

Supporting Information

Synthesis of tetrasubstituted furans through a Cu/base-mediated cascade reaction from terminal alkynes and 1,2- diketones

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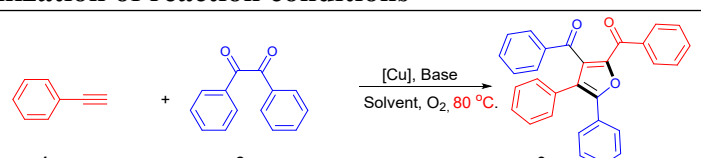
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1. General information:

All commercial materials were used as received unless otherwise noted. Commercial reagents were purchased from Alfa Aesar, TCI, Energy Chemical, and used without further purification. ^1H NMR spectra were recorded at 400 MHz or 500 MHz NMR spectrometers using TMS as an internal standard, ^{13}C NMR spectra were recorded at 100 MHz or 125 MHz NMR spectrometers using TMS as an internal standard and were fully decoupled by broad band proton decoupling. The multiplicities are reported as follows: singlet (s), doublet (d), doublet of doublets (dd), multiplet (m), triplet (t) and broad resonances (br). Melting points were measured on a hot-stage microscope (XT4-A) and are uncorrected. High resolution mass spectra (HRMS) were obtained on an APEXM Fourier transform mass spectrometry (APCI).

Table S1 Optimization of reaction conditions ^a

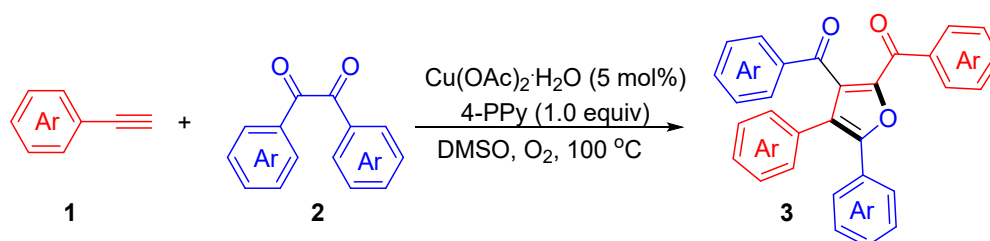


Entry	[Cu]	Base	Solvent	Yield (%) ^b
1	Cu(OAc) ₂ ·H ₂ O	DMAP	DMSO	45
2	CuBr ₂	DMAP	DMSO	38
3	CuCl	DMAP	DMSO	32
4	CuBr	DMAP	DMSO	36
5	CuI	DMAP	DMSO	25
6	Cu(OAc) ₂ ·H ₂ O	4-PPy	DMSO	55
7	Cu(OAc) ₂ ·H ₂ O	DABCO	DMSO	0
8	Cu(OAc) ₂ ·H ₂ O	Pyridine	DMSO	0
9	Cu(OAc) ₂ ·H ₂ O	Et ₃ N	DMSO	0
10	Cu(OAc) ₂ ·H ₂ O	DBU	DMSO	0
11	Cu(OAc) ₂ ·H ₂ O	K ₂ CO ₃	DMSO	0
12	Cu(OAc) ₂ ·H ₂ O	KOH	DMSO	0
13	Cu(OAc) ₂ ·H ₂ O	NaOH	DMSO	0
14	Cu(OAc) ₂ ·H ₂ O	Na ₂ CO ₃	DMSO	0
15	Cu(OAc) ₂ ·H ₂ O	4-PPy	DMF	0
16	Cu(OAc) ₂ ·H ₂ O	4-PPy	THF	0
17	Cu(OAc) ₂ ·H ₂ O	4-PPy	dioxane	10
18	Cu(OAc) ₂ ·H ₂ O	4-PPy	toluene	0
19	Cu(OAc) ₂ ·H ₂ O	4-PPy	NMP	0
20	Cu(OAc) ₂ ·H ₂ O	4-PPy	DMSO	63 ^c
21	Cu(OAc) ₂ ·H ₂ O	4-PPy	DMSO	75 ^d
22	Cu(OAc) ₂ ·H ₂ O	4-PPy	DMSO	74 ^e
23	Cu(OAc) ₂ ·H ₂ O	4-PPy	toluene	0 ^d

24	Cu(OAc) ₂ ·H ₂ O	4-PPy	THF	0 ^d
25	Cu(OAc) ₂ ·H ₂ O	4-PPy	NMP	trace ^d
26	Cu(OAc) ₂ ·H ₂ O	4-PPy	DMF	15 ^d

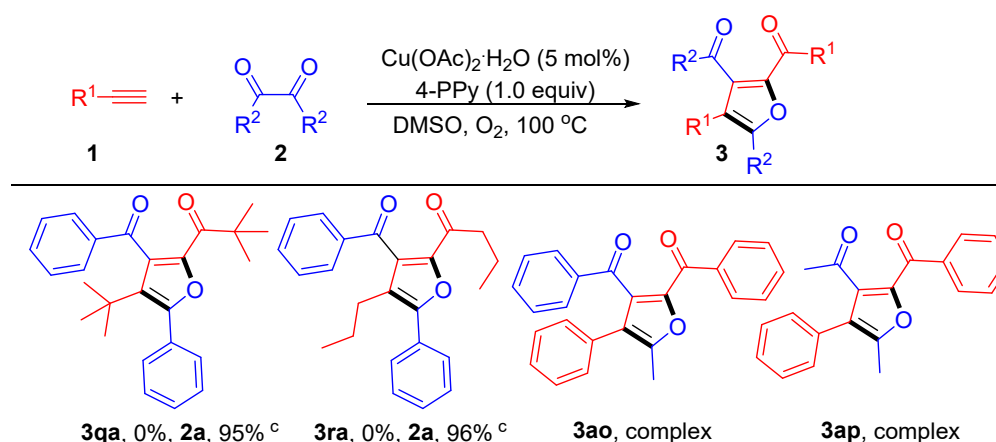
^a Reaction conditions: **1a** (0.5 mmol), **2a** (1.0 equiv.), [Cu] (5 mol%), Base (1.0 equiv.) solvent (1 mL), 72 h, O₂. ^b Isolated yield by flash column chromatography based on **1a**. 4-PPy = 4-Pyrrolidinopyridine. ^c 90 °C. ^d 100 °C. ^e 110 °C.

2. General procedure for synthesis of tetrasubstituted furans



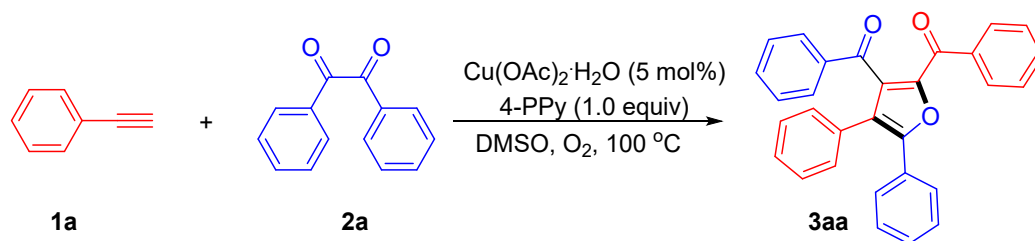
To a stirring mixture of terminal alkynes **1** (0.5 mmol), 1, 2-diketones **2** (0.5 mmol) and Cu(OAc)₂·H₂O (0.025 mmol) in 1.0 mL DMSO were added successively 4-pyrrolidinopyridine (0.5 mmol, 0.06 g). The reaction mixture was stirred at 100 °C under O₂ atmosphere for 72 h. After the completion of the reaction (monitored by TLC), the reaction mixture was quenched with saturated NH₄Cl and extracted with ethyl acetate (3 × 10 mL). The combined organics were dried over anhydrous Na₂SO₄ and the filtrate was concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (ethyl acetate /petroleum ether = 1/10) to afford products **3**.

3. Unsuccessful terminal alkyne and 1,2-diketones

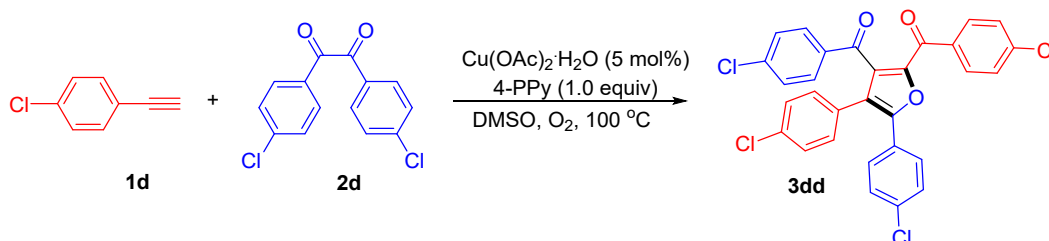


Reaction conditions: **1** (0.5 mmol), **2** (1.0 equiv.), Cu(OAc)₂·H₂O (5 mol%), 4-PPy (1.0 equiv.) DMSO (1 mL), 72 h, O₂. ^c Recovery of **2a**.

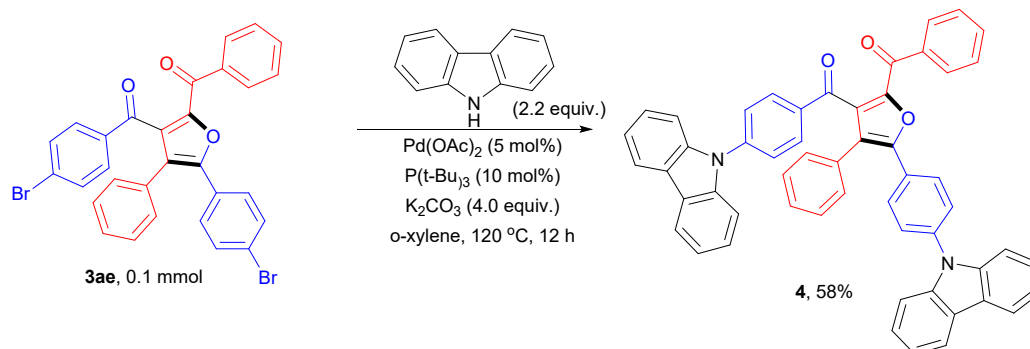
4. Gram-scale reaction and Applications



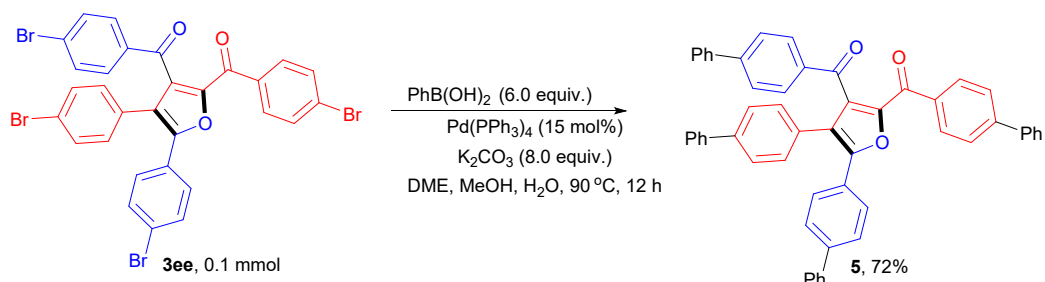
To a stirring mixture of ethynylbenzene **1a** (10.0 mmol, 1.02 g), benzil **2a** (10.0 mmol, 2.1 g) and Cu(OAc)₂·H₂O (0.5 mmol, 0.1g) in 10 mL DMSO were added successively 4-pyrrolidinopyridine (10.0 mmol, 1.48 g). The reaction mixture was stirred at 100 °C under O₂ atmosphere for 72 h. After the completion of the reaction (monitored by TLC), the reaction mixture was quenched with saturated NH₄Cl and extracted with ethyl acetate (3 × 10 mL). The combined organics were dried over anhydrous Na₂SO₄ and the filtrate was concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (ethyl acetate /petroleum ether = 1/10) to afford products **3aa**.



To a stirring mixture of 1-chloro-4-ethynylbenzene **1d** (10.0 mmol, 1.36 g), 1,2-bis(4-chlorophenyl)ethane-1,2-dione **2d** (10.0 mmol, 2.78 g) and Cu(OAc)₂·H₂O (0.5 mmol, 0.1g) in 10 mL DMSO were added successively 4-pyrrolidinopyridine (10.0 mmol, 1.48 g). The reaction mixture was stirred at 100 °C under O₂ atmosphere for 72 h. After the completion of the reaction (monitored by TLC), the reaction mixture was quenched with saturated NH₄Cl and extracted with ethyl acetate (3 × 10 mL). The combined organics were dried over anhydrous Na₂SO₄ and the filtrate was concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (ethyl acetate /petroleum ether = 1/10) to afford products **3ee**.



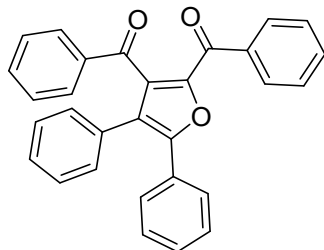
3ae (0.1 mmol), Pd(OAc)₂ (5 mol%), P(t-Bu)₃ (10 mol%), K₂CO₃ (0.4 mmol) and 9H-carbazole (0.22 mmol) were dissolved in o-xylene (2 ml) under Ar atmosphere, then the mixture was stirred at 120 °C for 12 hour. The solvent was removed in vacuo and the residue was chromatographed on silica gel (petroleum ether:diethyl ether 10:1) to yield in 4 (58% yield).



A Schlenk tube was charged with a solution of 3ae (0.1 mmol) and Pd(PPh₃)₄ (0.015 mmol) in DME (2 mL). A solution of K₂CO₃ (0.8 mmol) in H₂O (0.5 mL) and a solution of the naphthalen-1-ylboronic acid (0.6 mmol) in MeOH (1 mL) were sequentially added. The reaction mixture was stirred at 90 °C overnight (oil bath). After cooling to room temperature, the reaction mixture was quenched with H₂O (5 mL) and extracted with CH₂Cl₂ (3×5 mL). The combined organic layers were dried over Na₂SO₄, filtered, concentrated, and the residue was chromatographed on silica gel (petroleum ether:diethyl ether 10:1) to yield in 5 (72% yield).

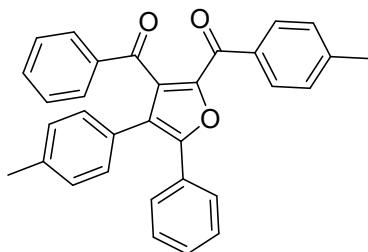
Analytic Data of Products

(4,5-diphenylfuran-2,3-diyl)bis(phenylmethanone) (**3aa**)



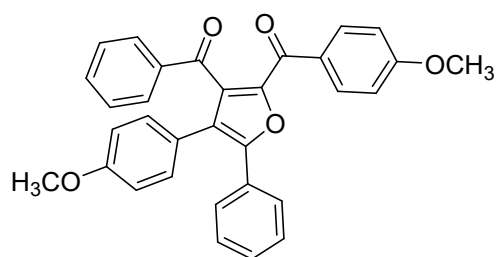
Yellow solid; m.p. 105-106 °C; (80.3 mg, yield: 75%); ¹H NMR (400 MHz, CDCl₃) δ 8.12 (d, *J* = 7.3 Hz, 2H), 7.87 (d, *J* = 7.3 Hz, 2H), 7.61 – 7.53 (m, 3H), 7.52 – 7.45 (m, 3H), 7.39 – 7.24 (m, 10H). ¹³C NMR (100 MHz, CDCl₃) δ 191.6, 181.2, 152.5, 147.8, 137.1, 136.4, 135.9, 133.6, 133.0, 130.7, 129.9, 129.7, 129.4, 129.2, 128.9, 128.8, 128.6, 128.5, 128.4, 126.9, 124.6. HRMS *m/z* (APCI) calcd for C₃₀H₂₁O₃ (M+H)⁺ 429.1485 found 429.1483.

(3-benzoyl-5-phenyl-4-(*p*-tolyl)furan-2-yl)(*p*-tolyl)methanone (**3ba**)

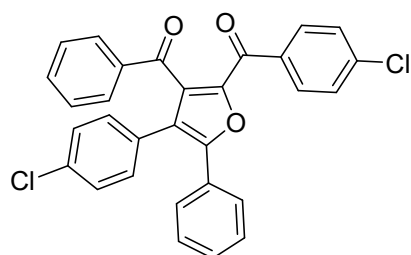


Yellow solid; m.p. 136-137 °C; (73 mg, yield: 64%); ¹H NMR (400 MHz, CDCl₃) δ 8.07 (d, *J* = 8.2 Hz, 2H), 7.91 – 7.86 (m, 2H), 7.61-7.58 (m, 2H), 7.52 – 7.47 (m, 1H), 7.41 – 7.32 (m, 5H), 7.30 (d, *J* = 8.1 Hz, 2H), 7.21 (d, *J* = 8.1 Hz, 2H), 7.09 (d, *J* = 7.9 Hz, 2H), 2.44 (s, 3H), 2.31 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 191.7, 180.7, 152.2, 148.0, 143.9, 138.1, 137.2, 135.8, 133.8, 133.5, 130.0, 129.6, 129.5, 129.4, 129.2, 129.21, 129.19, 128.7, 128.5, 127.7, 126.9, 124.6, 21.8, 21.3. HRMS *m/z* (APCI) calcd for C₃₂H₂₅O₃ (M+H)⁺ 457.1798 found 457.1796.

(3-benzoyl-4-(4-methoxyphenyl)-5-phenylfuran-2-yl)(4-methoxyphenyl)methanone (

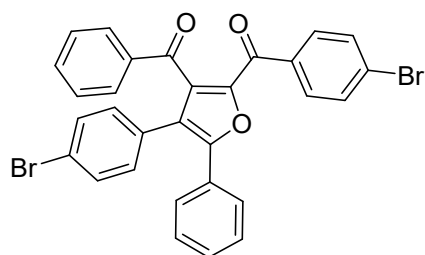
3ca)

Yellow solid; m.p. 143-144 °C; (70.8 mg, yield: 58%); ¹H NMR (400 MHz, CDCl₃) δ 8.19 (d, *J* = 8.8 Hz, 2H), 7.88 (d, *J* = 7.5 Hz, 2H), 7.59-7.57 (m, 2H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.40 – 7.34 (m, 5H), 7.22 (d, *J* = 8.6 Hz, 2H), 6.98 (d, *J* = 8.8 Hz, 2H), 6.81 (d, *J* = 8.6 Hz, 2H), 3.89 (s, 3H), 3.77 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 191.9, 179.5, 163.6, 159.5, 151.9, 148.1, 137.2, 135.7, 133.5, 132.3, 130.9, 129.5, 129.2, 129.1, 129.1, 128.8, 128.6, 126.8, 124.1, 122.8, 114.4, 113.8, 55.5, 55.2. HRMS *m/z* (APCI) calcd for C₃₂H₂₅O₅ (M+H)⁺ 489.1696 found 489.1692.

(3-benzoyl-4-(4-chlorophenyl)-5-phenylfuran-2-yl)(4-chlorophenyl)methanone (3da)

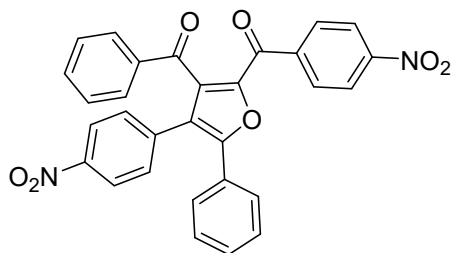
Yellow solid; m.p. 162-163 °C; (101.7 mg, yield: 82%); ¹H NMR (400 MHz, CDCl₃) δ 8.07 – 8.02 (m, 2H), 7.86 – 7.81 (m, 2H), 7.53 – 7.49 (m, 3H), 7.46-7.43 (m, 2H), 7.40 – 7.34 (m, 5H), 7.26 – 7.21 (m, 4H). ¹³C NMR (100 MHz, CDCl₃) δ 191.2, 179.7, 152.87, 147.6, 139.63, 136.9, 135.94, 134.6, 134.5, 133.9, 131.2, 131.0, 129.8, 129.3, 129.1, 129.0, 128.96, 128.9, 128.8, 128.7, 127.0, 123.4. HRMS *m/z* (APCI) calculated for C₃₀H₁₉Cl₂O₃ (M+H)⁺ 497.0705 found 497.0702.

(3-benzoyl-4-(4-bromophenyl)-5-phenylfuran-2-yl)(4-bromophenyl)methanone (**3ea**)



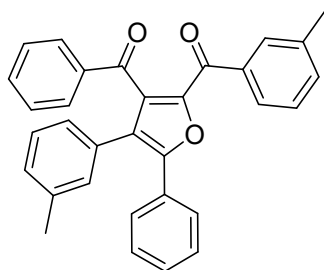
Yellow solid; m.p. 154-155 °C; (106.6 mg, yield: 73%); ¹H NMR (400 MHz, CDCl₃) δ 7.99 (d, *J* = 8.5 Hz, 2H), 7.86 (d, *J* = 7.4 Hz, 2H), 7.63 (d, *J* = 8.5 Hz, 2H), 7.56 – 7.49 (m, 3H), 7.44 – 7.35 (m, 7H), 7.18 (d, *J* = 8.3 Hz, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 191.2, 180.0, 152.9, 147.6, 136.9, 135.9, 135.0, 133.9, 132.2, 131.9, 131.3, 129.8, 129.5, 129.1, 129.0, 128.8, 128.7, 128.75, 128.4, 127.0, 123.4, 122.9. HRMS *m/z* (APCI) calcd for C₃₀H₁₉Br₂O₃ (M+H)⁺ 584.9695 found 584.9690.

(3-benzoyl-4-(4-nitrophenyl)-5-phenylfuran-2-yl)(4-nitrophenyl)methanone (**3fa**)



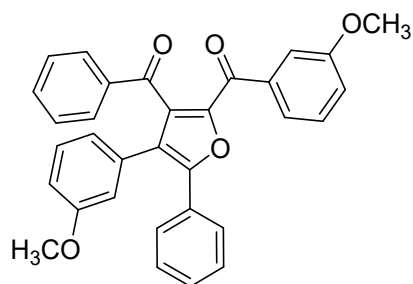
Yellow solid; m.p. 130-131 °C; (98.4 mg, yield: 76%); ¹H NMR (400 MHz, CDCl₃) δ 8.35 (d, *J* = 8.8 Hz, 2H), 8.25 (d, *J* = 8.8 Hz, 2H), 8.16 (d, *J* = 8.7 Hz, 2H), 7.86 (d, *J* = 7.4 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.52 – 7.47 (m, 4H), 7.46 – 7.37 (m, 5H). ¹³C NMR (100 MHz, CDCl₃) δ 190.92, 179.57, 154.57, 150.55, 148.13, 147.8, 141.24, 137.67, 136.83, 136.58, 134.74, 131.06, 131.01, 130.94, 129.62, 129.49, 129.33, 128.33, 127.61, 124.63, 124.08, 123.01. HRMS *m/z* (APCI) calcd for C₃₀H₁₉N₂O₇ (M+H)⁺ 519.1187 found 519.1184.

(3-benzoyl-5-phenyl-4-(*m*-tolyl)furan-2-yl)(*m*-tolyl)methanone (**3ga**)



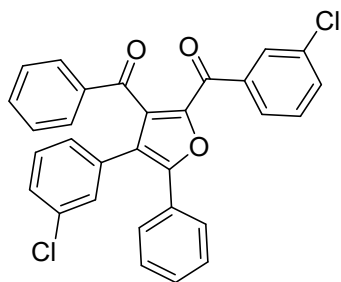
Yellow solid; m.p. 116-117 °C; (71.9 mg, yield: 63%); ^1H NMR (400 MHz, CDCl_3) δ 7.95 – 7.91 (m, 1H), 7.85 – 7.83 (m, 3H), 7.60 – 7.55 (m, 2H), 7.52 – 7.46 (m, 1H), 7.39 – 7.32 (m, 7H), 7.20 – 7.07 (m, 4H), 2.39 (s, 3H), 2.24 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 191.5, 181.5, 152.3, 147.8, 138.5, 138.3, 137.3, 136.5, 135.8, 133.7, 133.4, 130.6, 130.29, 129.3, 129.3, 129.2, 129.1, 128.7, 128.5, 128.3, 127.0, 126.8, 126.7, 124.7, 21.4, 21.4. HRMS m/z (APCI) calcd for $\text{C}_{32}\text{H}_{25}\text{O}_3$ ($\text{M}+\text{H}$) $^+$ 457.1798 found 457.1794.

(3-benzoyl-4-(3-methoxyphenyl)-5-phenylfuran-2-yl)(3-methoxyphenyl)methanone (**3ha**)



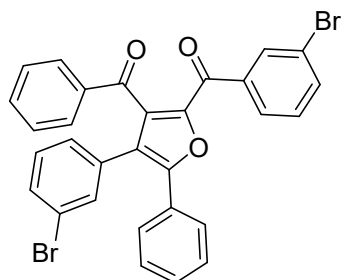
Yellow solid; m.p. 173-174 °C; (73.2 mg, yield: 60%); ^1H NMR (400 MHz, CDCl_3) δ 7.93 – 7.86 (m, 2H), 7.80 (d, $J = 7.7$ Hz, 1H), 7.65 – 7.56 (m, 3H), 7.53-7.49 (m, 1H), 7.43 – 7.32 (m, 6H), 7.19 (t, $J = 7.8$ Hz, 1H), 7.15 – 7.12 (m, 1H), 6.90 (d, $J = 7.6$ Hz, 1H), 6.84 – 6.81 (m, 2H), 3.82 (s, 3H), 3.63 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 191.5, 180.8, 159.7, 159.6, 152.6, 147.7, 137.6, 137.2, 136.1, 133.6, 131.9, 130.0, 129.5, 129.5, 129.2, 129.1, 128.8, 128.6, 126.9, 124.4, 122.6, 122.0, 120.1, 114.7, 114.5, 113.6, 55.4, 55.1. HRMS m/z (APCI) calcd for $\text{C}_{32}\text{H}_{25}\text{O}_5$ ($\text{M}+\text{H}$) $^+$ 489.1696 found 489.1693.

(3-benzoyl-4-(3-chlorophenyl)-5-phenylfuran-2-yl)(3-chlorophenyl)methanone (**3ia**)



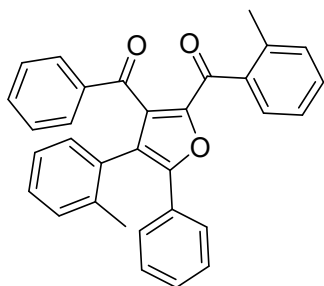
Yellow solid; m.p. 128-129 °C; (105.4 mg, yield: 85%); ^1H NMR (400 MHz, CDCl_3) δ 8.07 – 8.06 (m, 1H), 8.00 – 7.98 (m, 1H), 7.86 – 7.80 (m, 2H), 7.58 – 7.50 (m, 4H), 7.44 – 7.36 (m, 6H), 7.31 – 7.29 (m, 1H), 7.29 – 7.17 (m, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 190.9, 179.6, 153.2, 147.4, 137.8, 136.9, 136.1, 134.8, 134.7, 133.9, 133.0, 132.4, 130.3, 129.9, 129.9, 129.8, 129.7, 129.1, 129.0, 128.8, 128.7, 128.6, 128.0, 127.8, 127.0, 123.2. HRMS m/z (APCI) calculated for $\text{C}_{30}\text{H}_{19}\text{Cl}_2\text{O}_3$ ($\text{M}+\text{H}$) $^+$ 497.0705 found 497.0699.

(3-benzoyl-4-(3-bromophenyl)-5-phenylfuran-2-yl)(3-bromophenyl)methanone (**3ja**)



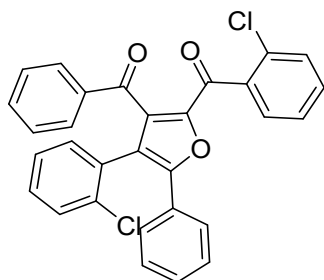
Yellow solid; m.p. 132-133 °C; (112.4 mg, yield: 77%); ^1H NMR (400 MHz, CDCl_3) δ 8.22 – 8.21 (m, 1H), 8.02 (d, $J = 7.8$ Hz, 1H), 7.86 – 7.79 (m, 2H), 7.73 – 7.66 (m, 1H), 7.58 – 7.51 (m, 3H), 7.48 – 7.35 (m, 8H), 7.26 – 7.23 (m, 1H), 7.18 – 7.14 (m, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 190.9, 179.5, 153.2, 147.4, 138.0, 136.9, 136.1, 135.9, 133.9, 132.7, 132.6, 132.5, 131.7, 130.5, 130.1, 129.9, 129.1, 129.0, 128.7, 128.6, 128.4, 128.2, 127.0, 123.1, 122.8, 122.7. HRMS m/z (APCI) calcd for $\text{C}_{30}\text{H}_{19}\text{Br}_2\text{O}_3$ ($\text{M}+\text{H}$) $^+$ 584.9695 found 584.9690.

(3-benzoyl-5-phenyl-4-(*o*-tolyl)furan-2-yl)(*o*-tolyl)methanone (**3ka**)



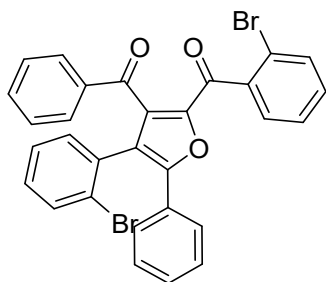
Yellow solid; m.p. 124-125 °C; (69.6 mg, yield: 61%); ^1H NMR (400 MHz, CDCl_3) δ 7.62 (d, $J = 7.3$ Hz, 2H), 7.51 (d, $J = 7.5$ Hz, 1H), 7.46 – 7.42 (m, 3H), 7.31 – 7.23 (m, 7H), 7.21 – 7.18 (m, 2H), 7.16 – 7.11 (m, 2H), 7.05 (d, $J = 7.6$ Hz, 1H), 2.26 (s, 3H), 2.15 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 190.6, 184.5, 152.6, 147.6, 137.7, 137.4, 136.9, 135.4, 133.3, 131.1, 131.0, 130.4, 130.4, 130.2, 129.3, 128.8, 128.8, 128.8, 128.3, 126.2, 125.8, 125.2, 123.8, 20.12, 19.88. HRMS m/z (APCI) calcd for $\text{C}_{32}\text{H}_{25}\text{O}_3$ ($\text{M}+\text{H}$) $^+$ 457.1798 found 457.1793.

(3-benzoyl-4-(2-chlorophenyl)-5-phenylfuran-2-yl)(2-chlorophenyl)methanone (**3la**)



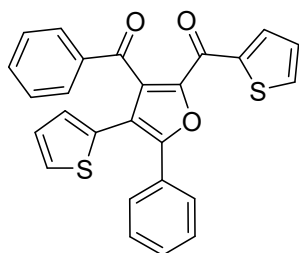
Yellow solid; m.p. 142-143 °C; (84.3 mg, yield: 68%); ^1H NMR (400 MHz, CDCl_3) δ 7.80 – 7.73 (m, 2H), 7.53 – 7.42 (m, 5H), 7.41 – 7.25 (m, 11H). ^{13}C NMR (100 MHz, CDCl_3) δ 190.2, 181.5, 154.0, 146.9, 136.9, 136.8, 135.3, 134.3, 133.6, 132.5, 132.2, 132.0, 130.2, 130.1, 130.0, 129.9, 129.7, 129.2, 129.0, 128.8, 128.4, 127.2, 126.6, 126.2, 121.80. HRMS m/z (APCI) calculated for $\text{C}_{30}\text{H}_{19}\text{Cl}_2\text{O}_3$ ($\text{M}+\text{H}$) $^+$ 497.0705 found 497.0701.

(3-benzoyl-4-(2-bromophenyl)-5-phenylfuran-2-yl)(2-bromophenyl)methanone (**3ma**)



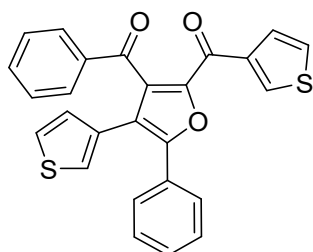
Yellow solid; m.p. 162-163 °C; (97.8 mg, yield: 67%); ^1H NMR (400 MHz, CDCl_3) δ 7.81 – 7.74 (m, 2H), 7.55 (d, $J = 8.0$ Hz, 1H), 7.50 – 7.41 (m, 5H), 7.40 – 7.38 (m, 1H), 7.36 – 7.23 (m, 8H), 7.23 – 7.17 (m, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 190.2, 182.3, 153.9, 146.4, 138.8, 136.7, 135.3, 133.7, 133.2, 133.1, 132.6, 132.0, 131.8, 130.4, 130.1, 129.7, 129.3, 129.0, 128.8, 128.4, 127.8, 127.1, 126.2, 124.7, 123.7, 120.5. HRMS m/z (APCI) calcd for $\text{C}_{30}\text{H}_{19}\text{Br}_2\text{O}_3$ ($\text{M}+\text{H}$) $^+$ 584.9695 found 584.9691.

(3-benzoyl-5-phenyl-4-(thiophen-2-yl)furan-2-yl)(thiophen-2-yl)methanone (**3na**)



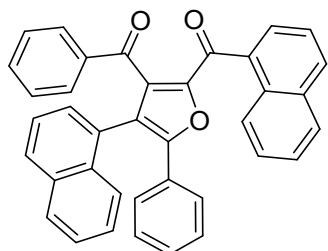
Yellow solid; m.p. 106-107 °C; (82.5 mg, yield: 75%); ^1H NMR (400 MHz, CDCl_3) δ 8.29 (s, 1H), 7.93 (d, $J = 7.5$ Hz, 2H), 7.74 – 7.69 (m, 3H), 7.55 – 7.51 (m, 1H), 7.43-7.41 (m, 5H), 7.27 – 7.21 (m, 2H), 7.01 (s, 1H), 6.96-6.95 (m, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 191.0, 172.1, 153.5, 141.2, 146.8, 136.9, 135.7, 134.9, 134.5, 133.8, 130.3, 129.8, 129.4, 129.3, 128.9, 128.8, 128.7, 128.4, 127.6, 127.3, 127.2, 117.6. HRMS m/z (APCI) calcd for $\text{C}_{26}\text{H}_{17}\text{S}_2\text{O}_3$ ($\text{M}+\text{H}$) $^+$ 441.0613 found 441.0611.

(3-benzoyl-5-phenyl-4-(thiophen-3-yl)furan-2-yl)(thiophen-3-yl)methanone (**3oa**)



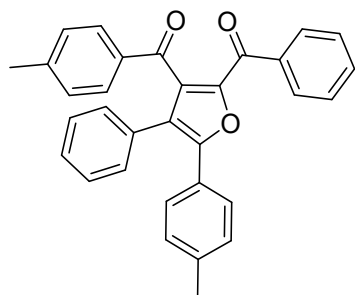
Yellow solid; m.p. 115-116 °C; (74.8 mg, yield: 68%); ¹H NMR (500 MHz, CDCl₃) δ 8.60-8.59 (m, 1H), 7.93 – 7.91 (m, 2H), 7.78 – 7.77 (m, 1H), 7.64 – 7.62 (m, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.43 – 7.41 (m, 5H), 7.37 – 7.35 (m, 1H), 7.26 – 7.22 (m, 2H), 6.98 – 6.95 (m, 1H). ¹³C NMR (125 MHz, CDCl₃) δ 192.1, 174.3, 153.0, 148.1, 139.9, 137.3, 135.8, 134.8, 134.1, 130.4, 130.0, 129.7, 129.6, 129.3, 129.1, 128.8, 128.6, 127.4, 126.7, 126.3, 125.5, 119.9. HRMS *m/z* (APCI) calcd for C₂₆H₁₇S₂O₃ (M+H)⁺ 441.0613 found 441.0610.

(2-(1-naphthoyl)-4-(naphthalen-1-yl)-5-phenylfuran-3-yl)(phenyl)methanone (**3pa**)



Yellow solid; m.p. 120-121 °C; (75.3 mg, yield: 57%); ¹H NMR (500 MHz, CDCl₃) δ 8.23 – 8.10 (m, 1H), 7.91 – 7.69 (m, 6H), 7.50-7.34 (m, 11H), 7.23– 7.06 (m, 4H), 7.00-6.94 (m, 2H). ¹³C NMR (125 MHz, CDCl₃) δ 190.9, 184.1, 154.2, 148.7, 137.2, 137.0, 135.0, 134.1, 133.9, 133.2, 132.9, 132.3, 130.7, 129.8, 129.6, 129.4, 129.3, 129.1, 129.1, 128.9, 128.8, 128.5, 128.3, 128.6, 127.8, 127.1, 126.8, 126.7, 126.6, 125.9, 125.9, 125.8, 124.5, 122.9. HRMS *m/z* (APCI) calcd for C₃₈H₂₅O₃ (M+H)⁺ 529.1798 found 529.1794.

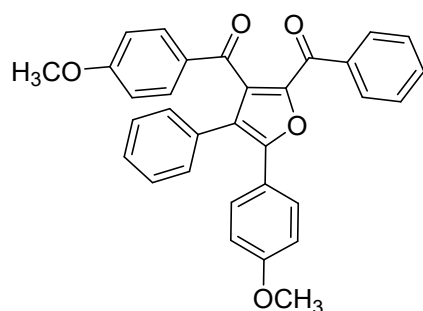
(2-benzoyl-4-phenyl-5-(*p*-tolyl)furan-3-yl)(*p*-tolyl)methanone (**3ab**)



Yellow solid; m.p. 172-173 °C; (75.3 mg, yield: 66%); ¹H NMR (400 MHz, CDCl₃) δ 8.12 (d, *J* = 7.9 Hz, 2H), 7.77 (d, *J* = 8.1 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.49 – 7.43

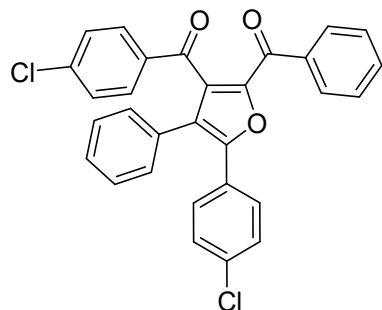
(m, 4H), 7.33 – 7.22 (m, 5H), 7.17 – 7.12 (m, 4H), 2.35 (d, $J = 2.3$ Hz, 6H). ^{13}C NMR (100 MHz, CDCl_3) δ 191.2, 181.1, 152.8, 147.5, 144.5, 139.6, 136.5, 136.2, 134.8, 132.8, 130.9, 129.8, 129.7, 129.5, 129.3, 128.8, 128.4, 128.2, 126.9, 126.5, 124.0, 21.8, 21.5. HRMS m/z (APCI) calcd for $\text{C}_{32}\text{H}_{25}\text{O}_3$ ($\text{M}+\text{H}$) $^+$ 457.1798 found 457.1796.

(2-benzoyl-5-(4-methoxyphenyl)-4-phenylfuran-3-yl)(4-methoxyphenyl)methanone (**3ac**)



Yellow solid; m.p. 166-167 °C; (70.8 mg, yield: 58%); ^1H NMR (400 MHz, CDCl_3) δ 8.12 (d, $J = 7.4$ Hz, 2H), 7.58 (t, $J = 7.4$ Hz, 1H), 7.48 (t, $J = 7.6$ Hz, 2H), 7.44 – 7.38 (m, 2H), 7.34 – 7.22 (m, 8H), 7.19 – 7.17 (m, 1H), 7.07 – 7.01 (m, 2H), 6.90 – 6.87 (m, 1H), 3.78 (s, 3H), 3.62 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 191.9, 179.5, 163.6, 159.5, 152.0, 148.1, 137.2, 135.7, 133.5, 132.3, 130.9, 129.5, 129.2, 129.2, 129.1, 128.8, 128.6, 126.8, 124.1, 122.9, 114.4, 113.8, 55.56, 55.21. HRMS m/z (APCI) calcd for $\text{C}_{32}\text{H}_{25}\text{O}_5$ ($\text{M}+\text{H}$) $^+$ 489.1696 found 489.1691.

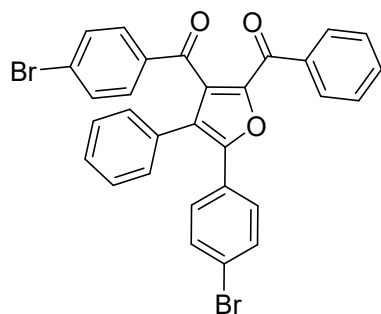
(2-benzoyl-5-(4-chlorophenyl)-4-phenylfuran-3-yl)(4-chlorophenyl)methanone (**3ad**)



Yellow solid; m.p. 131-132 °C; 95.9 mg, yield: 77%); ^1H NMR (400 MHz, CDCl_3) δ 8.12 – 8.05 (m, 2H), 7.79 (d, $J = 8.6$ Hz, 2H), 7.60 (t, $J = 7.4$ Hz, 1H), 7.52-7.46 (m, 4H), 7.37 – 7.23 (m, 10H). ^{13}C NMR (100 MHz, CDCl_3) δ 190.0, 181.1, 151.5, 148.0,

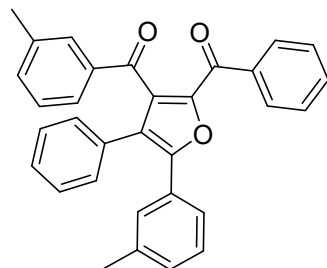
140.1, 136.1, 135.5, 135.4, 135.4, 133.2, 130.5, 130.2, 129.8, 129.5, 129.2, 129.1, 129.0, 128.7, 128.6, 128.1, 127.5, 124.8. HRMS m/z (APCI) calculated for $C_{30}H_{19}Cl_2O_3$ ($M+H$)⁺ 497.0705 found 497.0703.

(2-benzoyl-5-(4-bromophenyl)-4-phenylfuran-3-yl)(4-bromophenyl)methanone (**3ae**)



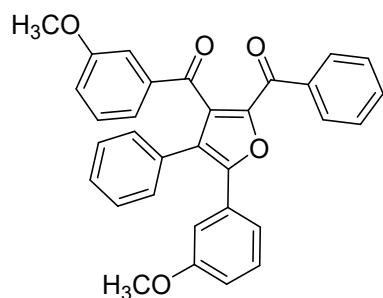
Yellow solid; m.p. 116-117 °C; (103.7 mg, yield: 71%); ¹H NMR (400 MHz, CDCl₃) δ 8.11 – 8.09 (m, 2H), 7.71 (d, J = 8.6 Hz, 2H), 7.61 (t, J = 7.4 Hz, 1H), 7.52 – 7.45 (m, 6H), 7.40 – 7.38 (m, 2H), 7.32 – 7.25 (m, 5H). ¹³C NMR (100 MHz, CDCl₃) δ 190.2, 181.1, 151.5, 148.0, 136.1, 135.8, 135.3, 133.3, 132.1, 132.0, 130.5, 130.2, 129.8, 129.5, 129.1, 129.0, 128.7, 128.6, 128.3, 128.0, 124.9, 123.8. HRMS m/z (APCI) calcd for $C_{30}H_{19}Br_2O_3$ ($M+H$)⁺ 584.9695 found 584.9693.

(2-benzoyl-4-phenyl-5-(*m*-tolyl)furan-3-yl)(*m*-tolyl)methanone (**3af**)



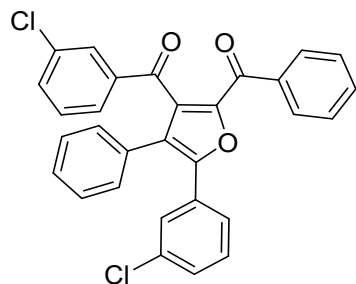
Yellow solid; m.p. 118-119 °C; (71.9 mg, yield: 63%); ¹H NMR (500 MHz, CDCl₃) δ 8.13 – 8.09 (m, 2H), 7.69 (s, 1H), 7.63 (d, J = 7.7 Hz, 1H), 7.59 (t, J = 7.4 Hz, 1H), 7.48 (t, J = 7.7 Hz, 2H), 7.40 (s, 1H), 7.34 – 7.28 (m, 7H), 7.24 – 7.16 (m, 3H), 2.33 (s, 3H), 2.30 (s, 3H). ¹³C NMR (125 MHz, CDCl₃) δ 192.1, 181.6, 153.1, 148.1, 138.9, 138.7, 137.5, 136.9, 136.4, 134.9, 133.3, 131.2, 130.6, 130.2, 130.1, 129.8, 129.5, 129.2, 129.0, 128.8, 128.7, 127.9, 127.1, 124.9, 124.6, 21.91, 21.71. HRMS m/z (APCI) calcd for $C_{32}H_{25}O_3$ ($M+H$)⁺ 457.1798 found 457.1796.

(2-benzoyl-5-(3-methoxyphenyl)-4-phenylfuran-3-yl)(3-methoxyphenyl)methanone
(3ag)



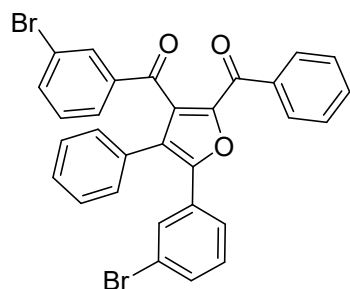
Yellow solid; m.p. 126-127 °C; (73.2 mg, yield: 60%); ¹H NMR (400 MHz, CDCl₃) δ 7.90 (d, *J* = 8.2 Hz, 2H), 7.81 (d, *J* = 7.6 Hz, 1H), 7.63 – 7.59 (m, 3H), 7.51 (t, *J* = 7.4 Hz, 1H), 7.42 – 7.34 (m, 6H), 7.20 (t, *J* = 7.9 Hz, 1H), 7.15 – 7.12 (m, 1H), 6.91 (d, *J* = 6.9 Hz, 1H), 6.88 – 6.79 (m, 2H), 3.82 (s, 3H), 3.63 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 191.2, 181.1, 159.8, 159.6, 152.3, 138.5, 136.4, 133.0, 130.70, 130.30, 129.90, 129.8, 129.8, 129.6, 128.9, 128.5, 128.4, 124.8, 122.5, 120.5, 119.3, 115.7, 112.5, 111.8, 55.4, 55.1. HRMS *m/z* (APCI) calcd for C₃₂H₂₅O₅ (M+H)⁺ 489.1696 found 489.1691.

(2-benzoyl-5-(3-chlorophenyl)-4-phenylfuran-3-yl)(3-chlorophenyl)methanone **(3ah)**



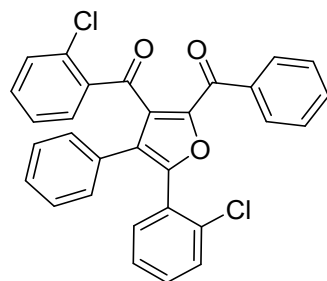
Yellow solid; m.p. 114-115 °C; (91.8 mg, yield: 74%); ¹H NMR (400 MHz, CDCl₃) δ 8.13 – 8.07 (m, 2H), 7.80 – 7.79 (m, 1H), 7.71 (d, *J* = 7.8 Hz, 1H), 7.62 (t, *J* = 7.4 Hz, 1H), 7.56 – 7.55 (m, 1H), 7.53 – 7.45 (m, 3H), 7.39 – 7.37 (m, 1H), 7.35 – 7.30 (m, 5H), 7.30 – 7.22 (m, 4H). ¹³C NMR (100 MHz, CDCl₃) δ 189.9, 181.2, 151.0, 148.2, 138.5, 136.0, 135.1, 135.0, 134.9, 133.6, 133.3, 130.7, 130.1, 123.0, 129.8, 129.5, 129.5, 129.1, 128.9, 128.8, 128.6, 127.3, 126.7, 125.3, 124.9. HRMS *m/z* (APCI) calculated for C₃₀H₁₉Cl₂O₃ (M+H)⁺ 497.0705 found 497.0707.

(2-benzoyl-5-(3-bromophenyl)-4-phenylfuran-3-yl)(3-bromophenyl)methanone (**3ai**)



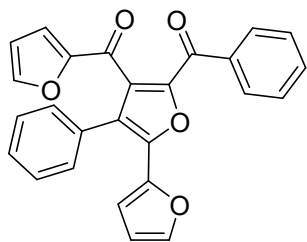
Yellow solid; m.p. 148-149 °C; (105.1 mg, yield: 72%); ¹H NMR (400 MHz, CDCl₃) δ 8.09 (d, *J* = 7.4 Hz, 2H), 7.95 (s, 1H), 7.77 – 7.69 (m, 2H), 7.64-7.60 (m, 2H), 7.534 – 7.47 (m, 3H), 7.42 (d, *J* = 7.9 Hz, 1H), 7.34 – 7.32 (m, 3H), 7.29 – 7.26 (m, 3H), 7.18 (t, *J* = 8.0 Hz, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 189.8, 181.2, 150.8, 138.7, 136.5, 136.0, 135.0, 133.3, 132.4, 131.8, 130.9, 130.3, 130.2, 129.9, 129.8, 129.6, 129.5, 129.1, 128.8, 128.6, 127.7, 125.4, 125.3, 123.0, 122.9. HRMS *m/z* (APCI) calcd for C₃₀H₁₉Br₂O₃ (M+H)⁺ 584.9695 found 584.9693.

(2-benzoyl-5-(2-chlorophenyl)-4-phenylfuran-3-yl)(2-chlorophenyl)methanone (**3aj**)



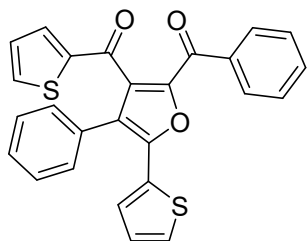
Yellow solid; m.p. 145-146 °C; (24.8 mg, yield: 20%); ¹H NMR (500 MHz, CDCl₃) δ 8.08 (d, *J* = 7.7 Hz, 2H), 7.79 (d, *J* = 7.7 Hz, 1H), 7.59 – 7.53 (m, 1H), 7.52 – 7.48 (m, 1H), 7.48 – 7.42 (m, 2H), 7.38 – 7.31 (m, 4H), 7.27 – 7.20 (m, 8H). ¹³C NMR (125 MHz, CDCl₃) δ 190.3, 182.1, 151.2, 149.7, 136.9, 136.4, 135.1, 134.7, 133.8, 133.6, 133.5, 132.9, 132.5, 131.6, 131.5, 130.8, 130.6, 130.3, 129.9, 128.9, 128.8, 128.4, 127.4, 127.2, 127.1. HRMS *m/z* (APCI) calculated for C₃₀H₁₉Cl₂O₃ (M+H)⁺ 497.0705 found 497.0704.

(5-benzoyl-3-phenyl-[2,2'-bifuran]-4-yl)(furan-2-yl)methanone (**3al**)



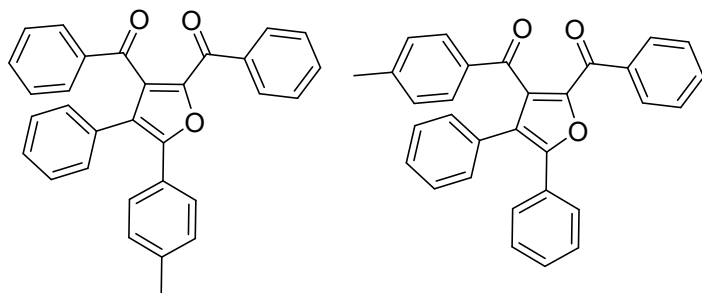
Yellow solid; m.p. 136-137 °C; (53.1 mg, yield: 52%); ¹H NMR (400 MHz, CDCl₃) δ 8.12 (d, *J* = 7.3 Hz, 2H), 7.59 (t, *J* = 7.4 Hz, 1H), 7.51 – 7.46 (m, 4H), 7.42 – 7.39 (m, 2H), 7.36 – 7.33 (m, 3H), 7.05 – 7.04 (m, 1H), 6.56 – 6.56 (m, 1H), 6.44 – 6.43 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 181.3, 177.9, 152.9, 147.3, 144.6, 144.3, 143.8, 136.3, 133.1, 129.8, 129.8, 129.7, 128.6, 128.5, 123.6, 119.6, 112.6, 111.8, 110.7. HRMS *m/z* (APCI) calcd for C₂₆H₁₇O₅ (M+H)⁺ 409.1070 found 409.1067.

(2-benzoyl-4-phenyl-5-(thiophen-2-yl)furan-3-yl)(thiophen-2-yl)methanone (**3am**)



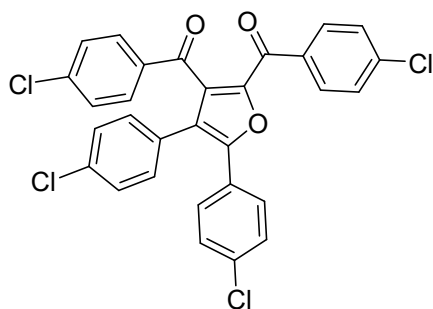
Yellow solid; m.p. 121-122 °C; (72.6 mg, yield: 66%); ¹H NMR (400 MHz, CDCl₃) δ 8.16 – 8.07 (m, 2H), 7.62 – 7.55 (m, 2H), 7.55 – 7.52 (m, 1H), 7.49 (t, *J* = 7.6 Hz, 2H), 7.42 – 7.39 (m, 2H), 7.38 – 7.33 (m, 3H), 7.33 – 7.30 (m, 1H), 7.28 – 7.25 (m, 1H), 7.01 – 6.98 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 182.8, 181.0, 148.6, 147.3, 144.4, 136.4, 135.3, 135.0, 134.3, 133.1, 131.0, 130.0, 129.8, 129.7, 128.9, 128.8, 128.5, 128.2, 127.8, 127.6, 127.0, 123.4. HRMS *m/z* (APCI) calcd for C₂₆H₁₇O₃S₂ (M+H)⁺ 441.0613 found 441.0609.

(4-phenyl-5-(*p*-tolyl)furan-2,3-diyl)bis(phenylmethanone) (**3an**)/ (2-benzoyl-4,5-diphenylfuran-3-yl)(*p*-tolyl)methanone (**3an'**)



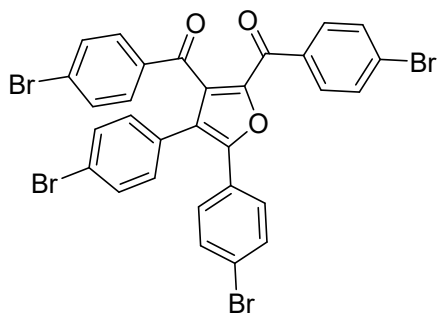
White solid; (75.2 mg, yield: 68%); ^1H NMR (400 MHz, CDCl_3) δ 8.16 – 8.07 (m, 4H), 7.87 (d, $J = 7.5$ Hz, 2H), 7.77 (d, $J = 8.2$ Hz, 2H), 7.58-7.54 (m, 4H), 7.49 – 7.43 (m, 7H), 7.37 – 7.25 (m, 14H), 7.17 – 7.12 (m, 4H), 2.34 (d, $J = 2.8$ Hz, 6H). ^{13}C NMR (100 MHz, Chloroform-d) δ 191.7, 191.2, 181.2, 181.1, 152.9, 147.7, 147.6, 144.6, 139.7, 137.1, 136.5, 136.0, 134.7, 133.6, 133.0, 132.9, 130.8, 130.8, 129.9, 129.8, 129.7, 129.7, 129.5, 129.4, 129.3, 129.3, 129.2, 128.9, 128.88, 128.8, 128.6, 128.5, 128.4, 128.3, 126.9, 126.91, 126.4, 124.0, 21.8, 21.5. HRMS m/z (APCI) calcd for $\text{C}_{31}\text{H}_{23}\text{O}_3$ ($\text{M}+\text{H}$) $^+$ 443.1641 found 443.1639.

(4,5-bis(4-chlorophenyl)furan-2,3-diyl)bis((4-chlorophenyl)methanone) (**3dd**)



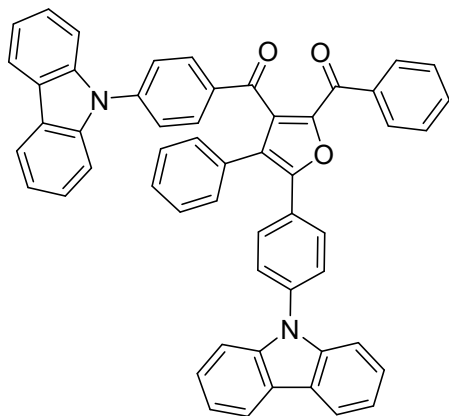
White solid; m.p. 146-147 °C; (102.9 mg, yield: 73%); ^1H NMR (400 MHz, CDCl_3) δ 8.06 (d, $J = 8.6$ Hz, 2H), 7.79 (d, $J = 8.5$ Hz, 2H), 7.49 (d, $J = 8.6$ Hz, 2H), 7.44 (d, $J = 8.6$ Hz, 2H), 7.38-7.33 (m, 4H), 7.29 (d, $J = 8.4$ Hz, 2H), 7.20 (d, $J = 8.5$ Hz, 2H). $\delta^{13}\text{C}$ NMR (125 MHz, CDCl_3) δ 190.1, 180.0, 152.2, 140.9, 140.3, 136.3, 135.8, 135.5, 135.3, 134.6, 131.5, 131.2, 130.8, 129.9, 129.7, 129.5, 129.4, 128.9, 128.5, 127.4, 124.0. HRMS m/z (APCI) calcd for $\text{C}_{30}\text{H}_{17}\text{Cl}_4\text{O}_3$ ($\text{M}+\text{H}$) $^+$ 564.9927 found 564.9923.

(4,5-bis(4-bromophenyl)furan-2,3-diyl)bis((4-bromophenyl)methanone) (**3ee**)



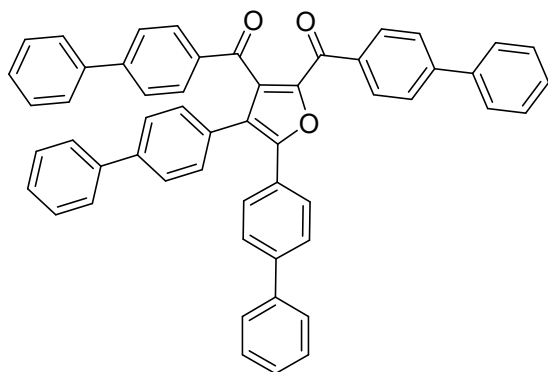
White solid; m.p. 141-142 °C; (114.7 mg, yield: 62%); ^1H NMR (500 MHz, CDCl_3) δ 7.97 (d, $J = 8.5$ Hz, 2H), 7.71 (d, $J = 8.5$ Hz, 2H), 7.66 (d, $J = 8.5$ Hz, 2H), 7.54 (d, $J = 8.5$ Hz, 2H), 7.51 (d, $J = 8.5$ Hz, 2H), 7.45 (d, $J = 8.3$ Hz, 2H), 7.37 (d, $J = 8.6$ Hz, 2H), 7.14 (d, $J = 8.3$ Hz, 2H). ^{13}C NMR (125 MHz, CDCl_3) δ 190.3, 180.2, 152.3, 148.2, 135.9, 135.7, 135.0, 132.9, 132.7, 132.6, 132.4, 131.6, 131.4, 130.9, 129.8, 129.4, 129.1, 128.7, 127.9, 124.7, 124.1, 123.6. HRMS m/z (APCI) calcd for $\text{C}_{30}\text{H}_{17}\text{Br}_4\text{O}_3$ ($\text{M}+\text{H}$) $^+$ 740.7905 found 740.7901.

(3-(4-(9H-carbazol-9-yl)benzoyl)-5-(4-(9H-carbazol-9-yl)phenyl)-4-phenylfuran-2-yl)(phenyl)methanone (**4**)



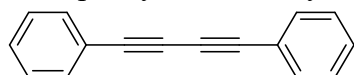
Yellow solid; m.p. 124-125 °C; (44.0 mg, yield: 58%); ^1H NMR (400 MHz, CDCl_3) δ 8.22 (d, $J = 7.3$ Hz, 2H), 8.17 – 8.10 (m, 6H), 7.83 (d, $J = 8.5$ Hz, 2H), 7.64 (d, $J = 8.3$ Hz, 3H), 7.61 – 7.55 (m, 4H), 7.48 (d, $J = 8.2$ Hz, 6H), 7.46 – 7.40 (m, 7H), 7.32 (t, $J = 7.3$ Hz, 4H). ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) δ 190.2, 181.4, 151.8, 148.1, 142.6, 140.4, 140.1, 138.7, 136.4, 135.8, 135.4, 133.3, 130.9, 130.5, 129.9, 129.8, 129.2, 128.8, 128.7, 128.2, 127.8, 127.0, 126.3, 126.2, 126.1, 125.0, 123.9, 123.7, 120.7, 120.5, 110.0, 109.8. HRMS m/z (APCI) calcd for $\text{C}_{54}\text{H}_{35}\text{N}_2\text{O}_3$ ($\text{M}+\text{H}$) $^+$ 759.2642 found 759.2638.

(4,5-di([1,1'-biphenyl]-4-yl)furan-2,3-diyl)bis([1,1'-biphenyl]-4-ylmethanone) (**5**)



Yellow solid; m.p. 115-116 °C; (52.7 mg, yield: 72%); ^1H NMR (400 MHz, CDCl_3) δ 8.27 (d, $J = 8.2$ Hz, 2H), 8.01 (d, $J = 8.2$ Hz, 2H), 7.77 – 7.69 (m, 4H), 7.66 (d, $J = 7.4$ Hz, 2H), 7.51 – 7.56 (m, 11H), 7.49-7.32 (m, 15H). ^{13}C NMR (100 MHz, CDCl_3) δ 191.2, 180.6, 152.5, 148.1, 146.3, 145.8, 142.1, 141.07, 140.3, 140.0, 139.94, 139.9, 136.1, 136.0, 135.1, 130.6, 130.1, 129.8, 129.7, 129.0, 128.99, 128.9, 128.86, 128.4, 128.3, 128.1, 127.9, 127.7, 127.6, 127.5, 127.4, 127.37, 127.2, 127.0, 127.03, 124.4. HRMS m/z (APCI) calcd for $\text{C}_{54}\text{H}_{37}\text{O}_3$ ($\text{M}+\text{H}$) $^+$ 733.2737 found 733.2733.

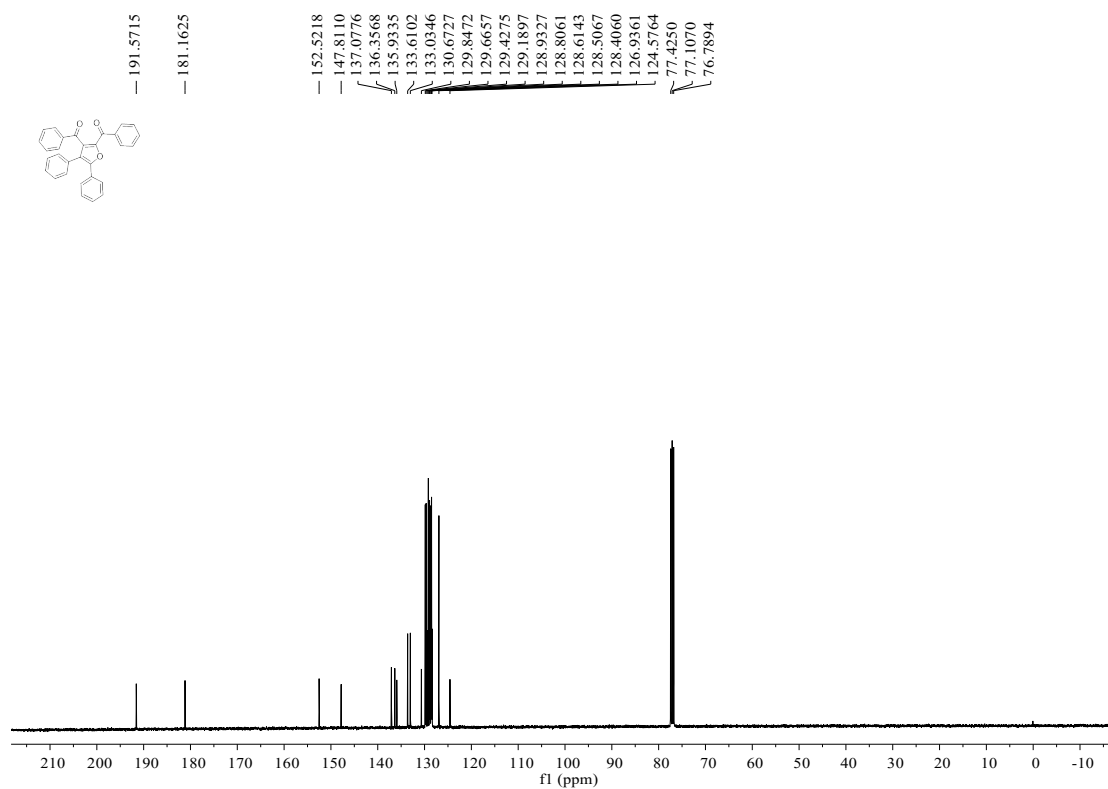
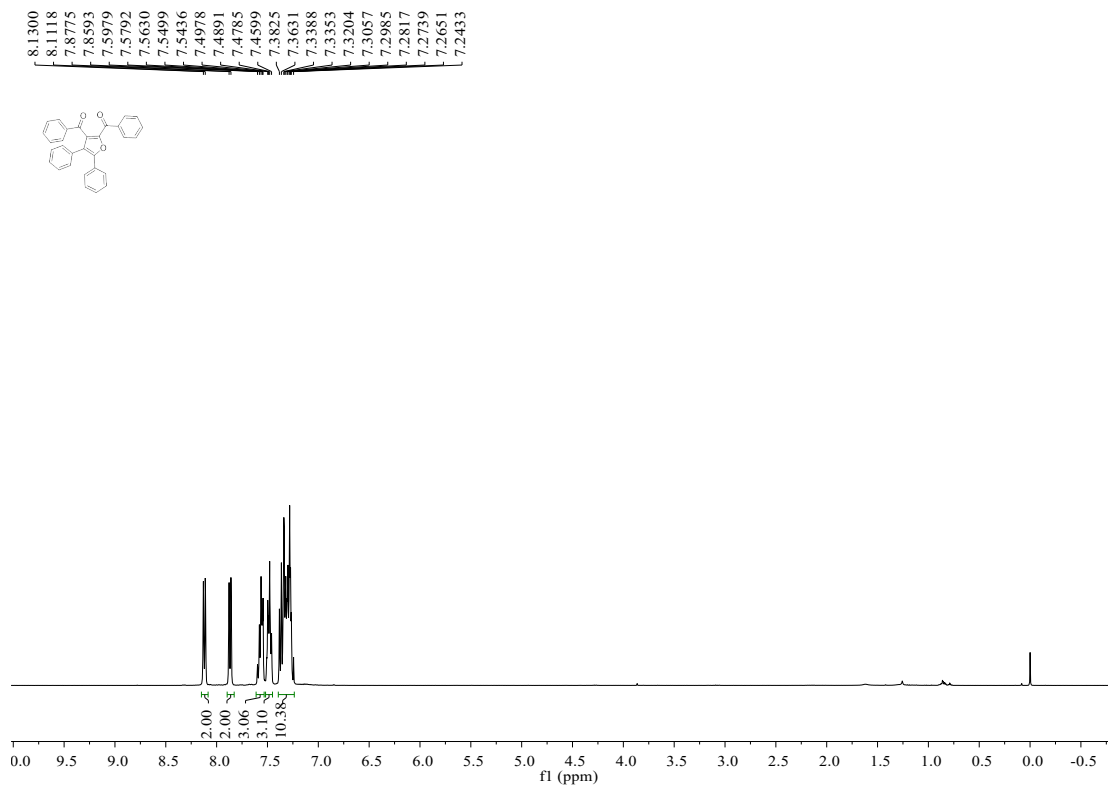
1,4-diphenylbuta-1,3-diyne (**A**)



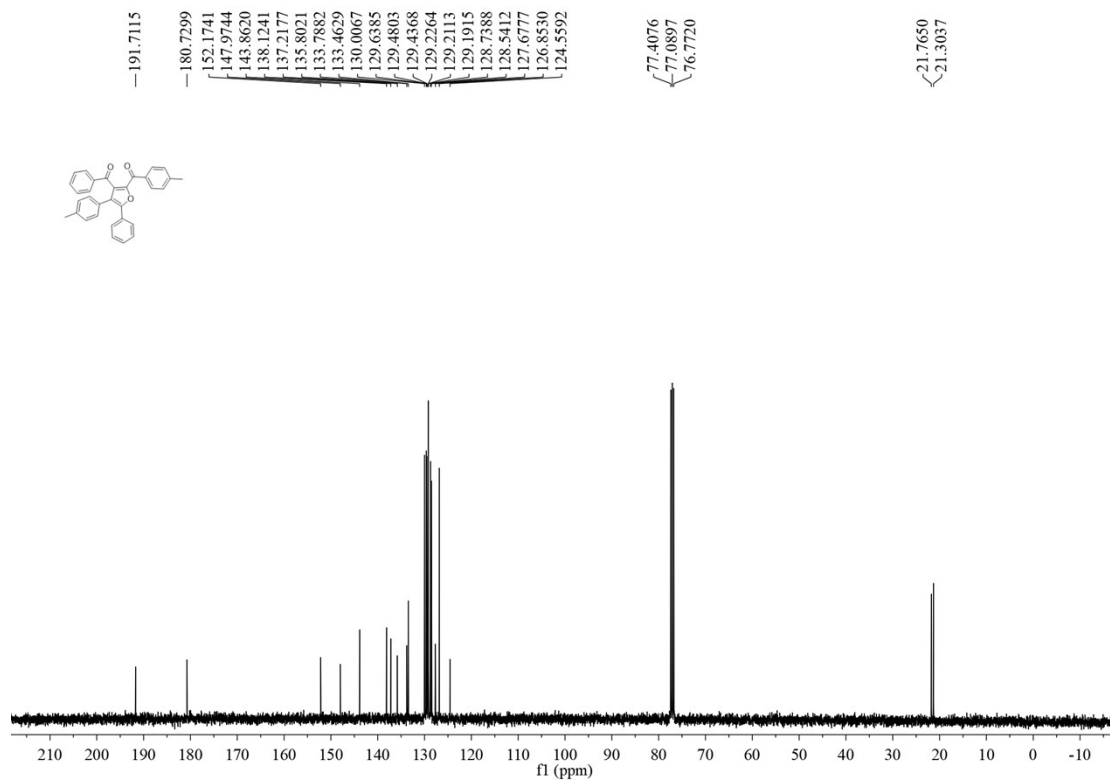
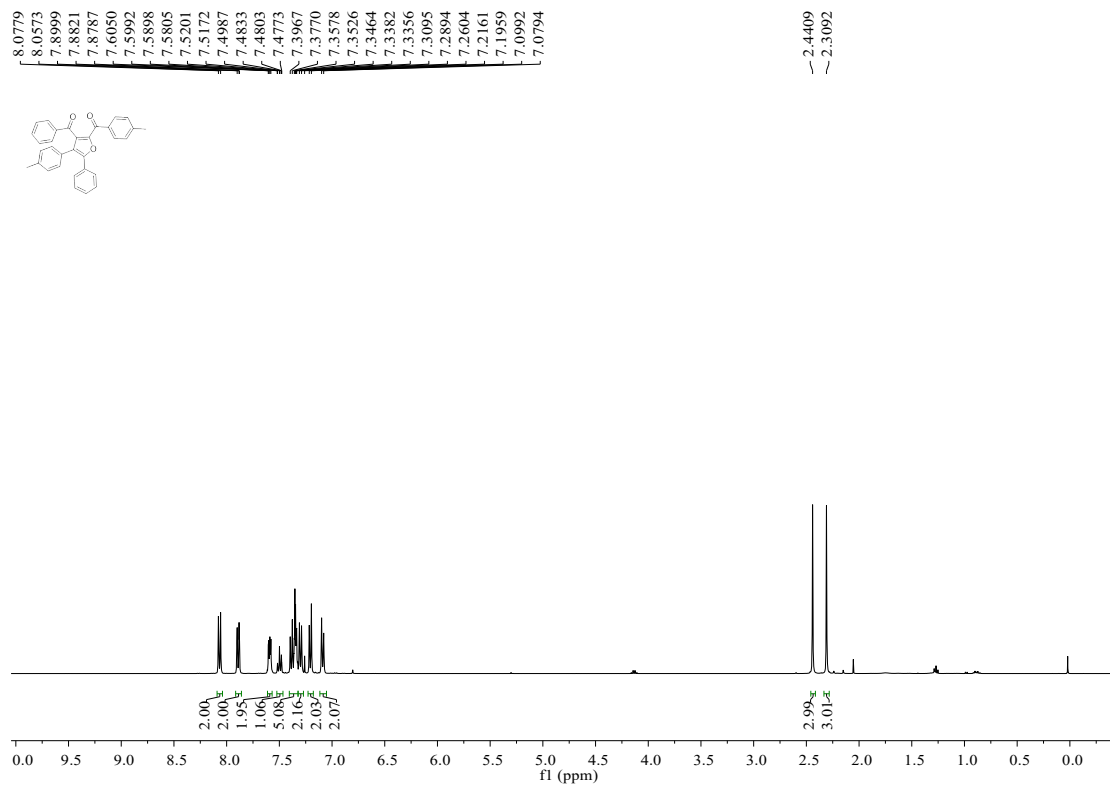
^1H NMR (400 MHz, CDCl_3) δ 7.55 – 7.47 (m, 4H), 7.37-7.29 (m, 6H). ^{13}C NMR (100 MHz, CDCl_3) δ 132.6, 129.3, 128.5, 121.8, 81.6, 74.0.

Copies of ^1H and ^{13}C Spectra

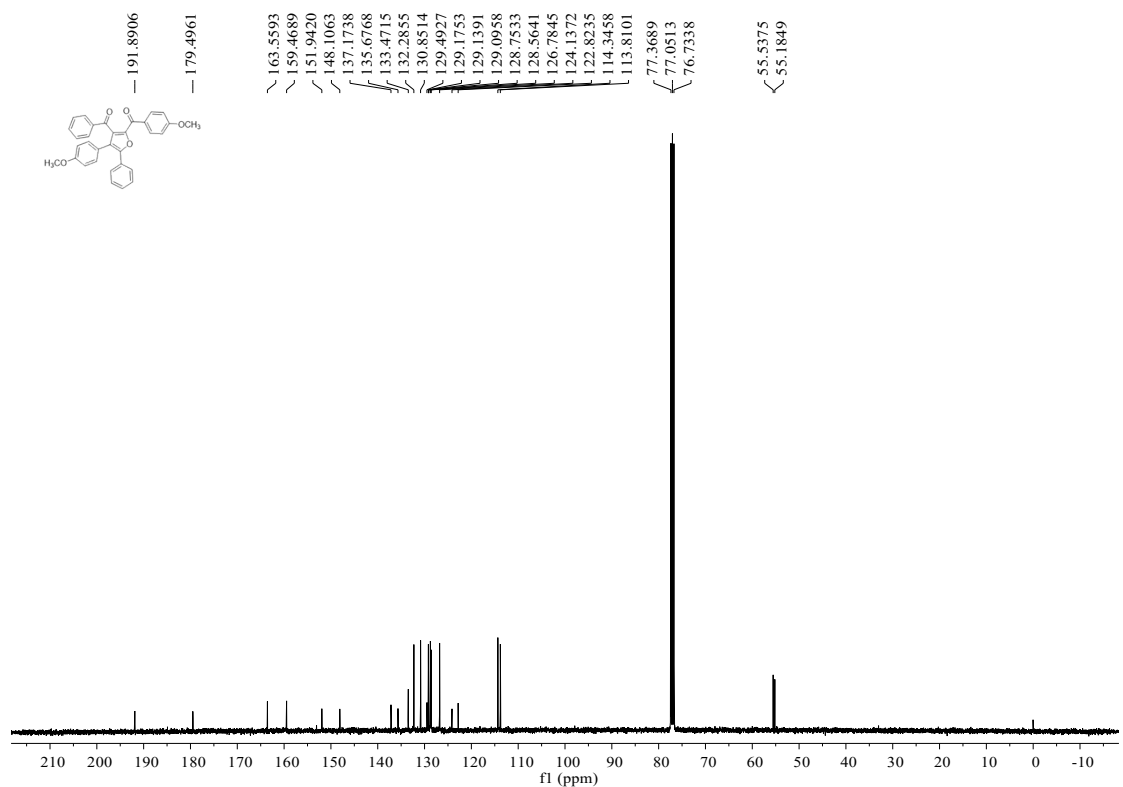
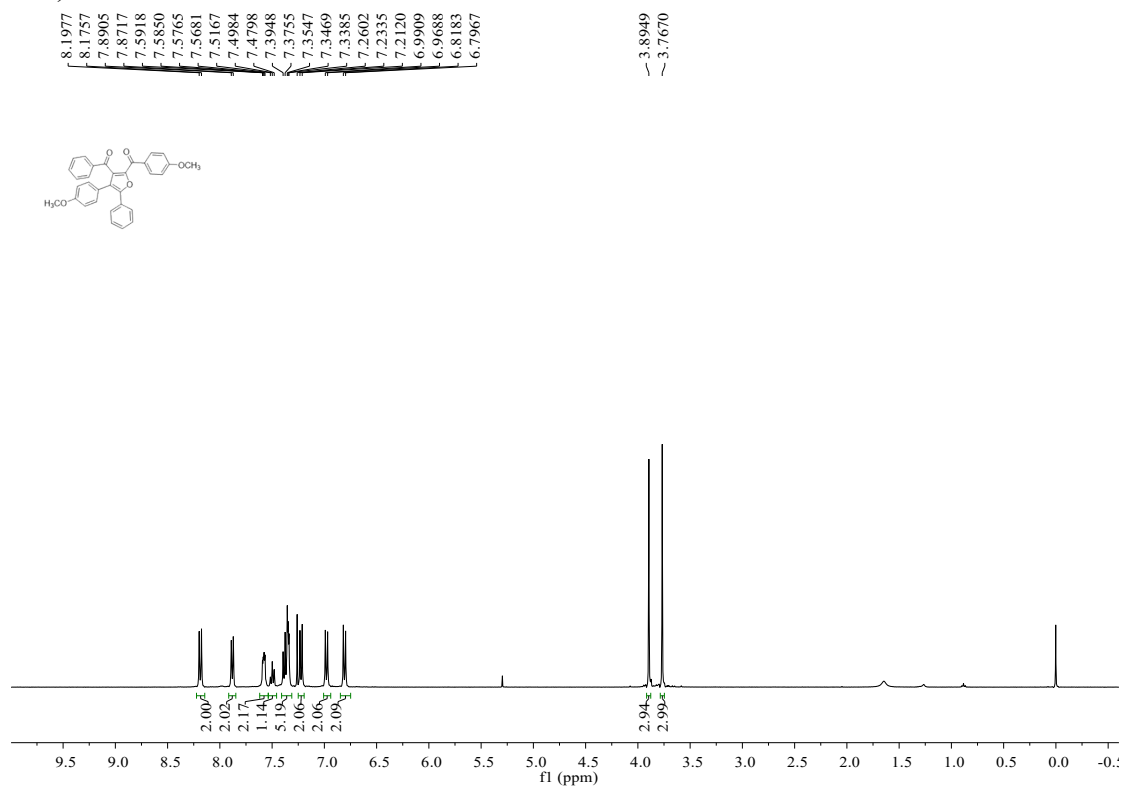
(4,5-diphenylfuran-2,3-diyl)bis(phenylmethanone) (**3aa**)



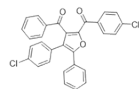
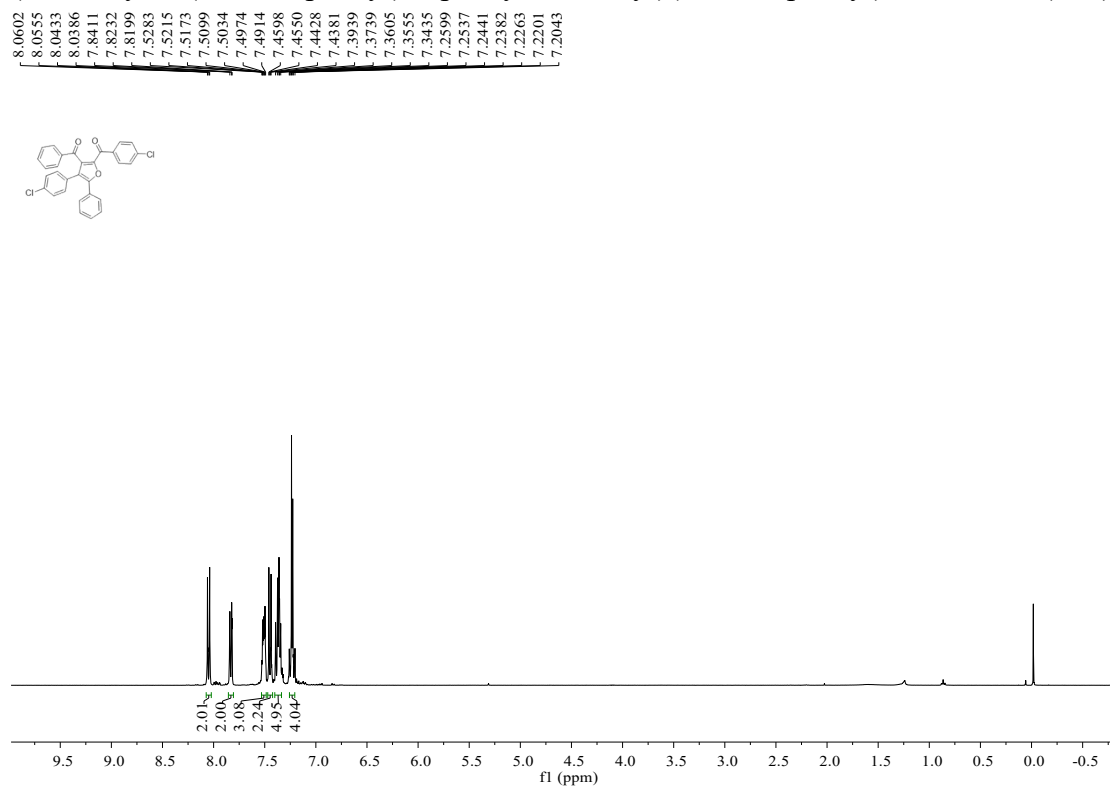
(3-benzoyl-5-phenyl-4-(p-tolyl)furan-2-yl)(p-tolyl)methanone (**3ba**)



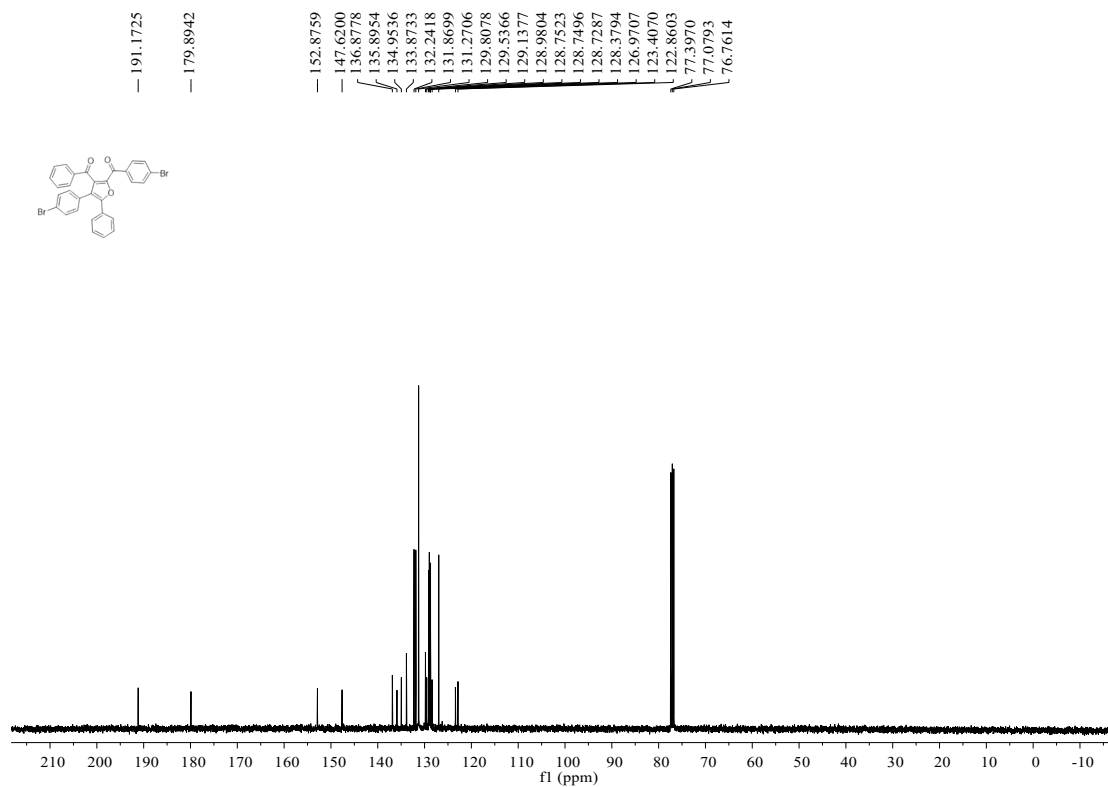
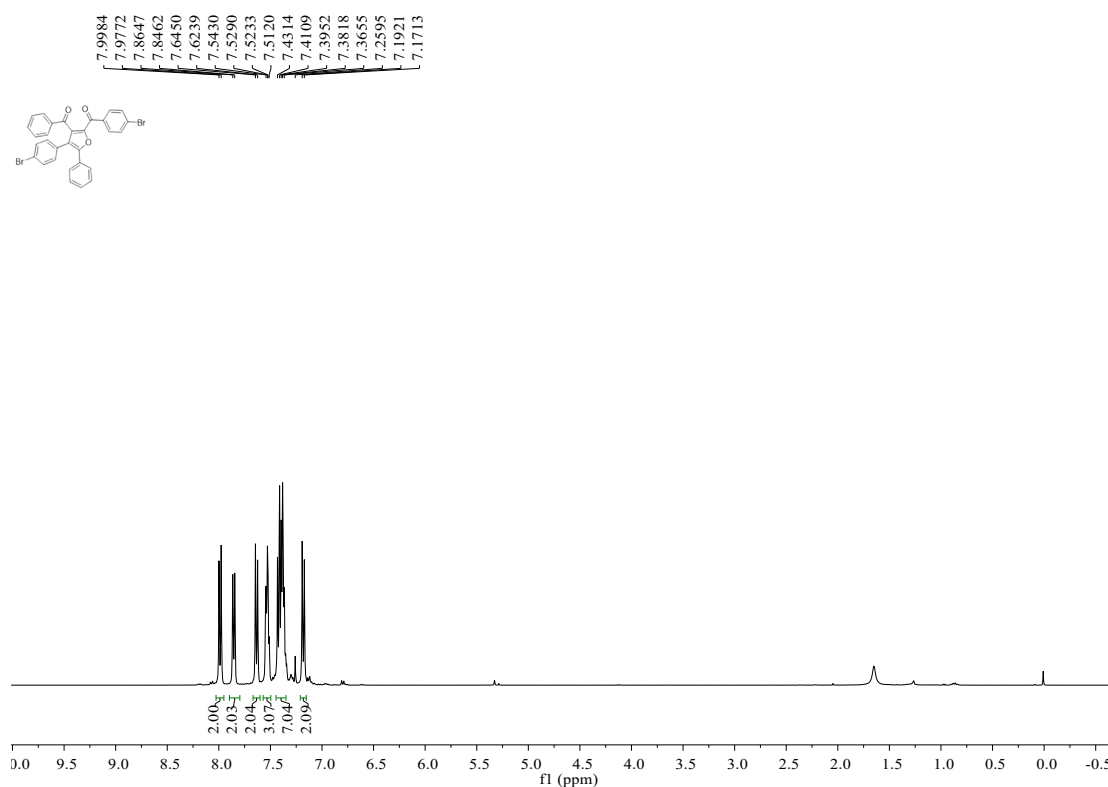
(3-benzoyl-4-(4-methoxyphenyl)-5-phenylfuran-2-yl)(4-methoxyphenyl)methanone (**3ca**)



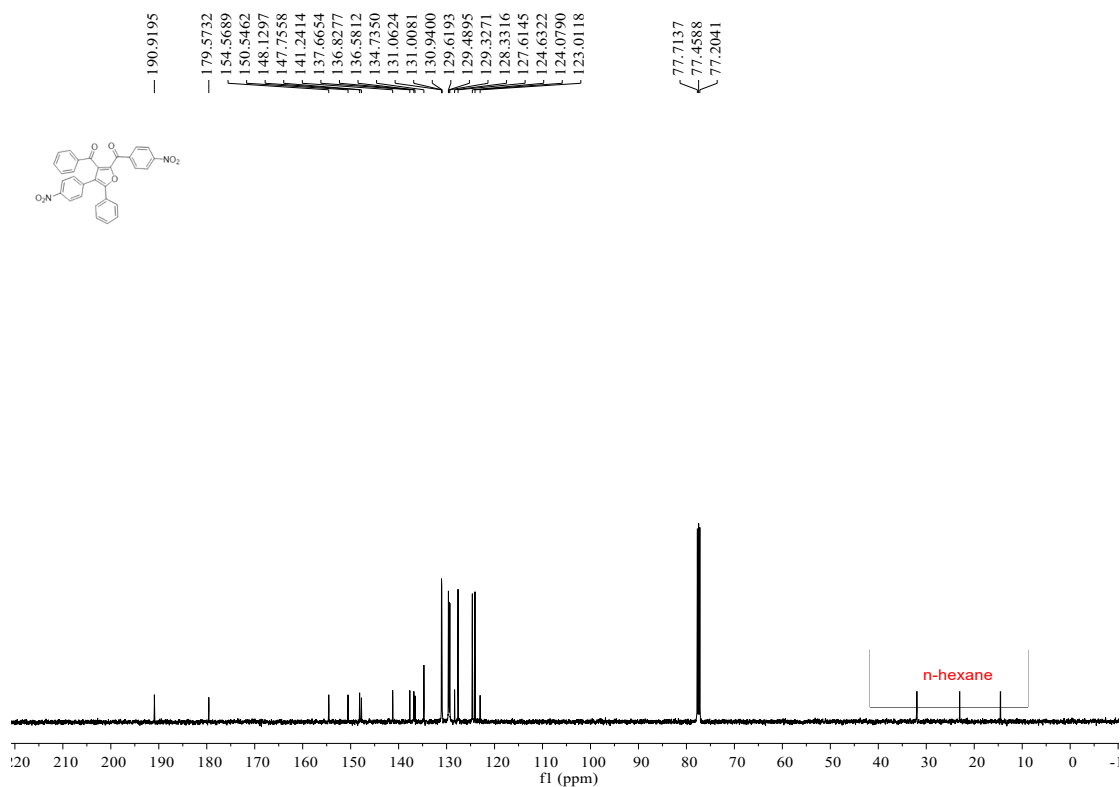
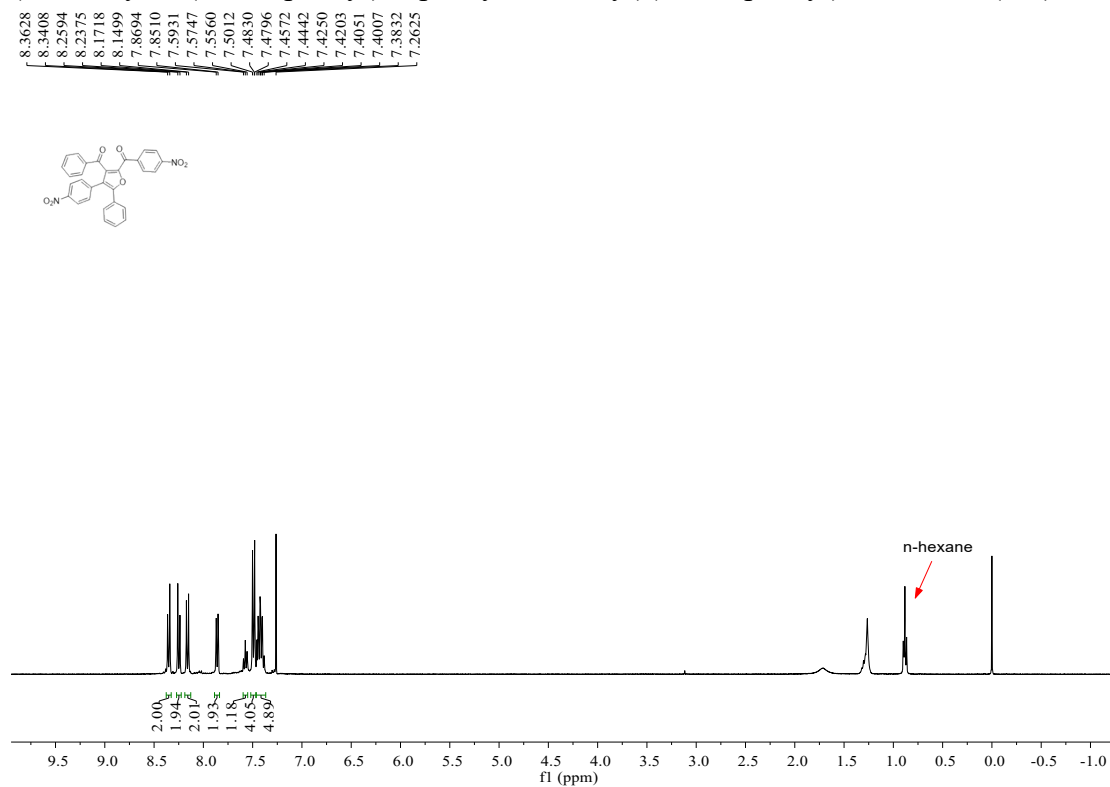
(3-benzoyl-4-(4-chlorophenyl)-5-phenylfuran-2-yl)(4-chlorophenyl)methanone (**3da**)



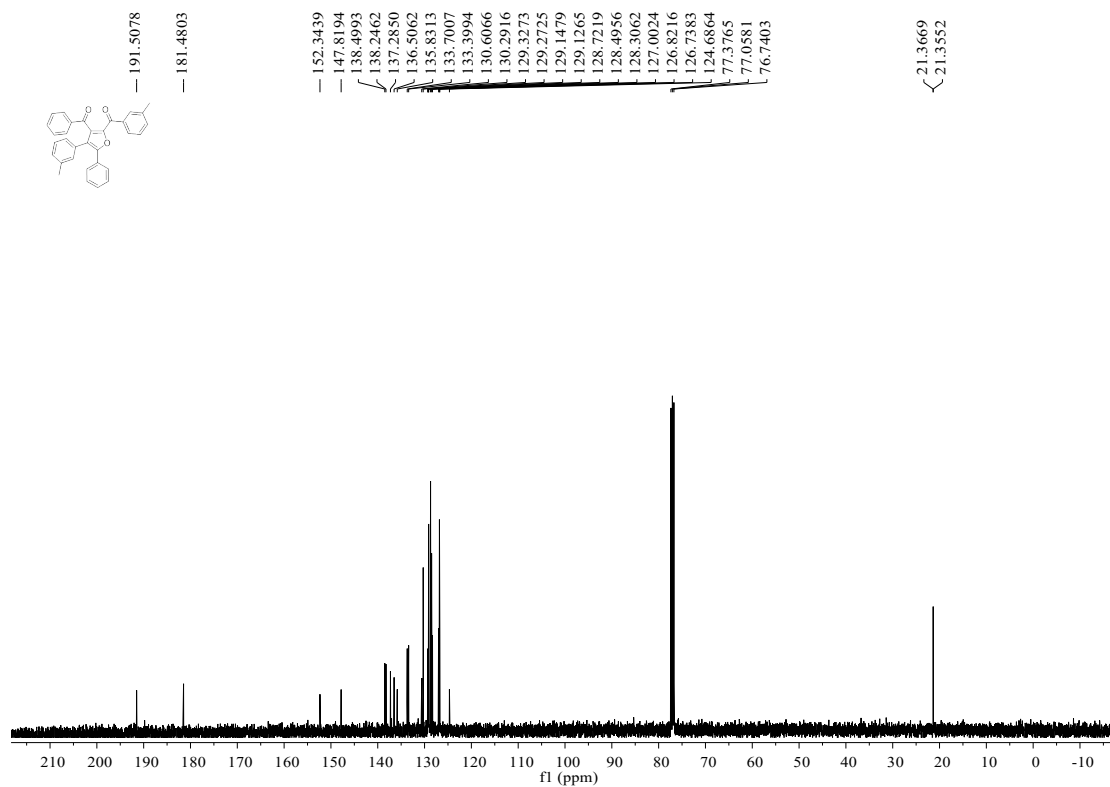
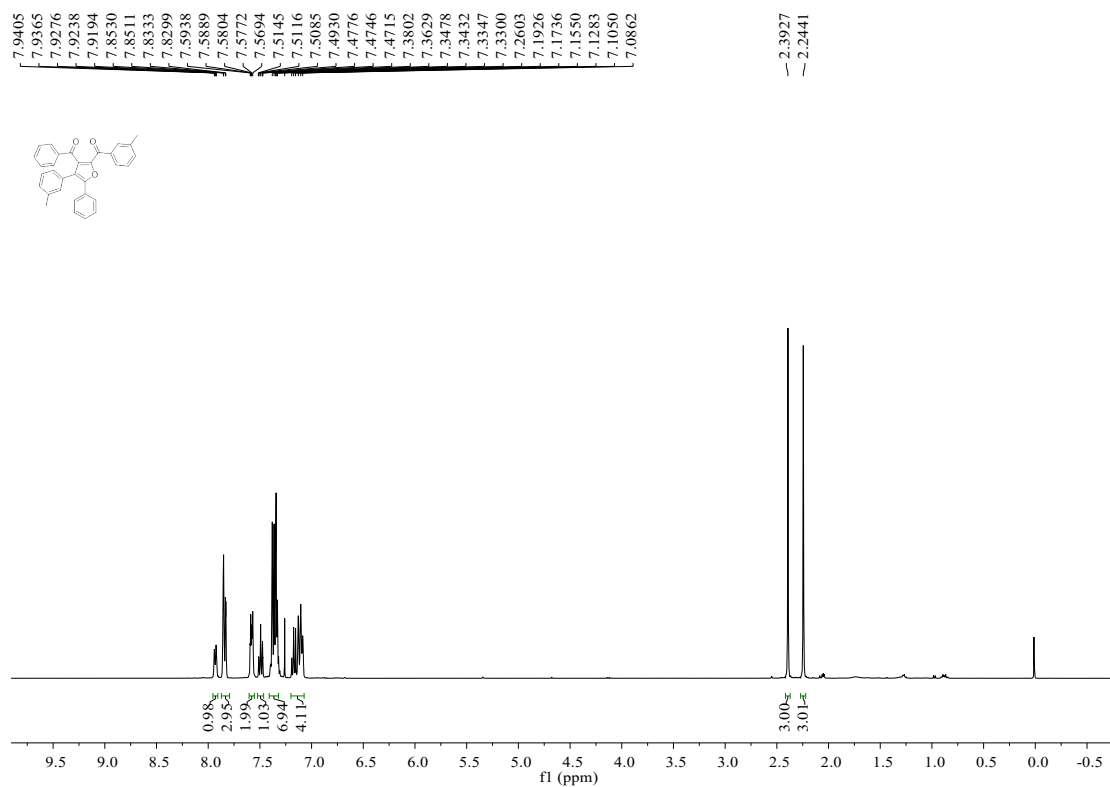
(3-benzoyl-4-(4-bromophenyl)-5-phenylfuran-2-yl)(4-bromophenyl)methanone (**3ea**)



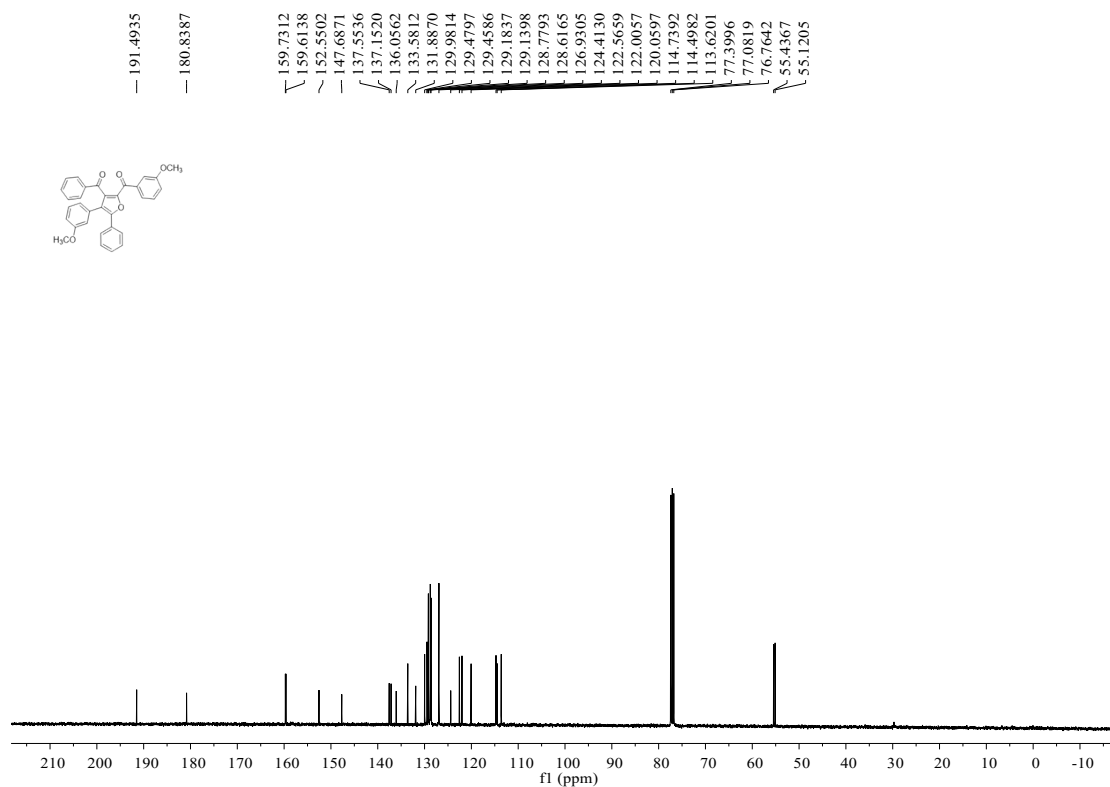
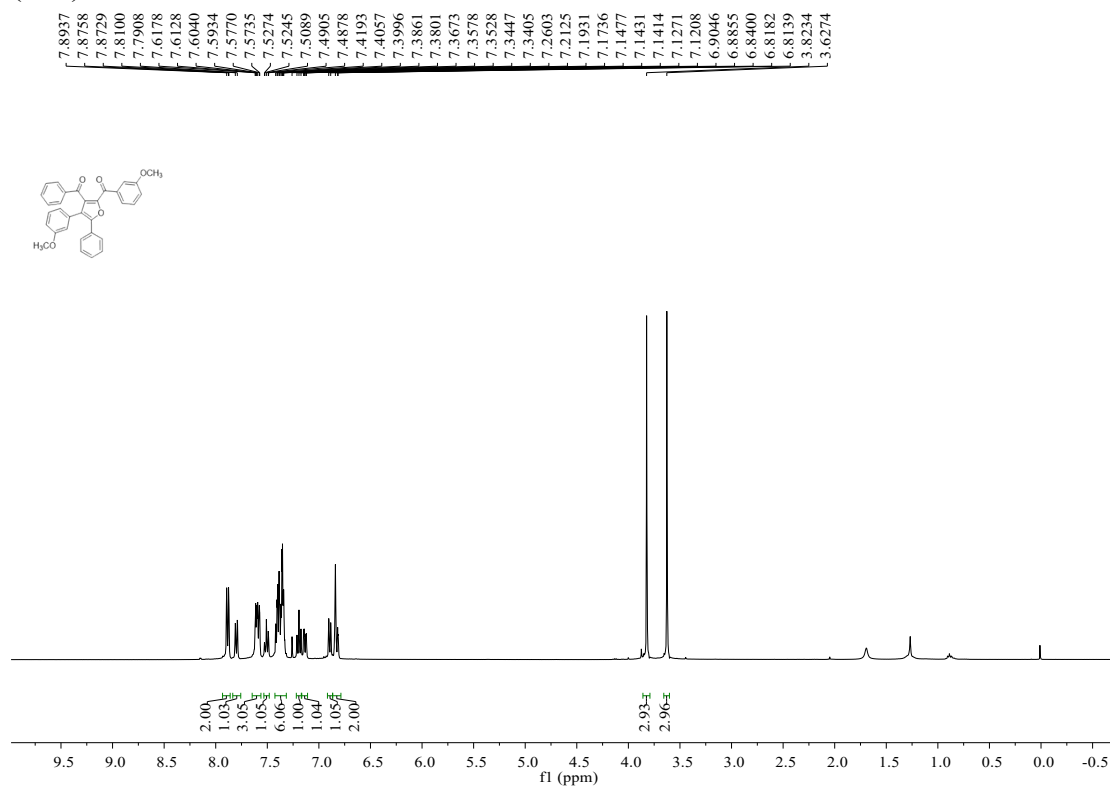
(3-benzoyl-4-(4-nitrophenyl)-5-phenylfuran-2-yl)(4-nitrophenyl)methanone (**3fa**)



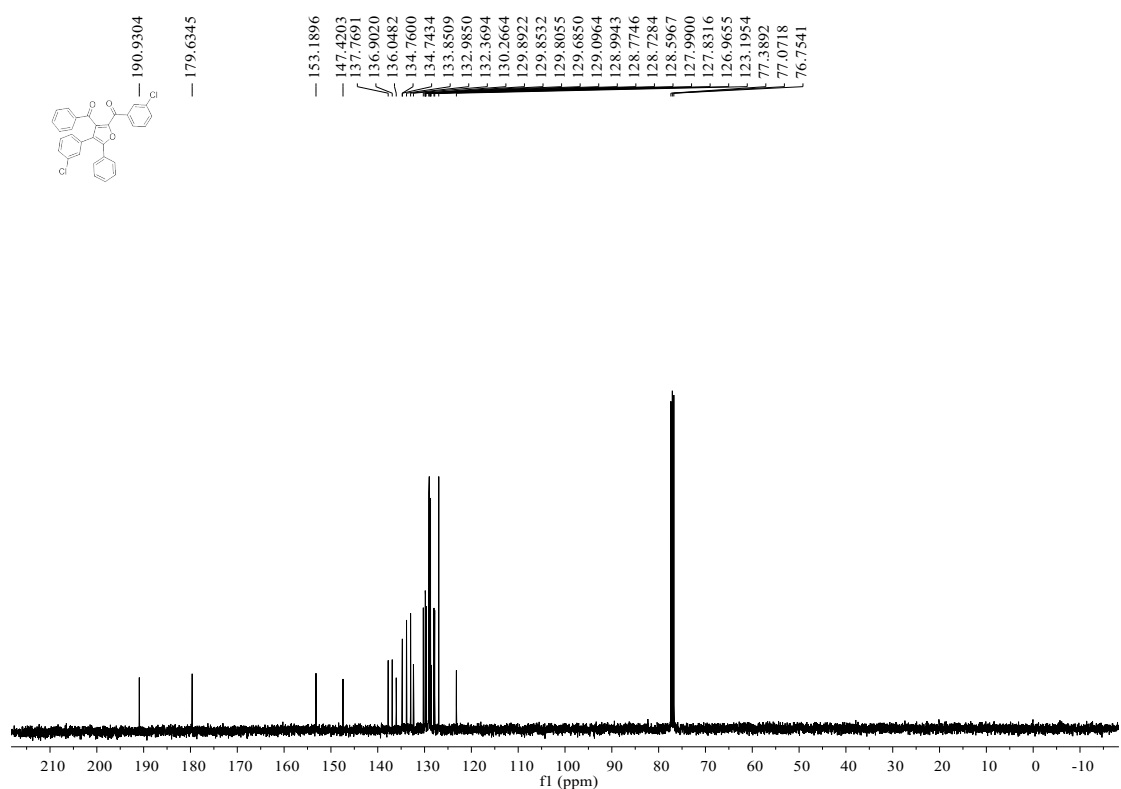
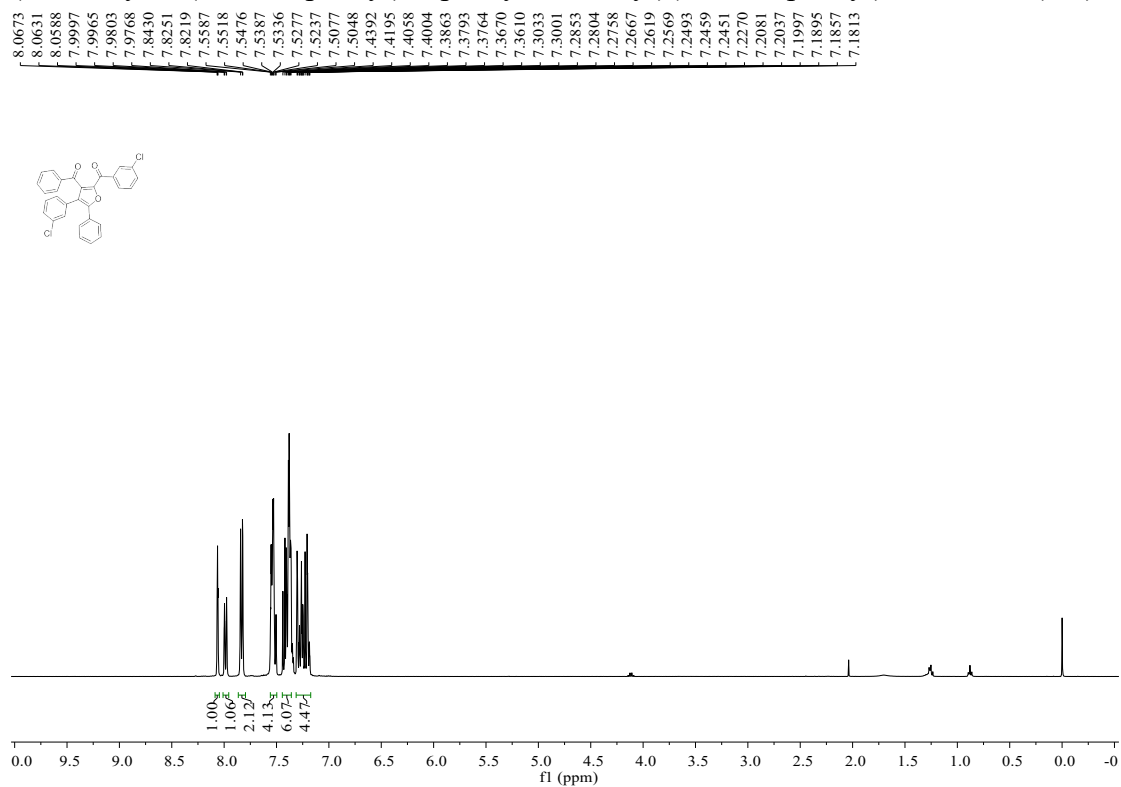
(3-benzoyl-5-phenyl-4-(m-tolyl)furan-2-yl)(m-tolyl)methanone (**3ga**)



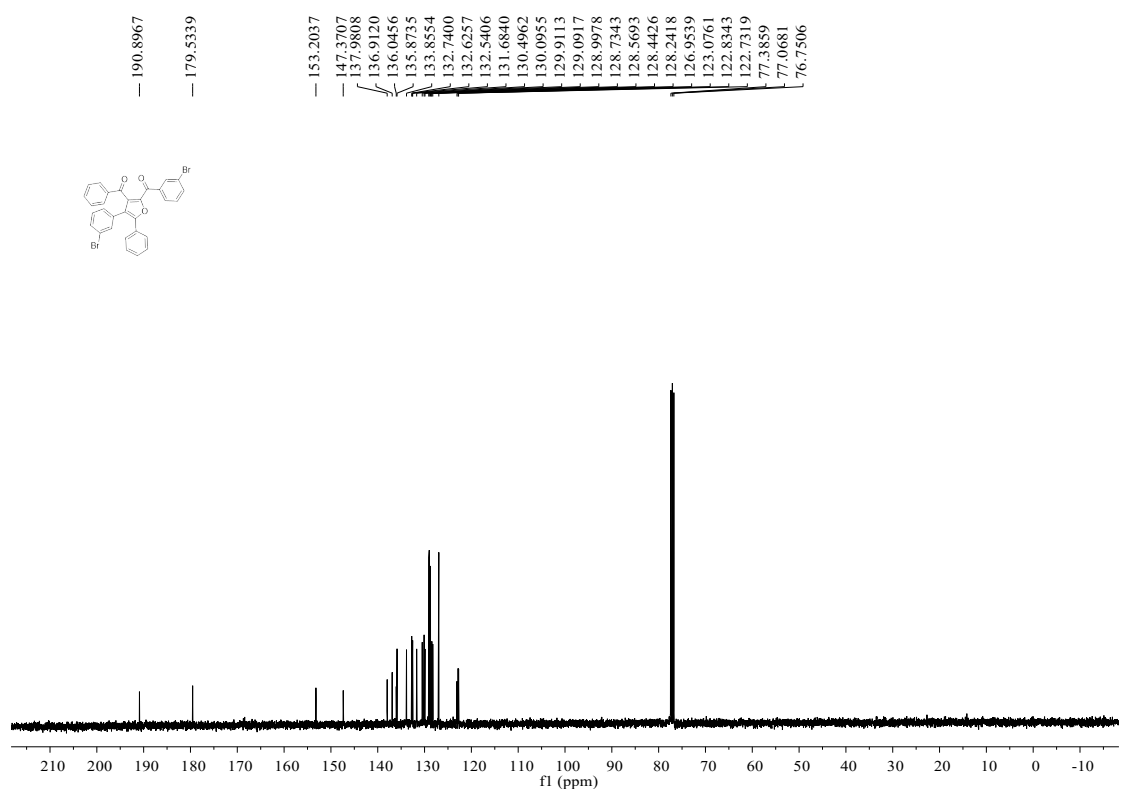
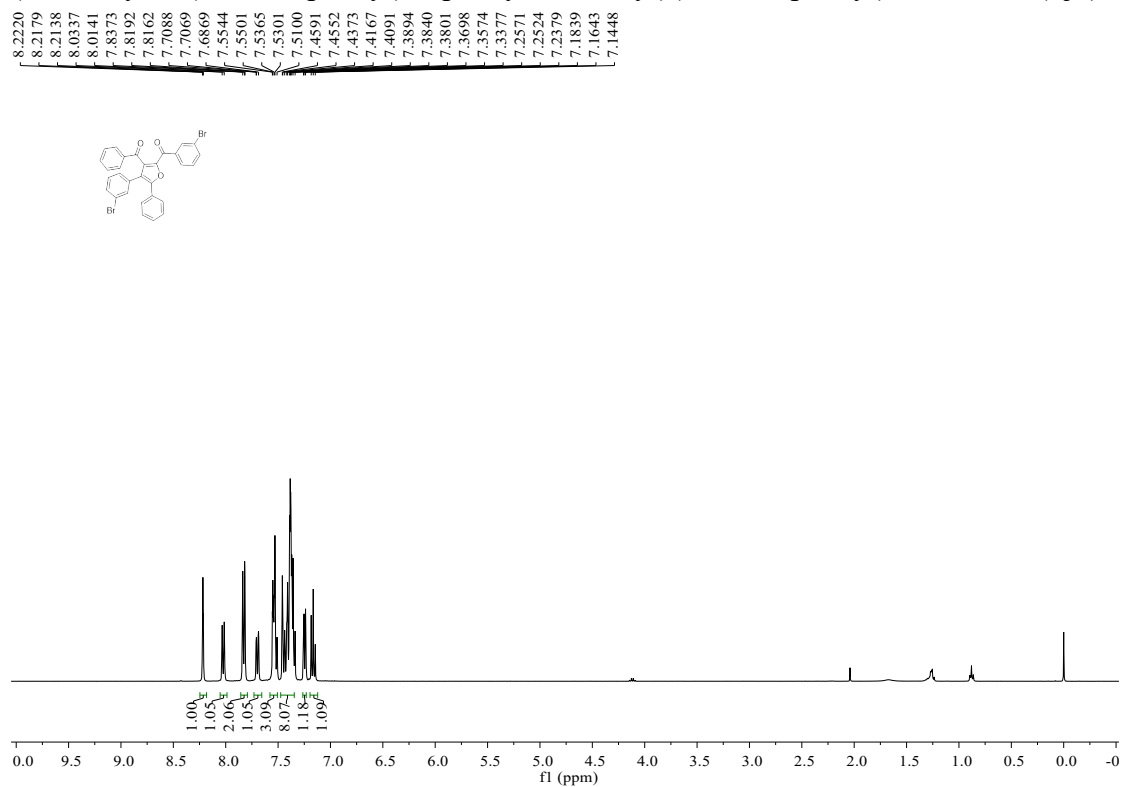
(3-benzoyl-4-(3-methoxyphenyl)-5-phenylfuran-2-yl)(3-methoxyphenyl)methanone
(3ha)



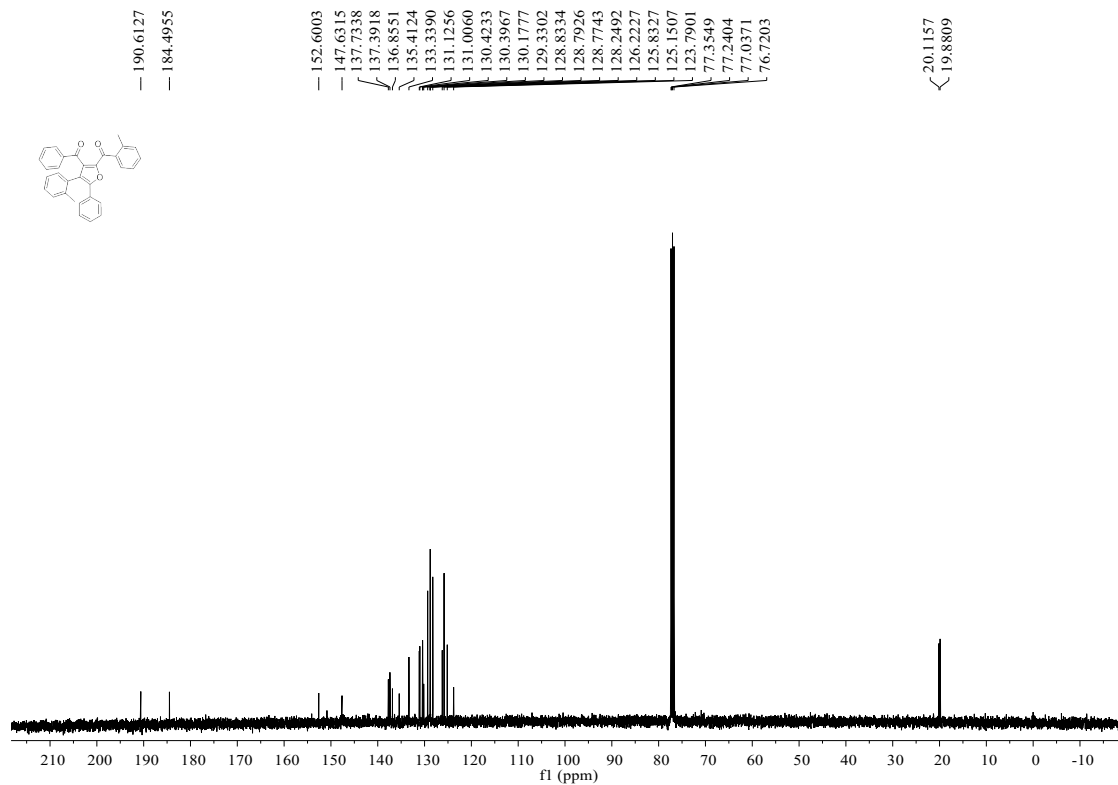
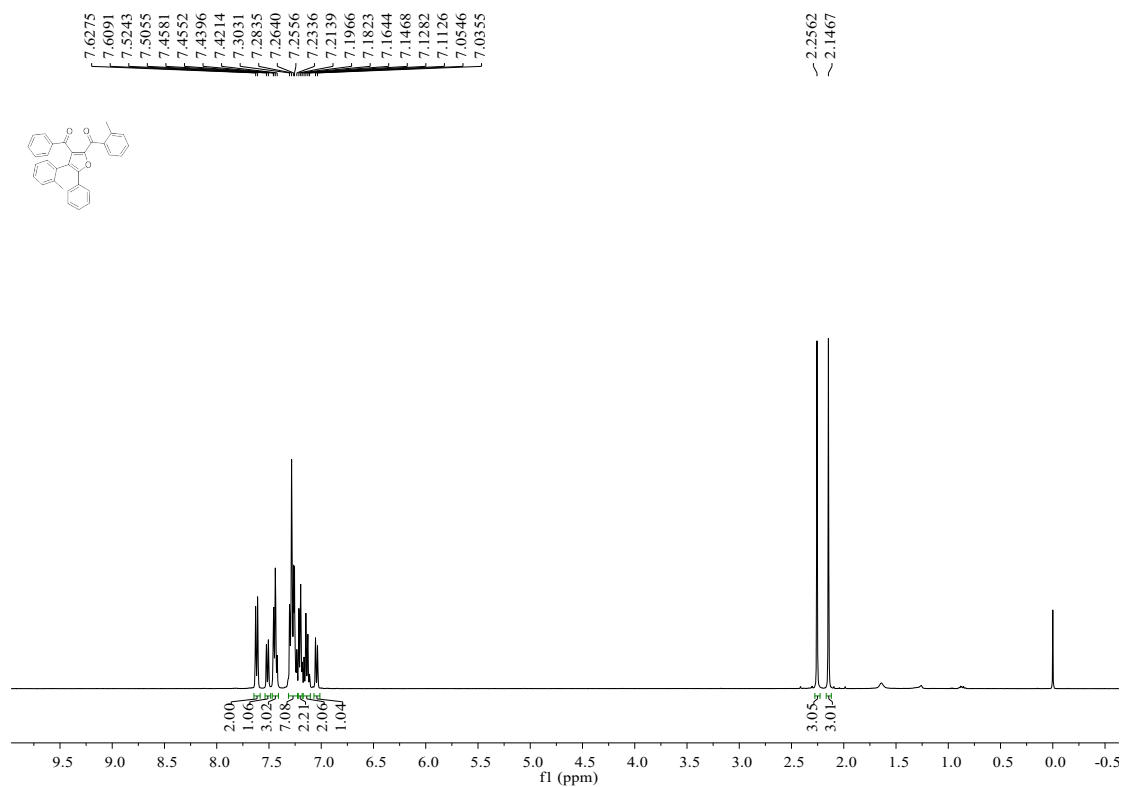
(3-benzoyl-4-(3-chlorophenyl)-5-phenylfuran-2-yl)(3-chlorophenyl)methanone (**3ia**)



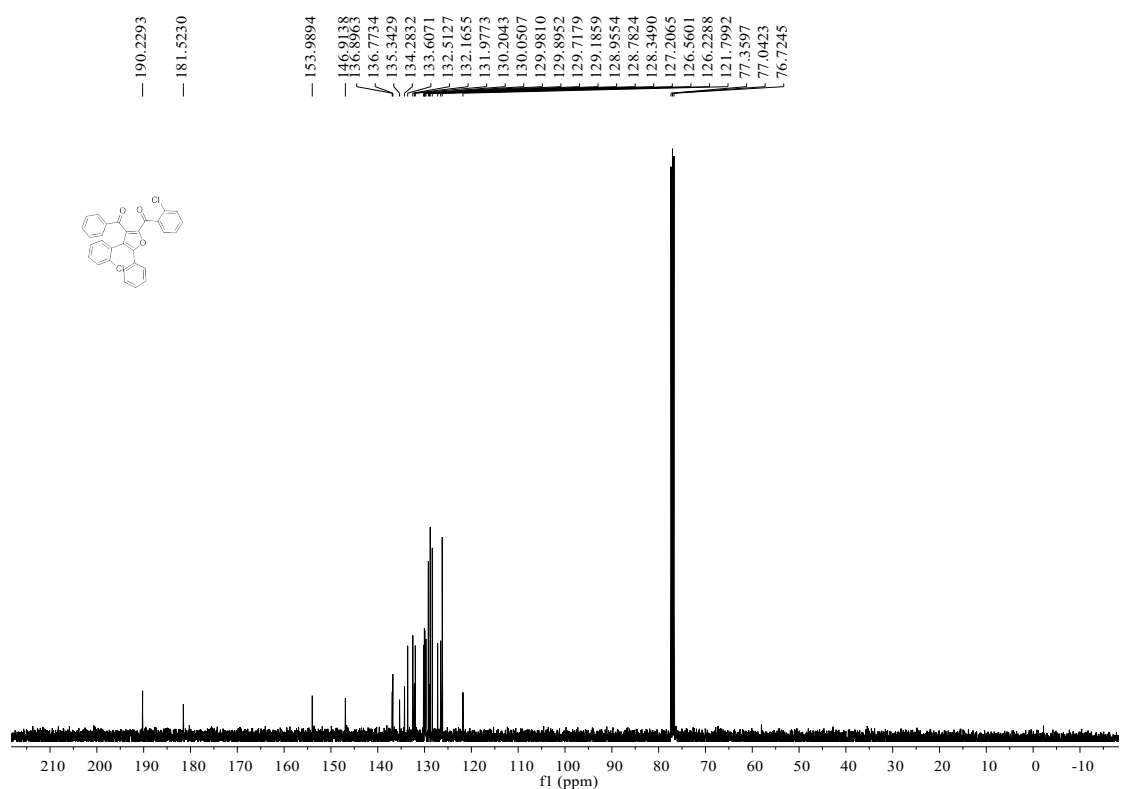
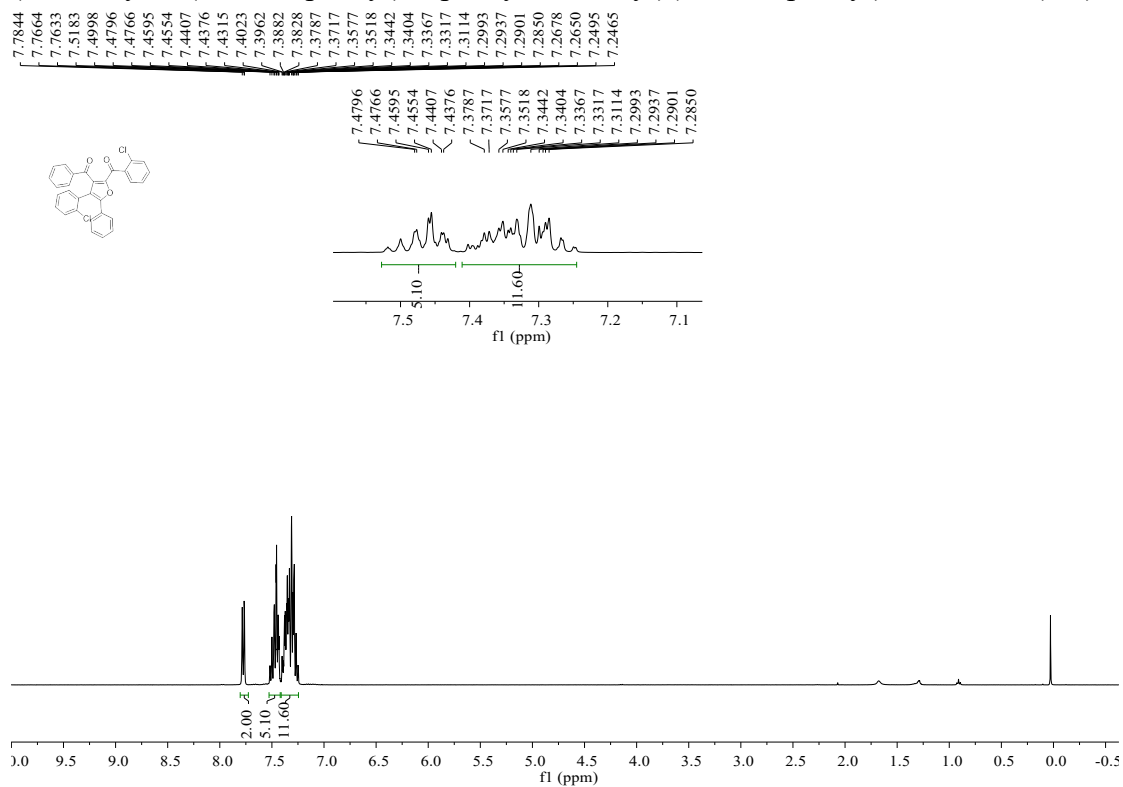
(3-benzoyl-4-(3-bromophenyl)-5-phenylfuran-2-yl)(3-bromophenyl)methanone (**3ja**)



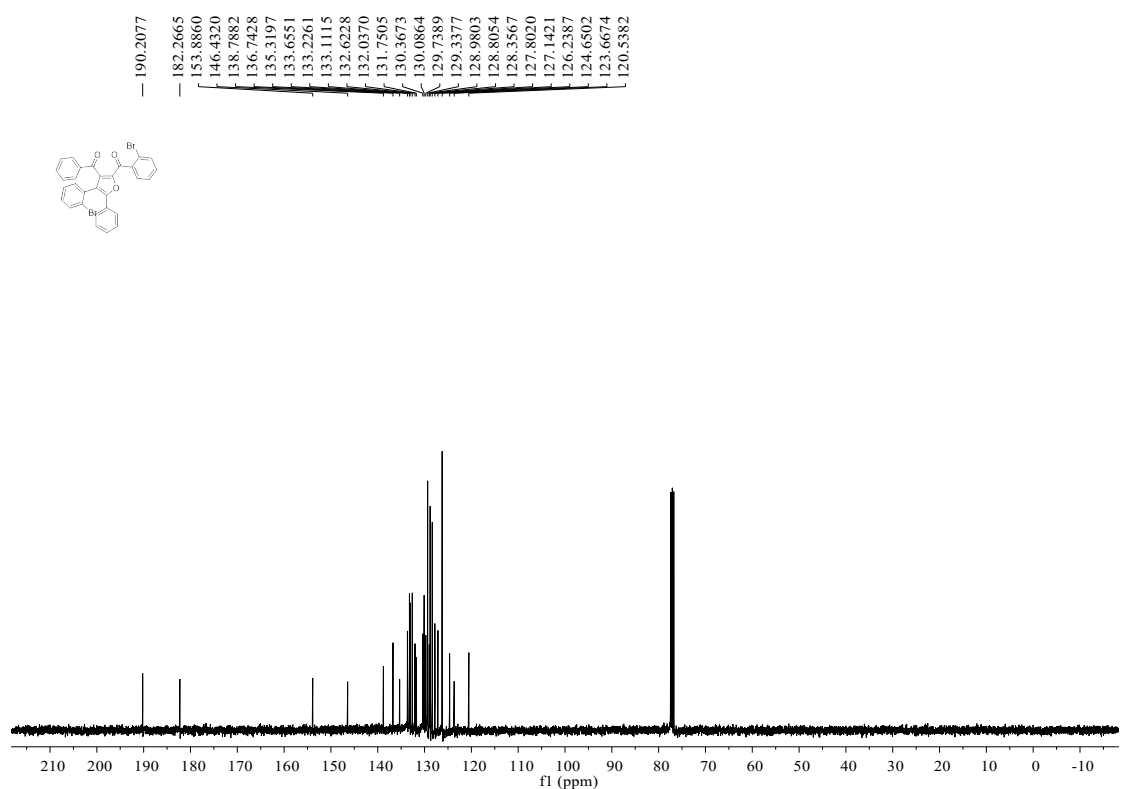
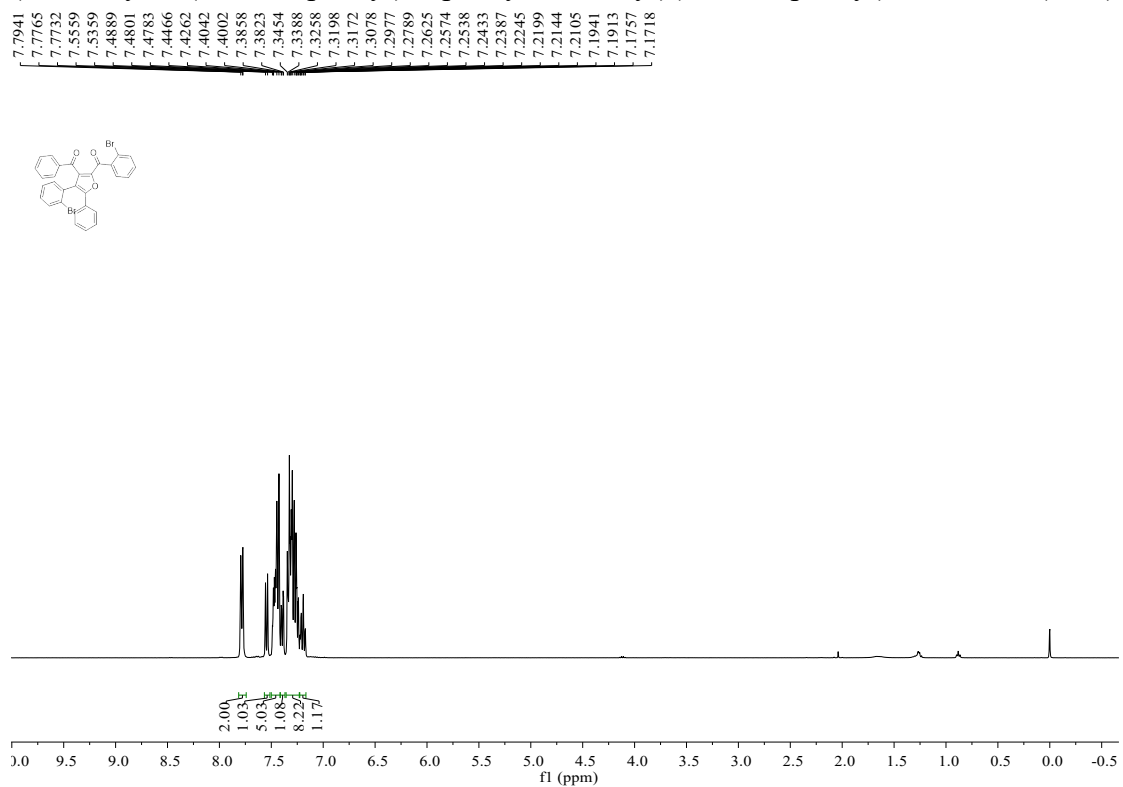
(3-benzoyl-5-phenyl-4-(o-tolyl)furan-2-yl)(o-tolyl)methanone (**3ka**)



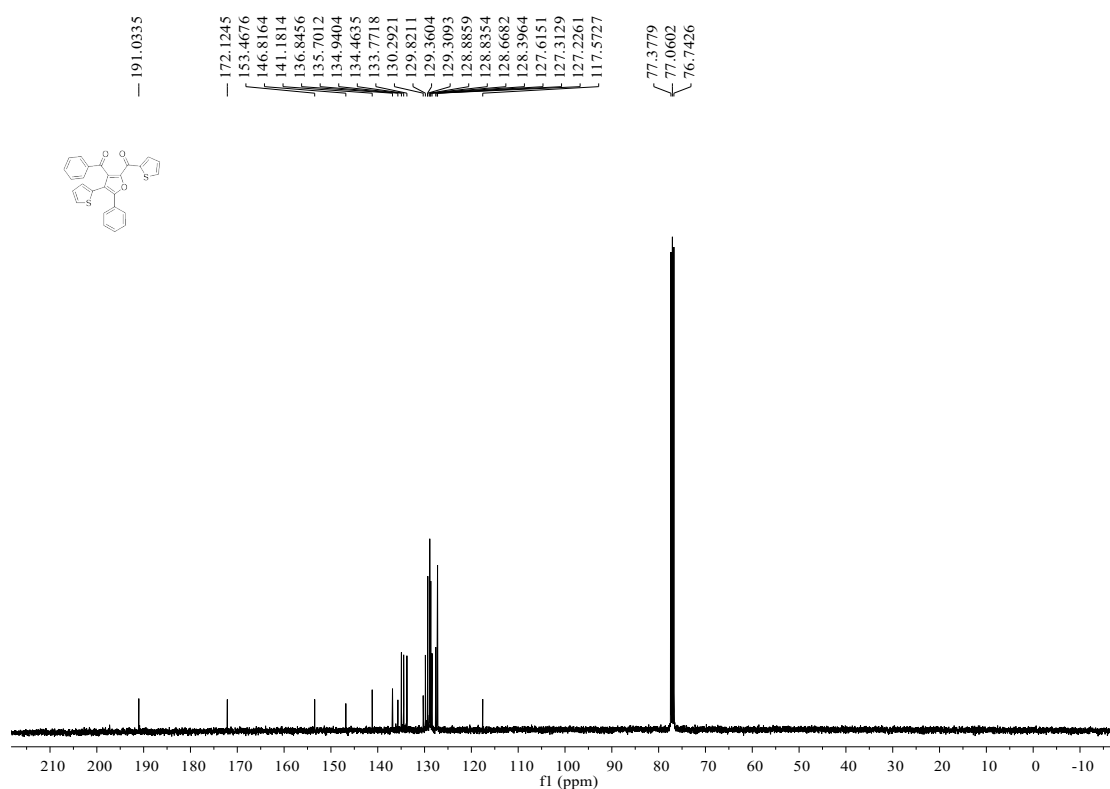
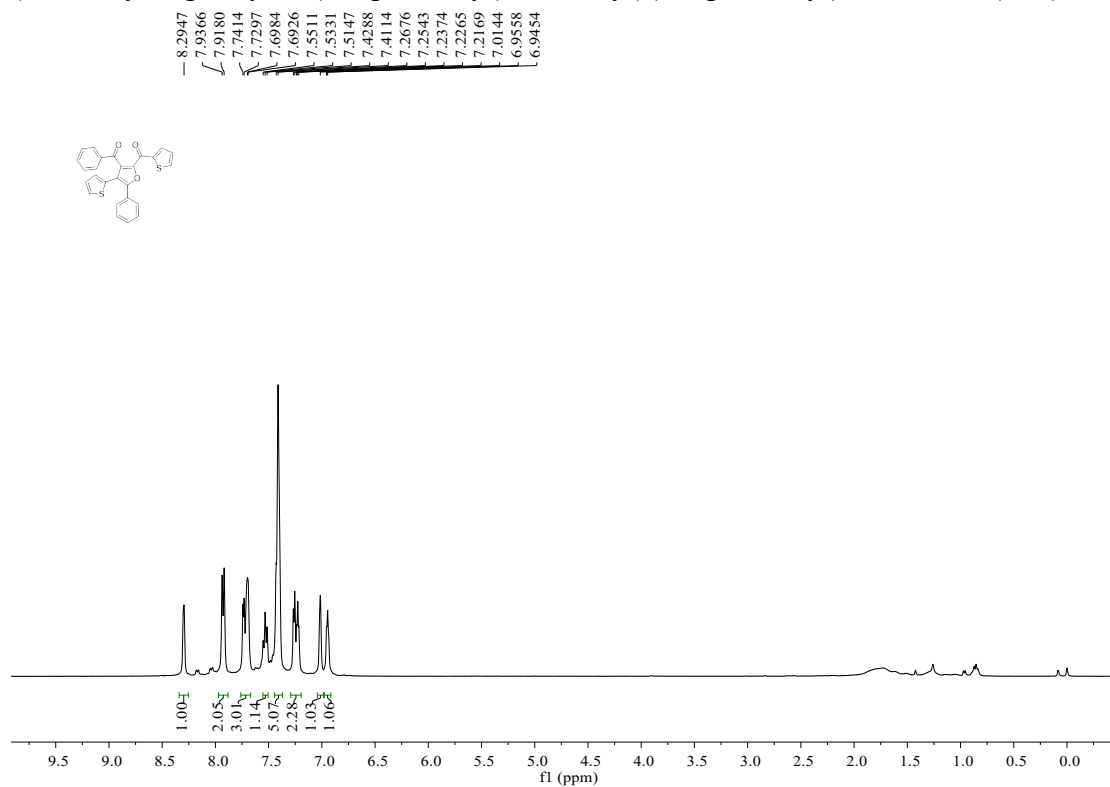
(3-benzoyl-4-(2-chlorophenyl)-5-phenylfuran-2-yl)(2-chlorophenyl)methanone (**31a**)



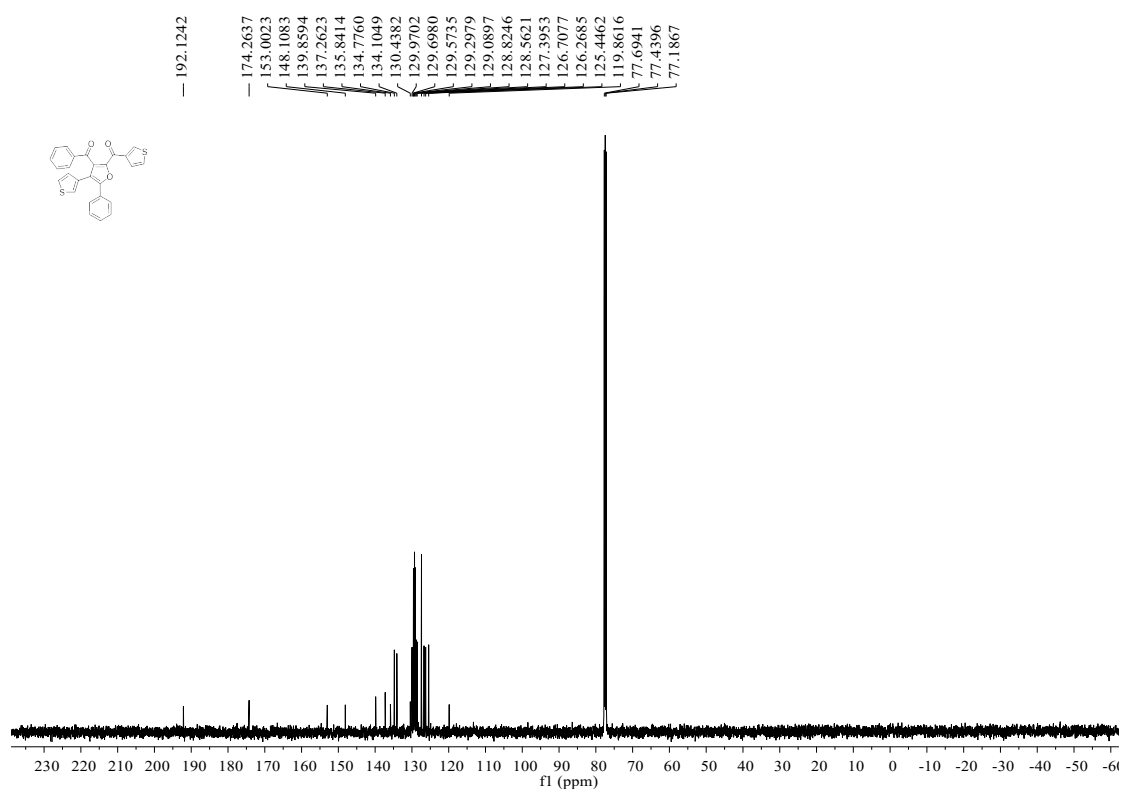
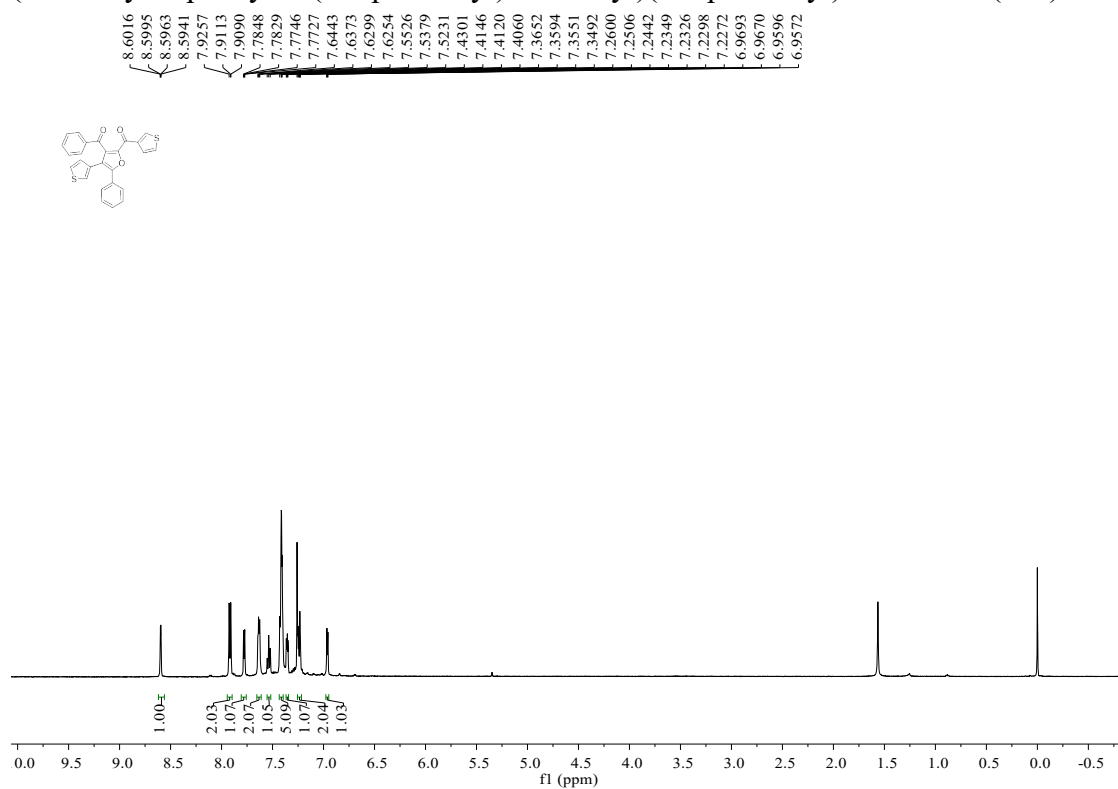
(3-benzoyl-4-(2-bromophenyl)-5-phenylfuran-2-yl)(2-bromophenyl)methanone (**3ma**)



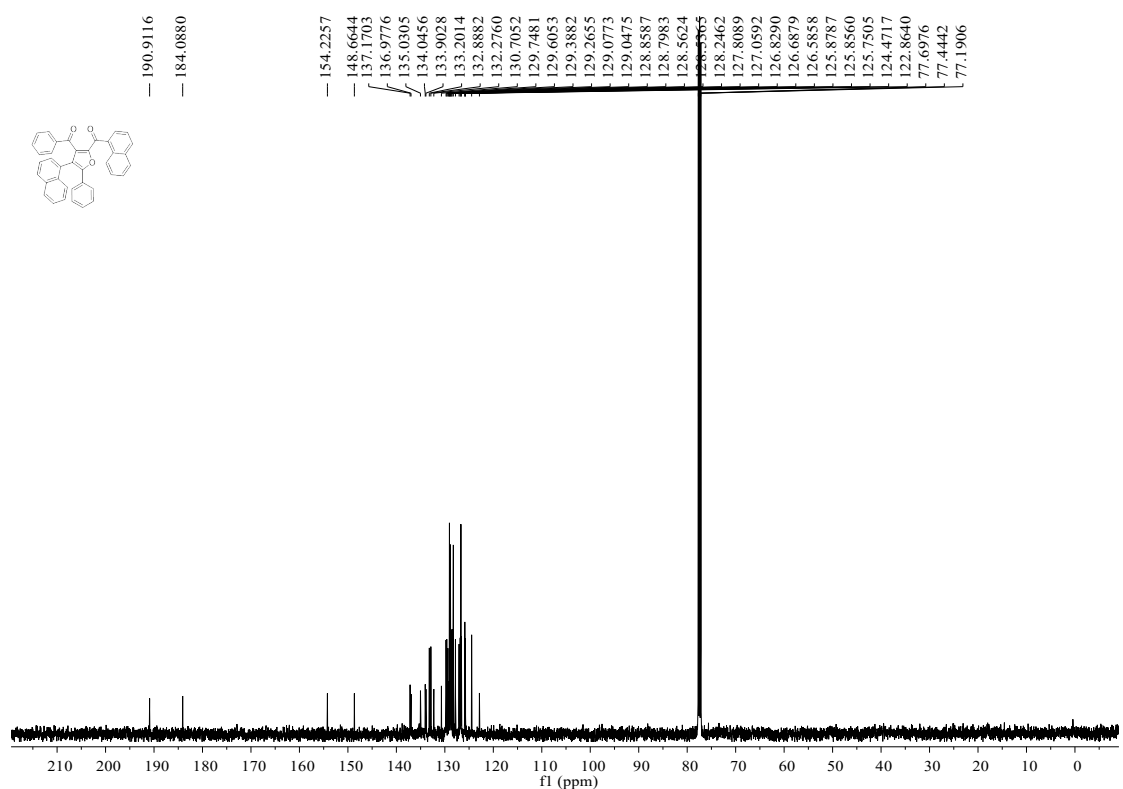
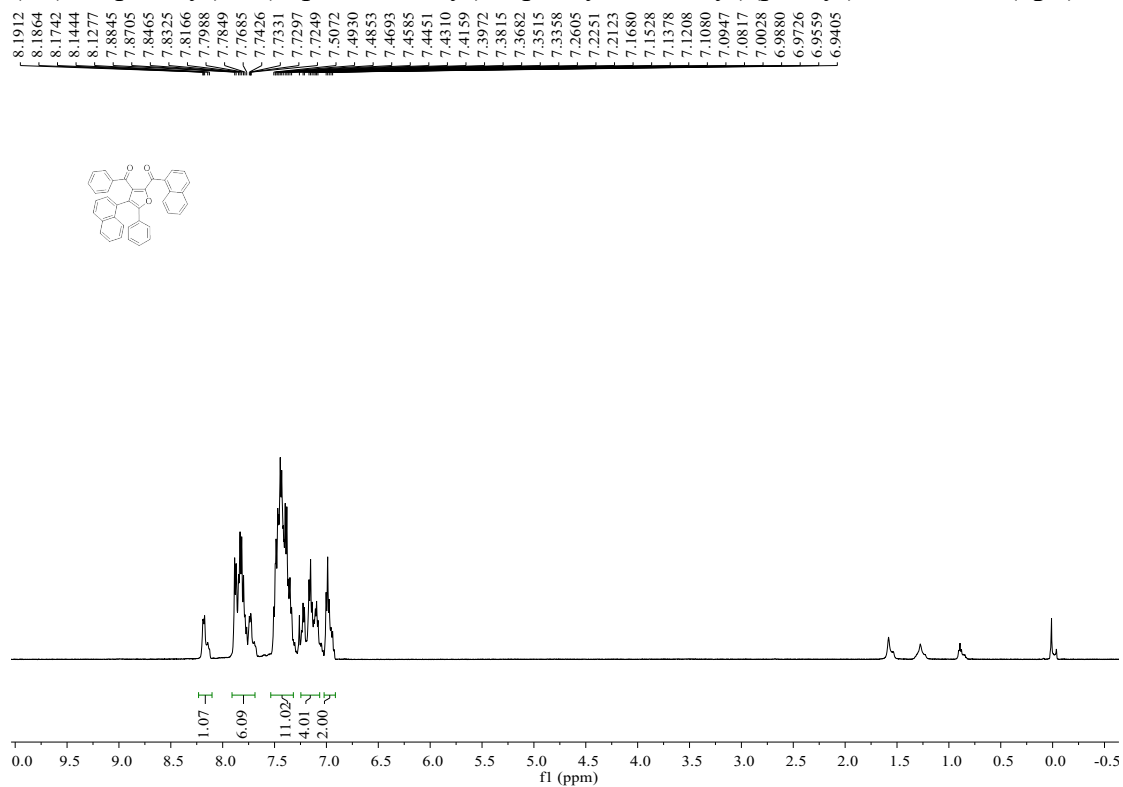
(3-benzoyl-5-phenyl-4-(thiophen-2-yl)furan-2-yl)(thiophen-2-yl)methanone (**3na**)



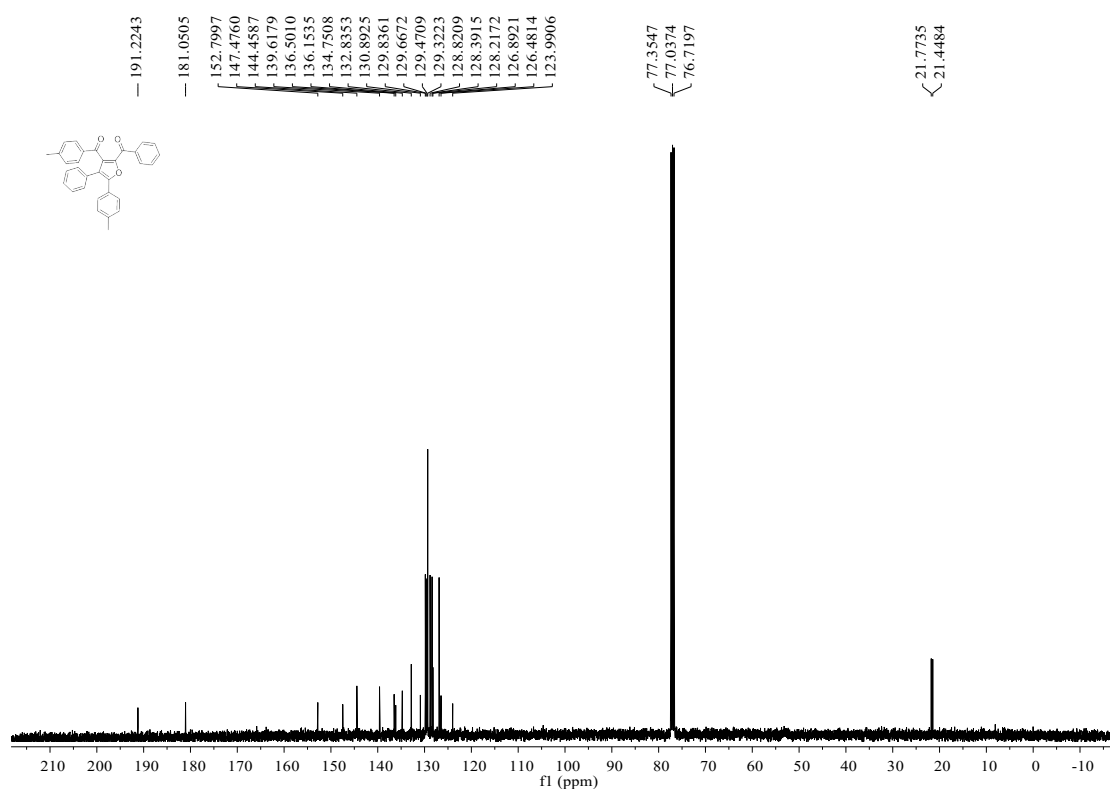
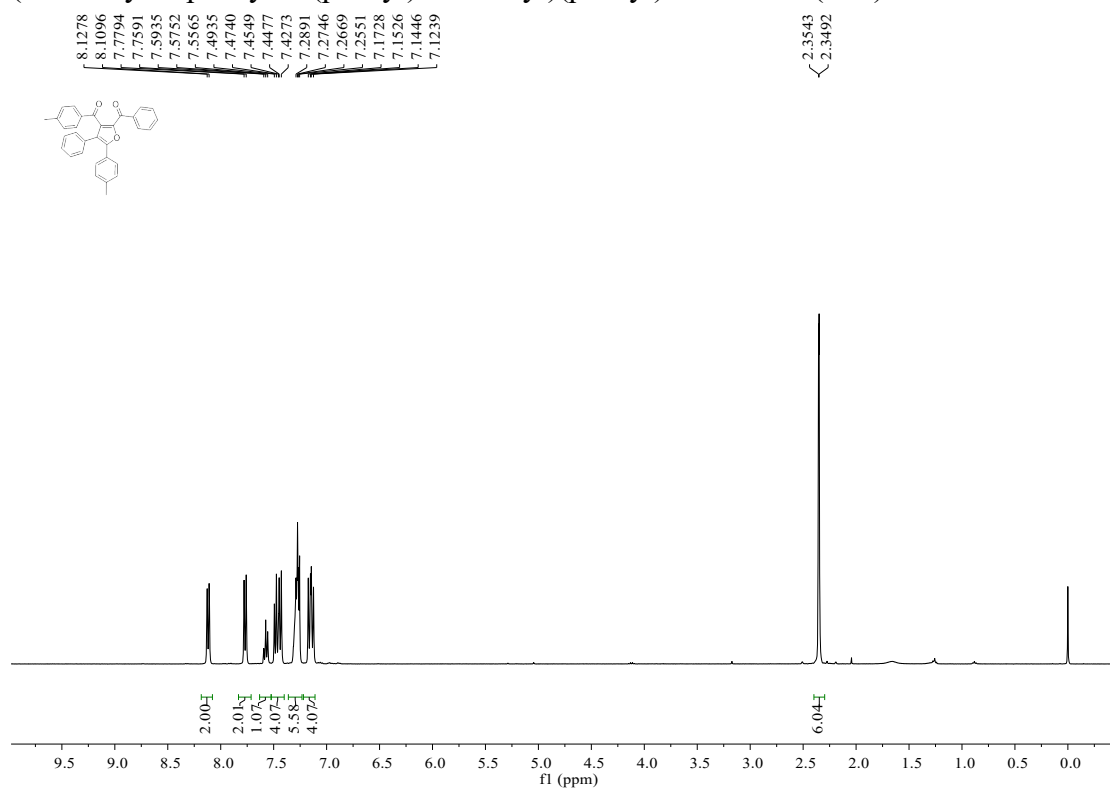
(3-benzoyl-5-phenyl-4-(thiophen-3-yl)furan-2-yl)(thiophen-3-yl)methanone (**30a**)



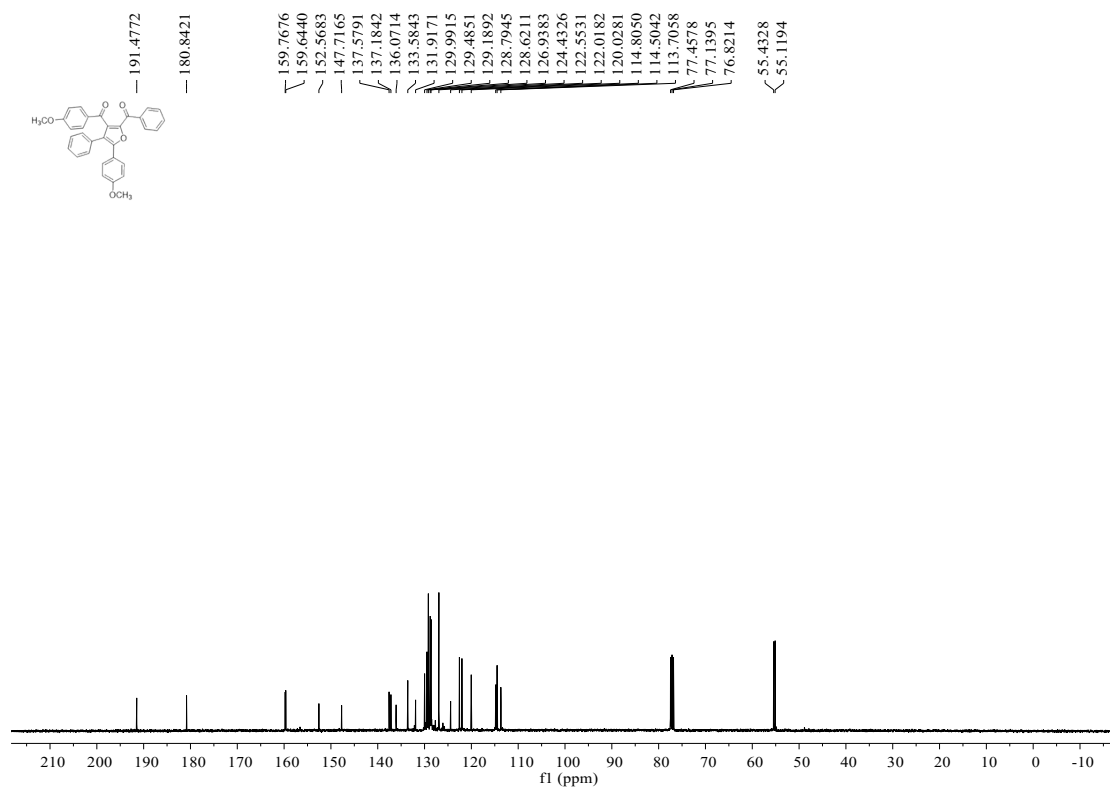
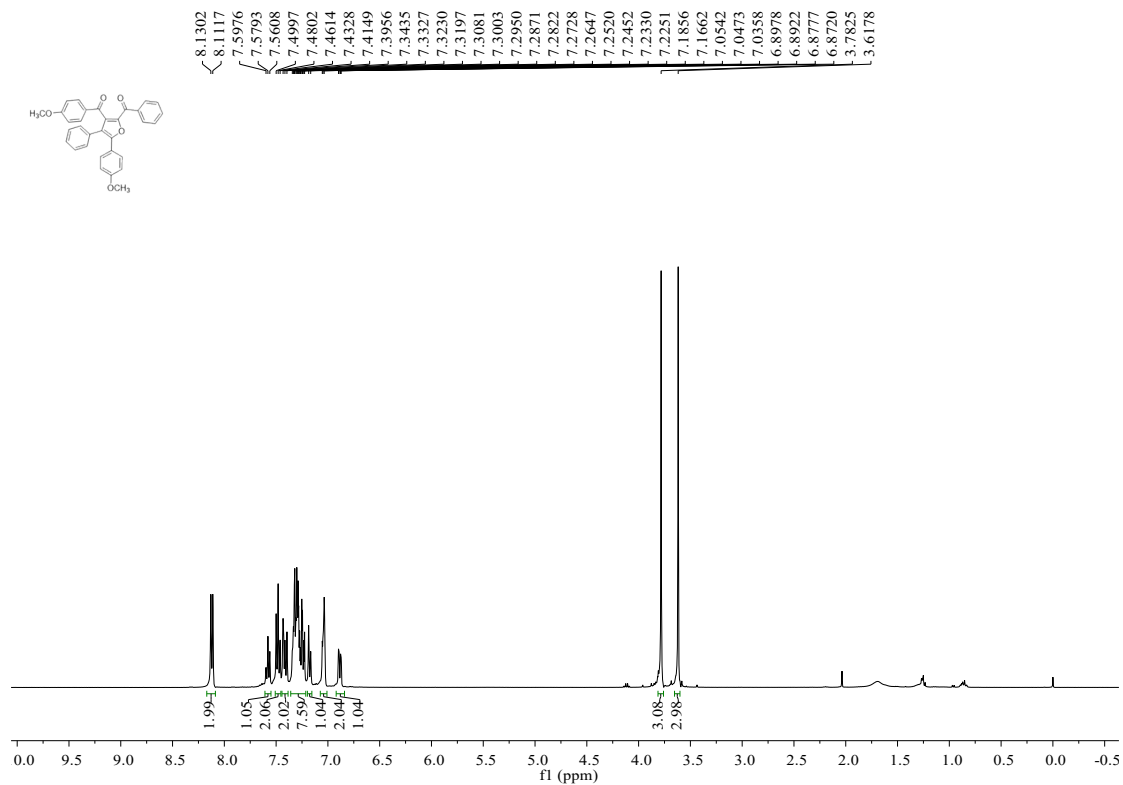
(2-(1-naphthoyl)-4-(naphthalen-1-yl)-5-phenylfuran-3-yl)(phenyl)methanone (**3pa**)



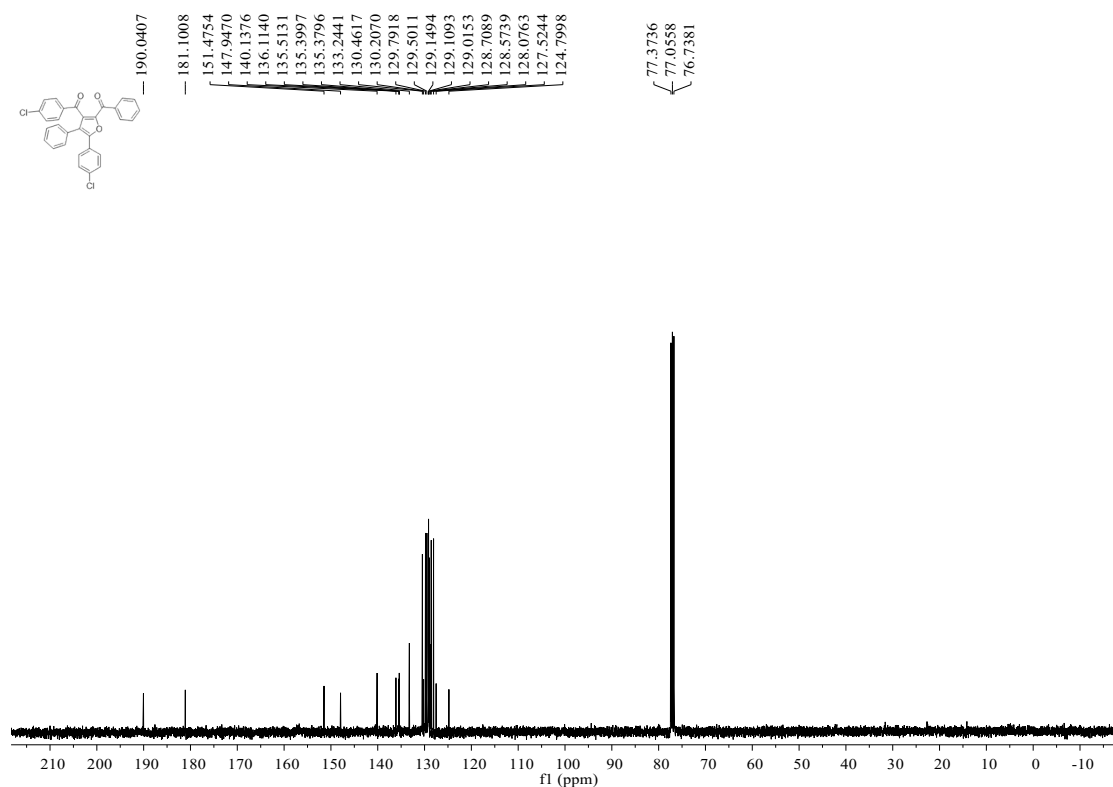
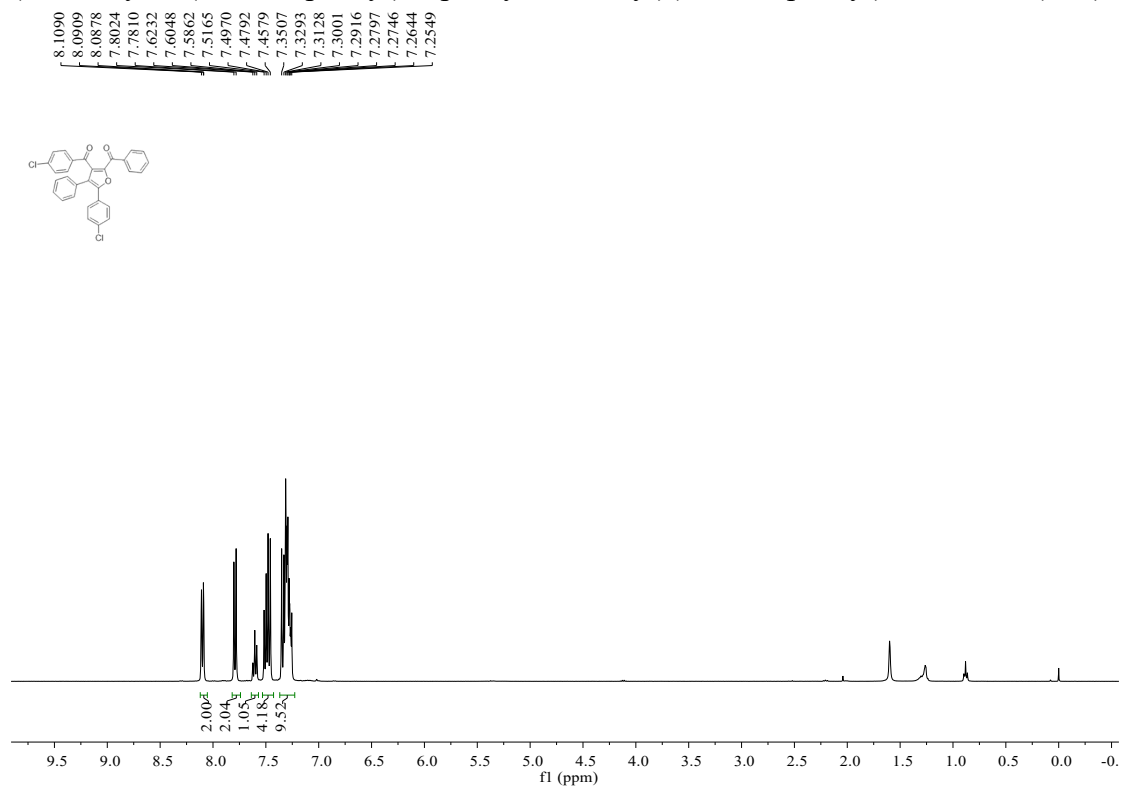
(2-benzoyl-4-phenyl-5-(p-tolyl)furan-3-yl)(p-tolyl)methanone (**3ab**)



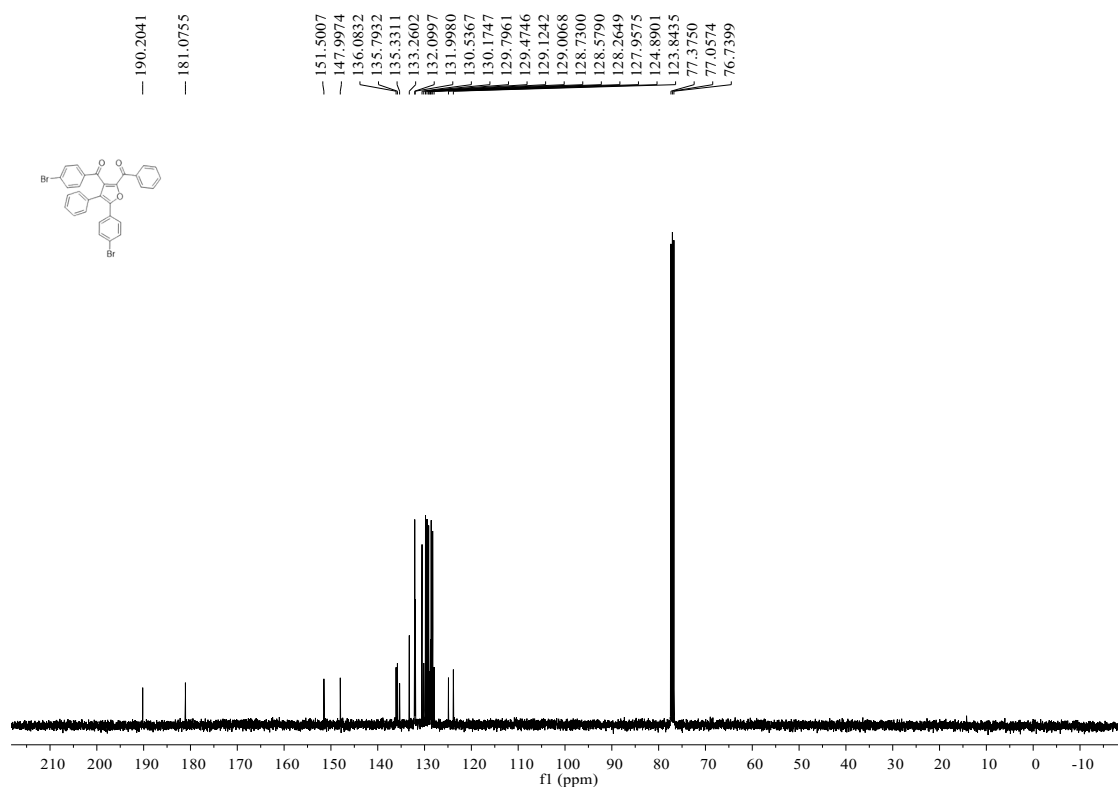
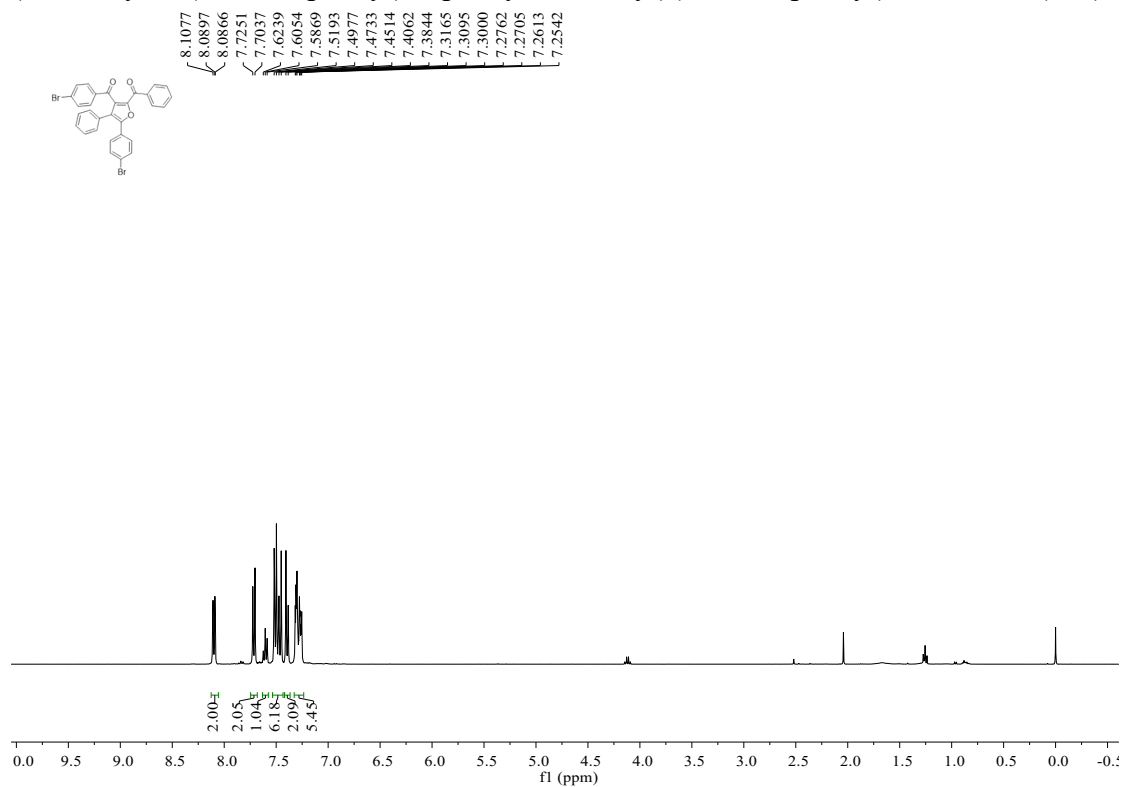
(2-benzoyl-5-(4-methoxyphenyl)-4-phenylfuran-3-yl)(4-methoxyphenyl)methanone
(3ac)



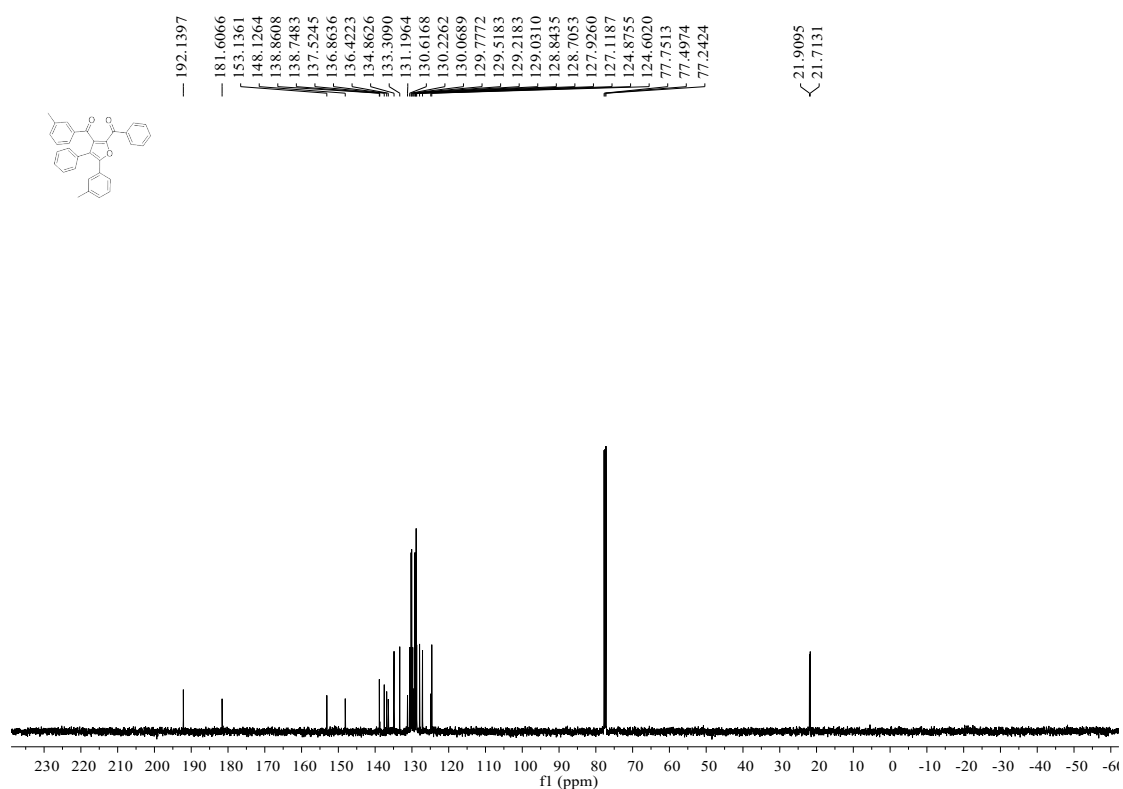
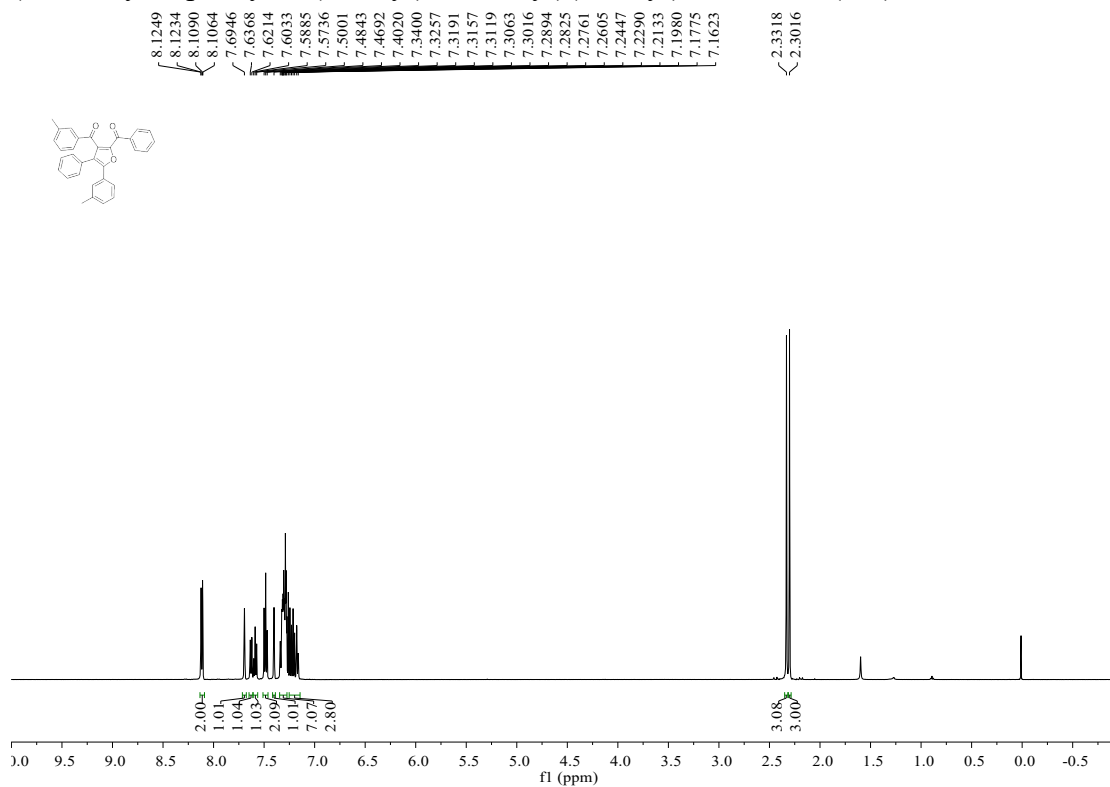
(2-benzoyl-5-(4-chlorophenyl)-4-phenylfuran-3-yl)(4-chlorophenyl)methanone (**3ad**)



(2-benzoyl-5-(4-bromophenyl)-4-phenylfuran-3-yl)(4-bromophenyl)methanone (**3ae**)

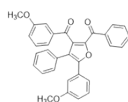
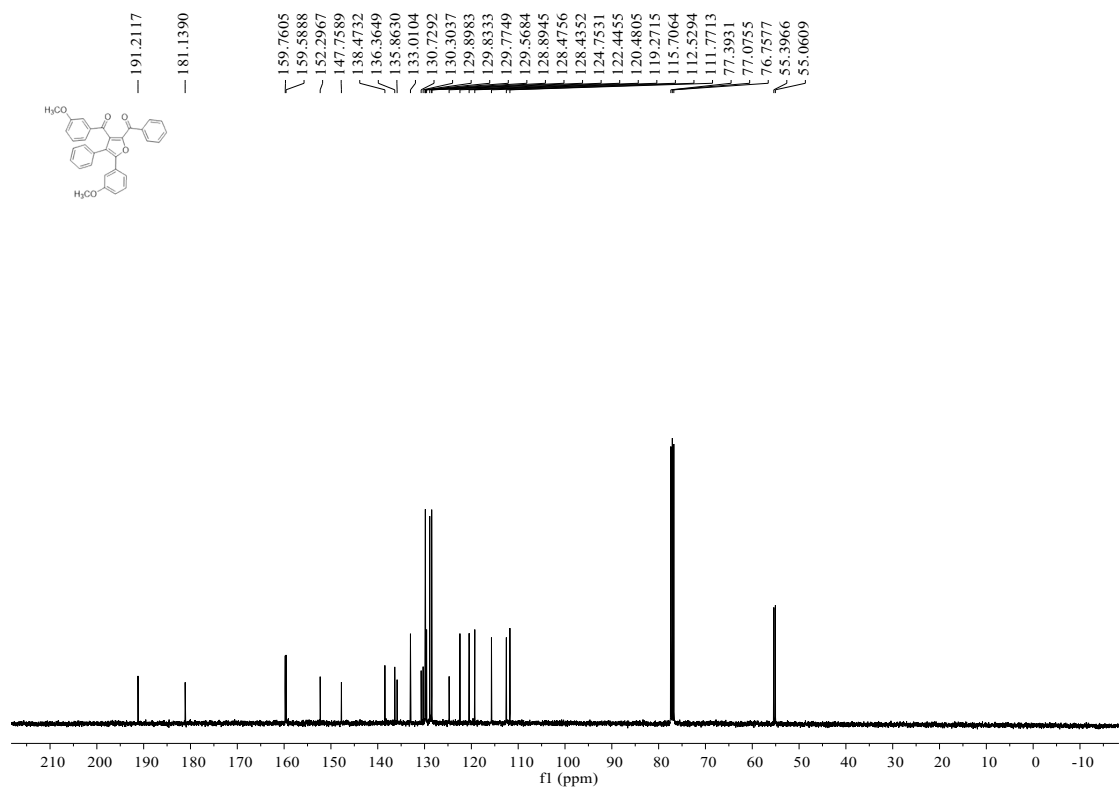
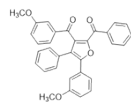
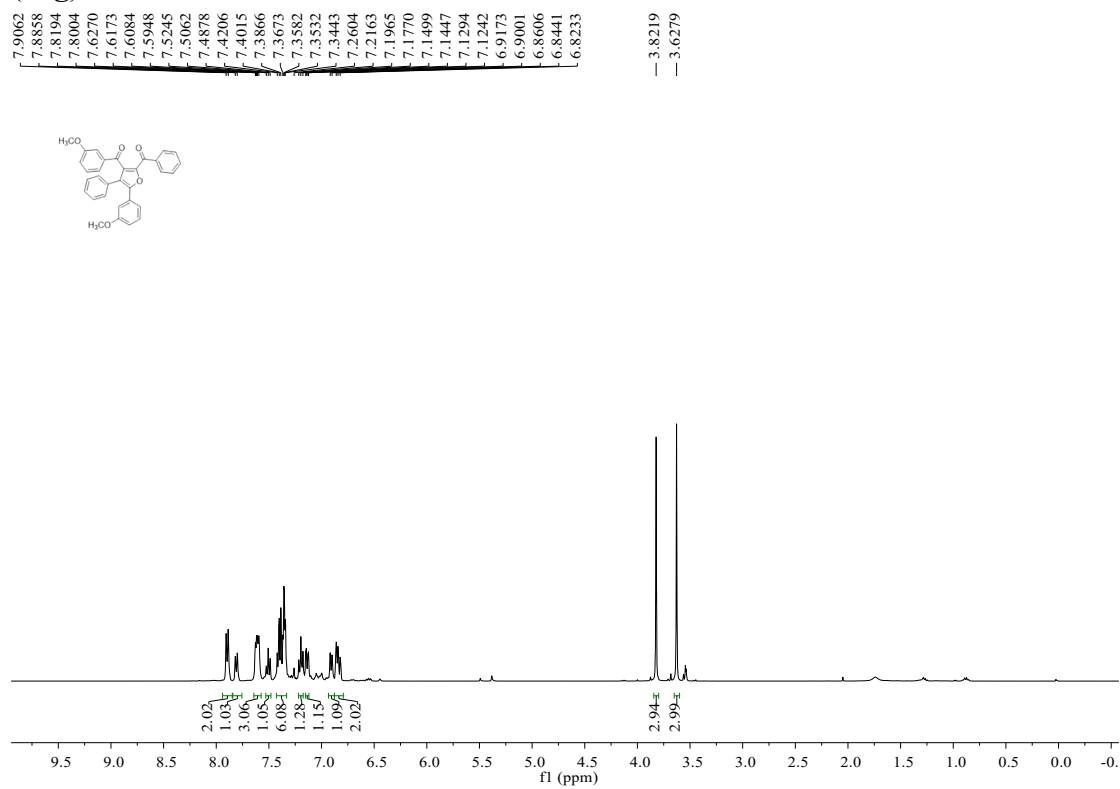


(2-benzoyl-4-phenyl-5-(m-tolyl)furan-3-yl)(m-tolyl)methanone (**3af**)

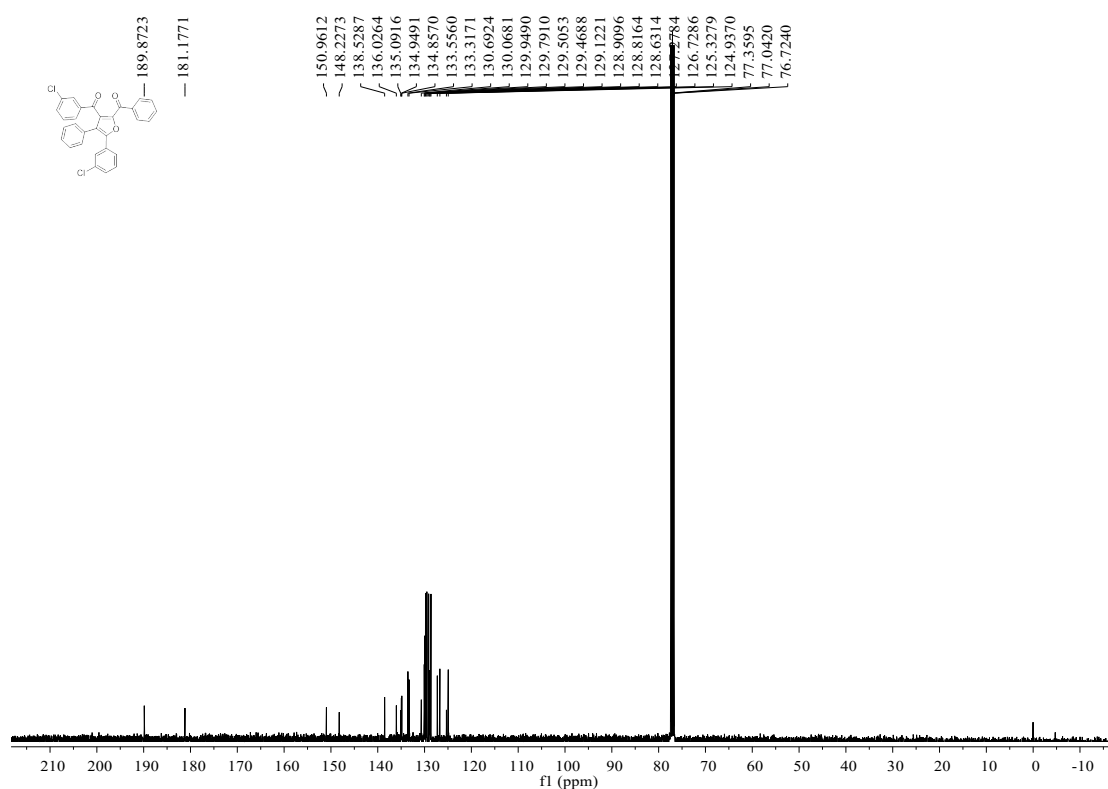
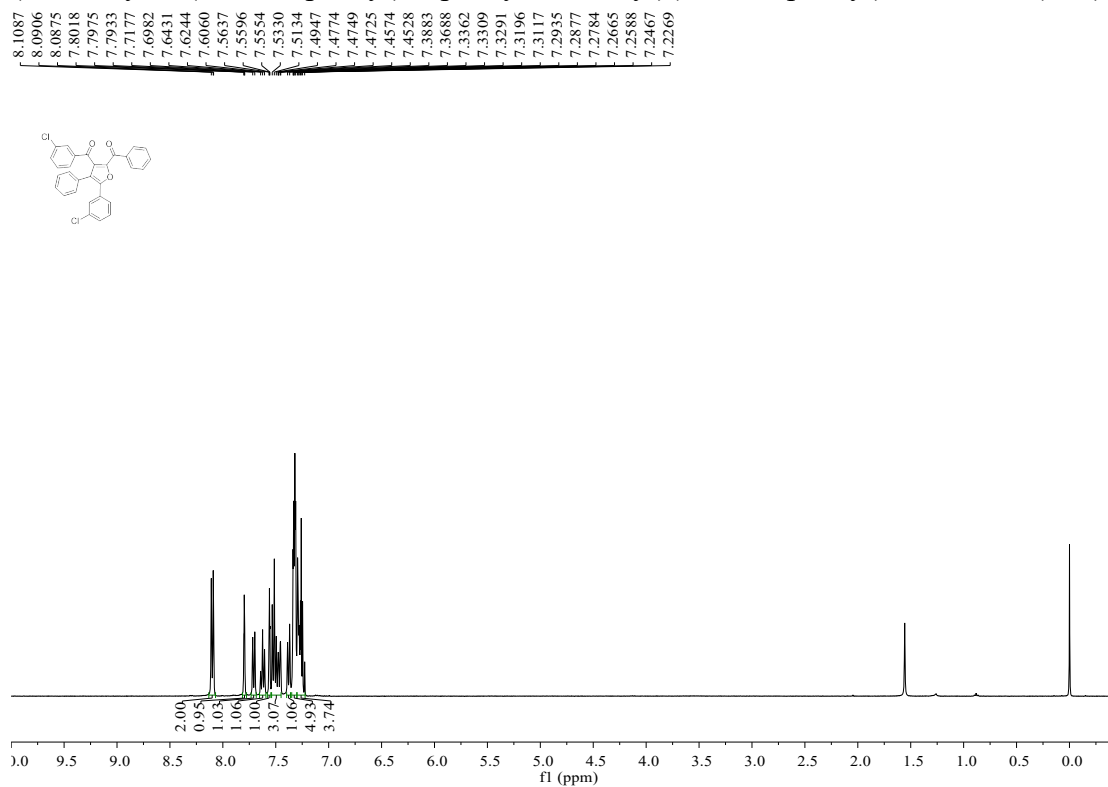


(2-benzoyl-5-(3-methoxyphenyl)-4-phenylfuran-3-yl)(3-methoxyphenyl)methanone

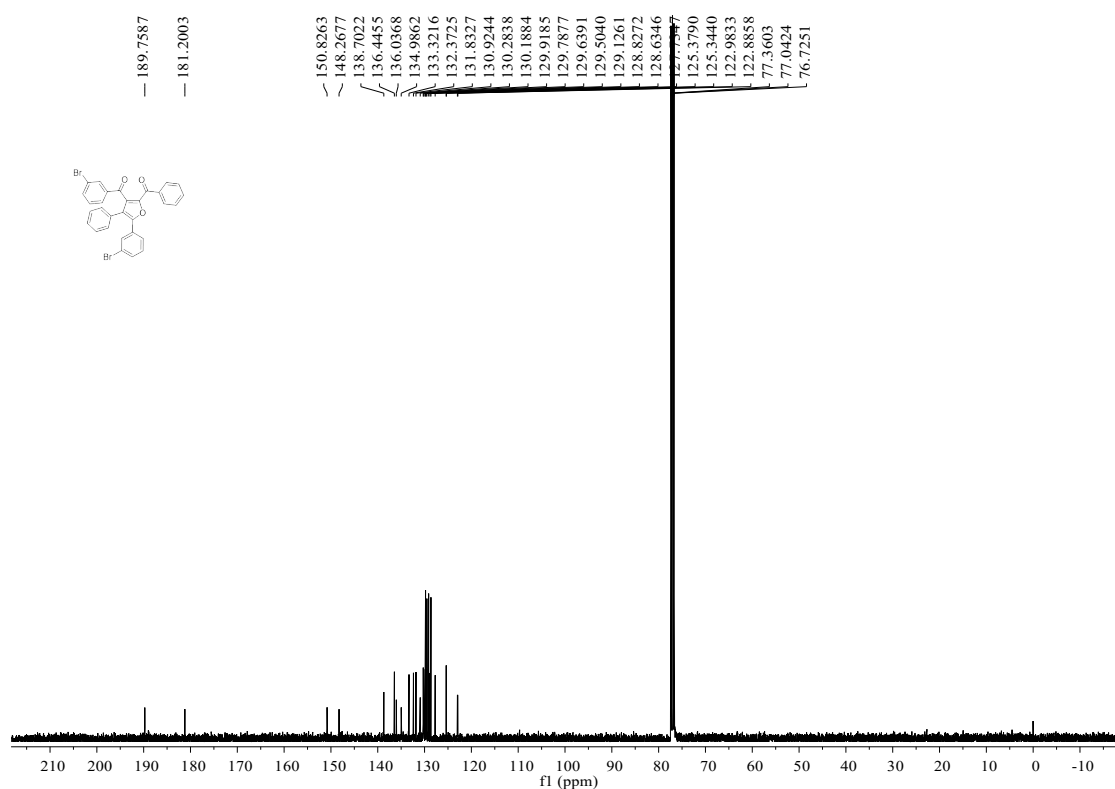
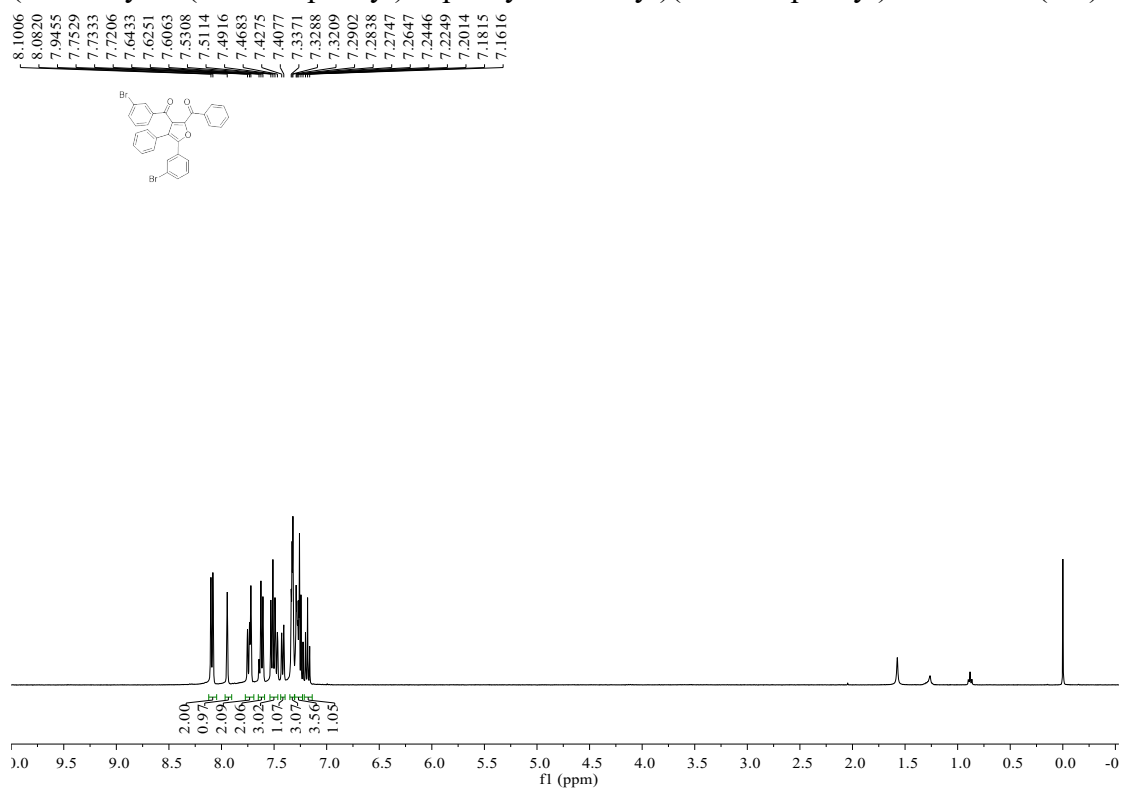
(3ag)



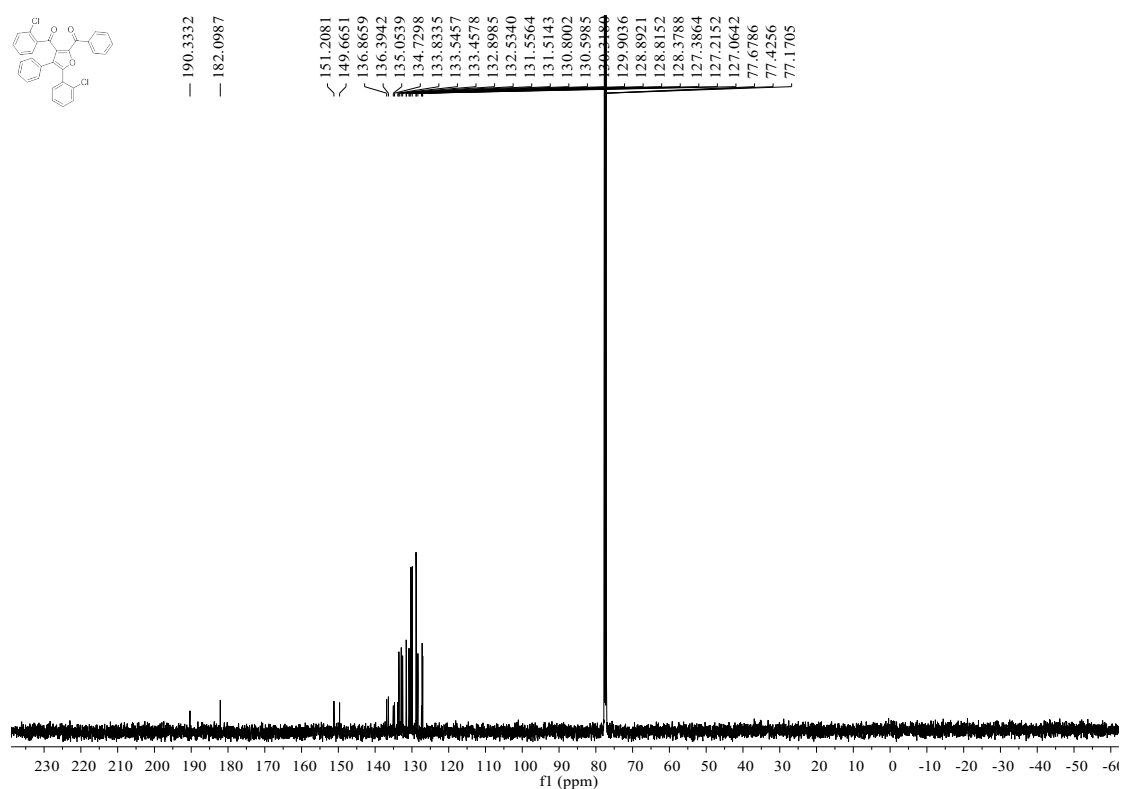
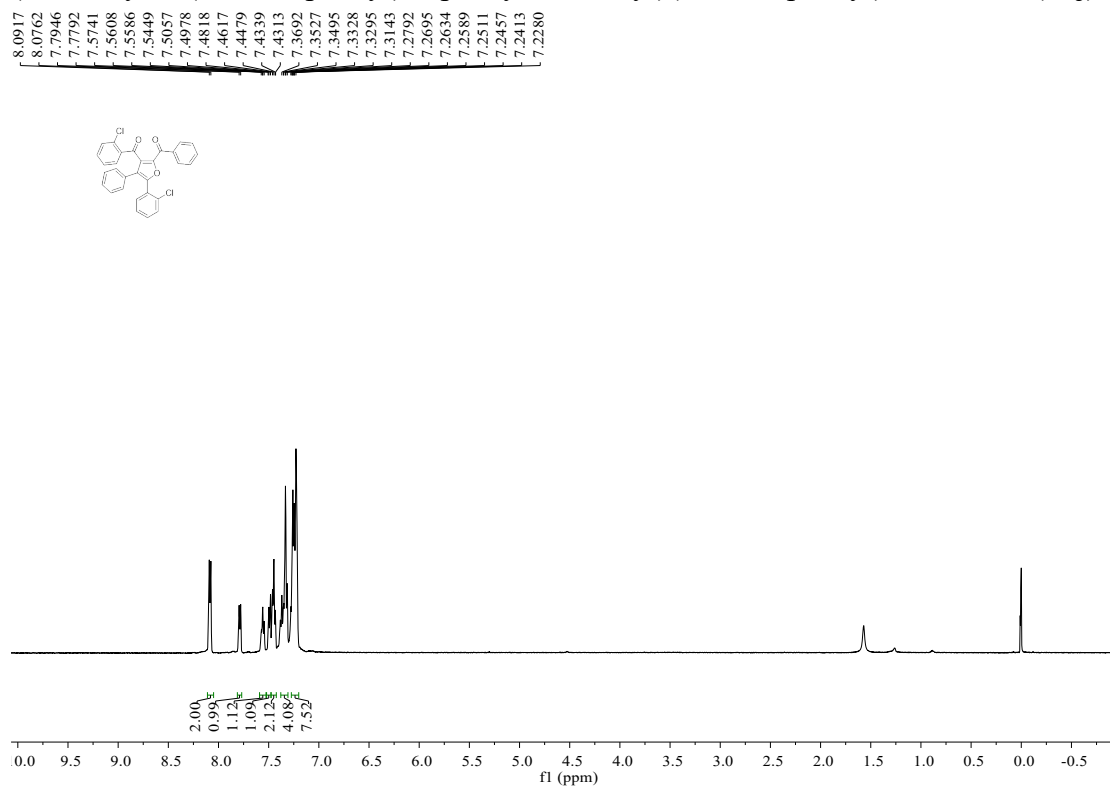
(2-benzoyl-5-(3-chlorophenyl)-4-phenylfuran-3-yl)(3-chlorophenyl)methanone (**3ah**)



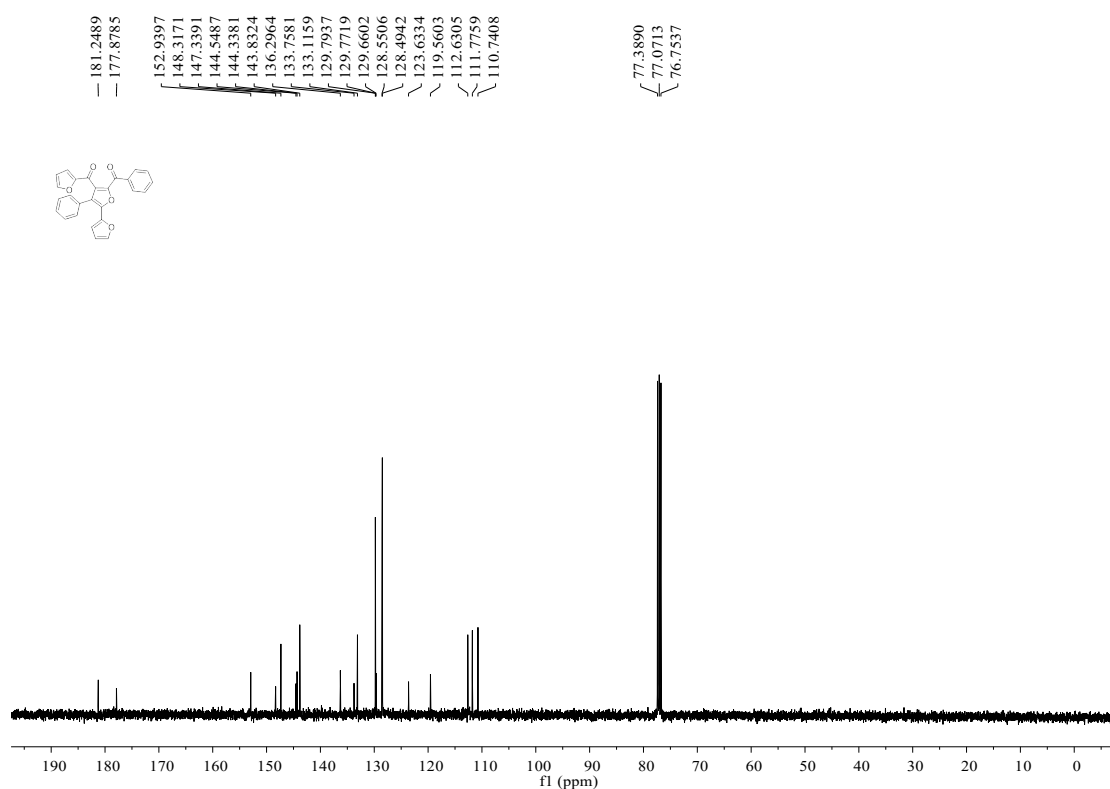
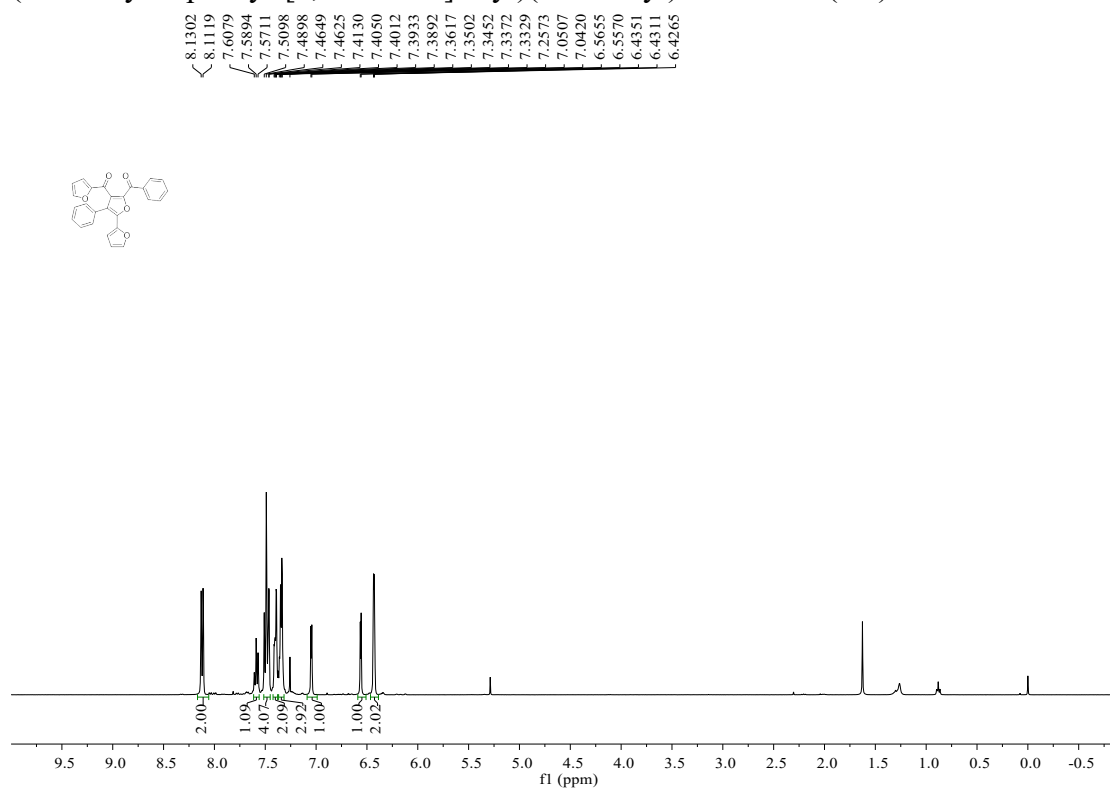
(2-benzoyl-5-(3-bromophenyl)-4-phenylfuran-3-yl)(3-bromophenyl)methanone (**3ai**)



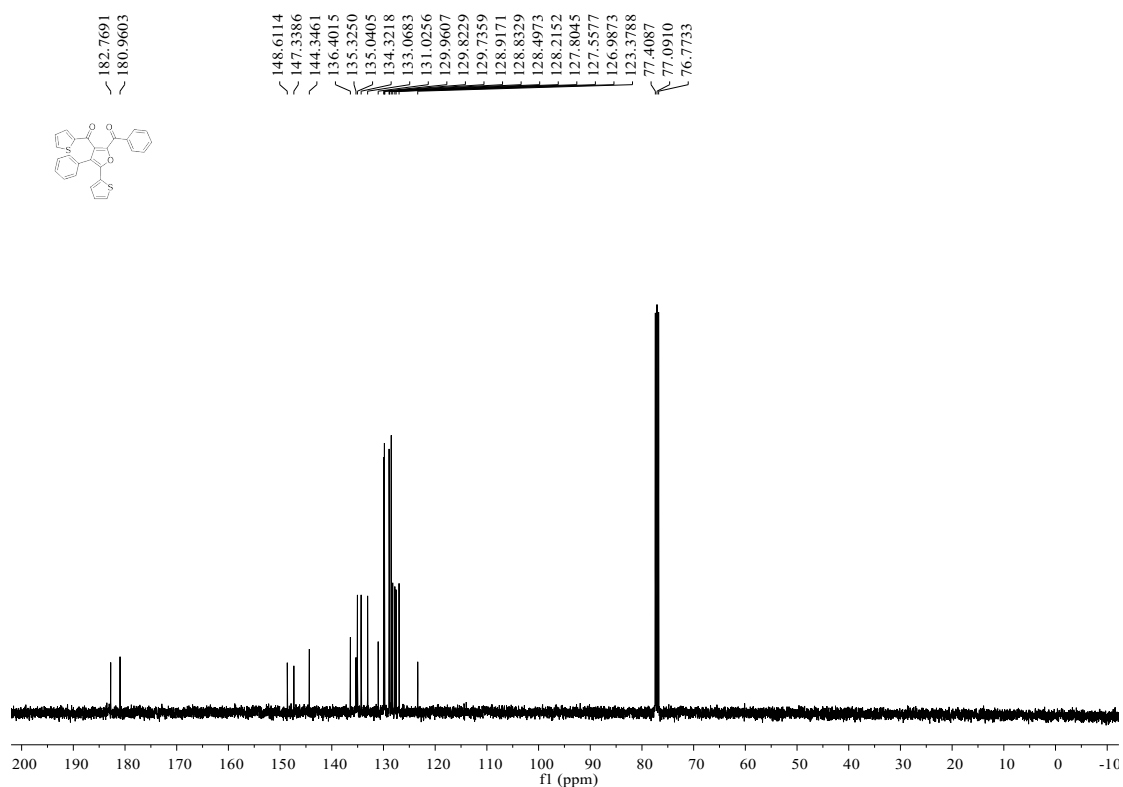
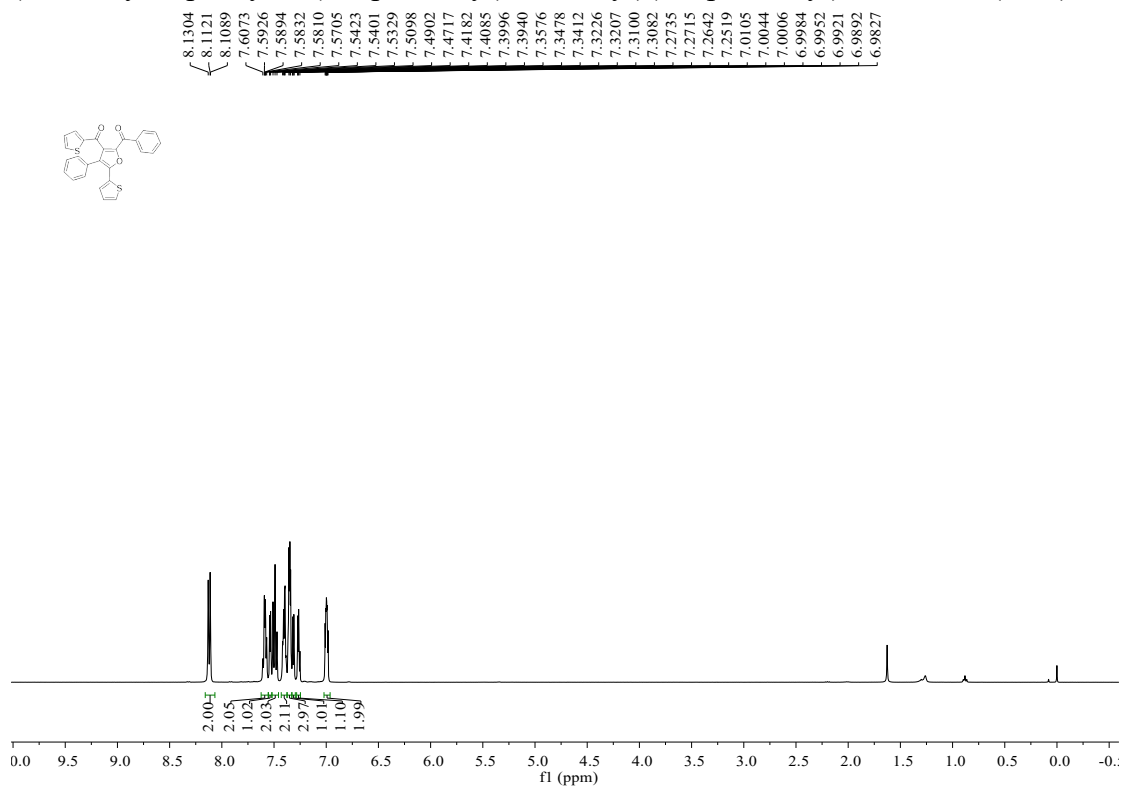
(2-benzoyl-5-(2-chlorophenyl)-4-phenylfuran-3-yl)(2-chlorophenyl)methanone (**3aj**)



(5-benzoyl-3-phenyl-[2,2'-bifuran]-4-yl)(furan-2-yl)methanone (**3al**)

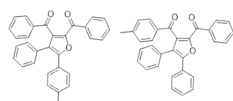
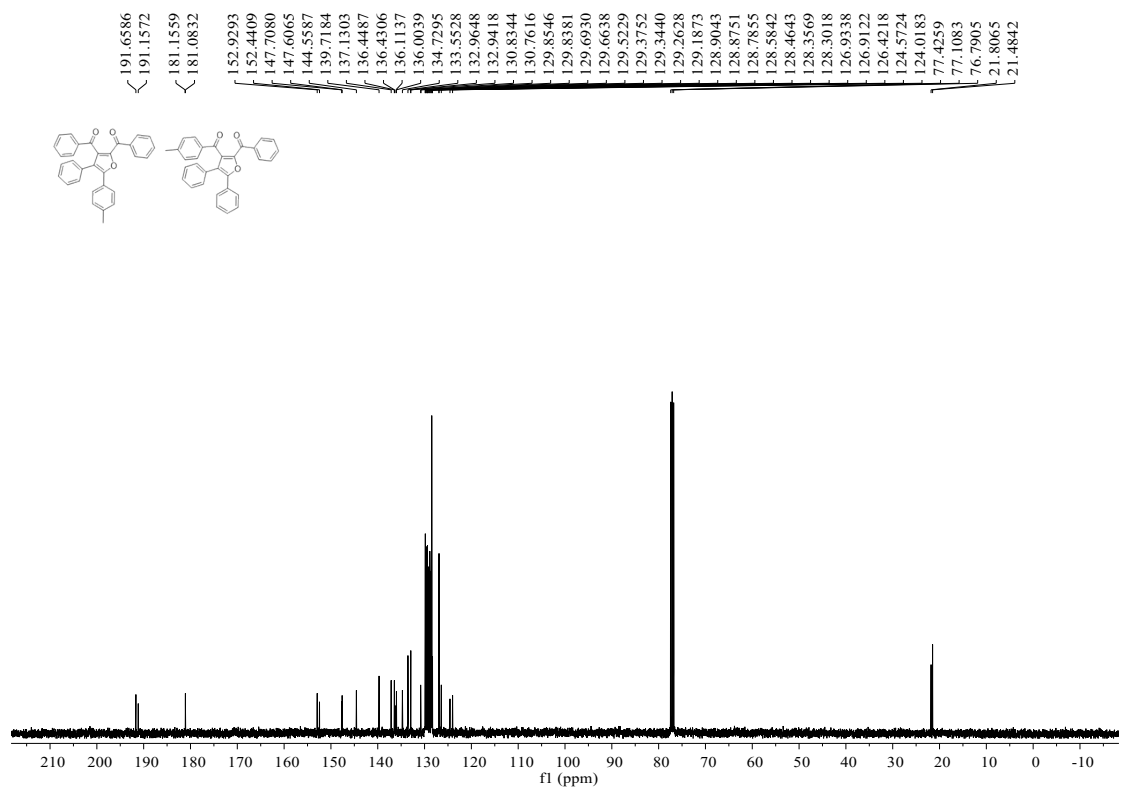
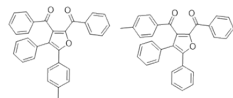
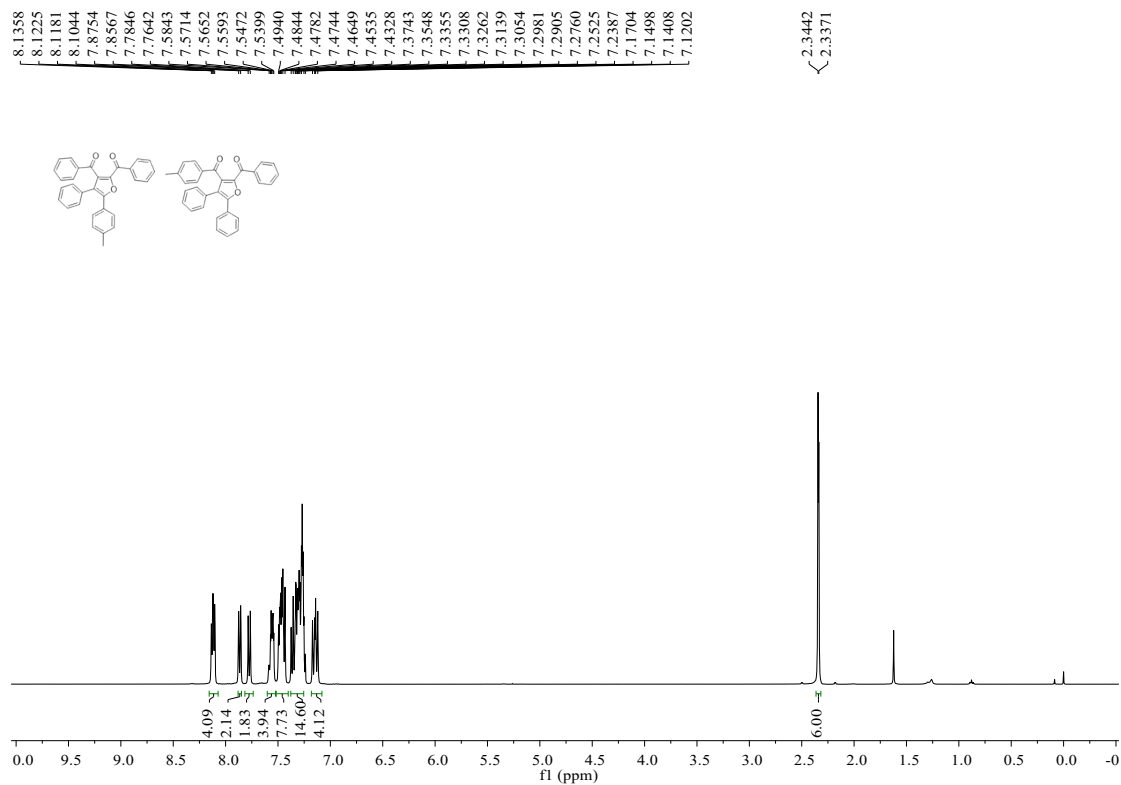


(2-benzoyl-4-phenyl-5-(thiophen-2-yl)furan-3-yl)(thiophen-2-yl)methanone (**3am**)

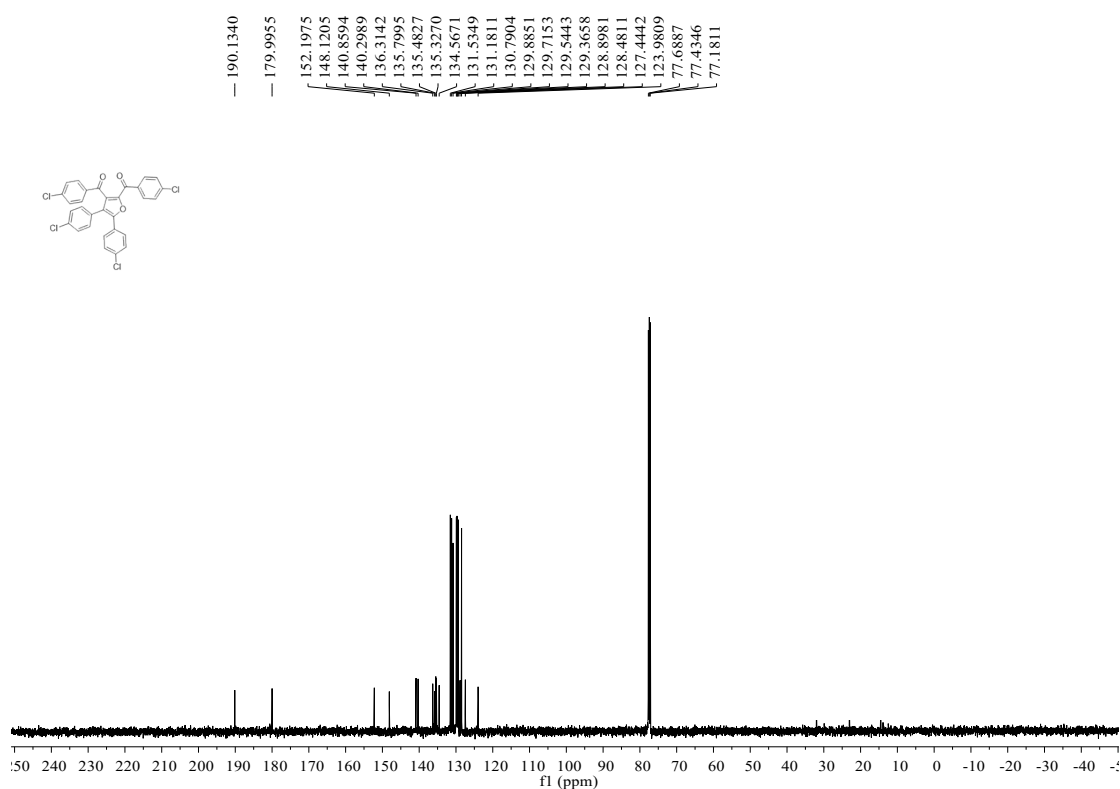
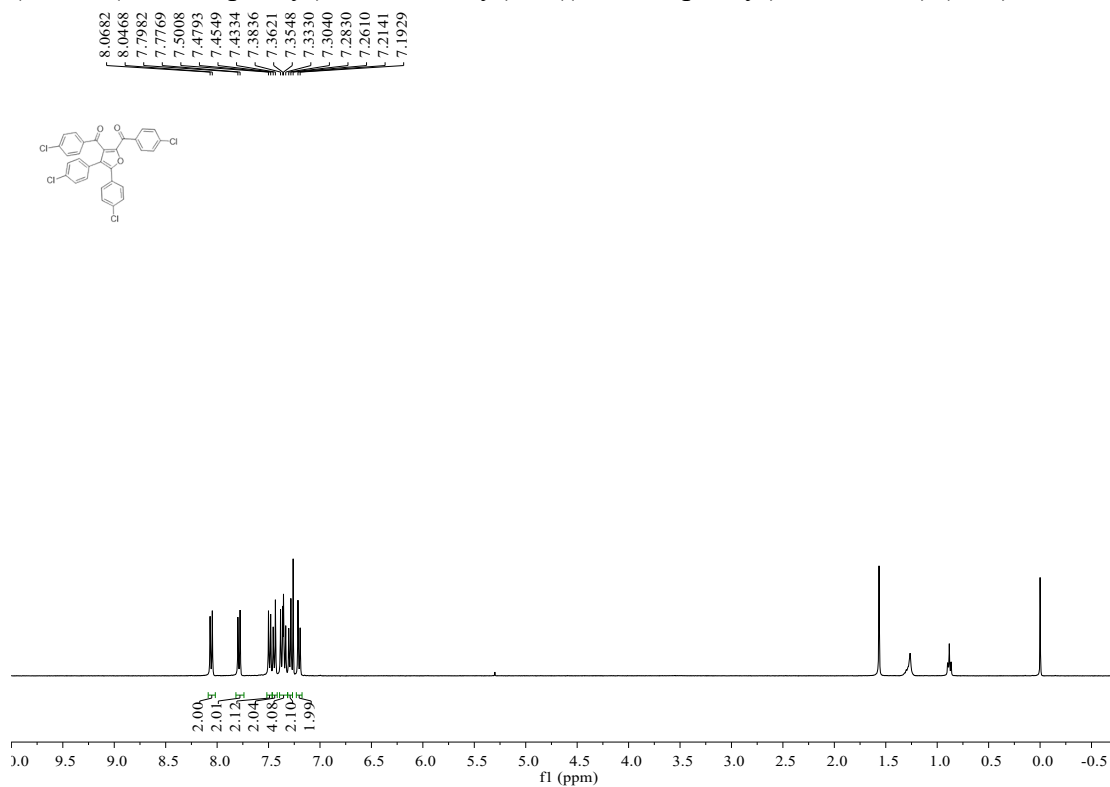


(4-phenyl-5-(p-tolyl)furan-2,3-diyl)bis(phenylmethanone) (**3an**)

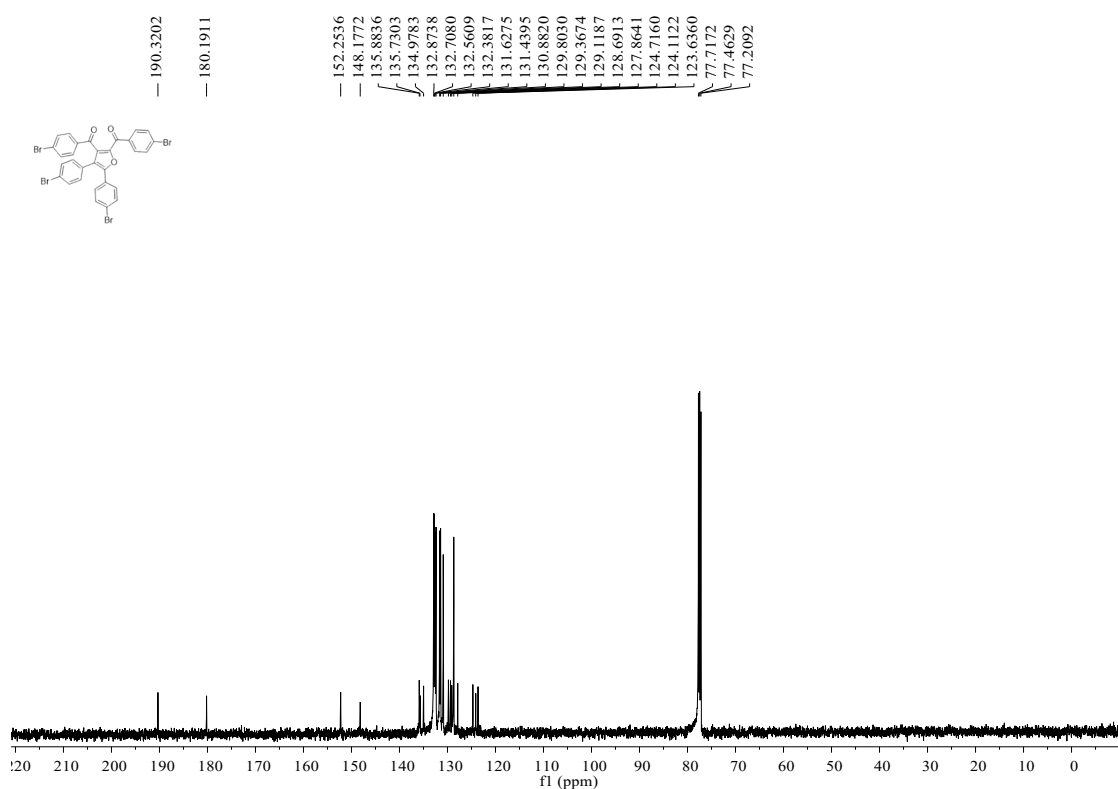
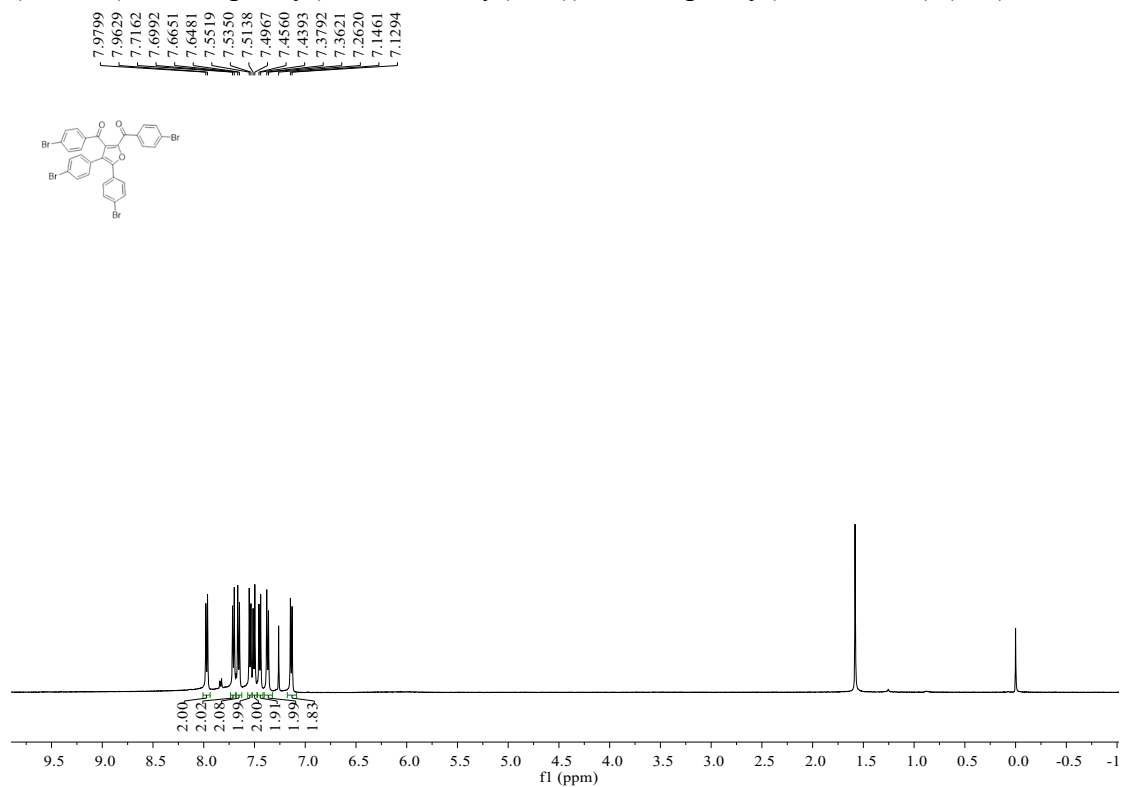
(2-benzoyl-4,5-diphenylfuran-3-yl)(p-tolyl)methanone (**3an'**)



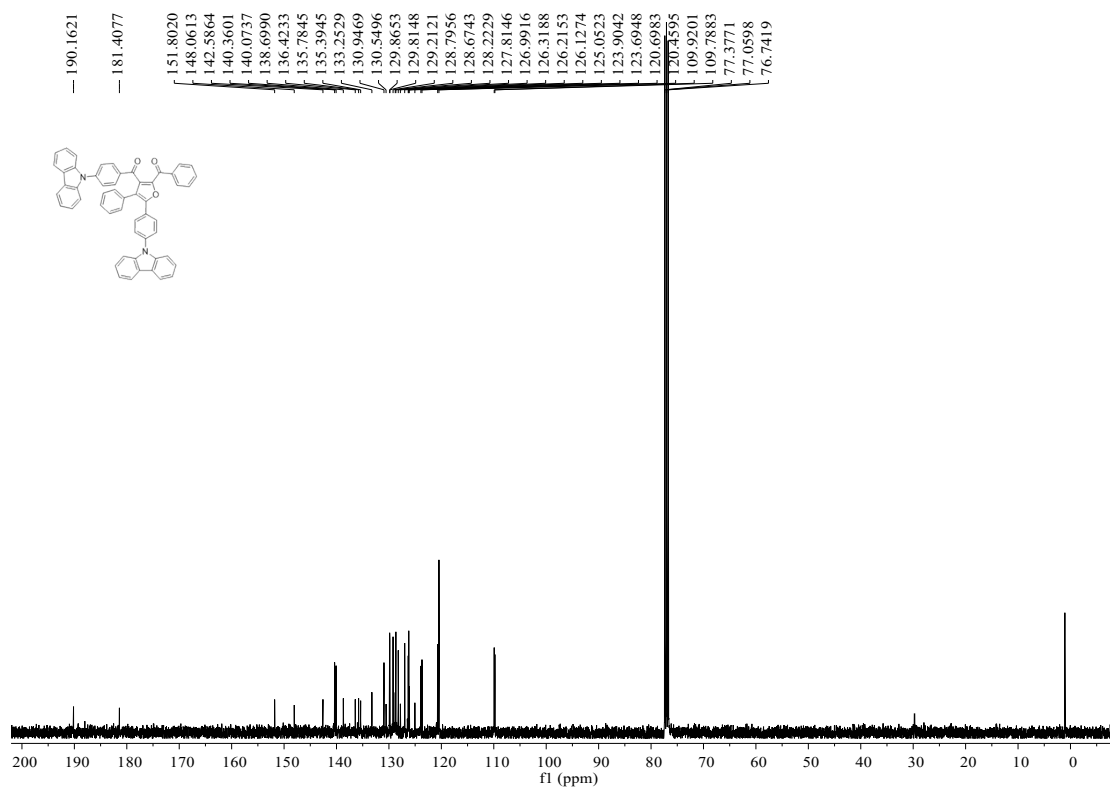
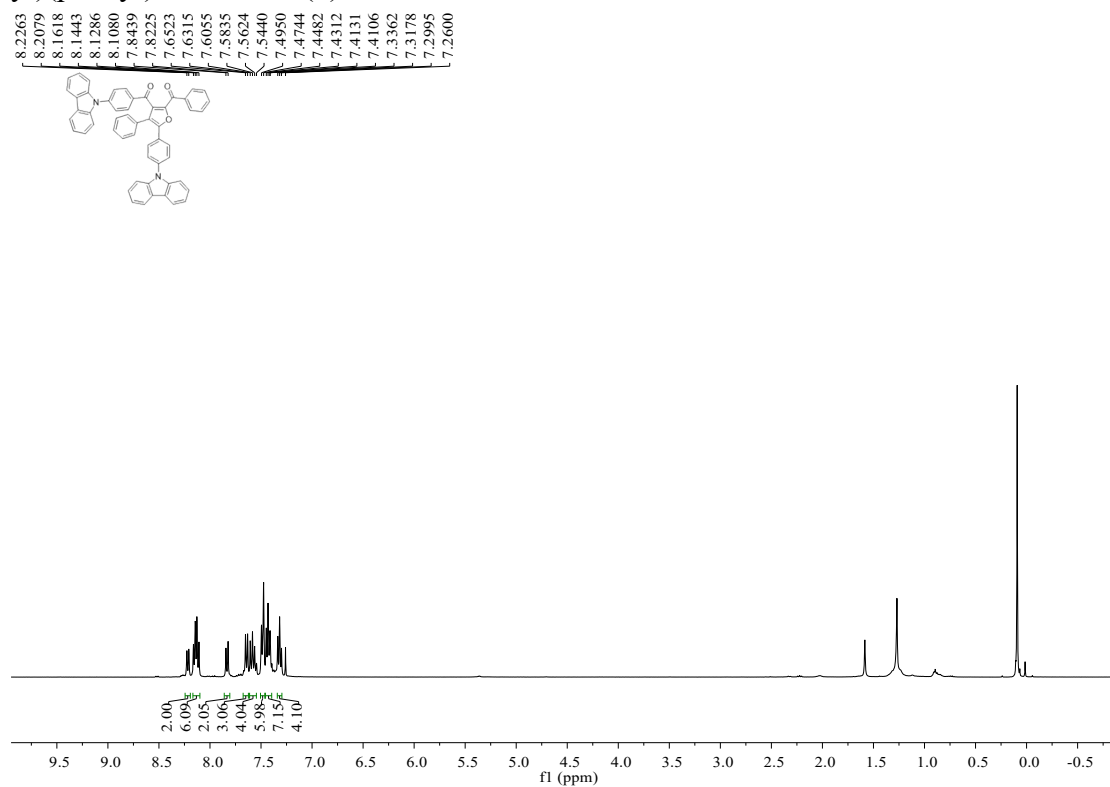
(4,5-bis(4-chlorophenyl)furan-2,3-diyl)bis((4-chlorophenyl)methanone) (**3dd**)



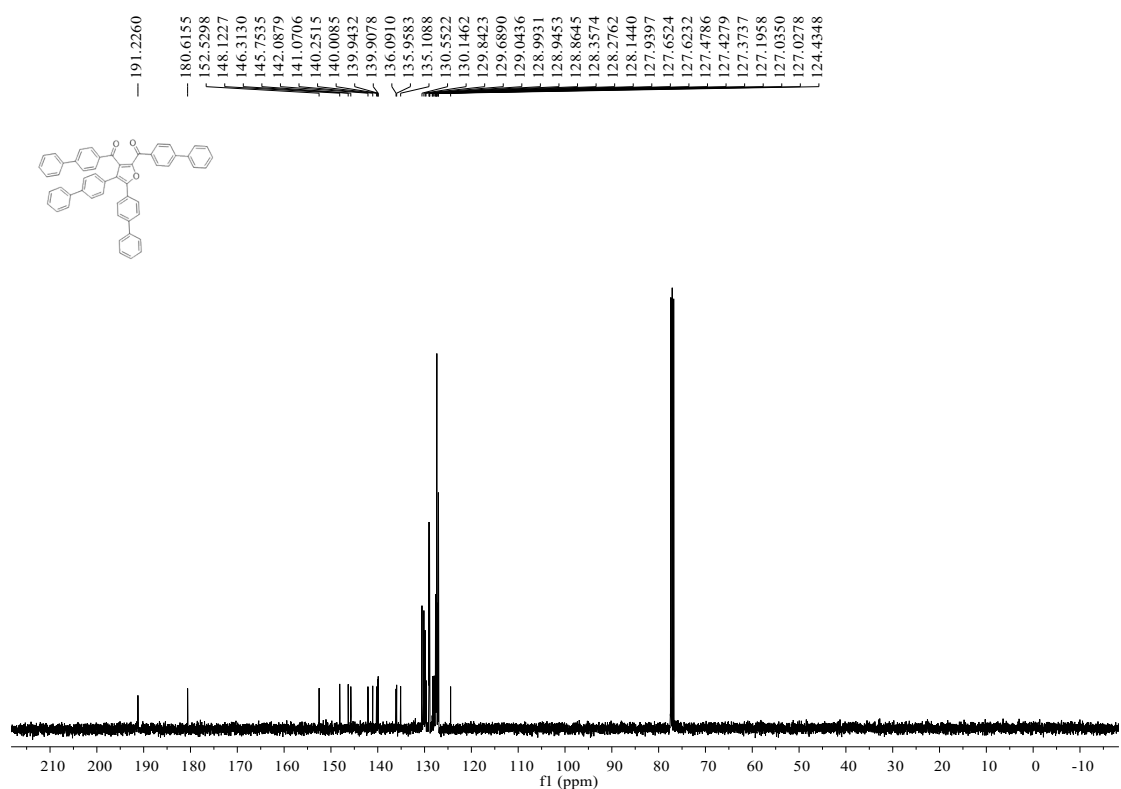
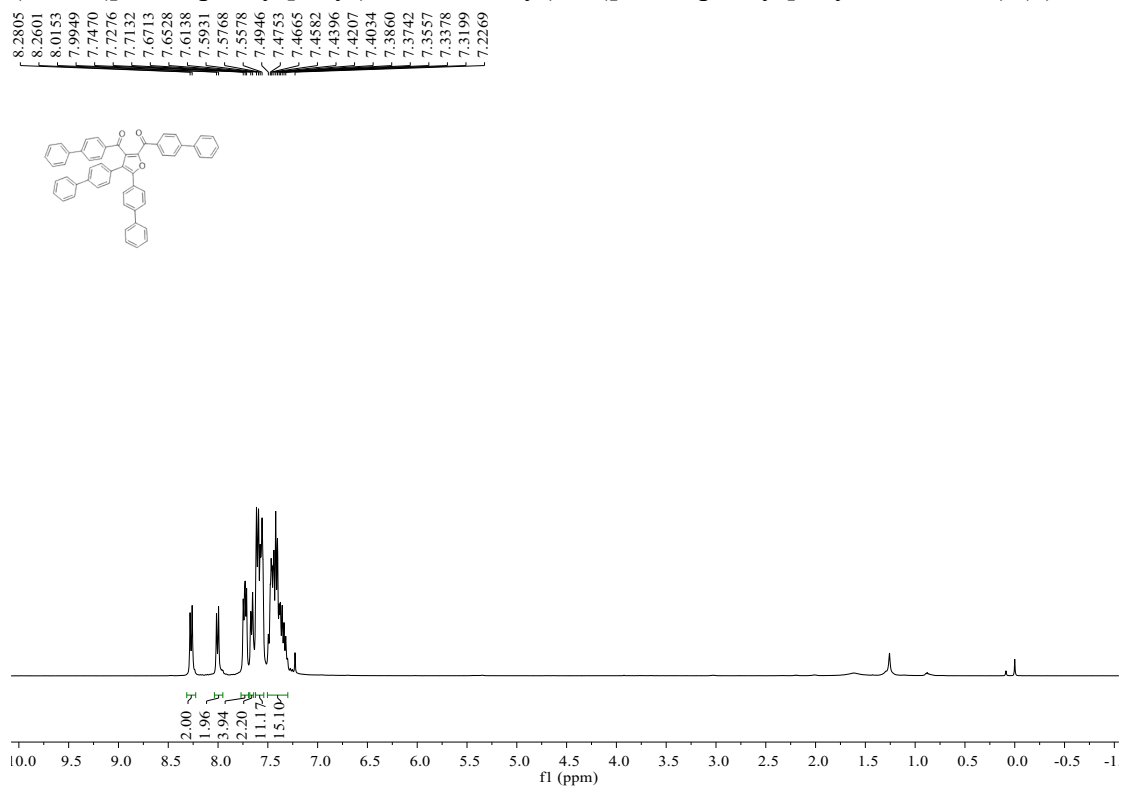
(4,5-bis(4-bromophenyl)furan-2,3-diyl)bis((4-bromophenyl)methanone) (**3ee**)



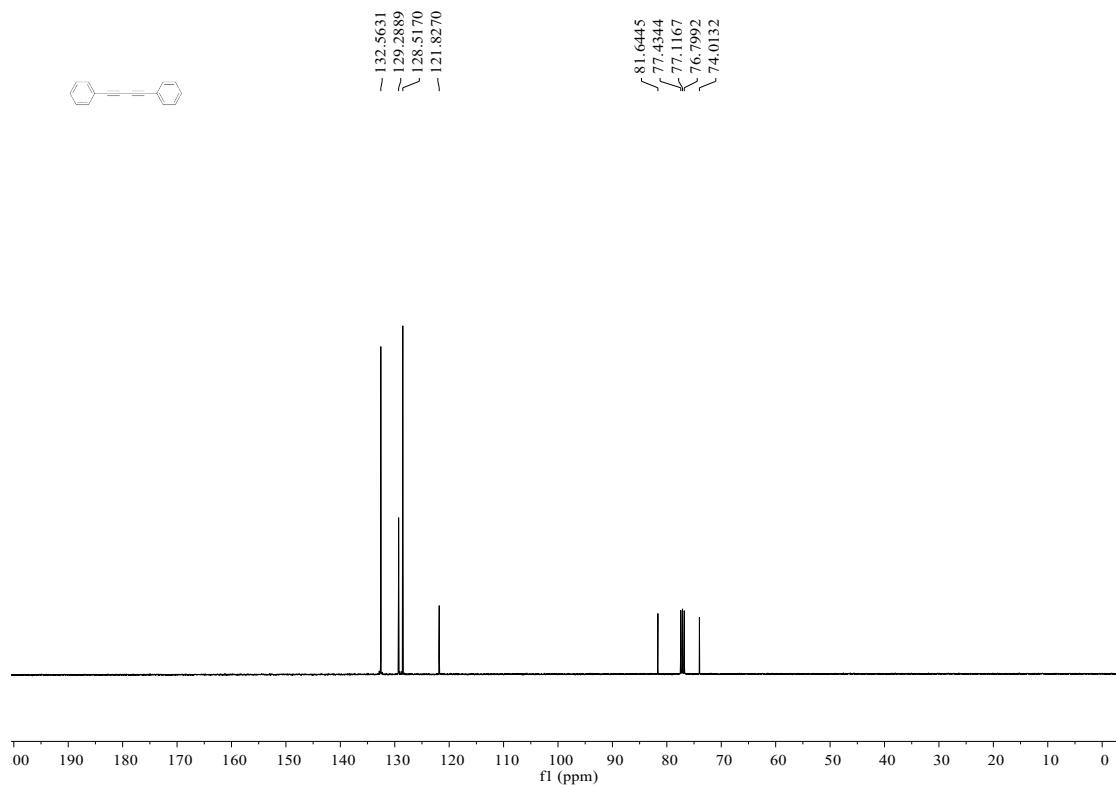
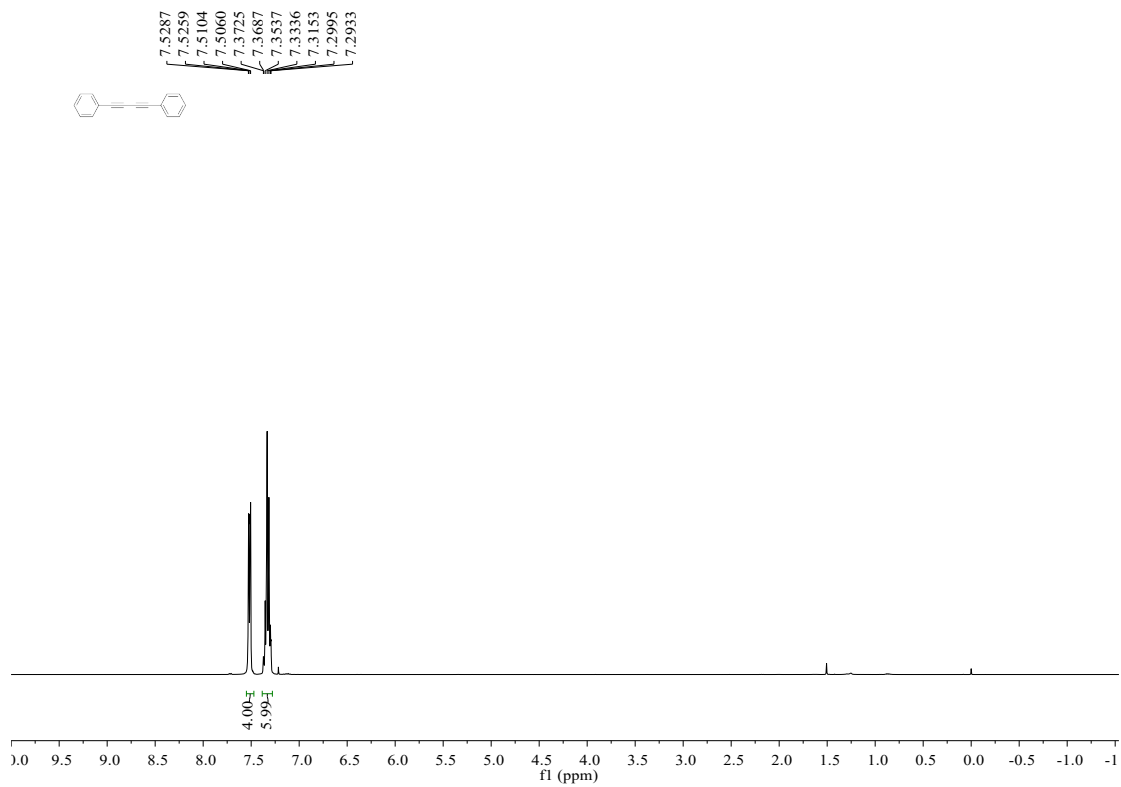
(3-(4-(9H-carbazol-9-yl)benzoyl)-5-(4-(9H-carbazol-9-yl)phenyl)-4-phenylfuran-2-yl)(phenyl)methanone (4)



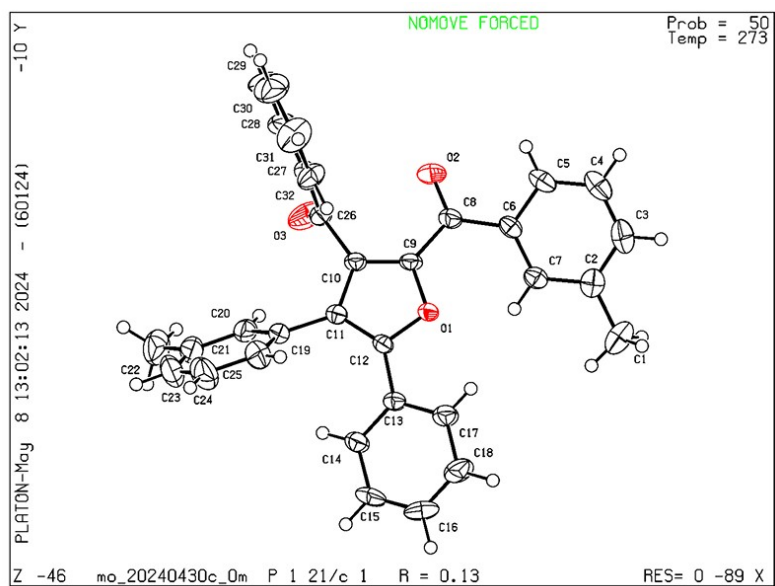
(4,5-di([1,1'-biphenyl]-4-yl)furan-2,3-diyl)bis([1,1'-biphenyl]-4-ylmethanone) (5)



1,4-diphenylbuta-1,3-diyne (A)



X-ray crystallographic data of **3ga** (CCDC 2386338)



ORTEP drawing of **3ga** showing thermal ellipsoid at the 50% probability level

Bond precision:	C-C = 0.0054 Å	Wavelength=0.71073	
Cell:	a=12.436 (17)	b=7.306 (8)	c=26.63 (4)
	alpha=90	beta=94.18 (5)	gamma=90
Temperature:	273 K		
	Calculated	Reported	
Volume	2413 (6)	2414 (5)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C32 H24 O3 [+ solvent]	C32 H24 O3, 0.05[C6H14]	
Sum formula	C32 H24 O3 [+ solvent]	C32 H24 O3	
Mr	456.51	456.51	
Dx, g cm ⁻³	1.257	1.256	
Z	4	4	
Mu (mm ⁻¹)	0.080	0.080	
F000	960.0	960.0	
F000'	960.44		
h, k, lmax	16, 9, 34	16, 9, 34	
Nref	5669	5645	
Tmin, Tmax	0.986, 0.988		
Tmin'	0.986		

Correction method= Not given

Data completeness= 0.996

Theta (max)= 27.726

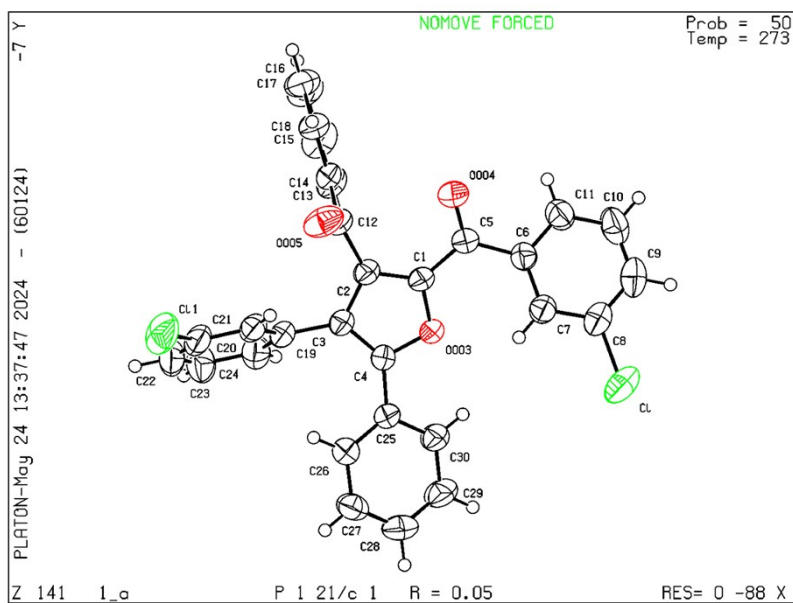
R(reflections)= 0.1266 (5254)

wR2 (reflections)=
0.2999 (5645)

S = 1.277

Npar= 318

X-ray crystallographic data of **3ia** (2386337)



ORTEP drawing of **3ia** showing thermal ellipsoid at the 50% probability level

Bond precision:	C-C = 0.0024 Å	Wavelength=0.71073
Cell:	a=12.5894 (8) alpha=90	b=7.3292 (4) beta=95.011 (2)
Temperature:	273 K	
	Calculated	Reported
Volume	2443.9 (3)	2443.9 (3)
Space group	P 21/c	P 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C30 H18 Cl2 O3	C30 H18 Cl2 O3
Sum formula	C30 H18 Cl2 O3	C30 H18 Cl2 O3
Mr	497.34	497.34
Dx, g cm ⁻³	1.352	1.352
Z	4	4
Mu (mm ⁻¹)	0.296	0.296
F000	1024.0	1024.0
F000'	1025.61	
h, k, lmax	16, 9, 34	16, 9, 34
Nref	5625	5488
Tmin, Tmax	0.962, 0.971	0.696, 0.746
Tmin'	0.943	
Correction method= # Reported T Limits: Tmin=0.696 Tmax=0.746		
AbsCorr = MULTI-SCAN		
Data completeness=	0.976	Theta (max)= 27.508
R(reflections)=	0.0472 (4716)	wR2(reflections)=
S =	1.063	0.1295 (5488)
Npar=	316	

Crystallization: Crystals of compound **3ga** and **3ia** suitable for X-ray analysis were grown from the solvent of ethyl acetate/hexane by slow evaporation method.

X-Ray Data Collection and structure Refinement Details: Diffraction was performed on a Bruker SMART APEX II CCD area detector diffractometer using graphite-monochromated Mo $K\alpha$ radiation ($\lambda = 0.71073 \text{ \AA}$) at 293(2) K, φ and ω scan technique. An empirical absorption correction was applied using the SADABS program.¹ The structure was solved by direct methods, completed by subsequent difference Fourier syntheses, and refined anisotropically for all nonhydrogen atoms by full-matrix least-squares calculations based on F^2 using the SHELXTL program package.² The hydrogen atom coordinates were calculated with SHELXTL by using an appropriate riding model with varied thermal parameters. The residual electron densities of solvent were squeezed by using PLATON.³ All crystal structural pictures drawn by IUCr web.

References

- [1] G. M. Sheldrick, SADABS: Program for Empirical Absorption Correction of Area Detector Data; University of Göttingen: Germany, 1996.
- [2] G. M. Sheldrick, Acta Cryst., 2015, A71, 3-8.
- [3] A. L. Spek, Acta Cryst., 2015, C71, 9-18.