Supporting Information

Transition-metal-free selective pyrimidines and pyridines formation from aromatic ketones, aldehydes and ammonium salts

Jinjin Chen[a], Huanxin Meng[a], Feng Zhang[a,b*], Fuhong Xiao[a], and Guo-Jun Deng[a*]

[a] Key Laboratory for Green Organic Synthesis and Application of Hunan Province, Key Laboratory of Environmentally Friendly Chemistry and Application of Ministry of Education, College of Chemistry, Xiangtan University, Xiangtan 411105, China. E-mail: gjdeng@xtu.edu.cn

[b] College of Science, Hunan Agricultural University, Changsha, 410128, China. E-mail: zhangf@iccas.ac.cn

Table of Contents

1. General information

All reactions were carried out under an atmosphere of oxygen unless otherwise noted. Column chromatography was performed using silica gel (200-300 mesh). ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker-AV (400 and 100 MHz, respectively) instrument internally referenced to tetramethylsilane (TMS) or chloroform. Mass spectra was measured on Agilent 5975 GC-MS instrument (EI). High-resolution mass spectra (HRMS) was conducted using electrospraying ionization (ESI) and was performed on a Thermo Scientific LTQ Orbitrap XL at Keecloud (Shanghai) Biotechnology co. LTD. The structure of known compounds were further corroborated by comparing their ^{1}H NMR, ^{13}C NMR data and MS data with those of literature. All reagents were obtained from commercial suppliers and used without further purification unless otherwise noted.

2. General procedure for the synthesis of pyrimidines

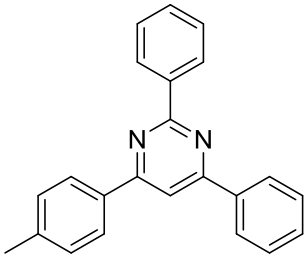
A 10 mL oven-dried reaction vessel was charged with aromatic ketones (0.2 mmol), aromatic aldehydes (0.6 mmol), ammonium acetate (0.6 mmol), $NaIO_4$ (0.08 mmol), DMSO (0.1 mmol) and chlorobenzene (0.8 mL). The reaction vessel was purged with oxygen for three times and stirred at 130 ^{o}C for 10 h. After cooling to room temperature, the volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel to give the products.

3. General procedure for the synthesis of pyridines

A 10 mL oven-dried reaction vessel was charged with aromatic ketones (0.6 mmol), aromatic aldehydes (0.2 mmol), ammonium iodide (0.4 mmol), DMSO (0.6 mmol) and chlorobenzene (0.8 mL). The reaction vessel was purged with oxygen for three times and stirred at 130 ^{o}C for 12 h. After cooling to room temperature, the volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel to give the products.

4. Characterization of products

2,4-Diphenyl-6-(*p*-tolyl)pyrimidine (3aa, CAS: 71103-76-9)[1]

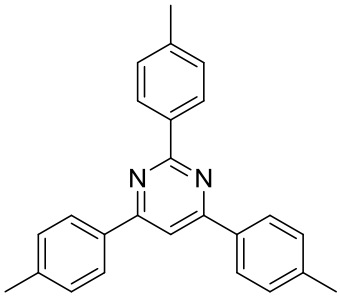


The reaction was conducted with 1-(*p*-tolyl)ethan-1-one (26.7 μL, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO

(7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3aa** as white solid; yield: 50.2 mg (78%), mp 143-146 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.72 (d, *J* = 6.3 Hz, 2H), 8.28 (d, *J* = 8.0 Hz, 2H), 8.20 (d, *J* = 8.2 Hz, 2H), 7.98 (s, 1H), 7.57-7.51(m, 6H), 7.36 (d, *J* = 8.0 Hz, 2H), 2.45 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 164.6, 164.5, 164.4, 141.1, 138.2, 137.6, 134.6, 130.7, 130.5, 129.6, 128.8, 128.4, 128.4, 127.2, 127.1, 109.9, 21.5.

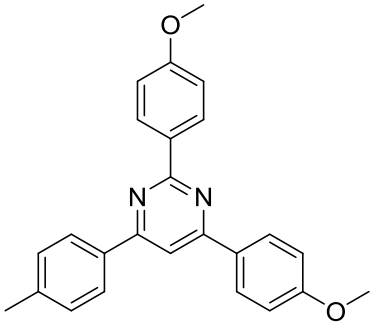
2,4,6-Tri-*p*-tolylpyrimidine (3ab)



The reaction was conducted with 1-(*p*-tolyl)ethan-1-one (26.7 μL, 0.2 mmol), 4-methylbenzaldehyde (71.0 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to give **3ab** as white solid; yield: 56.6 mg (81%), mp 238-240 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.61 (d, *J* = 8.0 Hz, 2H), 8.18 (d, *J* = 8.0 Hz, 4H), 7.93 (s, 1H), 7.34 (t, *J* = 7.9 Hz, 6H), 2.45 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 164.4, 164.4, 140.9, 140.6, 135.6, 134.9, 129.6, 129.1, 128.4, 127.1, 109.3, 21.5, 21.5; HRMS (ESI): *m/z* calcd for $C_{25}H_{23}N_2^+$ $[M+H]^+$ 351.1856, found 351.1855.

2,4-Bis(4-methoxyphenyl)-6-(*p*-tolyl)pyrimidine (3ac)

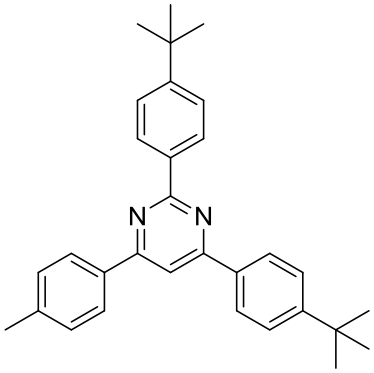


The reaction was conducted with 1-(*p*-tolyl)ethan-1-one (26.7 μL, 0.2 mmol), 4-methylbenzaldehyde (72.9 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column

chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to give **3ac** as white solid; yield: 53.5 mg (70%), mp 157-159 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.67 (d, *J* = 8.2 Hz, 2H), 8.25 (d, *J* = 8.3 Hz, 2H), 8.17 (d, *J* = 7.7 Hz, 2H), 7.86 (s, 1H), 7.35 (d, *J* = 7.8 Hz, 2H), 7.05 (t, *J* = 7.0 Hz, 4H), 3.91 (s, 6H), 2.45 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 164.2, 164.0, 163.9, 161.7, 161.6, 140.9, 134.9, 131.1, 130.1, 130.0, 129.5, 128.7, 127.1, 114.1, 113.6, 108.4, 55.4, 55.3, 21.6; HRMS (ESI): *m/z* calcd for $C_{25}H_{23}N_2O_2^+$ $[M+H]^+$ 383.1754, found 383.1752.

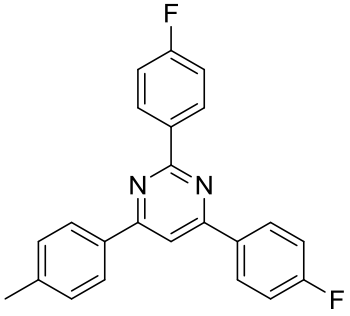
2,4-Bis(4-(*tert*-butyl)phenyl)-6-(*p*-tolyl)pyrimidine (3ad)



The reaction was conducted with 1-(*p*-tolyl)ethan-1-one (26.7 μL, 0.2 mmol), 4-(*tert*-butyl)benzaldehyde (100.3 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3ad** as white solid; yield: 53.5 mg (70%), mp 175-178 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.63 (d, *J* = 8.5 Hz, 2H), 8.20 (t, *J* = 8.9 Hz, 4H), 7.95 (s, 1H), 7.57 (t, *J* = 8.5 Hz, 4H), 7.36 (d, *J* = 8.0 Hz, 2H), 2.46 (s, 3H), 1.40 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 164.4, 164.4, 164.3, 154.0, 153.7, 140.9, 135.6, 134.9, 134.8, 129.5, 128.2, 127.1, 127.0, 125.8, 125.3, 109.4, 34.8, 34.8, 31.3, 31.2, 21.5; HRMS (ESI): *m/z* calcd for $C_{31}H_{35}N_2^+$ $[M+H]^+$ 435.2795, found 435.2798.

2,4-Bis(4-fluorophenyl)-6-(*p*-tolyl)pyrimidine (3ae)

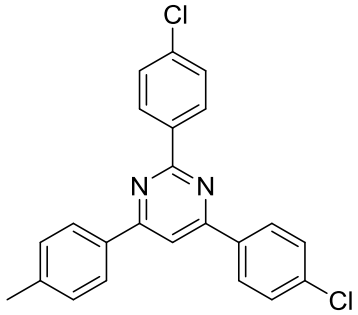


The reaction was conducted with 1-(*p*-tolyl)ethan-1-one (26.7 μL, 0.2 mmol), 4-fluorobenzaldehyde (64.4 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2

mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3ae** as white solid; yield: 54.4 mg (76%), mp 193-196 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.70 (dd, *J* = 8.8, 5.7 Hz, 2H), 8.26 (dd, *J* = 8.8, 5.4 Hz, 2H), 8.16 (d, *J* = 8.1 Hz, 2H), 7.91 (s, 1H), 7.35 (d, *J* = 8.0 Hz, 2H), 7.25-7.15 (m, 4H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 164.9, 164.8 (d, *J* = 248.7 Hz), 164.6 (d, *J* = 249.4 Hz), 163.6, 141.32, 134.60, 134.37, 133.72, 130.6 (d, *J* = 8.5 Hz), 129.7, 129.3 (d, *J* = 8.7 Hz), 127.2, 115.9 (d, *J* = 21.6 Hz), 115.3 (d, *J* = 21.5 Hz), 109.4, 21.4; HRMS (ESI): *m/z* calcd for $C_{23}H_{17}F_2N_2^+$ $[M+H]^+$ 359.1354, found 359.1358.

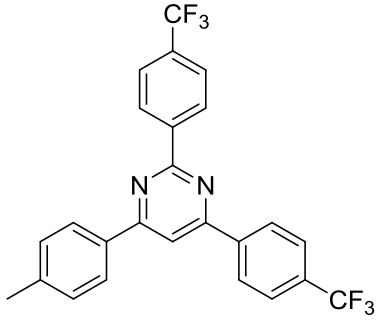
2,4-Bis(4-chlorophenyl)-6-(*p*-tolyl)pyrimidine (3af)



The reaction was conducted with 1-(*p*-tolyl)ethan-1-one (26.7 μL, 0.2 mmol), 4-chlorobenzaldehyde (84.3 mg, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to give **3af** as white solid; yield: 49.6 mg (64%), mp 146-148 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.63 (d, *J* = 8.6 Hz, 2H), 8.20 (d, *J* = 8.6 Hz, 2H), 8.16 (d, *J* = 8.1 Hz, 2H), 7.94 (s, 1H), 7.52 (d, *J* = 8.6 Hz, 2H), 7.49 (d, *J* = 8.6 Hz, 2H), 7.36 (d, *J* = 8.0 Hz, 2H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 165.0, 163.5, 163.4, 141.5, 137.0, 136.9, 136.5, 135.9, 134.3, 129.8, 129.7, 129.2, 128.7, 128.5, 127.2, 109.8, 21.5; HRMS (ESI): *m/z* calcd for $C_{23}H_{17}Cl_2N_2^+$ $[M+H]^+$ 391.0763, found 391.0768.

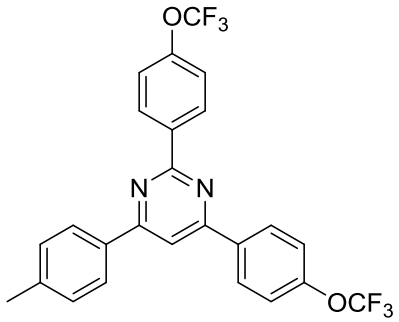
4-(*p*-Tolyl)-2,6-bis(4-(trifluoromethyl)phenyl)pyrimidine (3ag)



The reaction was conducted with 1-(*p*-tolyl)ethan-1-one (26.7 μL, 0.2 mmol), 4-(trifluoromethyl)benzaldehyde (81.9 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3ag** as white solid; yield: 45.3 mg (49%), mp 211-213 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.80 (d, *J* = 8.2 Hz, 2H), 8.37 (d, *J* = 8.1 Hz, 2H), 8.19 (d, *J* = 8.1 Hz, 2H), 8.04 (s, 1H), 7.82 (d, *J* = 8.3 Hz, 2H), 7.79 (d, *J* = 8.3 Hz, 2H), 7.38 (d, *J* = 8.1 Hz, 2H), 2.48 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 165.2, 163.2, 141.8, 141.1, 140.5, 133.9, 132.5 (q, *J* = 32.4 Hz), 132.3 (q, *J* = 32.1 Hz), 129.8, 128.7, 127.5, 127.2, 125.8 (q, *J* = 3.6 Hz), 125.3 (q, *J* = 3.7 Hz), 124.2 (q, *J* = 270.6 Hz), 123.9 (q, *J* = 270.7 Hz), 110.7, 21.5; HRMS (ESI): *m/z* calcd for $C_{25}H_{17}F_6N_2^+$ $[M+H]^+$ 459.1290, found 459.1296.

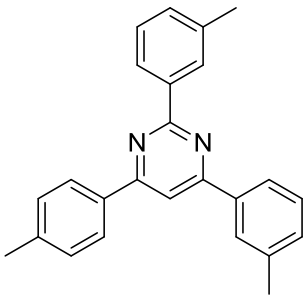
4-(*p*-Tolyl)-2,6-bis(4-(trifluoromethoxy)phenyl)pyrimidine (3ah)



The reaction was conducted with 1-(*p*-tolyl)ethan-1-one (26.7 μL, 0.2 mmol), 4-(trifluoromethoxy)benzaldehyde (85.7 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3ah** as white solid; yield: 41.2 mg (42%), mp 98-100 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.73 (d, *J* = 8.8 Hz, 2H), 8.30 (d, *J* = 8.7 Hz, 2H), 8.17 (d, *J* = 8.0 Hz, 2H), 7.96 (s, 1H), 7.42-7.35 (m, 6H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 164.9, 163.3, 163.2, 151.2, 151.2, 141.6, 136.5, 135.9, 134.2, 130.1, 129.7, 128.8, 127.1, 121.0, 120.5, 120.5 (q, *J* = 257.2 Hz), 120.4 (q, *J* = 256.4 Hz), 109.8, 21.5; HRMS (ESI): *m/z* calcd for $C_{25}H_{17}F_6N_2O_2^+$ $[M+H]^+$ 491.1189, found 491.1186.

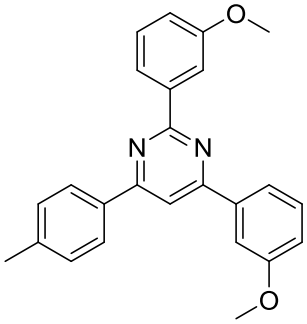
2,4-Di-*m*-tolyl-6-(*p*-tolyl)pyrimidine (3ai)



The reaction was conducted with 1-(*p*-tolyl)ethan-1-one (26.7 μL, 0.2 mmol), 3-methylbenzaldehyde (70.7 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to give **3ai** as white solid; yield: 51.5 mg (74%), mp 168-170 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.52 (d, *J* = 6.1 Hz, 2H), 8.20 (d, *J* = 8.1 Hz, 2H), 8.10-8.05 (m, 2H), 7.96 (s, 1H), 7.47-7.41 (m, 2H), 7.38-7.30 (m, 4H), 2.51 (s, 6H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 164.8, 164.8, 164.5, 141.1, 138.6, 138.2, 138.0, 137.6, 134.7, 131.4, 131.3, 129.6, 128.9, 128.8, 128.3, 127.9, 127.2, 125.7, 124.4, 110.0, 21.6, 21.5; HRMS (ESI): *m/z* calcd for $C_{25}H_{23}N_2^+$ $[M+H]^+$ 351.1856, found 351.1855.

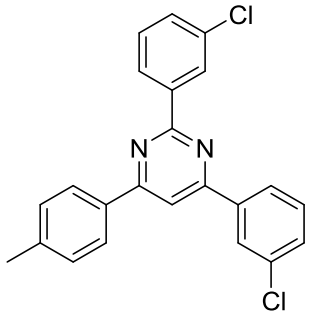
2,4-Bis(3-methoxyphenyl)-6-(*p*-tolyl)pyrimidine (3aj)



The reaction was conducted with 1-(*p*-tolyl)ethan-1-one (26.7 μL, 0.2 mmol), 3-methoxybenzaldehyde (73.1 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 20:1) to give **3aj** as white solid; yield: 47.9 mg (63%), mp 132-135 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.33 (d, *J* = 7.8 Hz, 1H), 8.28 (s, 1H), 8.19 (d, *J* = 8.2 Hz, 2H), 7.97 (s, 1H), 7.87 (s, 1H), 7.82 (d, *J* = 7.7 Hz, 1H), 7.49-7.44 (m, 2H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.10-7.06 (m, 2H), 3.96 (s, 3H), 3.94 (s, 3H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 164.6, 164.3, 164.1, 160.1, 159.8, 141.2, 139.6, 139.0, 134.6, 129.9, 129.6, 129.4, 127.2, 121.0, 119.6, 116.4, 116.2, 113.5, 112.7, 110.2, 55.4, 55.4, 21.5; HRMS (ESI): *m/z* calcd for $C_{25}H_{23}N_2O_2^+$ $[M+H]^+$ 383.1754, found 383.1752.

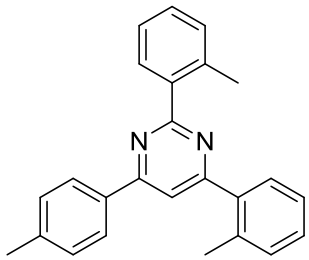
2,4-Bis(3-chlorophenyl)-6-(*p*-tolyl)pyrimidine (3ak)



The reaction was conducted with 1-(*p*-tolyl)ethan-1-one (26.7 μL, 0.2 mmol), 3-chlorobenzaldehyde (68.0 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to give **3ak** as white solid; yield: 46.8 mg (60%), mp 107-109 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.66 (s, 1H), 8.58 (d, *J* = 6.6 Hz, 1H), 8.23 (s, 1H), 8.17 (d, *J* = 8.1 Hz, 2H), 8.13 (d, *J* = 6.7 Hz, 1H), 7.94 (s, 1H), 7.53-7.43 (m, 4H), 7.37 (d, *J* = 8.1 Hz, 2H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 164.8, 163.0, 141.5, 139.7, 139.0, 135.0, 134.5, 133.9, 130.7, 130.6, 130.1, 129.6, 128.4, 127.2, 127.1, 126.5, 125.3, 110.1, 21.49; HRMS (ESI): *m/z* calcd for $C_{23}H_{17}Cl_2N_2^+$ $[M+H]^+$ 391.0763, found 391.0768.

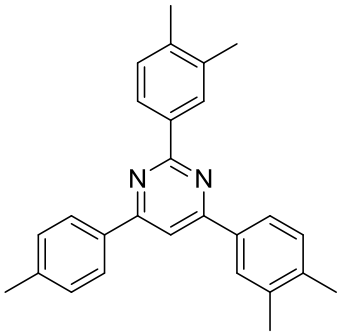
2,4-Di-*o*-tolyl-6-(*p*-tolyl)pyrimidine (3al)



The reaction was conducted with 1-(*p*-tolyl)ethan-1-one (26.7 μL, 0.2 mmol), 2-methylbenzaldehyde (69.4 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to give **3al** as white solid; yield: 31.6 mg (45%), mp 123-125 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.13 (d, *J* = 7.8 Hz, 2H), 8.02 (d, *J* = 7.3 Hz, 1H), 7.72 (s, 1H), 7.56 (d, *J* = 7.4 Hz, 1H), 7.40-7.33 (m, 8H), 2.72 (s, 3H), 2.54 (s, 3H), 2.44 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 167.8, 167.1, 163.7, 141.2, 138.7, 138.6, 137.5, 136.1, 134.4, 131.2, 131.1, 130.8, 129.7, 129.6, 129.2, 127.2, 126.1, 125.8, 113.4, 21.7, 21.4, 20.6; HRMS (ESI): *m/z* calcd for $C_{25}H_{23}N_2^+$ $[M+H]^+$ 351.1856, found 351.1855.

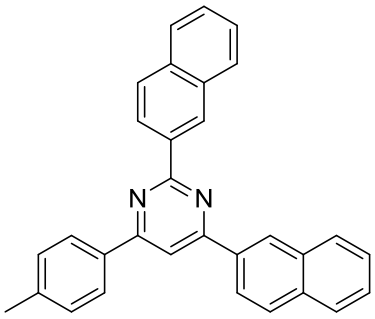
2,4-Bis(3,4-dimethylphenyl)-6-(*p*-tolyl)pyrimidine (3am)



The reaction was conducted with 1-(*p*-tolyl)ethan-1-one (26.7 μL, 0.2 mmol), 3,4-dimethylbenzaldehyde (79.6 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3am** as white solid; yield: 30.9 mg (41%), mp 196-198 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.47 (s, 1H), 8.44 (d, *J* = 7.9 Hz, 1H), 8.19 (d, *J* = 8.1 Hz, 2H), 8.05 (s, 1H), 8.00 (d, *J* = 7.8 Hz, 1H), 7.92 (s, 1H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.30 (t, *J* = 7.2 Hz, 2H), 2.46 (s, 3H), 2.41 (s, 6H), 2.36 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 164.6, 164.5, 164.3, 140.8, 139.6, 139.3, 137.1, 136.5, 136.0, 135.3, 135.0, 130.1, 129.7, 129.5, 129.4, 128.3, 127.1, 126.0, 124.7, 109.4, 21.5, 20.0, 20.0, 19.9, 19.8; HRMS (ESI): *m/z* calcd for $C_{27}H_{27}N_2^+$ $[M+H]^+$ 379.2169, found 379.2168.

2,4-Di(naphthalen-2-yl)-6-(*p*-tolyl)pyrimidine (3an)

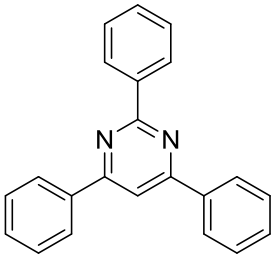


The reaction was conducted with 1-(*p*-tolyl)ethan-1-one (26.7 μL, 0.2 mmol), 2-naphthaldehyde (93.7 mg, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to give **3an** as white solid; yield: 57.4 mg (68%), mp 219-222 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 9.27 (s, 1H), 8.86 (d, *J* = 8.6 Hz, 1H), 8.80 (s, 1H), 8.43 (d, *J* = 8.5 Hz, 1H), 8.27 (d, *J* = 8.1 Hz, 2H), 8.13 (s, 1H), 8.10-8.00 (m, 4H), 7.94-7.91 (m, 2H), 7.60-7.53 (m, 4H), 7.40 (d, *J* = 7.9 Hz, 2H), 2.48 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ

164.8, 164.6, 164.5, 141.2, 135.7, 135.0, 134.7, 134.6, 133.4, 133.3, 129.7, 129.4, 129.3, 129.0, 128.7, 128.1, 128.0, 127.8, 127.7, 127.4, 127.3, 126.9, 126.6, 126.1, 125.6, 125.2, 124.3, 110.3, 21.5; HRMS (ESI): *m/z* calcd for $C_{31}H_{23}N_2^+$ $[M+H]^+$ 423.1856, found 423.1853.

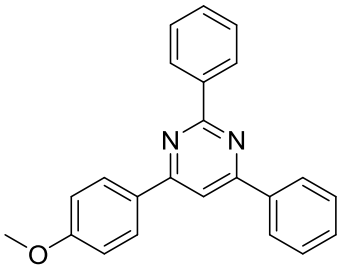
2,4,6-Triphenylpyrimidine (3ba, CAS: 1666-86-0)[1]



The reaction was conducted with acetophenone (23.4 μL, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3ba** as white solid; yield: 45.7 mg (74%), mp 190-191 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.74 (d, *J* = 7.0 Hz, 2H), 8.30 (d, *J* = 6.7 Hz, 4H), 8.02 (s, 1H), 7.56 (t, *J* = 6.7 Hz, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 164.7, 164.4, 138.1, 137.4, 130.8, 130.6, 128.9, 128.9, 128.4, 127.3, 110.3.

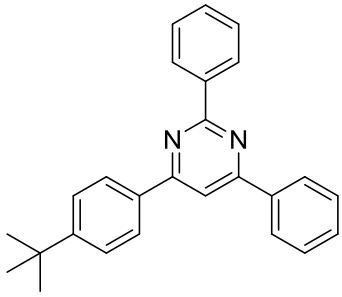
4-(4-Methoxyphenyl)-2,6-diphenylpyrimidine (3ca, CAS: 67073-24-9)[2]



The reaction was conducted with 1-(4-methoxyphenyl)ethan-1-one (30.0 mg, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to give **3ca** as white solid; yield: 37.4 mg (55%), mp 139-140 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.72 (d, *J* = 6.5 Hz, 2H), 8.28 (d, *J* = 7.9 Hz, 4H), 7.95 (s, 1H), 7.54 (t, *J* = 7.7 Hz, 6H), 7.07 (d, *J* = 8.4 Hz, 2H), 3.91 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 164.4, 164.3, 164.2, 161.9, 138.3, 137.7, 130.6, 130.5, 129.9, 128.8, 128.7, 128.4, 128.4, 127.2, 114.2, 109.4, 55.4.

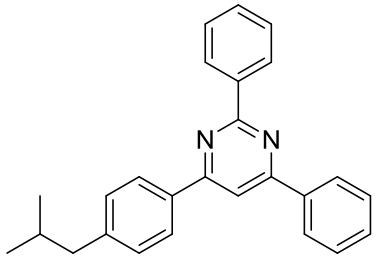
4-(4-(*tert*-Butyl)phenyl)-2,6-diphenylpyrimidine (3da)[2]



The reaction was conducted with 1-(4-(*tert*-butyl)phenyl)ethan-1-one (36.6 μL, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3da** as white solid; yield: 41.7 mg (57%), mp 132-134 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.73 (d, *J* = 7.7 Hz, 2H), 8.29 (d, *J* = 7.7 Hz, 2H), 8.23 (d, *J* = 7.7 Hz, 2H), 8.00 (s, 1H), 7.56 (q, *J* = 9.2 Hz, 8H), 1.40 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 164.7, 164.5, 164.4, 154.2, 138.2, 137.6, 134.7, 130.7, 130.5, 128.9, 128.4, 128.4, 127.2, 127.0, 125.9, 110.0, 34.9, 31.2.

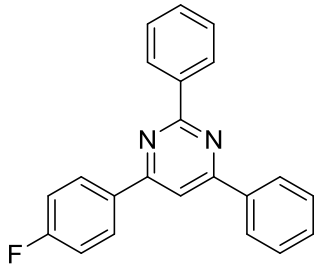
4-(4-Isobutylphenyl)-2,6-diphenylpyrimidine (3ea)



The reaction was conducted with 1-(4-isobutylphenyl)ethan-1-one (37.0 μL, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3ea** as white solid; yield: 47.3 mg (65%), mp 88-91 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.73 (d, *J* = 7.3 Hz, 2H), 8.29 (d, *J* = 7.1 Hz, 2H), 8.21 (d, *J* = 7.6 Hz, 2H), 8.00 (s, 1H), 7.54 (t, *J* = 6.9 Hz, 6H), 7.33 (d, *J* = 7.7 Hz, 2H), 2.58 (d, *J* = 7.1 Hz, 2H), 1.99-1.89 (m, 1H), 0.95 (d, *J* = 6.5 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 164.7, 164.4, 164.3, 144.9, 138.2, 137.5, 134.9, 130.6, 130.5, 129.6, 128.8, 128.4, 128.4, 127.2, 127.0, 109.9, 45.2, 30.2, 22.3; HRMS (ESI): *m/z* calcd for $C_{26}H_{25}N_2^+$ $[M+H]^+$ 365.2012, found 365.2012.

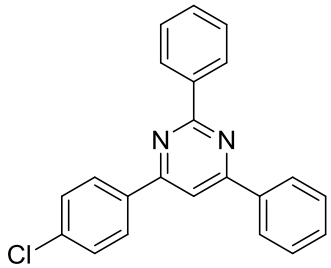
4-(4-Fluorophenyl)-2,6-diphenylpyrimidine (3fa)[1]



The reaction was conducted with 1-(4-fluorophenyl)ethan-1-one (24.2 μL, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3fa** as white solid; yield: 51.0 mg (78%), mp 166-167 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.71 (d, *J* = 7.9 Hz, 2H), 8.40-8.17 (m, 4H), 7.96 (s, 1H), 7.66-7.47 (m, 6H), 7.29-7.19 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ164.8, 164.6 (d, *J* = 249.6 Hz),164.4, 163.30, 138.0, 137.4, 133.6, 130.8 (d, *J* = 13.0 Hz), 129.3(d, *J* = 8.4 Hz), 128.9, 128.6, 128.4, 128.4, 127.2, 115.9 (d, *J* = 21.7 Hz), 109.8.

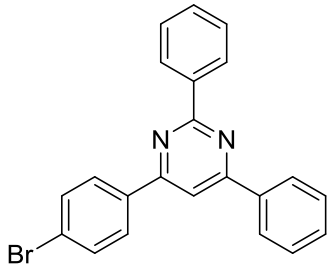
4-(4-Chlorophenyl)-2,6-diphenylpyrimidine (3ga)[2]



The reaction was conducted with 1-(4-chlorophenyl)ethan-1-one (25.9 μL, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3ga** as white solid; yield: 56.9 mg (83%), mp 165-166 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.71 (d, *J* = 7.9 Hz, 2H), 8.28 (d, *J* = 7.8 Hz, 2H), 8.24 (d, *J* = 8.6 Hz, 2H), 7.97 (s, 1H), 7.59-7.49 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 164.8, 164.4, 163.3, 137.9, 137.2, 136.9, 135.8, 130.8, 130.7, 129.0, 128.9, 128.5, 128.4, 128.5, 127.2, 109.8.

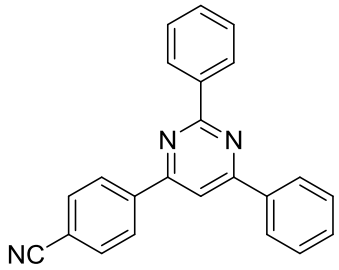
4-(4-Bromophenyl)-2,6-diphenylpyrimidine (3ha, CAS: 58536-46-2)[3]



The reaction was conducted with 1-(4-bromophenyl)ethan-1-one (39.8 mg, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3ha** as white solid; yield: 62.3 mg (81%), mp 169-171 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.71 (d, *J* = 7.9 Hz, 2H), 8.28 (d, *J* = 7.8 Hz, 2H), 8.17 (d, *J* = 8.4 Hz, 2H), 7.97 (s, 1H), 7.69 (d, *J* = 8.5 Hz, 2H), 7.60-7.50 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 164.9, 164.5, 163.5, 137.9, 137.2, 136.3, 132.1, 130.9, 130.8, 128.9, 128.7, 128.5, 128.4, 127.2, 125.4, 109.9.

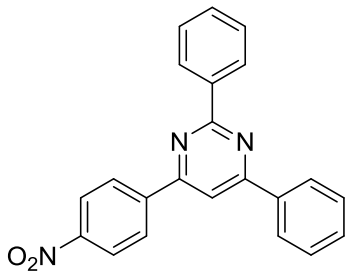
4-(2,6-Diphenylpyrimidin-4-yl)benzonitrile (3ia)



The reaction was conducted with 4-acetylbenzonitrile (29.0 mg, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to give **3ia** as white solid; yield: 41.3 mg (62%), mp 181-183 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.70 (d, *J* = 7.7 Hz, 2H), 8.39 (d, *J* = 8.4 Hz, 2H), 8.28 (d, *J* = 6.0 Hz, 2H), 8.01 (s, 1H), 7.85 (d, *J* = 8.4 Hz, 2H), 7.61-7.52 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 165.2, 164.6, 162.4, 141.5, 137.5, 136.9, 132.6, 131.1, 131.0, 129.0, 128.5, 128.4, 127.7, 127.2, 118.5, 114.0, 110.4; HRMS (ESI): *m/z* calcd for $C_{23}H_{16}N_3^+$ $[M+H]^+$ 334.1339, found 334.1338.

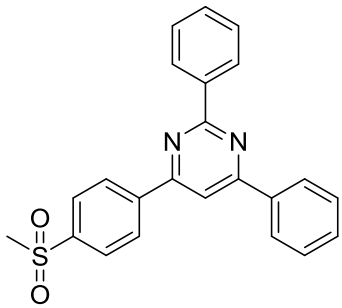
4-(4-Nitrophenyl)-2,6-diphenylpyrimidine (3ja, CAS: 13573-34-7)[4]



The reaction was conducted with 1-(4-nitrophenyl)ethan-1-one (33.0 mg, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to give **3ja** as yellow solid; yield: 30.3 mg (43%), mp 216-218 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.72 (d, *J* = 5.5 Hz, 2H), 8.51-8.39 (m, 4H), 8.31 (d, *J* = 5.9 Hz, 2H), 8.08 (s, 1H), 7.58 (d, *J* = 10.5 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 165.5, 164.9, 162.3, 149.2, 143.4, 137.5, 136.9, 131.2, 131.1, 129.0, 128.6, 128.5, 128.2, 127.3, 124.1, 110.8.

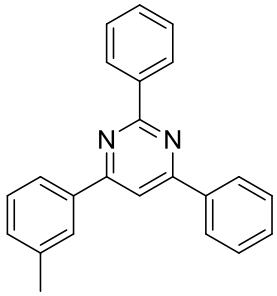
4-(4-(Methylsulfonyl)phenyl)-2,6-diphenylpyrimidine (3ka)



The reaction was conducted with 1-(4-(methylsulfonyl)phenyl)ethan-1-one (39.7 mg, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 4:1) to give **3ka** as yellow solid; yield: 28.1 mg (36%), mp 201-203 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.72 (d, *J* = 7.3 Hz, 2H), 8.47 (d, *J* = 7.2 Hz, 2H), 8.30 (d, *J* = 5.0 Hz, 2H), 8.14 (d, *J* = 7.3 Hz, 2H), 8.05 (s, 1H), 7.57 (d, *J* = 10.6 Hz, 6H), 3.14 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 165.4, 164.8, 162.7, 142.7, 142.0, 137.6, 136.9, 131.2, 131.0, 129.0, 128.5, 128.4, 128.2, 128.0, 127.3, 110.8, 44.5; HRMS (ESI): *m/z* calcd for $C_{23}H_{19}N_2O_2S^+$ $[M+H]^+$ 387.1162, found 387.1161.

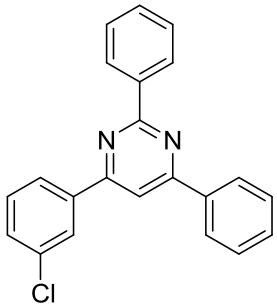
2,4-Diphenyl-6-(*m*-tolyl)pyrimidine (3la)[5]



The reaction was conducted with 1-(*m*-tolyl)ethan-1-one (27.2 μL, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3la** as white solid; yield: 41.5 mg (64%), mp 127-129 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.73 (d, *J* = 8.0 Hz, 2H), 8.30 (d, *J* = 8.0 Hz, 2H), 8.10 (s, 1H), 8.07 (d, *J* = 7.8 Hz, 1H), 8.01 (s, 1H), 7.58-7.52 (m, 6H), 7.45 (t, *J* = 7.6 Hz, 1H), 7.36 (d, *J* = 7.5 Hz, 1H), 2.51 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 164.8, 164.5, 164.4, 138.5, 138.1, 137.5, 137.4, 131.5, 130.7, 130.5, 128.8, 128.7, 128.4, 128.4, 127.8, 127.2, 124.4, 110.3, 21.6.

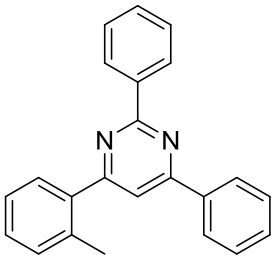
4-(3-Chlorophenyl)-2,6-diphenylpyrimidine (3ma)[3]



The reaction was conducted with 1-(3-chlorophenyl)ethan-1-one (26.0 μL, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3ma** as white solid; yield: 59.3 mg (87%), mp 152-154 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.72 (d, *J* = 7.9 Hz, 2H), 8.53 (s, 1H), 8.48 (d, *J* = 7.8 Hz, 1H), 8.31 (d, *J* = 7.9 Hz, 2H), 8.03 (s, 1H), 7.80 (d, *J* = 7.7 Hz, 1H), 7.70 (t, *J* = 7.8 Hz, 1H), 7.60-7.54 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 165.1, 164.6, 163.1, 138.3, 137.7, 137.1, 131.0, 130.9, 130.4, 129.4, 128.9, 128.5, 128.5, 127.3, 127.2, 124.0, 124.0, 110.2.

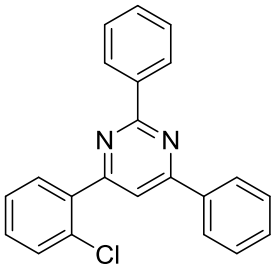
2,4-Diphenyl-6-(*o*-tolyl)pyrimidine (3na)[5]



The reaction was conducted with 1-(*o*-tolyl)ethan-1-one (26.2 μL, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3na** as yellow liquid; yield: 25.2 mg (39%).

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.67 (d, *J* = 7.9 Hz, 2H), 8.28 (d, *J* = 7.9 Hz, 2H), 7.74 (s, 1H), 7.62-7.50 (m, 7H), 7.42-7.33 (m, 3H), 2.58 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 168.1, 164.1, 164.0, 138.6, 138.1, 137.3, 136.5, 131.2, 130.8, 130.6, 129.6, 129.4, 128.9, 128.4, 127.2, 126.1, 114.3, 20.7.

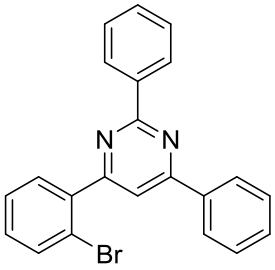
4-(2-Chlorophenyl)-2,6-diphenylpyrimidine (3oa)[3]



The reaction was conducted with 1-(2-chlorophenyl)ethan-1-one (30.9 mg, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3oa** as white solid; yield: 36.6 mg (53%), mp 124-126 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.67 (d, *J* = 8.0 Hz, 2H), 8.28 (d, *J* = 7.9 Hz, 2H), 8.02 (s, 1H), 7.85 (d, *J* = 7.7 Hz, 1H), 7.54 (dd, *J* = 13.4, 5.7 Hz, 7H), 7.48-7.41 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 164.6, 164.6, 163.8, 137.9, 137.5, 137.2, 132.4, 131.7, 130.9, 130.7, 130.6, 130.4, 128.9, 128.4, 128.4, 127.3, 127.2, 115.1.

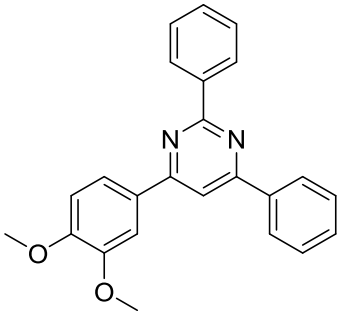
4-(2-Bromophenyl)-2,6-diphenylpyrimidine (3pa)



The reaction was conducted with 1-(2-bromophenyl)ethan-1-one (27.0 μL, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3pa** as white solid; yield: 31.8 mg (41%), mp 140-143 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.68 (d, *J* = 7.8 Hz, 2H), 8.29 (d, *J* = 7.8 Hz, 2H), 7.97 (s, 1H), 7.75 (d, *J* = 7.9 Hz, 2H), 7.58-7.47 (m, 7H), 7.35 (t, *J* = 7.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 166.0, 164.5, 163.8, 139.5, 137.9, 137.2, 133.7, 131.6, 130.9, 130.7, 130.7, 128.9, 128.5, 128.5, 127.7, 127.3, 121.6, 115.0; HRMS (ESI): *m/z* calcd for $C_{22}H_{16}BrN_2^+$ $[M+H]^+$ 387.0491, found 387.0490.

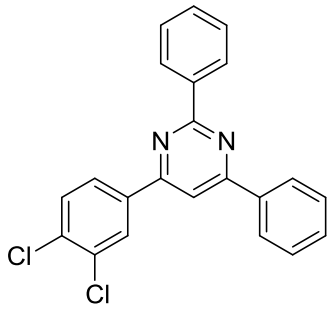
4-(3,4-Dimethoxyphenyl)-2,6-diphenylpyrimidine (3qa)



The reaction was conducted with 1-(3,4-dimethoxyphenyl)ethan-1-one (36.0 mg, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 10:1) to give **3qa** as yellow solid; yield: 37.0 mg (50%), mp 104-107 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.71 (d, *J* = 7.8 Hz, 2H), 8.29 (d, *J* = 7.7 Hz, 2H), 7.95 (s, 2H), 7.84 (d, *J* = 8.4 Hz, 1H), 7.55 (t, *J* = 7.5 Hz, 6H), 7.02 (d, *J* = 8.4 Hz, 1H), 4.07 (s, 3H), 3.98 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 164.3, 164.2, 164.1, 151.4, 149.2, 138.1, 137.5, 130.6, 130.5, 130.1, 128.8, 128.4, 128.3, 127.2, 120.2, 110.9, 109.9, 109.5, 56.0, 55.9; HRMS (ESI): *m/z* calcd for $C_{24}H_{21}N_2O_2^+$ $[M+H]^+$ 369.1598, found 369.1597.

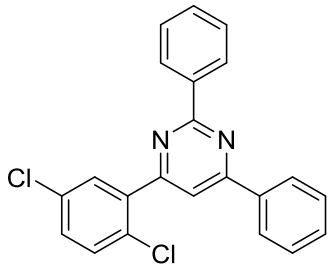
4-(3,4-Dichlorophenyl)-2,6-diphenylpyrimidine (3ra)



The reaction was conducted with 1-(3,4-dichlorophenyl)ethan-1-one (37.8 mg, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3ra** as white solid; yield: 55.0 mg (73%), mp 134-136 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.69 (d, *J* = 5.1 Hz, 2H), 8.39 (s, 1H), 8.28 (d, *J* = 3.9 Hz, 2H), 8.10 (d, *J* = 8.5 Hz, 1H), 7.94 (s, 1H), 7.62 (d, *J* = 8.3 Hz, 1H), 7.55 (d, *J* = 8.1 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.1, 164.6, 162.2, 137.6, 137.3, 137.0, 134.9, 133.3, 131.0, 130.9, 130.8, 129.1, 128.9, 128.5, 128.4, 127.3, 126.2, 109.9; HRMS (ESI): *m/z* calcd for $C_{22}H_{15}Cl_2N_2^+$ $[M+H]^+$ 377.0607, found 377.0606.

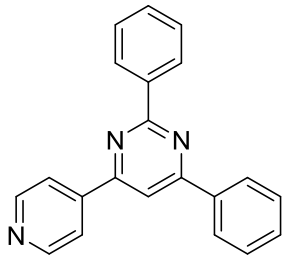
4-(2,5-Dichlorophenyl)-2,6-diphenylpyrimidine (3sa)



The reaction was conducted with 1-(2,5-dichlorophenyl)ethan-1-one (28.8 μL, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3sa** as white solid; yield: 42.2 mg (56%), mp 115-118 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.67 (d, *J* = 7.8 Hz, 2H), 8.28 (d, *J* = 7.7 Hz, 2H), 8.01 (s, 1H), 7.85 (s, 1H), 7.57-7.53 (m, 6H), 7.49 (d, *J* = 8.6 Hz, 1H), 7.41 (d, *J* = 8.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 164.7, 164.1, 163.3, 138.8, 137.6, 137.0, 133.2, 131.6, 131.5, 131.0, 130.9, 130.7, 130.6, 129.0, 128.5, 128.4, 127.4, 114.9; HRMS (ESI): *m/z* calcd for $C_{22}H_{15}Cl_2N_2^+$ $[M+H]^+$ 377.0607, found 377.0606.

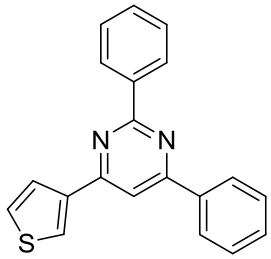
2,4-Diphenyl-6-(pyridin-4-yl)pyrimidine (3ta)[2]



The reaction was conducted with 4-acetylpyridine (22.1 μL, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to give **3ta** as yellow solid; yield: 36.9 mg (60%), mp 214-216 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.84 (d, *J* = 6.1 Hz, 2H), 8.72 (d, *J* = 7.8 Hz, 2H), 8.30 (d, *J* = 7.6 Hz, 2H), 8.14 (d, *J* = 6.1 Hz, 2H), 8.04 (s, 1H), 7.57 (dd, *J* = 9.1, 5.4 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 165.3, 164.8, 162.2, 150.6, 144.7, 137.5, 136.8, 131.1, 131.0, 129.0, 128.5, 128.4, 127.2, 121.1, 110.4.

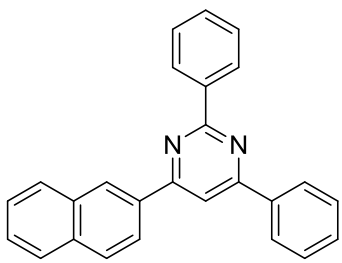
2,4-Diphenyl-6-(thiophen-3-yl)pyrimidine (3ua)[2]



The reaction was conducted with 3-acetylthiophene (25.2 mg, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3ua** as white solid; yield: 38.7 mg (62%), mp 169-171 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.70 (d, *J* = 7.9 Hz, 2H), 8.31 (d, *J* = 3.0 Hz, 1H), 8.28 (d, *J* = 7.9 Hz, 2H), 7.89 (d, *J* = 5.1 Hz, 1H), 7.85 (s, 1H), 7.55 (dd, *J* = 10.1, 7.2 Hz, 6H), 7.48 (dd, *J* = 5.0, 3.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 164.7, 164.5, 160.4, 140.8, 138.0, 137.4, 130.8, 130.6, 128.9, 128.4, 128.4, 127.2, 126.7, 126.6, 126.2, 110.1.

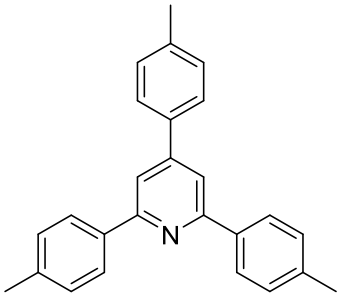
4-(Naphthalen-2-yl)-2,6-diphenylpyrimidine (3va)[6]



The reaction was conducted with 2-acetylnaphthalene (34.0 mg, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol), ammonium acetate (46.2 mg, 0.6 mmol), $NaIO_4$ (17.2 mg, 0.08 mmol) and DMSO (7.1 μL, 0.1 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3va** as white solid; yield: 46.2 mg (65%), mp 157-159 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.78 (s, 2H), 8.77 (s, 1H), 8.40 (d, *J* = 8.6 Hz, 1H), 8.34 (d, *J* = 8.0 Hz, 2H), 8.16 (s, 1H), 8.03 (t, *J* = 8.7 Hz, 2H), 7.92 (d, *J* = 6.0 Hz, 1H), 7.56 (q, *J* = 7.7 Hz, 8H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 164.8, 164.6, 164.5, 138.2, 137.5, 134.8, 134.6, 133.3, 130.8, 130.7, 129.0, 128.9, 128.7, 128.5, 128.5, 127.8, 127.4, 127.3, 126.6, 124.2, 110.5.

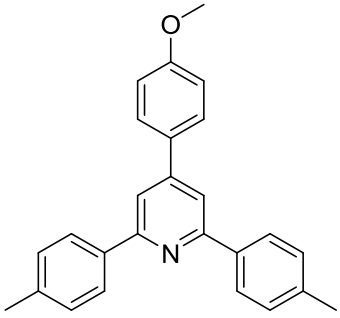
2,4,6-Tri-*p*-tolylpyridine (4ab, CAS: 16112-42-8)[7]



The reaction was conducted with 1-(*p*-tolyl)ethan-1-one (80.1 μL, 0.6 mmol), 4-methylbenzaldehyde (23.7 μL, 0.2 mmol), ammonium iodide (58.0 mg, 0.4 mmol) and DMSO (42.6 μL, 0.6 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **4ab** as white solid; yield: 52.5 mg (75%), mp 180-183 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.09 (d, *J* = 8.0 Hz, 4H), 7.83 (s, 2H), 7.65 (d, *J* = 8.0 Hz, 2H), 7.32 (t, *J* = 7.1 Hz, 6H), 2.44 (s, 3H), 2.43 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 157.3, 149.8, 138.9, 138.9, 136.9, 136.2, 129.8, 129.4, 127.0, 116.3, 21.3, 21.2.

4-(4-Methoxyphenyl)-2,6-di-*p*-tolylpyridine (4ac, CAS: 75573-10-3)[8]

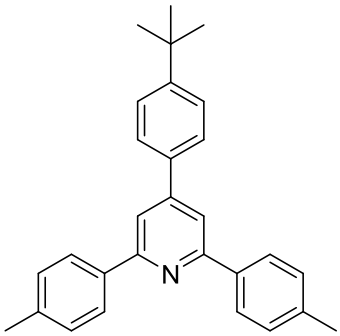


The reaction was conducted with 1-(*p*-tolyl)ethan-1-one (80.1 μL, 0.6 mmol), 4-methoxybenzaldehyde (24.3 μL, 0.2 mmol), ammonium iodide (58.0 mg, 0.4 mmol) and DMSO (42.6 μL, 0.6 mmol). The residue was purified by column chromatography on silica gel

(petroleum ether/ethyl acetate = 50:1) to give **4ac** as white solid; yield: 56.9 mg (78%), mp 156-159 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.09 (d, *J* = 7.9 Hz, 4H), 7.80 (s, 2H), 7.70 (d, *J* = 8.7 Hz, 2H), 7.31 (d, *J* = 7.9 Hz, 4H), 7.04 (d, *J* = 8.5 Hz, 2H), 3.88 (s, 3H), 2.43 (s, 6H);^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 160.3, 157.2, 149.3, 138.8, 136.9, 131.3, 129.3, 128.2, 126.9, 115.9, 114.4, 55.3, 21.3.

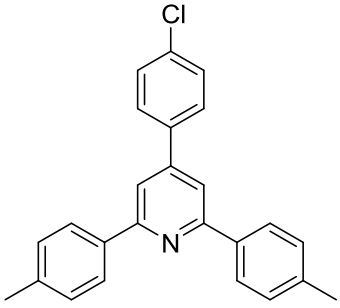
4-(4-(*tert*-Butyl)phenyl)-2,6-di-*p*-tolylpyridine (4ad)[9]



The reaction was conducted with 1-(*p*-tolyl)ethan-1-one (80.1 μL, 0.6 mmol), 4-(*tert*-butyl)benzaldehyde (33.4 μL, 0.2 mmol), ammonium iodide (58.0 mg, 0.4 mmol) and DMSO (42.6 μL, 0.6 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **4ad** as white solid; yield: 63.5 mg (81%), mp 137-140 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.09 (d, *J* = 6.5 Hz, 4H), 7.84 (s, 2H), 7.69 (d, *J* = 8.1 Hz, 2H), 7.55 (d, *J* = 8.1 Hz, 2H), 7.32 (d, *J* = 7.9 Hz, 4H), 2.43 (s, 6H), 1.39 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 157.2, 152.1, 149.8, 138.8, 136.9, 136.2, 129.4, 126.9, 126.8, 126.0, 116.4, 34.7, 31.3, 21.3.

4-(4-Chlorophenyl)-2,6-di-*p*-tolylpyridine (4af)[10]

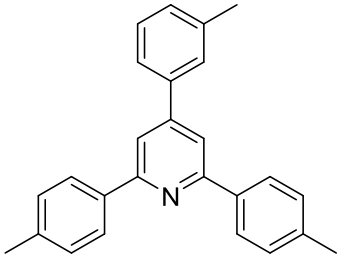


The reaction was conducted with 1-(*p*-tolyl)ethan-1-one (80.1 μL, 0.6 mmol), 4-chlorobenzaldehyde (28.1 mg, 0.2 mmol), ammonium iodide (58.0 mg, 0.4 mmol) and DMSO (42.6 μL, 0.6 mmol). The residue was purified by column chromatography on silica gel

(petroleum ether/ethyl acetate = 100:1) to give **4af** as white solid; yield: 47.9 mg (65%), mp 185-188 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.09 (d, *J* = 8.2 Hz, 4H), 7.79 (s, 2H), 7.67 (d, *J* = 8.4 Hz, 2H), 7.49 (d, *J* = 8.4 Hz, 2H), 7.32 (d, *J* = 7.9 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 157.5, 148.7, 139.1, 137.6, 136.6, 135.0, 129.4, 129.2, 128.4, 126.9, 116.1, 21.3.

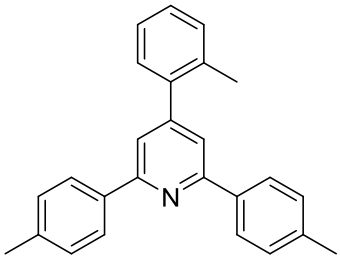
4-(*m*-Tolyl)-2,6-di-*p*-tolylpyridine (4ai)



The reaction was conducted with 1-(*p*-tolyl)ethan-1-one (80.1 μL, 0.6 mmol), 3-methylbenzaldehyde (23.6 μL, 0.2 mmol), ammonium iodide (58.0 mg, 0.4 mmol) and DMSO (42.6 μL, 0.6 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **4ai** as yellow solid; yield: 51.9 mg (74%), mp 106-108 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.10 (d, *J* = 7.8 Hz, 4H), 7.83 (s, 2H), 7.54 (d, *J* = 6.4 Hz, 2H), 7.41 (t, *J* = 7.9 Hz, 1H), 7.32 (d, *J* = 7.9 Hz, 4H), 7.28 (d, *J* = 7.7 Hz, 1H). 2.47 (s, 3H), 2.43 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 157.2, 150.1, 139.2, 138.9, 138.7, 136.9, 129.6, 129.3, 128.9, 127.8, 126.9, 124.2, 116.5, 21.5, 21.3; HRMS (ESI): *m/z* calcd for $C_{26}H_{24}N^+$ $[M+H]^+$ 350.1903, found 350.1901.

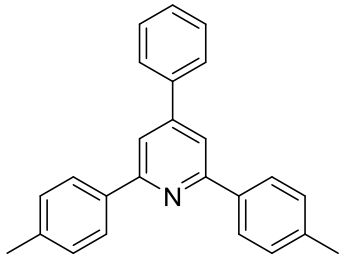
4-(*o*-Tolyl)-2,6-di-*p*-tolylpyridine (4al)



The reaction was conducted with 1-(*p*-tolyl)ethan-1-one (80.1 μL, 0.6 mmol), 2-methylbenzaldehyde (23.1 μL, 0.2 mmol), ammonium iodide (58.0 mg, 0.4 mmol) and DMSO (42.6 μL, 0.6 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **4al** as white solid; yield: 50.1 mg (72%), mp 122-125 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.07 (d, *J* = 8.0 Hz, 4H), 7.61 (s, 2H), 7.31 (t, *J* = 8.2 Hz, 8H), 2.42 (s, 6H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 156.6, 151.1, 139.9, 138.9, 136.7, 135.1, 130.6, 129.4, 129.2, 128.2, 126.9, 126.0, 118.7, 21.3, 20.4; HRMS (ESI): *m/z* calcd for $C_{26}H_{24}N^+$ $[M+H]^+$ 350.1903, found 350.1901.

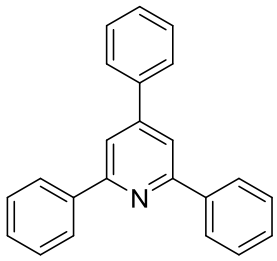
4-Phenyl-2,6-di-*p*-tolylpyridine (4aa, CAS: 16112-41-7)[11]



The reaction was conducted with 1-(*p*-tolyl)ethan-1-one (80.1 μL, 0.6 mmol), benzaldehyde (20.4 μL, 0.2 mmol), ammonium iodide (58.0 mg, 0.4 mmol) and DMSO (42.6 μL, 0.6 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **4aa** as yellow solid; yield: 51.3 mg (77%), mp 146-149 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.10 (d, *J* = 8.2 Hz, 4H), 7.84 (s, 2H), 7.74 (d, *J* = 7.0 Hz, 2H), 7.55-7.45 (m, 3H), 7.32 (d, *J* = 8.0 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 157.3, 149.9, 139.2, 138.9, 136.8, 129.4, 129.0, 128.8, 127.1, 126.9, 116.5, 21.3.

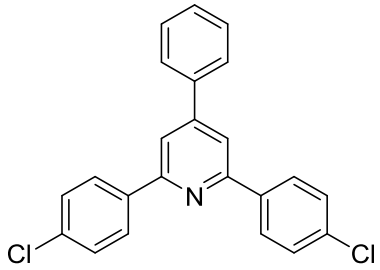
2,4,6-Triphenylpyridine (4ba, CAS: 580-35-8)[11]



The reaction was conducted with acetophenone (70.2 μL, 0.6 mmol), benzaldehyde (20.4 μL, 0.2 mmol), ammonium iodide (58.0 mg, 0.4 mmol) and DMSO (42.6 μL, 0.6 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **4ba** as white solid; yield: 50.4 mg (82%), mp 140-141 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.21 (d, *J* = 7.2 Hz, 4H), 7.90 (s, 2H), 7.76 (d, *J* = 7.0 Hz, 2H), 7.56-7.43 (m, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 157.4, 150.1, 139.5, 139.0, 129.1, 129.0, 128.9, 128.7, 127.1, 127.1, 117.1.

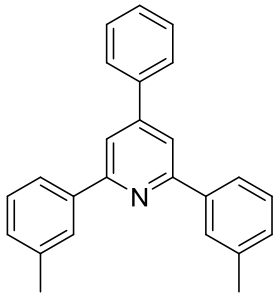
2,6-Bis(4-chlorophenyl)-4-phenylpyridine (4ga, CAS:72666-43-4)[12]



The reaction was conducted with 1-(4-chlorophenyl)ethan-1-one (77.7 μL, 0.6 mmol), benzaldehyde (20.4 μL, 0.2 mmol), ammonium iodide (58.0 mg, 0.4 mmol) and DMSO (42.6 μL, 0.6 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **4ga** as white solid; yield: 71.3 mg (95%), mp 186-188 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.13 (d, *J* = 8.5 Hz, 4H), 7.86 (s, 2H), 7.73 (d, *J* = 7.1 Hz, 2H), 7.56-7.26 (m, 7H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 156.3, 150.5, 138.6, 137.7, 135.2, 129.2, 129.2, 128.9, 128.3, 127.1, 117.1.

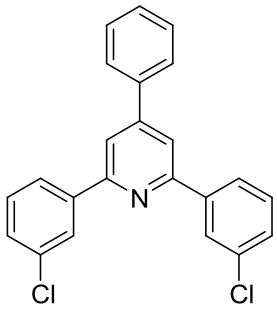
4-Phenyl-2,6-di-*m*-tolylpyridine (4la)[13]



The reaction was conducted with 1-(*m*-tolyl)ethan-1-one (81.6 μL, 0.6 mmol), benzaldehyde (20.4 μL, 0.2 mmol), ammonium iodide (58.0 mg, 0.4 mmol) and DMSO (42.6 μL, 0.6 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **4la** as white solid; yield: 58.9 mg (88%), mp 153-156 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.01 (s, 2H), 7.97 (d, *J* = 7.8 Hz, 2H), 7.87 (s, 2H), 7.76 (d, *J* = 7.2 Hz, 2H), 7.54 (t, *J* = 7.3 Hz, 2H), 7.48 (t, *J* = 7.3 Hz, 1H), 7.41 (t, *J* = 7.6 Hz, 2H), 7.26 (d, *J* = 9.7 Hz, 3H), 2.48 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 157.7, 150.0, 139.6, 139.0, 138.3, 129.8, 129.0, 128.9, 128.6, 127.8, 127.1, 124.3, 117.2, 21.6.

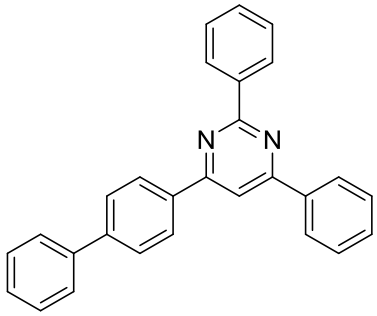
2,6-Bis(3-chlorophenyl)-4-phenylpyridine (4ma)[11]



The reaction was conducted with 1-(3-chlorophenyl)ethan-1-one (78.0 μL, 0.6 mmol), benzaldehyde (20.4 μL, 0.2 mmol), ammonium iodide (58.0 mg, 0.4 mmol) and DMSO (42.6 μL, 0.6 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **4ma** as white solid; yield: 68.5 mg (91%), mp 175-178 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.18 (s, 2H), 8.06 (d, *J* = 7.0 Hz, 2H), 7.88 (s, 2H), 7.74 (d, *J* = 6.9 Hz, 2H), 7.57-7.42 (m, 7H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 156.1, 150.6, 141.0, 138.4, 134.8, 130.0, 129.2, 129.2, 129.1, 127.2, 127.1, 125.2, 117.6.

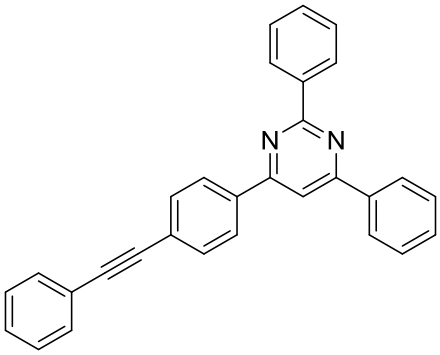
4-([1,1'-biphenyl]-4-yl)-2,6-diphenylpyrimidine (5a)



A 10 mL oven-dried reaction vessel was charged with 4-(4-bromophenyl)-2,6-diphenylpyrimidine (0.2 mmol, 77.2 mg), phenylboronic acid (0.26 mmol, 31.7 mg), $Pd(PPh_3)_4$ (0.01 mmol, 11.6 mg), Na_2CO_3 (1.4 mmol, 148.4mg), toluene (0.8 mL), H_2O (0.8 mL) and ethanol (0.2 mL). The reaction vessel was purged with argon for three times and stirred at 110 ^{o}C for 18 h. After cooling to room temperature, the volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **5a** as white solid; yield: 56.3 mg (73%), mp 177-179 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.75 (d, *J* = 7.8 Hz, 2H), 8.38 (d, *J* = 8.3 Hz, 2H), 8.31 (d, *J* = 7.8 Hz, 2H), 8.06 (s, 1H), 7.80 (d, *J* = 8.3 Hz, 2H), 7.69 (d, *J* = 7.4 Hz, 2H), 7.59-7.48 (m, 8H), 7.41 (t, *J* = 7.3 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 164.7, 164.5, 164.3, 143.6, 140.3, 138.1, 137.5, 136.3, 130.8, 130.6, 128.9, 128.5, 128. 5, 127.8, 127.7, 127.6, 127.3, 127.2, 110.1; HRMS (ESI): *m/z* calcd for $C_{28}H_{21}N_2^+$ $[M+H]^+$ 385.1699, found 385.1694.

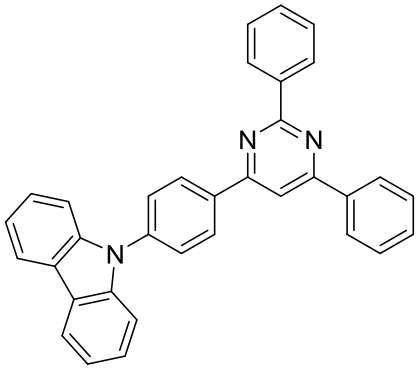
2,4-diphenyl-6-(4-(phenylethynyl)phenyl)pyrimidine (5b)



A 10 mL oven-dried reaction vessel was charged with 4-(4-bromophenyl)-2,6-diphenylpyrimidine (0.2 mmol, 77.2 mg), phenylacetylene (0.3 mmol, 33.0 μL), $PdCl_2$ (0.01 mmol, 1.8 mg), CuI (0.01 mmol, 2.0 mg), PPh_3 (0.03 mmol, 7.9 mg) and Et_3N (1.0 mL). The reaction vessel was purged with argon for three times and stirred at 80 ^oC for 12 h. After cooling to room temperature, the volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to give **5b** as white solid; yield: 77.0 mg (94%), mp 162-164 ℃.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 8.73 (d, *J* = 7.9 Hz, 2H), 8.31 (d, *J* = 8.2 Hz, 4H), 8.03 (s, 1H), 7.72 (d, *J* = 8.2 Hz, 2H), 7.63-7.49 (m, 8H), 7.43-7.30 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 164.8, 164.5, 163.7, 138.0, 137.4, 137.0, 132.0, 131.7, 130.8, 130.7, 128.9, 128.5, 128.4, 128.4, 127.3, 127.1, 125.7, 122.9, 110.1, 91.5, 89.1 HRMS (ESI): *m/z* calcd for $C_{30}H_{21}N_2^+$ $[M+H]^+$ 409.1699, found 409.1695.

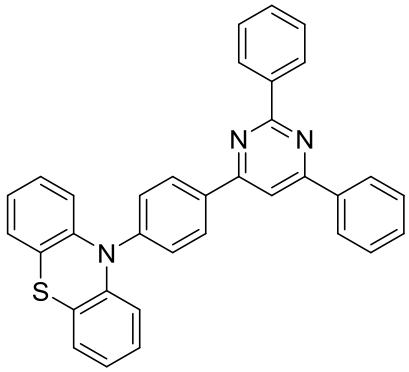
9-(4-(2,6-diphenylpyrimidin-4-yl)phenyl)-9H-carbazole (5c)



A 10 mL oven-dried reaction vessel was charged with 4-(4-bromophenyl)-2,6-diphenylpyrimidine (0.2 mmol, 77.2 mg), carbazole (0.3 mmol, 50.2 mg), $Pd(OAc)_2$ (0.02 mmol, 4.6 mg), P(*t*-Bu)$_3$HBF$_4$ (0.04 mmol, 11.6 mg), K_2CO_3 (0.6 mmol, 83 mg) and *o*-xylene (0.8 mL). The reaction vessel was purged with argon for three times and stirred at 140 ^oC for 16 h. After cooling to room temperature, the volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to give **5c** as white solid; yield: 81.4 mg (86%), mp 214-217 ℃.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 8.78 (d, *J* = 8.0 Hz, 2H), 8.55 (d, *J* = 8.4 Hz, 2H), 8.35 (d, *J* = 7.9 Hz, 2H), 8.18 (d, *J* = 7.7 Hz, 2H), 8.12 (s, 1H), 7.80 (d, *J* = 8.4 Hz, 2H), 7.62-7.52 (m, 8H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.33 (t, *J* = 7.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 165.0, 164.7, 163.9, 140.5, 140.1, 138.0, 137.4, 136.4, 130.9, 130.8, 129.0, 128. 9, 128.5, 128.5, 127.3, 127.2, 126.1, 123.7, 120.4, 120.3, 110.3, 109.8; HRMS (ESI): *m/z* calcd for $C_{34}H_{24}N_3^+$ $[M+H]^+$ 474.1965, found 474.1956.

10-(4-(2,6-diphenylpyrimidin-4-yl)phenyl)-10H-phenothiazine (5d)



A 10 mL oven-dried reaction vessel was charged with 4-(4-bromophenyl)-2,6-diphenylpyrimidine (0.2 mmol, 77.2 mg), phenothiazine (0.2 mmol, 39.8 mg), $Pd_2(dba)_3$ (0.004 mmol, 3.6 mg), P(*t*-Bu)$_3$HBF$_4$ (0.012 mmol, 3.4 mg), *t*-BuOK (0.26 mmol, 29.2 mg) and toluene (2.0 mL). The reaction vessel was purged with argon for three times and stirred at 110 ^{o}C for 10 h. After cooling to room temperature, the volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to give **5d** as yellow solid; yield: 90.2 mg (89%), mp 216-219 ℃

^{1}H NMR (400 MHz, DMSO-d_6, ppm) δ 8.73-8.64 (m, 4H), 8.60 (s, 1H), 8.52 (dd, *J* = 6.6, 2.9 Hz, 2H), 7.64-7.60 (m, 6H), 7.56 (d, *J* = 8.5 Hz, 2H), 7.23 (d, *J* = 7.6 Hz, 2H), 7.08 (t, *J* = 7.7 Hz, 2H), 6.99 (t, *J* = 7.4 Hz, 2H), 6.57 (d, *J* = 8.2 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6, ppm) δ 164.4, 163.5, 163.5, 144.1, 142.9, 137.5, 136.6, 135.0, 131.3, 131.1, 130.0, 129.1, 128.8, 128.1, 127.6, 127.5, 127.5, 127.3, 123.8, 122.5, 118.6, 110.6; HRMS (ESI): *m/z* calcd for $C_{34}H_{24}N_3S^+$ $[M+H]^+$ 506.1685, found 506.1678.

5. References

[1] L. B. Su, K. Sun, N. Pan, L. Liu, M. L. Sun, J. Y. Dong, Y. B. Zhou and S. F. Yin, *Org. Lett.*, 2018, **20**, 3399.

[2] D. Q. Liu, W. Guo, W. Q. Wu and H. F. Jiang, *J. Org. Chem.*, 2017, **82**, 13609.

[3] K. S. Vadagaonkar, H. P. Kalmode, S. Prakash, A. C. Chaskar, *New J. Chem.*, 2015, **39**, 3639.

[4] M. K. Gupta, A. K. Gupta, V. Gupta and K. C. Gupta, *J. Indian Chem. Soc.*, 2007, **84**, 299.

[5] T. C. Shi, F. Qin, Q. Li and W. Zhang, *Org. Biomol. Chem.*, 2018, **16**, 9487.

[6] M. Mastalir, M. Glatz, E. Pittenauer, G. Allmaier and K. Kirchner, *J. Am. Chem. Soc.*, 2016, **138**, 15543.

[7] X. Zhang, Z. Q. Wang, K. Xu, Y. Q. Feng, W. Zhao, X. F. Xu, Y. L. Yan and W. Yi, *Green Chem.*, 2016, *18*, 2313.

[8] R. S. Rohokale, B. Koenig and D. D. Dhavale, *J. Org. Chem.*, 2016, **81**, 7121.

[9] A. A. Buelt, N. C. Osti, Y. Htet, C. A. Conrad, M. F. Shehata, R. Potai, A. G. Tennyson, D. Perahia and R. C. Smith, *J. Mater. Chem. C*, 2014, **2**, 8113.

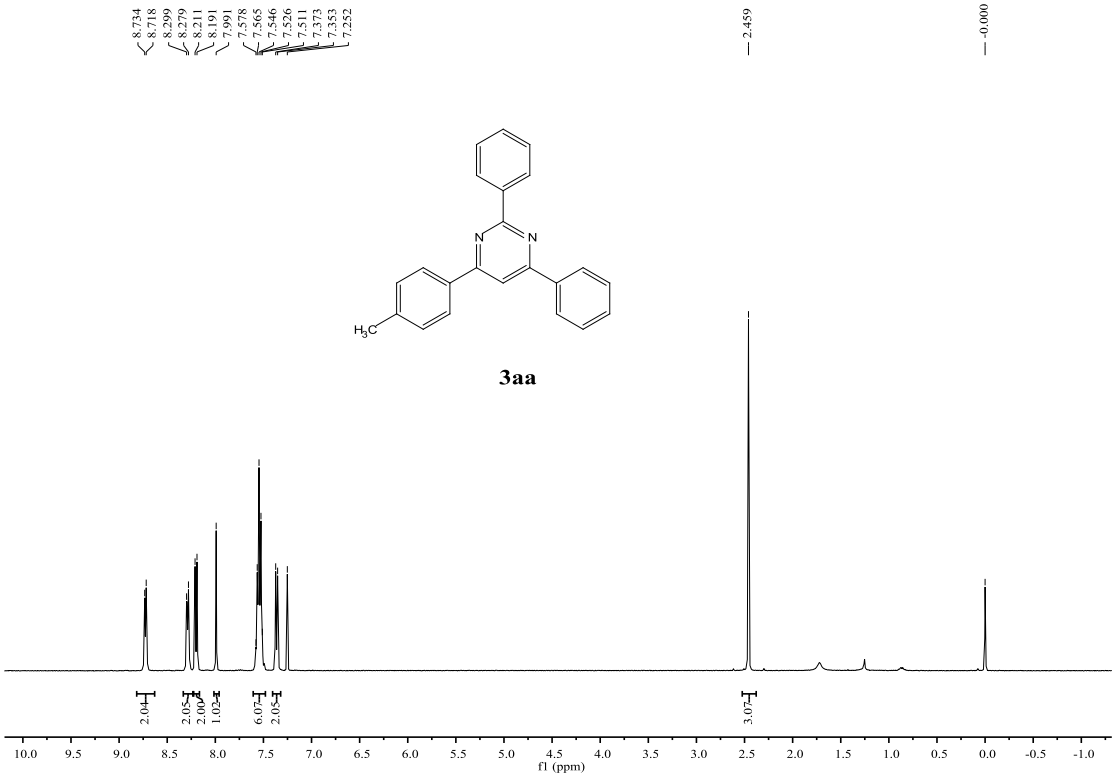
[10] S. J. Tu, T. J. Li, F. Shi, Q. Wang, J. P. Zhang, J. N. Xu, X. T. Zhu, X. J. Zhang, S. L. Zhu and D. Q. Shi, *Synthesis*, 2005, **18**. 3045.

[11] Z. Y. Mao, X. Y. Liao, H. S. Wang, C. G. Wang, K. B. Huang and Y. M. Pan, *RSC Adv.*, 2017, **7**, 13123.

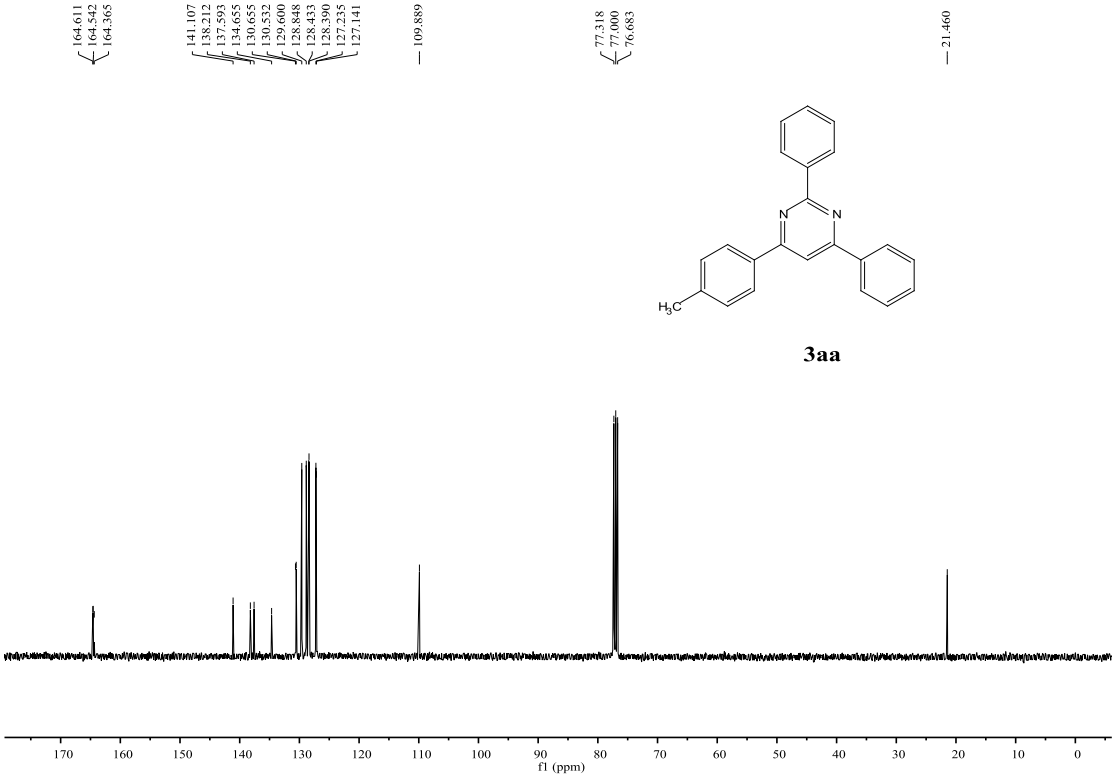
[12] Y. K. Yi, M. N. Zhao, Z. H. Ren, Y. Y. Wang and Z. H. Guan, *Green Chem.*, 2017, **19**, 1023.

[13] Y. J. Fu, P. P. Wang, X. Guo, P. Wu, X. Meng and B. H. Chen, *J. Org. Chem.*, 2016, **81**, 11671.

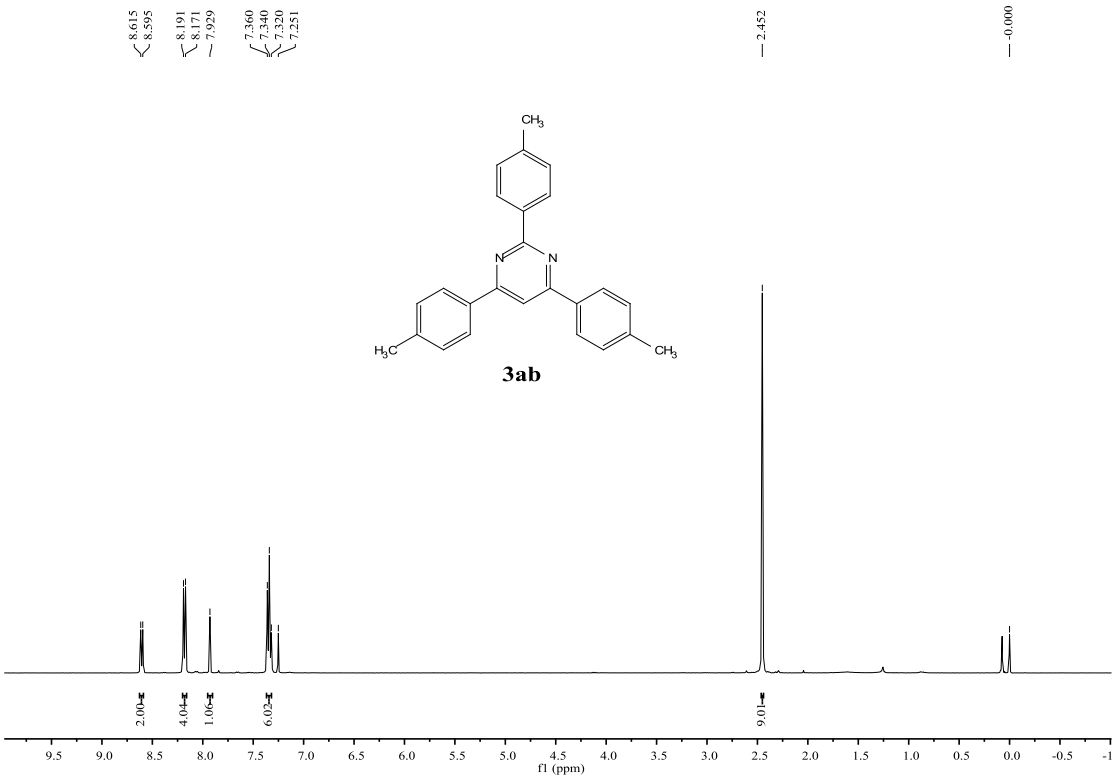
6. ^{1}H NMR and ^{13}C NMR spectra of all products

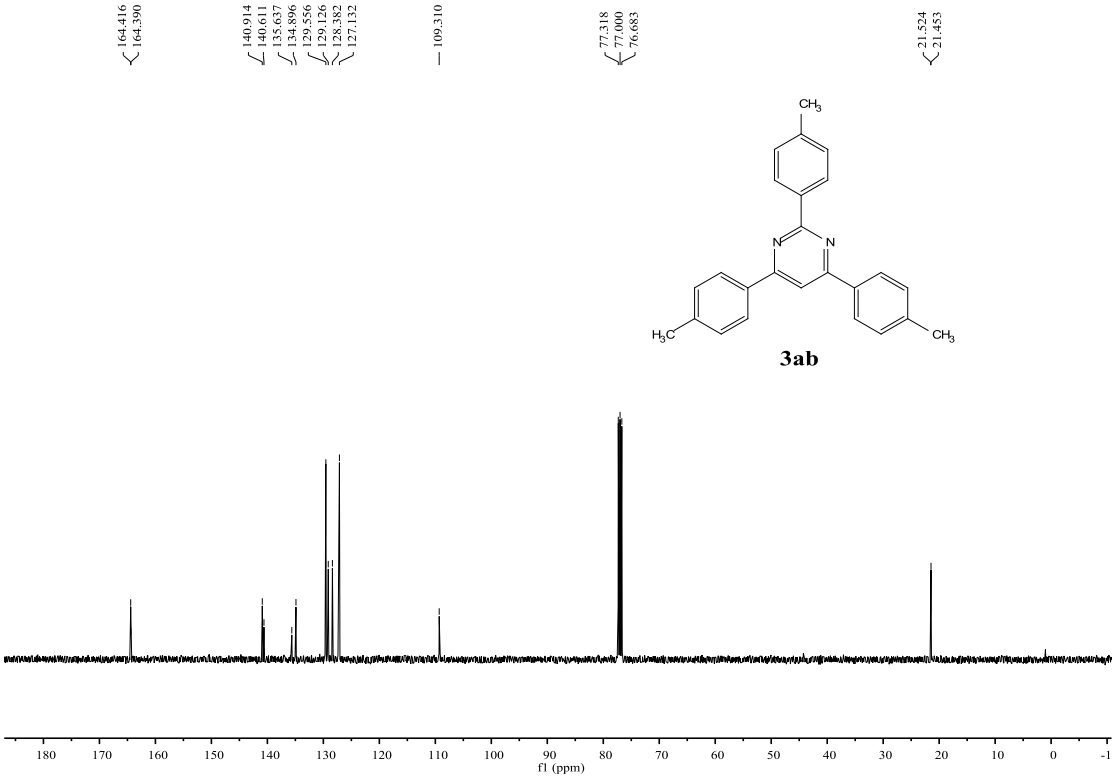


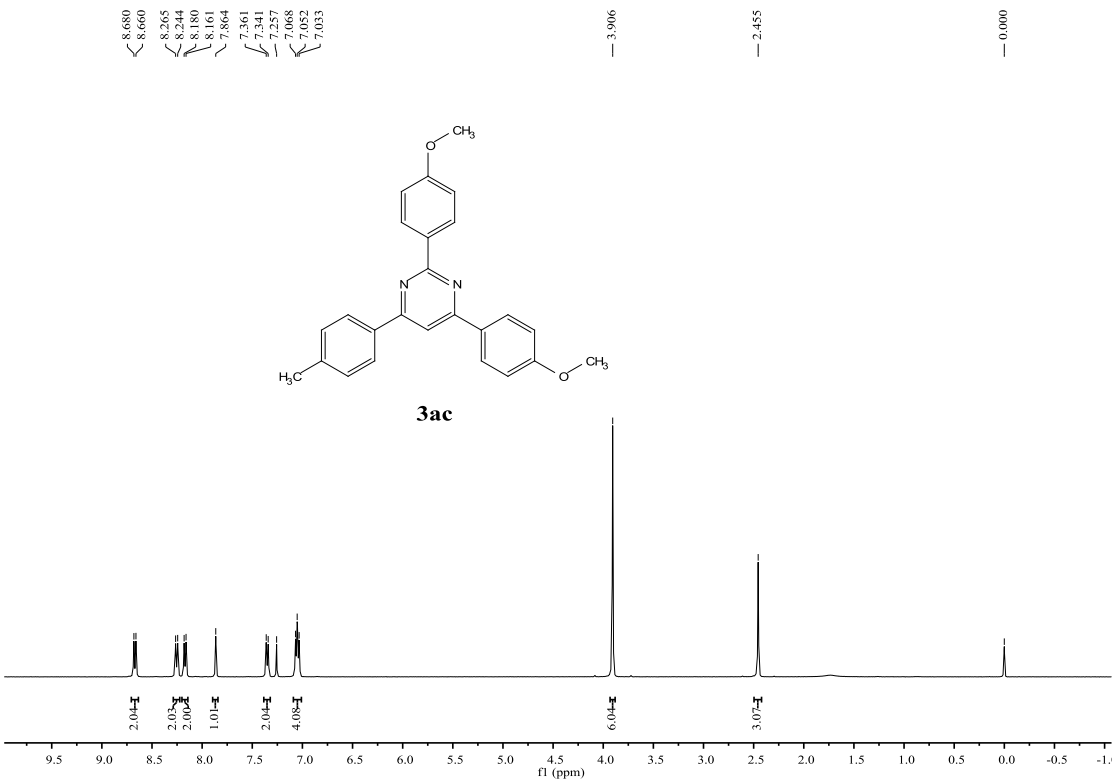
3aa



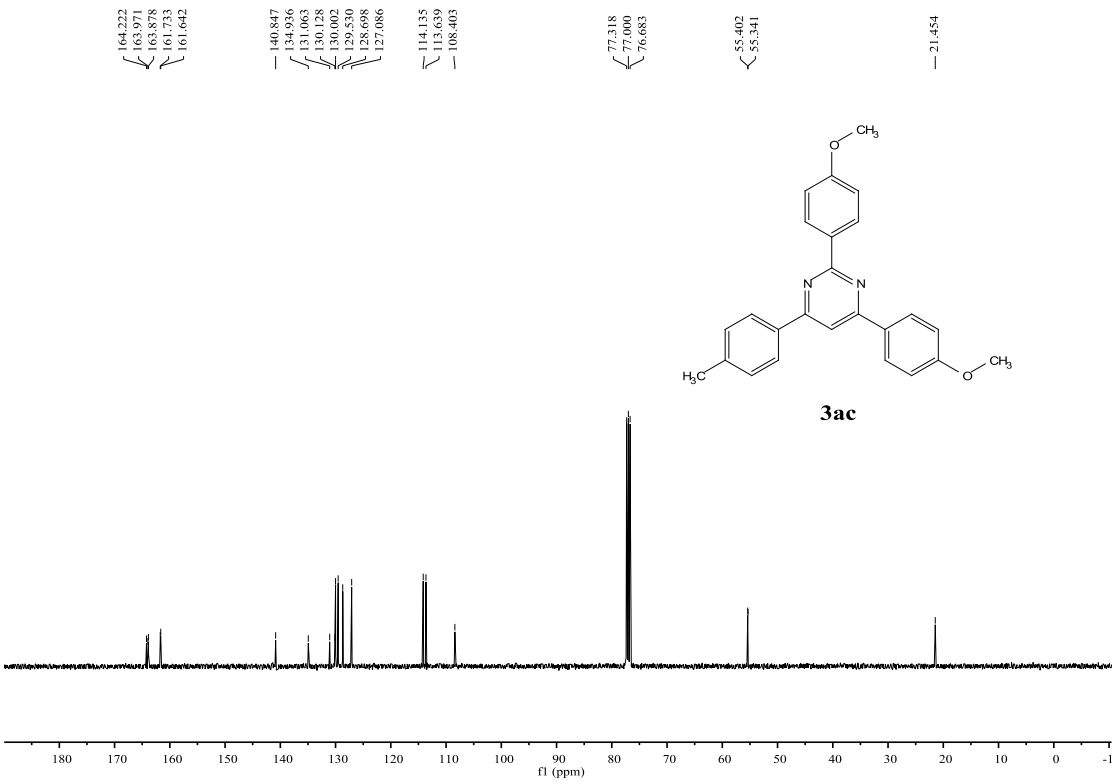
3aa


8.615
8.595
8.191
8.171
7.929
7.360
7.340
7.320
7.251
2.452
0.000
CH3
N
N
H3C
CH3
3ab
2.00
4.04
1.06
6.02
9.01
f1 (ppm)

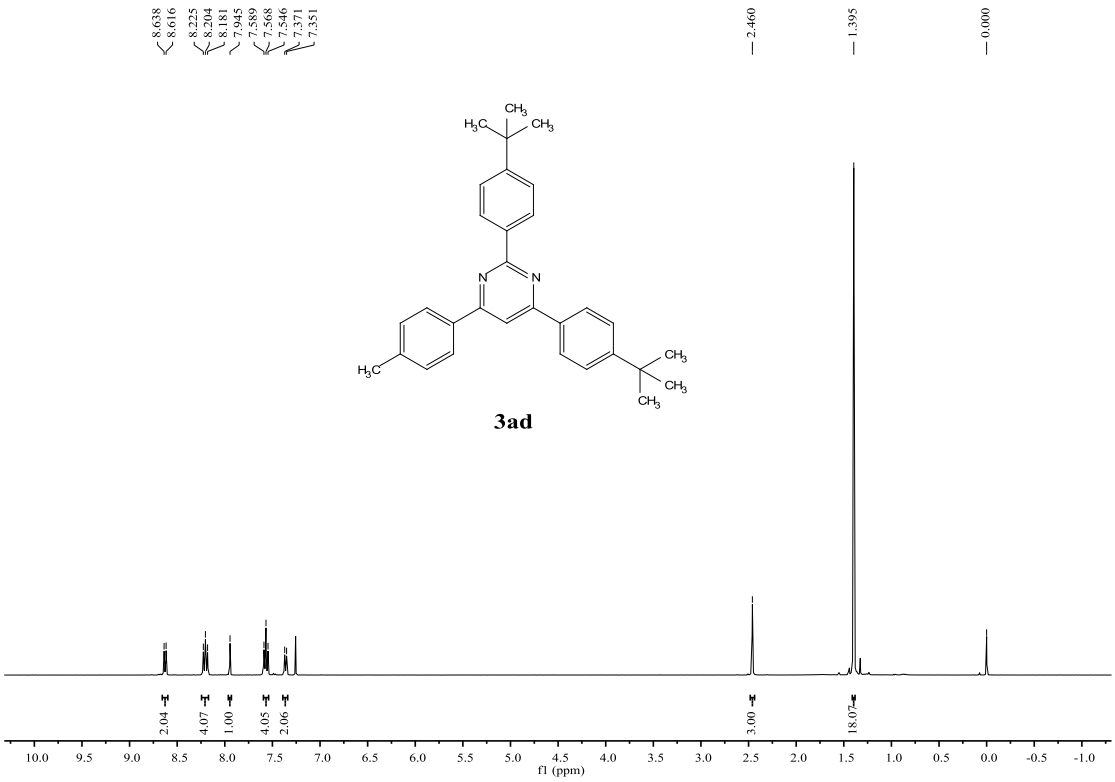

164.416
164.390
140.914
140.611
135.637
134.896
129.556
129.126
128.382
127.132
109.310
77.318
77.000
76.683
21.524
21.453
CH3
N
N
H3C
CH3
3ab
f1 (ppm)

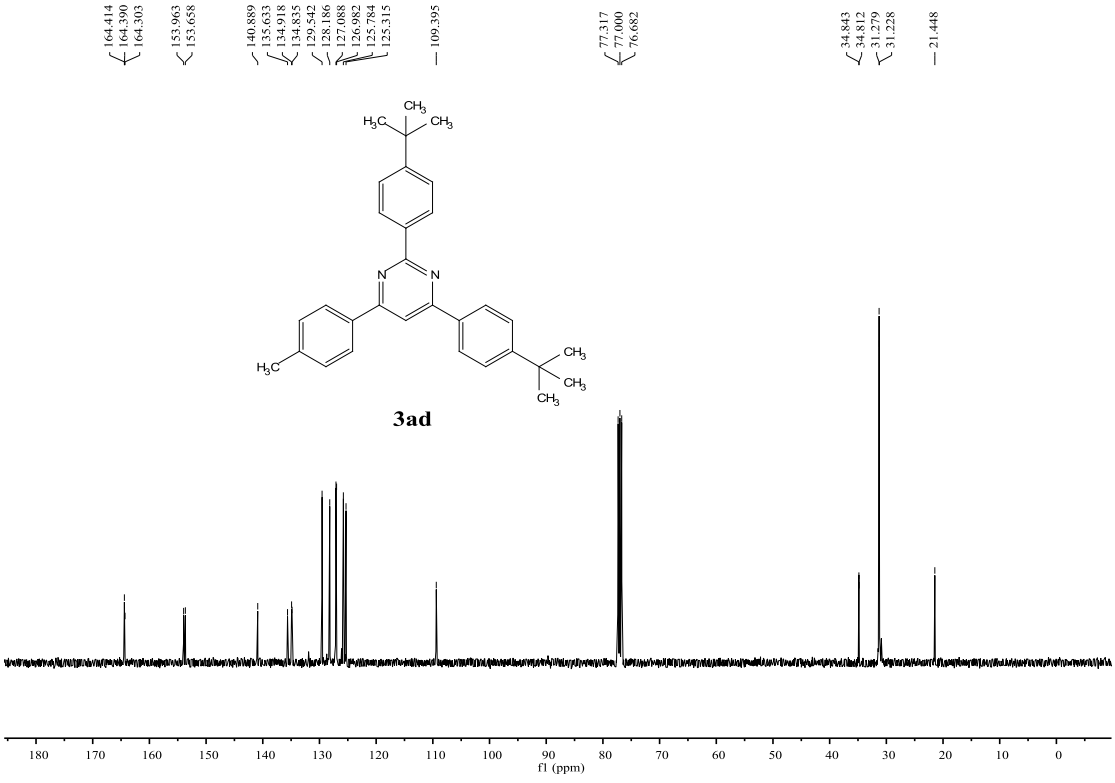

8.680
8.660
8.265
8.244
8.180
8.161
7.864
7.361
7.341
7.257
7.068
7.052
7.033
3.906
2.455
0.000
CH3
O
N
N
H3C
O
CH3
2.04
2.03
2.00
1.01
2.04
4.08
6.04
3.07
f1 (ppm)

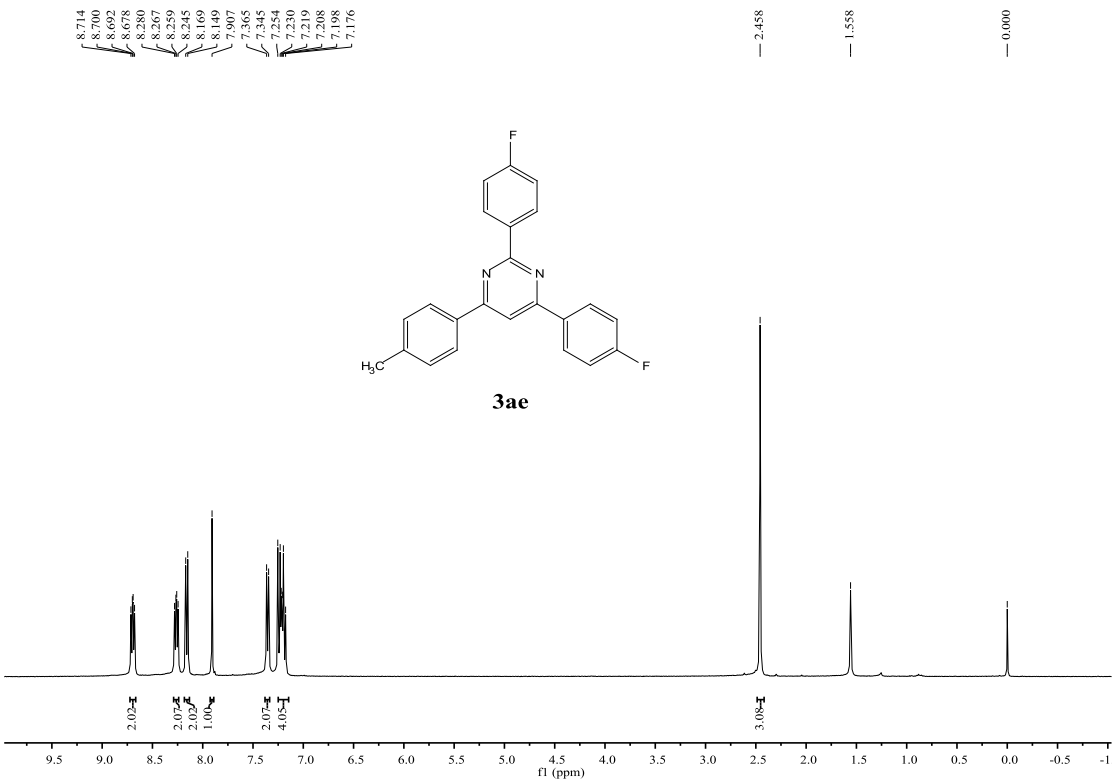
3ac

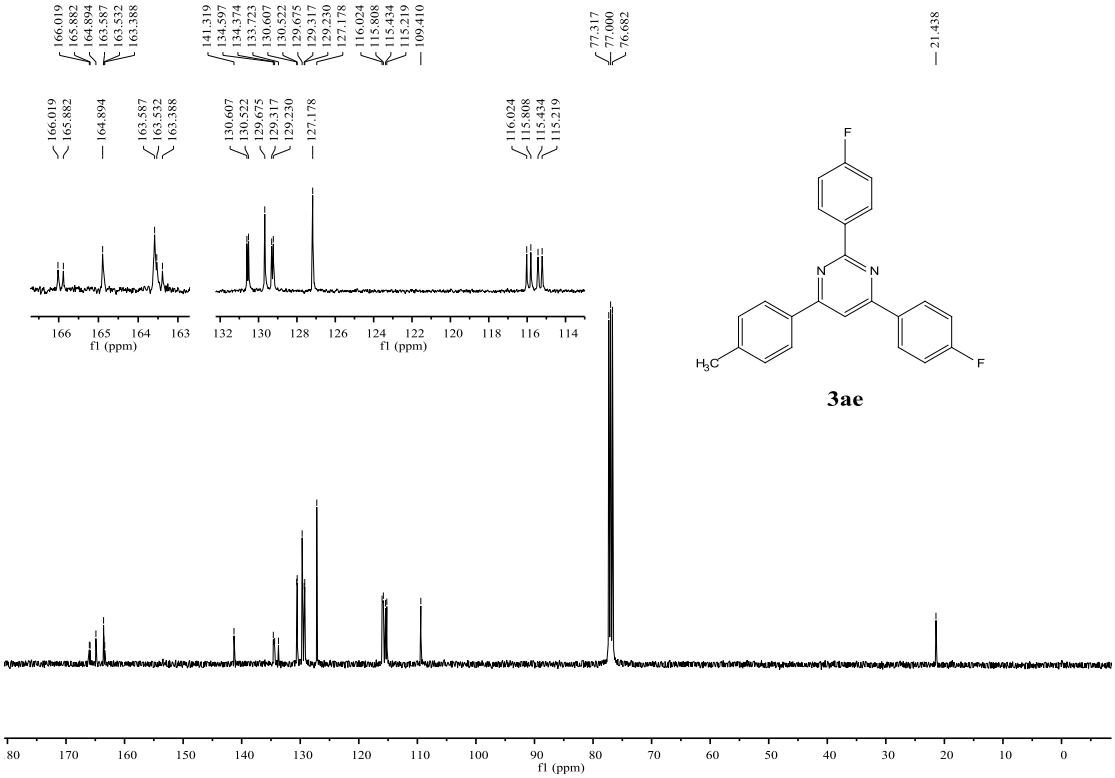

164.222
163.971
163.878
161.733
161.642
140.847
134.936
131.063
130.128
130.002
129.530
128.698
127.086
114.135
113.639
108.403
77.318
77.000
76.683
55.402
55.341
21.454
CH3
O
N
N
H3C
O
CH3
f1 (ppm)

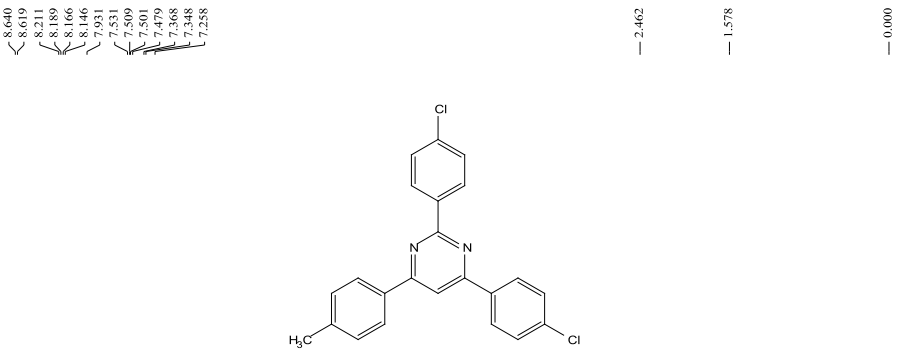
3ac


8.638
8.616
8.225
8.204
8.181
7.945
7.589
7.568
7.546
7.371
7.351
2.460
1.395
0.000
3ad
2.04
4.07
1.00
4.05
2.06
3.00
18.07
f1 (ppm)

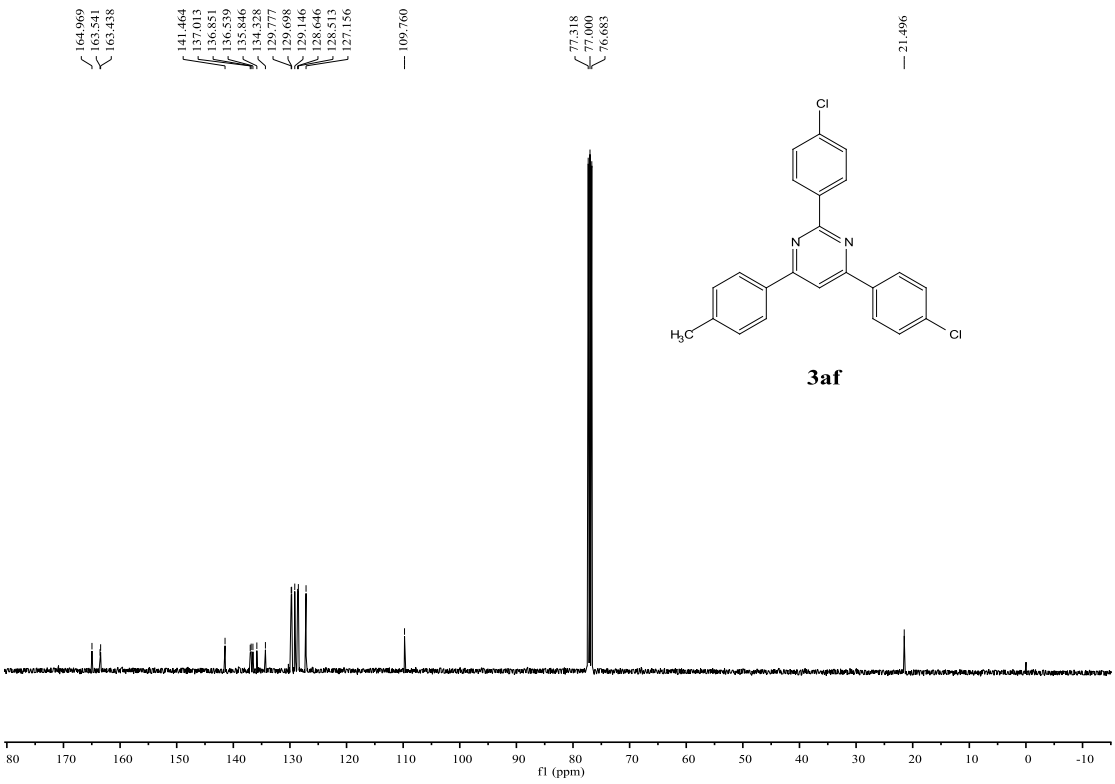

164.414
164.390
164.303
153.963
153.658
140.889
135.633
134.918
134.835
129.542
128.186
127.088
126.982
125.784
125.315
109.395
77.317
77.000
76.682
34.843
34.812
31.279
31.228
21.448
3ad
f1 (ppm)


8.714
8.700
8.692
8.678
8.280
8.267
8.259
8.245
8.169
8.149
7.907
7.365
7.345
7.254
7.230
7.219
7.208
7.198
7.176
2.458
1.558
0.000
F
N
N
H3C
F
3ae
2.02
2.07
2.02
1.00
2.07
4.05
3.08
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

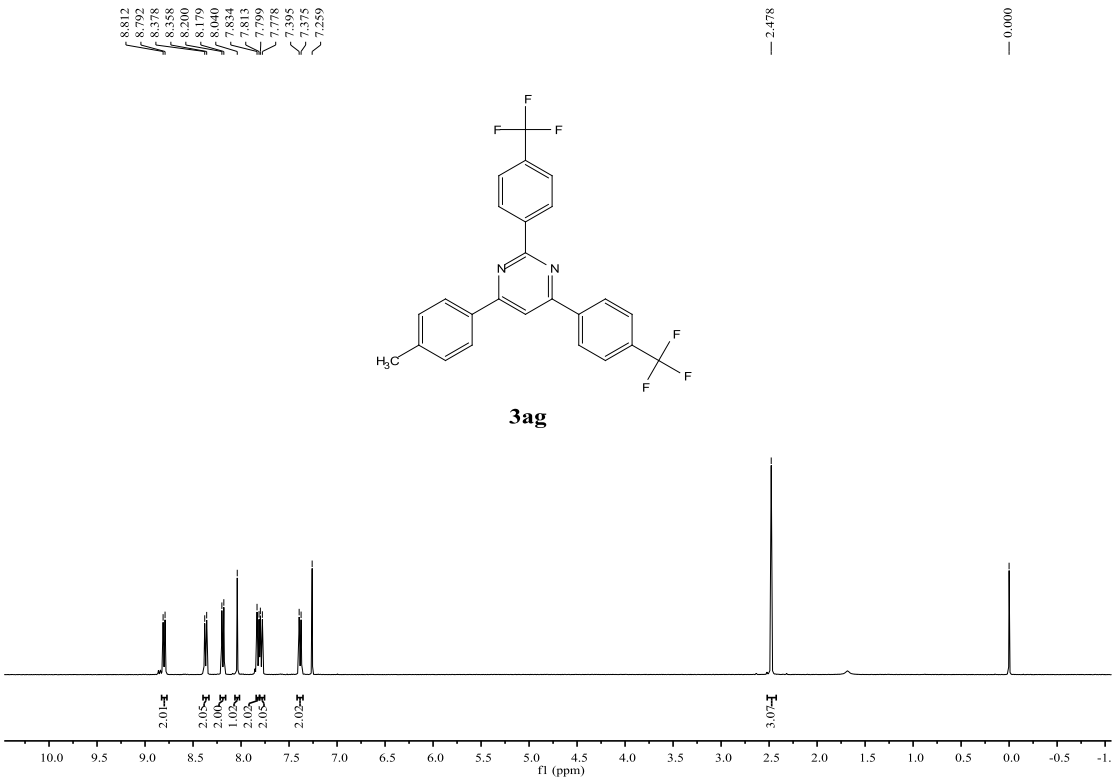

166.019
165.882
164.894
163.587
163.532
163.388
141.319
134.597
134.374
133.723
130.607
130.522
129.675
129.317
129.230
127.178
116.024
115.808
115.434
115.219
109.410
77.317
77.000
76.682
21.438
166 165 164 163
f1 (ppm)
132 130 128 126 124 122 120 118 116 114
f1 (ppm)
F
N
N
H3C
F
3ae
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.640
8.619
8.211
8.189
8.166
8.146
7.931
7.531
7.509
7.501
7.479
7.368
7.348
7.258
2.462
1.578
0.000
Cl
N
N
H3C
Cl
2.08
2.06
2.03
1.03
2.06
2.00
2.04
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

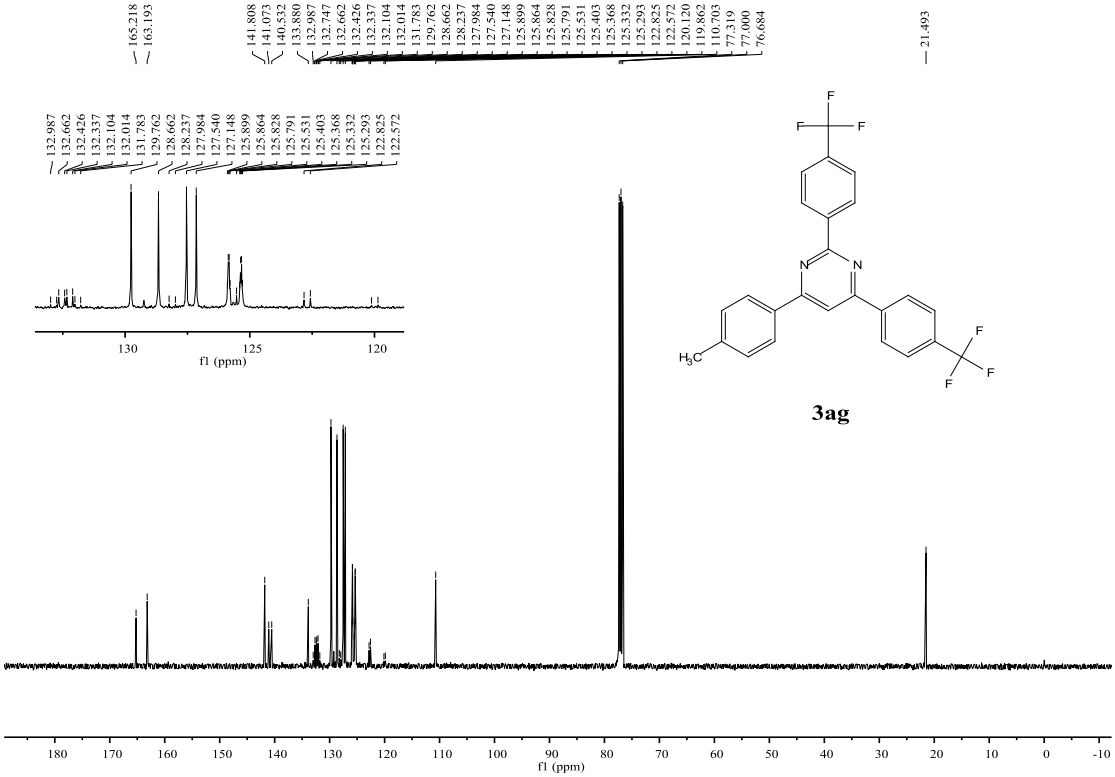
3af


164.969
163.541
163.438
141.464
137.013
136.851
136.539
135.846
134.328
129.777
129.698
129.146
128.646
128.513
127.156
109.760
77.318
77.000
76.683
21.496
Cl
N
N
H3C
Cl
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

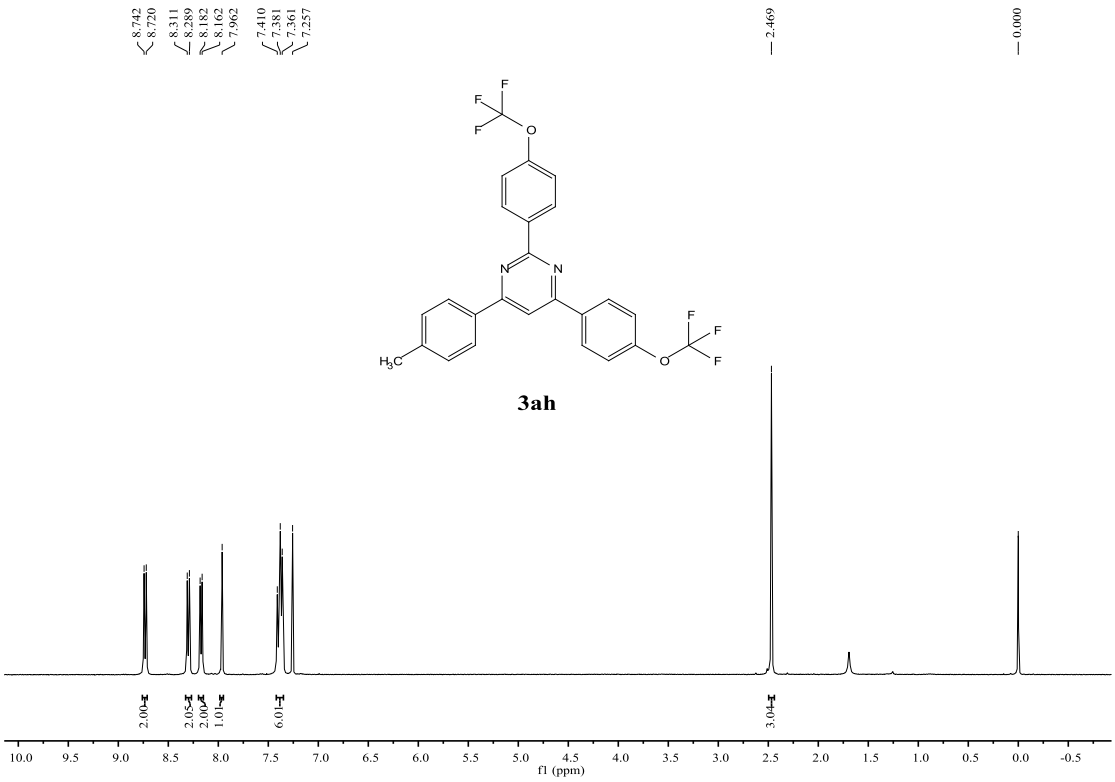
3af

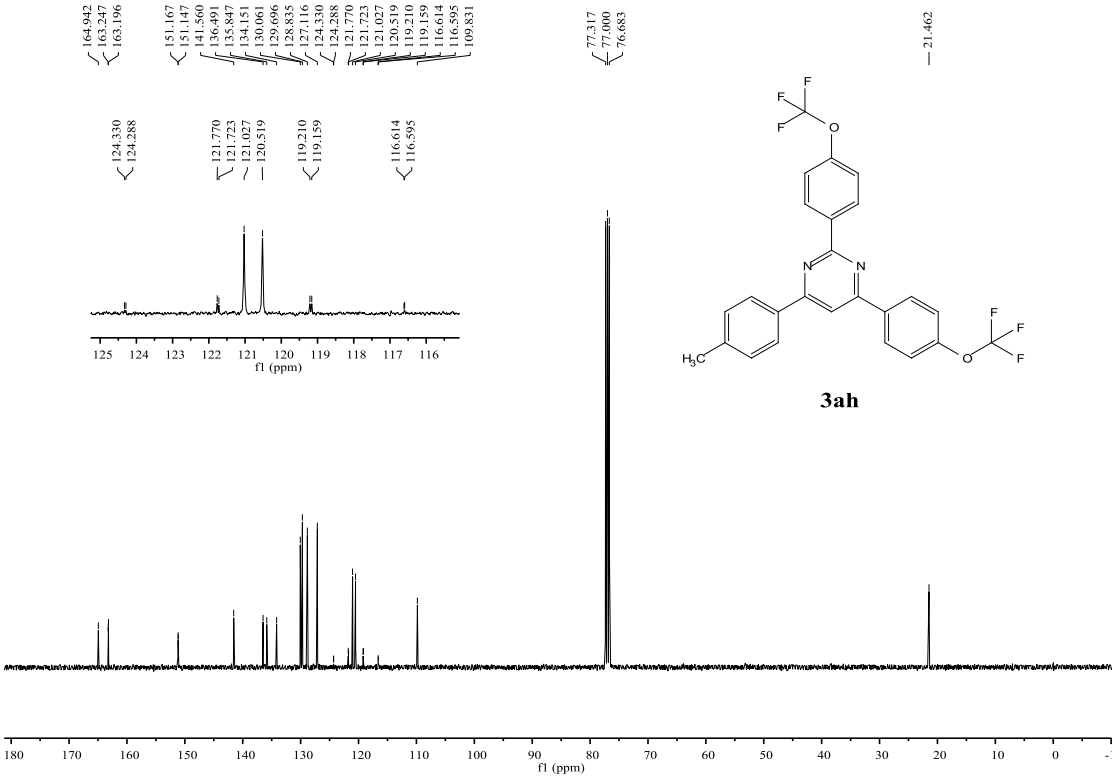

8.812
8.792
8.378
8.358
8.200
8.179
8.040
7.834
7.813
7.799
7.778
7.395
7.375
7.259
2.478
0.000
F
F
F
N
N
H3C
F
F
F
2.01
2.05
2.00
1.02
2.03
2.05
2.02
3.07
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.
f1 (ppm)

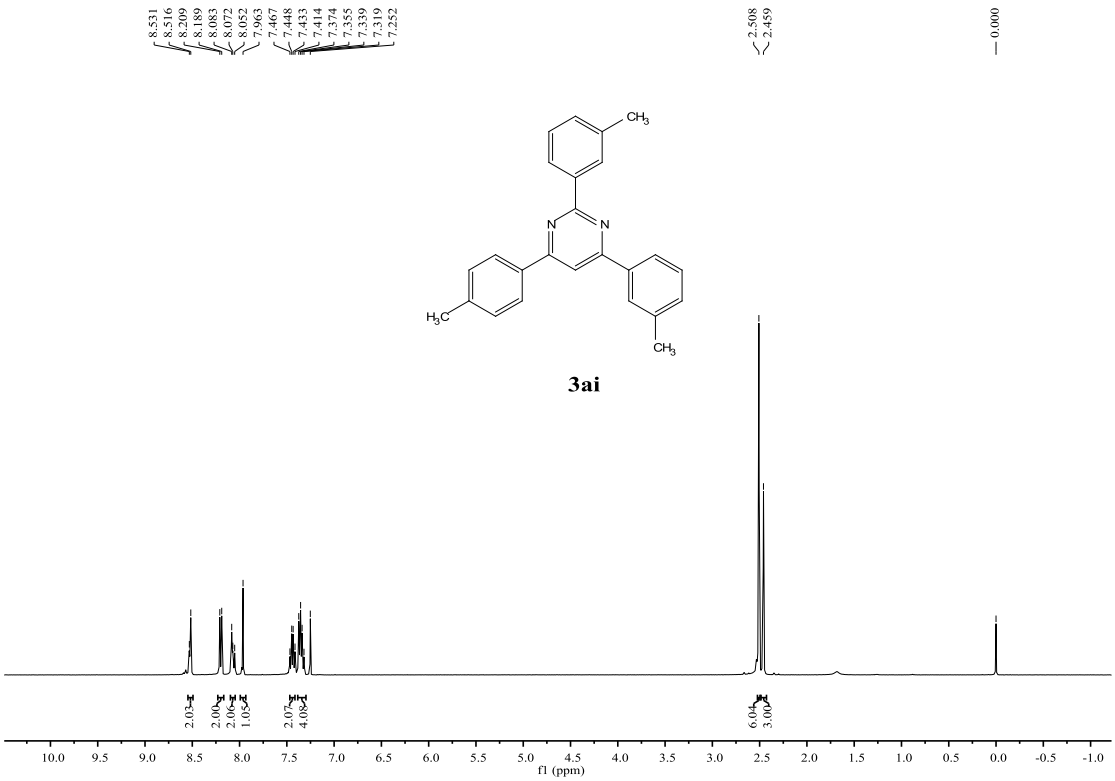
3ag


165.218
163.193
141.808
141.073
140.532
133.880
132.987
132.747
132.662
132.426
132.337
132.104
132.014
131.783
129.762
128.662
128.237
127.984
127.540
127.148
125.899
125.864
125.828
125.791
125.531
125.403
125.368
125.332
125.293
122.825
122.572
120.120
119.862
110.703
77.319
77.000
76.684
21.493
130
125
120
f1 (ppm)
F
F
F
N
N
H3C
F
F
F
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

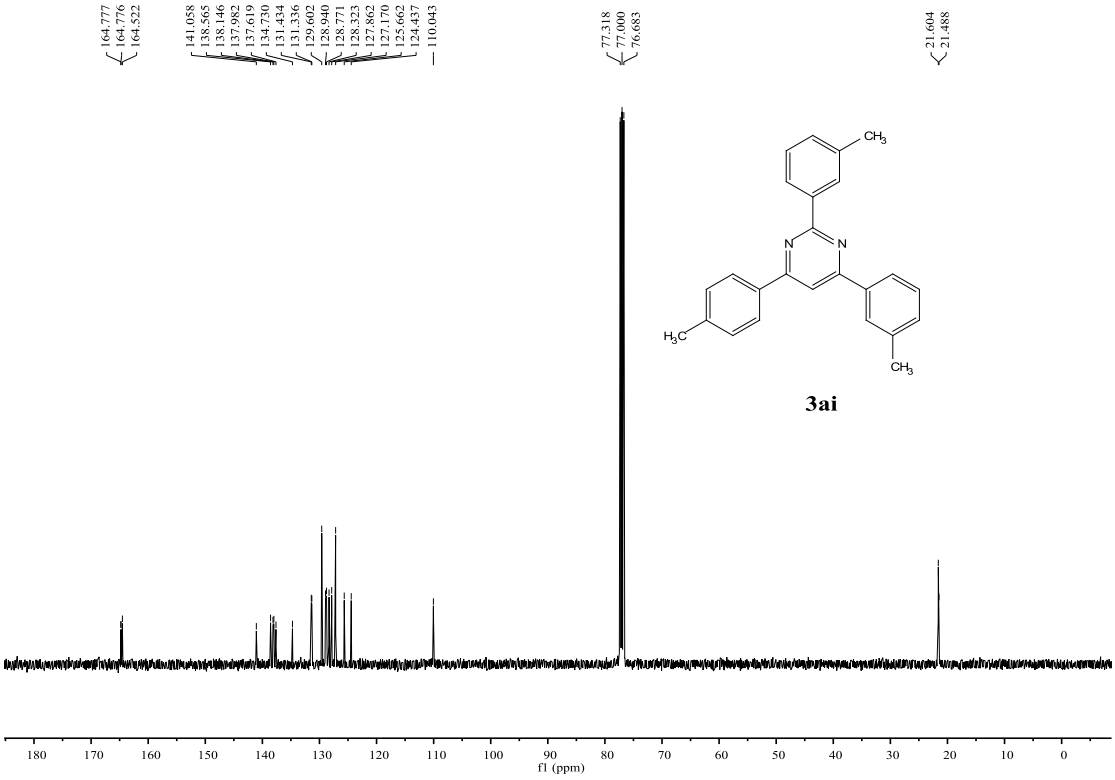
3ag


8.742
8.720
8.311
8.289
8.182
8.162
7.962
7.410
7.381
7.361
7.257
2.469
0.000
3ah
2.00
2.05
2.00
1.01
6.01
3.04
f1 (ppm)

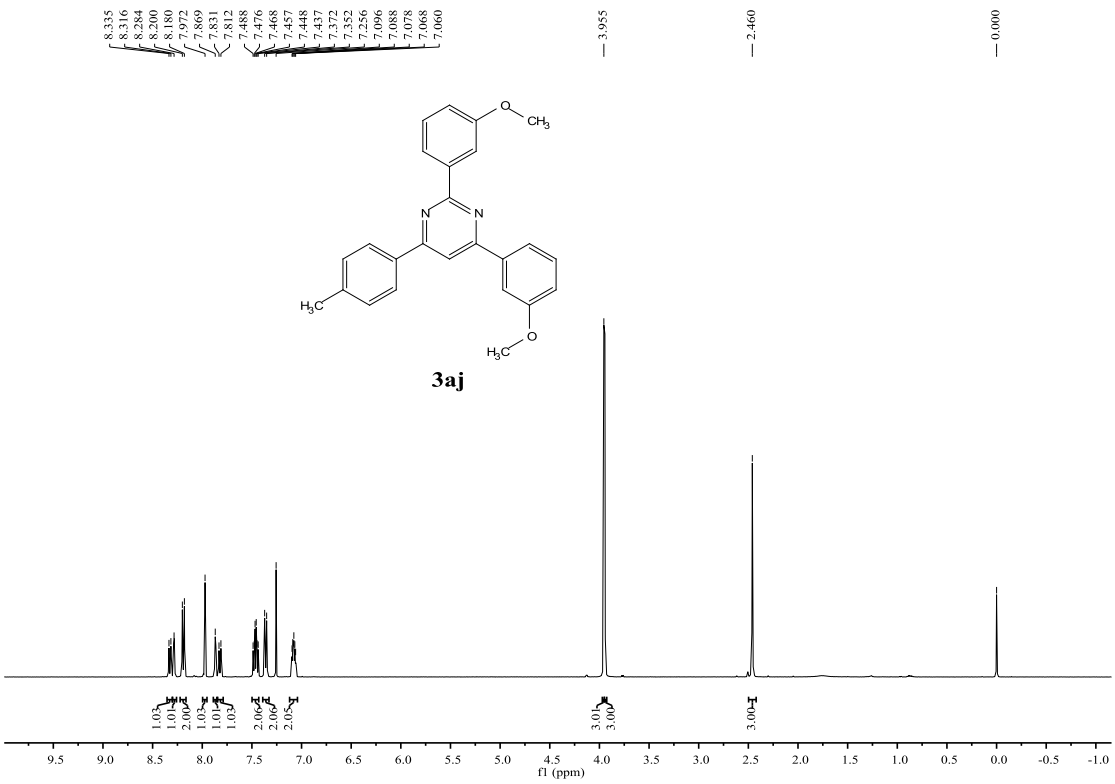

164.942
163.247
163.196
151.167
151.147
141.560
136.491
135.847
134.151
130.061
129.696
128.835
127.116
124.330
124.288
121.770
121.723
121.027
120.519
119.210
119.159
116.614
116.595
109.831
77.317
77.000
76.683
21.462
3ah
f1 (ppm)


8.531
8.516
8.209
8.189
8.083
8.072
8.052
7.963
7.467
7.448
7.433
7.414
7.374
7.355
7.339
7.319
7.252
2.508
2.459
0.000
CH3
N
N
H3C
CH3
2.03
2.00
2.06
1.05
2.07
4.08
6.04
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

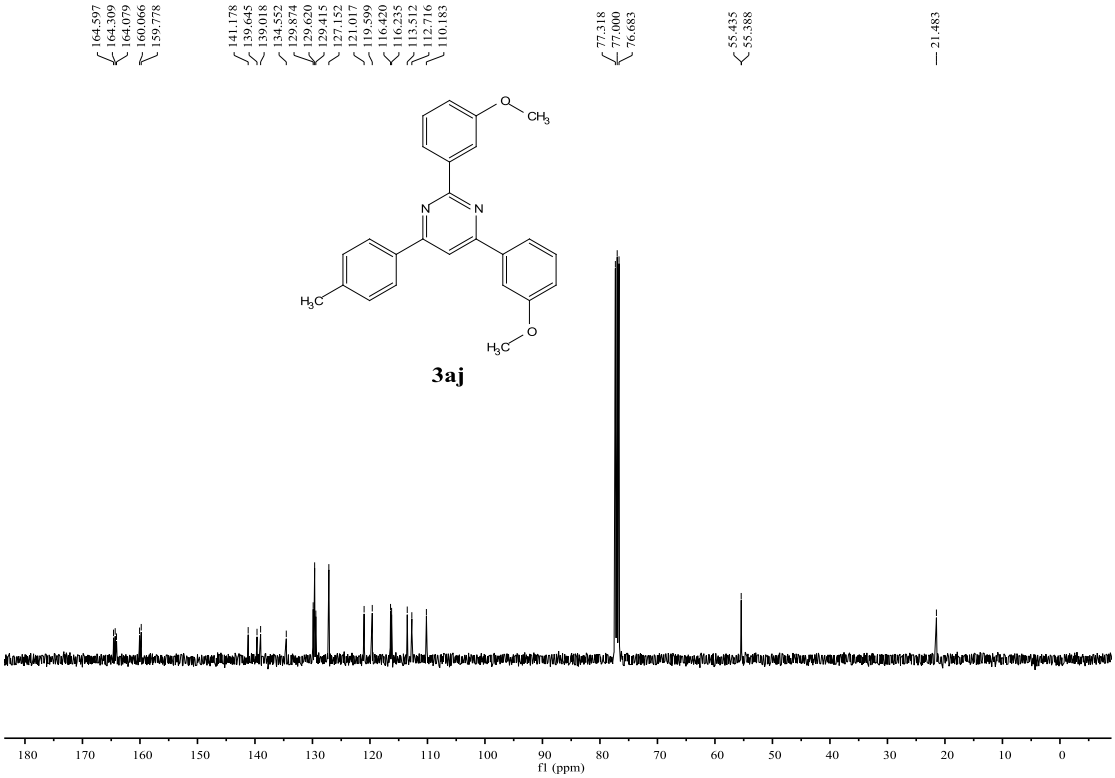
3ai


164.777
164.776
164.522
141.058
138.565
138.146
137.982
137.619
134.730
131.434
131.336
129.602
128.940
128.771
128.323
127.862
127.170
125.662
124.437
110.043
77.318
77.000
76.683
21.604
21.488
CH3
N
N
H3C
CH3
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

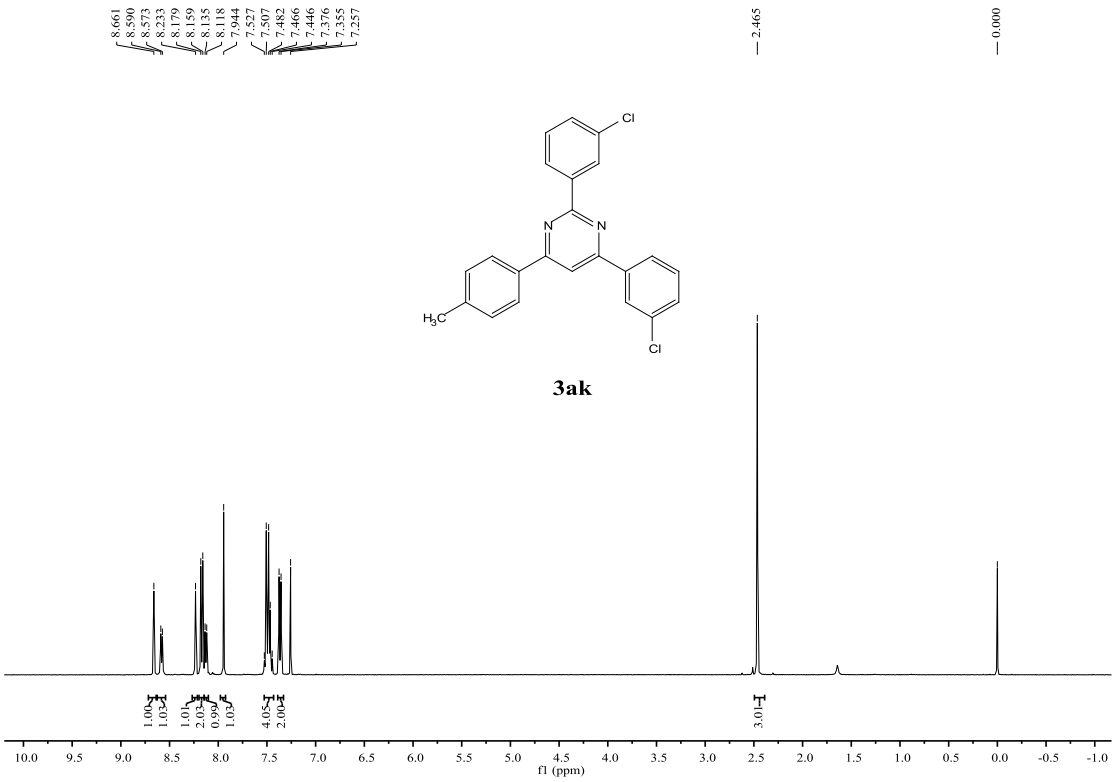
3ai


8.335
8.316
8.284
8.200
8.180
7.972
7.869
7.831
7.812
7.488
7.476
7.468
7.457
7.448
7.437
7.372
7.352
7.256
7.096
7.088
7.078
7.068
7.060
3.955
2.460
0.000
O
CH3
N
N
H3C
O
H3C
1.03
1.01
2.00
1.03
1.01
1.03
2.06
2.06
2.05
3.01
3.00
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

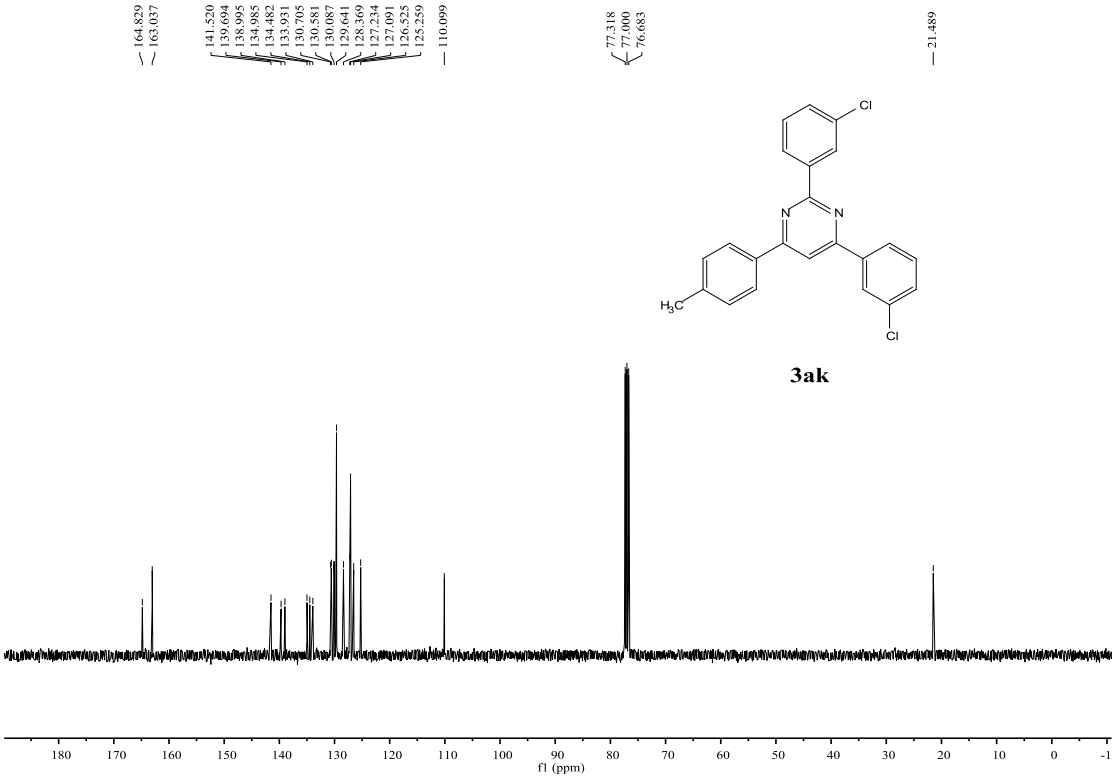
3aj


164.597
164.309
164.079
160.066
159.778
141.178
139.645
139.018
134.552
129.874
129.620
129.415
127.152
121.017
119.599
116.420
116.235
113.512
112.716
110.183
77.318
77.000
76.683
55.435
55.388
21.483
O
CH3
N
N
H3C
O
H3C
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

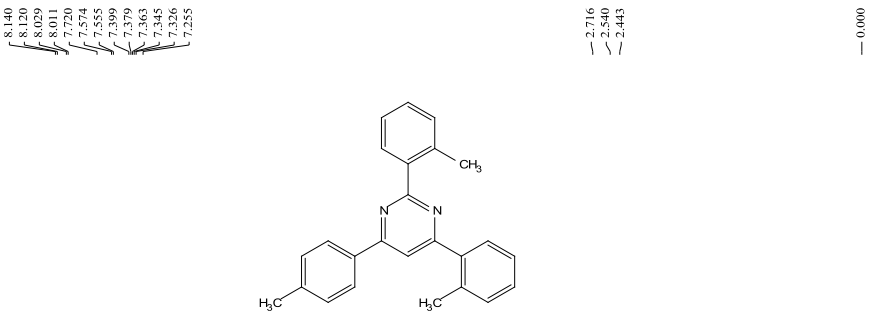
3aj


8.661
8.590
8.573
8.233
8.179
8.159
8.135
8.118
7.944
7.527
7.507
7.482
7.466
7.446
7.376
7.355
7.257
2.465
0.000
Cl
N
N
H3C
Cl
1.00
1.03
1.01
2.03
0.99
1.03
4.05
2.00
3.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

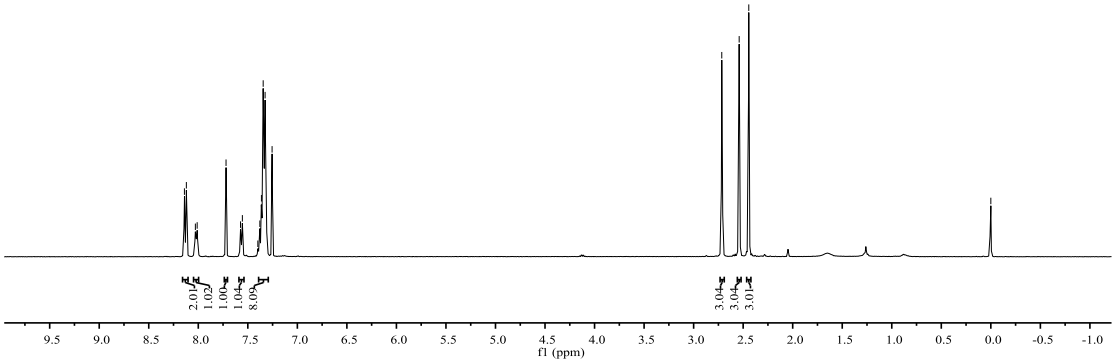
3ak


164.829
163.037
141.520
139.694
138.995
134.985
134.482
133.931
130.705
130.581
130.087
129.641
128.369
127.234
127.091
126.525
125.259
110.099
77.318
77.000
76.683
21.489
Cl
N
N
H3C
Cl
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

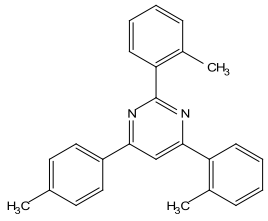
3ak


8.140
8.120
8.029
8.011
7.720
7.574
7.555
7.399
7.379
7.363
7.345
7.326
7.255
2.716
2.540
2.443
0.000
CH3
N
N
H3C
H3C

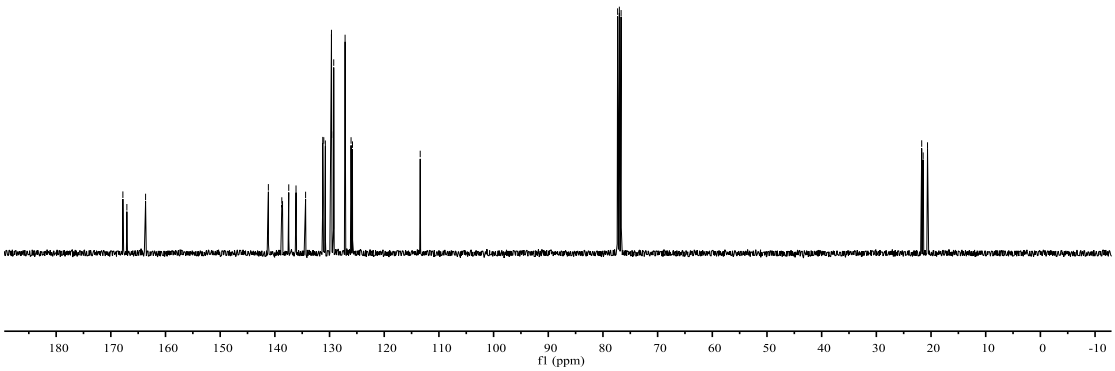
3al

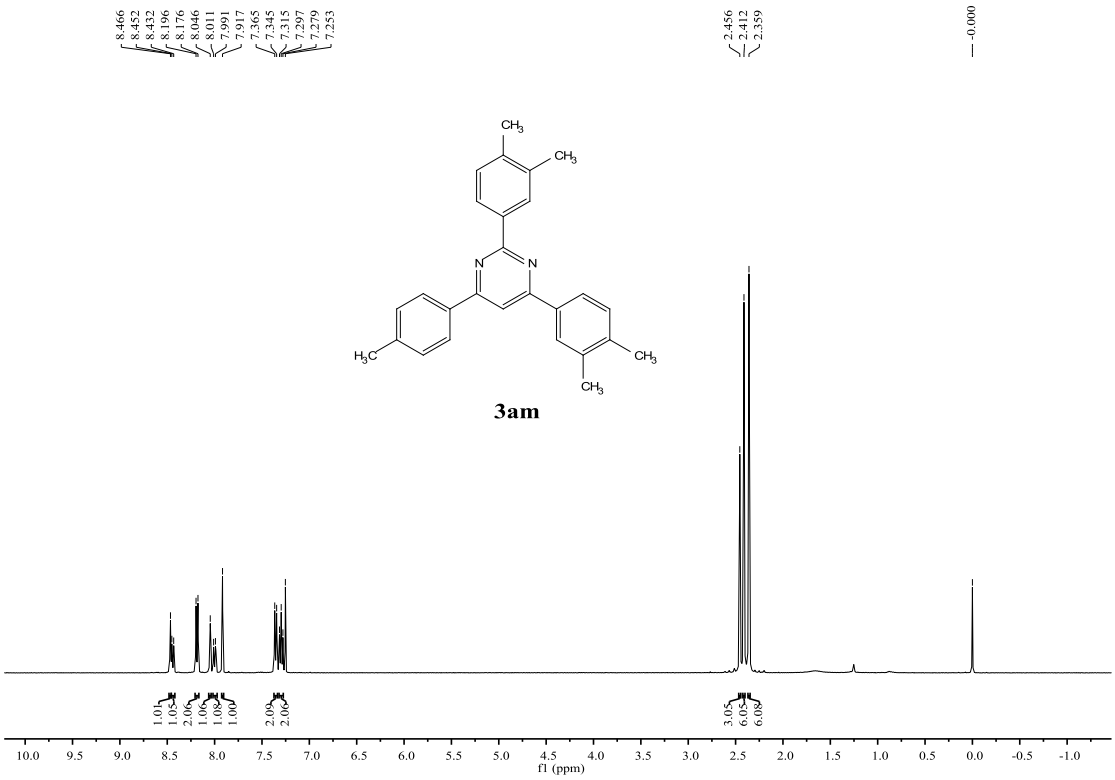

2.01
1.03
1.00
1.04
8.09
3.04
3.04
3.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

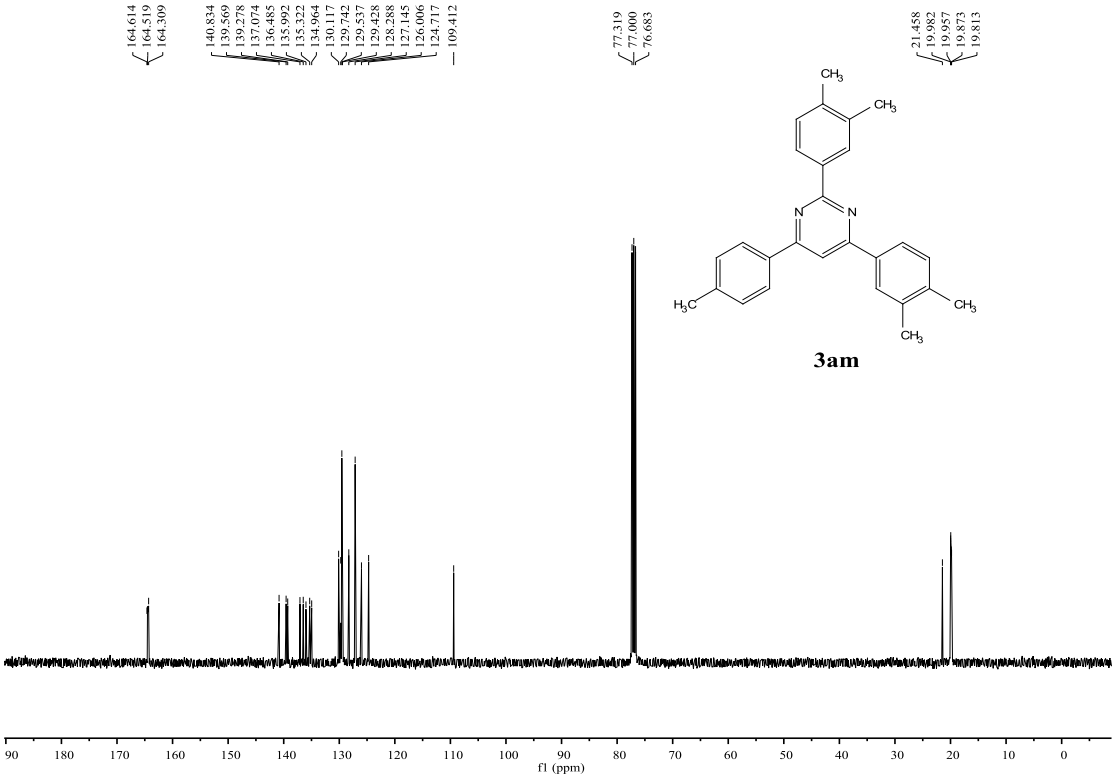

167.797
167.068
163.646
141.187
138.729
138.597
137.461
136.132
134.381
131.242
131.053
130.770
129.650
129.615
129.238
127.160
126.066
125.806
113.421
77.318
77.000
76.682
21.705
21.439
20.642

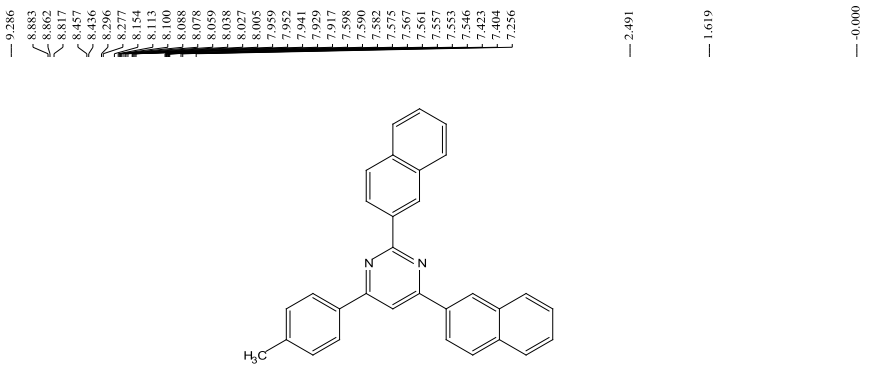

CH3
N
N
H3C
H3C

3al

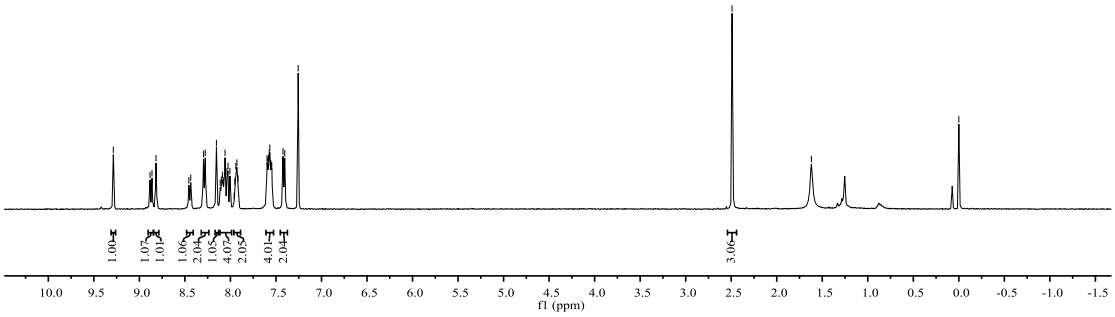

180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

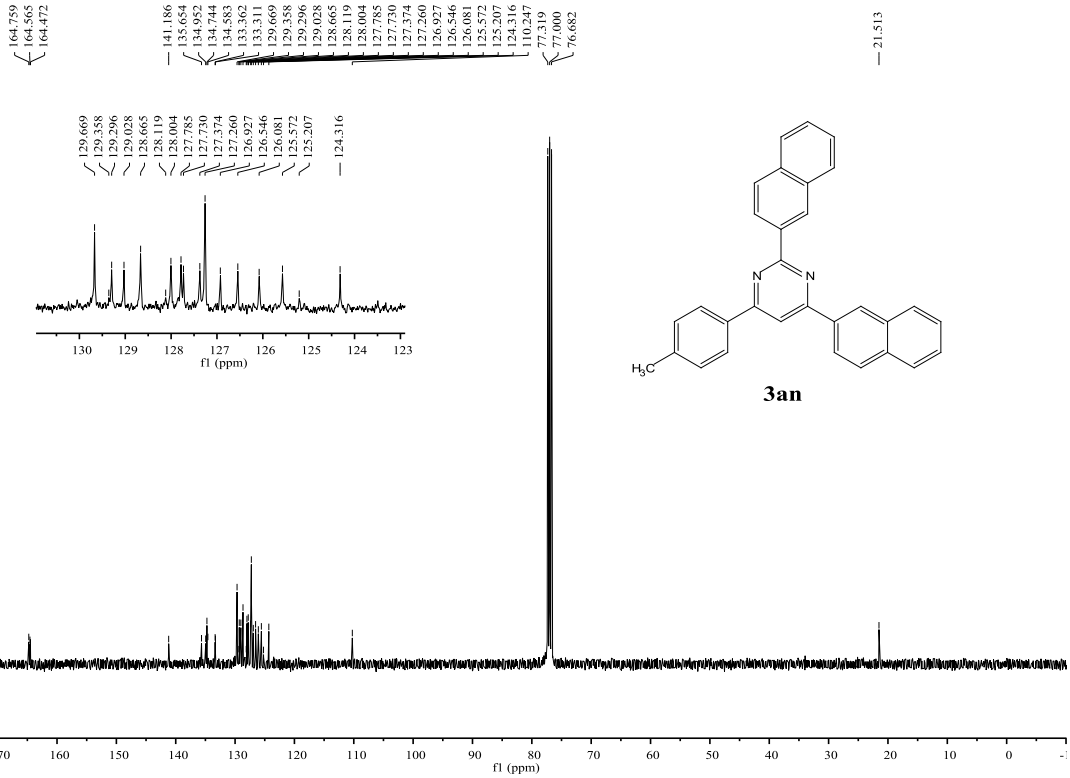

8.466
8.452
8.432
8.196
8.176
8.046
8.011
7.991
7.917
7.365
7.345
7.315
7.297
7.279
7.253
2.456
2.412
2.359
-0.000
3am
1.01
1.05
2.06
1.06
1.08
1.00
2.09
2.00
3.05
6.05
6.08
f1 (ppm)


164.614
164.519
164.309
140.834
139.569
139.278
137.074
136.485
135.992
135.322
134.964
130.117
129.742
129.537
129.428
128.288
127.145
126.006
124.717
109.412
77.319
77.000
76.683
21.458
19.982
19.957
19.873
19.813
3am
f1 (ppm)

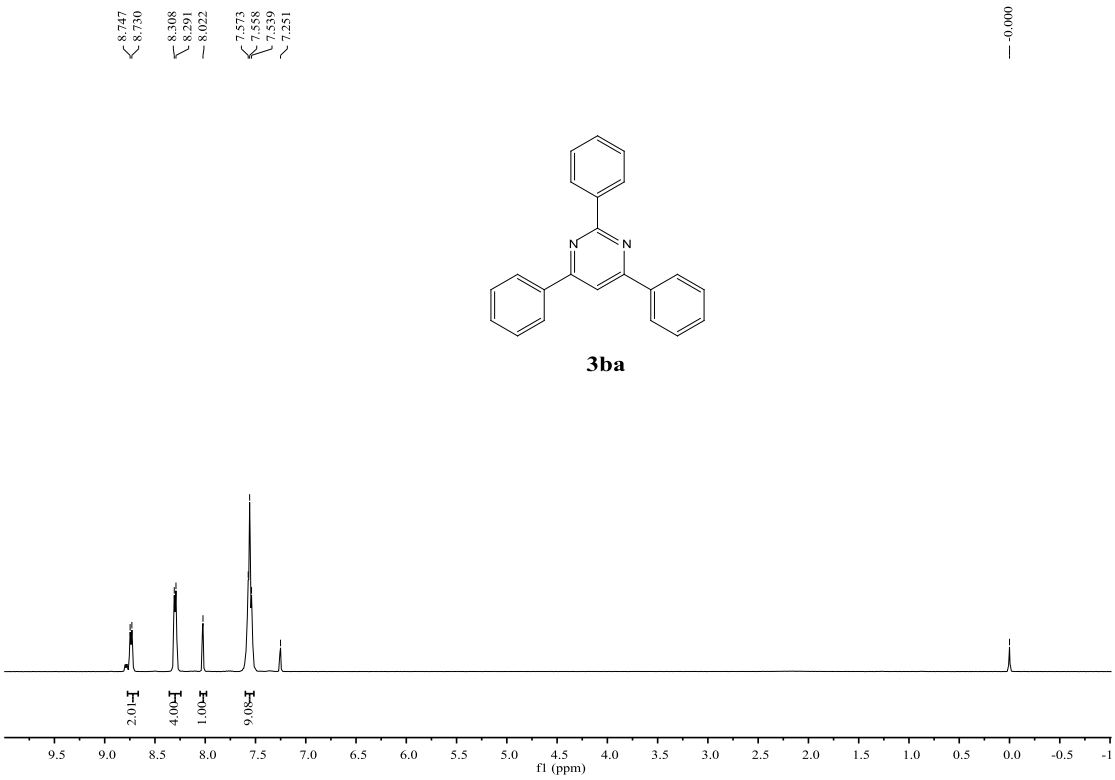

9.286
8.883
8.862
8.817
8.457
8.436
8.296
8.277
8.154
8.113
8.100
8.088
8.078
8.059
8.038
8.027
8.005
7.959
7.952
7.941
7.929
7.917
7.598
7.590
7.582
7.575
7.567
7.561
7.557
7.553
7.546
7.423
7.404
7.256
2.491
1.619
-0.000
N
N
H3C

3an

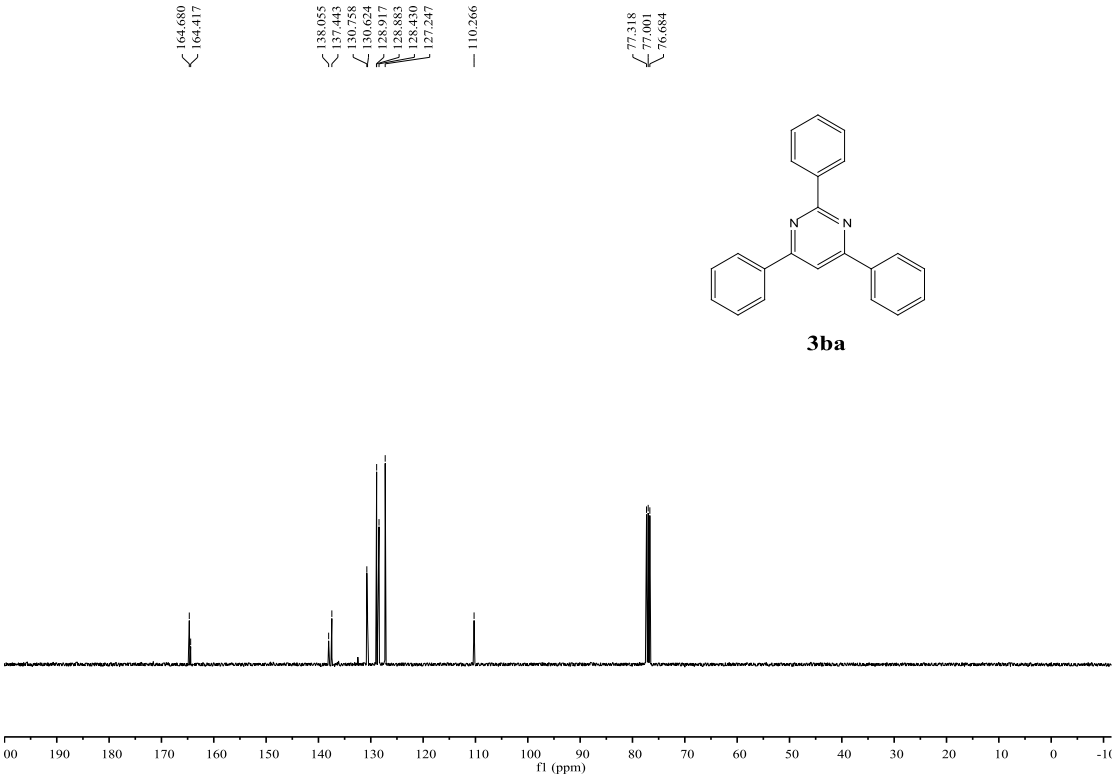

1.00
1.07
1.01
1.06
2.04
1.05
4.07
2.05
4.01
2.04
3.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)


164.759
164.565
164.472
141.186
135.654
134.952
134.744
134.583
133.362
133.311
129.669
129.358
129.296
129.028
128.665
128.119
128.004
127.785
127.730
127.374
127.260
126.927
126.546
126.081
125.572
125.207
124.316
110.247
77.319
77.000
76.682
21.513
129.669
129.358
129.296
129.028
128.665
128.119
128.004
127.785
127.730
127.374
127.260
126.927
126.546
126.081
125.572
125.207
124.316
130 129 128 127 126 125 124 123
f1 (ppm)
N
N
H3C
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

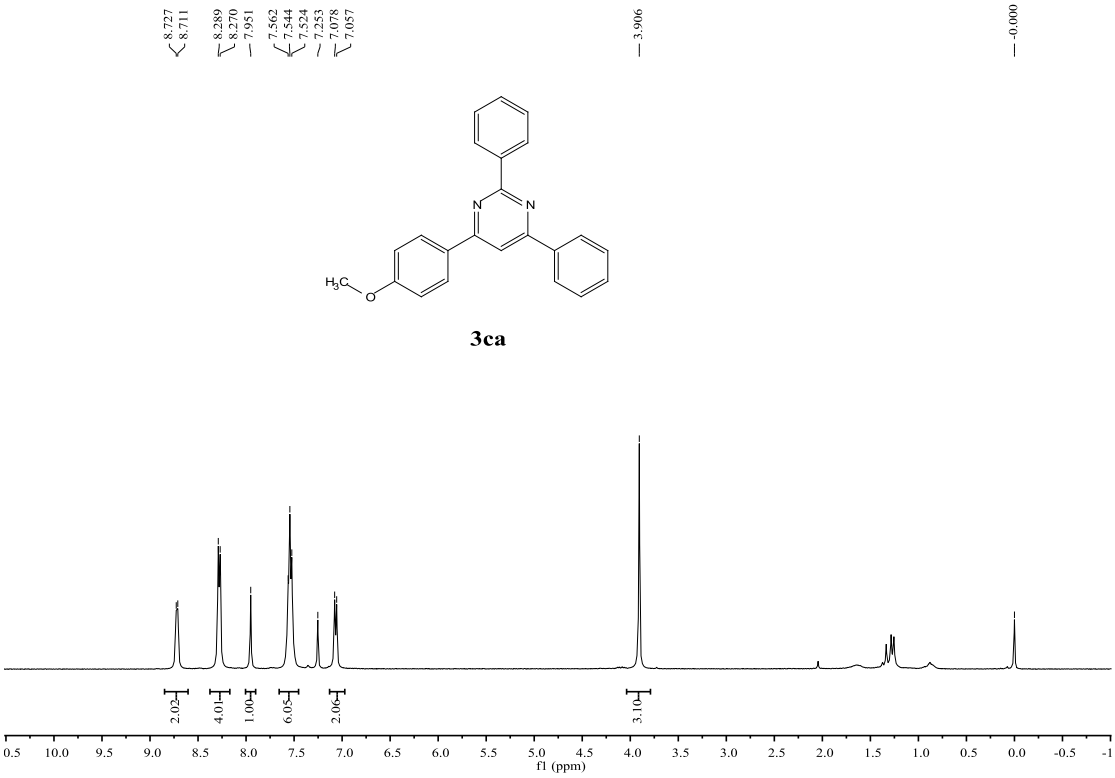
3an


8.747
8.730
8.308
8.291
8.022
7.573
7.558
7.539
7.251
-0.000
N
N
2.01
4.00
1.00
9.08
f1 (ppm)

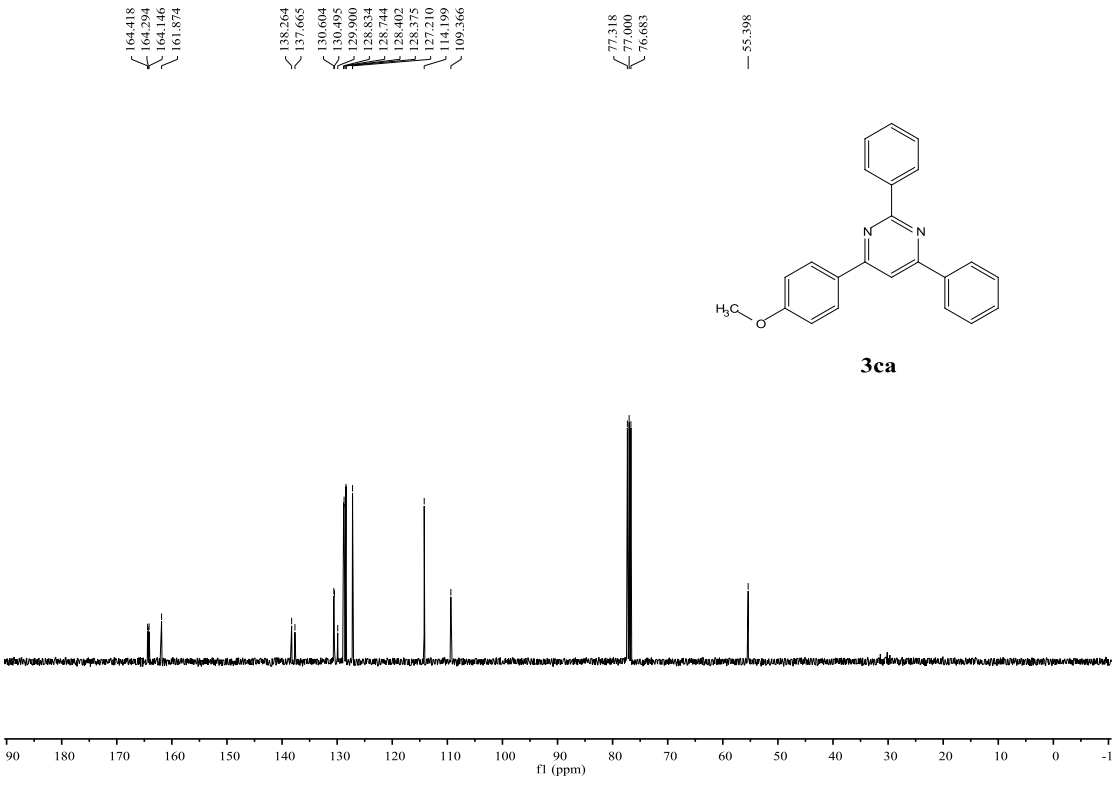
3ba


164.680
164.417
138.055
137.443
130.758
130.624
128.917
128.883
128.430
127.247
110.266
77.318
77.001
76.684
N
N
f1 (ppm)

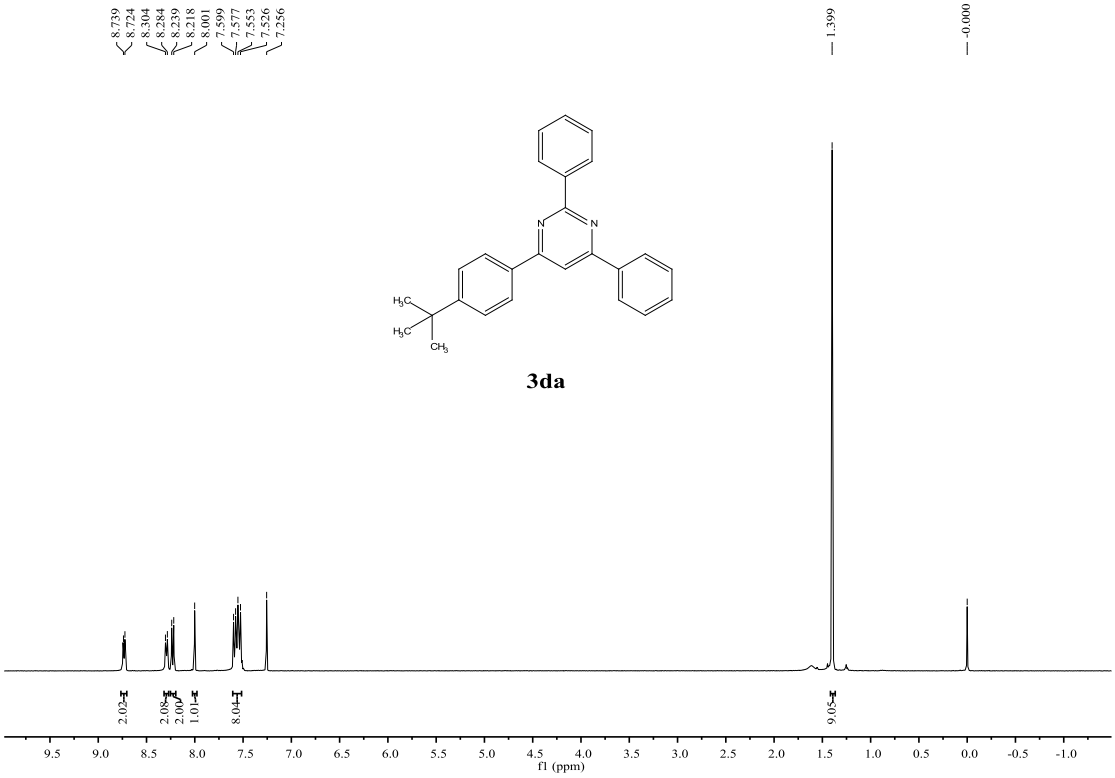
3ba


8.727
8.711
8.289
8.270
7.951
7.562
7.544
7.524
7.253
7.078
7.057
3.906
-0.000
N
N
H3C
O
2.02
4.01
1.00
6.05
2.06
3.10
f1 (ppm)

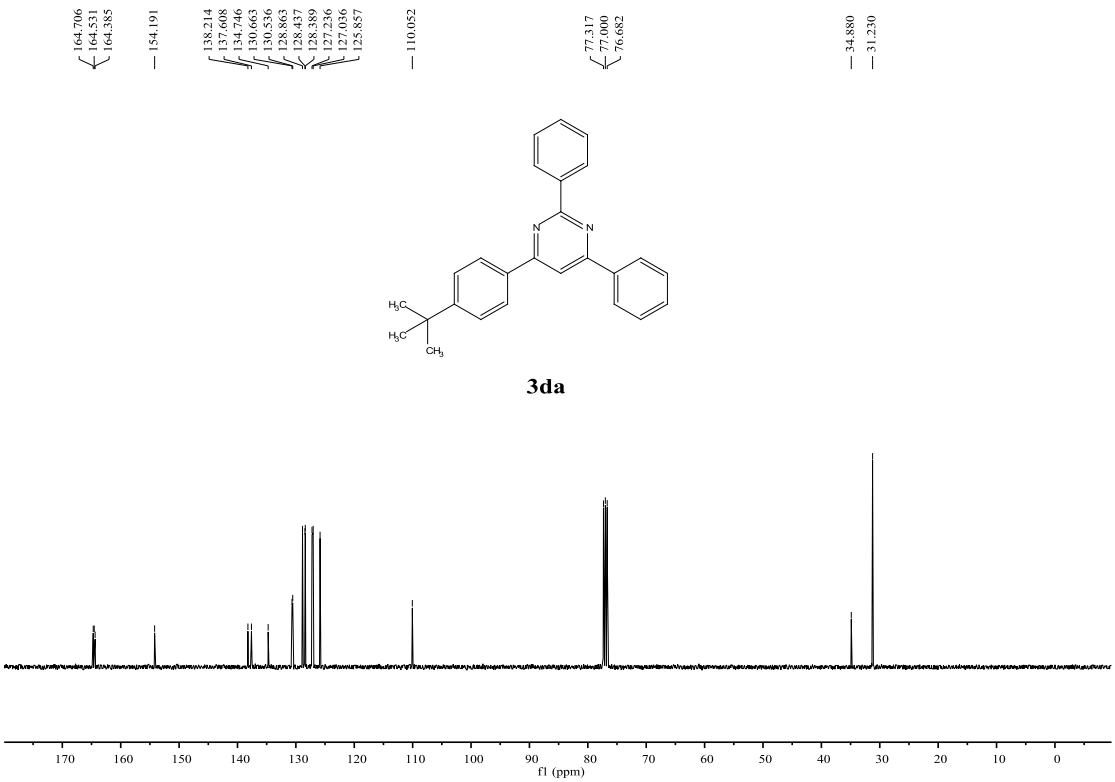
3ca


164.418
164.294
164.146
161.874
138.264
137.665
130.604
130.495
129.900
128.834
128.744
128.402
128.375
127.210
114.199
109.366
77.318
77.000
76.683
55.398
N
N
H3C
O
f1 (ppm)

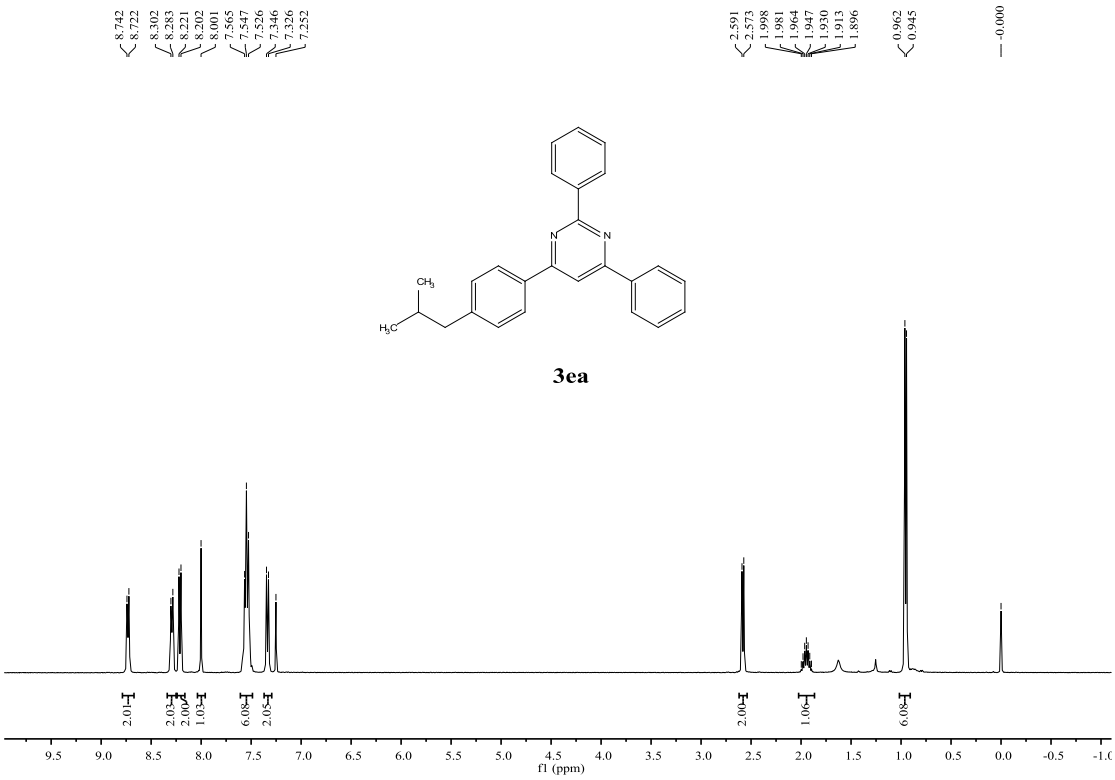
3ca


8.739
8.724
8.304
8.284
8.239
8.218
8.001
7.599
7.577
7.553
7.526
7.256
1.399
-0.000
N
N
H3C
H3C
CH3
2.02
2.08
2.00
1.01
8.04
9.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

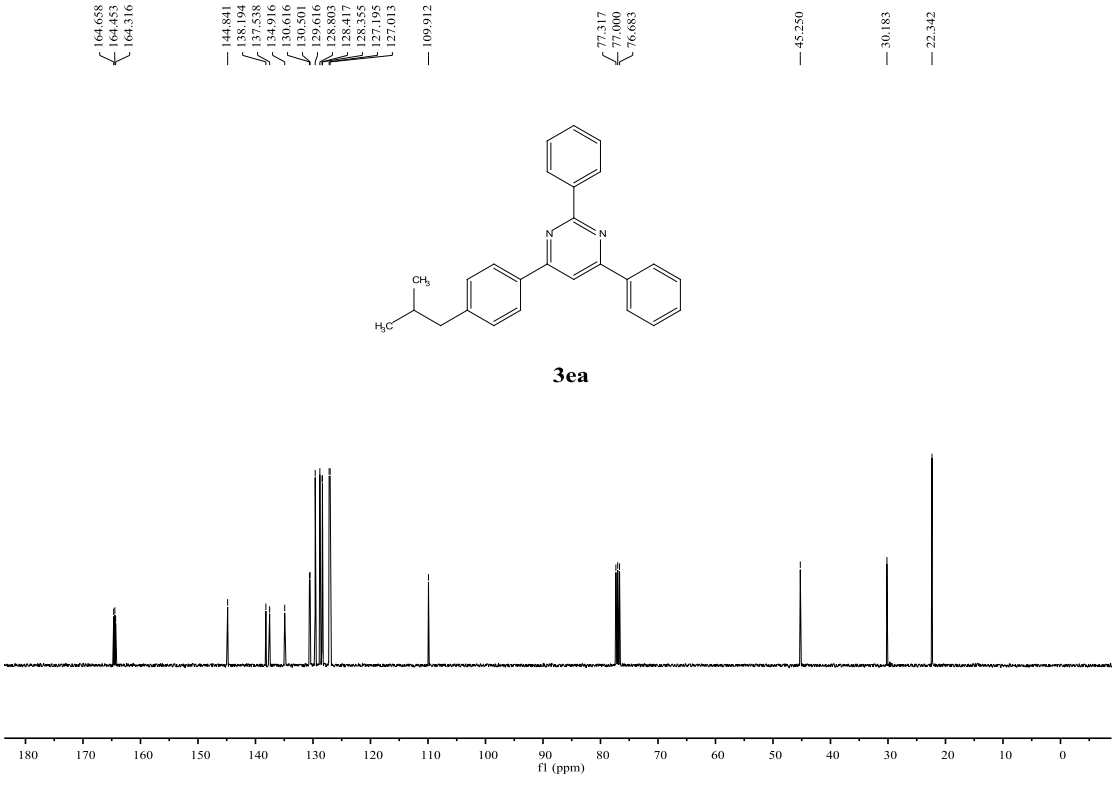
3da


164.706
164.531
164.385
154.191
138.214
137.608
134.746
130.663
130.536
128.863
128.437
128.389
127.236
127.036
125.857
110.052
77.317
77.000
76.682
34.880
31.230
N
N
H3C
H3C
CH3
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

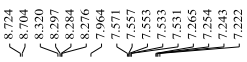
3da


8.742
8.722
8.302
8.283
8.221
8.202
8.001
7.565
7.547
7.526
7.346
7.326
7.252
2.591
2.573
1.998
1.981
1.964
1.947
1.930
1.913
1.896
0.962
0.945
-0.000
N
N
CH3
H3C
2.01
2.03
2.00
1.03
6.08
2.05
2.00
1.06
6.08
f1 (ppm)

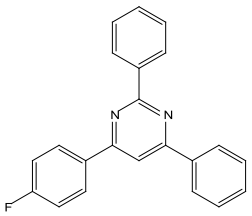
3ea


164.658
164.453
164.316
144.841
138.194
137.538
134.916
130.616
130.501
129.616
128.803
128.417
128.355
127.195
127.013
109.912
77.317
77.000
76.683
45.250
30.183
22.342
N
N
CH3
H3C
f1 (ppm)

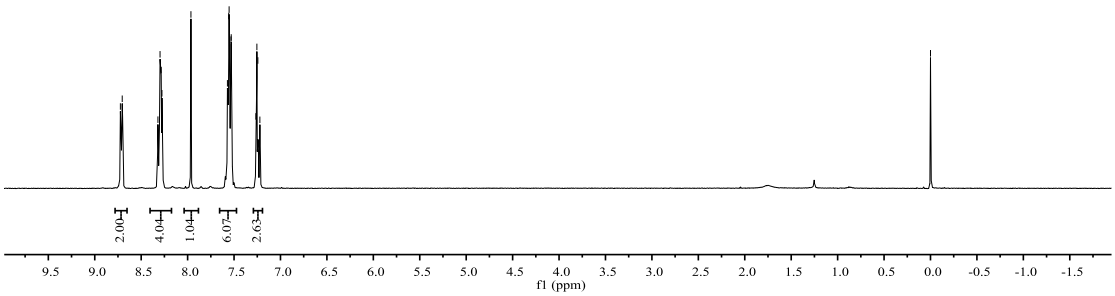
3ea

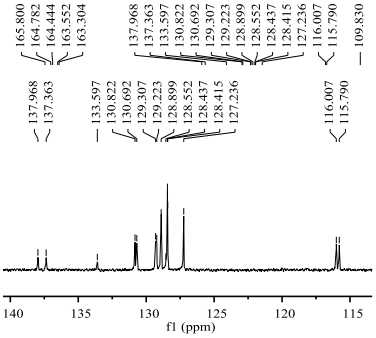

8.724
8.704
8.320
8.297
8.284
8.276
7.964
7.571
7.557
7.553
7.533
7.531
7.265
7.254
7.243
7.222

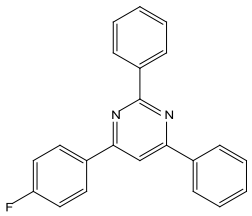
-0.000


N
N
F

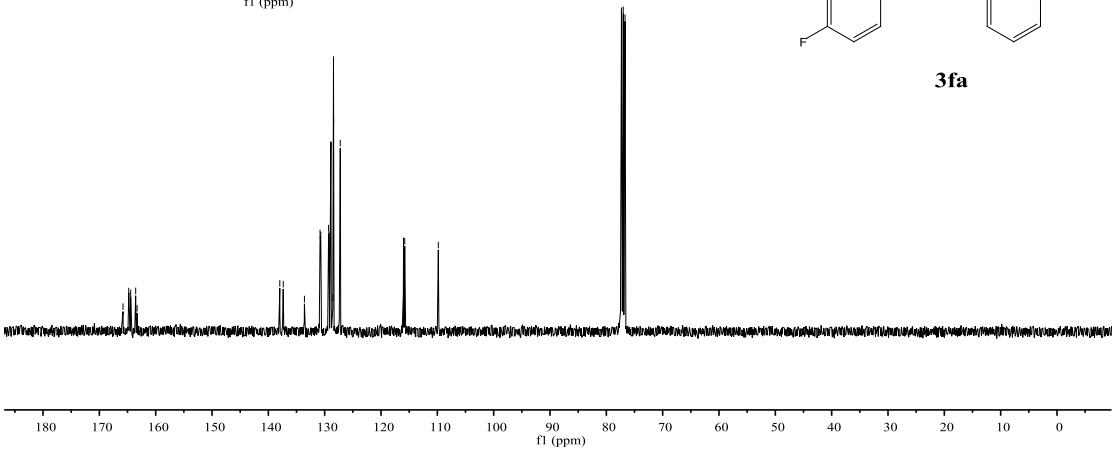
3fa

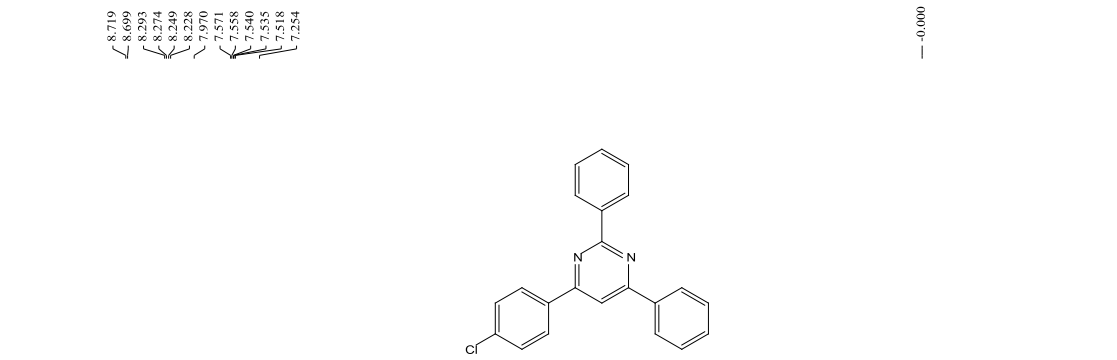

2.00
4.04
1.04
6.07
2.63
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)


165.800
164.782
164.444
163.552
163.304
137.968
137.363
133.597
130.822
130.692
129.307
129.223
128.899
128.552
128.437
128.415
127.236
116.007
115.790
109.830
77.319
77.000
76.684
140 135 130 125 120 115
f1 (ppm)

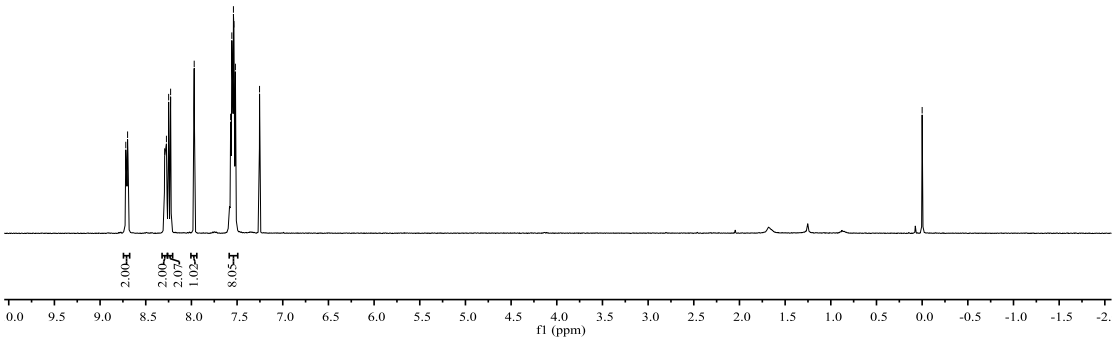

N
N
F

3fa

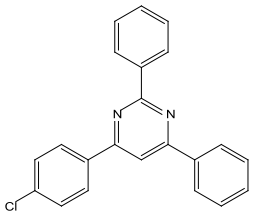

180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.719
8.699
8.293
8.274
8.249
8.228
7.970
7.571
7.558
7.540
7.535
7.518
7.254
-0.000
N
N
Cl

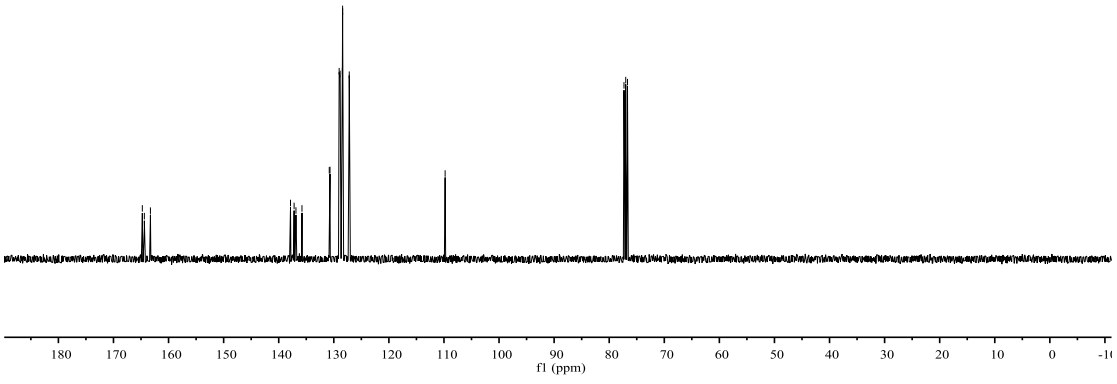
3ga

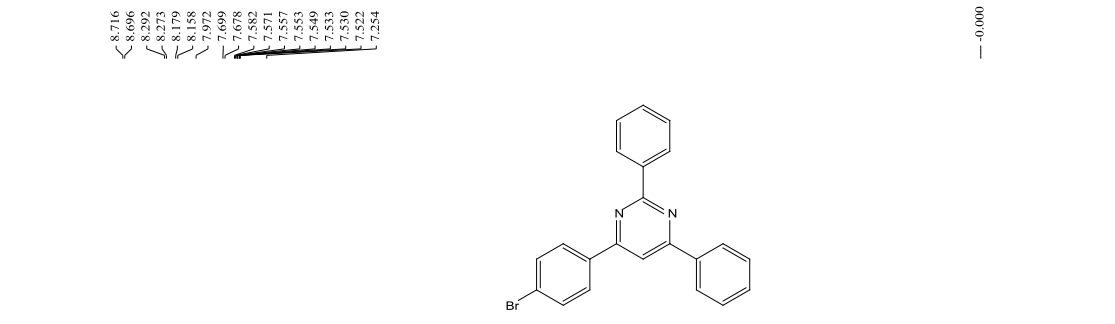

2.00
2.00
2.07
1.02
8.05
f1 (ppm)


164.762
164.394
163.292
137.860
137.208
136.871
135.778
130.824
130.691
129.029
128.847
128.451
128.400
128.395
127.195
109.788
77.318
77.000
76.682

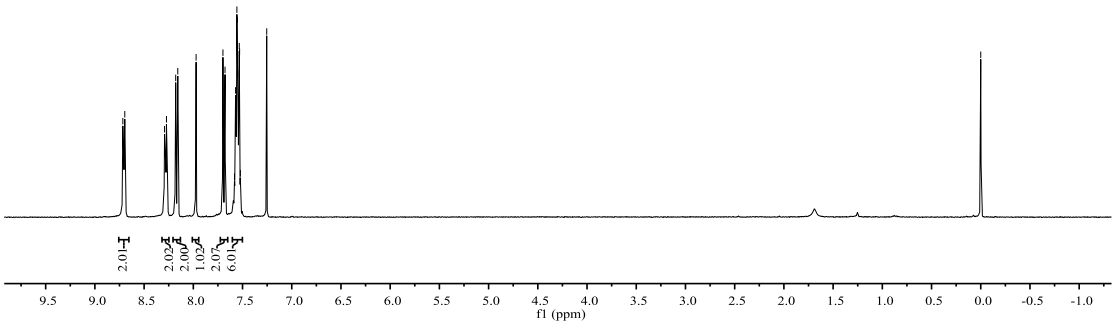

N
N
Cl

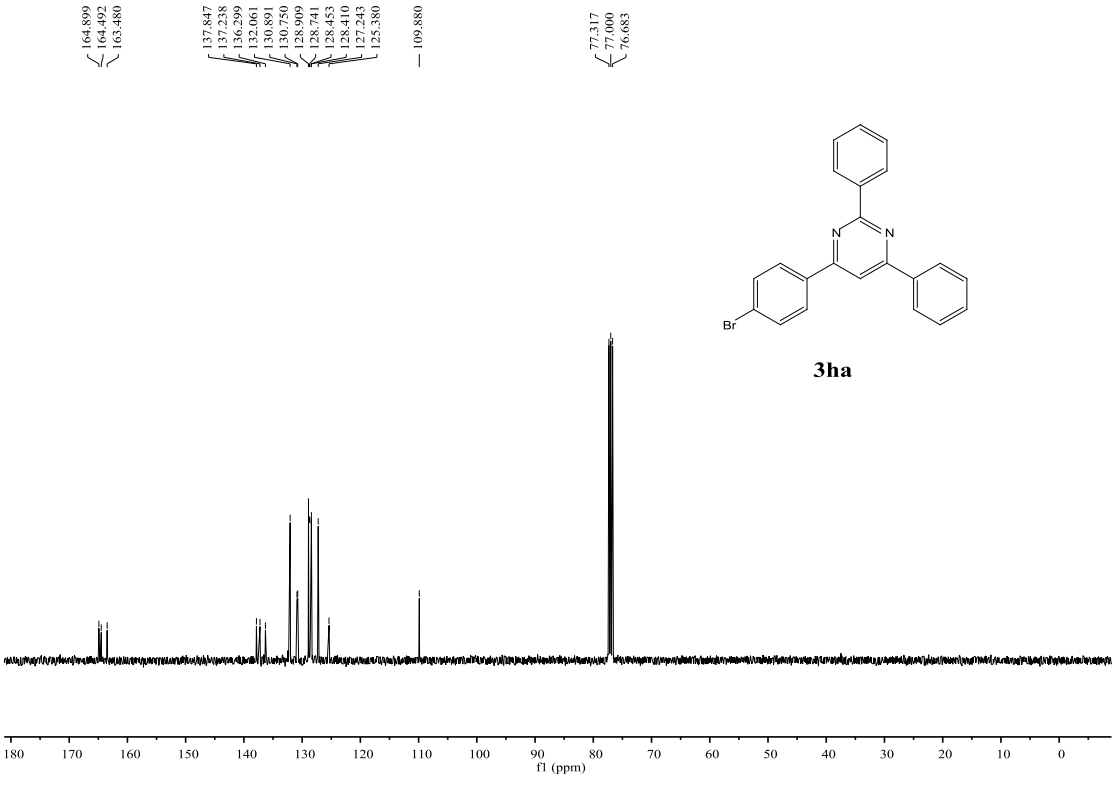
3ga


f1 (ppm)

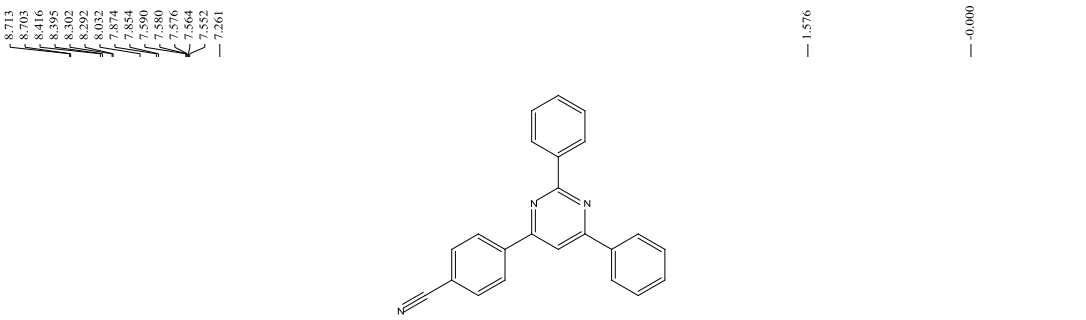

8.716
8.696
8.292
8.273
8.179
8.158
7.972
7.699
7.678
7.582
7.571
7.557
7.553
7.549
7.533
7.530
7.522
7.254
-0.000
N
N
Br

3ha

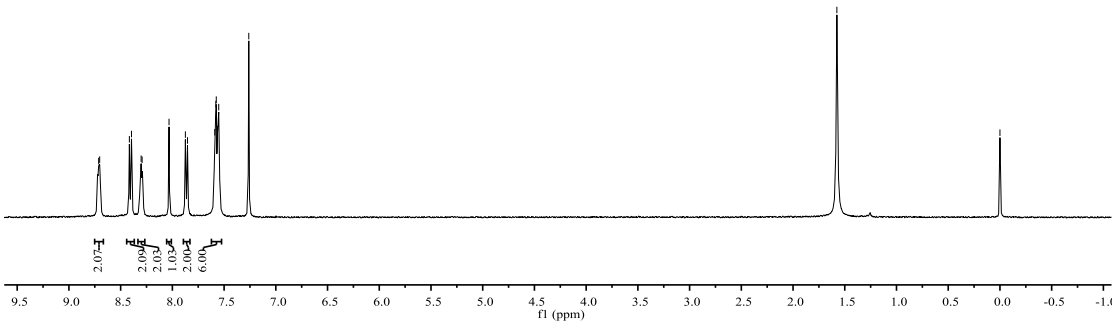

2.01
2.02
2.00
1.02
2.07
6.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

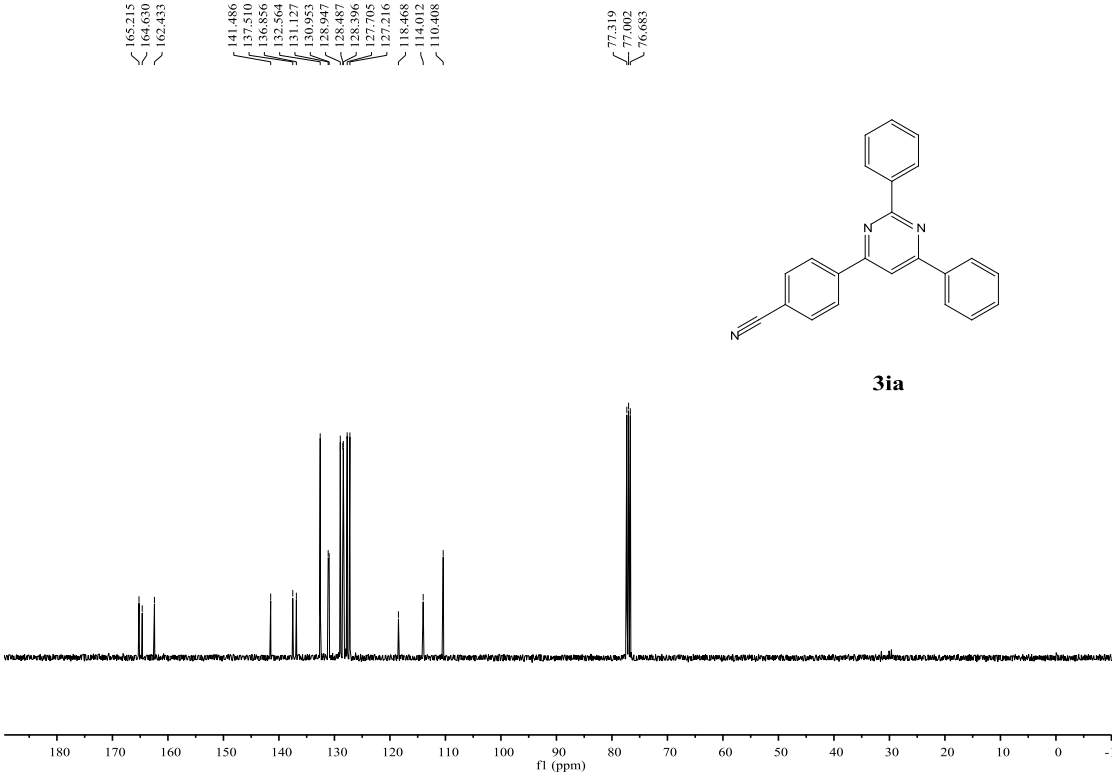

164.899
164.492
163.480
137.847
137.238
136.299
132.061
130.891
130.750
128.909
128.741
128.453
128.410
127.243
125.380
109.880
77.317
77.000
76.683
N
N
Br
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3ha

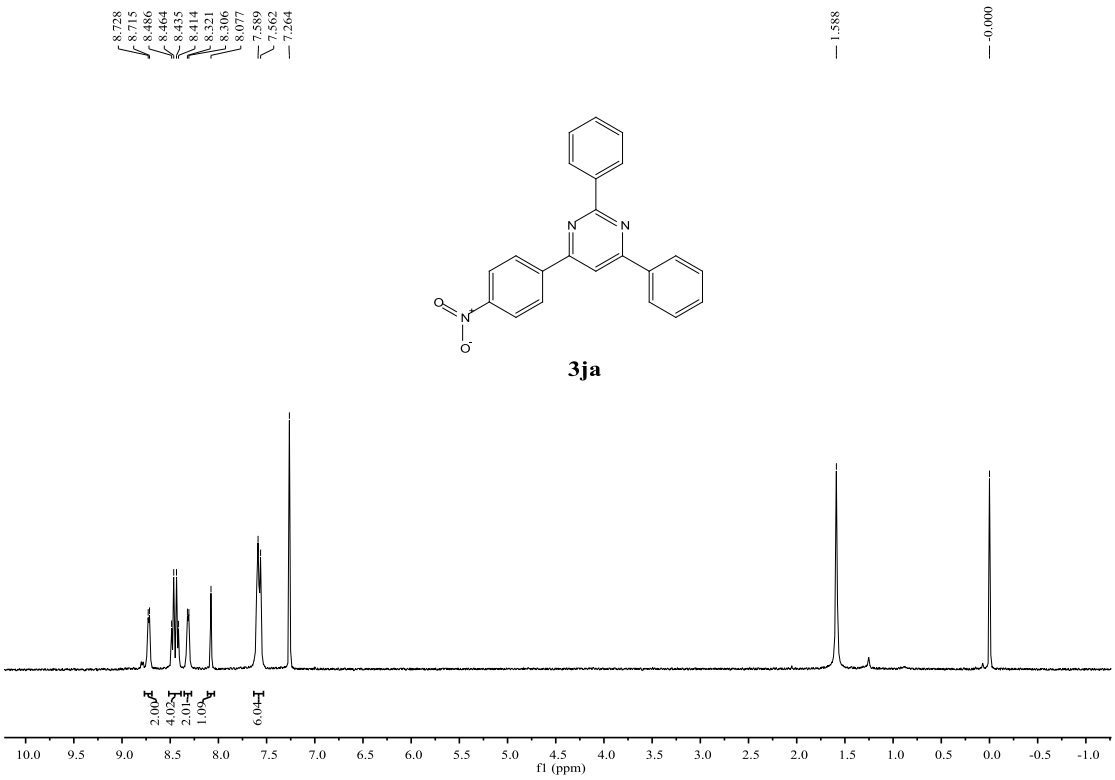

8.713
8.703
8.416
8.395
8.302
8.292
8.032
7.874
7.854
7.590
7.580
7.576
7.564
7.552
7.261
1.576
-0.000
N
N
N

3ia

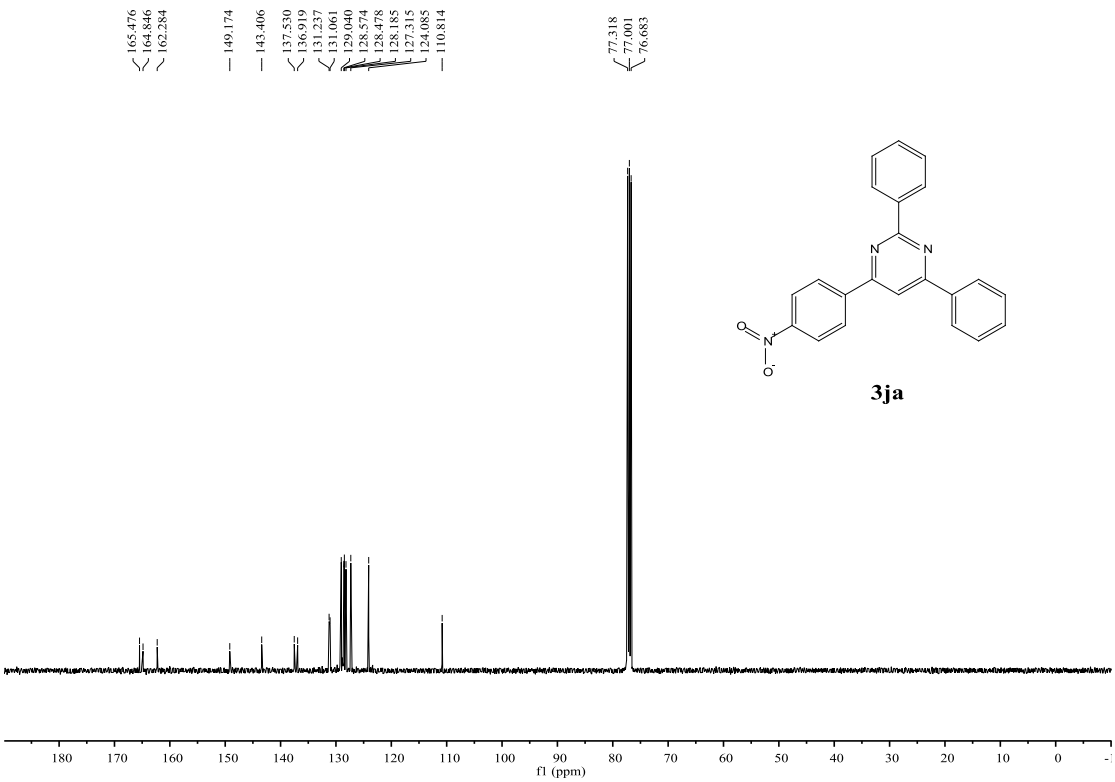

2.07
2.09
2.03
1.03
2.00
6.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


165.215
164.630
162.433
141.486
137.510
136.856
132.564
131.127
130.953
128.947
128.487
128.396
127.705
127.216
118.468
114.012
110.408
77.319
77.002
76.683
N
N
N
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

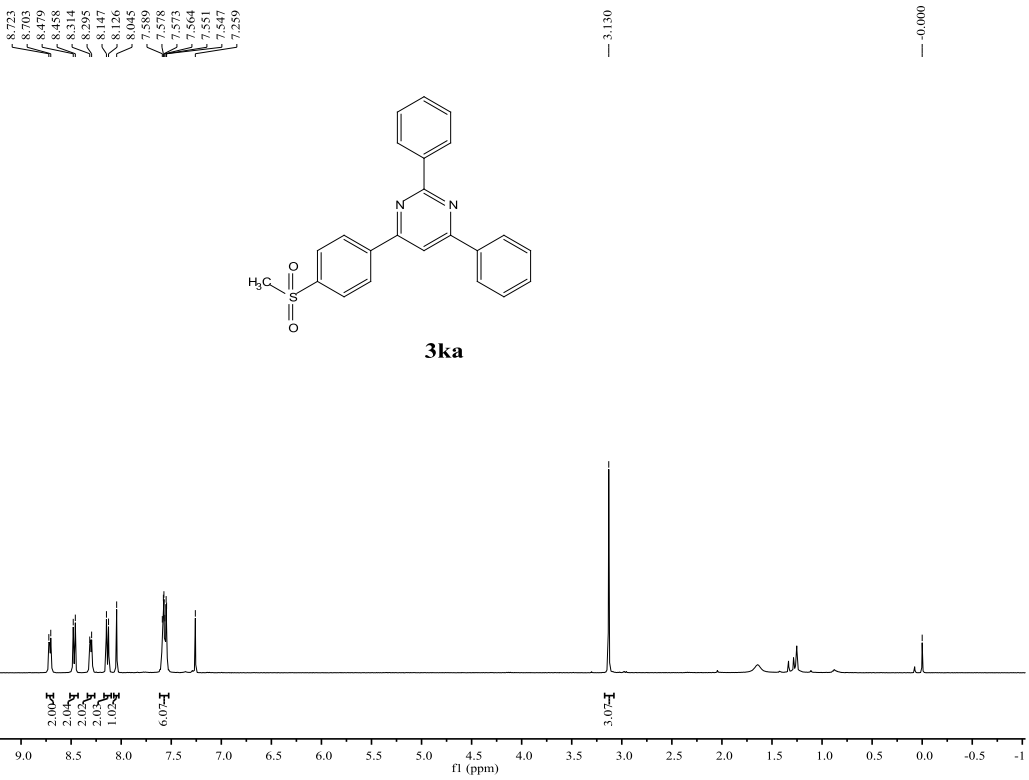
3ia


8.728
8.715
8.486
8.464
8.435
8.414
8.321
8.306
8.077
7.589
7.562
7.264
1.588
0.000
2.00
4.02
2.01
1.09
6.04
f1 (ppm)

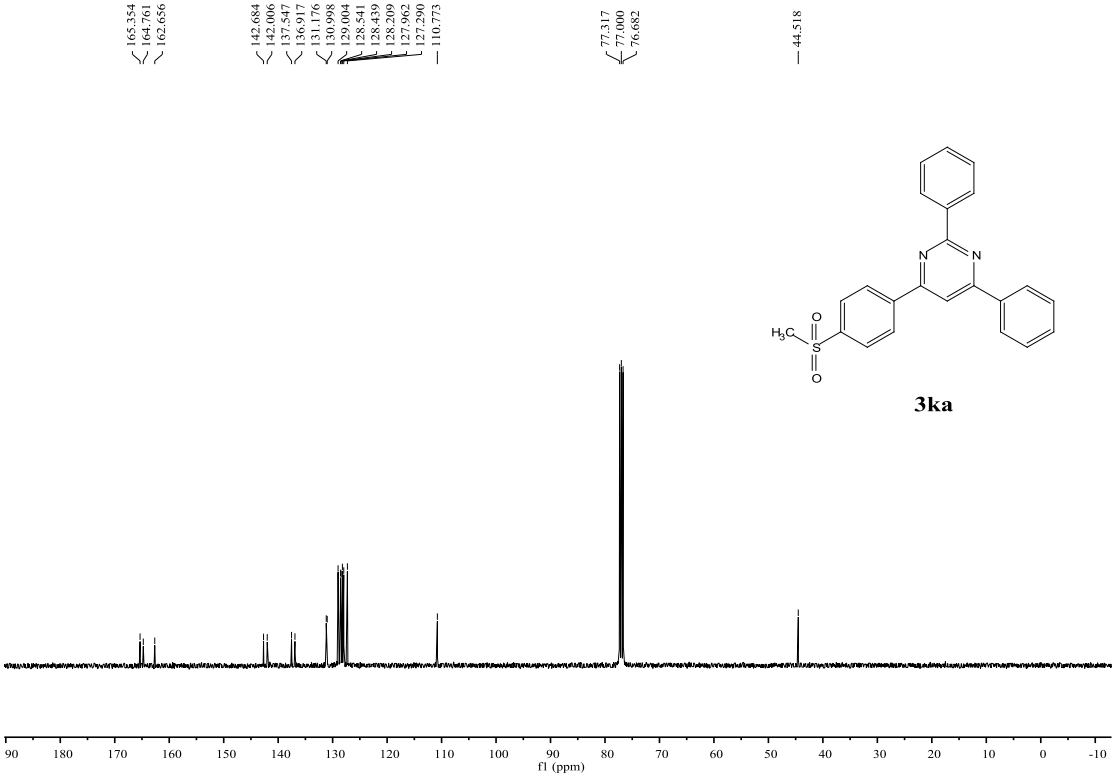
3ja


165.476
164.846
162.284
149.174
143.406
137.530
136.919
131.237
131.061
129.040
128.574
128.478
128.185
127.315
124.085
110.814
77.318
77.001
76.683
f1 (ppm)

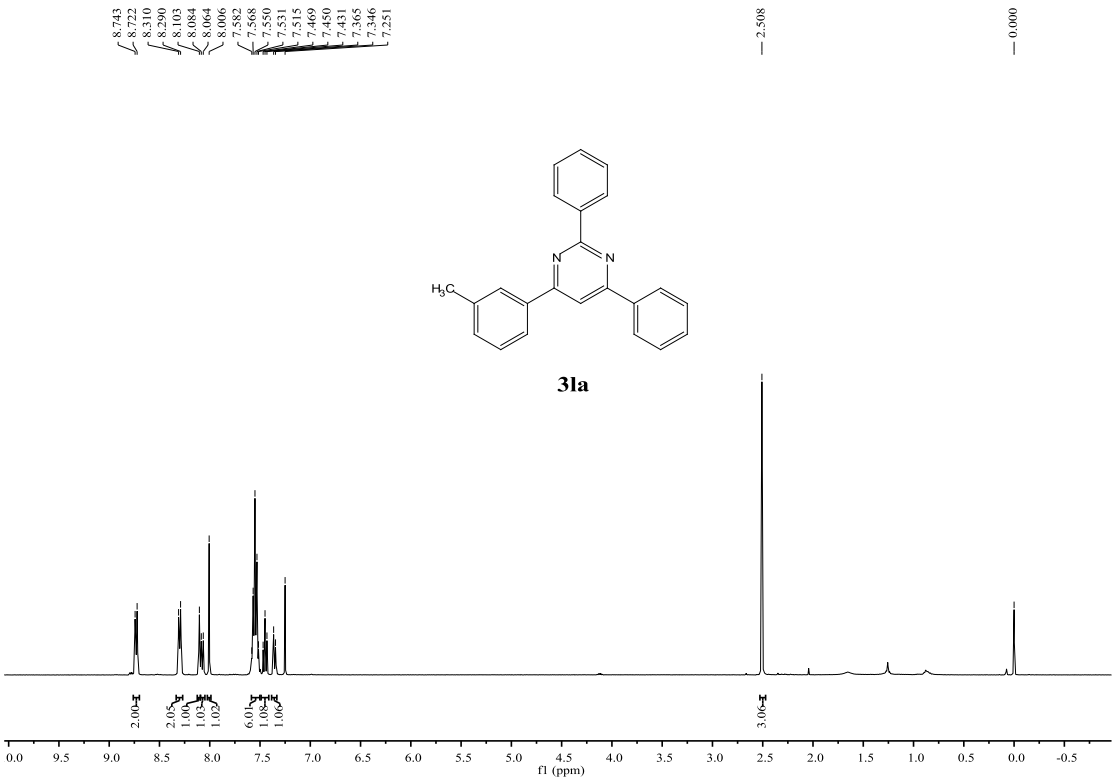
3ja


8.723
8.703
8.479
8.458
8.314
8.295
8.147
8.126
8.045
7.589
7.578
7.573
7.564
7.551
7.547
7.259
3.130
-0.000
N
N
O
S
O
H3C
2.00
2.04
2.02
2.03
1.02
6.07
3.07
f1 (ppm)

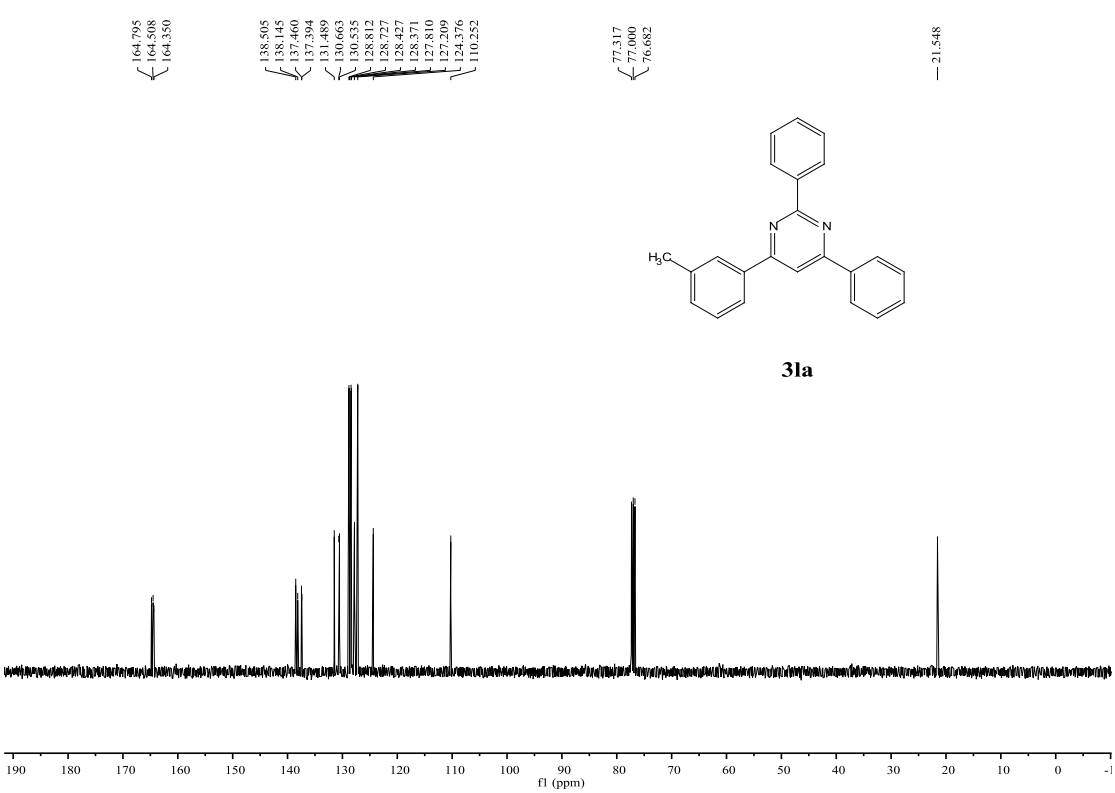
3ka


165.354
164.761
162.656
142.684
142.006
137.547
136.917
131.176
130.998
129.004
128.541
128.439
128.209
127.962
127.290
110.773
77.317
77.000
76.682
44.518
N
N
O
S
O
H3C
f1 (ppm)

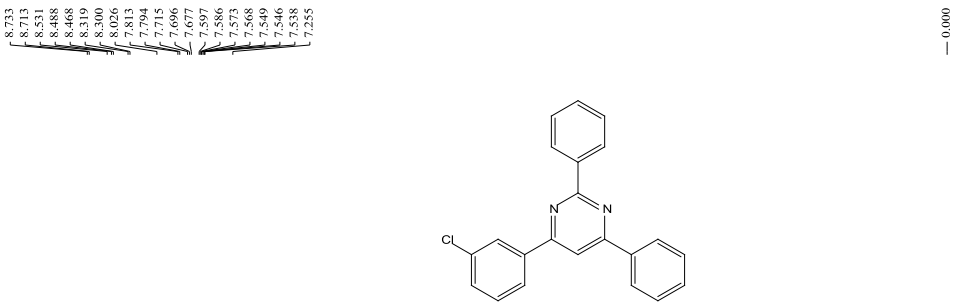
3ka


8.743
8.722
8.310
8.290
8.103
8.084
8.064
8.006
7.582
7.568
7.550
7.531
7.515
7.469
7.450
7.431
7.365
7.346
7.251
2.508
0.000
N
N
H3C
2.00
2.05
1.00
1.03
1.02
6.01
1.08
1.06
3.06
f1 (ppm)

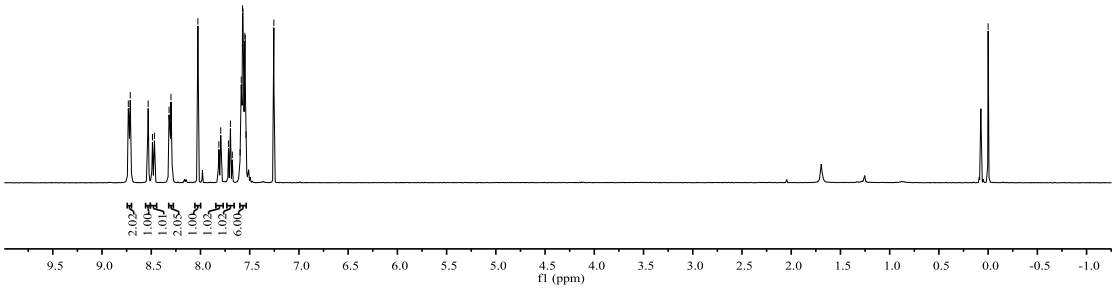
3la


164.795
164.508
164.350
138.505
138.145
137.460
137.394
131.489
130.663
130.535
128.812
128.727
128.427
128.371
127.810
127.209
124.376
110.252
77.317
77.000
76.682
21.548
N
N
H3C
f1 (ppm)

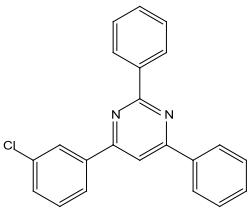
3la


8.733
8.713
8.531
8.488
8.468
8.319
8.300
8.026
7.813
7.794
7.715
7.696
7.677
7.597
7.586
7.573
7.568
7.549
7.546
7.538
7.255
0.000
N
N
Cl

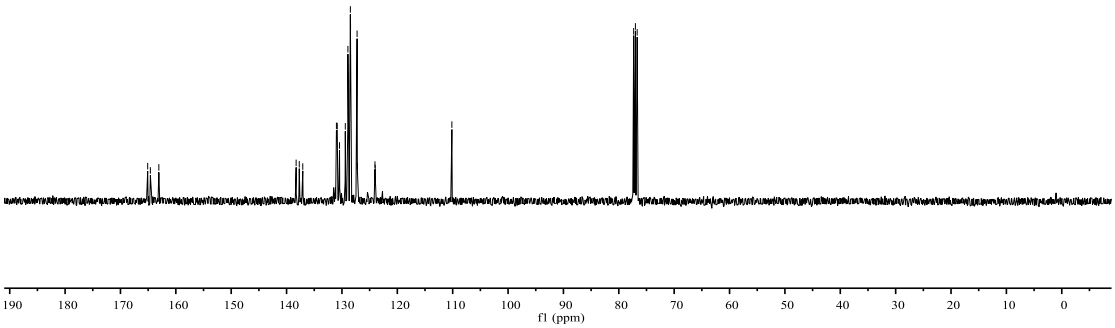
3ma

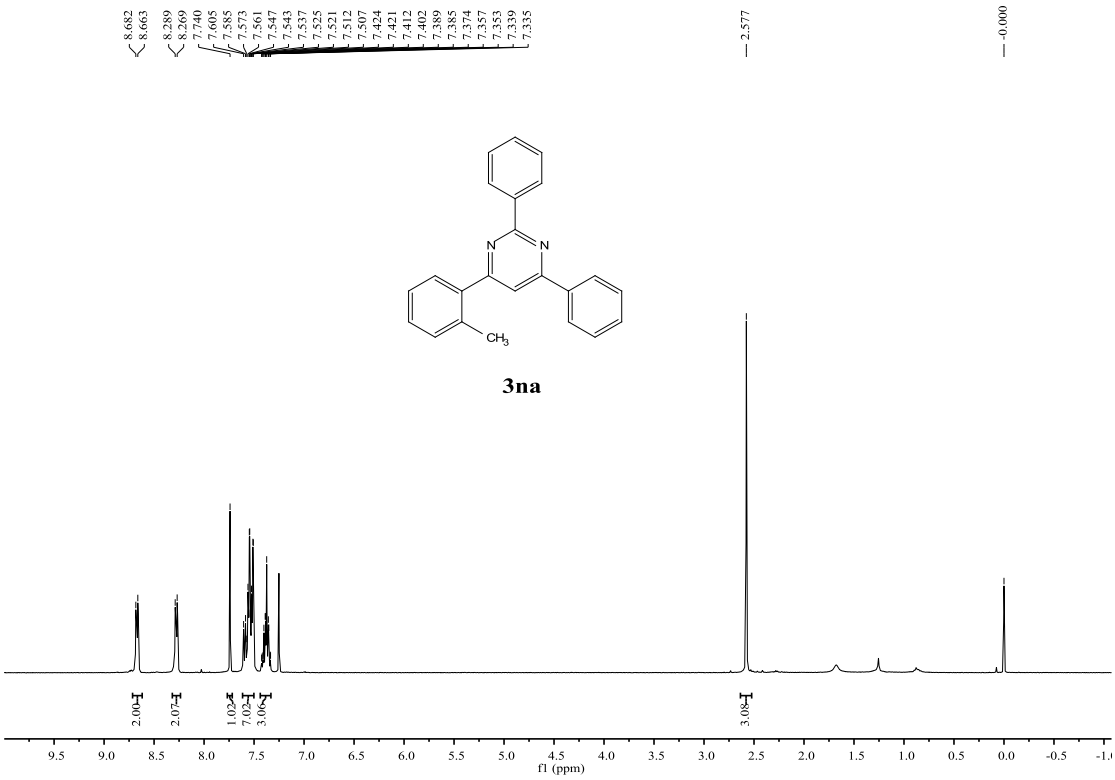

2.02
1.00
1.01
2.05
1.00
1.03
1.03
6.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


165.084
164.600
163.069
138.275
137.711
137.075
130.998
130.849
130.440
129.394
128.923
128.482
128.449
127.268
127.200
124.038
123.999
110.147
77.318
77.000
76.683

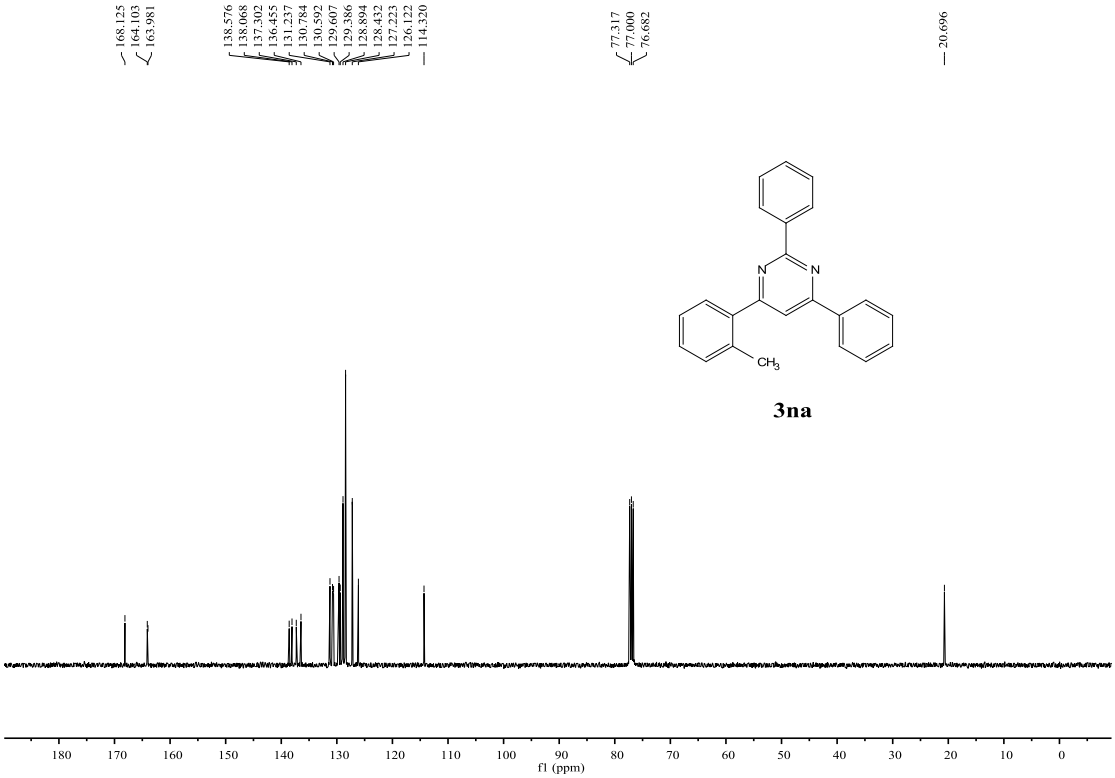

N
N
Cl

3ma

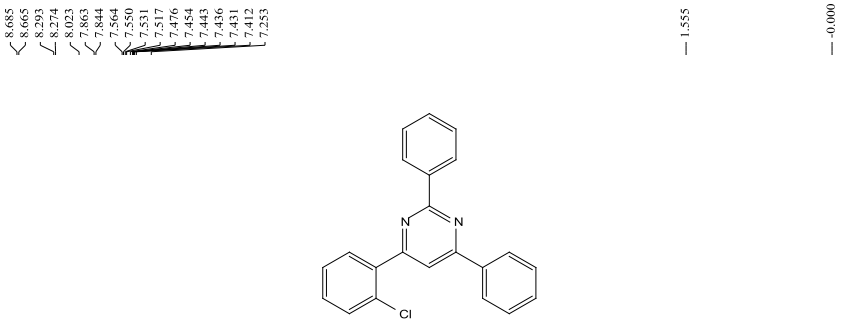

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.682
8.663
8.289
8.269
7.740
7.605
7.585
7.573
7.561
7.547
7.543
7.537
7.525
7.521
7.512
7.507
7.424
7.421
7.412
7.402
7.389
7.385
7.374
7.357
7.353
7.339
7.335
2.577
-0.000
N
N
CH3
2.00
2.07
1.02
7.02
3.06
3.08
f1 (ppm)

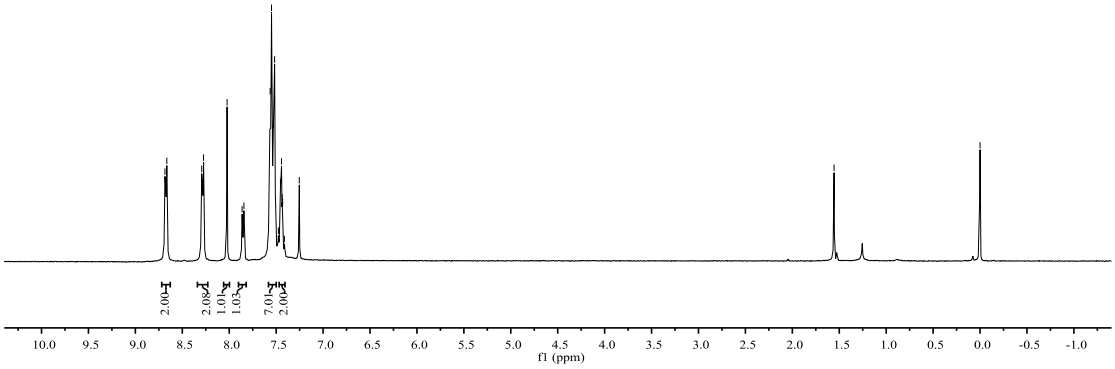
3na

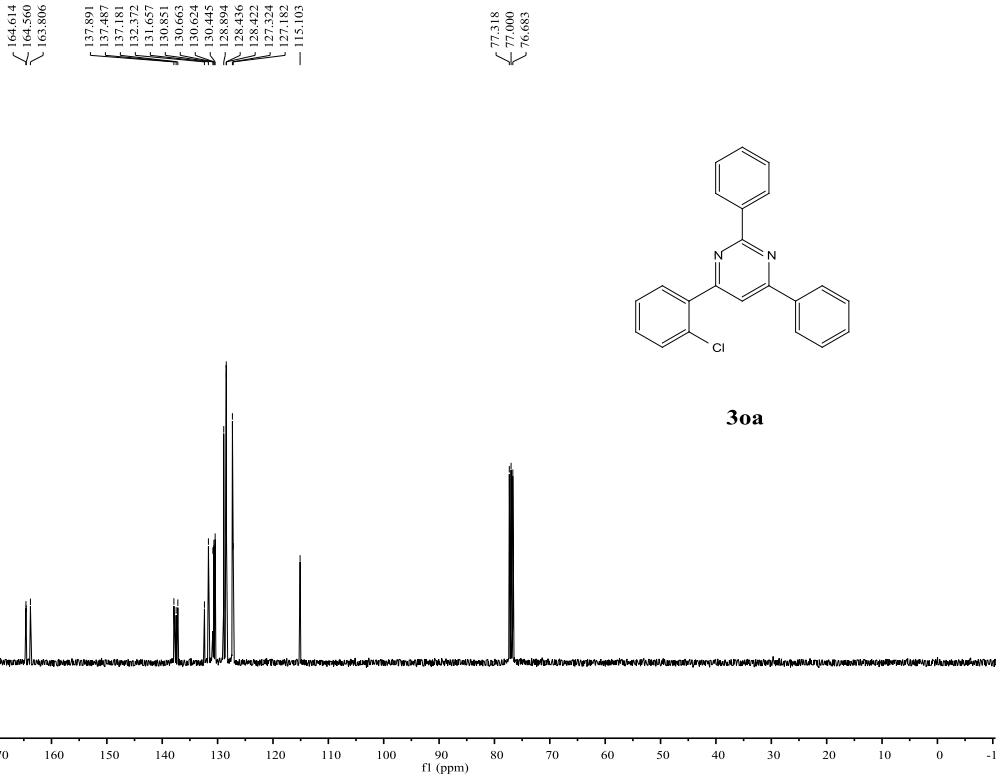

168.125
164.103
163.981
138.576
138.068
137.302
136.455
131.237
130.784
130.592
129.607
129.386
128.894
128.432
127.223
126.122
114.320
77.317
77.000
76.682
20.696
N
N
CH3
f1 (ppm)

3na

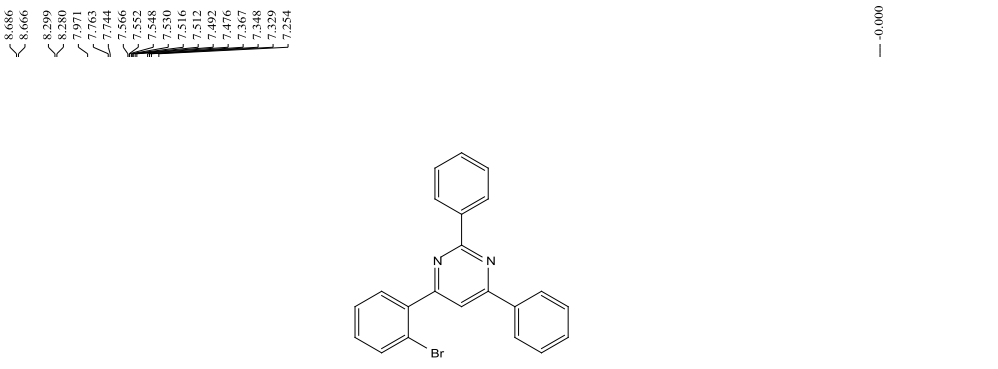

8.685
8.665
8.293
8.274
8.023
7.863
7.844
7.564
7.550
7.531
7.517
7.476
7.454
7.443
7.436
7.431
7.412
7.253
1.555
-0.000
N
N
Cl

3oa

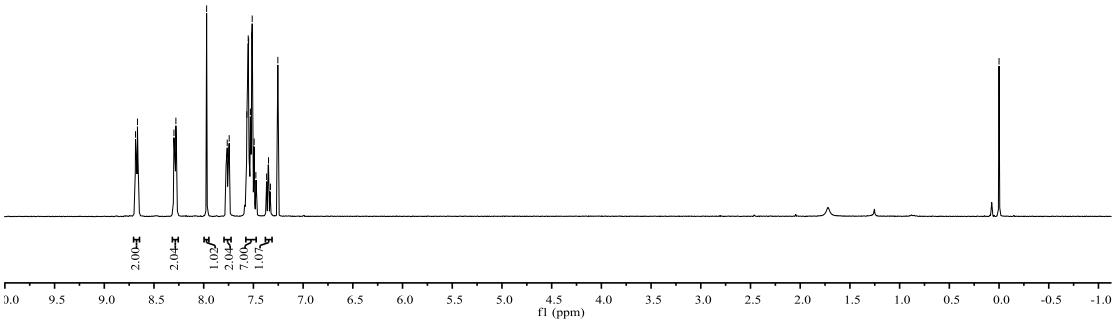

2.00
2.08
1.01
1.03
7.01
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

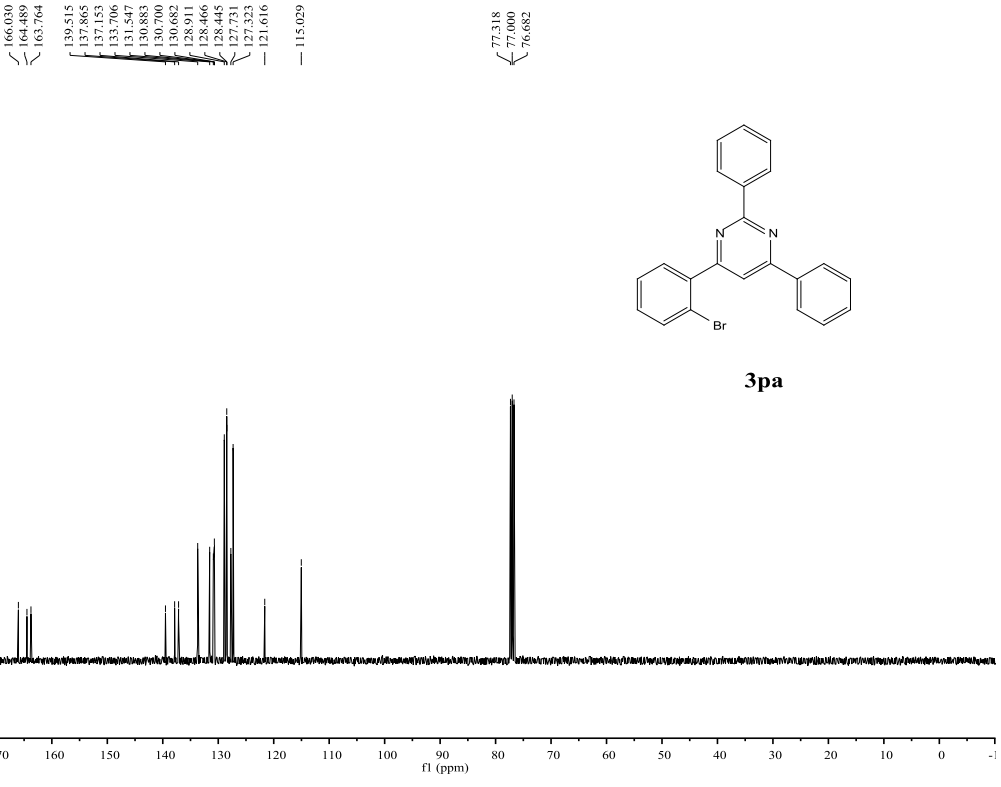

164.614
164.560
163.806
137.891
137.487
137.181
132.372
131.657
130.851
130.663
130.624
130.445
128.894
128.436
128.422
127.324
127.182
115.103
77.318
77.000
76.683
N
N
Cl
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

3oa

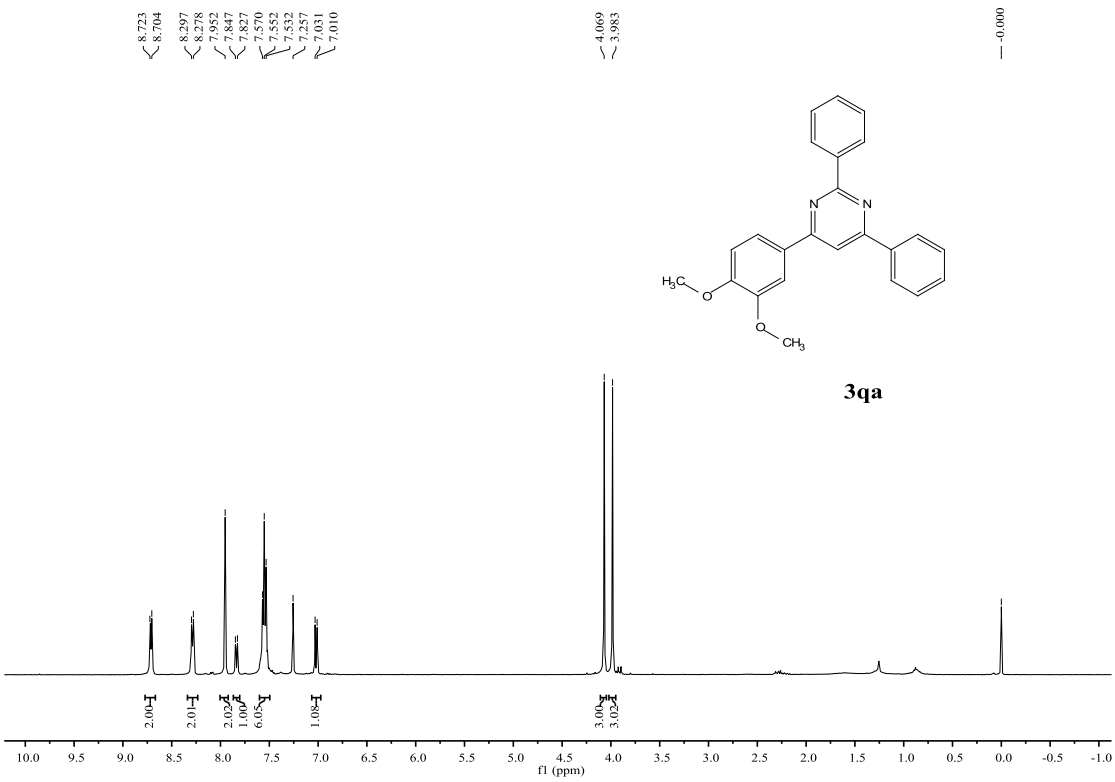

8.686
8.666
8.299
8.280
7.971
7.763
7.744
7.566
7.552
7.548
7.530
7.516
7.512
7.492
7.476
7.367
7.348
7.329
7.254
-0.000
N
N
Br

3pa

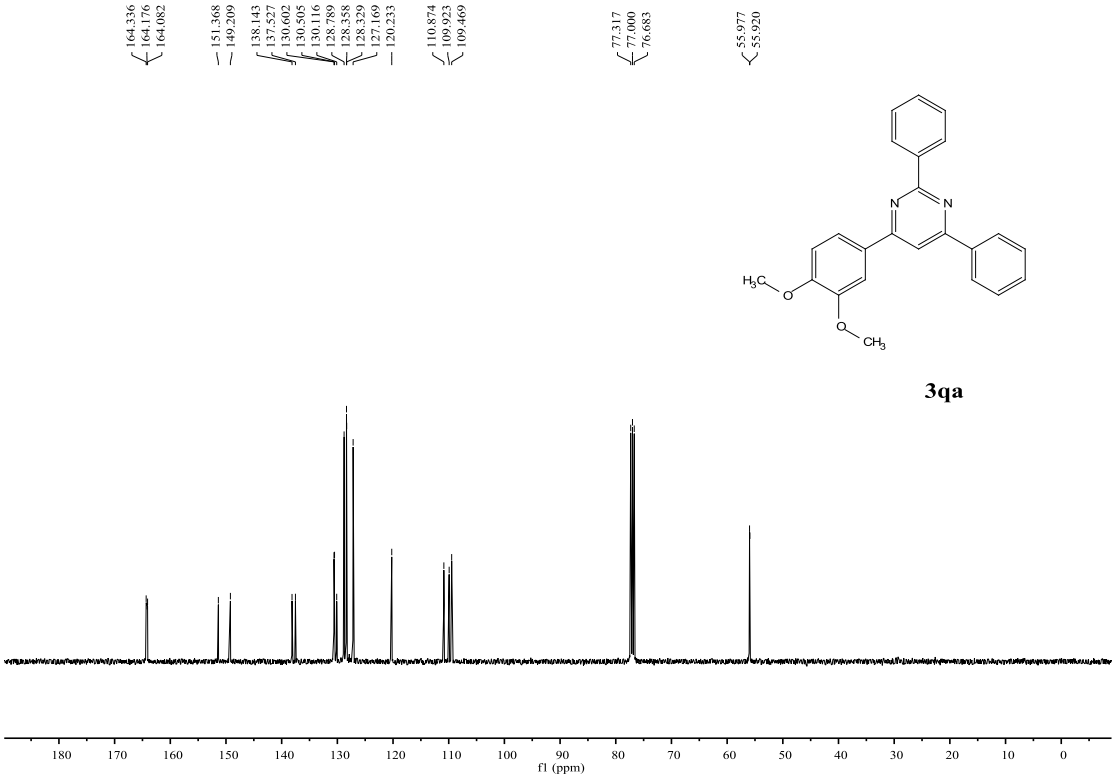

2.00
2.04
1.02
2.04
7.00
1.07
f1 (ppm)


166.030
164.489
163.764
139.515
137.865
137.153
133.706
131.547
130.883
130.700
130.682
128.911
128.466
128.445
127.731
127.323
121.616
115.029
77.318
77.000
76.682
N
N
Br
f1 (ppm)

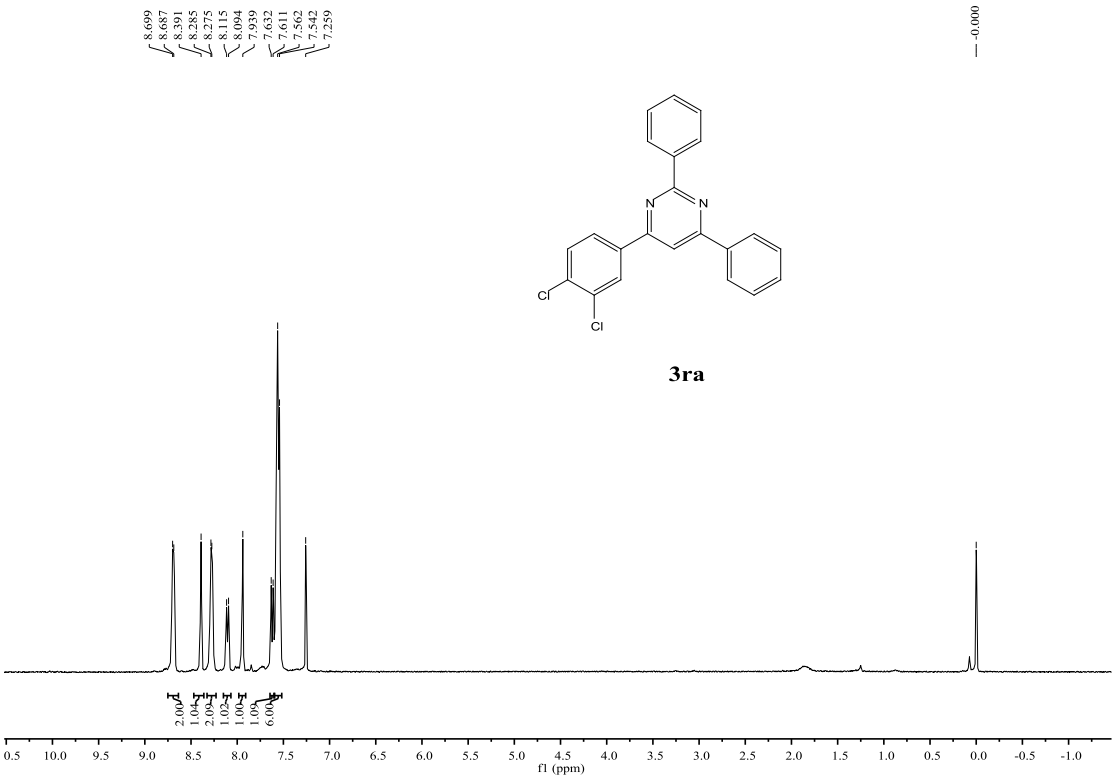
3pa


8.723
8.704
8.297
8.278
7.952
7.847
7.827
7.570
7.552
7.532
7.257
7.031
7.010
4.069
3.983
-0.000
N
N
H3C
O
O
CH3
2.00
2.01
2.02
1.00
6.05
1.08
3.00
3.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

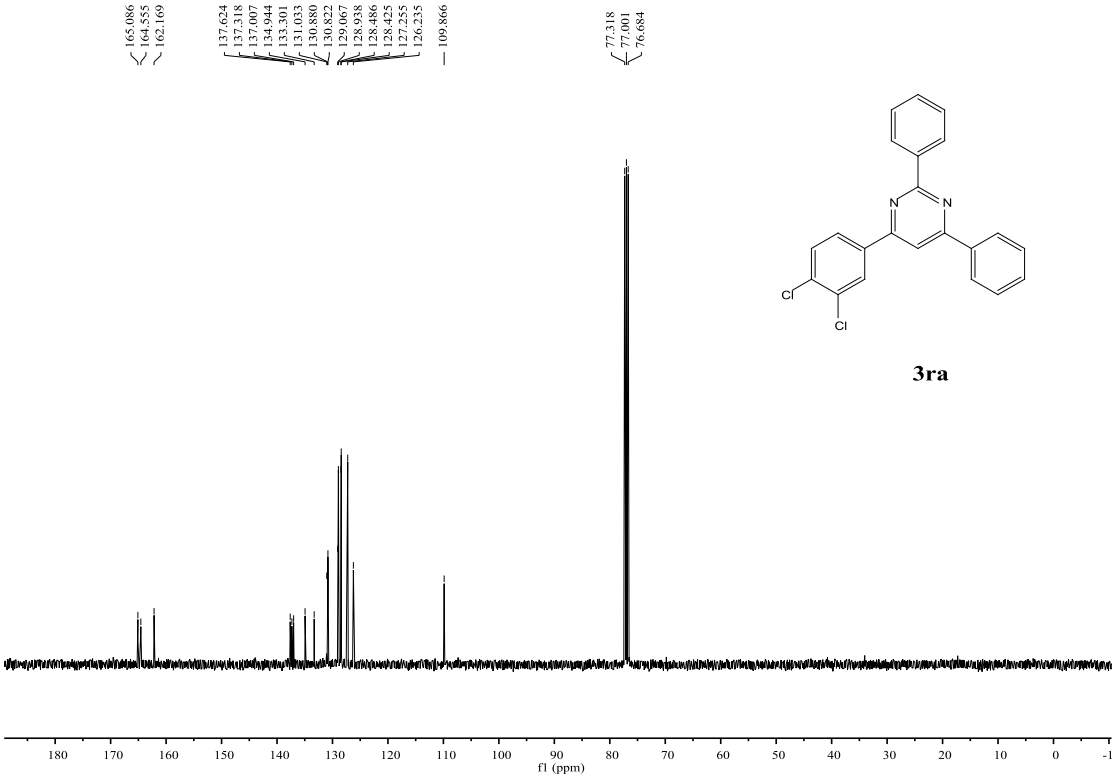
3qa


164.336
164.176
164.082
151.368
149.209
138.143
137.527
130.602
130.505
130.116
128.789
128.358
128.329
127.169
120.233
110.874
109.923
109.469
77.317
77.000
76.683
55.977
55.920
N
N
H3C
O
O
CH3
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

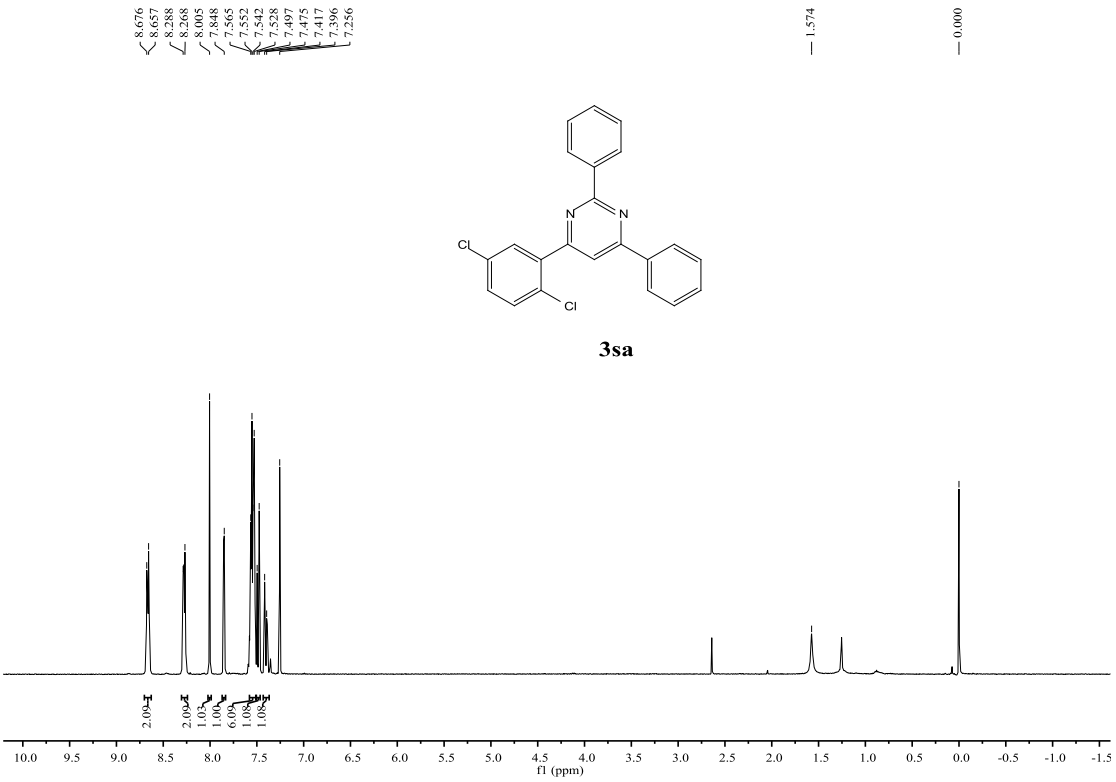
3qa


8.699
8.687
8.391
8.285
8.275
8.115
8.094
7.939
7.632
7.611
7.562
7.542
7.259
-0.000
N
N
Cl
Cl
2.00
1.04
2.09
1.02
1.00
1.09
6.00
f1 (ppm)

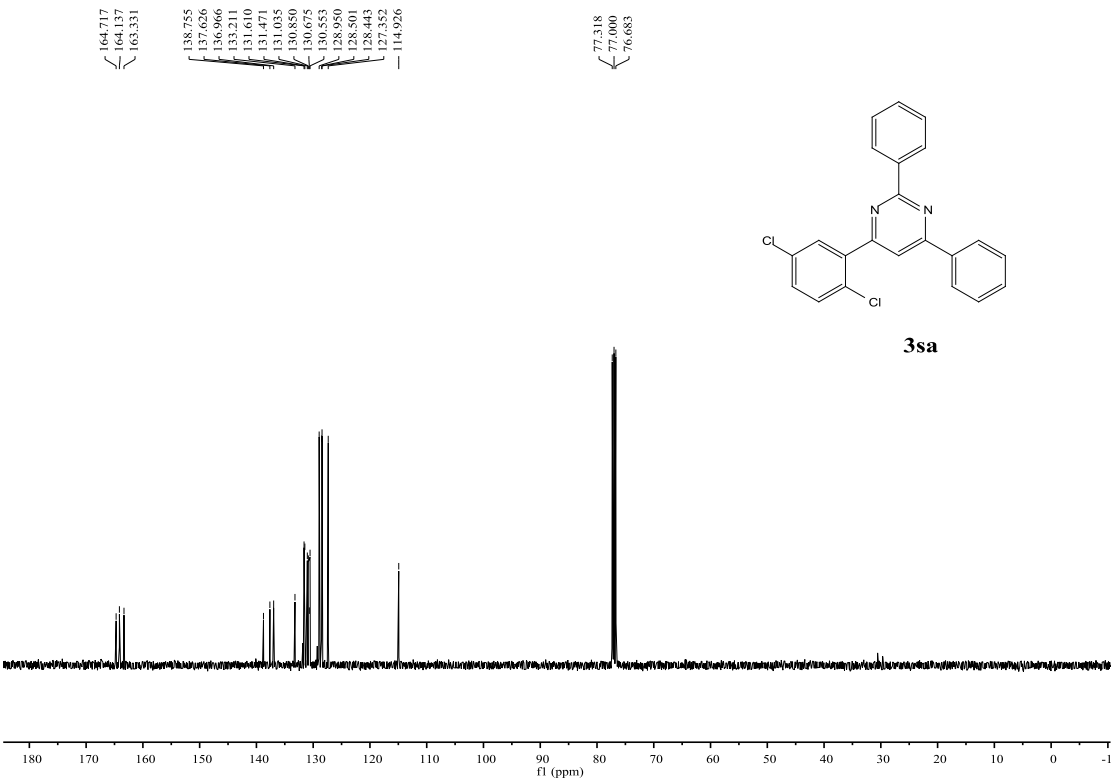
3ra


165.086
164.555
162.169
137.624
137.318
137.007
134.944
133.301
131.033
130.880
130.822
129.067
128.938
128.486
128.425
127.255
126.235
109.866
77.318
77.001
76.684
N
N
Cl
Cl
f1 (ppm)

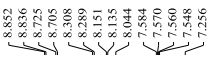
3ra

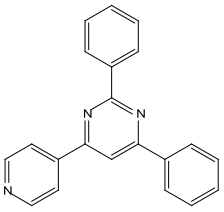

8.676
8.657
8.288
8.268
8.005
7.848
7.565
7.552
7.542
7.528
7.497
7.475
7.417
7.396
7.256
1.574
0.000
N
N
Cl
Cl
2.09
2.09
1.03
1.00
6.09
1.08
1.08
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)

3sa

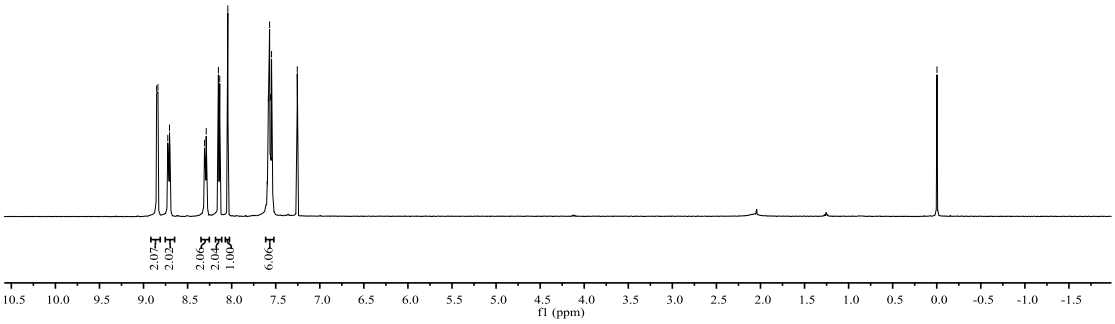

164.717
164.137
163.331
138.755
137.626
136.966
133.211
131.610
131.471
131.035
130.850
130.675
130.553
128.950
128.501
128.443
127.352
114.926
77.318
77.000
76.683
N
N
Cl
Cl
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

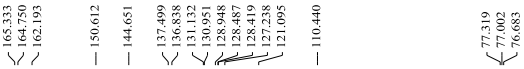
3sa

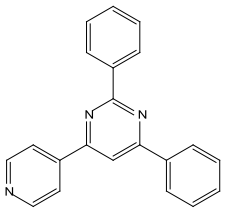

8.852
8.836
8.725
8.705
8.308
8.289
8.151
8.135
8.044
7.584
7.570
7.560
7.548
7.256
-0.003


N
N
N

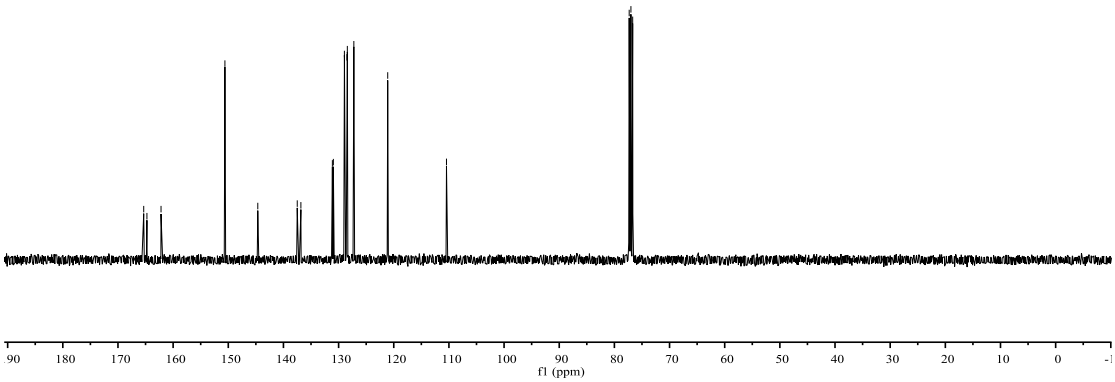
3ta

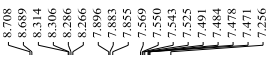

2.07
2.03
2.06
2.04
1.00
6.06
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)


165.333
164.750
162.193
150.612
144.651
137.499
136.838
131.132
130.951
128.948
128.487
128.419
127.238
121.095
110.440
77.319
77.002
76.683

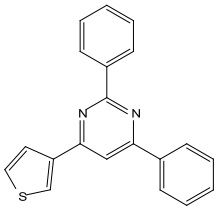

N
N
N

3ta

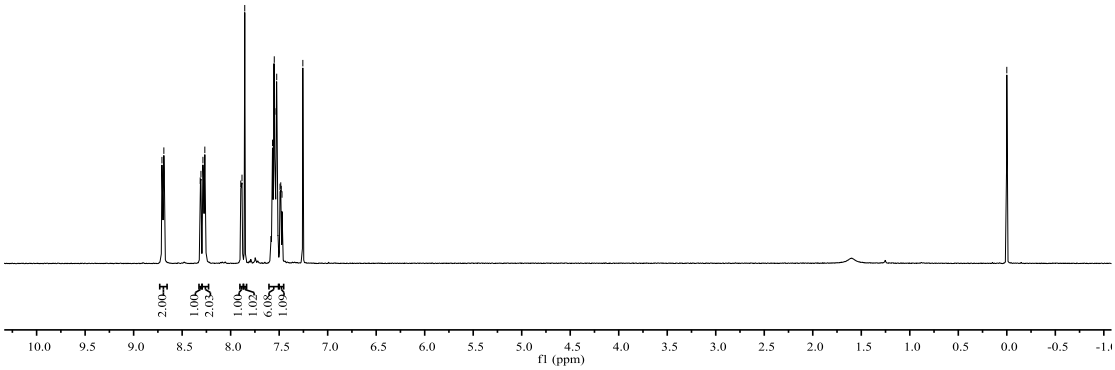

90 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

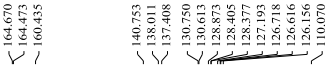

8.708
8.689
8.314
8.306
8.286
8.266
7.896
7.883
7.855
7.569
7.550
7.543
7.525
7.491
7.484
7.478
7.471
7.256

-0.000


N
N
S

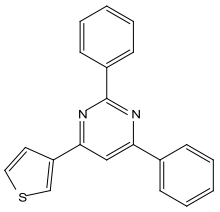
3ua


2.00
1.00
2.03
1.00
1.02
6.08
1.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

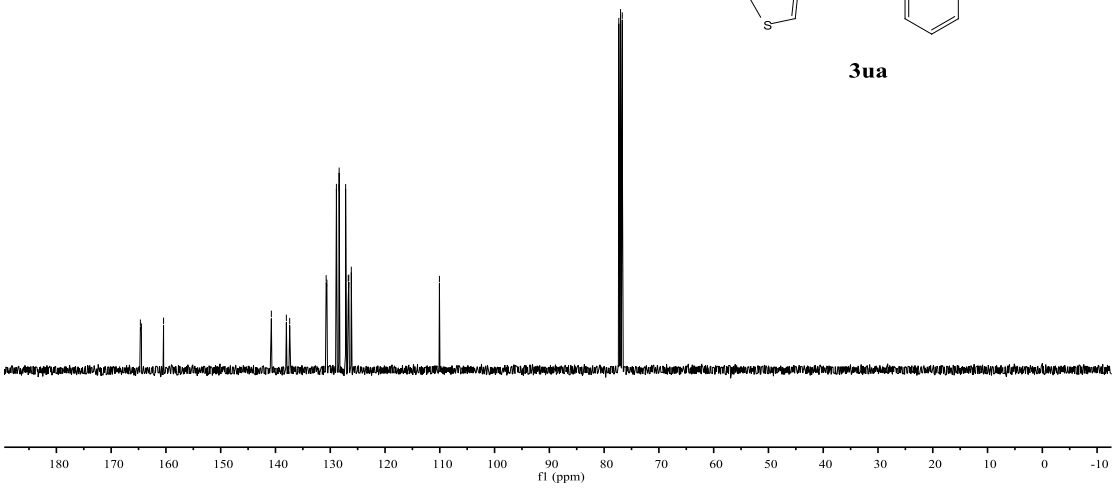

164.670
164.473
160.435

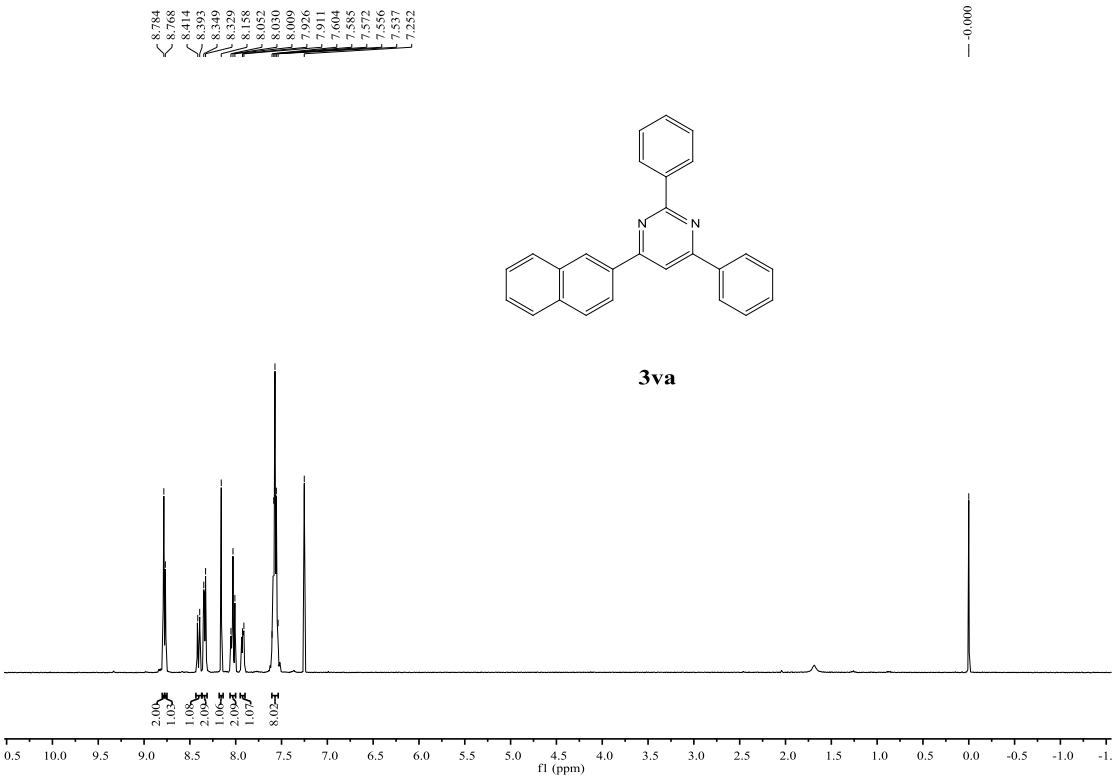
140.753
138.011
137.408
130.750
130.613
128.873
128.405
128.377
127.193
126.718
126.616
126.156
110.070

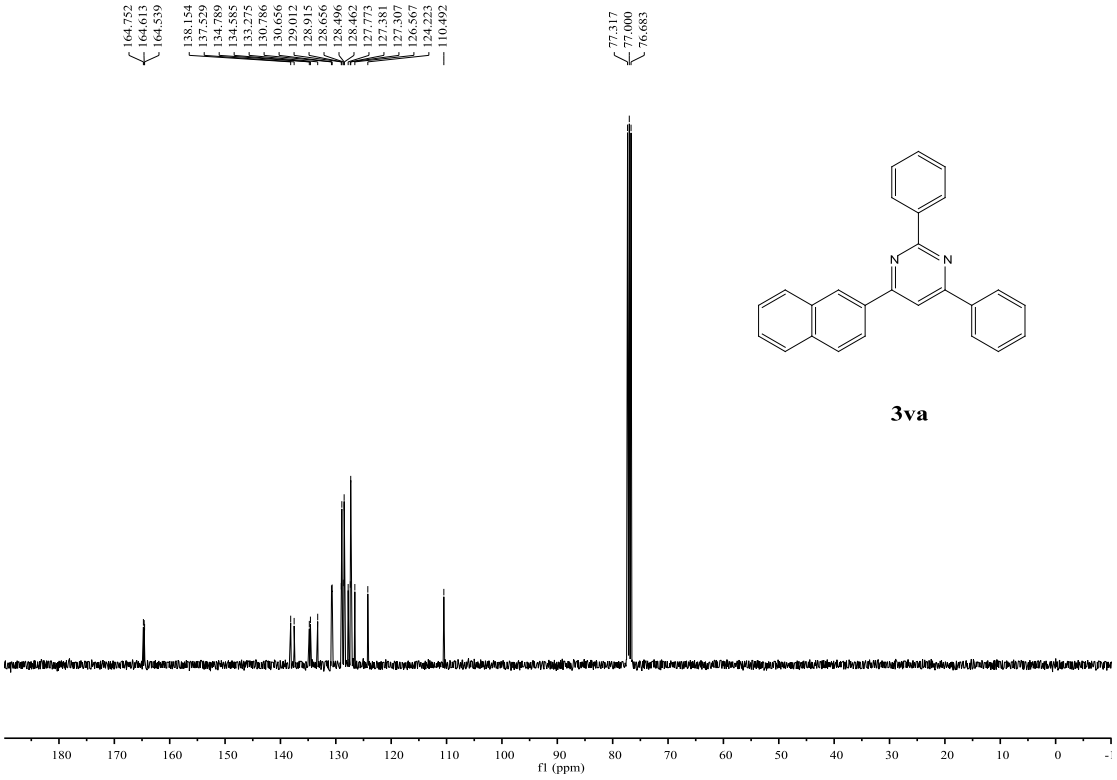

77.318
77.001
76.683

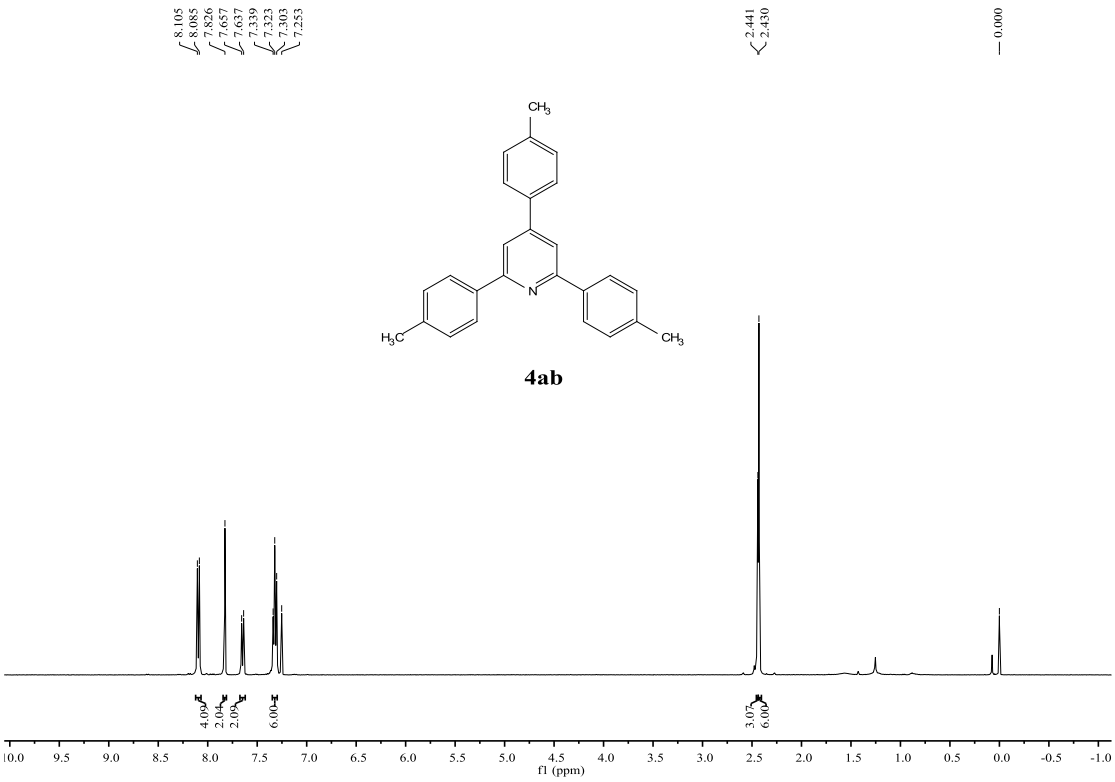

N
N
S

3ua

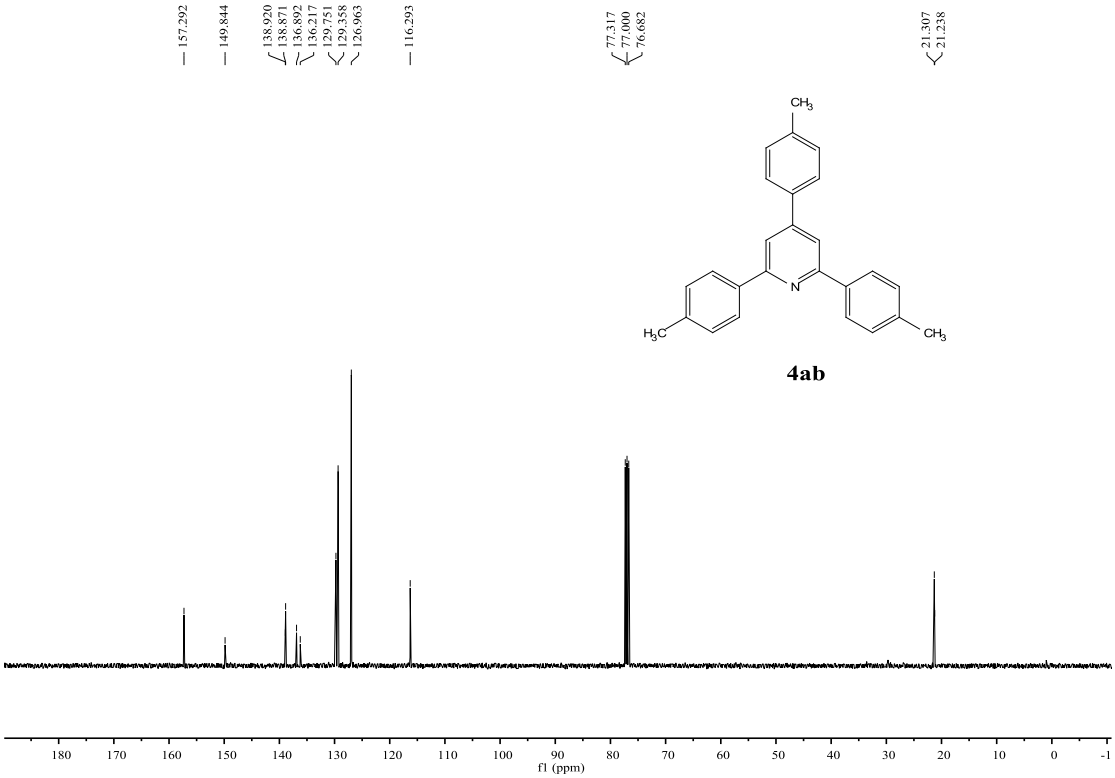

180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.784
8.768
8.414
8.393
8.349
8.329
8.158
8.052
8.030
8.009
7.926
7.911
7.604
7.585
7.572
7.556
7.537
7.252
-0.000
N
N
3va
2.00
1.03
1.08
2.04
1.06
2.04
1.07
8.02
f1 (ppm)

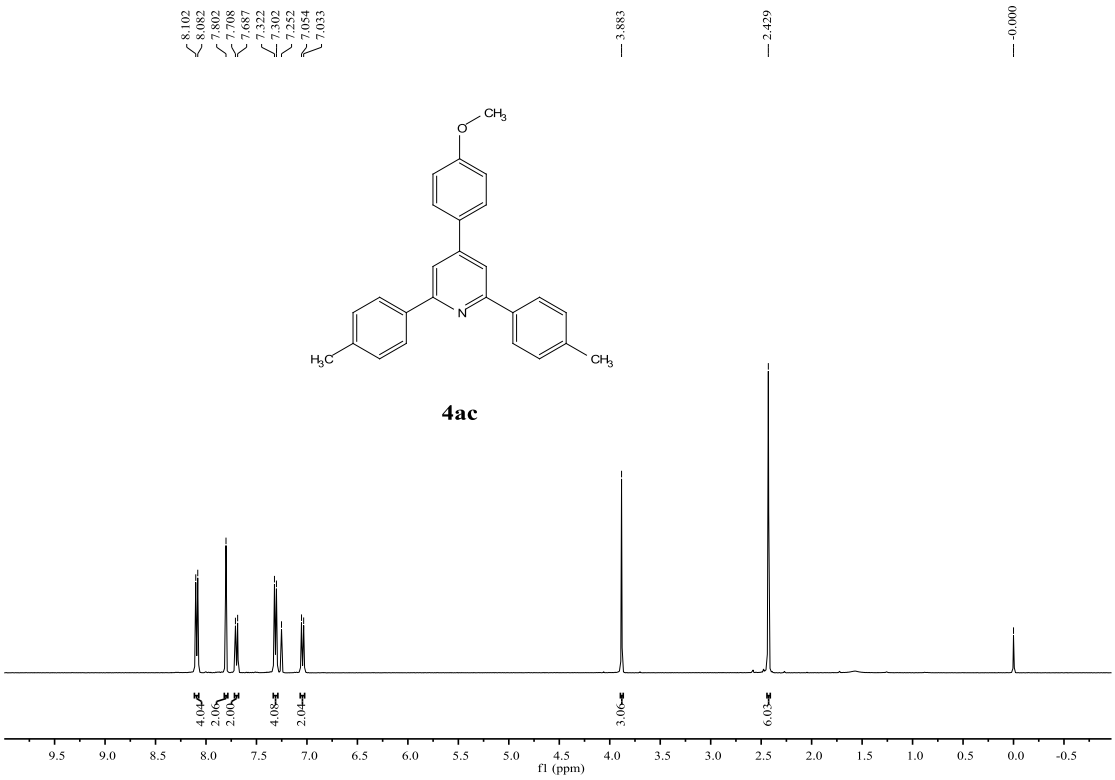

164.752
164.613
164.539
138.154
137.529
134.789
134.585
133.275
130.786
130.656
129.012
128.915
128.656
128.496
128.462
127.773
127.381
127.307
126.567
124.223
110.492
77.317
77.000
76.683
N
N
3va
f1 (ppm)


8.105
8.085
7.826
7.657
7.637
7.339
7.323
7.303
7.253
2.441
2.430
0.000
CH3
N
H3C
CH3
4.09
2.04
2.09
6.00
3.07
6.00
f1 (ppm)

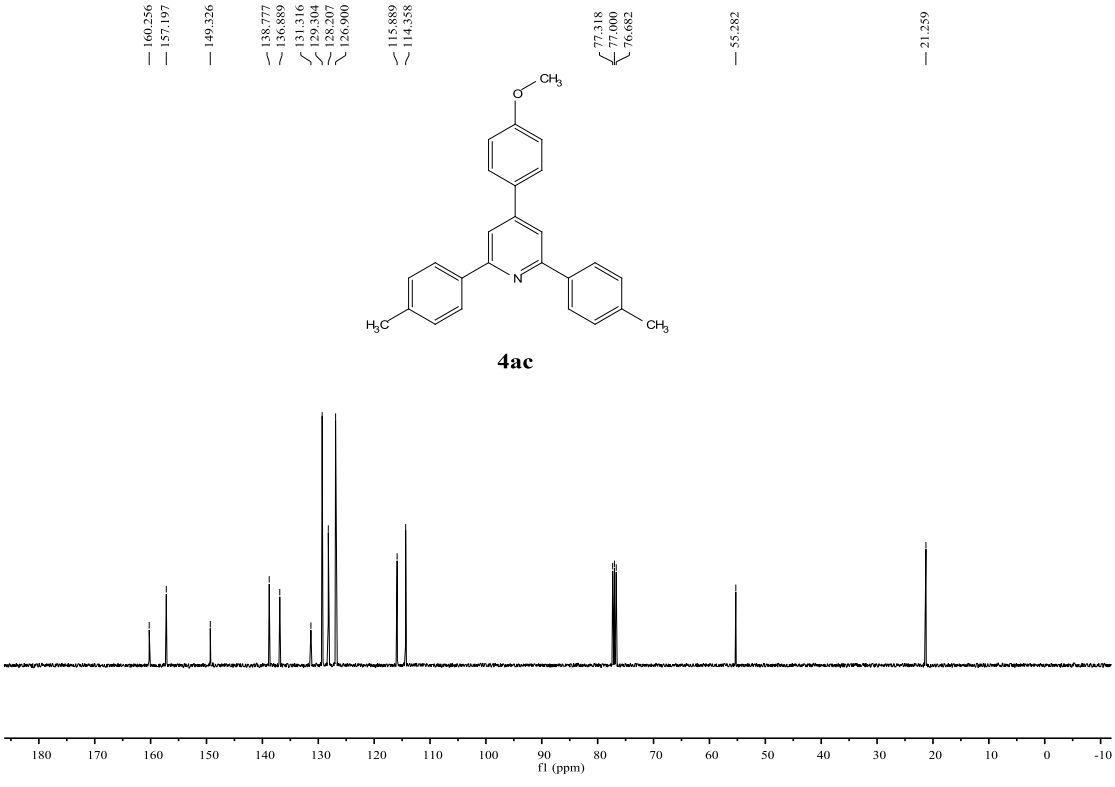
4ab


157.292
149.844
138.920
138.871
136.892
136.217
129.751
129.358
126.963
116.293
77.317
77.000
76.682
21.307
21.238
CH3
N
H3C
CH3
f1 (ppm)

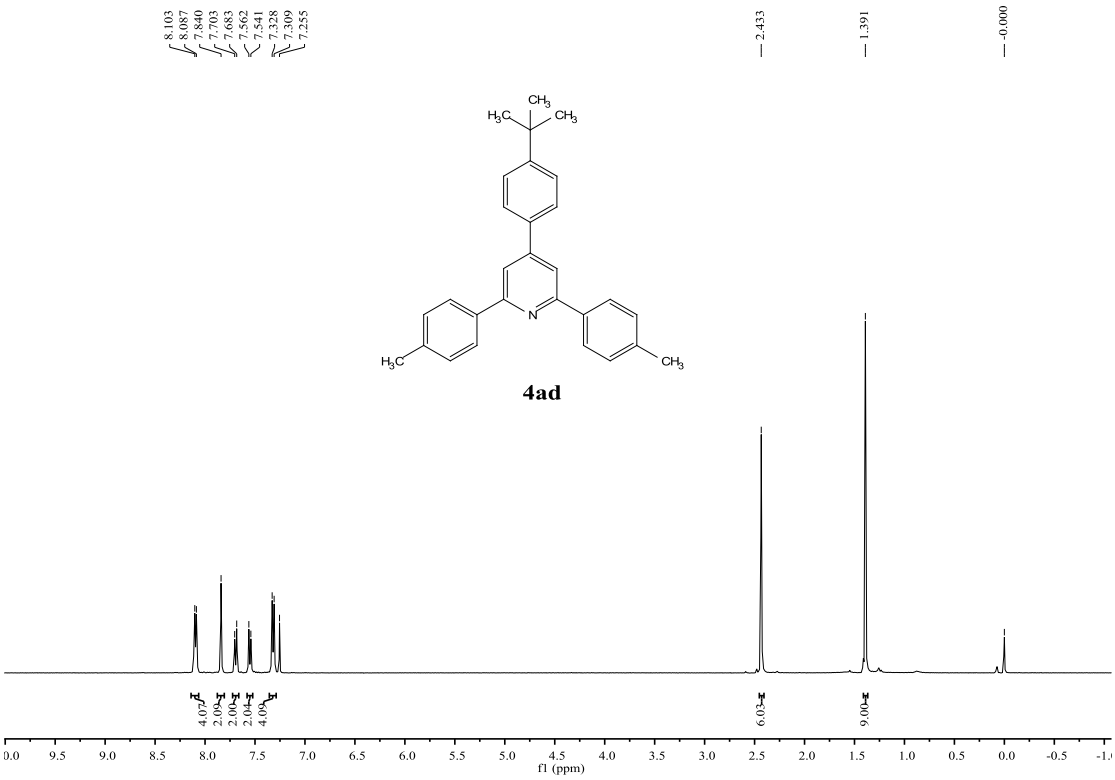
4ab


8.102
8.082
7.802
7.708
7.687
7.322
7.302
7.252
7.054
7.033
3.883
2.429
-0.000
O
CH3
N
H3C
CH3
4.04
2.06
2.00
4.08
2.04
3.06
6.03
f1 (ppm)

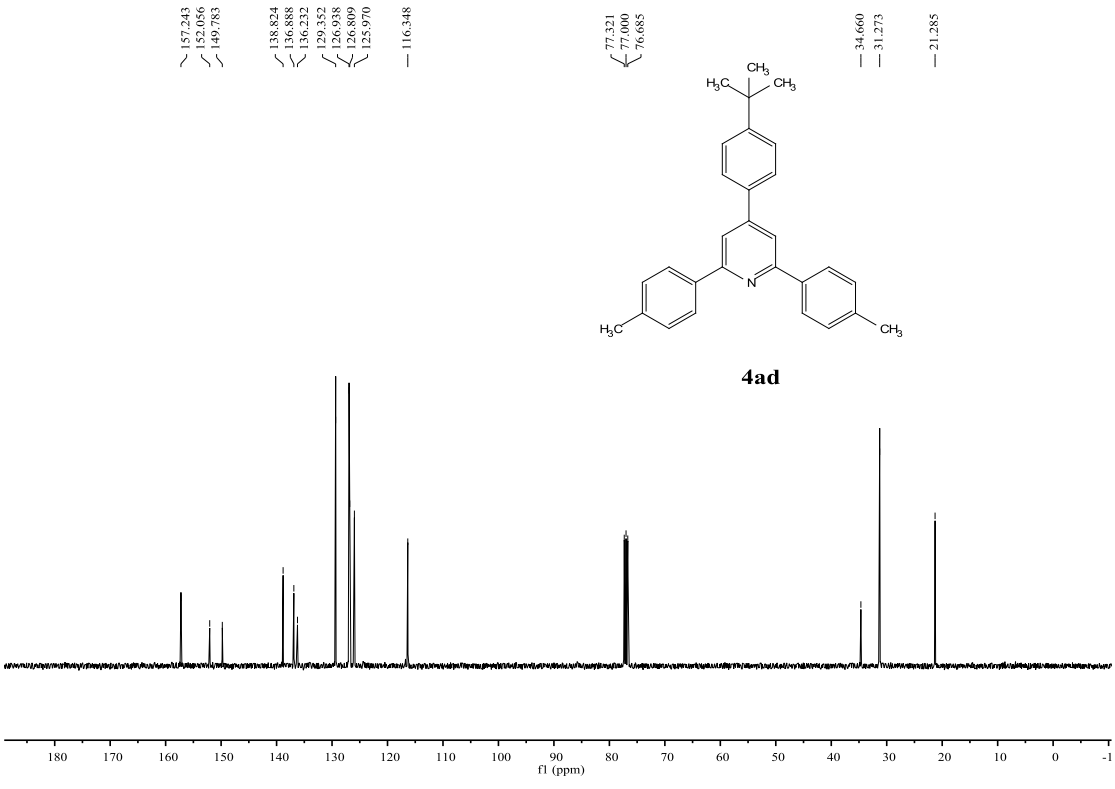
4ac


160.256
157.197
149.326
138.777
136.889
131.316
129.304
128.207
126.900
115.889
114.358
77.318
77.000
76.682
55.282
21.259
O
CH3
N
H3C
CH3
f1 (ppm)

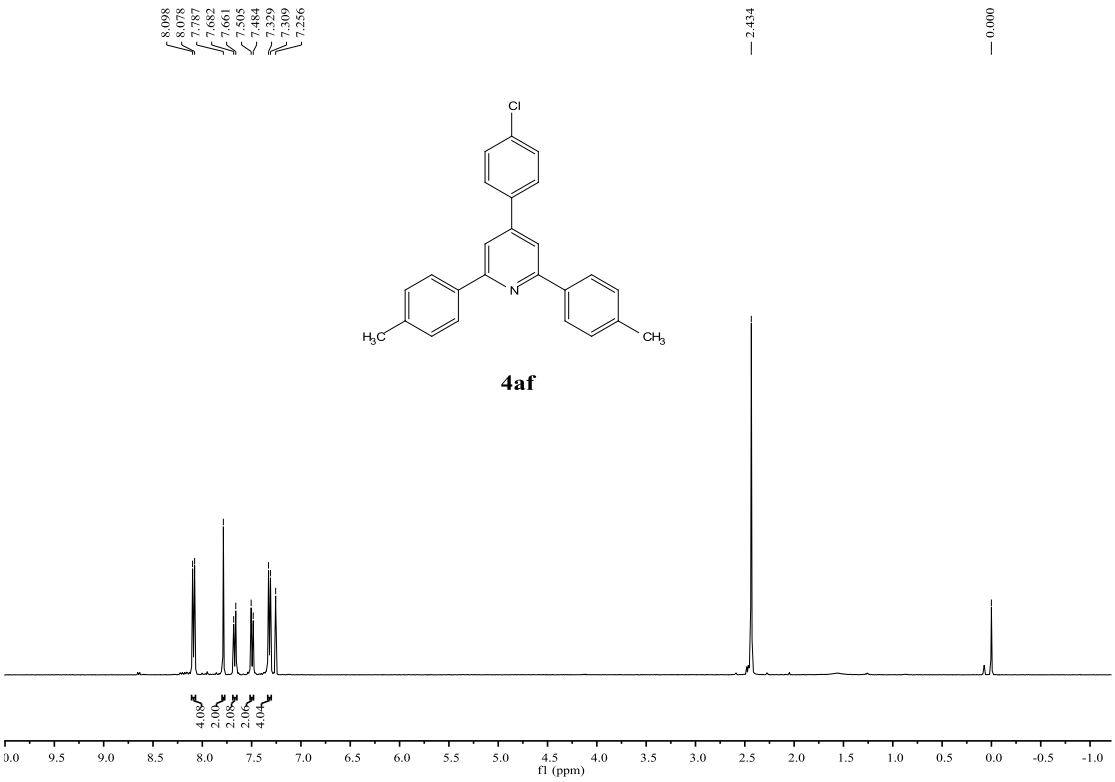
4ac


8.103
8.087
7.840
7.703
7.683
7.562
7.541
7.328
7.309
7.255
2.433
1.391
-0.000
4.07
2.09
2.00
2.04
4.00
6.03
9.00
f1 (ppm)

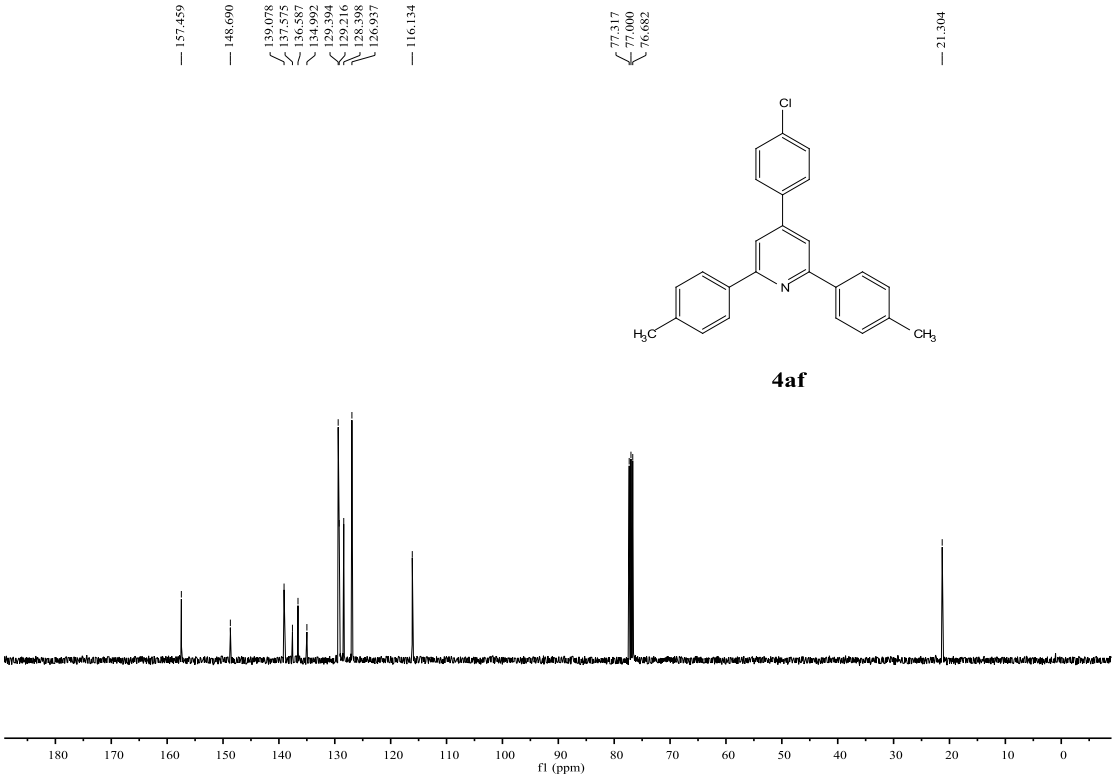
4ad


157.243
152.056
149.783
138.824
136.888
136.232
129.352
126.938
126.809
125.970
116.348
77.321
77.000
76.685
34.660
31.273
21.285
f1 (ppm)

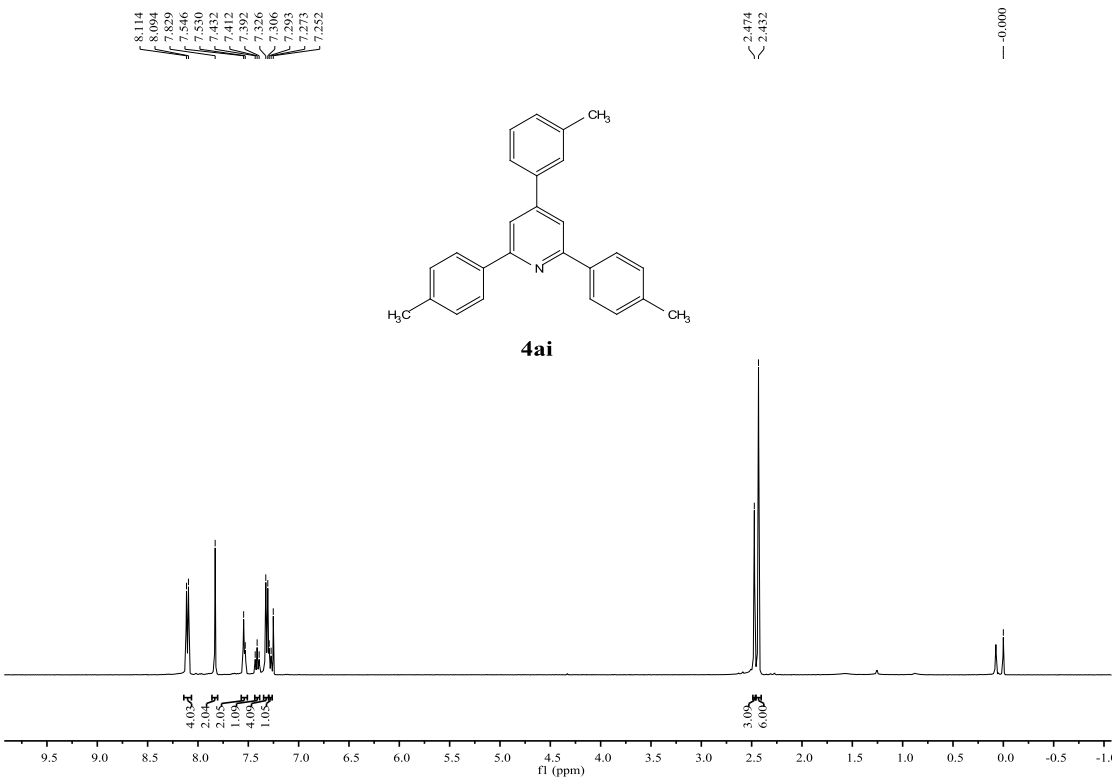
4ad


8.098
8.078
7.787
7.682
7.661
7.505
7.484
7.329
7.309
7.256
2.434
0.000
Cl
N
H3C
CH3
4.09
2.00
2.08
2.06
4.04
f1 (ppm)

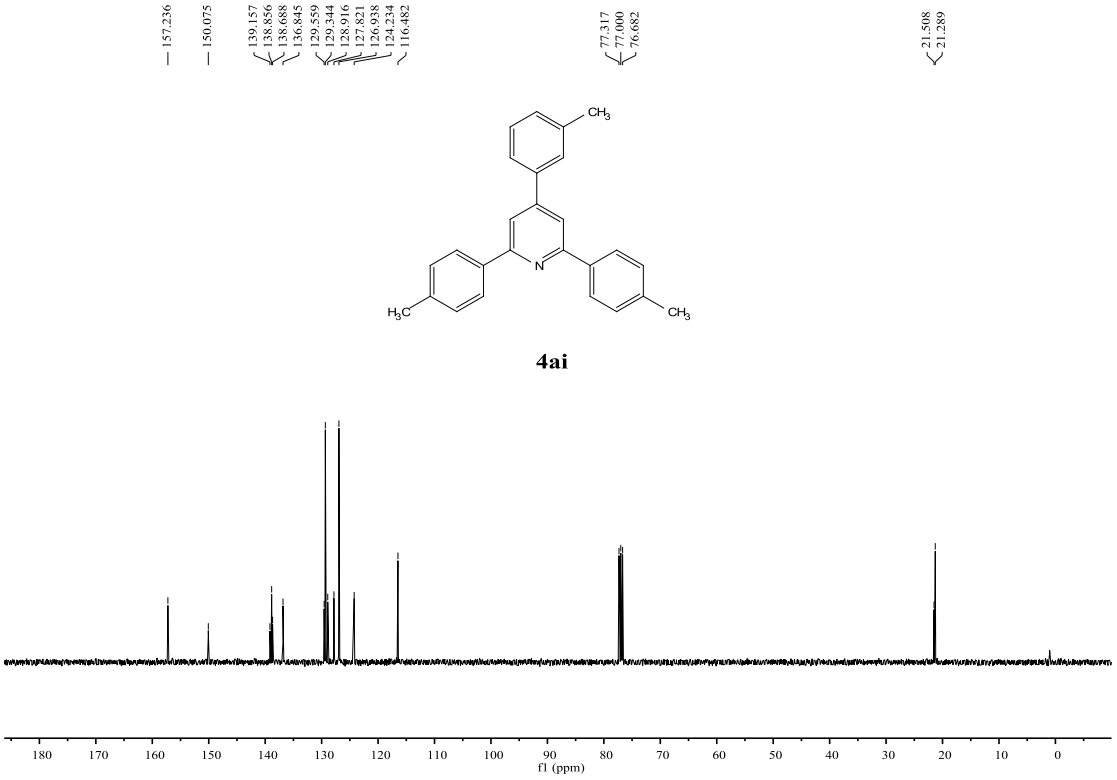
4af


157.459
148.690
139.078
137.575
136.587
134.992
129.394
129.216
128.398
126.937
116.134
77.317
77.000
76.682
21.304
Cl
N
H3C
CH3
f1 (ppm)

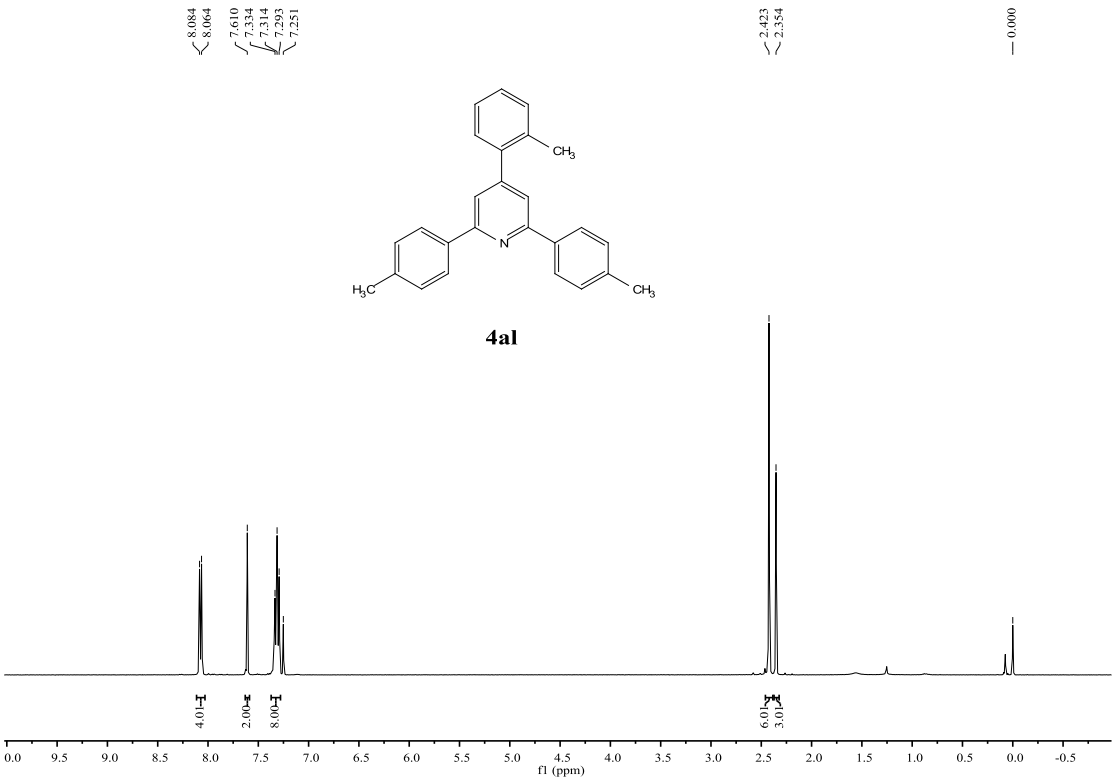
4af


8.114
8.094
7.829
7.546
7.530
7.432
7.412
7.392
7.326
7.306
7.293
7.273
7.252
2.474
2.432
-0.000
CH3
N
H3C
CH3
4.03
2.04
2.05
1.09
4.09
1.05
3.00
6.00
f1 (ppm)

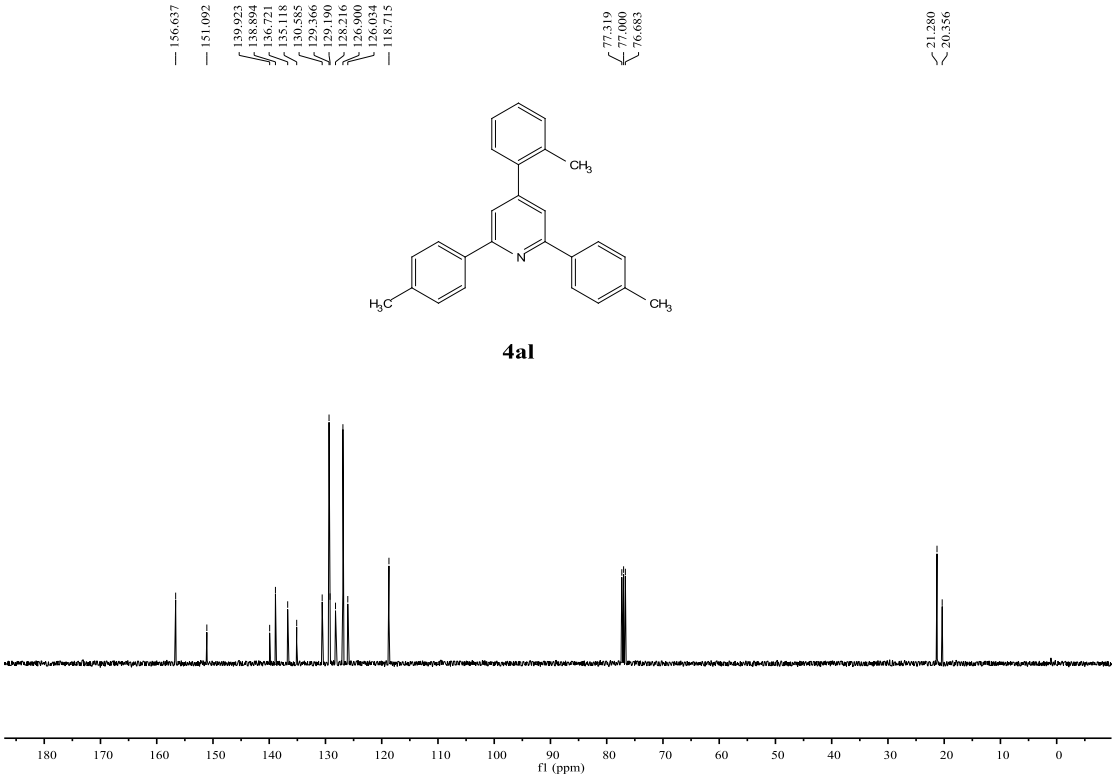
4ai


157.236
150.075
139.157
138.856
138.688
136.845
129.559
129.344
128.916
127.821
126.938
124.234
116.482
77.317
77.000
76.682
21.508
21.289
CH3
N
H3C
CH3
f1 (ppm)

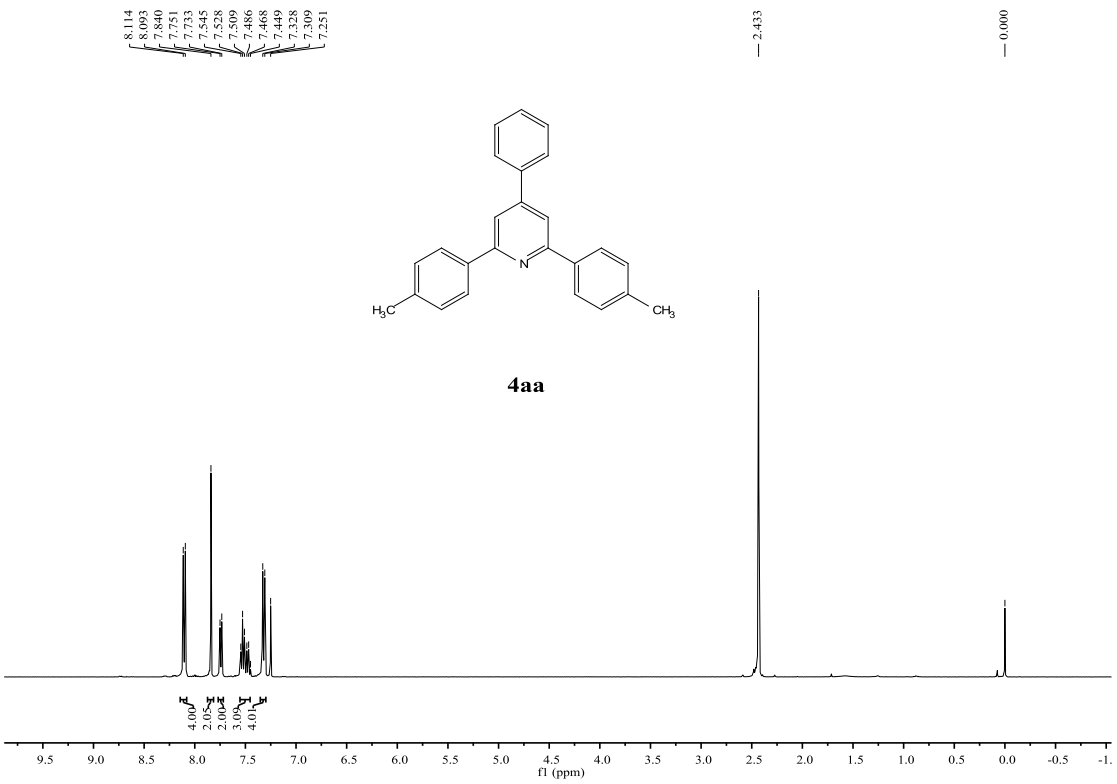
4ai


8.084
8.064
7.610
7.334
7.314
7.293
7.251
2.423
2.354
0.000
CH3
N
H3C
CH3
4.01
2.00
8.00
6.01
3.01
f1 (ppm)

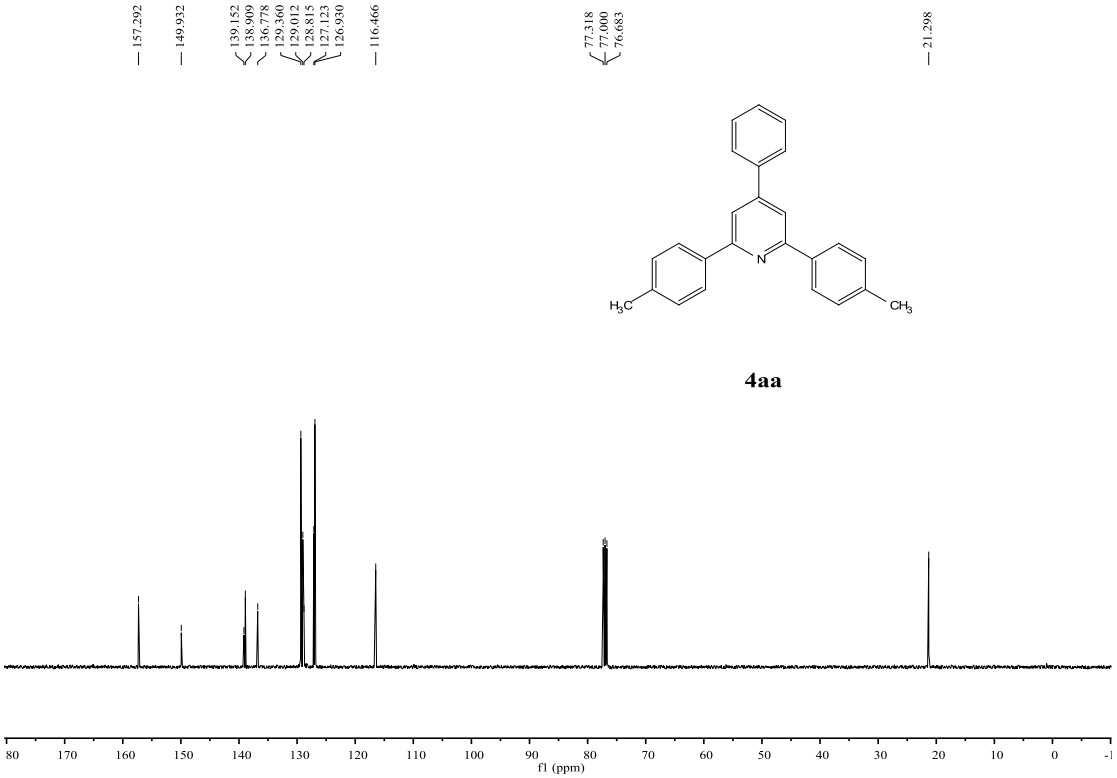
4al


156.637
151.092
139.923
138.894
136.721
135.118
130.585
129.366
129.190
128.216
126.900
126.034
118.715
77.319
77.000
76.683
21.280
20.356
CH3
N
H3C
CH3
f1 (ppm)

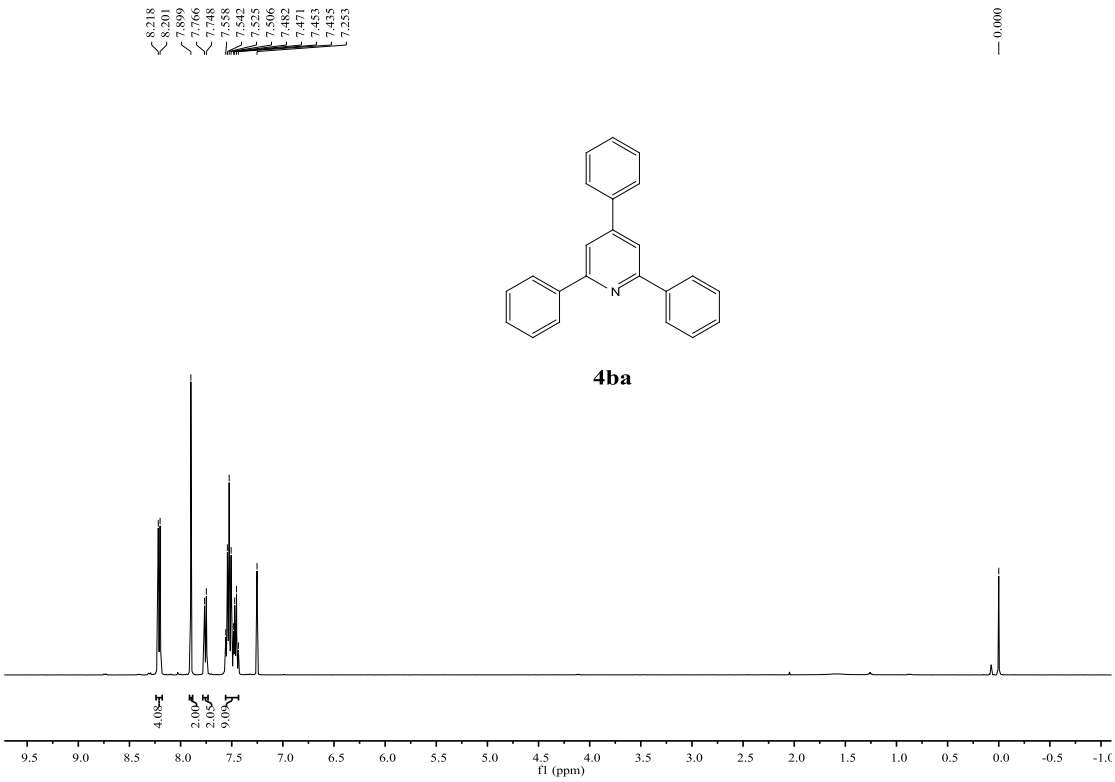
4al


8.114
8.093
7.840
7.751
7.733
7.545
7.528
7.509
7.486
7.468
7.449
7.328
7.309
7.251
2.433
0.000
N
H3C
CH3
4.00
2.05
2.00
3.09
4.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)

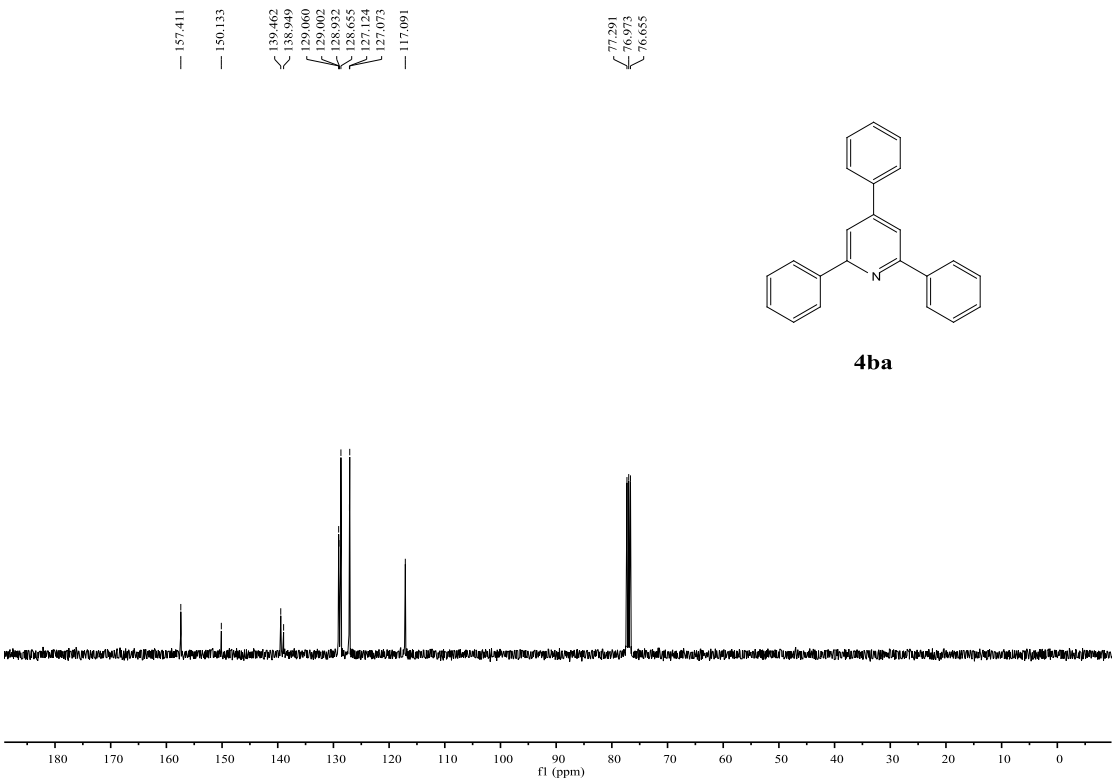
4aa


157.292
149.932
139.152
138.909
136.778
129.360
129.012
128.815
127.123
126.930
116.466
77.318
77.000
76.683
21.298
N
H3C
CH3
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

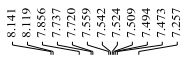
4aa


8.218
8.201
7.899
7.766
7.748
7.558
7.542
7.525
7.506
7.482
7.471
7.453
7.435
7.253
0.000
N
4.08
2.00
2.05
9.09
f1 (ppm)

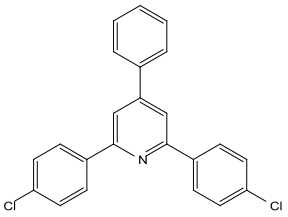
4ba


157.411
150.133
139.462
138.949
129.060
129.002
128.932
128.655
127.124
127.073
117.091
77.291
76.973
76.655
N
f1 (ppm)

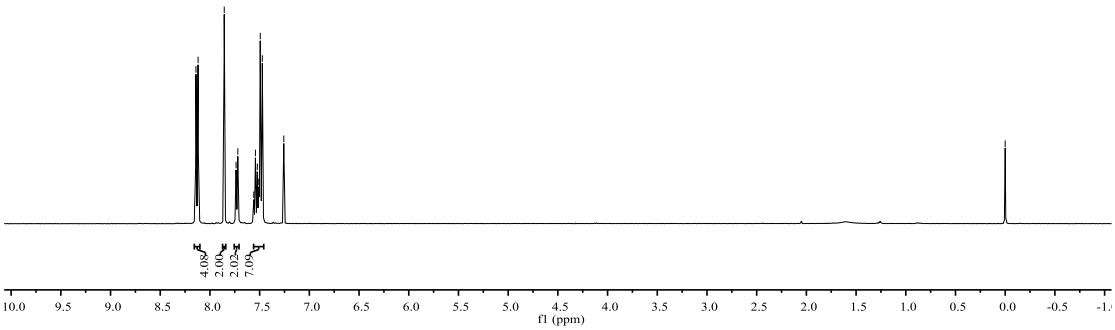
4ba

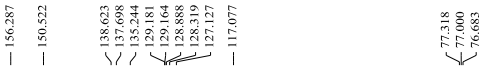

8.141
8.119
7.856
7.737
7.720
7.559
7.542
7.524
7.509
7.494
7.473
7.257

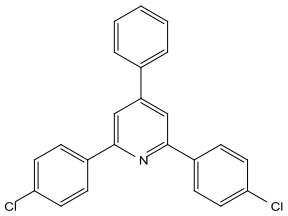
0.000


N
Cl
Cl

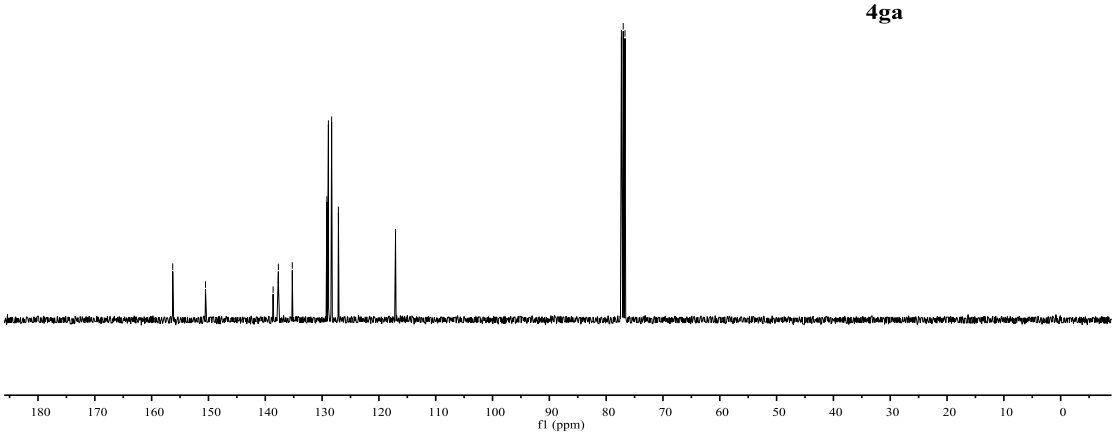
4ga

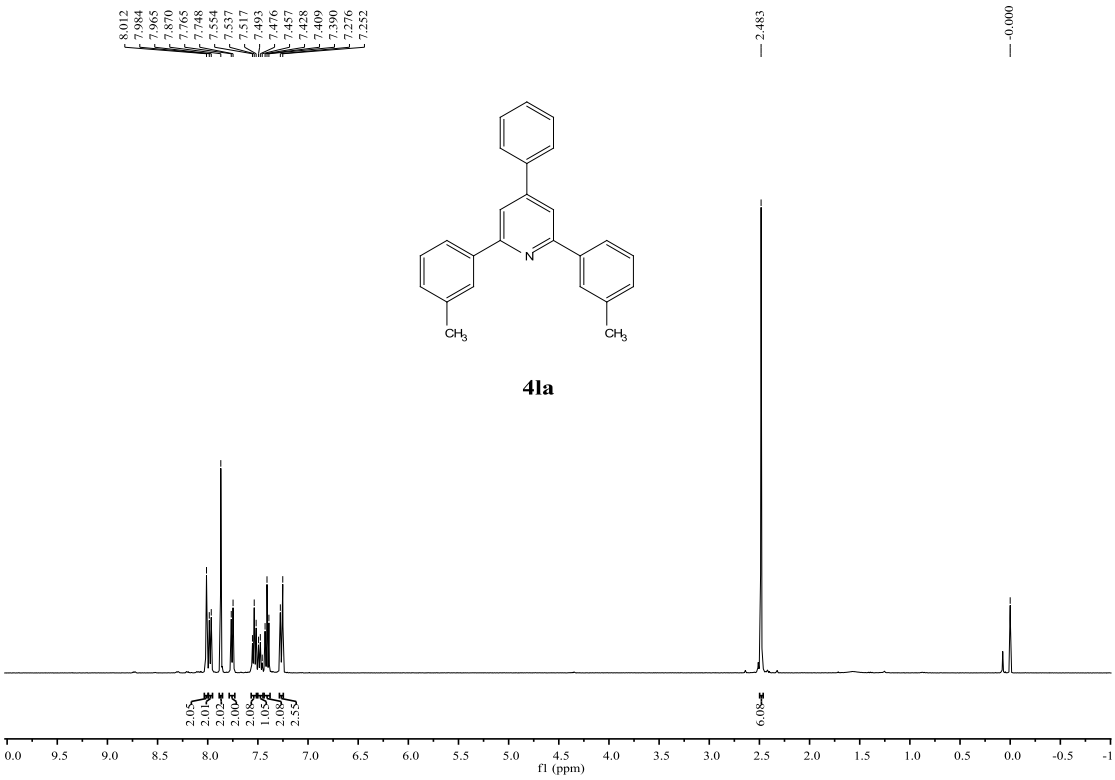

4.08
2.00
2.02
7.09
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


156.287
150.522
138.623
137.698
135.244
129.181
129.164
128.888
128.319
127.127
117.077
77.318
77.000
76.683

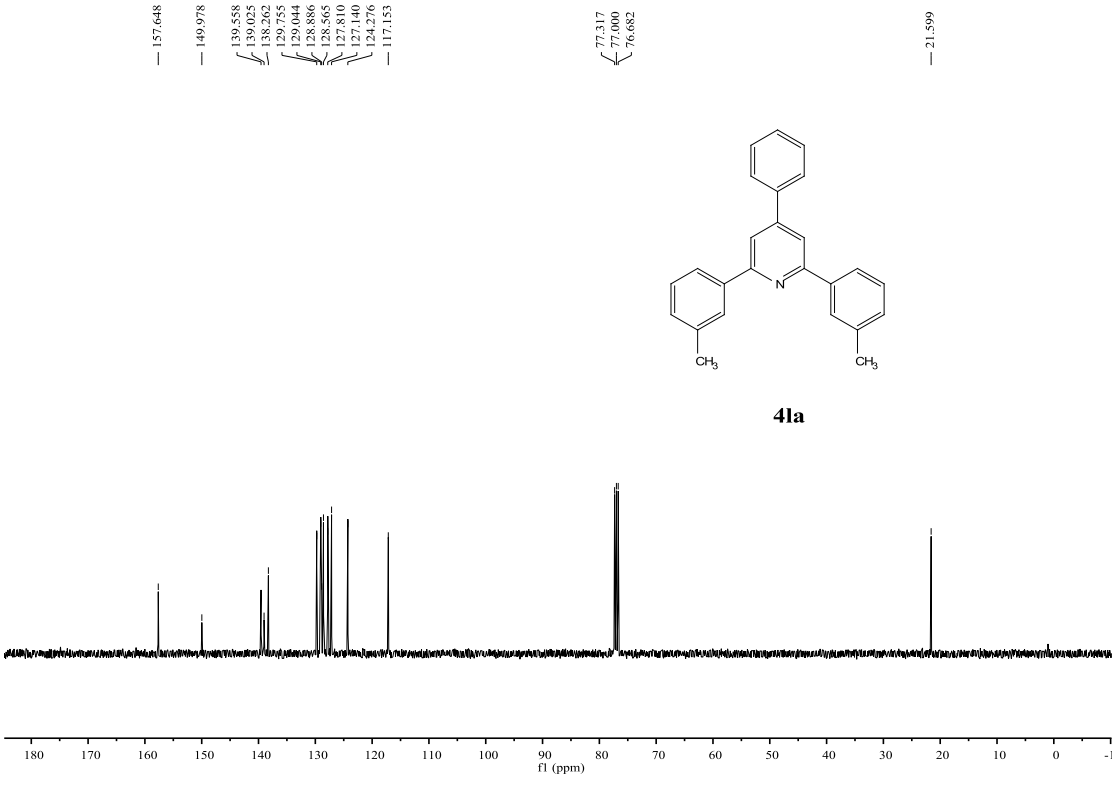

N
Cl
Cl

4ga

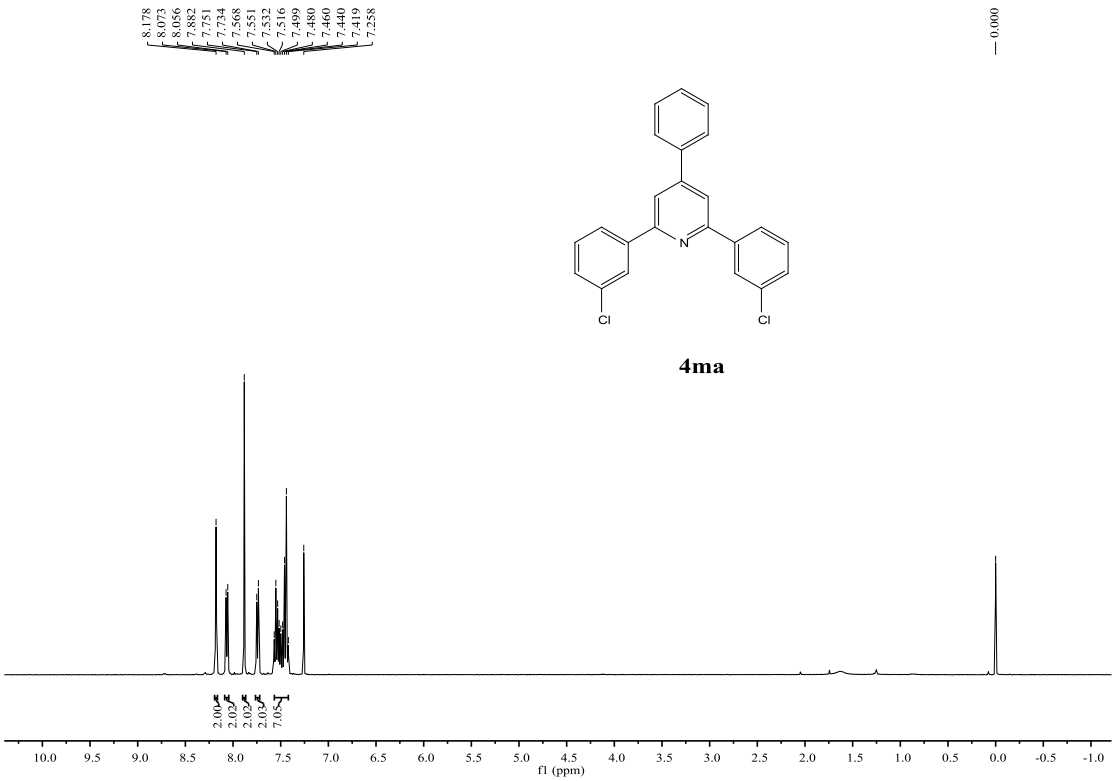

180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.012
7.984
7.965
7.870
7.765
7.748
7.554
7.537
7.517
7.493
7.476
7.457
7.428
7.409
7.390
7.276
7.252
2.483
-0.000
N
CH3
CH3
2.05
2.01
2.02
2.00
2.08
1.05
2.09
2.59
6.08
f1 (ppm)

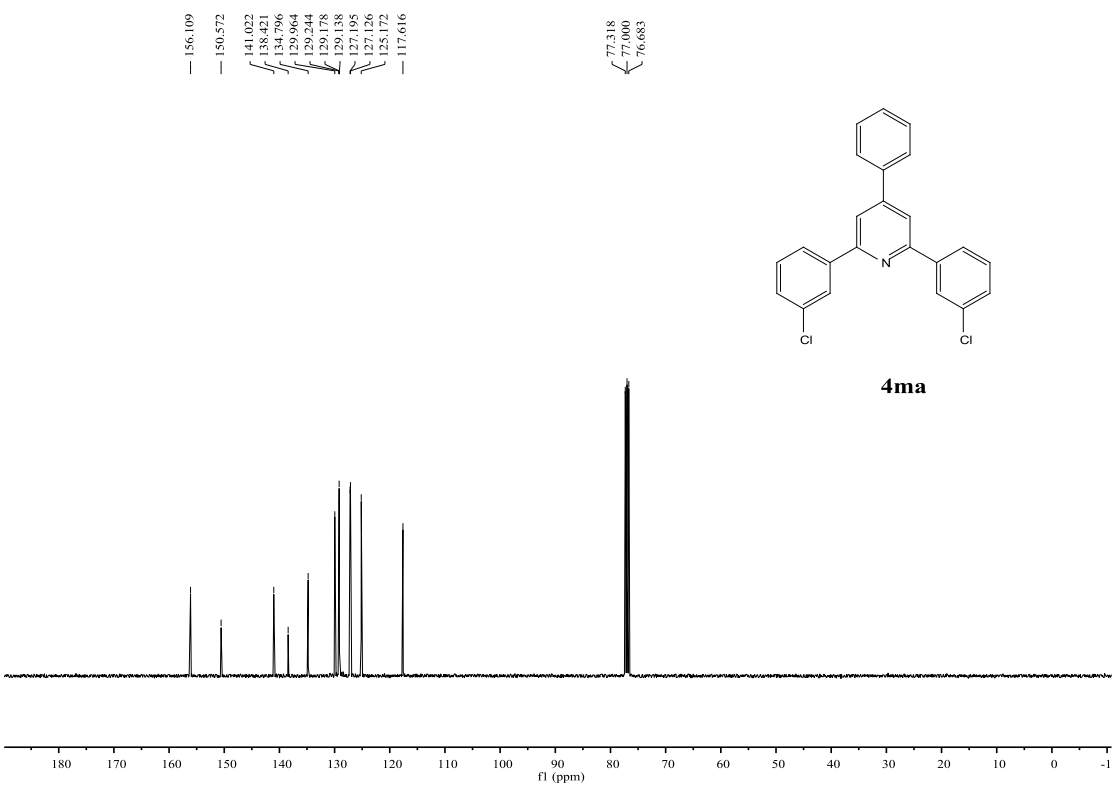
4la


157.648
149.978
139.558
139.025
138.262
129.755
129.044
128.886
128.565
127.810
127.140
124.276
117.153
77.317
77.000
76.682
21.599
N
CH3
CH3
f1 (ppm)

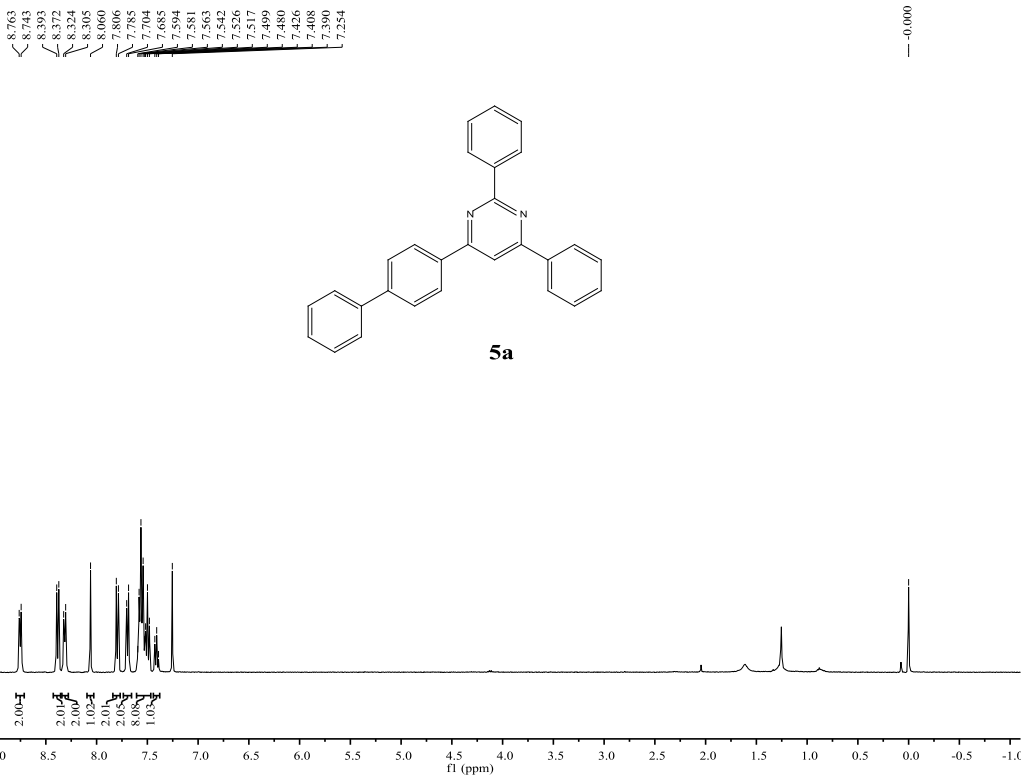
4la

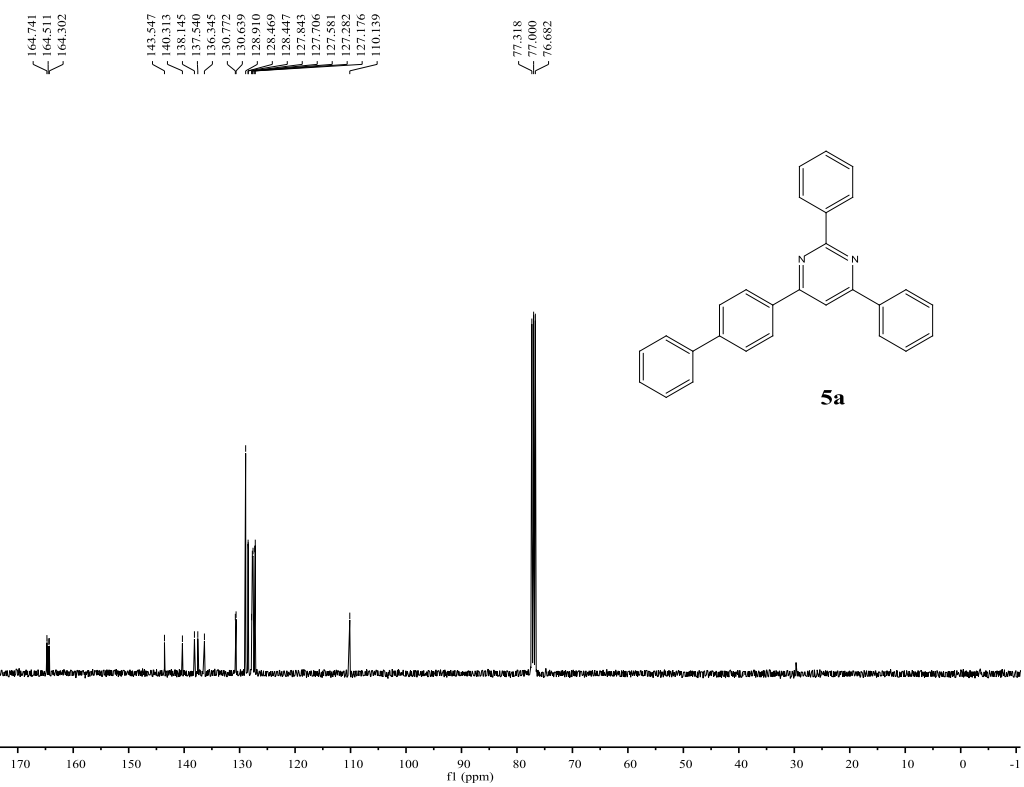

8.178
8.073
8.056
7.882
7.751
7.734
7.568
7.551
7.532
7.516
7.499
7.480
7.460
7.440
7.419
7.258
0.000
Cl
Cl
N
2.00
2.02
2.02
2.03
7.05
f1 (ppm)

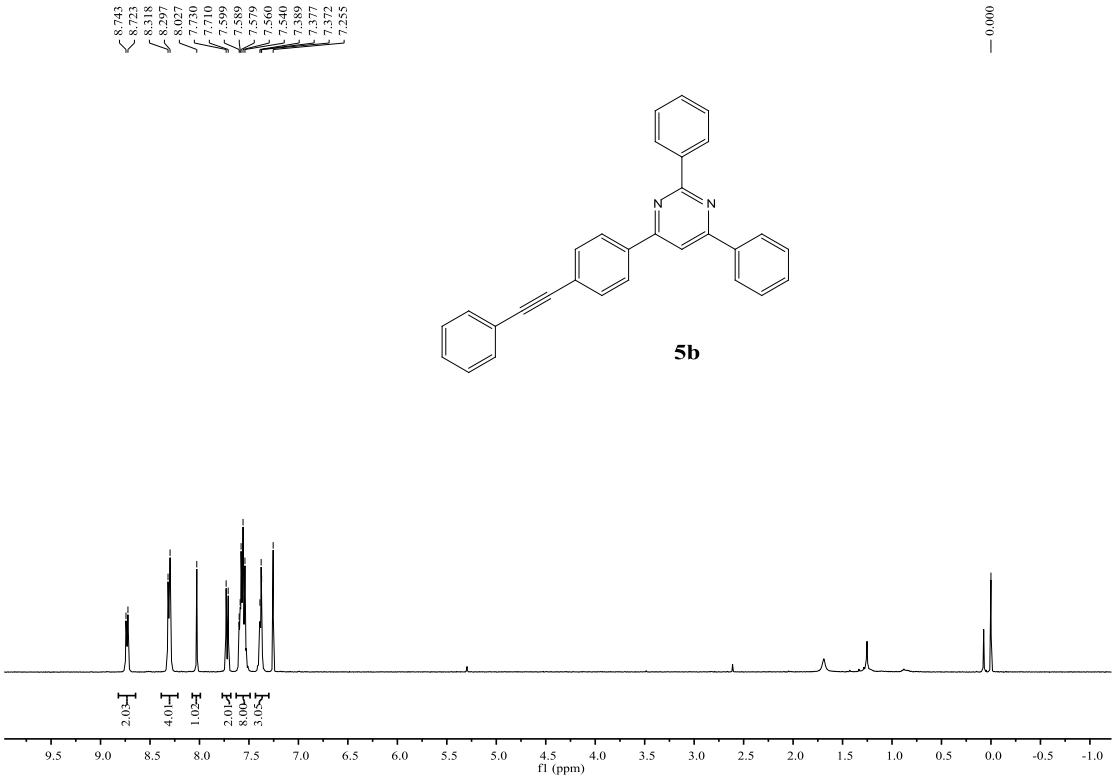
4ma

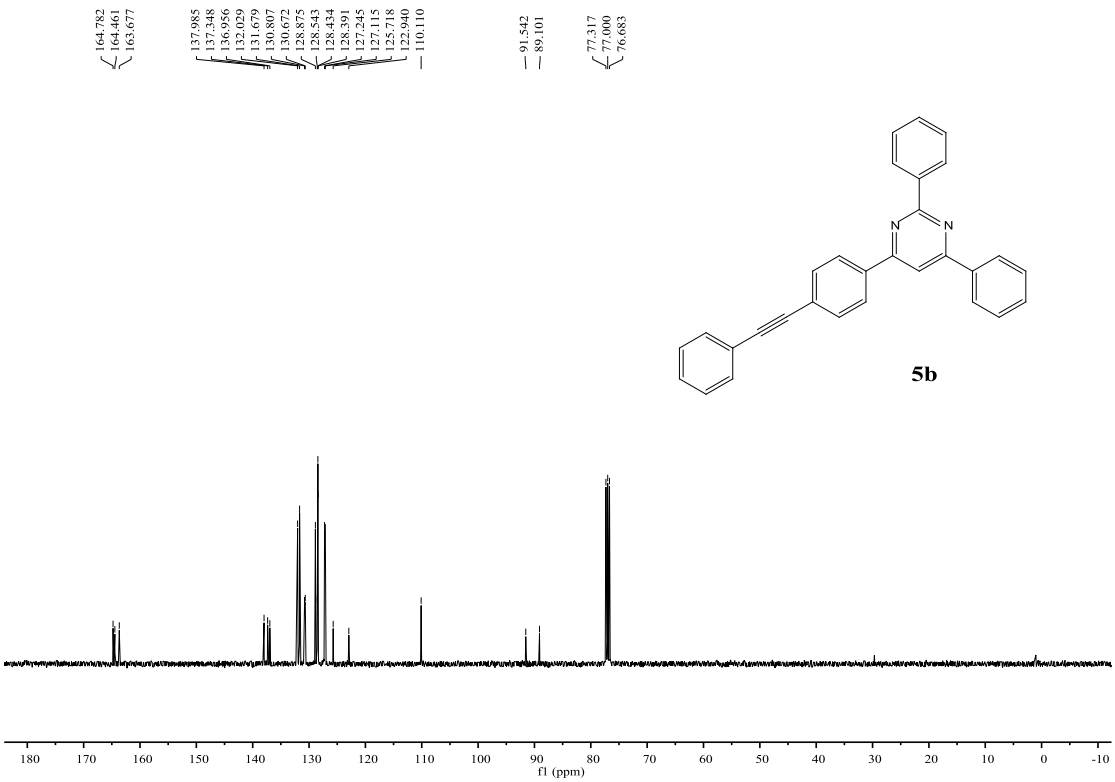

156.109
150.572
141.022
138.421
134.796
129.964
129.244
129.178
129.138
127.195
127.126
125.172
117.616
77.318
77.000
76.683
Cl
Cl
N
f1 (ppm)

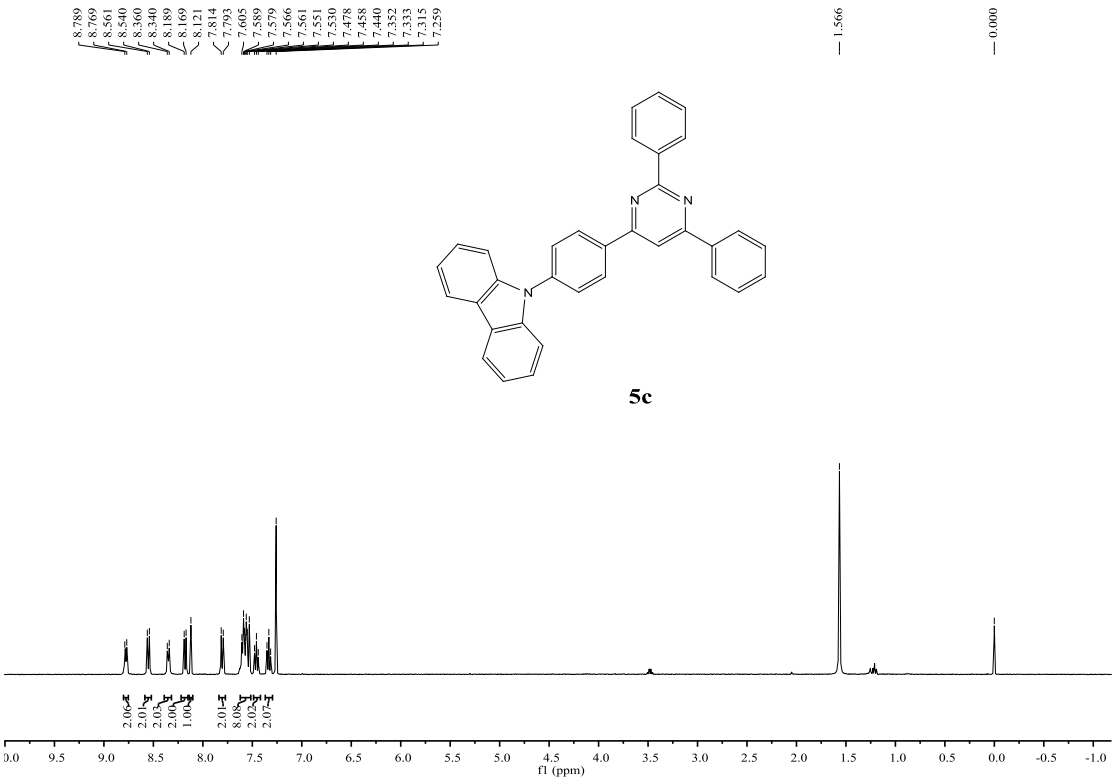
4ma

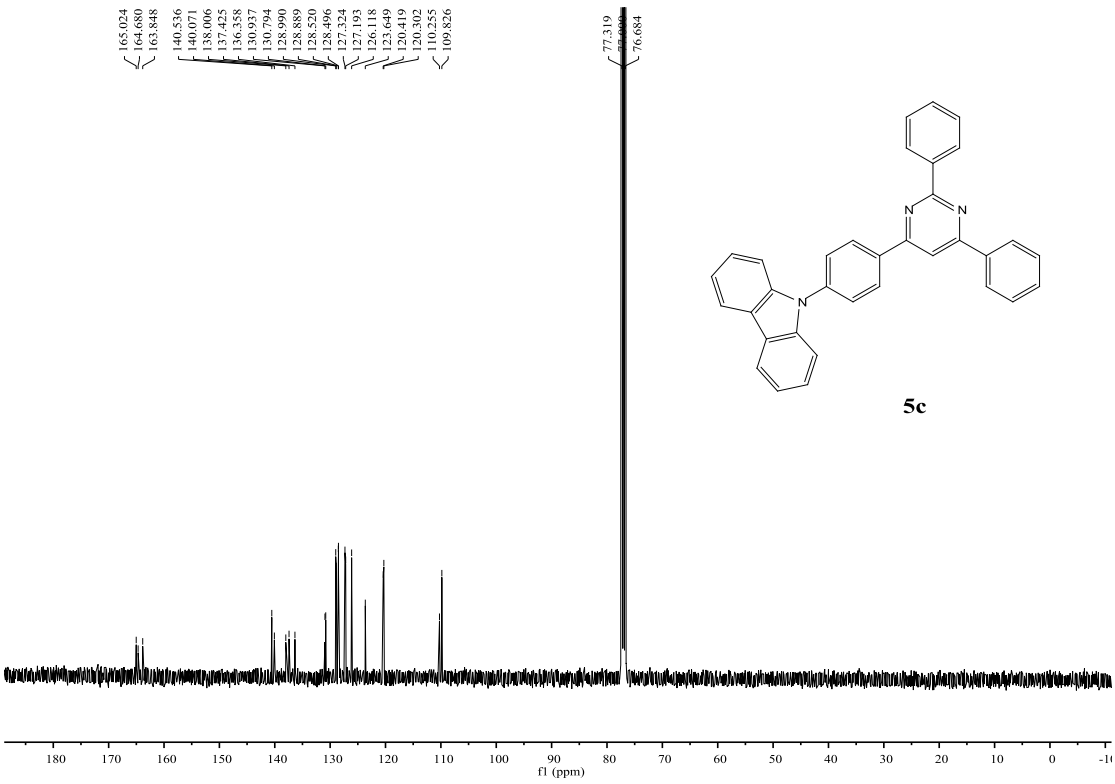

8.763
8.743
8.393
8.372
8.324
8.305
8.060
7.806
7.785
7.704
7.685
7.594
7.581
7.563
7.542
7.526
7.517
7.499
7.480
7.426
7.408
7.390
7.254
-0.000
5a
2.00
2.01
2.00
1.02
2.01
2.05
8.08
1.03
f1 (ppm)

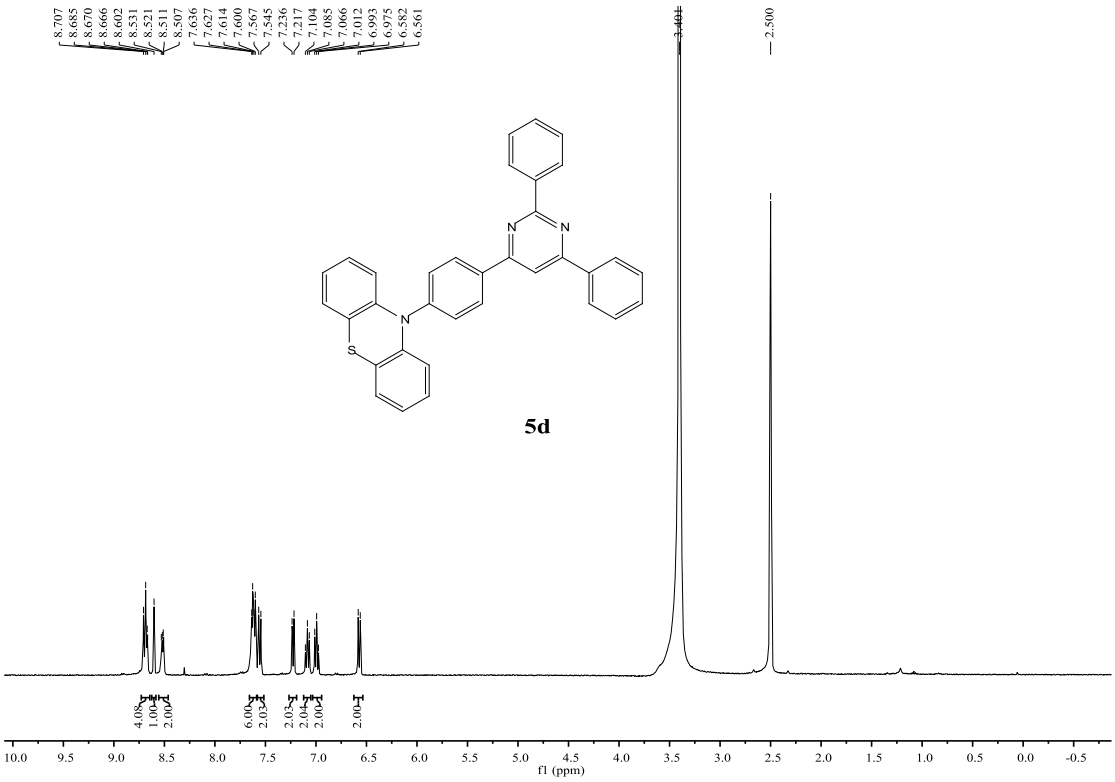

164.741
164.511
164.302
143.547
140.313
138.145
137.540
136.345
130.772
130.639
128.910
128.469
128.447
127.843
127.706
127.581
127.282
127.176
110.139
77.318
77.000
76.682
5a
f1 (ppm)


8.743
8.723
8.318
8.297
8.027
7.730
7.710
7.599
7.589
7.579
7.560
7.540
7.389
7.377
7.372
7.255
0.000
N
N
5b
2.03
4.01
1.02
2.01
8.00
3.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

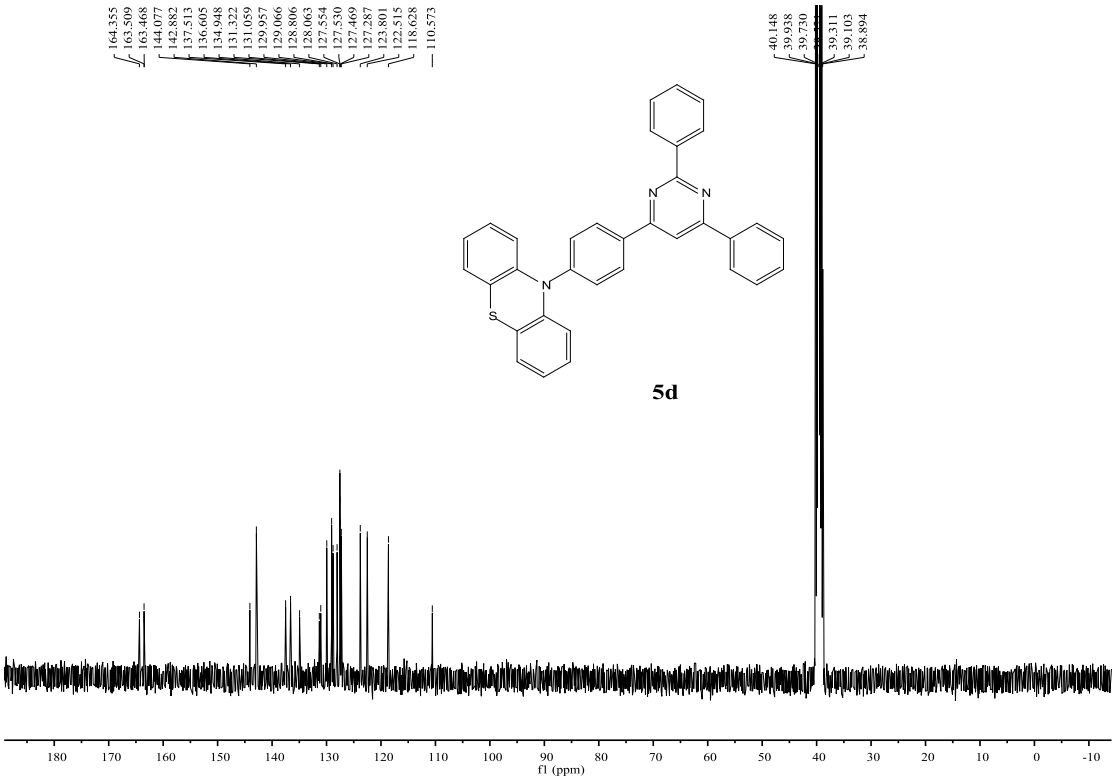

164.782
164.461
163.677
137.985
137.348
136.956
132.029
131.679
130.807
130.672
128.875
128.543
128.434
128.391
127.245
127.115
125.718
122.940
110.110
91.542
89.101
77.317
77.000
76.683
N
N
5b
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.789
8.769
8.561
8.540
8.360
8.340
8.189
8.169
8.121
7.814
7.793
7.605
7.589
7.579
7.566
7.561
7.551
7.530
7.478
7.458
7.440
7.352
7.333
7.315
7.259
1.566
0.000
N
N
N
5c
2.06
2.01
2.03
2.00
1.00
2.01
8.08
2.02
2.07
f1 (ppm)


165.024
164.680
163.848
140.536
140.071
138.006
137.425
136.358
130.937
130.794
128.990
128.889
128.520
128.496
127.324
127.193
126.118
123.649
120.419
120.302
110.255
109.826
77.319
77.000
76.684
N
N
N
5c
f1 (ppm)


8.707
8.685
8.670
8.666
8.602
8.531
8.521
8.511
8.507
7.636
7.627
7.614
7.600
7.567
7.545
7.236
7.217
7.104
7.085
7.066
7.012
6.993
6.975
6.582
6.561
3.401
2.500
4.08
1.00
2.00
6.00
2.03
2.03
2.04
2.00
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

5d


164.355
163.509
163.468
144.077
142.882
137.513
136.605
134.948
131.322
131.059
129.957
129.066
128.806
128.063
127.554
127.530
127.469
127.287
123.801
122.515
118.628
110.573
40.148
39.938
39.730
39.311
39.103
38.894
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

5d