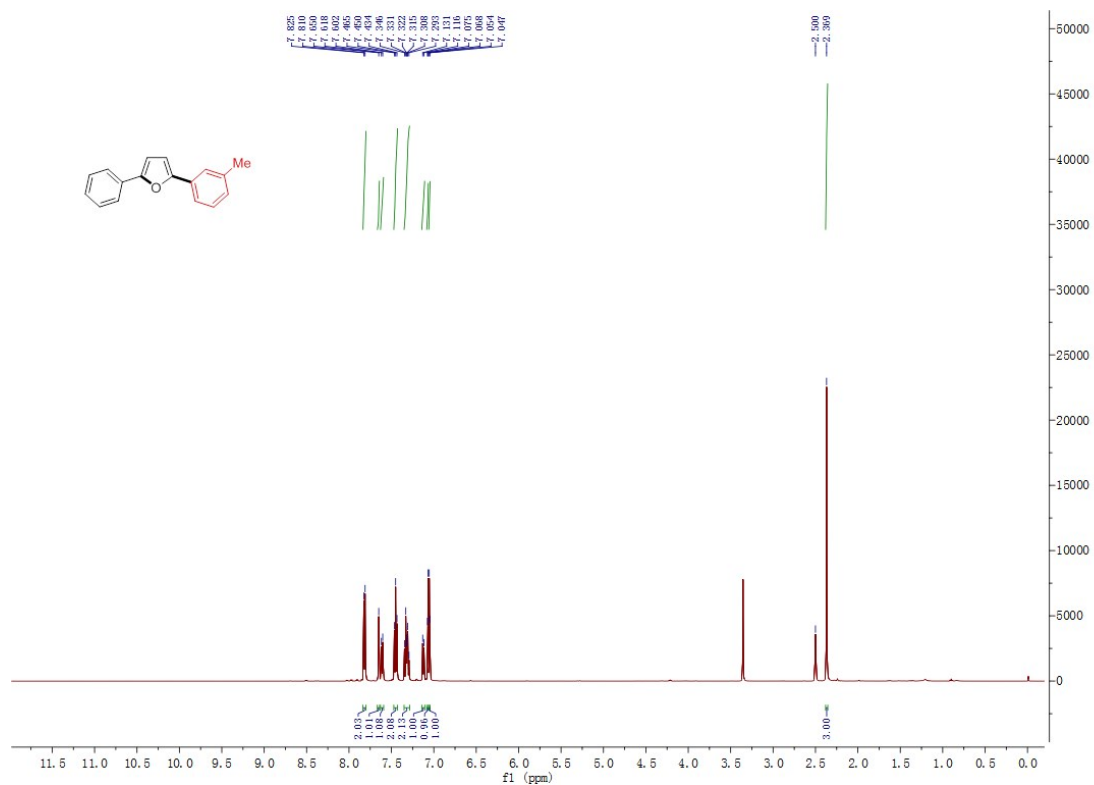
^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) of compound **3a**



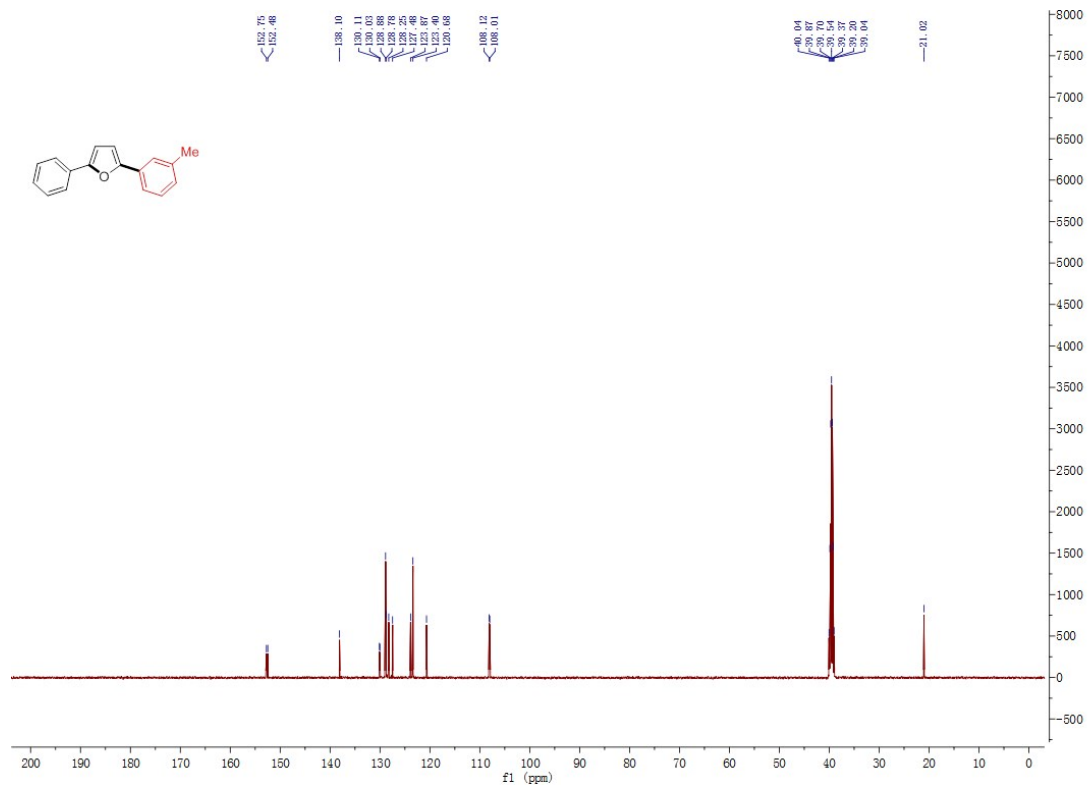
^1H NMR (500 MHz, $\text{DMSO-}d_6$) of compound **3b**



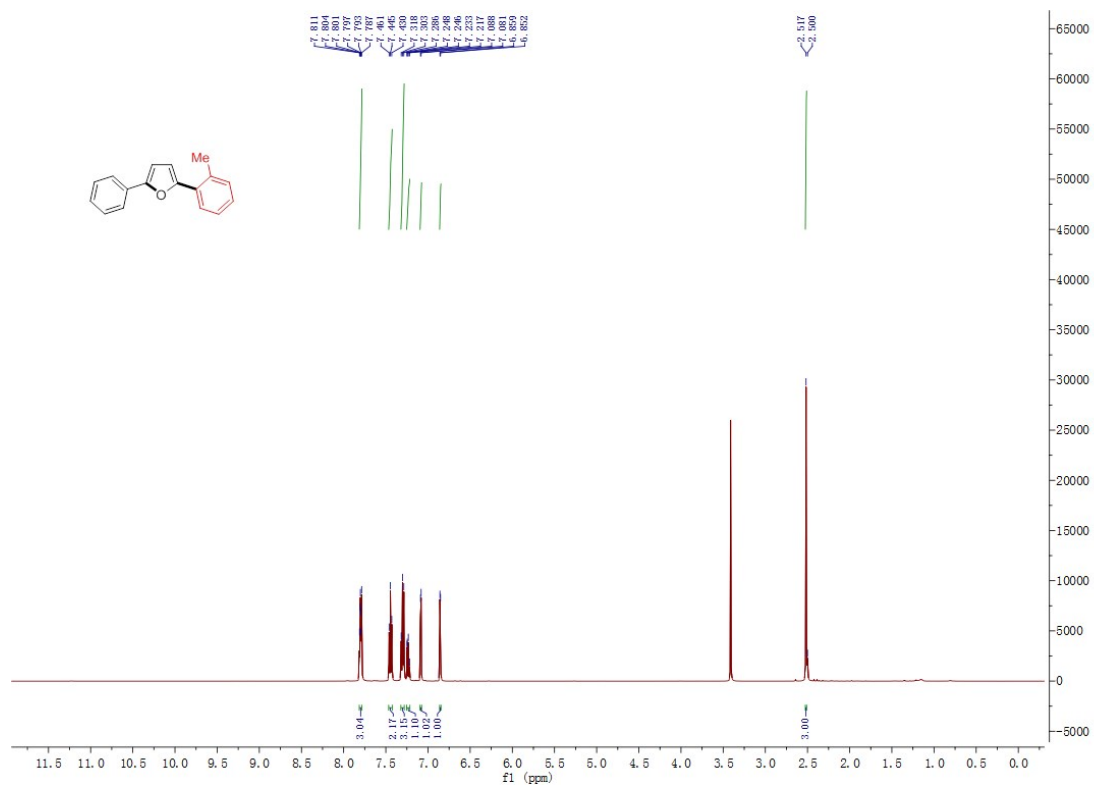
^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) of compound **3b**



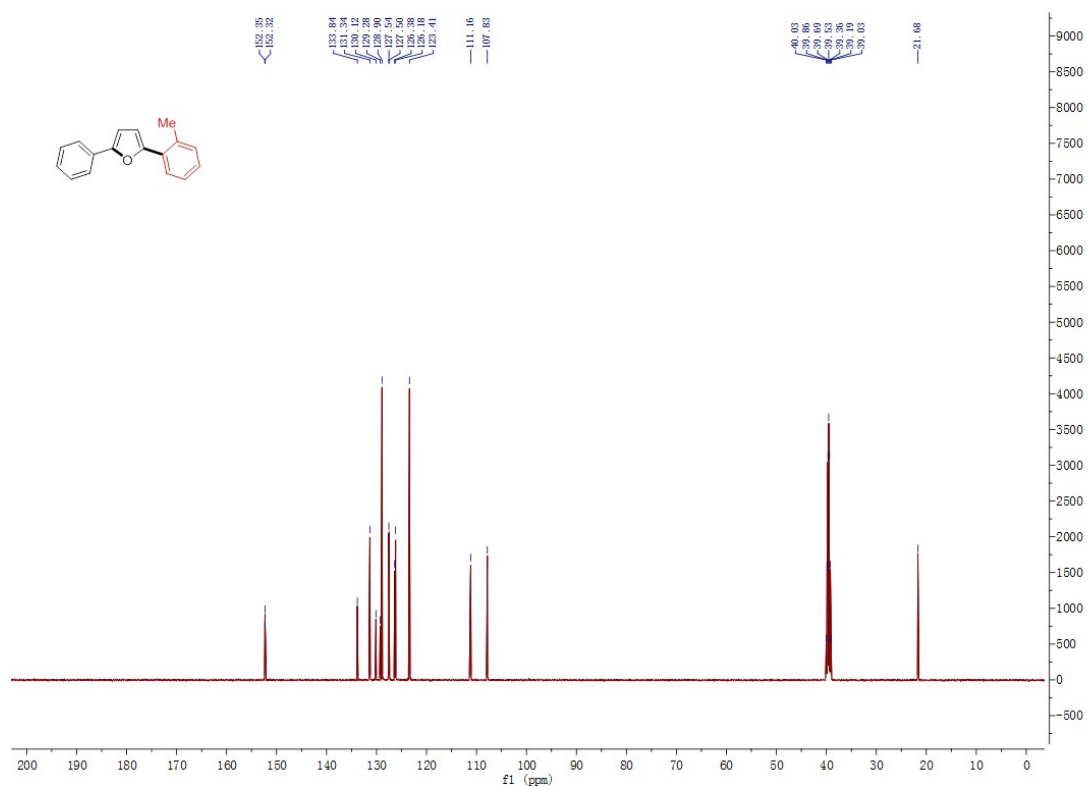
^1H NMR (500 MHz, $\text{DMSO-}d_6$) of compound **3b**



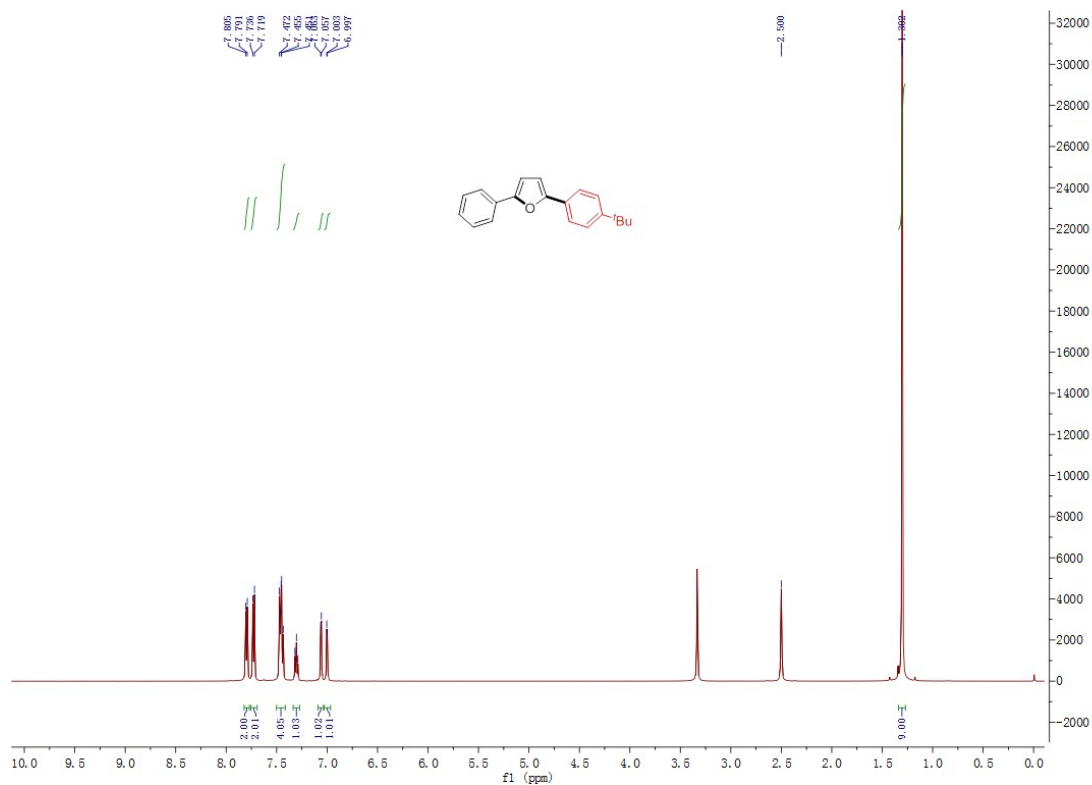
¹³C NMR (125 MHz, DMSO-*d*₆) of compound **3c**



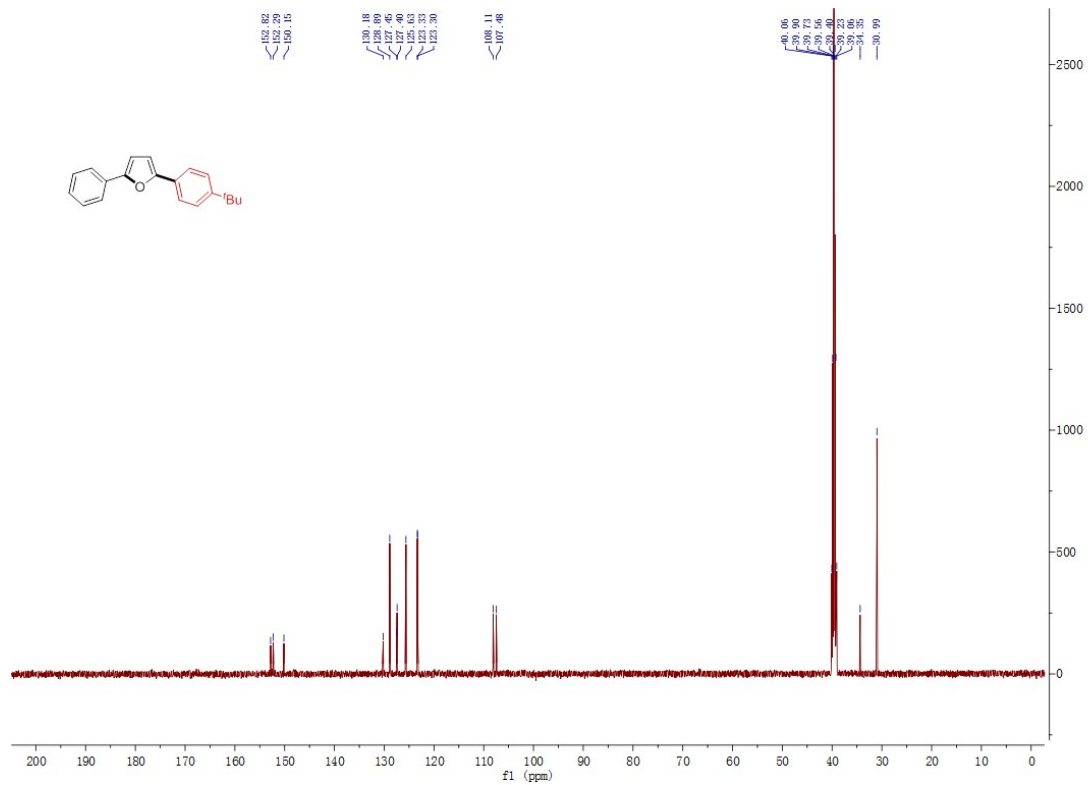
¹H NMR (500 MHz, DMSO-*d*₆) of compound **3d**



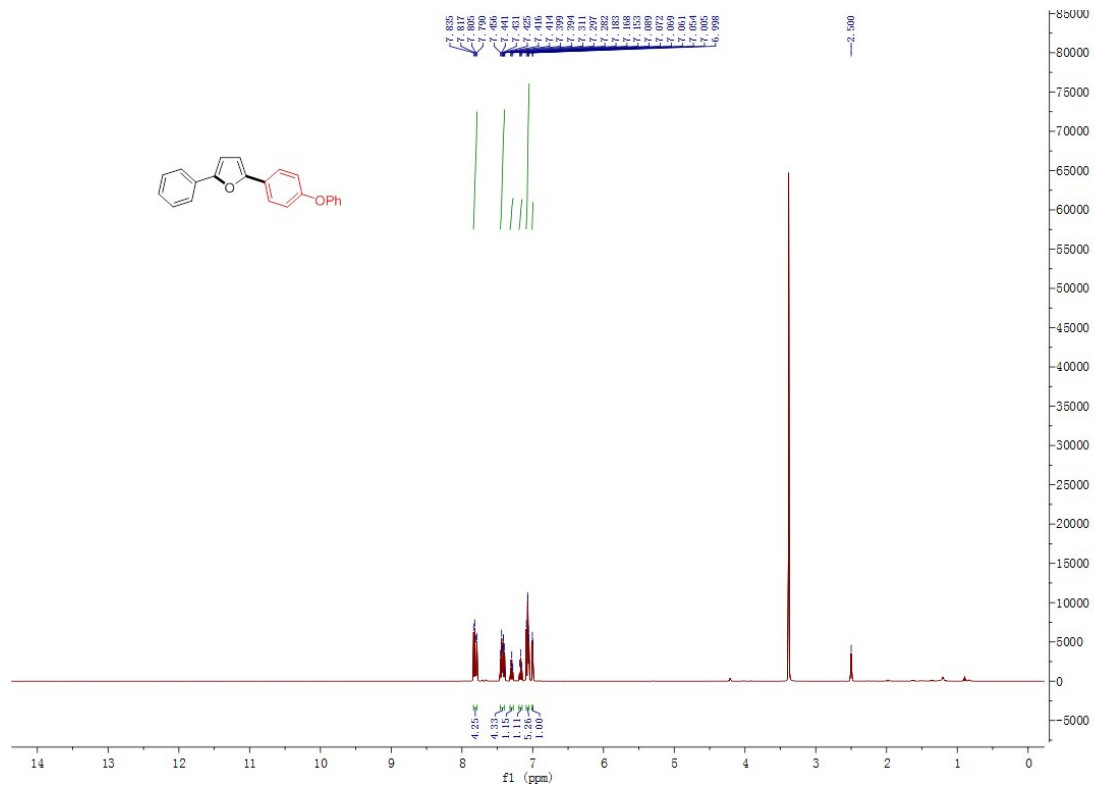
¹³C NMR (125 MHz, DMSO-*d*₆) of compound 3d



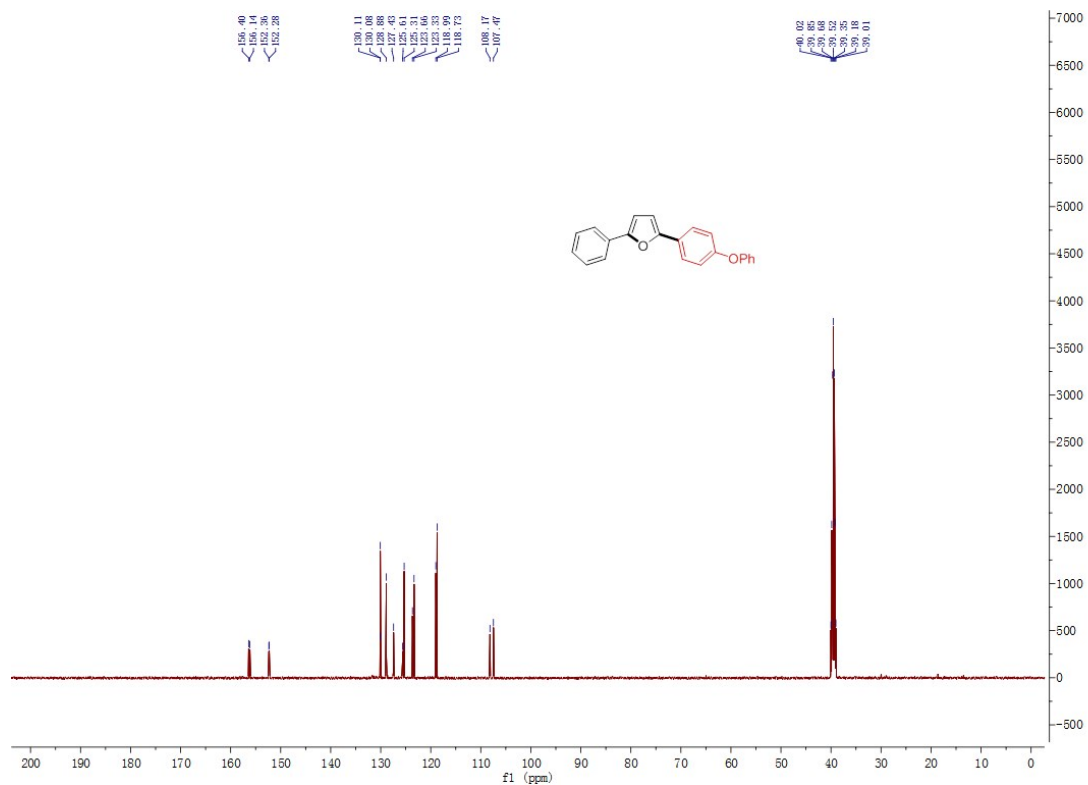
¹H NMR (500 MHz, DMSO-*d*₆) of compound 3e



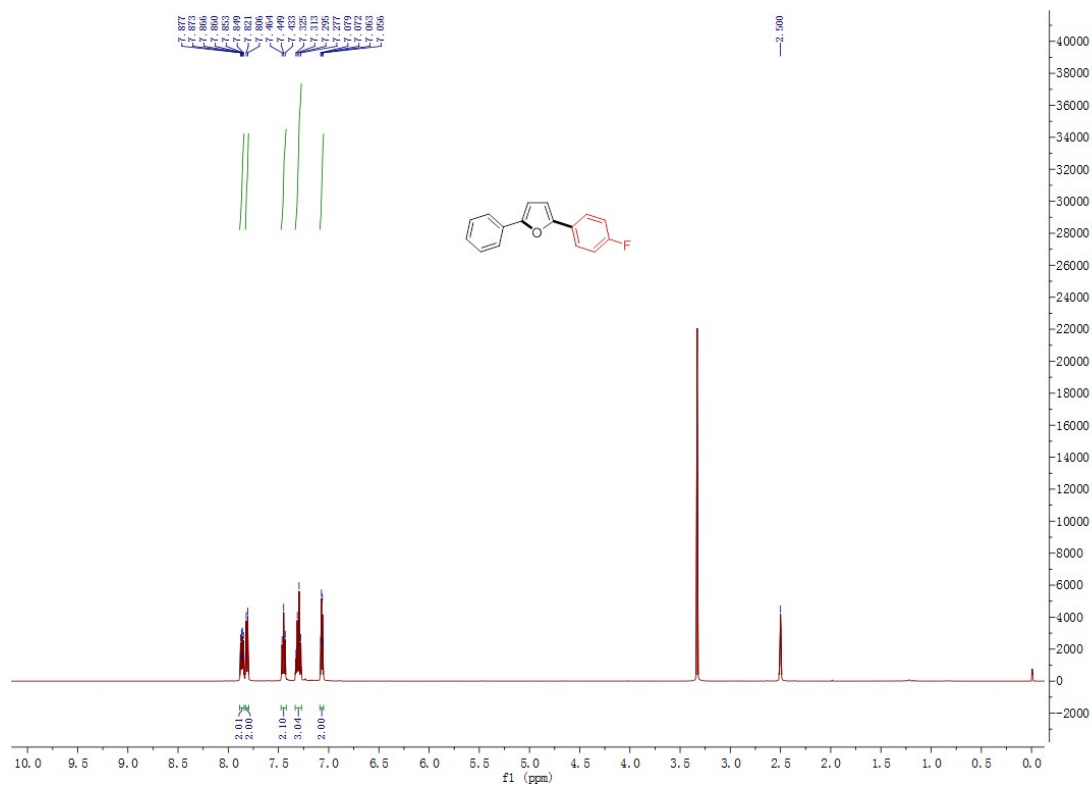
^{13}C NMR (125 MHz, DMSO- d_6) of compound 3e



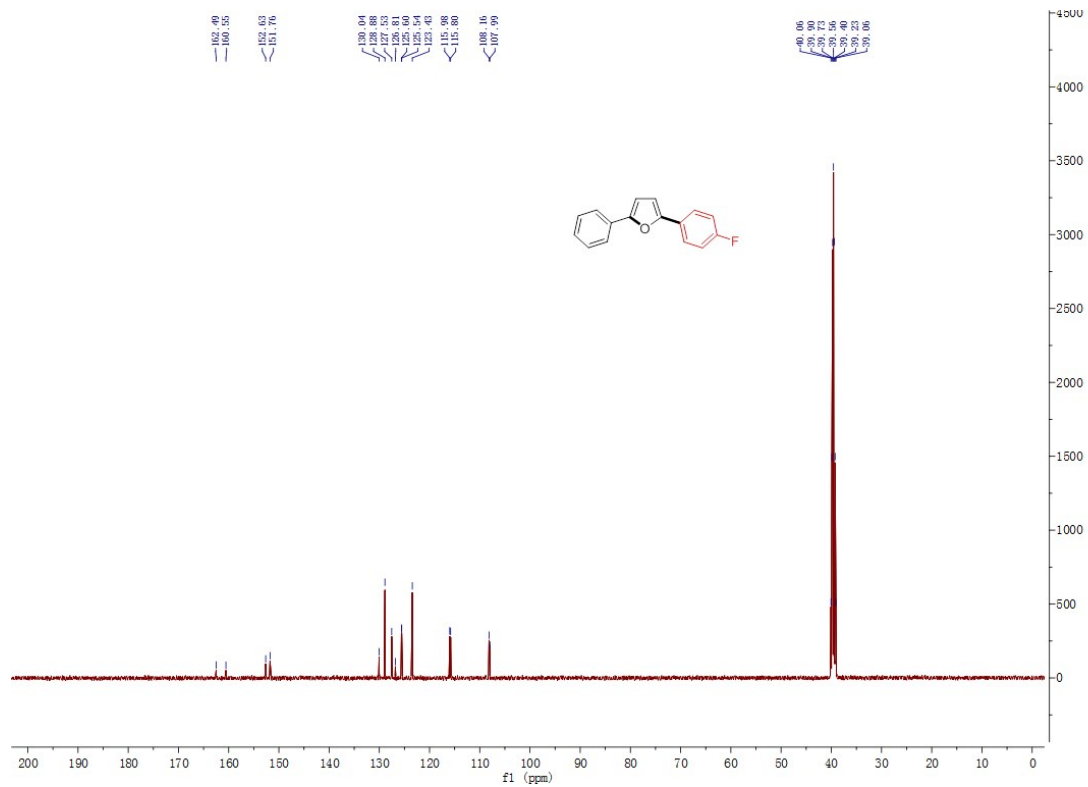
^1H NMR (500 MHz, DMSO- d_6) of compound 3f



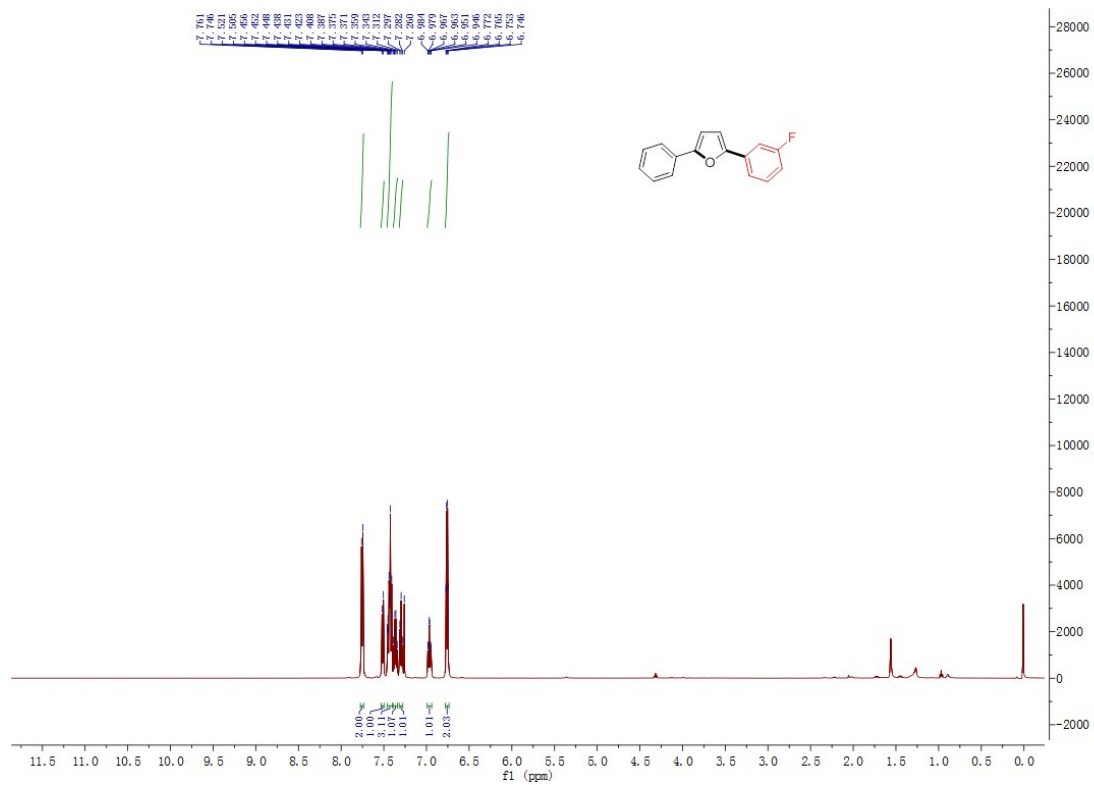
^{13}C NMR (125 MHz, DMSO- d_6) of compound **3f**

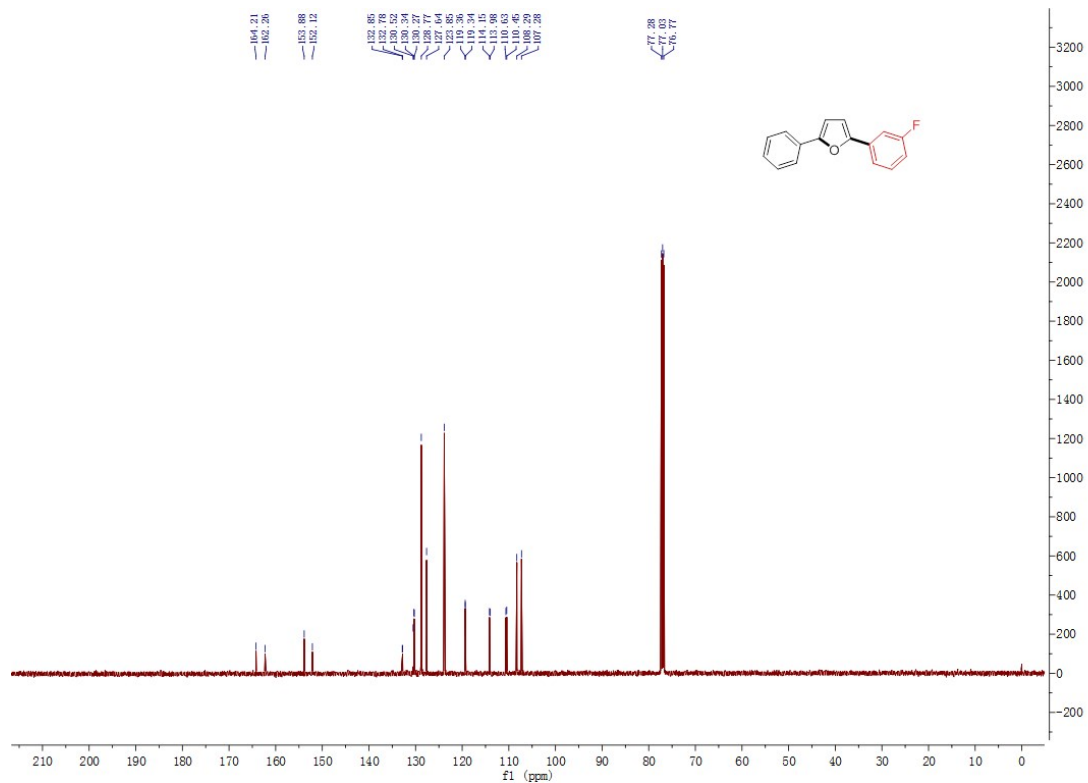


^1H NMR (500 MHz, DMSO- d_6) of compound **3g**

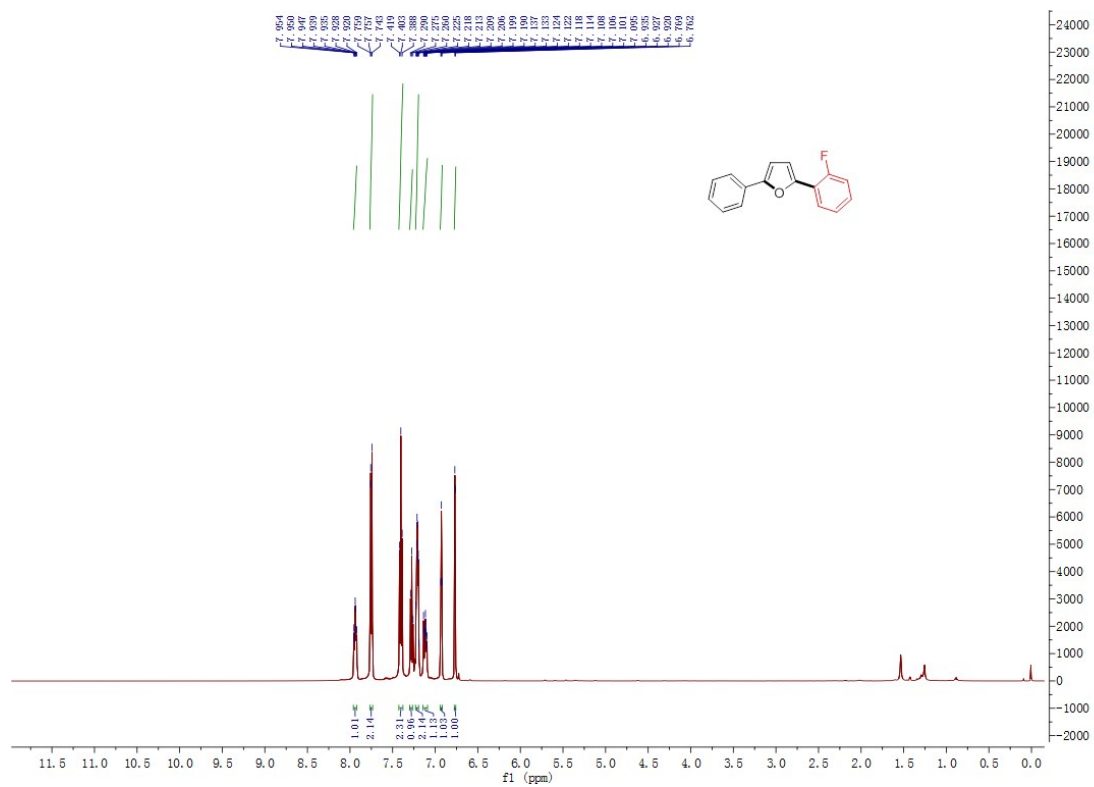


¹³C NMR (125 MHz, DMSO-*d*₆) of compound **3g**

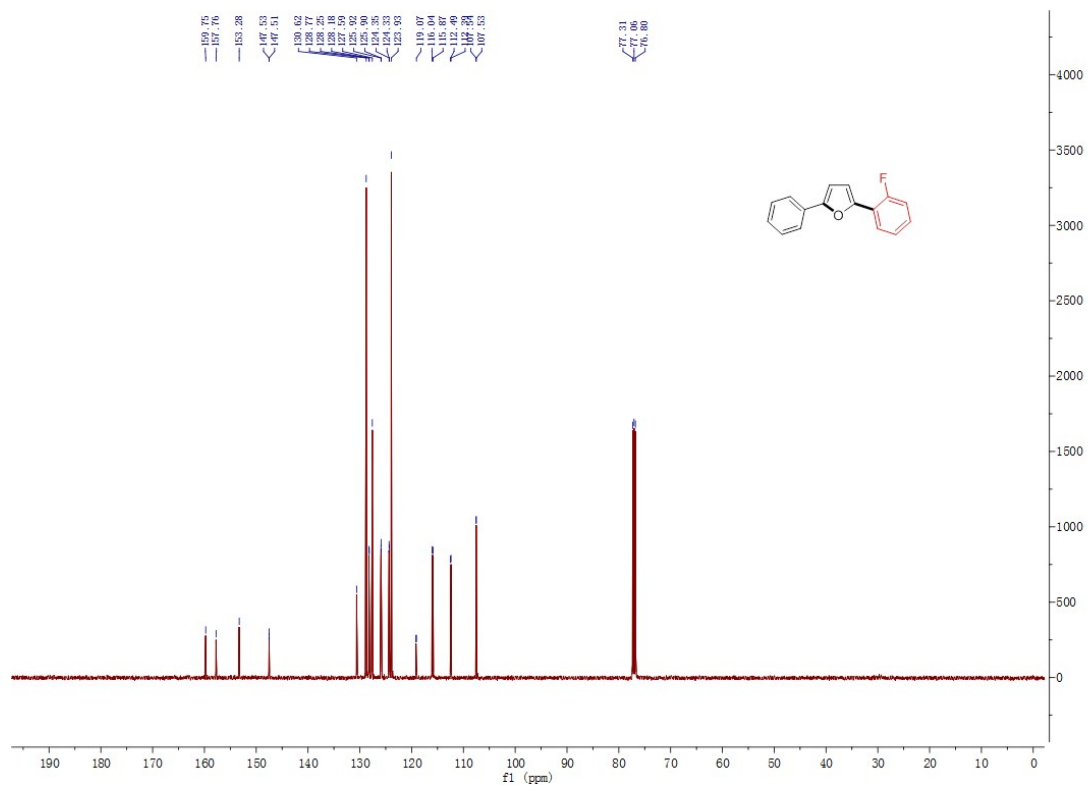




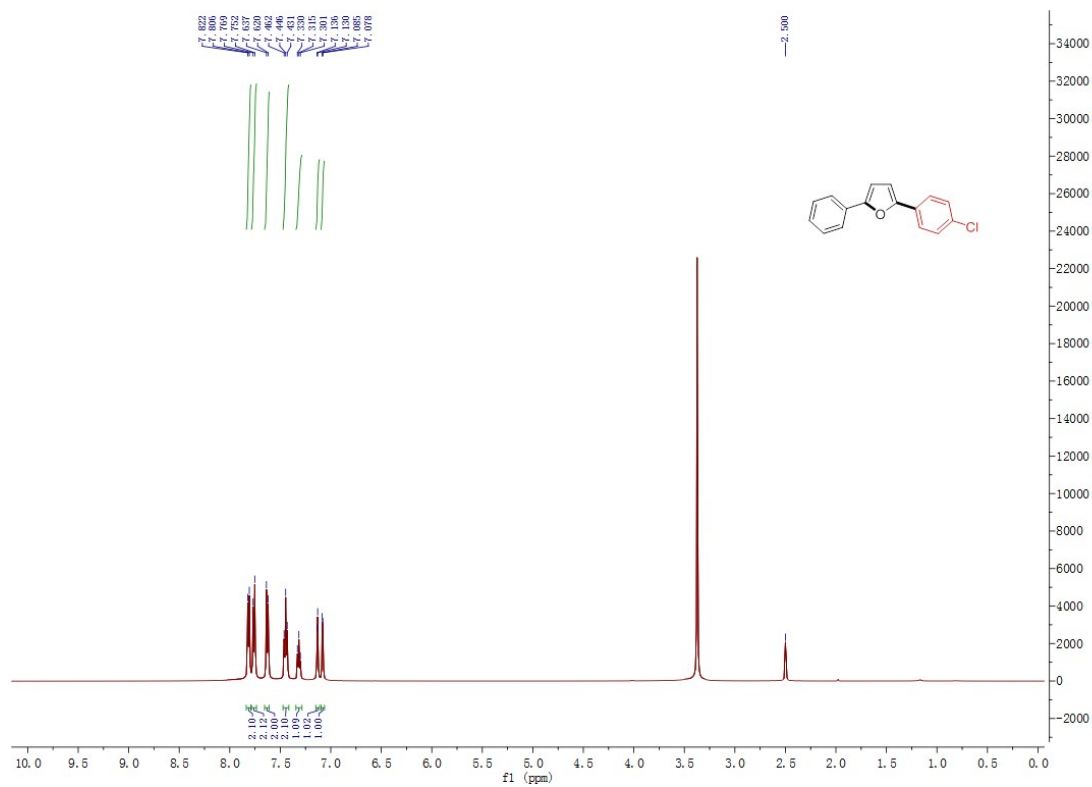
¹³C NMR (125 MHz, CDCl₃) of compound **3h**



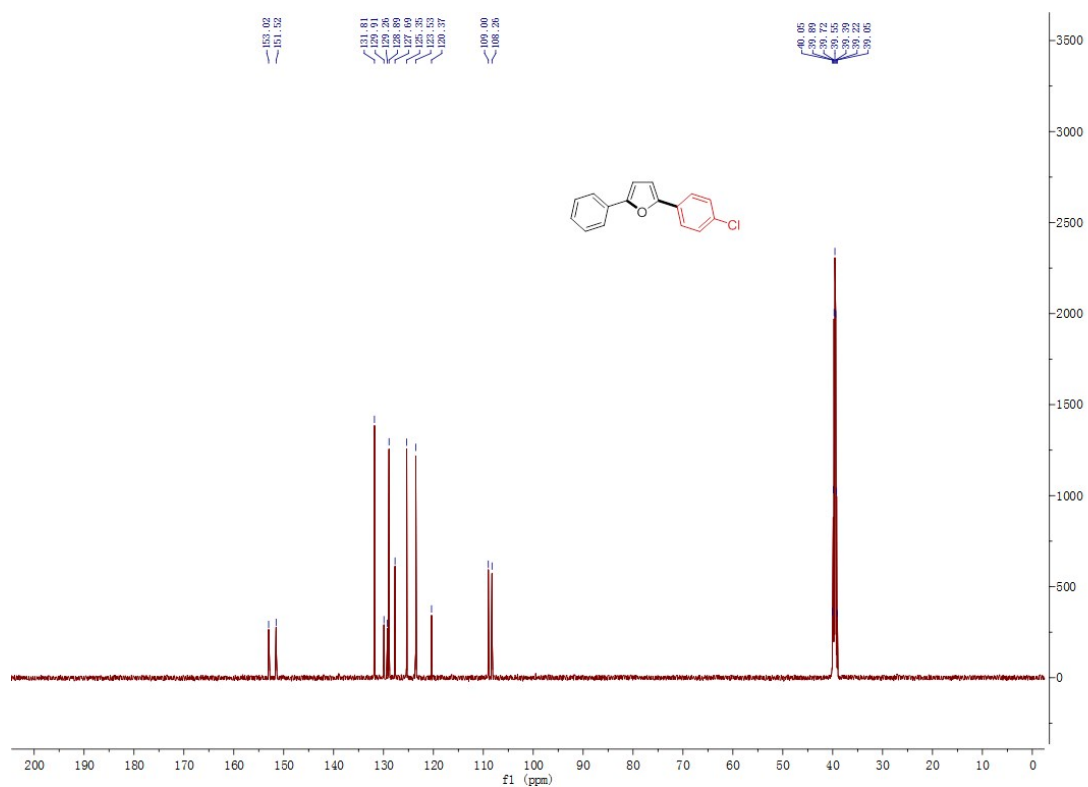
¹H NMR (500 MHz, CDCl₃) of compound **3i**



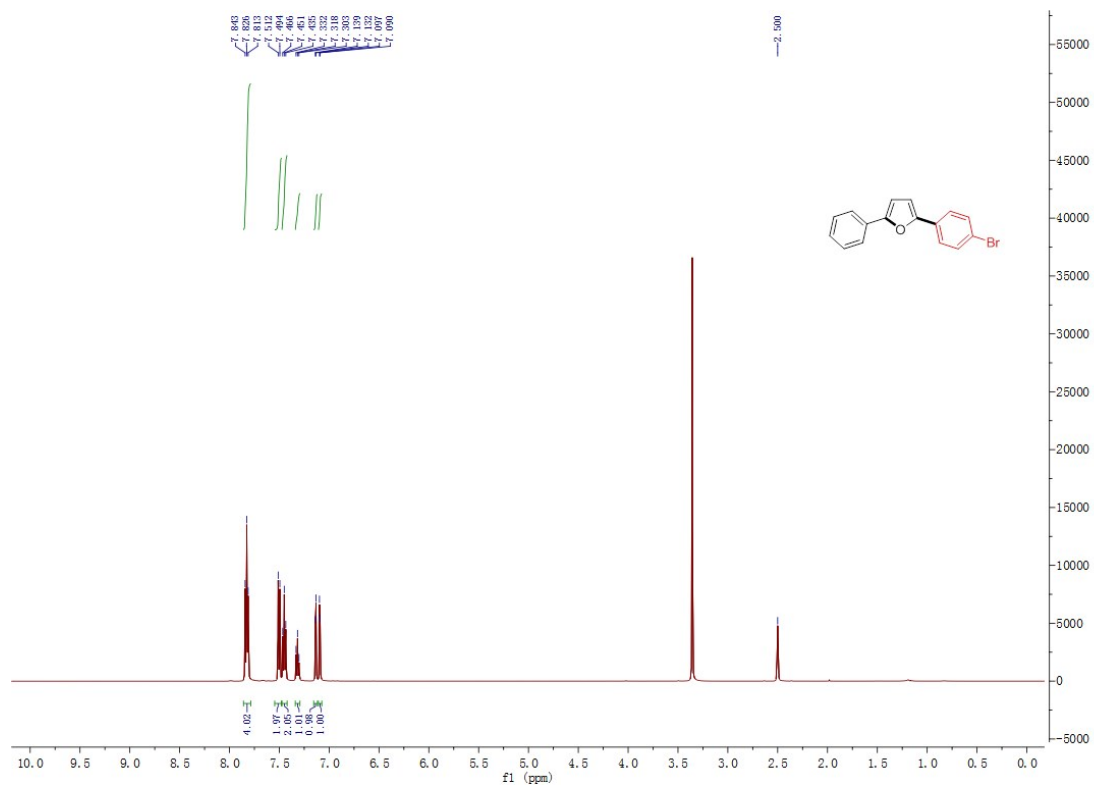
^{13}C NMR (125 MHz, CDCl_3) of compound **3i**



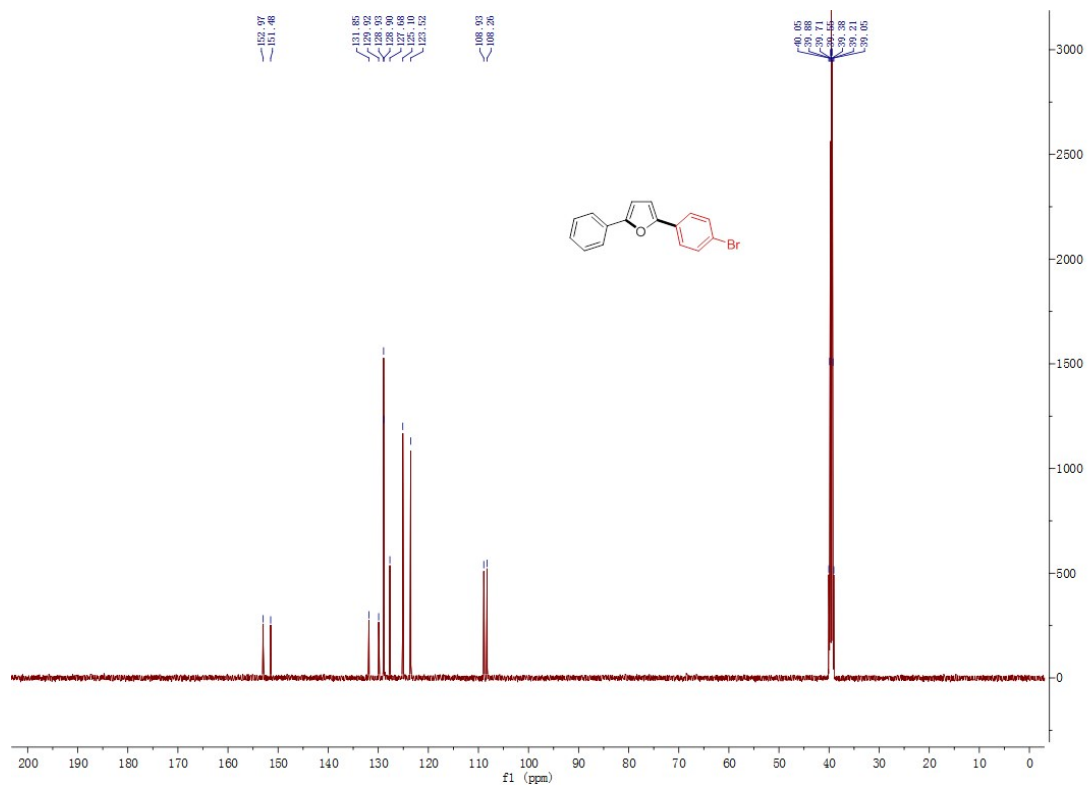
^1H NMR (500 MHz, $\text{DMSO}-d_6$) of compound **3j**



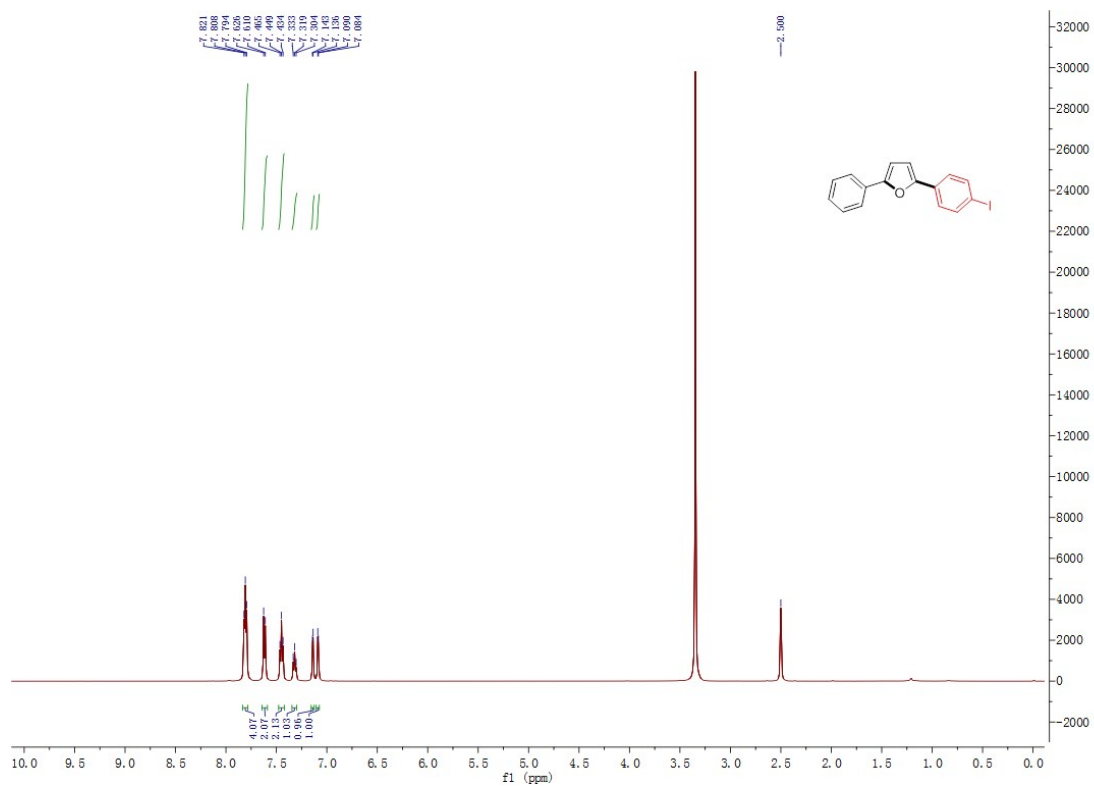
^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) of compound **3j**



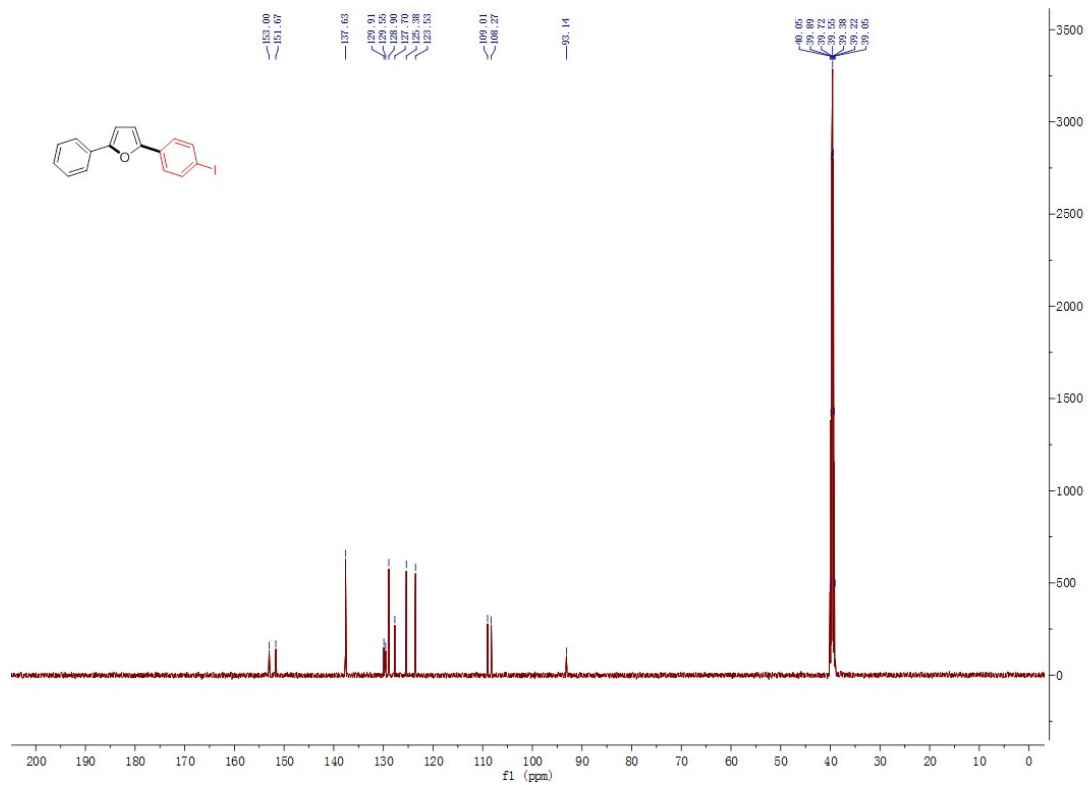
^1H NMR (500 MHz, $\text{DMSO-}d_6$) of compound **3k**



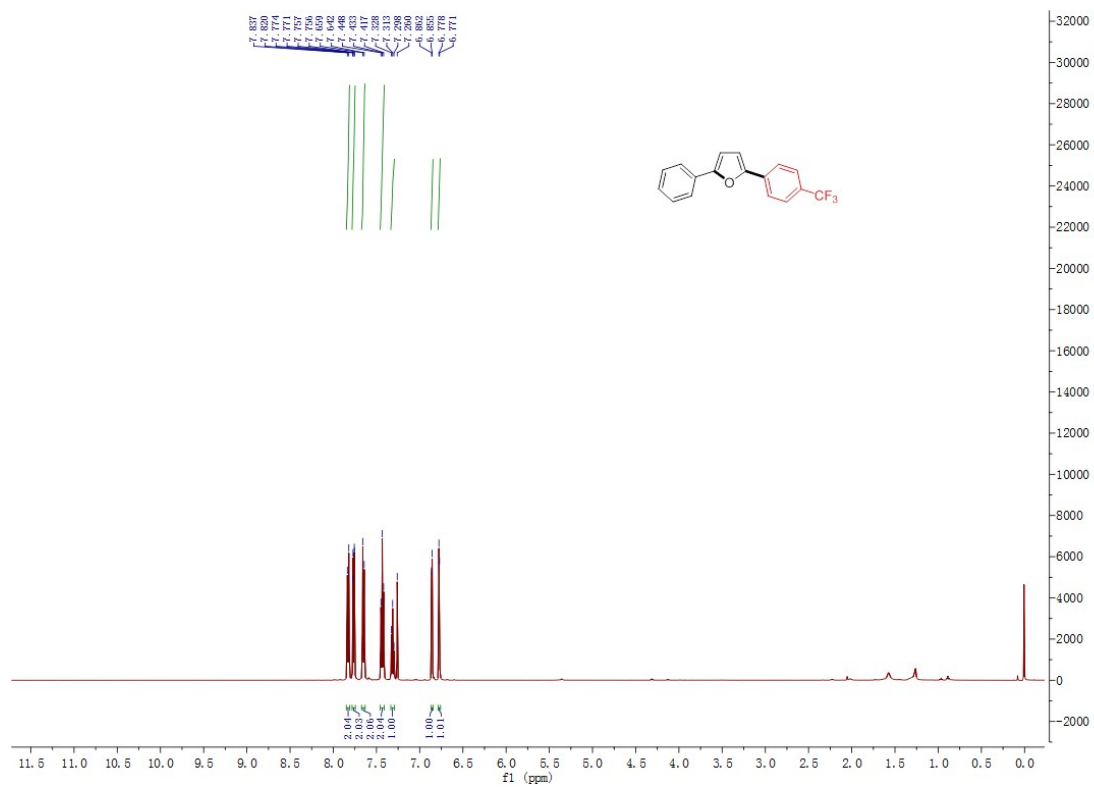
^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) of compound **3k**



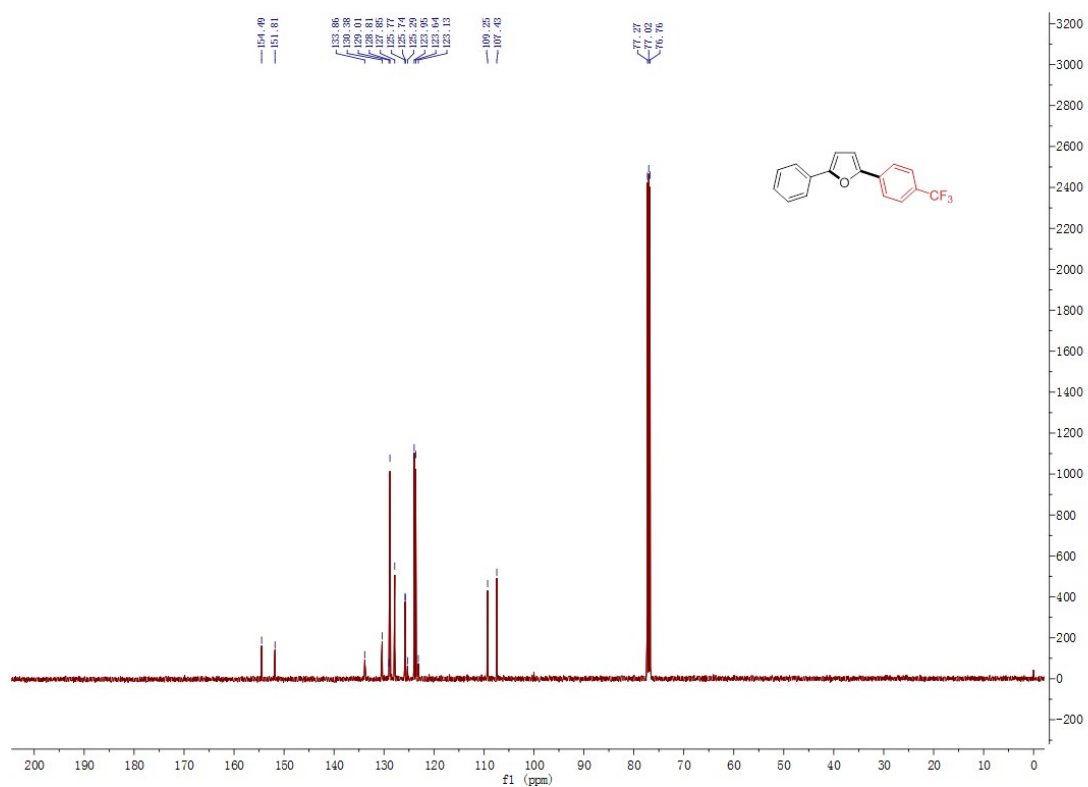
^1H NMR (500 MHz, $\text{DMSO-}d_6$) of compound **3l**



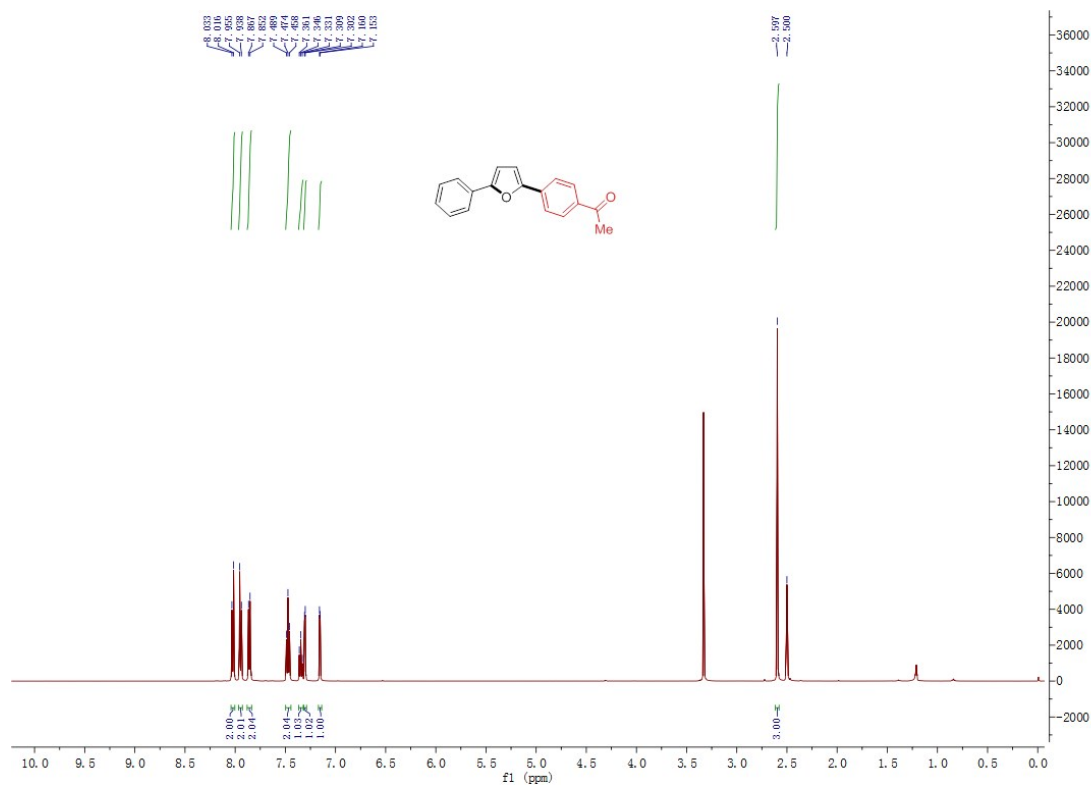
^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) of compound 31



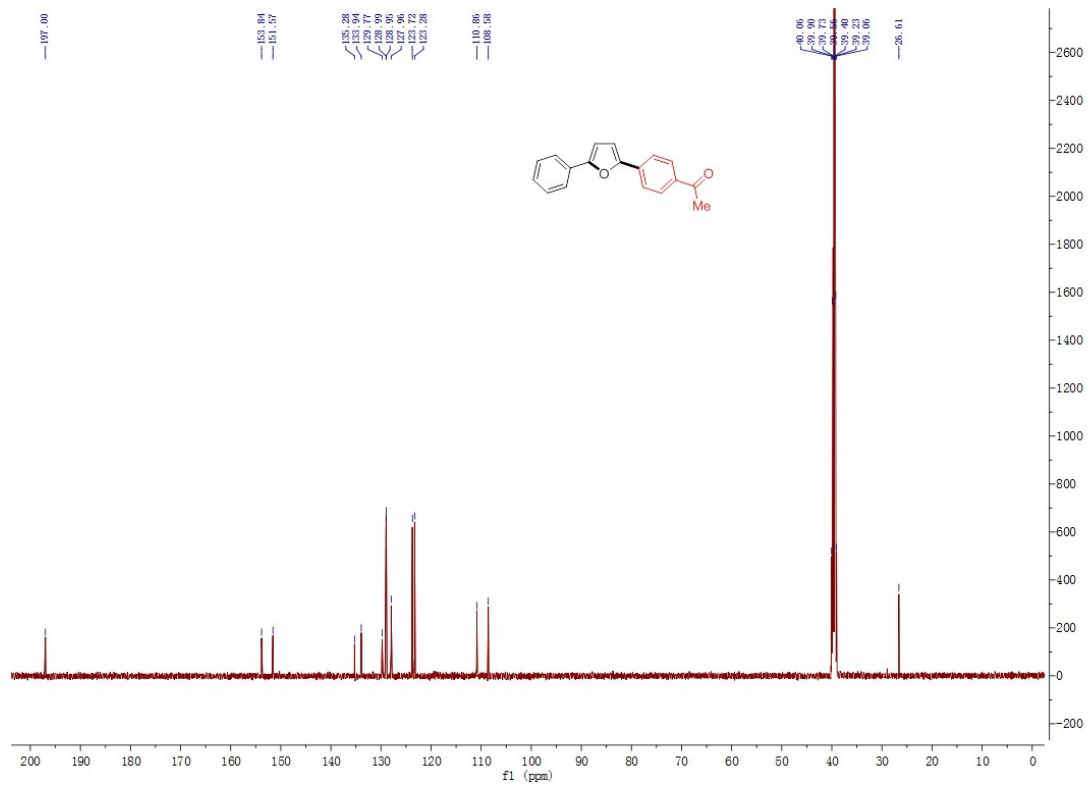
^1H NMR (500 MHz, CDCl_3) of compound 3m



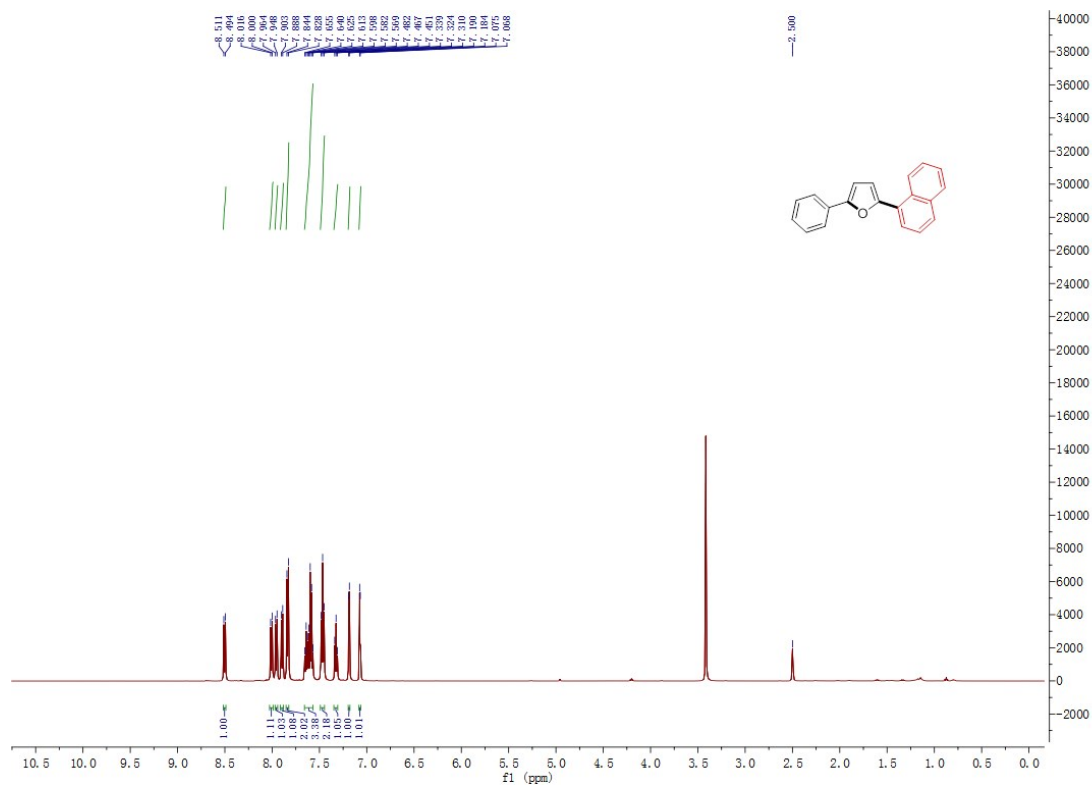
¹³C NMR (125 MHz, CDCl₃) of compound **3m**



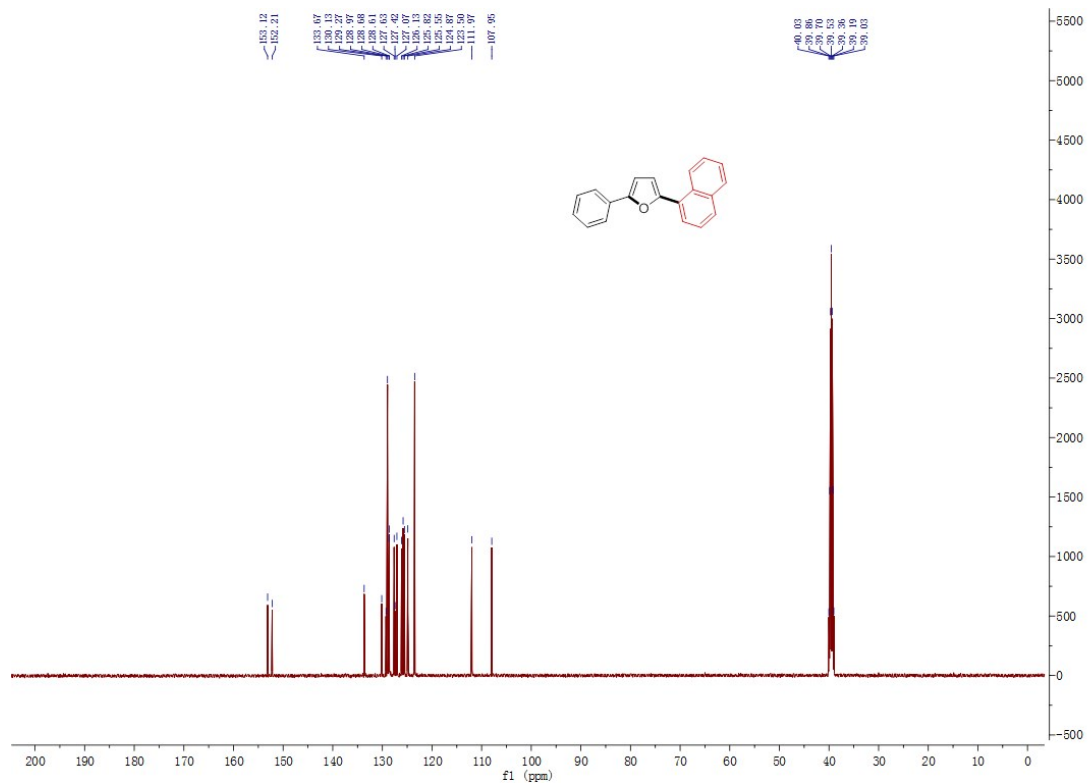
¹H NMR (500 MHz, DMSO-*d*₆) of compound **3n**

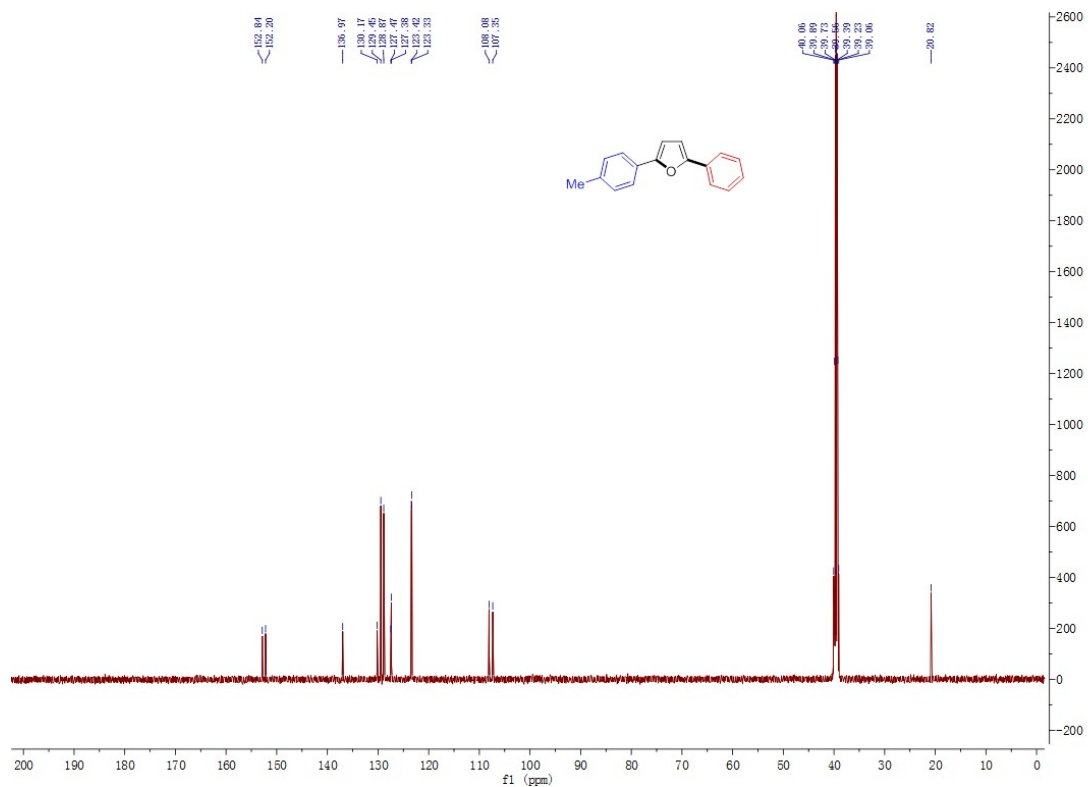


^{13}C NMR (125 MHz, DMSO- d_6) of compound **3n**

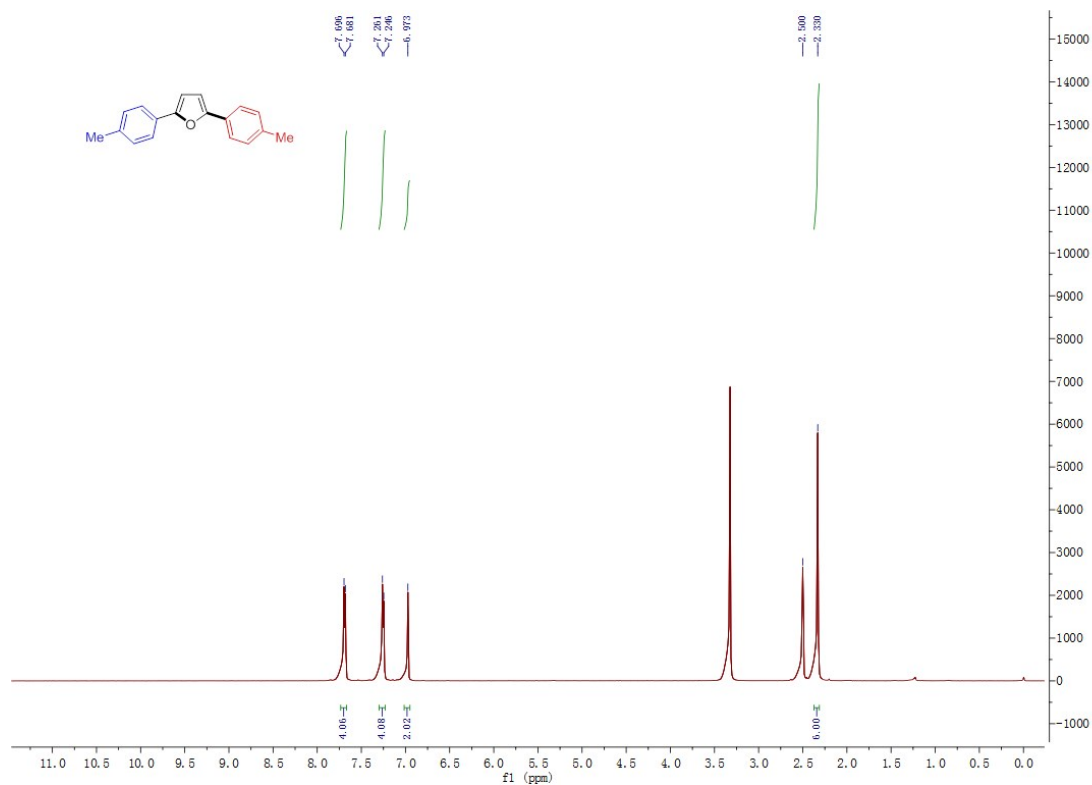


^1H NMR (500 MHz, DMSO- d_6) of compound **3o**

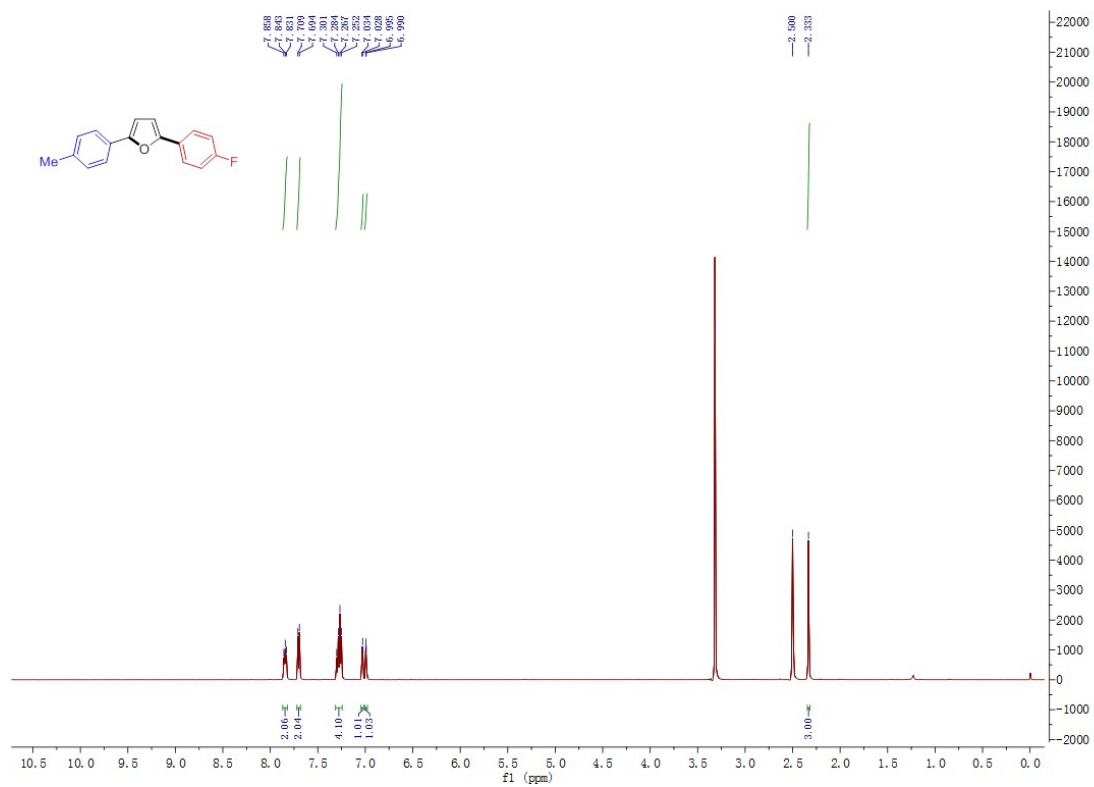
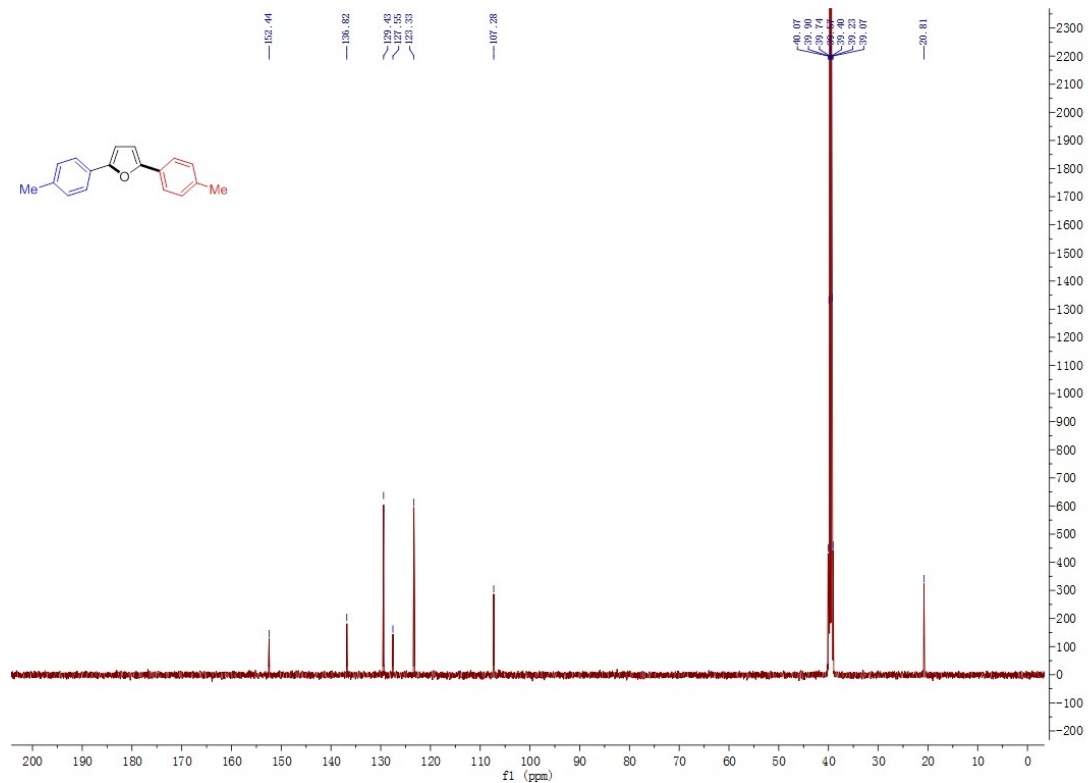


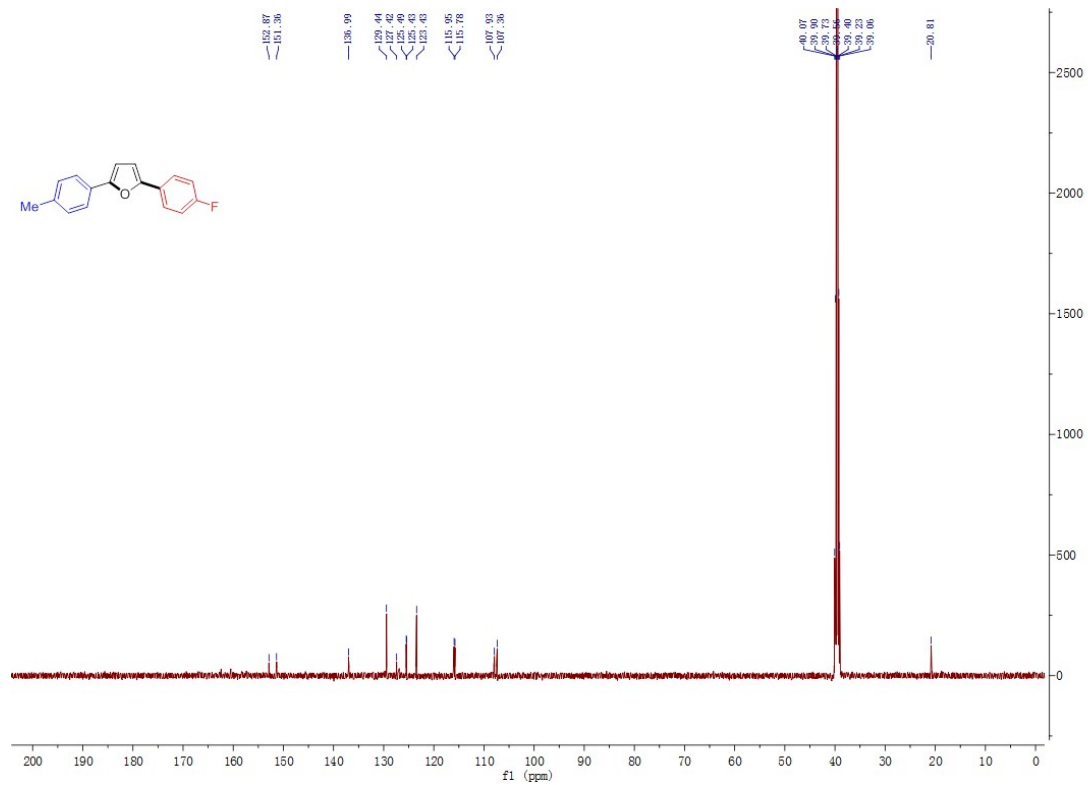


^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) of compound **3p**

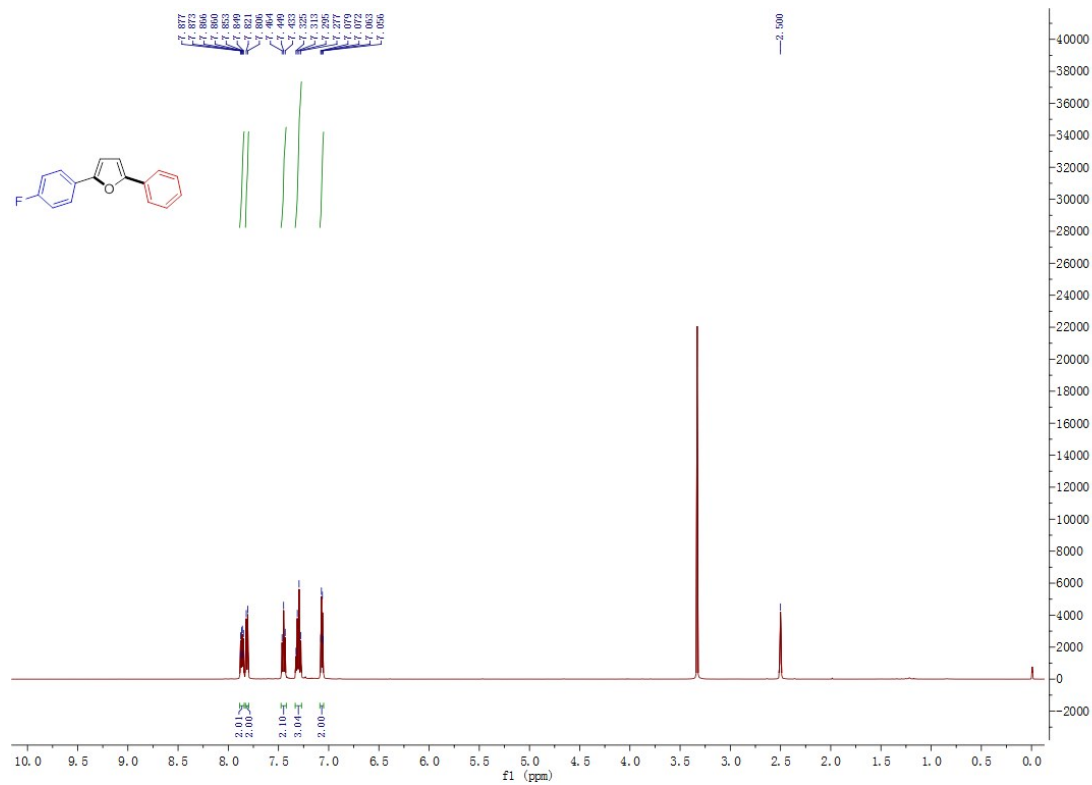


^1H NMR (500 MHz, $\text{DMSO-}d_6$) of compound **3q**

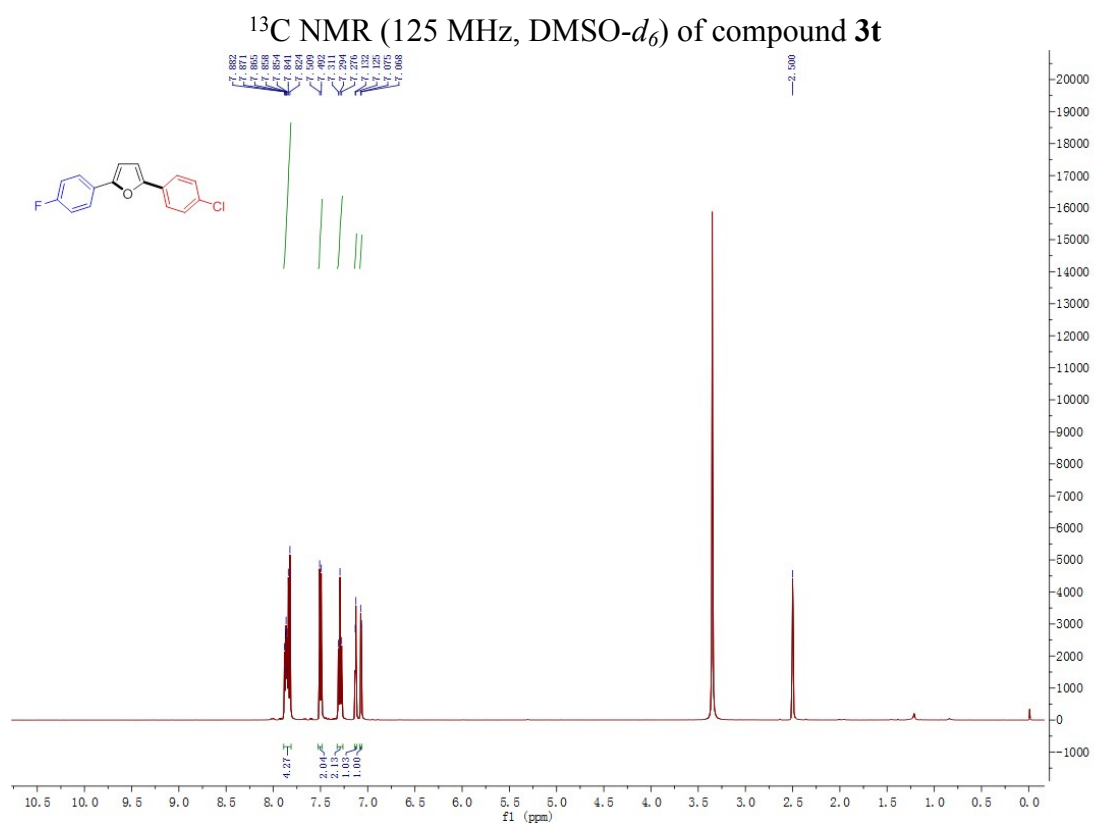
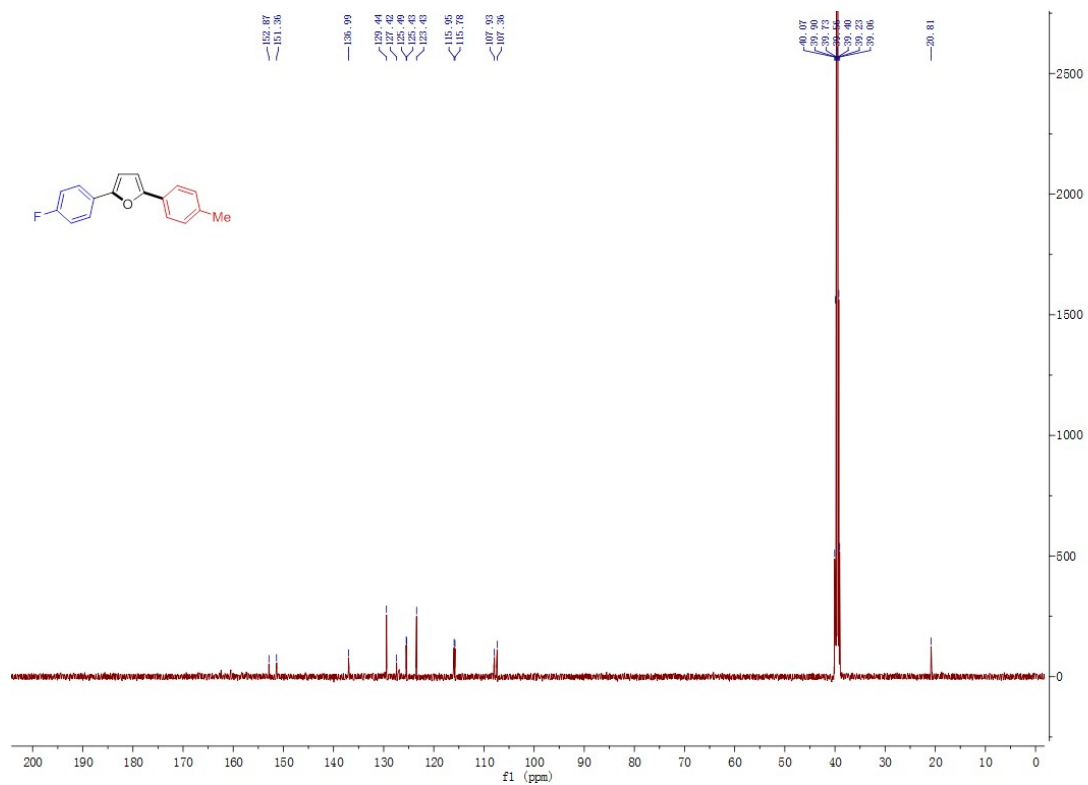




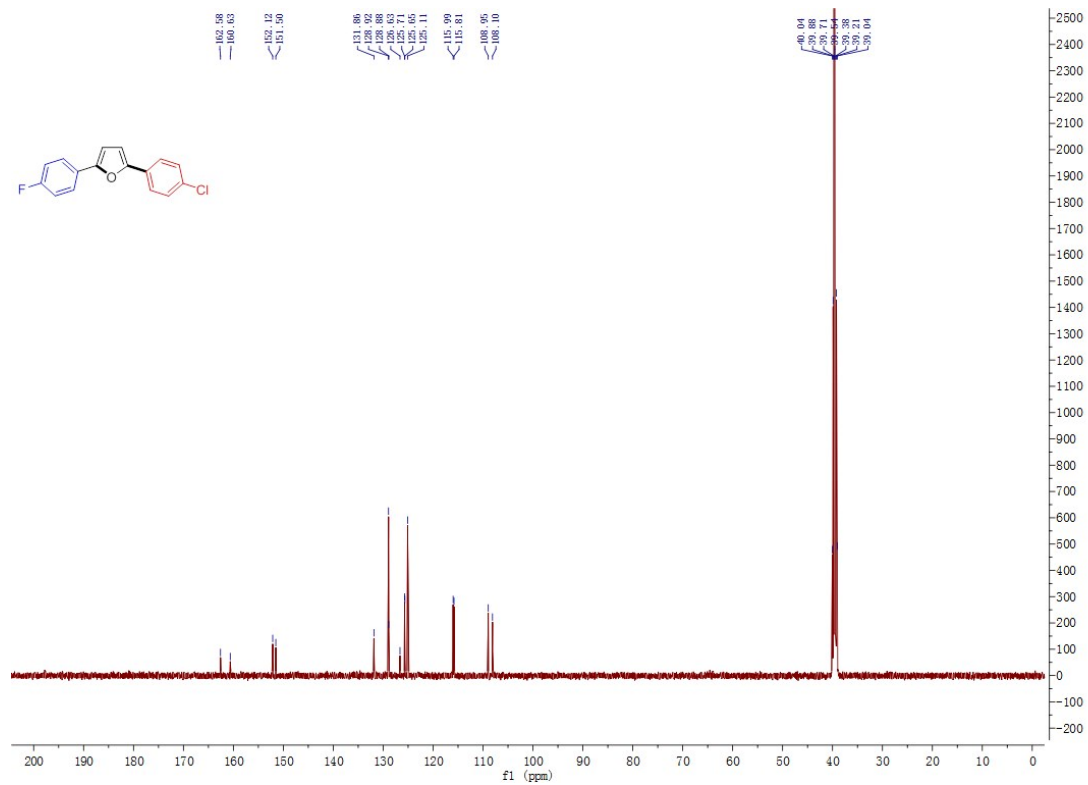
¹³C NMR (125 MHz, DMSO-*d*₆) of compound 3r



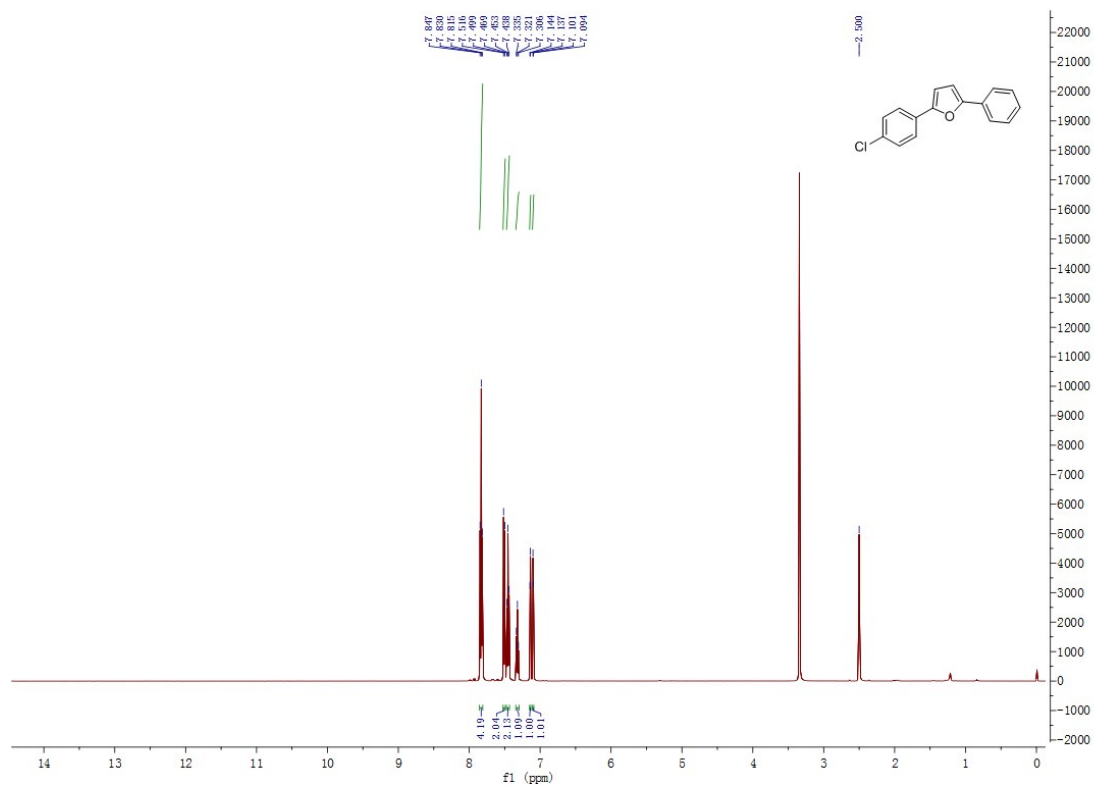
¹H NMR (500 MHz, DMSO-*d*₆) of compound 3s



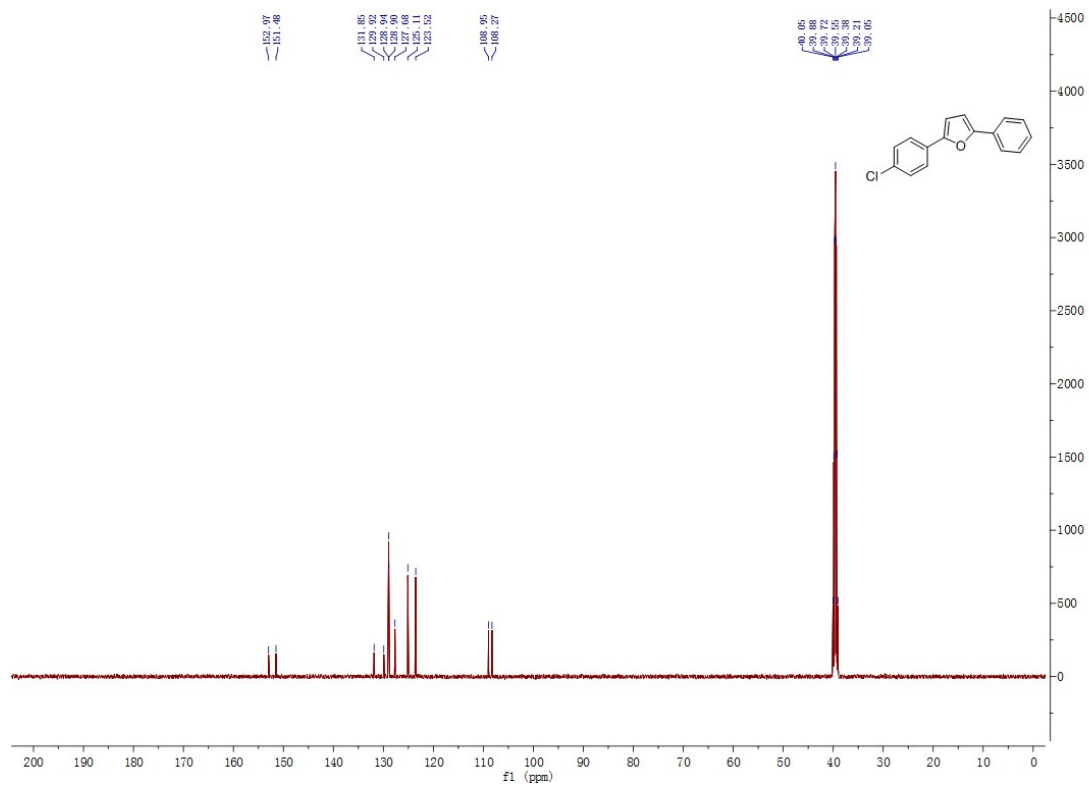
^1H NMR (500 MHz, $\text{DMSO-}d_6$) of compound **3u**



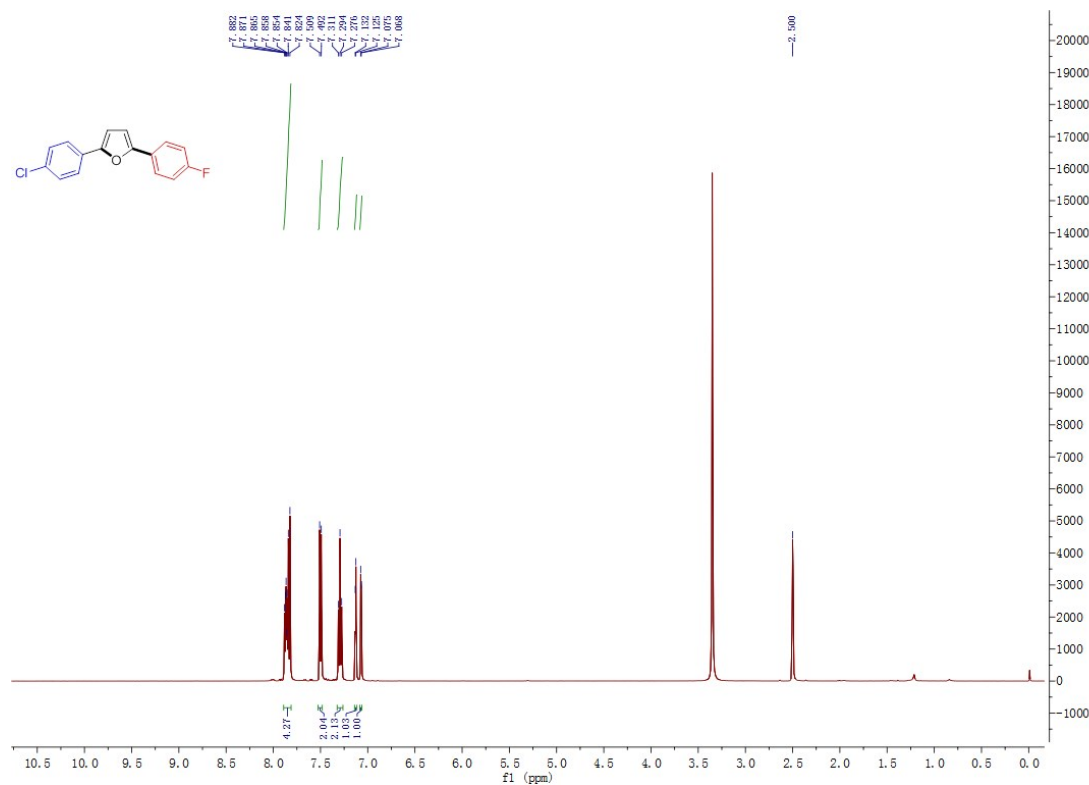
¹³C NMR (125 MHz, DMSO-*d*₆) of compound **3u**



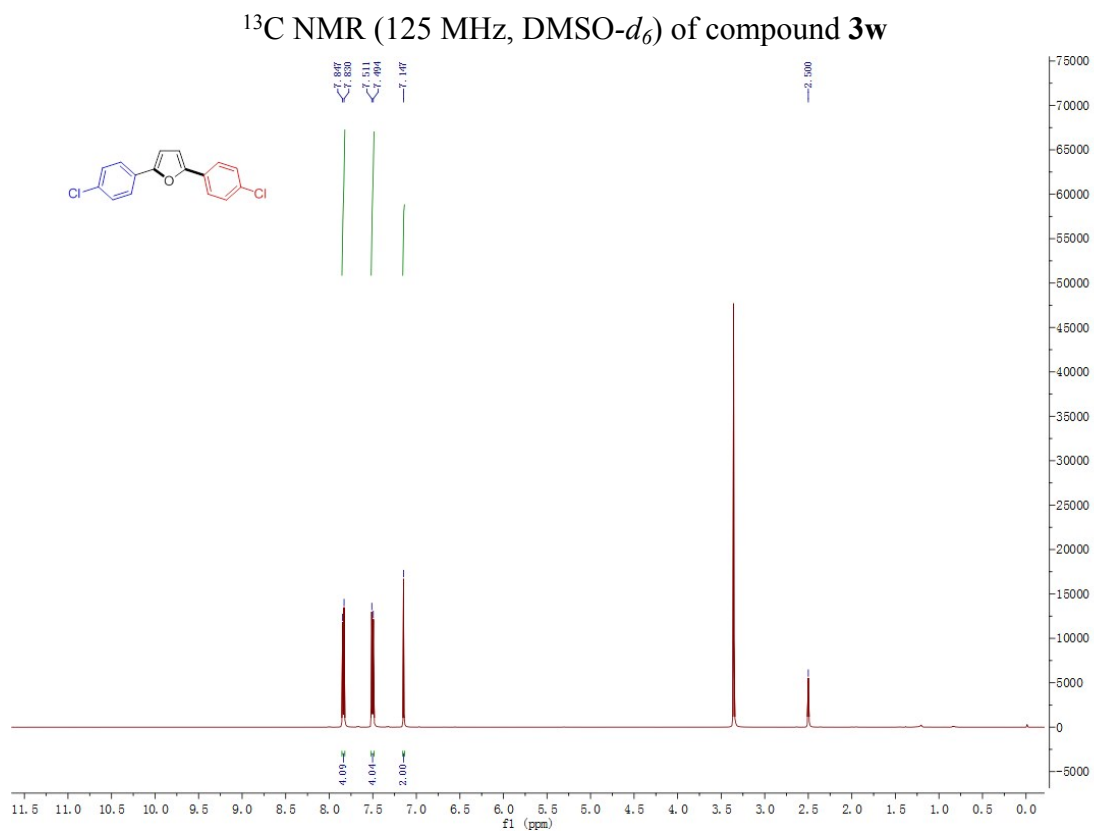
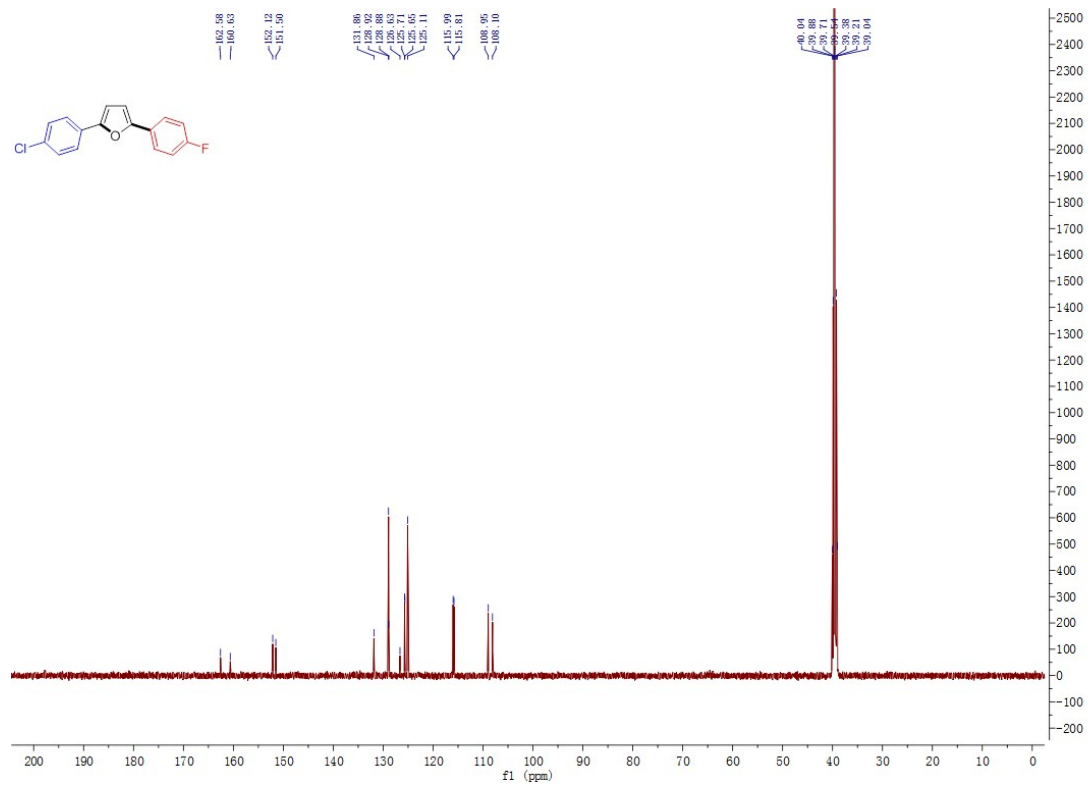
¹H NMR (500 MHz, DMSO-*d*₆) of compound **3v**

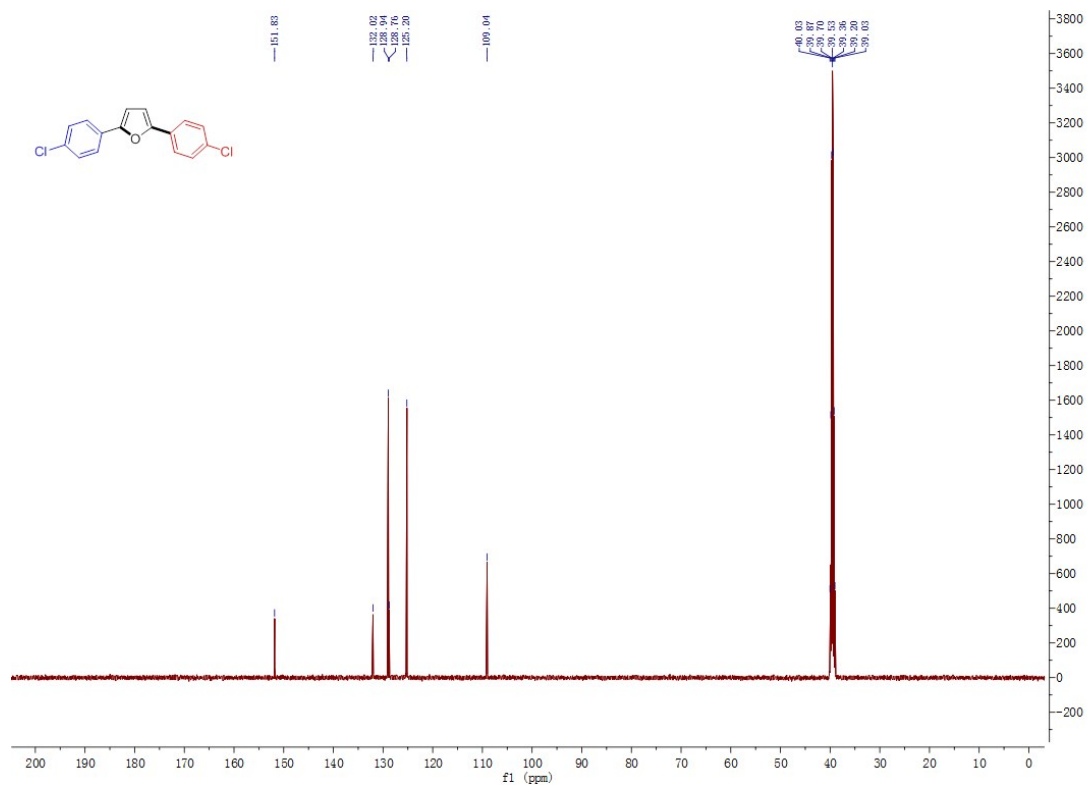


¹³C NMR (125 MHz, DMSO-*d*₆) of compound **3v**

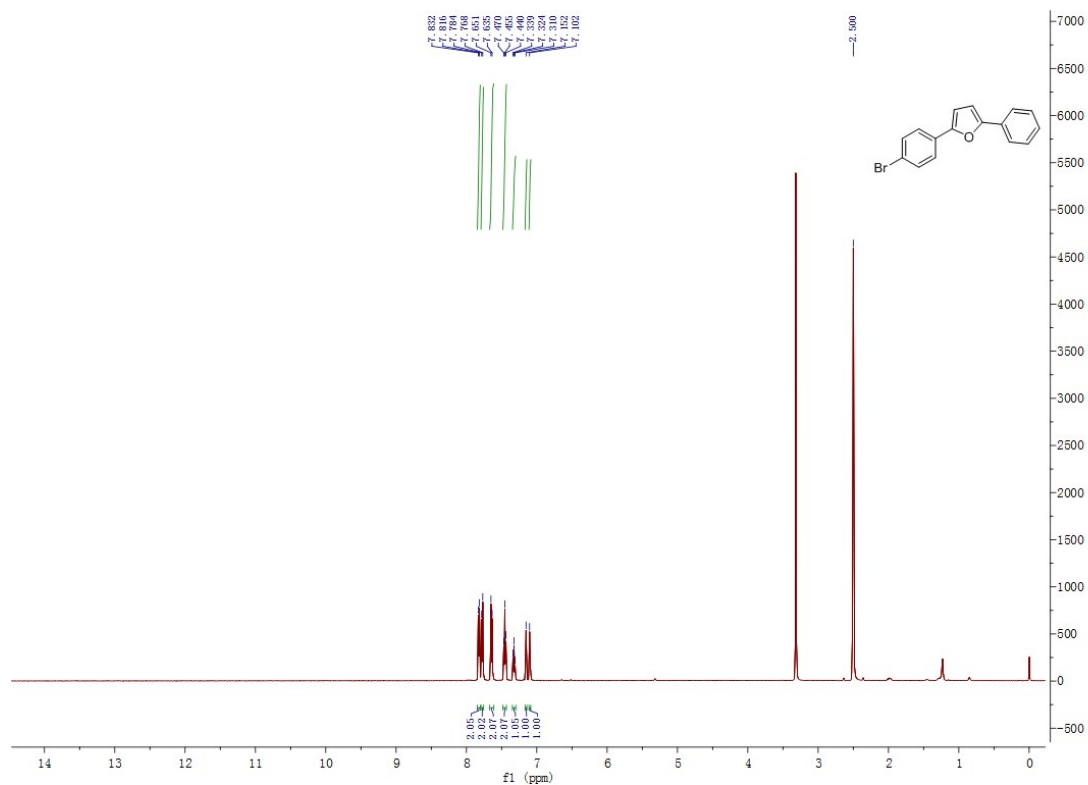


¹H NMR (500 MHz, DMSO-*d*₆) of compound **3w**

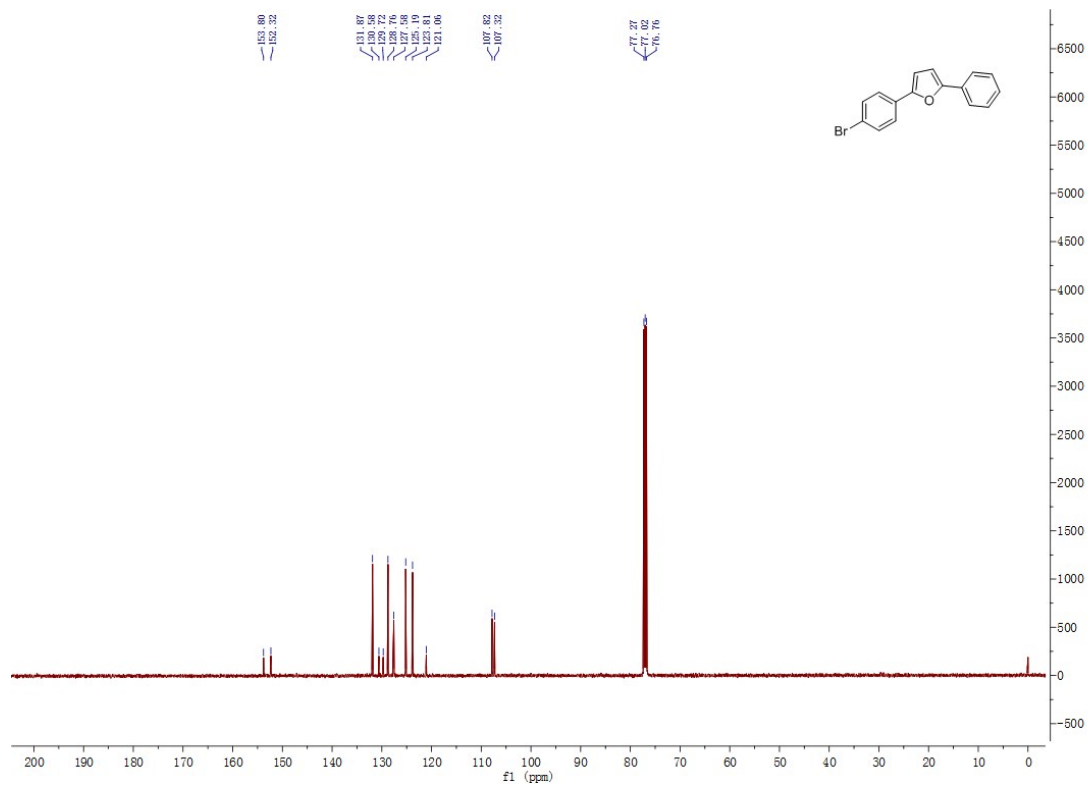




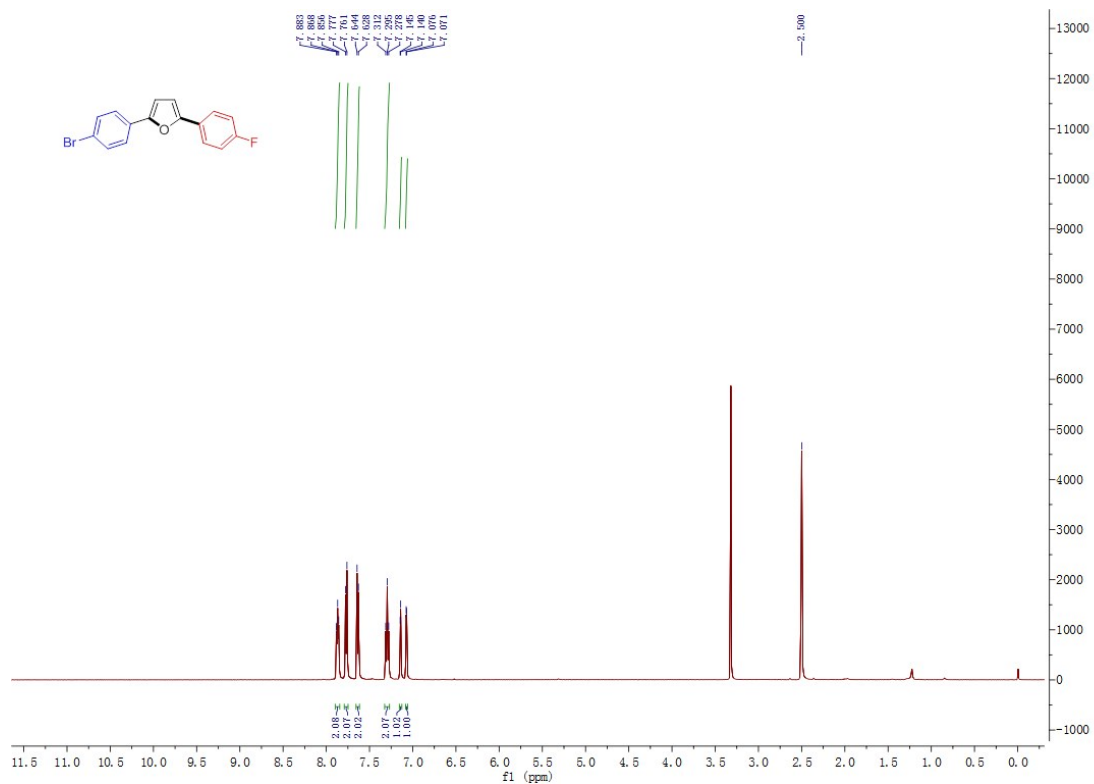
^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) of compound **3x**



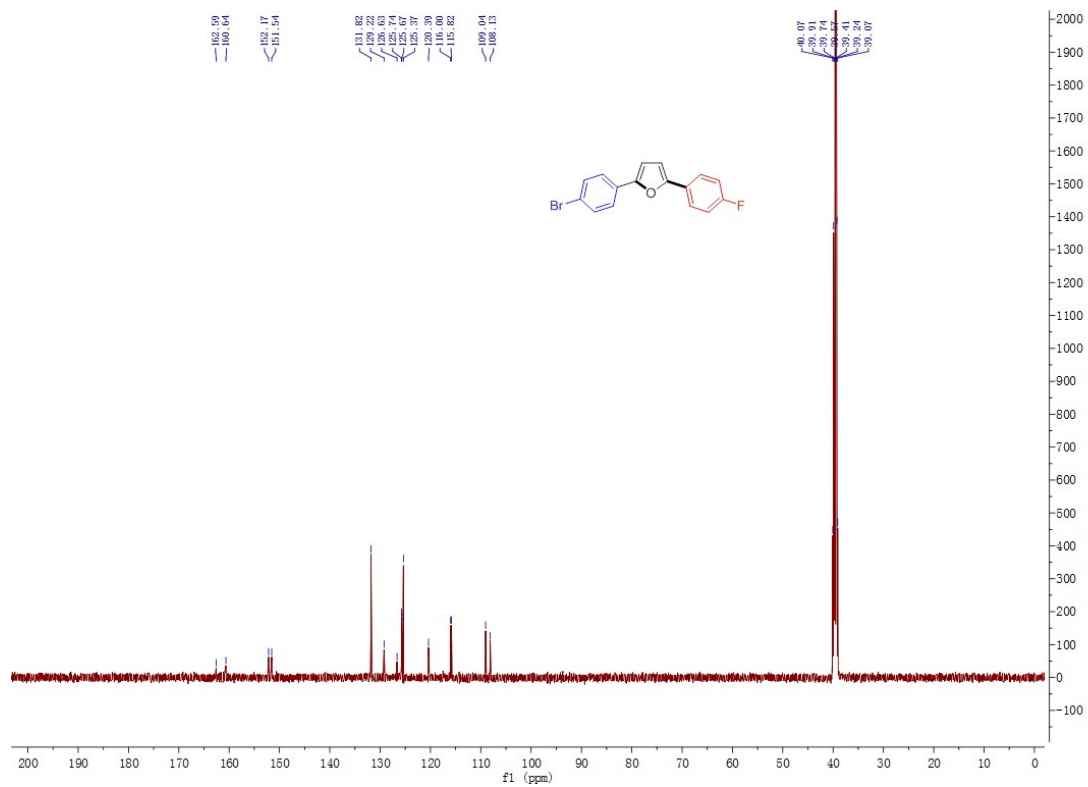
^1H NMR (500 MHz, $\text{DMSO-}d_6$) of compound **3y**



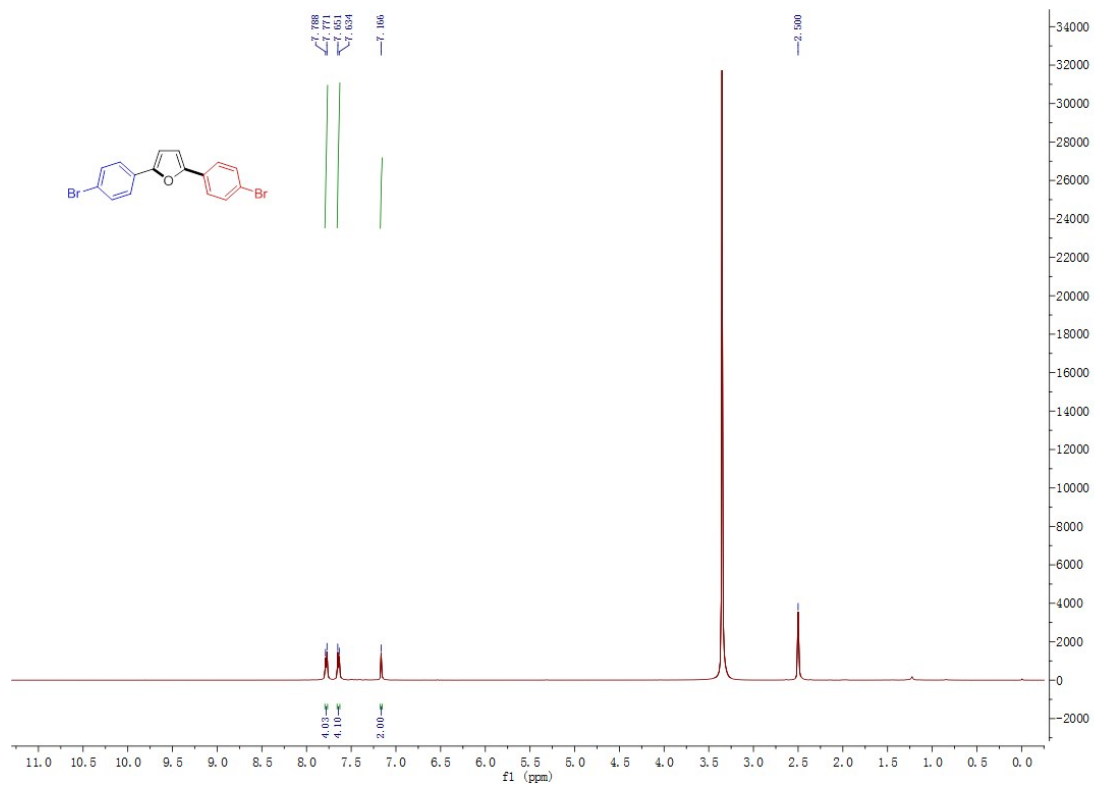
^{13}C NMR (125 MHz, CDCl_3) of compound **3y**



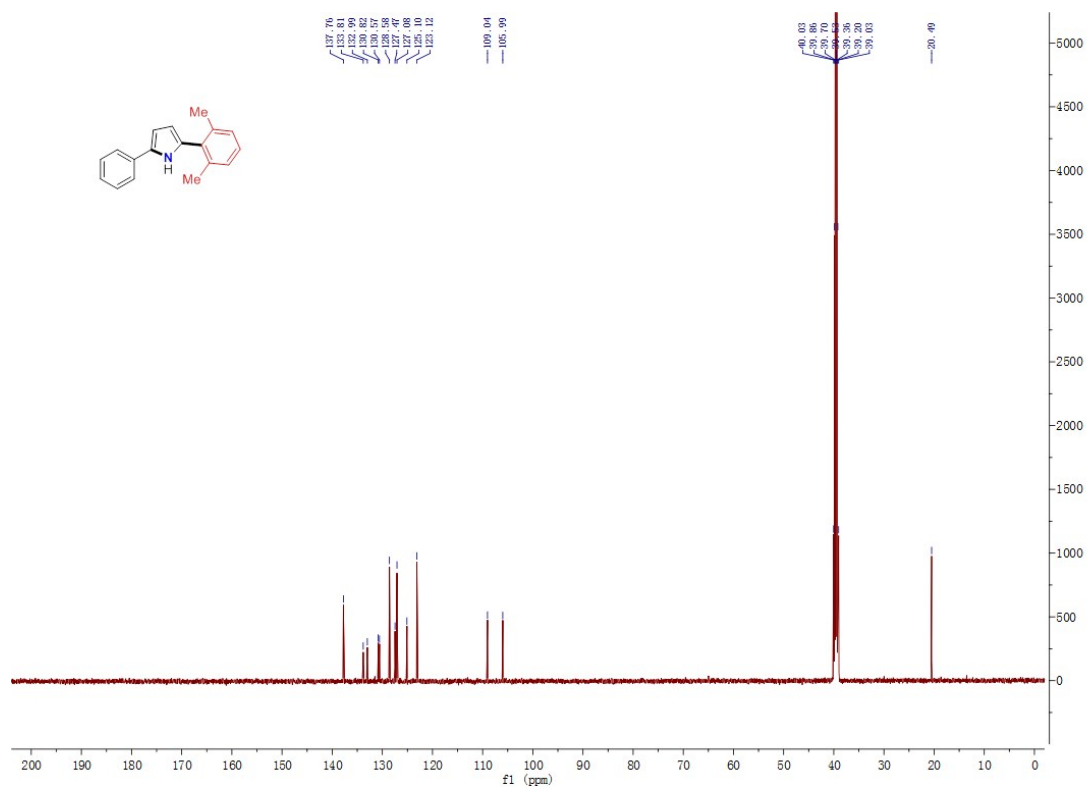
^1H NMR (500 MHz, $\text{DMSO}-d_6$) of compound **3z**



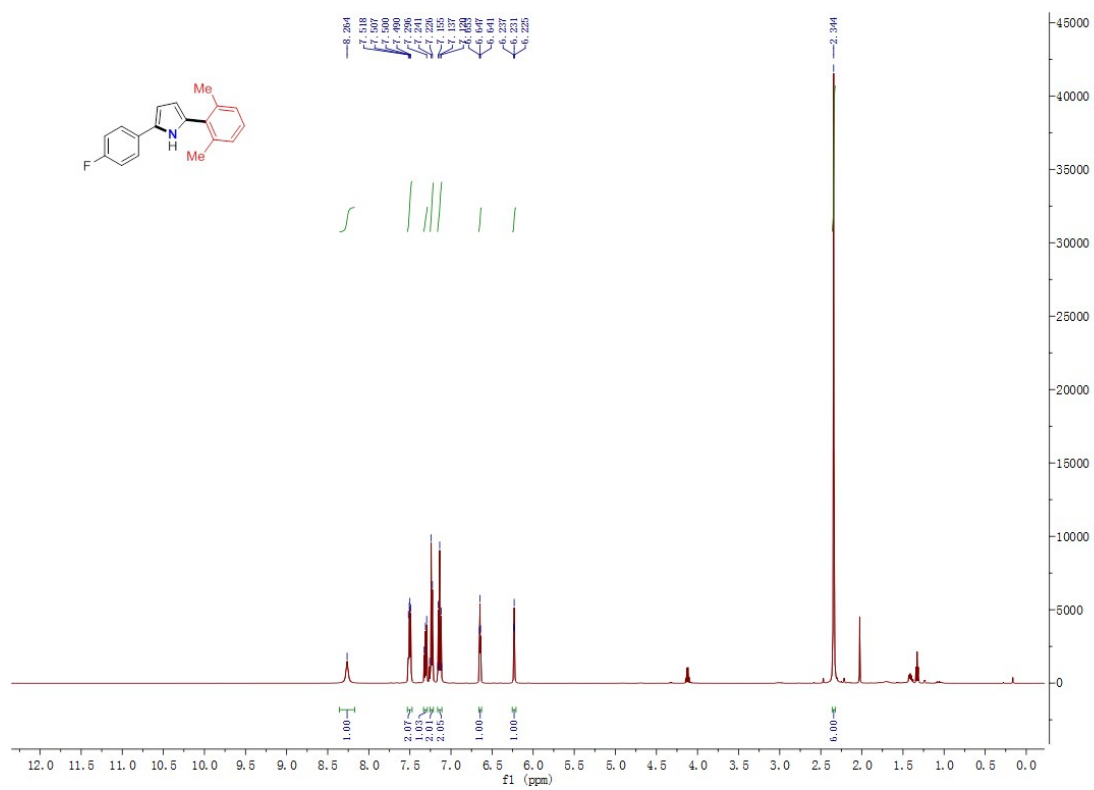
¹³C NMR (125 MHz, DMSO-*d*₆) of compound 3z



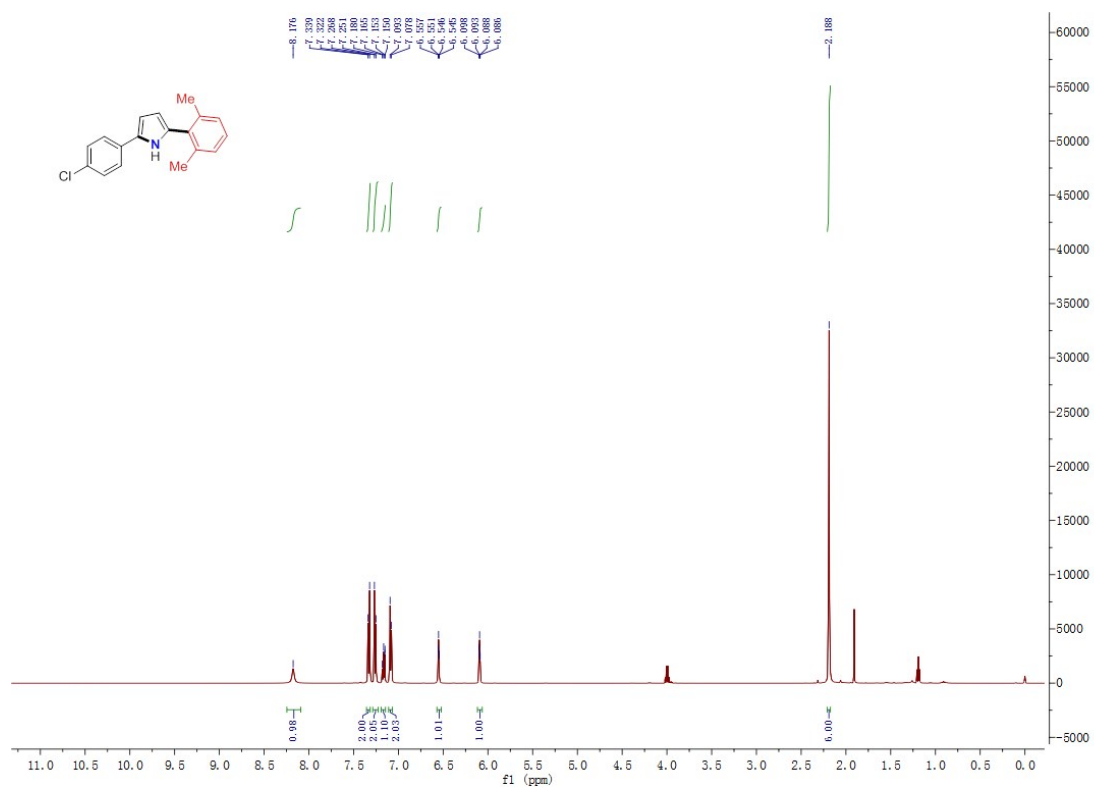
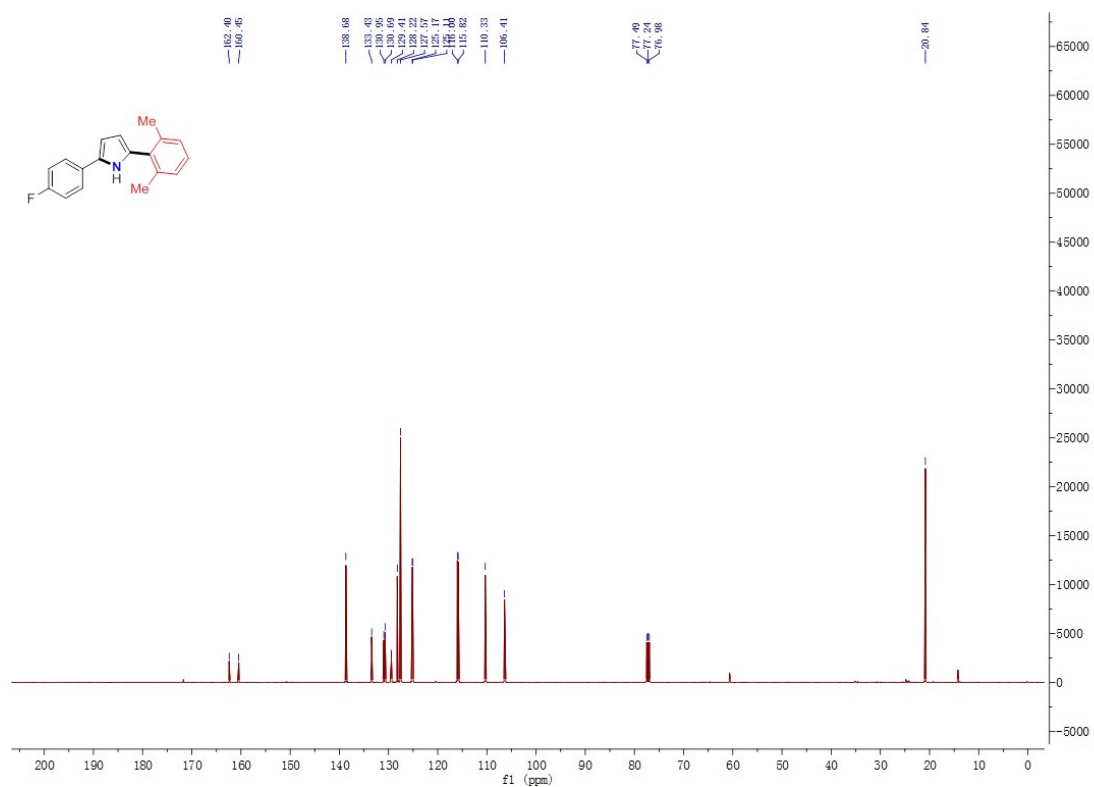
¹H NMR (500 MHz, DMSO-*d*₆) of compound 3aa

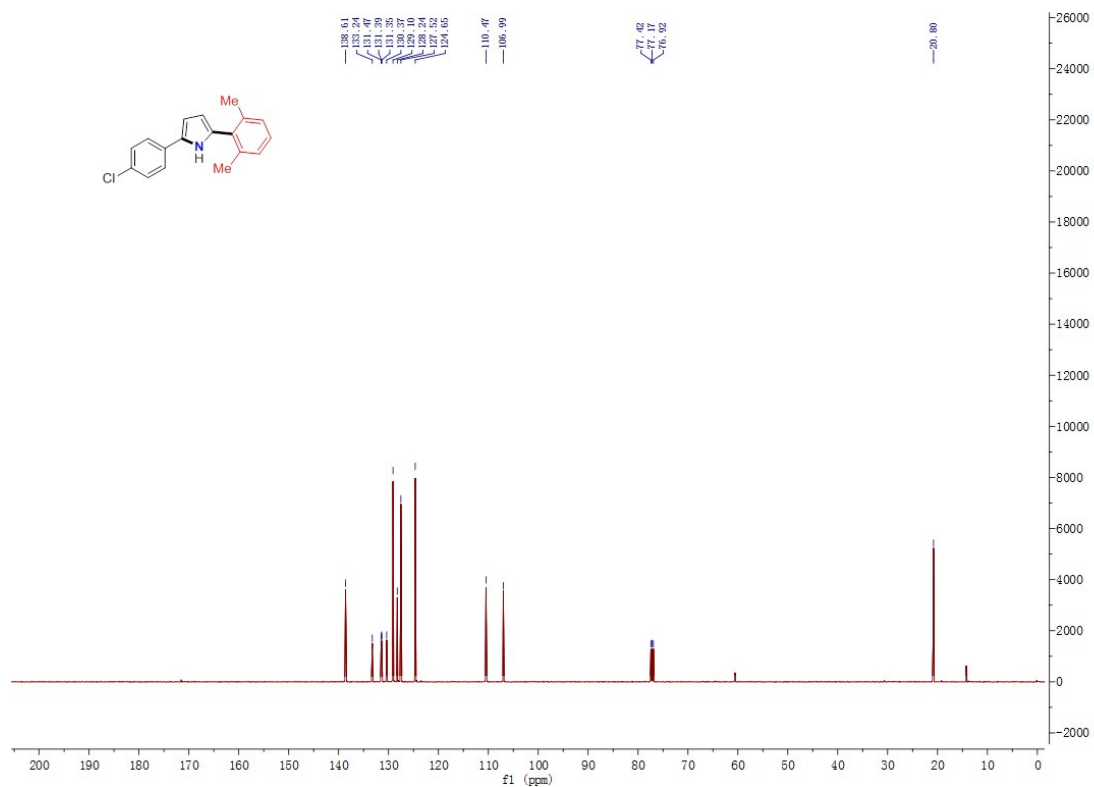


^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) of compound **4a**

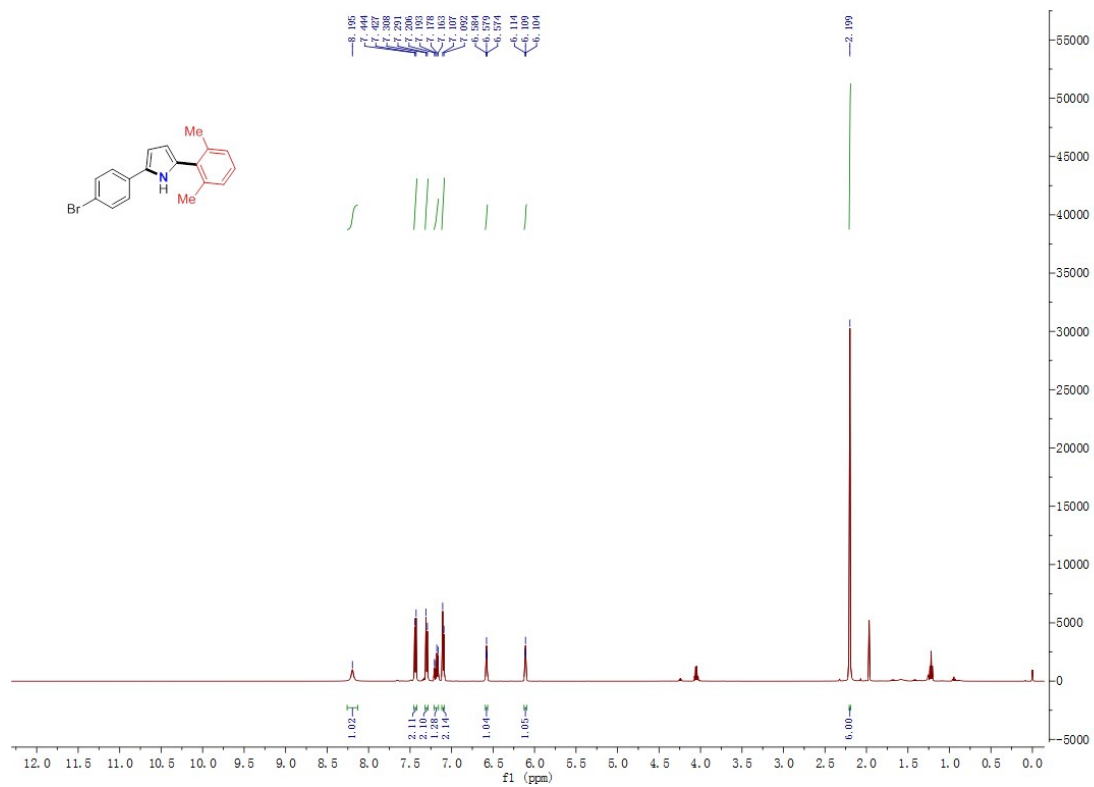


^1H NMR (500 MHz, CDCl_3) of compound **4b**

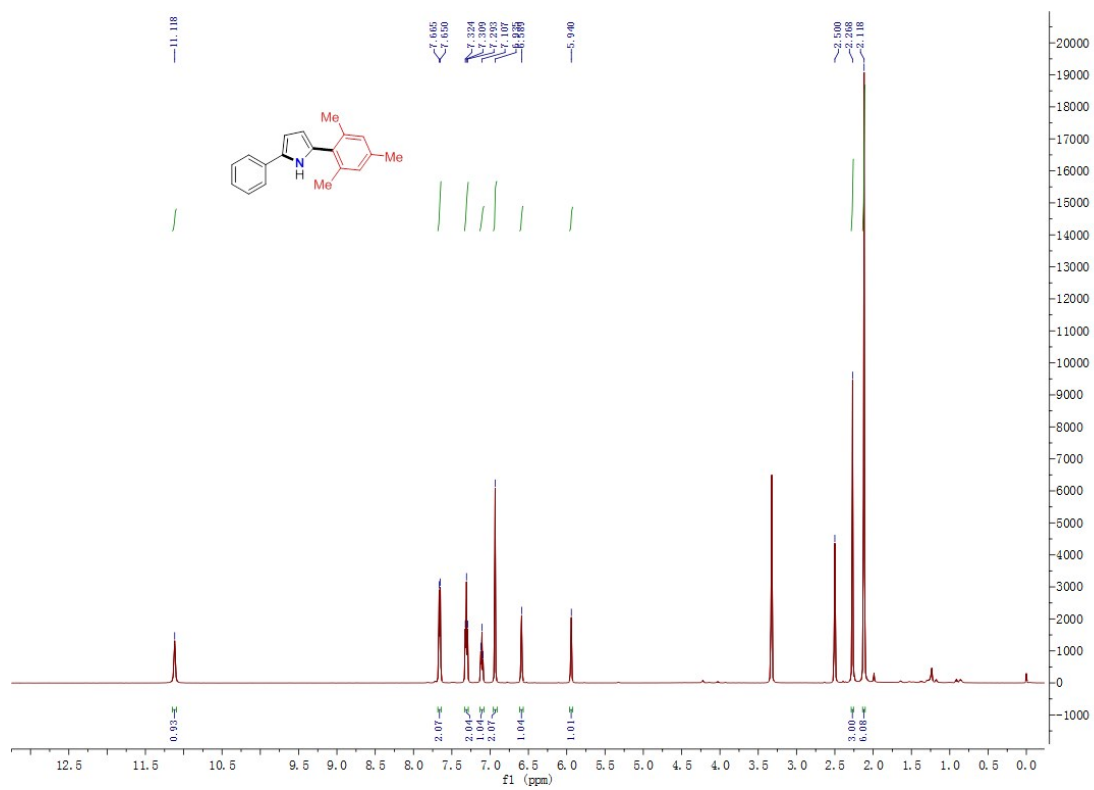
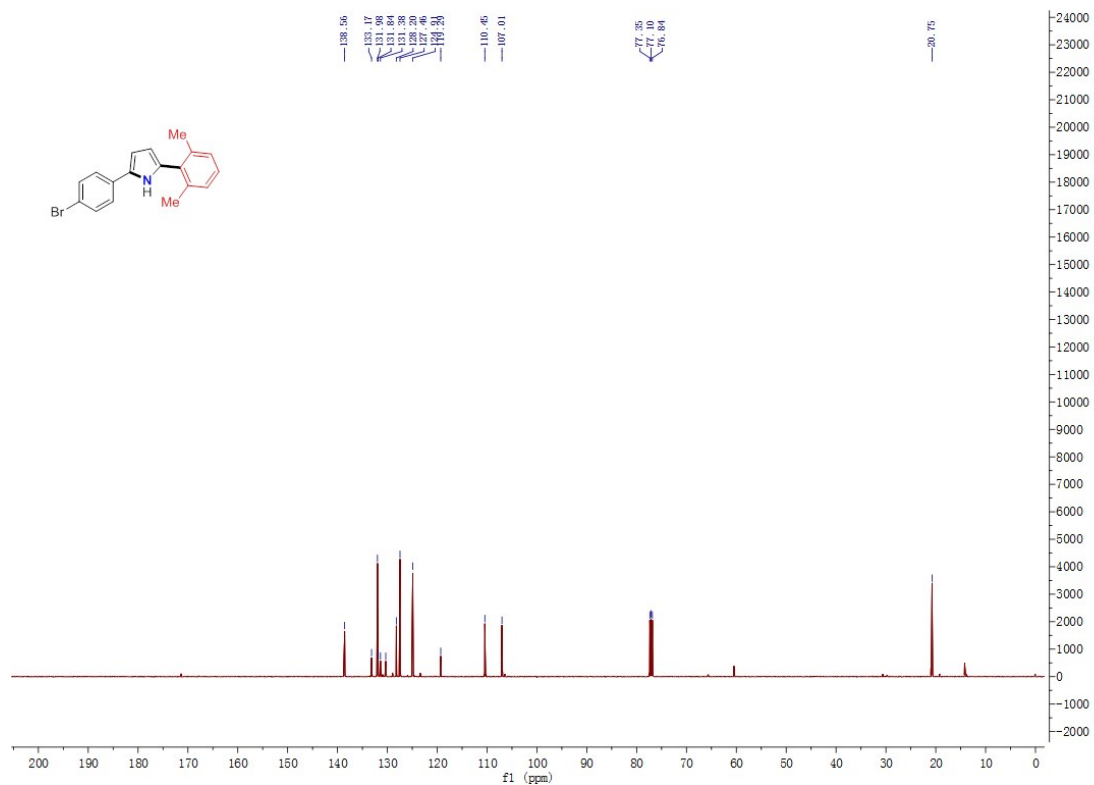


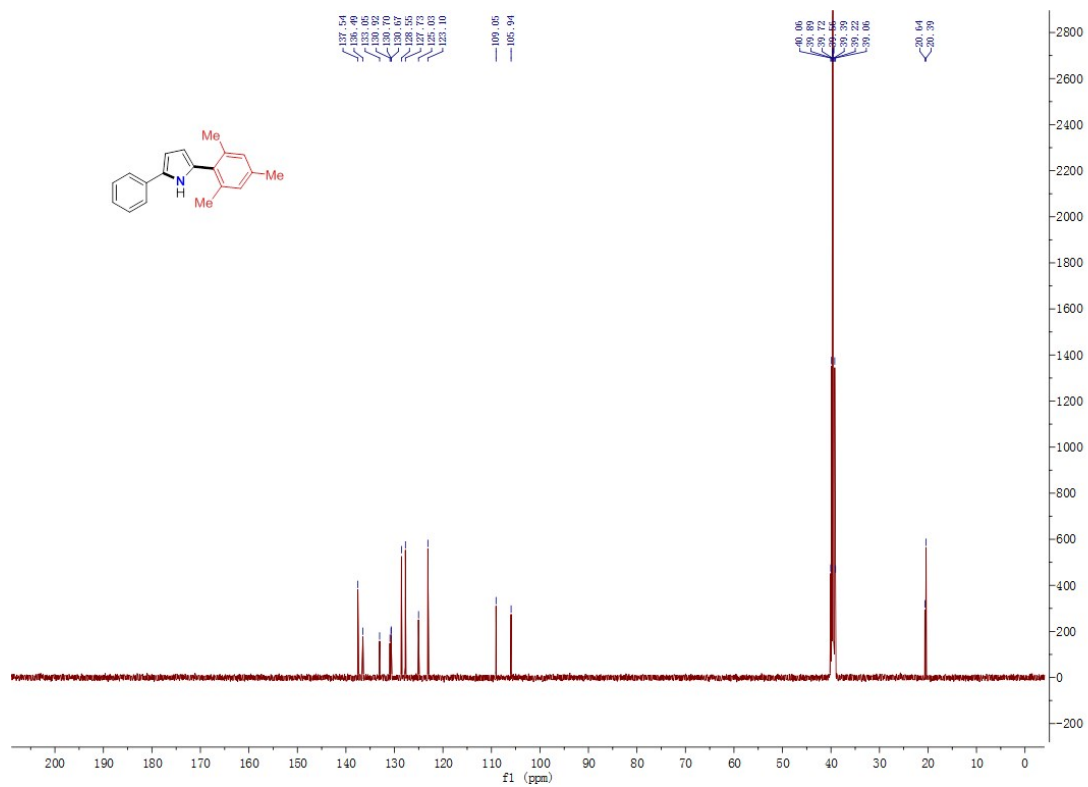


¹³C NMR (125 MHz, CDCl₃) of compound 4c

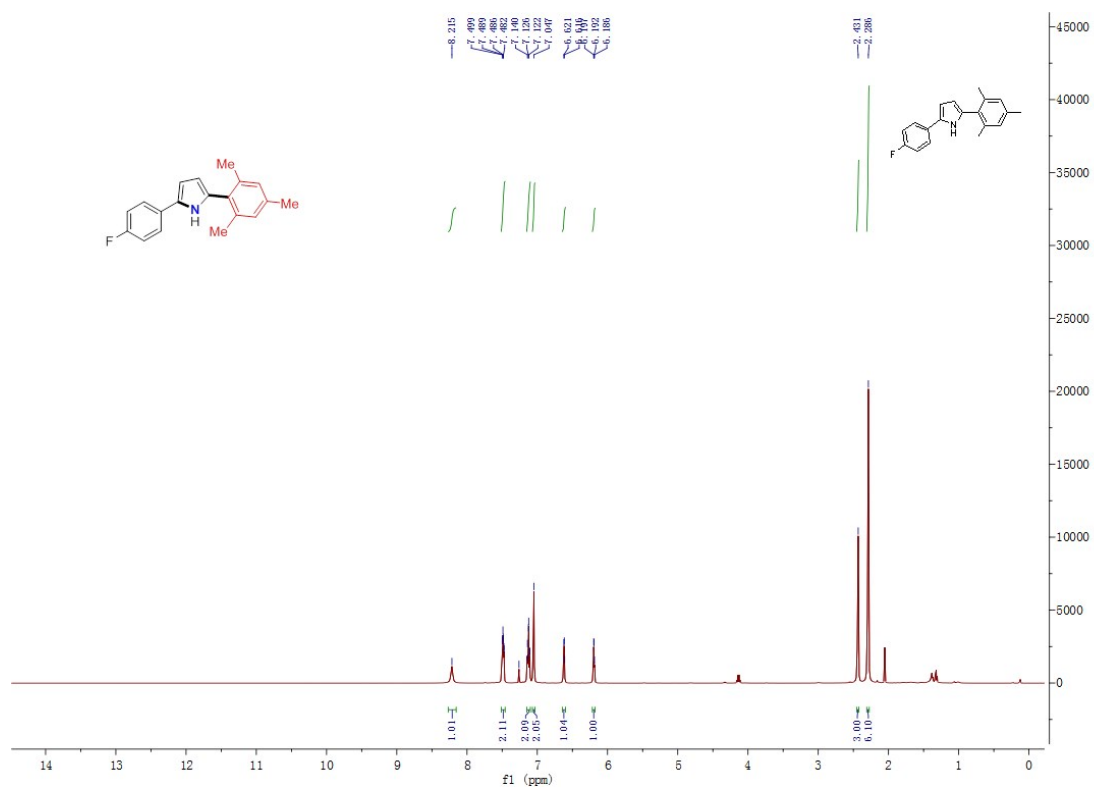


¹H NMR (500 MHz, CDCl₃) of compound 4d

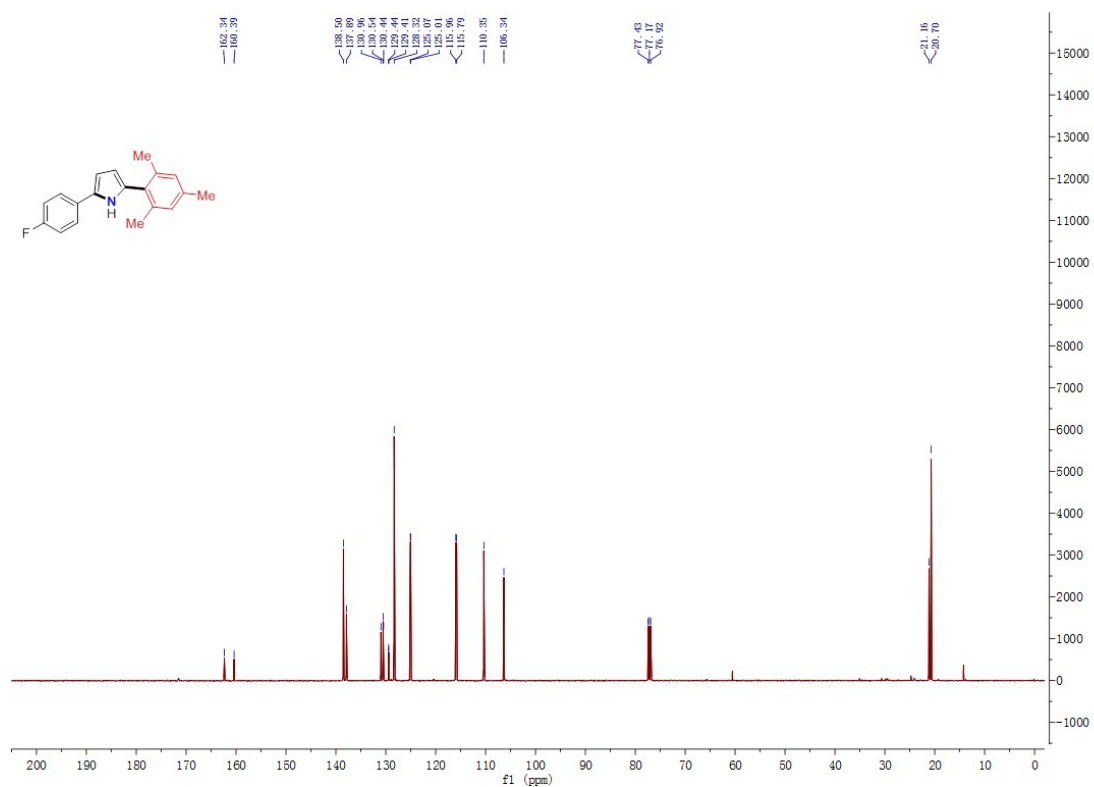




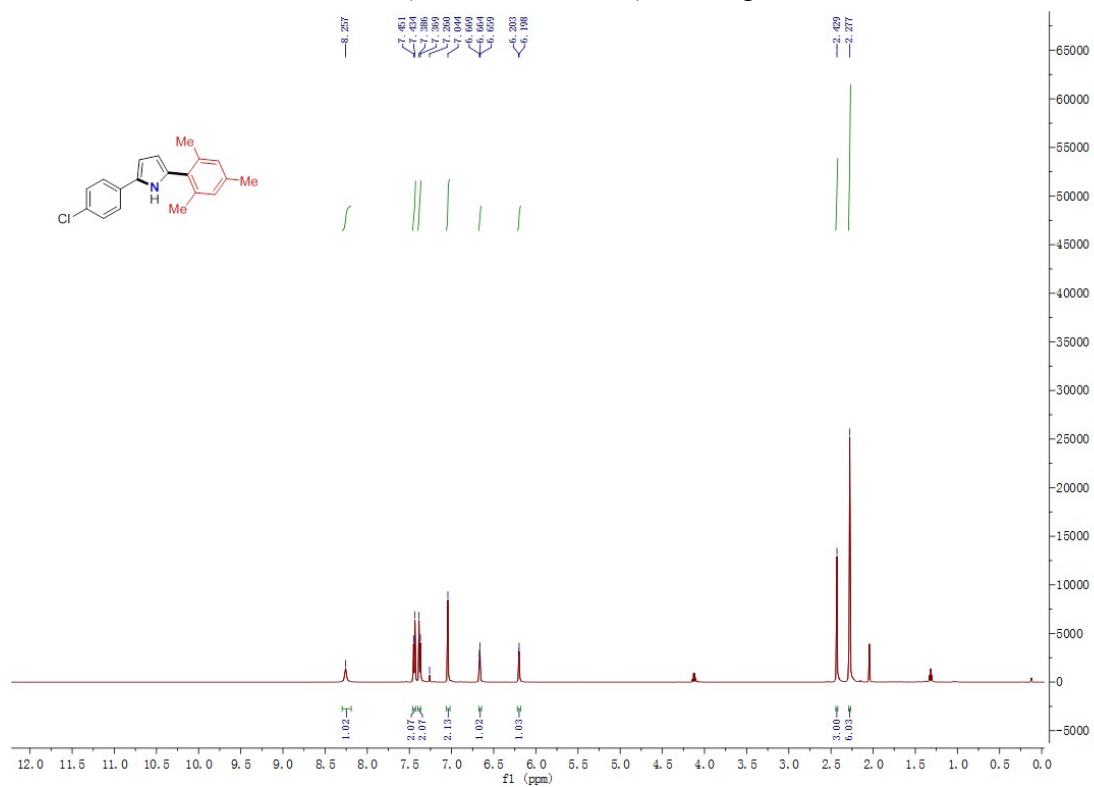
^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) of compound 4e



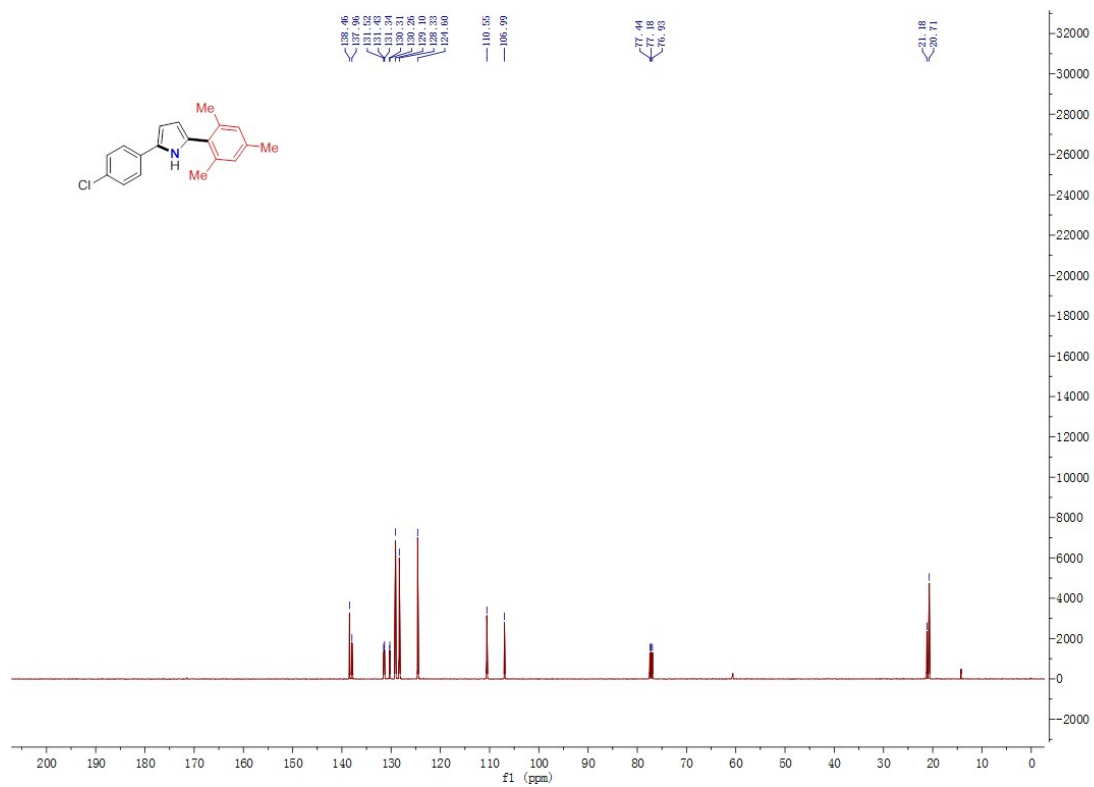
^1H NMR (500 MHz, CDCl_3) of compound 4f



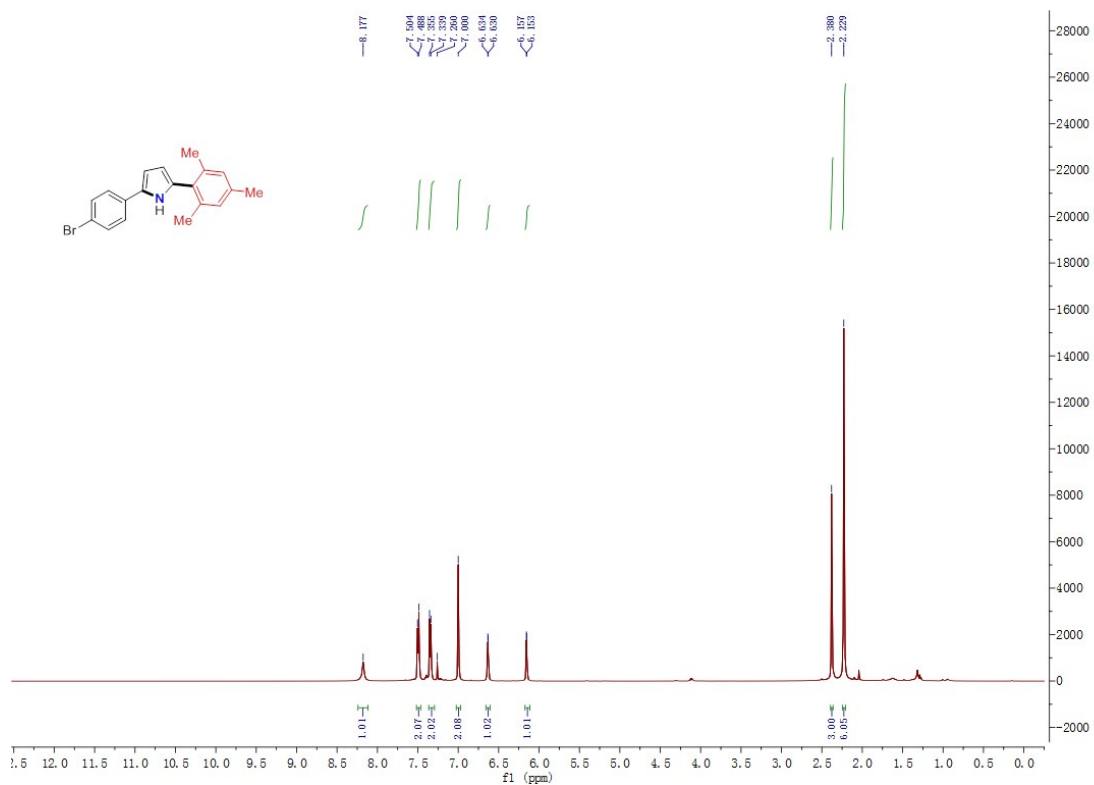
^{13}C NMR (125 MHz, CDCl_3) of compound **4f**



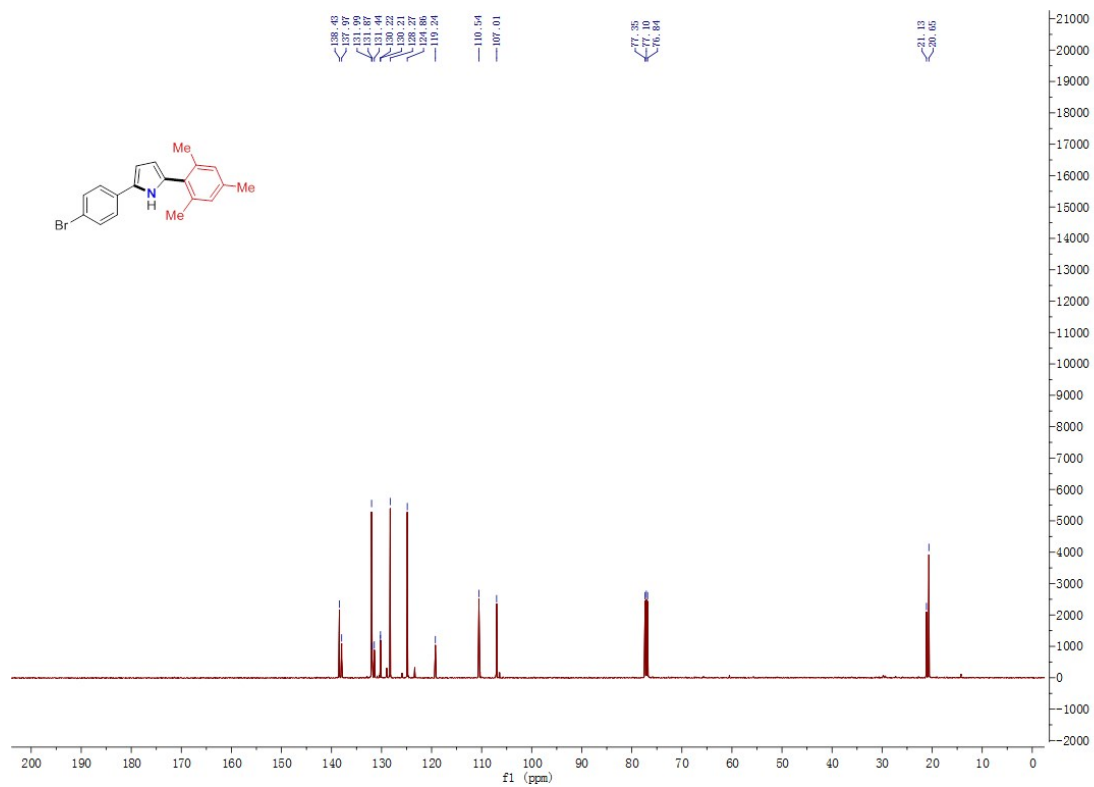
^1H NMR (500 MHz, CDCl_3) of compound **4g**



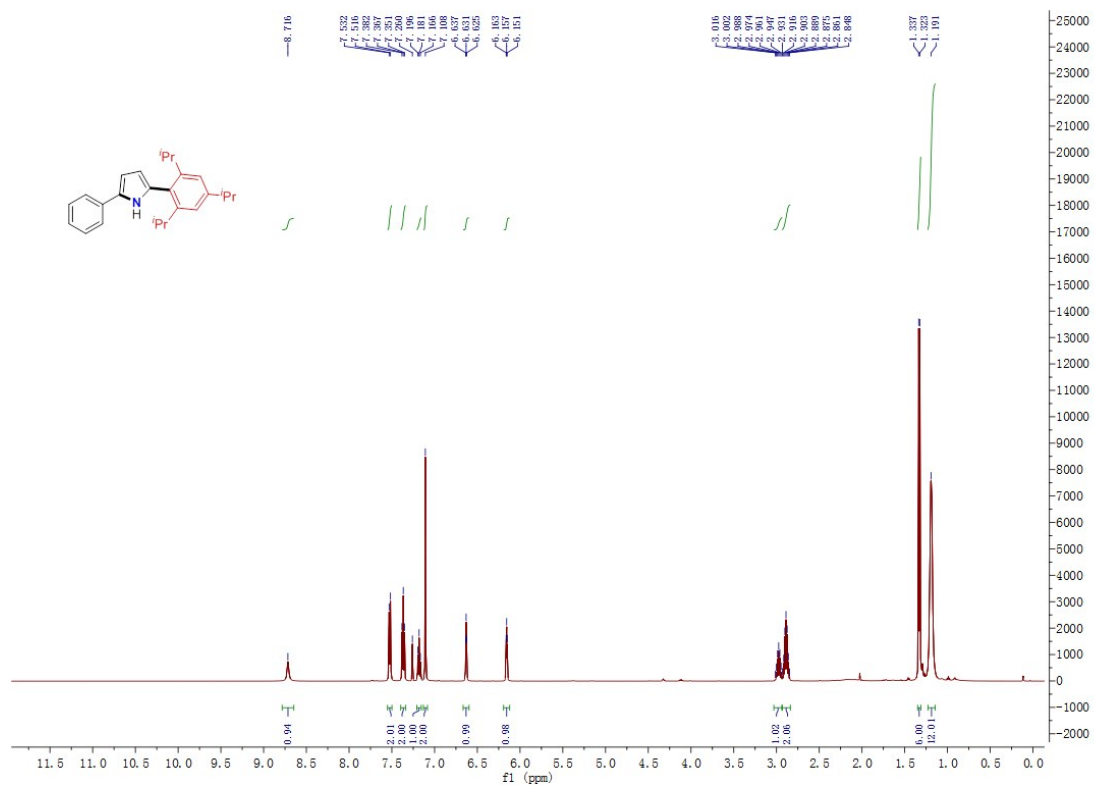
^{13}C NMR (125 MHz, CDCl_3) of compound **4g**



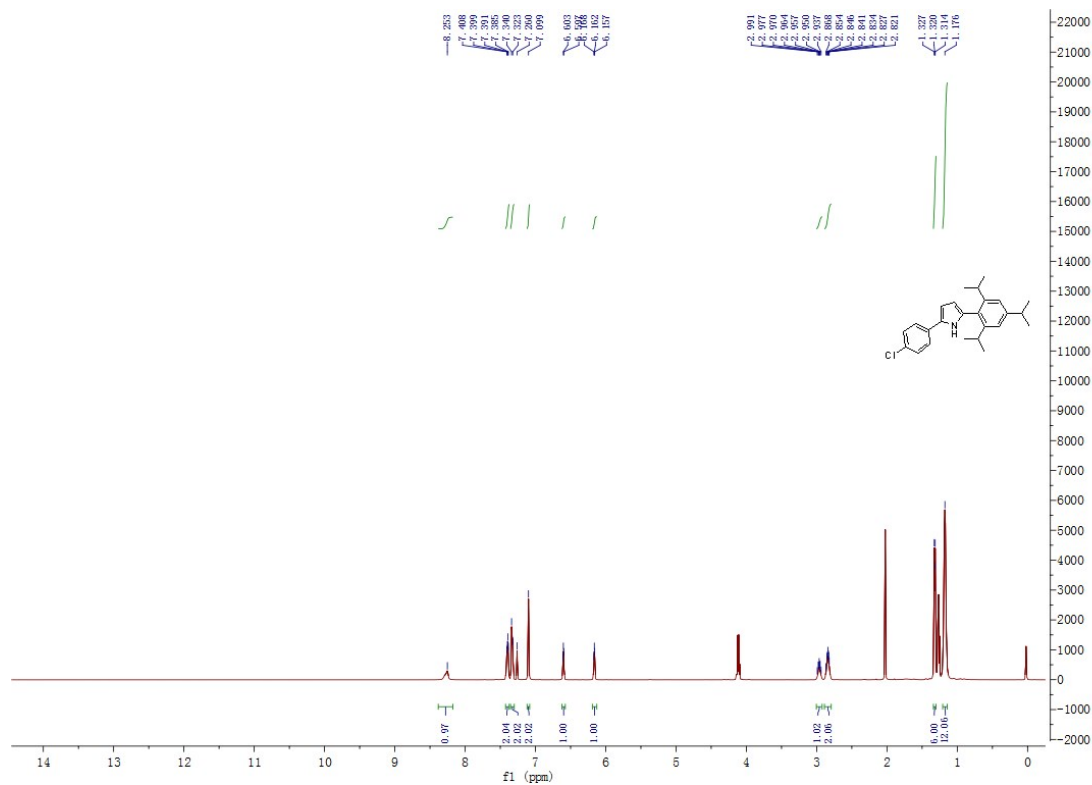
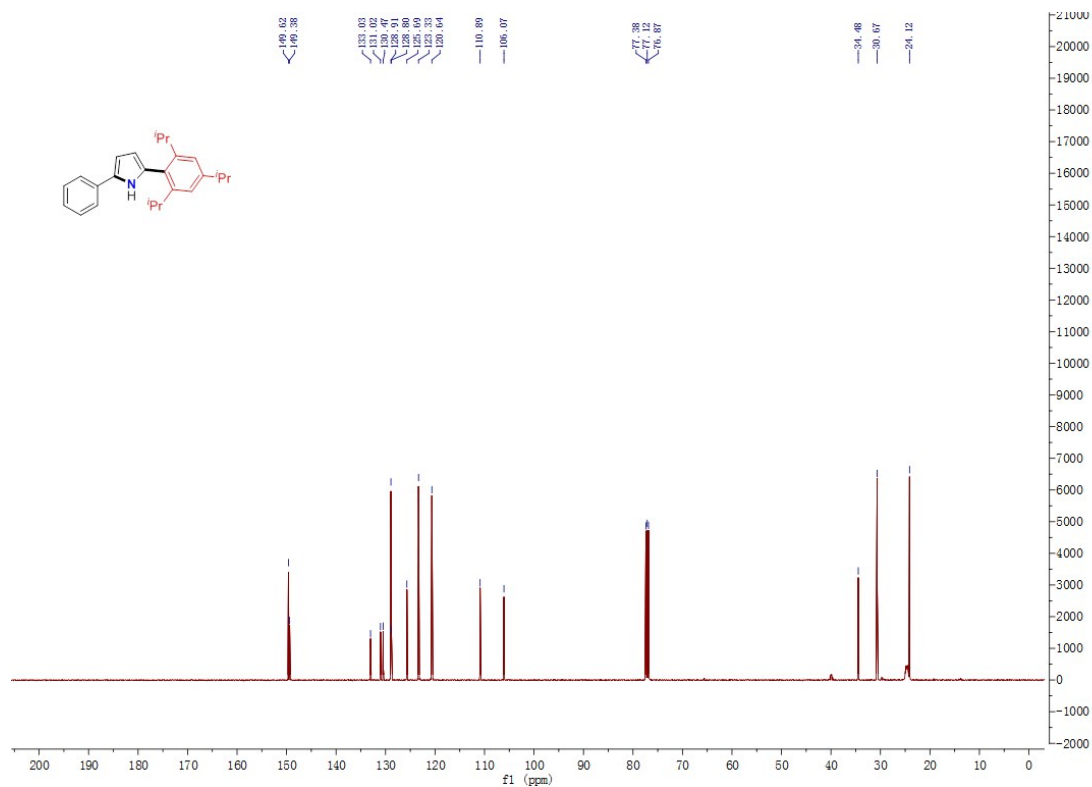
^1H NMR (500 MHz, CDCl_3) of compound **4h**

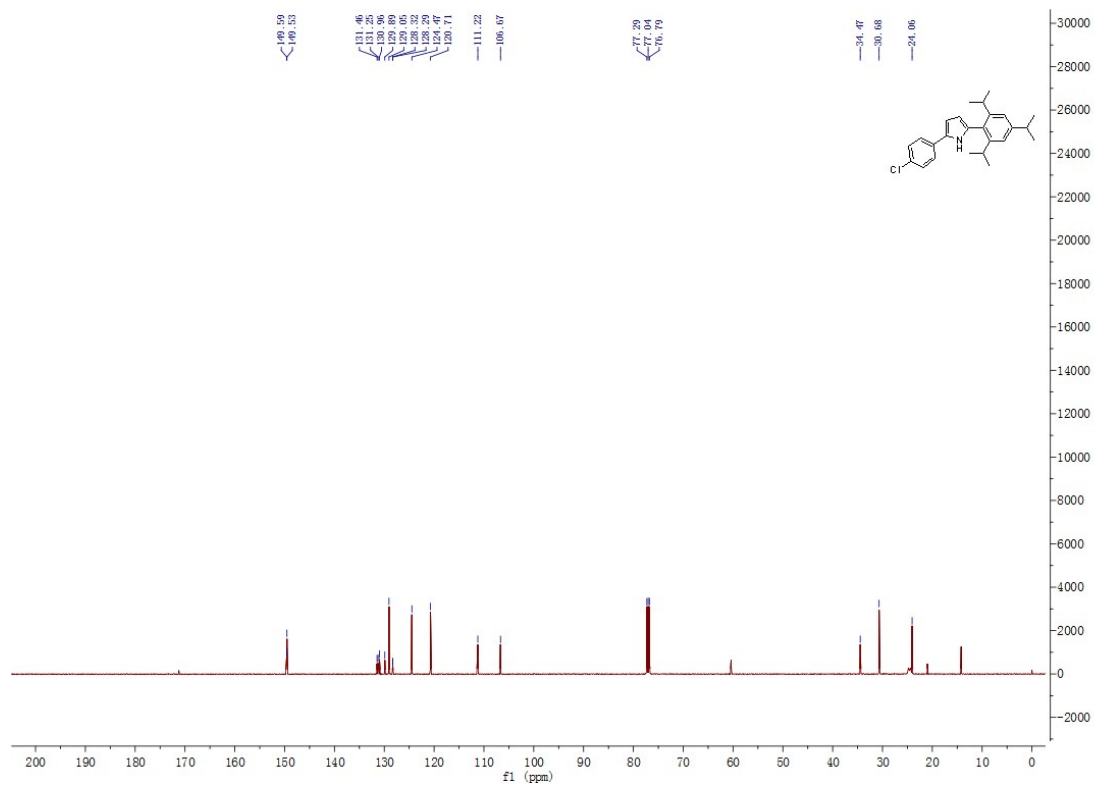


^{13}C NMR (125 MHz, CDCl_3) of compound **4h**

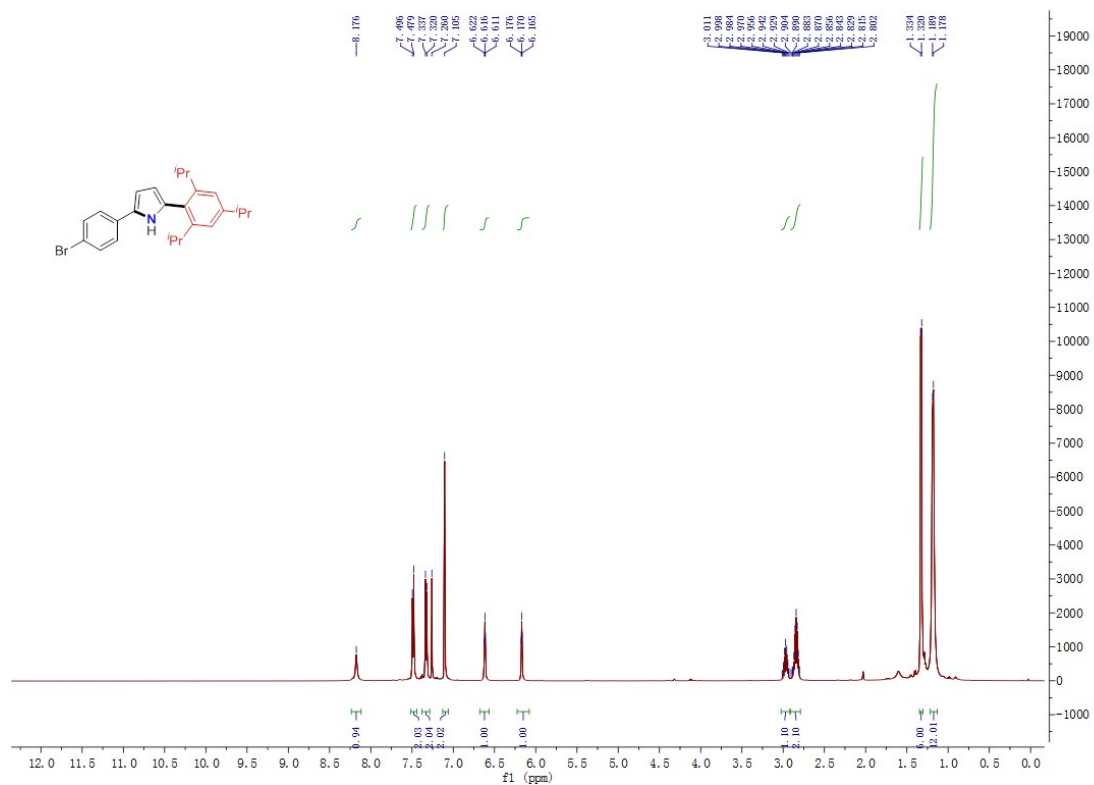


^1H NMR (500 MHz, CDCl_3) of compound **4i**





^{13}C NMR (125 MHz, CDCl_3) of compound **4j**



^1H NMR (500 MHz, CDCl_3) of compound **4k**

