Supporting Information

Construction of 1,2-Dihydro-1,3,5-triazines *via* the Reaction Involving Amidines

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1. General

Unless otherwise noted, all reagents and solvents obtained from commercial sources were used without further purification. Deuterated solvents were purchased from Sigma-Aldrich. Column chromatography was performed on silica gel (200−300 mesh) using petroleum ether/ethyl acetate. The known compounds were partly characterized by ^{1}H NMR, and compared to authentic samples or the literature data. ^{1}H NMR spectra were taken on a Bruker AVANCE III 400 MHz NMR spectrometer. The chemical shifts are reported in ppm downfield to the $CDCl_3$ resonance (δ = 7.27). Spectra are reported as follows: chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz), integration, and assignment. $^{13}C\{^1H\}$ NMR data were collected at 100 MHz with complete proton decoupling. The chemical shifts are reported in ppm downfield to the central $CDCl_3$ resonance (δ = 77.0). High-resolution mass spectra (HRMS) were performed on a micrOTOF-Q II instrument with an ESI source. Melting points were measured with a RD-II melting point apparatus and are uncorrected.

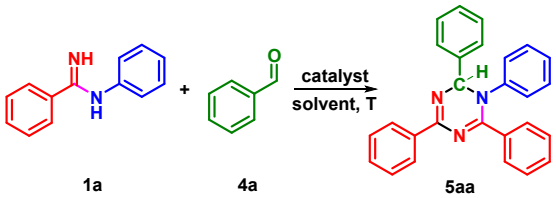
2. Optimization of reaction conditions

2.1. Optimization for the reaction of amidines with aldehydes

Initially, we used the reaction of *N*-phenylbenzylamidine **1a** and benzaldehyde **4a** as the model reaction to screen the optimal reaction conditions and the experimental results are shown in Table 1. The investigation of catalysts showed that catalysts had a great influence on the yield (Table S1, entries 1−10). Most catalysts had low catalytic activity for the reaction and the yields were less than 40% (Table S1, entries 1−8). $Cu(OAc)_2$, $CuSO_4$ and $Cu(OTf)_2$ as catalysts showed higher catalytic activity than $Pd(OAc)_2$ and $AlCl_3$. Furthermore, other catalysts containing Cu(I) such as $(CuOTf)_2{\cdot}Ph$, CuBr and CuCl were screened. However, no higher yield was obtained. Subsequently, the use of I_2 improved catalytic activity and 42% yield could be obtained (Table S1, entry 9). Based on these experimental results, the examination of ZnI_2 increased the yield to 57% (Table S1, entry 10). Unfortunately, increasing or decreasing the amount of ZnI_2 could not improve the yield (Table S1, entries 11 and 12 *vs.* 10). Subsequently, the effect of solvents was examined. It was found that the solvents had a great effect on the yield, too. For most solvents, the yield was less than 30% (Table S1, entries 13−18). 1,4-Dioxane, CH_3CH_2OH and CH_3CN as solvents led

to lower yields due to the occurrence of more side-reactions and more surplus starting materials (Table S1, entries 15, 18 and 19). Because of more side reactions and more by-products, Toluene and DCE gave lower yields (Table S1, entries 13 and 14). Only trace of product was observed when DMF and CH_3NO_2 were adopted as solvents due to low activity (Table S1, entries 16 and 17). To our delight, 57% yield could be obtained (Table S1, entry 10). Therefore, EtOAc was selected as the best solvent. Through examination of the effect of solvent dosage (Table S1, entries 20−22), the yield was increased to 73% when 1.5 mL EtOAc was used (Table S1, entry 21). Finally, when the molar ratio of **1a**/**4a** was 2.1:1, the yield was increased to 76% (Table S1, entry 23).

Table S1 Screening of reaction conditions[a]



1a **4a** **5aa**

Entry	Catalyst	Solvent	**1a**:**4a**	Yield[b] (%)
1	$Cu(OAc)_2$	EtOAc	2:1	34
2	$CuSO_4$	EtOAc	2:1	26
3	$Cu(OTf)_2$	EtOAc	2:1	24
4	$(CuOTf)_2{\cdot}Ph$	EtOAc	2:1	23
5	CuBr	EtOAc	2:1	29
6	CuCl	EtOAc	2:1	24
7	$Pd(OAc)_2$	EtOAc	2:1	16
8	$AlCl_3$	EtOAc	2:1	10
9	I_2	EtOAc	2:1	42
10	ZnI_2	EtOAc	2:1	57
11[c]	ZnI_2	EtOAc	2:1	41
12[d]	ZnI_2	EtOAc	2:1	42
13	ZnI_2	Toluene	2:1	21
14	ZnI_2	DCE	2:1	26
15	ZnI_2	1,4-Dioxane	2:1	16
16	ZnI_2	DMF	2:1	trace[e]
17	ZnI_2	CH_3NO_2	2:1	trace
18	ZnI_2	EtOH	2:1	25
19	ZnI_2	CH_3CN	2:1	45
20[f]	ZnI_2	EtOAc	2:1	61
21[g]	ZnI_2	EtOAc	2:1	73
22[h]	ZnI_2	EtOAc	2:1	67
23[g]	**ZnI_2**	**EtOAc**	**2.1:1**	**76(11[i])**
24[g]	ZnI_2	EtOAc	2.2:1	72

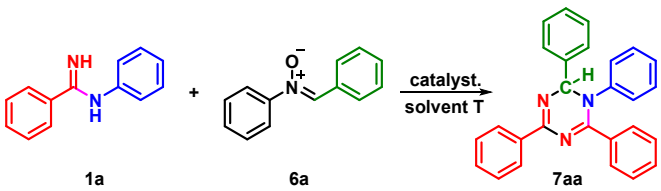
[a] Unless otherwise noted, all reactions were carried out with benzaldehyde **4a** (0.2 mmol), *N*-

phenylbenzylamidine **1a** (2 equiv) and 10 mol% catalyst in a solvent (1.0 mL) at 80 °C for 36 h. [b] Isolated yield by silica gel chromatography. [c] 5 mol% ZnI_2 was used. [d] 15 mol% ZnI_2 was used. [e] trace = Detected by TLC, not obtained by column chromatography. [f] 1.2 mL EtOAc was used. [g] 1.5 mL EtOAc was used. [h] 1.8 mL EtOAc was used. [i] When the reaction was performed with benzaldehyde **4a** (0.2 mmol), *N*-phenylbenzylamidine **1a** (2.2 equiv) and 25 mol% $Cu(OAc)_2$ in 1.0 mL EA at 80 °C for 16 h, the yield was 11%.

2.2. Optimization for the reaction of amidines with nitrones

Initially, we selected the reaction of *N*-phenylbenzylamidine **1a** and *N*-phenylnitrone **6a** as template reaction to optimize the reaction conditions. As shown in Table 2, 10 mol% Lewis acids as catalysts were screened in 1.0 mL DCE at 60 °C for 12 h. The results indicated that when $CuCl_2·2H_2O$ and $CuCl_2$ was employed as catalysts, the 31% and 30% yields were obtained, respectively (Table S2, entries 1 and 2). Other catalysts gave the lower yields (Table S2, entries 3−8). However, no product was observed when $ZnCl_2$ was used as a catalyst (Table S2, entry 9). Considering that $CuCl_2$ easily deliquesce in air and the price is higher than $CuCl_2·2H_2O$, the latter was selected as the best catalyst. Next, the effect of solvents was investigated. The experimental results showed that when acetonitrile and *N*,*N*-dimethylformamide (DMF) were used, no product or trace amount of product **7aa** was observed, respectively (Table S2, entries 13 and 14). When bromobenzene, 1,4-dioxane and anisole were utilized as solvents, 34%, 29% and 29% yields were provided (Table S2, entries 10−12). Gratifyingly, chloroform could give 53% yield (Table S2, entry 15). Then, when the reaction system was stirred at 50 °C for 20 h, the yield could be basically maintained (Table S2, entry 16). The investigation of catalyst loading and solvent dosage indicated that 10 mol% $CuCl_2·2H_2O$ (Table S2, entry 16 *vs.* 17−19) and 1.0 mL $CHCl_3$ (Table S2, entry 16 *vs.* 20 and 21) were more suitable. Finally, when the molar ratio of **1a**/**6a** was 1.8:1, the yield was increased to 75% (Table S2, entry 23 *vs.* 16, 22, 24 and 25).

Table S2 Screening of reaction conditions[a]



1a 6a 7aa

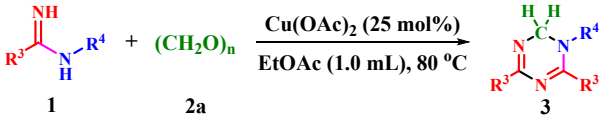
Entry	Catalyst	Solvent	**1a**:**6a**	Yield[b] (%)
1	$CuCl_2·2H_2O$	DCE	1:1	31
2	$CuCl_2$	DCE	1:1	30
3	$CuSO_4$	DCE	1:1	23
4	$Cu(OAc)_2$	DCE	1:1	11

5	$Cu(OTf)_2$	DCE	1:1	24
6	CuCl	DCE	1:1	8
7	$(CuOTf)_2 \cdot Ph$	DCE	1:1	13
8	$FeCl_3$	DCE	1:1	10
9	$ZnCl_2$	DCE	1:1	N.D.[c]
10	$CuCl_2 \cdot 2H_2O$	Bromobenzene	1:1	34
11	$CuCl_2 \cdot 2H_2O$	1,4-Dioxane	1:1	29
12	$CuCl_2 \cdot 2H_2O$	Anisole	1:1	29
13	$CuCl_2 \cdot 2H_2O$	DMF	1:1	N.D.
14	$CuCl_2 \cdot 2H_2O$	CH_3CN	1:1	trace[d]
15[e]	$CuCl_2 \cdot 2H_2O$	$CHCl_3$	1:1	53
16[f]	$CuCl_2 \cdot 2H_2O$	$CHCl_3$	1:1	41(54[g])
17[g,h]	$CuCl_2 \cdot 2H_2O$	$CHCl_3$	1:1	51
18[g,i]	$CuCl_2 \cdot 2H_2O$	$CHCl_3$	1:1	54
19[g,j]	$CuCl_2 \cdot 2H_2O$	$CHCl_3$	1:1	39
20[g,k]	$CuCl_2 \cdot 2H_2O$	$CHCl_3$	1:1	34
21[g,l]	$CuCl_2 \cdot 2H_2O$	$CHCl_3$	1:1	43
22[g]	$CuCl_2 \cdot 2H_2O$	$CHCl_3$	1.5:1	62
23[g]	**$CuCl_2 \cdot 2H_2O$**	**$CHCl_3$**	**1.8:1**	**75**
24[g]	$CuCl_2 \cdot 2H_2O$	$CHCl_3$	2:1	71
25[g]	$CuCl_2 \cdot 2H_2O$	$CHCl_3$	1:1.5	60

[a] Unless otherwise noted, all reactions were performed with *N*-phenylnitrone **6a** (0.1 mmol), *N*-phenylbenzamidine **1a** (0.1 mmol) and 10 mol% catalyst in a solvent (1.0 mL) at 60 °C for 12 h. [b] Isolated yield by silica gel chromatography. [c] N.D. = Not detected. [d] trace = Detected by TLC, not obtained by column chromatography. [e] The reaction was stirred at 60 °C. [f] The reaction was stirred at 50 °C for 12 h. [g] The reaction was stirred at 50 °C for 20 h. [h] 5 mol% $CuCl_2 \cdot 2H_2O$ was used. [i] 15 mol% $CuCl_2 \cdot 2H_2O$ was used. [j] 20 mol% $CuCl_2 \cdot 2H_2O$ was used. [k] 0.8 mL $CHCl_3$ was used. [l] 1.2 mL $CHCl_3$ was used.

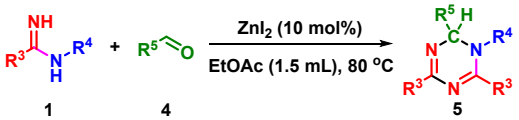
3 Three procedures for the preparation of 1,2-dihydro-1,3,5-triazine compounds

3.1 1,2-dihydro-1,3,5-triazine compounds were synthesized from the reaction of paraformaldehyde with amidines



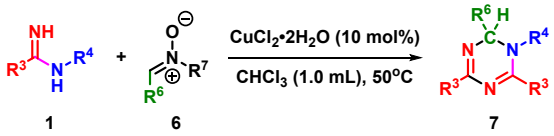
To an oven-dried glass tube were added paraformaldehyde **2a** (18 mg, 0.2 mmol), amidine **1** (0.44 mmol, 2.2 equiv), $Cu(OAc)_2$ (9.1 mg, 0.05 mmol, 25 mol%) and 1.0 mL ethyl acetate in turn. The reaction system was then stirred at 80 °C until the amount of amidine **1** was no longer consumed as monitored by TLC. Finally, the mixture was purified by silica gel column chromatography to afford the target product **3**.

3.2 1,2-dihydro-1,3,5-triazine compounds were synthesized from the reaction of aldehydes with amidines



To an oven-dried glass tube were added aldehyde **4** (0.2 mmol), amidine **1** (0.42 mmol, 2.1 equiv), ZnI_2 (6.4 mg, 1.4 μL, 0.02 mmol, 10 mol%) and 1.5 mL ethyl acetate in turn. The reaction system was then stirred at 80 °C until aldehyde **4** was completely consumed as monitored by TLC. Finally, the mixture was purified by silica gel column chromatography to offer the target product **5**.

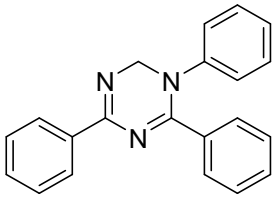
3.3 1,2-dihydro-1,3,5-triazine compounds were synthesized from the reaction of nitrones with amidines



To an oven-dried glass tube were added *N*-arylnitrone **6** (0.1 mmol), amidine **1** (0.18 mmol, 1.8 equiv), $CuCl_2 \cdot 2H_2O$ (1.7 mg, 0.01 mmol, 10 mol%) and 1.0 mL chloroform in turn. The reaction system was then stirred at 50 °C until amidine **1** was completely consumed as monitored by TLC. Finally, the mixture was purified by silica gel column chromatography to provide the target product **7**.

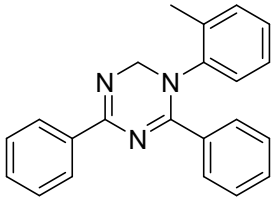
4. Characterization data for products 3

1,4,6-triphenyl-1,2-dihydro-1,3,5-triazine (3aa)



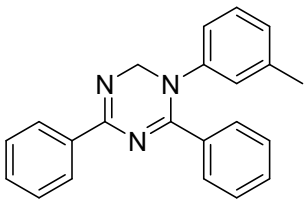
yellow solid (mp: 105−106 °C), (54.7 mg, 88%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.39−8.38 (m, 2H), 7.64−7.62 (m, 2H), 7.43 (t, J = 3.2 Hz, 3H), 7.31−7.27 (m, 1H), 7.22 (t, J = 6.8 Hz, 2H), 7.12−7.07 (m, 2H), 7.02−7.00 (m, 1H), 6.87−6.86 (m, 2H), 5.44 (s, 2H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 162.4, 161.5, 143.3, 136.3, 134.1, 131.4, 130.7, 130.6, 129.1, 128.4, 128.3, 128.1, 125.7, 124.7, 66.9 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{21}H_{18}N_3^+$ 312.1495, found: 312.1495.

4,6-diphenyl-1-(*o*-tolyl)-1,2-dihydro-1,3,5-triazine (3ba)



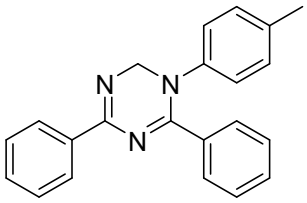
yellow solid (mp: 108−109 °C), (42.2 mg, 65%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.37−8.35 (m, 2H), 7.65−7.63 (m, 2H), 7.47−7.44 (m, 3H), 7.36 (tt, J = 7.2, 1.2 Hz, 1H), 7.26−7.22 (m, 2H), 7.09−7.06 (m, 4H), 5.36 (s, 2H), 2.16 (s, 3H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 163.3, 162.3, 142.5, 136.4, 134.4, 134.3, 131.4, 131.3, 130.5, 130.1, 128.2, 128.1, 128.0, 127.6, 127.4, 126.9, 67.4, 18.5 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{22}H_{20}N_3^+$ 326.1652, found: 326.1657.

4,6-diphenyl-1-(*m*-tolyl)-1,2-dihydro-1,3,5-triazine (3ca)



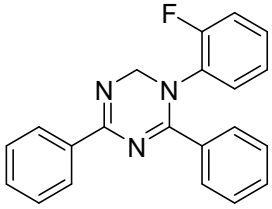
viscous liquid, (48.7 mg, 75%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.36−8.34 (m, 2H), 7.67−7.65 (m, 2H), 7.46−7.44 (m, 3H), 7.38 (t, J = 7.6 Hz, 1H), 7.29 (t, J = 8.0 Hz, 2H), 7.06 (t, J = 7.6 Hz, 1H), 6.91 (d, J = 7.6 Hz, 1H), 6.79 (s, 1H), 6.72 (d, J = 15.6 Hz, 1H), 5.47 (s, 2H), 2.22 (s, 3H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 162.4, 161.5, 143.2, 139.0, 136.2, 134.2, 131.2, 130.5, 129.3, 128.7, 128.3, 128.2, 127.9, 126.5, 125.2, 122.0, 66.9, 21.3 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{22}H_{20}N_3^+$ 326.1652, found: 326.1654.

4,6-diphenyl-1-(*p*-tolyl)-1,2-dihydro-1,3,5-triazine (3da)



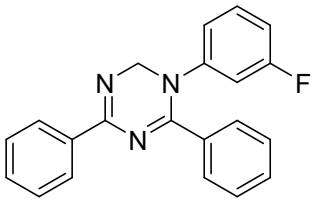
yellow solid (mp: 62−64 °C), (51.7 mg, 80%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.36−8.33 (m, 2H), 7.66−7.63 (m, 2H), 7.46−7.44 (m, 3H), 7.37−7.34 (m, 1H), 7.29 (t, J = 8.0 Hz, 2H), 6.99 (d, J = 8.0 Hz, 2H), 6.84 (d, J = 8.4 Hz, 2H), 5.47 (s, 2H), 2.25 (s, 3H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 162.3, 161.5, 140.7, 136.3, 135.6, 134.2, 131.2, 130.5, 130.4, 129.6, 128.3, 128.2, 127.9, 124.6, 67.0, 20.9 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{22}H_{20}N_3^+$ 326.1652, found: 326.1660.

1-(2-fluorophenyl)-4,6-diphenyl-1,2-dihydro-1,3,5-triazine (3ea)



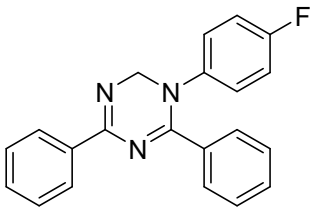
yellow solid (mp: 126−127 °C), (45.4 mg, 69%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.36−8.33 (m, 2H), 7.67 (s, 1H), 7.65 (d, J = 1.6 Hz, 1H), 7.46−7.45 (m, 3H), 7.40−7.35 (m ,1H), 7.30 (t, J = 8.0 Hz, 2H), 7.15−7.09 (m, 1H), 7.04 (t, J = 8.8 Hz, 1H), 6.94−6.93 (m, 2H), 5.42 (d, J = 0.8 Hz, 2H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 163.0 (d, J = 132.3 Hz), 158.3 (d, J = 247.4 Hz), 136.2, 133.8, 131.5 (d, J = 150.8 Hz), 131.4 (d, J = 11.8 Hz), 130.0, 128.9, 128.3, 128.2, 128.1, 128.0, 127.9, 124.6 (d, J = 3.8 Hz), 116.7 (d, J = 19.6 Hz), 67.0, 69.9 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{21}H_{17}FN_3^+$ 330.1401, found: 330.1407.

1-(3-fluorophenyl)-4,6-diphenyl-1,2-dihydro-1,3,5-triazine (3fa)



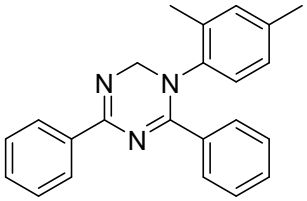
yellow solid (mp: 78−79 °C), (57.1 mg, 87%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.35−8.33 (m, 2H), 7.67 (d, J = 7.2 Hz, 2H), 7.46−7.45 (m, 2H), 7.40 (d, J = 7.2 Hz, 1H), 7.32 (d, J = 7.6 Hz, 2H), 7.15−7.09 (m, 1H), 6.81−6.77 (m, 1H), 6.69−6.65 (m, 2H), 5.45 (s, 2H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 163.9 (d, J = 246.4 Hz), 162.2 (d, J = 83.7 Hz), 144.9 (d, J = 9.6 Hz), 135.9, 133.6, 131.6, 130.7, 130.4, 130.2, 130.1, 128.5, 128.2, 128.0, 120.3 (d, J = 2.9 Hz), 112.7 (d, J = 20.9 Hz), 111.8 (d, J = 23.8 Hz), 66.7 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{21}H_{17}FN_3^+$ 330.1401, found: 330.1413.

1-(4-fluorophenyl)-4,6-diphenyl-1,2-dihydro-1,3,5-triazine (3ga)



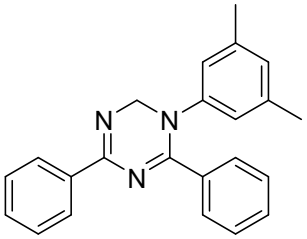
yellow solid (mp: 57−58 °C), (56.6 mg, 86%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.36−8.33 (m, 2H), 7.64−7.62 (m, 2H), 7.48−7.43 (m, 3H), 7.40−7.36 (m, 1H), 7.31 (t, J = 8.0 Hz, 2H), 6.91−6.86 (m, 4H), 5.46 (s, 2H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 162.3 (d, J = 85.4 Hz), 161.5 (d, J = 96.5 Hz), 139.5 (d, J = 3.0 Hz), 136.1, 133.8, 131.4, 130.6, 130.5, 128.4, 128.2, 127.9, 126.3 (d, J = 8.4 Hz), 116.1, 115.9, 67.1 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{21}H_{17}FN_3^+$ 330.1401, found: 330.1411.

1-(2,4-dimethylphenyl)-4,6-diphenyl-1,2-dihydro-1,3,5-triazine (3ha)



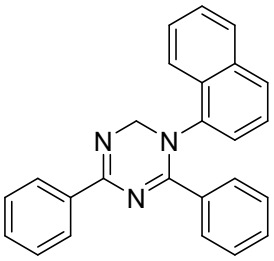
yellow solid (mp: 58−59 °C), (24.9 mg, 37%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.36−8.34 (m, 2H), 7.66 (s, 1H), 7.64 (d, J = 1.6 Hz, 1H), 7.47−7.42 (m, 3H), 7.37−7.32 (m ,1H), 7.27−7.23 (m, 2H), 6.96 (t, J = 8.4 Hz, 1H), 6.89 (s, 2H), 5.34 (d, J = 2.4 Hz, 2H) 2.24 (s, 3H), 2.12 (s, 3H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 163.3, 162.2, 139.9, 137.3, 136.5, 134.4, 134.1, 132.0, 131.2, 130.4, 130.1, 128.1, 128.0, 127.9, 127.6, 127.4, 67.6, 20.9, 18.3 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{23}H_{22}N_3^+$ 340.1808, found: 340.1805.

1-(3,5-dimethylphenyl)-4,6-diphenyl-1,2-dihydro-1,3,5-triazine (3ia)



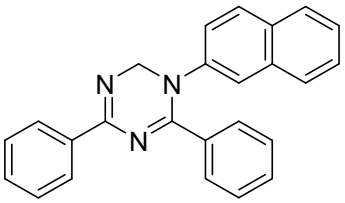
yellow solid (mp: 141−142 °C), (36.7 mg, 68%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.35−8.34 (m, 2H), 7.68 (d, J = 8.0 Hz, 2H), 7.45−7.44 (m, 3H), 7.38−7.34 (m, 1H), 7.29 (t, J = 7.6 Hz, 2H), 6.72 (s, 1H), 6.56 (s, 2H), 5.45 (s, 2H), 2.16 (s, 6H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 162.4, 161.5, 143.2, 138.7, 136.3, 134.3, 131.2, 130.5, 128.2, 128.1, 127.9, 127.5, 122.6, 67.2, 21.2 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{23}H_{22}N_3^+$ 340.1808, found: 340.1811.

1-(naphthalen-1-yl)-4,6-diphenyl-1,2-dihydro-1,3,5-triazine (3ja)



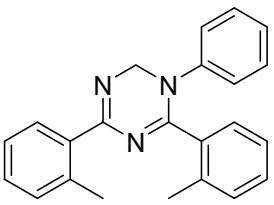
yellow solid (mp: 66−68 °C), (53.8 mg, 75%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.42−8.40 (m, 2H), 8.02 (d, J = 8.4 Hz, 1H), 7.85 (d, J = 8.0 Hz, 1H), 7.69−7.65 (m, 3H), 7.62−7.58 (m, 1H), 7.54−7.52 (m, 1H), 7.49−7.47 (m, 3H), 7.26−7.19 (m, 2H), 7.13 (t, J = 7.6 Hz, 2H), 7.07−7.05 (m, 1H), 5.61 (d, J = 11.6 Hz, 1H), 5.47 (d, J = 11.6 Hz, 1H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 164.1, 162.3, 140.1, 136.4, 134.5, 134.3, 131.4, 130.6, 130.1, 129.7, 128.8, 128.2, 128.1, 128.0, 127.9, 127.4, 126.7, 125.7, 125.3, 122.9, 67.9 ppm; **HRMS** (ESI) m/z [M + H]$^+$ calcd for $C_{25}H_{20}N_3^+$ 362.1652, found: 362.1663.

1-(naphthalen-2-yl)-4,6-diphenyl-1,2-dihydro-1,3,5-triazine (3ka)



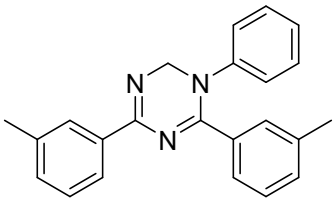
yellow solid (mp: 83−84 °C), (36.7 mg, 51%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.39−8.37 (m ,2H), 7.72 (t, J = 6.8 Hz, 4H), 7.58 (d, J = 8.8 Hz, 1H), 7.47−7.46 (m, 3H), 7.43−7.38 (m, 3H), 7.35−7.31 (m, 1H), 7.25 (t, J = 7.6 Hz, 2H), 6.99 (dd, J = 8.8, 2.0 Hz, 1H), 5.61 (s, 2H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 162.3, 161.4, 140.9, 136.2, 134.1, 133.4, 131.4, 131.1, 130.6, 130.5, 128.7, 128.4, 128.2, 128.0, 127.7, 127.5, 126.9, 126.0, 123.9, 121.5, 67.2 ppm; **HRMS** (ESI) m/z [M + H]$^+$ calcd for $C_{25}H_{20}N_3^+$ 362.1652, found: 362.1658.

1-phenyl-4,6-di-*o*-tolyl-1,2-dihydro-1,3,5-triazine (3ma)



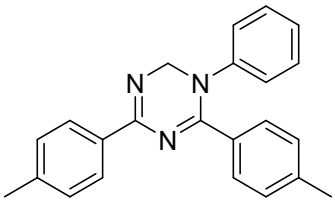
yellow solid (mp: 120−121 °C), (36.6 mg, 54%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 7.80 (d, J = 6.8 Hz, 1H), 7.46 (d, J = 7.6 Hz, 1H), 7.29−7.22 (m, 4H), 7.19−7.10 (m, 3H), 7.07 (t, J = 7.6 Hz, 1H), 7.01 (d, J = 7.6 Hz, 1H), 6.93 (d, J = 7.6 Hz, 2H), 5.52 (s, 2H), 2.61 (s, 3H), 2.24 (s, 3H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 164.1, 163.2, 141.9, 137.2, 136.8, 136.3, 134.4, 130.9, 130.6, 130.5, 130.2, 129.3, 129.0, 128.7, 125.9, 125.8, 125.6, 124.2, 65.8, 29.7, 21.3, 19.9 ppm; **HRMS** (ESI) m/z [M + H]$^+$ calcd for $C_{23}H_{22}N_3^+$ 340.1808, found: 340.1811.

1-phenyl-4,6-di-*m*-tolyl-1,2-dihydro-1,3,5-triazine (3na)



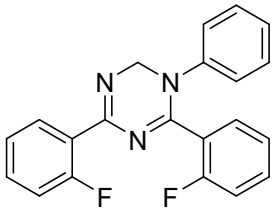
viscous liquid, (52.2.mg, 77%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.17−8.15 (m, 2H), 7.56 (s, 1H), 7.37−7.32 (m, 2H), 7.29 (d, J = 7.2 Hz, 2H), 7.20 (t, J = 8 Hz, 3H), 7.12−7.05 (m, 2H), 5.48 (s, 2H), 2.43 (s, 3H), 2.29 (s, 3H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 162.6, 161.6, 143.4, 138.1, 137.8, 136.2, 134.0, 132.1, 131.3, 131.0, 129.0, 128.4, 128.1, 128.0, 127.8, 125.6, 125.2, 124.6, 66.8, 21.5, 21.4 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{23}H_{22}N_3^+$ 340.1808, found: 340.1810.

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



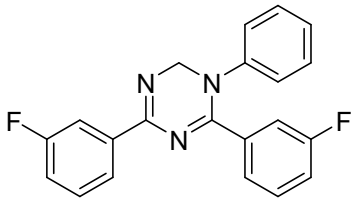
yellow solid (mp: 117−118 °C), (56.8 mg, 84%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.25 (d, J = 8.4 Hz, 2H), 7.56 (d, J = 8.4 Hz, 2H), 7.26 (d, J = 8.0 Hz, 2H), 7.20 (t, J = 7.6 Hz, 2H), 7.09 (t, J = 7.2 Hz, 3H), 6.94−6.92 (m, 2H), 5.45 (s, 2H), 2.40 (s, 3H), 2.31 (s, 3H), ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 162.2, 161.6, 143.5, 141.8, 140.6, 133.5, 131.1, 130.5, 129.5, 129.1, 129.0, 128.9, 127.9, 125.4, 124.6, 66.8, 21.5 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{23}H_{22}N_3^+$ 340.1808, found: 340.1817.

4,6-bis(2-fluorophenyl)-1-phenyl-1,2-dihydro-1,3,5-triazine (3pa)



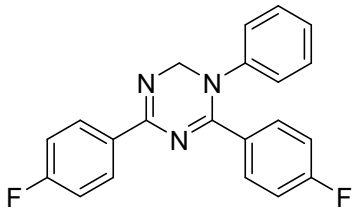
viscous liquid, (36.4 mg, 53%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.06 (td, J = 7.6, 1.6 Hz, 1H), 7.82 (td, J = 7.6, 2.0 Hz, 1H), 7.42−7.32 (m, 2H), 7.21−7.17 (m, 4H), 7.14−7.09 (m, 2H), 6.99 (d, J = 8.0 Hz, 2H), 6.83 (t, J = 9.2 Hz, 1H), 5.53 (s, 2H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 162.6 (d, J = 165.3 Hz), 160.3 (d, J = 4.3 Hz), 160.0 (d, J = 164.3 Hz), 159.2, 141.8, 133.2 (d, J = 8.5 Hz), 132.2 (d, J = 2.1 Hz), 131.6 (d, J = 7.5 Hz), 128.7, 126.3, 125.1 (d, J = 9.6 Hz), 124.6 (d, J = 3.6 Hz), 124.4, 123.8 (d, J = 3.7 Hz), 122.6 (d, J = 12.9 Hz), 116.7 (d, J = 22.4 Hz), 115.9 (d, J = 21.6 Hz), 65.9, 29.7 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{21}H_{16}F_2N_3^+$ 348.1307, found: 348.1311.

4,6-bis(3-fluorophenyl)-1-phenyl-1,2-dihydro-1,3,5-triazine (3qa)



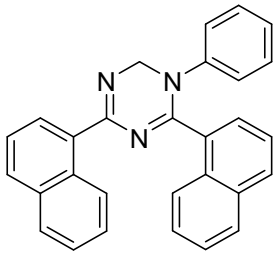
viscous liquid, (37.9 mg, 55%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.10 (d, J = 7.6 Hz, 1H), 8.02 (d, J = 10.4 Hz, 1H), 7.43−7.38 (m, 2H), 7.36 (d, J = 8.0 Hz, 1H), 7.23−7.21 (m, 3H), 7.16 (d, J = 7.6 Hz, 2H), 7.10 (td, J = 8.4, 2.0 Hz, 1H), 6.96 (d, J = 7.6 Hz, 2H), 5.50 (s, 2H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 164.1 (d, J = 41.7 Hz), 161.6 (d, J = 43.7 Hz), 161.4 (d, J = 2.5 Hz), 142.8, 138.4 (d, J = 7.8 Hz), 136.2 (d, J = 7.5 Hz), 129.9 (d, J = 8.0 Hz), 129.7 (d, J = 7.8 Hz), 129.3, 129.2, 126.3, 126.2, 124.7, 123.6 (d, J = 2.7 Hz), 118.5 (d, J = 21.2 Hz), 117.6 (d, J = 38.5 Hz), 117.4 (d, J = 6.1 Hz), 115.0 (d, J = 23.1 Hz), 66.9 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{21}H_{16}F_2N_3^+$ 348.1307, found: 348.1313.

4,6-bis(4-fluorophenyl)-1-phenyl-1,2-dihydro-1,3,5-triazine (3ra)



viscous liquid, (54.1 mg, 78%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.33−8.30 (m, 2H), 7.66−7.62 (m, 2H), 7.24 (t, J = 7.6 Hz, 2H), 7.14−7.09 (m, 3H), 6.98−6.92 (m, 4H), 5.46 (s, 2H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 165.8 (d, J = 4.8 Hz), 163.3 (d, J = 7.7 Hz), 161.4, 160.5, 143.1, 132.8 (d, J = 8.8 Hz), 132.3 (d, J = 2.9 Hz), 130.9 (d, J = 9.3 Hz), 130.1 (d, J = 8.6 Hz), 129.6 (d, J = 2.6 Hz), 129.1, 125.9, 124.7, 116.1 (d, J = 22.3 Hz), 115.6 (d, J = 66.3 Hz), 115.4 (d, J = 23.0 Hz), 66.8 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{21}H_{16}F_2N_3^+$ 348.1307, found: 348.1309.

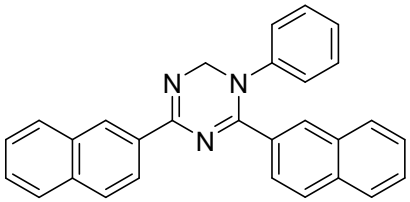
4,6-di(naphthalen-1-yl)-1-phenyl-1,2-dihydro-1,3,5-triazine (3sa)



yellow solid (mp: 82−83 ^{o}C), (28.7 mg, 35%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 9.03 (d, J = 8.8 Hz, 1H), 8.26−8.23 (m, 2H), 7.91−7.86 (m, 2H), 7.80−7.74 (m, 2H), 7.64 (d, J = 6.8 Hz, 1H), 7.59−7.54 (m, 1H), 7.52−7.46 (m, 2H), 7.44−7.40 (m, 1H), 7.36−7.32 (m, 1H), 7.05 (t, J = 7.6 Hz, 2H), 6.98−6.94 (m, 3H), 5.79 (s, 2H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 163.3, 162.7, 142.2, 134.4, 134.1, 133.5, 132.0, 131.2, 130.9, 130.8, 130.3, 129.5, 128.8, 128.5, 128.4, 128.2, 127.1, 126.6, 126.5, 126.2, 126.1, 125.7, 125.1, 124.9, 124.2, 124.1, 66.5 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd

for $C_{29}H_{22}N_3^+$ 412.1808, found: 412.1803.

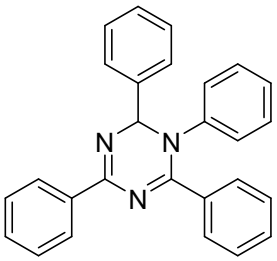
4,6-di(naphthalen-2-yl)-1-phenyl-1,2-dihydro-1,3,5-triazine (3ta)



yellow solid (mp: 79−80 °C), (34.4 mg, 42%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.89 (s, 1H), 8.43 (d, J = 8.4 Hz, 1H), 8.38 (s, 1H), 8.05−8.03 (m, 1H), 7.93 (d, J = 8.8 Hz, 1H), 7.90−7.85 (m, 2H), 7.79 (d, J = 7.6 Hz, 1H), 7.71 (d, J = 8.4 Hz, 1H), 7.62 (dd, J = 8.4, 1.6 Hz, 1H), 7.54−7.53 (m, 1H), 7.52−7.46 (m, 3H), 7.19 (t, J = 7.6 Hz, 2H), 7.09 (t, J = 7.2 Hz, 1H), 7.02−6.99 (m, 2H), 5.61 (s, 2H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 162.4, 161.5, 143.3, 134.7, 134.6, 133.6, 133.1, 132.8, 131.7, 131.5, 129.2, 129.1, 129.0, 128.5, 128.0, 127.9, 127.8, 127.7, 126.9, 126.6, 126.5, 126.2, 125.7, 124.9, 124.7, 67.1, 29.7 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{29}H_{22}N_3^+$ 412.1808, found: 412.1812.

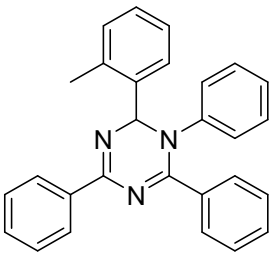
5. Characterization data for products 5 and 7

1,2,4,6-tetraphenyl-1,2-dihydro-1,3,5-triazine (5aa and **7aa)**[1]



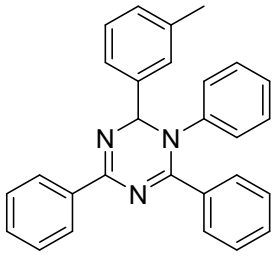
yellow solid (mp: 146−147 °C), (**5aa**: 58.8 mg, 76%; **7aa**: 29.1 mg, 75%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.39−8.37 (m, 2H), 7.79−7.67 (m, 2H), 7.72 (d, J = 7.6 Hz, 2H), 7.45−7.43 (m, 3H), 7.41−7.33 (m, 4H), 7.32 (t, J = 7.6 Hz, 2H), 7.18−7.15 (m, 2H), 7.11 (t, J = 7.2 Hz, 1H), 7.00 (d, J = 7.2 Hz, 2H), 6.41 (s, 1H) ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{27}H_{22}N_3^+$ 388.1808, found: 388.1805.

1,4,6-triphenyl-2-(*o*-tolyl)-1,2-dihydro-1,3,5-triazine (5ab and **7ab)**



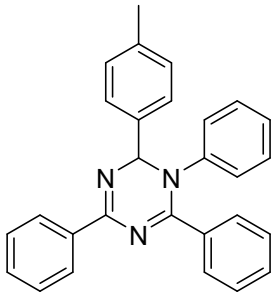
yellow solid (mp: 124−125 °C), (**5ab**: 54.4 mg, 68%; **7ab**: 20.1mg, 50%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.34−8.32 (m, 2H), 7.82 (d, J = 8.1 Hz, 2H), 7.63 (d, J = 7.6 Hz, 1H), 7.41−7.38 (m, 4H), 7.34 (d, J = 7.8 Hz, 2H), 7.30−7.22 (m, 3H), 7.19 (t, J = 7.4 Hz, 1H), 7.14−7.05 (m, 2H), 6.89 (d, J = 7.6 Hz, 2H), 6.56 (s, 1H), 2.72 (s, 3H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 161.0, 157.4, 144.3, 139.6, 136.8, 135.2, 134.8, 131.2, 131.1, 130.2, 128.9, 128.4, 128.2, 128.0, 128.0, 126.6, 126.0, 125.4, 124.9, 76.7, 19.6 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{28}H_{24}N_3^+$ 402.1965, found: 402.1970.

1,4,6-triphenyl-2-(*m*-tolyl)-1,2-dihydro-1,3,5-triazine (5ac and **7ac)**



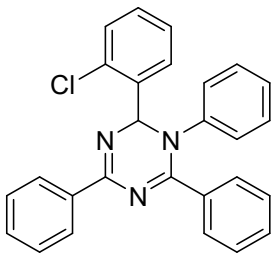
yellow solid (mp: 141−142 °C), (**5ac**: 56.0 mg, 70%; **7ac**: 26.5 mg, 66%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.44−8.42 (m, 2H), 7.84 (d, J = 7.6 Hz, 2H), 7.57 (d, J = 7.5 Hz, 2H), 7.50−7.49 (m, 3H), 7.45 (t, J = 7.3 Hz, 1H), 7.37 (q, J = 7.8 Hz, 3H), 7.23 (t, J = 7.7 Hz, 3H), 7.16 (t, J = 7.1 Hz, 1H), 7.05 (d, J = 7.6 Hz, 2H), 6.42 (s, 1H), 2.40 (s, 3H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 160.8, 158.2, 144.2, 141.8, 138.6, 136.6, 134.9, 131.2, 130.4, 130.2, 129.3, 128.9, 128.8, 128.4, 128.1, 126.8, 125.9, 124.9, 123.2, 78.8, 21.6 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{28}H_{24}N_3^+$ 402.1965, found: 402.1962.

1,4,6-triphenyl-2-(*p*-tolyl)-1,2-dihydro-1,3,5-triazine (5ad and **7ad)**



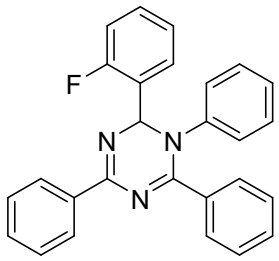
yellow solid (mp: 72−73 °C), (**5ad**: 58.1 mg, 73%; **7ad**: 31.3 mg, 78%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.39−8.37 (m, 2H), 7.78−7.75 (m, 2H), 7.61−7.59 (m, 2H), 7.44 (d, J = 5.2 Hz, 3H), 7.39 (t, J = 7.6 Hz, 1H), 7.30 (t, J = 7.2 Hz, 2H), 7.20 (t, J = 7.2 Hz, 2H), 7.17 (t, J = 7.2 Hz, 2H), 7.10 (t, J = 7.2 Hz, 1H), 7.00 (d, J = 7.2 Hz, 2H), 6.37 (s, 1H), 2.33 (s, 3H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 160.7, 158.2, 144.2, 139.0, 138.3, 136.6, 134.9, 131.2, 130.4, 130.2, 129.6, 128.9, 128.3, 128.1, 126.1, 125.9, 124.9, 78.6, 21.2 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{28}H_{24}N_3^+$ 402.1965, found: 402.1968.

2-(2-chlorophenyl)-1,4,6-triphenyl-1,2-dihydro-1,3,5-triazine (5ae)



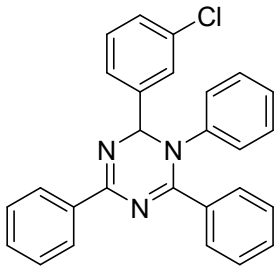
yellow solid (mp: 151−152 °C), (38.0 mg, 45%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.36−8.34 (m, 2H), 7.76 (s, 1H), 7.75−7.72 (m, 2H), 7.51 (dd, J = 8.0, 1.2 Hz, 1H), 7.44−7.38 (m, 4H), 7.34−7.28 (m, 3H), 7.26−7.22 (m, 1H), 7.17−7.08 (m, 3H), 6.90−6.88 (m, 2H), 6.83 (s, 1H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 161.6, 158.3, 143.9, 139.5, 135.0, 131.6, 131.3, 130.6, 130.5, 130.2, 129.8, 129.1, 128.5, 128.2, 128.1, 128.0, 127.9, 126.4, 125.3, 76.3 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{27}H_{21}ClN_3^+$ 422.1419, found: 422.1416.

2-(2-fluorophenyl)-1,4,6-triphenyl-1,2-dihydro-1,3,5-triazine (7ae)



white solid (mp: 146−147 °C), (17.8 mg, 44%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.40−8.38 (m, 2H), 7.74 (d, J = 7.6 Hz, 2H), 7.64 (t, J = 7.6 Hz, 1H), 7.44−7.41 (m, 3H), 7.38−7.26 (m, 5H), 7.16−7.07 (m, 5H), 6.98 (d, J = 8.2 Hz, 2H), 6.76 (s, 1H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 161.4, 160.3, 158.8, 157.8, 143.9, 136.5, 134.8, 131.2, 130.6, 130.4, 130.3, 130.1, 129.0, 128.8, 128.7, 128.4, 128.1, 128.1, 126.2, 125.2, 124.9, 124.9, 116.3, 116.0, 73.3, 73.3 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{27}H_{21}FN_3^+$ 406.1714, found: 406.1710.

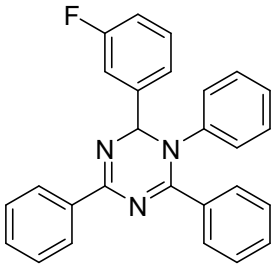
2-(3-chlorophenyl)-1,4,6-triphenyl-1,2-dihydro-1,3,5-triazine (5af)



yellow solid (mp: 135−136 °C), (47.5 mg, 67%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.38−8.36 (m, 2H), 7.80 (d, J = 7.6 Hz, 2H), 7.69 (s, 1H), 7.60−7.59 (m, 1H), 7.46−7.44 (m, 3H), 7.41 (d, J = 7.2 Hz, 1H), 7.34−7.31 (m, 4H), 7.21 (t, J = 7.2 Hz, 2H), 7.14 (t, J = 7.2 Hz, 1H), 6.99 (d, J = 7.6 Hz, 2H), 6.39 (s, 1H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 160.8, 158.9, 144.1, 143.7, 134.9, 134.6, 131.5, 130.7, 130.3, 130.2, 129.2, 128.5, 128.2, 128.2, 126.5, 126.2, 124.8, 124.3, 120.9, 78.1 ppm;

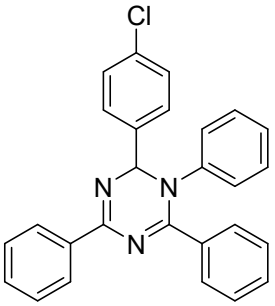
HRMS (ESI) m/z $[M + H]^+$ calcd for $C_{27}H_{21}ClN_3^+$ 422.1419, found: 422.1425.

2-(3-fluorophenyl)-1,4,6-triphenyl-1,2-dihydro-1,3,5-triazine (7af)



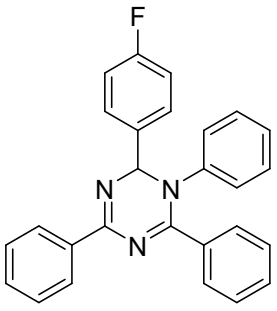
white solid (mp: 179−180 °C), (26.4 mg, 65%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.40−8.37 (m, 2H), 7.80 (d, J = 7.3 Hz, 2H), 7.51 (d, J = 7.8 Hz, 1H), 7.47−7.39 (m, 4H), 7.38−7.29 (m, 4H), 7.20−7.16 (m, 3H), 7.05 (dd, J = 8.3, 2.0 Hz, 1H), 7.00−6.98 (m, 2H), 6.41 (s, 1H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 164.3, 161.8, 160.6, 158.8, 144.1, 136.3, 134.5, 131.4, 130.6, 130.5, 130.4, 130.2, 129.1, 128.4, 128.1, 128.1, 126.1, 124.7, 121.7, 121.7, 115.5, 115.3, 113.5, 113.2, 78.0, 77.9 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{27}H_{21}FN_3^+$ 406.1714, found: 406.1711.

2-(4-chlorophenyl)-1,4,6-triphenyl-1,2-dihydro-1,3,5-triazine (5ag and **7al)**



yellow solid (mp: 69−70 °C), (**5ag**: 63.4 mg, 76%; **7al**: 31.2 mg, 74%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.38−8.36 (m, 2H), 7.77 (d, J = 7.1 Hz, 2H), 7.65 (d, J = 8.3 Hz, 2H), 7.45−7.42 (m, 3H), 7.38 (t, J = 6.7 Hz, 3H), 7.31 (t, J = 7.8 Hz, 2H), 7.19 (t, J = 7.1 Hz, 2H), 7.12−7.08 (m, 1H), 6.98 (d, J = 7.8 Hz, 2H), 6.38 (s, 1H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 160.7, 158.6, 144.1, 140.3, 136.4, 134.5, 134.3, 131.4, 130.6, 130.1, 129.1, 128.4, 128.1, 128.1, 127.6, 126.1, 124.8, 78.1 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{27}H_{21}ClN_3^+$ 422.1419, found: 422.1408.

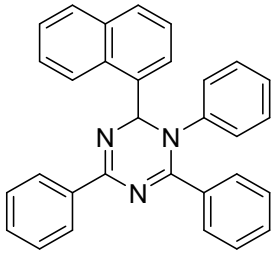
2-(4-fluorophenyl)-1,4,6-triphenyl-1,2-dihydro-1,3,5-triazine (5ah and **7ag)**



white solid (mp: 125−126 °C), (**5ah**: 55.3 mg, 69%; **7ag**: 32.4 mg, 80%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.39−8.37 (m, 2H), 7.77 (d, J = 8.1 Hz, 2H), 7.70−7.66 (m, 2H),

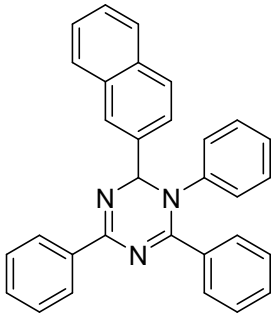
7.46−7.44 (m, 3H), 7.41−7.37 (m, 1H), 7.32 (t, *J* = 7.8 Hz, 2H), 7.20−7.16 (m, 2H), 7.13−7.05 (m, 3H), 6.99 (d, *J* = 7.7 Hz, 2H), 6.38 (s, 1H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) *δ* 164.0, 161.5, 160.6, 158.5, 144.1, 137.7, 137.7, 136.4, 134.6, 131.1, 130.6, 130.1, 129.1, 128.4, 128.1, 128.1, 128.0, 127.9, 126.1, 124.8, 115.9, 115.7, 78.0 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{27}H_{21}FN_3^+$ 406.1714, found: 406.1710.

2-(naphthalen-1-yl)-1,4,6-triphenyl-1,2-dihydro-1,3,5-triazine (5ai and **7ai)**



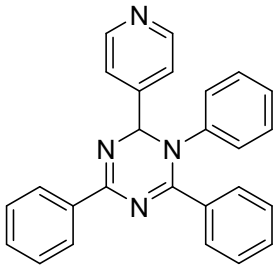
yellow solid (mp: 146−147 °C), (**5ai**: 22.3 mg, 26%; **7ai**: 25.4 mg, 58%); **^{1}H NMR** ($CDCl_3$, 400 MHz) *δ* 8.83 (d, *J* = 8.5 Hz, 1H), 8.32−8.30 (m, 2H), 7.94−7.89 (m, 3H), 7.85 (d, *J* = 8.2 Hz, 1H), 7.81 (d, *J* = 7.1 Hz, 1H), 7.68−7.64 (m, 1H), 7.57 (t, *J* = 7.2 Hz, 1H), 7.46−7.35 (m, 7H), 7.14−7.06 (m, 4H), 6.93 (d, *J* = 6.8 Hz, 2H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) *δ* 160.9, 157.6, 144.3, 136.6, 136.2, 134.7, 134.3, 131.3, 130.4, 130.3, 130.1, 128.9, 128.9, 128.5, 128.5, 128.1, 128.0, 126.4, 126.0, 125.5, 125.3, 124.8, 122.7, 77.1 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{31}H_{24}N_3^+$ 438.1965, found: 438.1968.

2-(naphthalen-2-yl)-1,4,6-triphenyl-1,2-dihydro-1,3,5-triazine (5aj and **7ah)**



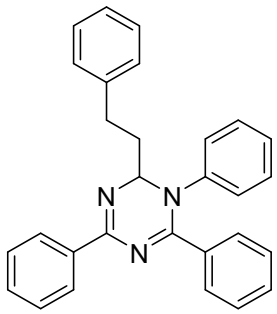
yellow solid (mp: 74−75 °C), (**5aj**: 25.7 mg, 30%; **7ah**: 29.3 mg, 67%); **^{1}H NMR** ($CDCl_3$, 400 MHz) *δ* 8.40−8.38 (m, 2H), 8.11 (s, 1H), 7.88 (s, 2H), 7.84−7.80 (m, 4H), 7.48−7.43 (m, 5H), 7.39 (d, *J* = 7.0 Hz, 1H), 7.33 (t, *J* = 7.1 Hz, 2H), 7.18 (t, *J* = 7.1 Hz, 2H), 7.11 (t, *J* = 7.0 Hz, 1H), 7.03 (d, *J* = 7.9 Hz, 2H), 6.56 (s, 1H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) *δ* 160.9, 158.5, 144.2, 139.2, 136.6, 134.9, 133.4, 133.3, 131.2, 130.5, 130.2, 129.1, 129.0, 128.4, 128.3, 128.1, 128.1, 127.7, 126.3, 126.3, 126.0, 125.0, 124.9, 124.4, 79.1 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{31}H_{24}N_3^+$ 438.1965, found: 438.1972.

1,4,6-triphenyl-2-(pyridin-4-yl)-1,2-dihydro-1,3,5-triazine (5ak)



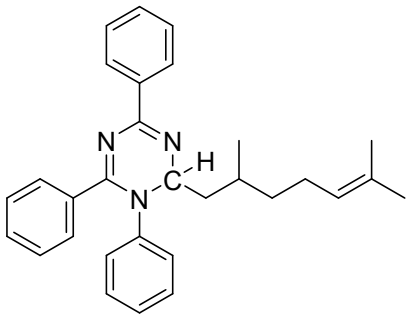
yellow solid (mp: 118−119 °C), (32.0 mg, 25%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.80 (d, J = 4.0 Hz, 3H), 8.59 (dd, J = 4.4 Hz, J = 1.2 Hz, 3H), 8.11 (d, J = 5.6 Hz, 1H), 7.95 (d, J = 5.2 Hz, 1H), 7.86−7.83 (m, 1H), 7.69−7.68 (m, 3H), 7.52−7.20 (m, 2H), 7.48−7.42 (m, 5H), 7.18 (s, 1H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 165.9, 160.4, 152.1, 150.3, 145.2, 137.8, 134.1, 130.9, 128.7, 128.7, 127.7, 126.1, 124.4, 121.3 ppm; **HRMS** (ESI) m/z [M + H]$^+$ calcd for $C_{26}H_{21}N_4^+$ 389.1761, found: 389.1768.

2-phenethyl-1,4,6-triphenyl-1,2-dihydro-1,3,5-triazine (5al)



viscous liquid, (56.3 mg, 68%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.40−8.38 (m, 2H), 7.74−7.72 (m, 2H), 7.47−7.46 (m, 3H), 7.38 (t, J = 7.2 Hz, 1H), 7.30−7.27 (m, 6H), 7.20−7.17 (m, 1H), 7.16 (t, J = 7.6 Hz, 2H), 7.06 (t, J = 7.6 Hz, 1H), 6.93 (d, J = 7.6 Hz, 2H), 5.53−5.49 (m, 1H), 3.10−2.98 (m, 2H), 2.54−2.45 (m, 1H), 2.27−2.18 (m, 1H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 160.5, 158.9, 144.1, 141.5, 136.6, 135.0, 131.3, 130.5, 130.2, 129.1, 128.6, 128.5, 128.4, 128.2, 128.0, 126.1, 125.5, 124.5, 76.4, 36.4, 31.2 ppm; **HRMS** (ESI) m/z [M + H]$^+$ calcd for $C_{29}H_{26}N_4^+$ 416.2121, found: 416.2125.

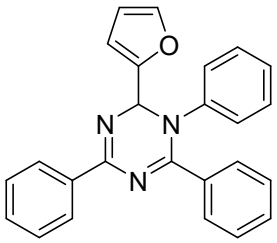
2-(2,6-dimethylhept-5-en-1-yl)-1,4,6-triphenyl-1,2-dihydro-1,3,5-triazine (5an)



yellow oil (38.8 mg, 45%), dr = 1:1; **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.38−8.36 (m, 4H), 7.77−7.73 (m, 4H), 7.47−7.45 (m, 6H), 7.39 (t, J = 7.2 Hz, 2H), 7.31 (t, J = 7.2 Hz, 4H), 7.19 (t, J = 7.8 Hz, 4H), 7.10−7.07 (m, 2H), 6.98 (t, J = 7.2 Hz, 4H),

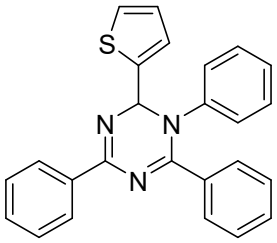
5.59−5.54 (m, 2H), 5.15 (t, *J* = 7.2 Hz, 1H), 5.09 (t, *J* = 6.6 Hz, 1H), 2.30−2.26 (m, 1H), 2.10−1.97 (m, 8H), 1.93−1.89 (m, 1H), 1.70 (s, 3H), 1.64 (s, 3H), 1.60 (s, 3H), 1.56 (s, 3H), 1.48−1.43 (m, 1H), 1.37−1.30 (m, 3H), 1.20 (d, *J* = 6.6 Hz, 3H), 1.12 (d, *J* = 6.6 Hz, 3H) ppm.

2-(furan-2-yl)-1,4,6-triphenyl-1,2-dihydro-1,3,5-triazine (7aj)



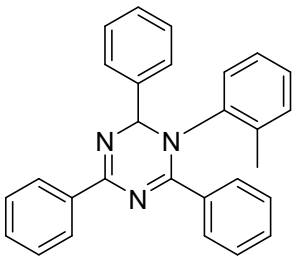
white solid, (20.8 mg, 55%); **^{1}H NMR** ($CDCl_3$, 400 MHz) *δ* 8.45−8.42 (m, 2H), 7.67−7.65 (m, 2H), 7.50−7.47 (m, 4H), 7.36−7.32 (m, 1H), 7.27 (dd, *J* = 6.6, 1.4 Hz, 2H), 7.23 (d, *J* = 4.3 Hz, 4H), 7.15−7.10 (m, 1H), 6.54 (s, 1H), 6.42 (d, *J* = 3.3 Hz, 1H), 6.33 (q, *J* = 1.8 Hz, 1H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) *δ* 160.8, 160.0, 152.0, 143.6, 143.0, 136.2, 134.5, 131.2, 130.7, 130.3, 129.0, 128.3, 128.2, 128.2, 125.8, 125.1, 110.6, 108.8, 72.4 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{25}H_{20}N_3O^+$ 378.1601, found: 378.1597.

1,4,6-triphenyl-2-(thiophen-2-yl)-1,2-dihydro-1,3,5-triazine (7ak)



white solid (mp: 102−103 °C), (13.0 mg, 33%); **^{1}H NMR** ($CDCl_3$, 400 MHz) *δ* 8.42−8.40 (m, 2H), 7.77(d, 2H, *J* = 8 Hz), 7.48−7.45 (m, 3H), 7.40−7.36 (m, 1H), 7.32−7.20(m, 6H), 7.13−7.10(m, 3H), 6.99(t, *J* = 8 Hz, 1H), 6.66 (s, 1H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) *δ* 160.2, 159.6, 144.8, 143.7, 136.3, 134.5, 131.3, 130.6, 130.3, 129.1, 128.3, 128.2, 128.1, 126.7, 125.9, 125.4, 125.1, 124.6, 74.8 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{25}H_{20}N_3S^+$ 394.1372, found: 394.1368.

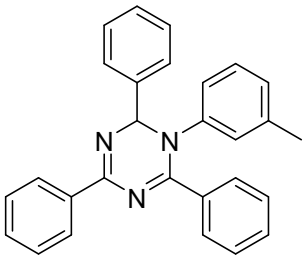
2,4,6-triphenyl-1-(*o*-tolyl)-1,2-dihydro-1,3,5-triazine (5ba and **7ba)**



yellow solid (mp: 78−79 °C), (**5ba**: 37.0 mg, 46%; **7ba**: 13.7 mg, 34%); **^{1}H NMR** ($CDCl_3$, 400 MHz) *δ* 8.38−8.35 (m, 2H), 7.74 (d, *J* = 7.4 Hz, 2H), 7.67 (d, *J* = 6.7 Hz, 2H), 7.45−7.31 (m, 8H), 7.24 (d, *J* = 7.1 Hz, 2H), 7.12−7.10 (m, 2H), 7.00−6.99 (m, 1H), 6.12 (s, 1H), 2.06 (s, 3H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) *δ* 162.0, 158.9,

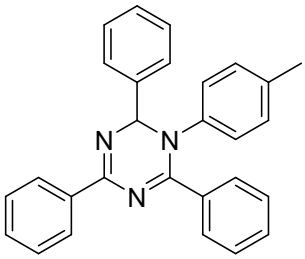
142.9, 142.2, 136.9, 135.1, 134.9, 131.4, 131.1, 130.3, 130.0, 128.9, 128.6, 128.3, 128.1, 128.0, 127.9, 126.7, 126.6, 79.6, 18.0 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{28}H_{24}N_3^+$ 402.1965, found: 402.1959.

2,4,6-triphenyl-1-(*m*-tolyl)-1,2-dihydro-1,3,5-triazine (5ca and **7ca)**



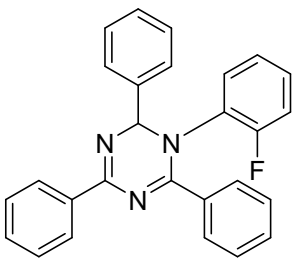
yellow solid (mp: 146−147 °C), (**5ca**: 57.6 mg, 72%; **7ca**: 22.5 mg, 56%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.43−8.41 (m, 2H), 7.85 (d, J = 7.5 Hz, 2H), 7.77 (d, J = 7.4 Hz, 2H), 7.49−7.47 (m, 3H), 7.45 (t, J = 7.1 Hz, 3H), 7.39−7.33 (m, 3H), 7.10 (t, J = 7.7 Hz, 1H), 6.97 (d, J = 7.5 Hz, 2H), 6.87 (s, 1H), 6.84 (d, J = 7.9 Hz, 1H), 6.44 (s, 1H), 2.24 (s, 3H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 160.7, 158.5, 144.2, 141.8, 139.0, 136.6, 134.8, 131.2, 130.4, 130.2, 128.9, 128.7, 128.4, 128.3, 128.1, 126.8, 126.1, 125.3, 122.2, 78.6, 21.3 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{28}H_{24}N_3^+$ 402.1965, found: 402.1967.

2,4,6-triphenyl-1-(*p*-tolyl)-1,2-dihydro-1,3,5-triazine (5da and **7da)**



yellow solid (mp: 138−139 °C), (**5da**: 61.2 mg, 77%; **7da**: 30.1 mg, 75%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.44−8.42 (m, 2H), 7.84 (d, J = 7.3 Hz, 2H), 7.77 (d, J = 7.3 Hz, 2H), 7.49−7.40 (m, 6H), 7.38−7.33 (m, 3H), 7.02 (d, J = 8.2 Hz, 2H), 6.94 (d, J = 8.3 Hz, 2H), 6.42 (s, 1H), 2.29 (s, 3H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 160.7, 158.4, 141.9, 141.7, 136.6, 135.9, 134.9, 131.1, 130.4, 130.2, 129.6, 128.9, 128.4, 128.3, 128.1, 126.2, 124.8, 78.8, 20.9 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{28}H_{24}N_3^+$ 402.1965, found: 402.1963.

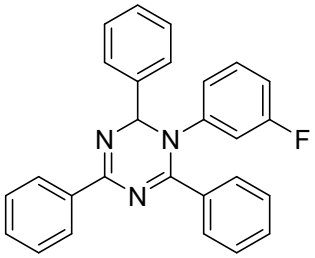
1-(2-fluorophenyl)-2,4,6-triphenyl-1,2-dihydro-1,3,5-triazine (5ea and **7ea)**



yellow solid (mp: 137−138 °C), (**5ea**: 37.7 mg, 47%; **7ea**: 19.1 mg, 47%); **^{1}H NMR**

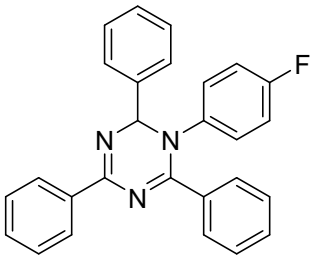
($CDCl_3$, 400 MHz) δ 8.43−8.41 (m, 2H), 7.82 (d, J = 7.6 Hz, 2H), 7.73 (d, J = 7.3 Hz, 2H), 7.49−7.38 (m, 7H), 7.36 (t, J = 7.6 Hz, 2H), 7.17−7.13 (m, 2H), 7.06 (d, J = 7.6 Hz, 1H), 6.94 (t, J = 9.6 Hz, 1H), 6.34 (s, 1H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 161.9, 158.6, 141.5, 136.6, 134.6, 132.2, 132.1, 131.4, 130.5, 129.6, 128.8, 128.5, 128.4, 128.4, 128.2, 128.1, 128.1, 126.4, 124.7, 124.7, 116.6, 116.4, 79.0 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{27}H_{21}FN_3^+$ 406.1714, found: 406.1719.

1-(3-fluorophenyl)-2,4,6-triphenyl-1,2-dihydro-1,3,5-triazine (5fa and **7fa)**



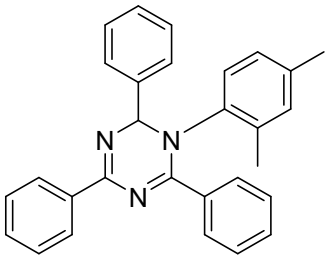
yellow solid (mp: 126−127 °C), (**5fa**: 51.0 mg, 63%; **7fa**: 21.5 mg, 53%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.43−8.41 (m, 2H), 7.84 (d, J = 7.6 Hz, 2H), 7.74 (d, J = 7.4 Hz, 2H), 7.50−7.42 (m, 6H), 7.40 (t, J = 7.8 Hz, 3H), 7.18 (q, J = 7.8 Hz, 1H), 6.88−6.77 (m, 3H), 6.45 (s, 1H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 163.8, 161.3, 160.5, 158.2, 145.8, 145.7, 141.2, 136.3, 134.4, 131.6, 130.6, 130.1, 130.1, 130.0, 129.0, 128.6, 128.5, 128.1, 128.1, 126.0, 120.5, 120.5, 112.9, 112.7, 112.0, 111.7, 78.6 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{27}H_{21}FN_3^+$ 406.1714, found: 406.1713.

1-(4-fluorophenyl)-2,4,6-triphenyl-1,2-dihydro-1,3,5-triazine (5ga and **7ga)**



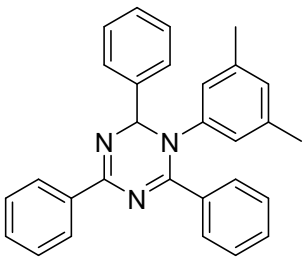
yellow solid (mp: 63−64 °C), (**5ga**: 65.3 mg, 81%; **7ga**: 27.6 mg, 68%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.42−8.41 (m, 2H), 7.80 (d, J = 7.6 Hz, 2H), 7.74 (d, J = 7.5 Hz, 2H), 7.49−7.34 (m, 9H), 7.02−6.98 (m, 2H), 6.93 (t, J = 8.2 Hz, 2H), 6.39 (s, 1H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 161.7, 160.7, 159.3, 158.3, 141.6, 140.3, 140.3, 136.4, 134.5, 131.3, 130.5, 130.1, 129.0, 128.6, 128.4, 128.1, 128.1, 126.6, 126.6, 126.1, 116.0, 115.8, 79.0 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{27}H_{21}FN_3^+$ 406.1714, found: 406.1721.

1-(2,4-dimethylphenyl)-2,4,6-triphenyl-1,2-dihydro-1,3,5-triazine (5ha and **7ia)**



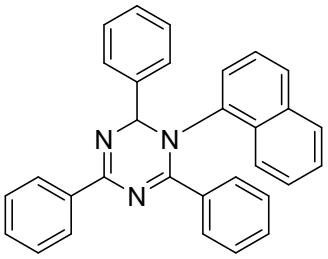
yellow solid (mp: 72−73 °C), (**5ha**: 19.9 mg, 24%; **7ia**: 15.0 mg, 36%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.37−8.34 (m, 2H), 7.74 (d, J = 7.3 Hz, 2H), 7.65 (d, J = 7.9 Hz, 2H), 7.44−7.32 (m, 7H), 7.25 (d, J = 7.2 Hz, 2H), 7.00 (d, J = 8.0 Hz, 1H), 6.89 (d, J = 8.2 Hz, 1H), 6.80 (s, 1H), 6.07 (s, 1H), 2.22 (s, 3H), 2.02 (s, 3H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 162.1, 158.8, 142.3, 140.3, 137.7, 137.0, 135.2, 134.5, 132.0, 131.0, 130.3, 129.9, 128.9, 128.6, 128.2, 128.1, 128.0, 128.0, 127.4, 126.7, 79.8, 20.9, 17.9 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{29}H_{26}N_3^+$ 416.2121, found: 416.2128.

1-(3,5-dimethylphenyl)-2,4,6-triphenyl-1,2-dihydro-1,3,5-triazine (5ia and **7ha)**



yellow solid (mp: 133−134 °C), (**5ia**: 36.2 mg, 44%; **7ha**: 17.0 mg, 41%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.42−8.40 (m, 2H), 7.86 (d, J = 7.3 Hz, 2H), 7.75 (d, J = 7.4 Hz, 2H), 7.48−7.46 (m, 3H), 7.44 (t, J = 7.2 Hz, 3H), 7.38 (q, J = 6.8 Hz, 3H), 6.78 (s, 1H), 6.65 (s, 2H), 6.41 (s, 1H), 2.18 (s, 6H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 160.7, 158.6, 144.2, 141.8, 138.6, 136.6, 134.9, 131.1, 130.4, 130.1, 128.8, 128.3, 128.3, 128.1, 128.0, 127.7, 126.1, 122.7, 78.5, 21.2 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{29}H_{26}N_3^+$ 416.2121, found: 416.2119.

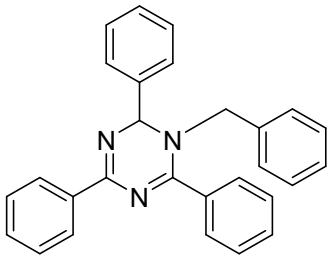
1-(naphthalen-1-yl)-2,4,6-triphenyl-1,2-dihydro-1,3,5-triazine (5ja)



yellow solid (mp: 138−139 °C), (51.7 mg, 59%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.94 (s, 1H), 7.96−7.93 (m, 3H), 7.72 (d, J = 8.0 Hz, 1H), 7.56−7.52 (m, 1H), 7.47−7.41 (m, 7H), 7.40−7.37 (m, 3H), 7.33−7.24 (m, 4H), 6.90 (d, J = 8.4 Hz, 1H), 5.94 (s, 1H), 5.80 (s, 1H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 153.1, 145.7, 135.5, 133.8, 130.9, 129.1, 128.7, 128.3, 127.5, 127.4, 126.8, 126.2, 125.9, 124.6, 124.6, 29.8 ppm;

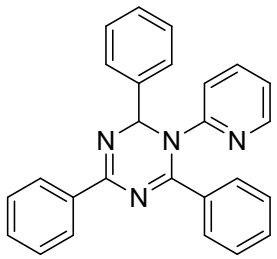
HRMS (ESI) m/z $[M + H]^+$ calcd for $C_{31}H_{24}N_3^+$ 438.1965, found: 438.1961.

1-benzyl-2,4,6-triphenyl-1,2-dihydro-1,3,5-triazine (5ka and **7ka)**



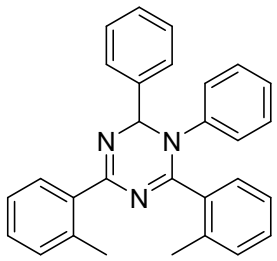
yellow solid (mp: 141−142 °C), (**5ka**: 44.9 mg, 56%; **7ka**: 18.9 mg, 47%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.28−8.26 (m, 2H), 7.64−7.62 (m, 2H), 7.57 (d, J = 6.8 Hz, 2H), 7.46−7.43 (m, 3H), 7.42−7.36 (m, 7H), 7.30−7.26 (m, 2H), 7.22 (d, J = 7.0 Hz, 2H), 5.99 (s, 1H), 4.97 (d, J = 15.4 Hz, 1H), 4.17 (d, J = 15.4 Hz, 1H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 164.1, 158.9, 141.3, 137.0, 135.6, 134.7, 130.8, 130.3, 129.0, 129.0, 128.8, 128.8, 128.7, 128.1, 128.1, 127.9, 127.4, 126.7, 74.0, 53.0 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{28}H_{24}N_3^+$ 402.1965, found: 402.1957.

2,4,6-triphenyl-1-(pyridin-2-yl)-1,2-dihydro-1,3,5-triazine (5la)



yellow solid (mp: 152−153 °C), (32.0 mg, 41%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.46−8.44 (m, 3H), 7.82 (d, J = 7.6 Hz, 2H), 7.74−7.72 (m, 2H), 7.49−7.47 (m, 3H), 7.43 (t, J = 7.6 Hz, 1H), 7.36−7.27 (m, 6H), 7.18 (s, 1H), 6.99−6.96 (m, 1H), 6.59 (d, J = 8.0 Hz, 1H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 159.8, 159.7, 155.1, 148.8, 140.1, 136.9, 136.2, 135.3, 134.7, 131.8, 130.8, 129.8, 128.2, 127.0, 125.1, 119.6, 118.5, 73.3 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{26}H_{21}N_4^+$ 389.1761, found: 389.1763.

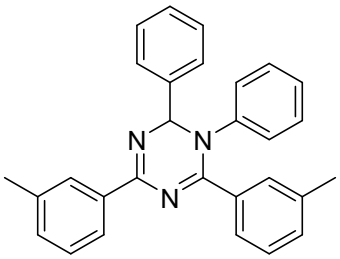
1,2-diphenyl-4,6-di-*o*-tolyl-1,2-dihydro-1,3,5-triazine (5ma and **7la)**



yellow solid (mp: 115−116 °C), (**5na**: 53.9 mg, 65%; **7la**: 19.1 mg, 46%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 7.70−7.68 (m, 1H), 7.62−7.59 (m, 2H), 7.37−7.31 (m, 3H), 7.20−7.09 (m, 4H), 7.06−6.97 (m, 5H), 6.94 (t, J = 7.6 Hz, 1H), 6.85−6.83 (m, 2H), 6.27 (s, 1H), 2.43 (s, 3H), 2.33 (s, 3H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ

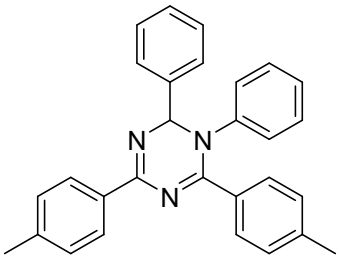
162.2, 161.3, 142.6, 142.4, 137.8, 137.0, 136.9, 134.6, 130.9, 130.8, 129.6, 129.5, 129.0, 128.9, 126.9, 126.3, 125.5, 79.7, 21.0, 20.2 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{29}H_{26}N_3^+$ 416.2121, found: 416.2115.

1,2-diphenyl-4,6-di-*m*-tolyl-1,2-dihydro-1,3,5-triazine (5na and **7ma)**



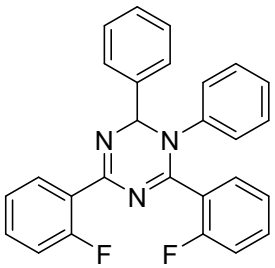
yellow solid (mp: 114−115 °C), (**5oa**: 48.5 mg, 58%; **7ma**: 24.9 mg, 60%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.20 (d, J = 9.6 Hz, 2H), 7.71 (t, J = 7.6 Hz, 3H), 7.45 (d, J = 7.2 Hz, 1H), 7.40 (t, J = 7.2 Hz, 2H), 7.34−7.31 (m, 2H), 7.27 (d, J = 7.2 Hz, 1H), 7.18−7.13 (m, 4H), 7.11−7.06 (m, 1H), 6.99 (d, J = 7.6 Hz, 2H), 6.39 (s, 1H), 2.41 (s, 3H), 2.31 (s, 3H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 160.9, 158.6, 144.4, 141.9, 138.3, 137.7, 136.6, 134.7, 132.1, 131.3, 130.7, 128.9, 128.6, 128.5, 128.1, 128.0, 127.4, 126.2, 125.9, 125.4, 124.9, 78.8, 21.5, 21.4 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{29}H_{26}N_3^+$ 416.2121, found: 416.2124.

1,2-diphenyl-4,6-di-p-tolyl-1,2-dihydro-1,3,5-triazine (5oa and **7na)**



yellow solid (mp: 72−73 °C), (**5pa**: 58.9 mg, 71%; **7na**: 31.2 mg, 75%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.27−8.25 (m, 2H), 7.70 (t, J = 8.4 Hz, 4H), 7.38 (t, J = 7.2 Hz, 2H), 7.33 (t, J = 7.2 Hz, 1H), 7.24 (m, 2H), 7.18−7.14 (m, 2H), 7.10 (d, J = 7.6 Hz, 3H), 7.00 (d, J = 8.0 Hz, 2H), 6.38 (s, 1H), 2.39 (s, 3H), 2.32 (s, 3H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 160.5, 158.5, 144.6, 141.9, 141.7, 140.6, 133.9, 131.9, 130.2, 129.1, 128.9, 128.8, 128.4, 128.1, 126.2, 125.7, 124.8, 78.6, 21.6, 21.5 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{29}H_{26}N_3^+$ 416.2121, found: 416.2110.

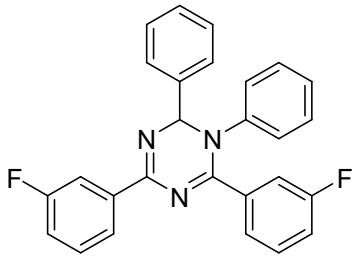
4,6-bis(2-fluorophenyl)-1,2-diphenyl-1,2-dihydro-1,3,5-triazine (5pa)



yellow solid (mp: 122−123 °C), (36.4 mg, 43%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 7.98

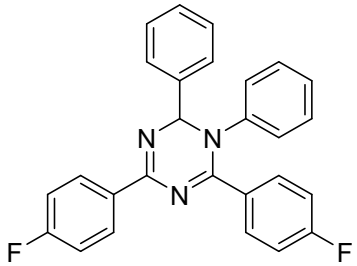
(td, *J* = 7.6, 1.6 Hz, 1H), 7.89 (td, *J* = 7.2, 1.2 Hz, 1H), 7.79 (d, *J* = 7.2 Hz, 2H), 7.45−7.41 (m, 2H), 7.39−7.31 (m, 3H), 7.20−7.09 (m, 6H), 7.02−7.00 (m, 2H), 6.85−6.81 (m, 1H), 6.43 (s, 1H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) *δ* 162.6, 160.1, 158.6, 158.1, 157.6 (d, *J* = 4.1 Hz), 142.7, 141.3, 133.1 (d, *J* = 8.6 Hz), 132.2 (d, *J* = 2.2 Hz), 131.6 (d, *J* = 1.9 Hz), 131.4 (d, *J* = 8.6 Hz), 128.9, 128.7, 128.6, 126.8, 126.6 (d, *J* = 2.2 Hz), 125.7 (d, *J* = 10.1 Hz), 125.4, 124.7 (d, *J* = 3.5 Hz), 123.8 (d, *J* = 3.7 Hz), 123.1 (d, *J* = 12.4 Hz), 116.7 (d, *J* = 22.5 Hz), 116.1 (d, *J* = 21.8 Hz), 78.9 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{27}H_{20}F_2N_3^+$ 424.1620, found: 424.1617.

4,6-bis(3-fluorophenyl)-1,2-diphenyl-1,2-dihydro-1,3,5-triazine (5qa and **7oa)**



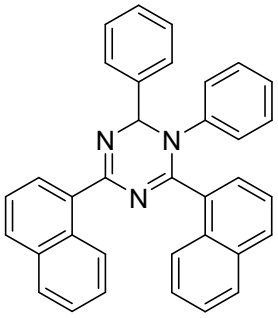
yellow solid (mp: 156−157 °C), (**5ra**: 47.4 mg, 56%; **7oa**: 26.3 mg, 62%); **^{1}H NMR** ($CDCl_3$, 400 MHz) *δ* 8.07 (d, *J* = 7.6 Hz, 1H), 7.98 (d, *J* = 10.4 Hz, 1H), 7.59 (d, *J* = 7.2 Hz, 2H), 7.44 (t, *J* = 8.4 Hz, 2H), 7.35−7.30 (m, 4H), 7.20−7.15 (m, 1H), 7.14−7.08 (m, 3H), 7.07 (d, *J* = 1.6 Hz, 1H), 7.04−6.98 (m ,1H), 6.92 (d, *J* = 7.6 Hz, 2H), 6.31 (s, 1H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) *δ* 164.1 (d, *J* = 29.5 Hz), 161.6 (d, *J* = 32.0 Hz), 159.8 (d, *J* = 2.8 Hz), 157.2 (d, *J* = 3.2 Hz), 143.7, 141.5, 138.9 (d, *J* = 7.6 Hz), 137.0 (d, *J* = 7.7 Hz), 130.0 (d, *J* = 7.9 Hz), 129.6 (d, *J* = 7.8 Hz), 129.2, 129.1, 128.8, 126.5, 125.9 (d, *J* = 2.9 Hz), 124.9, 123.8 (d, *J* = 2.8 Hz), 118.5 (d, *J* = 21.2 Hz), 117.5 (d, *J* = 59.7 Hz), 117.3, 117.2, 115.1, 114.9, 78.8 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{27}H_{20}F_2N_3^+$ 424.1620, found: 424.1629.

4,6-bis(4-fluorophenyl)-1,2-diphenyl-1,2-dihydro-1,3,5-triazine (5ra and **7pa)**



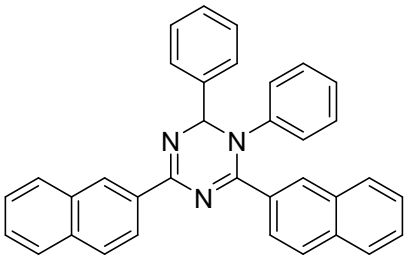
yellow solid (mp: 177−178 °C), (**5sa**: 65.5 mg, 78%; **7pa**: 30.9 mg, 73%); **^{1}H NMR** ($CDCl_3$, 400 MHz) *δ* 8.29−8.26 (m, 2H), 7.70−7.67 (m, 2H), 7.60 (d, *J* = 7.2 Hz, 2H), 7.34−7.27 (m, 3H), 7.13 (t, *J* = 7.2 Hz, 2H), 7.07−7.00 (m, 3H), 6.93−6.89 (m, 4H), 6.29 (s, 1H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) *δ* 165.8 (d, *J* = 5.3 Hz), 163.3 (d, *J* = 8.4 Hz), 159.8, 157.4, 144.0, 141.7, 132.7 (d, *J* = 2.7 Hz), 132.4 (d, *J* = 8.9 Hz), 130.8 (d, *J* = 2.9 Hz), 130.2 (d, *J* = 8.5 Hz), 129.2, 129.0, 128.6, 126.2, 126.1, 124.9, 115.7 (d, *J* = 63.7 Hz), 115.5 (d, *J* = 63.4 Hz), 78.8 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{27}H_{20}F_2N_3^+$ 424.1620, found: 424.1611.

4,6-di(naphthalen-1-yl)-1,2-diphenyl-1,2-dihydro-1,3,5-triazine (5sa)



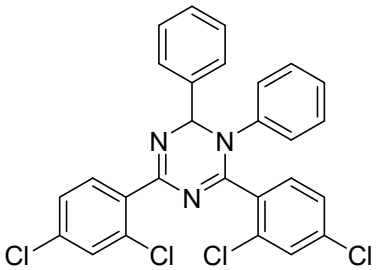
yellow solid (mp: 68−69 °C), (46.1 mg, 43%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.91 (d, J = 8.0 Hz, 1H), 8.44 (d, J = 8.4 Hz, 1H), 8.22 (d, J = 7.2 Hz, 1H), 7.90 (d, J = 8.0 Hz, 1H), 7.85 (d, J = 7.6 Hz, 3H), 7.77−7.73 (m, 2H), 7.53−7.51 (m, 4H), 7.49−7.48 (m, 2H), 7.46−7.43 (m, 3H), 7.29 (t, J = 7.6 Hz, 1H), 7.01−6.96 (m, 5H), 6.55 (s, 1H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 161.7, 160.6, 142.8, 142.4, 134.9, 134.1, 133.7, 132.4, 131.4, 130.5, 130.2, 129.3, 129.2, 128.8, 128.4, 128.3, 128.2, 128.1, 126.9, 126.8, 126.5, 126.2, 126.1, 125.6, 125.3, 125.0, 124.7, 79.7 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{35}H_{26}N_3^+$ 488.2121, found: 488.2127.

4,6-di(naphthalen-2-yl)-1,2-diphenyl-1,2-dihydro-1,3,5-triazine (5ta)



yellow solid (mp: 73−74 °C), (58.2 mg, 60%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.92 (s, 1H), 8.41−8.35 (m, 2H), 7.94−7.92 (m, 1H), 7.83−7.76 (m, 3H), 7.72−7.68 (m, 4H), 7.65 (d, J = 8.4 Hz, 1H), 7.44−7.40 (m, 3H), 7.39−7.36 (m, 1H), 7.35 (t, J = 7.6 Hz, 2H), 7.28 (t, J = 6.8 Hz, 1H), 7.07 (t, J = 7.6 Hz, 2H), 6.99−6.96 (m, 3H), 6.42 (s, 1H) ppm; **^{13}C{^{1}H} NMR** ($CDCl_3$, 100 MHz) δ 160.8, 160.5, 158.5, 144.3, 141.9, 134.7, 134.6, 134.1, 133.2, 132.8, 132.3, 131.4, 129.2, 129.1, 129.0, 128.9, 128.8, 128.6, 128.1, 127.8, 127.7, 126.9, 126.6, 126.3, 126.2, 126.1, 126.0, 125.9, 125.1, 124.9, 79.1 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{35}H_{26}N_3^+$ 488.2121, found: 488.2123.

4,6-bis(2,4-dichlorophenyl)-1,2-diphenyl-1,2-dihydro-1,3,5-triazine (7qa)



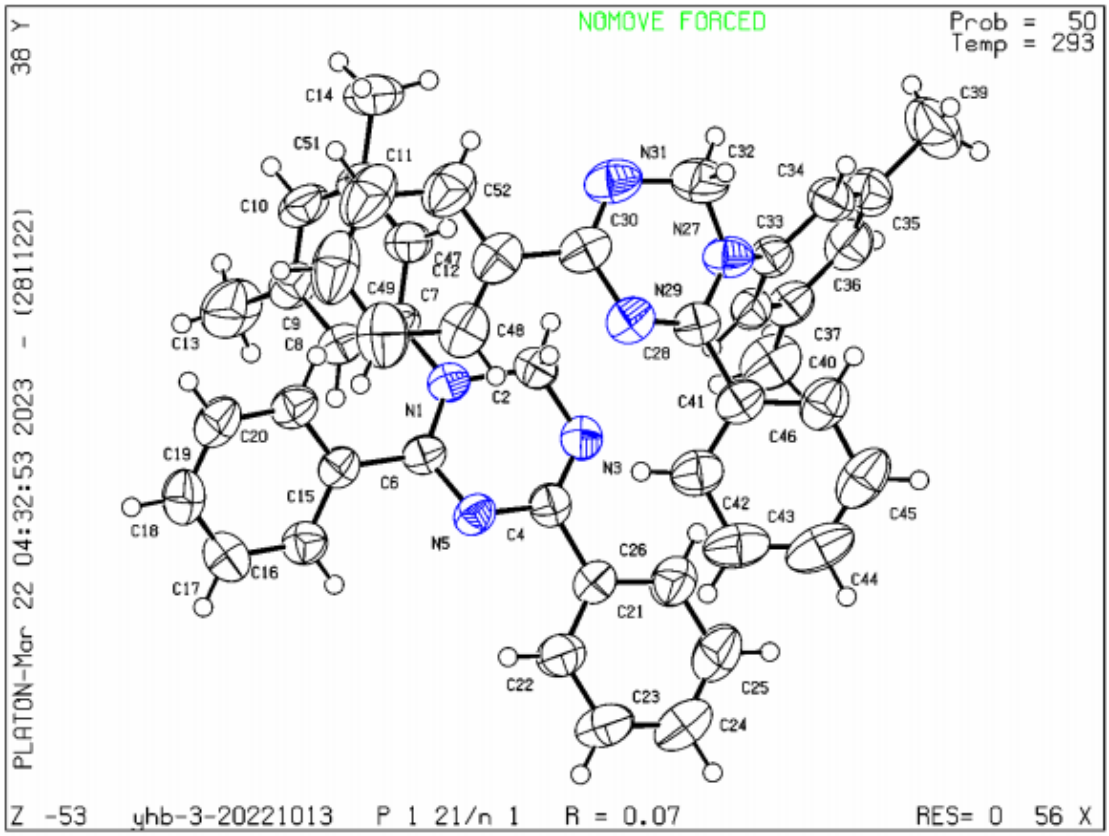
yellow oil (32.0 mg, 61%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 7.66−7.61 (m, 3H), 7.43−7.41 (m, 4H), 7.38 (d, J = 8.3 Hz, 1H), 7.26−7.24 (m, 1H), 7.20 (d, J = 1.8 Hz,

1H), 7.14−7.12 (m, 4H), 7.00−6.95 (m, 2H), 6.33 (s, 1H) ppm; **$^{13}C\{^{1}H\}$ NMR** ($CDCl_3$, 100 MHz) δ 160.0, 158.8, 141.3, 141.1, 136.3, 136.0, 135.2, 133.4, 133.4, 132.5, 131.7, 131.4, 130.0, 129.9, 129.4, 129.0, 128.9, 128.0, 127.3, 127.1, 127.0, 126.9, 80.2 ppm; **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{27}H_{18}Cl_4N_3^+$ 526.0220, found: 526.0215.

6. Reference

[1] X. Meng, X. Bi, Y. Wang, G. Chen, B. Chen, Z. Jing and P. Zhao, *Catal. Commun.,* 2017, **89**, 34.

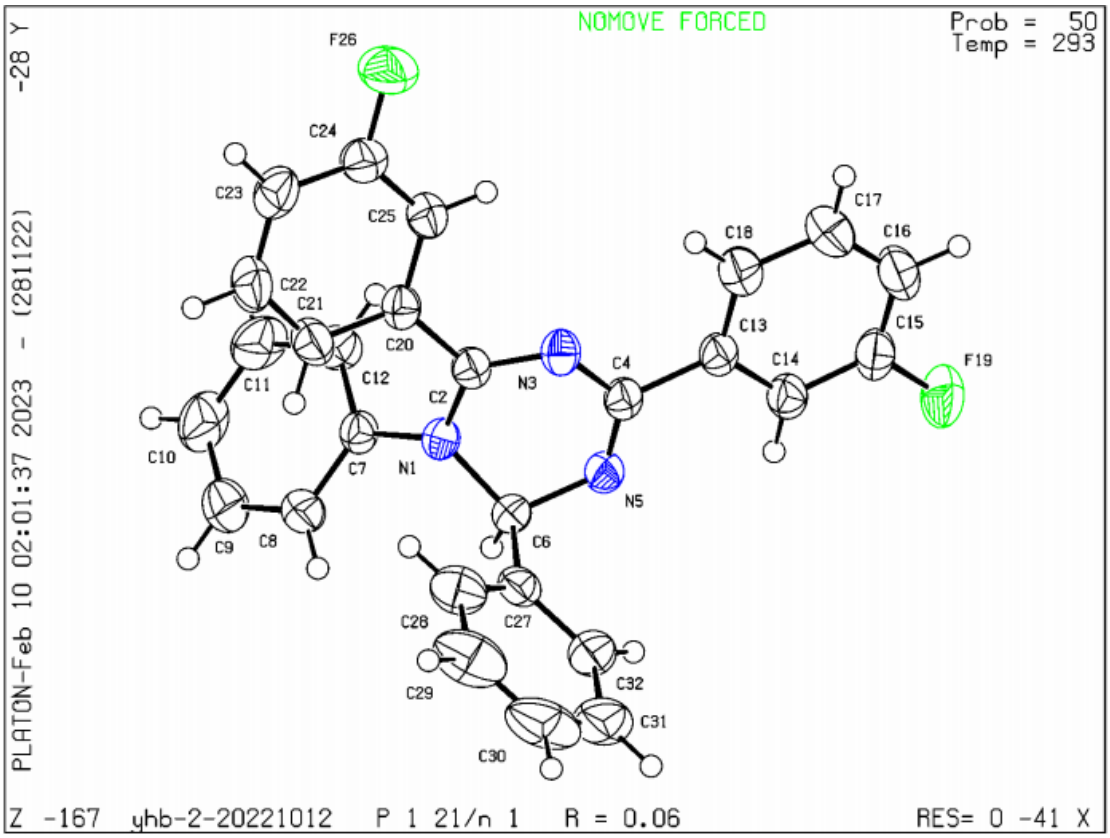
7. Crystal structure of compound 3ia (CCDC 2224587)



CCDC number	2224587
Identification code	**3ia**
Moiety formula	$2(C_{23}H_{21}N_3)$
Sum formula	$C_{46}H_{42}N_6$
Formula weight	678.85
Temperature/K	293
Crystal system	monoclinic
Space group	P 1 21/n 1
a,b,c (Å)	9.5634(5), 33.8247(15), 12.5950(7)
α,β,γ (°)	90, 111.385(6), 90
Volume/Å^3	3793.7(4)
Z	4
ρ_{calc}g/cm^3	1.189
μ/mm^{-1}	0.071
F(000)	1440.0
Crystal size/mm^3	0.21×0.18×0.16
Radiation type	Mo *K*α
Radiation wavelength	0.71073
Index ranges	$-8 \le h \le 11$, $-26 \le k \le 42$, $-16 \le l \le 16$
Reflections collected	14633

Independent reflections	8234
Data/restraints/parameters	8234/0/473
Goodness-of-fit on F^2	1.047
Final R indexes [I>=2σ (I)]	R_1 = 0.0702, wR_2 = 0.1906
Final R indexes [all data]	R_1 = 0.1084, wR_2 = 0.2186
Largest diff. peak/hole / e $Å^{-3}$	0.197/-0.189

8. Crystal structure of compound 7oa (CCDC 2224582)

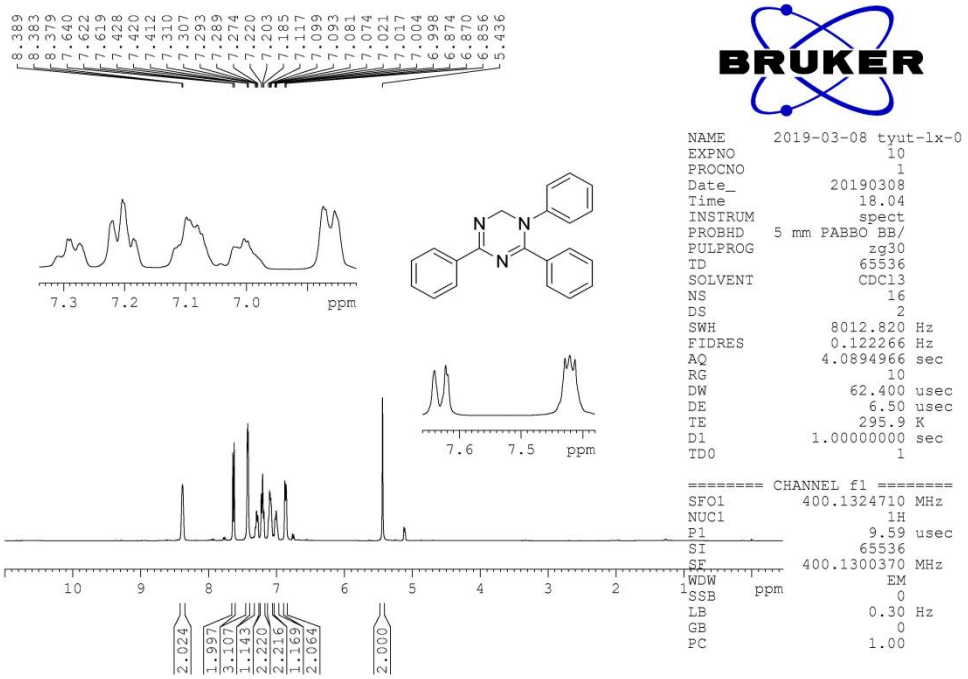


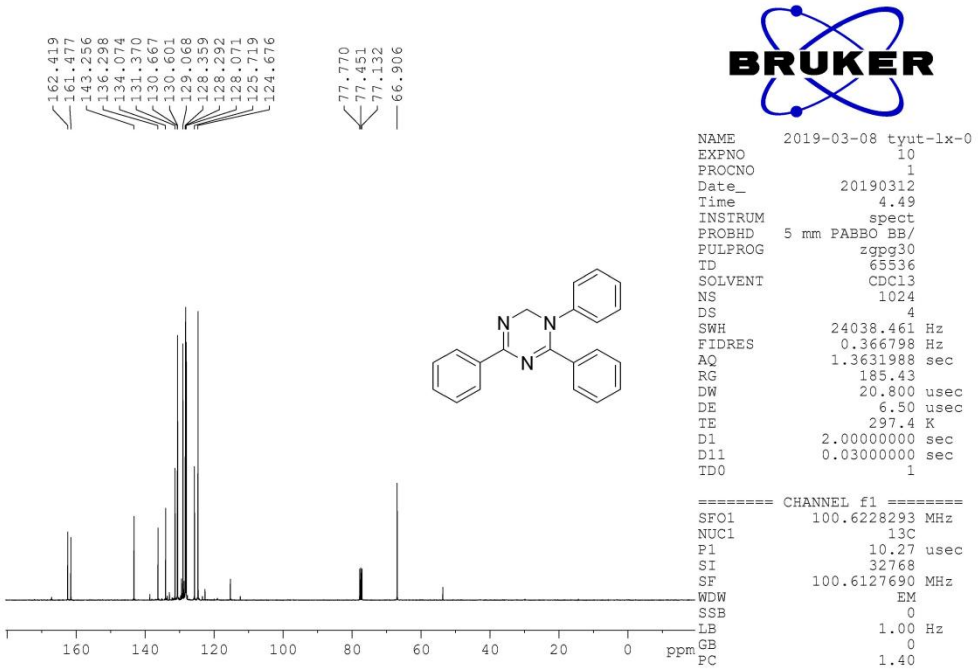
CCDC number	2224582
Identification code	**7oa**
Moiety formula	$C_{27}H_{19}F_2N_3$
Sum formula	$C_{27}H_{19}F_2N_3$
Formula weight	423.45
Temperature/K	293
Crystal system	monoclinic
Space group	P 1 21/n 1
a,b,c (Å)	10.1865(2), 11.3004(2), 19.1635(4)
α,β,γ (°)	90, 103.307(2), 90
Volume/$Å^3$	2146.71(7)

Z	4
ρ_{calc}g/cm^3	1.310
μ/mm^{-1}	0.737
F(000)	880.0
Crystal size/mm^3	0.22×0.18×0.16
Radiation type	Cu *K*α
Radiation wavelength	1.54184
Index ranges	$-9 \leq h \leq 12$, $-13 \leq k \leq 13$, $-23 \leq l \leq 20$
Reflections collected	10518
Independent reflections	4088
Data/restraints/parameters	4088/0/289
Goodness-of-fit on F^2	1.094
Final R indexes [I>=2σ (I)]	R_1 = 0.0577, wR_2 = 0.1510
Final R indexes [all data]	R_1 = 0.0637, wR_2 = 0.1572
Largest diff. peak/hole / e Å^{-3}	0.254/-0.413

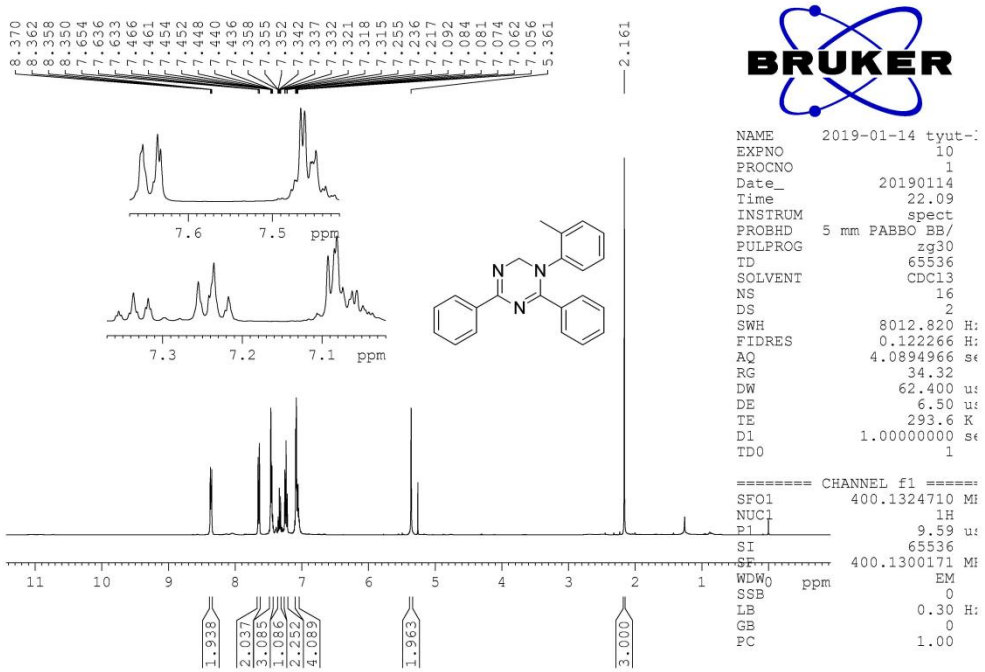
9. ^{1}H NMR and ^{13}C NMR for products 3

3aa





3ba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7.654
7.636
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7.461
7.454
7.452
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7.436
7.358
7.355
7.352
7.342
7.337
7.332
7.321
7.318
7.315
7.255
7.236
7.217
7.092
7.084
7.081
7.074
7.062
7.056
5.361
2.161
7.6
7.5
ppm
7.3
7.2
7.1
ppm
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.938
2.037
3.085
1.086
2.252
4.089
1.963
3.000
BRUKER
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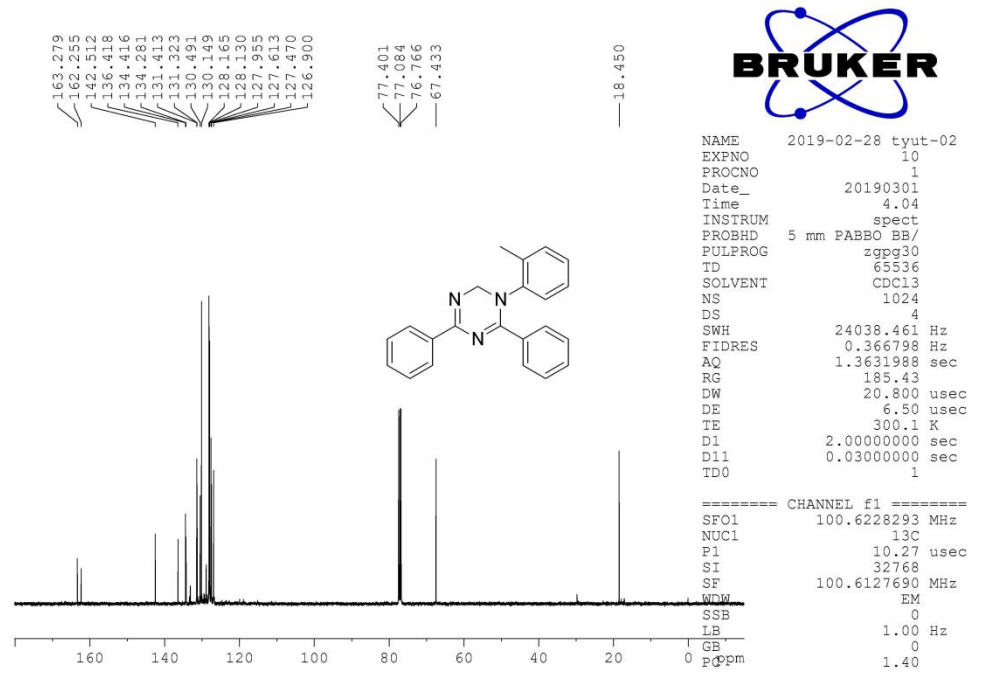
EXPNO 10
PROCNO 1
Date_ 20190114
Time 22.09
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 34.32
DW 62.400 usec
DE 6.50 usec
TE 293.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ======
SFO1 400.1324710 MHz
NUC1 1H
P1 9.59 usec
SI 65536
SF 400.1300171 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00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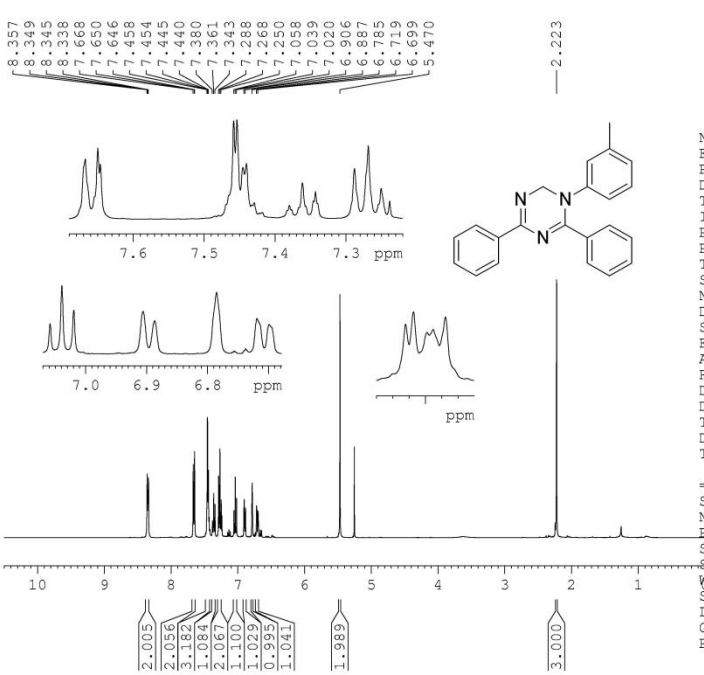
134.281
131.413
131.323
130.491
130.149
128.165
128.130
127.955
127.613
127.470
126.900
77.401
77.084
76.766
67.433
18.450
160
140
120
100
80
60
40
20
0
ppm
BRUKER
NAME 2019-02-28 tyut-02
EXPNO 10
PROCNO 1
Date_ 20190301
Time 4.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 185.43
DW 20.800 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.27 usec
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3ca



BRUKER

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EXPNO                   10
PROCNO                   1
Date_              20190114
Time                 22.20
INSTRUM              spect
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PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH               8012.820 Hz
FIDRES               0.122266 Hz
AQ                4.0894966 sec
RG                    34.32
DW                  62.400 usec
DE                   6.50 usec
TE                  293.6 K
D1                1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1            400.1324710 MHz
NUC1                    1H
P1                   9.59 usec
SI                  65536
SF              400.1300186 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
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PC                    1.00
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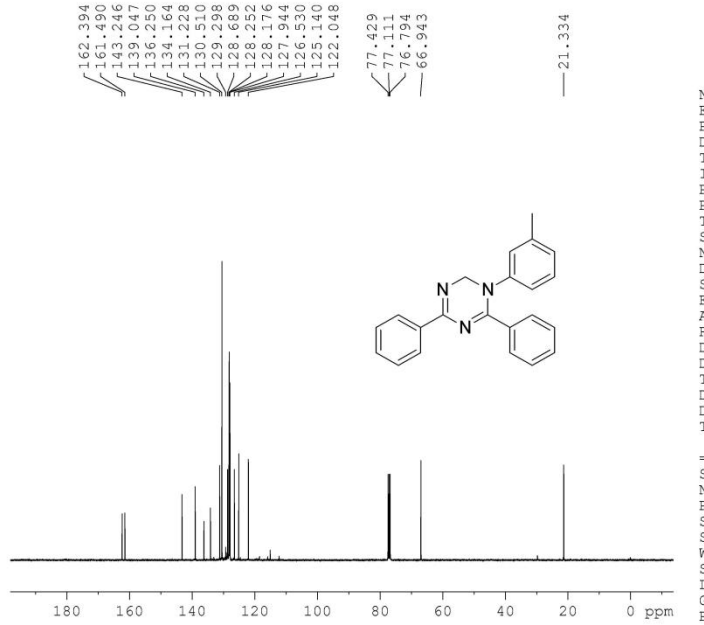

BRUKER

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EXPNO                   10
PROCNO                   1
Date_              20190301
Time                  1.01
INSTRUM              spect
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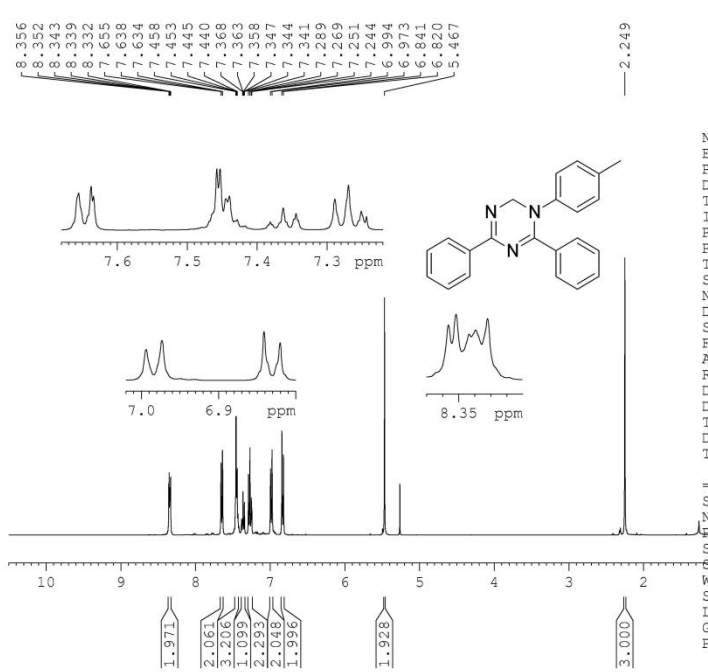
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   1024
DS                      4
SWH              24038.461 Hz
FIDRES               0.366798 Hz
AQ                1.3631988 sec
RG                   185.43
DW                  20.800 usec
DE                   6.50 usec
TE                  300.3 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1            100.6228293 MHz
NUC1                    13C
P1                  10.27 usec
SI                  32768
SF              100.6127690 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

3da



BRUKER

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NAME          2019-01-14 tyut-lx-0
EXPNO                   10
PROCNO                   1
Date_              20190114
Time                 22.16
INSTRUM              spect
PROBHD     5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8012.820 Hz
FIDRES                0.122266 Hz
AQ                 4.0894966 sec
RG                      34.32
DW                     62.400 usec
DE                      6.50 usec
TE                     293.6 K
D1                 1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1             400.1324710 MHz
NUC1                     1H
P1                     9.59 usec
SI                    65536
SF               400.1300165 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
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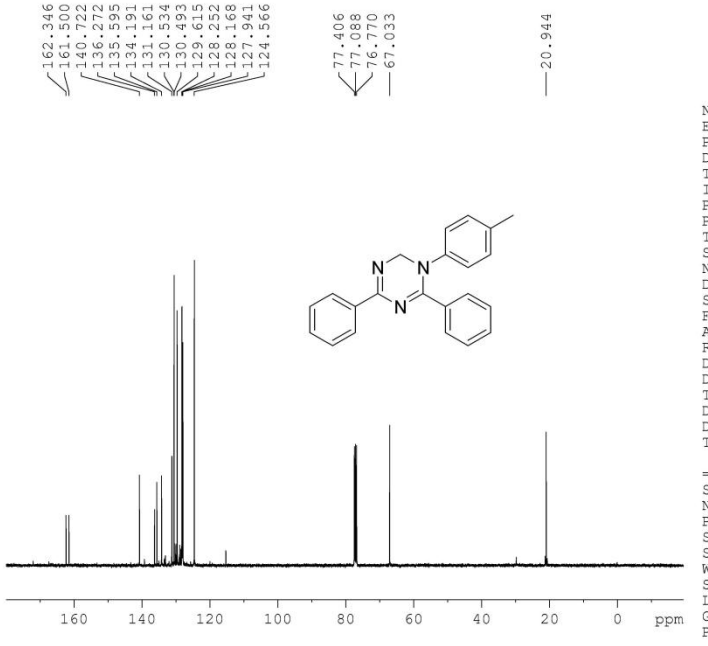

BRUKER

```
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EXPNO                   10
PROCNO                   1
Date_              20190301
Time                  2.02
INSTRUM              spect
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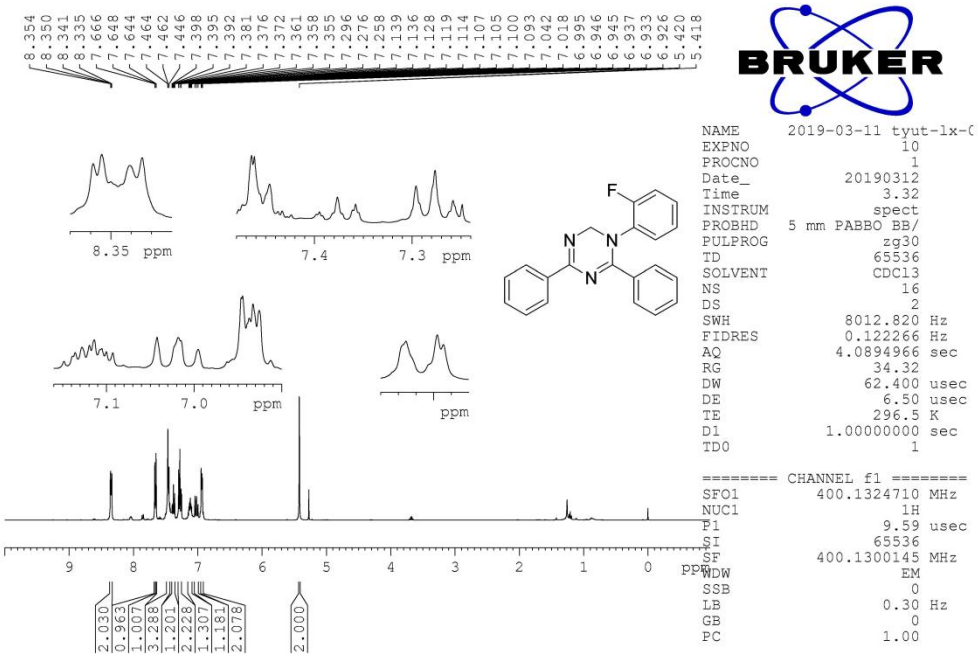
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES                0.366798 Hz
AQ                 1.3631988 sec
RG                     185.43
DW                     20.800 usec
DE                      6.50 usec
TE                     300.2 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1             100.6228293 MHz
NUC1                     13C
P1                    10.27 usec
SI                    32768
SF               100.6127690 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

3ea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7.464
7.462
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7.398
7.395
7.392
7.381
7.376
7.372
7.361
7.358
7.355
7.296
7.276
7.258
7.139
7.136
7.128
7.119
7.114
7.107
7.105
7.100
7.093
7.042
7.018
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6.946
6.945
6.937
6.933
6.926
5.420
5.418
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7.4
7.3 ppm
7.1
7.0
ppm
ppm
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N
N
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8
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6
5
4
3
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BRUKER
NAME 2019-03-11 tyut-lx-(
EXPNO 10
PROCNO 1
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Time 3.32
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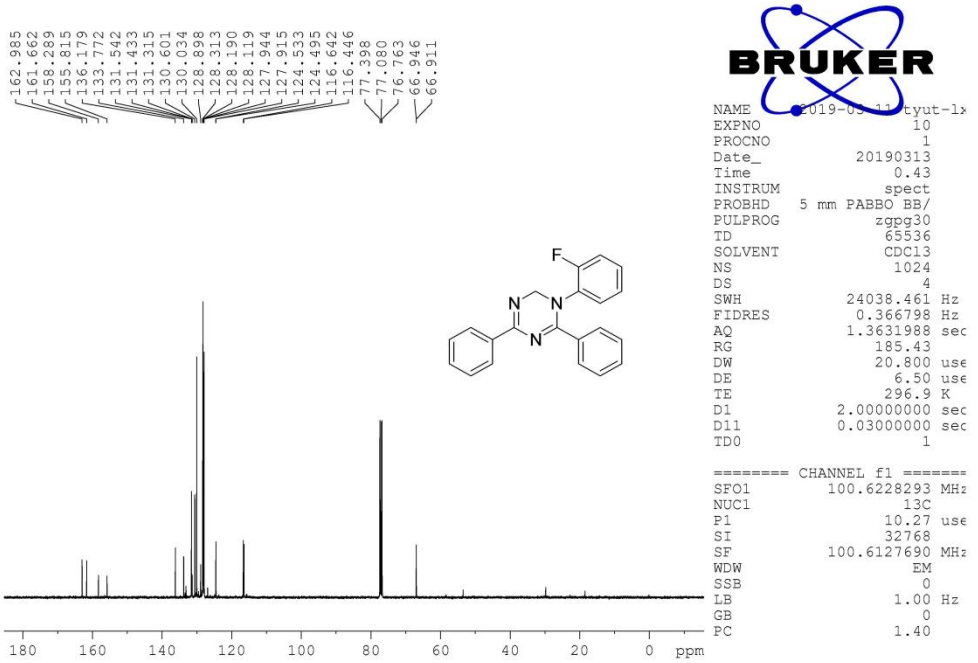
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 34.32
DW 62.400 usec
DE 6.50 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.59 usec
SI 65536
SF 400.1300145 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00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130.601
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128.190
128.119
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127.915
124.533
124.495
116.642
116.446
77.398
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66.946
66.911
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80
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40
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ppm
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NAME 2019-03-11 tyut-lx
EXPNO 10
PROCNO 1
Date_ 20190313
Time 0.43
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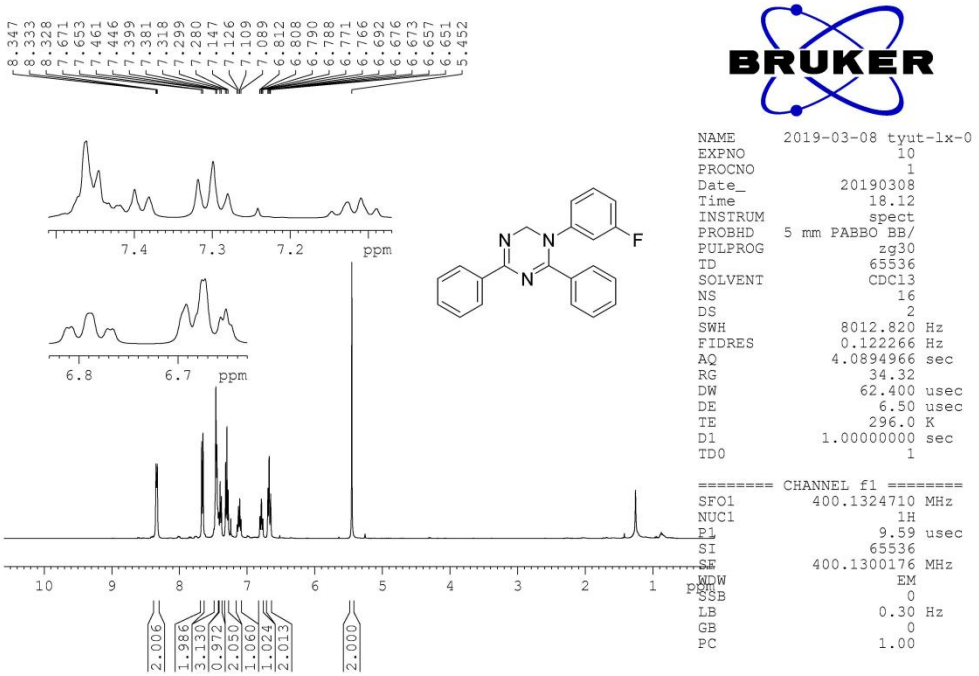
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 185.43
DW 20.800 use
DE 6.50 use
TE 296.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 =======
SFO1 100.6228293 MHz
NUC1 13C
P1 10.27 use
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3fa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7.399
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7.147
7.126
7.109
7.089
6.812
6.808
6.790
6.788
6.771
6.766
6.692
6.676
6.673
6.657
6.651
5.452
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7.3
7.2
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6.8
6.7
ppm
10
9
8
7
6
5
4
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2
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ppm
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2.000
BRUKER
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EXPNO 10
PROCNO 1
Date_ 20190308
Time 18.12
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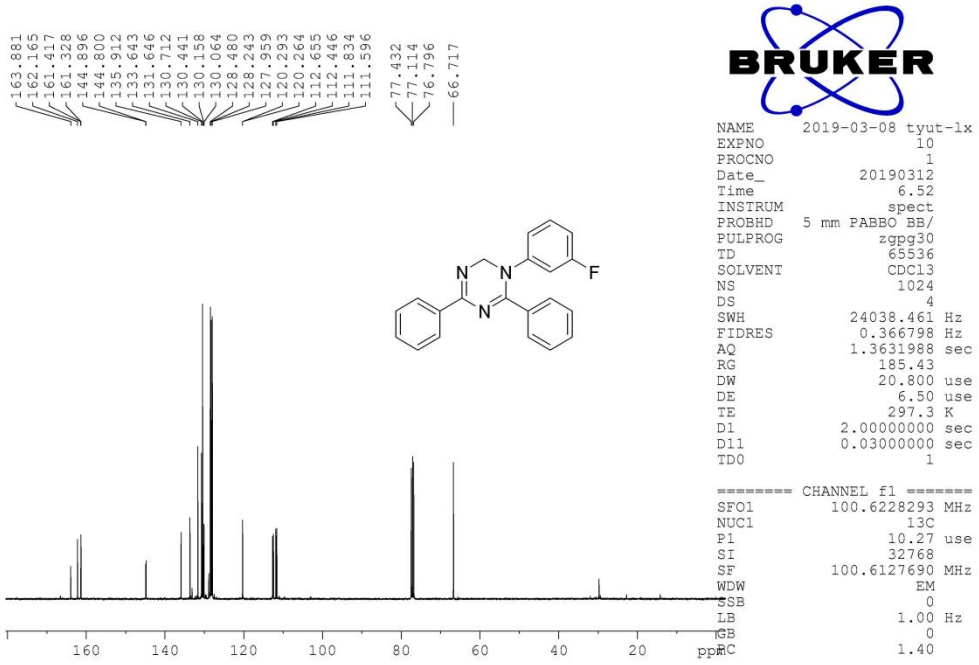
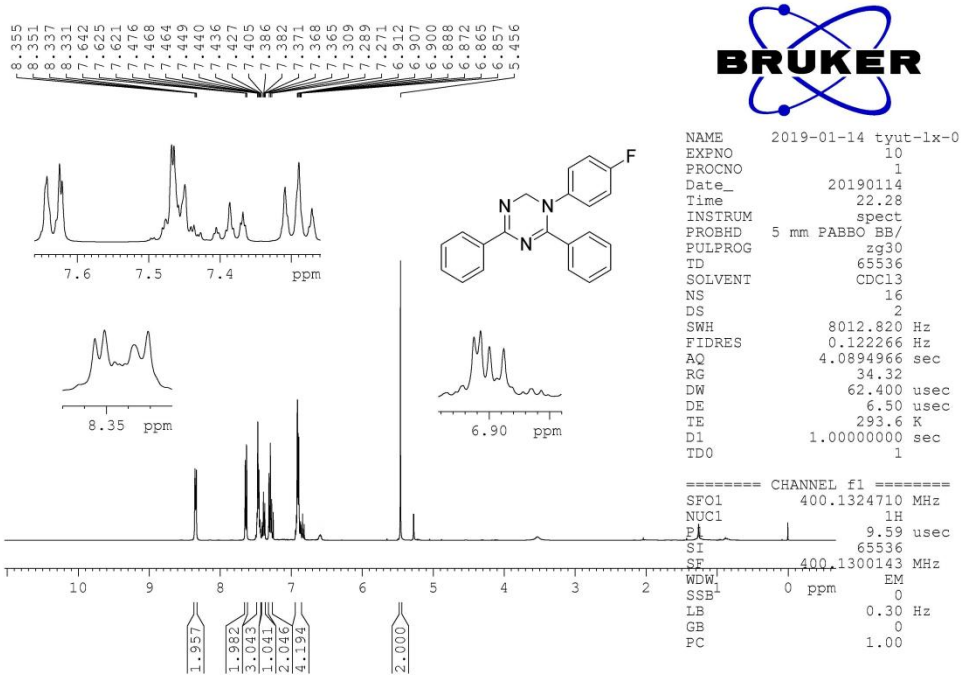
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 34.32
DW 62.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.59 usec
SI 65536
SF 400.1300176 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

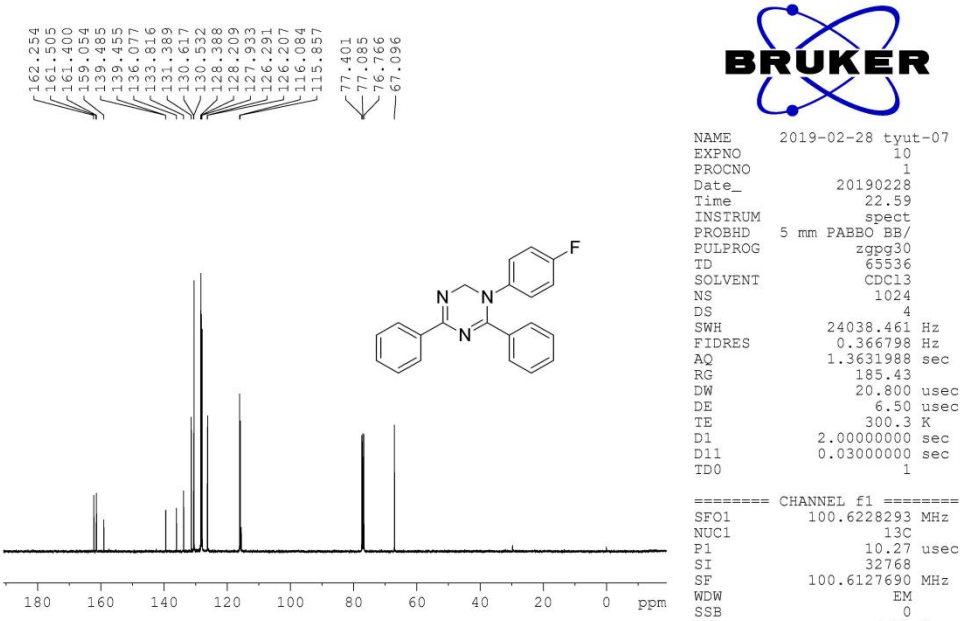

163.881
162.165
161.417
161.328
144.896
144.800
135.912
133.643
131.646
130.712
130.441
130.158
130.064
128.480
128.243
127.959
120.293
120.264
112.655
112.446
111.834
111.596
77.432
77.114
76.796
66.717
160
140
120
100
80
60
40
20
ppm
BRUKER
NAME 2019-03-08 tyut-lx
EXPNO 10
PROCNO 1
Date_ 20190312
Time 6.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 185.43
DW 20.800 use
DE 6.50 use
TE 297.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 =======
SFO1 100.6228293 MHz
NUC1 13C
P1 10.27 use
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3ga



BRUKER

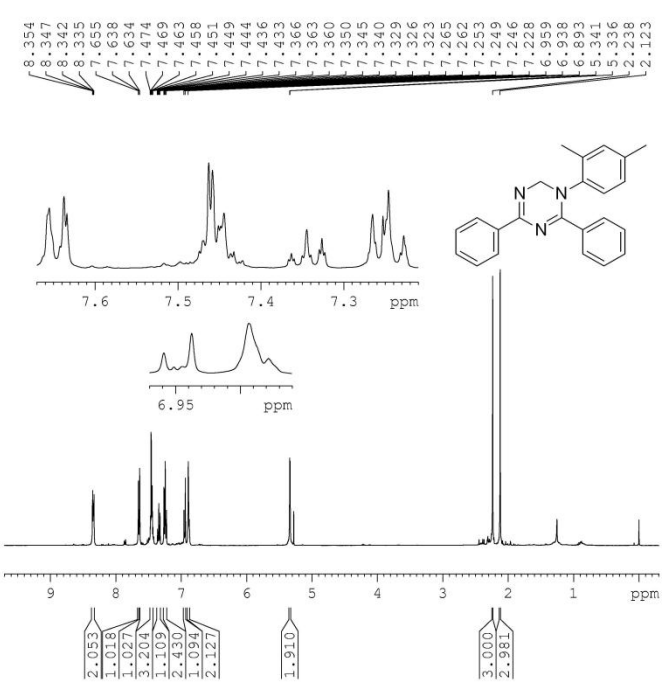
NAME	2019-01-14 tyut-1x-0
EXPNO	10
PROCNO	1
Date_	20190114
Time	22.28
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	34.32
DW	62.400 usec
DE	6.50 usec
TE	293.6 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1324710 MHz
NUC1	1H
P1	9.59 usec
SI	65536
SF	400.1300143 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

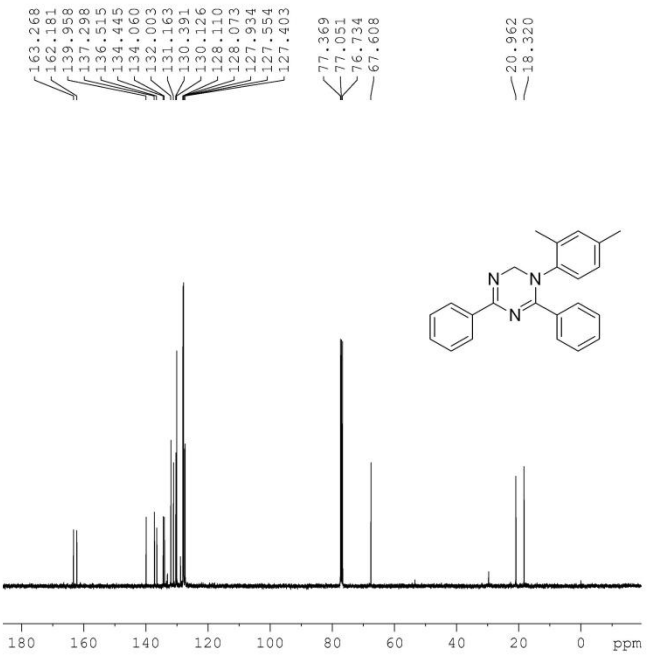
NAME	2019-02-28 tyut-07
EXPNO	10
PROCNO	1
Date_	20190228
Time	22.59
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	185.43
DW	20.800 usec
DE	6.50 usec
TE	300.3 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228293 MHz
NUC1	13C
P1	10.27 usec
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

3ha




```
NAME          2019-03-11 tyut-lx-0
EXPNO                   10
PROCNO                   1
Date_             20190312
Time                 3.36
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH               8012.820 Hz
FIDRES               0.122266 Hz
AQ                4.0894966 sec
RG                    57.76
DW                  62.400 usec
DE                    6.50 usec
TE                   296.4 K
D1                1.00000000 sec
TD0                     1

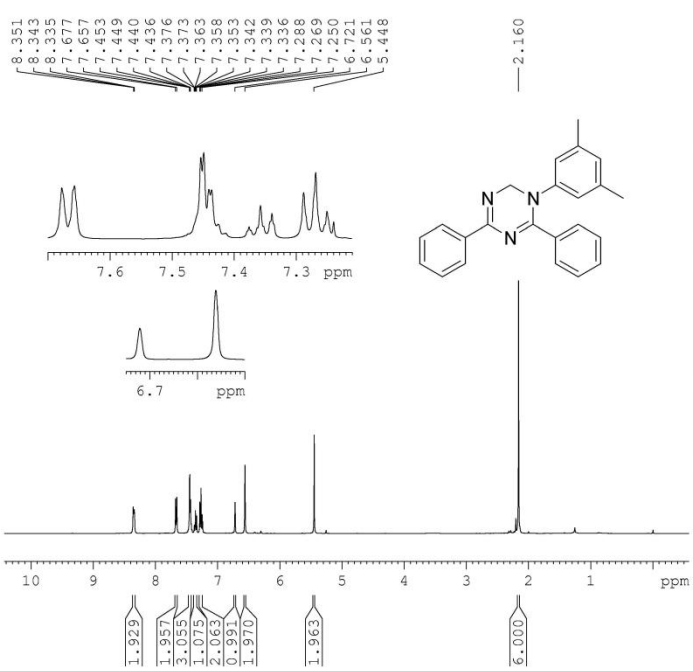
======== CHANNEL f1 ========
SFO1           400.1324710 MHz
NUC1                   1H
P1                   9.59 usec
SI                  65536
SF             400.1300130 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```




```
NAME          2019-03-11 tyut-lx-C-0
EXPNO                   10
PROCNO                   1
Date_             20190313
Time                 1.44
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   1024
DS                      4
SWH              24038.461 Hz
FIDRES               0.366798 Hz
AQ                1.3631988 sec
RG                   185.43
DW                  20.800 usec
DE                    6.50 usec
TE                   296.8 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                     1

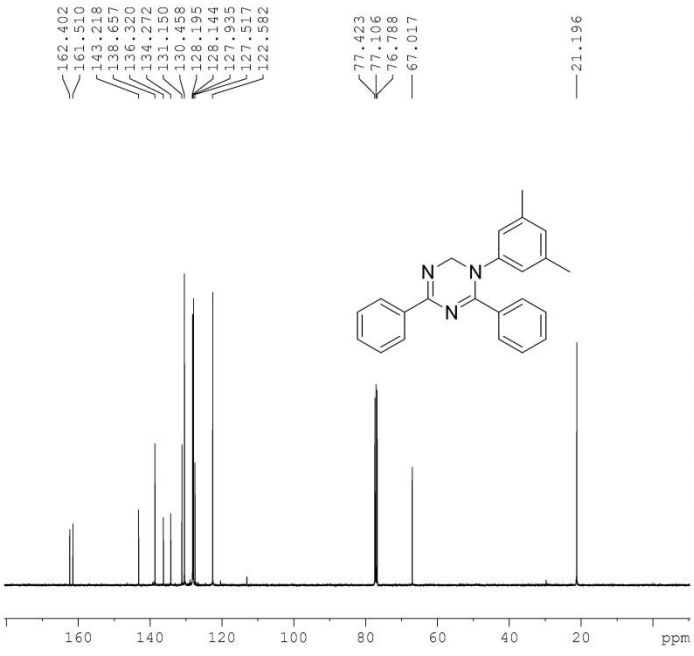
======== CHANNEL f1 ========
SFO1           100.6228293 MHz
NUC1                   13C
P1                  10.27 usec
SI                  32768
SF             100.6127690 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

3ia




```
NAME        2019-03-13 tyut-lx-(
EXPNO                   10
PROCNO                   1
Date_             20190314
Time                 2.11
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH               8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894966 sec
RG                    34.32
DW                  62.400 usec
DE                   6.50 usec
TE                  295.6 K
D1                1.00000000 sec
TD0                     1

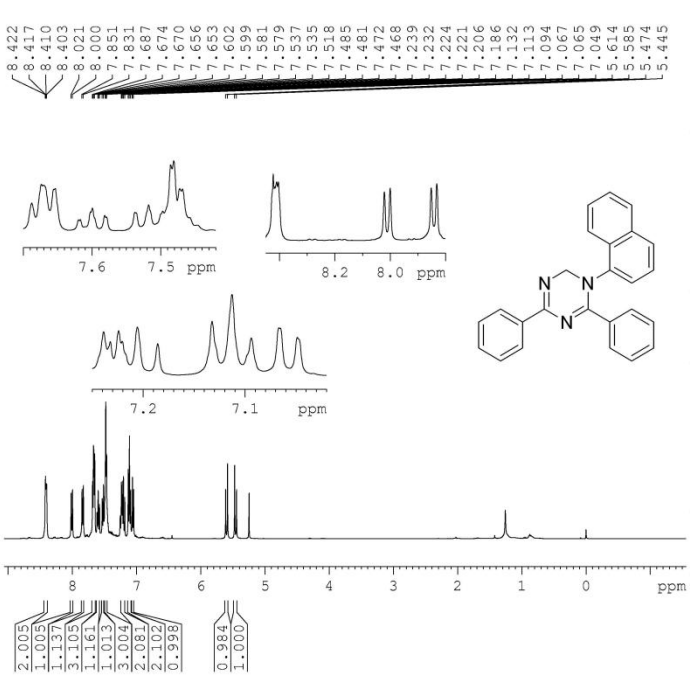
======== CHANNEL f1 ========
SFO1           400.1324710 MHz
NUC1                   1H
P1                   9.59 usec
SI                  65536
SF             400.1300181 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```




```
NAME        2019-03-13 tyut-lx-(
EXPNO                   10
PROCNO                   1
Date_             20190315
Time                10.38
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   1024
DS                      4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                   185.43
DW                  20.800 usec
DE                   6.50 usec
TE                  296.2 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                     1

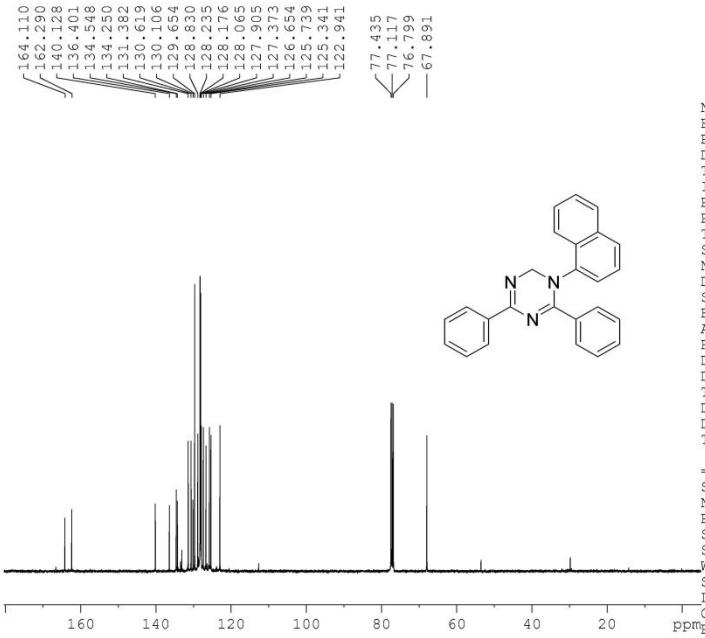
======== CHANNEL f1 ========
SFO1           100.6228293 MHz
NUC1                   13C
P1                  10.27 usec
SI                  32768
SF             100.6127690 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

3ja



```
NAME          2019-03-08 tyut-lx-0
EXPNO                   10
PROCNO                   1
Date_             20190308
Time                 18.16
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH                8012.820 Hz
FIDRES                0.122266 Hz
AQ                 4.0894966 sec
RG                      34.32
DW                    62.400 usec
DE                     6.50 usec
TE                    296.0 K
D1                 1.00000000 sec
TD0                      1

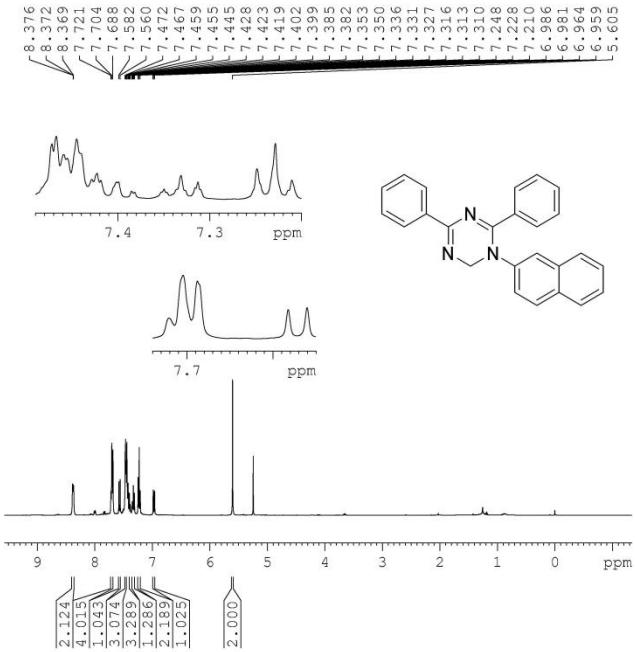
======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                    1H
P1                    9.59 usec
SI                   65536
SF            400.1300212 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



```
NAME          2019-03-08 tyut-lx-0
EXPNO                   10
PROCNO                   1
Date_             20190312
Time                  7.53
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG            zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH               24038.461 Hz
FIDRES                0.366798 Hz
AQ                 1.3631988 sec
RG                     185.43
DW                    20.800 usec
DE                     6.50 usec
TE                    297.3 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                      1

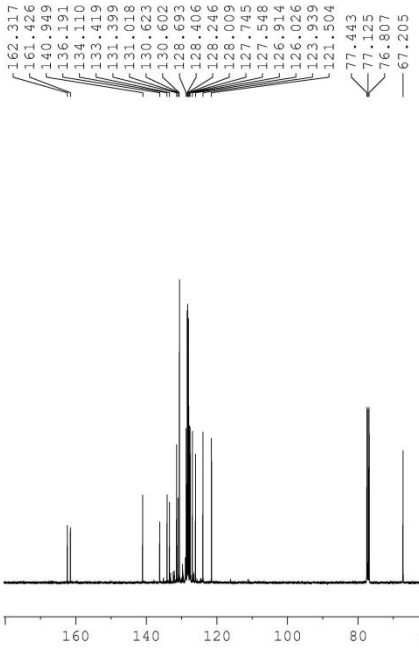
======== CHANNEL f1 ========
SFO1          100.6228293 MHz
NUC1                    13C
P1                   10.27 usec
SI                   32768
SF            100.6127690 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

3ka



```
NAME          2019-03-11 tyut-lx-0
EXPNO                 10
PROCNO                 1
Date_           20190312
Time                3.43
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES             0.122266 Hz
AQ              4.0894966 sec
RG                 34.32
DW                 62.400 usec
DE                  6.50 usec
TE                296.4 K
D1              1.00000000 sec
TD0                    1

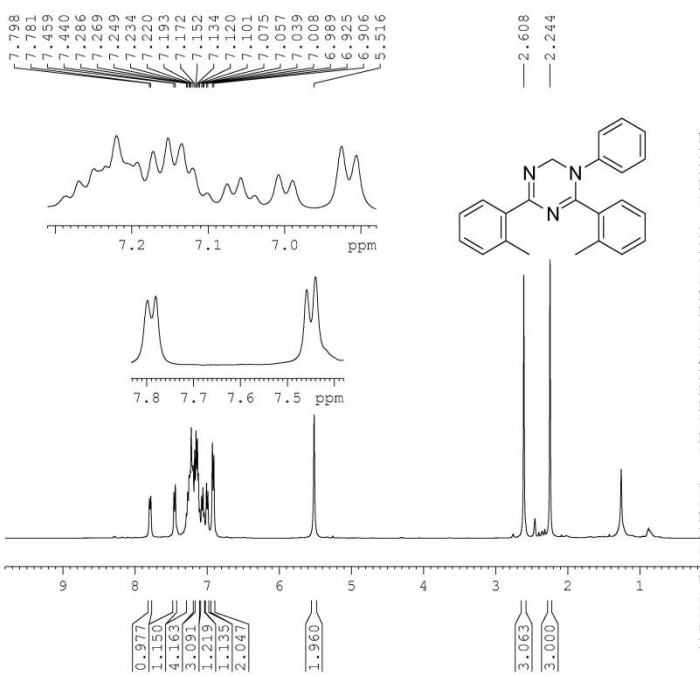
======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                  1H
P1                  9.59 usec
SI                 65536
SF            400.1300228 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

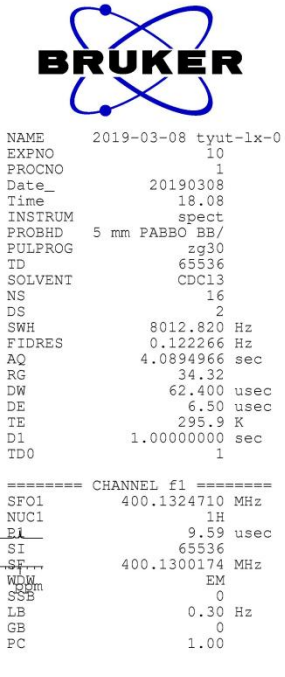


```
NAME          2019-03-11 tyut-lx-0
EXPNO                 10
PROCNO                 1
Date_           20190313
Time                3.46
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES             0.366798 Hz
AQ              1.3631988 sec
RG                 185.43
DW                 20.800 usec
DE                  6.50 usec
TE                296.7 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1

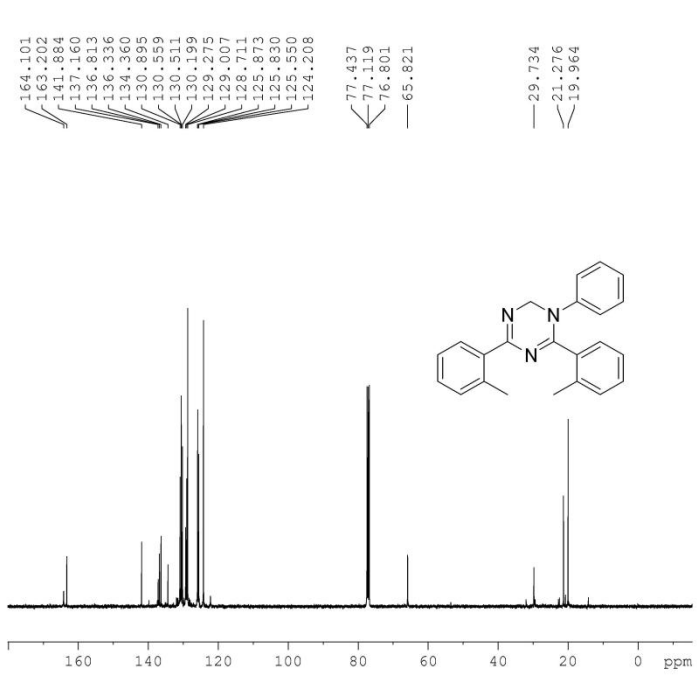
======== CHANNEL f1 ========
SFO1          100.6228293 MHz
NUC1                  13C
P1                 10.27 usec
SI                 32768
SF            100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

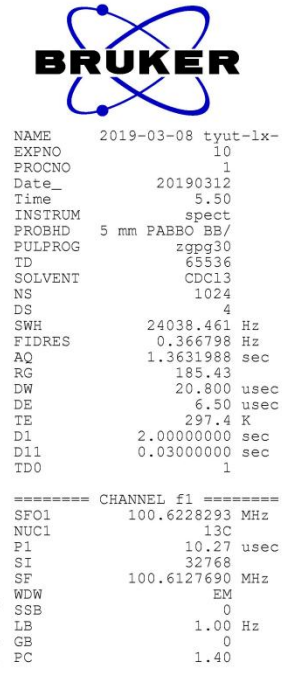
3ma





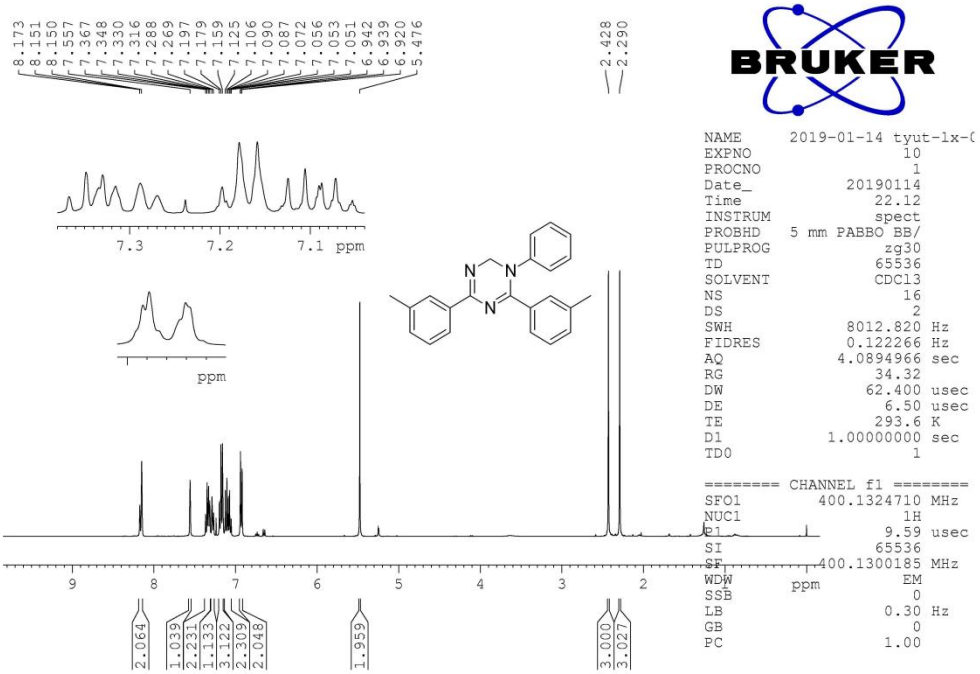
NAME	2019-03-08 tyut-lx-0
EXPNO	10
PROCNO	1
Date_	20190308
Time	18.08
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	34.32
DW	62.400 usec
DE	6.50 usec
TE	295.9 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1324710 MHz
NUC1	1H
P1	9.59 usec
SI	65536
SF	400.1300174 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

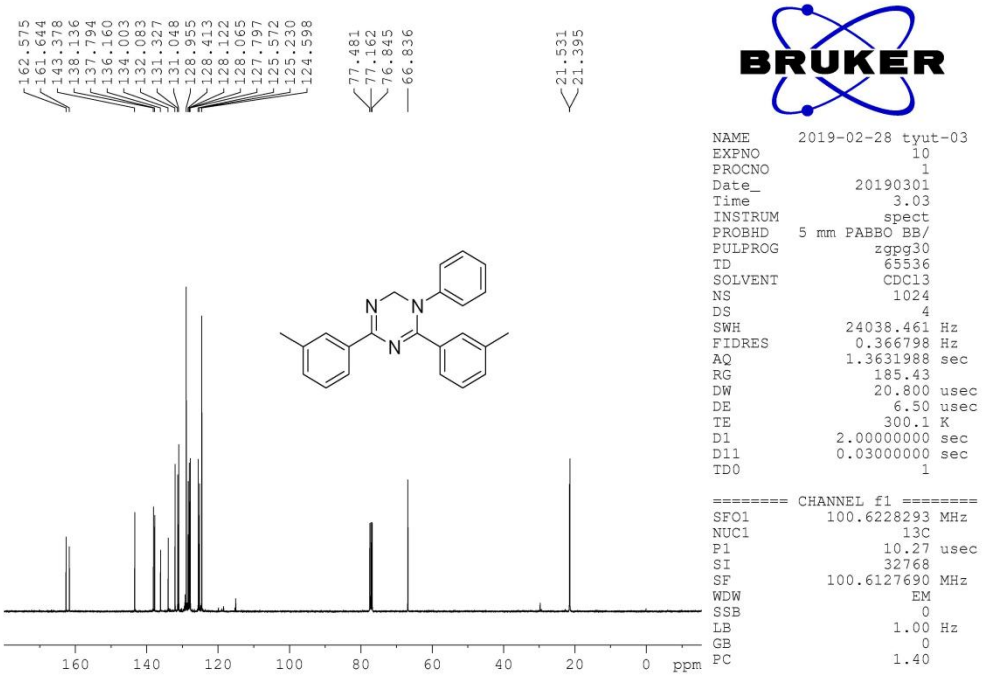




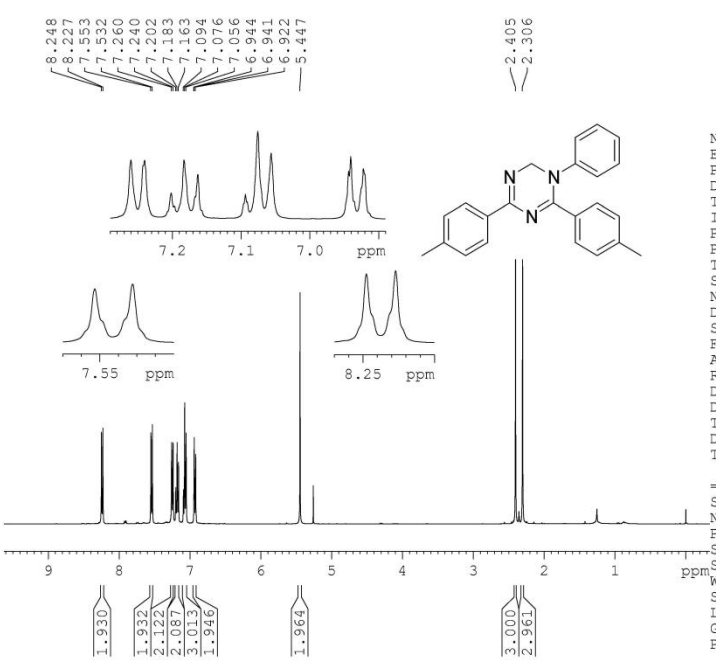
NAME	2019-03-08 tyut-lx-
EXPNO	10
PROCNO	1
Date_	20190312
Time	5.50
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	185.43
DW	20.800 usec
DE	6.50 usec
TE	297.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228293 MHz
NUC1	13C
P1	10.27 usec
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

3na


8.173
8.151
8.150
7.557
7.367
7.348
7.330
7.316
7.288
7.269
7.197
7.179
7.159
7.125
7.106
7.090
7.087
7.072
7.056
7.053
7.051
6.942
6.939
6.920
5.476
2.428
2.290
7.3
7.2
7.1 ppm
ppm
9 8 7 6 5 4 3 2 1 ppm
2.064
1.039
2.231
1.133
3.122
2.309
2.048
1.959
3.000
3.027
NAME 2019-01-14 tyut-lx-(
EXPNO 10
PROCNO 1
Date_ 20190114
Time 22.12
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 34.32
DW 62.400 usec
DE 6.50 usec
TE 293.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.59 usec
SI 65536
SF 400.1300185 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


162.575
161.644
143.378
138.136
137.794
136.160
134.003
132.083
131.327
131.048
128.955
128.413
128.122
128.065
127.797
125.572
125.230
124.598
77.481
77.162
76.845
66.836
21.531
21.395
160 140 120 100 80 60 40 20 0 ppm
NAME 2019-02-28 tyut-03
EXPNO 10
PROCNO 1
Date_ 20190301
Time 3.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 185.43
DW 20.800 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.27 usec
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

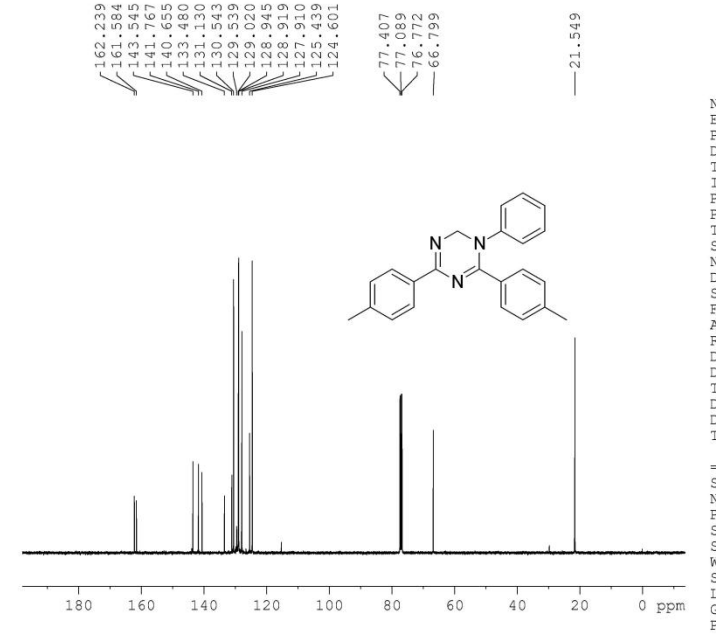
3oa



BRUKER

```
NAME          2019-01-14 tyut-lx-
EXPNO                 10
PROCNO                 1
Date_           20190114
Time               22.24
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES             0.122266 Hz
AQ              4.0894966 sec
RG                 34.32
DW                 62.400 usec
DE                  6.50 usec
TE                293.6 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                  1H
P1                  9.59 usec
SI                 65536
SF            400.1300167 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

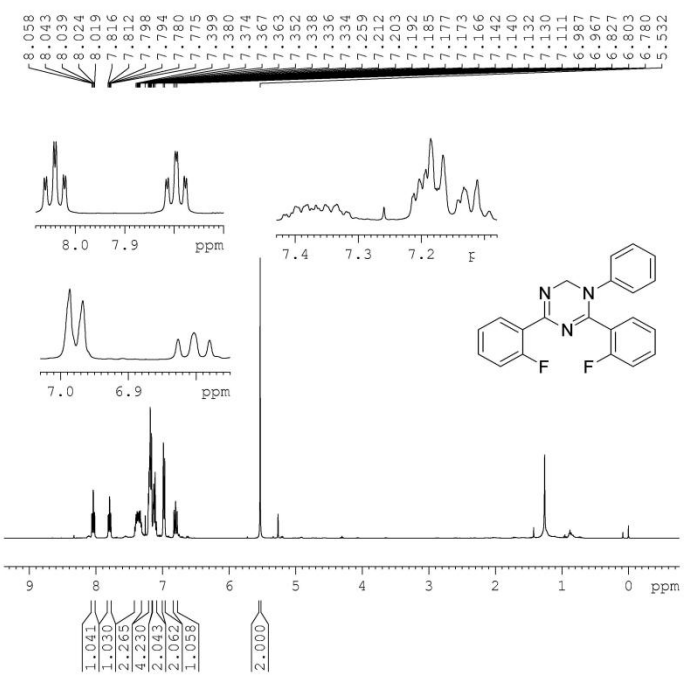


BRUKER

```
NAME          2019-02-28 tyut-06
EXPNO                 10
PROCNO                 1
Date_           20190301
Time                0.00
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES             0.366798 Hz
AQ              1.3631988 sec
RG                 185.43
DW                 20.800 usec
DE                  6.50 usec
TE                300.3 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1

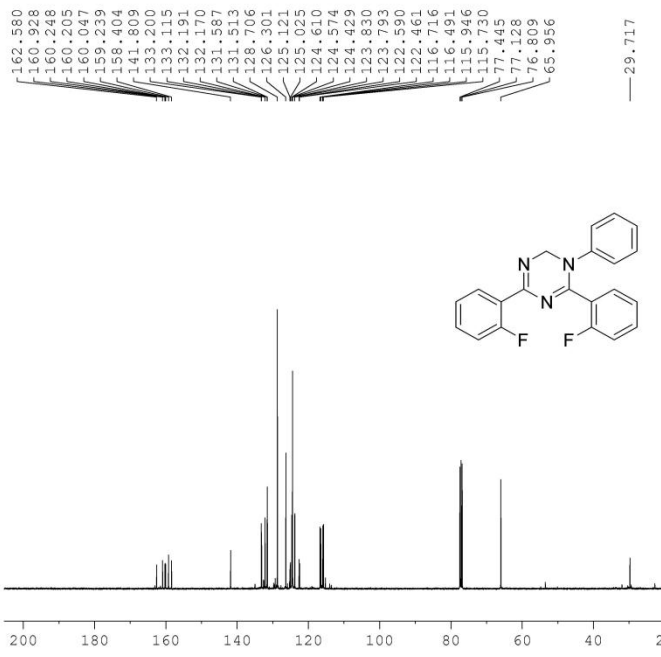
======== CHANNEL f1 ========
SFO1          100.6228293 MHz
NUC1                  13C
P1                 10.27 usec
SI                 32768
SF            100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

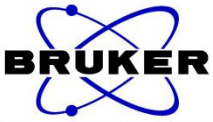
3pa



```
NAME        2019-03-11 tyut-lx-0
EXPNO                        10
PROCNO                        1
Date_                  20190312
Time                       3.47
INSTRUM                   spect
PROBHD    5 mm PABBO BB/
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                   8012.820 Hz
FIDRES                0.122266 Hz
AQ                    4.0894966 sec
RG                        34.32
DW                       62.400 usec
DE                        6.50 usec
TE                       296.4 K
D1                    1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1           400.1324710 MHz
NUC1                       1H
P1                       9.59 usec
SI                      65536
SF               400.1300104 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
```

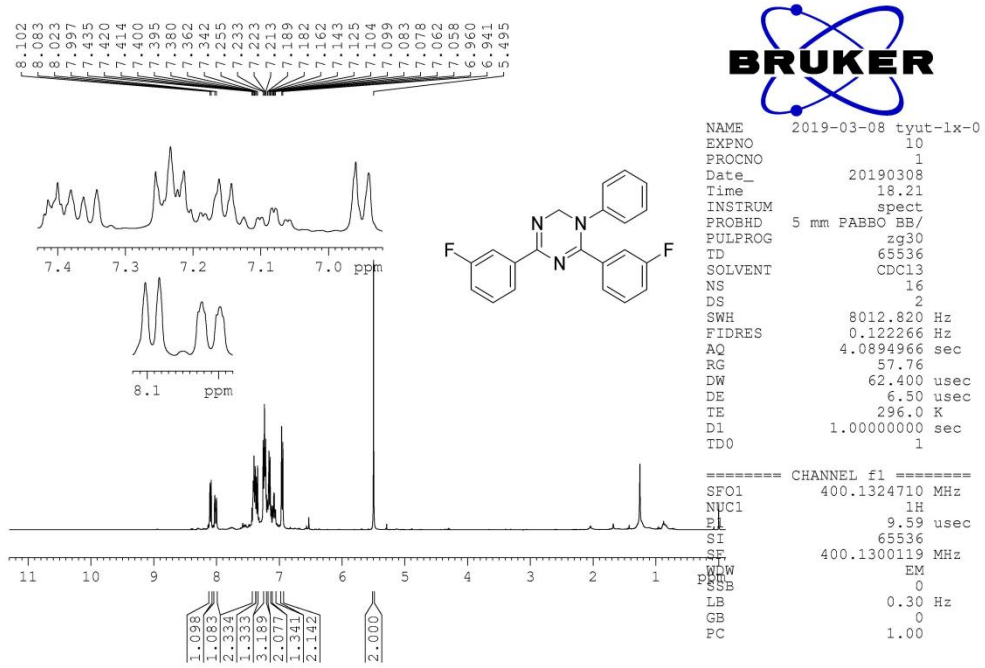


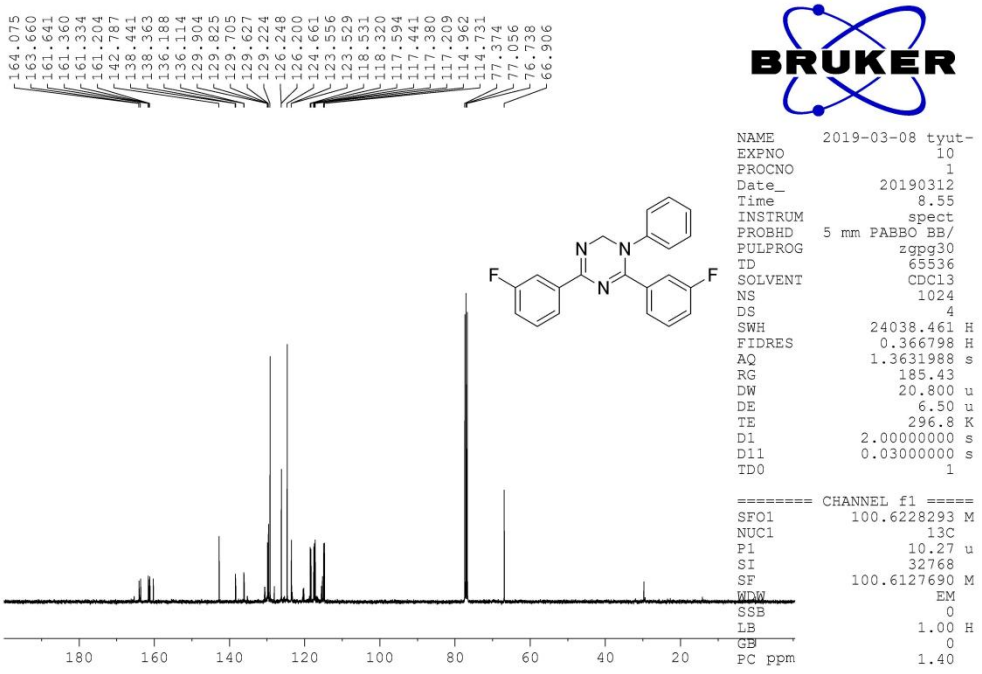


```
NAME        2019-03-11 tyut-l:
EXPNO                        10
PROCNO                        1
Date_                  20190313
Time                       4.47
INSTRUM                   spect
PROBHD    5 mm PABBO BB/
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                        1024
DS                           4
SWH                  24038.461 Hz
FIDRES                0.366798 Hz
AQ                    1.3631988 se
RG                       185.43
DW                       20.800 us
DE                        6.50 us
TE                       296.6 K
D1                    2.00000000 se
D11                   0.03000000 se
TD0                          1

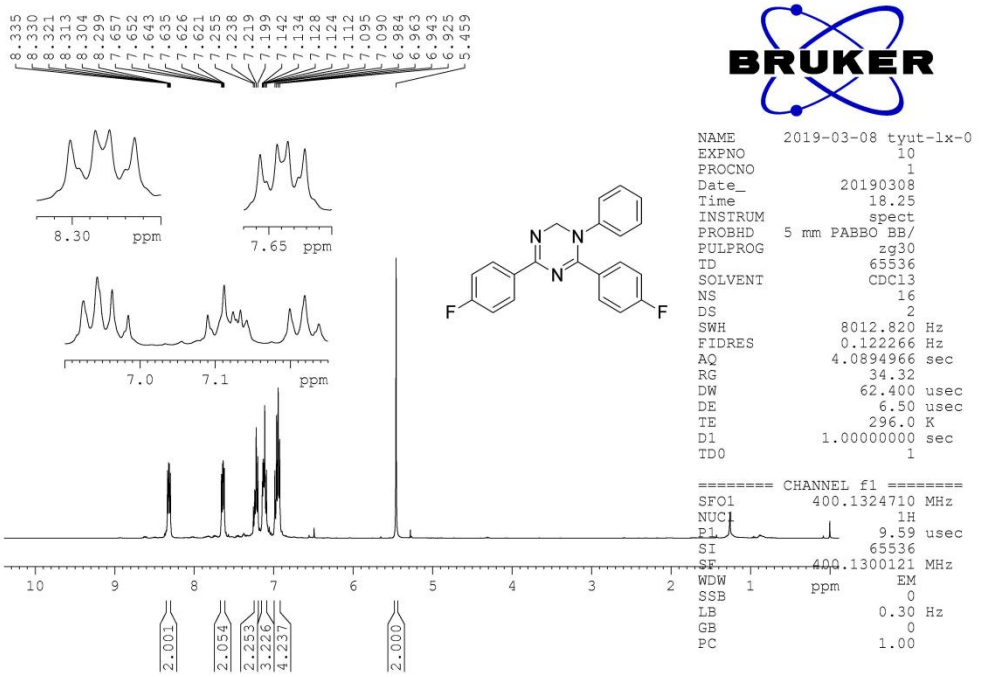
======== CHANNEL f1 =======
SFO1           100.6228293 MH:
NUC1                       13C
P1                       10.27 us
SI                      32768
SF               100.6127690 MH:
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```

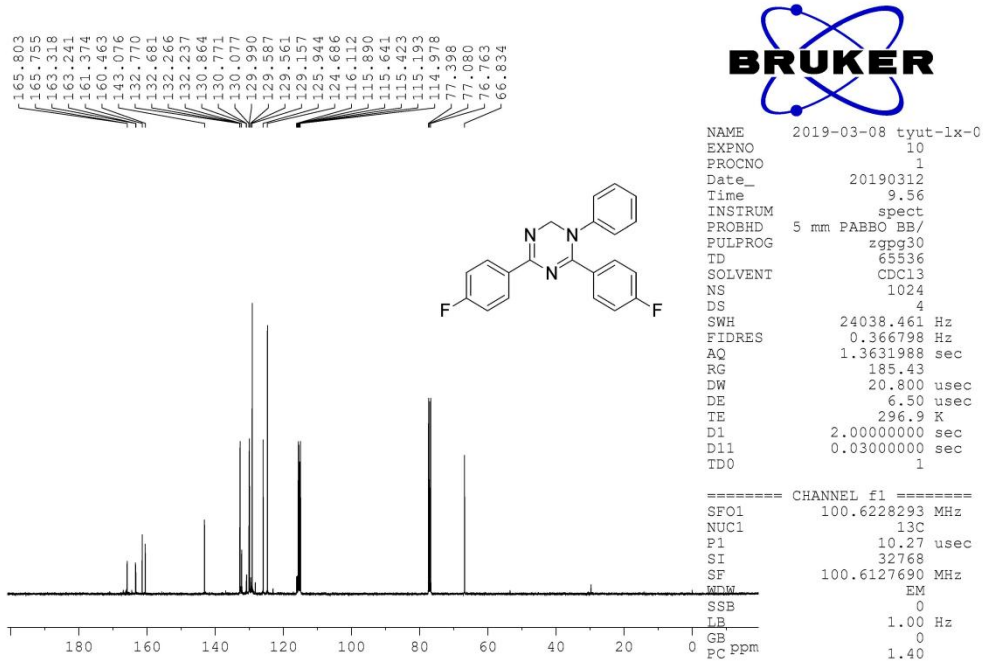
3qa


8.102
8.083
8.023
7.997
7.435
7.420
7.414
7.400
7.395
7.380
7.362
7.342
7.255
7.233
7.223
7.213
7.189
7.182
7.162
7.143
7.125
7.104
7.099
7.083
7.078
7.062
7.058
6.960
6.941
5.495
7.4
7.3
7.2
7.1
7.0 ppm
8.1 ppm
F
N
N
N
F
11
10
9
8
7
6
5
4
3
2
1
ppm
1.098
1.083
2.334
1.333
3.189
2.077
1.341
2.142
2.000
BRUKER
NAME 2019-03-08 tyut-1x-0
EXPNO 10
PROCNO 1
Date_ 20190308
Time 18.21
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 57.76
DW 62.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.59 usec
SI 65536
SF 400.1300119 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

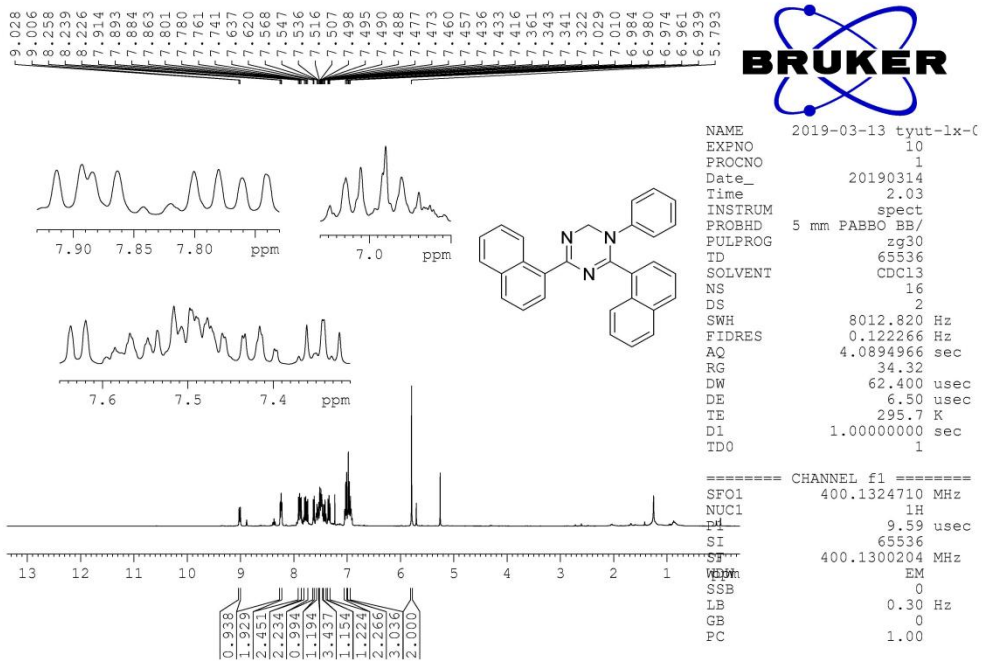

164.075
163.660
161.641
161.360
161.334
161.204
142.787
138.441
138.363
136.188
136.114
129.904
129.825
129.705
129.627
129.224
126.248
126.200
124.661
123.556
123.529
118.531
118.320
117.594
117.441
117.380
117.209
114.962
114.731
77.374
77.056
76.738
66.906
N
N
N
F
F
180
160
140
120
100
80
60
40
20
BRUKER
NAME 2019-03-08 tyut-
EXPNO 10
PROCNO 1
Date_ 20190312
Time 8.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 H
FIDRES 0.366798 H
AQ 1.3631988 s
RG 185.43
DW 20.800 u
DE 6.50 u
TE 296.8 K
D1 2.00000000 s
D11 0.03000000 s
TD0 1
======== CHANNEL f1 =====
SFO1 100.6228293 M
NUC1 13C
P1 10.27 u
SI 32768
SF 100.6127690 M
WDW EM
SSB 0
LB 1.00 H
GB 0
PC ppm 1.40

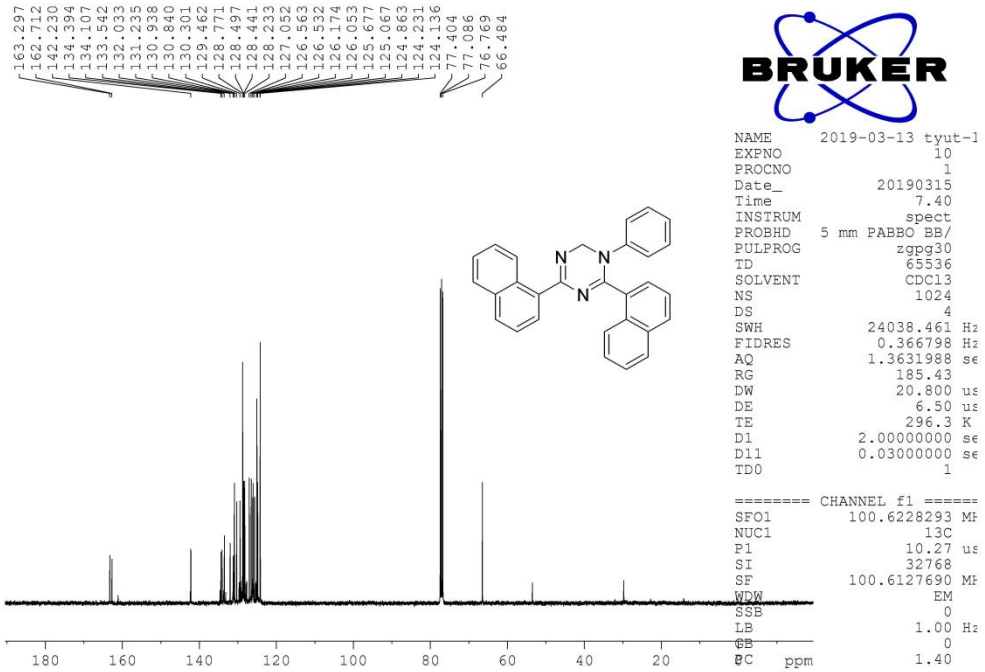
3ra


8.335
8.330
8.321
8.313
8.304
8.299
7.657
7.652
7.643
7.635
7.626
7.621
7.255
7.238
7.219
7.199
7.142
7.134
7.128
7.124
7.112
7.095
7.090
6.984
6.963
6.943
6.925
5.459
8.30 ppm
7.65 ppm
7.0 7.1 ppm
10 9 8 7 6 5 4 3 2 1 ppm
2.001
2.054
2.253
3.226
4.237
2.000
F
F
BRUKER
NAME 2019-03-08 tyut-lx-0
EXPNO 10
PROCNO 1
Date_ 20190308
Time 18.25
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 34.32
DW 62.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.59 usec
SI 65536
SF 400.1300121 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

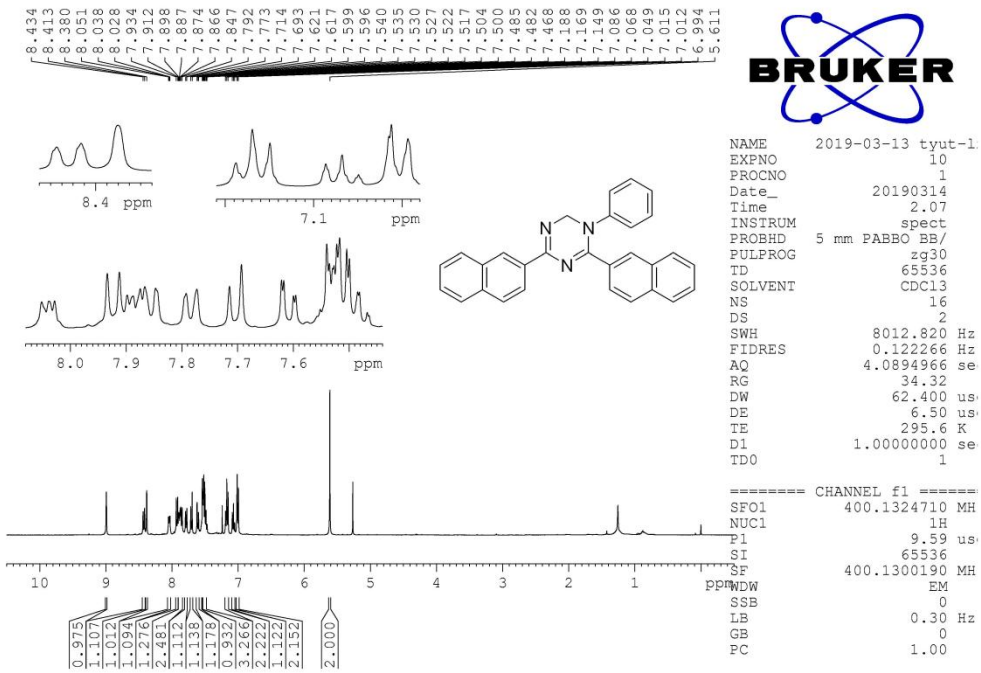

165.803
165.755
163.318
163.241
161.374
160.463
143.076
132.770
132.681
132.266
132.237
130.864
130.771
130.077
129.990
129.587
129.561
129.157
125.944
124.686
116.112
115.890
115.641
115.423
115.193
114.978
77.398
77.080
76.763
66.834
180 160 140 120 100 80 60 40 20 0 ppm
F
F
BRUKER
NAME 2019-03-08 tyut-lx-0
EXPNO 10
PROCNO 1
Date_ 20190312
Time 9.56
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 185.43
DW 20.800 usec
DE 6.50 usec
TE 296.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.27 usec
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

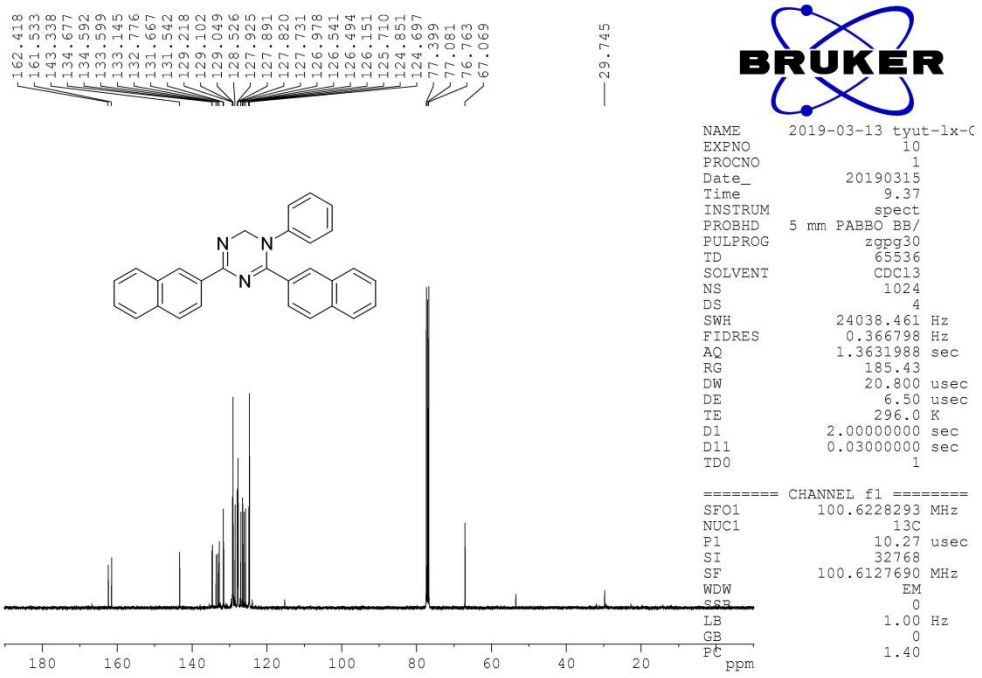
3sa


9.028
9.006
8.258
8.239
8.226
7.914
7.893
7.884
7.863
7.801
7.780
7.761
7.741
7.637
7.620
7.568
7.547
7.536
7.516
7.507
7.498
7.495
7.490
7.488
7.477
7.473
7.460
7.457
7.436
7.433
7.416
7.361
7.343
7.341
7.322
7.029
7.010
6.984
6.980
6.974
6.961
6.939
5.793
7.90 7.85 7.80 ppm
7.0 ppm
7.6 7.5 7.4 ppm
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.938
1.929
2.451
2.234
0.994
1.194
3.437
1.154
1.224
2.266
3.036
2.000
BRUKER
NAME 2019-03-13 tyut-1x-(
EXPNO 10
PROCNO 1
Date_ 20190314
Time 2.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 34.32
DW 62.400 usec
DE 6.50 usec
TE 295.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.59 usec
SI 65536
SF 400.1300204 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


163.297
162.712
142.230
134.394
134.107
133.542
132.033
131.235
130.938
130.840
130.301
129.462
128.771
128.497
128.441
128.233
127.052
126.563
126.532
126.174
126.053
125.677
125.067
124.863
124.231
124.136
77.404
77.086
76.769
66.484
180 160 140 120 100 80 60 40 20 0 ppm
BRUKER
NAME 2019-03-13 tyut-1
EXPNO 10
PROCNO 1
Date_ 20190315
Time 7.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 se
RG 185.43
DW 20.800 us
DE 6.50 us
TE 296.3 K
D1 2.00000000 se
D11 0.03000000 se
TD0 1
======== CHANNEL f1 ======
SFO1 100.6228293 MH
NUC1 13C
P1 10.27 us
SI 32768
SF 100.6127690 MH
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

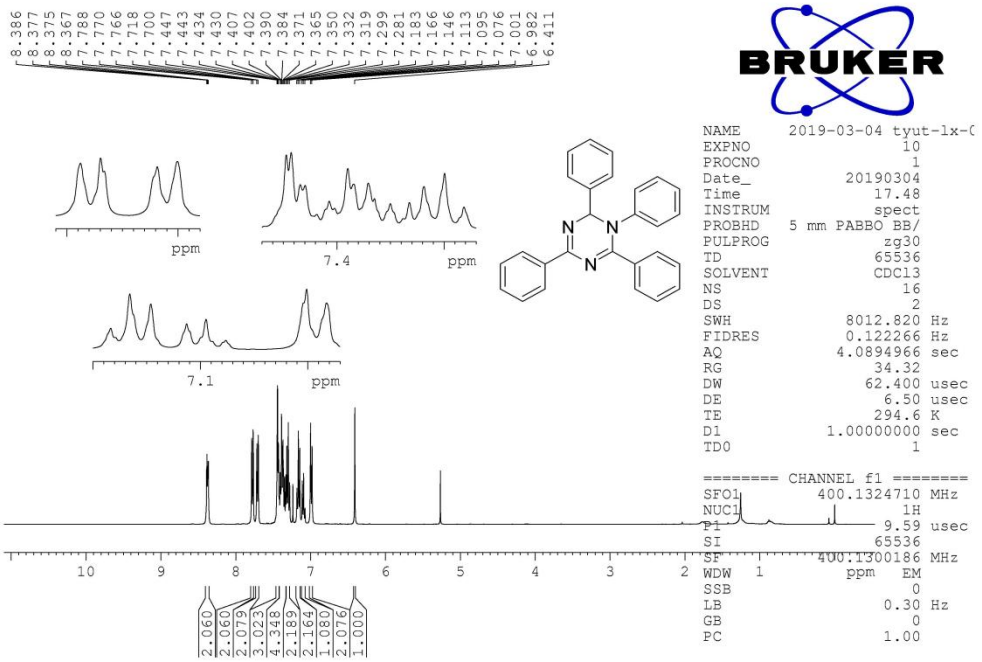
3ta


8.434
8.413
8.380
8.051
8.038
8.028
7.934
7.912
7.898
7.887
7.874
7.866
7.847
7.792
7.773
7.714
7.693
7.621
7.617
7.599
7.596
7.540
7.535
7.530
7.527
7.522
7.517
7.504
7.500
7.485
7.482
7.468
7.188
7.169
7.149
7.086
7.068
7.049
7.015
7.012
6.994
5.611
8.4 ppm
7.1 ppm
8.0 7.9 7.8 7.7 7.6 ppm
10 9 8 7 6 5 4 3 2 1 ppm
0.975
1.107
1.012
1.094
1.276
2.481
1.112
1.138
1.178
0.932
3.266
2.222
1.122
2.152
2.000
BRUKER
NAME 2019-03-13 tyut-1
EXPNO 10
PROCNO 1
Date_ 20190314
Time 2.07
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 se
RG 34.32
DW 62.400 us
DE 6.50 us
TE 295.6 K
D1 1.00000000 se
TD0 1
======== CHANNEL f1 ======
SFO1 400.1324710 MH
NUC1 1H
P1 9.59 us
SI 65536
SF 400.1300190 MH
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

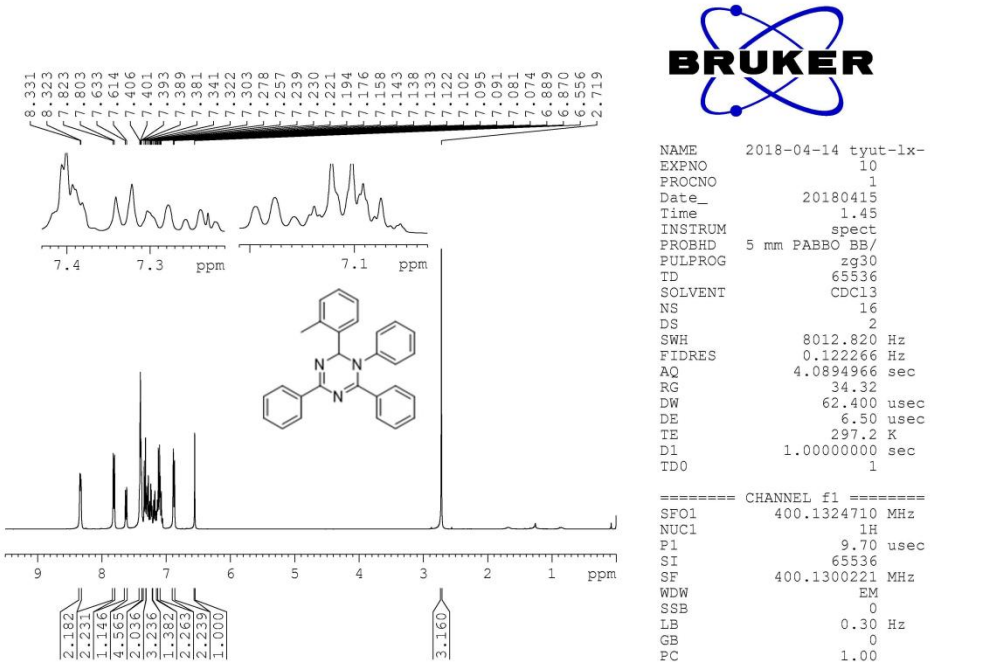

162.418
161.533
143.338
134.677
134.592
133.599
133.145
132.776
131.667
131.542
129.218
129.102
129.049
128.526
127.925
127.891
127.820
127.731
126.978
126.541
126.494
126.151
125.710
124.851
124.697
77.399
77.081
76.763
67.069
29.745
180 160 140 120 100 80 60 40 20 ppm
BRUKER
NAME 2019-03-13 tyut-1x-C
EXPNO 10
PROCNO 1
Date_ 20190315
Time 9.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 185.43
DW 20.800 usec
DE 6.50 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.27 usec
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

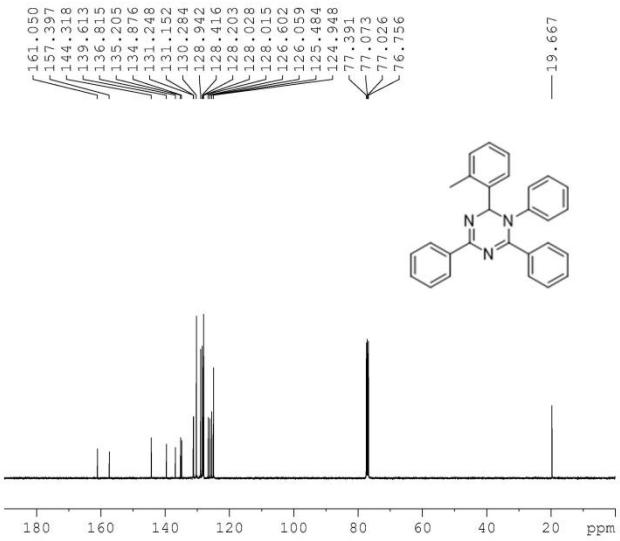
10. ^{1}H NMR and ^{13}C NMR for products 5 and 7

5aa and **7aa**



5ab and **7ab**

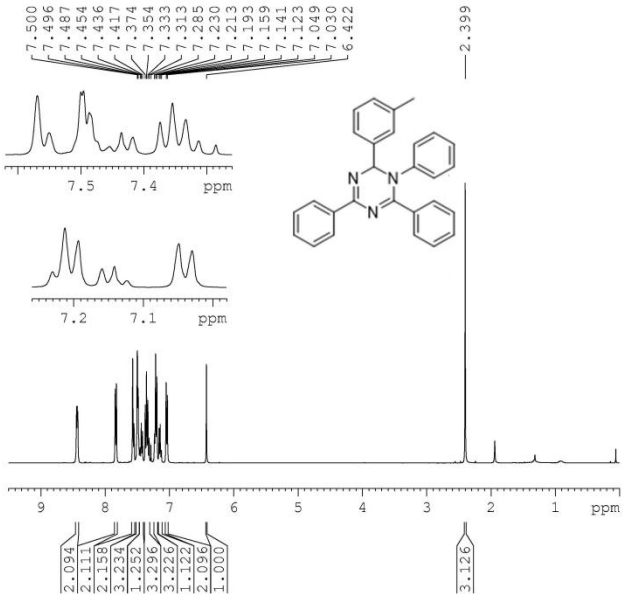




```
NAME          2018-04-14 tyut-lx-
EXPNO                 11
PROCNO                 1
Date_           20180415
Time                2.44
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                185.43
DW                20.800 usec
DE                 6.50 usec
TE                297.9 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

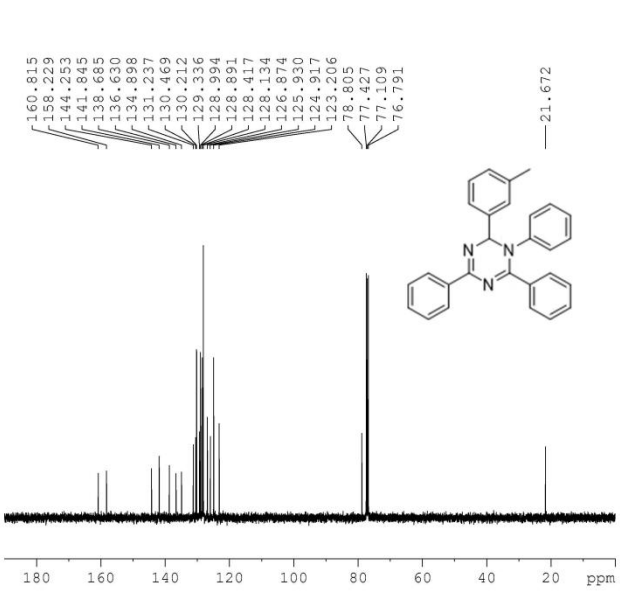
======== CHANNEL f1 ========
SFO1          100.6228293 MHz
NUC1                13C
P1                 9.50 usec
SI                32768
SF           100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

5ac and **7ac**



```
NAME                  54
EXPNO                  1
PROCNO                 1
Date_           20180326
Time               17.09
INSTRUM            spect
PROBHD    5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     0
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9846387 sec
RG                    64
DW                60.800 usec
DE                 6.50 usec
TE                291.9 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.00 usec
PL1               -3.13 dB
PL1W          20.50172997 W
SFO1          400.1324710 MHz
SI                32768
SF            400.1300000 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
```

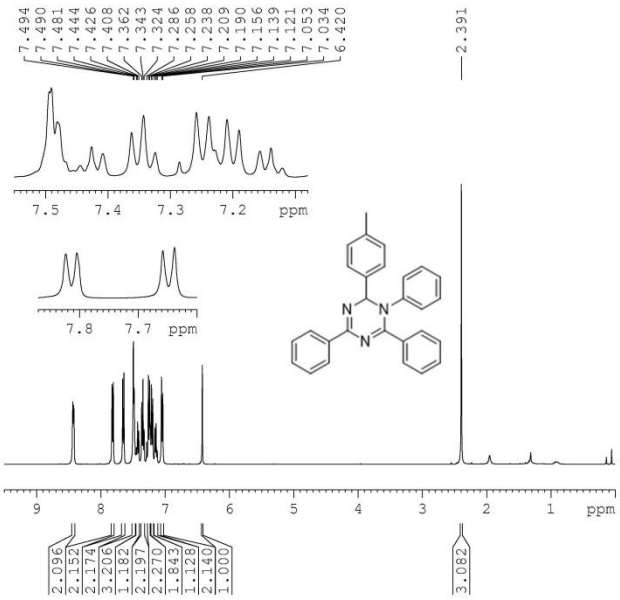



```
NAME                   54
EXPNO                   2
PROCNO                  1
Date_            20180326
Time                17.13
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    64
DS                     4
SWH             24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                 32800
DW                20.800 usec
DE                 6.50 usec
TE                293.4 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 10.00 usec
PL1                -2.04 dB
PL1W         55.04534149 W
SFO1        100.6238364 MHz

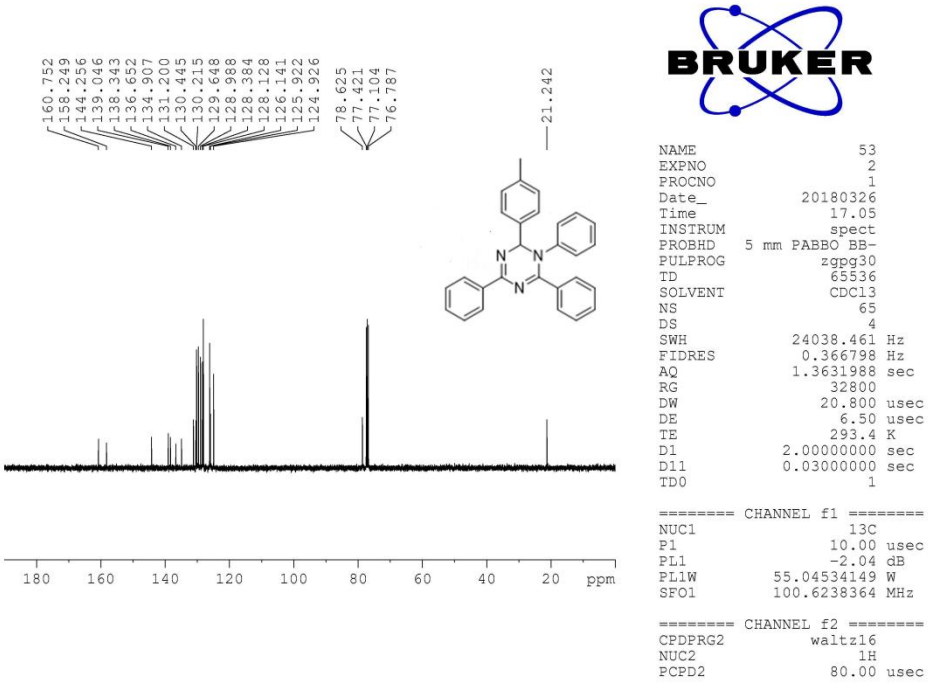
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              80.00 usec
```

5ad and **7ad**




```
NAME                   53
EXPNO                   1
PROCNO                  1
Date_            20180326
Time                17.01
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     0
SWH              8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                    64
DW                60.800 usec
DE                 6.50 usec
TE                292.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 14.00 usec
PL1                -3.13 dB
PL1W         20.50172997 W
SFO1        400.1324710 MHz
SI                 32768
SF          400.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
```

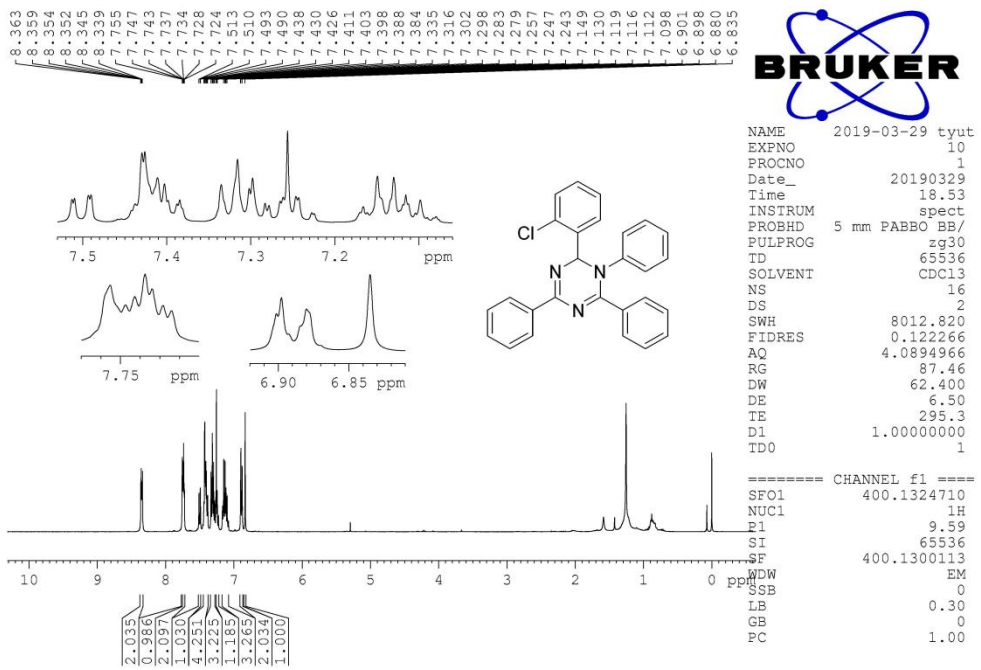



```
NAME                  53
EXPNO                  2
PROCNO                 1
Date_           20180326
Time               17.05
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   65
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                32800
DW               20.800 usec
DE                6.50 usec
TE               293.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -2.04 dB
PL1W        55.04534149 W
SFO1       100.6238364 MHz

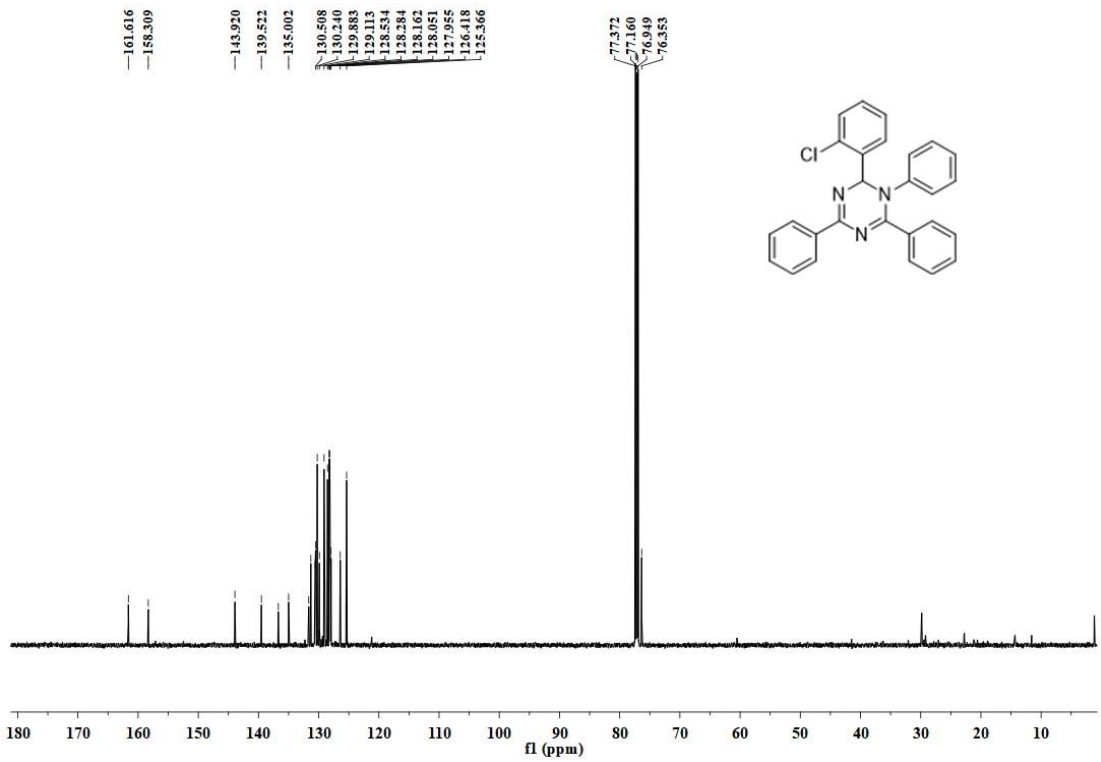
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
```

5ae

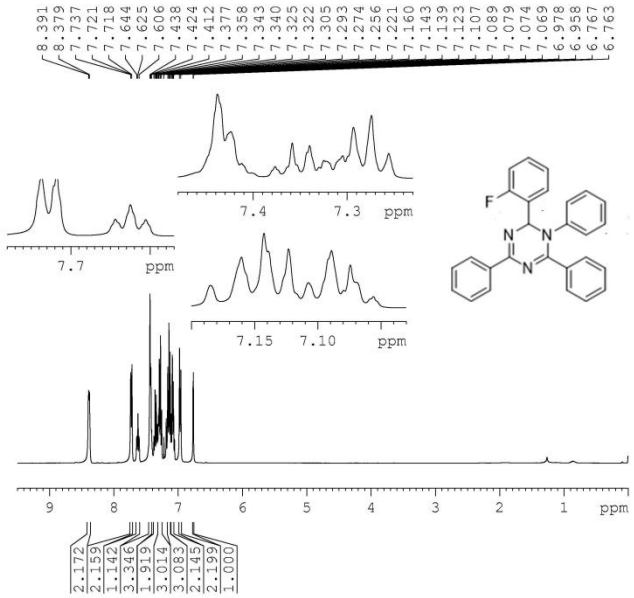



```
NAME       2019-03-29 tyut
EXPNO                  10
PROCNO                  1
Date_            20190329
Time                18.53
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH               8012.820
FIDRES            0.122266
AQ               4.0894966
RG                   87.46
DW                  62.400
DE                    6.50
TE                   295.3
D1             1.00000000
TD0                     1

======== CHANNEL f1 ====
SFO1          400.1324710
NUC1                   1H
P1                   9.59
SI                  65536
SF            400.1300113
WDW                   EM
SSB                    0
LB                  0.30
GB                     0
PC                  1.00
```

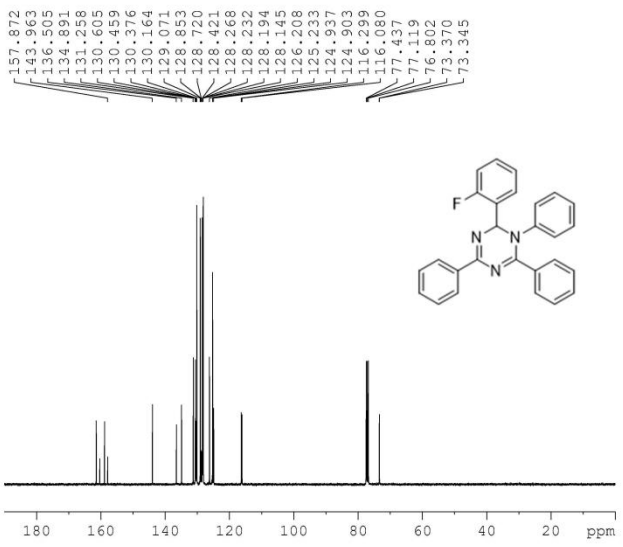


7ae




```
NAME          2018-04-14 tyut-lx-
EXPNO                 10
PROCNO                 1
Date_           20180415
Time                2.48
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894966 sec
RG                 34.32
DW                62.400 usec
DE                 6.50 usec
TE                297.2 K
D1             1.00000000 sec
TD0                    1

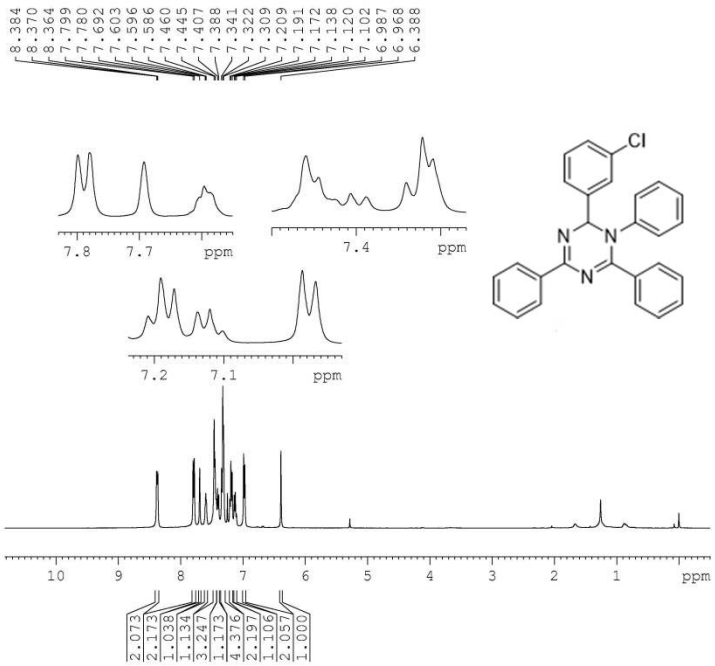
======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                  1H
P1                 9.70 usec
SI                 65536
SF            400.1300257 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




```
NAME      2018-04-14 tyut-lx-
EXPNO                 11
PROCNO                 1
Date_           20180415
Time                3.47
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                185.43
DW                20.800 usec
DE                 6.50 usec
TE                297.9 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

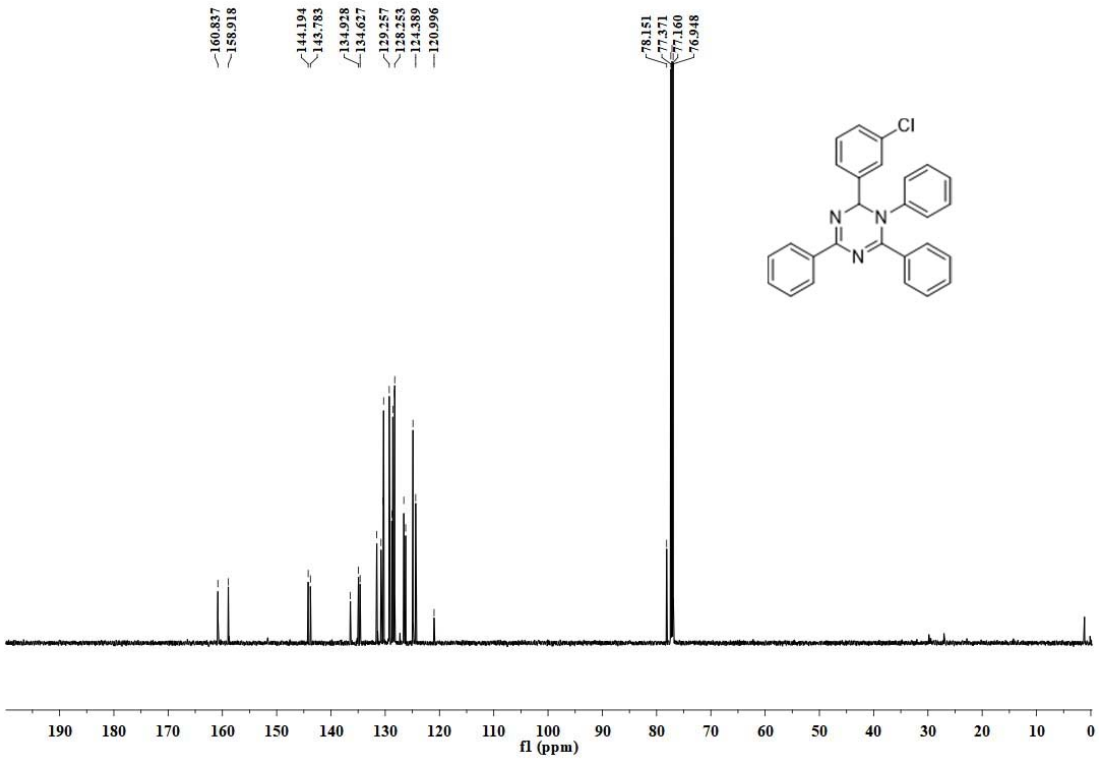
======== CHANNEL f1 ========
SFO1         100.6228293 MHz
NUC1               13C
P1                9.50 usec
SI                32768
SF           100.6127690 MHz
WDW                EM
SSB                 0
LB                1.00 Hz
GB                  0
PC                1.40
```

5af

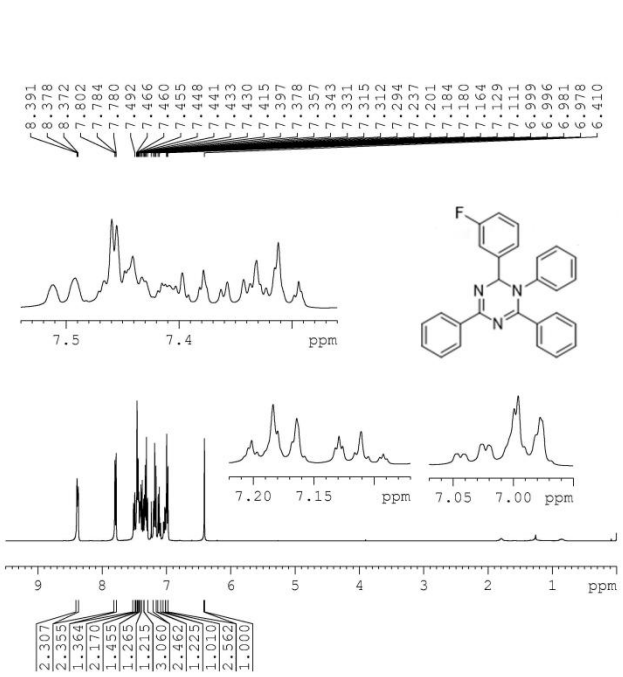


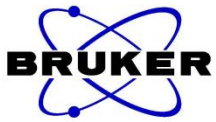

```
NAME      2019-03-29 tyut-l
EXPNO                 10
PROCNO                 1
Date_           20190329
Time               18.49
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894966 se
RG                 60.71
DW                62.400 us
DE                 6.50 us
TE                295.3 K
D1             1.00000000 se
TD0                    1

======== CHANNEL f1 ======
SFO1          400.1324710 MH
NUC1                1H
P1                 9.59 us
SI                65536
SF           400.1300147 MH
WDW                EM
SSB                 0
LB                0.30 Hz
GB                  0
PC                1.00
```



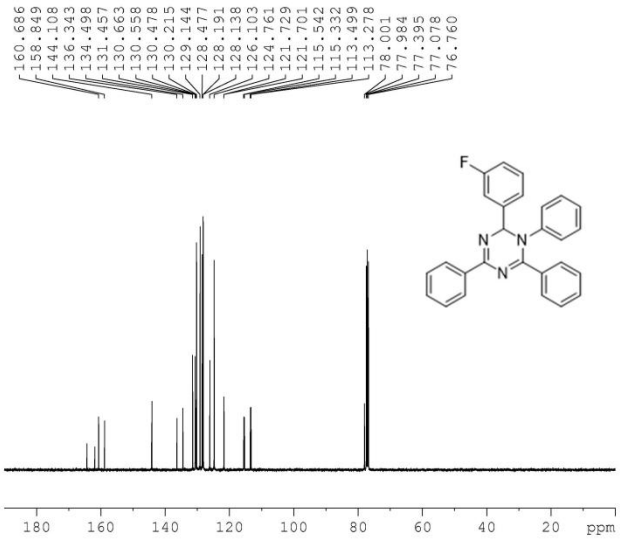
7af






```
NAME          2018-04-18 tyut-lx-
EXPNO                 20
PROCNO                 1
Date_           20180420
Time                0.13
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES             0.122266 Hz
AQ              4.0894966 sec
RG                 34.32
DW                 62.400 usec
DE                  6.50 usec
TE                294.9 K
D1             1.00000000 sec
TD0                    1

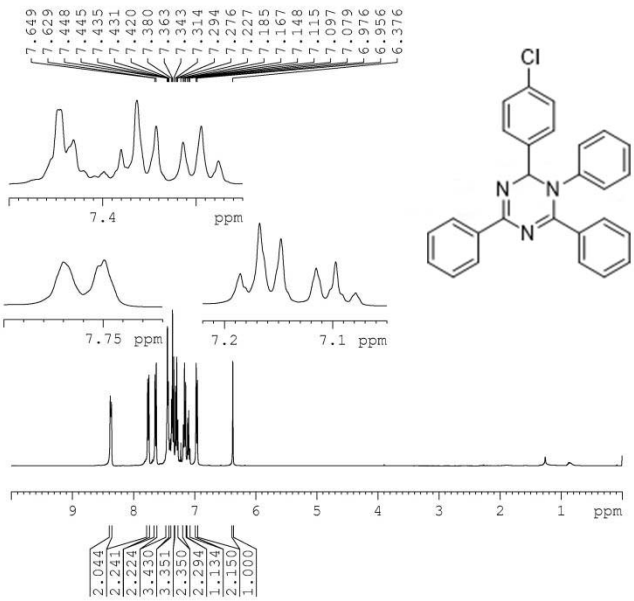
======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                  1H
P1                  9.70 usec
SI                 65536
SF            400.1300190 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




```
NAME      2018-04-18 tyut-lx-
EXPNO                 21
PROCNO                 1
Date_           20180420
Time                1.12
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                185.43
DW                20.800 usec
DE                 6.50 usec
TE                295.9 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

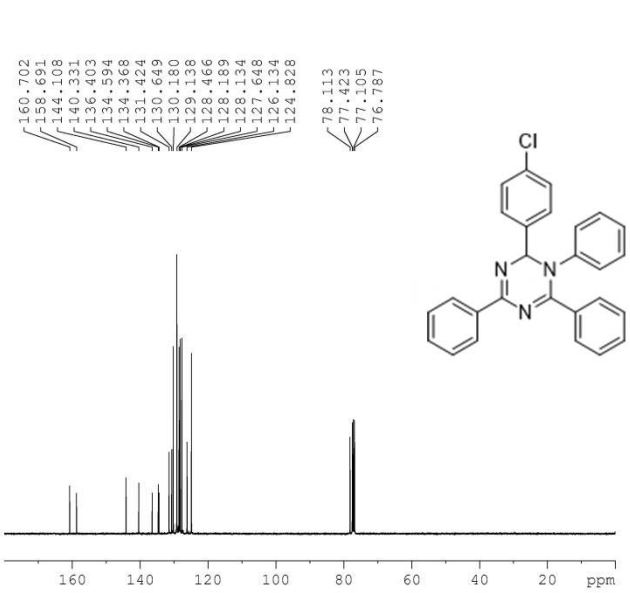
======== CHANNEL f1 ========
SFO1         100.6228293 MHz
NUC1                13C
P1                 9.50 usec
SI                32768
SF           100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

5ag and **7al**




```
NAME          2018041206
EXPNO                 10
PROCNO                 1
Date_           20180413
Time                5.44
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894966 sec
RG                 34.32
DW                62.400 usec
DE                 6.50 usec
TE                297.8 K
D1             1.00000000 sec
TD0                    1

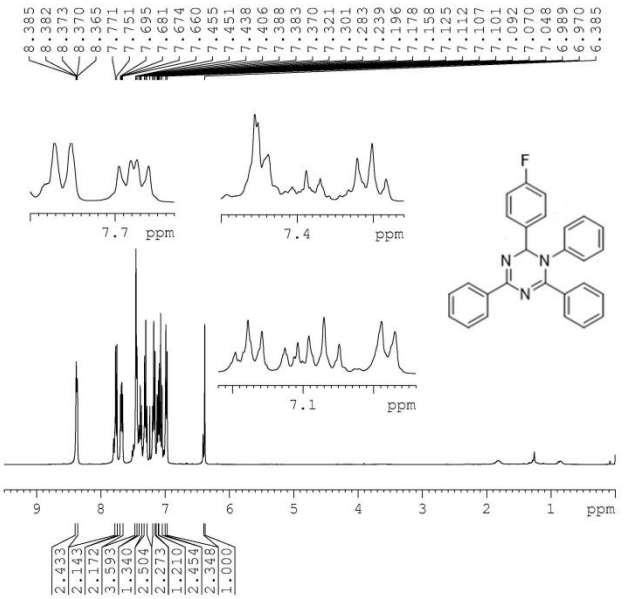
======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                 1H
P1                 9.70 usec
SI                65536
SF           400.1300235 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```




```
NAME          2018041206
EXPNO                 11
PROCNO                 1
Date_           20180413
Time                6.43
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG               185.43
DW               20.800 usec
DE                6.50 usec
TE               298.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

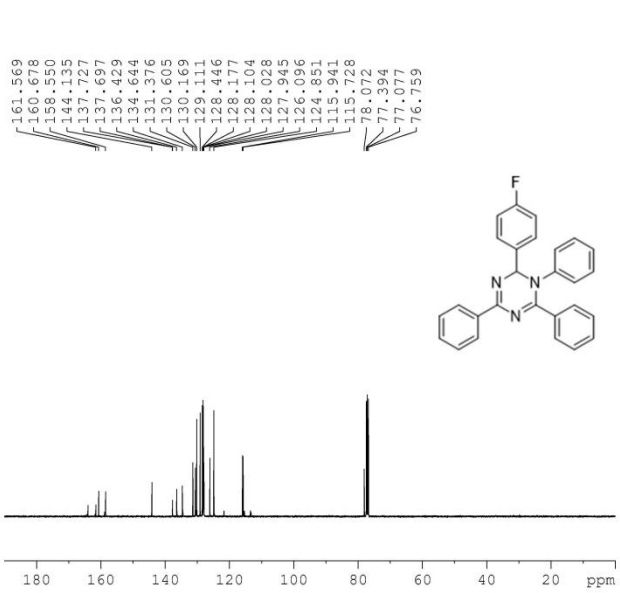
======== CHANNEL f1 ========
SFO1        100.6228293 MHz
NUC1               13C
P1                9.50 usec
SI               32768
SF          100.6127690 MHz
WDW                EM
SSB                 0
LB                1.00 Hz
GB                  0
PC                1.40
```

7ag




```
NAME      2018-04-18 tyut-lx-
EXPNO                 10
PROCNO                 1
Date_           20180420
Time                3.39
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ            4.0894966 sec
RG                34.32
DW               62.400 usec
DE                6.50 usec
TE               294.9 K
D1            1.00000000 sec
TD0                    1

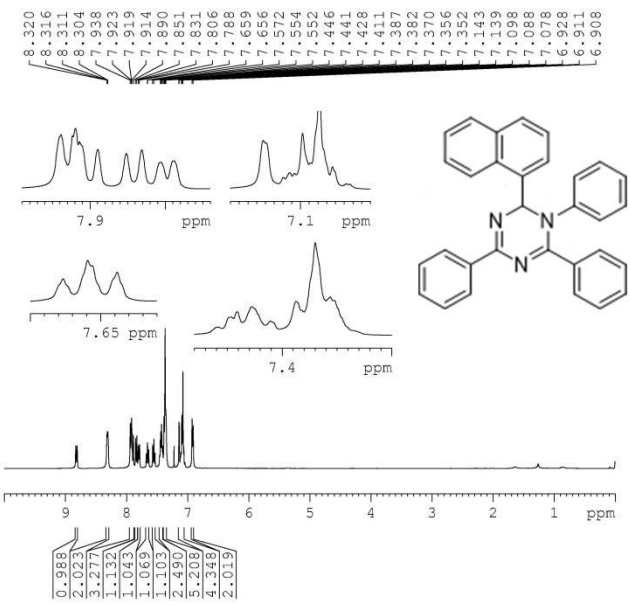
======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1               1H
P1                9.70 usec
SI               65536
SF          400.1300182 MHz
WDW                EM
SSB                 0
LB                0.30 Hz
GB                  0
PC                1.00
```




```
NAME      2018-04-18 tyut-lx-
EXPNO                 12
PROCNO                 1
Date_           20180420
Time                4.38
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                185.43
DW                20.800 usec
DE                 6.50 usec
TE                295.8 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

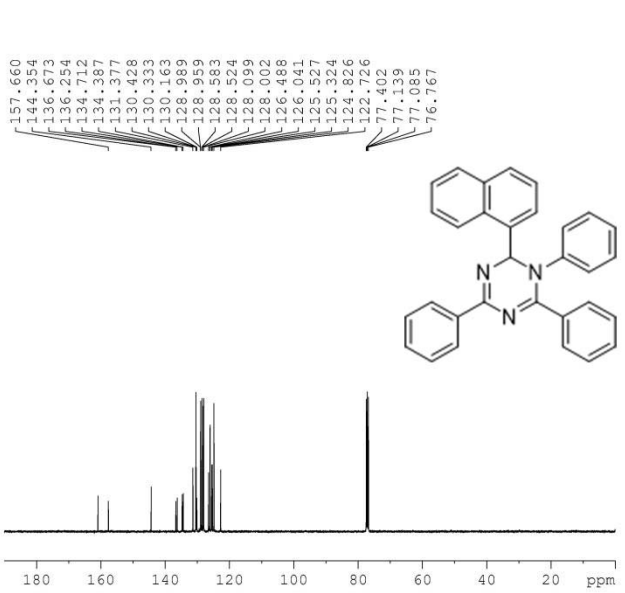
======== CHANNEL f1 ========
SFO1         100.6228293 MHz
NUC1                13C
P1                 9.50 usec
SI                32768
SF           100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

5ai and **7ai**




```
NAME      2018-04-14 tyut-lx-
EXPNO                 10
PROCNO                 1
Date_           20180415
Time                0.42
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894966 sec
RG                 34.32
DW                62.400 usec
DE                 6.50 usec
TE                297.2 K
D1             1.00000000 sec
TD0                    1

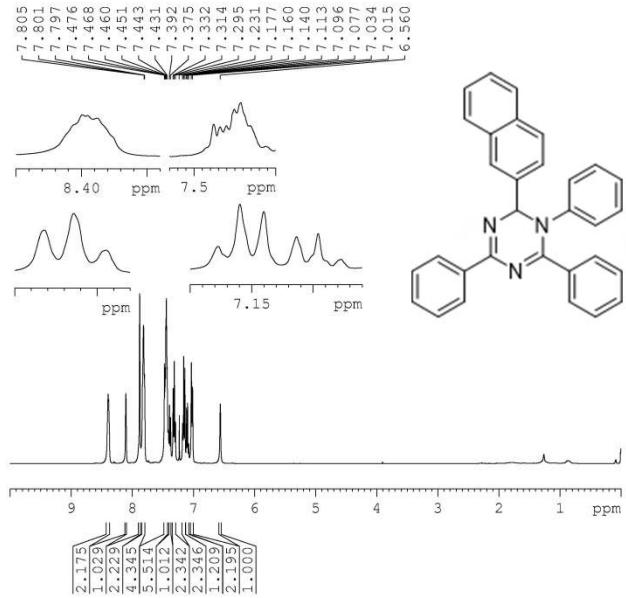
======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                 1H
P1                 9.70 usec
SI                65536
SF           400.1300248 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```




```
NAME      2018-04-14 tyut-lx-
EXPNO                 11
PROCNO                 1
Date_           20180415
Time                1.41
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                185.43
DW                20.800 usec
DE                 6.50 usec
TE                297.9 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

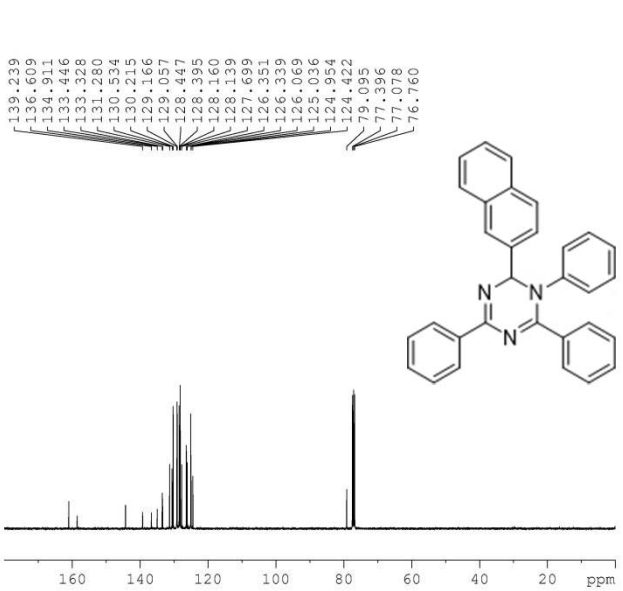
======== CHANNEL f1 ========
SFO1          100.6228293 MHz
NUC1                 13C
P1                  9.50 usec
SI                 32768
SF           100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

5aj and **7ah**




```
NAME          2018041205
EXPNO                 10
PROCNO                 1
Date_           20180413
Time                4.41
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894966 sec
RG                 34.32
DW                62.400 usec
DE                 6.50 usec
TE                297.8 K
D1             1.00000000 sec
TD0                    1

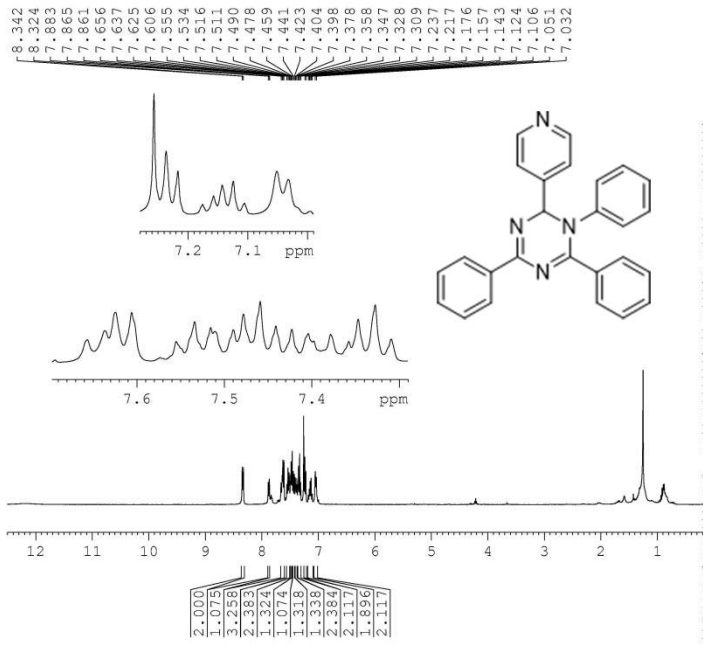
======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                  1H
P1                  9.70 usec
SI                 65536
SF           400.1300216 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



NAME 2018041205
EXPNO 11
PROCNO 1
Date_ 20180413
Time 5.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 185.43
DW 20.800 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

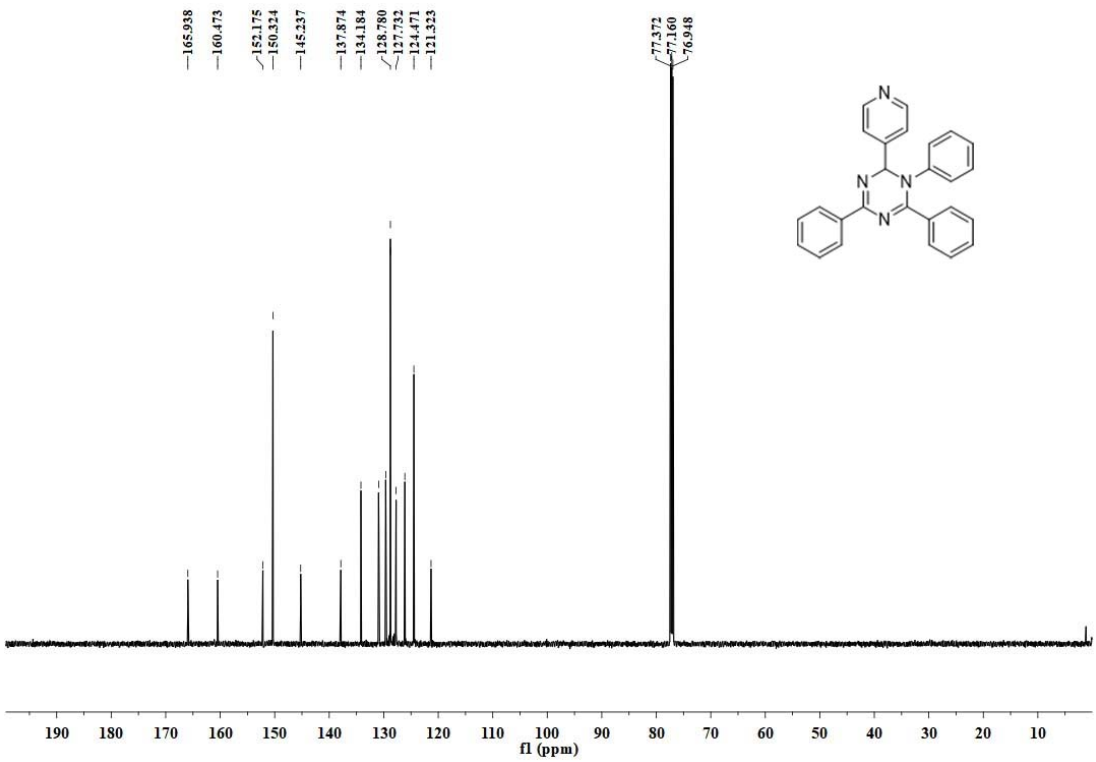
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 9.50 usec
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

5ak

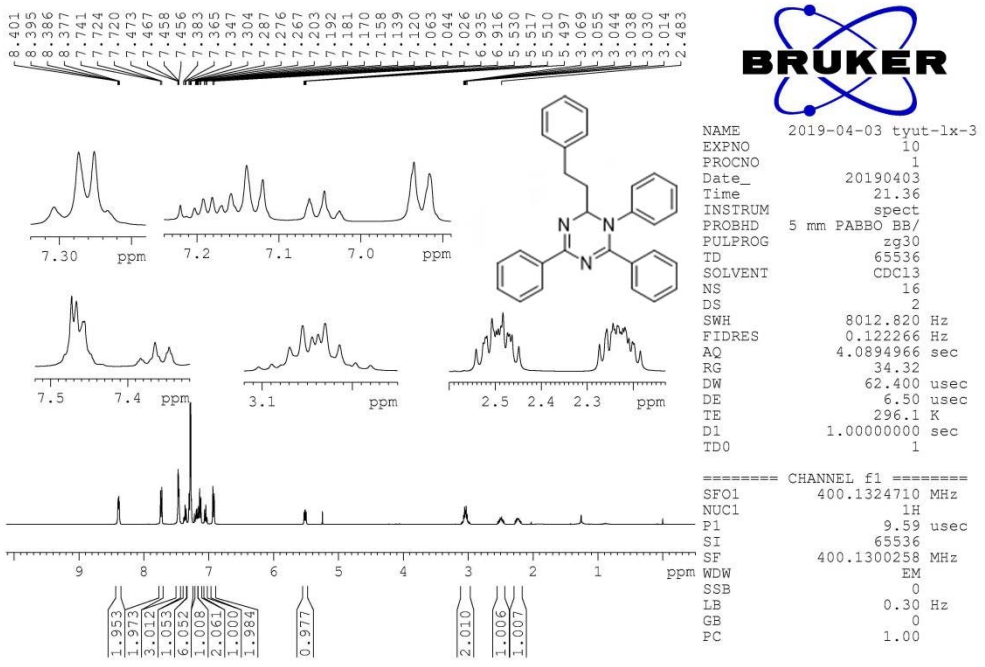


NAME 2019-03-29 tyut-lx-1
EXPNO 10
PROCNO 1
Date_ 20190329
Time 18.58
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 74.25
DW 62.400 usec
DE 6.50 usec
TE 295.3 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.59 usec
SF 400.1300109 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

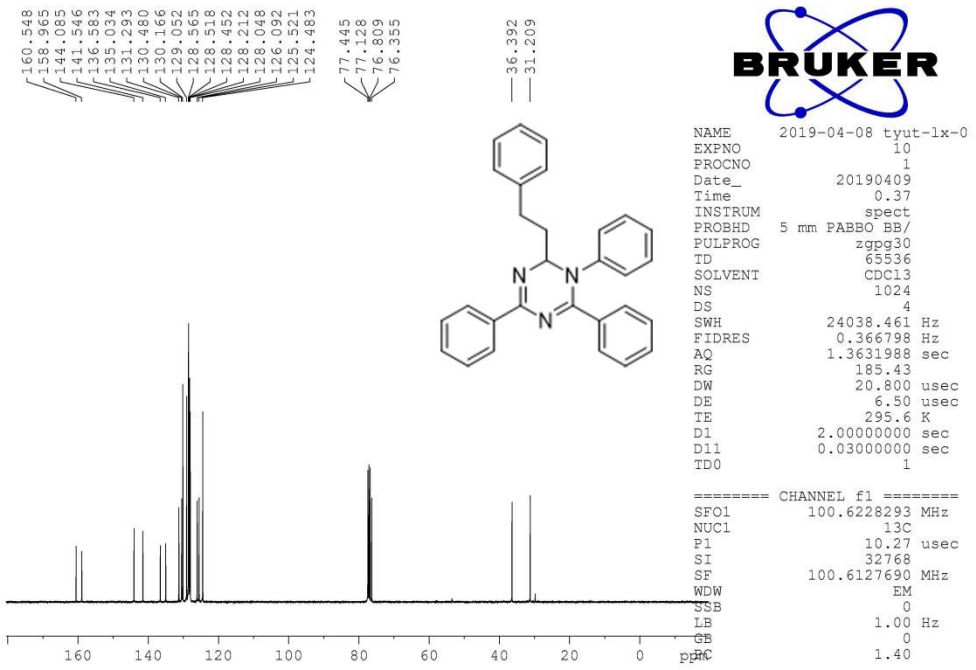


5al

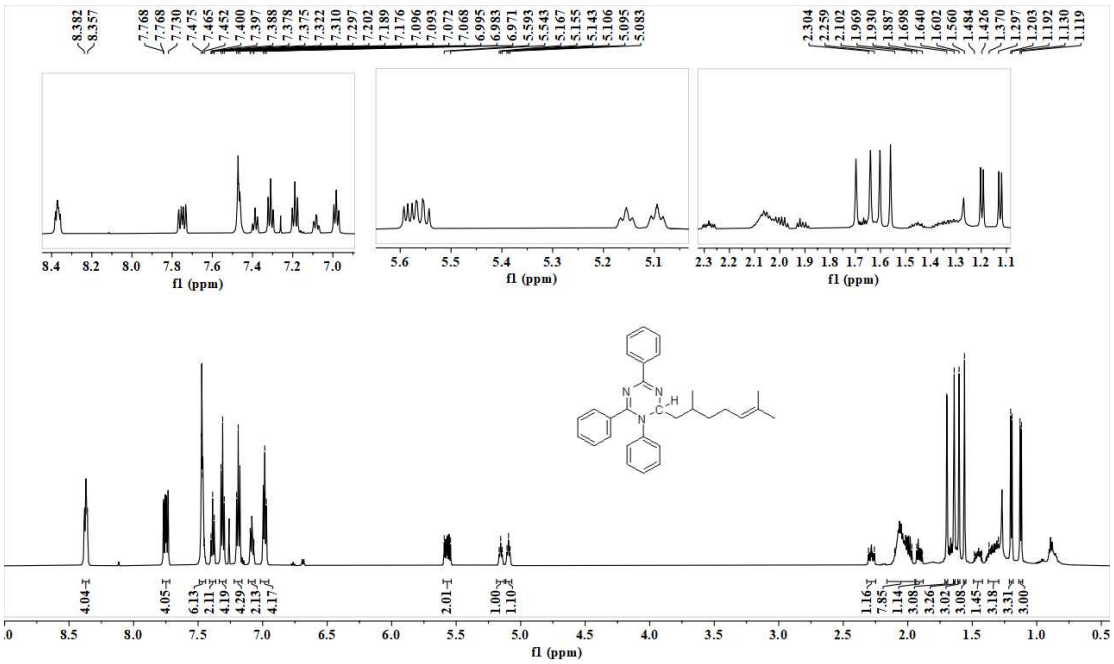


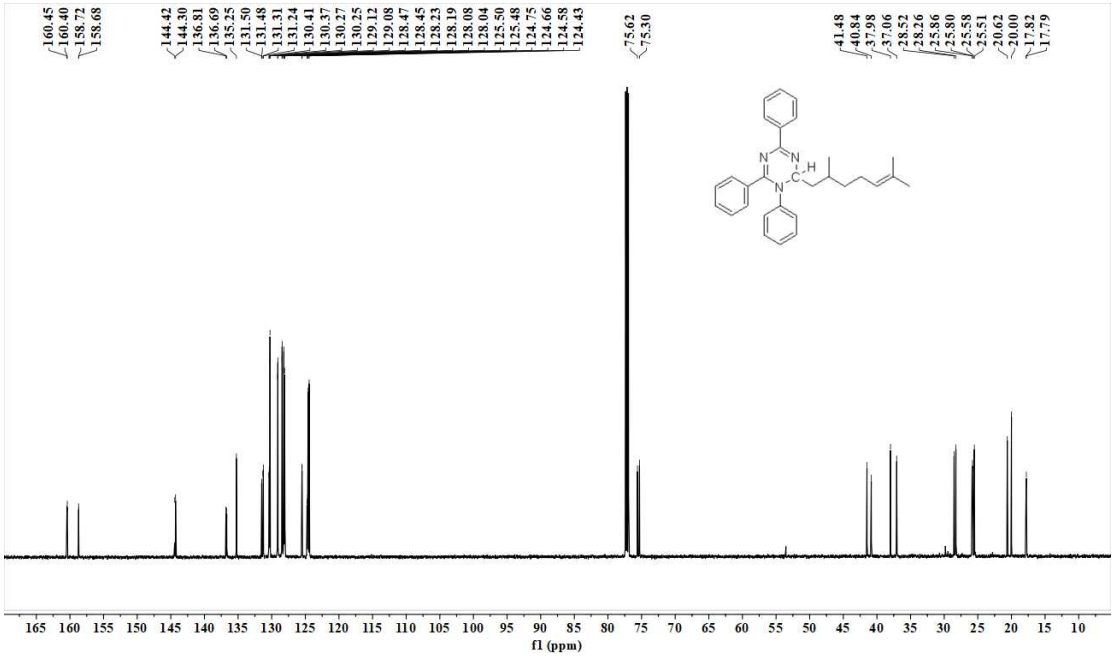

```
NAME          2019-04-03 tyut-lx-3
EXPNO                   10
PROCNO                   1
Date_             20190403
Time                 21.36
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDC13
NS                     16
DS                      2
SWH               8012.820 Hz
FIDRES               0.122266 Hz
AQ                4.0894966 sec
RG                     34.32
DW                   62.400 usec
DE                    6.50 usec
TE                   296.1 K
D1               1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1            400.1324710 MHz
NUC1                    1H
P1                    9.59 usec
SI                  65536
SF              400.1300258 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

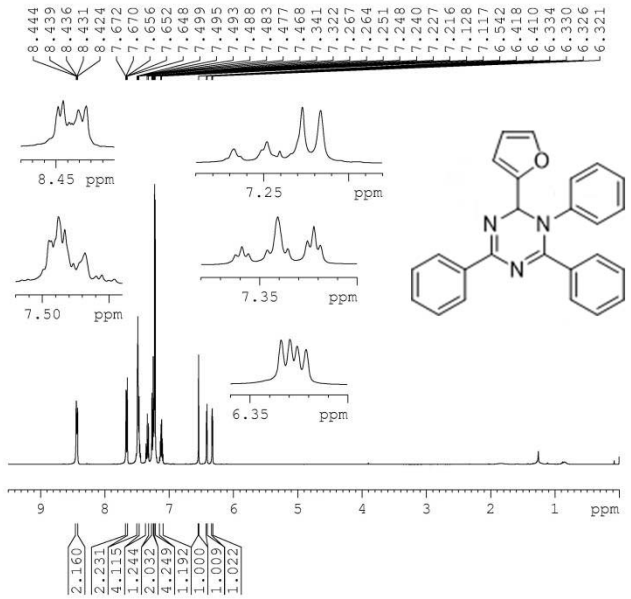

160.548
158.965
144.085
141.546
136.583
135.034
131.293
130.480
130.166
129.052
128.565
128.518
128.452
128.212
128.048
126.092
125.521
124.483
77.445
77.128
76.809
76.355
36.392
31.209
BRUKER
NAME 2019-04-08 tyut-lx-0
EXPNO 10
PROCNO 1
Date_ 20190409
Time 0.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 185.43
DW 20.800 usec
DE 6.50 usec
TE 295.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.27 usec
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
160 140 120 100 80 60 40 20 0 ppm

5an


8.382
8.357
7.768
7.730
7.475
7.465
7.452
7.400
7.397
7.388
7.378
7.375
7.322
7.310
7.297
7.202
7.189
7.176
7.096
7.093
7.072
7.068
6.995
6.983
6.971
5.593
5.543
5.167
5.155
5.143
5.106
5.095
5.083
2.304
2.259
2.102
1.969
1.930
1.887
1.698
1.640
1.602
1.560
1.484
1.426
1.370
1.297
1.203
1.192
1.130
1.119
f1 (ppm)
4.04
4.05
6.13
2.11
4.19
4.29
2.13
4.17
2.01
1.00
1.10
1.16
7.85
1.14
3.08
3.26
3.02
3.08
1.45
3.18
3.31
3.00

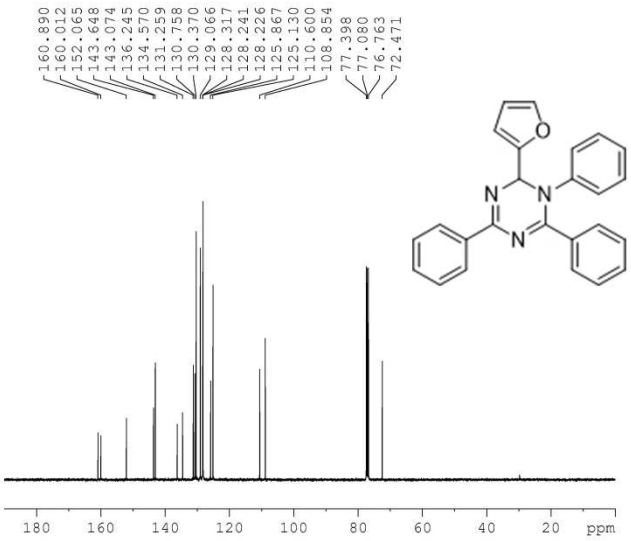


7aj




```
NAME        2018-04-18 tyut-lx-
EXPNO                   10
PROCNO                   1
Date_             20180420
Time                  4.41
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH                8012.820 Hz
FIDRES                0.122266 Hz
AQ                 4.0894966 sec
RG                    34.32
DW                   62.400 usec
DE                    6.50 usec
TE                   295.2 K
D1                1.00000000 sec
TD0                      1

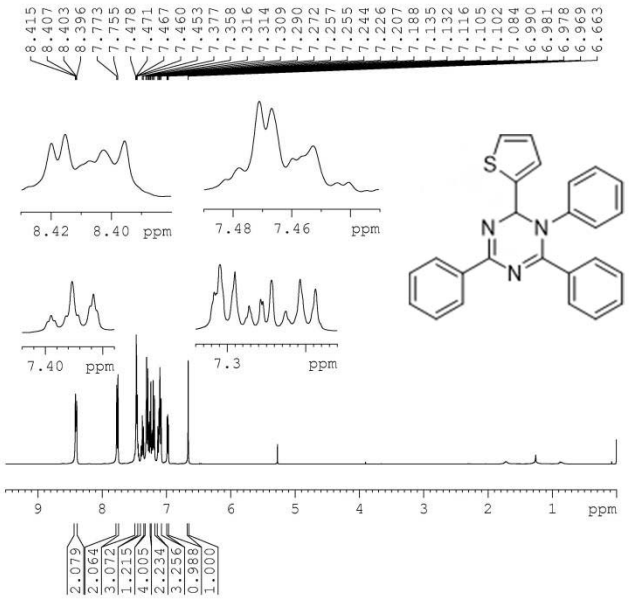
======== CHANNEL f1 ========
SFO1             400.1324710 MHz
NUC1                     1H
P1                    9.70 usec
SI                   65536
SF               400.1300176 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```




```
NAME      2018-04-18 tyut-lx-
EXPNO                 11
PROCNO                 1
Date_           20180420
Time                5.40
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                185.43
DW                20.800 usec
DE                 6.50 usec
TE                295.9 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

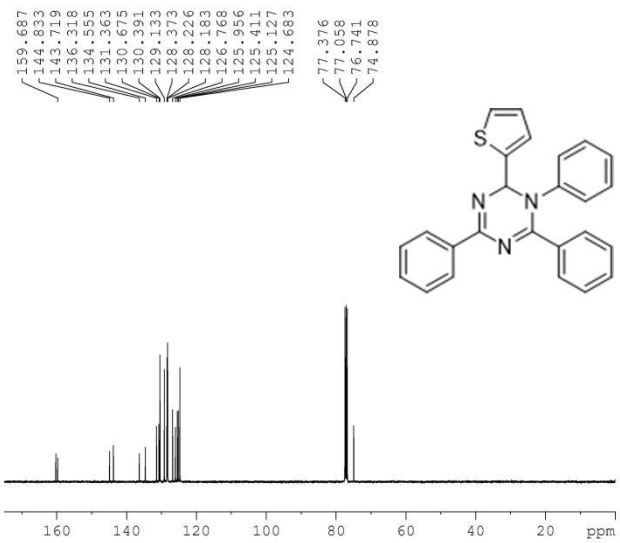
======== CHANNEL f1 ========
SFO1          100.6228293 MHz
NUC1                 13C
P1                  9.50 usec
SI                 32768
SF            100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

7ak




```
NAME          2018041204
EXPNO                 10
PROCNO                 1
Date_           20180413
Time                3.37
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894966 sec
RG                 60.71
DW                62.400 usec
DE                 6.50 usec
TE                297.8 K
D1             1.00000000 sec
TD0                    1

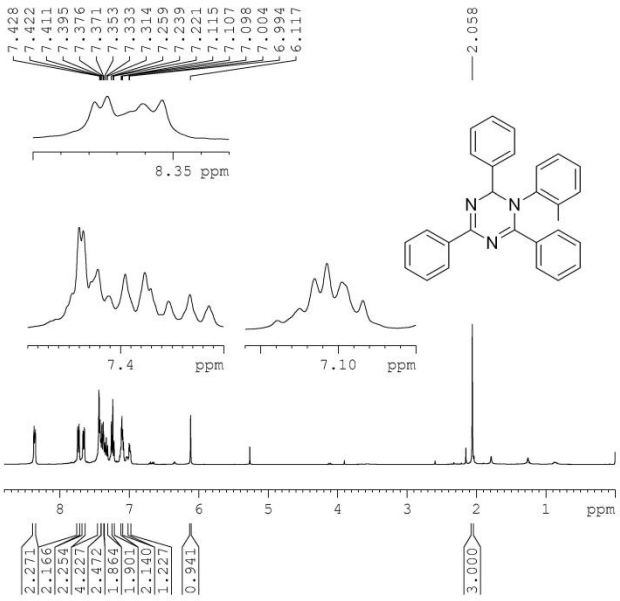
======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                  1H
P1                  9.70 usec
SI                 65536
SF            400.1300167 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



```
NAME          2018041204
EXPNO                 11
PROCNO                 1
Date_           20180413
Time                4.36
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                185.43
DW                20.800 usec
DE                 6.50 usec
TE                298.5 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

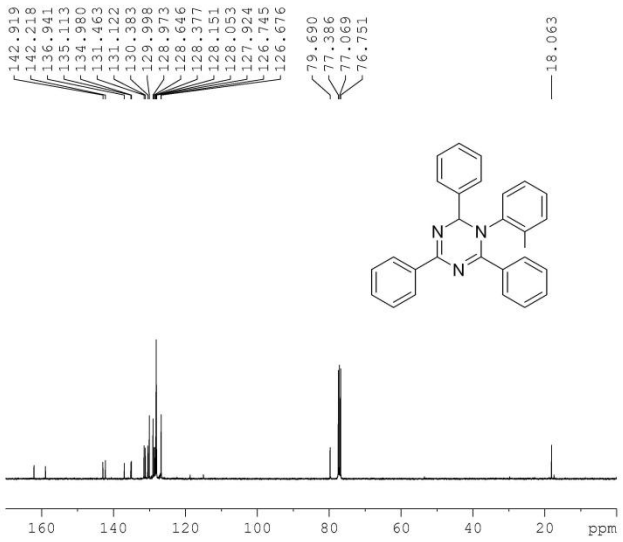
======== CHANNEL f1 ========
SFO1          100.6228293 MHz
NUC1                 13C
P1                  9.50 usec
SI                 32768
SF            100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

5ba and **7ba**



```
NAME          2018041203
EXPNO                 10
PROCNO                 1
Date_           20180413
Time                2.34
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894966 sec
RG                 34.32
DW                62.400 usec
DE                 6.50 usec
TE                297.8 K
D1             1.00000000 sec
TD0                    1

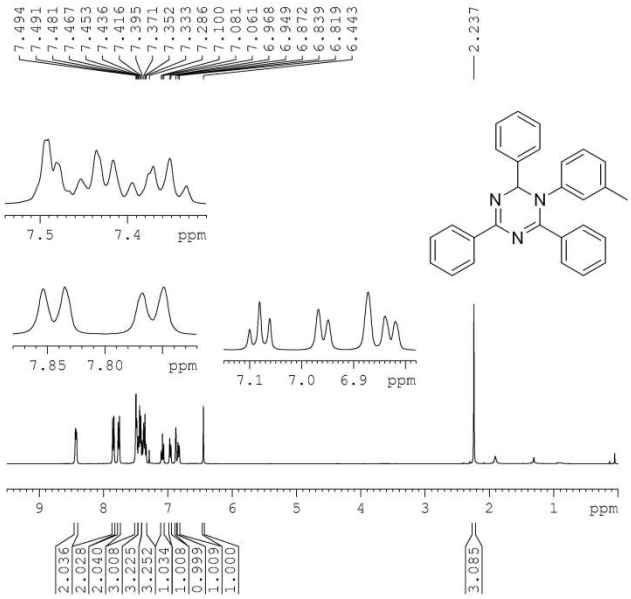
======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                  1H
P1                  9.70 usec
SI                 65536
SF            400.1300189 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




```
NAME          2018041203
EXPNO                 11
PROCNO                 1
Date_           20180413
Time                3.33
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG               185.43
DW               20.800 usec
DE                6.50 usec
TE               298.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

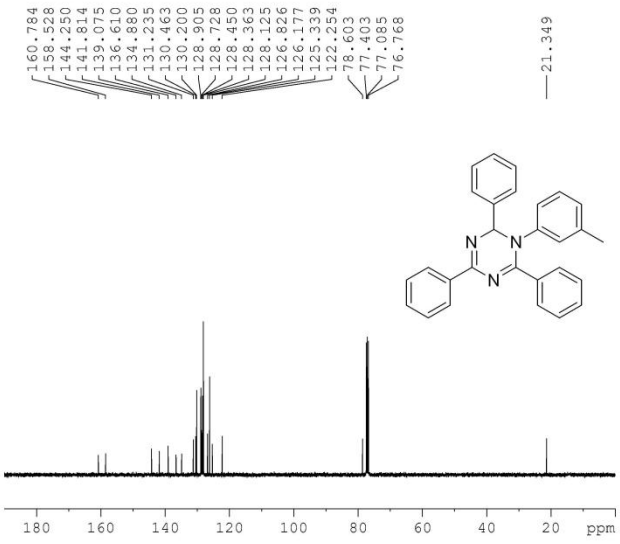
======== CHANNEL f1 ========
SFO1        100.6228293 MHz
NUC1                13C
P1                 9.50 usec
SI                32768
SF          100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

5ca and **7ca**




```
NAME                  29
EXPNO                  1
PROCNO                 1
Date_           20180326
Time               15.07
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                65536
SOLVENT           CDCl3
NS                    8
DS                    0
SWH            8223.685 Hz
FIDRES         0.125483 Hz
AQ            3.9846387 sec
RG                 71.8
DW               60.800 usec
DE                6.50 usec
TE               291.6 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.00 usec
PL1                -3.13 dB
PL1W         20.50172997 W
SFO1        400.1324710 MHz
SI                32768
SF          400.1300000 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
```

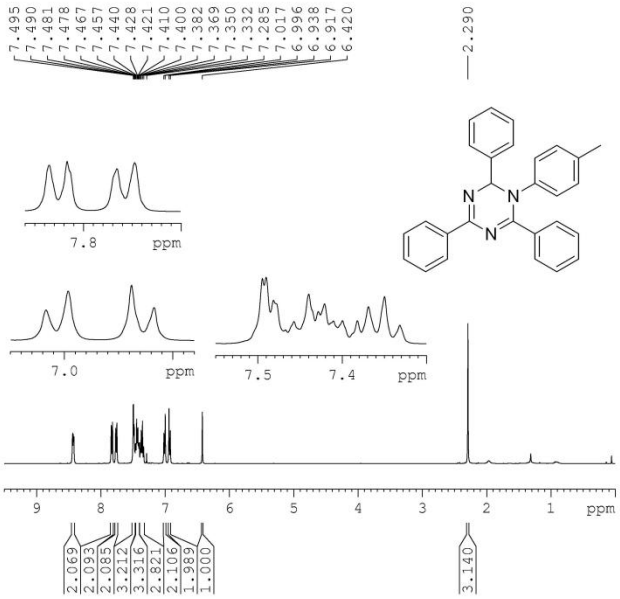



```
NAME                  29
EXPNO                  2
PROCNO                 1
Date_           20180326
Time               15.17
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  160
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                32800
DW               20.800 usec
DE                6.50 usec
TE                293.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.00 usec
PL1                -2.04 dB
PL1W        55.04534149 W
SFO1       100.6238364 MHz

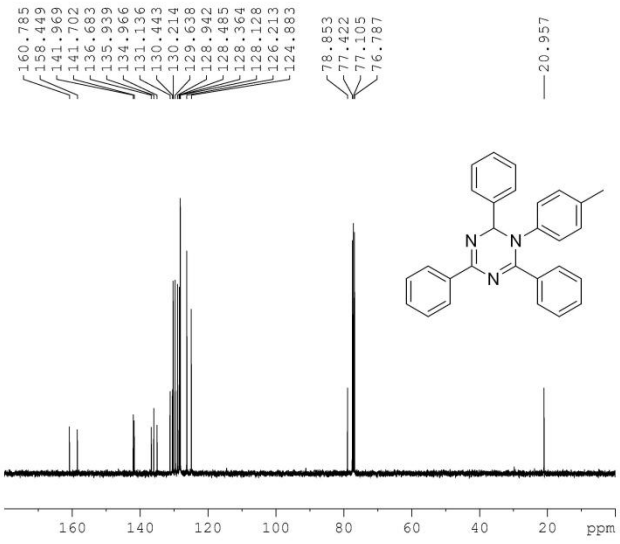
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              80.00 usec
```

5da and **7da**




```
NAME                  30
EXPNO                  1
PROCNO                 1
Date_           20180326
Time               15.20
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                65536
SOLVENT           CDCl3
NS                    8
DS                    0
SWH            8223.685 Hz
FIDRES         0.125483 Hz
AQ            3.9846387 sec
RG                   57
DW               60.800 usec
DE                6.50 usec
TE                291.8 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                 14.00 usec
PL1                -3.13 dB
PL1W        20.50172997 W
SFO1       400.1324710 MHz
SI                32768
SF         400.1300000 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
```

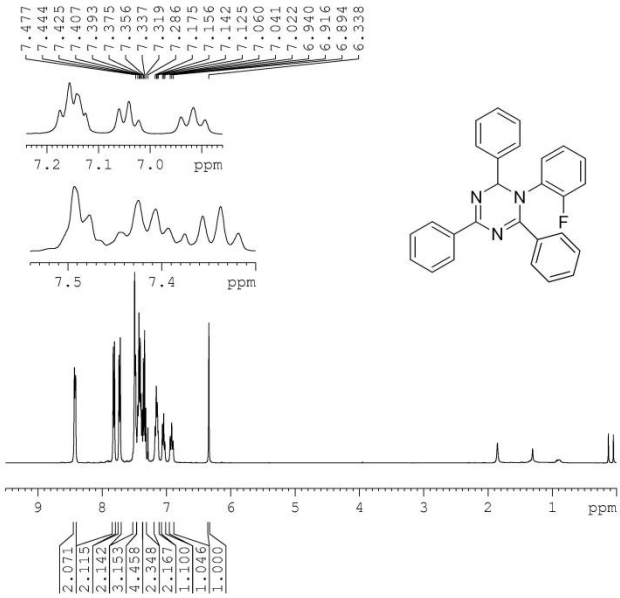



```
NAME                  30
EXPNO                  2
PROCNO                 1
Date_           20180326
Time               15.30
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  168
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                32800
DW               20.800 usec
DE                6.50 usec
TE               293.3 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.00 usec
PL1                -2.04 dB
PL1W        55.04534149 W
SFO1       100.6238364 MHz

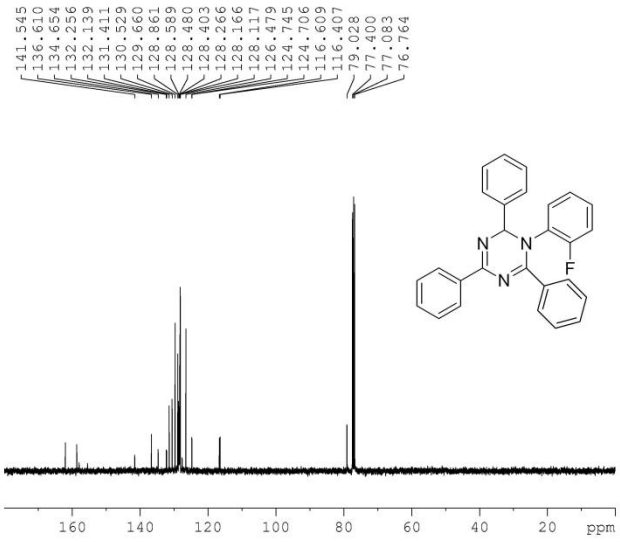
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              80.00 usec
```

5ea and **7ea**




```
NAME                  49
EXPNO                  1
PROCNO                 1
Date_           20180326
Time               15.34
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                65536
SOLVENT           CDCl3
NS                    8
DS                    0
SWH            8223.685 Hz
FIDRES         0.125483 Hz
AQ             3.9846387 sec
RG                71.8
DW               60.800 usec
DE                6.50 usec
TE               291.7 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                 14.00 usec
PL1                -3.13 dB
PL1W        20.50172997 W
SFO1       400.1324710 MHz
SI                32768
SF         400.1300000 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
```

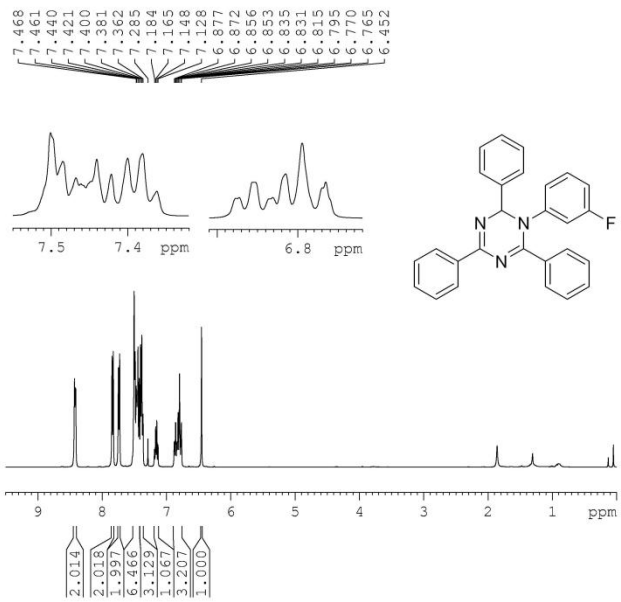



```
NAME                   49
EXPNO                   2
PROCNO                  1
Date_            20180326
Time                15.45
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   179
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                 32800
DW                20.800 usec
DE                 6.50 usec
TE                293.6 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.00 usec
PL1                -2.04 dB
PL1W         55.04534149 W
SFO1        100.6238364 MHz

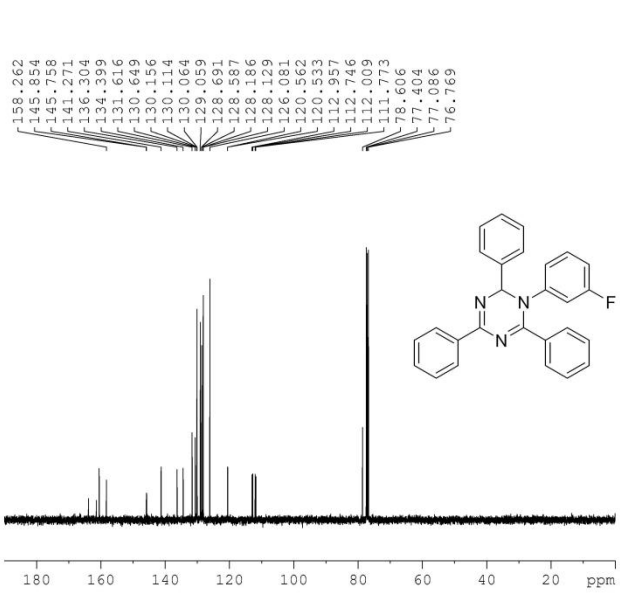
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              80.00 usec
```

5fa and **7fa**




```
NAME                   50
EXPNO                   1
PROCNO                  1
Date_            20180326
Time                15.49
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     0
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                  71.8
DW                60.800 usec
DE                 6.50 usec
TE                291.9 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 1H
P1                 14.00 usec
PL1                -3.13 dB
PL1W         20.50172997 W
SFO1        400.1324710 MHz
SI                 32768
SF          400.1300000 MHz
WDW                  EM
SSB                  0
LB                0.30 Hz
GB                   0
```

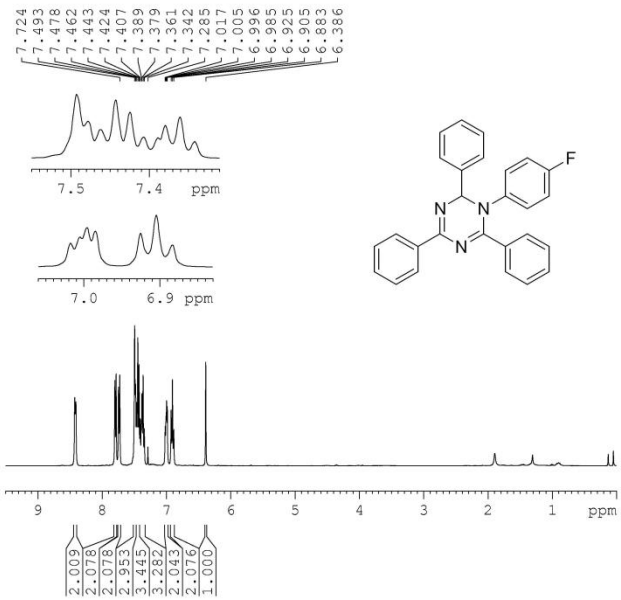



```
NAME                   50
EXPNO                   2
PROCNO                  1
Date_            20180326
Time                15.56
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   112
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                 32800
DW                20.800 usec
DE                 6.50 usec
TE                293.3 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 10.00 usec
PL1                -2.04 dB
PL1W         55.04534149 W
SFO1        100.6238364 MHz

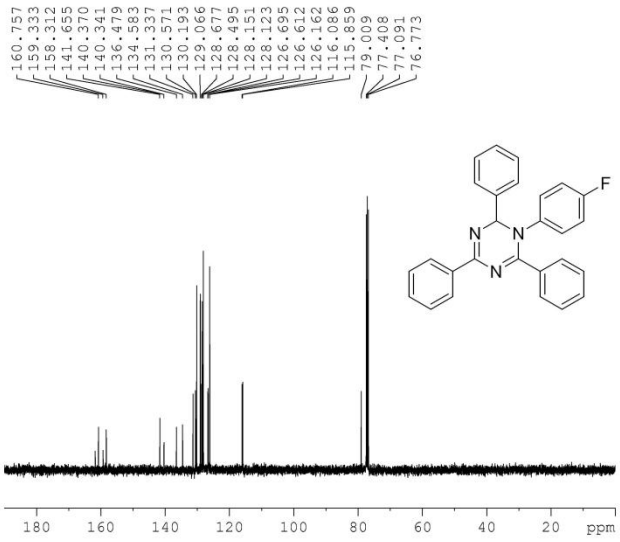
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              80.00 usec
```

5ga and **7ga**




```
NAME                   51
EXPNO                   1
PROCNO                  1
Date_            20180326
Time                16.38
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     0
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                  71.8
DW                60.800 usec
DE                 6.50 usec
TE                292.6 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 14.00 usec
PL1                -3.13 dB
PL1W         20.50172997 W
SFO1        400.1324710 MHz
SI                 32768
SF          400.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
```

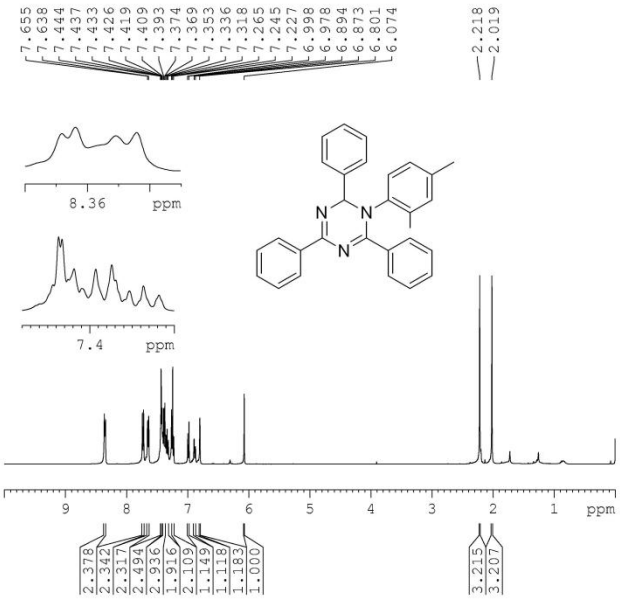



```
NAME                  51
EXPNO                  2
PROCNO                 1
Date_           20180326
Time               16.43
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   73
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                32800
DW               20.800 usec
DE                6.50 usec
TE                293.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -2.04 dB
PL1W        55.04534149 W
SFO1       100.6238364 MHz

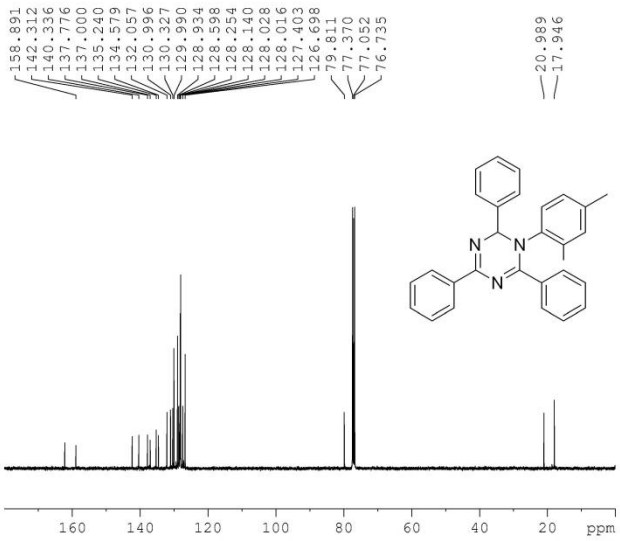
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
```

5ha and **7ia**




```
NAME      2018-04-13 tyut-lx-
EXPNO                 10
PROCNO                 1
Date_           20180413
Time               22.57
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ            4.0894966 sec
RG                57.76
DW               62.400 usec
DE                6.50 usec
TE                297.6 K
D1           1.00000000 sec
TD0                   1

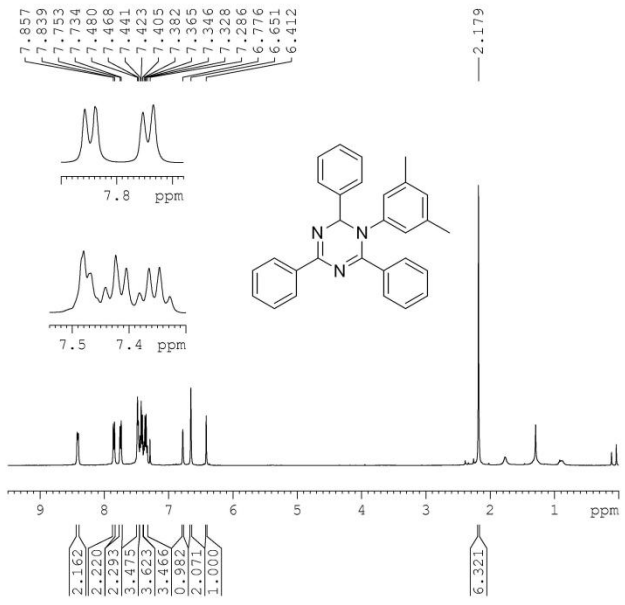
======== CHANNEL f1 ========
SFO1       400.1324710 MHz
NUC1                 1H
P1                9.70 usec
SI                65536
SF         400.1300160 MHz
WDW                  EM
SSB                   0
LB                0.30 Hz
GB                    0
PC                1.00
```




```
NAME      2018-04-13 tyut-lx-
EXPNO                 11
PROCNO                 1
Date_           20180413
Time                23.56
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   1024
DS                      4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                 185.43
DW                 20.800 usec
DE                  6.50 usec
TE                 298.3 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

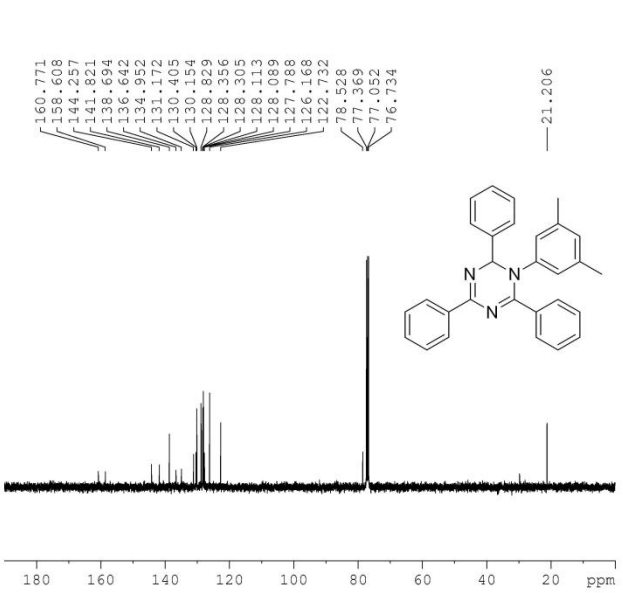
======== CHANNEL f1 ========
SFO1         100.6228293 MHz
NUC1                13C
P1                 9.50 usec
SI                32768
SF           100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

5ia and **7ha**




```
NAME                  52
EXPNO                  1
PROCNO                 1
Date_           20180326
Time                16.48
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      8
DS                      0
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9846387 sec
RG                  90.5
DW                 60.800 usec
DE                  6.50 usec
TE                 292.1 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                   1H
P1                 14.00 usec
PL1                -3.13 dB
PL1W          20.50172997 W
SFO1         400.1324710 MHz
SI                32768
SF           400.1300000 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
```

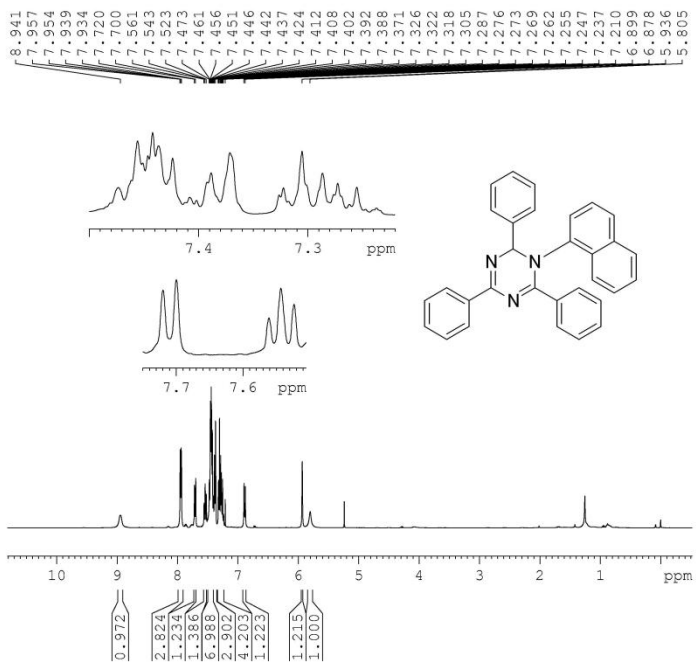


```
NAME                  52
EXPNO                  2
PROCNO                 1
Date_           20180326
Time               16.56
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  137
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                32800
DW               20.800 usec
DE                6.50 usec
TE               293.8 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -2.04 dB
PL1W        55.04534149 W
SFO1       100.6238364 MHz

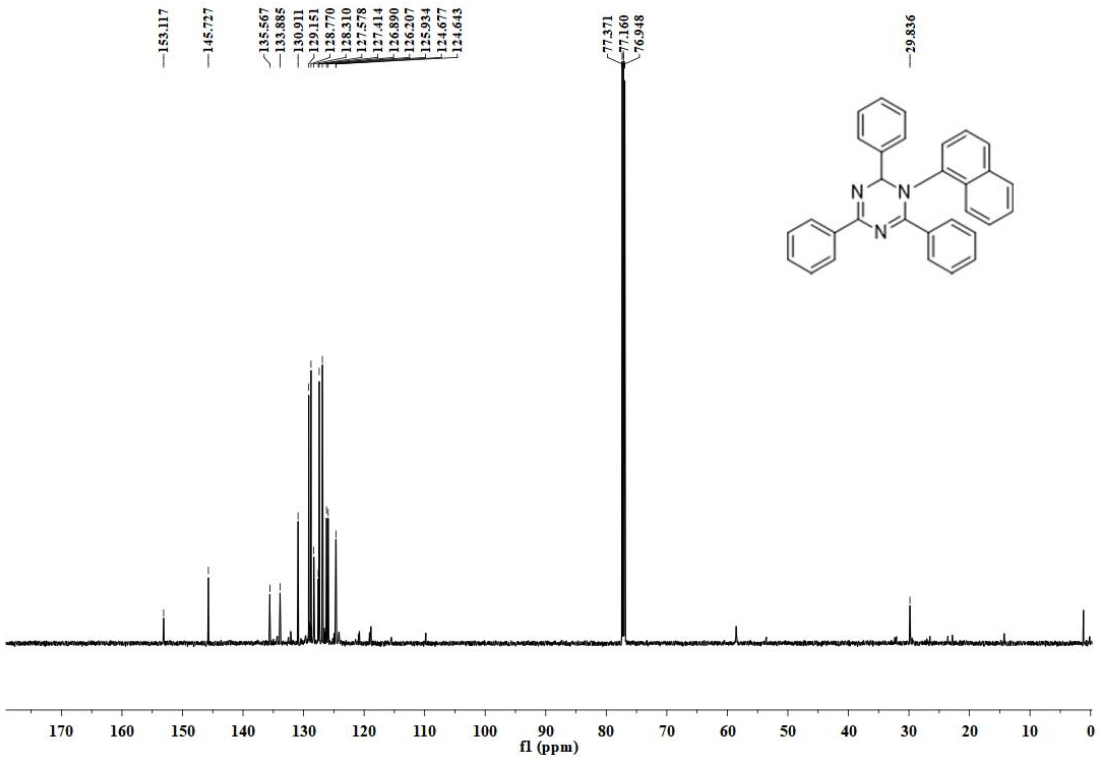
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
```

5ja

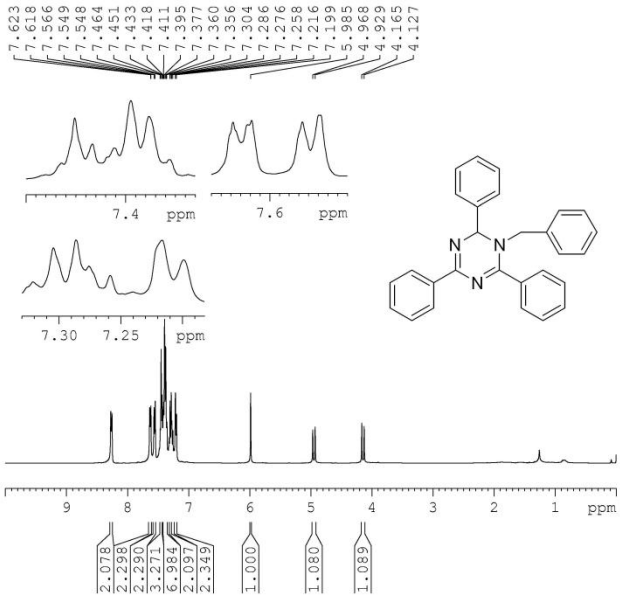


```
NAME      2019-04-01 tyut-lx-(
EXPNO                   10
PROCNO                   1
Date_             20190402
Time                 18.03
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH               8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894966 sec
RG                   34.32
DW                  62.400 usec
DE                   6.50 usec
TE                  295.4 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                    1H
P1                   9.59 usec
SI                  65536
SF            400.1300299 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

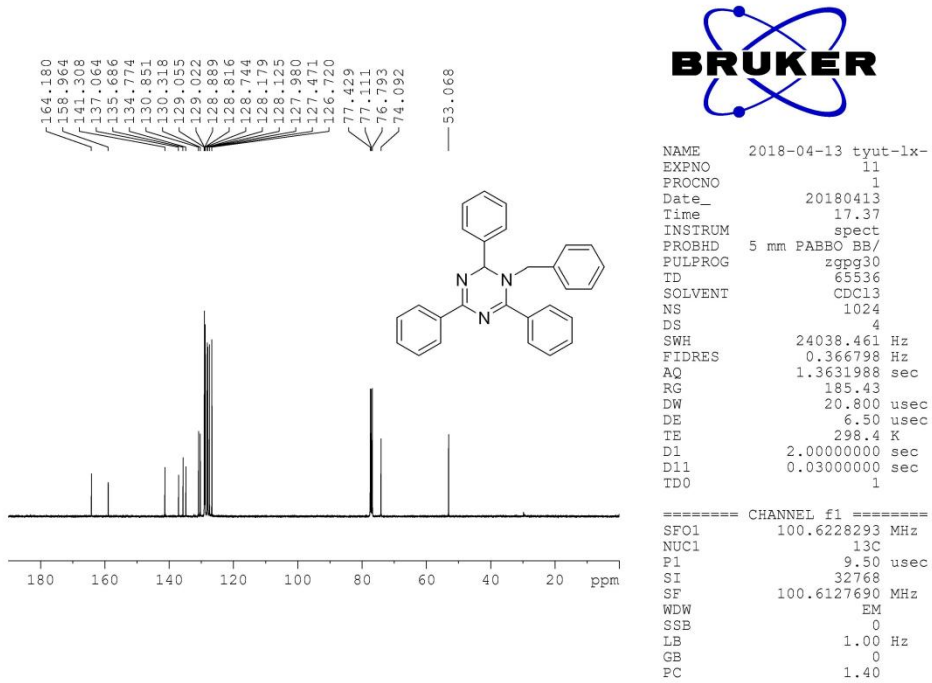


5ka and **7ka**

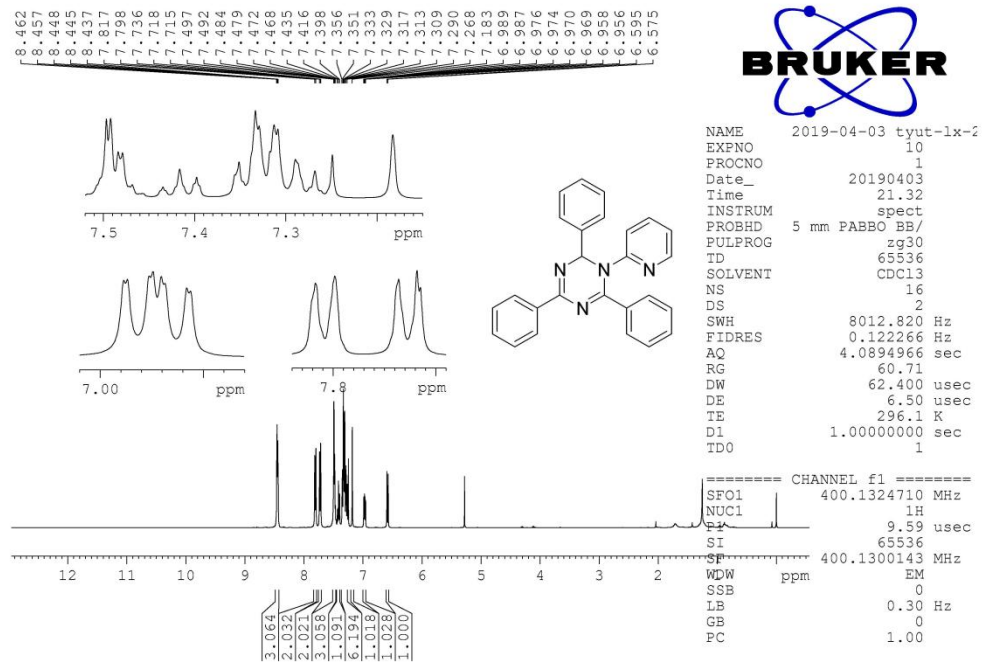


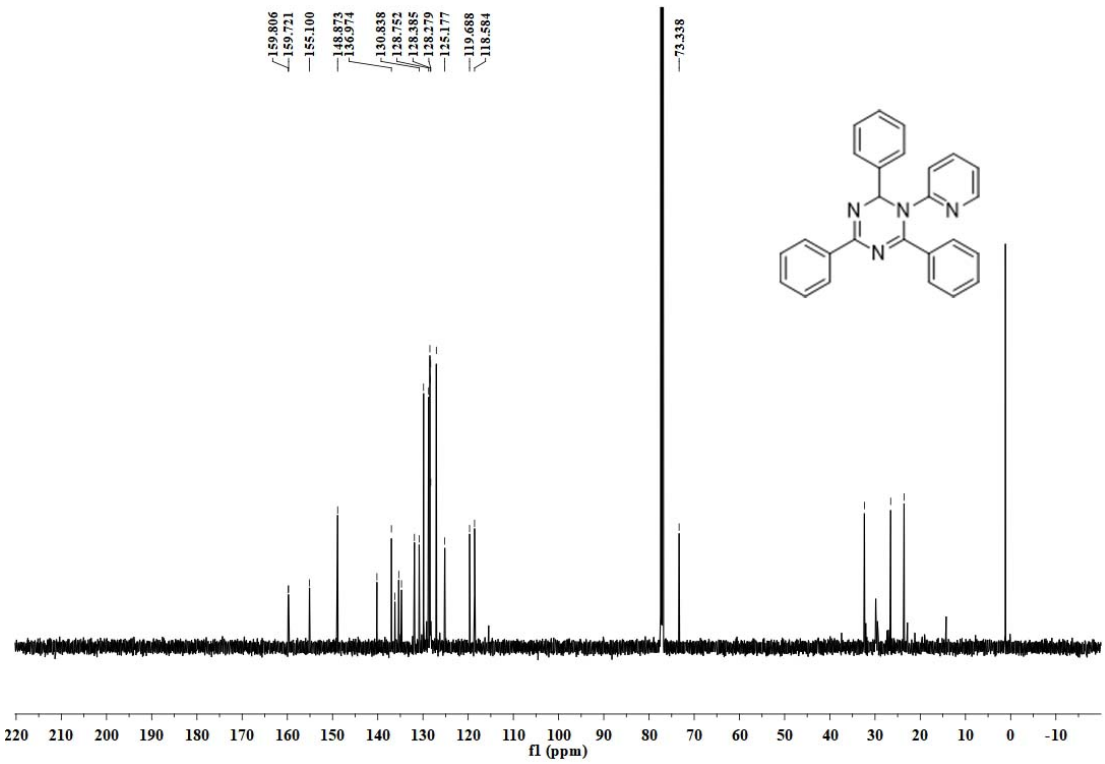

```
NAME          2018-04-13 tyut-lx-
EXPNO                 10
PROCNO                 1
Date_           20180413
Time               16.38
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES             0.122266 Hz
AQ              4.0894966 sec
RG                 34.32
DW                62.400 usec
DE                 6.50 usec
TE                297.4 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                  1H
P1                 9.70 usec
SI                 65536
SF            400.1300251 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

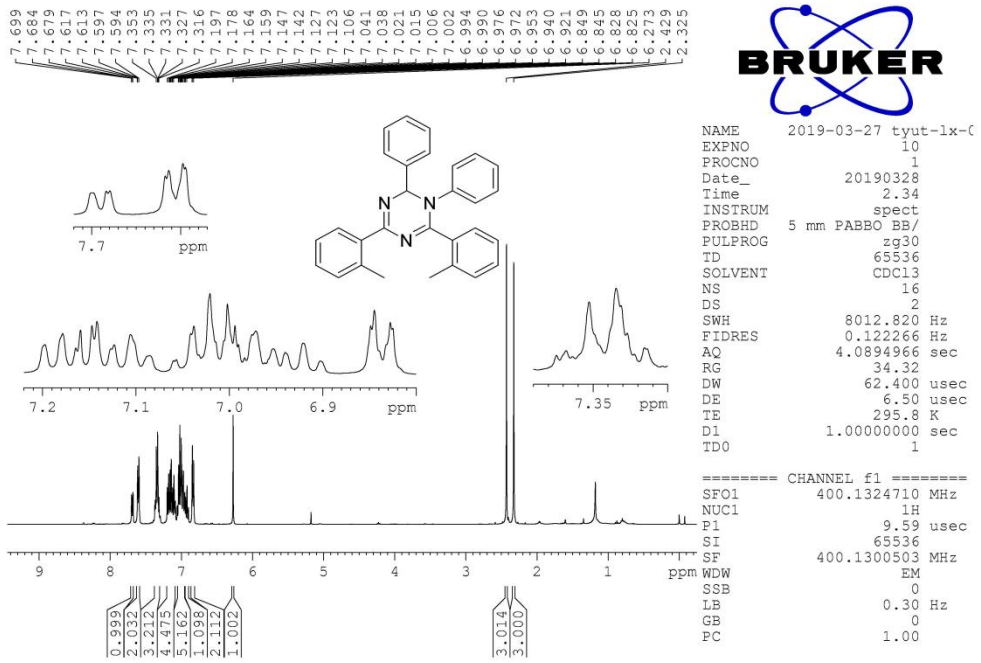

164.180
158.964
141.308
137.064
135.686
134.774
130.851
130.318
129.055
129.022
128.889
128.816
128.744
128.179
128.125
127.980
127.471
126.720
77.429
77.111
76.793
74.092
53.068
180
160
140
120
100
80
60
40
20
ppm
BRUKER
NAME 2018-04-13 tyut-lx-
EXPNO 11
PROCNO 1
Date_ 20180413
Time 17.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 185.43
DW 20.800 usec
DE 6.50 usec
TE 298.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 9.50 usec
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

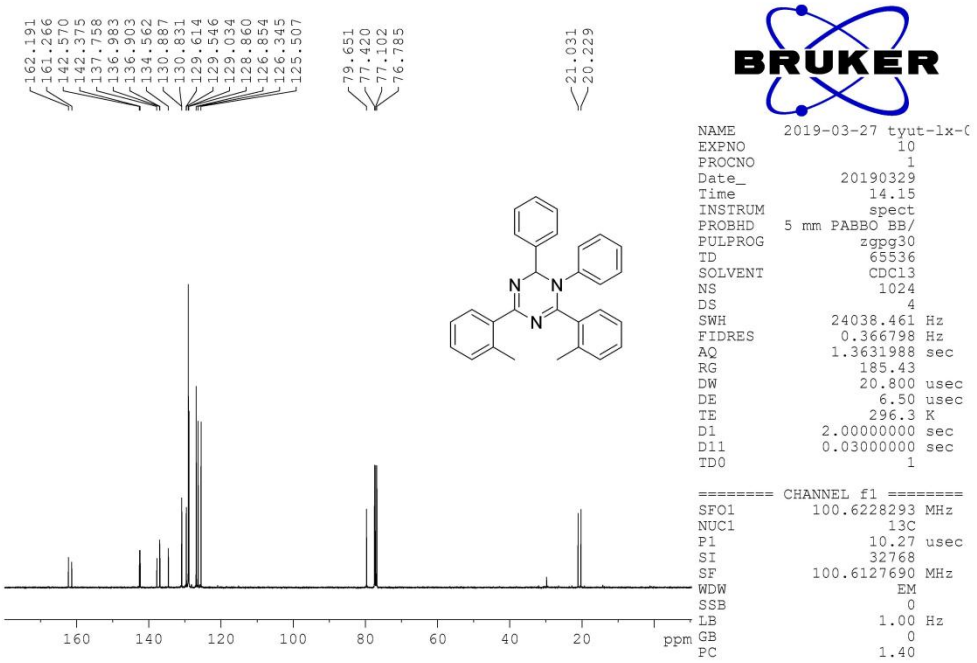
5la


8.462
8.457
8.448
8.445
8.437
7.817
7.798
7.736
7.718
7.715
7.497
7.492
7.484
7.479
7.472
7.468
7.435
7.416
7.398
7.356
7.351
7.333
7.329
7.317
7.313
7.309
7.290
7.268
7.183
6.989
6.987
6.976
6.974
6.970
6.969
6.958
6.956
6.595
6.575
7.5
7.4
7.3
ppm
7.00
ppm
7.8
ppm
12
11
10
9
8
7
6
5
4
3
2
ppm
3.064
2.032
2.021
3.058
1.091
6.194
1.018
1.028
1.000
BRUKER
NAME 2019-04-03 tyut-lx-2
EXPNO 10
PROCNO 1
Date_ 20190403
Time 21.32
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 60.71
DW 62.400 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.59 usec
SI 65536
SF 400.1300143 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

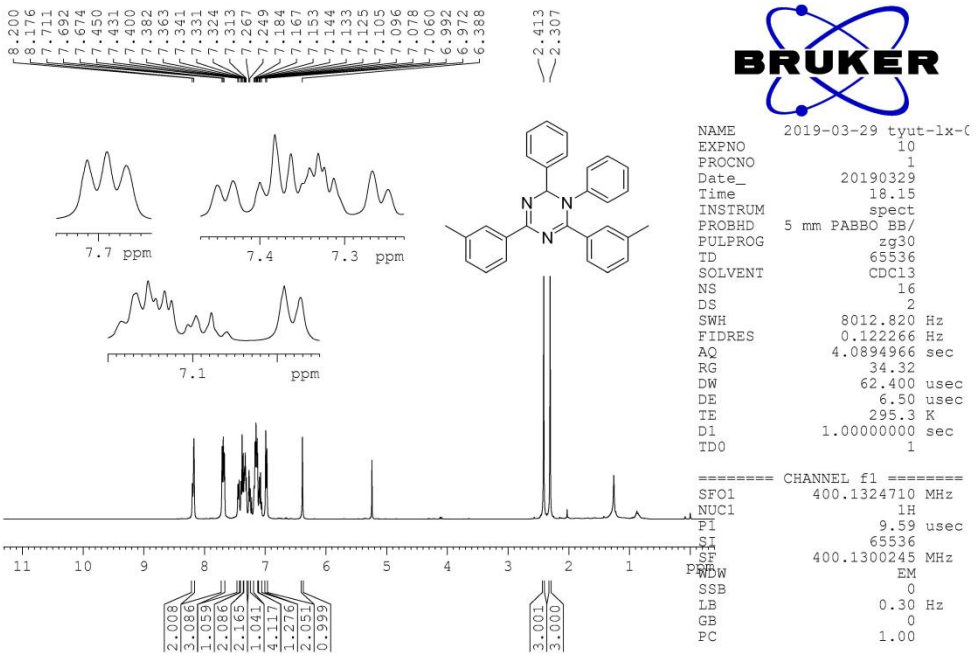

159.806
159.721
155.100
148.873
136.974
130.838
128.752
128.385
128.279
125.177
119.688
118.584
73.338
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

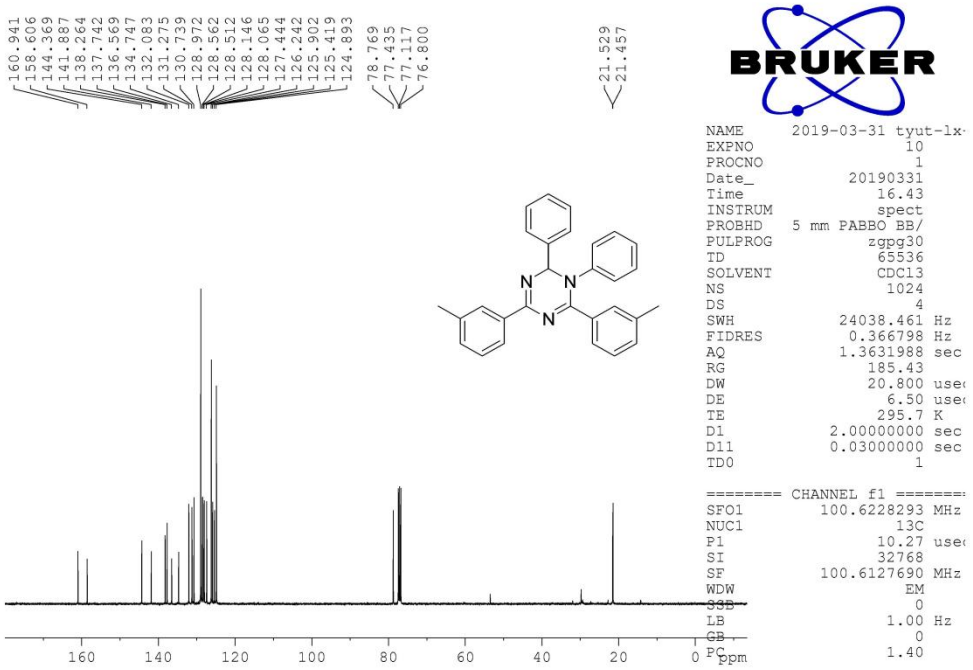
5ma and **7la**


7.699
7.684
7.679
7.617
7.613
7.597
7.594
7.353
7.335
7.331
7.327
7.316
7.197
7.178
7.164
7.159
7.147
7.142
7.127
7.123
7.106
7.041
7.038
7.021
7.015
7.006
7.002
6.994
6.990
6.976
6.972
6.953
6.940
6.921
6.849
6.845
6.828
6.825
6.273
2.429
2.325
7.7 ppm
7.2 7.1 7.0 6.9 ppm
7.35 ppm
9 8 7 6 5 4 3 2 1 ppm
0.999
2.032
3.212
4.475
5.162
1.098
2.112
1.002
3.014
3.000
BRUKER
NAME 2019-03-27 tyut-1x-(
EXPNO 10
PROCNO 1
Date_ 20190328
Time 2.34
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 34.32
DW 62.400 usec
DE 6.50 usec
TE 295.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.59 usec
SI 65536
SF 400.1300503 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

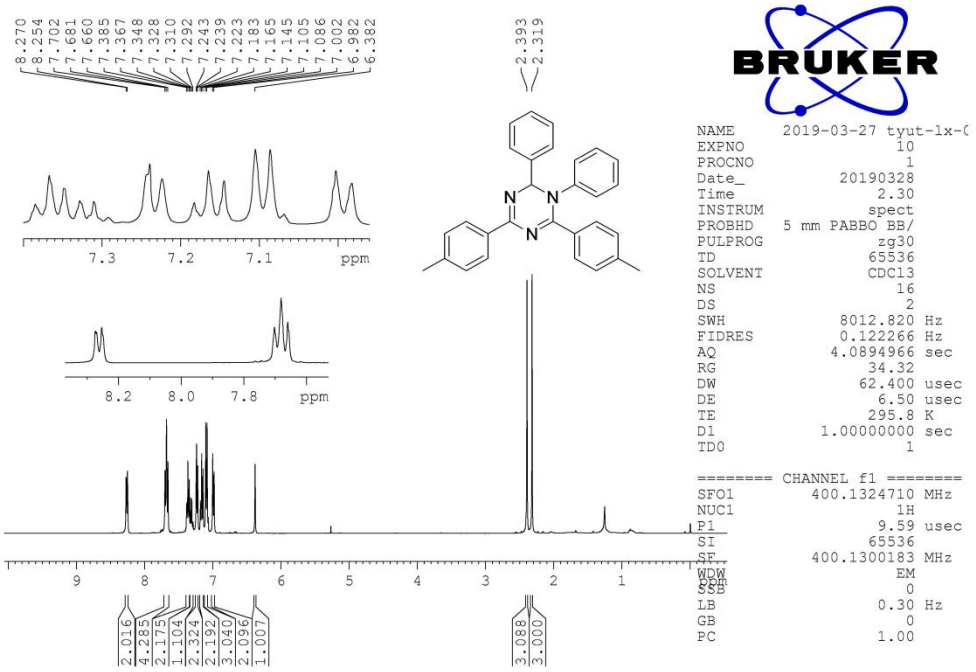

162.191
161.266
142.570
142.375
137.758
136.983
136.903
134.562
130.887
130.831
129.614
129.546
129.034
128.860
126.854
126.345
125.507
79.651
77.420
77.102
76.785
21.031
20.229
160
140
120
100
80
60
40
20
ppm
BRUKER
NAME 2019-03-27 tyut-lx-(
EXPNO 10
PROCNO 1
Date_ 20190329
Time 14.15
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 185.43
DW 20.800 usec
DE 6.50 usec
TE 296.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.27 usec
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

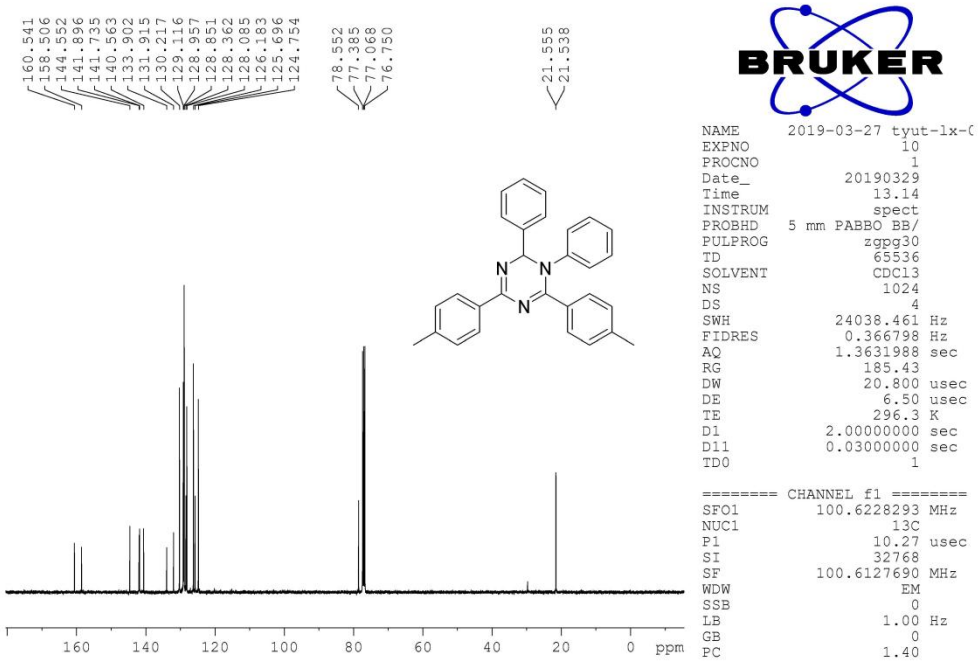
5na and **7ma**


8.200
8.176
7.711
7.692
7.674
7.450
7.431
7.400
7.382
7.363
7.341
7.331
7.324
7.313
7.267
7.249
7.184
7.167
7.153
7.144
7.133
7.125
7.105
7.096
7.078
7.060
6.992
6.972
6.388
2.413
2.307
7.7 ppm
7.4
7.3 ppm
7.1
ppm
11
10
9
8
7
6
5
4
3
2
1
ppm
2.008
3.086
1.059
2.086
2.165
1.041
4.117
1.276
2.051
0.999
3.001
3.000
BRUKER
NAME 2019-03-29 tyut-lx-(
EXPNO 10
PROCNO 1
Date_ 20190329
Time 18.15
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 34.32
DW 62.400 usec
DE 6.50 usec
TE 295.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.59 usec
SI 65536
SF 400.1300245 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

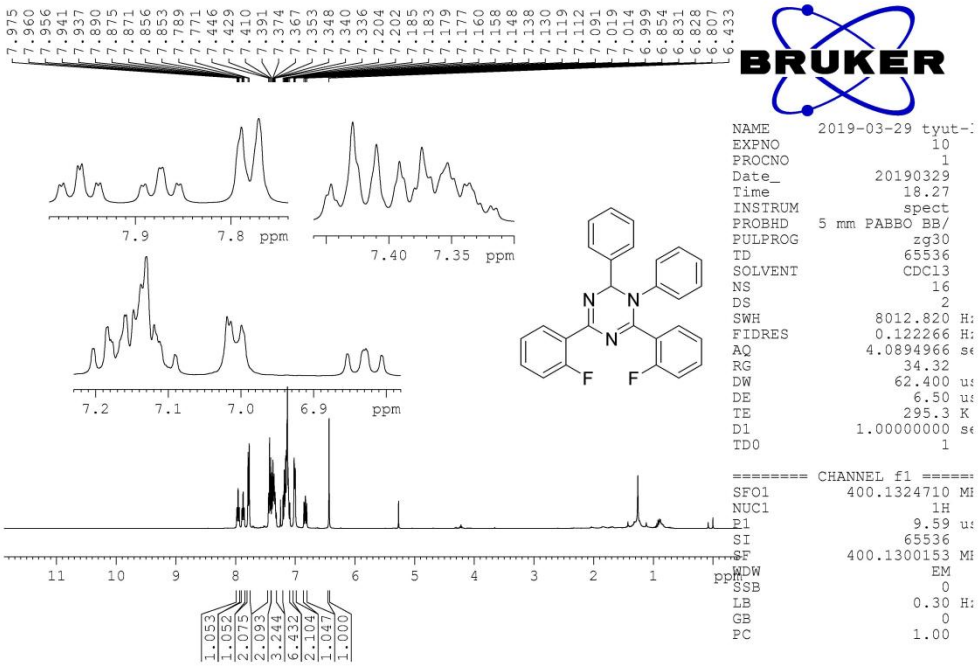

160.941
158.606
144.369
141.887
138.264
137.742
136.569
134.747
132.083
131.275
130.739
128.972
128.562
128.512
128.146
128.065
127.444
126.242
125.902
125.419
124.893
78.769
77.435
77.117
76.800
21.529
21.457
160
140
120
100
80
60
40
20
0
ppm
NAME 2019-03-31 tyut-lx
EXPNO 10
PROCNO 1
Date_ 20190331
Time 16.43
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 185.43
DW 20.800 use
DE 6.50 use
TE 295.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.27 use
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

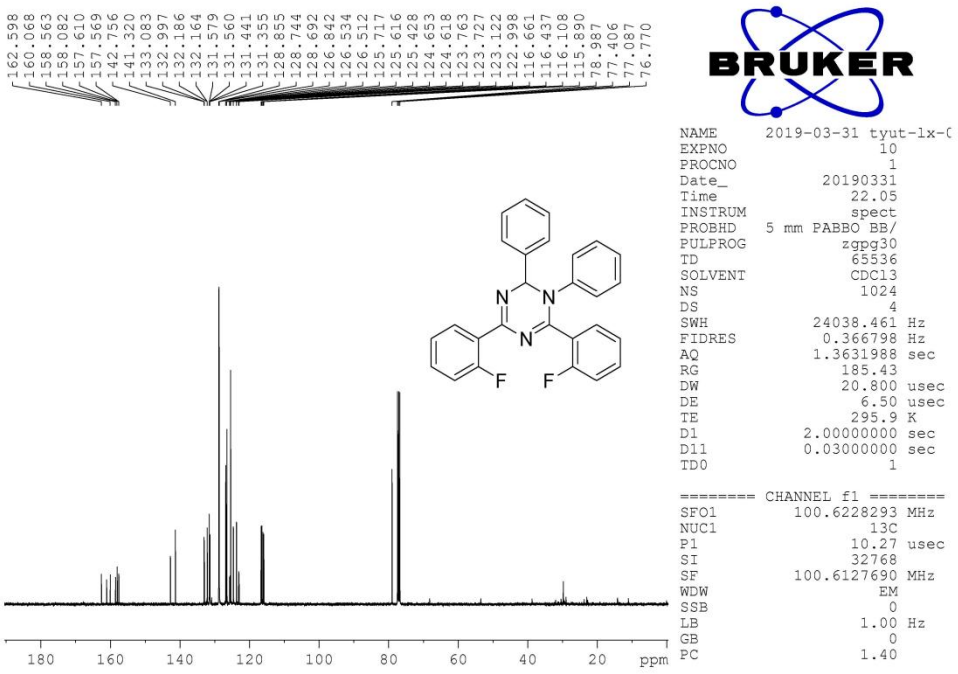
5oa and **7na**


8.270
8.254
7.702
7.681
7.660
7.385
7.367
7.348
7.328
7.310
7.292
7.243
7.239
7.223
7.183
7.165
7.145
7.105
7.086
7.002
6.982
6.382
2.393
2.319
7.3
7.2
7.1
ppm
8.2
8.0
7.8
ppm
9
8
7
6
5
4
3
2
1
2.016
4.285
2.175
1.104
2.324
2.192
3.040
2.096
1.007
3.088
3.000
NAME 2019-03-27 tyut-lx-(
EXPNO 10
PROCNO 1
Date_ 20190328
Time 2.30
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 34.32
DW 62.400 usec
DE 6.50 usec
TE 295.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.59 usec
SI 65536
SF 400.1300183 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


160.541
158.506
144.552
141.896
141.735
140.563
133.902
131.915
130.217
129.116
128.957
128.851
128.362
128.085
126.183
125.696
124.754
78.552
77.385
77.068
76.750
21.555
21.538
BRUKER
NAME 2019-03-27 tyut-1x-(
EXPNO 10
PROCNO 1
Date_ 20190329
Time 13.14
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 185.43
DW 20.800 usec
DE 6.50 usec
TE 296.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.27 usec
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
160 140 120 100 80 60 40 20 0 ppm

5pa

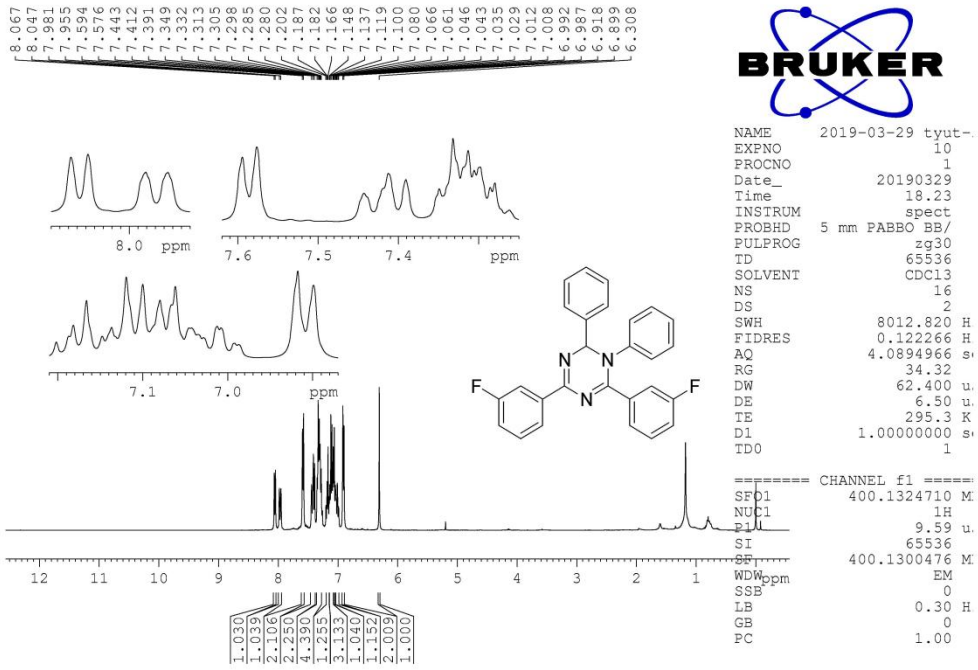

7.975
7.960
7.956
7.941
7.937
7.890
7.875
7.871
7.856
7.853
7.789
7.771
7.446
7.429
7.410
7.391
7.374
7.367
7.353
7.348
7.340
7.336
7.204
7.202
7.185
7.183
7.179
7.177
7.160
7.158
7.148
7.138
7.130
7.119
7.112
7.091
7.019
7.014
6.999
6.854
6.831
6.828
6.807
6.433
BRUKER
NAME 2019-03-29 tyut-1
EXPNO 10
PROCNO 1
Date_ 20190329
Time 18.27
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 34.32
DW 62.400 usec
DE 6.50 usec
TE 295.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ======
SFO1 400.1324710 MHz
NUC1 1H
P1 9.59 usec
SI 65536
SF 400.1300153 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.9 7.8 ppm
7.40 7.35 ppm
7.2 7.1 7.0 6.9 ppm
11 10 9 8 7 6 5 4 3 2 1 ppm
1.053
1.052
2.075
2.093
3.244
6.432
2.104
1.047
1.000



BRUKER

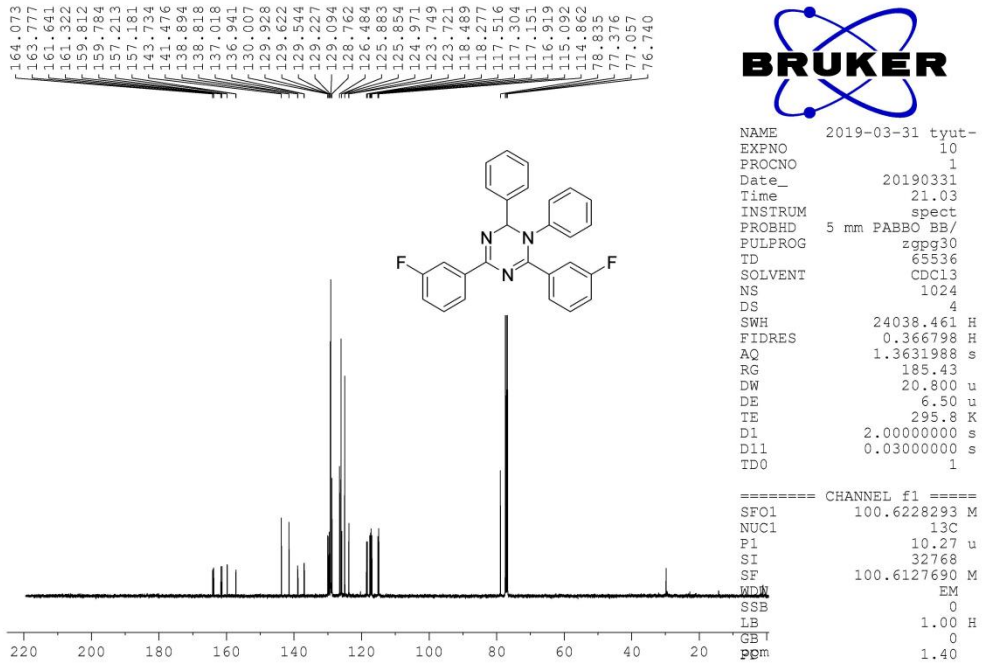
NAME	2019-03-31 tyut-lx-(
EXPNO	10
PROCNO	1
Date_	20190331
Time	22.05
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	185.43
DW	20.800 usec
DE	6.50 usec
TE	295.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228293 MHz
NUC1	13C
P1	10.27 usec
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

5qa and **7oa**

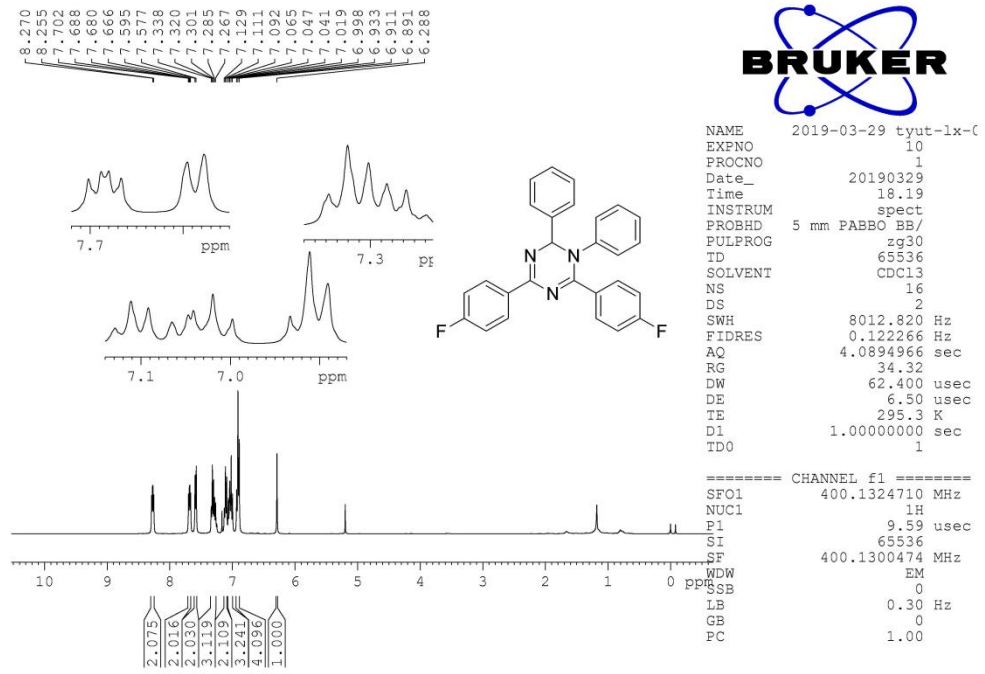


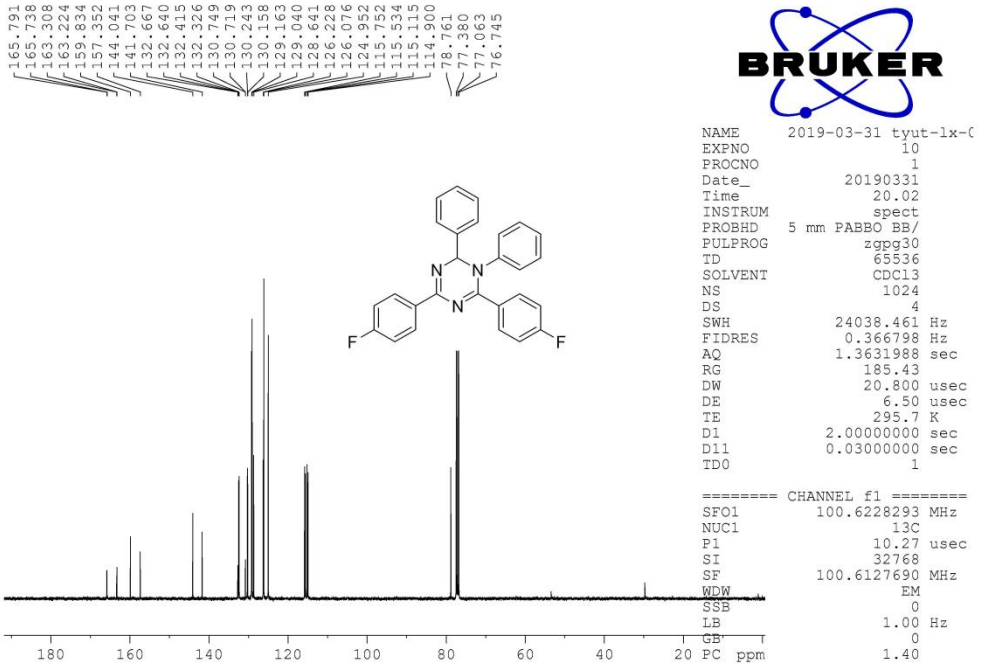
BRUKER

NAME	2019-03-29 tyut-.
EXPNO	10
PROCNO	1
Date_	20190329
Time	18.23
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8012.820 H
FIDRES	0.122266 H
AQ	4.0894966 s
RG	34.32
DW	62.400 u
DE	6.50 u
TE	295.3 K
D1	1.00000000 s
TD0	1
======== CHANNEL f1 ======	
SFO1	400.1324710 M
NUC1	1H
P1	9.59 u
SI	65536
SF	400.1300476 M
WDW	EM
SSB	0
LB	0.30 H
GB	0
PC	1.00


164.073
163.777
161.641
161.322
159.812
159.784
157.213
157.181
143.734
141.476
138.894
138.818
137.018
136.941
130.007
129.928
129.622
129.544
129.227
129.094
128.762
126.484
125.883
125.854
124.971
123.749
123.721
118.489
118.277
117.516
117.304
117.151
116.919
115.092
114.862
78.835
77.376
77.057
76.740
N
N
N
F
F
220
200
180
160
140
120
100
80
60
40
20
ppm
BRUKER
NAME 2019-03-31 tyut-
EXPNO 10
PROCNO 1
Date_ 20190331
Time 21.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 H
FIDRES 0.366798 H
AQ 1.3631988 s
RG 185.43
DW 20.800 u
DE 6.50 u
TE 295.8 K
D1 2.00000000 s
D11 0.03000000 s
TD0 1
======== CHANNEL f1 =====
SFO1 100.6228293 M
NUC1 13C
P1 10.27 u
SI 32768
SF 100.6127690 M
WDW EM
SSB 0
LB 1.00 H
GB 0
PC 1.40

5ra and **7pa**

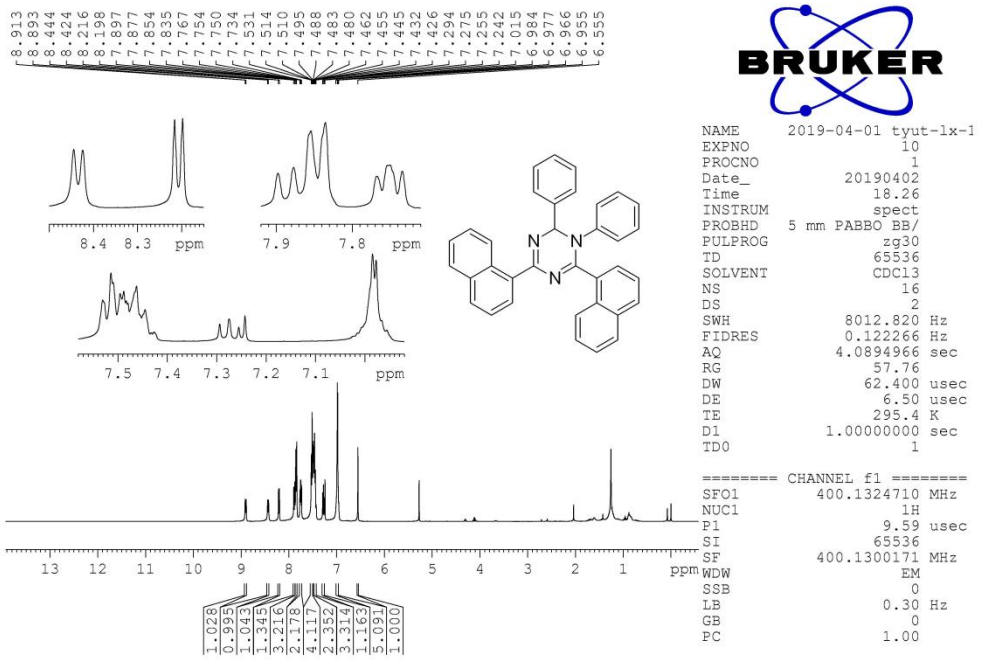

8.270
8.255
7.702
7.688
7.680
7.666
7.595
7.577
7.338
7.320
7.301
7.285
7.267
7.129
7.111
7.092
7.065
7.047
7.041
7.019
6.998
6.933
6.911
6.891
6.288
7.7
ppm
7.3
pp
7.1
7.0
ppm
N
N
N
F
F
10
9
8
7
6
5
4
3
2
1
0 ppm
2.075
2.016
2.030
3.119
2.109
3.241
4.096
1.000
BRUKER
NAME 2019-03-29 tyut-1x-(
EXPNO 10
PROCNO 1
Date_ 20190329
Time 18.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 34.32
DW 62.400 usec
DE 6.50 usec
TE 295.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.59 usec
SI 65536
SF 400.1300474 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER

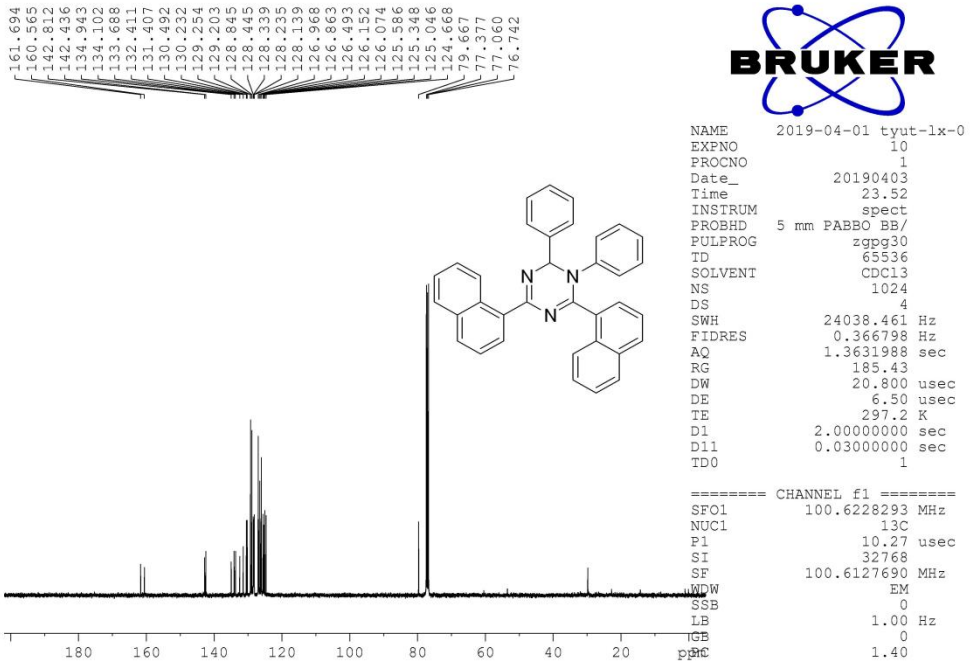
NAME	2019-03-31 tyut-lx-(
EXPNO	10
PROCNO	1
Date_	20190331
Time	20.02
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	185.43
DW	20.800 usec
DE	6.50 usec
TE	295.7 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228293 MHz
NUC1	13C
P1	10.27 usec
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC ppm	1.40

5sa



BRUKER

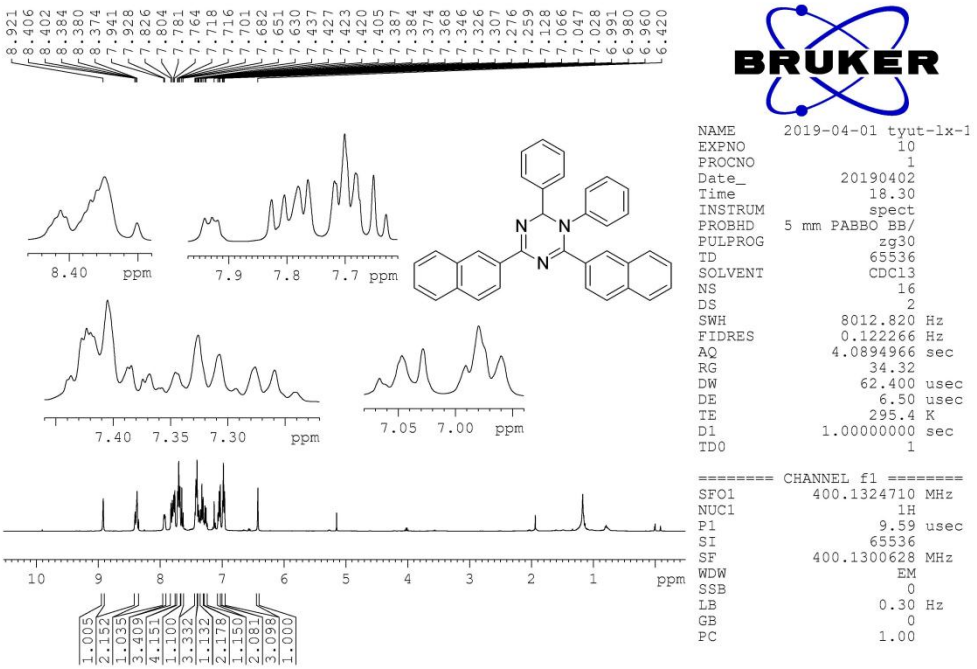
NAME	2019-04-01 tyut-lx-1
EXPNO	10
PROCNO	1
Date_	20190402
Time	18.26
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	57.76
DW	62.400 usec
DE	6.50 usec
TE	295.4 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1324710 MHz
NUC1	1H
P1	9.59 usec
SI	65536
SF	400.1300171 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



NAME 2019-04-01 tyut-1x-0
EXPNO 10
PROCNO 1
Date_ 20190403
Time 23.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 185.43
DW 20.800 usec
DE 6.50 usec
TE 297.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

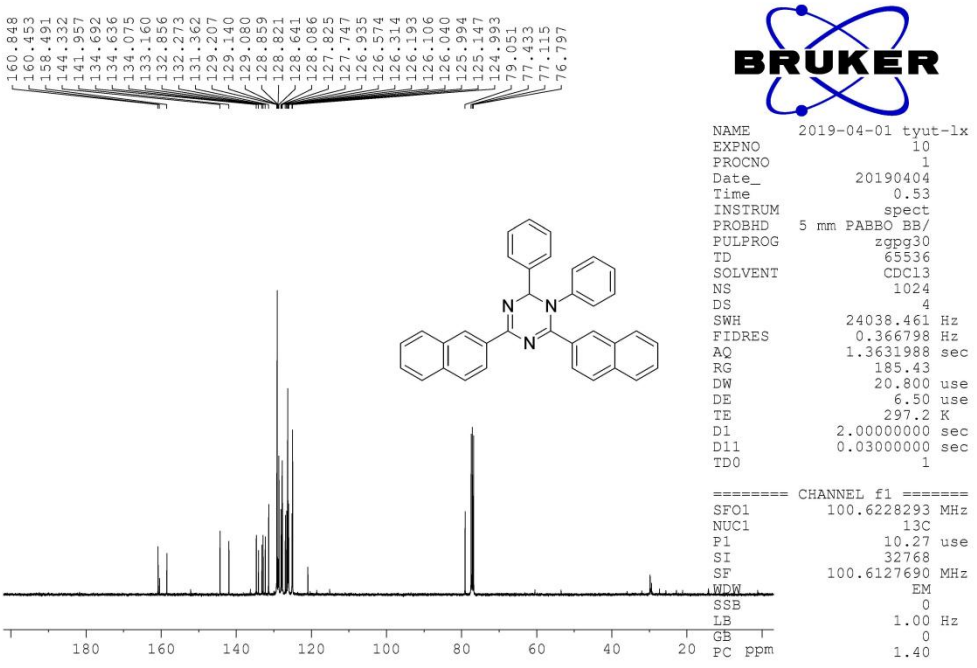
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.27 usec
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

5ta

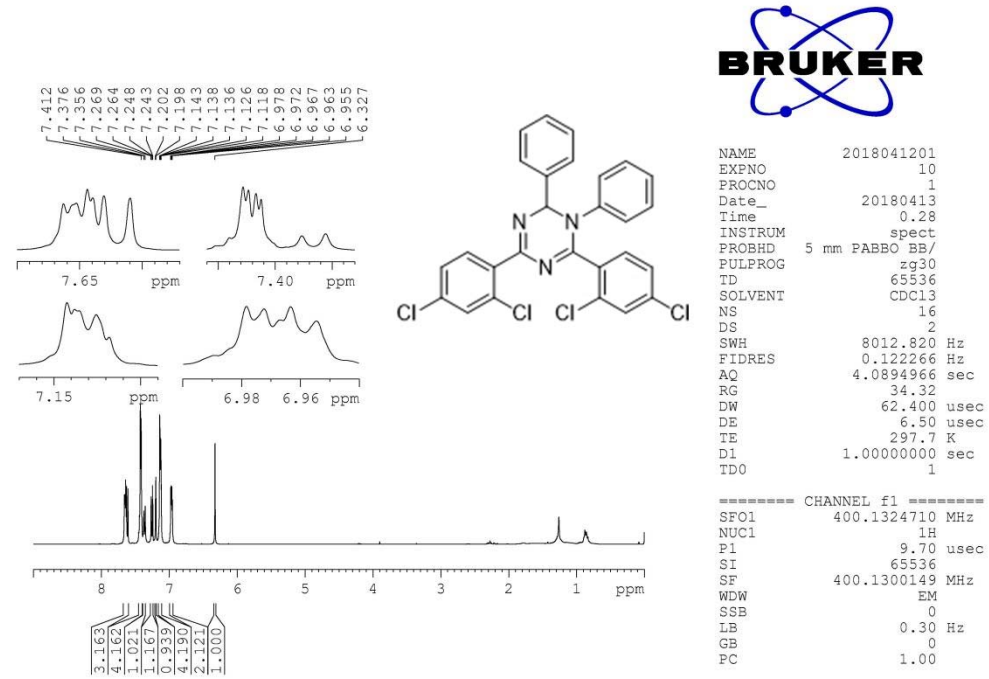


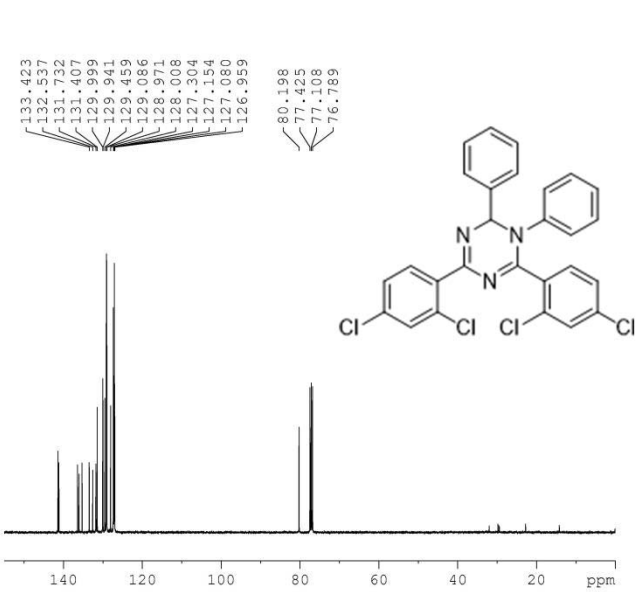
NAME 2019-04-01 tyut-1x-1
EXPNO 10
PROCNO 1
Date_ 20190402
Time 18.30
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 34.32
DW 62.400 usec
DE 6.50 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.59 usec
SI 65536
SF 400.1300628 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


160.848
160.453
158.491
144.332
141.957
134.692
134.636
134.075
133.160
132.856
132.273
131.362
129.207
129.140
129.080
128.859
128.821
128.641
128.086
127.825
127.747
126.935
126.574
126.314
126.193
126.106
126.040
125.994
125.147
124.993
79.051
77.433
77.115
76.797
N
N
N
180
160
140
120
100
80
60
40
20
ppm
BRUKER
NAME 2019-04-01 tyut-lx
EXPNO 10
PROCNO 1
Date_ 20190404
Time 0.53
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 185.43
DW 20.800 use
DE 6.50 use
TE 297.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 =======
SFO1 100.6228293 MHz
NUC1 13C
P1 10.27 use
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC ppm 1.40

7qa


7.412
7.376
7.356
7.269
7.264
7.248
7.243
7.202
7.198
7.143
7.138
7.136
7.126
7.118
6.978
6.972
6.967
6.963
6.955
6.327
7.65 ppm
7.40 ppm
7.15 ppm
6.98 6.96 ppm
N
N
N
Cl
Cl
Cl
Cl
8
7
6
5
4
3
2
1
ppm
3.163
4.162
1.021
1.167
0.939
4.130
2.121
1.000
BRUKER
NAME 2018041201
EXPNO 10
PROCNO 1
Date_ 20180413
Time 0.28
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 34.32
DW 62.400 usec
DE 6.50 usec
TE 297.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.70 usec
SI 65536
SF 400.1300149 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER

NAME	2018041201
EXPNO	11
PROCNO	1
Date_	20180413
Time	1.27
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	185.43
DW	20.800 usec
DE	6.50 usec
TE	298.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228293 MHz
NUC1	13C
P1	9.50 usec
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40