

Supporting Information

**A facile metal-free one-flask synthesis of multi-substituted furans *via* a  $\text{BF}_3\cdot\text{Et}_2\text{O}$  mediated formal [4+1] reaction of 3-chloro-3-phenyldiazirines and  $\alpha$ ,  $\beta$ -alkenyl ketones**

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## Contents

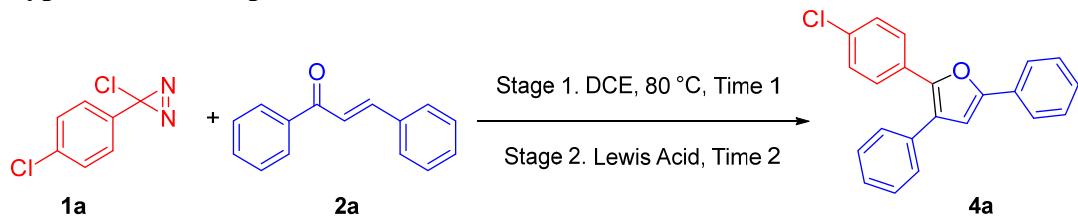
1.	General information .....	3
2.	Typical procedure.....	3
3.	Synthesis of starting materials .....	4
4.	Details for reaction conditions screening and scope test.....	9
5.	The spectral data .....	16
6.	The NMR Charts.....	30
7.	References.....	71

## 1. General information

All the solvents are dried before use. Thin-layer chromatography (TLC) was performed with silica gel GF254 plates. Column chromatography was performed on silica gel (300 ~ 400 mesh) with petroleum ether/ethyl acetate for the gradient elution. All melting points were measured without correction. Nuclear magnetic resonance (NMR) spectra were recorded on a Bruker Advance III HD 500 spectrometer at 500 MHz (<sup>1</sup>H NMR) and 126 MHz (<sup>13</sup>C NMR) respectively. The chemical shifts are reported relative to CHCl<sub>3</sub> ( $\delta$  = 7.26 for <sup>1</sup>H NMR and  $\delta$  = 77.16 for <sup>13</sup>C NMR). The infrared spectra were recorded on a Nicolet iS 50 FT-IR spectrometer. Mass spectra (ESI-MS) were obtained on an Agilent 1240/6460 LC-MS system. HRMS spectra were obtained on Thermo Fisher HRMS, Q Exactive instrument.

## 2. Typical procedure

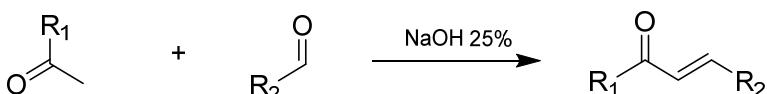
### Typical one-flask procedure for **4a**:



To a 38 mL Schlenk tube covered with aluminum foil, 37.5 mg **1a** (0.2 mmol), 41.6 mg chalcone **2a** (0.2 mmol) and 5 mL DCE was charged. The mixture was heated to 80 °C for 2 h until the diazirine **1a** was consumed by UV monitoring on the specific absorption of diazirine between 330-400 nm. Then 28.4 mg BF<sub>3</sub>·Et<sub>2</sub>O (0.2 mmol) was added in the same reaction vessel and continued heating for 17 h until the reaction completed by TLC monitoring. The mixture was separated between water and 10 mL DCM, and the water phase was extracted with 10 mL DCM for twice. The combined organic phase was then dried over Na<sub>2</sub>SO<sub>4</sub>, filtered and concentrated to give oily crude product. After silica gel chromatography, 45.2 mg furan **4a** obtained in 68% yield.

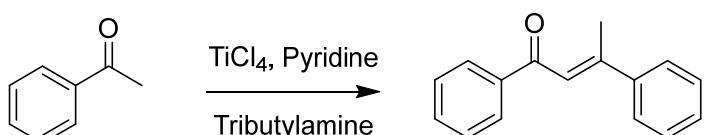
### 3. Synthesis of starting materials

#### Synthesis of chalcones 2a-2u<sup>1</sup>



To a round bottom flask, the appropriate ketone (25 mmol) and the corresponding aldehyde (30 mmol) were solved in EtOH (15 mL). Then, a NaOH aqueous solution (25%, 25 mL) was slowly added at 0 °C. The reaction mixture was stirring at room temperature for 4 h. In all cases the compound precipitated and was collected by filtration. The residue was purified by recrystallization in MeOH to afford the pure chalcones.

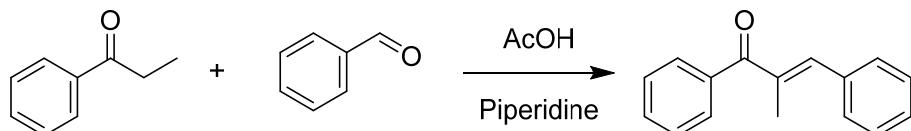
#### Synthesis of (E)-1,3-diphenylbut-2-en-1-one<sup>2</sup>



To a flame-dried two-necked 50 mL flask containing 0.58 mL of acetophenone (5.0 mmol) and 10 mL of CH<sub>2</sub>Cl<sub>2</sub> were added TiCl<sub>4</sub> (0.60 mL, 5.5 mmol) and 1.4 mL of tributylamine (6.0 mmol), and the whole mixture was stirred for 30 min at room temperature. After addition of 0.58 mL of acetophenone (5.0 mmol) and stirring for 1 h at the same temperature, 2.0 mL of pyridine (25.0 mmol) was added and the mixture was stirred for 5 h at room temperature. Filtration of the reaction mixture after addition of Et<sub>2</sub>O and hexane (25 mL each) with the aid of Celite and concentration of the organic phase furnished crude mixture which was chromatographed on silica gel using a mixture of Hex: AcOEt = 10:1 as an eluent to give 0.35 g of the title compound (1.6 mmol, 32% yield) as a yellow oil.

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.02 – 7.98 (m, 2H), 7.59 – 7.54 (m, 3H), 7.48 (m, 2H), 7.45 – 7.40 (m, 3H), 7.18 (d, *J* = 1.2 Hz, 1H), 2.61 (d, *J* = 1.2 Hz, 3H).

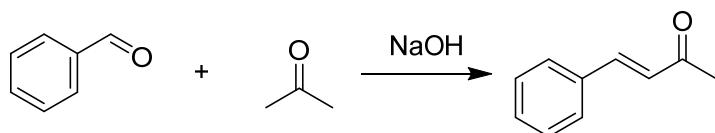
#### Synthesis of (E)-2-methyl-1,3-diphenylprop-2-en-1-one<sup>3</sup>



A solution of phenylacetone (14.8 g, 0.076 mol), benzaldehyde (11.6 g, 0.078 mol), piperidine (15 mL), and acetic acid (7.5 mL) in ethanol (80 mL) was heated at reflux. After 18 h the solvent was removed and the residue was chromatographed on a flash silica gel column using 25% EtOAc in hexane as eluent.

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.62 – 7.58 (m, 2H), 7.41 – 7.37 (m, 1H), 7.31 (t, *J* = 7.5 Hz, 2H), 7.27 (s, 2H), 7.26 – 7.23 (m, 1H), 7.19 (m, 1H), 7.11 (s, 1H), 7.03 (d, *J* = 1.3 Hz, 1H), 2.12 (d, *J* = 1.4 Hz, 3H).

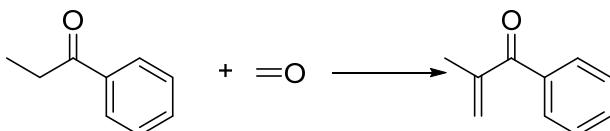
### Synthesis of (E)-4-phenylbut-3-en-2-one<sup>4</sup>



Benzaldehyde (36 mmol, 1.0 eq) was suspended in a mixture of acetone/water (5 mL/5 mL). A 1% aqueous solution of sodium hydroxide (10 mL) was slowly added to the reaction mixture. The reaction mixture was heated to 65 °C and stirred until no benzaldehyde was detected by TLC. The reaction mixture was cooled to ambient temperature, water (20 mL) and toluene (20 mL) were added to the flask. The organic phase was separated, washed with brine. The combined organic layer was dried with MgSO<sub>4</sub> and concentrated to dryness, and the residue was purified by flash chromatography on silica gel to give the product (96% yield).

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.56 – 7.53 (m, 2H), 7.51 (d, *J* = 16.3 Hz, 1H), 7.42 – 7.39 (m, 3H), 6.72 (d, *J* = 16.3 Hz, 1H), 2.38 (s, 3H).

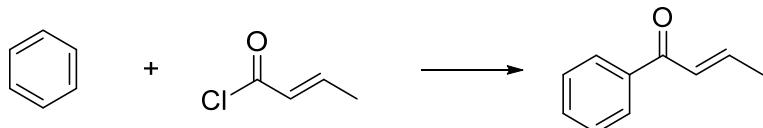
### Synthesis of 2-methyl-1-phenylprop-2-en-1-one<sup>5</sup>



Add paraformaldehyde (1.80 g, 60.0 mmol), piperidine (0.13 mL, 1.3 mmol) and AcOH (0.13 mL, 2.2 mmol) sequentially to a stirred solution of propiophenone (1.34 g, 10.0 mmol) in DMF (25 mL). Heat the resulting mixture at 90 °C for 24 hours. Cool down the reaction mixture. Add water (60 mL) to the residue. Extract the reaction mixture with Et<sub>2</sub>O (3 × 60 mL). Wash the combined organic layers with water (60 mL). Dry the residue over anhydrous Na<sub>2</sub>SO<sub>4</sub> and filter. Concentrate the reaction mixture to obtain the crude product. Purify the crude product by silica gel column chromatography using ethyl acetate/petroleum ether as eluent to obtain 2-methyl-1-phenylprop-2-en-one as a colorless oil (0.8 g, 55%).

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.75 – 7.71 (m, 2H), 7.55 – 7.50 (m, 1H), 7.45 – 7.41 (m, 2H), 5.93 – 5.89 (m, 1H), 5.64 – 5.61 (m, 1H), 2.09 – 2.06 (m, 3H).

### Synthesis of (E)-1-phenylbut-2-en-1-one<sup>6</sup>

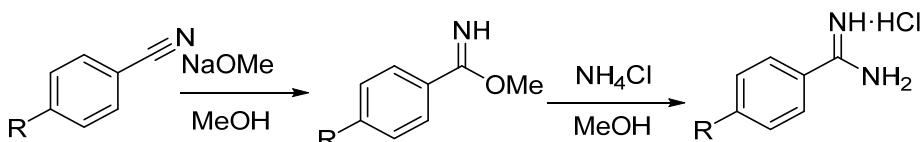


Aluminium trichloride (freshly ground, 5.48 g, 41.1 mmol) was suspended in benzene (20 ml), then stirred vigorously at room temperature while *trans*-crotonyl chloride (3.09 ml, 32.1 mmol) was added dropwise over 5 min. After a further 15 min the resulting clear solution was poured onto a mixture of ice (100 ml) and hydrochloric acid solution (2 M, 50 ml). The resulting mixture was extracted with ether (2 × 30 ml), washed with sodium hydroxide solution (4 M, 30 ml), dried (MgSO<sub>4</sub>) and concentrated *in vacuo*.

The crude material was purified by distillation to give the (E)-1-phenylbut-2-en-1-one as a clear oil (2.86 g, 61%).

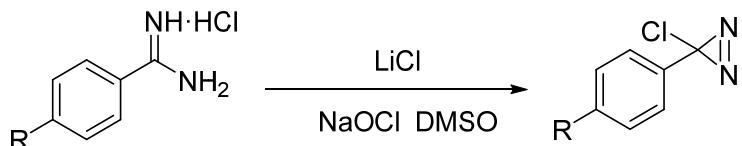
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.94 – 7.91 (m, 2H), 7.57 – 7.52 (m, 1H), 7.48 – 7.44 (m, 2H), 7.07 (dq, *J* = 15.2, 6.8 Hz, 1H), 6.91 (dq, *J* = 15.3, 1.6 Hz, 1H), 2.00 (dd, *J* = 6.8, 1.6 Hz, 3H).

### Synthesis of benzamidine<sup>7</sup>



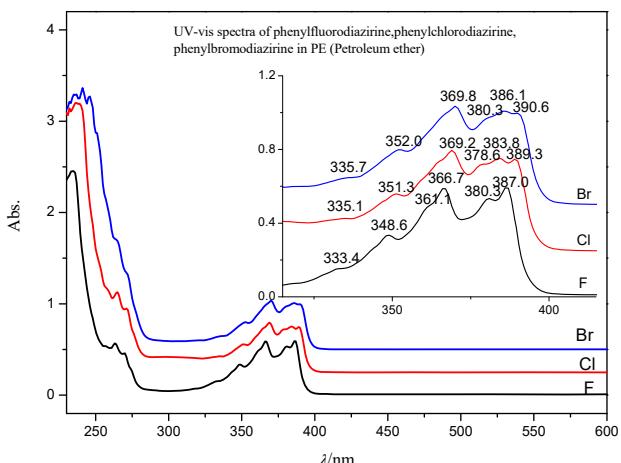
A 1 L round-bottom flask was charged with 500 mL of MeOH (dried over Na metal), 0.5 mol of the appropriate nitrile, and 0.05 mol of sodium methoxide. The contents of the flask were protected from moisture and stirred magnetically for 48 h. Then, 0.5 mol of NH<sub>4</sub>Cl was added and stirring was continued for 24 h. Unreacted NH<sub>4</sub>Cl was filtered, and methanol was stripped from the filtrate to afford the crude products. These were washed free of unreacted aryl nitriles with ether. The recovered nitrile was recycled, whereas the product was directly used in the Graham diazirine synthesis.

### Synthesis of 3-chloro-3-phenyldiazirine: Graham reaction (1a-1g)<sup>8</sup>

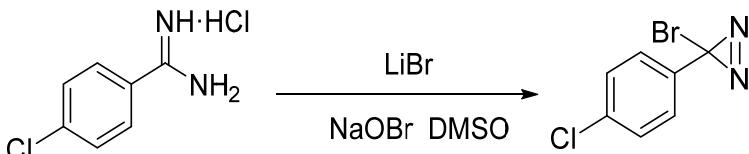


In a 500 mL round-bottom flask, were combined 2 g of LiCl, 1.0 g of amidine, and 40 mL of DMSO. The mixture was stirred magnetically until most of the LiCl had dissolved. Then 80 mL of pentane was added, followed by the slow addition of 300 mL of 12 wt% aqueous NaOCl (saturated with NaCl). The reaction mixture was stirred during the addition of the NaOCl, and the reaction temperature was kept below 40 °C by a cold water bath. Stirring was continued at room temperature for 40 min after the addition. The pentane layer was collected and combined with a (2 × 50 mL) pentane extract of the aqueous phase. The combined pentane solution was washed twice with 200 mL portions of ice water and then dried over sodium sulfate. The desiccant was filtered, the pentane solution was concentrated to about 5 mL on the rotary evaporator, and the concentrate was chromatographed over a short silica column using 10:1 pentane/ether as the eluent. The diazirines were obtained as pale-yellow oil in 50-70% yields. Spectra data of 3-phenyl-3-chloro diazirine: <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.43 – 7.36 (m, 3H), 7.15 – 7.08 (m, 2H). The semi-stable diazirine is usually quickly characterized by UV-vis spectra, which showed a characteristic absorption in the region of 330-400 nm as below.

Typical UV/vis spectra for diazirines:

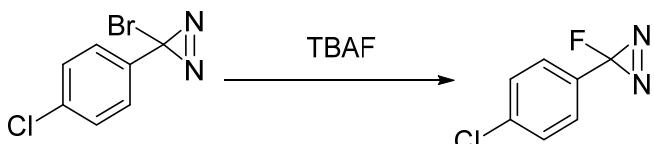


### Synthesis of 3-bromo-3-(4-chlorophenyl)diazirine<sup>7</sup>



A three-neck, 1 L, round-bottom flask was fitted with a mechanical stirrer, a dropping funnel, and a thermometer. It was charged with 0.05 mol of the appropriate amidine salt, 210 mL of DMSO, and 21 g of LiBr. After the salts had dissolved (stirring), 100 mL of hexane was added, and the reaction mixture was cooled to 5 °C with an ice-salt mixture. A fresh solution of NaOBr (0.47 mol) was prepared by the slow addition of 24 mL of bromine to a stirred and cooled (10 °C) solution of 50 g of NaOH and 155 g of NaBr in 360 mL of water. The cooled hypobromite solution was added rapidly through the dropping funnel to the vigorously stirred arylamidine reaction mixture. The reaction temperature was maintained below 30 °C by a cooling bath. After the addition was completed, the reaction mixture was stirred for an additional hour, diluted with 200 mL of water, and transferred to a large separatory funnel. The hexane layer was separated, and the aqueous layer was extracted with 4 × 50 mL of hexane. The combined hexane portions were dried ( $\text{MgSO}_4$ ), filtered, and concentrated *in vacuo* (1 mmHg) at 25 °C. The oily residue was chromatographed on a 20 cm column of 200 ~ 300 mesh silica using hexane as eluent. The diazirines eluted in the first fraction (light yellow). The 3-bromo-3-(4-chlorophenyl)-diazirine was obtained as a slightly yellow oil (6.8g, 59%).

### Synthesis of 3-fluoro-3-(4-chlorophenyl)diazirine<sup>7</sup>

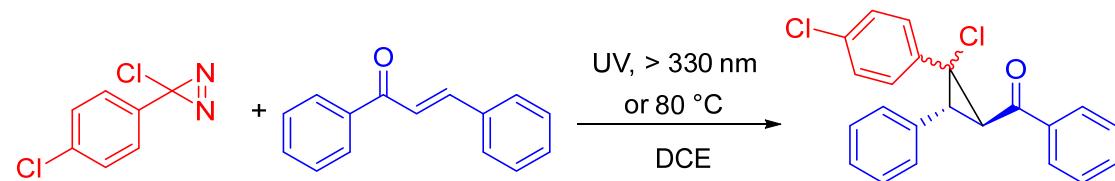


Molten n-Bu<sub>4</sub>N<sup>+</sup>F<sup>-</sup> was prepared from 4 g of the trihydrate in a 25 mL round bottom flask as described above. The fluoride melt was cooled to 25 °C, and 1 g of bromodiazirine was added. The reaction mixture was stirred magnetically at 25 °C in

the dark for 4 h. (Crystals of n-Bu<sub>4</sub>N<sup>+</sup>Br<sup>-</sup> were usually observed to form after 10 min.) The reaction product was quenched with 20 mL of water and the resulting solution was extracted with 65 mL of pentane. The combined pentane extract was dried (MgSO<sub>4</sub>), filtered, and concentrated. The oily residue was chromatographed on a 20 cm column of 200 ~ 300 mesh silica using PE (b.p. 30-60 °C) as eluent. The diazirines eluted in the first fraction. The 3-(4-chlorophenyl)-3-fluoro-diazirine was obtained as a slightly yellow oil (0.37 g, 50%).

#### 4. Details for reaction conditions screening and scope test

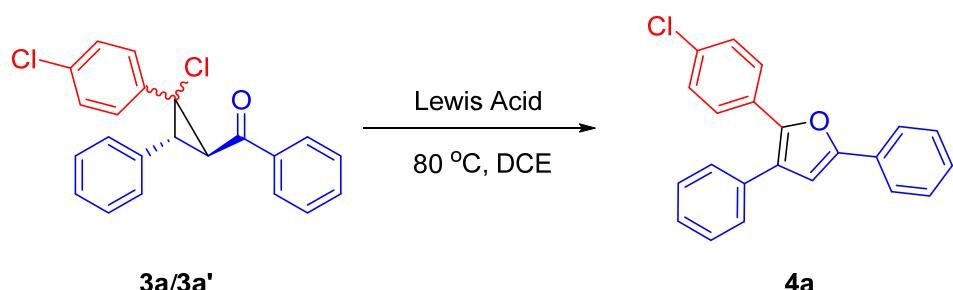
**Table S1** Optimization of cyclopropanes **3a/3a'**. <sup>a</sup>



Entry	1a	2a	3a/3a'	Yield, %	d. r.	
Entry	Solvent	Temp, °C	Agitation method	Time, h		
1	DCE	rt~32	UV, > 330 nm <sup>b</sup>	4.5	77	68:32
2	Et <sub>2</sub> O	rt~32	UV, > 330 nm <sup>b</sup>	11	48	79:21
3	Hexane	rt~32	UV, > 330 nm <sup>b</sup>	24	60	88:12
4	Chlorobenzene	110	In dark.	0.18	30	59:41
5	DCE	Reflux (83.5)	In dark.	0.8	78	57:43
6	DCE	80	In dark.	2	79	59:41
7	DCE	60	In dark.	28	76	61:39
8	DCE	25	In dark.	72	72	62:38
9 <sup>d</sup>	DCE	80	In dark.	2	79	60:40

<sup>a</sup> Reagents and conditions: 3-Chloro-3-(4-chlorophenyl)diazirine **1a** (0.2 mmol) and **2a** (0.2 mmol) were dissolved in DCE (5 mL), degassed and then subjected to irradiation or heating. <sup>b</sup> Under the irradiation of 250 W medium-pressure mercury lamp with 10% NaNO<sub>3</sub> filter. <sup>c</sup> Isolated yield of **3a** and **3a'**. <sup>d</sup> With 4 Å molecular sieves.

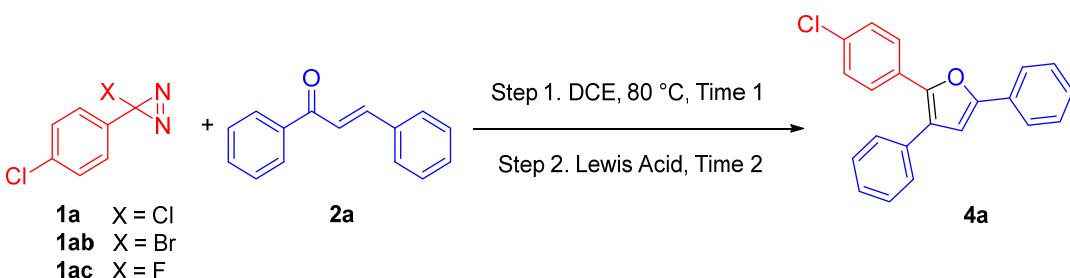
**Table S2** optimizing conditions for cyclopropyl ketone to furan **4a**.<sup>a</sup>



Entry	Reactant	Lewis Acid	Temp, °C	Time (h)	Yield, % <sup>b</sup>
1	<b>3a</b>	TiCl <sub>4</sub> , 1 eq	80	0.16	86
2	<b>3a</b>	FeCl <sub>2</sub> ·4H <sub>2</sub> O, 1 eq	80	0.5	96
3	<b>3a</b>	FeCl <sub>3</sub> ·6H <sub>2</sub> O, 1 eq	80	0.08	86
4	<b>3a</b>	AlCl <sub>3</sub> , 1 eq	80	17	90
5	<b>3a</b>	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	80	15	98
6	<b>3a</b>	SnCl <sub>4</sub> , 1 eq	80	21	87
7	<b>3a</b>	Sc(OTf) <sub>3</sub> , 1 eq	80	45	86
8	<b>3a</b>	PTSA, 1 eq	80	36	90
9	<b>3a</b>	BiCl <sub>3</sub> , 1 eq	80	72	68 <sup>c</sup>
10	<b>3a</b>	CrCl <sub>3</sub> ·6H <sub>2</sub> O, 1 eq	80	72	26 <sup>d</sup>
11	<b>3a</b>	Ferrocene, 1 eq	80	8	NR
12	<b>3a</b>	CuI, 1 eq	80	8	NR
13	<b>3a</b>	CoCl <sub>2</sub> , 1 eq	80	5	NR
14	<b>3a</b>	NiCl <sub>2</sub> , 1 eq	80	5	NR
15	<b>3a</b>	ZnCl <sub>2</sub> , 1 eq	80	5	NR
16	<b>3a</b>	FeCl <sub>2</sub> ·4H <sub>2</sub> O, 0.5 eq	80	0.7	94
17	<b>3a</b>	FeCl <sub>2</sub> ·4H <sub>2</sub> O, 0.2 eq	80	1	97
18	<b>3a</b>	FeCl <sub>2</sub> ·4H <sub>2</sub> O, 0.1 eq	80	8	97
19	<b>3a</b>	FeCl <sub>2</sub> ·4H <sub>2</sub> O, 2 eq	100 <sup>f</sup>	0.16	97
20	<b>3a</b>	FeCl <sub>2</sub> ·4H <sub>2</sub> O, 2 eq	60	1	92
21	<b>3a</b>	BF <sub>3</sub> ·Et <sub>2</sub> O, 2 eq	80	6	98
22	<b>3a</b>	BF <sub>3</sub> ·Et <sub>2</sub> O, 0.5 eq	80	67	94
23	<b>3a</b>	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	100 <sup>f</sup>	4.5	94
24	<b>3a</b>	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	60	28	94
25	<b>3a</b>	No LA	80	24	NR
26 <sup>e</sup>	<b>3a'</b>	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	80	16	98
27 <sup>e</sup>	<b>3a'</b>	FeCl <sub>2</sub> ·4H <sub>2</sub> O, 0.2 eq	80	1	97

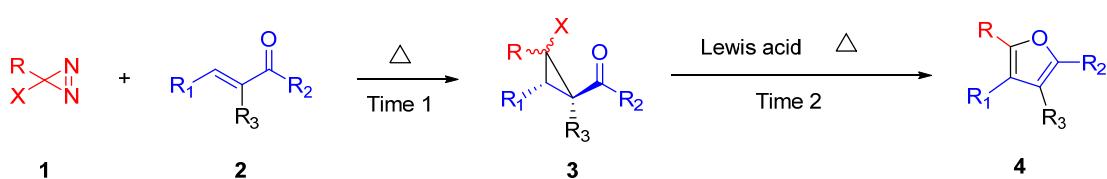
<sup>a</sup> Reagents and conditions: Cyclopropyl ketone **3a** (0.06 mmol), Lewis acid (0.06 mmol) in 5 mL DCE was heated at 80 °C in a 38 mL reaction tube with condenser until the reaction was completed. NR = No reaction. RSM = Recovery of Starting Material. <sup>b</sup> Isolated yield. <sup>c</sup> RSM = 16%. <sup>d</sup> RSM = 60%. <sup>e</sup> **3a'** was used as starting material. <sup>f</sup> Chlorobenzene was used as solvent instead of DCE.

**Table S3** One-flask reaction sequence for **4a** from diazirines (**1a**, **1ab**, **1ac**).<sup>a</sup>

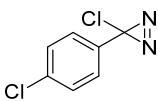
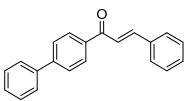
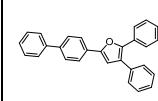
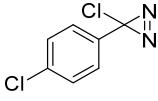
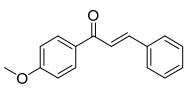
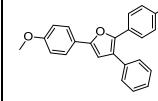
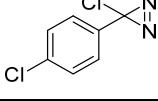
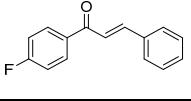
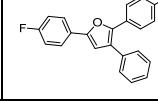
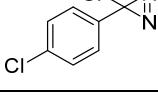
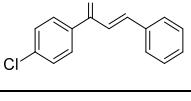
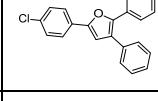
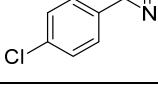
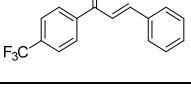
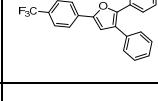
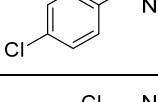
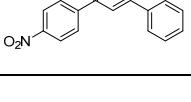
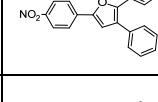
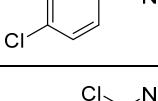
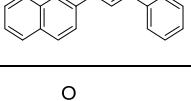
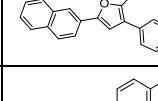
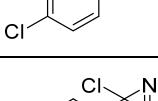
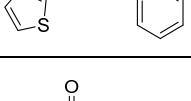
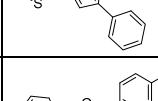
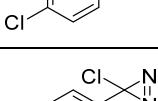
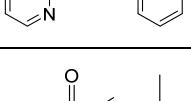
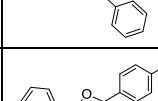
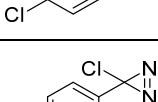
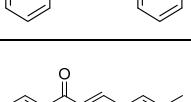
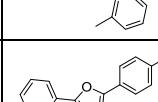
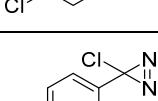
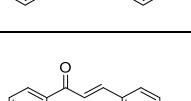
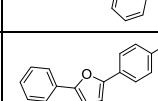
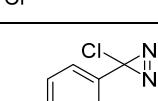
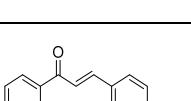
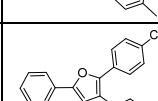
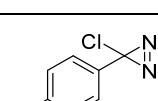
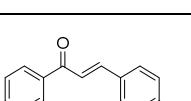
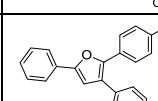


Entry	Diazirine	Time 1, h	Lewis acid	Time 2, h	Yield, % <sup>b</sup>
1	<b>1a</b>	2	TiCl <sub>4</sub> , 1 eq	3	53
2	<b>1a</b>	2	FeCl <sub>3</sub> ·6H <sub>2</sub> O, 1 eq	3.5	56
3	<b>1a</b>	2	FeCl <sub>2</sub> ·4H <sub>2</sub> O, 1 eq	12	61
4	<b>1a</b>	2	AlCl <sub>3</sub> , 1 eq	13	64
5	<b>1a</b>	2	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	17	68
6	<b>1a</b>	2	BF <sub>3</sub> ·Et <sub>2</sub> O, 0.5 eq	72	68
7	<b>1a</b>	2	BF <sub>3</sub> ·Et <sub>2</sub> O, 2 eq	5	70
8	<b>1a</b>	2	FeCl <sub>2</sub> ·4H <sub>2</sub> O, 0.2 eq	25	64
9	<b>1a</b>	2	FeCl <sub>2</sub> ·4H <sub>2</sub> O, 0.5 eq	20	61
10 <sup>c</sup>	<b>1a</b>	/	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	7	11
11 <sup>c, d</sup>	<b>1a</b>	/	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	8	10
12	<b>1ab</b>	2	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	17	62
13	<b>1ac</b>	48	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	2	40

<sup>a</sup> Reagents and conditions: 3-Halo-3-(4-chlorophenyl)diazirine **1a** (0.2 mmol), chalcone **2a** (0.2 mmol) in 5 mL DCE was heated at 80 °C in a 38 mL reaction tube with condenser until the reaction was completed. NR = No reaction. <sup>b</sup> Isolated overall yield. <sup>c</sup> Lewis acid was added in the beginning. <sup>d</sup> Molecular sieve (4 Å) was added.

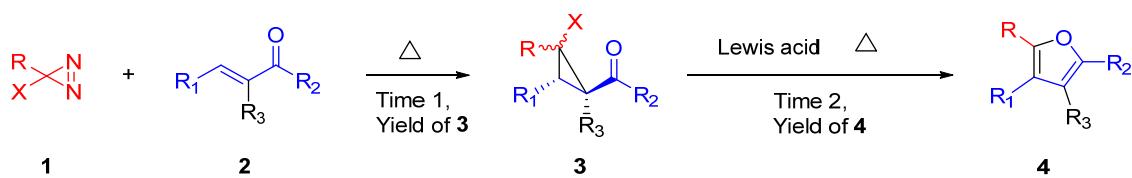
**Table S4** Scope of substrates.<sup>a, b</sup>

Entry	Diazirine 1	Alkenyl ketone 2	Time 1, h	Lewis acid	Time 2, h	Product	Yield d, %
1			2	$\text{BF}_3 \cdot \text{Et}_2\text{O}$ , 1 eq	17		68
			2	$\text{FeCl}_2 \cdot 4\text{H}_2\text{O}$ , 0.2 eq	25		64
2			2	$\text{BF}_3 \cdot \text{Et}_2\text{O}$ , 1 eq	17		71
			2	$\text{FeCl}_2 \cdot 4\text{H}_2\text{O}$ , 0.2 eq	25		62
3			2	$\text{BF}_3 \cdot \text{Et}_2\text{O}$ , 1 eq	16.5		65
			2	$\text{FeCl}_2 \cdot 4\text{H}_2\text{O}$ , 0.2 eq	24		61
4			2	$\text{BF}_3 \cdot \text{Et}_2\text{O}$ , 1 eq	17.5		66
			2	$\text{FeCl}_2 \cdot 4\text{H}_2\text{O}$ , 0.2 eq	25		62
5			2	$\text{BF}_3 \cdot \text{Et}_2\text{O}$ , 1 eq	18		57
			2	$\text{FeCl}_2 \cdot 4\text{H}_2\text{O}$ , 0.2 eq	26		52
6			2	$\text{BF}_3 \cdot \text{Et}_2\text{O}$ , 1 eq	32		21
			2	$\text{BF}_3 \cdot \text{Et}_2\text{O}$ , 5 eq	7		43 <sup>c</sup>
			2	$\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$ , 0.5 eq	13		57
7			2	$\text{BF}_3 \cdot \text{Et}_2\text{O}$ , 5 eq	14		42 <sup>c</sup>
			2	$\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$ , 1 eq	26		55
8			2	$\text{BF}_3 \cdot \text{Et}_2\text{O}$ , 1 eq	16		74
9			2	$\text{BF}_3 \cdot \text{Et}_2\text{O}$ , 1 eq	18		80
10			2	$\text{BF}_3 \cdot \text{Et}_2\text{O}$ , 1 eq	16		71

11			2	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	18		74
12			2	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	19		73
13			2	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	17		80
14			2	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	17		77
15			2	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	17		74
16			2	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	18		79
17			2	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	17		78
18			2	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	24		67
19			2	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	5		40
20			2	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	17		73
21			2	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	17		79
22			2	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	20		75
23			2	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	15		71
24			2	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	17		75

25			2	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	18		78
26			2	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	34		77
27			2	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	17		76
28			2	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	17		62
29			2	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	5		60
30			2	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	4		63
31			2	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	6		67
32			1	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	1		45
33 <sup>d</sup>			2	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	14.5		29
34			2	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	1.5		50
35			2	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	12		29
36 <sup>e</sup>			12	BF <sub>3</sub> ·Et <sub>2</sub> O, 1 eq	23		42

<sup>a</sup> Reagents and conditions: 3-Chloro-3-phenyldiazirine **1** (0.2 mmol), alkenyl ketone **2** (0.2 mmol) in 5 mL DCE was heated at 80 °C in a 38 mL reaction tube with a condenser until the reaction was completed (usually 2 h). Then Lewis acid BF<sub>3</sub>·Et<sub>2</sub>O (0.2 mmol, 1 eq) was added in and kept on heating to complete the transformation. <sup>b</sup> Isolated yield of one-flask reaction. <sup>c</sup> Reacted at 120 °C in *n*-Octane and BF<sub>3</sub>·Et<sub>2</sub>O (5 eq) was used. <sup>d</sup> **1a** (0.2 mmol) was reacted with 2 eq alkenyl ketone (0.4 mmol). <sup>e</sup> Two equivalents of alkenyl ketone were used and reactions were performed at 60 °C in both steps.

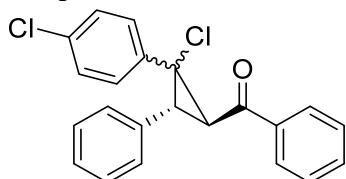
**Table S5** Step-by-step yield. <sup>a, b</sup>

Entr y	Diazirine <b>1</b>	Vinyl ketone <b>2</b>	Time 1, h	Yield of <b>3</b> , %	Time 2, h	Yield of <b>4</b> from <b>3</b> , %	Yield of one- flask reaction, %
1			2	61	17	97	57
2 <sup>c</sup>			2	67.2	12	86	57
3 <sup>c</sup>			2	72	24	85.6	54.8
4			2	47.5	3	95	40
5			2	69.7	15	91	62
6			1	57.4	0.5	89	45
7			2	35	15	92.8	29
8			2	39.5	5	78.5	29.4
9 <sup>d</sup>			11	48.1	5	94.8	42

<sup>a</sup> Reagents and conditions: 3-Halo-3-(4-chlorophenyl)diazirine **1** (0.2 mmol), alkenyl ketone **2** (0.2 mmol) in 5 mL DCE was heated at 80 °C in a 38 mL reaction tube with condenser until the reaction was completed (usually 2 h). Then the cyclopropylketone **3** was separated to determine the yield. The cyclopropylketone **3** was further transformed to furan **4** in the presence of 1 eq BF<sub>3</sub>·Et<sub>2</sub>O at 80 °C and the yield was given. NR = No reaction. <sup>b</sup> Isolated yield of one-flask reaction. <sup>c</sup> FeCl<sub>3</sub>·6H<sub>2</sub>O was used as Lewis acid. <sup>d</sup> **1a** (0.2 mmol) was reacted with 2 eq alkenyl ketone (0.4 mmol) at 60 °C in step 1.

## 5. The spectral data

All the known compounds' (**4a**, **4c**, **4d**, **4e**, **4f**, **4g**, **5o**, **5r**, **6a**, **6b**, **6d**, **6h**) spectral data (<sup>1</sup>H NMR, <sup>13</sup>C NMR, IR, MS) agree with the reported references. The unreported compounds were characterized by <sup>1</sup>H NMR, <sup>13</sup>C NMR, IR and HRMS.



**3a/3a'**

The diastereoisomers **3a/3a'** were separated by silica gel chromatography with a gradient elution of petroleum ether/dichloromethane from 100: 0 to 91: 9.

**2-Chloro-2-(4-chlorophenyl)-3-phenylcyclopropyl(phenyl)methanone (3a)**

Obtained as a white solid in 47% yield (34.0 mg); mp 129–131 °C (DCM/PE = 1:2); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.10 – 8.06 (m, 2H), 7.68 – 7.63 (m, 1H), 7.58 – 7.53 (m, 2H), 7.46 – 7.40 (m, 4H), 7.38 – 7.32 (m, 3H), 7.26 – 7.23 (m, 2H), 3.93 (d, *J* = 7.6 Hz, 1H), 3.84 (d, *J* = 7.6 Hz, 1H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 193.2, 137.5, 136.6, 134.6, 134.5, 133.7, 130.5, 129.3, 129.0, 128.9, 128.42, 128.37, 127.6, 56.8, 40.2, 35.2.

IR(KBr)  $\nu_{\text{max}}$ : 3063, 3039, 3009, 2926, 2858, 1679, 1596, 1494, 1450, 1413, 1329, 1264, 1222, 1211, 1090, 1014, 824, 796, 746, 694, 657, 600, 533 cm<sup>-1</sup>.

HRMS: (ESI) calcd for C<sub>22</sub>H<sub>15</sub>Cl<sub>2</sub>O [M-H] 365.05054; found 365.05035.

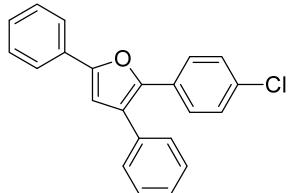
**3a'**, diastereomer of **3a** was obtained as a white solid in 32% yield (24.0 mg); mp 128–130 °C (DCM/PE = 1:2);

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.20 – 8.15 (m, 2H), 7.68 – 7.65 (m, 1H), 7.61 – 7.56 (m, 2H), 7.30 – 7.27 (m, 2H), 7.25 – 7.21 (m, 2H), 7.19 – 7.12 (m, 3H), 6.96 – 6.91 (m, 2H), 3.86 (d, *J* = 7.5 Hz, 1H), 3.83 (d, *J* = 7.5 Hz, 1H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 192.6, 137.9, 136.4, 134.52, 134.47, 133.7, 130.7, 129.1, 129.0, 128.6, 128.4, 128.2, 127.3, 53.1, 38.4, 36.3.

IR(KBr)  $\nu_{\text{max}}$ : 3087, 3066, 3027, 1678, 1597, 1581, 1494, 1448, 1413, 1399, 1333, 1303, 1263, 1214, 1180, 1149, 1092, 1032, 1014, 1001, 822, 796, 746, 732, 712, 692, 658, 600, 533 cm<sup>-1</sup>.

HRMS: (ESI) calcd for C<sub>22</sub>H<sub>15</sub>Cl<sub>2</sub>O [M-H] 365.05054; found 365.05035.



**2-(4-Chlorophenyl)-3,5-diphenylfuran (4a)**

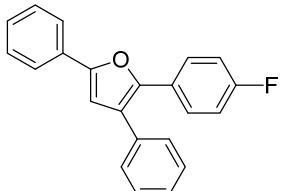
Obtained as a white solid in 68% yield (46.0 mg); mp 101–103 °C (lit<sup>9</sup> 100–102 °C) (DCM/PE = 1:2);

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.76 (d, *J* = 7.5 Hz, 2H), 7.55 – 7.52 (m, 2H), 7.46 –

7.38 (m, 6H), 7.36 (d,  $J = 7.2$  Hz, 1H), 7.31 (t,  $J = 7.4$  Hz, 1H), 7.29 – 7.26 (m, 2H), 6.81 (s, 1H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  153.0, 146.9, 134.2, 133.3, 130.5, 129.7, 128.94, 128.92, 128.8(2C), 127.9, 127.7, 127.4, 125.2, 124.0, 109.7.

IR(KBr)  $\nu_{\text{max}}$ : 3063, 3030, 1500, 1488, 1476, 1449, 1146, 1094, 1012, 953, 932, 830, 759, 743, 719, 699, 664, 532, 495  $\text{cm}^{-1}$ .



#### 2-(4-Fluorophenyl)-3,5-diphenylfuran (**4b**)

Obtained as a white solid in 70% yield (44.3 mg); mp 86–88 °C (DCM/PE = 1:2);

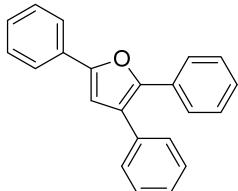
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.77 – 7.74 (m, 2H), 7.60 – 7.56 (m, 2H), 7.46 – 7.38 (m, 6H), 7.36 – 7.32 (m, 1H), 7.30 (t,  $J = 7.4$  Hz, 1H), 7.01 (t,  $J = 8.8$  Hz, 2H), 6.81 (s, 1H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  162.3 (d,  $J = 247.6$  Hz), 152.7, 147.2, 134.2, 130.6, 128.9, 128.8, 128.1 (d,  $J = 8.0$  Hz), 127.7, 127.54, 127.49 (d,  $J = 3.3$  Hz), 124.4, 123.9, 115.6 (d,  $J = 21.8$  Hz), 109.5.

$^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -113.69.

IR(KBr)  $\nu_{\text{max}}$ : 3078, 3057, 3027, 1606, 1509, 1489, 1449, 1234, 1158, 1146, 953, 932, 836, 813, 759, 723, 712, 692, 665, 612, 585  $\text{cm}^{-1}$ .

HRMS: (ESI) calcd for  $\text{C}_{22}\text{H}_{16}\text{FO}^+ [\text{M}+\text{H}]^+$  315.11797; found 315.11761.



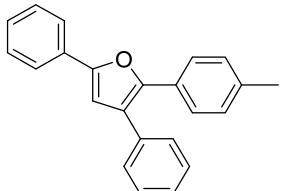
#### 2,3,5-Triphenylfuran (**4c**)

Obtained as a white solid in 64% yield (38.2 mg); mp 90–92 °C (lit<sup>9</sup> 91–93 °C) (DCM/PE = 1:2);

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.77 (dd,  $J = 8.2, 1.0$  Hz, 2H), 7.63 – 7.60 (m, 2H), 7.47 (dt,  $J = 3.0, 1.8$  Hz, 2H), 7.44 – 7.37 (m, 4H), 7.36 – 7.29 (m, 4H), 7.28 – 7.24 (m, 1H), 6.82 (s, 1H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  152.7, 148.0, 134.5, 131.2, 130.7, 128.9, 128.84, 128.82, 128.6, 127.7, 127.6, 127.4, 126.3, 124.7, 124.0, 109.6.

IR(KBr)  $\nu_{\text{max}}$ : 3063, 3030, 1602, 1593, 1502, 1488, 1444, 1145, 1073, 1054, 1027, 953, 932, 912, 815, 761, 722, 694, 674, 664, 593, 503, 481  $\text{cm}^{-1}$ .



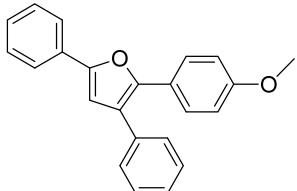
#### 3,5-Diphenyl-2-(p-tolyl)furan (**4d**)

Obtained as a white solid in 66% yield (41.0 mg); mp 107-109 °C (lit<sup>9</sup> 108-110 °C) (DCM/PE = 1:2);

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.77 (d, *J* = 8.2 Hz, 2H), 7.54 – 7.50 (m, 2H), 7.48 (dd, *J* = 7.1, 1.2 Hz, 2H), 7.44 – 7.37 (m, 4H), 7.35 – 7.27 (m, 2H), 7.13 (d, *J* = 7.8 Hz, 2H), 6.82 (s, 1H), 2.36 (s, 3H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 152.4, 148.3, 137.6, 134.6, 130.8, 129.3, 128.9, 128.80, 128.77, 128.5, 127.5, 127.3, 126.3, 124.0, 123.9, 109.5, 21.5.

IR(KBr) ν<sub>max</sub>: 3083, 3060, 3030, 2930, 2863, 1608, 1593, 1512, 1489, 1449, 1145, 1114, 1073, 1055, 1027, 953, 932, 821, 758, 719, 694, 664, 587, 505, 485 cm<sup>-1</sup>.



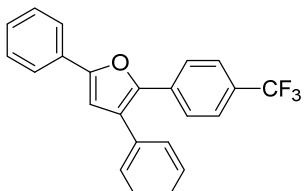
#### 2-(4-Methoxyphenyl)-3,5-diphenylfuran (4e)

Obtained as a white solid in 57% yield (37.0 mg); mp 56-58 °C<sup>10</sup> (DCM/PE = 1:2);

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.75 (dd, *J* = 8.3, 1.1 Hz, 2H), 7.56 – 7.53 (m, 2H), 7.46 (dt, *J* = 3.0, 1.7 Hz, 2H), 7.43 – 7.36 (m, 4H), 7.34 – 7.26 (m, 2H), 6.88 – 6.84 (m, 2H), 6.81 (s, 1H), 3.82 (s, 3H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 159.3, 152.2, 148.2, 134.6, 130.8, 128.8, 128.78, 128.77, 127.8, 127.4, 127.2, 124.1, 123.8, 123.2, 114.0, 109.4, 55.4.

IR(KBr) ν<sub>max</sub>: 3060, 3003, 2953, 2938, 2908, 2837, 1608, 1570, 1511, 1489, 1463, 1450, 1442, 1299, 1250, 1177, 1145, 1055, 1033, 953, 932, 833, 759, 729, 712, 695, 663, 614, 586 cm<sup>-1</sup>.



#### 3,5-Diphenyl-2-(4-(trifluoromethyl) phenyl) furan (4f)

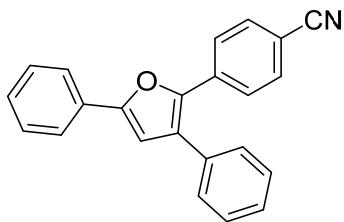
Obtained as a white solid in 43% yield (31.2 mg); mp 79-81 °C (lit<sup>11</sup> 85-86 °C) (DCM/PE = 1:2);

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.78 (d, *J* = 7.6 Hz, 2H), 7.70 (d, *J* = 8.3 Hz, 2H), 7.54 (d, *J* = 8.4 Hz, 2H), 7.47 – 7.36 (m, 7H), 7.33 (t, *J* = 7.2 Hz, 1H), 6.83 (s, 1H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 153.6, 146.4, 134.5, 134.0, 130.3, 129.2 (q, *J* = 32.6 Hz), 129.0, 128.90, 128.86, 128.1, 128.0, 126.7, 125.9, 125.5 (q, *J* = 3.7 Hz), 124.4 (q, *J* = 268.4 Hz), 124.2, 110.0.

<sup>19</sup>F NMR (471 MHz, CDCl<sub>3</sub>) δ -62.64.

IR(KBr) ν<sub>max</sub>: 3060, 3030, 2923, 1618, 1490, 1449, 1412, 1385, 1324, 1166, 1123, 1110, 1070, 1016, 953, 932, 843, 759, 719, 694, 665, 605, 473 cm<sup>-1</sup>.



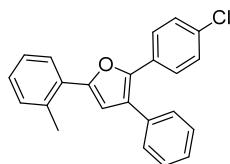
**4-(3,5-Diphenylfuran-2-yl)benzonitrile (4g)**

Obtained as a yellow solid in 42% yield (26.8 mg); mp 112-114 °C (lit<sup>11</sup> 105-106 °C) (DCM/PE = 1:2);

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.77 (d, *J* = 7.3 Hz, 2H), 7.68 (d, *J* = 8.6 Hz, 2H), 7.55 (d, *J* = 8.6 Hz, 2H), 7.48 – 7.39 (m, 7H), 7.34 (t, *J* = 7.4 Hz, 1H), 6.82 (s, 1H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 154.1, 145.7, 135.2, 133.7, 132.4, 130.0, 129.1, 129.0, 128.8, 128.4, 128.2, 128.0, 125.8, 124.2, 119.1, 110.3, 110.2.

IR(KBr) ν<sub>max</sub>: 3108, 2221, 1606, 1508, 1489, 1448, 1180, 951, 930, 839, 760, 709, 697, 667, 599, 566, 552 cm<sup>-1</sup>.



**2-(4-Chlorophenyl)-3-phenyl-5-(o-tolyl)furan (5a)**

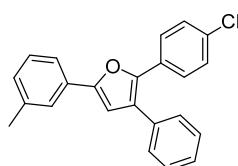
Obtained as a white solid in 74% yield (51.0 mg); mp 148-150 °C (DCM/PE = 1:2);

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.80 (d, *J* = 7.5 Hz, 1H), 7.52 (d, *J* = 8.4 Hz, 2H), 7.46 (d, *J* = 7.2 Hz, 2H), 7.40 (t, *J* = 7.4 Hz, 2H), 7.36 – 7.33 (m, 1H), 7.30 – 7.23 (m, 5H), 6.70 (s, 1H), 2.58 (s, 3H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 152.7, 146.5, 134.8, 134.3, 133.2, 131.5, 129.74, 129.70, 128.9, 128.85, 128.80, 127.9, 127.6, 127.3, 127.1, 126.2, 124.8, 113.2, 22.3.

IR(KBr) ν<sub>max</sub>: 3060, 3024, 29265, 2860. 1601, 1499, 1481, 1446, 1403, 1384, 1149, 1122, 1094, 1039, 1012, 954, 932, 830, 759, 741, 720, 698, 597, 535, 493, 450 cm<sup>-1</sup>.

HRMS: (ESI) calcd for C<sub>23</sub>H<sub>18</sub>ClO<sup>+</sup> [M+H]<sup>+</sup> 345.10406; found 345.10394.



**2-(4-Chlorophenyl)-3-phenyl-5-(m-tolyl)furan (5b)**

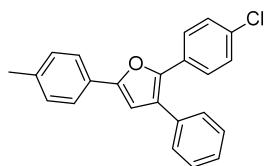
Obtained as a white solid in 80% yield (55.3 mg); mp 72-74 °C (DCM/PE = 1:2);

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.59 – 7.53 (m, 4H), 7.47 – 7.44 (m, 2H), 7.40 (t, *J* = 7.3 Hz, 2H), 7.37 – 7.30 (m, 2H), 7.29 – 7.26 (m, 2H), 7.13 (d, *J* = 7.5 Hz, 1H), 6.80 (s, 1H), 2.43 (s, 3H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 153.1, 146.8, 138.5, 134.2, 133.2, 130.4, 129.7, 128.9, 128.82, 128.79, 128.77, 128.7, 127.6, 127.4, 125.2, 124.6, 121.2, 109.6, 21.7.

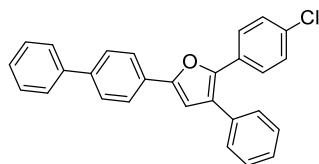
IR(KBr) ν<sub>max</sub>: 3060, 3027, 2930, 2855, 1609, 1588, 1563, 1500, 1482, 1446, 1402, 1384, 1145, 1094, 1063, 1012, 953, 830, 783, 764, 740, 719, 698, 596, 494, 438 cm<sup>-1</sup>.

HRMS: (ESI) calcd for  $C_{23}H_{18}ClO^+ [M+H]^+$  345.10406; found 345.10391.



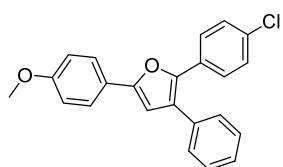
**2-(4-Chlorophenyl)-3-phenyl-5-(p-tolyl)furan (5c)**

Obtained as a white solid in 70% yield (41.8 mg); mp 98–100 °C (DCM/PE = 1:2);  
 $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  7.65 (d,  $J$  = 7.4 Hz, 2H), 7.53 (dd,  $J$  = 8.5, 1.2 Hz, 2H),  
7.46 – 7.43 (m, 2H), 7.42 – 7.38 (m, 2H), 7.36 – 7.33 (m, 1H), 7.27 (d,  $J$  = 7.5 Hz, 2H),  
7.23 (d,  $J$  = 7.9 Hz, 2H), 6.75 (s, 1H), 2.39 (s, 3H).  
 $^{13}C$  NMR (126 MHz,  $CDCl_3$ )  $\delta$  153.2, 146.5, 137.8, 134.3, 133.1, 129.8, 129.6, 128.9,  
128.80, 128.76, 127.8, 127.6, 127.3, 125.2, 124.0, 109.0, 21.5.  
IR(KBr)  $\nu_{max}$ : 3057, 3030, 2920, 2857, 1600, 1499, 1478, 1446, 1402, 1385, 1145, 1093,  
1053, 1028, 1012, 953, 933, 830, 808, 764, 741, 719, 699, 667, 593, 524, 494  $cm^{-1}$ .  
HRMS: (ESI) calcd for  $C_{23}H_{18}ClO^+ [M+H]^+$  345.10406; found 345.10391.



**5-([1,1'-Diphenyl]-4-yl)-2-(4-chlorophenyl)-3-phenylfuran (5d)**

Obtained as a white feather in 74% yield (60.2 mg); mp 166–168 °C (DCM/PE = 1:2);  
 $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  7.82 (d,  $J$  = 8.3 Hz, 2H), 7.67 (d,  $J$  = 8.5 Hz, 2H), 7.65  
(d,  $J$  = 7.6 Hz, 2H), 7.55 (d,  $J$  = 8.6 Hz, 2H), 7.48 – 7.44 (m, 4H), 7.41 (t,  $J$  = 7.4 Hz,  
2H), 7.39 – 7.34 (m, 2H), 7.28 (d,  $J$  = 8.6 Hz, 2H), 6.85 (s, 1H).  
 $^{13}C$  NMR (126 MHz,  $CDCl_3$ )  $\delta$  152.7, 147.0, 140.7, 140.5, 134.1, 133.3, 129.7, 129.4,  
129.00, 128.96, 128.8, 127.7, 127.61, 127.59, 127.4, 127.1, 125.3, 124.4, 109.9.  
IR(KBr)  $\nu_{max}$ : 3060, 3027, 1599, 1499, 1485, 1446, 1410, 1385, 1146, 1094, 1056, 1012,  
952, 932, 831, 762, 738, 725, 696, 667  $cm^{-1}$ .  
HRMS: (ESI) calcd for  $C_{28}H_{20}ClO^+ [M+H]^+$  407.11971; found 407.11929.

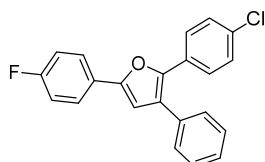


**2-(4-Chlorophenyl)-5-(4-methoxyphenyl)-3-phenylfuran (5e)**

Obtained as a yellow solid in 73% yield (53.0 mg); mp 89–91 °C (DCM/PE = 1:2);  
 $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  7.68 (d,  $J$  = 8.8 Hz, 2H), 7.51 (d,  $J$  = 8.6 Hz, 2H), 7.44  
(d,  $J$  = 7.0 Hz, 2H), 7.39 (t,  $J$  = 7.3 Hz, 2H), 7.34 (t,  $J$  = 7.2 Hz, 1H), 7.27 – 7.25 (m,  
2H), 6.96 (d,  $J$  = 8.8 Hz, 2H), 6.67 (s, 1H), 3.86 (s, 3H).  
 $^{13}C$  NMR (126 MHz,  $CDCl_3$ )  $\delta$  159.5, 153.1, 146.2, 134.3, 133.0, 129.8, 128.9, 128.79,  
128.75, 127.6, 127.2, 125.5, 125.2, 123.5, 114.4, 108.2, 55.5.  
IR(KBr)  $\nu_{max}$ : 3057, 3000, 2952, 2837, 1612, 1499, 1441, 1303, 1249, 1175, 1110, 1093,

1054, 1031, 1012, 953, 933, 831, 764, 740, 699, 614, 509 cm<sup>-1</sup>.

HRMS: (ESI) calcd for C<sub>23</sub>H<sub>18</sub>ClO<sub>2</sub><sup>+</sup> [M+H]<sup>+</sup> 361.09898; found 361.09860.



**2-(4-Chlorophenyl)-5-(4-fluorophenyl)-3-phenylfuran (5f)**

Obtained as a white solid in 80% yield (56.2 mg); mp 110-112 °C (DCM/PE = 1:2);

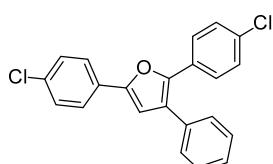
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.74 – 7.70 (m, 2H), 7.51 (d, J = 8.5 Hz, 2H), 7.43 (t, J = 7.0 Hz, 3H), 7.39 (d, J = 7.6 Hz, 1H), 7.36 (d, J = 7.0 Hz, 1H), 7.28 – 7.25 (m, 2H), 7.12 (t, J = 8.6 Hz, 2H), 6.74 (s, 1H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 162.5 (d, J = 247.8 Hz), 152.1, 146.9, 134.0, 133.4, 129.6, 129.0, 128.81, 128.76, 127.7, 127.4, 126.8 (d, J = 3.2 Hz), 125.8 (d, J = 8.1 Hz), 125.2, 116.0 (d, J = 22.0 Hz), 109.4.

<sup>19</sup>F NMR (471 MHz, CDCl<sub>3</sub>) δ -114.09.

IR(KBr) ν<sub>max</sub>: 3057, 3024, 1604, 1497, 1478, 1446, 1402, 1232, 1157, 1146, 1094, 1053, 1012, 953, 933, 831, 812, 765, 741, 720, 699, 612, 593, 503 cm<sup>-1</sup>.

HRMS: (ESI) calcd for C<sub>22</sub>H<sub>15</sub>ClFO<sup>+</sup> [M+H]<sup>+</sup> 349.07899; found 349.07874.



**2,5-Dis(4-chlorophenyl)-3-phenylfuran (5g)**

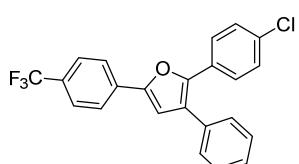
Obtained as a white needle in 77% yield (56.5 mg); mp 108-110 °C (DCM/PE = 1:2);

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.75 (d, J = 7.4 Hz, 2H), 7.51 (d, J = 8.6 Hz, 2H), 7.43 (t, J = 7.7 Hz, 2H), 7.37 (s, 4H), 7.32 (d, J = 7.4 Hz, 1H), 7.31 – 7.28 (m, 2H), 6.77 (s, 1H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 153.2, 147.1, 133.59, 133.55, 132.6, 130.3, 130.1, 129.4, 129.2, 129.0, 128.9, 128.0, 127.5, 124.0, 123.9, 109.3.

IR(KBr) ν<sub>max</sub>: 3081, 3066, 3027, 1603, 1498, 1485, 1447, 1400, 1384, 1146, 1092, 1053, 1027, 1012, 953, 932, 830, 763, 749, 720, 699, 664, 594, 553, 496 cm<sup>-1</sup>.

HRMS: (ESI) calcd for C<sub>22</sub>H<sub>15</sub>Cl<sub>2</sub>O<sup>+</sup> [M+H]<sup>+</sup> 365.04944; found 365.04926.



**2-(4-Chlorophenyl)-3-phenyl-5-(4-(trifluoromethyl) phenyl)furan (5h)**

Obtained as a white solid in 74% yield (59.3 mg); mp 128-130 °C (DCM/PE = 1:2);

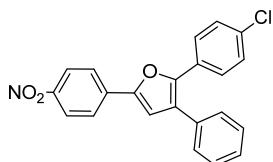
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.77 – 7.74 (m, 2H), 7.65 (d, J = 8.1 Hz, 2H), 7.56 (d, J = 8.1 Hz, 2H), 7.52 – 7.48 (m, 2H), 7.43 (t, J = 7.7 Hz, 2H), 7.34 – 7.29 (m, 3H), 6.82 (s, 1H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 151.4, 148.0, 133.8, 133.7, 133.6, 129.4 (q, *J* = 32.5 Hz), 129.3, 129.0, 128.9, 128.8, 127.9, 127.6, 126.0 (q, *J* = 3.8 Hz), 125.4, 124.3(q, *J* = 271.8 Hz), 123.9, 111.6.

<sup>19</sup>F NMR (471 MHz, CDCl<sub>3</sub>) δ -62.58.

IR(KBr)  $\nu_{\text{max}}$ : 3060, 3027, 1618, 1500, 1477, 1324, 1166, 1124, 1109, 1096, 1069, 1050, 1014, 953, 933, 843, 831, 765, 742, 720, 699, 674, 594, 497 cm<sup>-1</sup>.

HRMS: (ESI) calcd for C<sub>23</sub>H<sub>15</sub>ClF<sub>3</sub>O<sup>+</sup> [M+H]<sup>+</sup> 399.07580; found 399.07535.



### 2-(4-Chlorophenyl)-5-(4-nitrophenyl)-3-phenylfuran (**5i**)

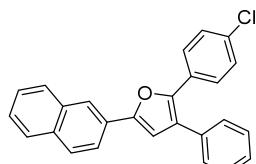
Obtained as the orange needle in 79% yield (59.3 mg); mp 157-159 °C (DCM/PE = 1:2);

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.28 (d, *J* = 8.8 Hz, 2H), 7.86 (d, *J* = 8.8 Hz, 2H), 7.56 – 7.52 (m, 2H), 7.44 – 7.36 (m, 5H), 7.32 – 7.28 (m, 2H), 7.03 (s, 1H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 150.6, 149.2, 146.7, 136.0, 134.2, 133.3, 129.1, 129.0, 128.9, 128.7, 128.1, 127.7, 125.8, 124.6, 124.0, 113.5.

IR(KBr)  $\nu_{\text{max}}$ : 3104, 3066, 3027, 2926, 1598, 1514, 1486, 1473, 1386, 1335, 1182, 1151, 1109, 1093, 1012, 953, 933, 852, 832, 766, 753, 745, 720, 699, 678, 495 cm<sup>-1</sup>.

HRMS: (ESI) calcd for C<sub>22</sub>H<sub>15</sub>ClNO<sub>3</sub><sup>+</sup> [M+H]<sup>+</sup> 376.07349; found 376.07300.



### 2-(4-Chlorophenyl)-5-(naphthalen-2-yl)-3-phenylfuran (**5j**)

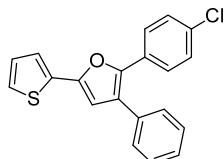
Obtained as a yellow solid in 78% yield (59.6 mg); mp 130-132 °C (DCM/PE = 1:2);

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.23 (s, 1H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.88 (d, *J* = 8.7 Hz, 1H), 7.83 (dd, *J* = 6.4, 2.1 Hz, 2H), 7.60 – 7.57 (m, 2H), 7.53 – 7.47 (m, 4H), 7.43 – 7.40 (m, 2H), 7.38 – 7.35 (m, 1H), 7.32 – 7.29 (m, 2H), 6.93 (s, 1H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 153.0, 147.2, 134.1, 133.7, 133.4, 133.0, 129.7, 129.0, 128.83, 128.81, 128.7, 128.3, 128.0, 127.8, 127.7, 127.5, 126.8, 126.2, 125.4, 122.41, 122.35, 110.4.

IR(KBr)  $\nu_{\text{max}}$ : 3060, 3030, 1629, 1601, 1500, 1480, 1446, 1393, 1265, 1147, 1093, 1012, 964, 953, 929, 890, 856, 831, 812, 765, 741, 719, 699, 531, 493, 473 cm<sup>-1</sup>.

HRMS: (ESI) calcd for C<sub>26</sub>H<sub>18</sub>ClO<sup>+</sup> [M+H]<sup>+</sup> 381.10406; found 381.10388.



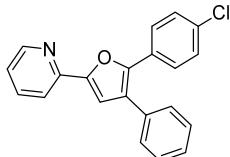
### 2-(4-Chlorophenyl)-3-phenyl-5-(thiophen-2-yl)furan (**5k**)

Obtained as a pale green solid in 67% yield (45.0 mg); mp 89-91 °C (DCM/PE = 1:2);  
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.51 – 7.48 (m, 2H), 7.41 (dt, *J* = 7.9, 1.8 Hz, 2H), 7.40 – 7.36 (m, 2H), 7.35 – 7.32 (m, 2H), 7.27 – 7.25 (m, 2H), 7.24 (d, *J* = 2.1 Hz, 1H), 7.07 (dd, *J* = 5.0, 3.6 Hz, 1H), 6.65 (s, 1H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 148.6, 146.5, 133.9, 133.36, 133.35, 129.4, 129.0, 128.79, 128.78, 127.9, 127.8, 127.4, 125.1, 124.8, 123.2, 109.6.

IR(KBr) ν<sub>max</sub>: 3104, 3060, 3024, 1601, 1499, 1477, 1446, 1424, 1385, 1139, 1093, 1012, 952, 897, 847, 829, 764, 739, 718, 696, 530, 493 cm<sup>-1</sup>.

HRMS: (ESI) calcd for C<sub>20</sub>H<sub>14</sub>ClOS<sup>+</sup> [M+H]<sup>+</sup> 337.04448; found 337.04443.



*2-(5-(4-Chlorophenyl)-4-phenylfuran-2-yl) pyridine (5l)*

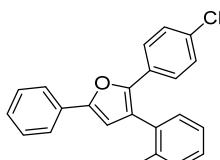
Obtained as a yellow solid in 40% yield (26.5 mg); mp 78-80 °C (DCM/PE = 1:2);

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.63 (d, *J* = 4.8 Hz, 1H), 7.80 (d, *J* = 7.9 Hz, 1H), 7.75 (td, *J* = 7.7, 1.6 Hz, 1H), 7.57 – 7.54 (m, 2H), 7.46 – 7.44 (m, 2H), 7.39 (t, *J* = 7.3 Hz, 2H), 7.35 (dd, *J* = 6.1, 3.8 Hz, 1H), 7.29 (dd, *J* = 8.9, 2.0 Hz, 2H), 7.24 (s, 1H), 7.21 – 7.17 (m, 1H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 152.6, 149.9, 149.2, 148.2, 136.8, 133.79, 133.77, 129.4, 129.0, 128.84, 128.76, 127.76, 127.75, 125.5, 122.3, 118.8, 113.0.

IR(KBr) ν<sub>max</sub>: 3060, 2926, 2854, 1582, 1500, 1478, 1425, 1148, 1095, 952, 831, 780, 765, 713, 699 cm<sup>-1</sup>.

HRMS: (ESI) calcd for C<sub>21</sub>H<sub>15</sub>ClNO<sup>+</sup> [M+H]<sup>+</sup> 332.08366; found 332.08334.



*3-(4-Chlorophenyl)-5-phenyl-2-(o-tolyl) furan (5m)*

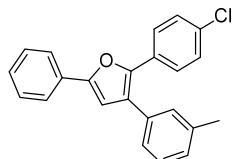
Obtained as a white feather in 72% yield (50.1 mg); mp 99-101 °C (DCM/PE = 1:2);

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.75 – 7.72 (m, 2H), 7.41 (t, *J* = 7.8 Hz, 2H), 7.36 (d, *J* = 7.6 Hz, 1H), 7.34 – 7.27 (m, 3H), 7.26 – 7.19 (m, 5H), 6.93 (s, 1H), 2.25 (s, 3H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 153.4, 149.2, 137.8, 132.7, 132.4, 130.9, 130.8, 130.7, 130.6, 129.2, 128.90, 128.87, 128.8, 127.8, 126.0, 123.9, 123.8, 106.6, 20.5.

IR(KBr) ν<sub>max</sub>: 3060, 3030, 2959, 2920, 1607, 1553, 1489, 1450, 1408, 1381, 1142, 1117, 1092, 1072, 1052, 1036, 1014, 953, 932, 834, 808, 761, 740, 725, 690, 665, 598, 522, 505, 453 cm<sup>-1</sup>.

HRMS: (ESI) calcd for C<sub>23</sub>H<sub>18</sub>ClO<sup>+</sup> [M+H]<sup>+</sup> 345.10406; found 345.10388.



*2-(4-Chlorophenyl)-5-phenyl-3-(*m*-tolyl)furan (**5n**)*

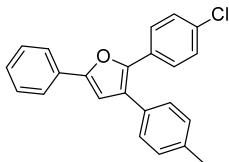
Obtained as a white solid in 79% yield (54.4 mg); mp 76–78 °C (DCM/PE = 1:2);

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.75 (d, *J* = 8.2 Hz, 2H), 7.54 (d, *J* = 8.0 Hz, 2H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.32 – 7.29 (m, 1H), 7.29 – 7.26 (m, 4H), 7.23 (d, *J* = 7.2 Hz, 1H), 7.17 (d, *J* = 7.1 Hz, 1H), 6.80 (s, 1H), 2.38 (s, 3H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 152.9, 146.8, 138.6, 134.1, 133.2, 130.5, 129.8, 129.4, 128.9, 128.82, 128.75, 128.4, 127.8, 127.3, 125.9, 125.3, 124.0, 109.8, 21.6.

IR(KBr) ν<sub>max</sub>: 3063, 3039, 2920, 2863, 1606, 1560, 1488, 1448, 1402, 1384, 1264, 1180, 1143, 1093, 1056, 1027, 1013, 970, 932, 909, 829, 787, 760, 740, 719, 704, 690, 667, 533, 505, 485 cm<sup>-1</sup>.

HRMS: (ESI) calcd for C<sub>23</sub>H<sub>18</sub>ClO<sup>+</sup> [M+H]<sup>+</sup> 345.10406; found 345.10391.



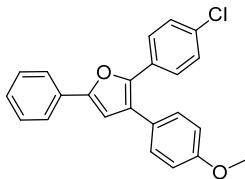
*2-(4-Chlorophenyl)-5-phenyl-3-(*p*-tolyl)furan (**5o**)*

Obtained as a white solid in 75% yield (51.5 mg); mp 82–84 °C<sup>12</sup> (DCM/PE = 1:2);

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.78 – 7.74 (m, 2H), 7.57 – 7.54 (m, 2H), 7.43 (t, *J* = 7.7 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 7.31 (d, *J* = 7.4 Hz, 1H), 7.29 – 7.27 (m, 2H), 7.22 (d, *J* = 7.8 Hz, 2H), 6.79 (s, 1H), 2.42 (s, 3H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 152.8, 146.7, 137.4, 133.2, 131.1, 130.5, 129.8, 129.6, 128.9, 128.7, 128.6, 127.8, 127.3, 125.2, 124.0, 109.8, 21.4.

IR(KBr) ν<sub>max</sub>: 3063, 3030, 2923, 2855, 1610, 1511, 1489, 1448, 1401, 1384, 1145, 1093, 1055, 1012, 953, 932, 824, 811, 760, 740, 723, 689, 665, 589, 529, 499 cm<sup>-1</sup>.



*2-(4-Chlorophenyl)-3-(4-methoxyphenyl)-5-phenylfuran (**5p**)*

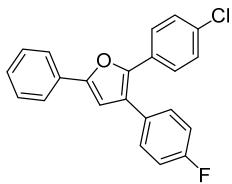
Obtained as a yellow solid in 71% yield (51.4 mg); mp 126–128 °C (DCM/PE = 1:2);

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.75 (d, *J* = 7.6 Hz, 2H), 7.52 (d, *J* = 8.8 Hz, 2H), 7.44 – 7.38 (m, 4H), 7.35 (d, *J* = 8.5 Hz, 2H), 7.29 (t, *J* = 7.4 Hz, 1H), 6.88 (d, *J* = 8.8 Hz, 2H), 6.78 (s, 1H), 3.83 (s, 3H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 159.4, 152.4, 148.4, 133.1, 133.0, 130.6, 130.0, 129.0, 128.9, 127.9, 127.6, 123.8, 123.7, 122.0, 114.1, 108.9, 55.4.

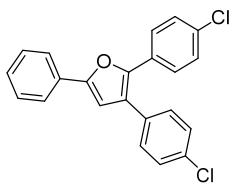
IR(KBr) ν<sub>max</sub>: 3006, 2962, 2929, 2908, 2831, 1608, 1571, 1509, 1489, 1463, 1441, 1300, 1251, 1176, 1145, 1091, 1053, 1030, 1015, 953, 932, 832, 812, 798, 761, 730, 690, 590, 529, 511 cm<sup>-1</sup>.

HRMS: (ESI) calcd for C<sub>23</sub>H<sub>18</sub>ClO<sub>2</sub><sup>+</sup> [M+H]<sup>+</sup> 361.09898; found 361.09875.



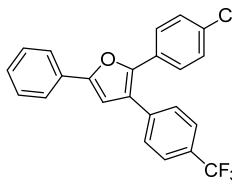
**2-(4-Chlorophenyl)-3-(4-fluorophenyl)-5-phenylfuran (5q)**

Obtained as a white solid in 75% yield (53.0 mg); mp 90-92 °C (DCM/PE = 1:2);  
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.75 (d, *J* = 8.2 Hz, 2H), 7.51 (d, *J* = 8.5 Hz, 2H), 7.45 – 7.39 (m, 4H), 7.35 – 7.30 (m, 1H), 7.29 (d, *J* = 8.6 Hz, 2H), 7.10 (t, *J* = 8.7 Hz, 2H), 6.77 (s, 1H).  
<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 162.4 (d, *J* = 247.0 Hz), 153.0, 146.9, 133.4, 130.4 (d, *J* = 8.0 Hz), 130.3, 130.1 (d, *J* = 3.4 Hz), 129.5, 128.93, 128.86, 127.9, 127.3, 124.1, 124.0, 116.0 (d, *J* = 21.5 Hz), 109.6.  
<sup>19</sup>F NMR (471 MHz, CDCl<sub>3</sub>) δ -114.36.  
IR(KBr) ν<sub>max</sub>: 3063, 3042, 1606, 1548, 1509, 1489, 1448, 1401, 1384, 1226, 1157, 1146, 1093, 1056, 1012, 954, 933, 830, 814, 760, 742, 725, 717, 690, 666, 609, 587, 529, 507, 488 cm<sup>-1</sup>.  
HRMS: (ESI) calcd for C<sub>22</sub>H<sub>15</sub>ClFO<sup>+</sup> [M+H]<sup>+</sup> 349.07899; found 349.07870.



**2,3-Dis(4-chlorophenyl)-5-phenylfuran (5r)**

Obtained as a white solid in 78% yield (57.2 mg); mp 134-136 °C (lit<sup>13</sup> 128-130 °C) (DCM/PE = 1:2);  
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.76 – 7.73 (m, 2H), 7.52 – 7.49 (m, 2H), 7.43 (t, *J* = 7.8 Hz, 2H), 7.37 (s, 4H), 7.34 – 7.31 (m, 1H), 7.31 – 7.28 (m, 2H), 6.77 (s, 1H).  
<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 153.2, 147.1, 133.59, 133.55, 132.6, 130.3, 130.1, 129.4, 129.2, 129.0, 128.9, 128.0, 127.5, 124.0, 123.9, 109.3.  
IR(KBr) ν<sub>max</sub>: 3084, 3066, 3036, 1605, 1545, 1497, 1488, 1477, 1448, 1400, 1147, 1093, 1056, 1014, 953, 933, 830, 812, 761, 740, 724, 715, 691, 665, 593, 530, 499, 488 cm<sup>-1</sup>.



**2-(4-Chlorophenyl)-5-phenyl-3-(4-(trifluoromethyl) phenyl)furan (5s)**

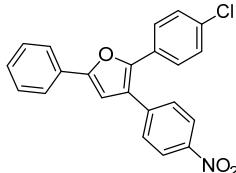
Obtained as a white solid in 77% yield (61.7 mg); mp 132-134 °C (DCM/PE = 1:2);  
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.77 – 7.74 (m, 2H), 7.65 (d, *J* = 8.2 Hz, 2H), 7.56 (d, *J* = 8.0 Hz, 2H), 7.52 – 7.49 (m, 2H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.35 – 7.30 (m, 3H), 6.82 (s, 1H).  
<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 153.5, 147.6, 137.9, 133.9, 130.2, 129.7 (q, *J* = 32.5 Hz), 129.2, 129.02, 129.00, 128.1, 127.7, 125.9 (q, *J* = 3.7 Hz), 124.3 (q, *J* = 272.3 Hz),

124.1, 123.7, 123.2, 109.1.

<sup>19</sup>F NMR (471 MHz, CDCl<sub>3</sub>) δ -62.51.

IR(KBr) ν<sub>max</sub>: 3057, 1619, 1490, 1480, 1402, 1325, 1166, 1125, 1107, 1095, 1069, 1018, 954, 933, 848, 831, 813, 761, 719, 691, 677, 666, 610, 500, 478 cm<sup>-1</sup>.

HRMS: (ESI) calcd for C<sub>23</sub>H<sub>15</sub>ClF<sub>3</sub>O<sup>+</sup> [M+H]<sup>+</sup> 399.07580; found 399.07547.



**2-(4-Chlorophenyl)-3-(4-nitrophenyl)-5-phenylfuran (5t)**

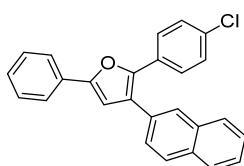
Obtained as a yellow solid in 76% yield (56.9 mg); mp 135-138 °C (DCM/PE = 1:2);

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.25 (d, *J* = 8.8 Hz, 2H), 7.76 (d, *J* = 7.4 Hz, 2H), 7.61 (d, *J* = 8.8 Hz, 2H), 7.50 (d, *J* = 8.6 Hz, 2H), 7.44 (t, *J* = 7.7 Hz, 2H), 7.34 (t, *J* = 7.4 Hz, 3H), 6.85 (s, 1H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 153.9, 148.3, 147.1, 141.1, 134.4, 129.9, 129.3, 129.2, 129.0, 128.9, 128.4, 128.0, 124.3, 124.1, 123.0, 108.5.

IR(KBr) ν<sub>max</sub>: 3057, 2956, 2840, 1599, 1546, 1515, 1488, 1447, 1342, 1292, 1147, 1109, 1095, 1053, 1013, 953, 932, 853, 833, 766, 755, 691, 665, 594, 484 cm<sup>-1</sup>.

HRMS: (ESI) calcd for C<sub>22</sub>H<sub>15</sub>ClNO<sub>3</sub><sup>+</sup> [M+H]<sup>+</sup> 376.07349; found 376.07303.



**2-(4-Chlorophenyl)-3-(naphthalen-2-yl)-5-phenylfuran (5u)**

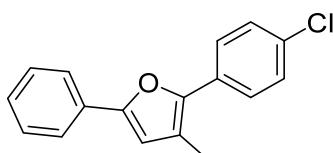
Obtained as a white solid in 62% yield (47.4 mg); mp 140-142 °C (DCM/PE = 1:2);

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.94 (s, 1H), 7.90 – 7.81 (m, 3H), 7.81 – 7.76 (m, 2H), 7.58 – 7.53 (m, 2H), 7.53 – 7.50 (m, 2H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.34 – 7.30 (m, 1H), 7.28 – 7.24 (m, 3H), 6.91 (s, 1H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 153.1, 147.2, 133.8, 133.4, 132.8, 131.6, 130.5, 129.7, 129.0, 128.8, 128.6, 128.1, 127.91, 127.90, 127.5, 127.4, 127.0, 126.5, 126.3, 125.1, 124.0, 109.8.

IR(KBr) ν<sub>max</sub>: 3060, 3033, 2953, 2920, 2852, 1636, 1598, 1529, 1477, 1446, 1133, 1093, 1072, 1012, 977, 952, 830, 763, 749, 730, 719, 691, 675, 574, 524, 493 cm<sup>-1</sup>.

HRMS: (ESI) calcd for C<sub>26</sub>H<sub>18</sub>ClO<sup>+</sup> [M+H]<sup>+</sup> 381.10406; found 381.10373.



**2-(4-Chlorophenyl)-3-methyl-5-phenylfuran (6a)**

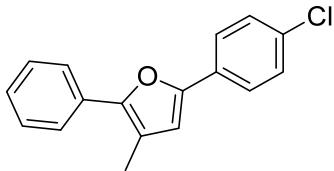
Obtained as a white solid in 60% yield (32.0 mg); mp 68-70 °C (lit<sup>14</sup> 77-78 °C) (DCM/PE = 1:2);

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.72 – 7.69 (m, 2H), 7.66 – 7.62 (m, 2H), 7.42 – 7.37

(m, 4H), 7.29 – 7.25 (m, 1H), 6.61 (s, 1H), 2.32 (s, 3H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 152.1, 147.3, 132.4, 130.7, 130.4, 128.9, 128.8, 127.5, 126.4, 123.9, 119.3, 111.0, 12.3.

IR(KBr) ν<sub>max</sub>: 2953, 2926, 1612, 1489, 1448, 1391, 1098, 1071, 1009, 932, 826, 810, 797, 756, 710, 687, 666, 518, 485 cm<sup>-1</sup>.



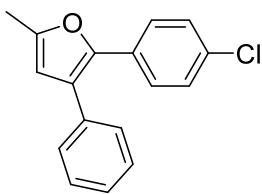
**5-(4-Chlorophenyl)-3-methyl-2-phenylfuran (6b)**

Obtained as a white solid in 63% yield (33.7 mg); mp 72-74 °C (lit<sup>15</sup> 80-82 °C) (DCM/PE = 1:2);

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.70 (m, 2H), 7.65 – 7.62 (m, 2H), 7.44 (m, 2H), 7.37 – 7.34 (m, 2H), 7.28 (t, J = 7.4 Hz, 1H), 6.60 (s, 1H), 2.33 (s, 3H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 150.8, 148.7, 132.9, 131.7, 129.4, 129.0, 128.7, 127.0, 125.4, 125.0, 118.9, 111.4, 12.2.

IR(KBr) ν<sub>max</sub>: 3058, 2965, 2925, 2863, 1610, 1601, 1493, 1478, 1444, 1411, 1094, 1060, 1013, 933, 830, 809, 796, 758, 706, 699, 688, 665, 503, 485 cm<sup>-1</sup>.



**2-(4-Chlorophenyl)-5-methyl-3-phenylfuran (6c)**

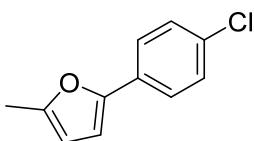
Obtained as a white solid in 67% yield (36.1 mg); mp 50-52 °C (DCM/PE = 1:2);

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.43 (d, J = 8.5 Hz, 2H), 7.37 (q, J = 7.7 Hz, 4H), 7.31 (dd, J = 8.4, 5.1 Hz, 1H), 7.23 (d, J = 8.5 Hz, 2H), 6.16 (s, 1H), 2.39 (s, 3H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 151.8, 145.8, 134.6, 132.8, 130.0, 128.8, 128.69, 128.66, 127.3, 127.2, 123.9, 110.5, 13.7.

IR(KBr) ν<sub>max</sub>: 3057, 3036, 2959, 2917, 2852, 1602, 1571, 1553, 1500, 1481, 1445, 1384, 1130, 1093, 1071, 1054, 1013, 998, 951, 830, 764, 748, 698, 578, 516, 491 cm<sup>-1</sup>.

HRMS: (ESI) calcd for C<sub>17</sub>H<sub>14</sub>ClO<sup>+</sup> [M+H]<sup>+</sup> 269.07276; found 269.07254.



**2-(4-Chlorophenyl)-5-methylfuran (6d)**

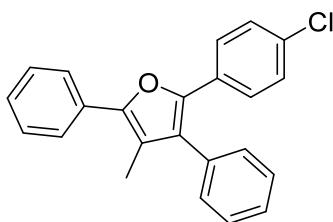
Obtained as a colorless oily<sup>16</sup> in 45% yield (17.2 mg);

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.55 (d, J = 8.6 Hz, 2H), 7.32 (d, J = 8.6 Hz, 2H), 6.52 (d, J = 3.2 Hz, 1H), 6.05 (dd, J = 3.2, 1.1 Hz, 1H), 2.36 (s, 3H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 152.4, 151.4, 132.4, 129.8, 128.9, 124.6, 108.0, 106.5, 13.9.

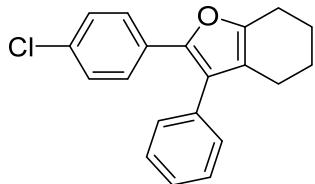
IR(KBr) ν<sub>max</sub>: 2953, 2923, 2855, 1482, 1409, 1102, 1025, 919, 834, 822, 786, 748, 497

$\text{cm}^{-1}$ .



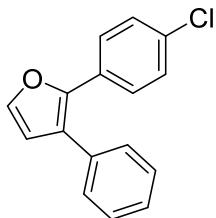
**2-(4-Chlorophenyl)-4-methyl-3,5-diphenylfuran (6e)**

Obtained as a white solid in 29% yield (20.0 mg); mp 82–84 °C (DCM/PE = 1:2);  
 $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.75 (d,  $J$  = 7.6 Hz, 2H), 7.46 (t,  $J$  = 7.9 Hz, 4H), 7.41 (d,  $J$  = 7.1 Hz, 1H), 7.39 (d,  $J$  = 8.5 Hz, 2H), 7.33 (d,  $J$  = 6.5 Hz, 2H), 7.31 (d,  $J$  = 7.6 Hz, 1H), 7.20 (d,  $J$  = 8.5 Hz, 2H), 2.14 (s, 3H).  
 $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  148.2, 146.3, 133.7, 132.8, 131.6, 130.2, 129.7, 129.1, 128.8, 128.7, 127.8, 127.2, 126.7, 126.6, 125.7, 119.1, 10.6.  
IR(KBr)  $\nu_{\text{max}}$ : 3081, 3057, 2953, 2920, 2875, 1598, 1493, 1481, 1443, 1383, 1090, 1071, 1012, 944, 914, 830, 781, 764, 753, 724, 695, 669, 494  $\text{cm}^{-1}$ .  
HRMS: (ESI) calcd for  $\text{C}_{23}\text{H}_{18}\text{ClO}^+ [\text{M}+\text{H}]^+$  345.10406; found 345.10379.



**2-(4-Chlorophenyl)-3-phenyl-4,5,6,7-tetrahydrobenzofuran (6f)**

Obtained as a white solid in 50% yield (31.1 mg); mp 98–100 °C (DCM/PE = 1:2);  
 $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.40 – 7.35 (m, 4H), 7.34 – 7.29 (m, 3H), 7.21 – 7.16 (m, 2H), 2.70 (tt,  $J$  = 6.3, 1.6 Hz, 2H), 2.35 (tt,  $J$  = 6.0, 1.6 Hz, 2H), 1.93 – 1.87 (m, 2H), 1.78 – 1.72 (m, 2H).  
 $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  150.7, 145.7, 134.0, 132.3, 130.2, 129.5, 128.8, 128.6, 127.3, 126.8, 123.1, 119.9, 23.5, 23.2, 23.1, 21.5.  
IR(KBr)  $\nu_{\text{max}}$ : 2935, 2849, 1602, 1575, 1554, 1498, 1479, 1442, 1400, 1288, 1089, 1069, 1053, 1012, 966, 956, 927, 827, 758, 722, 710, 698, 655, 598, 513, 494  $\text{cm}^{-1}$ .  
HRMS: (ESI) calcd for  $\text{C}_{20}\text{H}_{18}\text{ClO}^+ [\text{M}+\text{H}]^+$  309.10407; found 309.10400.

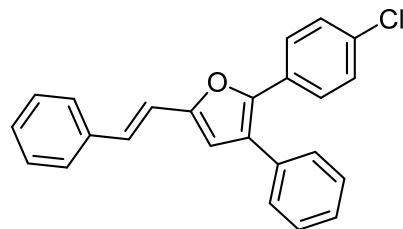


**2-(4-Chlorophenyl)-3-phenylfuran (6g)**

Obtained as a yellow solid in 29% yield (15.0 mg); mp 95–98 °C (DCM/PE = 1:2);  
 $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.50 (d,  $J$  = 1.8 Hz, 1H), 7.47 – 7.43 (m, 2H), 7.40 – 7.35 (m, 4H), 7.34 – 7.30 (m, 1H), 7.27 – 7.23 (m, 2H), 6.55 (d,  $J$  = 1.8 Hz, 1H).  
 $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  147.6, 141.9, 134.2, 133.4, 129.8, 128.9, 128.78, 128.75, 127.54, 127.49, 122.9, 114.3.

IR(KBr)  $\nu_{\text{max}}$ : 2920, 2858, 1591, 1483, 1398, 1224, 1097, 1012, 922, 834, 827, 734  $\text{cm}^{-1}$ .

HRMS: (ESI) calcd for  $\text{C}_{16}\text{H}_{12}\text{ClO}^+ [\text{M}+\text{H}]^+$  255.05712; found 255.05678.



*(E)-2-(4-Chlorophenyl)-3-phenyl-5-styrylfuran (6h)*

Obtained as a yellow solid in 42% yield (30.1 mg); mp 122-124 °C (lit<sup>17</sup> 121-123 °C) (DCM/PE=1:2);

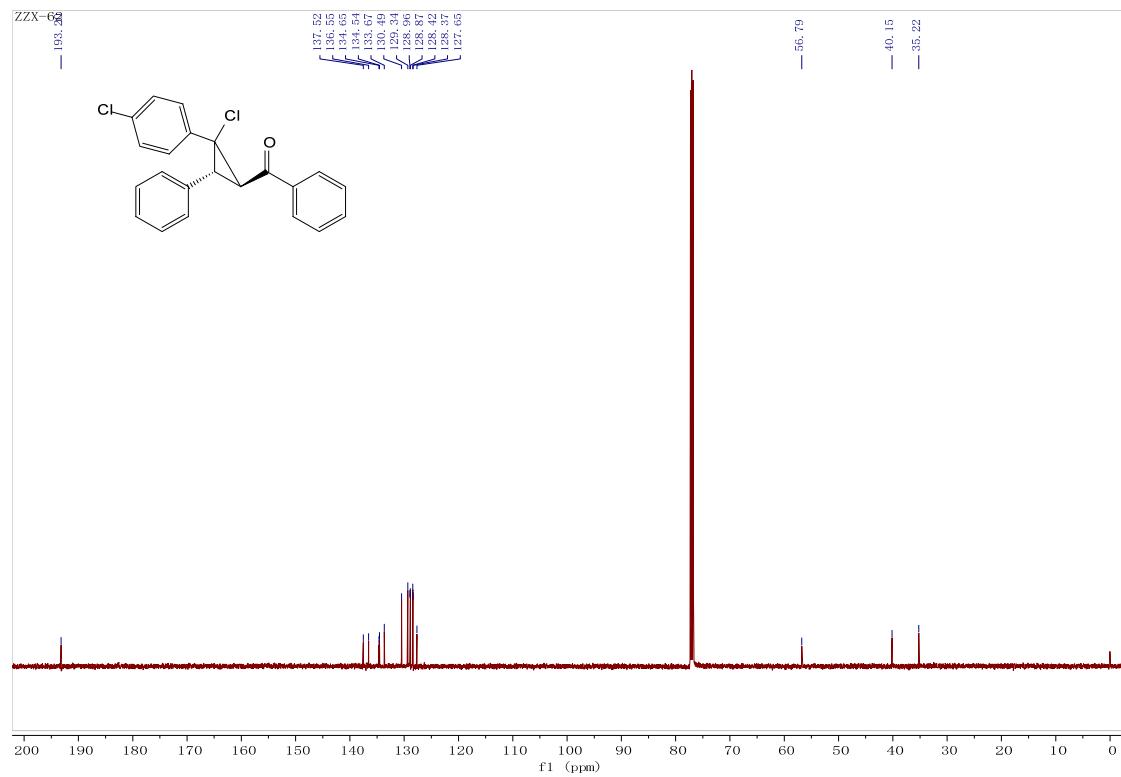
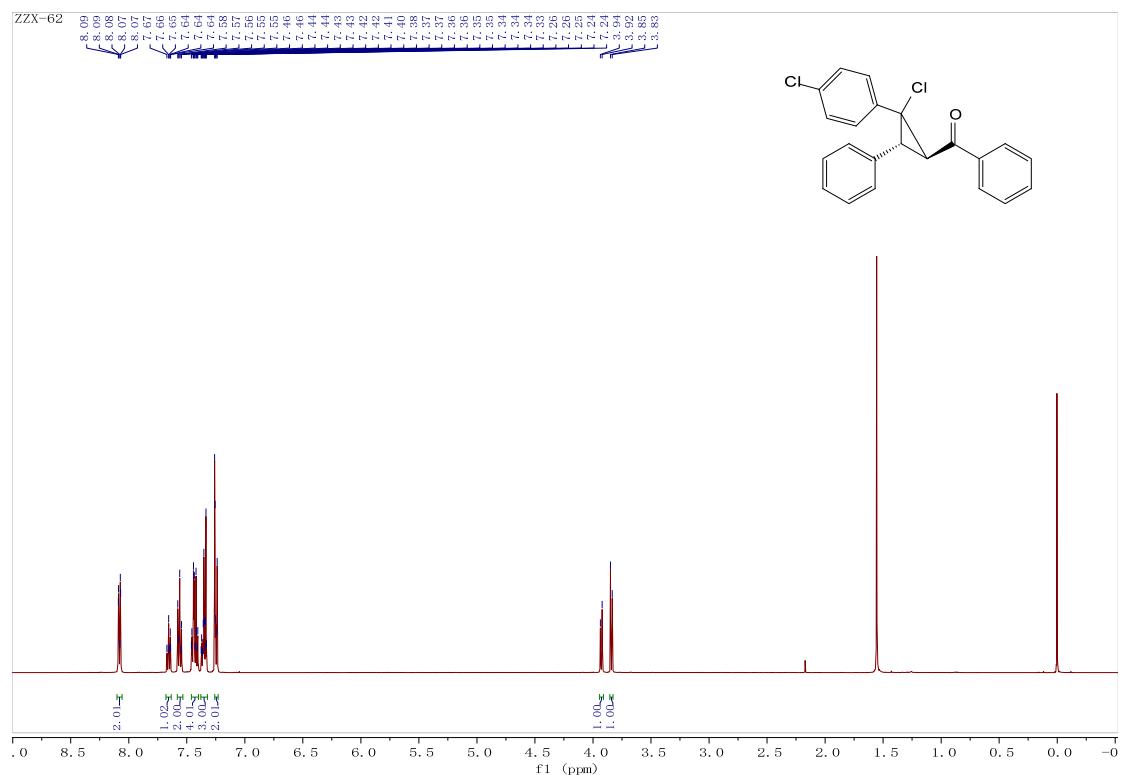
<sup>1</sup>H NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.53 – 7.50 (m, 4H), 7.43 – 7.32 (m, 8H), 7.29 – 7.27 (m, 2H), 7.15 (d,  $J$  = 16.2 Hz, 1H), 6.93 (d,  $J$  = 16.2 Hz, 1H), 6.51 (s, 1H).

<sup>13</sup>C NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  152.3, 147.0, 137.0, 134.0, 133.4, 129.6, 128.94, 128.90, 128.80, 128.77, 128.0, 127.9, 127.7, 127.5, 126.6, 125.2, 116.1, 113.3.

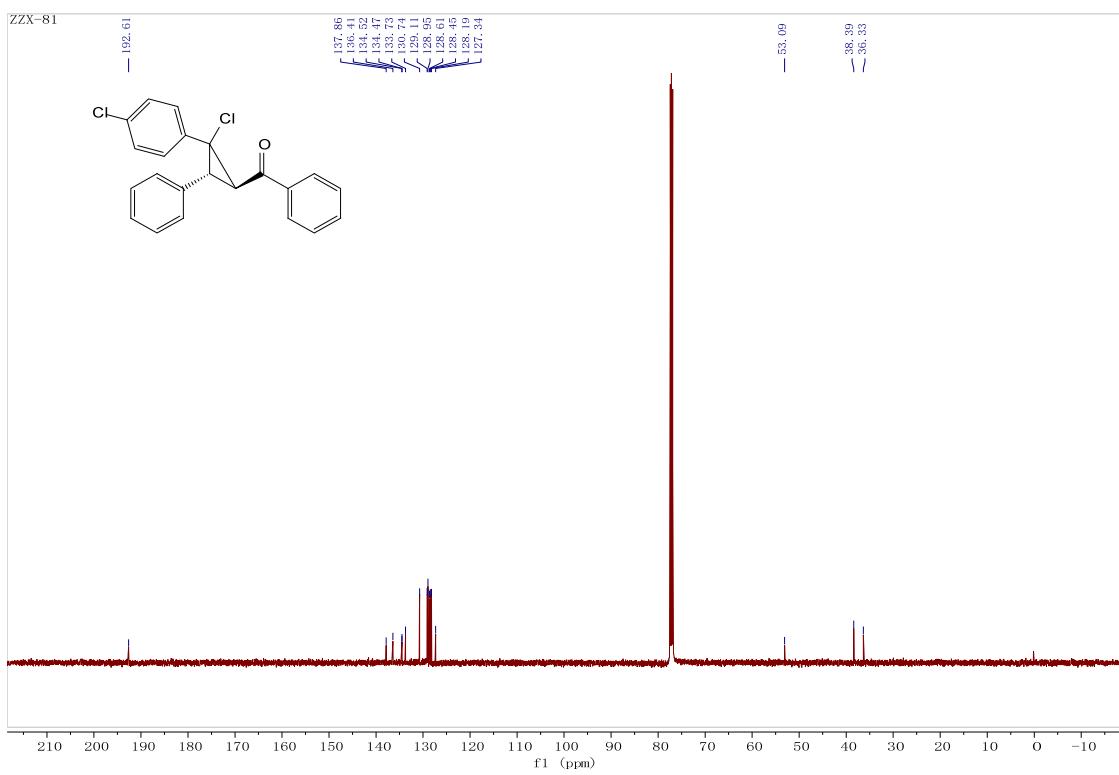
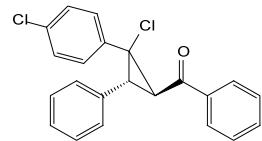
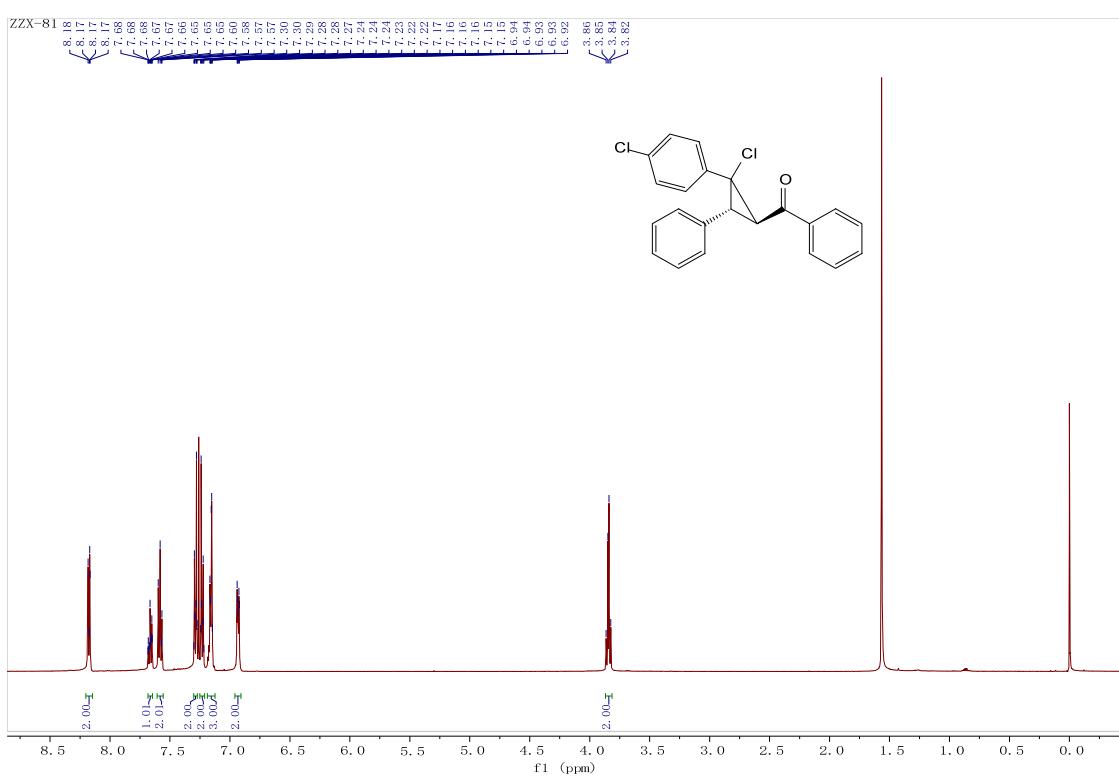
IR(KBr)  $\nu_{\text{max}}$ : 3081, 3060, 3030, 2959, 2923, 2852, 1636, 1598, 1529, 1498, 1477, 1446, 1385, 1133, 1093, 1072, 1012, 977, 952, 830, 763, 749, 730, 719, 691, 675, 574, 524, 493  $\text{cm}^{-1}$ .

## 6. The NMR Charts

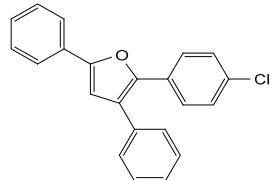
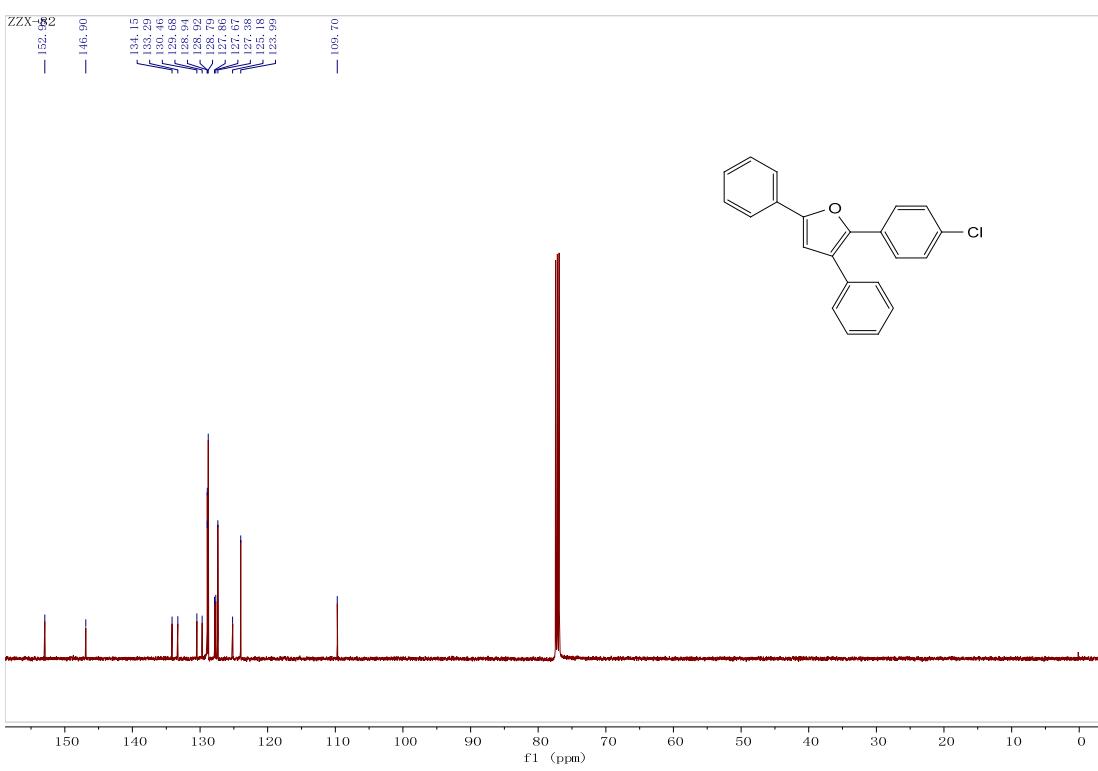
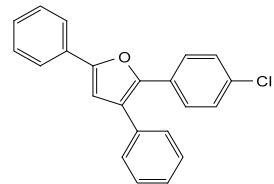
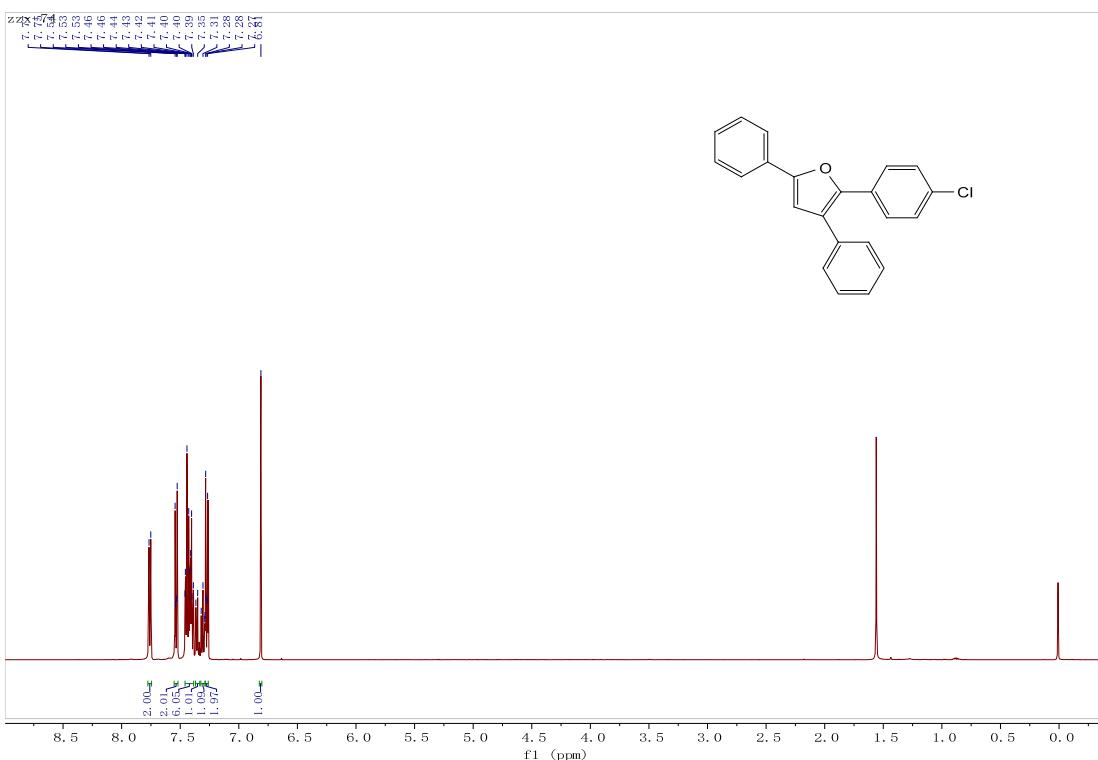
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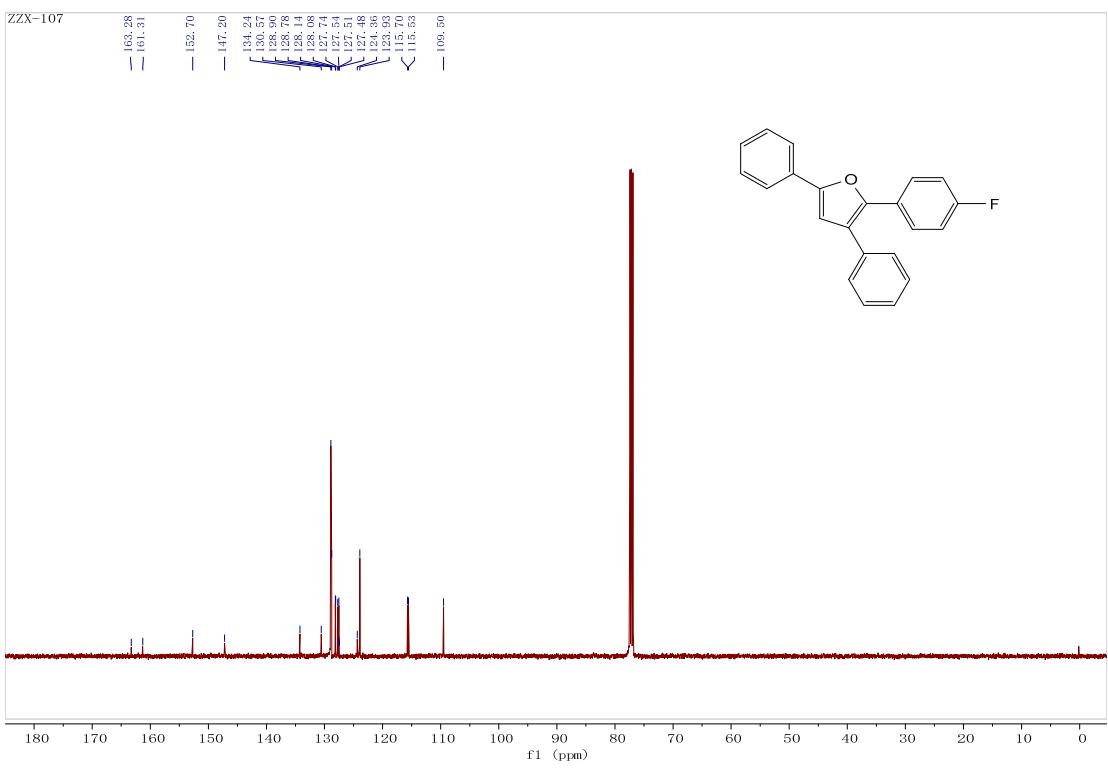
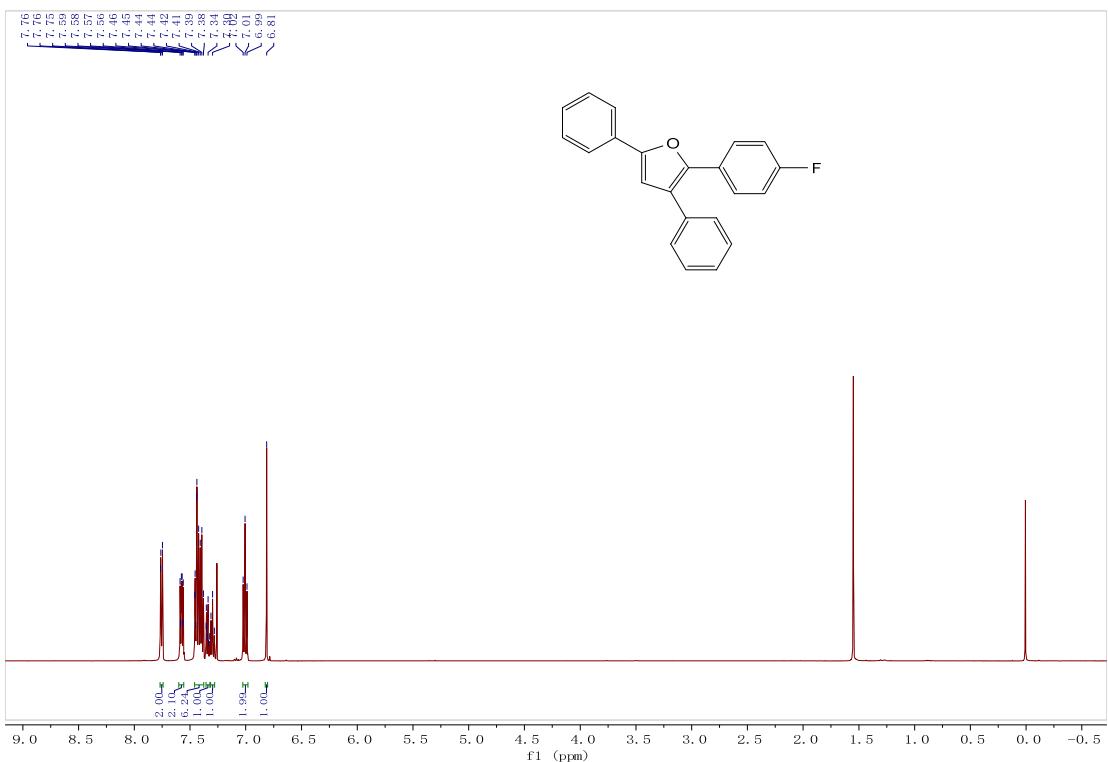
3a'



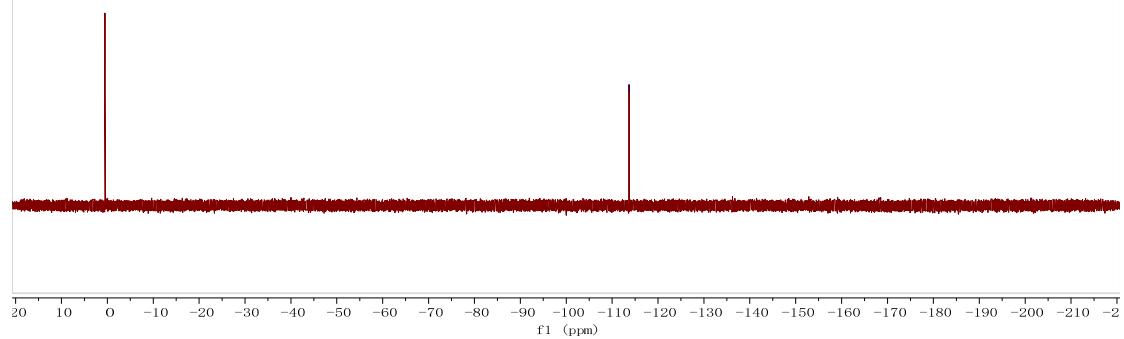
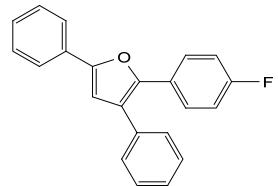
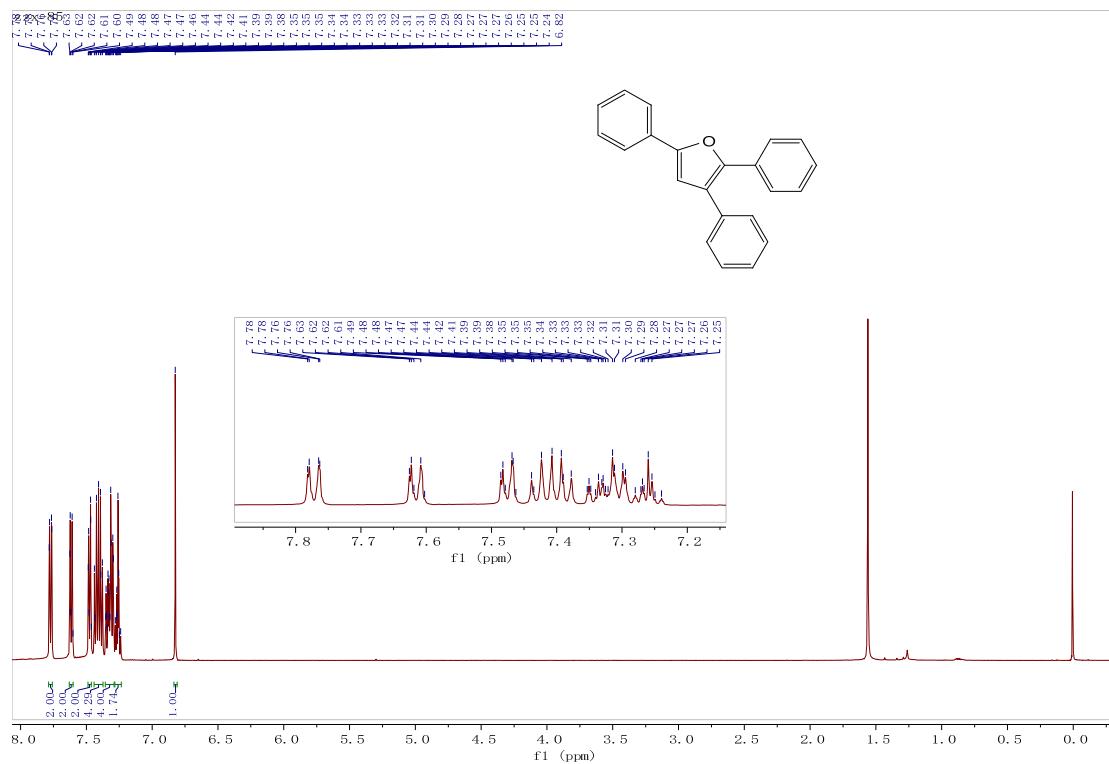
4a

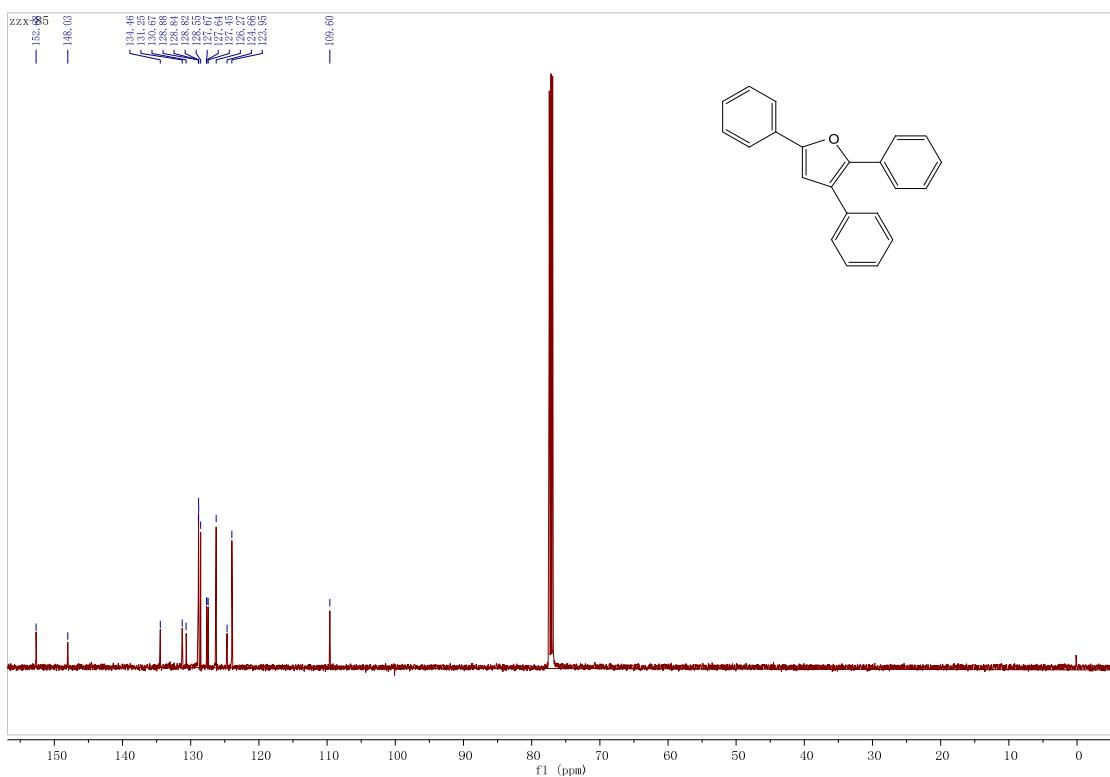


4b

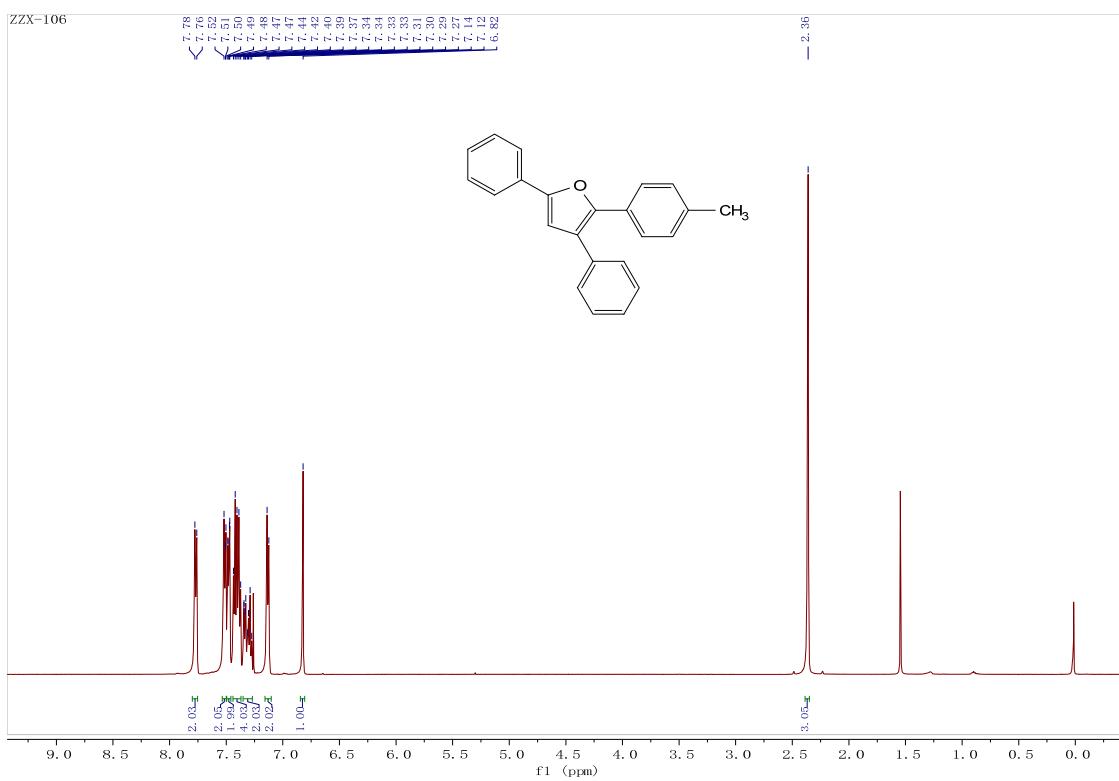


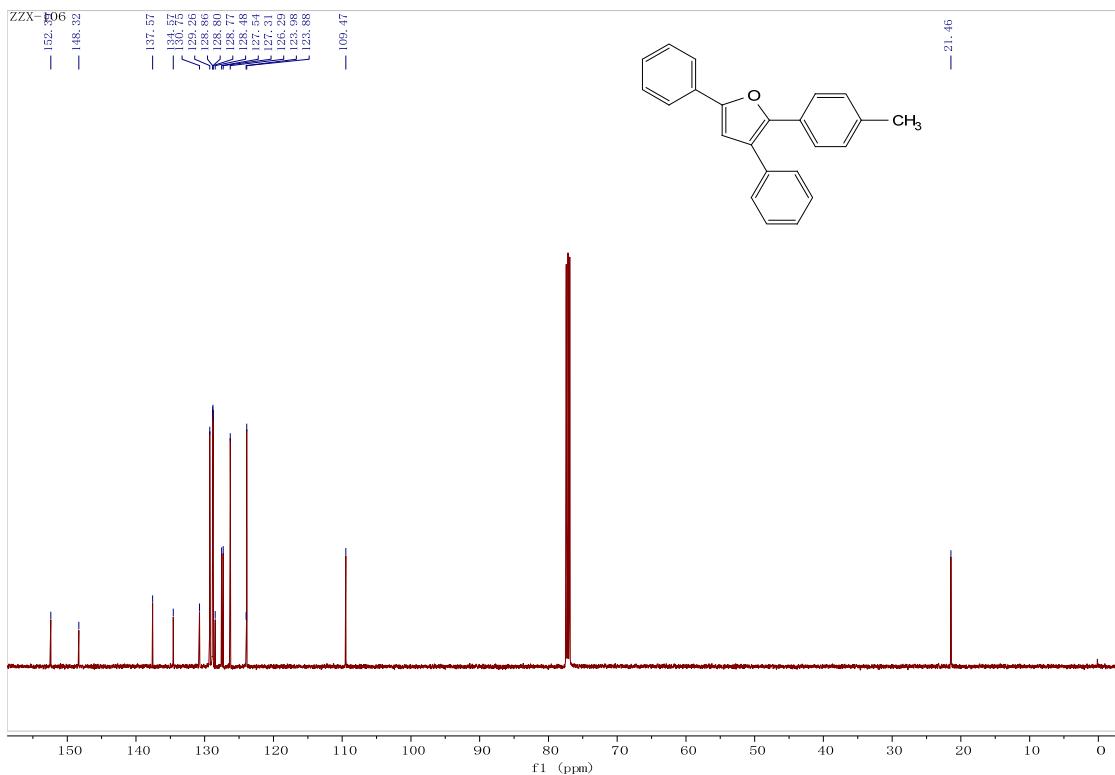
—113.69

**4c**

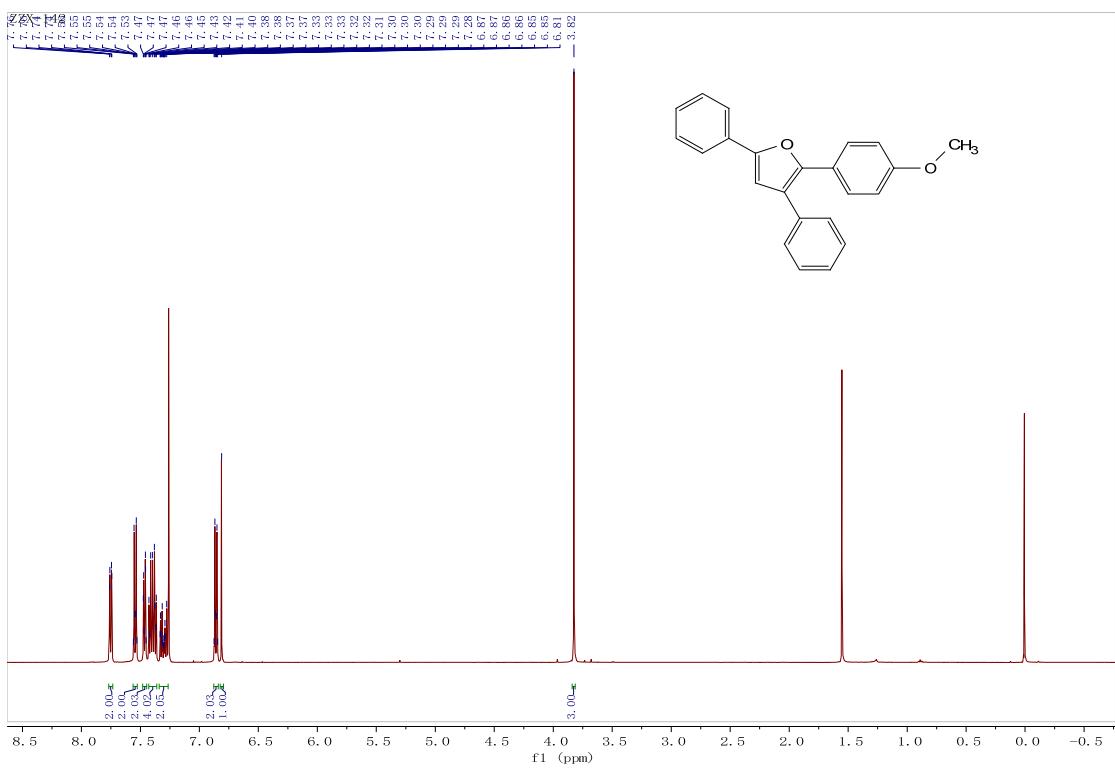


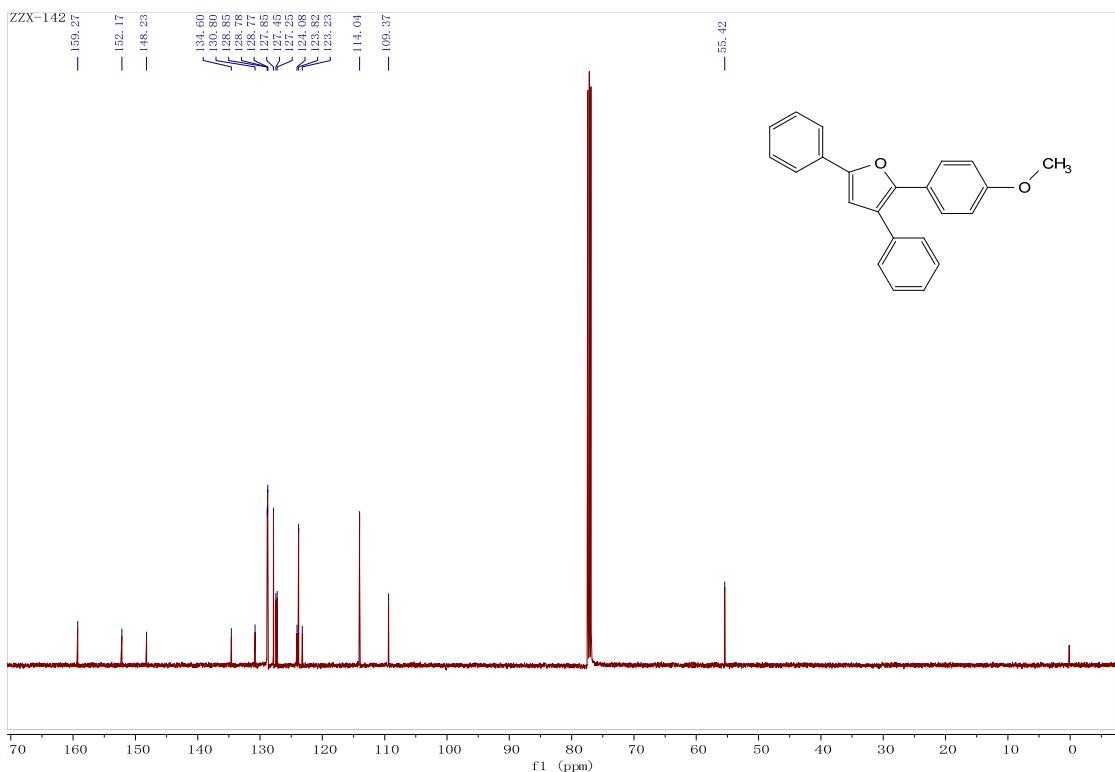
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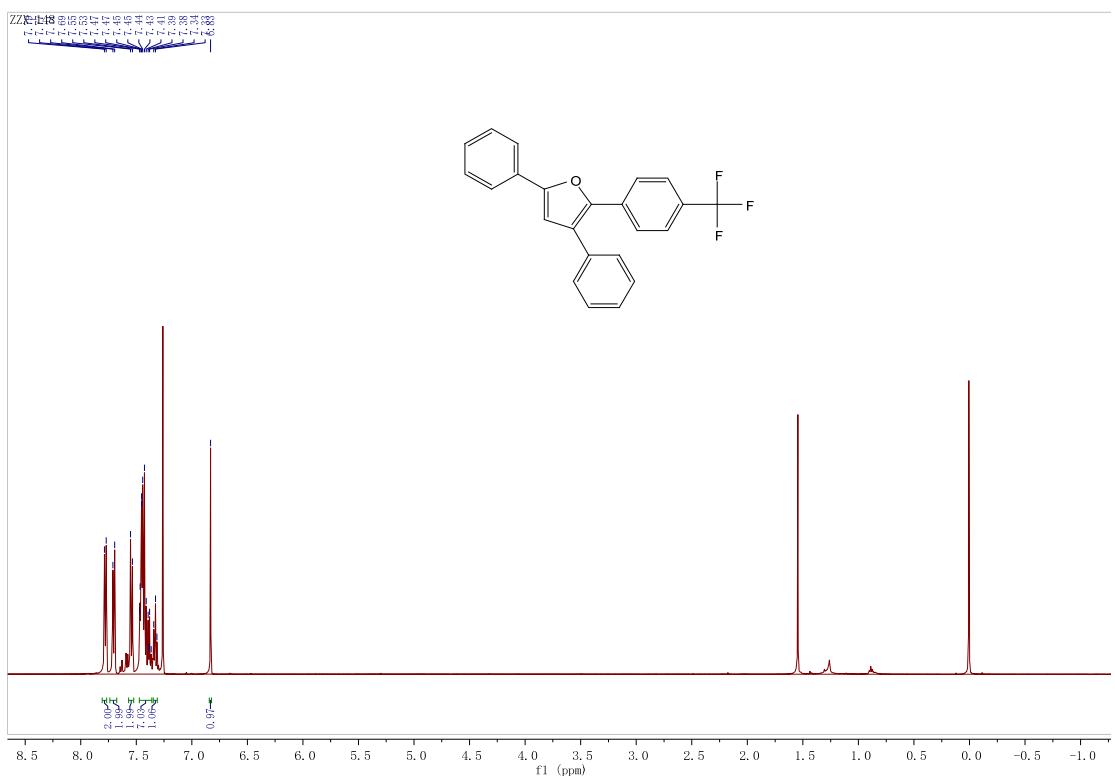


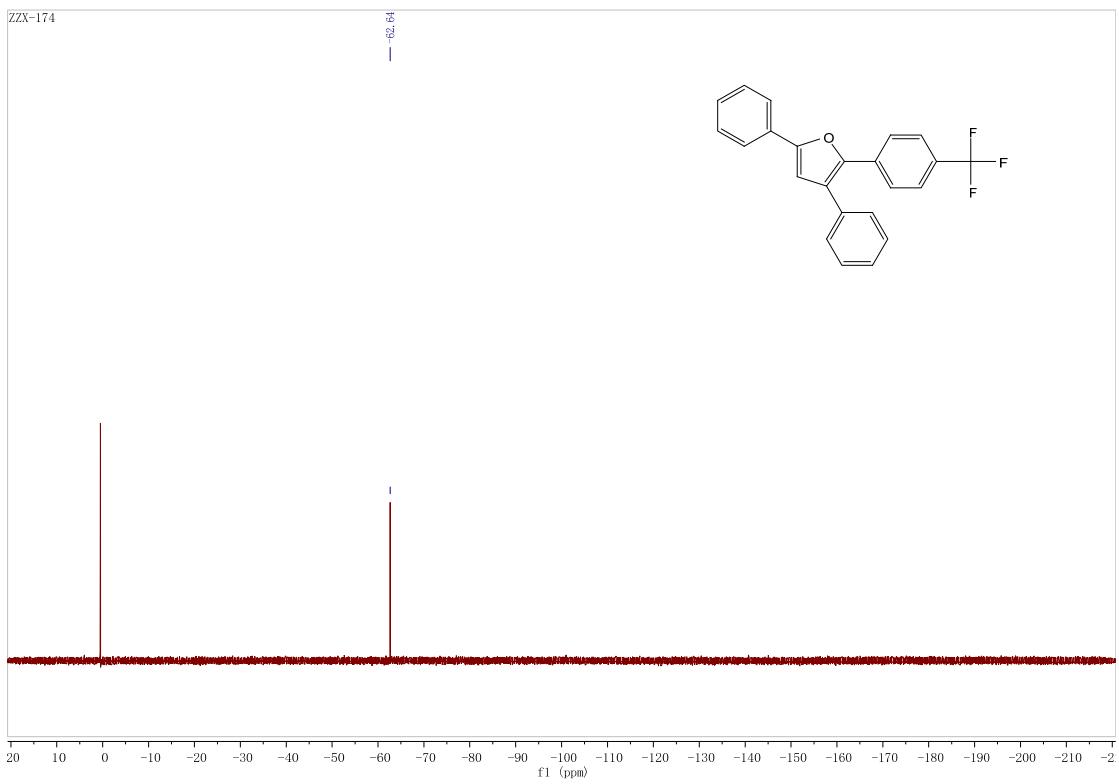
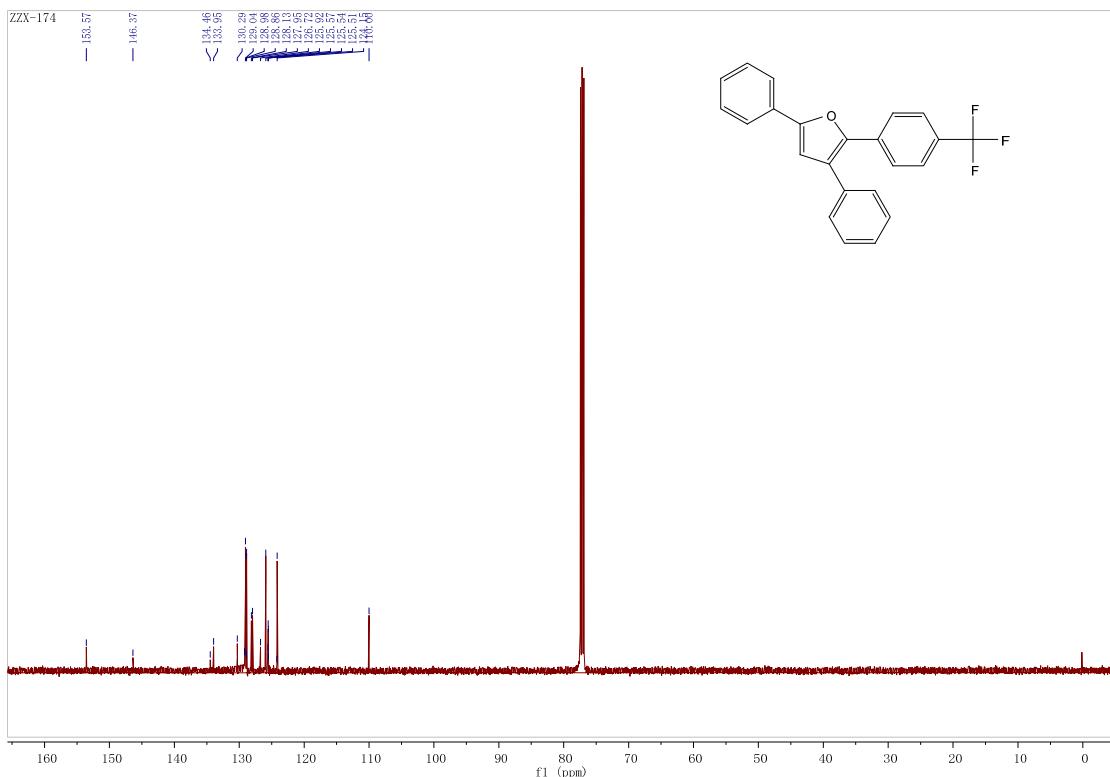
**4e**



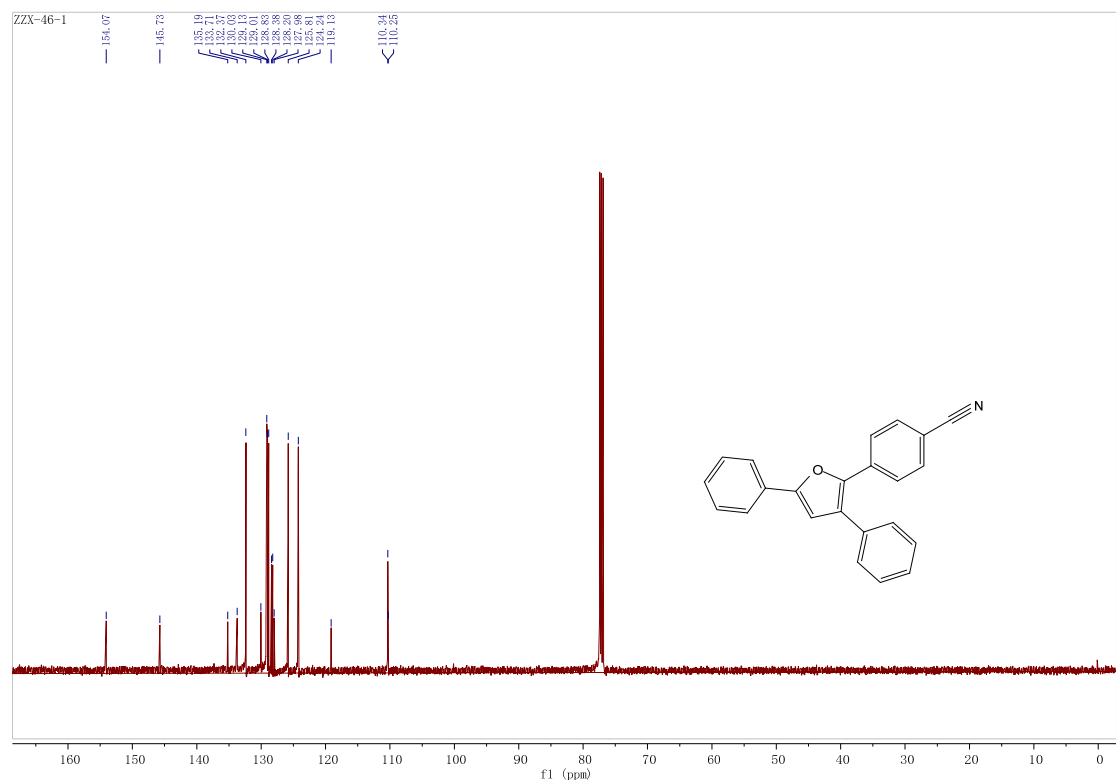
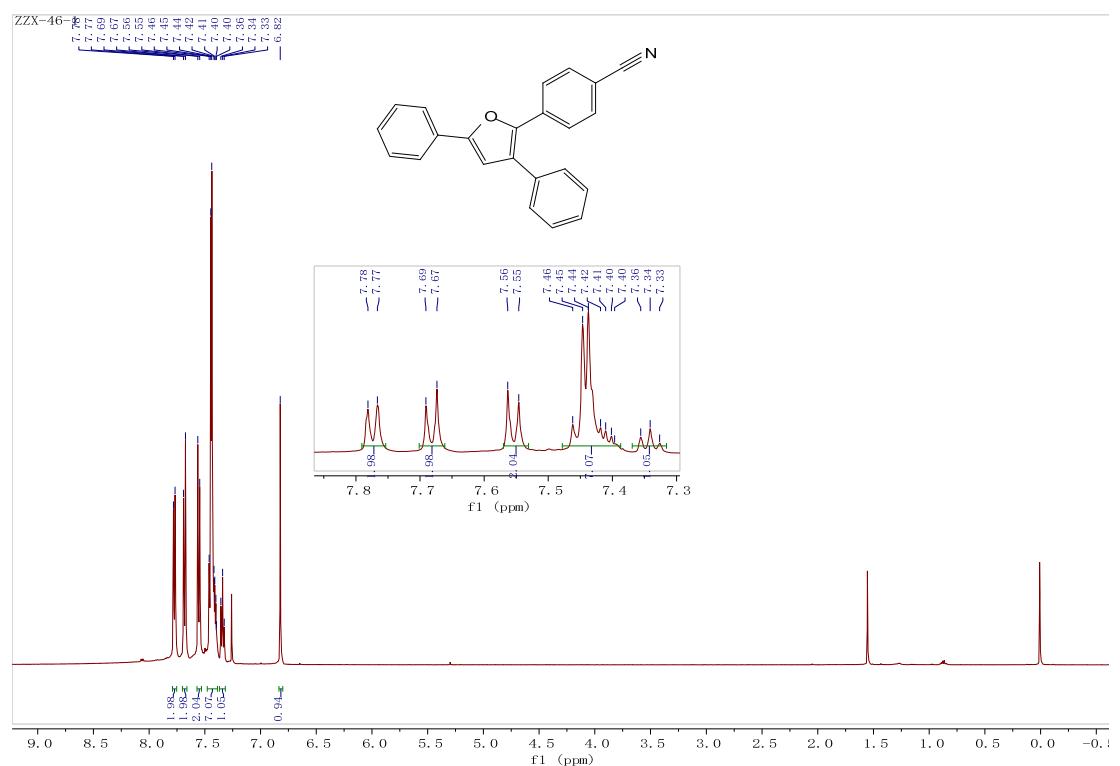


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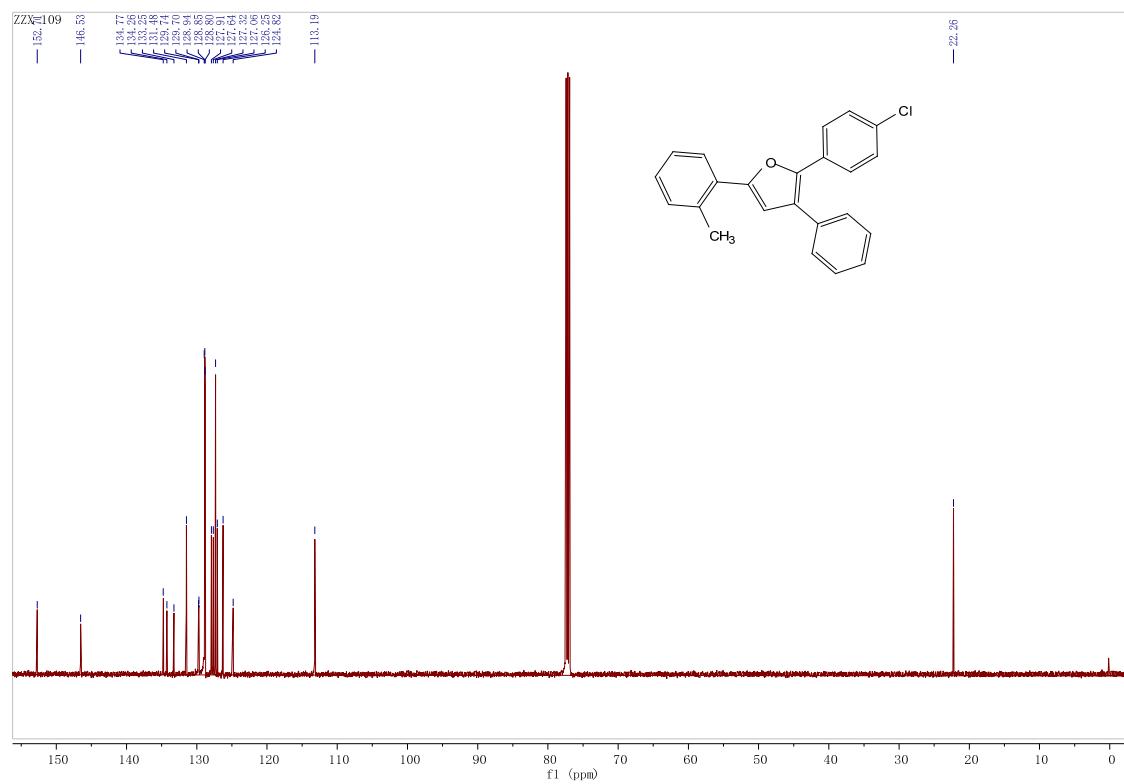
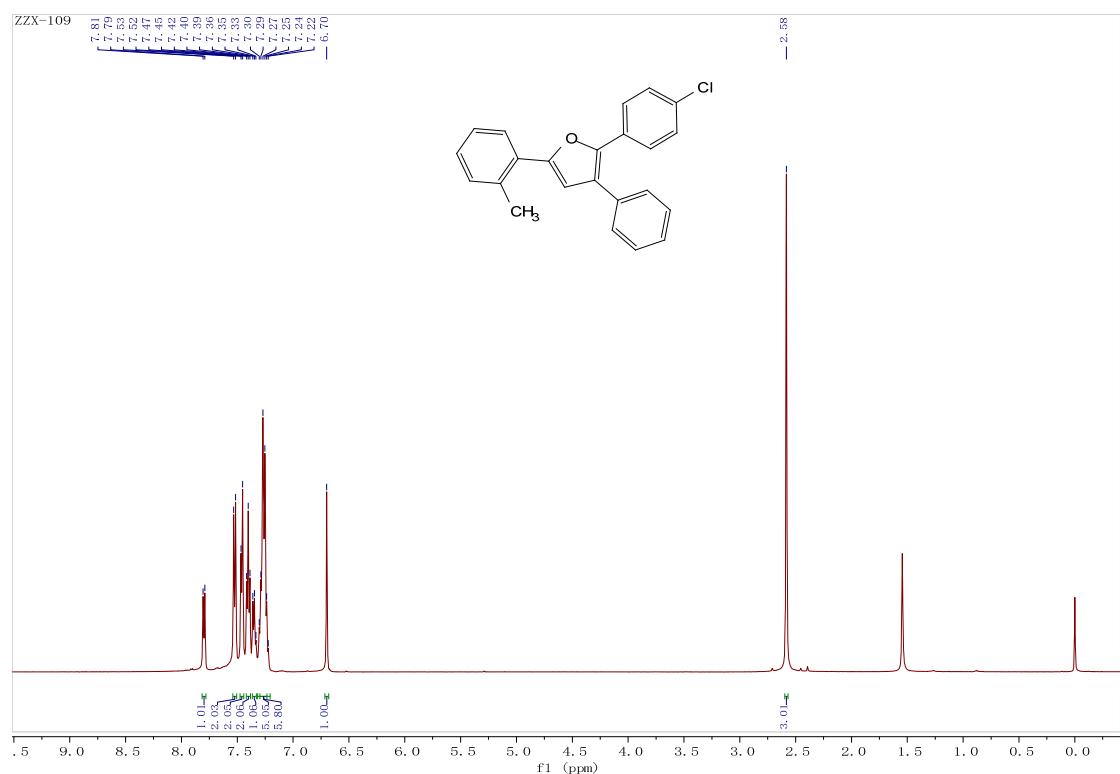




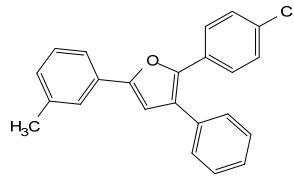
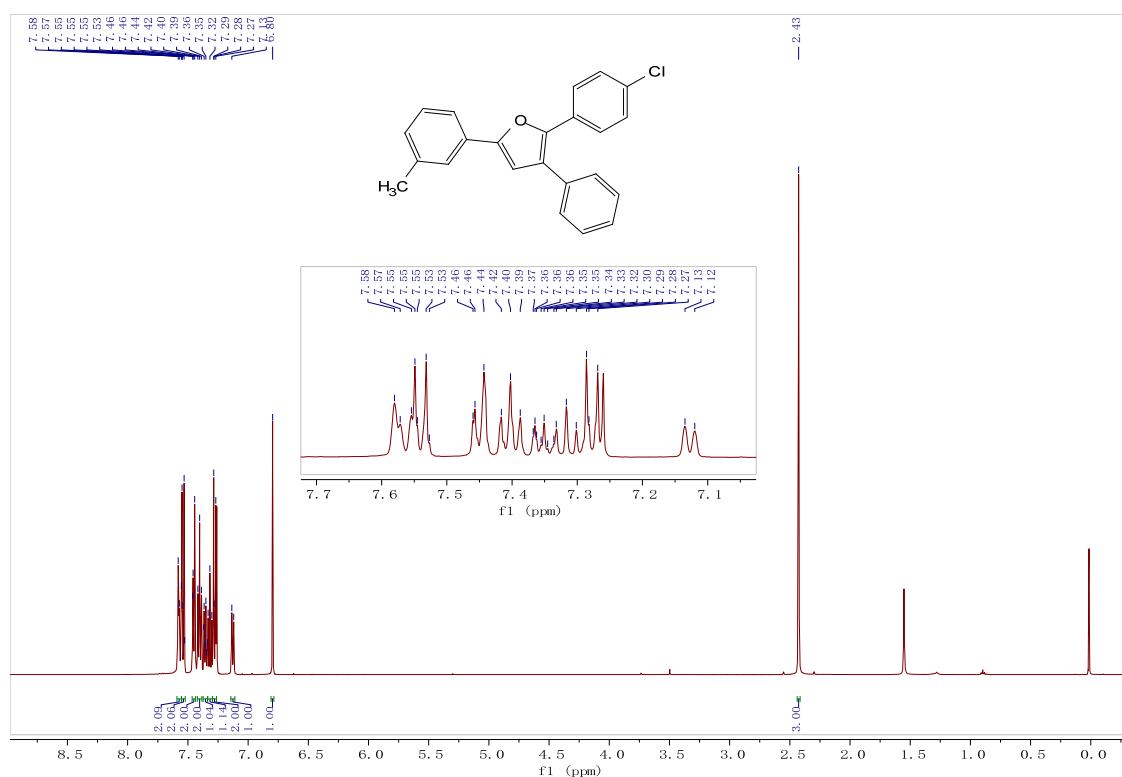
**4g**



**5a**



5b

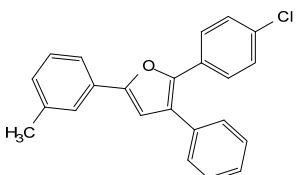
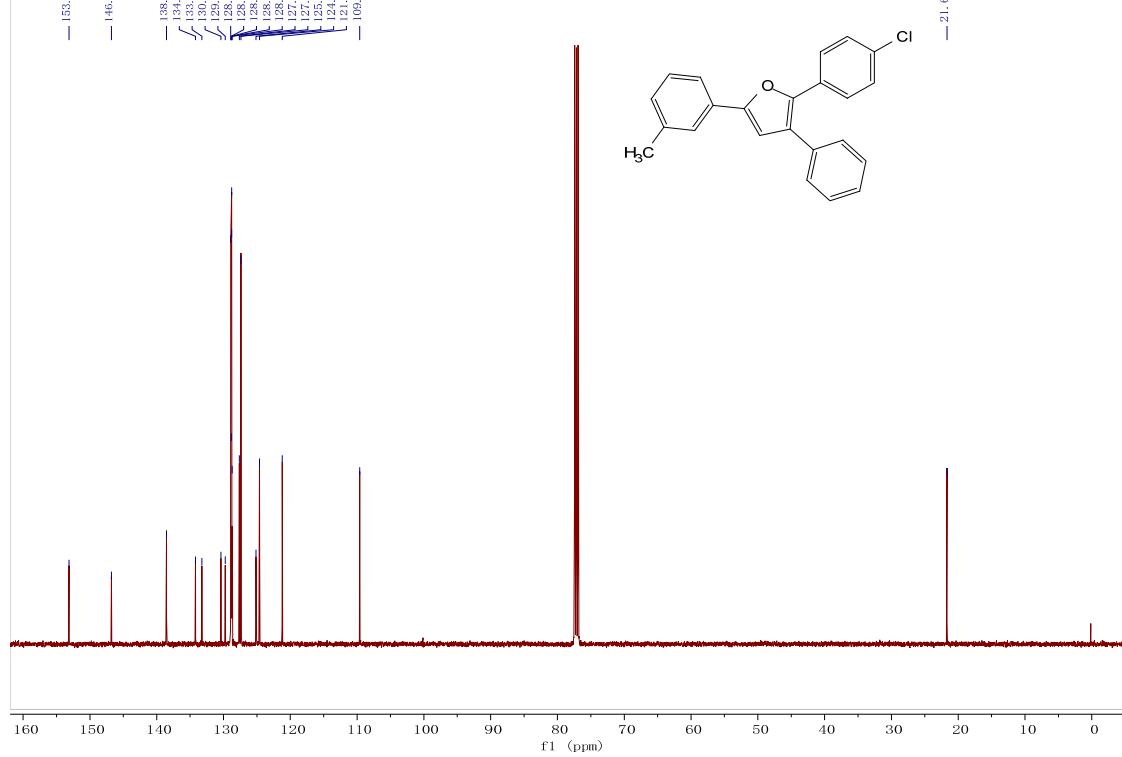


243

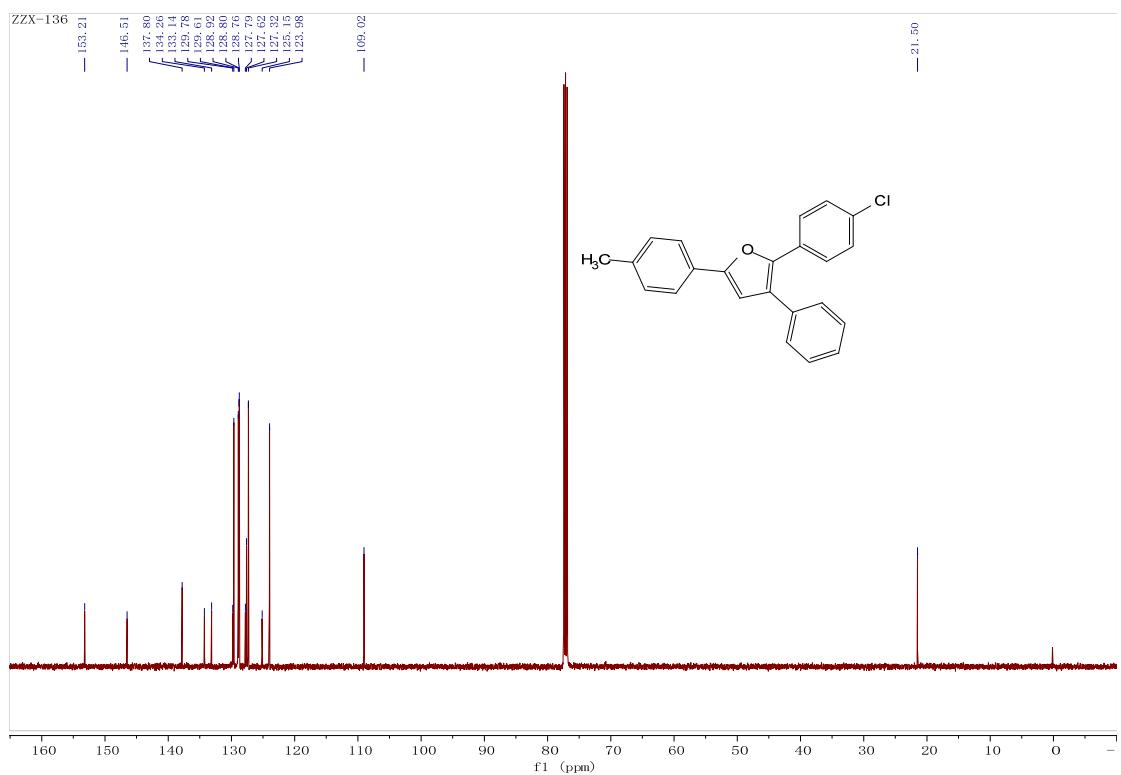
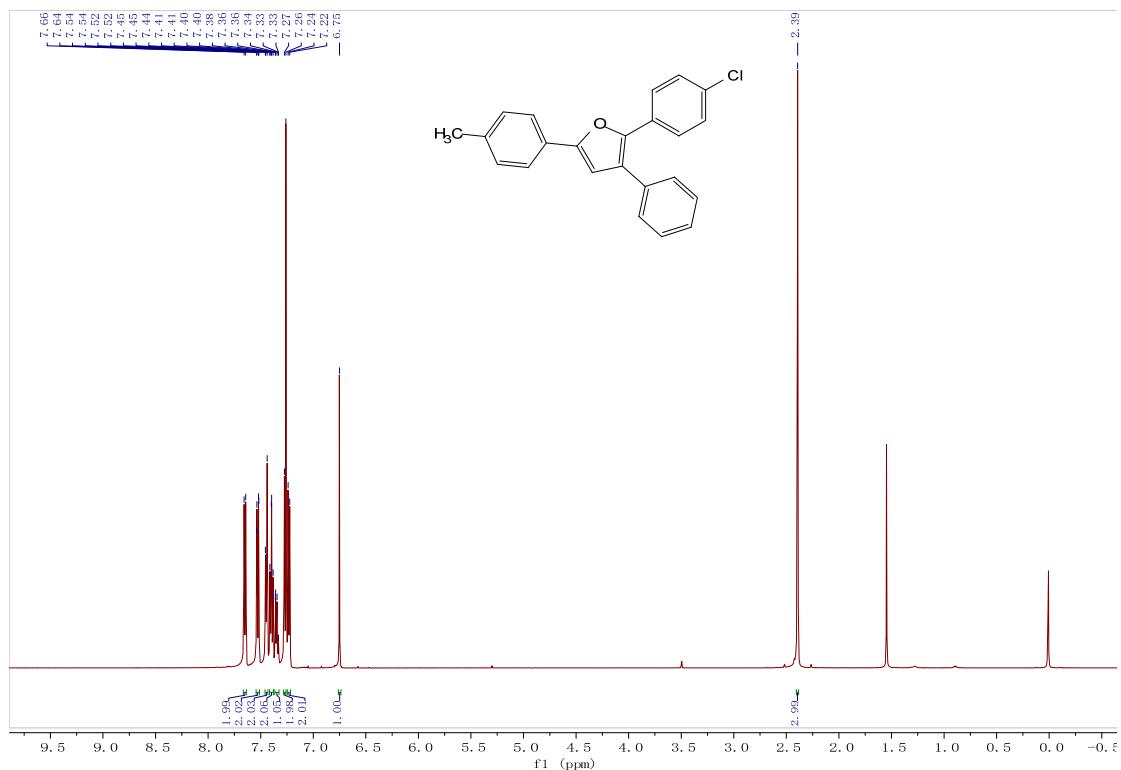
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21. 68

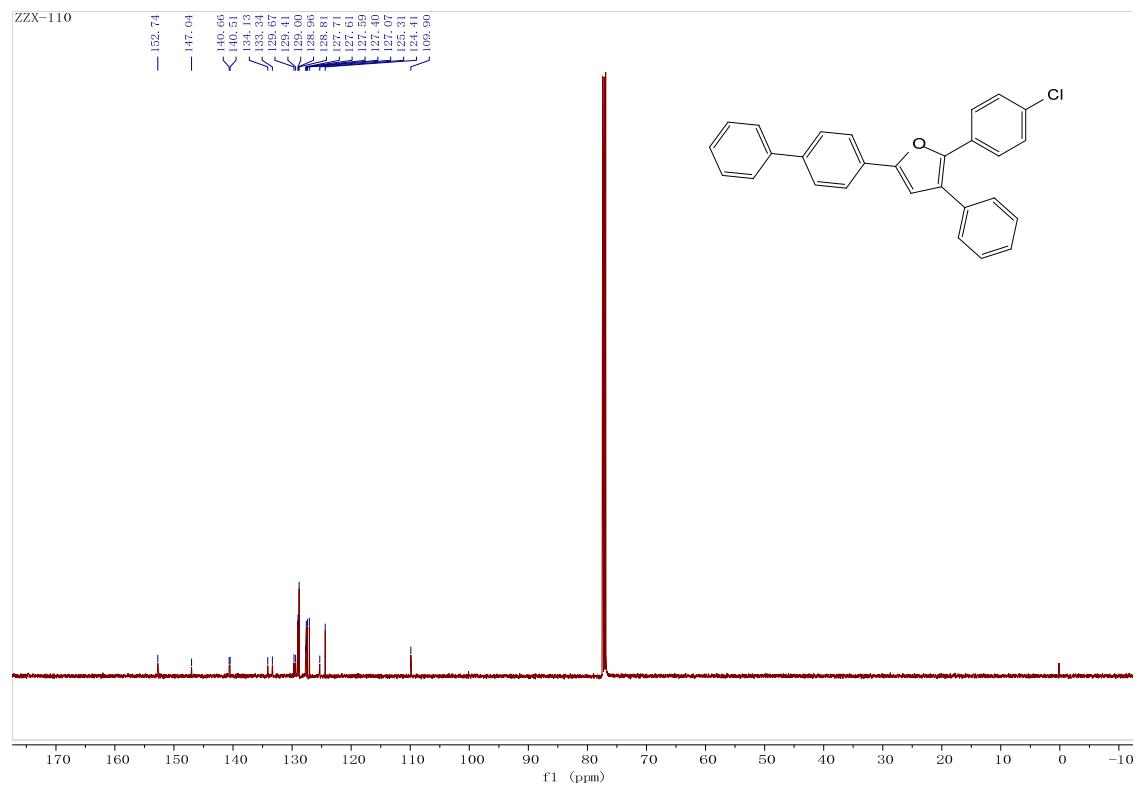
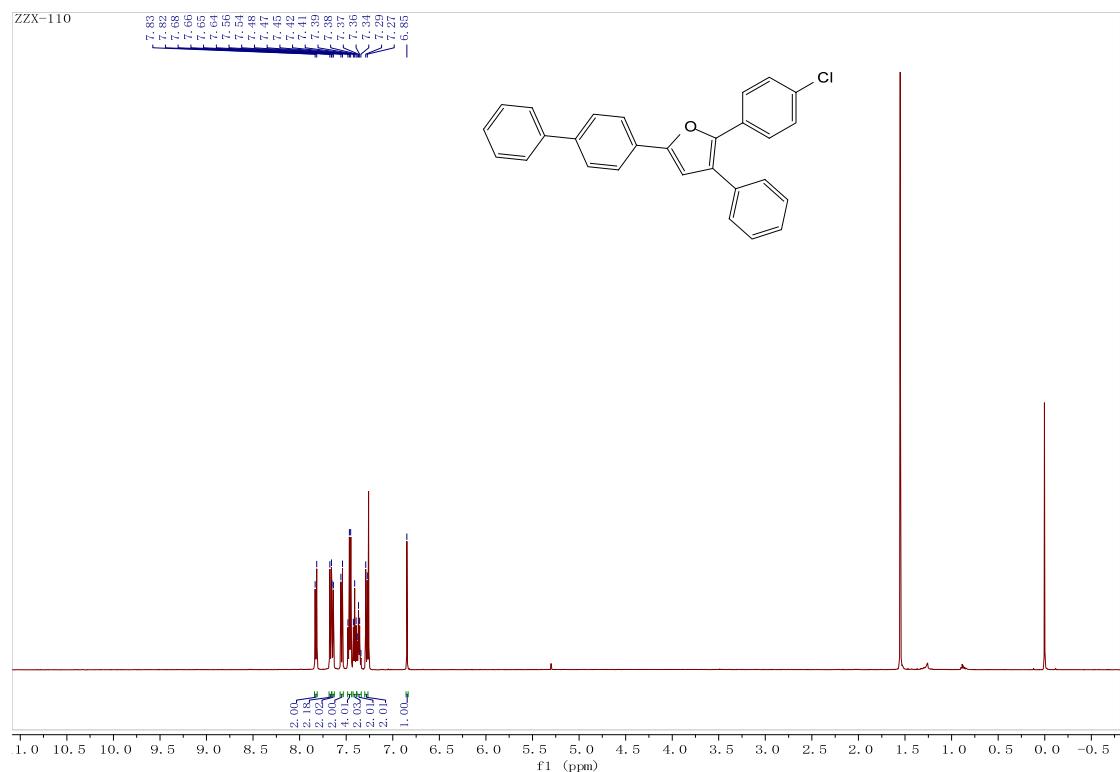
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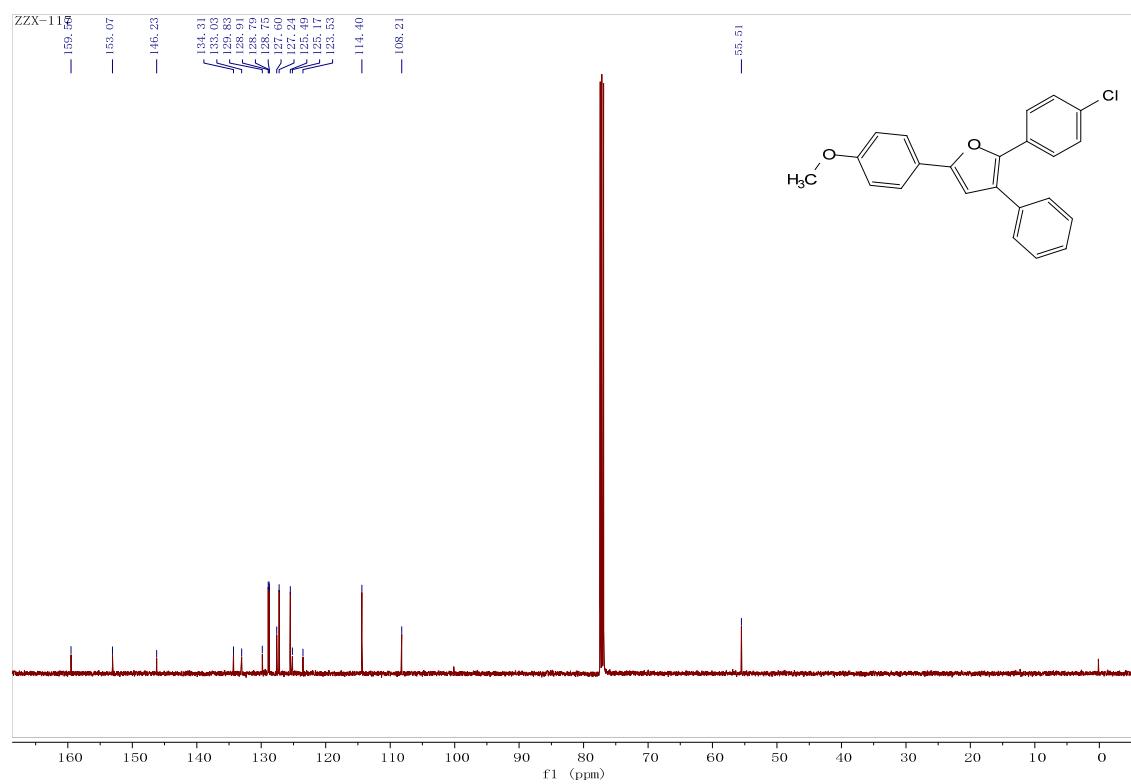
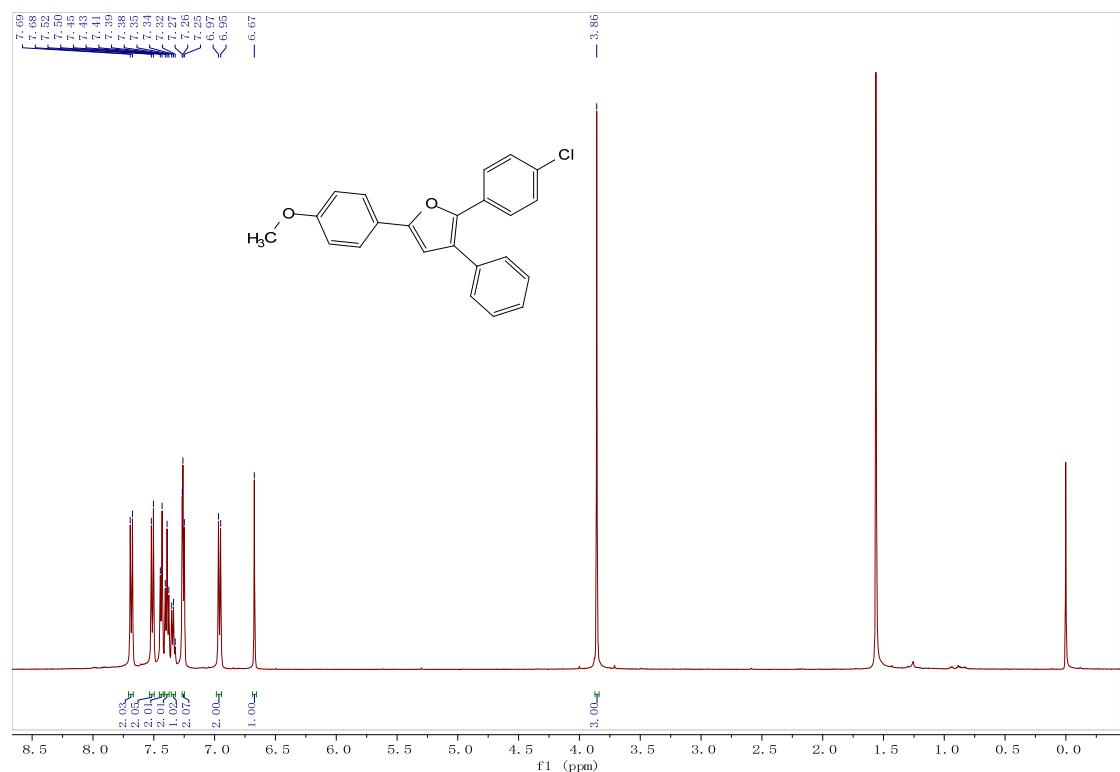
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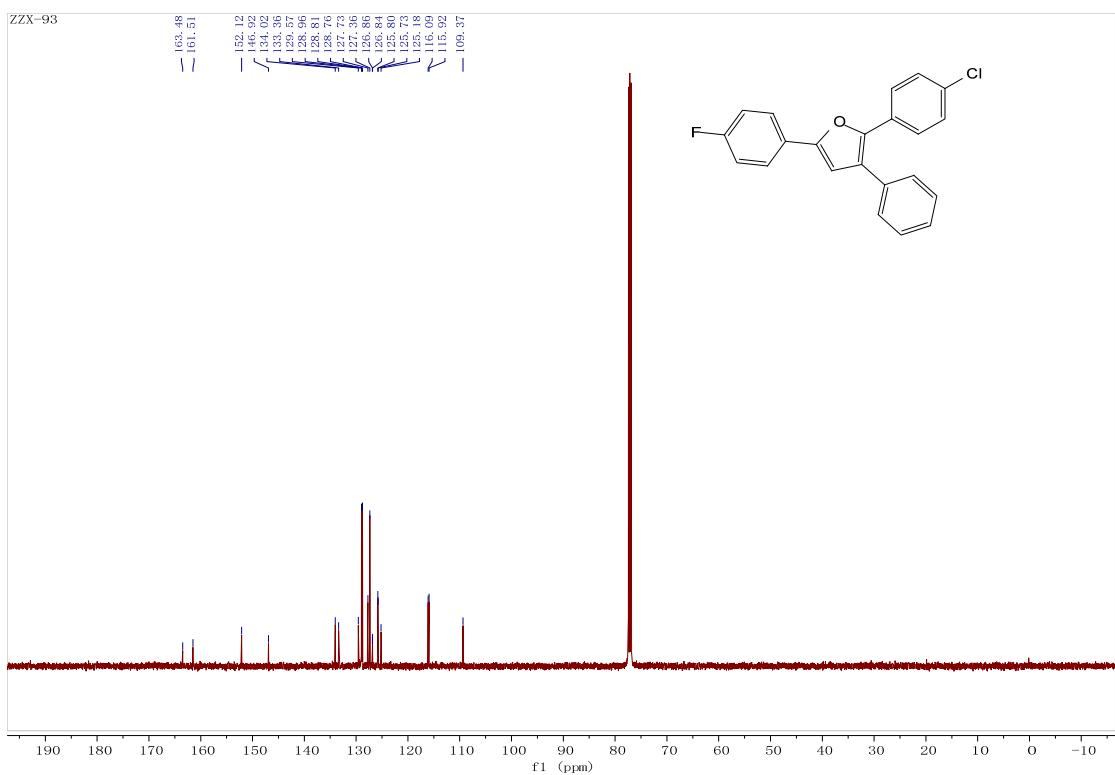
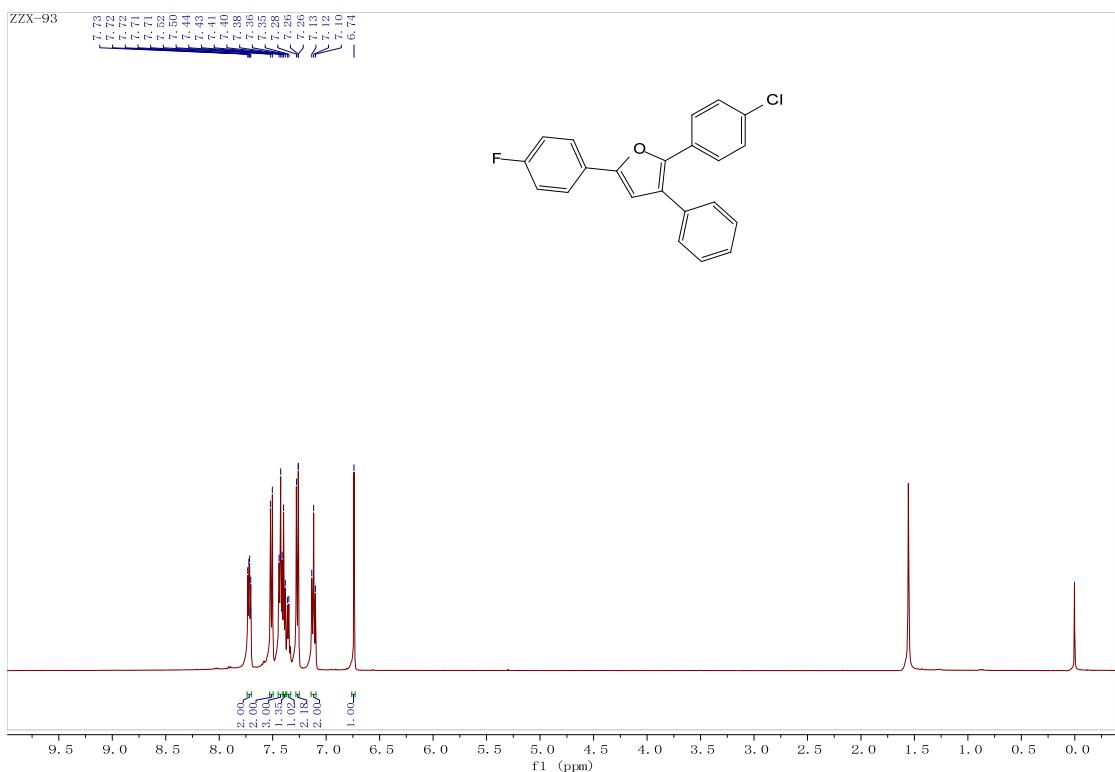
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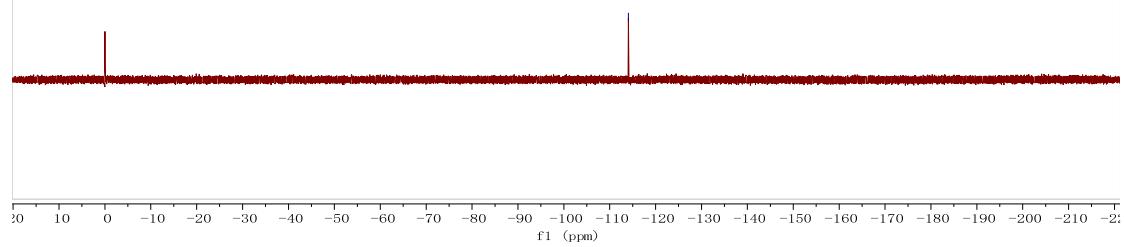
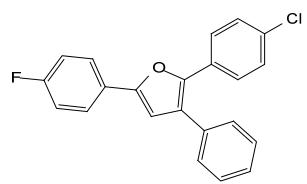


**5f**



ZZX-150

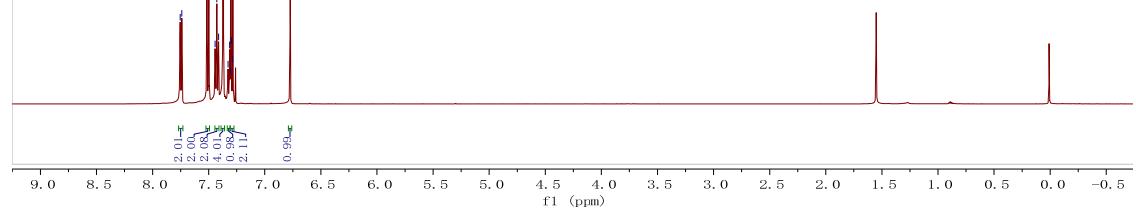
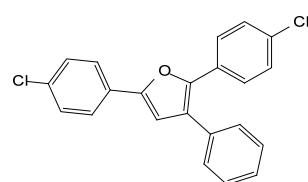
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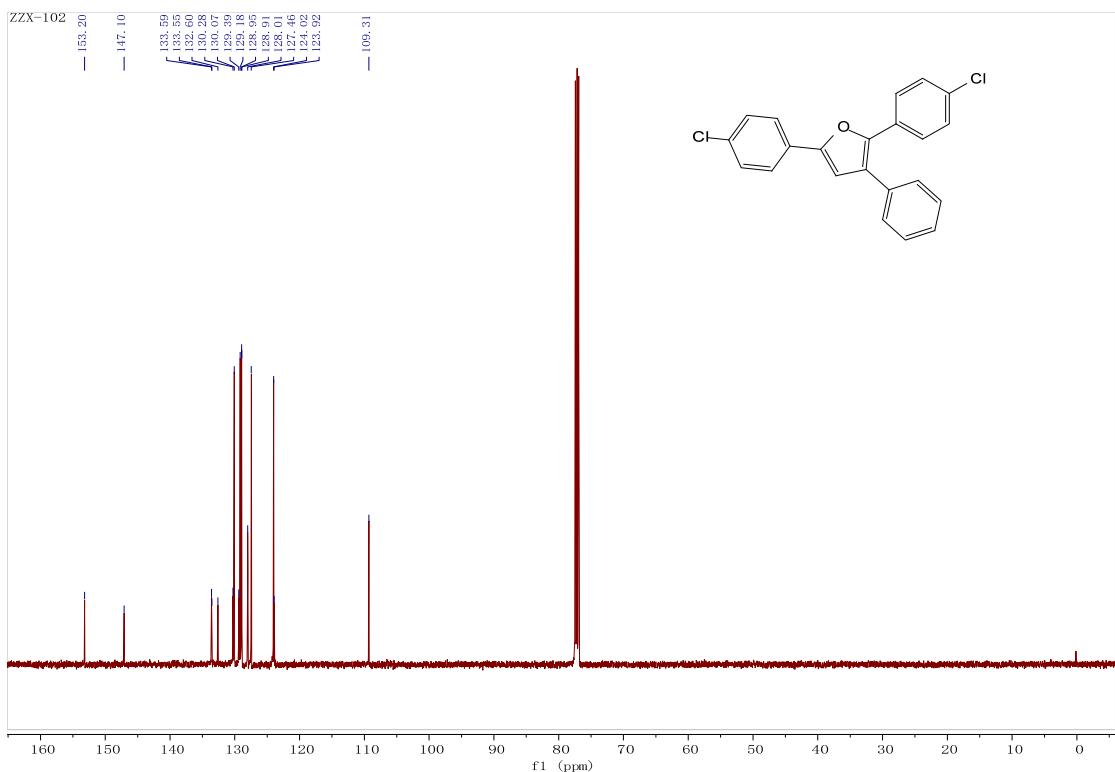


**5g**

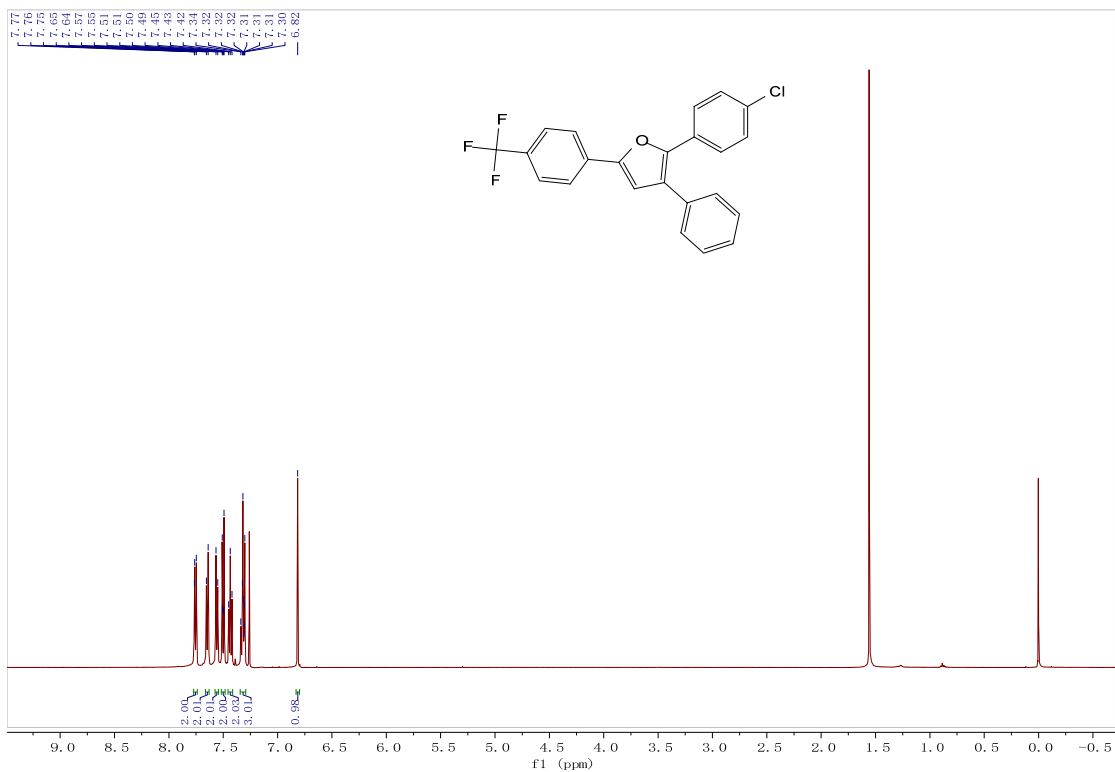
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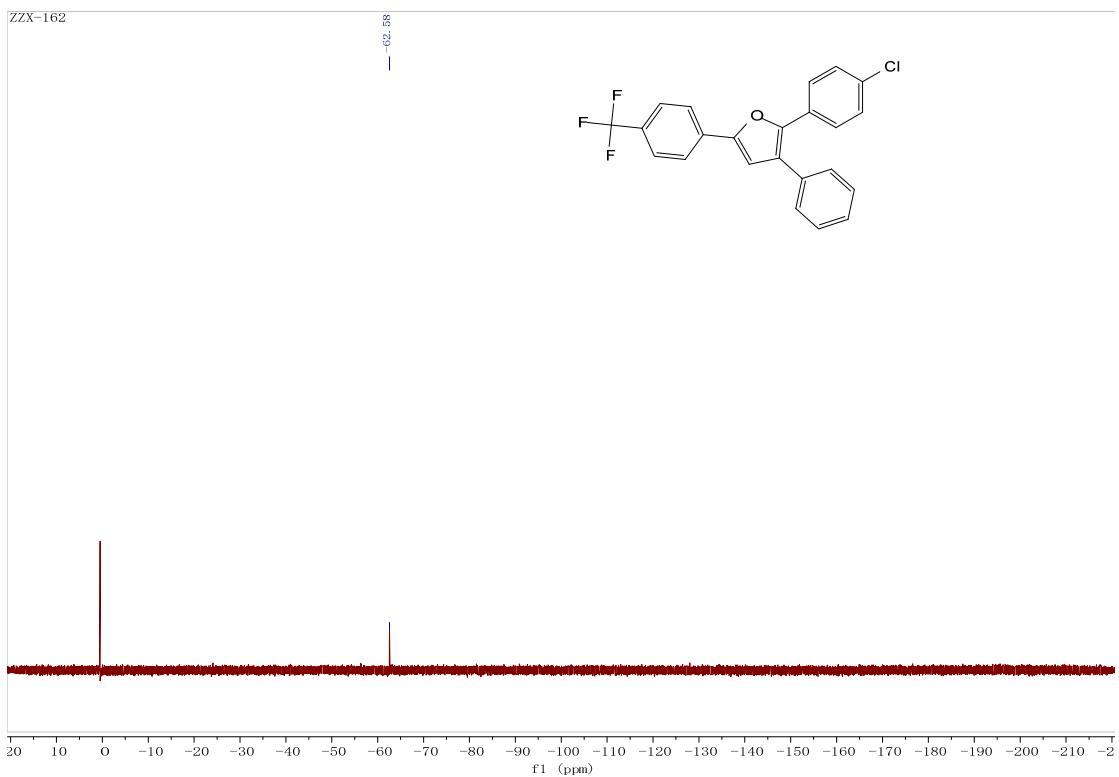
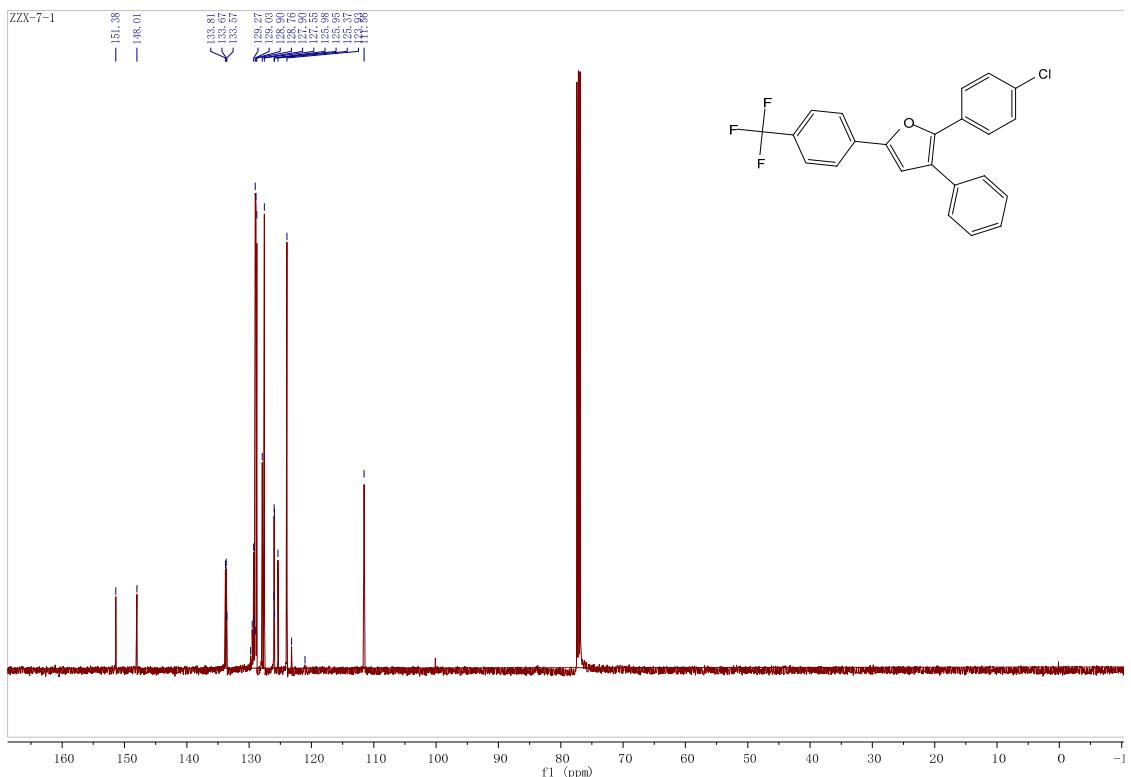
7.35  
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7.14



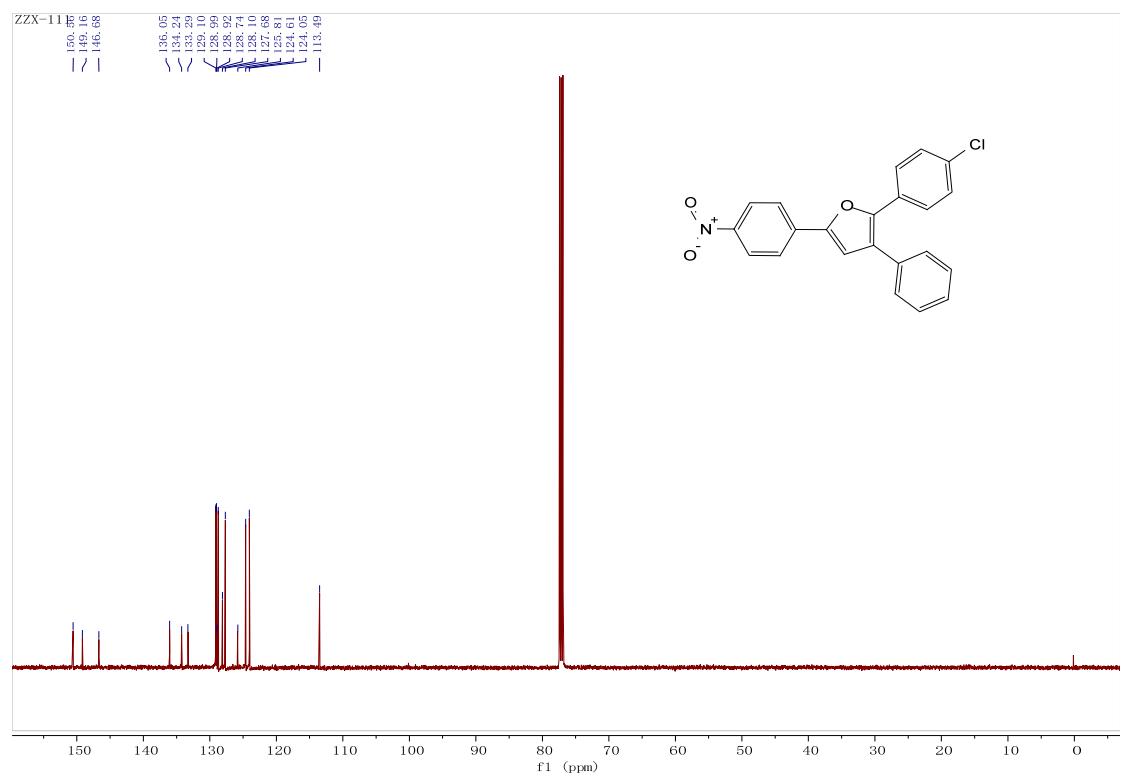
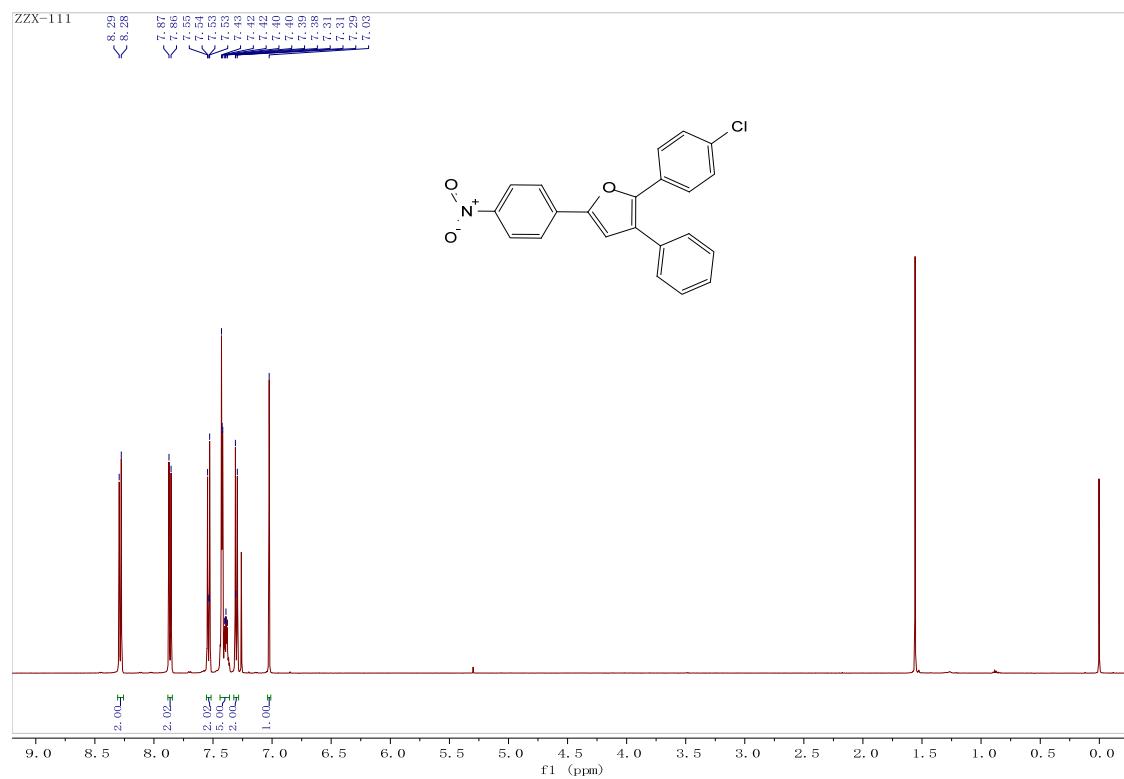


**5h**

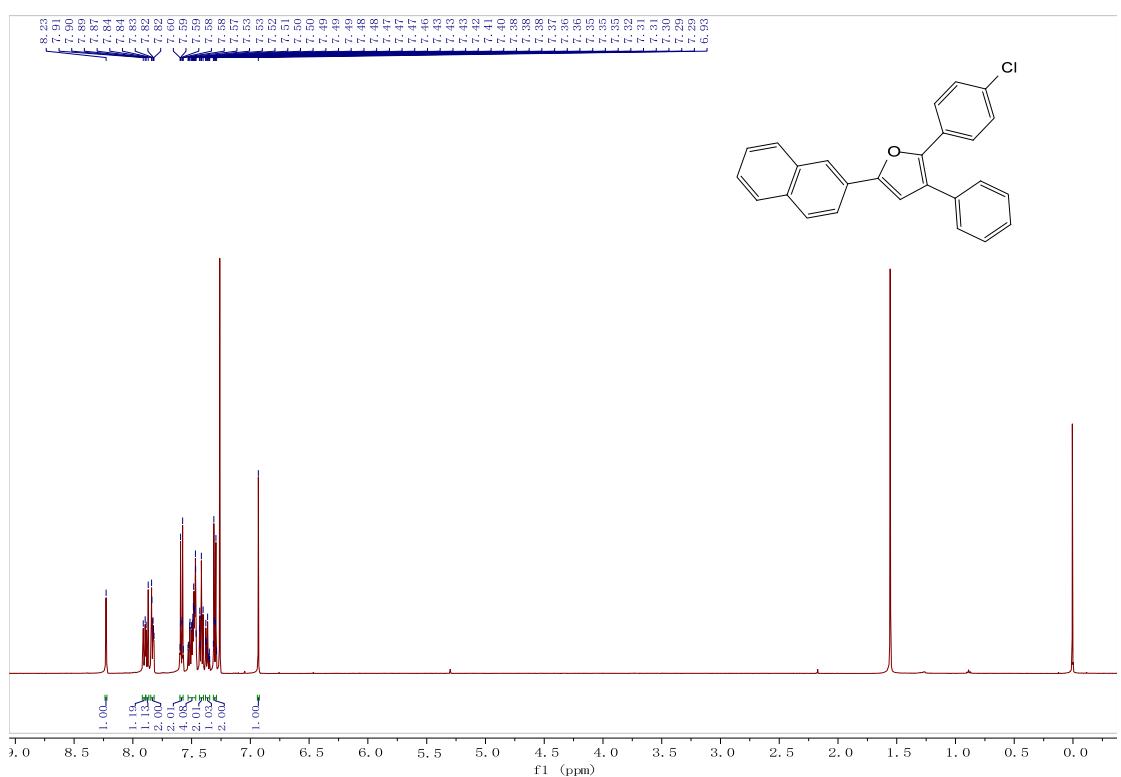




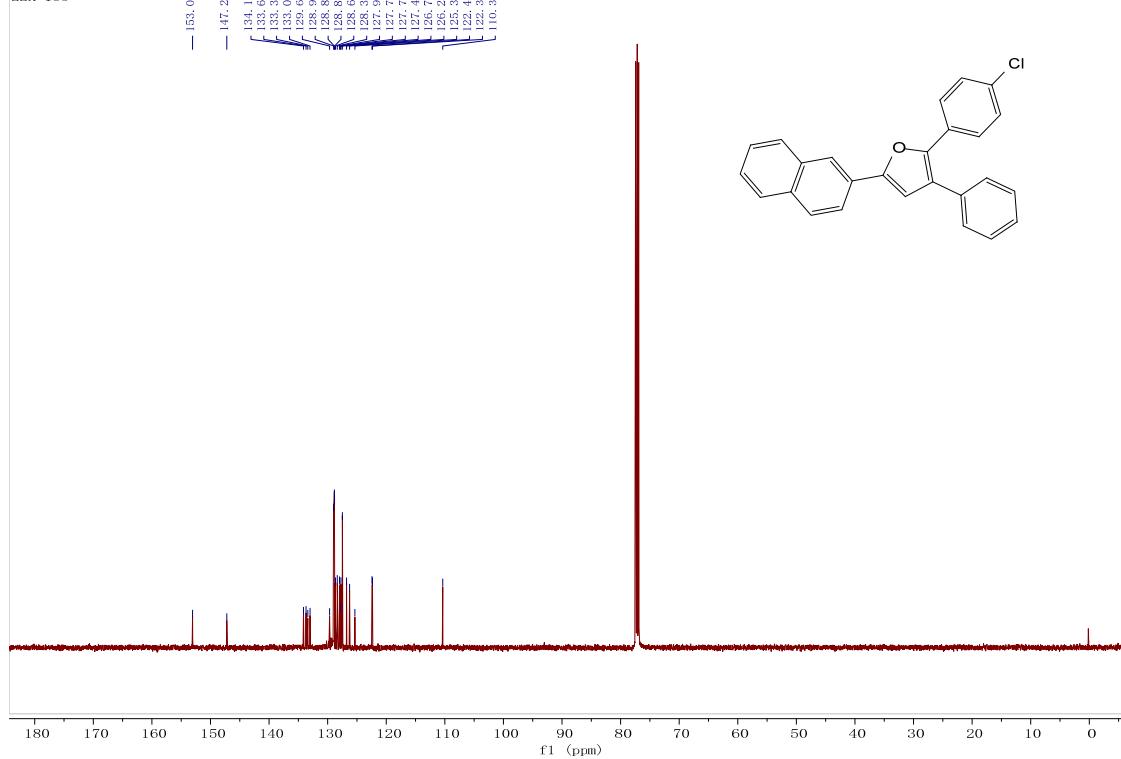
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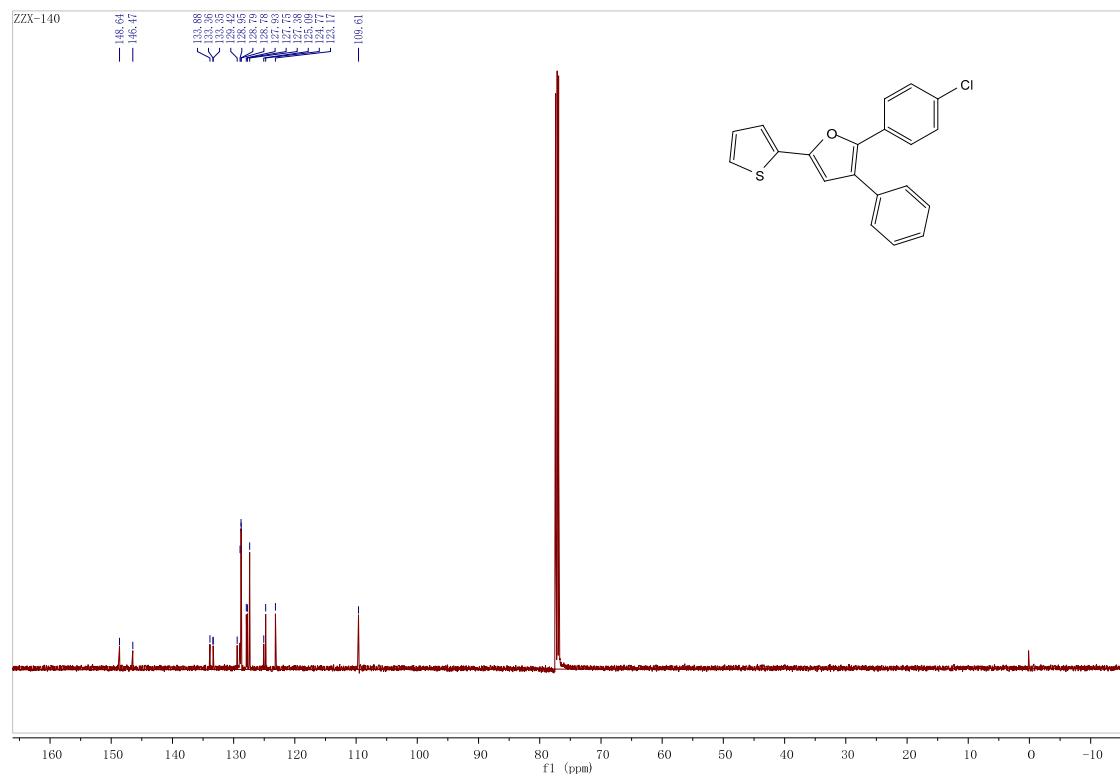
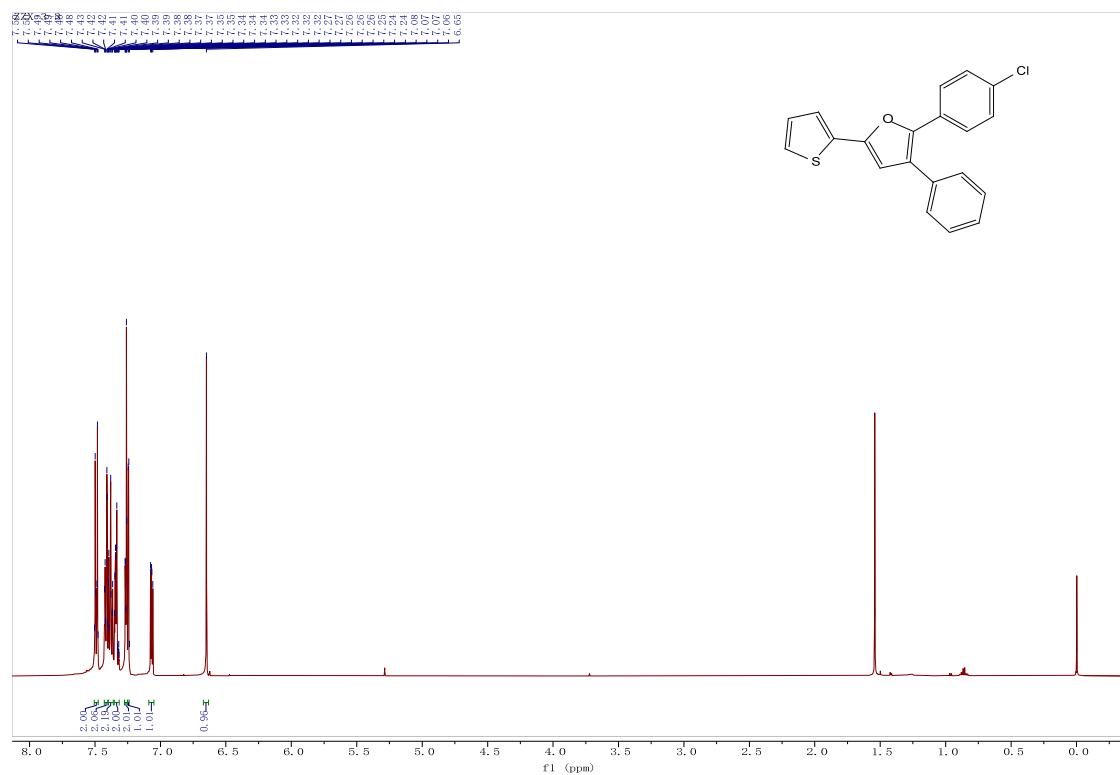
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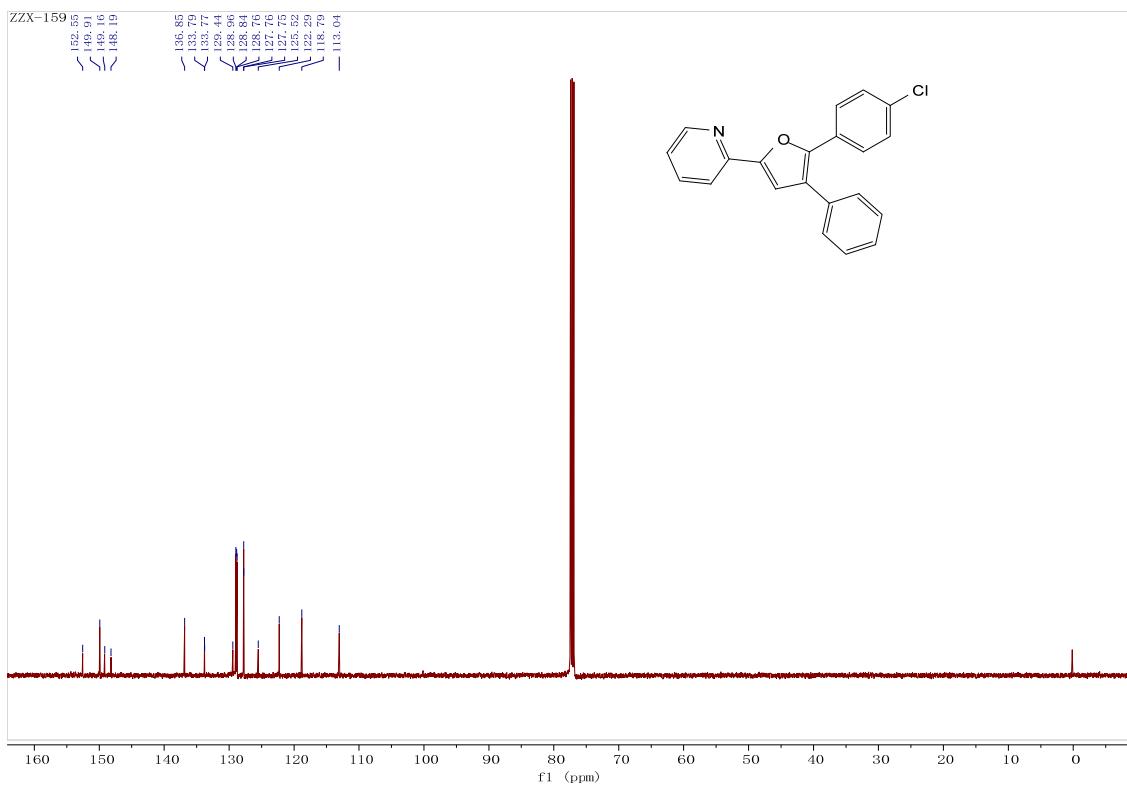
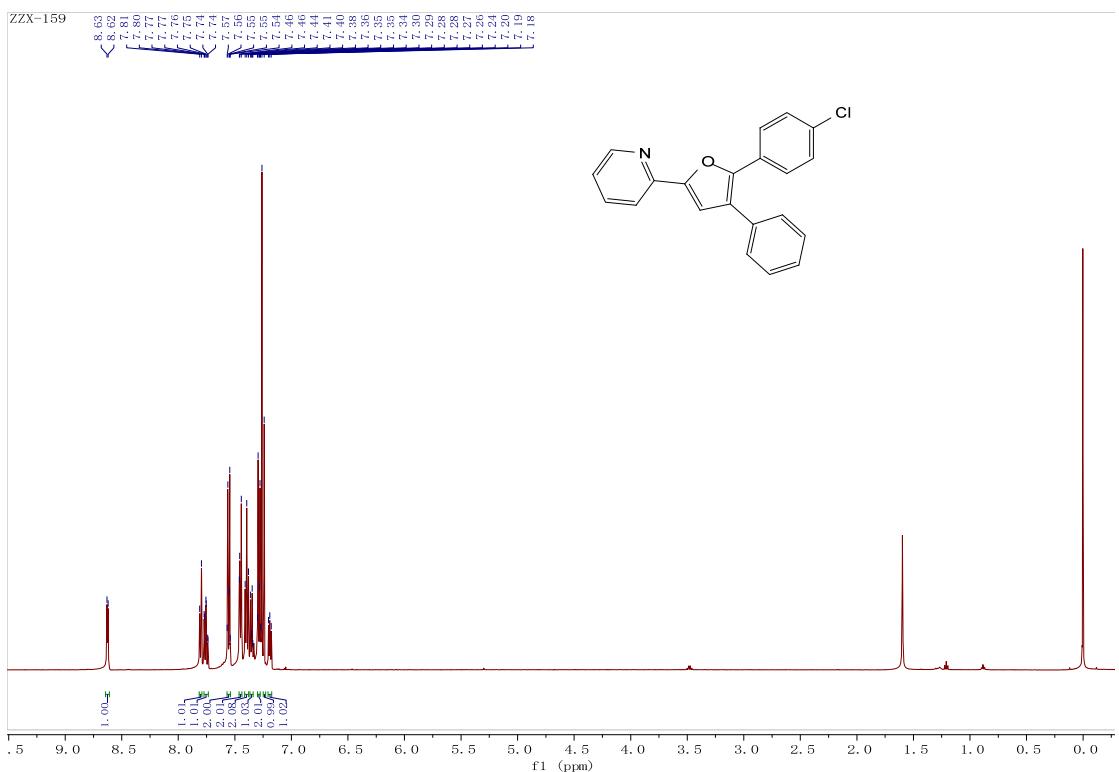


ZZX-135

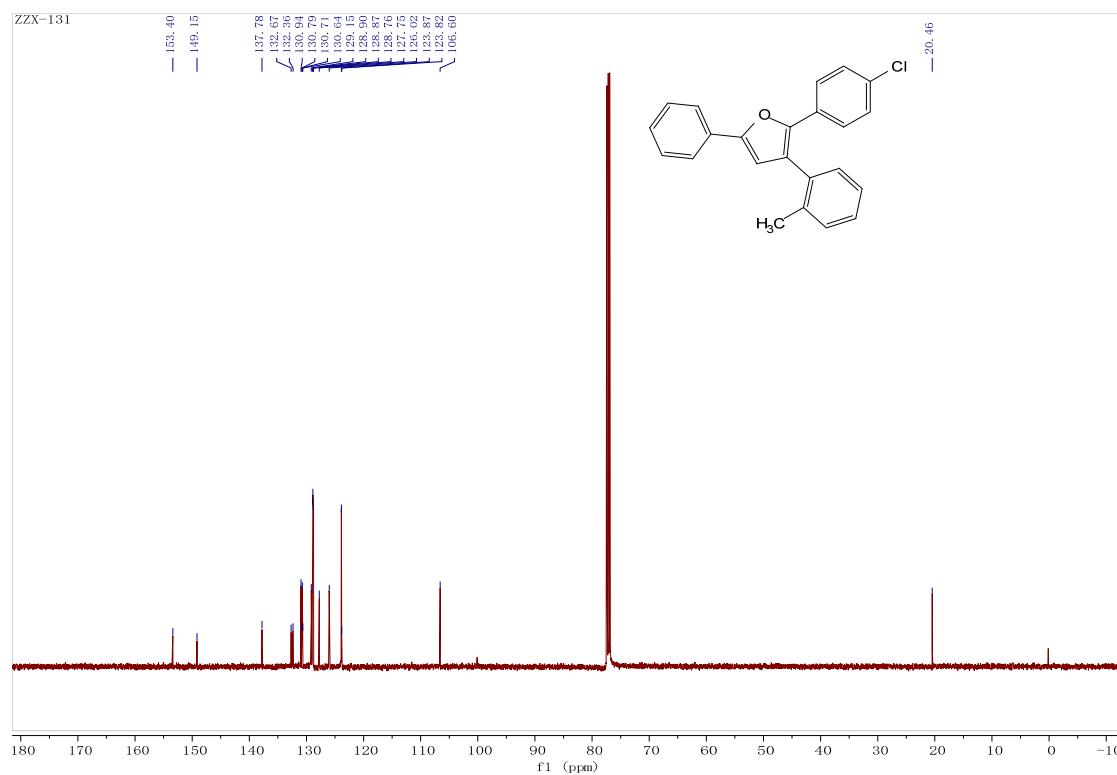
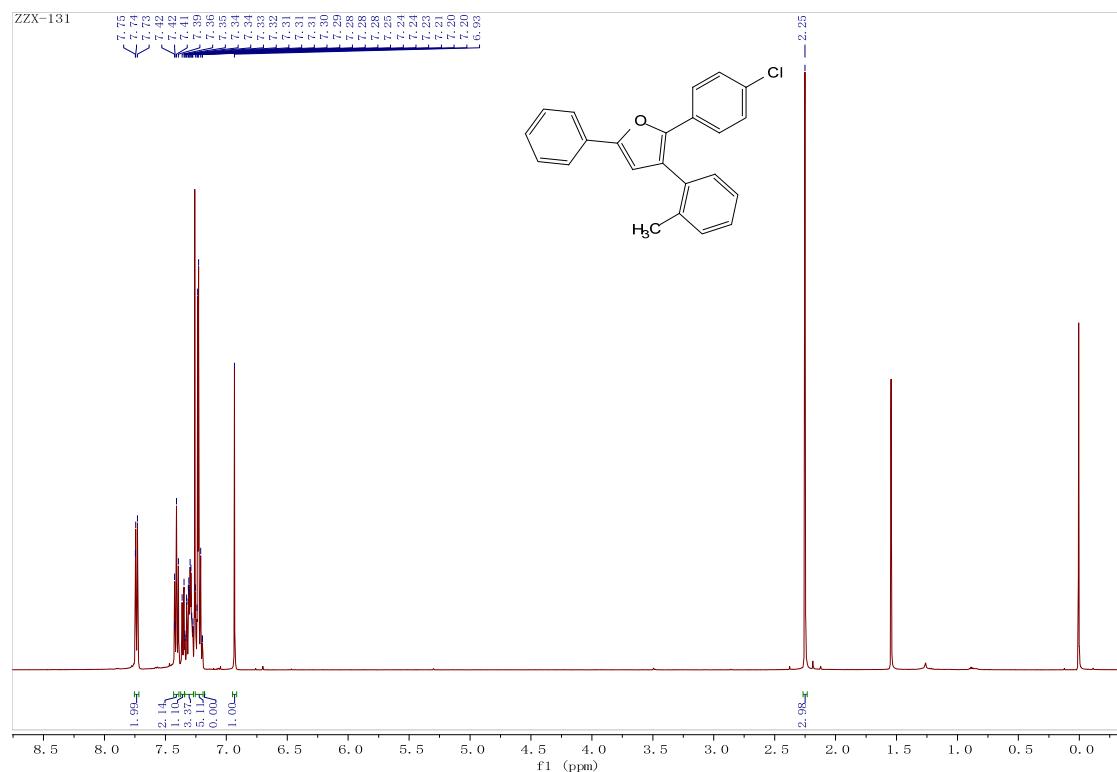


**5k**

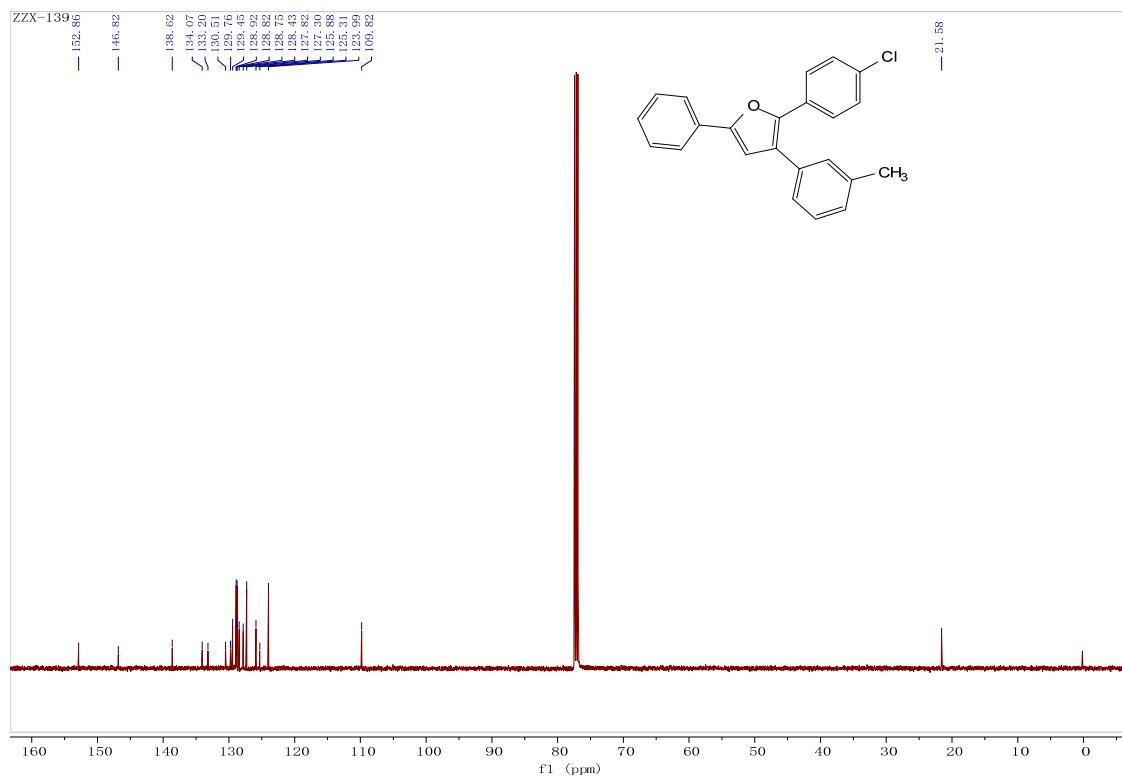
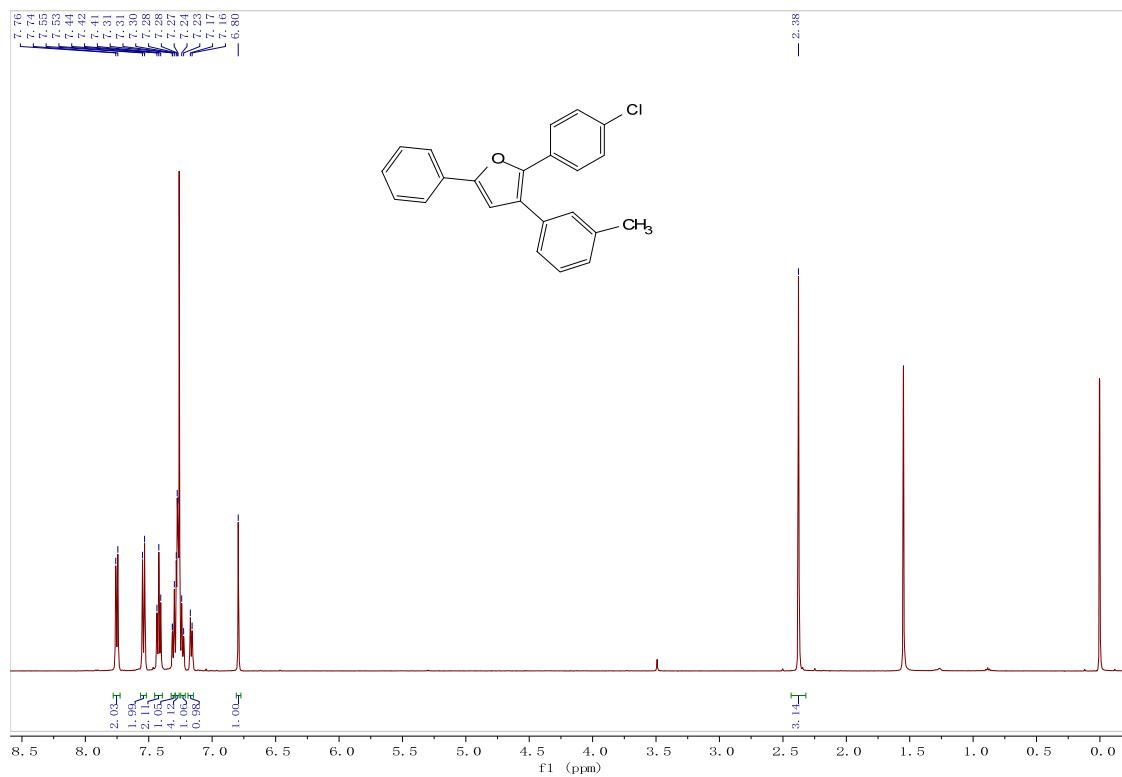


**5l**

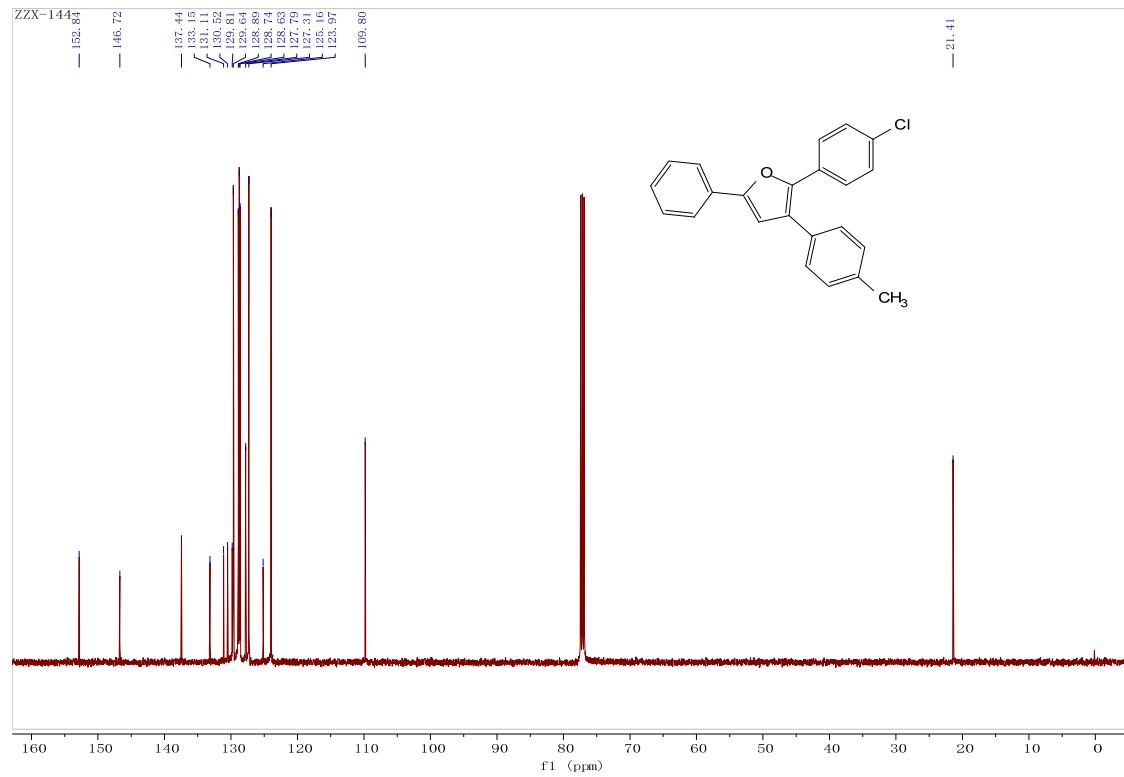
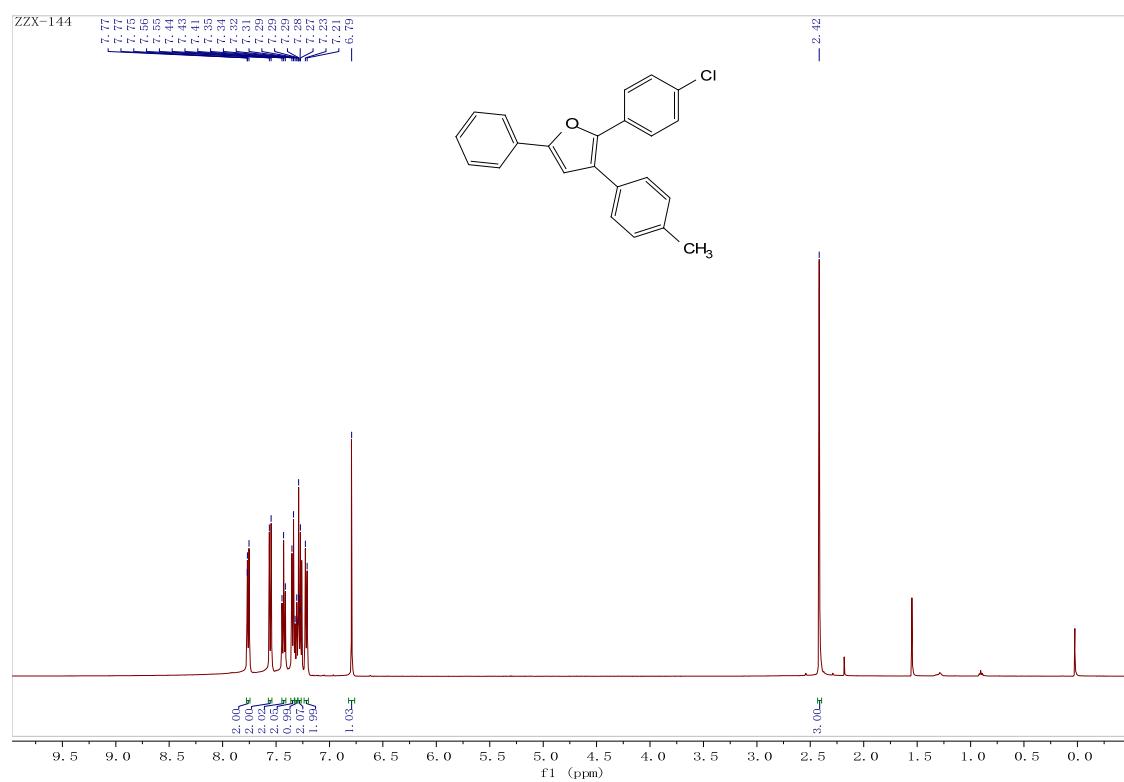
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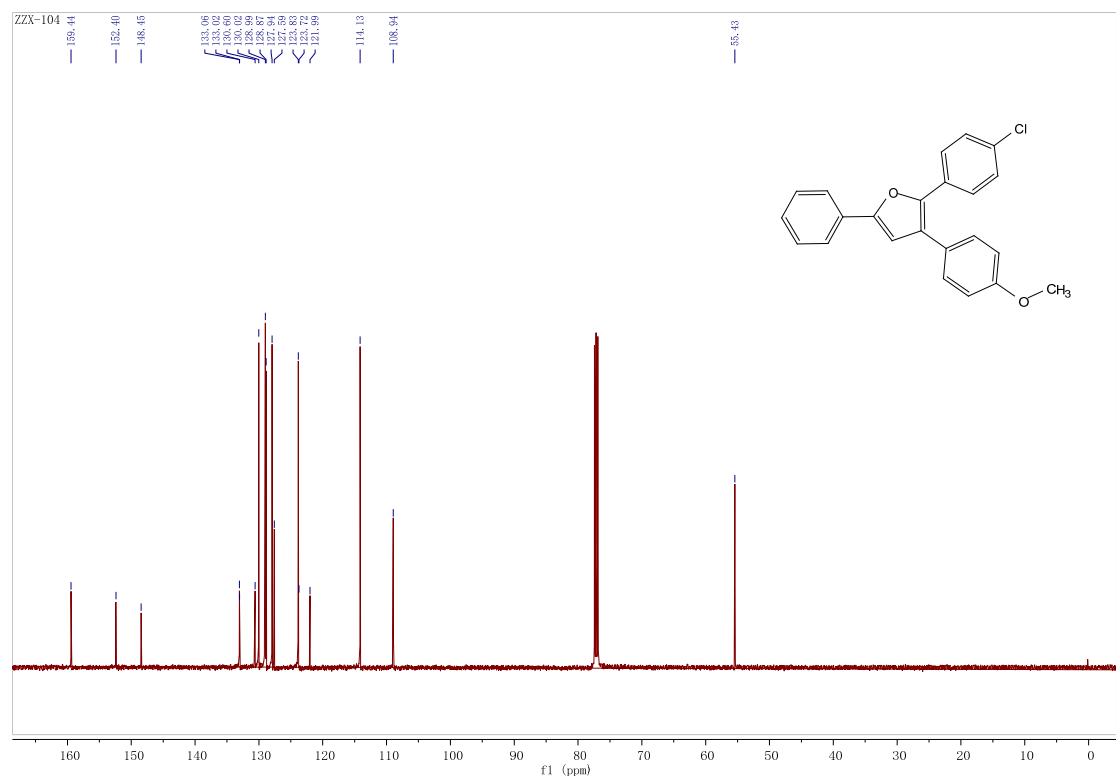
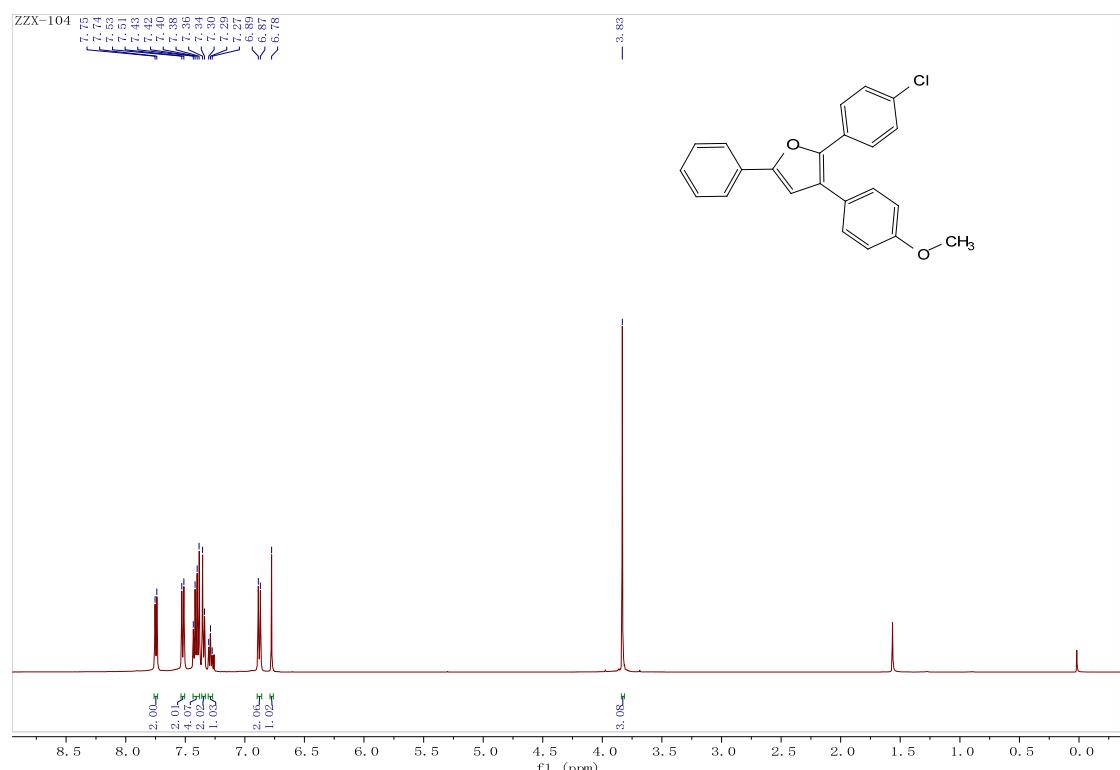


5n

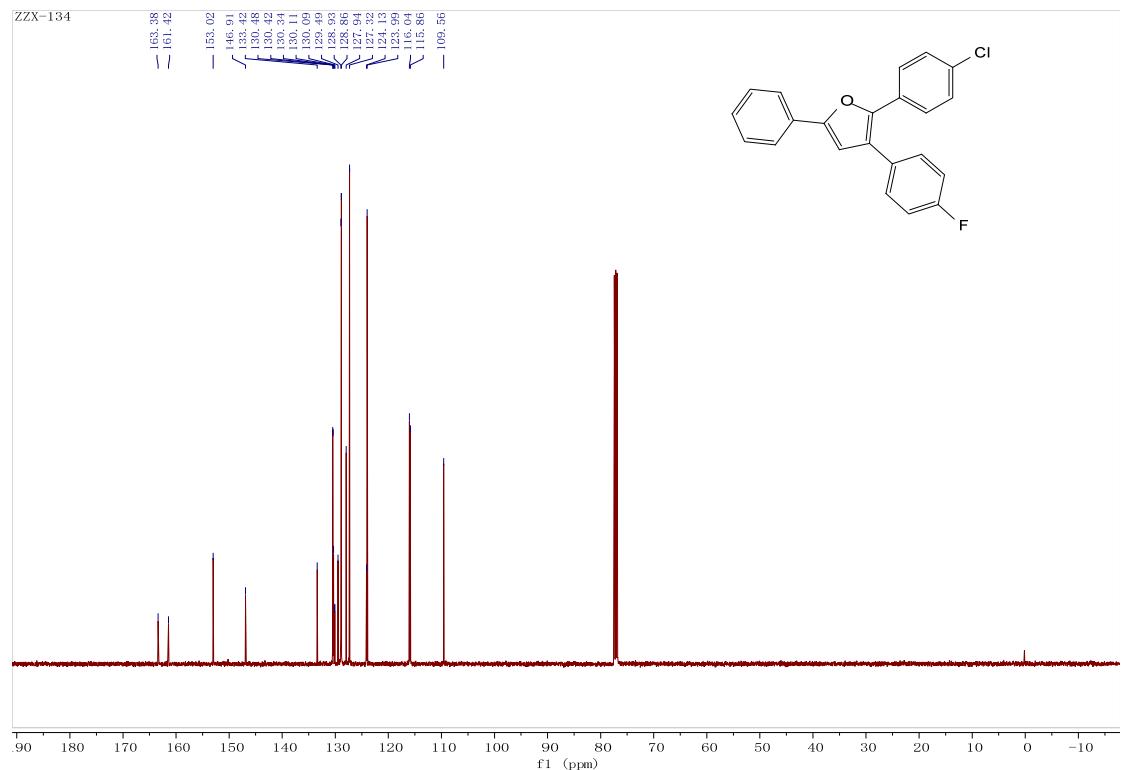
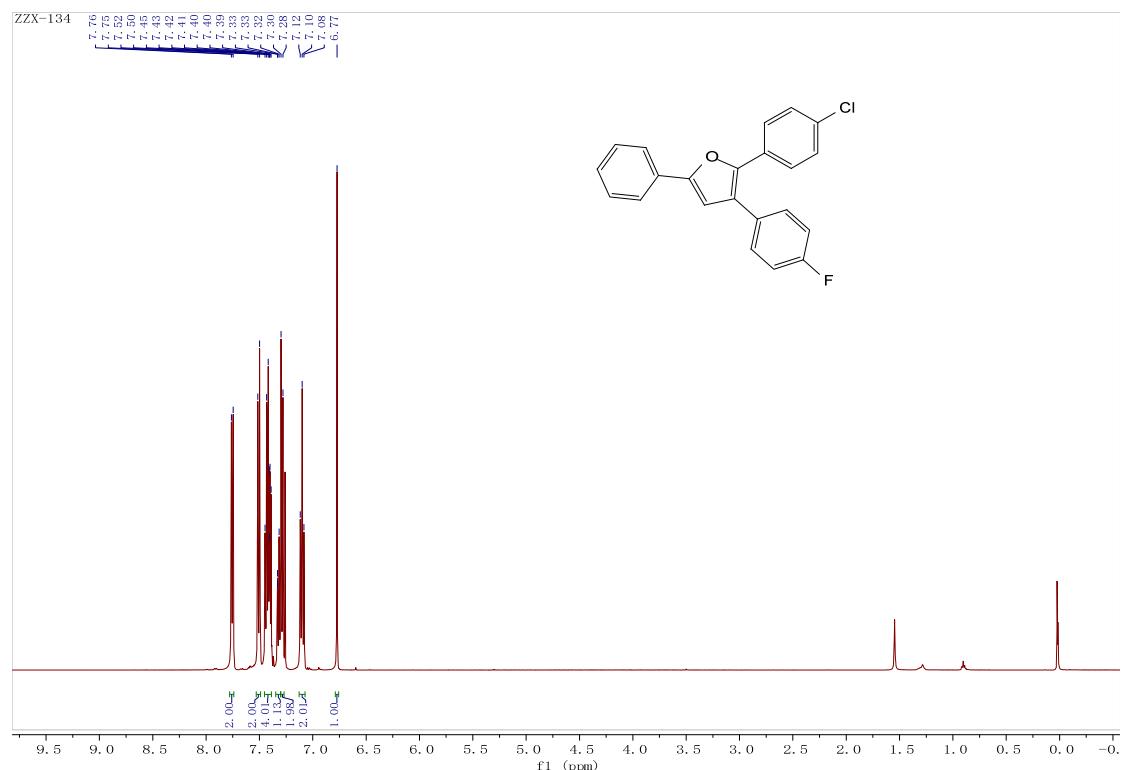


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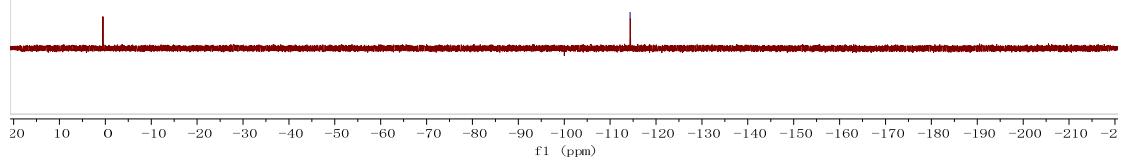
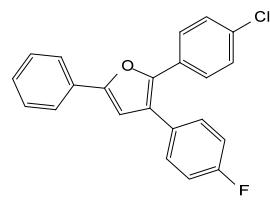


**5p**

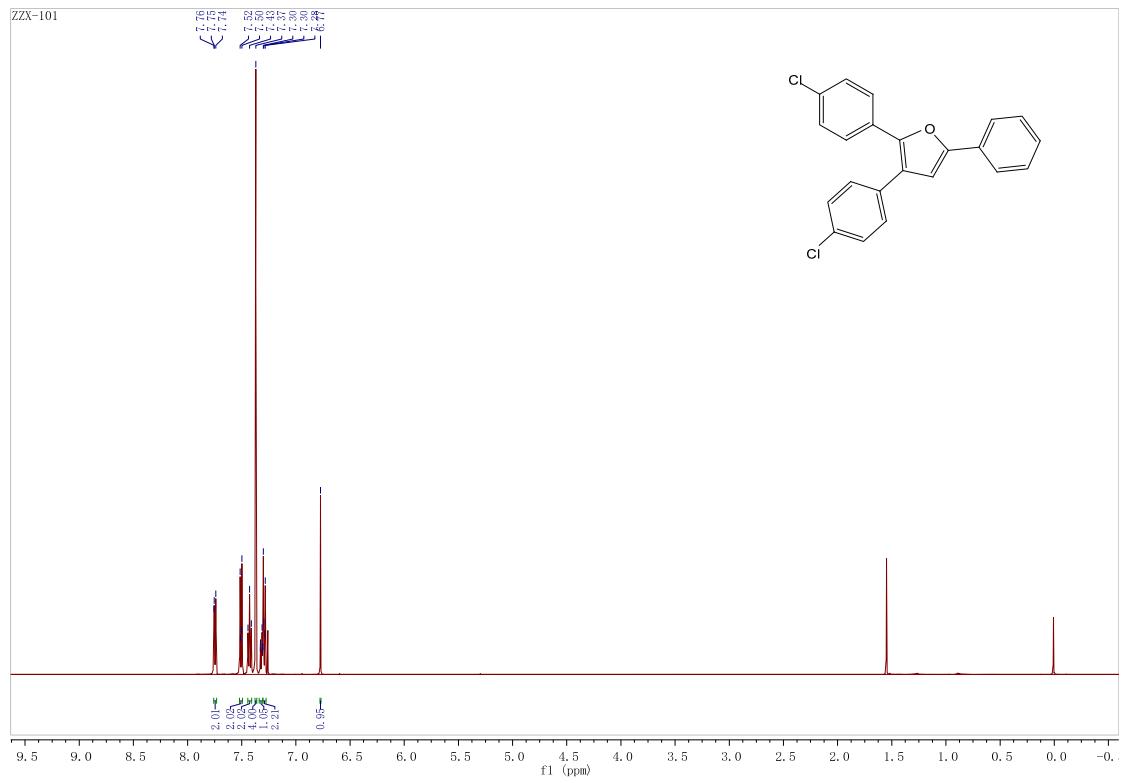
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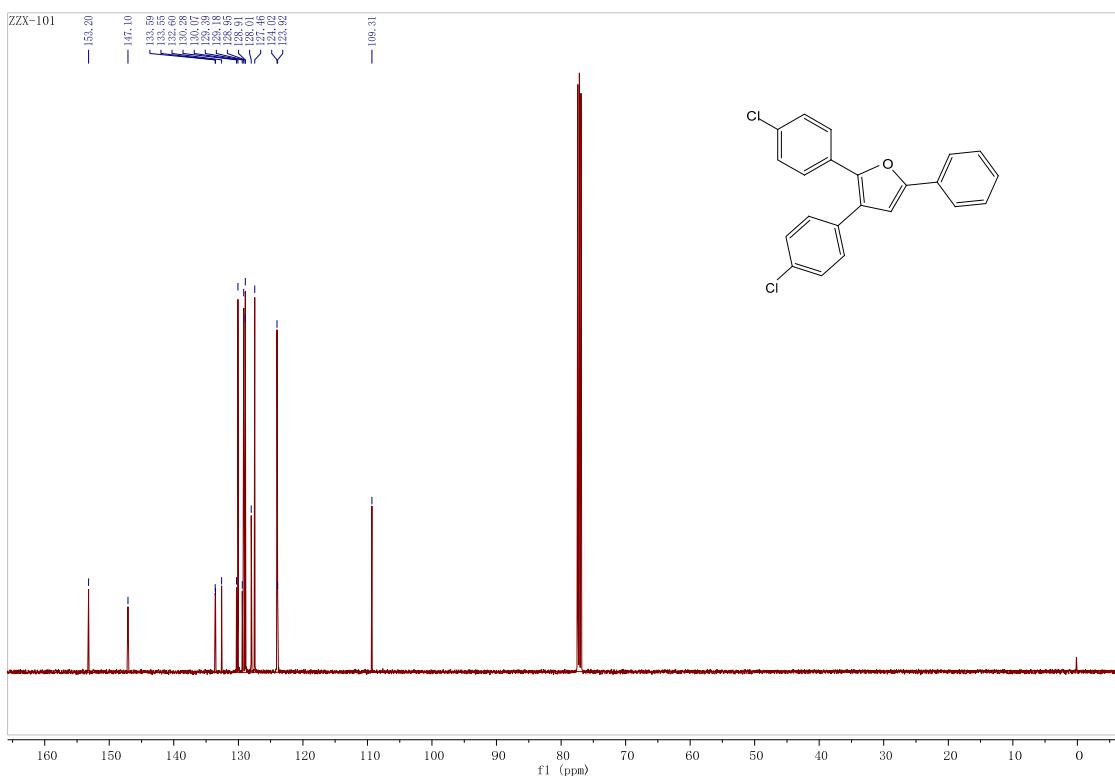


ZZ-152

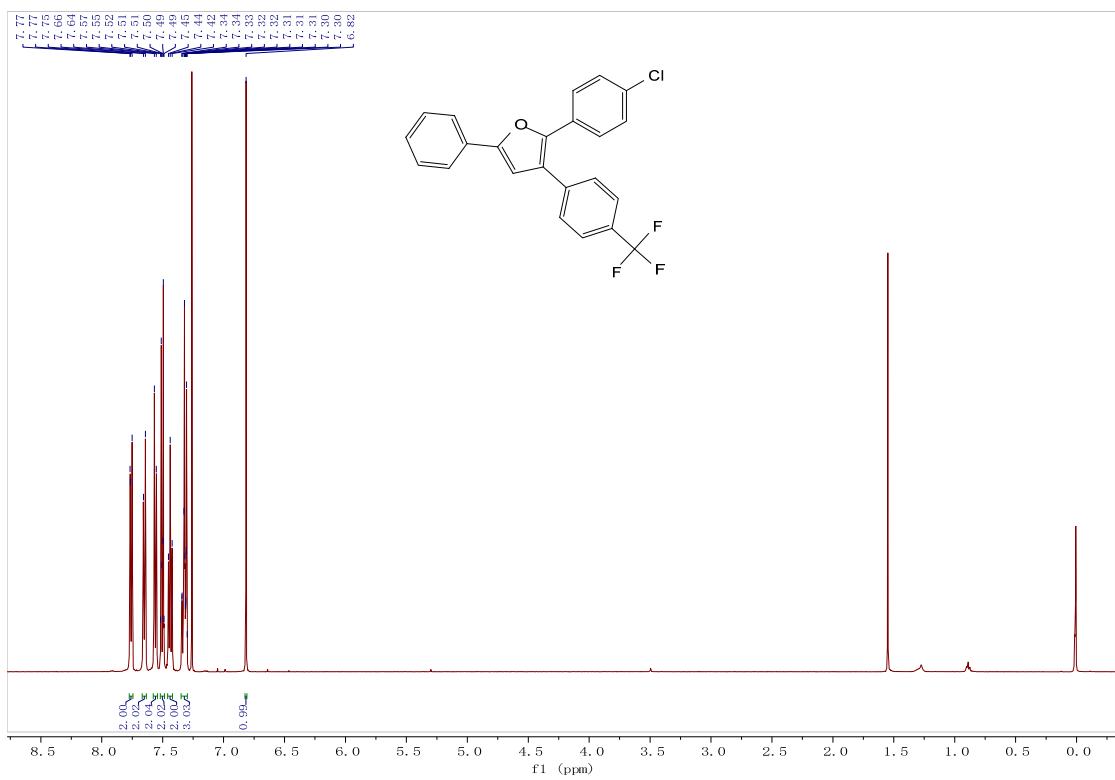


5r

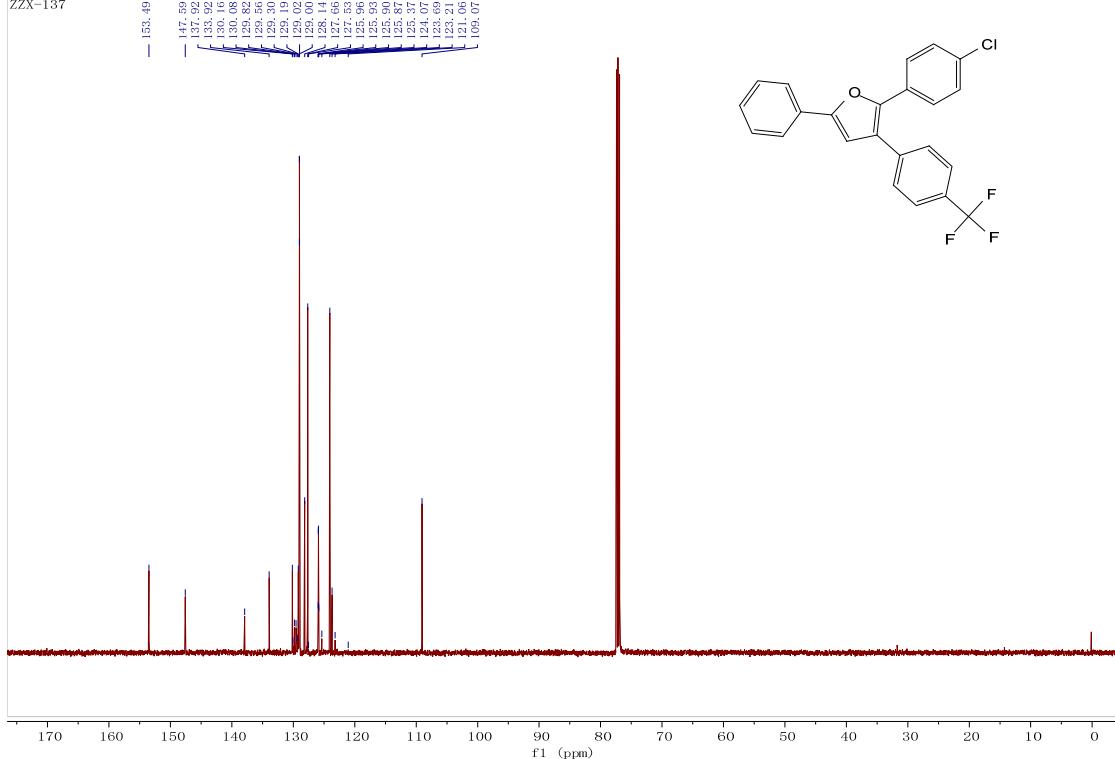




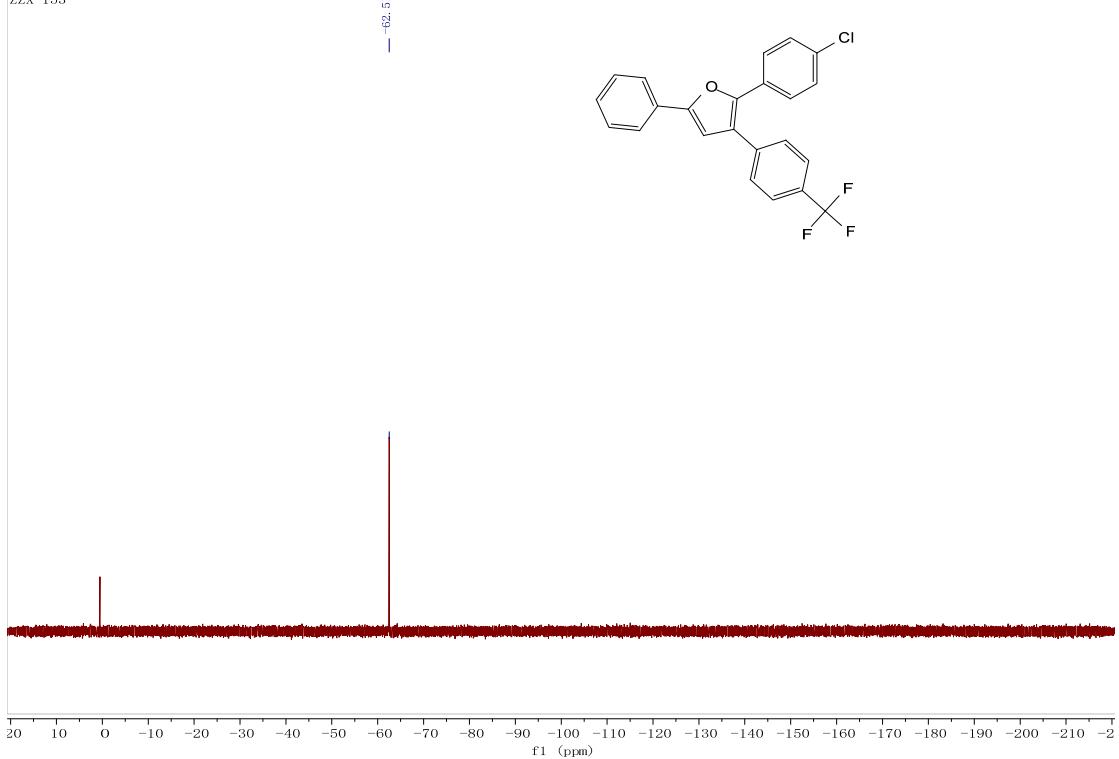
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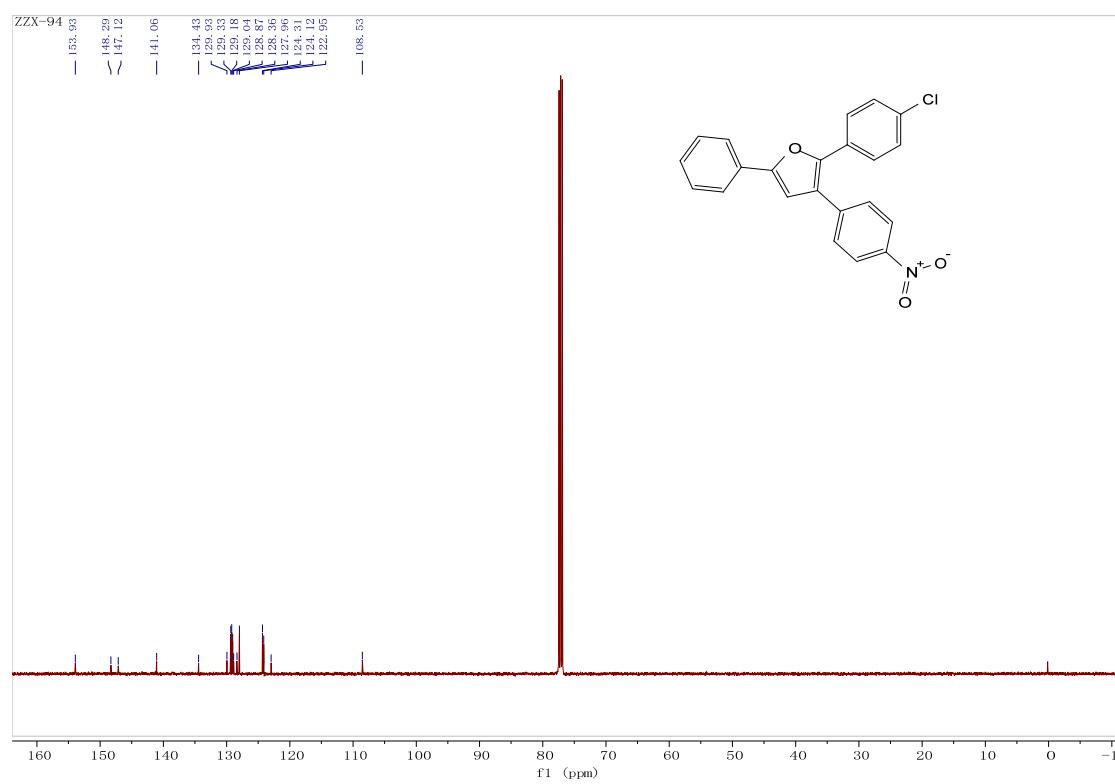
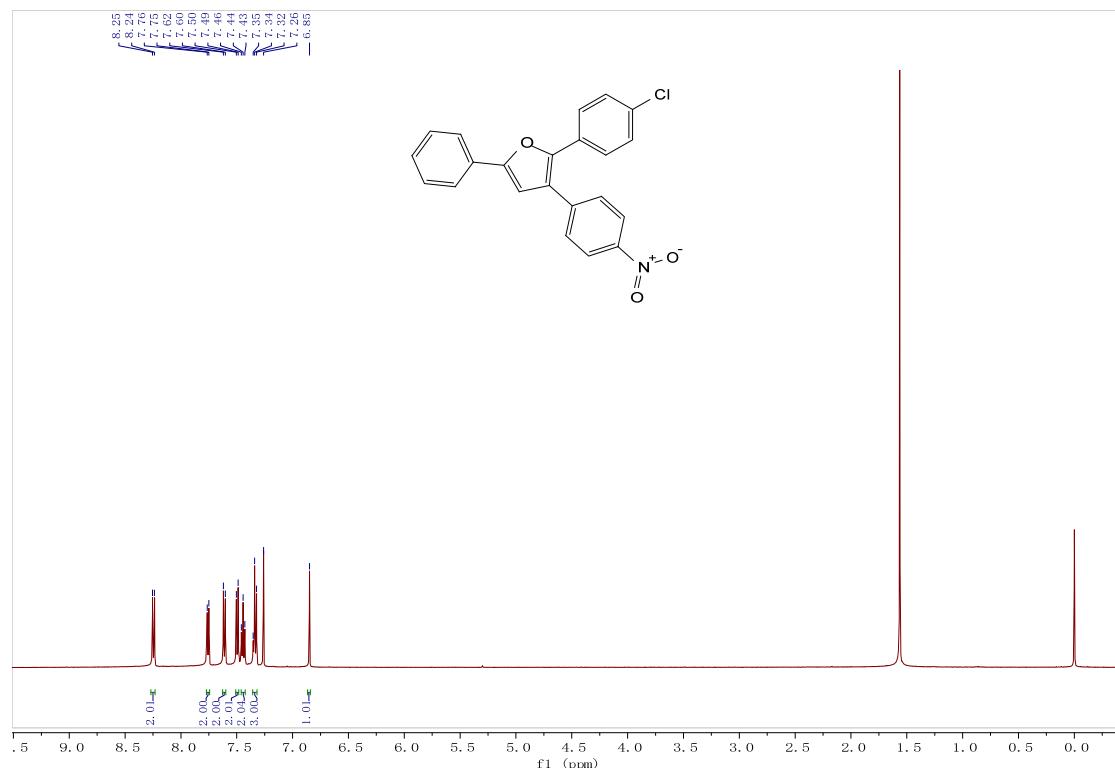
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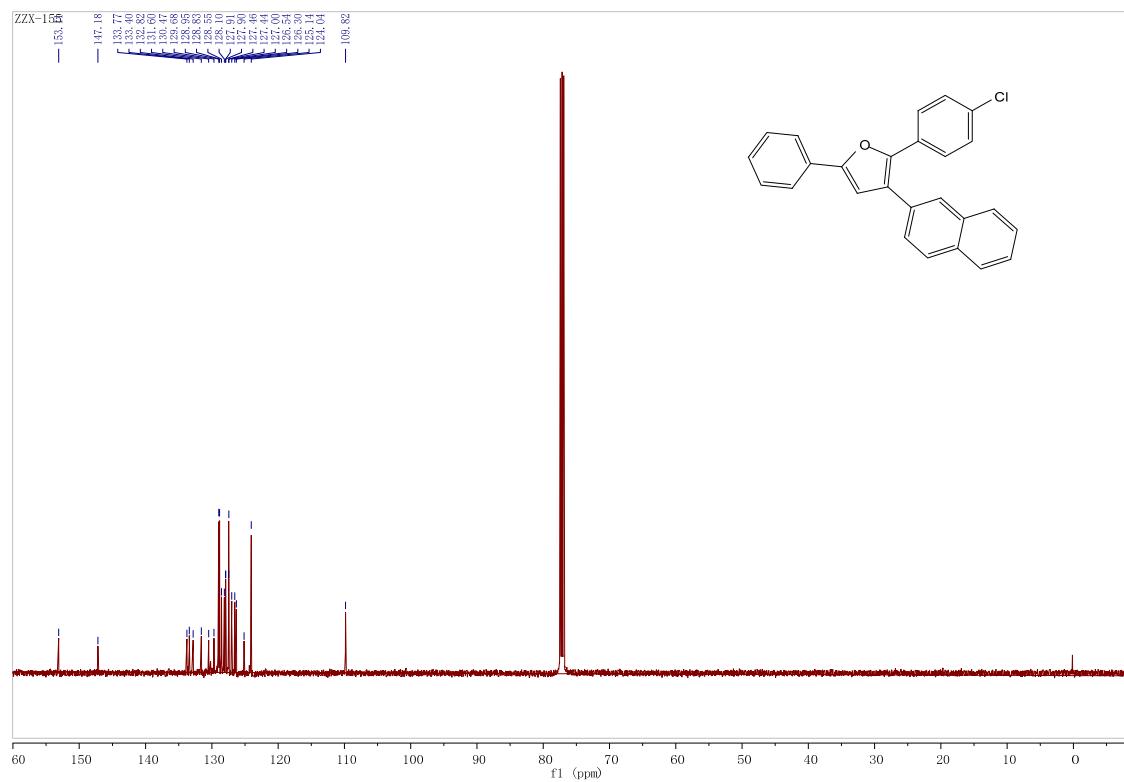
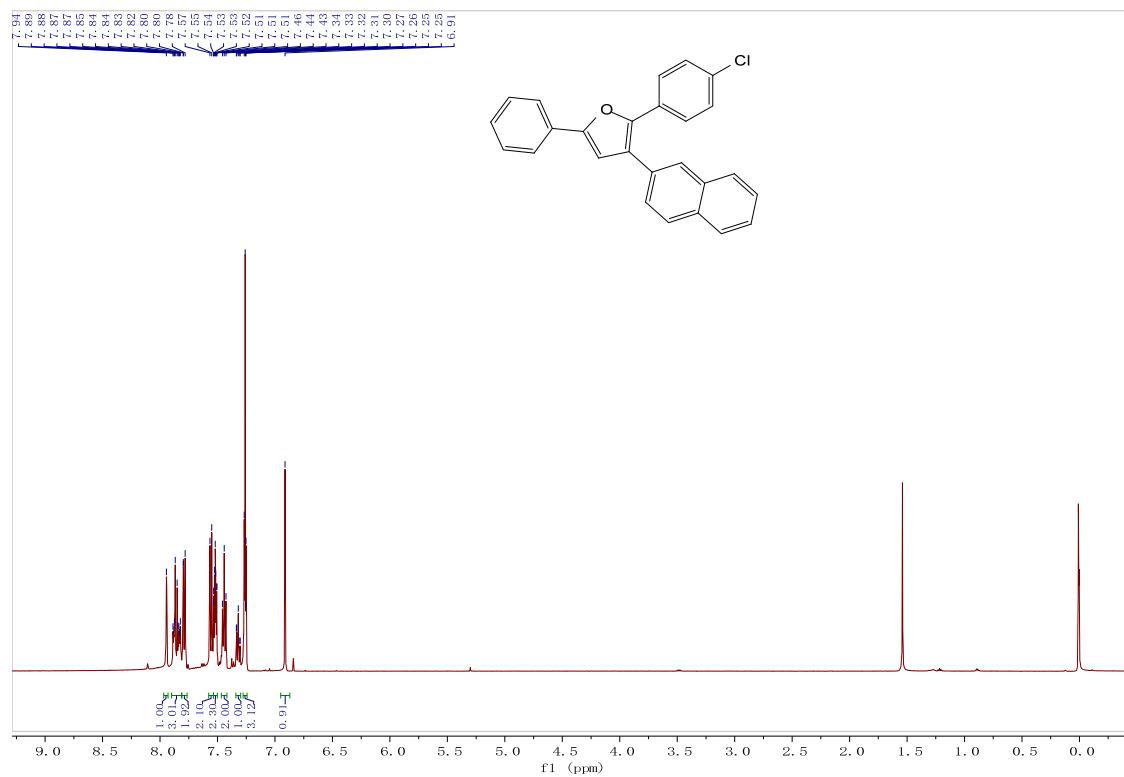
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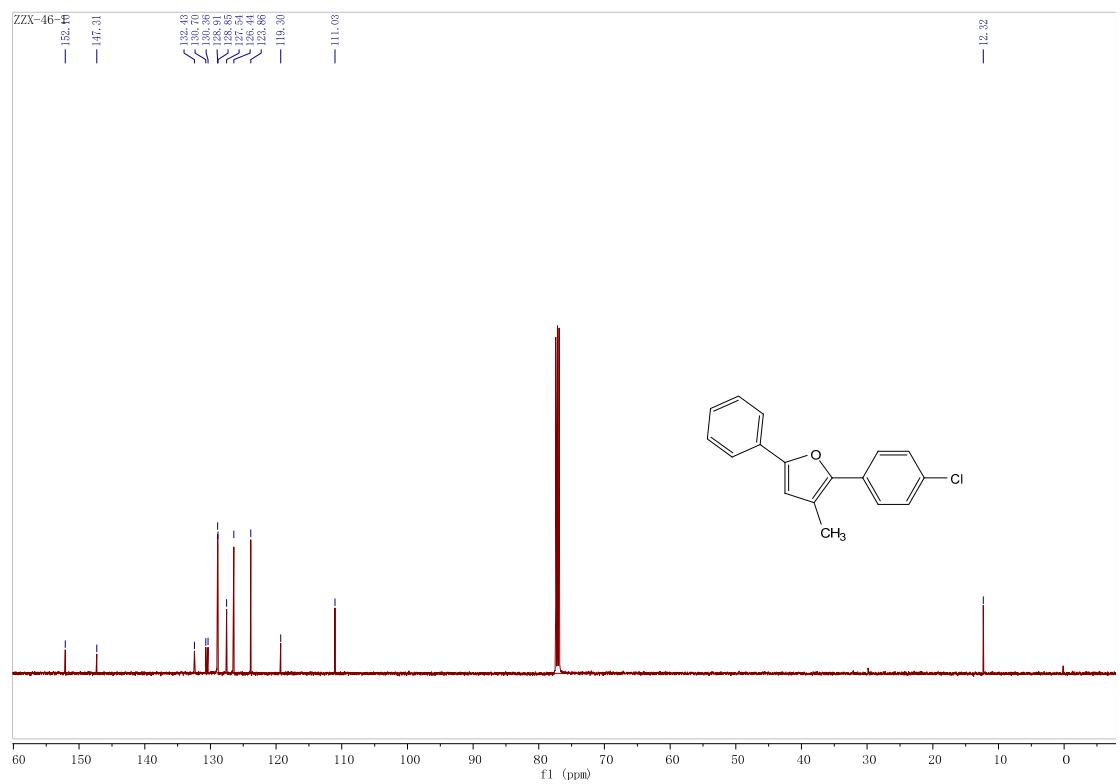
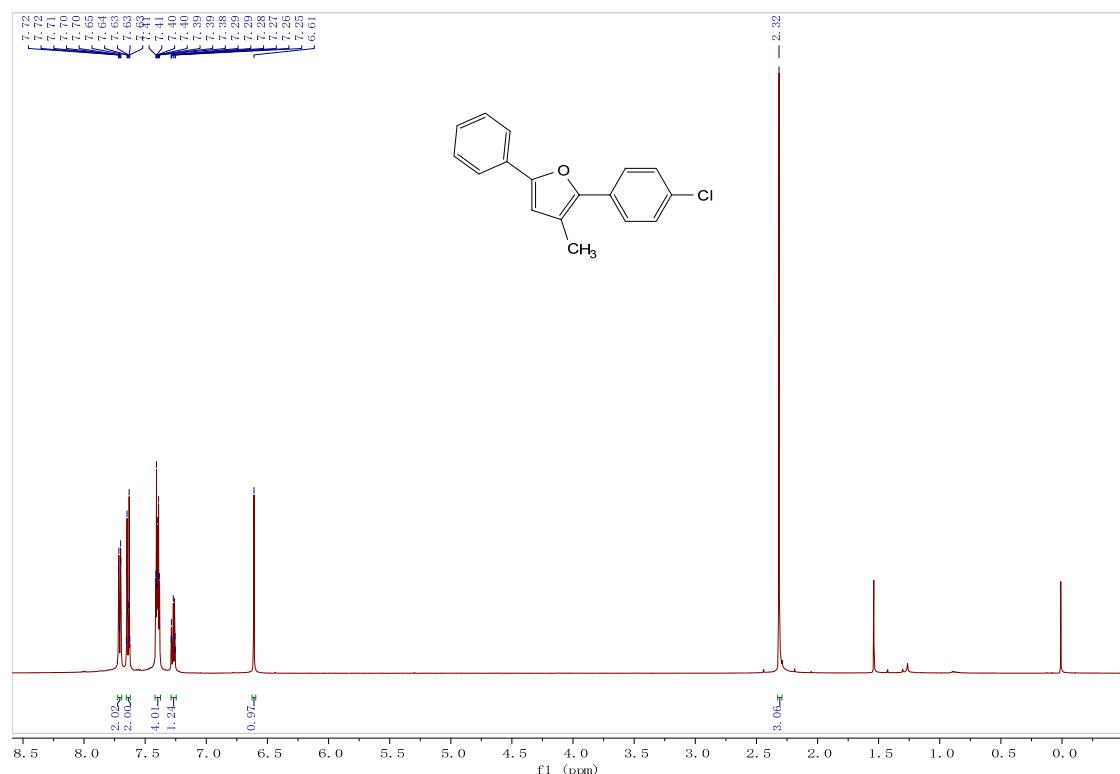
**5t**

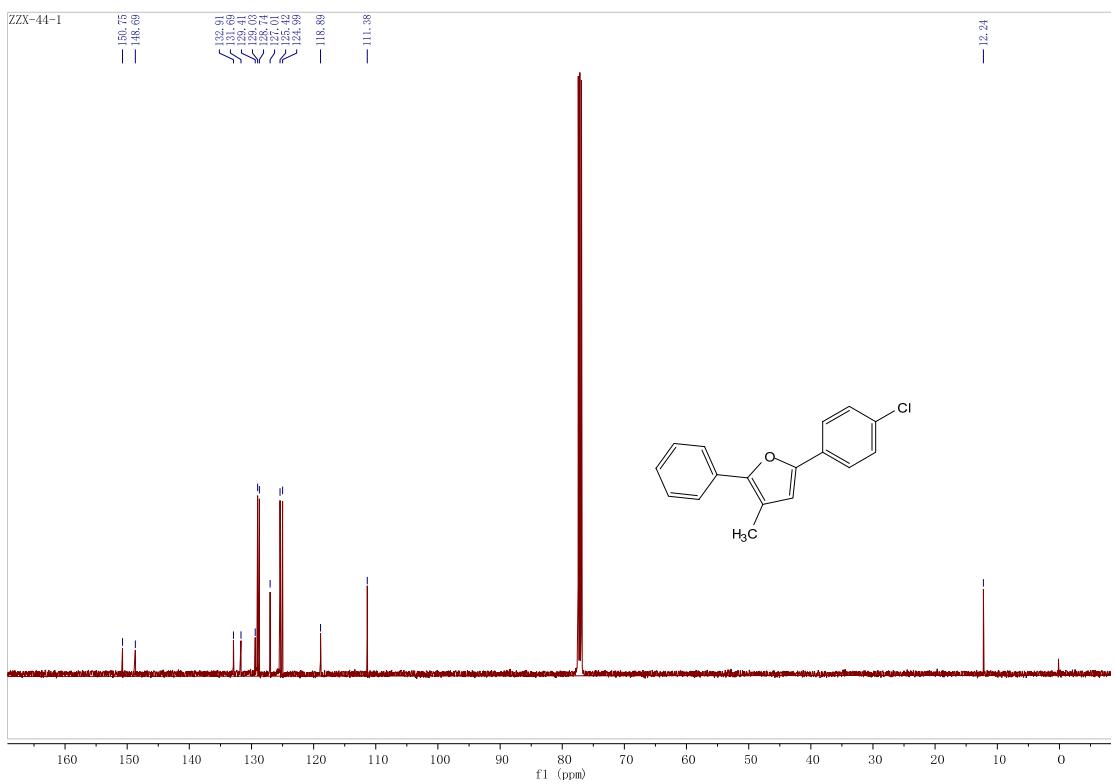
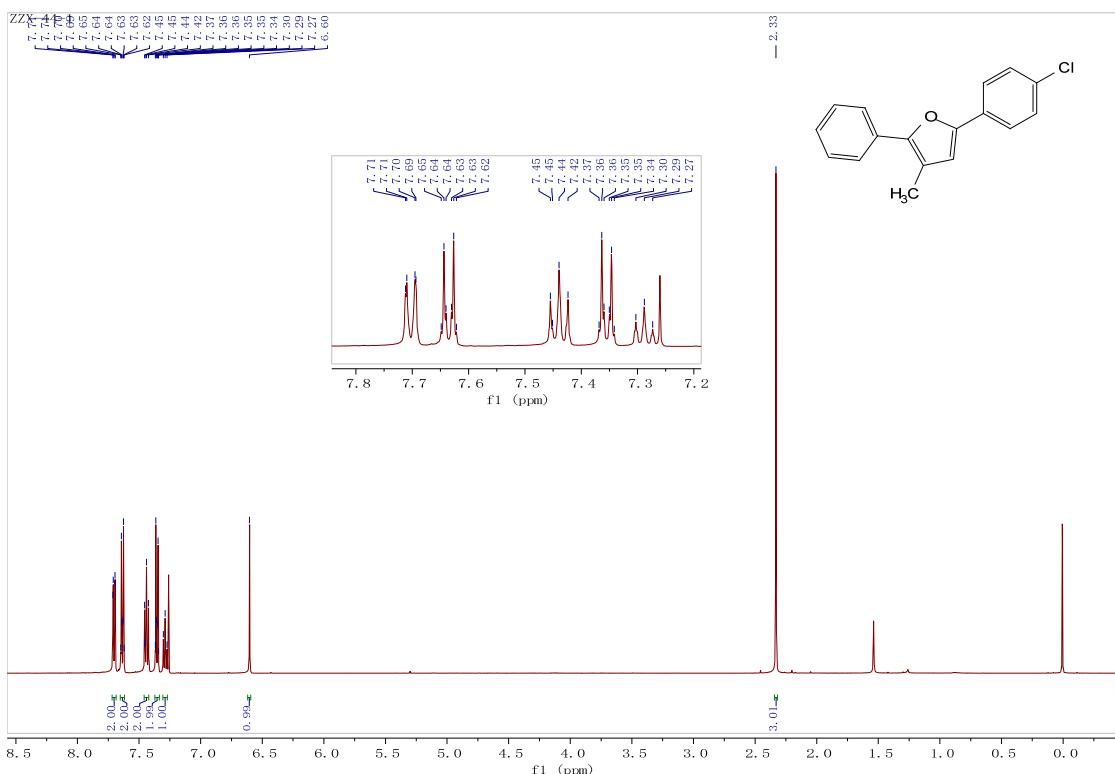


**5u**

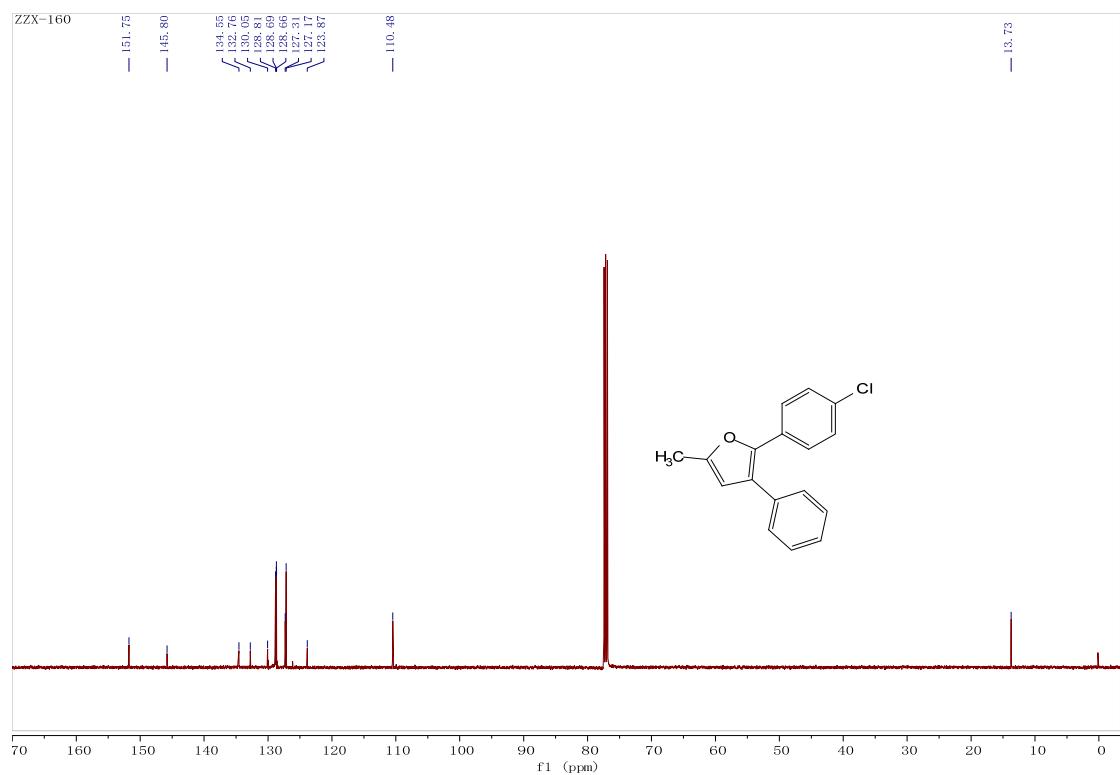
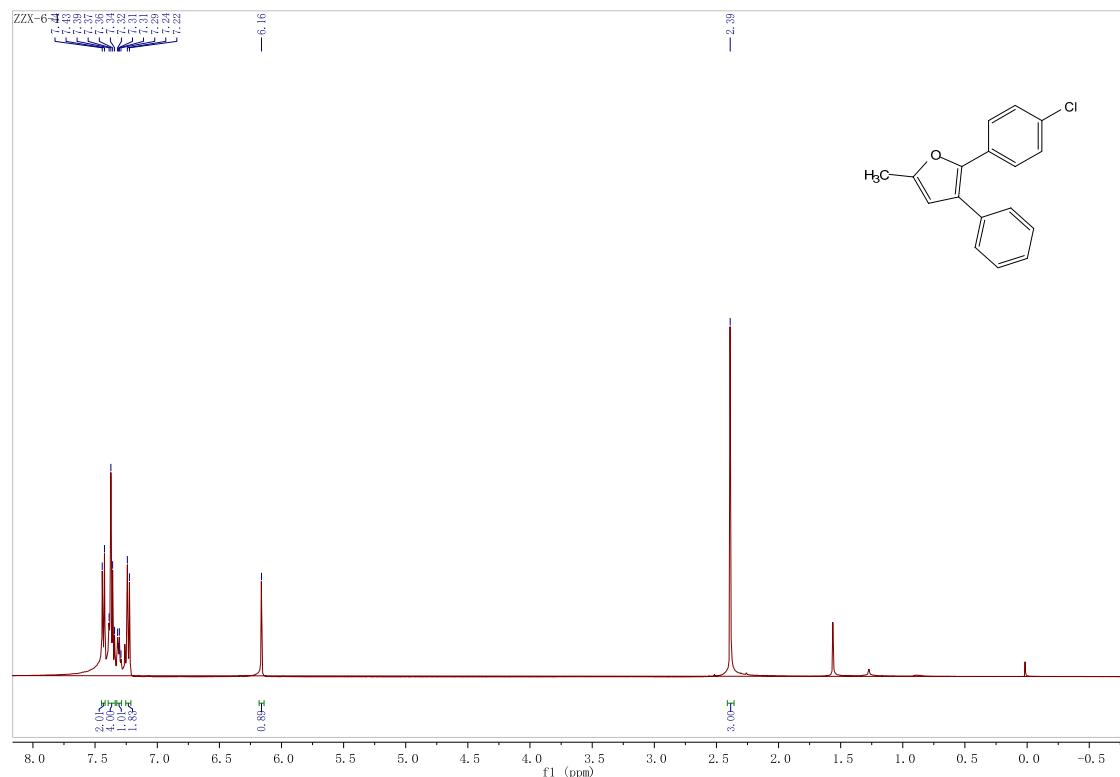


**6a**

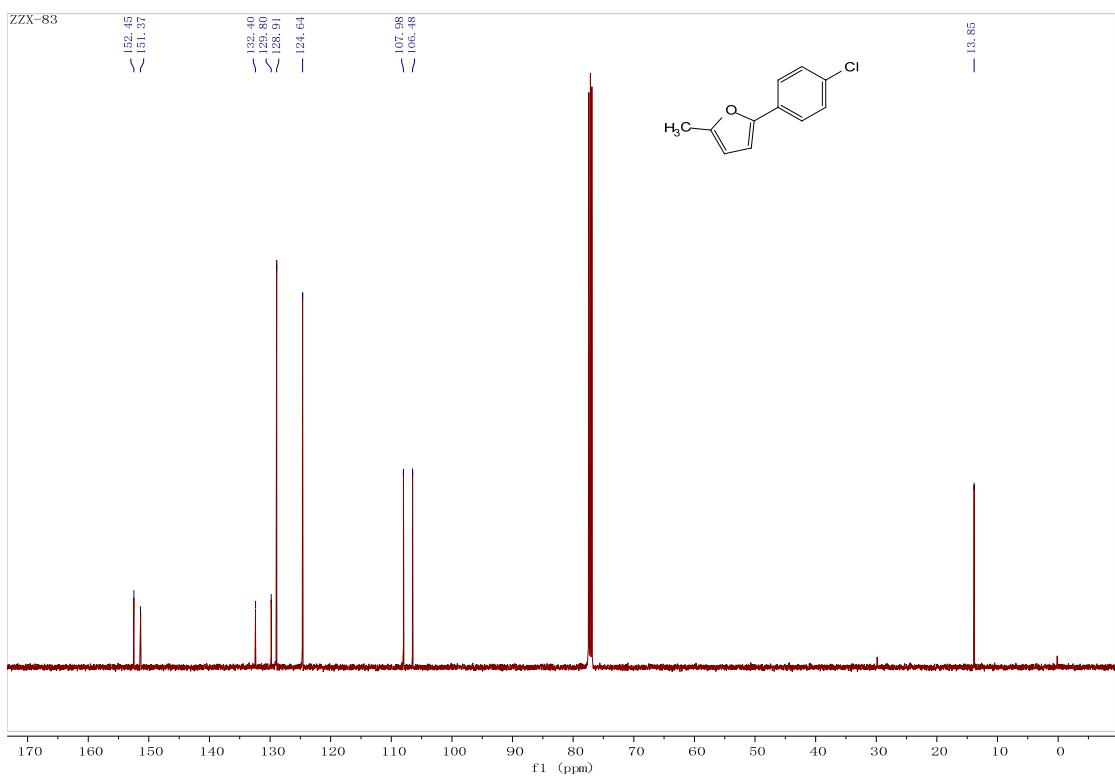
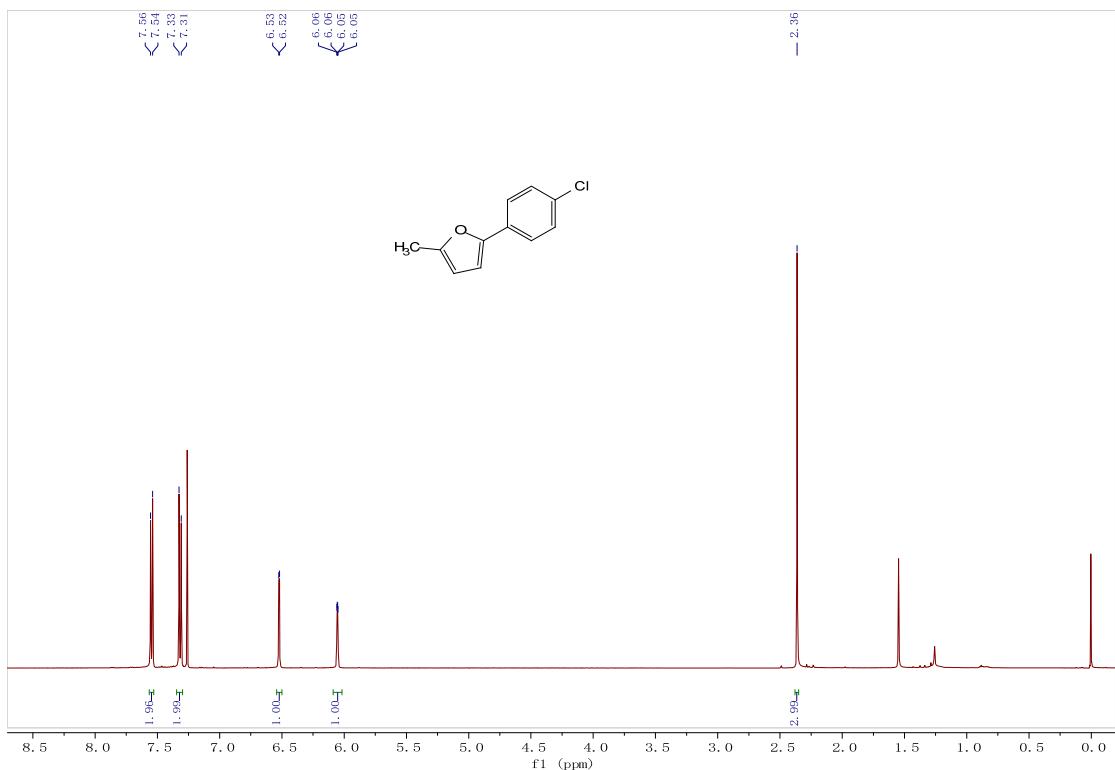


**b**

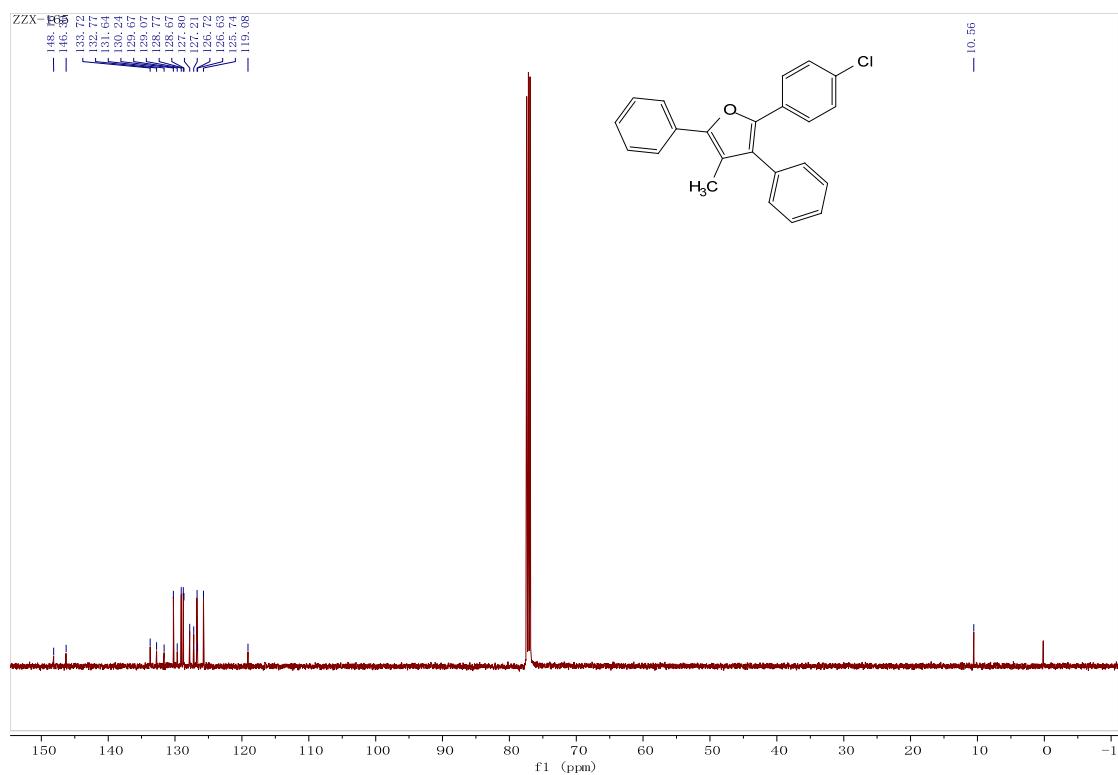
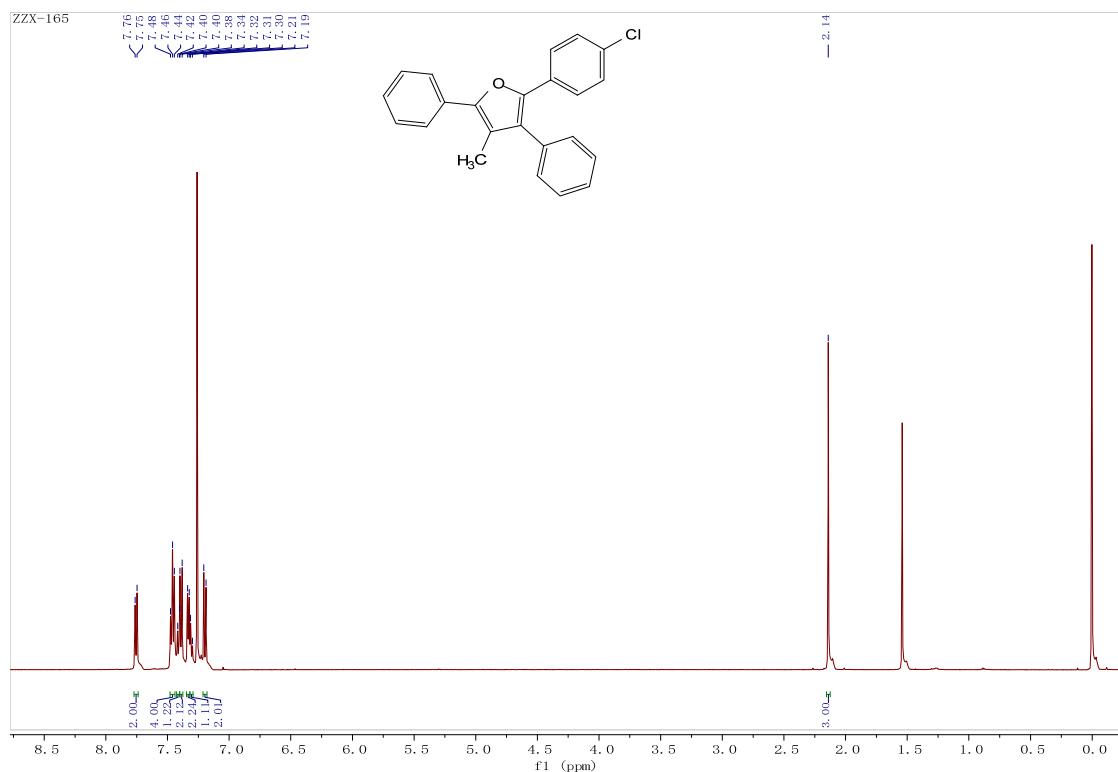
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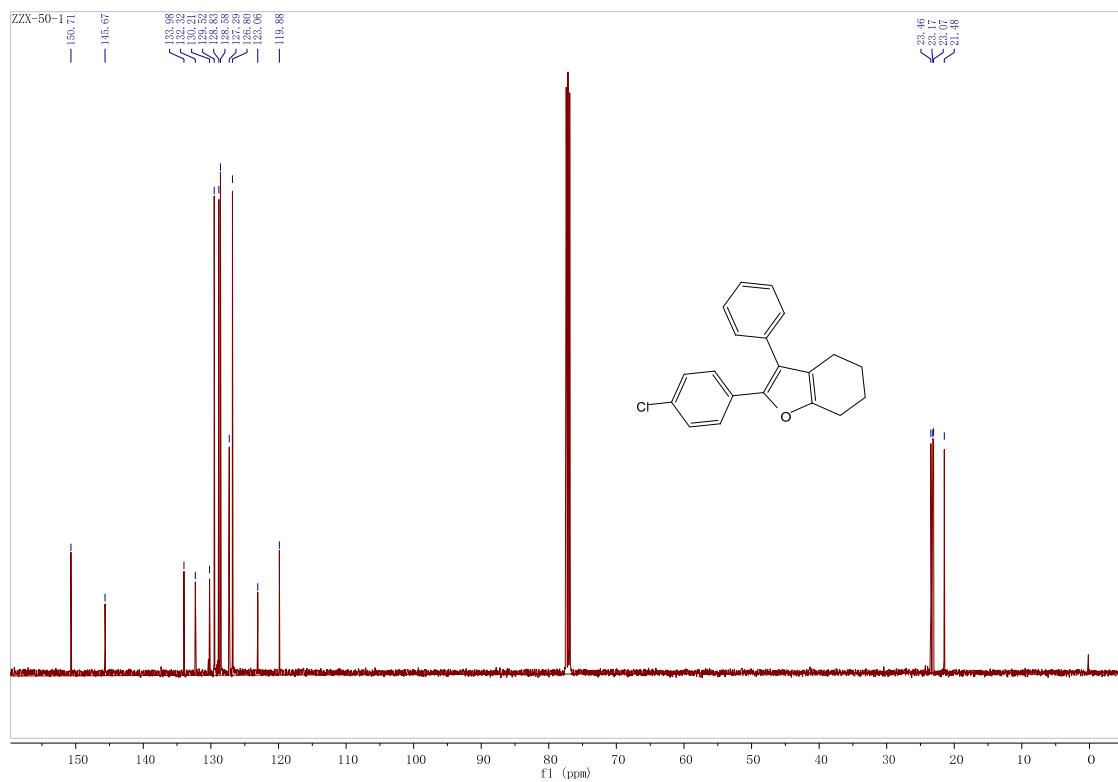
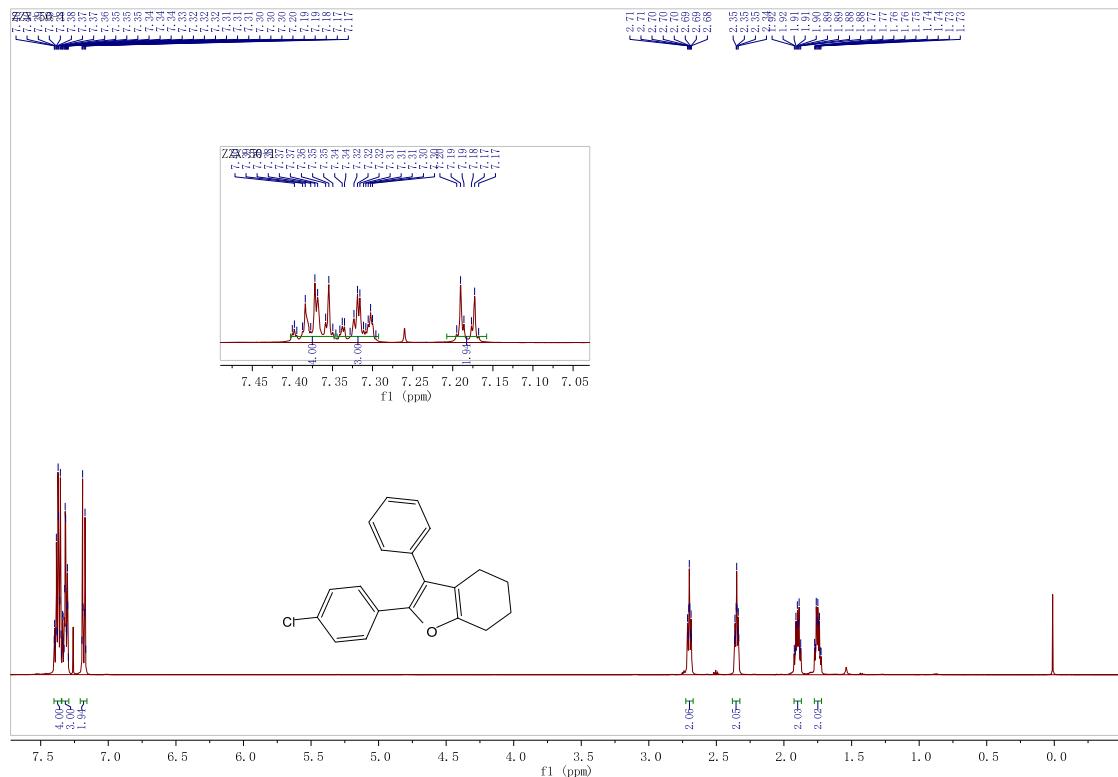
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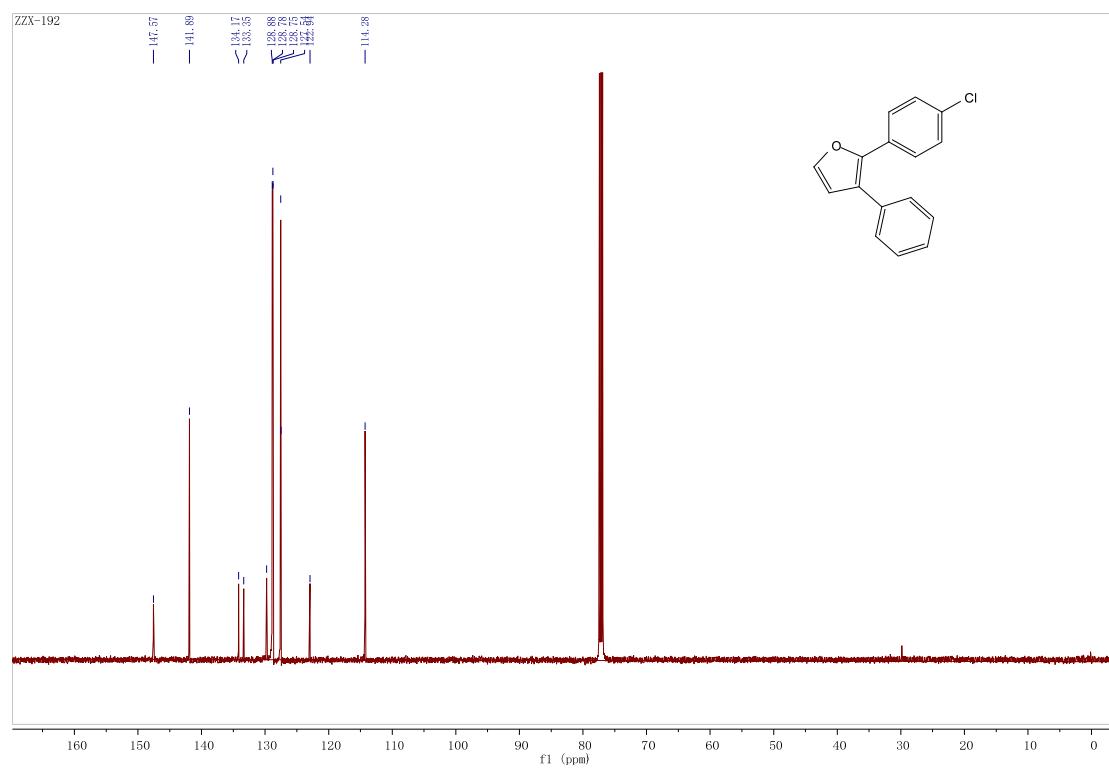
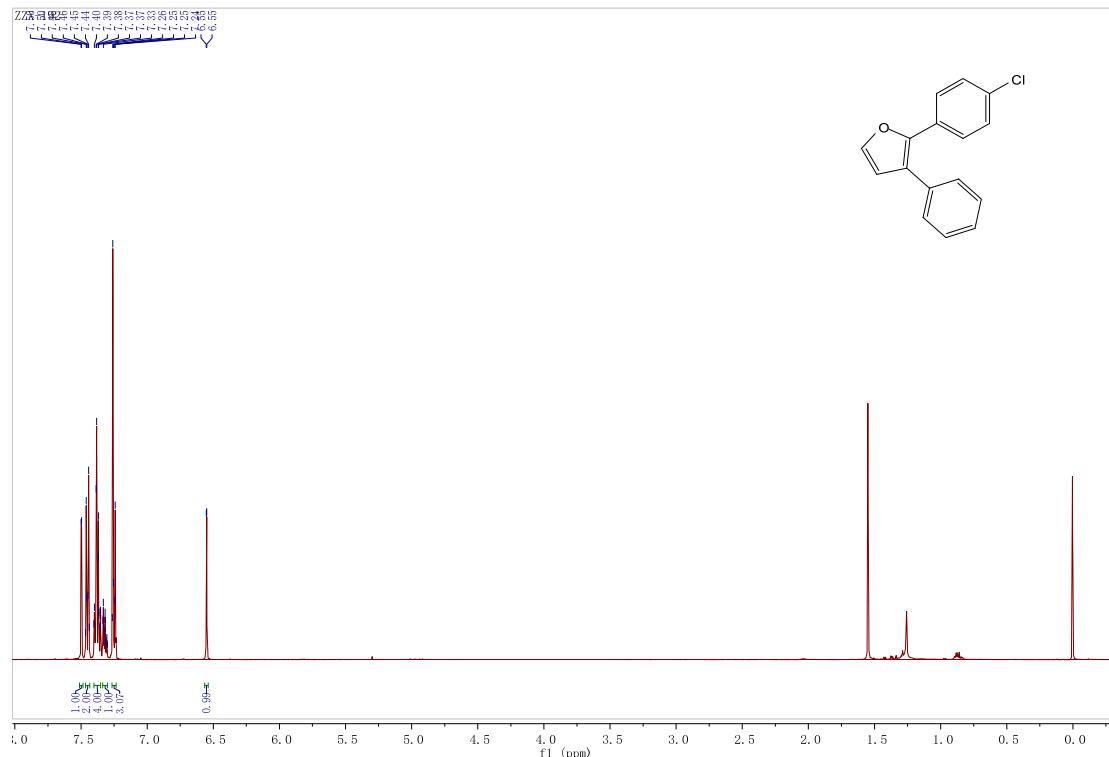
**6e**



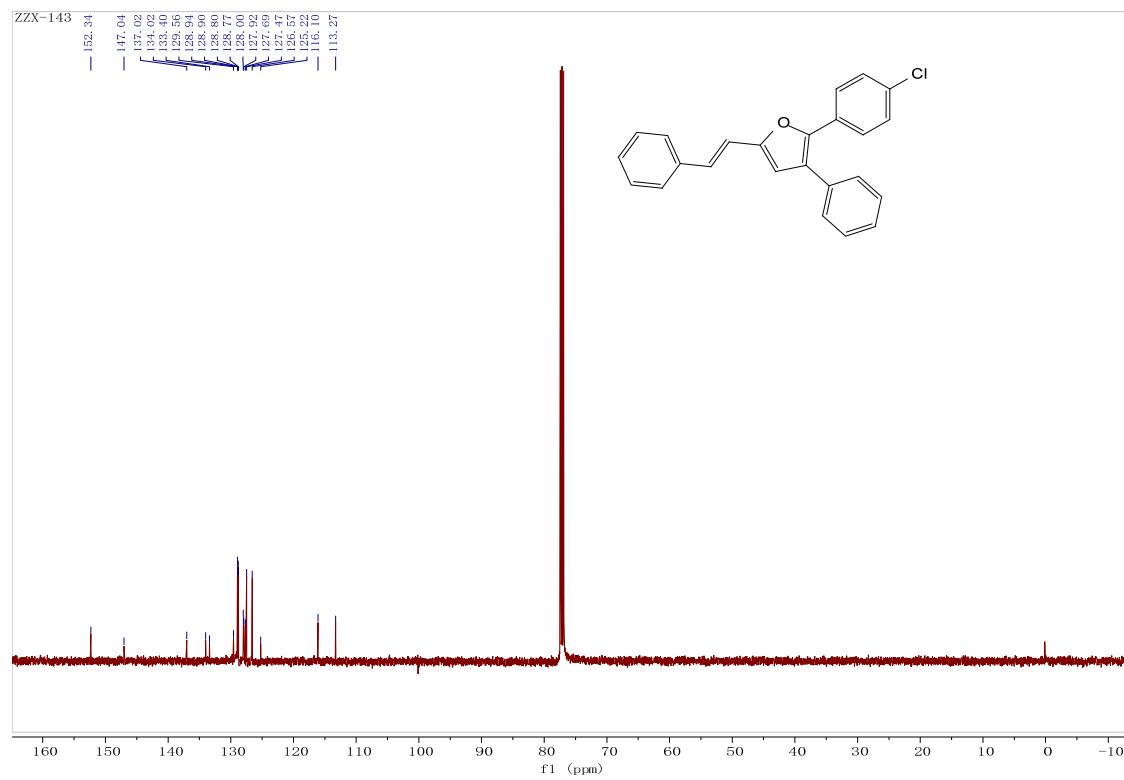
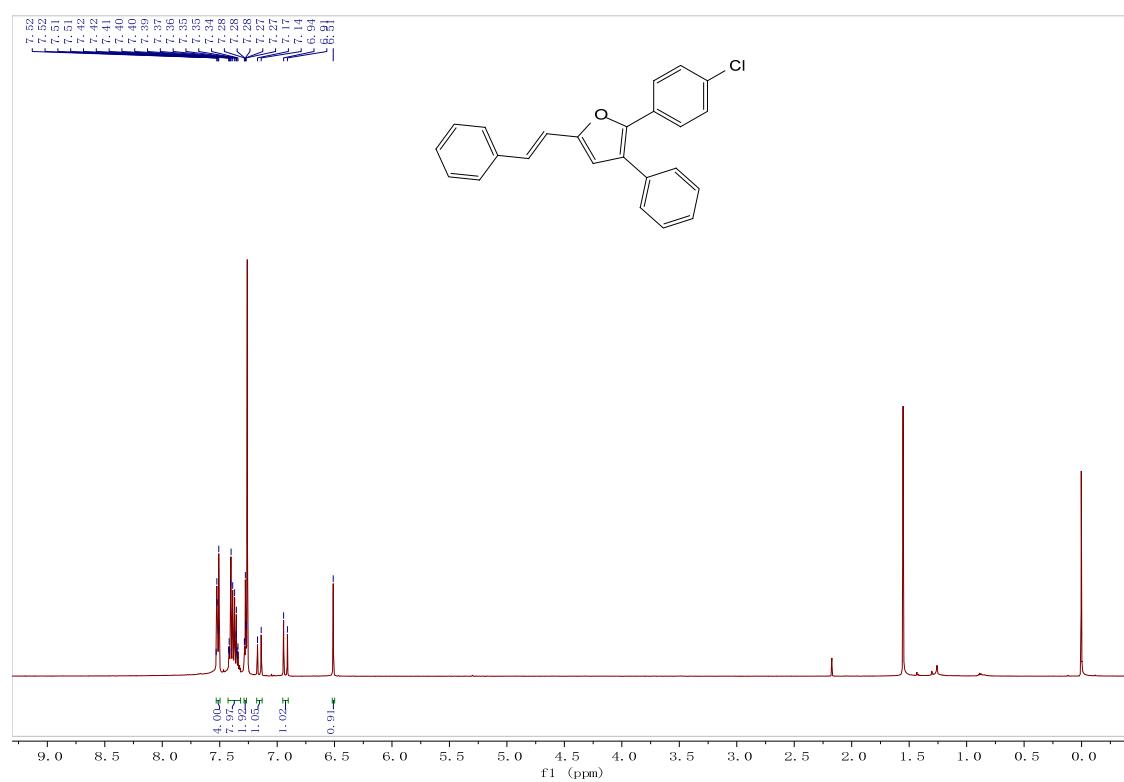
6f



**6g**



**6h**



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