

# Efficient Ruthenium-Catalyzed Dehydrogenative Synthesis of 2,4,6-triaryl-1,3,5-triazines from Aryl Methanols and Amidines

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## Supplementary Information

### Table of contents

General information	2
Typical procedure for synthesis of 2,4,6-triphenyl-1,3,5-triazine (3a).	2
Analytical data of the obtained compounds	2-9
NMR spectra of the obtained compounds	10-21
Reference	21-22

## General information

All the obtained products were characterized by melting points (m.p), <sup>1</sup>H-NMR, infrared spectra (IR), and high resolution mass spectra (HRMS). The <sup>1</sup>H-NMR spectra of known compounds were found to be identical with ones reported in the literatures. Additionally, all the new compounds were further characterized by <sup>13</sup>C-NMR. Melting points were measured on an Electrothemal SGW-X4 microscopy digital melting point apparatus and are uncorrected; IR spectra were recorded on a FTLA2000 spectrometer; <sup>1</sup>H-NMR spectra were obtained on Bruker-400; High-resolution mass spectra (HRMS) were recorded on a JEOL JMS-600 spectrometer. Chemical shifts were reported in parts per million (ppm,  $\delta$ ) downfield from tetramethylsilane. Proton coupling patterns are described as singlet (s), doublet (d), triplet (t), multiplet (m); TLC was performed using commercially prepared 100-400 mesh silica gel plates (GF254), and visualization was effected at 254 nm; All the reagents were purchased from commercial sources (J&KChemic, TCI, Fluka, Acros, SCRC), and used without further purification.

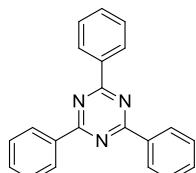
It is noteworthy that the solubility of all the obtained products is very poor in all the tested solvents (e.g. CHCl<sub>3</sub>, CH<sub>2</sub>Cl<sub>2</sub>, DMF, DMSO, acetone, hexane, toluene). Even the best solvent CHCl<sub>3</sub> can only slightly dissolve the compounds. Herein we selected CDCl<sub>3</sub> for NMR detection. And it is unavoidable to show the peaks of water (around 1.6 ppm), petroleum ether (around 1.2 and 0.8 ppm), and tetramethylsilane (0 ppm) in NMR spectrum owing to the low sample concentration.

## Typical procedure for synthesis of 2,4,6-triphenyl-1,3,5-triazine (3a).

To a solution of benzyl alcohol (0.162 g, 1.5 mmol) and benzamidine hydrochloride (0.156 g, 1 mmol) in DMSO (1mL) were added [RuCl<sub>2</sub>-(*p*-Cymene)]<sub>2</sub> (0.015 mmol, 4.5 mg) and Cs<sub>2</sub>CO<sub>3</sub> (0.325 g, 1 mmol). The reaction mixture was heated at 110 °C for the 16 h in a sealed tube without insert any gas protection. Afterwards, water (10 mL) and dichloromethane (20 mL) were added, the layers were separated, then the aqueous layer was extracted with dichloromethane (2×10 mL). The combined organic layers were dried with anhydrous Na<sub>2</sub>SO<sub>4</sub>, and concentrated under vacuum. The residue was directly purified by flash chromatography on silica gel eluting with petroleum ether (60-90 °C): ethyl acetate (15:1) to give 2,4,6-triphenyl-1,3,5-triazine 3a as a white solid (0.123 g, 85%).

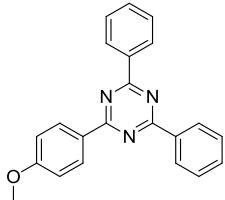
## Analytical data of the obtained compounds

### 2,4,6-triphenyl-1,3,5-triazine (3a)



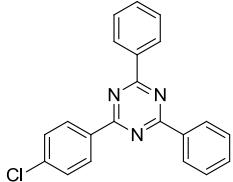
White solid, m.p: 233-234 °C (Lit<sup>1c</sup>, 231-233 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.78-8.67 (m, 6H), 7.58-7.48 (m, 9H); IR (KBr): 3062, 1586, 1527, 1362, 1253, 1022, 739, 677 cm<sup>-1</sup>; HRMS (ESI): Calcd. for C<sub>21</sub>H<sub>15</sub>N<sub>3</sub> [M+1]<sup>+</sup>: 309.1266; found: 309.1265.

### **2-(4-methoxyphenyl)-4,6-di-phenyl-1,3,5-triazine (3b)**



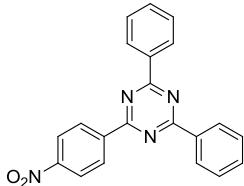
White solid, m.p: 158-160 °C (Lit<sup>1b</sup>, 157-158 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) : δ 8.73-8.64 (m, 6H), 7.56-7.46 (m, 6H), 7.03-6.97 (m, 2H), 3.85 (s, 3H); IR (KBr): 3045, 2922, 2850, 1583, 1524, 1371, 1262, 823, 761, 729 cm<sup>-1</sup>; HRMS (ESI): Calcd. for C<sub>21</sub>H<sub>15</sub>N<sub>3</sub> [M+1]<sup>+</sup>: 339.1372; found: 339.1369.

### **2-(4-chlorophenyl)-4,6-diphenyl-1,3,5-triazine (3c)**



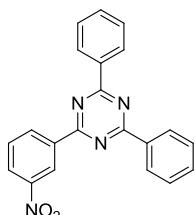
White solid, m.p: 199-200 °C (Lit<sup>2</sup>, 197-198 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.73-8.60 (m, 6H), 7.59-7.43 (m, 8H); IR (KBr): 3072, 1591, 1524, 1370, 819, 765, 726, 681 cm<sup>-1</sup>; HRMS (ESI): Calcd. for C<sub>21</sub>H<sub>14</sub>ClN<sub>3</sub> [M+1]<sup>+</sup>: 343.0876; found: 343.0871.

### **2-(4-nitrophenyl)-4,6-diphenyl-1,3,5-triazine (3d)**



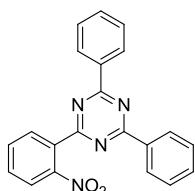
Yellow solid, m.p: 216-218 °C (Lit<sup>1b</sup>, 217-218 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.84 (d, J = 8.7 Hz, 2H), 8.68 (d, J = 7.1 Hz, 4H), 8.31 (d, J = 8.8 Hz, 2H), 7.60-7.46 (m, 6H); IR (KBr): 3045, 1589, 1530, 1340, 832, 748, 683 cm<sup>-1</sup>; HRMS (ESI): Calcd. for C<sub>21</sub>H<sub>14</sub>N<sub>4</sub>O<sub>2</sub> [M+1]<sup>+</sup>: 354.1117; found: 354.1117.

### **2-(3-nitrophenyl)-4,6-diphenyl-1,3,5-triazine (3e)**



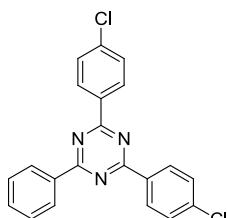
Light yellow solid, m.p: 196-199 °C (Lit<sup>3</sup>, 203-204 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 9.53 (d, *J* = 1.2 Hz, 1H), 9.07 (dd, *J* = 7.8, 1.1 Hz, 1H), 8.75 (dd, *J* = 5.3, 3.0 Hz, 4H), 8.47-8.39 (m, 1H), 7.74 (t, *J* = 8.0 Hz, 1H), 7.66-7.53 (m, 6H); IR (KBr): 3040, 1586, 1524, 1371, 1352, 776, 736, 692 cm<sup>-1</sup>; HRMS (ESI): Calcd. for C<sub>21</sub>H<sub>14</sub>N<sub>4</sub>O<sub>2</sub> [M+1]<sup>+</sup>: 354.1117; found: 354.1103.

### **2-(2-nitrophenyl)-4,6-diphenyl-1,3,5-triazine (3f)**



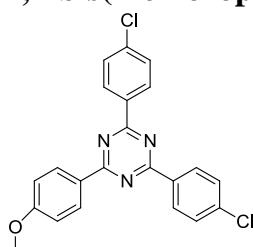
Yellow solid, m.p: 143-146 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) : δ 8.73-8.60 (m, 4H), 8.41 (dd, *J* = 7.6, 1.3 Hz, 1H), 7.79 (dt, *J* = 11.5, 5.7 Hz, 1H), 7.77-7.63 (m, 2H), 7.62-7.50 (m, 6H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 171.90, 170.29, 151.01, 135.52, 132.94, 131.89, 131.71, 130.81, 129.16, 128.78, 127.27, 123.86; IR (KBr): 3054, 1583, 1521, 1446, 1371, 832, 770, 739, 686 cm<sup>-1</sup>; HRMS (ESI): Calcd. for C<sub>21</sub>H<sub>14</sub>N<sub>4</sub>O<sub>2</sub> [M+1]<sup>+</sup>: 354.1117; found: 354.1109.

### **2,4-bis(4-chlorophenyl)-6-phenyl-1,3,5-triazine (3g)**



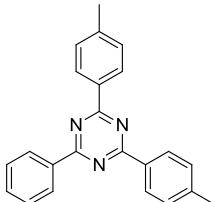
White solid, m.p: 240-243 °C (Lit<sup>1a</sup>, 240-241 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.80-8.59 (m, 6H), 7.69-7.47 (m, 7H); IR (KBr): 3062, 1583, 1514, 1367, 1089, 1014, 808, 752, 777, 632 cm<sup>-1</sup>; HRMS (ESI): Calcd. for C<sub>21</sub>H<sub>13</sub>Cl<sub>2</sub>N<sub>3</sub> [M+1]<sup>+</sup>: 377.0486; found: 377.0482.

### **2,4-bis(4-chlorophenyl)-6-(4-methoxyphenyl)-1,3,5-triazine (3h)**



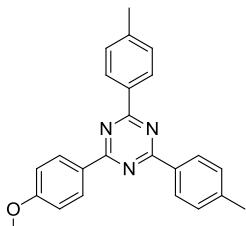
White solid, m.p: 266-269 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) :  $\delta$  8.60 (d,  $J = 8.7$  Hz, 6H), 7.49 (d,  $J = 8.5$  Hz, 4H), 7.03 (s, 2H), 3.91 (s, 3H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  171.24, 170.45, 163.60, 138.74, 134.70, 130.98, 130.19, 128.85, 128.34, 113.99, 55.47; IR (KBr): 3034, 2917, 2849, 1585, 1523, 1403, 1370, 1254, 1087, 845, 805  $\text{cm}^{-1}$ ; HRMS (ESI): Calcd. for  $\text{C}_{22}\text{H}_{15}\text{Cl}_2\text{N}_3\text{O}$  [ $\text{M}+1$ ] $^+$ : 407.0592; found: 407.0587.

### **2-phenyl-4,6-di-p-tolyl-1,3,5-triazine (3i)**



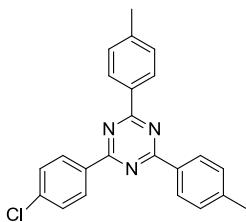
White solid, m.p: 213-216 °C (Lit<sup>1a</sup>, 215-216 °C);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.82-8.71 (m, 2H), 8.65 (d,  $J = 8.2$  Hz, 4H), 7.66-7.51 (m, 3H), 7.36 (d,  $J = 8.2$  Hz, 4H), 2.47 (s, 6H); IR (KBr): 3067, 2917, 2849, 1612, 1586, 1369, 1178, 1021, 814, 775, 695  $\text{cm}^{-1}$ ; HRMS (ESI): Calcd. for  $\text{C}_{23}\text{H}_{19}\text{N}_3$  [ $\text{M}+1$ ] $^+$ : 337.1579; found: 337.1578.

### **2-(4-methoxyphenyl)-4,6-di-p-tolyl-1,3,5-triazine (3j)**



White solid, m.p: 196-199 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.74-8.67 (m, 2H), 8.62 (d,  $J = 8.2$  Hz, 4H), 7.34 (d,  $J = 8.0$  Hz, 4H), 7.05 (dd,  $J = 9.5, 6.8$  Hz, 2H), 3.90 (s, 3H), 2.46 (s, 6H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  171.27, 170.97, 163.19, 142.78, 133.86, 130.80, 129.31, 129.05, 128.89, 113.89, 55.44, 21.72; IR (KBr): 3078, 2917, 2849, 1609, 1584, 1370, 1253, 1170, 1033, 854, 802, 769  $\text{cm}^{-1}$ ; HRMS (ESI): Calcd. for  $\text{C}_{24}\text{H}_{21}\text{N}_3\text{O}$  [ $\text{M}+1$ ] $^+$ : 367.1685; found: 367.1689.

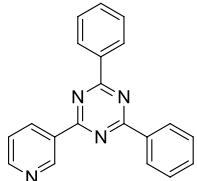
### **2-(4-chlorophenyl)-4,6-di-p-tolyl-1,3,5-triazine (3k)**



White solid, m.p: 282-285 °C (Lit<sup>3</sup>, 279-280 °C);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.71-8.66 (m, 2H), 8.62 (d,  $J = 8.2$  Hz, 4H), 7.58-7.46 (m, 2H), 7.35 (d,  $J = 8.0$  Hz, 4H).

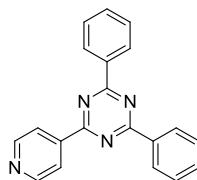
Hz, 4H), 2.47 (s, 6H); IR (KBr): 3056, 2918, 2849, 1609, 1585, 1368, 1177, 1088, 848, 800 cm<sup>-1</sup>; HRMS (ESI): Calcd. for C<sub>23</sub>H<sub>18</sub>ClN<sub>3</sub> [M+1]<sup>+</sup>: 371.1189; found: 371.1186.

### **2,4-di-phenyl-6-(pyridin-3-yl)-1,3,5-triazine (3n)**



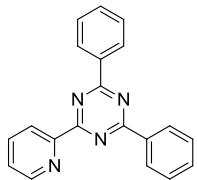
White solid, m.p: 254-256 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 9.92 (d, *J* = 1.3 Hz, 1H), 8.97 (dd, *J* = 6.2, 1.7 Hz, 1H), 8.82 (dt, *J* = 12.4, 6.2 Hz, 1H), 8.75 (d, *J* = 6.9 Hz, 4H), 7.69-7.53 (m, 6H), 7.50 (dd, *J* = 7.9, 4.9 Hz, 1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 171.83, 170.26, 152.94, 150.62, 136.19, 135.82, 132.82, 131.88, 129.03, 128.73, 123.46; IR (KBr): 3040, 1580, 1530, 1452, 1368, 1032, 764, 692 cm<sup>-1</sup>; HRMS (ESI): Calcd. for C<sub>20</sub>H<sub>14</sub>N<sub>4</sub> [M+1]<sup>+</sup>: 310.1218; found: 310.1214.

### **2,4-di-phenyl-6-(pyridin-4-yl)-1,3,5-triazine (3o)**



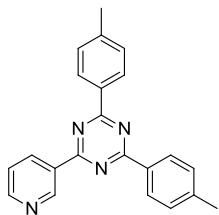
White solid, m.p: 258-260 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.88 (d, *J* = 5.9 Hz, 2H), 8.82-8.70 (m, 4H), 8.55 (d, *J* = 5.9 Hz, 2H), 7.67-7.54 (m, 6H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 171.12, 169.14, 149.67, 142.62, 134.64, 131.92, 128.04, 127.74, 121.28; IR (KBr): 3056, 1520, 1370, 1261, 1101, 827, 803, 759, 688 cm<sup>-1</sup>; HRMS (ESI): Calcd. for C<sub>20</sub>H<sub>14</sub>N<sub>4</sub> [M+1]<sup>+</sup>: 310.1218; found: 310.1219.

### **2,4-di-phenyl-6-(pyridin-2-yl)-1,3,5-triazine (3p)**



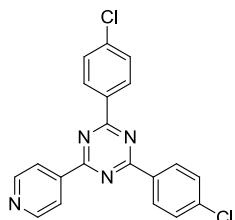
Yellow solid, m.p: 230-231 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.97 (t, *J* = 8.2 Hz, 1H), 8.88-8.73 (m, 5H), 7.95 (td, *J* = 7.8, 1.6 Hz, 1H), 7.66- 7.54 (m, 6H), 7.54-7.49 (m, 1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 172.39, 171.09, 153.97, 150.46, 137.02, 135.83, 132.78, 129.25, 128.67, 126.11, 124.81; IR (KBr): 3068, 1369, 1254, 1067, 749, 688, 655 cm<sup>-1</sup>; HRMS (ESI): Calcd. for C<sub>20</sub>H<sub>14</sub>N<sub>4</sub> [M+1]<sup>+</sup>: 310.1218; found: 310.1220.

**2-(pyridin-3-yl)-4,6-di-p-tolyl-1,3,5-triazine (3q)**



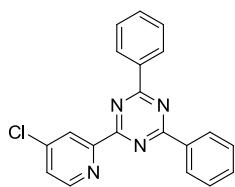
White solid, m.p: 198-200 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  9.92 (s, 1H), 9.12-8.54 (m, 6H), 7.58-7.26 (m, 5H), 2.49 (s, 6H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  171.64, 170.29, 152.90, 152.70, 150.54, 143.37, 136.16, 133.22, 129.44, 128.99, 123.41, 21.76; IR (KBr): 3064, 2922, 2852, 1584, 1522, 1367, 1175, 1021, 848, 796, 701  $\text{cm}^{-1}$ ; HRMS (ESI): Calcd. for  $\text{C}_{22}\text{H}_{18}\text{N}_4$  [ $\text{M}+1$ ] $^+$ : 338.1531; found: 338.1530.

**2,4-bis(4-chlorophenyl)-6-(pyridin-4-yl)-1,3,5-triazine (3r)**



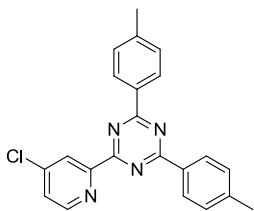
White solid, m.p: 268-270 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.89 (d,  $J = 5.5$  Hz, 2H), 8.66 (t,  $J = 8.9$  Hz, 4H), 8.51 (d,  $J = 5.7$  Hz, 2H), 7.54 (t,  $J = 8.4$  Hz, 4H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  171.34, 170.00, 150.76, 143.11, 139.53, 133.93, 130.37, 129.13, 122.26; IR (KBr): 3042, 1582, 1517, 1403, 1370, 1090, 1012, 846, 802, 654  $\text{cm}^{-1}$ ; HRMS (ESI): Calcd. for  $\text{C}_{20}\text{H}_{12}\text{Cl}_2\text{N}_4$  [ $\text{M}+1$ ] $^+$ : 378.0439; found: 378.0438.

**2-(4-chloropyridin-2-yl)-4,6-di-phenyl-1,3,5-triazine (3s)**



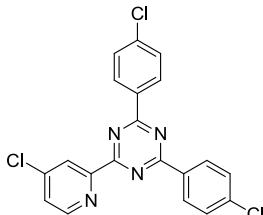
Light Yellow solid, m.p: 203-206 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.83 (d,  $J = 5.2$  Hz, 1H), 8.81-8.74 (m, 5H), 7.64 -7.54 (m, 6H), 7.52 (dd,  $J = 5.2, 2.0$  Hz, 1H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  172.52, 170.13, 155.51, 151.20, 145.35, 135.59, 132.94, 129.27, 128.72, 126.24, 125.11; IR (KBr): 3056, 1589, 1447, 1371, 1350, 1209, 1172, 834, 775, 739, 687  $\text{cm}^{-1}$ ; HRMS (ESI): Calcd. for  $\text{C}_{20}\text{H}_{13}\text{ClN}_4$  [ $\text{M}+1$ ] $^+$ : 344.0829; found: 344.0828.

**2-(4-chloropyridin-2-yl)-4,6-di-p-tolyl-1,3,5-triazine (3t)**



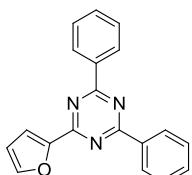
Yellow solid, m.p: 221-224 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.80-8.71 (m, 1H), 8.68 (s, 1H), 8.58 (d,  $J = 8.1$  Hz, 4H), 7.47-7.39 (m, 1H), 7.28 (d,  $J = 8.0$  Hz, 4H), 2.40 (d,  $J = 7.4$  Hz, 6H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  172.34, 169.81, 155.72, 151.14, 145.30, 143.57, 132.98, 129.46, 129.26, 126.11, 125.05, 21.78; IR (KBr): 3072, 2923, 2852, 1609, 1571, 1366, 1344, 1171, 1018, 808, 732  $\text{cm}^{-1}$ ; HRMS (ESI): Calcd. for  $\text{C}_{22}\text{H}_{17}\text{ClN}_4$   $[\text{M}+1]^+$ : 372.1142; found: 372.1141.

**2-(4-chloropyridin-2-yl)-4,6-bis(4-chlorophenyl)-1,3,5-triazine (3u)**



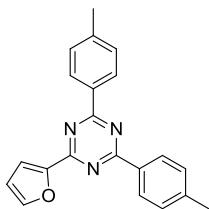
White solid, m.p: 246-247 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.82 (d,  $J = 5.2$  Hz, 1H), 8.73-8.61 (m, 5H), 7.52 (d,  $J = 8.4$  Hz, 5H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  171.62, 170.20, 155.04, 151.24, 145.43, 139.52, 133.81, 130.56, 129.06, 126.46, 125.13; IR (KBr): 3034, 1583, 1520, 1406, 1370, 1171, 1091, 1015, 845, 811, 751, 686  $\text{cm}^{-1}$ ; HRMS (ESI): Calcd. for  $\text{C}_{20}\text{H}_{11}\text{Cl}_3\text{N}_4$   $[\text{M}+1]^+$ : 412.0049; found: 412.0046.

**2-(furan-2-yl)-4,6-di-phenyl-1,3,5-triazine (3v)**



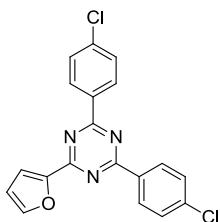
White solid, m.p: 195-197 °C(Lit<sup>3</sup>, 194-195 °C);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.72 (dd,  $J = 8.2, 1.4$  Hz, 4H), 7.79-7.75 (m, 1H), 7.70 (dd,  $J = 3.5, 0.7$  Hz, 1H), 7.64-7.52 (m, 6H), 6.67 (dd,  $J = 3.5, 1.7$  Hz, 1H); IR (KBr): 3134, 3115, 1589, 1519, 1355, 1168, 1049, 761, 676  $\text{cm}^{-1}$ ; HRMS (ESI): Calcd. for  $\text{C}_{19}\text{H}_{13}\text{N}_3\text{O}$   $[\text{M}+1]^+$ : 299.1059; found: 299.1058.

**2-(furan-2-yl)-4,6-di-p-tolyl-1,3,5-triazine (3w)**



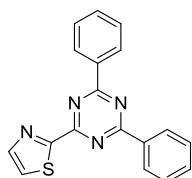
White solid, m.p: 139-142 °C (Lit<sup>3</sup>, 157-158 °C); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.60 (d, *J* = 8.2 Hz, 4H), 7.75 (d, *J* = 0.7 Hz, 1H), 7.68 (dd, *J* = 3.4, 0.6 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 4H), 6.65 (dd, *J* = 3.4, 1.7 Hz, 1H), 2.47 (s, 6H); IR (KBr): 3133, 2923, 1586, 1521, 1383, 1174, 1090, 1010, 845, 808, 760 cm<sup>-1</sup>; HRMS (ESI): Calcd. for C<sub>21</sub>H<sub>17</sub>N<sub>3</sub>O [M+1]<sup>+</sup>: 327.1372; found: 327.1373.

### **2,4-bis(4-chlorophenyl)-6-(furan-2-yl)-1,3,5-triazine (3x)**



Light yellow solid, m.p: 177-180 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.65- 8.54 (m, 4H), 7.75 (dd, *J* = 1.6, 0.8 Hz, 1H), 7.65 (dd, *J* = 3.5, 0.7 Hz, 1H), 7.54-7.45 (m, 4H), 6.65 (dd, *J* = 3.5, 1.7 Hz, 1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 170.79, 164.27, 150.96, 146.85, 139.07, 134.18, 130.27, 128.93, 117.47, 112.69; IR (KBr): 3133, 3113, 1586, 1521, 1419, 1353, 1174, 1090, 1010, 845, 808, 760 cm<sup>-1</sup>; HRMS (ESI): Calcd. for C<sub>19</sub>H<sub>11</sub>Cl<sub>2</sub>N<sub>3</sub>O [M+1]<sup>+</sup>: 367.0279; found: 367.0262.

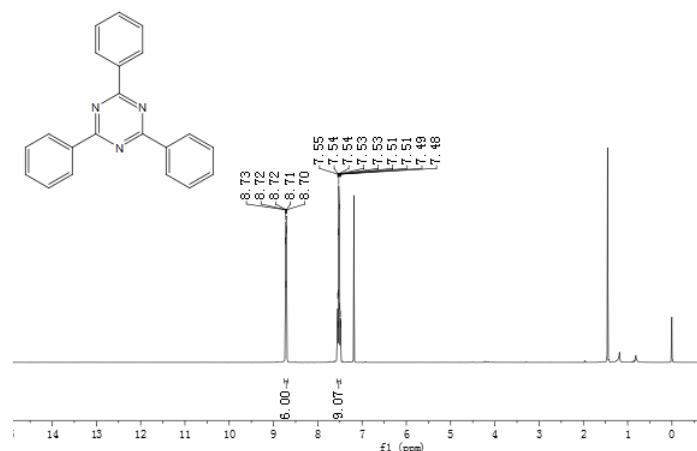
### **2,4-diphenyl-6-(thiazol-2-yl)-1,3,5-triazine (3y)**



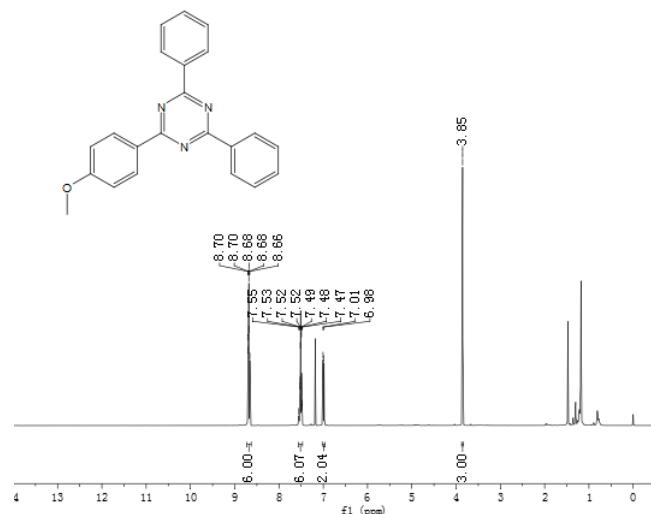
Yellow solid, m.p: 223-224 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.80-8.70 (m, 4H), 8.19 (d, *J* = 3.1 Hz, 1H), 7.67 (d, *J* = 3.1 Hz, 1H), 7.65-7.53 (m, 6H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 172.42, 166.51, 166.17, 145.91, 135.26, 133.06, 129.28, 128.71, 124.55; IR (KBr): 3046, 1525, 1384, 1371, 1119, 832, 765, 704, 683 cm<sup>-1</sup>; HRMS (ESI): Calcd. for C<sub>18</sub>H<sub>12</sub>N<sub>4</sub>S [M+1]<sup>+</sup>: 316.0783; found: 316.0773.

**NMR spectra of the obtained compounds**

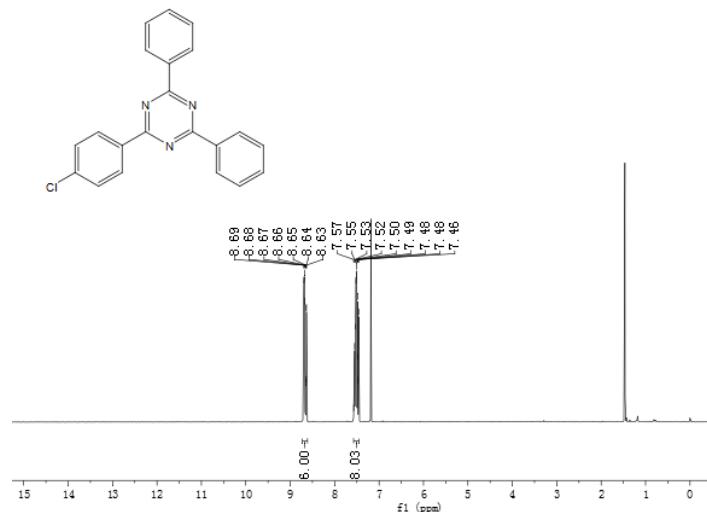
**$^1\text{H}$ - NMR spectrum of 2,4,6-triphenyl-1,3,5-triazine (3a)**



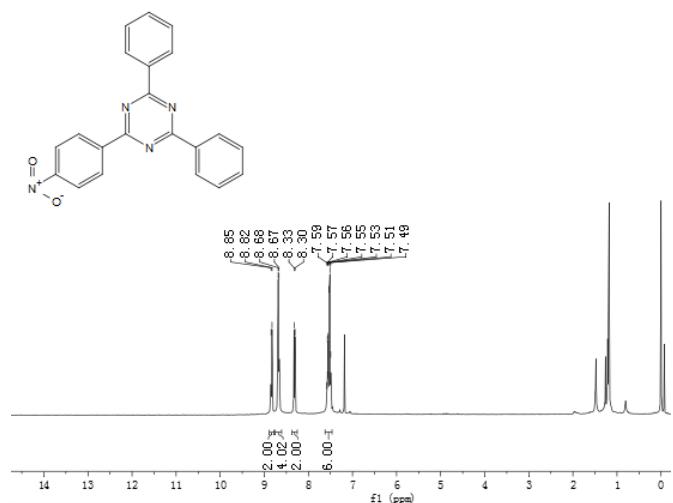
**$^1\text{H}$ - NMR spectrum of 2-(4-methoxyphenyl)-4,6-diphenyl-1,3,5-triazine (3b)**



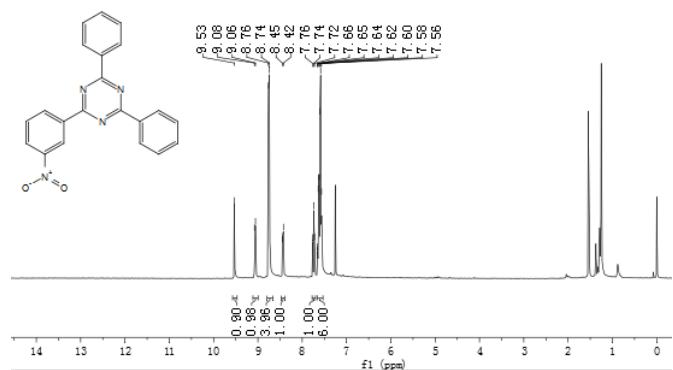
**$^1\text{H}$ - NMR spectrum of 2-(4-chlorophenyl)-4,6-diphenyl-1,3,5-triazine (3c)**



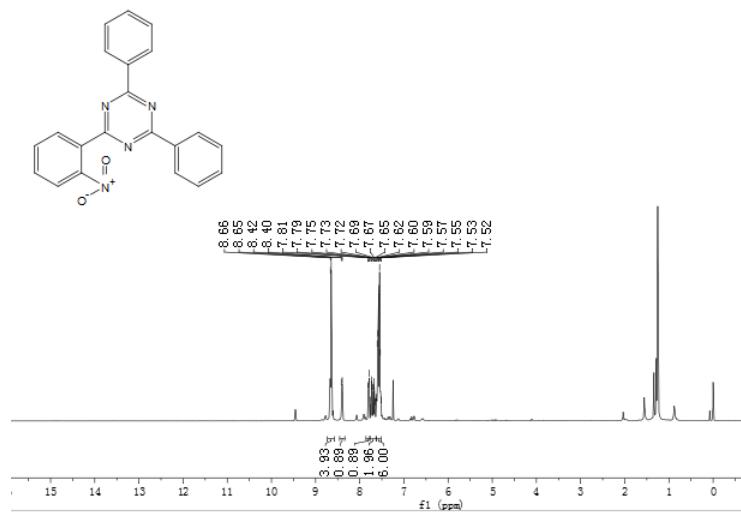
**<sup>1</sup>H- NMR spectrum of 2-(4-nitrophenyl)-4,6-diphenyl-1,3,5-triazine(3d)**



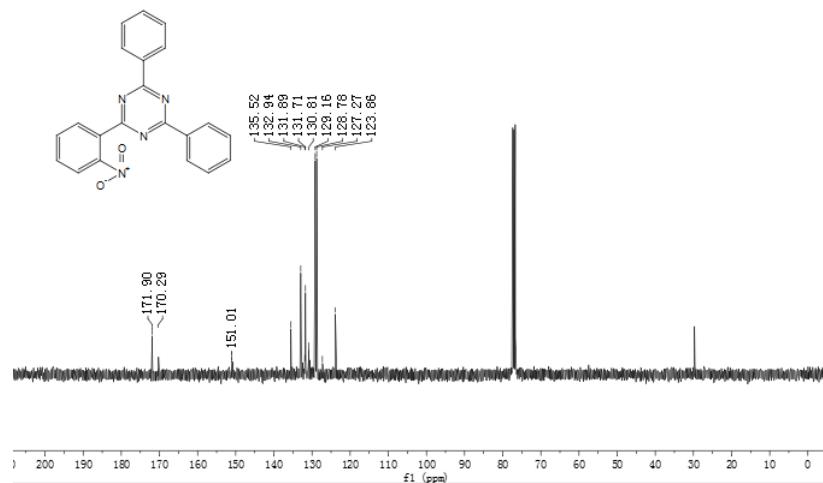
**<sup>1</sup>H-NMR spectrum of 2-(3-nitrophenyl)-4,6-diphenyl-1,3,5-triazine (3e)**



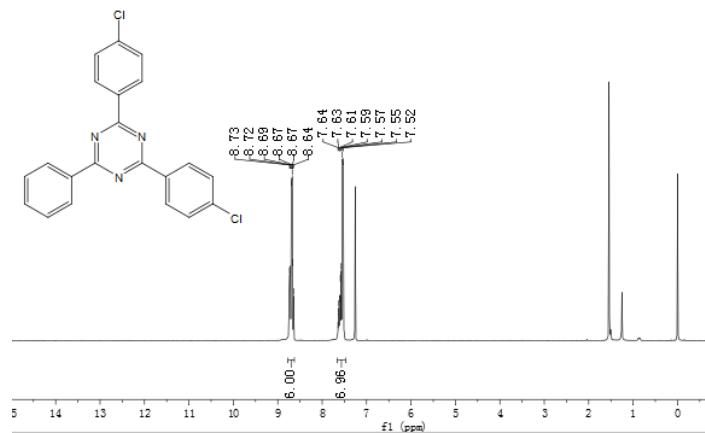
**<sup>1</sup>H- NMR spectrum of 2-(2-nitrophenyl)-4,6-diphenyl-1,3,5-triazine (3f)**



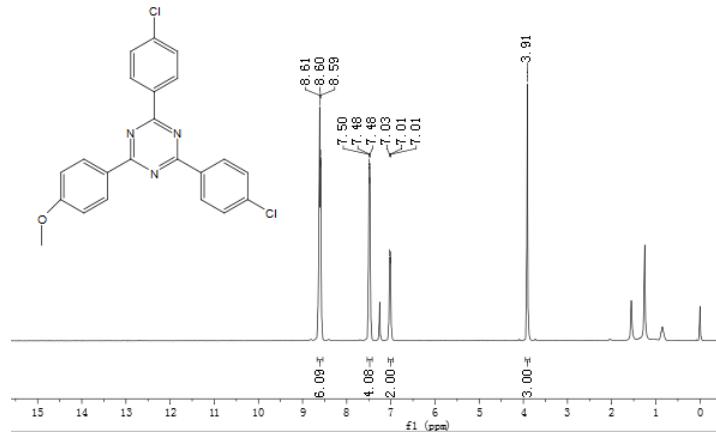
### <sup>13</sup>C-NMR spectrum of 2-(2-nitrophenyl)-4,6-diphenyl-1,3,5-triazine



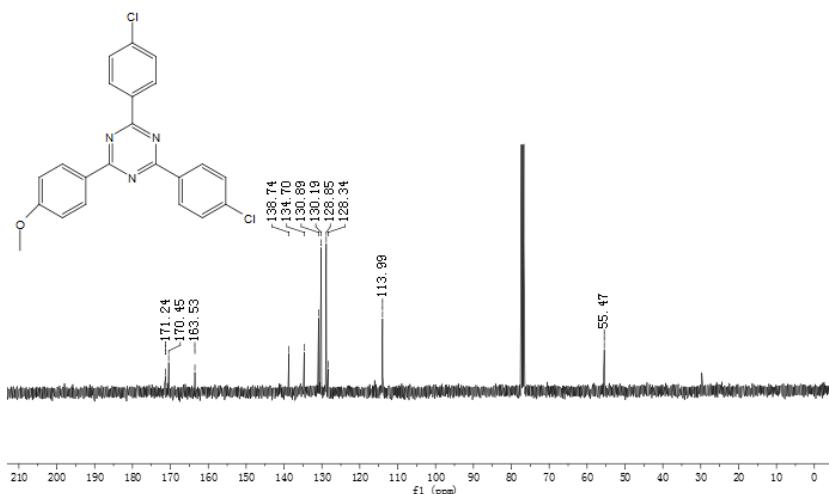
<sup>1</sup>H-NMR spectrum of 2,4-bis(4-chlorophenyl)-6-phenyl-1,3,5-triazine (3g)



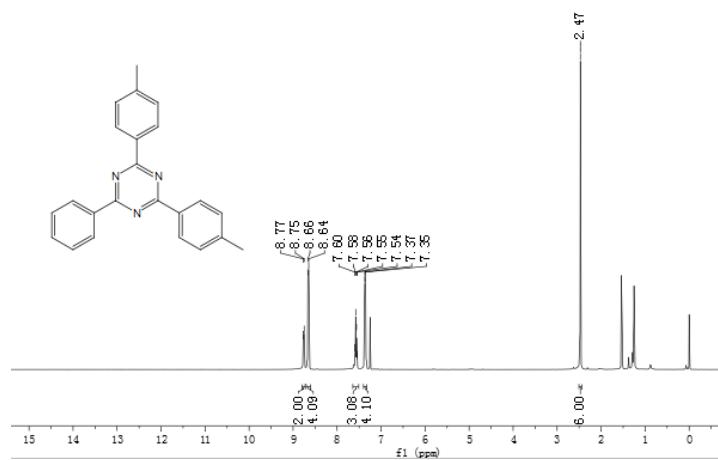
**<sup>1</sup>H- NMR spectrum of  
2,4-bis(4-chlorophenyl)-6-(4-methoxyphenyl)-1,3,5-triazine (3h)**



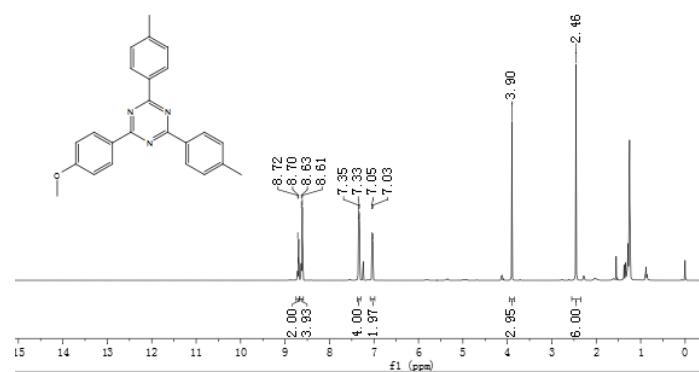
**$^{13}\text{C}$ -NMR spectrum of  
2,4-bis(4-chlorophenyl)-6-(4-methoxyphenyl)-1,3,5-triazine**



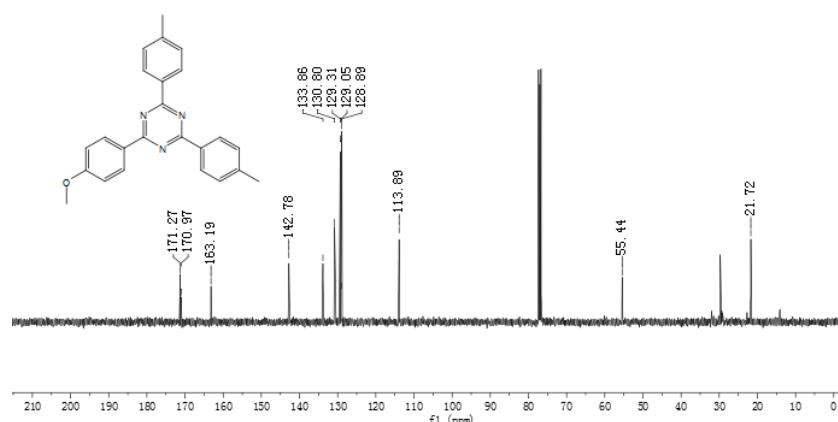
**$^1\text{H}$ - NMR spectrum of 2-phenyl-4,6-di-p-tolyl-1,3,5-triazine (3i)**



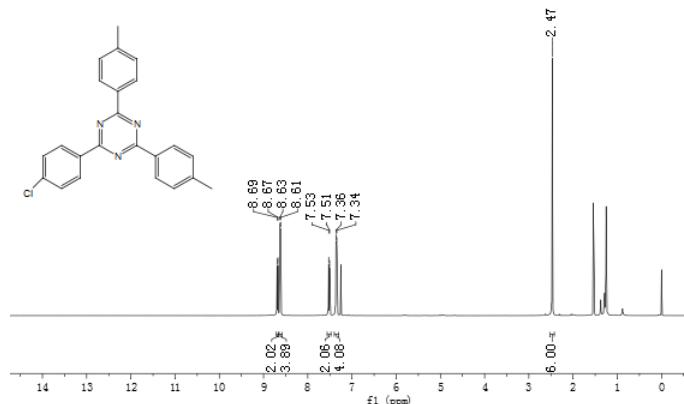
**$^1\text{H}$ - NMR spectrum of 2-(4-methoxyphenyl)-4,6-di-p-tolyl-1,3,5-triazine (3j)**



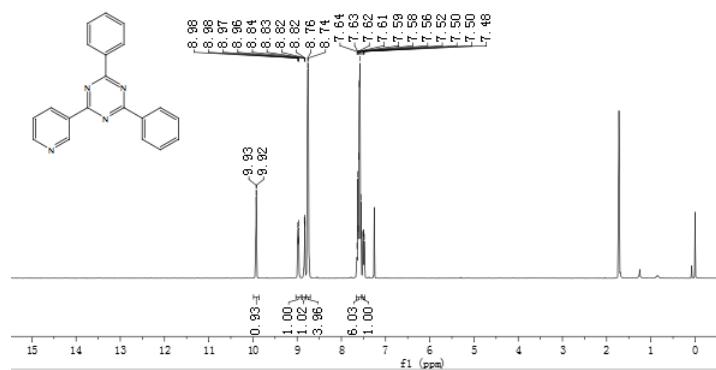
<sup>13</sup>C-NMR spectrum of 2-(4-methoxyphenyl)-4,6-di-p-tolyl-1,3,5-triazine



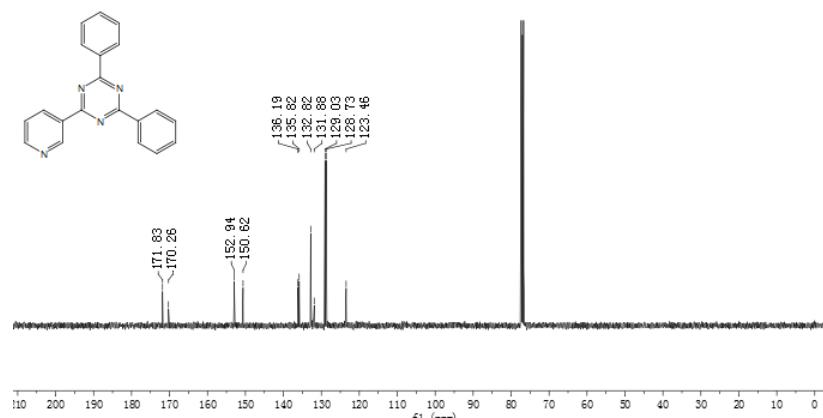
<sup>1</sup>H-NMR spectrum of 2-(4-chlorophenyl)-4,6-di-p-tolyl-1,3,5-triazine (3k)



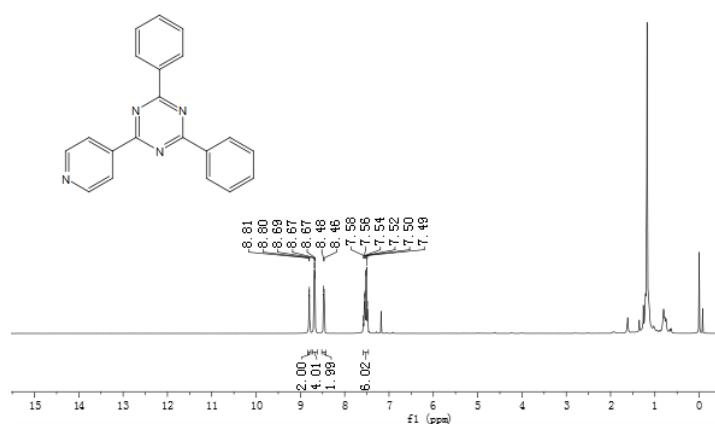
**<sup>1</sup>H- NMR spectrum of 2,4-di-phenyl-6-(pyridin-3-yl)-1,3,5-triazine (3n)**



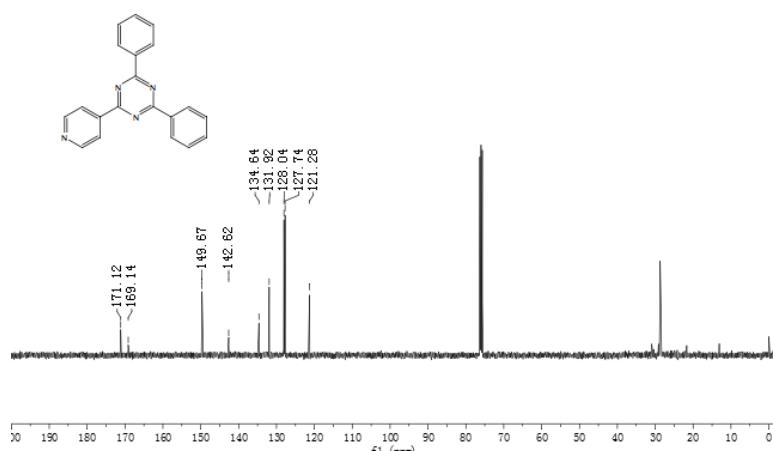
**$^{13}\text{C}$ -NMR spectrum of 2,4-di-phenyl-6-(pyridin-3-yl)-1,3,5-triazine**



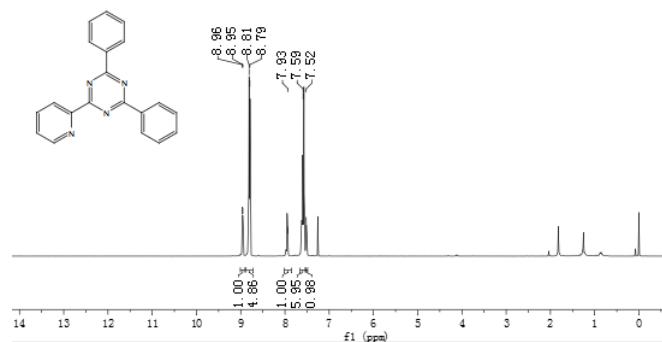
**$^1\text{H}$ - NMR spectrum of 2,4-diphenyl-6-(pyridin-4-yl)-1,3,5-triazine (3o)**



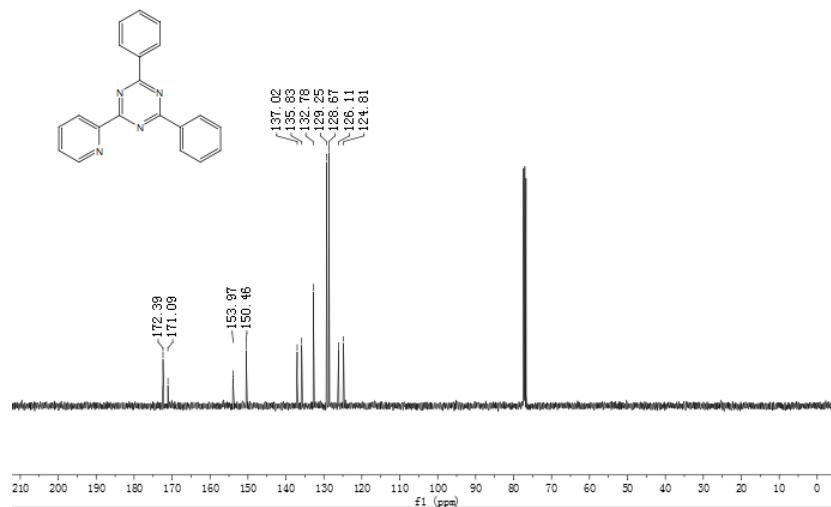
**$^{13}\text{C}$ -NMR spectrum of 2,4-diphenyl-6-(pyridin-4-yl)-1,3,5-triazine**



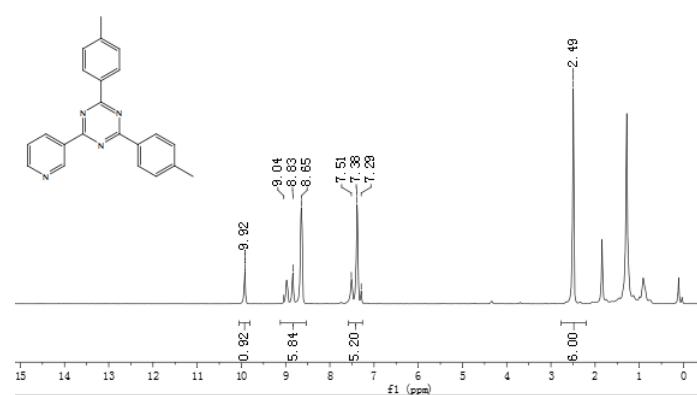
**<sup>1</sup>H- NMR spectrum of 2,4-diphenyl-6-(pyridin-2-yl)-1,3,5-triazine (3p)**



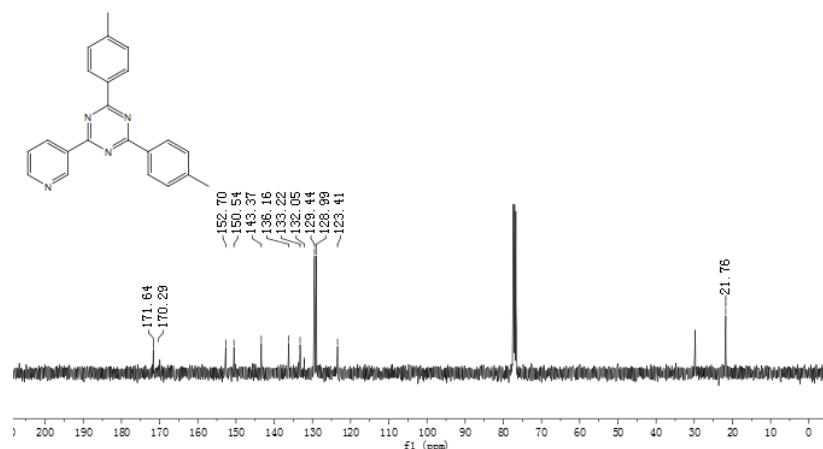
**<sup>13</sup>C-NMR spectrum of 2,4-diphenyl-6-(pyridin-2-yl)-1,3,5-triazine**



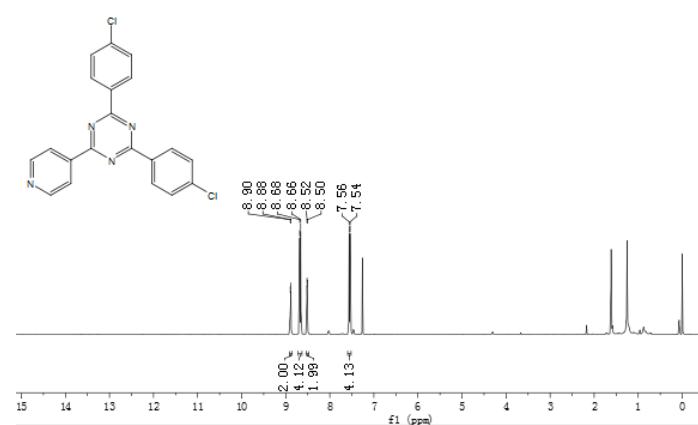
**<sup>1</sup>H- NMR spectrum of 2-(pyridin-3-yl)-4,6-di-p-tolyl-1,3,5-triazine (3q)**



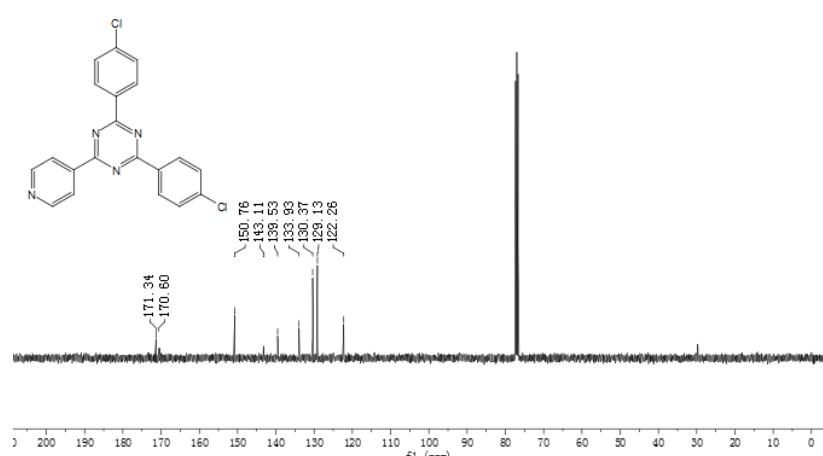
**$^{13}\text{C}$ -NMR spectrum of 2-(pyridin-3-yl)-4,6-di-p-tolyl-1,3,5-triazine**



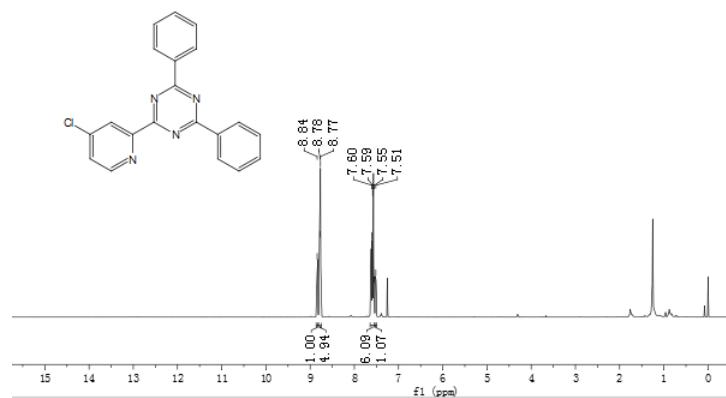
**$^1\text{H}$ - NMR spectrum of 2,4-bis(4-chlorophenyl)-6-(pyridin-4-yl)-1,3,5-triazine (3r)**



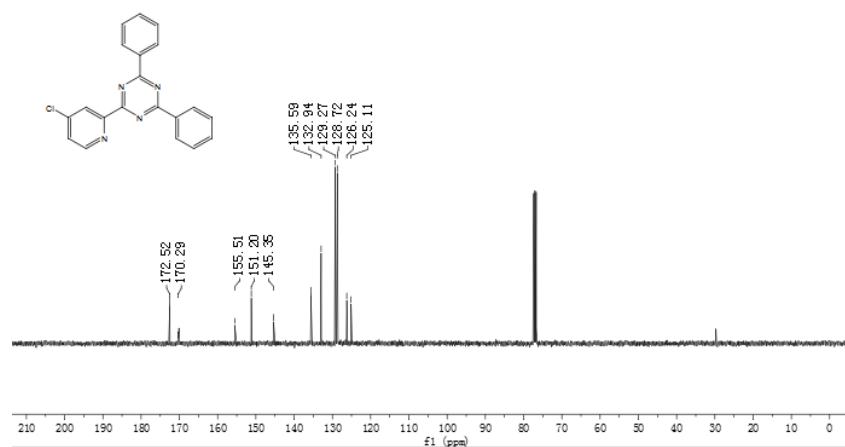
**$^{13}\text{C}$ -NMR spectrum of 2,4-bis(4-chlorophenyl)-6-(pyridin-4-yl)-1,3,5-triazine**



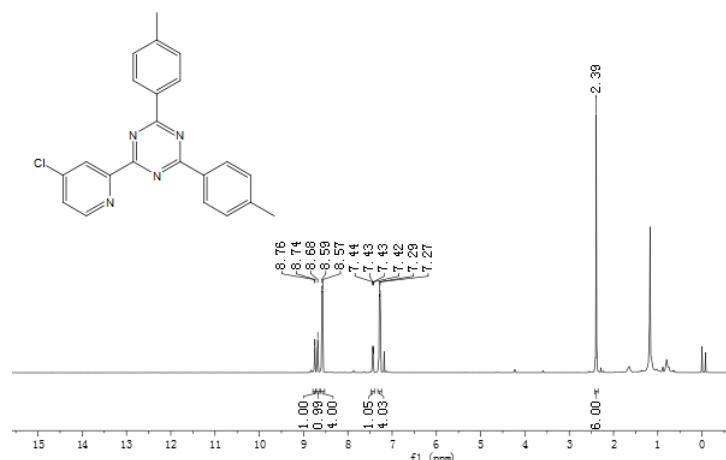
**<sup>1</sup>H- NMR spectrum of 2-(4-chloropyridin-2-yl)-4,6-diphenyl-1,3,5-triazine (3s)**



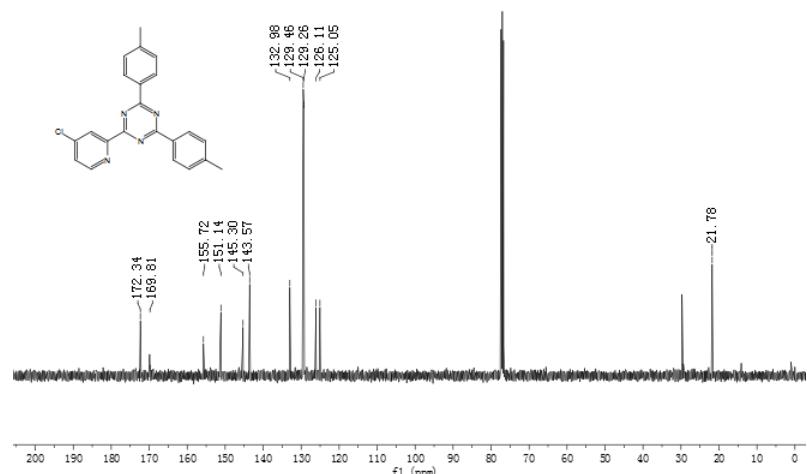
**<sup>13</sup>C-NMR spectrum of 2-(4-chloropyridin-2-yl)-4,6-diphenyl-1,3,5-triazine**



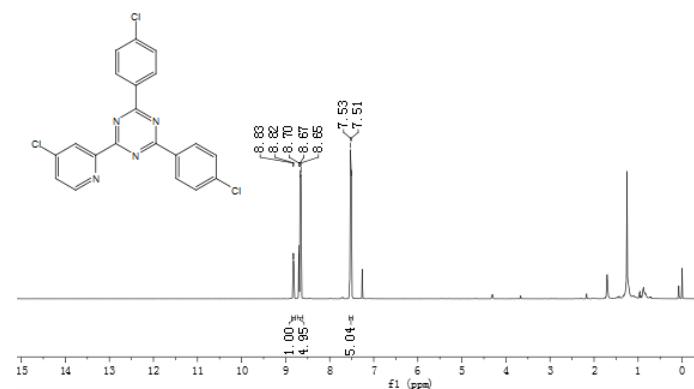
**<sup>1</sup>H- NMR spectrum of 2-(4-chloropyridin-2-yl)-4,6-di-p-tolyl-1,3,5-triazine (3t)**



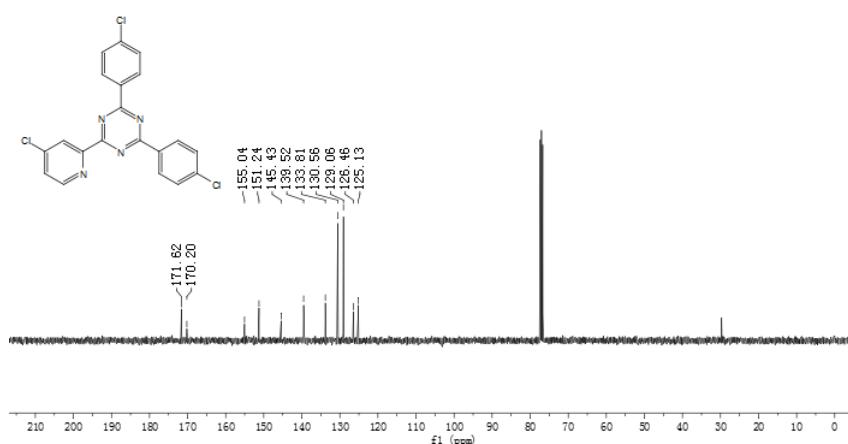
**$^{13}\text{C}$ -NMR spectrum of 2-(4-chloropyridin-2-yl)-4,6-di-p-tolyl-1,3,5-triazine**



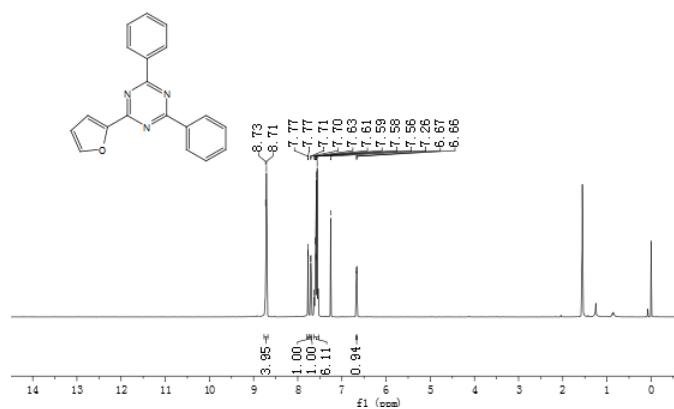
**$^1\text{H}$ -NMR spectrum of  
2-(4-chloropyridin-2-yl)-4,6-bis(4-chlorophenyl)-1,3,5-triazine (3u)**



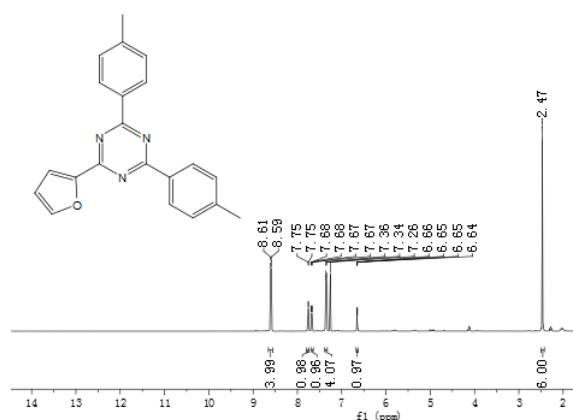
**$^{13}\text{C}$ -NMR spectrum of  
2-(4-chloropyridin-2-yl)-4,6-bis(4-chlorophenyl)-1,3,5-triazine**



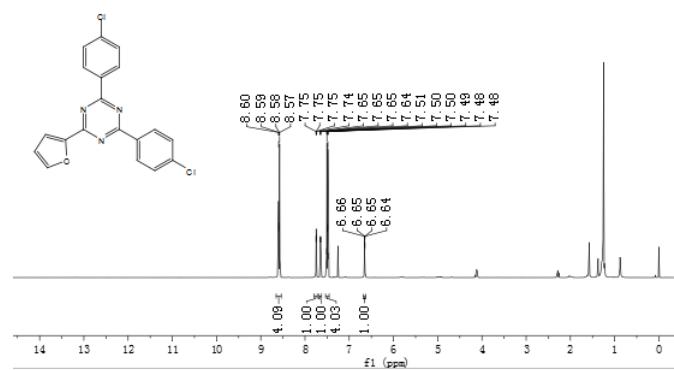
**<sup>1</sup>H- NMR spectrum of 2-(furan-2-yl)-4,6-diphenyl-1,3,5-triazine (3v)**



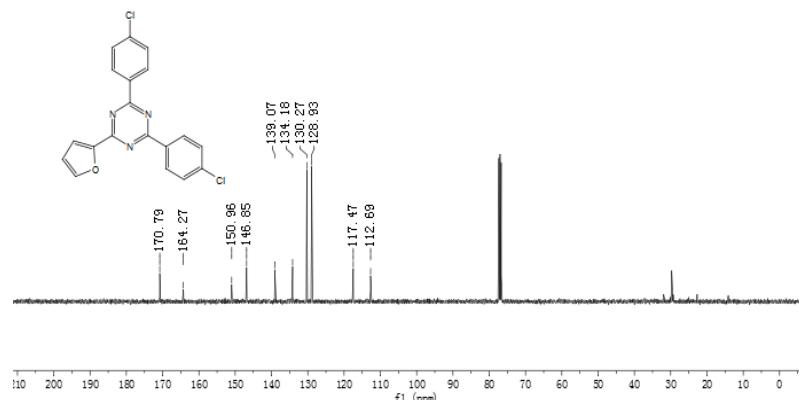
**<sup>1</sup>H- NMR spectrum of 2-(furan-2-yl)-4,6-di-p-tolyl-1,3,5-triazine (3w)**



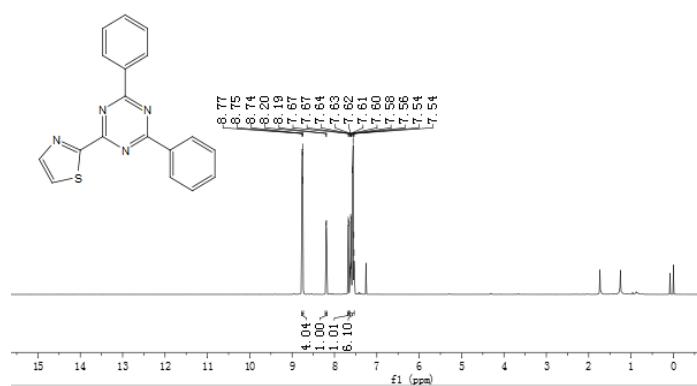
**<sup>1</sup>H-NMR spectrum of 2,4-bis(4-chlorophenyl)-6-(furan-2-yl)-1,3,5-triazine (3x)**



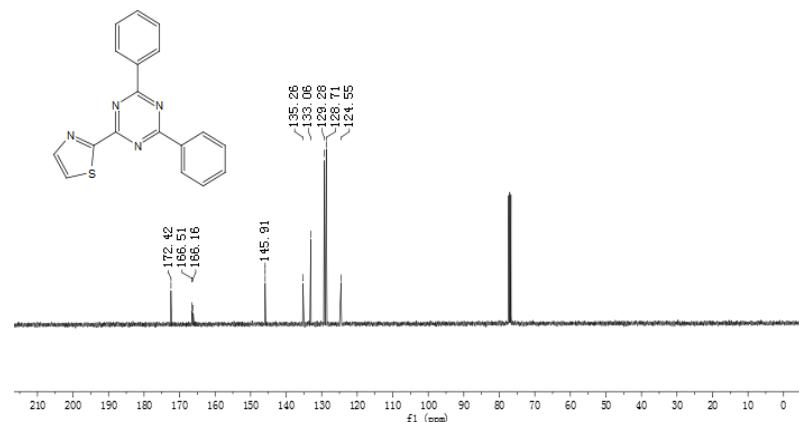
<sup>13</sup>C-NMR spectrum of 2,4-bis(4-chlorophenyl)-6-(furan-2-yl)-1,3,5-triazine



<sup>1</sup>H-NMR spectrum of 2,4-diphenyl-6-(thiazol-2-yl)-1,3,5-triazine (3y)



### <sup>13</sup>C-NMR spectrum of 2,4-diphenyl-6-(thiazol-2-yl)-1,3,5-triazine



## References:

1. (a) N. A. Kapran, V. G. Lukmanov, L. M. Yagupol'skii and V. M. Cherkasov, *Khim. Geterotsikl. Soedin.*, 1977, 122-123; (b) E. F. Silversmith, *J. Org. Chem.*, 1963, **28**, 3568-3569; (c) F. C. Schaefer, *J. Org. Chem.*, 1962, **27**, 3608-3613.

2. R. D. Spencer and B. H. Beggs, *Anal. Chem.*, 1963, **35**, 1633-1636.
3. E. Haruki, T. Inaike, E. Imoto, *Nippon Kagaku Zasshi*. 1966, **87**, 206-208.