

**Direct oxidative coupling of amidine hydrochlorides and  
methylarenes: TBHP-mediated synthesis of substituted 1,3,5-  
triazines under metal-free conditions**

Wei Guo<sup>a,b</sup>\*

<sup>a</sup> School of Chemistry and Chemical Engineering, South China University of Technology, Guangzhou 510640, China. \*E-mail: guoweigw@126.com

<sup>b</sup> Key laboratory of organo-pharmaceutical chemistry of Jiangxi province, Gannan Normal University, Ganzhou, 341000, China

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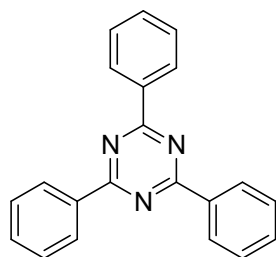
## A. General methods

Melting points were measured using a melting point instrument and are uncorrected.  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were recorded on a 400 MHz NMR spectrometer. IR spectra were obtained with an infrared spectrometer on either potassium bromide pellets or liquid films between two potassium bromide pellets. GC–MS data were obtained using electron ionization. HRMS was carried out on a high-resolution mass spectrometer (LCMS-IT-TOF). TLC was performed using commercially available 100–400 mesh silica gel plates (GF254). Unless otherwise noted, purchased chemicals were used without further purification.

## B. Typical experimental procedure for the synthesis of **3**

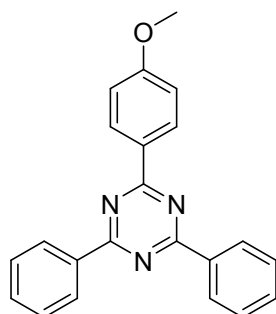
A mixture of amidine hydrochloride **1** (0.25 mmol), toluene derivatives **2** (1 mL),  $\text{Cs}_2\text{CO}_3$  (159 mg, 2 equiv), 70% TBHP (96 mg, 3 equiv) in a test tube (10 mL) equipped with a magnetic stirring bar. The mixture was stirred at 100 °C for 24 h. After the reaction was completed, 10 mL ethyl acetate (3×10 mL) was added into the tube. The combined organic layers were washed with brine to neutral, dried over anhydrous  $\text{MgSO}_4$ , and concentrated in vacuum. Purification of the residue on a preparative TLC afforded **3** with white solid.

## C. Characterization data



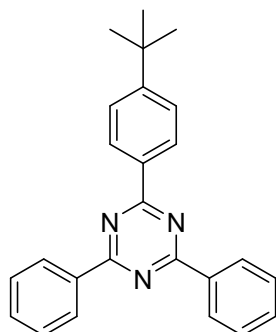
### 2,4,6-Triphenyl-1,3,5-triazine (3aa)<sup>[1]</sup>

Yield: 0.056 g (73%), white solid, m.p. 170-172 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm): δ = 8.78 (d, 6H, J = 8.0 Hz), 7.63-7.56 (m, 9H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm): δ = 171.7, 136.3, 132.5, 129.0, 128.6; IR (KBr, cm<sup>-1</sup>): ν = 3063, 1556, 1522, 789, 737, 674. HRMS (ESI) calc. C<sub>21</sub>H<sub>16</sub>N<sub>3</sub> [M+H]<sup>+</sup>: 310.1339, found: 310.1339.



### 2-(4-Methoxyphenyl)-4,6-diphenyl-1,3,5-triazine (3ab)<sup>[2]</sup>

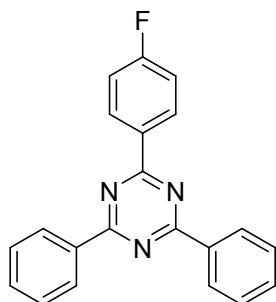
Yield: 0.065 g (77%), white solid, m.p. 157-159 °C; <sup>1</sup>H NMR (400 Hz, CDCl<sub>3</sub>, ppm): δ = 8.59-8.52 (dd, J = 8.0 Hz, J = 8.0 Hz, 6H), 7.43-7.40 (m, 6H), 6.86 (d, J = 8.0 Hz, 2H), 3.70 (s, 3H); <sup>13</sup>C NMR (100 Hz, CDCl<sub>3</sub>, ppm): δ = 171.30, 171.11, 163.31, 136.48, 132.30, 130.87, 128.94, 128.79, 128.55, 113.91, 55.40; IR (KBr, cm<sup>-1</sup>): ν = 3077, 2913, 2840, 1603, 1558, 1521, 1377, 1251, 1178, 1034, 855, 801, 784, 734, 675; HRMS (ESI) calc. C<sub>22</sub>H<sub>18</sub>N<sub>3</sub>O [M+H]<sup>+</sup>: 340.1444, found: 340.1442.



### 2-(4-(*tert*-Butyl)phenyl)-4,6-diphenyl-1,3,5-triazine (3ac)

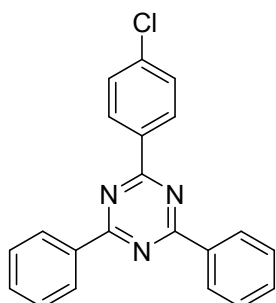
Yield: 0.068 g (74%), white solid, m.p. 164-166 °C; <sup>1</sup>H NMR (400 Hz, CDCl<sub>3</sub>, ppm): δ = 8.86-8.76 (m, 6H), 7.69-7.64 (m, 8H), 1.51 (s, 9H); <sup>13</sup>C NMR (100 Hz, CDCl<sub>3</sub>,

ppm):  $\delta = 171.67, 171.53, 156.10, 136.46, 133.66, 132.42, 129.02, 128.94, 128.62, 125.64, 35.15, 31.32$ ; IR (KBr,  $\text{cm}^{-1}$ ):  $\nu = 3067, 2916, 2844, 1612, 1578, 1521, 1369, 1249, 1178, 1024, 843, 811, 776, 685$ ; HRMS (ESI) calc.  $\text{C}_{25}\text{H}_{23}\text{N}_3\text{Na}$   $[\text{M}+\text{Na}]^+$ : 388.1784, found: 388.1781.



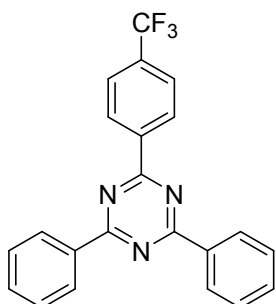
**2-(4-Fluorophenyl)-4,6-diphenyl-1,3,5-triazine (3ad)** <sup>[3]</sup>

Yield: 0.056 g (69%), white solid; m.p. 247-248 °C;  $^1\text{H}$  NMR (400 Hz,  $\text{CDCl}_3$ , ppm):  $\delta = 8.80-8.74$  (m, 6H), 7.58-7.55 (m, 6H), 7.23-7.21 (m, 2H);  $^{13}\text{C}$  NMR (100 Hz,  $\text{CDCl}_3$ , ppm):  $\delta = 171.66, 170.67, 165.83$  (d,  $J = 252$  Hz), 136.15, 132.56, 132.44 (d,  $J = 2$  Hz), 131.30 (d,  $J = 9$  Hz), 128.96, 128.64, 115.69 (d,  $J = 22$  Hz); IR (KBr,  $\text{cm}^{-1}$ ):  $\nu = 3036, 1584, 1525, 1366, 832, 763, 681$ ; HRMS (ESI) calc.  $\text{C}_{21}\text{H}_{15}\text{FN}_3$   $[\text{M}+\text{H}]^+$ : 328.1250, found: 328.1243.



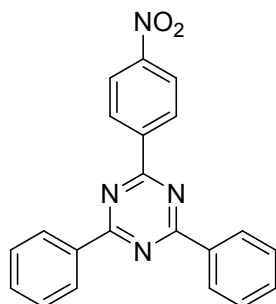
**2-(4-Chlorophenyl)-4,6-diphenyl-1,3,5-triazine (3ae)** <sup>[1]</sup>

Yield: 0.057 g (66%), white solid, m.p. 200-201 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , ppm):  $\delta = 8.74-8.62$  (m, 6H), 7.58-7.47 (m, 8H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , ppm):  $\delta = 171.6, 170.6, 136.8, 136.3, 136.1, 132.6, 132.5, 130.3, 129.0, 128.6$ ; IR (KBr,  $\text{cm}^{-1}$ ):  $\nu = 3044, 1585, 1520, 1365, 830, 760, 683$ ; HRMS (ESI) calc.  $\text{C}_{21}\text{H}_{15}\text{ClN}_3$   $[\text{M}+\text{H}]^+$ : 344.0949, found: 344.0953.



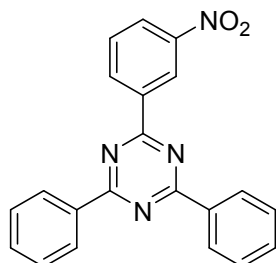
**2,4-Diphenyl-6-(4-(trifluoromethyl)phenyl)-1,3,5-triazine (3af)** [3]

Yield: 0.057 g (61%), white solid, m.p. 186-187 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm): δ = 8.72-8.58 (m, 6H), 7.73-7.50 (m, 8H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm): δ = 171.7, 170.2, 139.5, 135.8, 133.8, 132.7, 129.2, 129.0, 128.6, 125.4, 124.0 (CF<sub>3</sub>); IR (KBr, cm<sup>-1</sup>): ν = 3037, 1521, 1367, 1323, 1122, 1067, 835, 771, 686; HRMS (ESI) calc. C<sub>22</sub>H<sub>15</sub>F<sub>3</sub>N<sub>3</sub> [M+H]<sup>+</sup>: 378.1213, found: 378.1220.



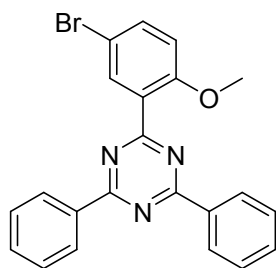
**2-(4-Nitrophenyl)-4,6-diphenyl-1,3,5-triazine (3ag)** [1]

Yield: 0.048 g (54%), yellow solid, m.p. 216-218 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm): δ = 8.92 (d, 2H, *J* = 8.0 Hz), 8.76 (d, 4H, *J* = 8.0 Hz), 8.40 (d, 2H, *J* = 8.0 Hz), 7.61-7.57 (m, 6H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm): δ = 172.1, 169.8, 150.4, 142.0, 135.7, 133.0, 129.8, 129.1, 128.8, 123.7; IR (KBr, cm<sup>-1</sup>): ν = 3036, 1525, 1360, 834, 782, 742, 683; HRMS (ESI) calc. C<sub>21</sub>H<sub>14</sub>N<sub>4</sub>O<sub>2</sub>Na [M+Na]<sup>+</sup>: 377.1009, found: 377.1011.



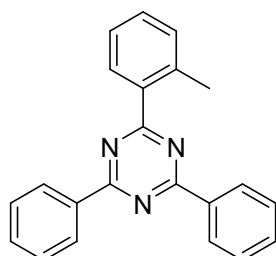
**2-(3-Nitrophenyl)-4,6-diphenyl-1,3,5-triazine (3ah)** [2]

Yield: 0.056 g (63%), yellow solid, m.p. 200-202 °C; <sup>1</sup>H NMR (400 Hz, CDCl<sub>3</sub>, ppm): δ = 9.50 (s, 1H), 9.03 (d, *J* = 8.0 Hz, 1H), 8.73 (d, *J* = 8.0 Hz, 4H), 8.43 (d, *J* = 8.0 Hz, 1H), 7.75-7.57 (m, 7H); <sup>13</sup>C NMR (100 Hz, CDCl<sub>3</sub>, ppm): δ = 171.95, 169.52, 148.75, 138.09, 135.55, 134.48, 132.93, 129.60, 129.04, 128.72, 126.73, 123.75; IR (KBr, cm<sup>-1</sup>): ν = 3045, 1587, 1533, 1359, 833, 784, 746, 681; HRMS (ESI) calc. C<sub>21</sub>H<sub>14</sub>N<sub>4</sub>NaO<sub>2</sub> [M+Na]<sup>+</sup>: 377.1009, found: 377.1009.



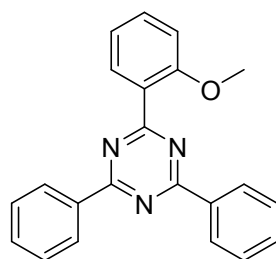
**2-(5-Bromo-2-methoxyphenyl)-4,6-diphenyl-1,3,5-triazine (3ai)**

Yield: 0.059 g (57%), white solid, m.p. 176-179 °C; <sup>1</sup>H NMR (400 Hz, CDCl<sub>3</sub>, ppm): δ = 8.66 (d, *J* = 8.0 Hz, 4H), 8.22 (s, 1H), 7.51-7.47 (m, 7H), 6.86 (d, *J* = 8.0 Hz, 1H), 3.86 (s, 3H); <sup>13</sup>C NMR (100 Hz, CDCl<sub>3</sub>, ppm): δ = 171.96, 171.53, 158.39, 136.16, 135.03, 134.72, 132.60, 129.11, 128.68, 128.51, 114.68, 113.04, 56.61; IR (KBr, cm<sup>-1</sup>): ν = 3034, 2928, 2835, 1607, 1561, 1531, 1380, 1252, 1179, 1033, 857, 783, 734, 677; HRMS (ESI) calc. C<sub>22</sub>H<sub>16</sub>BrN<sub>3</sub>NaO [M+Na]<sup>+</sup>: 440.0369, found: 440.0364.



**2,4-Diphenyl-6-(*o*-tolyl)-1,3,5-triazine (3aj)** <sup>[3]</sup>

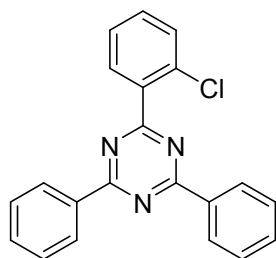
Yield: 0.034 g (42%), white solid, m.p. 121-123 °C; <sup>1</sup>H NMR (400 Hz, CDCl<sub>3</sub>, ppm): δ = 8.70-8.69 (m, 4H), 8.32 (d, *J* = 8.0 Hz, 1H), 7.52-7.31 (m, 9H), 3.03 (s, 3H); <sup>13</sup>C NMR (100 Hz, CDCl<sub>3</sub>, ppm): δ = 174.51, 171.32, 139.24, 136.37, 136.13, 132.54, 131.99, 131.41, 131.08, 129.07, 128.71, 126.13, 22.59; IR (KBr, cm<sup>-1</sup>): ν = 3068, 2917, 2845, 1613, 1579, 1523, 1368, 1179, 1024, 845, 815, 778, 689; HRMS (ESI) calc. C<sub>22</sub>H<sub>17</sub>N<sub>3</sub>Na [M+Na]<sup>+</sup>: 346.1315, found: 346.1313.



**2-(2-Methoxyphenyl)-4,6-diphenyl-1,3,5-triazine (3ak)**

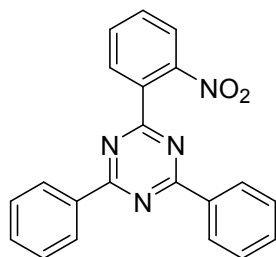
Yield: 0.040 g (47%), white solid, m.p. 134-136 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm): δ = 8.71 (d, 4H, *J* = 8.0 Hz), 8.14 (d, 1H, *J* = 8.0 Hz), 7.52-7.44 (m, 7H), 7.10 (t, 1H, *J* = 8.0 Hz), 7.04 (d, 1H, *J* = 8.0 Hz), 3.92 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm): δ = 173.3, 171.5, 159.3, 136.5, 132.6, 132.5, 132.4, 129.1, 128.7, 126.9, 120.8, 112.9, 56.4; IR (KBr, cm<sup>-1</sup>): ν = 3063, 2931, 2825, 1592, 1516, 1448, 1360, 1249, 1165, 1021, 846, 748, 695, 634; HRMS (ESI) calc. C<sub>22</sub>H<sub>18</sub>N<sub>3</sub>O [M+H]<sup>+</sup>: 340.1444,

found: 340.1453.



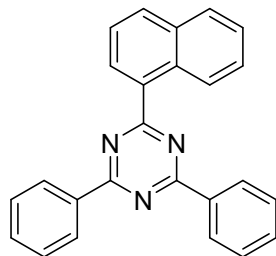
**2-(2-Chlorophenyl)-4,6-diphenyl-1,3,5-triazine (3al)** <sup>[3]</sup>

Yield: 0.035 g (41%), white solid, m.p. 133-135 °C; <sup>1</sup>H NMR (400 Hz, CDCl<sub>3</sub>, ppm): δ = 8.72 (d, *J* = 8.0 Hz, 4H), 8.15 (d, *J* = 8.0 Hz, 1H), 7.59-7.43 (m, 9H); <sup>13</sup>C NMR (100 Hz, CDCl<sub>3</sub>, ppm): δ = 172.80, 171.65, 136.00, 135.92, 133.85, 132.70, 132.43, 131.64, 131.27, 129.15, 128.71, 126.87; IR (KBr, cm<sup>-1</sup>): ν = 3056, 1588, 1519, 1363, 834, 756, 689; HRMS (ESI) calc. C<sub>21</sub>H<sub>14</sub>ClN<sub>3</sub>Na [M+Na]<sup>+</sup>: 366.0768, found: 366.0776.



**2-(2-Nitrophenyl)-4,6-diphenyl-1,3,5-triazine (3am)** <sup>[2]</sup>

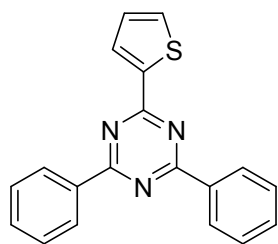
Yield: 0.029 g (33%), yellow solid, m.p. 144-146 °C; <sup>1</sup>H NMR (400 Hz, CDCl<sub>3</sub>, ppm): δ = 8.50 (d, *J* = 8.0 Hz, 4H), 8.24 (d, *J* = 8.0 Hz, 1H), 7.62 (d, *J* = 8.0 Hz, 1H) 7.56-7.37 (m, 8H); <sup>13</sup>C NMR (100 Hz, CDCl<sub>3</sub>, ppm): δ = 171.82, 170.11, 150.79, 135.49, 132.95, 131.90, 131.71, 131.69, 130.63, 129.16, 128.78, 123.81; IR (KBr, cm<sup>-1</sup>): ν = 3062, 1591, 1520, 1447, 1368, 844, 776, 691; HRMS (ESI) calc. C<sub>21</sub>H<sub>14</sub>N<sub>4</sub>NaO<sub>2</sub> [M+Na]<sup>+</sup>: 377.1009, found: 377.1005.



**2-(Naphthalen-1-yl)-4,6-diphenyl-1,3,5-triazine (3an)**

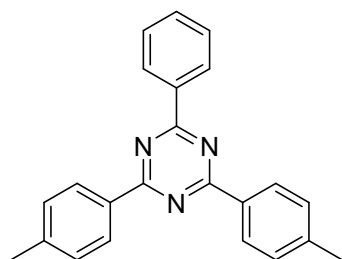
Yield: 0.040 g (45%), white solid, m.p. 258-260 °C; <sup>1</sup>H NMR (400 Hz, CDCl<sub>3</sub>, ppm): δ = 9.14 (d, *J* = 8.0 Hz, 1H), 8.75-8.74 (m, 4H), 8.50 (d, *J* = 8.0 Hz, 1H), 7.99 (d, *J* = 8.0 Hz, 1H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.59-7.50 (m, 9H); <sup>13</sup>C NMR (100 Hz, CDCl<sub>3</sub>, ppm): δ = 174.40, 171.54, 136.27, 134.33, 134.03, 132.66, 132.38, 131.47, 130.84,

129.14, 128.77, 127.30, 126.24, 126.13, 125.21; IR (KBr,  $\text{cm}^{-1}$ ):  $\nu = 3067, 1567, 1541, 834, 799, 737, 686$ ; HRMS (ESI) calc.  $\text{C}_{25}\text{H}_{17}\text{N}_3\text{Na}$   $[\text{M}+\text{Na}]^+$ : 382.1315, found: 382.1315.



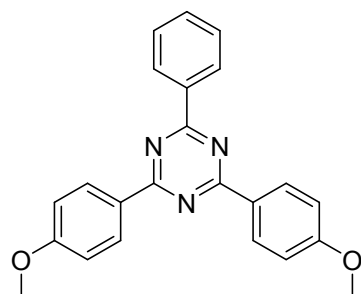
**2,4-Diphenyl-6-(thiophen-2-yl)-1,3,5-triazine (3ao)**

Yield: 0.020 g (25%), white solid, m.p. 255-257 °C;  $^1\text{H}$  NMR (400 Hz,  $\text{CDCl}_3$ , ppm):  $\delta = 8.71$  (d,  $J = 8.0$  Hz, 4H), 8.36-8.35 (m, 1H), 7.63-7.53 (m, 7H), 7.24-7.21 (m, 1H);  $^{13}\text{C}$  NMR (100 Hz,  $\text{CDCl}_3$ , ppm):  $\delta = 171.56, 168.11, 142.20, 135.97, 132.55, 132.13, 131.49, 128.96, 128.61, 128.46$ ; IR (KBr,  $\text{cm}^{-1}$ ):  $\nu = 3045, 1526, 1391, 1121, 832, 789, 766, 685$ ; HRMS (ESI) calc.  $\text{C}_{19}\text{H}_{13}\text{N}_3\text{NaS}$   $[\text{M}+\text{Na}]^+$ : 338.0722, found: 338.0731.



**2-Phenyl-4,6-di-*p*-tolyl-1,3,5-triazine (3ba)** <sup>[2]</sup>

Yield: 0.061 g (72%), white solid, m.p. 215-217 °C;  $^1\text{H}$  NMR (400 Hz,  $\text{CDCl}_3$ , ppm):  $\delta = 8.79$  (d,  $J = 8.0$  Hz, 2H), 8.68 (d,  $J = 8.0$  Hz, 4H), 7.63-7.58 (m, 3H), 7.39 (d,  $J = 8.0$  Hz, 4H), 2.50 (s, 6H);  $^{13}\text{C}$  NMR (100 Hz,  $\text{CDCl}_3$ , ppm):  $\delta = 171.52, 171.41, 142.96, 136.51, 133.69, 132.28, 129.36, 128.96, 128.93, 128.56, 21.72$ ; IR (KBr,  $\text{cm}^{-1}$ ):  $\nu = 3066, 2911, 2832, 1611, 1574, 1512, 1370, 1177, 1023, 845, 812, 779, 685$ ; HRMS (ESI) calc.  $\text{C}_{23}\text{H}_{20}\text{N}_3$   $[\text{M}+\text{H}]^+$ : 338.1652, found: 338.1656.

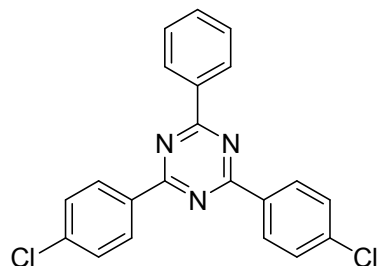


**2,4-Bis(4-methoxyphenyl)-6-phenyl-1,3,5-triazine (3ca)**

Yield: 0.063 g (68%), white solid, m.p. 209-211 °C;  $^1\text{H}$  NMR (400 Hz,  $\text{CDCl}_3$ , ppm):  $\delta = 8.72$ -8.66 (m, 6H), 7.57-7.51 (m, 3H), 7.02 (d,  $J = 8.0$  Hz, 4H), 3.87 (s, 6H);  $^{13}\text{C}$  NMR (100 Hz,  $\text{CDCl}_3$ , ppm):  $\delta = 171.10, 170.91, 163.21, 136.63, 132.16, 130.78,$

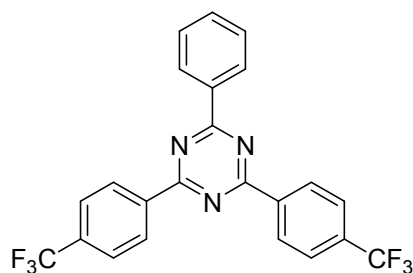


128.99, 128.85, 128.51, 113.88, 55.42; IR (KBr,  $\text{cm}^{-1}$ ):  $\nu = 3064, 2928, 2812, 1594, 1516, 1438, 1359, 1244, 1162, 1024, 844, 749, 693$ ; HRMS (ESI) calc.  $\text{C}_{23}\text{H}_{20}\text{N}_3\text{O}_2$   $[\text{M}+\text{H}]^+$ : 370.1550, found: 370.1548.



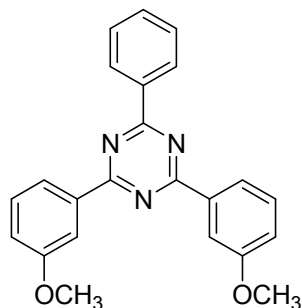
**2,4-Bis(4-chlorophenyl)-6-phenyl-1,3,5-triazine (3da)** <sup>[2]</sup>

Yield: 0.057 g (61%), white solid, m.p. 239-241 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , ppm):  $\delta = 8.78\text{-}8.65$  (m, 6H), 7.58-7.51 (m, 7H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , ppm):  $\delta = 171.7, 170.7, 138.8, 136.1, 134.8, 132.6, 130.3, 129.0, 128.9, 128.7$ ; IR (KBr,  $\text{cm}^{-1}$ ):  $\nu = 3059, 1583, 1515, 1368, 829, 768, 682$ ; HRMS (ESI) calc.  $\text{C}_{21}\text{H}_{14}\text{Cl}_2\text{N}_3$   $[\text{M}+\text{H}]^+$ : 378.0559, found: 378.0562.



**2-Phenyl-4,6-bis(4-(trifluoromethyl)phenyl)-1,3,5-triazine (3ea)** <sup>[3]</sup>

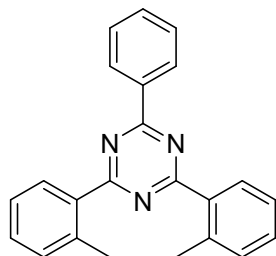
Yield: 0.061 g (54%), white solid, m.p. 169-171 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , ppm):  $\delta = 8.47\text{-}8.41$  (m, 6H), 7.61-7.39 (m, 7H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , ppm):  $\delta = 171.7, 170.1, 138.7, 135.1, 133.9, 133.0, 128.9, 128.8, 128.6, 125.4, 124.0$  ( $\text{CF}_3$ ); IR (KBr,  $\text{cm}^{-1}$ ):  $\nu = 3053, 2923, 1588, 1521, 1366, 1316, 1121, 1063, 824, 778, 689$ ; HRMS (ESI) calc.  $\text{C}_{23}\text{H}_{14}\text{F}_6\text{N}_3$   $[\text{M}+\text{H}]^+$ : 446.1086, found: 446.1089.



**2,4-Bis(3-methoxyphenyl)-6-phenyl-1,3,5-triazine (3fa)**

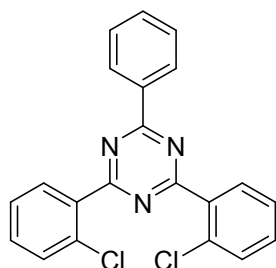
Yield: 0.057 g (62%), white solid, m.p. 186-188 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{d}^6\text{-DMSO}$ , ppm):  $\delta = 8.73$  (d, 2H,  $J = 8.0$  Hz), 8.31 (d, 2H,  $J = 8.0$  Hz), 8.22 (s, 2H), 7.74-7.65 (m, 3H), 7.58 (t, 2H,  $J = 8.0$  Hz), 7.29 (d, 2H,  $J = 8.0$  Hz), 3.93 (s, 6H);  $^{13}\text{C}$  NMR

(100 MHz, d<sup>6</sup>-DMSO, ppm):  $\delta$  = 171.0, 170.8, 159.7, 136.8, 133.1, 130.1, 129.0, 128.7, 118.8, 113.5, 99.5, 55.3; IR (KBr, cm<sup>-1</sup>):  $\nu$  = 3064, 3010, 2949, 2830, 1594, 1520, 1453, 1357, 1236, 1132, 1032, 770, 683, 639; HRMS (ESI) calc. C<sub>23</sub>H<sub>20</sub>N<sub>3</sub>O<sub>2</sub> [M+H]<sup>+</sup>: 370.1550, found: 370.1554.



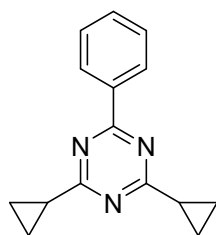
**2-Phenyl-4,6-di-*o*-tolyl-1,3,5-triazine (3ga)**

Yield: 0.048 g (57%), white solid, m.p. 175-176 °C; <sup>1</sup>H NMR (400 Hz, CDCl<sub>3</sub>, ppm):  $\delta$  = 8.68 (d, *J* = 8.0 Hz, 2H), 8.28 (d, *J* = 8.0 Hz, 2H), 7.56-7.50 (m, 3H), 7.39-7.32 (m, 6H), 2.82 (s, 6H); <sup>13</sup>C NMR (100 Hz, CDCl<sub>3</sub>, ppm):  $\delta$  = 174.28, 170.88, 139.11, 136.38, 136.18, 132.56, 131.93, 131.36, 131.00, 129.07, 128.76, 126.12, 22.47; IR (KBr, cm<sup>-1</sup>):  $\nu$  = 3034, 2956, 2812, 1604, 1579, 1512, 1366, 1180, 1022, 847, 813, 772, 689; HRMS (ESI) calc. C<sub>23</sub>H<sub>20</sub>N<sub>3</sub> [M+H]<sup>+</sup>: 338.1652, found: 338.1652.



**2,4-Bis(2-chlorophenyl)-6-phenyl-1,3,5-triazine (3ha)**

Yield: 0.046 g (49%), white solid, m.p. 195-197 °C; <sup>1</sup>H NMR (400 Hz, CDCl<sub>3</sub>, ppm):  $\delta$  = 8.71 (d, *J* = 8.0 Hz, 2H), 8.14-8.10 (m, 2H), 7.59-7.51 (m, 5H), 7.44-7.40 (m, 4H); <sup>13</sup>C NMR (100 Hz, CDCl<sub>3</sub>, ppm):  $\delta$  = 172.78, 171.58, 135.70, 135.64, 133.77, 132.95, 132.55, 131.79, 131.23, 129.39, 128.80, 126.96; IR (KBr, cm<sup>-1</sup>):  $\nu$  = 3056, 1584, 1516, 1369, 832, 769, 686; HRMS (ESI) calc. C<sub>21</sub>H<sub>13</sub>Cl<sub>2</sub>N<sub>3</sub>Na [M+Na]<sup>+</sup>: 400.0379, found: 400.0370.



**2,4-Dicyclopropyl-6-phenyl-1,3,5-triazine (3ia)**

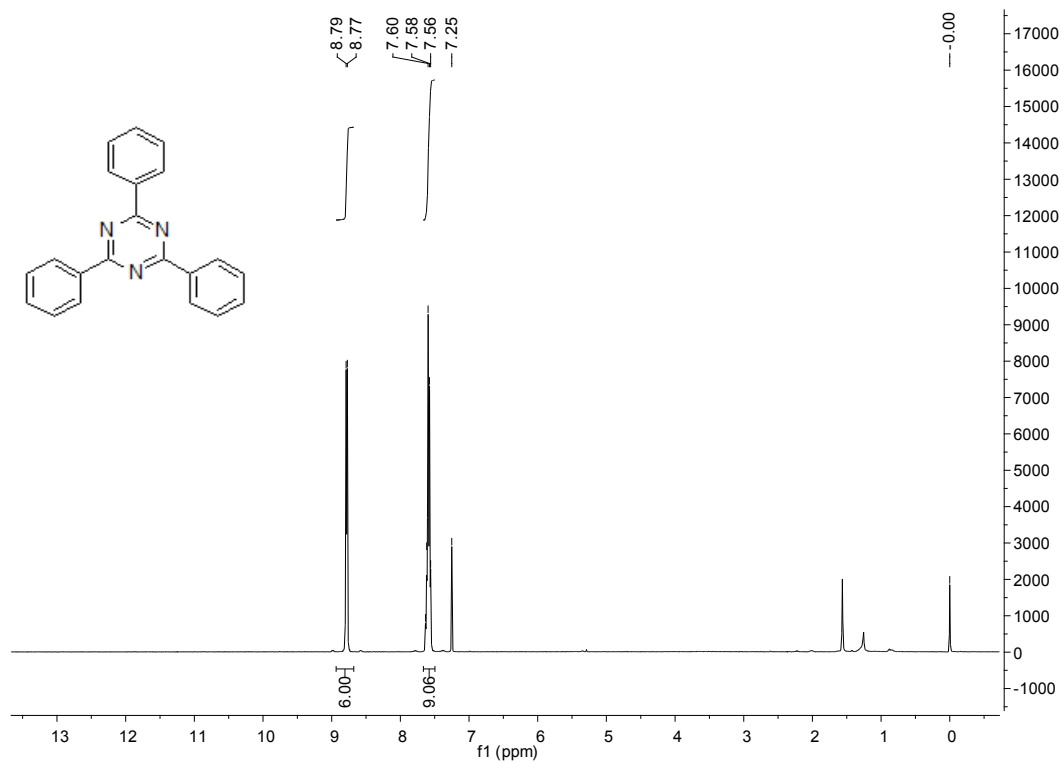
Yield: 0.020 g (34%), white solid, m.p. 126-127 °C; <sup>1</sup>H NMR (400 Hz, CDCl<sub>3</sub>, ppm):  $\delta$  = 8.45 (d, *J* = 8.0 Hz, 2H), 7.51-7.42 (m, 3H), 2.18-2.11 (m, 2H), 1.30-1.26 (m, 4H),

1.11-1.07 (m, 4H);  $^{13}\text{C}$  NMR (100 Hz,  $\text{CDCl}_3$ , ppm):  $\delta = 179.73, 169.80, 136.11, 132.03, 128.67, 128.42, 17.95, 11.37$ ; IR (KBr,  $\text{cm}^{-1}$ ):  $\nu = 3066, 2934, 2812, 1579, 1514, 1367, 1172, 1031, 849, 779, 684$ ; HRMS (ESI) calc.  $\text{C}_{15}\text{H}_{16}\text{N}_3$   $[\text{M}+\text{H}]^+$ : 238.1339, found: 238.1337.

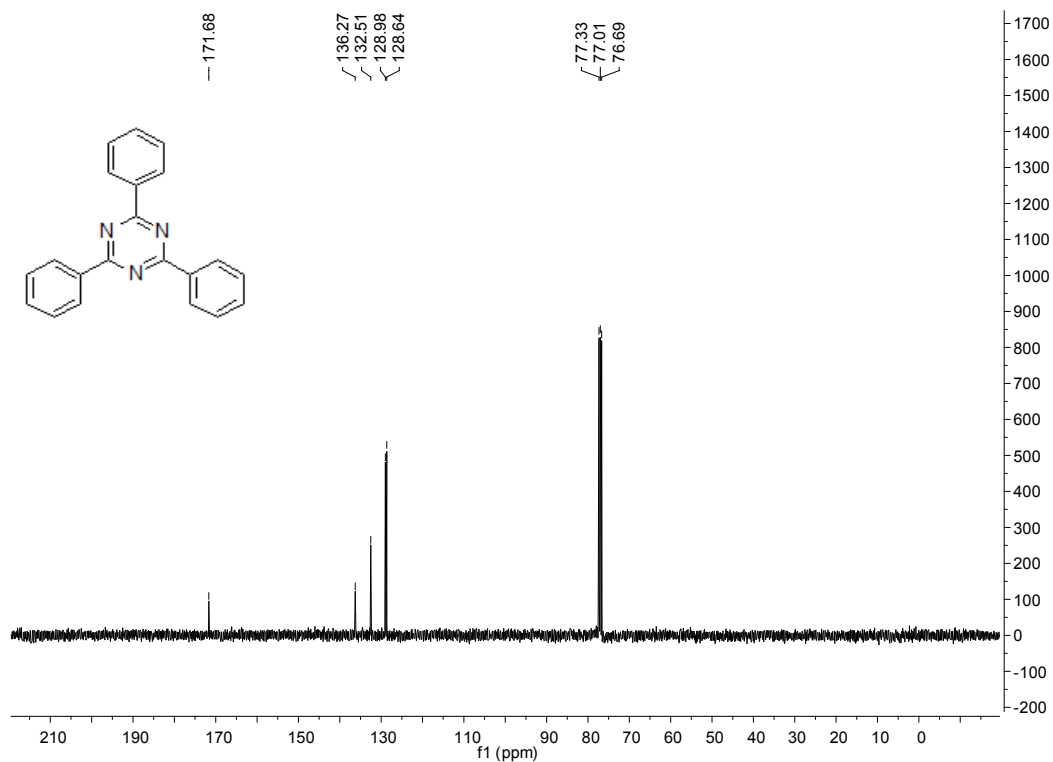
## D. Reference

- [1] S. Biswas, S. Batra, *Eur. J. Org. Chem.* **2012**, *18*, 3492
- [2] F. Xie, M. Chen, X. Wang, H. Jiang, M. Zhang, *Org. Biomol. Chem.*, 2014, **12**, 2761-2768;
- [3] Q. You, F. Wang, C. Wu, T. Shi, D. Min, H. Chen, W. Zhang, *Org. Biomol. Chem.*, 2015, **13**, 6723-6727.

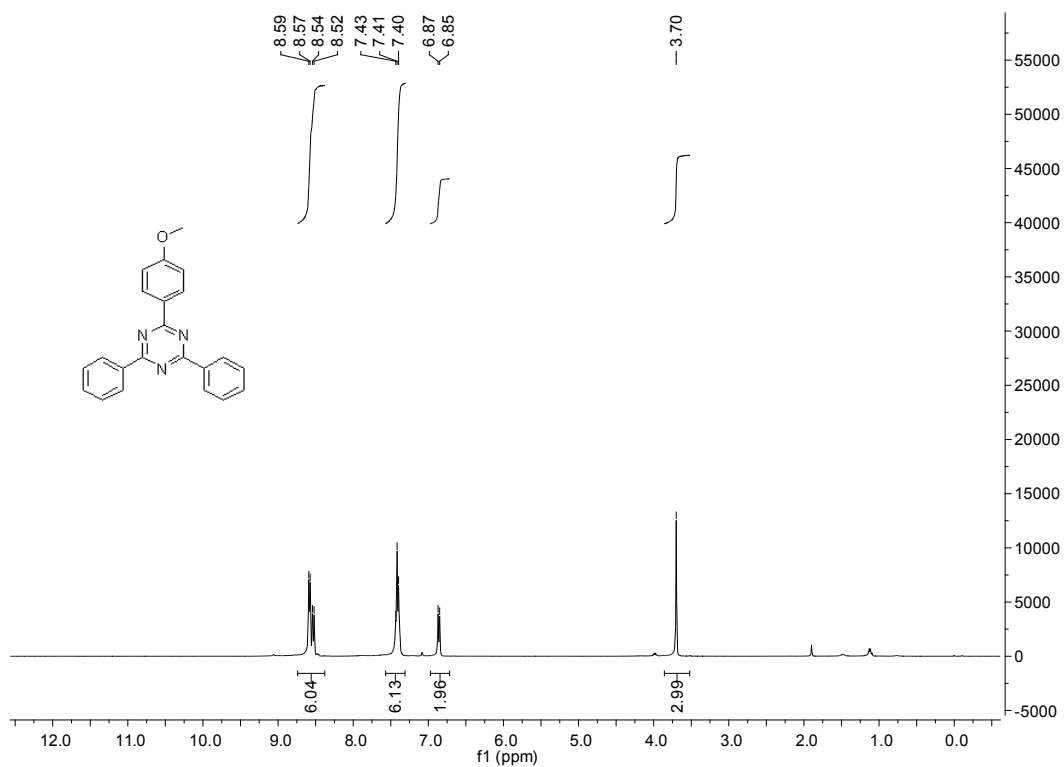
## E. NMR Spectra



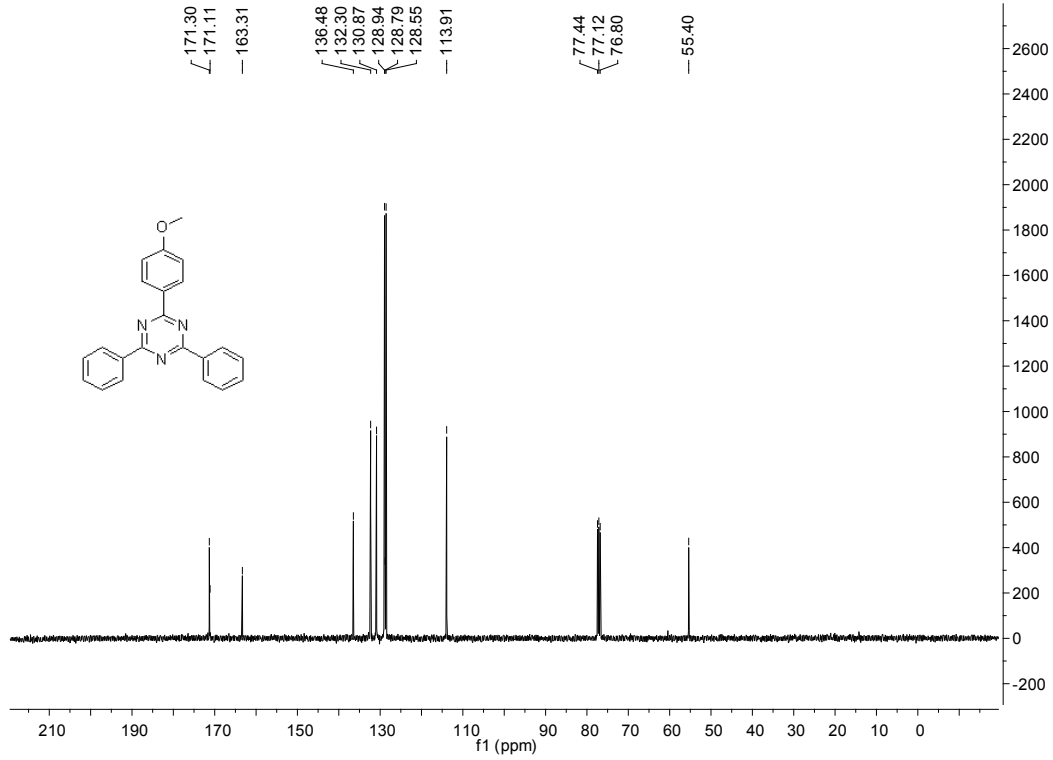
$^1\text{H}$  NMR of **3aa**



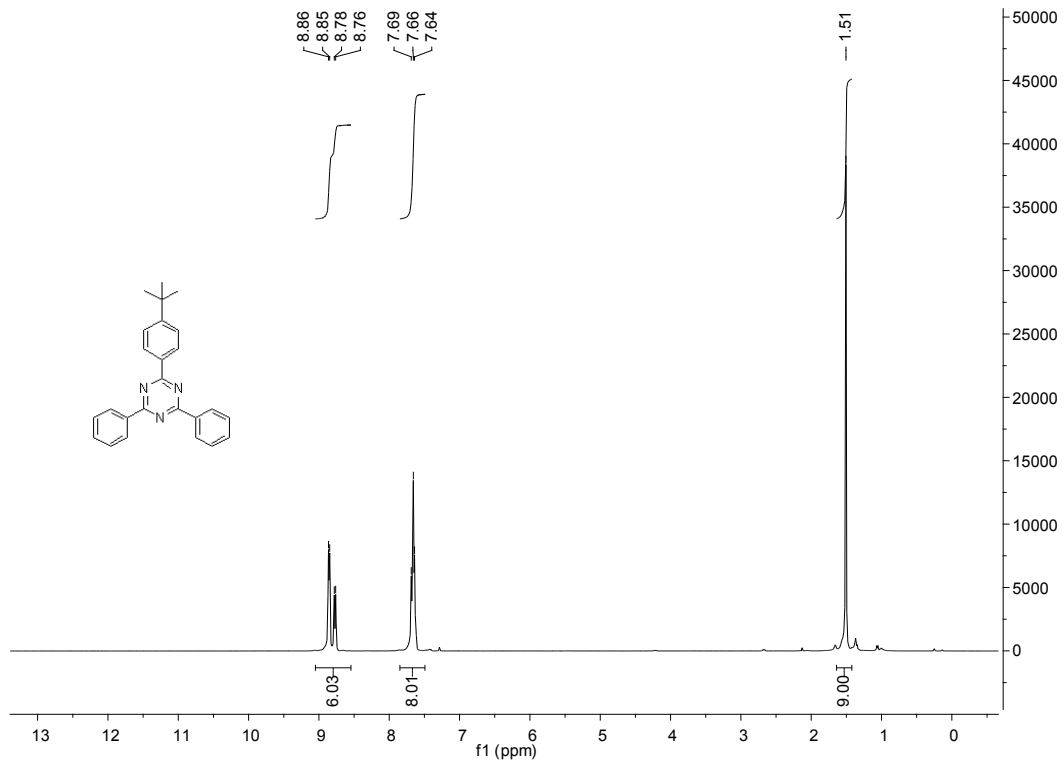
$^{13}\text{C}$  NMR of 3aa



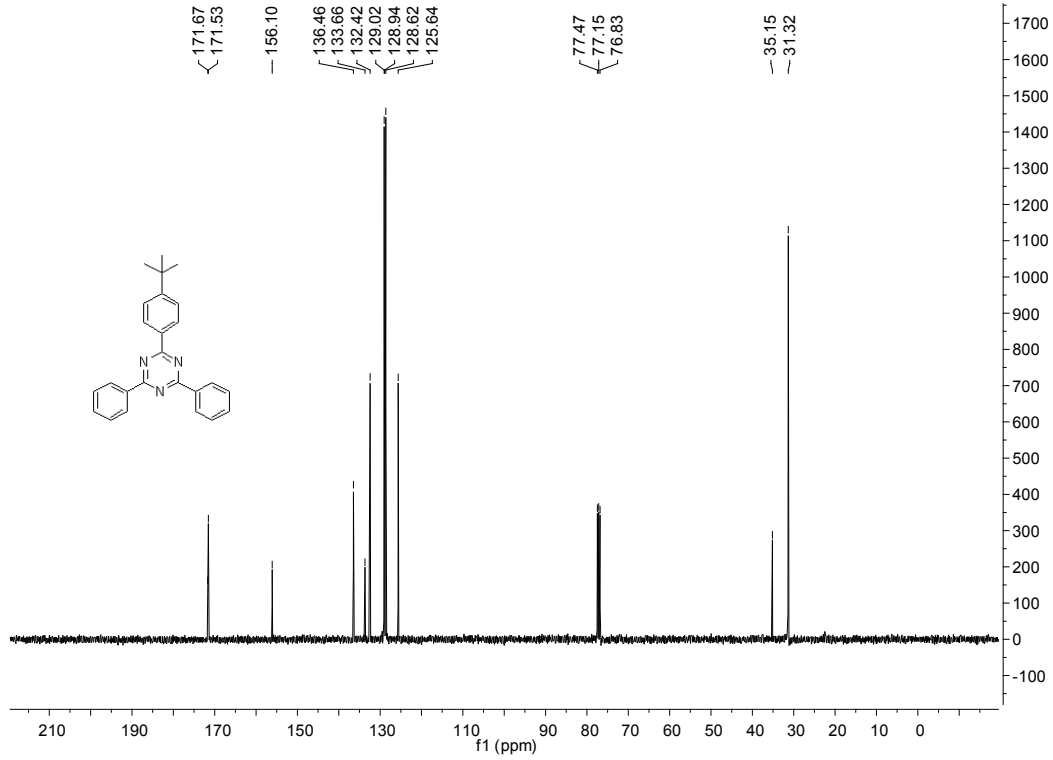
$^1\text{H}$  NMR of 3ab



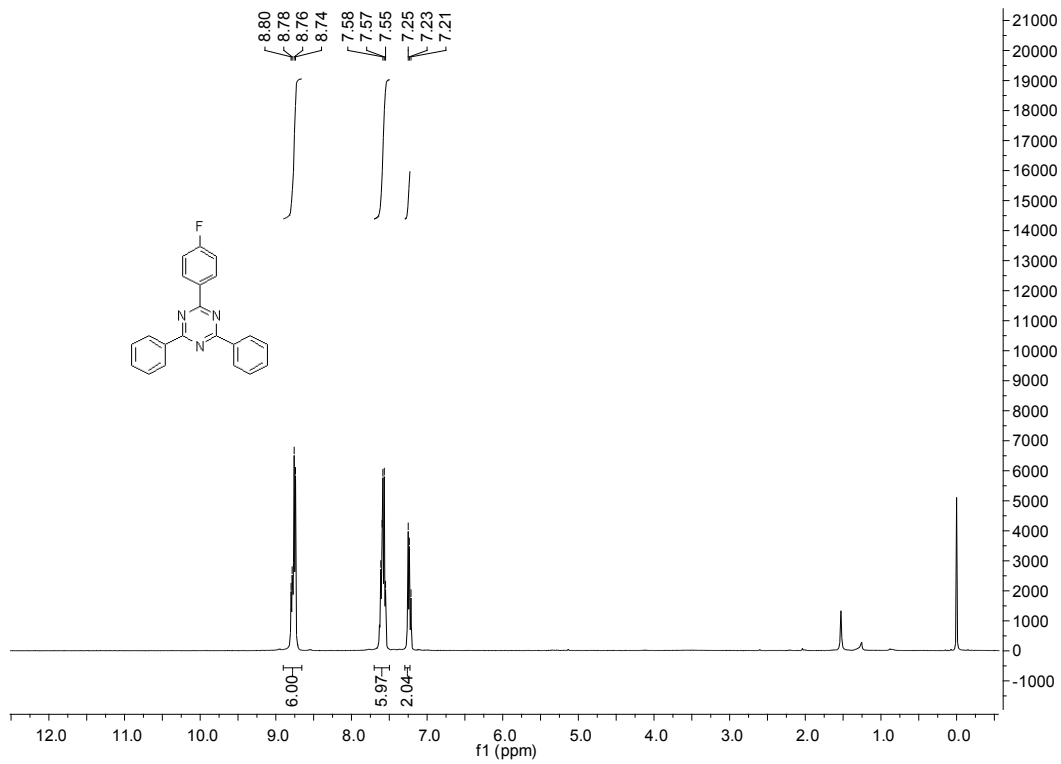
<sup>13</sup>C NMR of 3ab



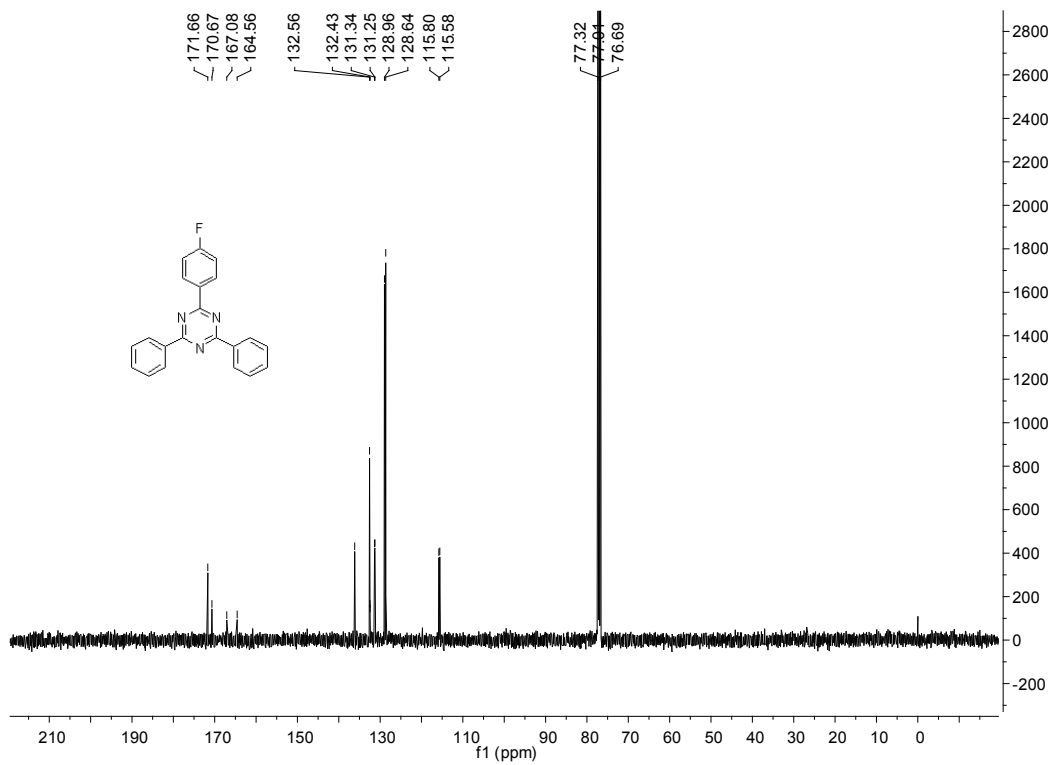
<sup>1</sup>H NMR of 3ac



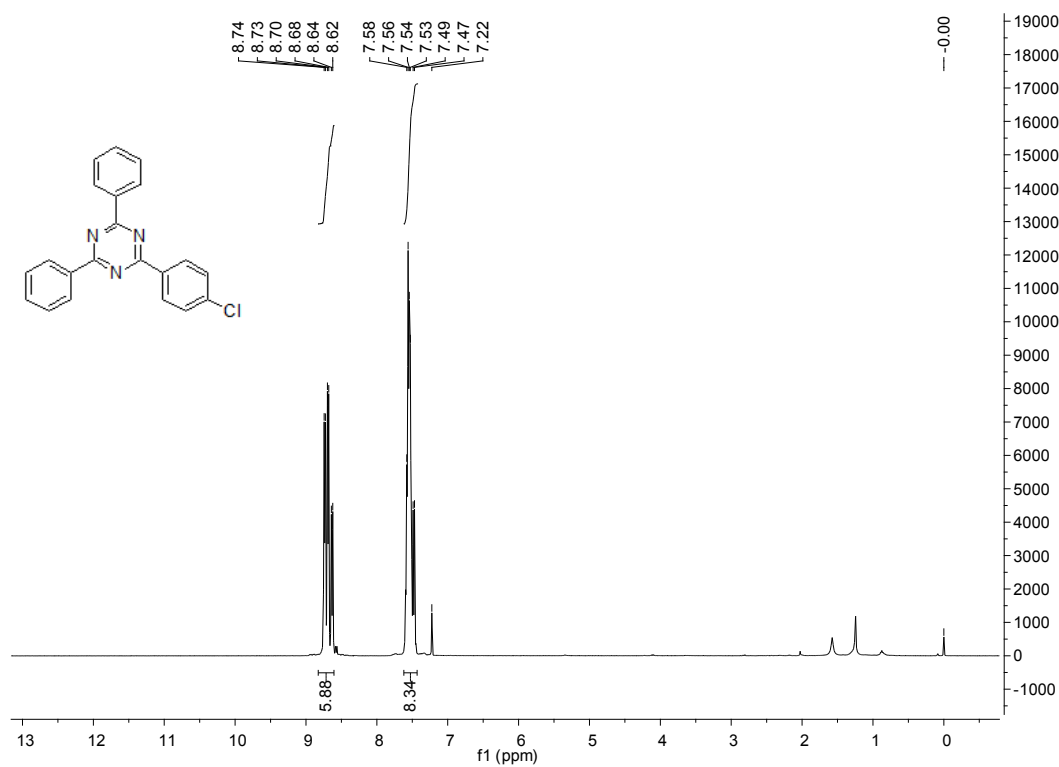
<sup>13</sup>C NMR of 3ac



<sup>1</sup>H NMR of 3ad

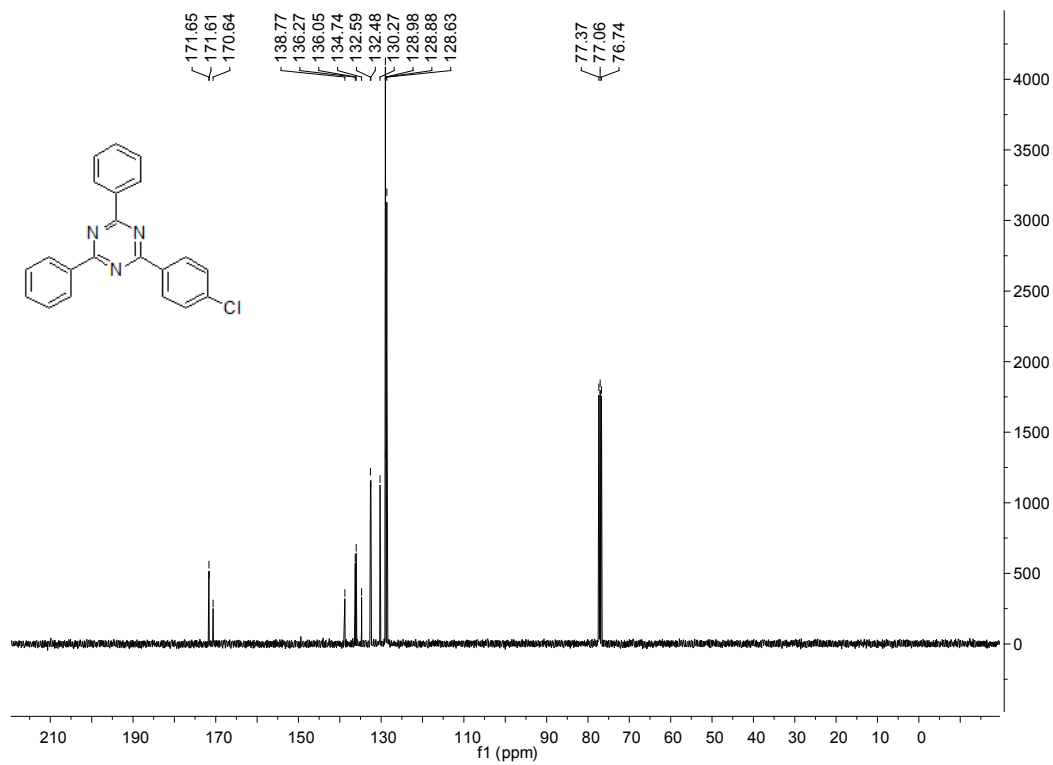


$^{13}\text{C}$  NMR of 3ad

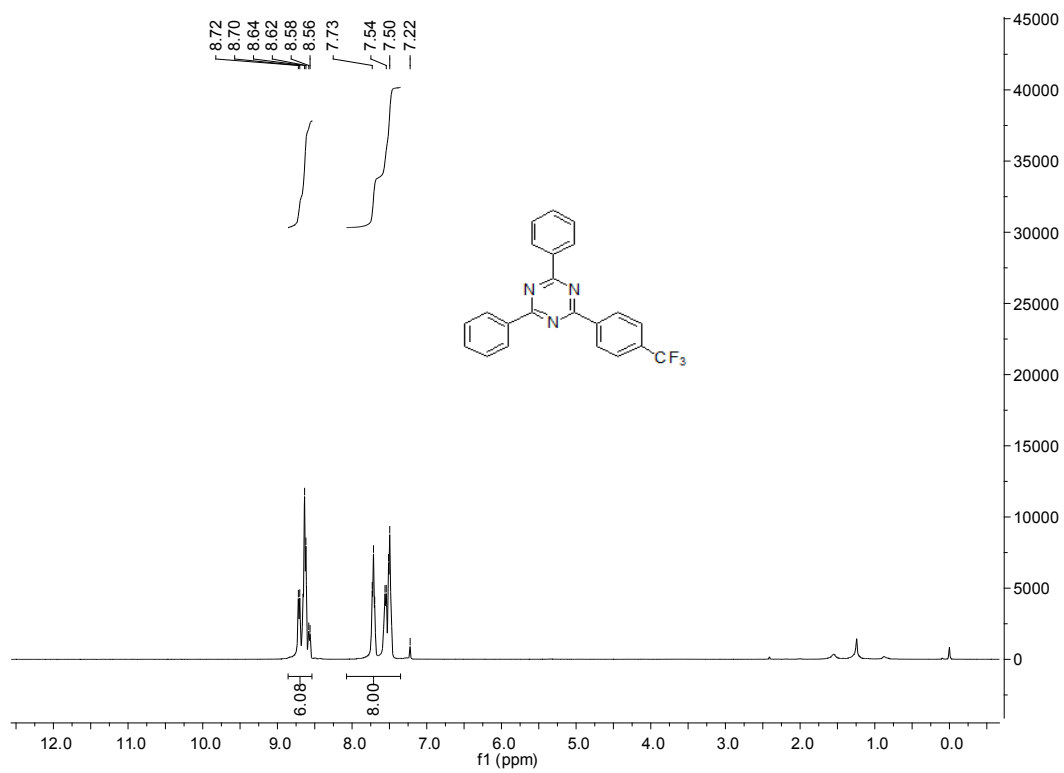


$^1\text{H}$  NMR of 3ae

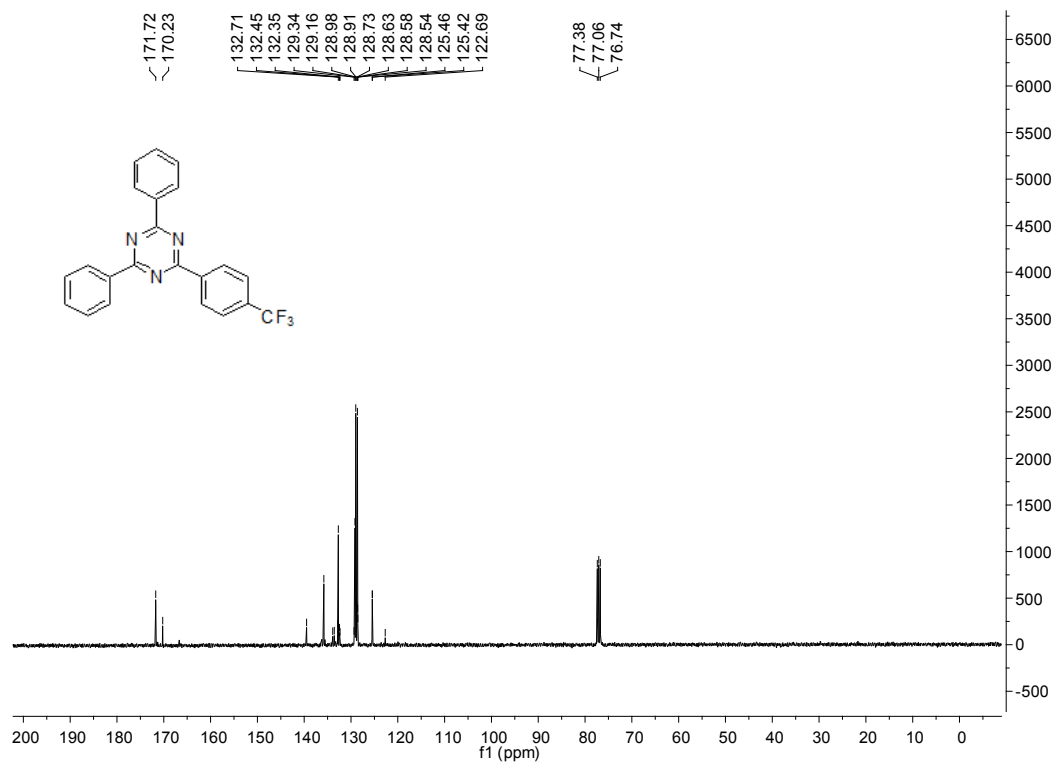




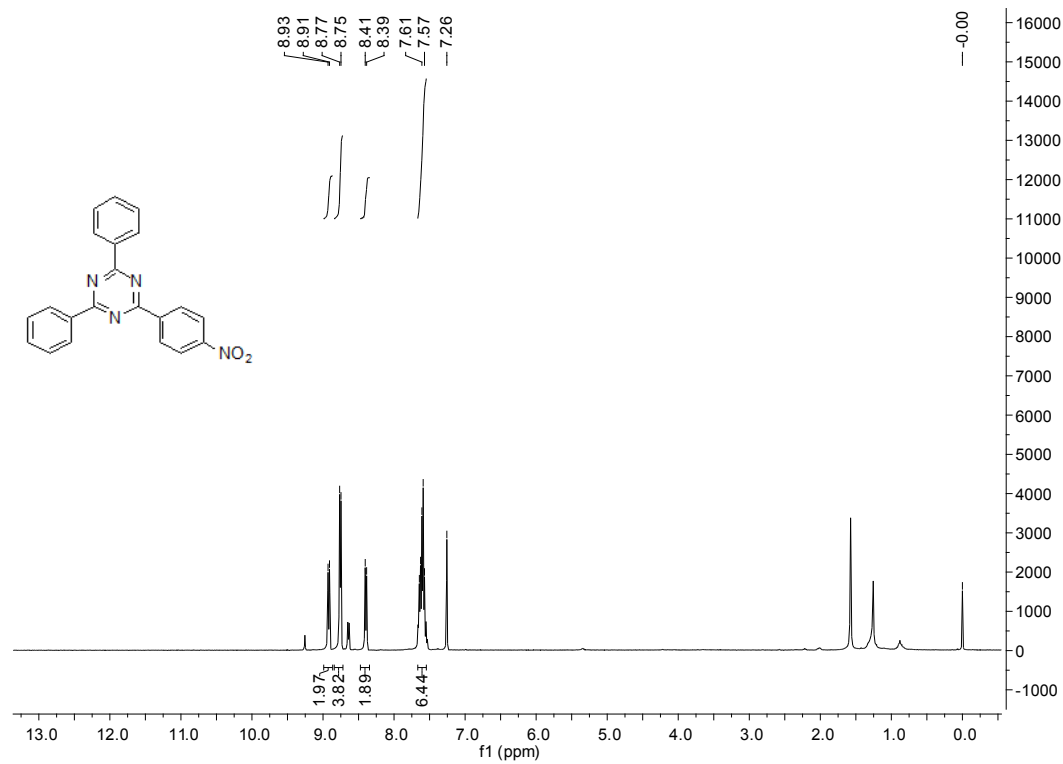
<sup>13</sup>C NMR of 3ae



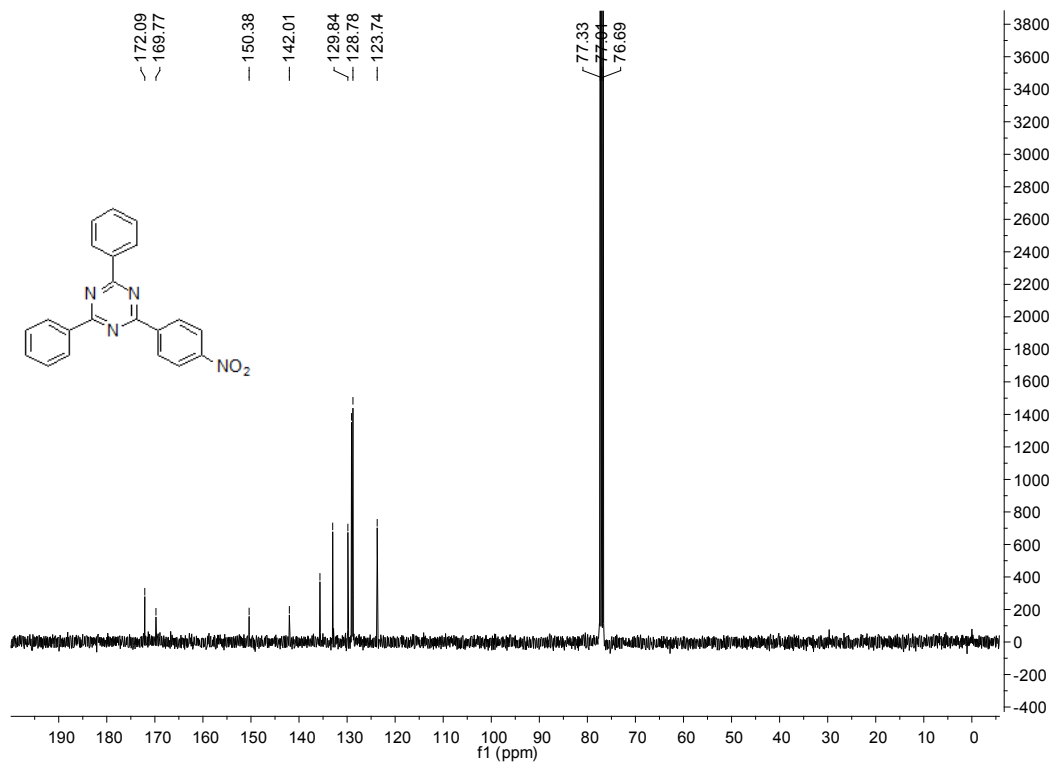
<sup>1</sup>H NMR of 3af



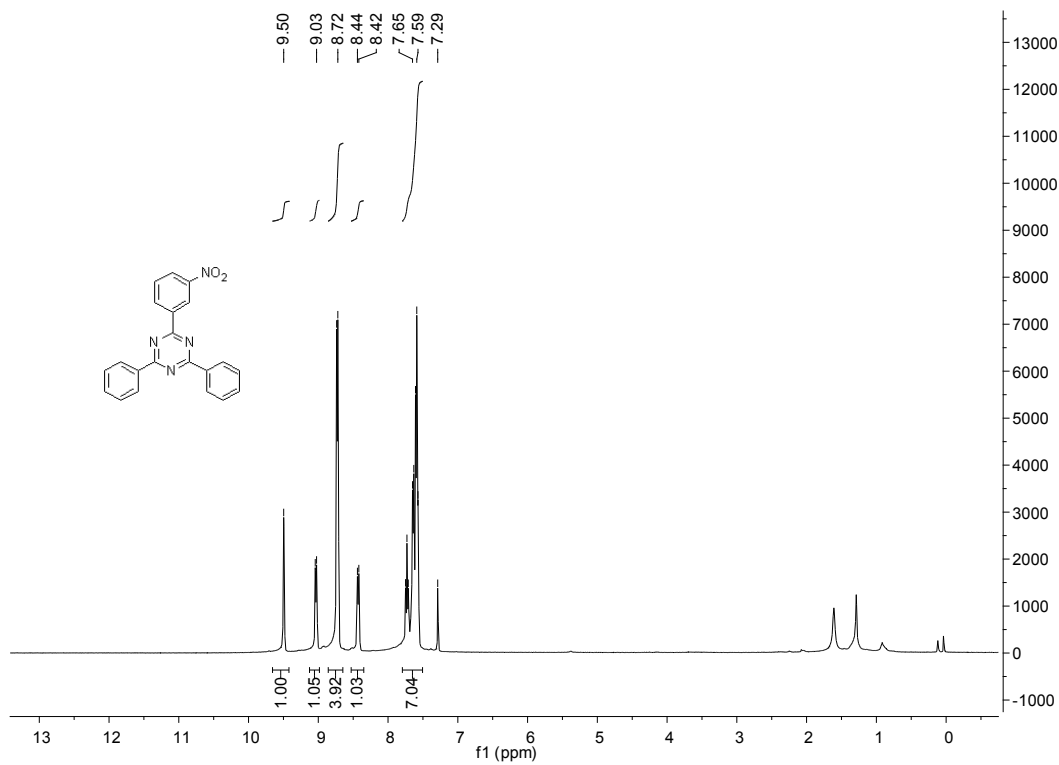
<sup>13</sup>C NMR of 3af



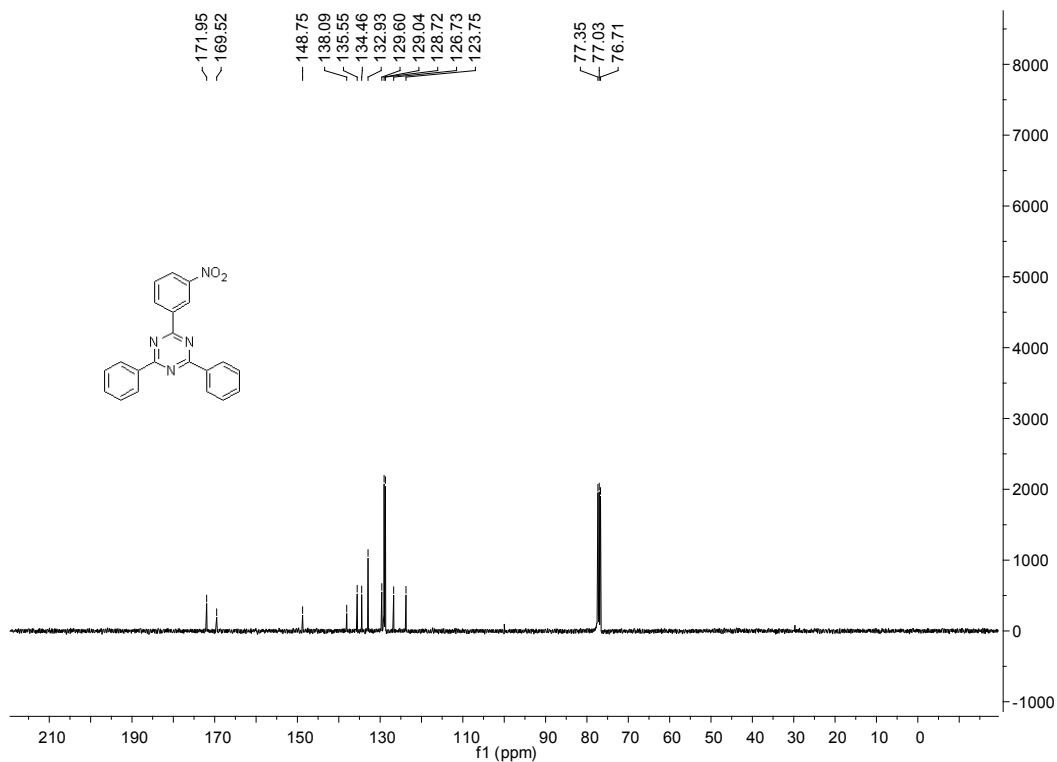
<sup>1</sup>H NMR of 3ag



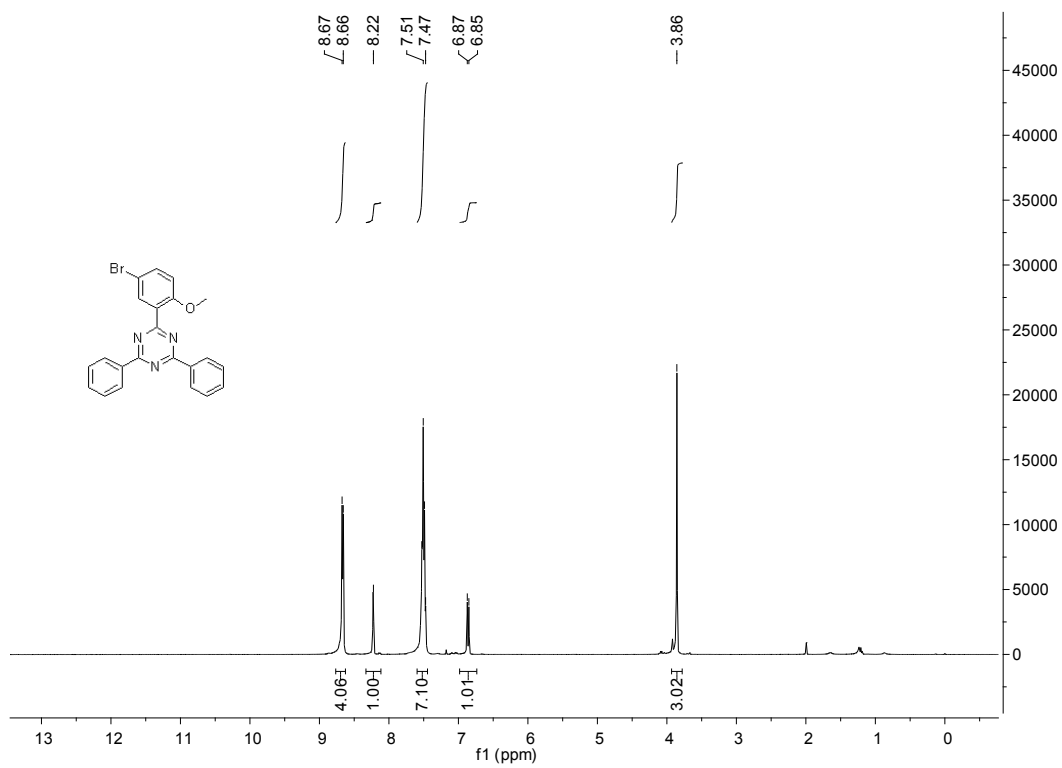
<sup>13</sup>C NMR of **3ag**



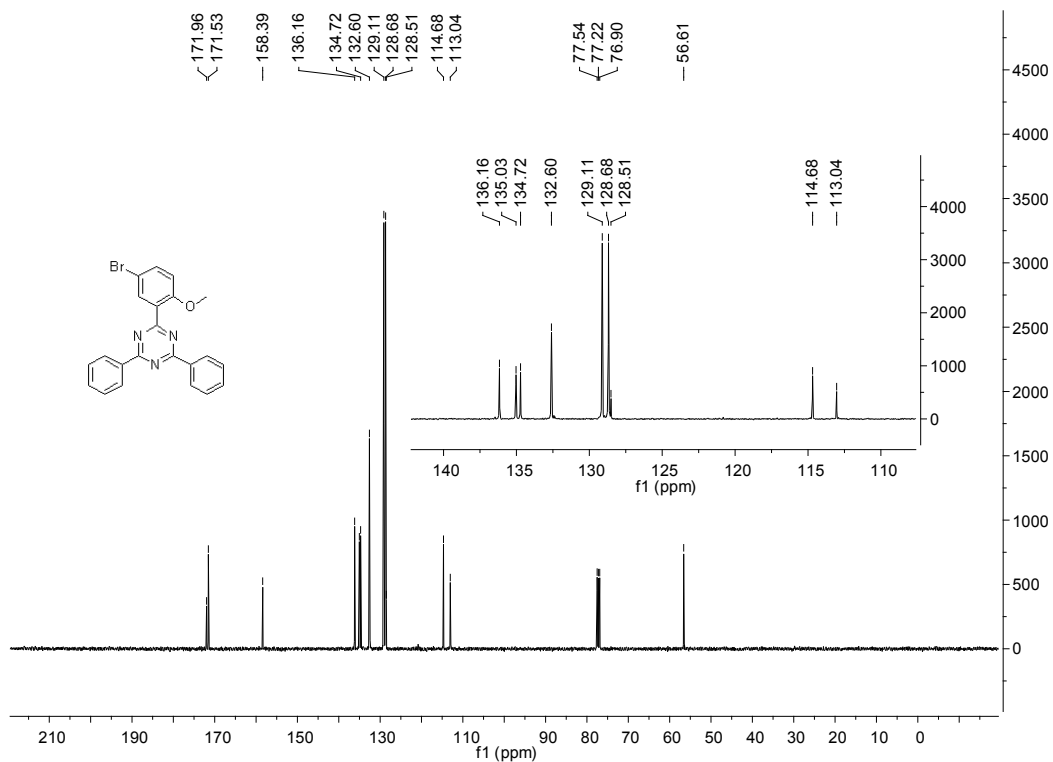
<sup>1</sup>H NMR of **3ah**



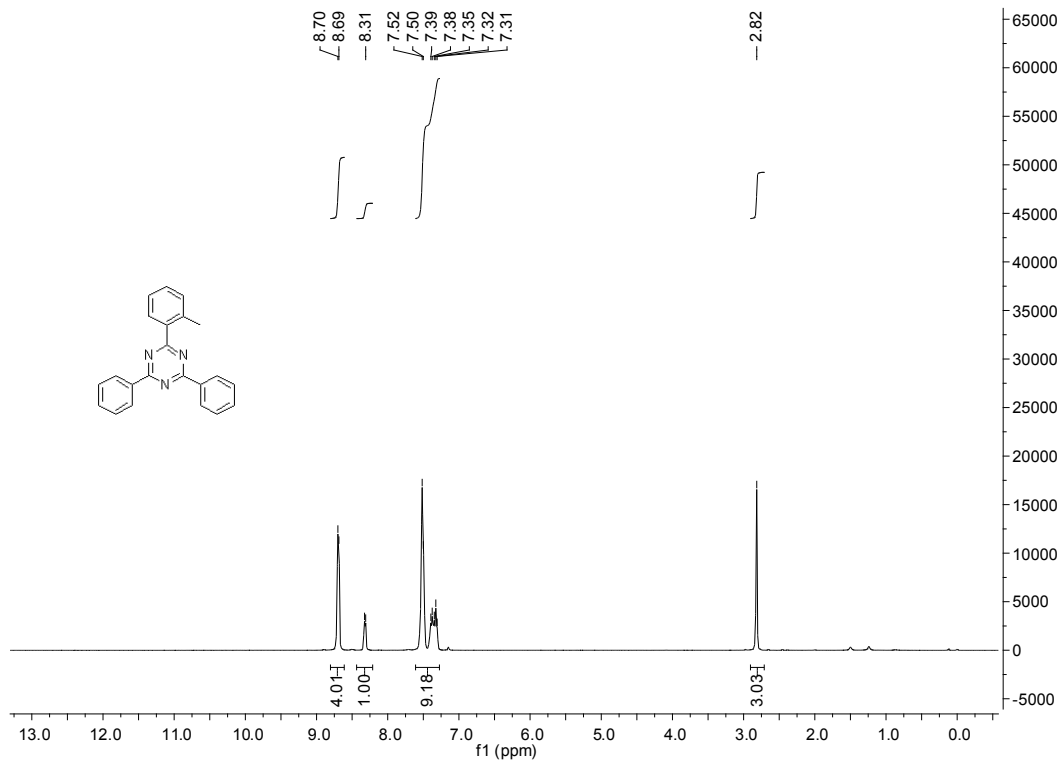
$^{13}\text{C}$  NMR of 3ah



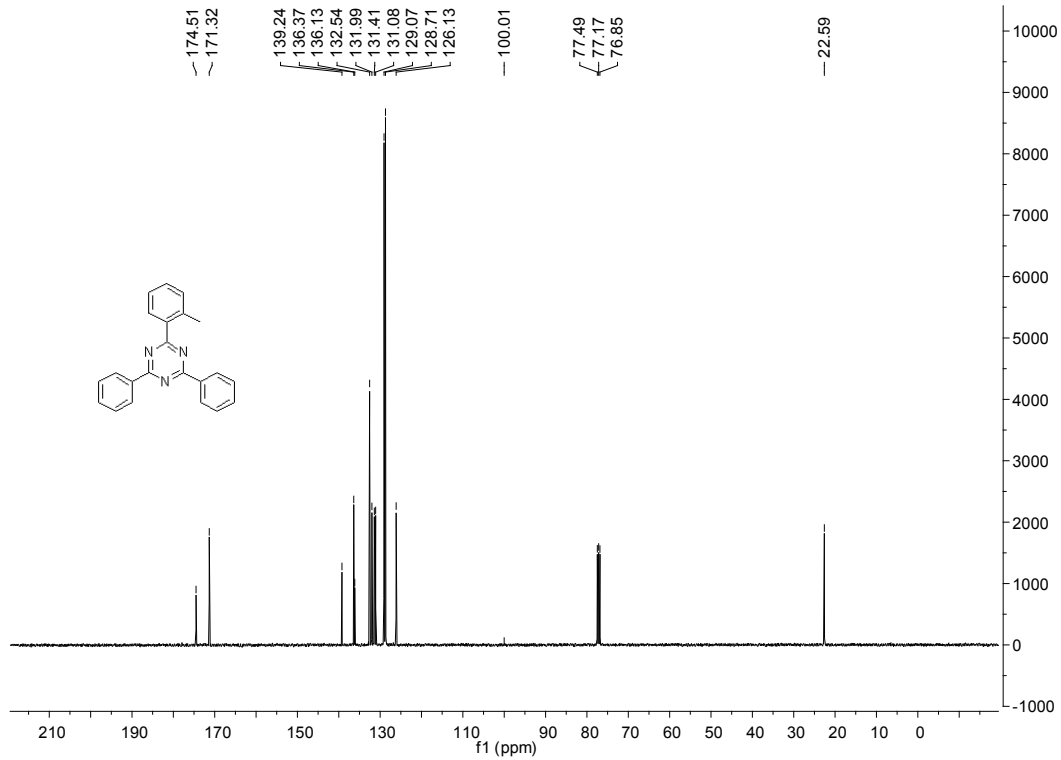
$^1\text{H}$  NMR of 3ai



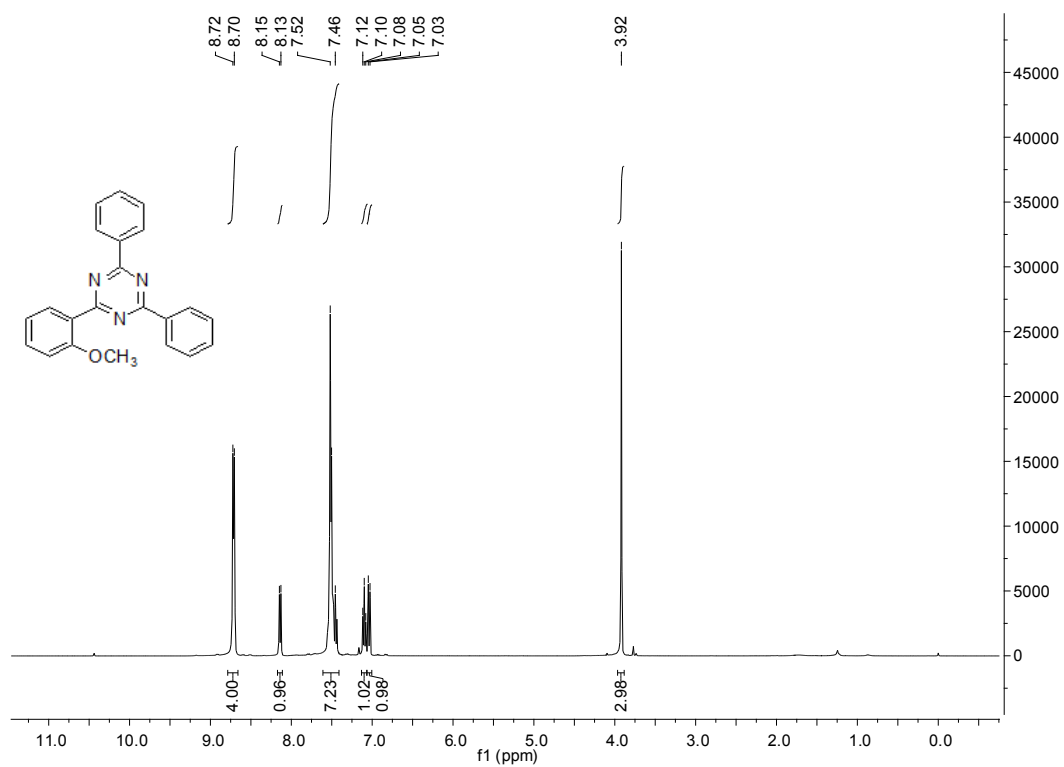
$^{13}\text{C}$  NMR of **3ai**



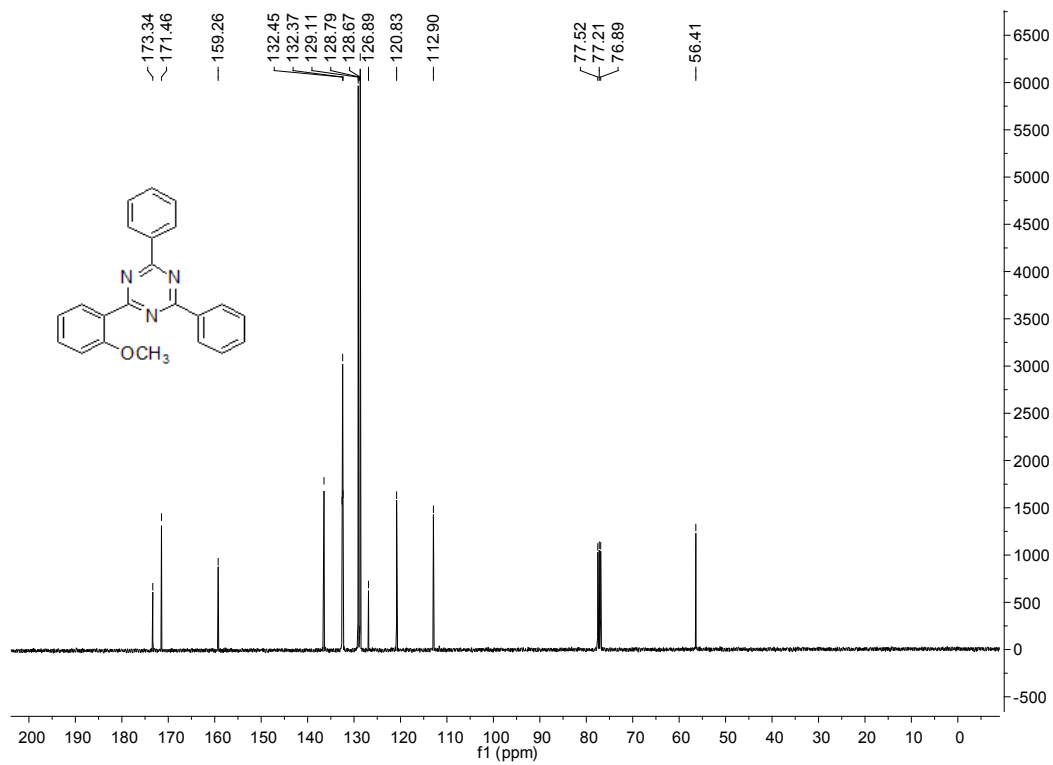
$^1\text{H}$  NMR of **3aj**



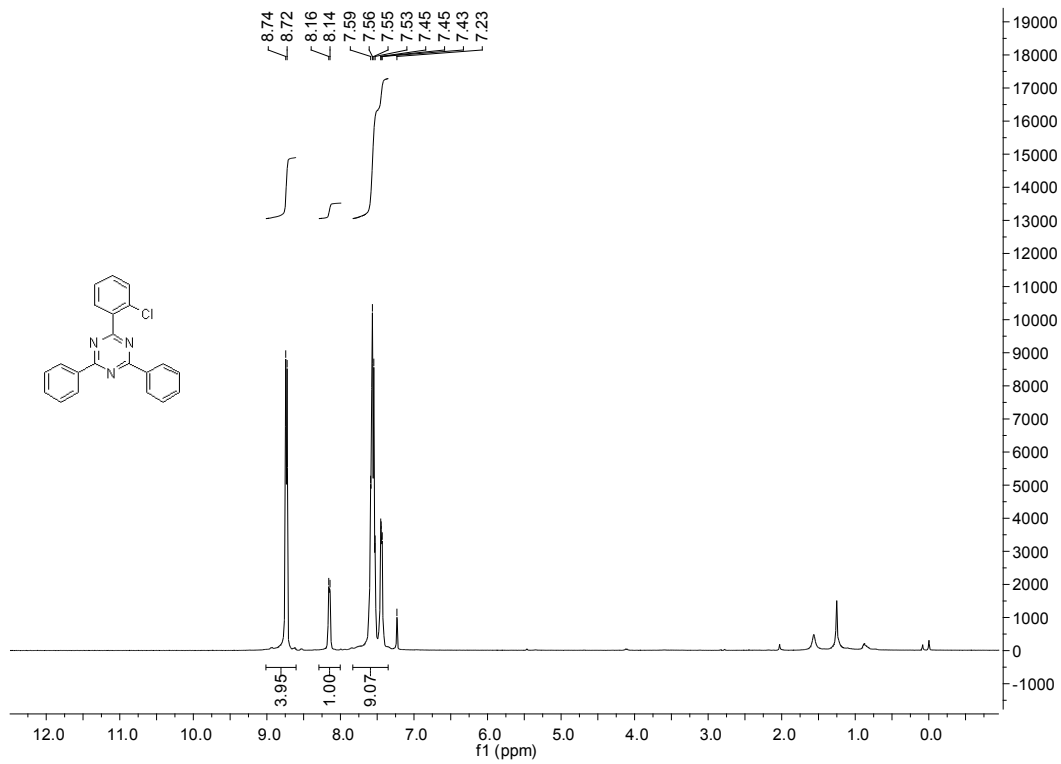
<sup>13</sup>C NMR of **3aj**



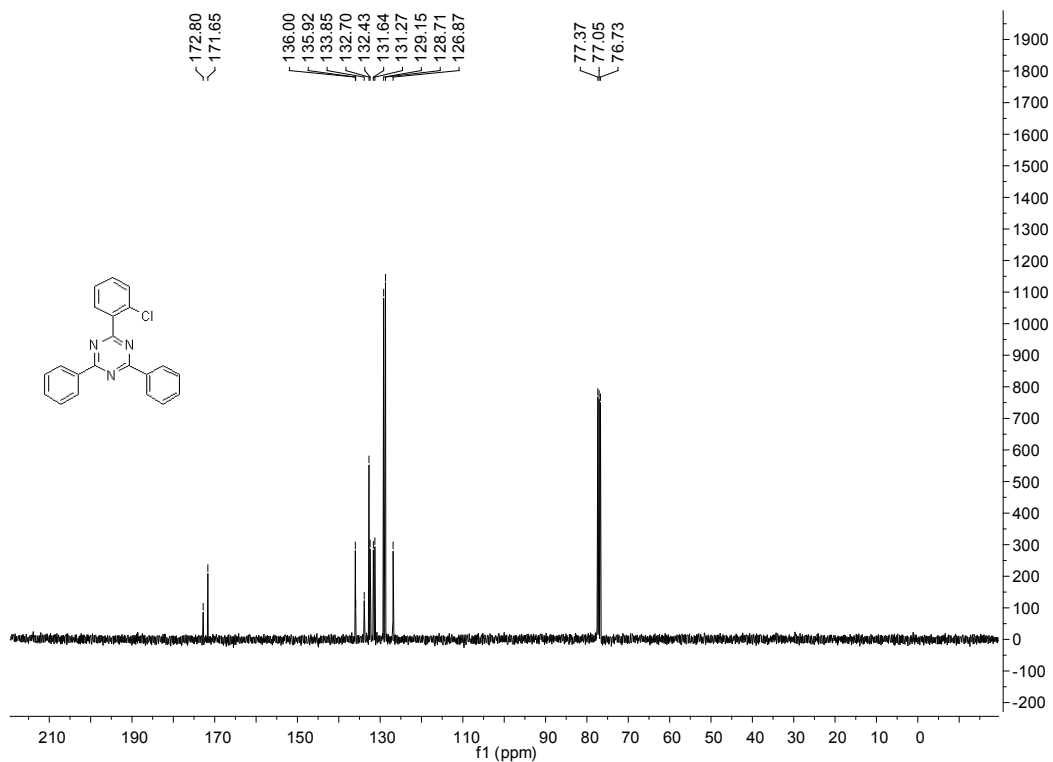
<sup>1</sup>H NMR of **3ak**



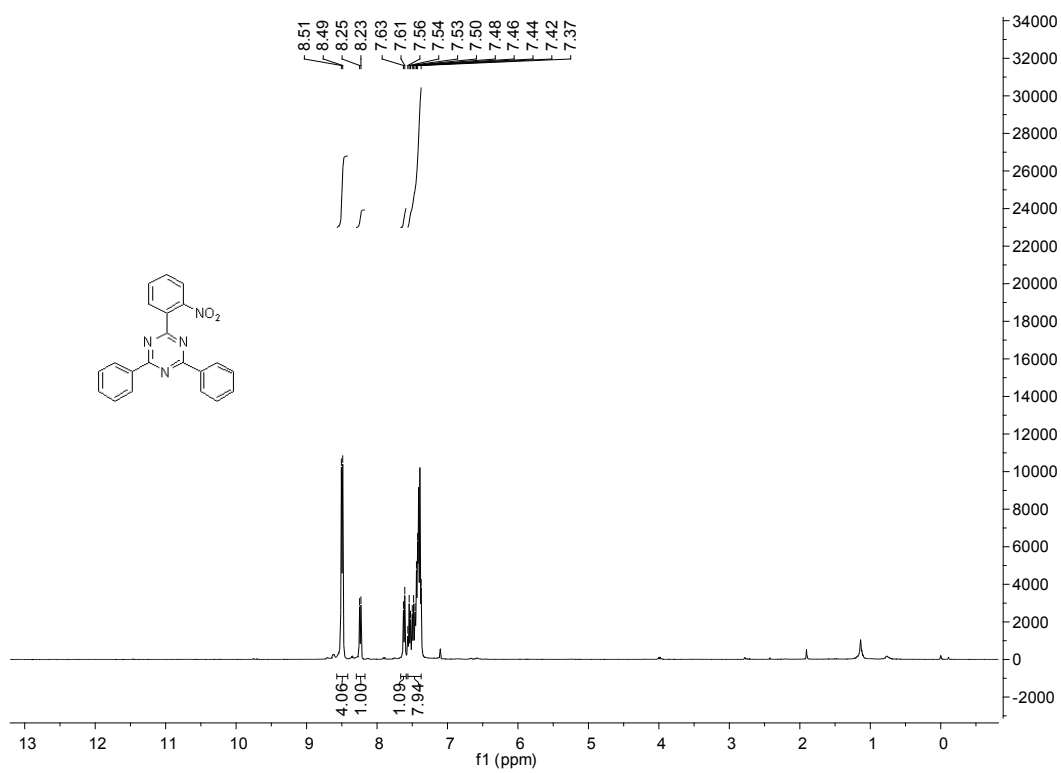
$^{13}\text{C}$  NMR of 3ak



$^1\text{H}$  NMR of 3al

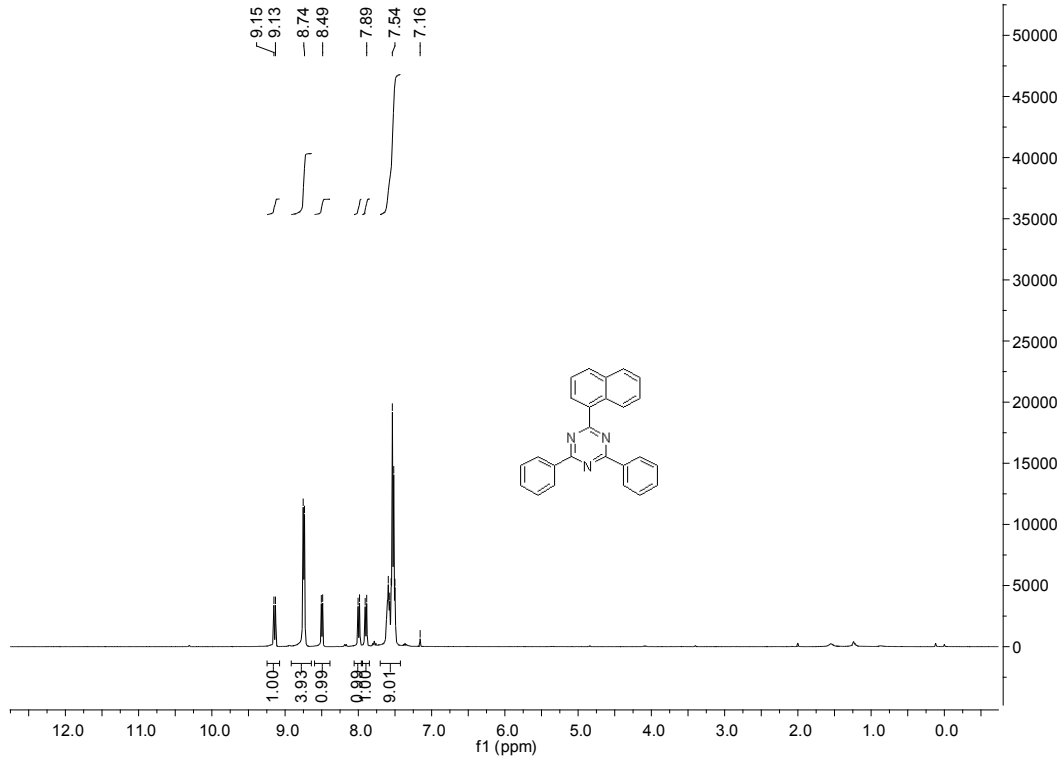
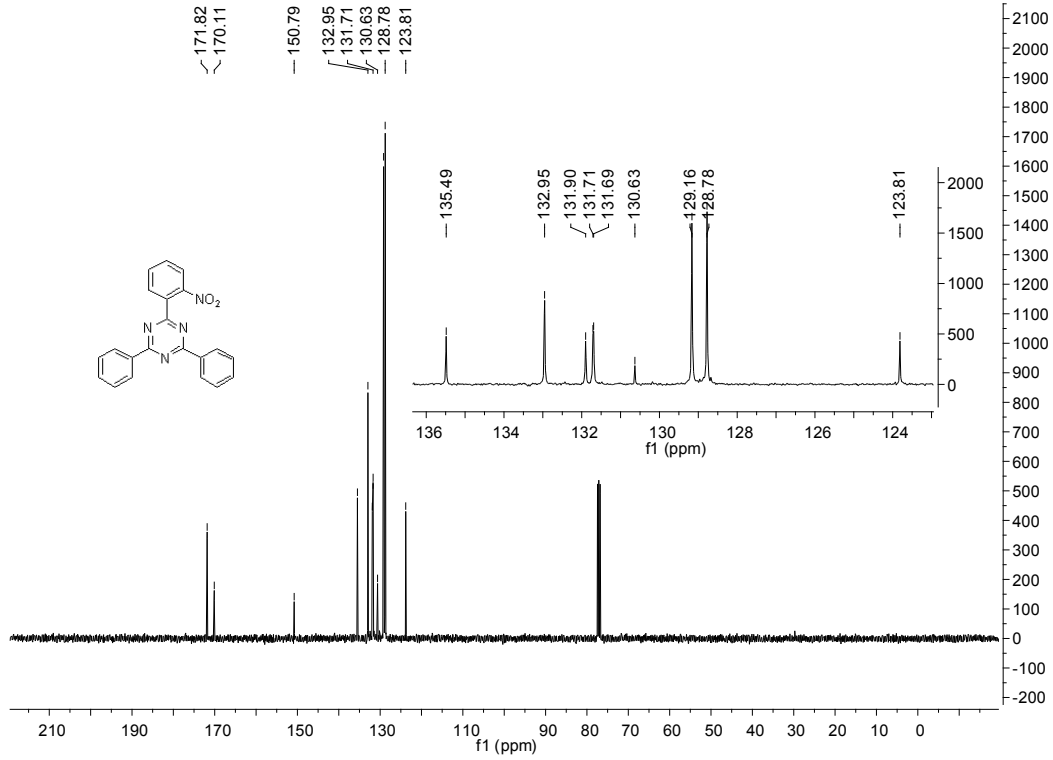


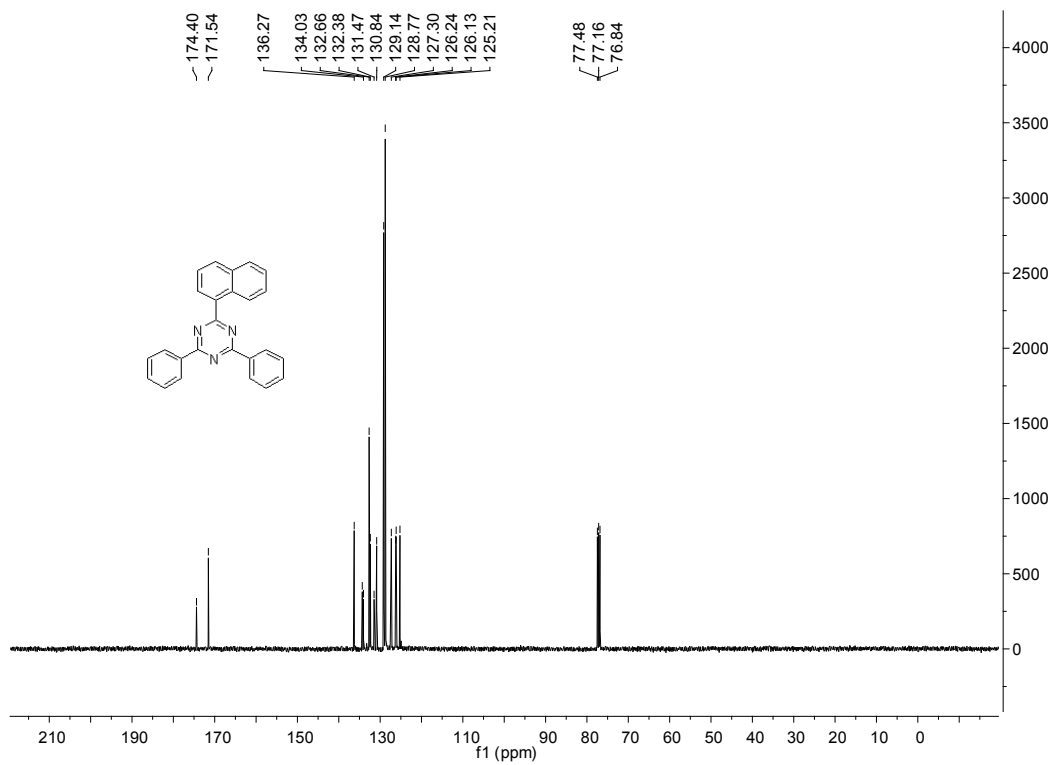
<sup>13</sup>C NMR of 3al



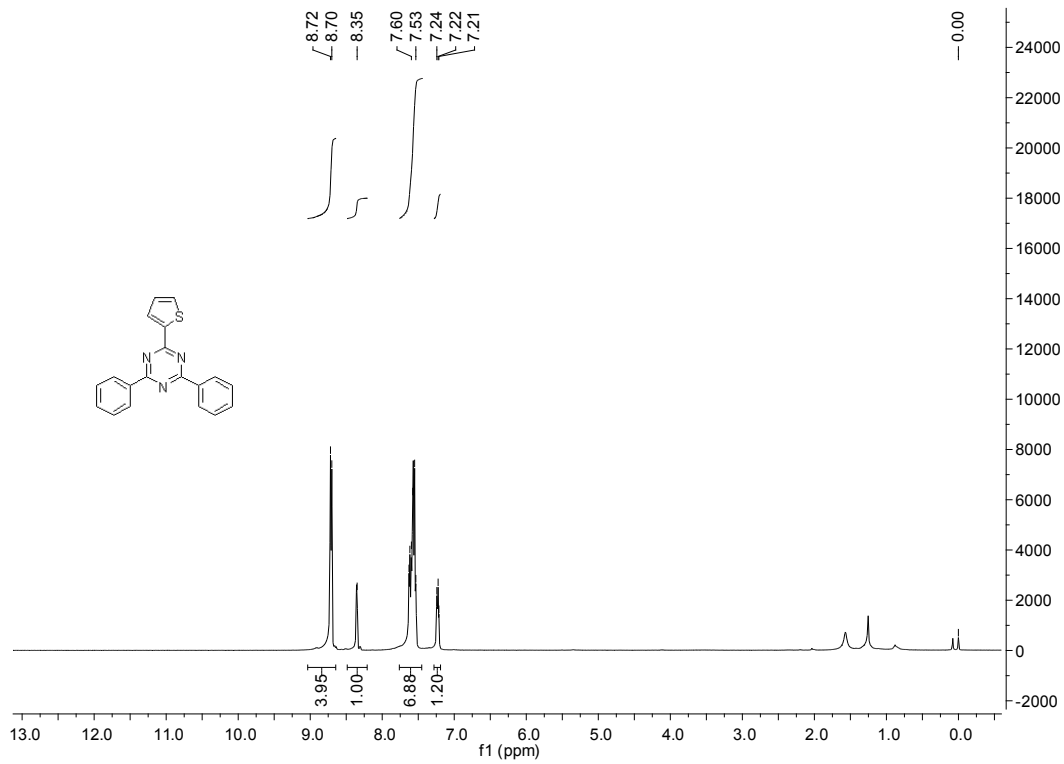
<sup>1</sup>H NMR of 3am



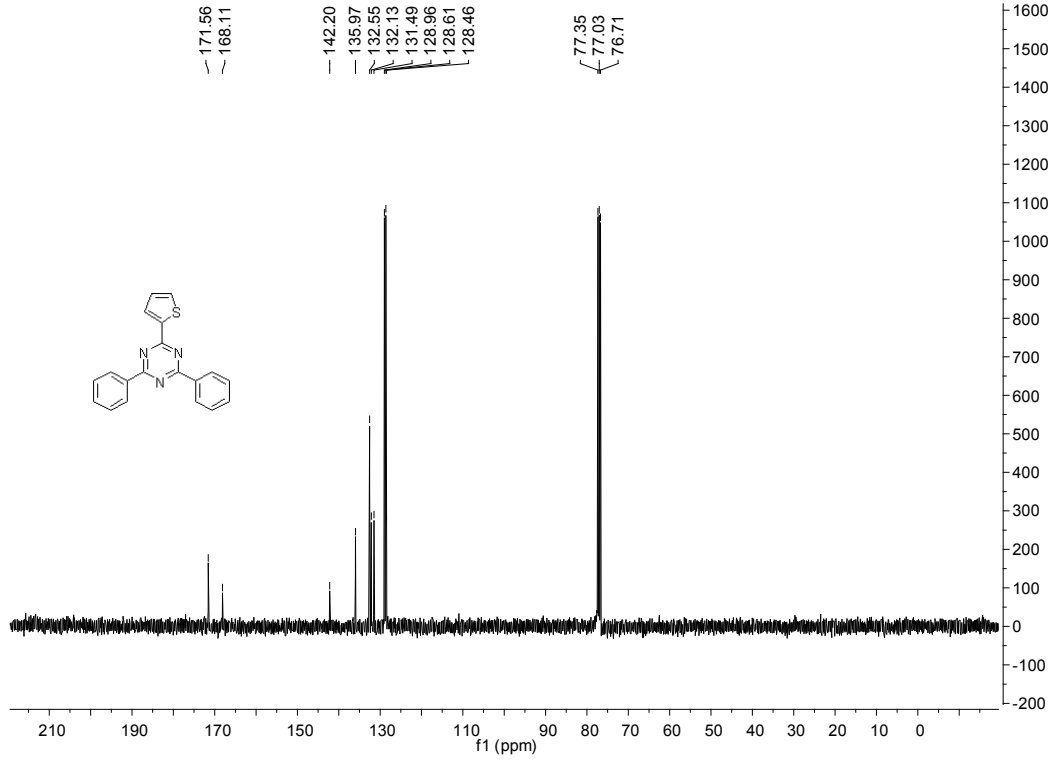




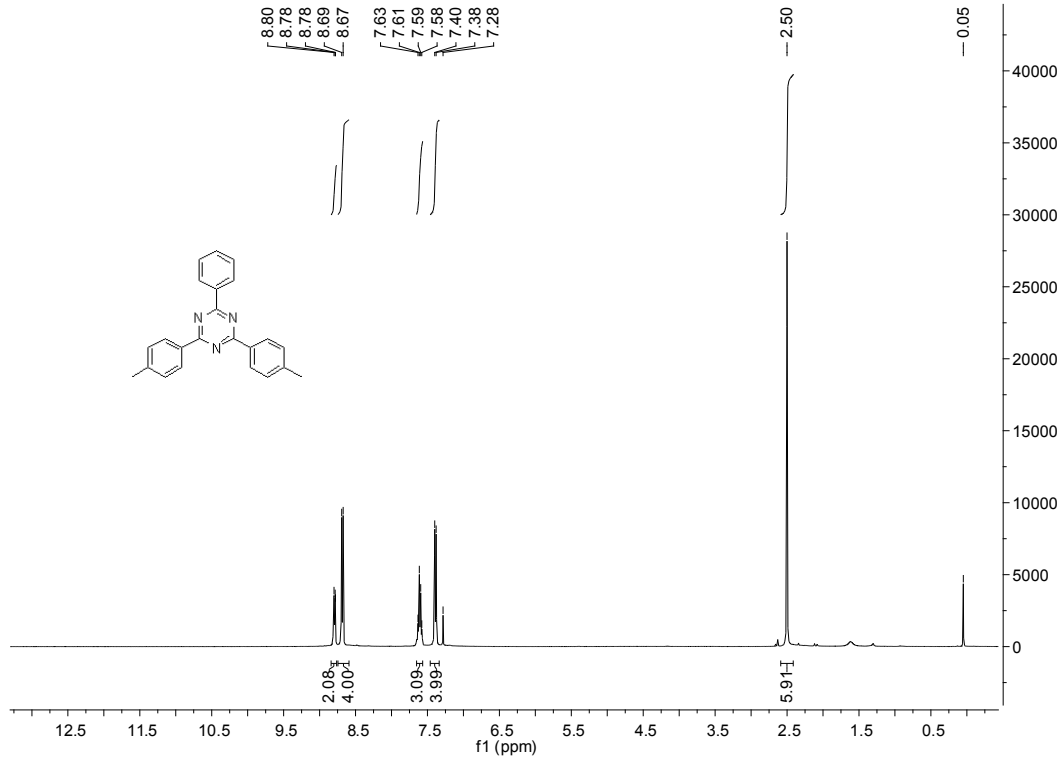
$^{13}\text{C}$  NMR of 3an



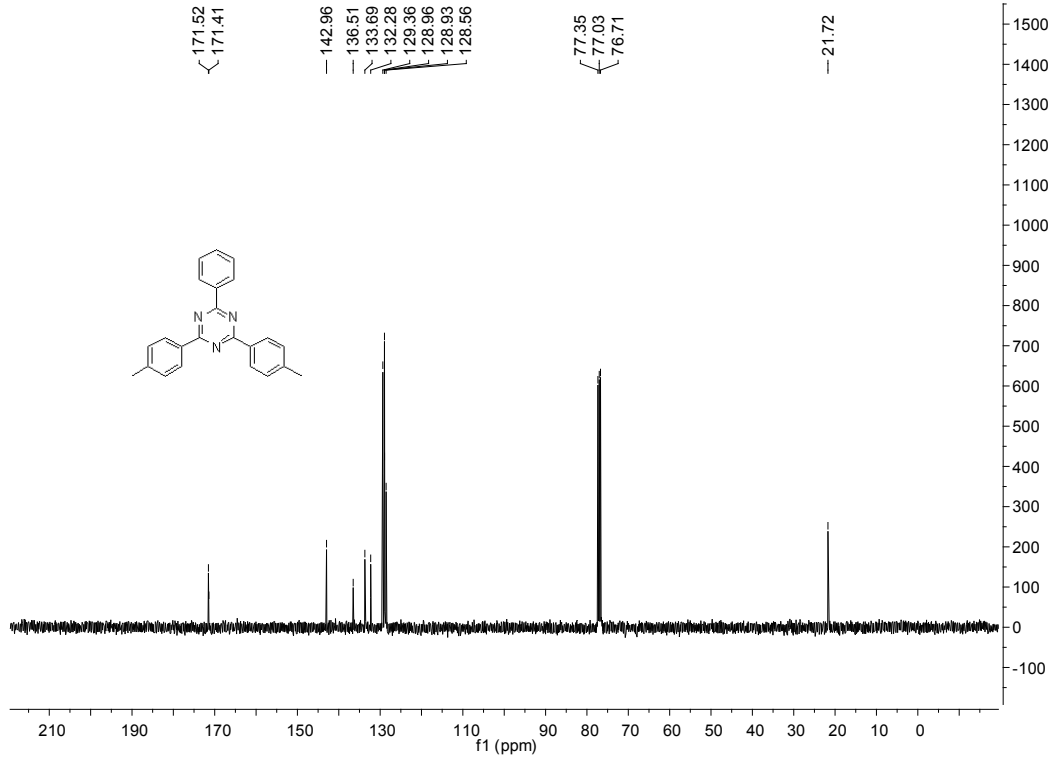
$^1\text{H}$  NMR of 3ao



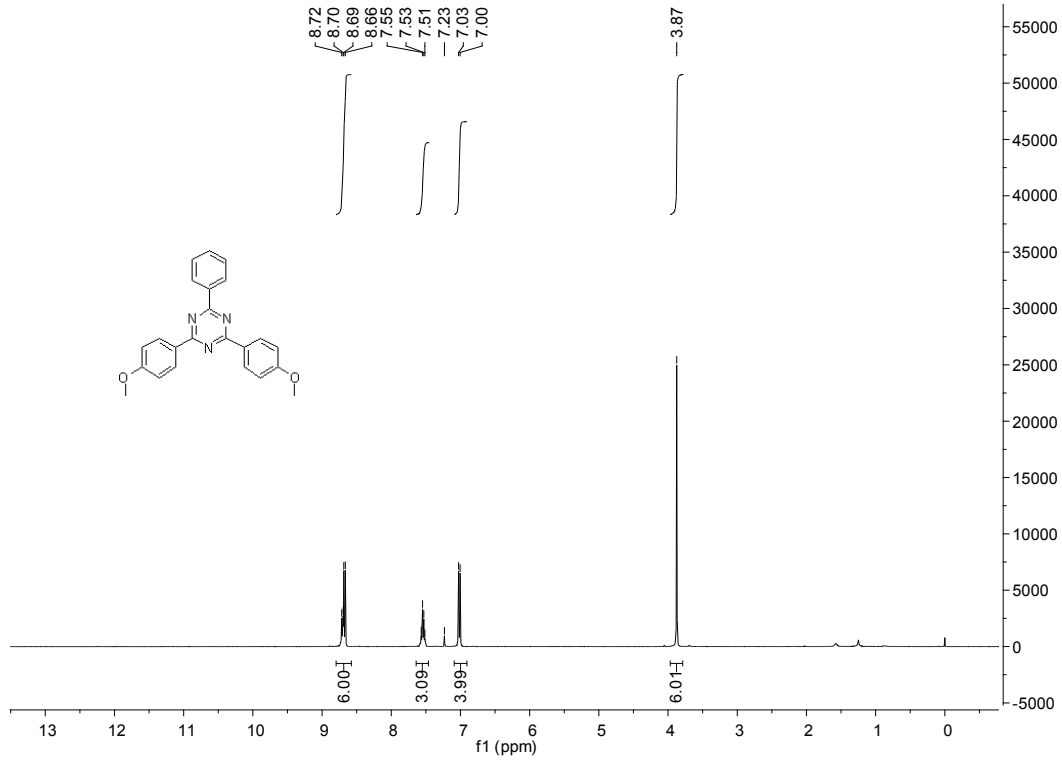
<sup>13</sup>C NMR of **3ao**



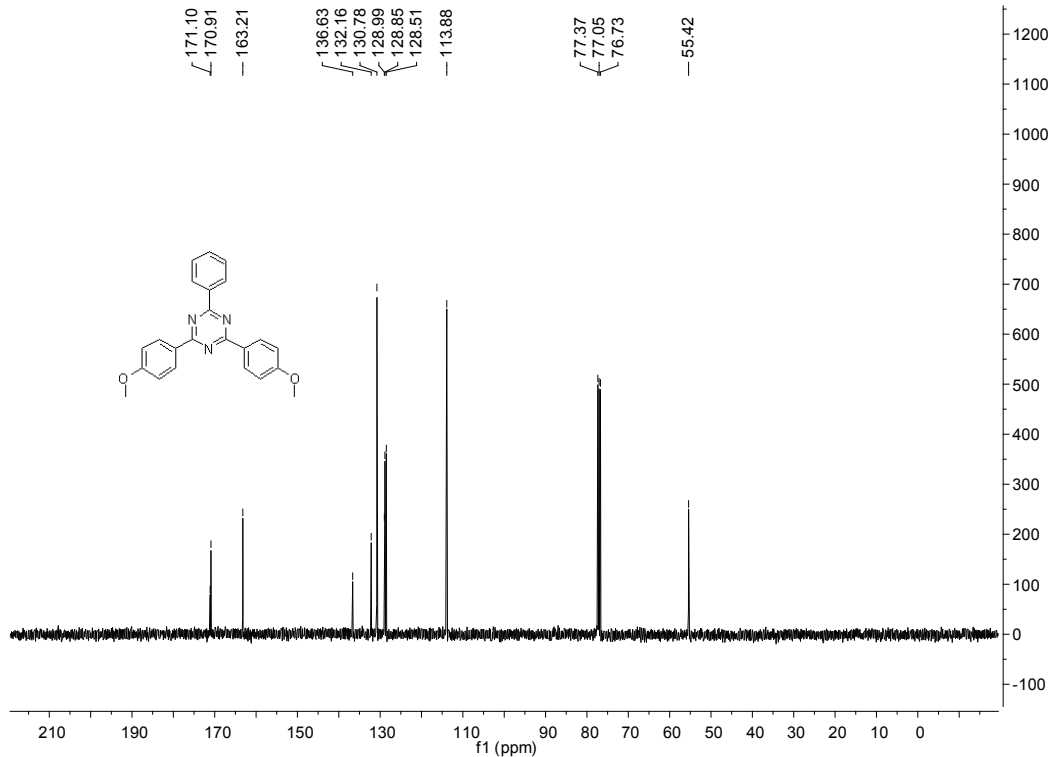
<sup>1</sup>H NMR of **3ba**



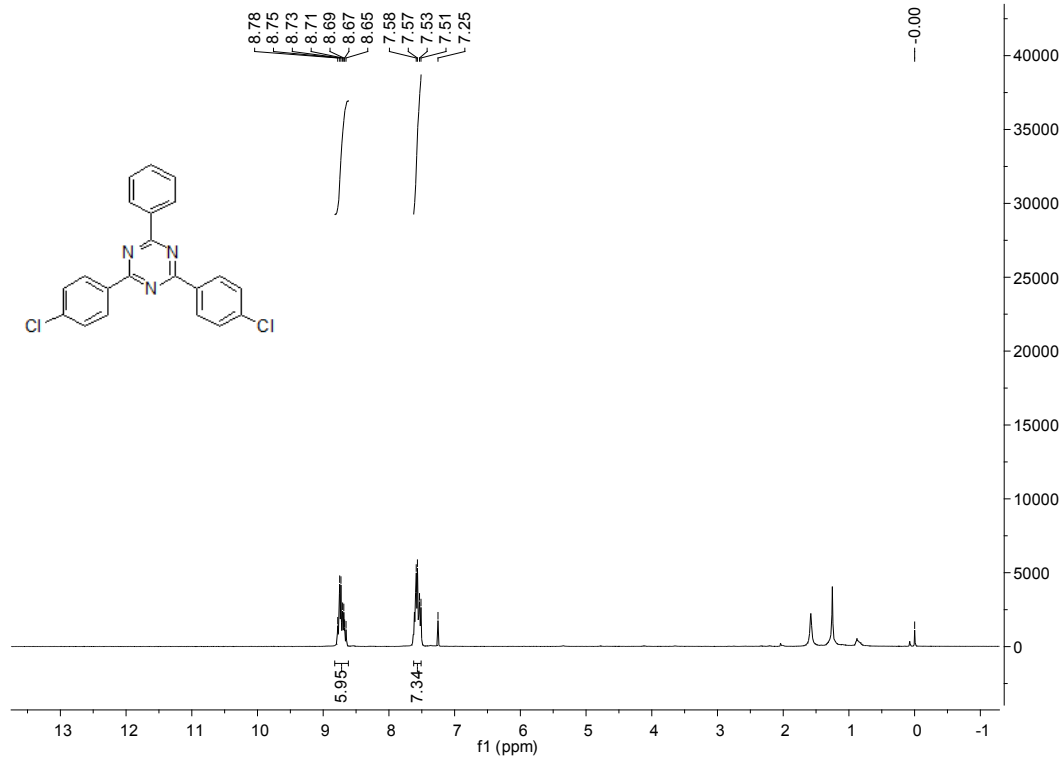
$^{13}\text{C}$  NMR of 3ba



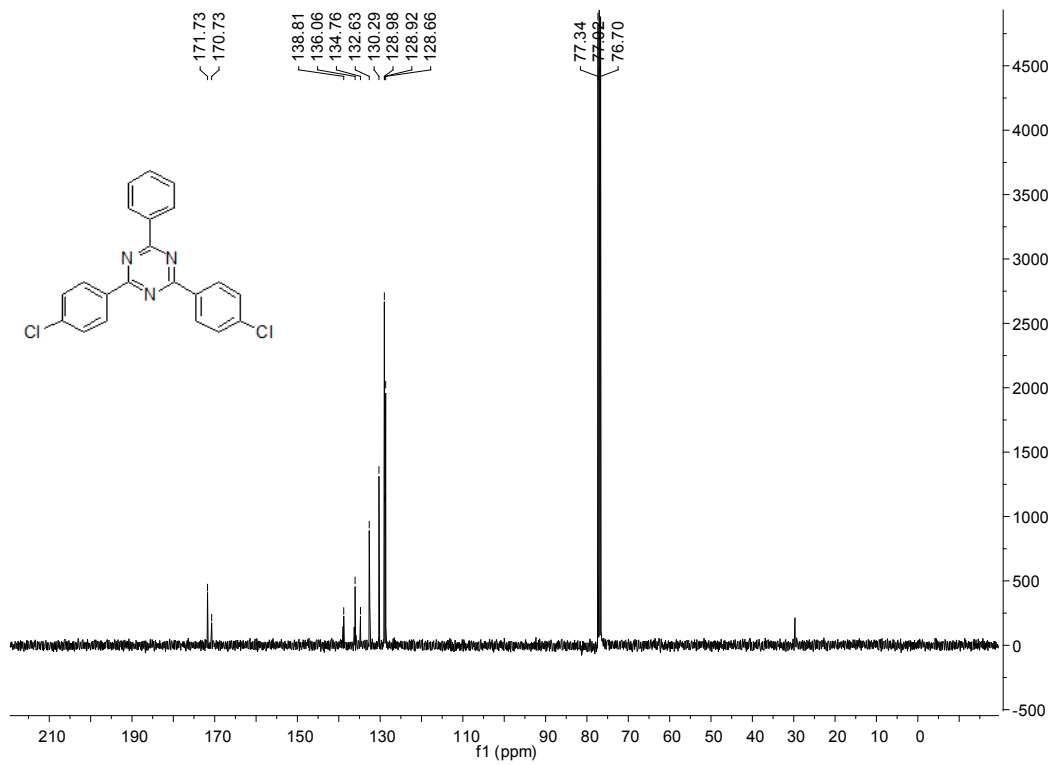
$^1\text{H}$  NMR of 3ca



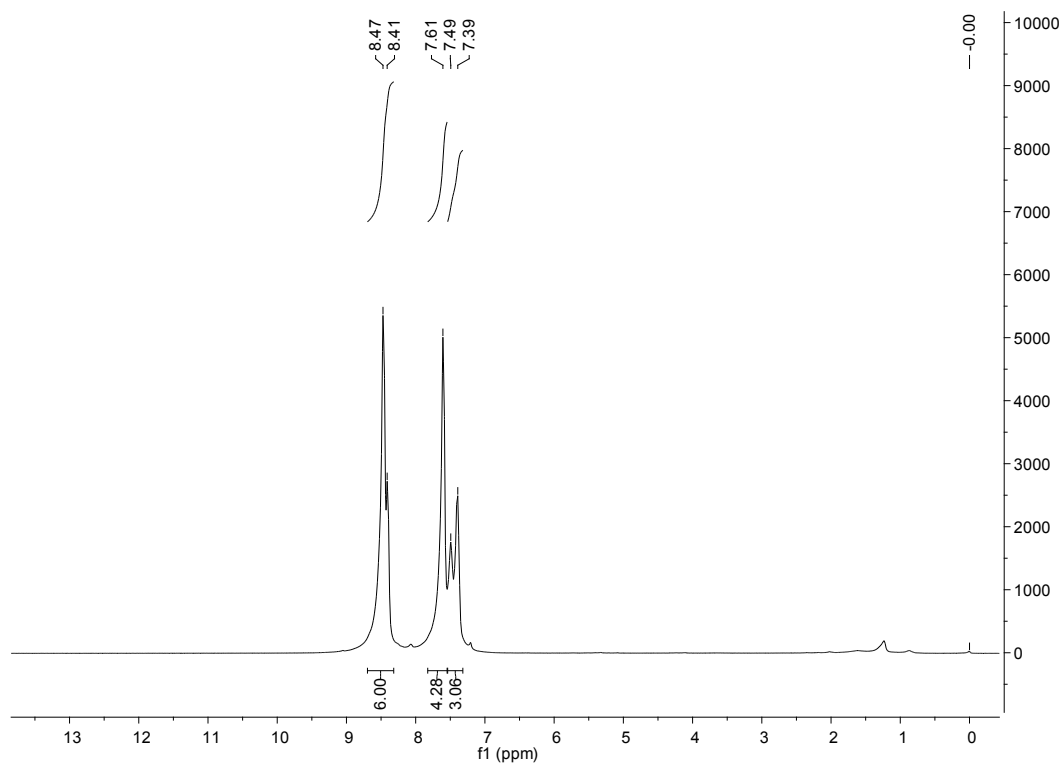
<sup>13</sup>C NMR of 3ca



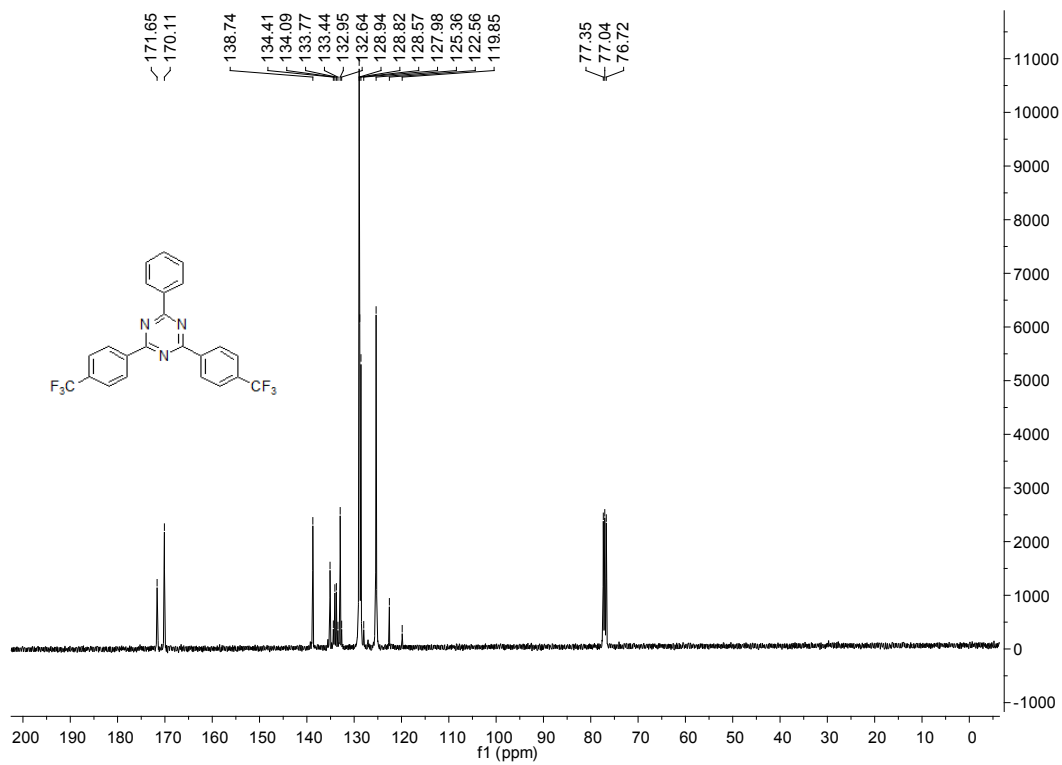
<sup>1</sup>H NMR of 3da



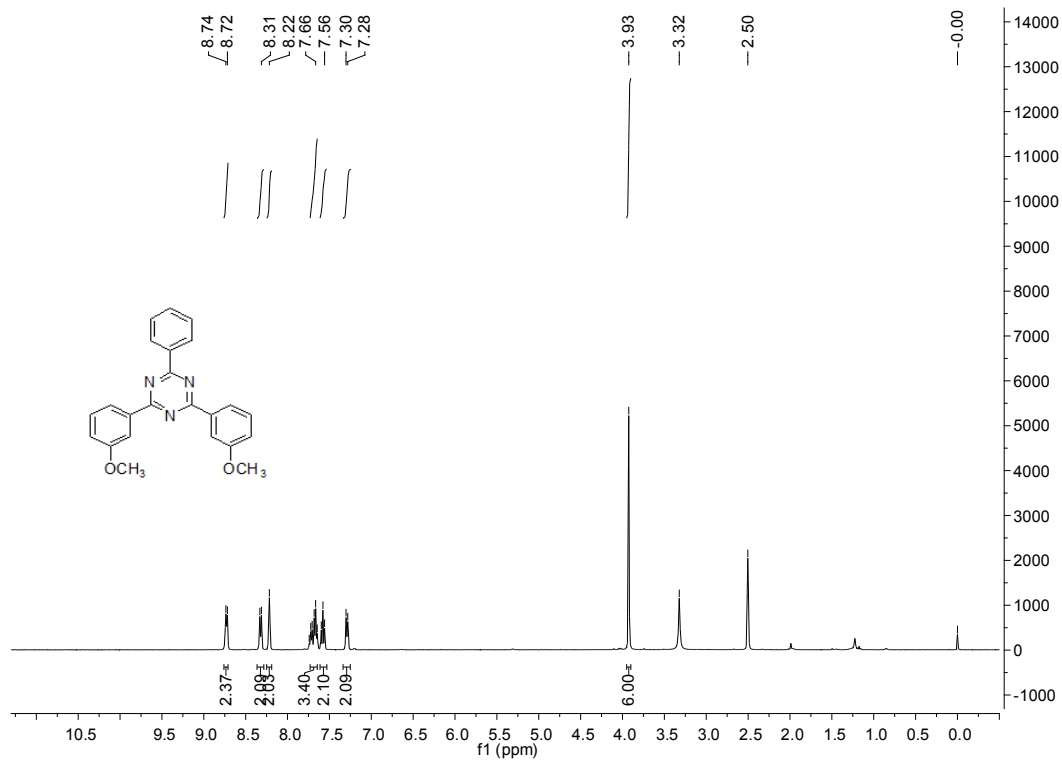
<sup>13</sup>C NMR of 3da



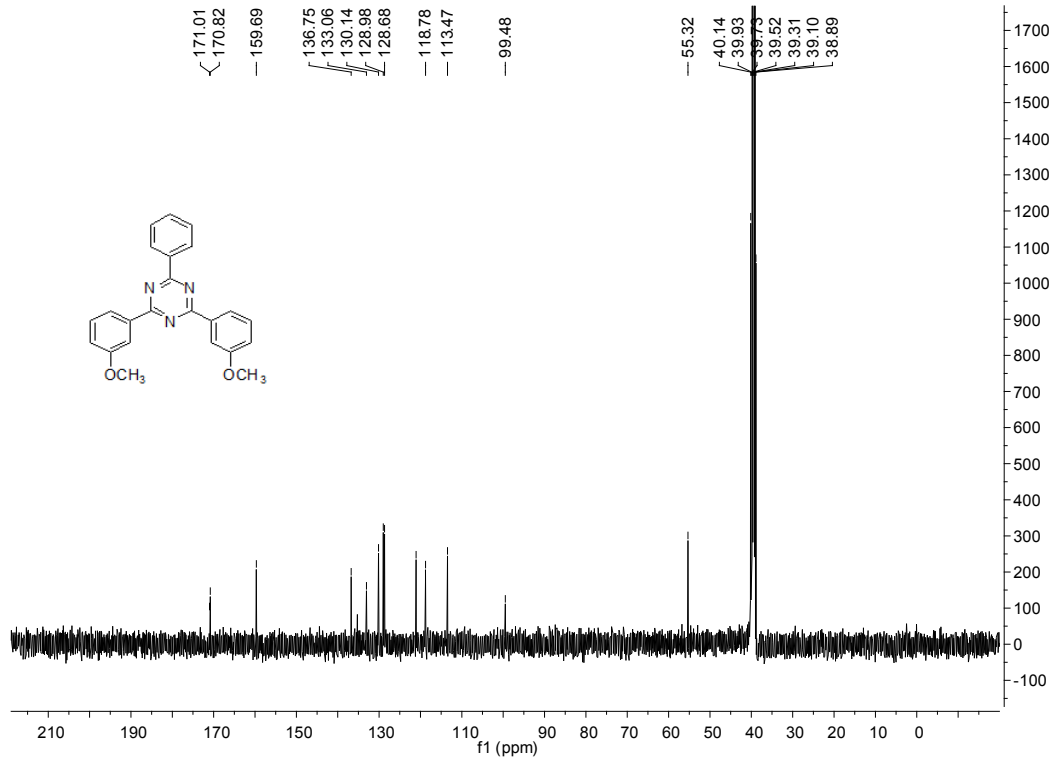
<sup>1</sup>H NMR of 3ea



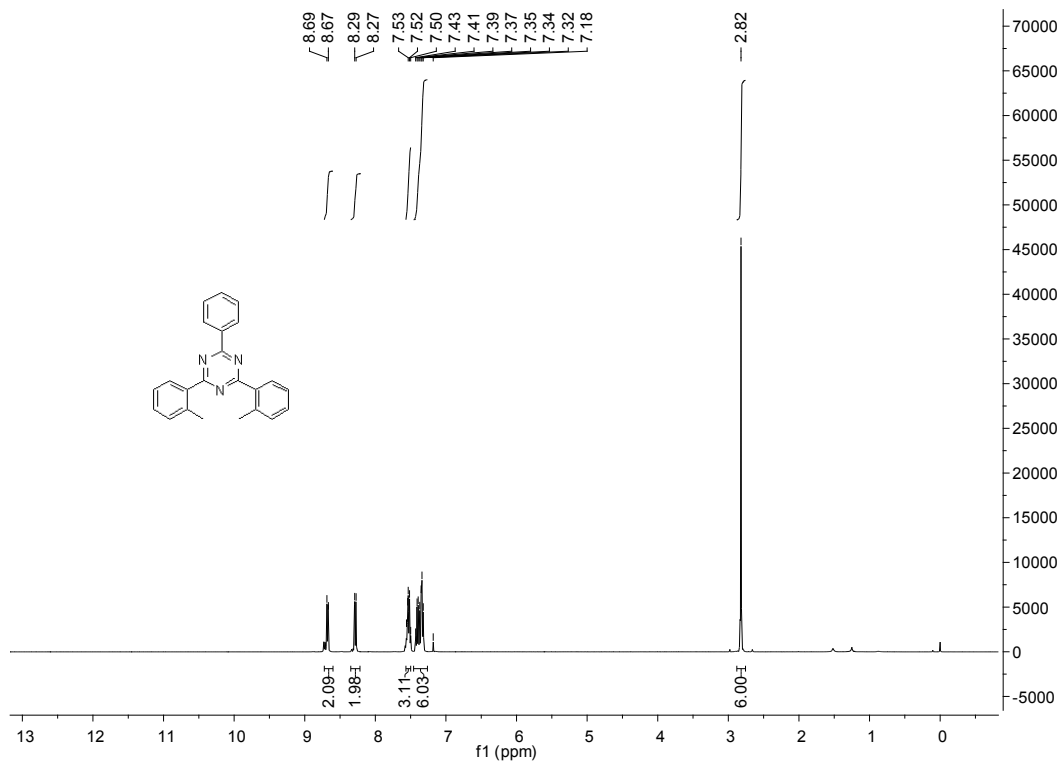
**<sup>13</sup>C NMR of 3ea**



**<sup>1</sup>H NMR of 3fa**

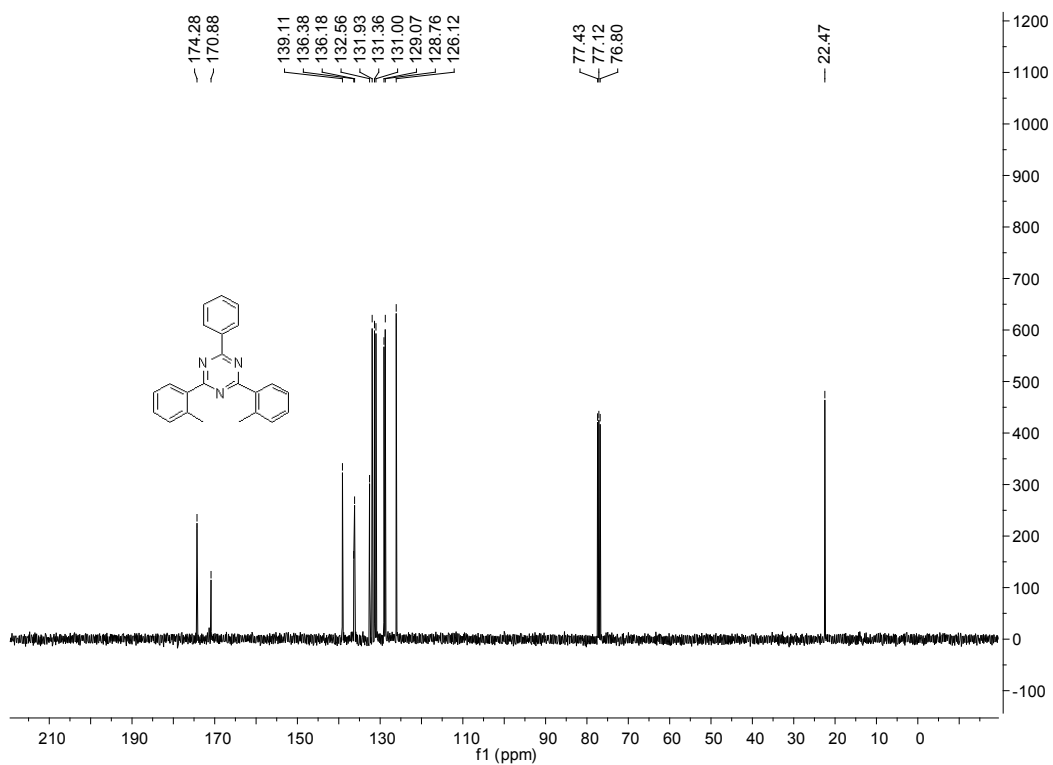


<sup>13</sup>C NMR of 3fa

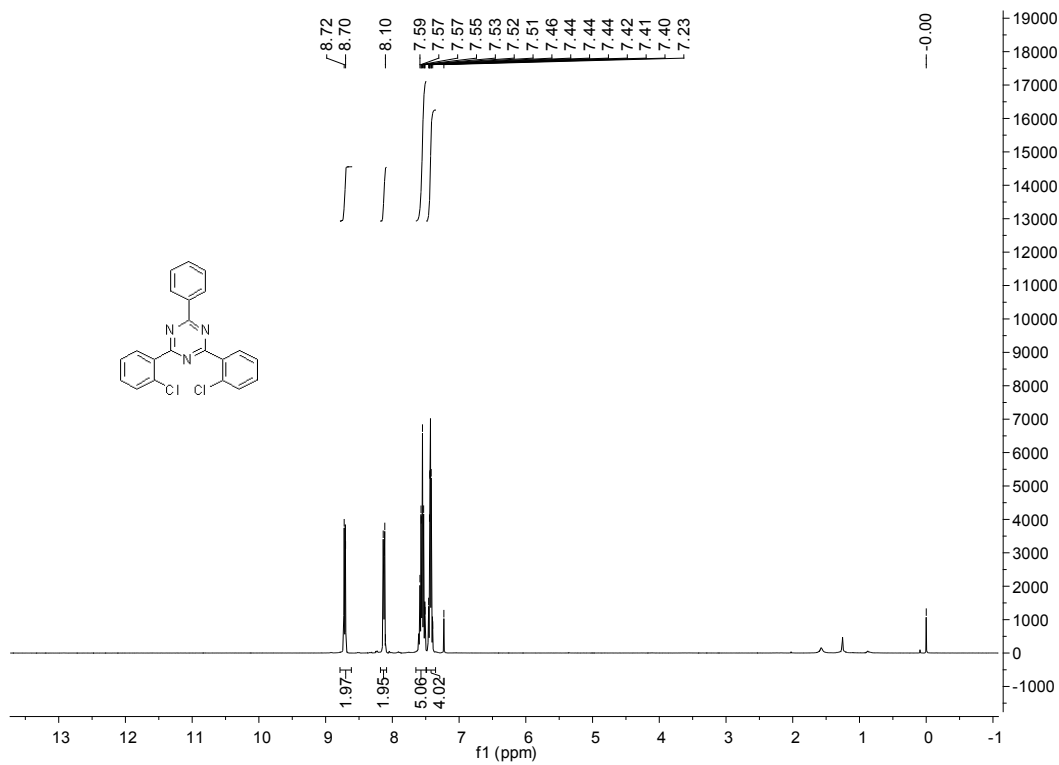


<sup>1</sup>H NMR of 3ga

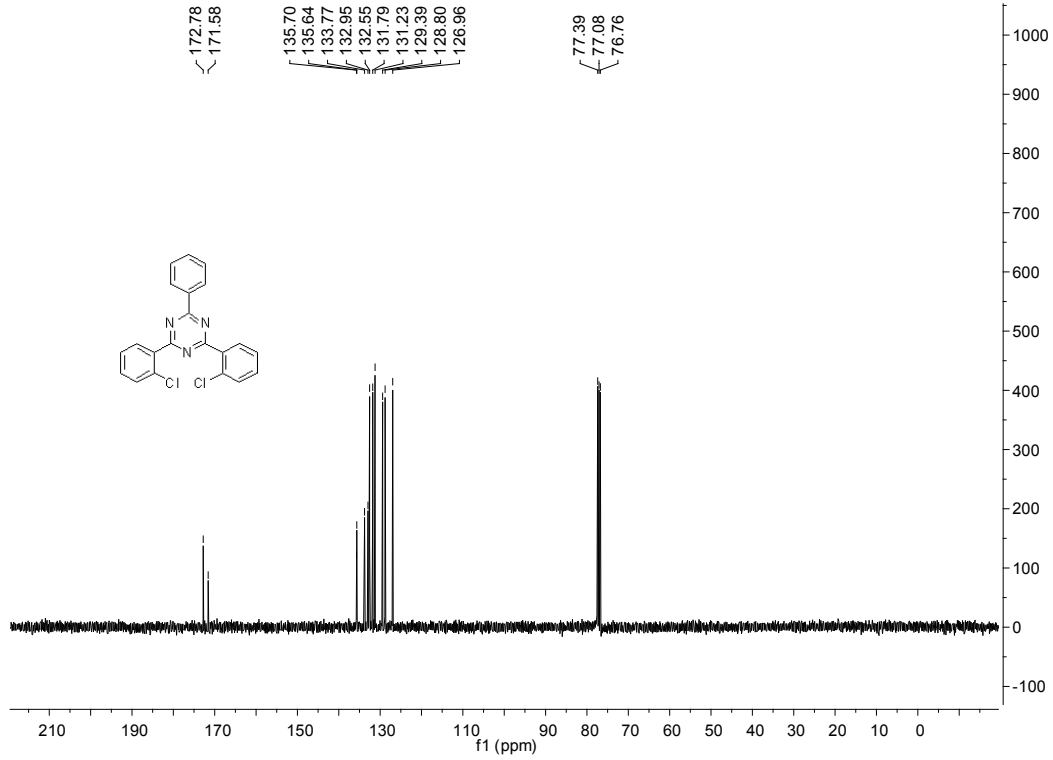




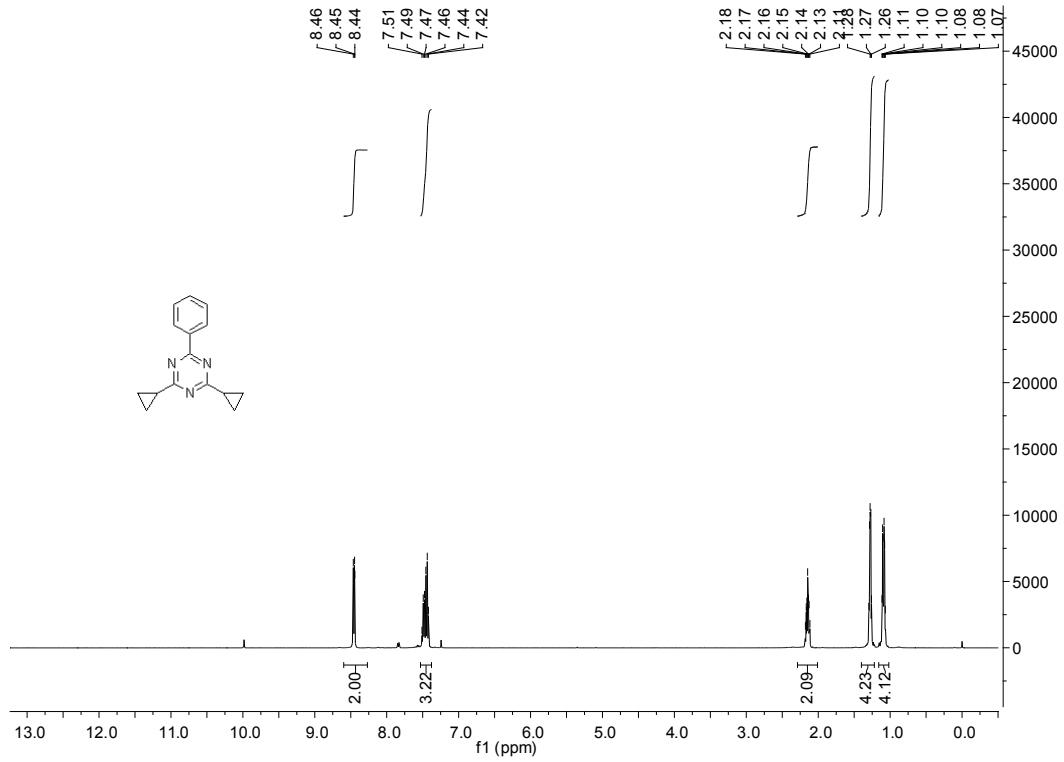
$^{13}\text{C}$  NMR of **3ga**



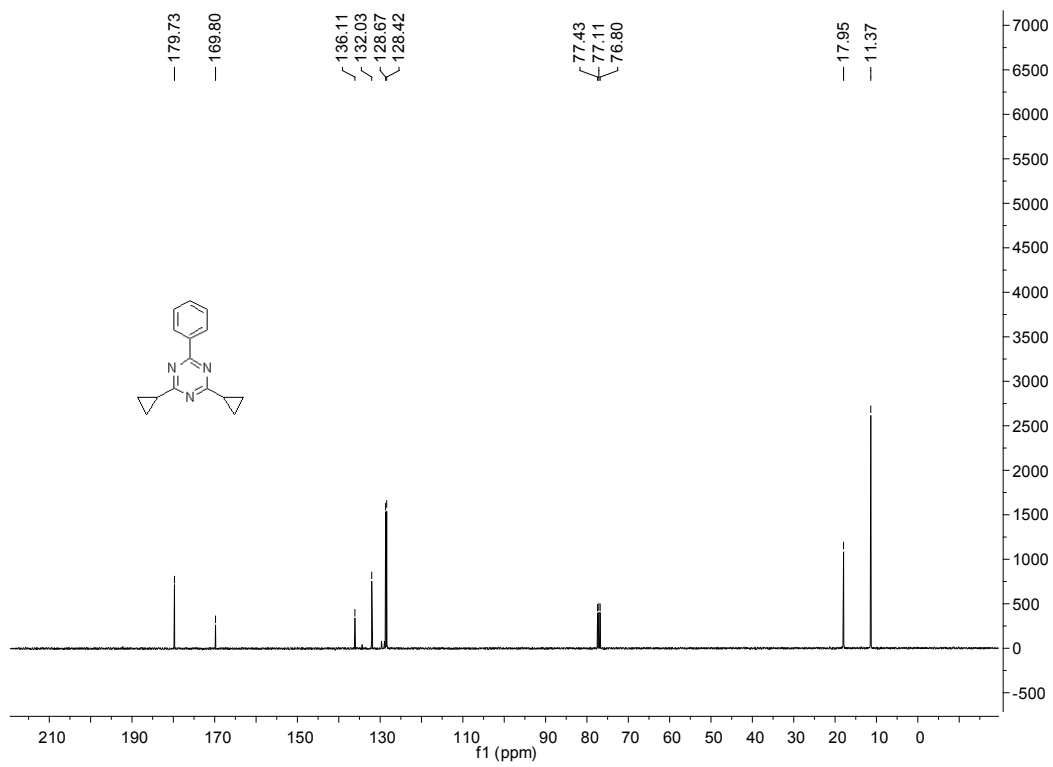
$^1\text{H}$  NMR of **3ha**



$^{13}\text{C}$  NMR of **3ha**



$^1\text{H}$  NMR of **3ia**



$^{13}\text{C}$  NMR of **3ia**