# Supporting Information

## Four-component quinazolines synthesis from simple anilines, aromatic aldehydes and ammonium iodide under metal-free conditions

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**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 were recorded at Keecloud (Shanghai) Biotechnology co. LTD. HRMS was conducted using electrospraying ionization (ESI) and was performed on a Thermo Scientific LTQ Orbitrap XL. 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 quinazolines from anilines**

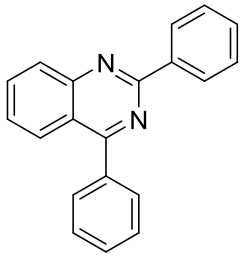
A 10 mL oven-dried reaction vessel was charged with anilines (0.2 mmol), benzaldehydes (0.6 mmol), ammonium iodide (0.24 mmol), DMSO (0.2 mmol) and chlorobenzene (0.5 mL). The reaction vessel was purged with oxygen for three times and stirred at 150 $^{o}$C for 12 h. After cooling to room temperature, the volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel to give the products.

**3. General procedure for the synthesis of quinazolines from nitroarenes**

A 10 mL oven-dried reaction vessel was charged with nitrobenzene (0.2 mmol), benzaldehydes (0.6 mmol), ammonium iodide (0.24 mmol), iron powder (0.4 mmol) and chlorobenzene (0.5 mL). The reaction vessel was stirred at 150 $^{o}$C for 12 h under air. 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 desired product.

**4. Characterization of products**

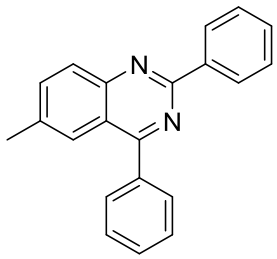
**2,4-Diphenylquinazoline (3aa, CAS: 31730-65-1)[1]**




The reaction was conducted with aniline (18.2 μL, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3aa** as white solid; yield: 47.5 mg (85%), mp 114-116 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.71 (d, *J* = 7.1 Hz, 2H), 8.19 (d, *J* = 8.5 Hz, 1H), 8.14 (d, *J* = 8.5 Hz, 1H), 7.90 (s, 3H), 7.64-7.49 (m, 7H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 168.2, 160.2, 151.9, 138.2, 137.6, 133.5, 130.5, 130.1, 129.9, 129.1, 128.6, 128.5, 127.0, 121.6.

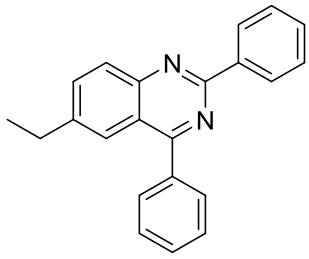
**6-Methyl-2,4-diphenylquinazoline (3ba, CAS: 16107-83-8)[1]**



The reaction was conducted with 4-methylaniline (21.4 mg, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to give **3ba** as yellow solid; yield: 45.1 mg (76%), mp 173-176 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.68 (d, *J* = 6.8 Hz, 2H), 8.08 (d, *J* = 8.3 Hz, 1H), 7.88 (s, 3H), 7.73 (d, *J* = 8.4 Hz, 1H), 7.60 (s, 3H), 7.53-7.51 (m, 3H), 2.52 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 167.5, 159.5, 150.5, 138.3, 137.8, 137.1, 135.7, 130.2, 130.1, 129.7, 128.8, 128.5, 125.5, 121.6, 21.8.

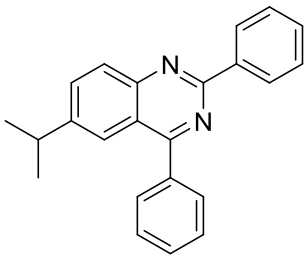
**6-Ethyl-2,4-diphenylquinazoline (3ca)**



The reaction was conducted with 4-ethylaniline (25.0 μL, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to give **3ca** as white solid; yield: 55.2 mg (89%), mp 102-105 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.68 (d, *J* = 7.1 Hz, 2H), 8.10 (d, *J* = 8.3 Hz, 1H), 7.90 (s, 3H), 7.77 (d, *J* = 8.6 Hz, 1H), 7.61 (s, 3H), 7.53-7.51 (m, 3H), 2.82 (q, *J* = 7.1 Hz, 2H), 1.30 (t, *J* = 7.0 Hz, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 167.6, 159.6, 150.7, 143.3, 138.3, 137.8, 134.6, 130.2, 130.1, 129.7, 128.9, 128.5, 124.3, 121.6, 29.1, 15.4; HRMS (m/z): calcd for $C_{22}H_{19}N_2$ $[M+H]^+$ 311.1543, found 311.1541.

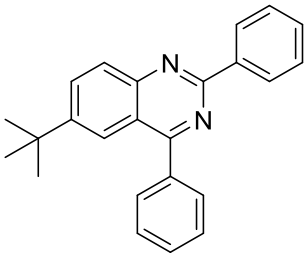
**6-Isopropyl-2,4-diphenylquinazoline (3da, CAS: 106910-93-4)[2]**



The reaction was conducted with 4-isopropylaniline (27.5 μL, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to give **3da** as yellow solid; yield: 58.5 mg (90%), mp 58-60 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.69 (d, *J* = 6.6 Hz, 2H), 8.16 (d, *J* = 7.2 Hz, 1H), 7.91 (d, *J* = 8.3 Hz, 3H), 7.83 (d, *J* = 8.4 Hz, 1H), 7.61 (s, 3H), 7.52 (d, *J* = 8.6 Hz, 3H), 3.08 (m, 1H), 1.32 (d, *J* = 6.6 Hz, 6H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 167.7, 159.6, 150.8, 147.8, 138.3, 137.8, 133.2, 130.2, 130.1, 129.8, 129.0, 128.5, 128.5, 128.4, 123.0, 121.6, 34.3, 23.7.

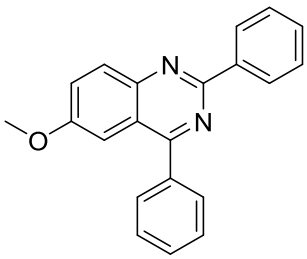
**6-(*tert*-Butyl)-2,4-diphenylquinazoline (3ea)**



The reaction was conducted with 4-(*tert*-butyl)aniline (31.8 μL, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to give **3ea** as yellow liquid; yield: 64.3 mg (95%).

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.69 (d, *J* = 6.9 Hz, 2H), 8.14 (d, *J* = 7.9 Hz, 1H), 8.09 (s, 1H), 8.01 (d, *J* = 8.9 Hz, 1H), 7.93 (d, *J* = 5.7 Hz, 2H), 7.61 (s, 3H), 7.53 (d, *J* = 8.5 Hz, 3H), 1.39 (s, 9H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 167.8, 159.8, 150.5, 145.0, 138.3, 137.8, 132.4, 130.2, 130.1, 129.8, 128.9, 128.6, 128.5, 128.4, 121.7, 121.2, 35.1, 31.0; HRMS (m/z): calcd for $C_{24}H_{23}N_2$ $[M+H]^+$ 339.1856, found 339.1852.

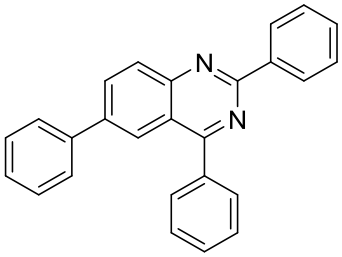
**6-Methoxy-2,4-diphenylquinazoline (3fa, CAS: 1315314-52-3)[1]**



The reaction was conducted with 4-methoxyaniline (24.6 mg, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 20:1) to give **3fa** as yellow solid; yield: 53.6 mg (86%), mp 138-140 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.66 (d, *J* = 7.1 Hz, 2H), 8.11 (d, *J* = 8.4 Hz, 1H), 7.91 (d, *J* = 5.8 Hz, 2H), 7.75 – 7.46 (m, 7H), 7.40 (s, 1H), 3.86 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 166.5, 158.5, 157.9, 148.0, 138.2, 137.9, 130.5, 130.0, 129.8, 129.7, 128.5, 128.4, 128.2, 126.1, 122.3, 104.2, 55.5.

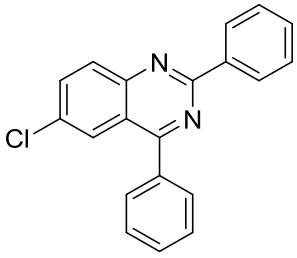
**2,4,6-Triphenylquinazoline (3ga)**




The reaction was conducted with [1,1'-biphenyl]-4-amine (34.0 mg, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30:1) to give **3ga** as white solid; yield: 58.5 mg (82%), mp 143-145 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.72 (d, *J* = 6.6 Hz, 2H), 8.31 (s, 1H), 8.26 (d, *J* = 8.7 Hz, 1H), 8.17 (d, *J* = 8.6 Hz, 1H), 7.94 (d, *J* = 5.6 Hz, 2H), 7.67-7.60 (m, 5H), 7.57-7.45 (m, 5H), 7.40 (t, *J* = 7.1 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 168.3, 160.1, 151.3, 139.9, 139.8, 138.1, 137.6, 133.2, 130.5, 130.2, 129.9, 129.5, 129.0, 128.6, 128.6, 128.5, 127.9, 127.3, 124.5, 121.8; HRMS (m/z): calcd for $C_{26}H_{19}N_2$ $[M+H]^+$ 359.1543, found 359.1550.

**6-Chloro-2,4-diphenylquinazoline (3ha, CAS: 30169-34-7)[1]**

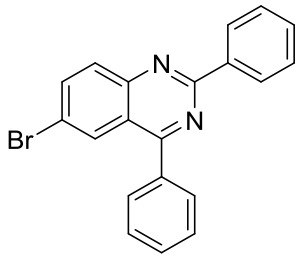



The reaction was conducted with 4-chloroaniline (25.5 mg, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3ha** as white solid; yield: 40.1 mg (63%), mp 193-195 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.69 (d, *J* = 7.9 Hz, 2H), 8.18-8.07 (m, 2H), 7.87 (d, *J* = 3.7 Hz, 2H), 7.83 (d, *J* = 9.0 Hz, 1H), 7.66-7.61 (m, 3H), 7.56-7.50 (m, 3H);$^{13}$C NMR (100 MHz,

$CDCl_3$, ppm) δ 167.5, 160.4, 150.4, 137.7, 137.0, 134.5, 132.6, 130.8, 130.7, 130.2, 130.0, 128.7, 128.6, 128.5, 125.7, 122.1.

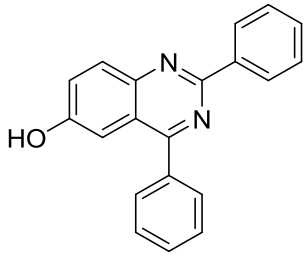
**6-Bromo-2,4-diphenylquinazoline (3ia, CAS: 1229609-99-7)[1]**




The reaction was conducted with 4-bromoaniline (34.0 mg, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3ia** as white solid; yield: 49.8 mg (69%), mp 202-204 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.69 (d, *J* = 7.9 Hz, 2H), 8.27 (s, 1H), 8.06 (d, *J* = 8.9 Hz, 1H), 7.96 (d, *J* = 9.0 Hz, 1H), 7.87 (d, *J* = 3.6 Hz, 2H), 7.67-7.61 (m, 3H), 7.57-7.49 (m, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 167.4, 160.4, 150.6, 137.7, 137.0, 137.0, 130.9, 130.8, 130.2, 130.0, 129.1, 128.7, 128.7, 128.6, 122.6, 120.6.

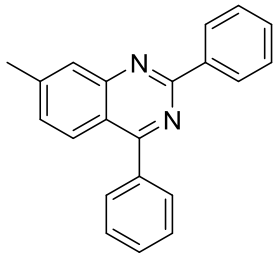
**2,4-Diphenylquinazolin-6-ol (3ja)**




The reaction was conducted with 4-aminophenol (21.8 mg, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 10:1) to give **3ja** as yellow solid; yield: 29.5 mg (49%), mp 213-216 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.58 (d, *J* = 6.5 Hz, 2H), 8.10 (t, *J* = 9.3 Hz, 2H), 7.78 (d, *J* = 3.7 Hz, 2H), 7.52-7.45 (m, 7H), 7.36 (d, *J* = 2.6 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 171.8, 166.9, 158.4, 154.7, 137.9, 137.5, 133.8, 130.2, 129.8, 129.3, 128.5, 128.5, 128.4, 125.9, 122.5, 108.4; HRMS (m/z): calcd for $C_{20}H_{15}N_2O$ $[M+H]^+$ 299.1179, found 299.1180.

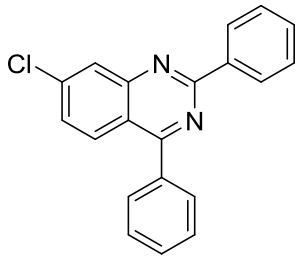
**7-Methyl-2,4-diphenylquinazoline (3ka, CAS: 16151-75-0)[1]**



The reaction was conducted with 3-methylaniline (21.6 μL, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to give **3ka** as white solid; yield: 44.6 mg (75%), mp 159-162 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.69 (d, *J* = 6.9 Hz, 2H), 8.02 (d, *J* = 8.4 Hz, 1H), 7.97 (s, 1H), 7.89 (d, *J* = 3.2 Hz, 2H), 7.59 (s, 3H), 7.52 (d, *J* = 7.1 Hz, 3H), 7.38 (d, *J* = 8.5 Hz, 1H), 2.61 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 167.6, 160.2, 152.1, 144.4, 138.2, 137.7, 130.3, 130.1, 129.7, 129.2, 128.5, 128.5, 128.4, 128.0, 126.5, 119.7, 21.99.

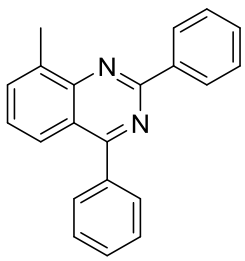
**7-Chloro-2,4-diphenylquinazoline (3la)[3]**



The reaction was conducted with 3-chloroaniline (21.0 μL, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to give **3la** as white solid; yield: 41.2 mg (65%), mp 156-158 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.70 (d, *J* = 7.8 Hz, 2H), 8.20 (s, 1H), 8.07 (d, *J* = 8.9 Hz, 1H), 7.86 (d, *J* = 6.7 Hz, 2H), 7.61 (s, 3H), 7.56-7.48 (m, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 168.2, 161.0, 152.5, 139.7, 137.6, 137.2, 130.8, 130.2, 130.1, 128.7, 128.6, 128.5, 128.4, 128.0, 127.9, 120.0.

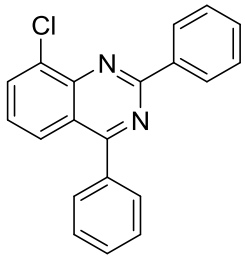
**8-Methyl-2,4-diphenylquinazoline (3ma, CAS: 106910-91-2)[4]**



The reaction was conducted with 2-methylaniline (21.3 μL, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to give **3ma** as yellow solid; yield: 43.2 mg (73%), mp 106-109 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.75 (d, *J* = 7.1 Hz, 2H), 7.95 (d, *J* = 8.6 Hz, 1H), 7.88 (d, *J* = 3.5 Hz, 2H), 7.73 (d, *J* = 6.7 Hz, 1H), 7.61-7.50 (m, 6H), 7.43 (t, *J* = 7.7 Hz, 1H), 2.92 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 168.3, 158.9, 150.8, 138.5, 138.0, 137.3, 133.2, 130.3, 130.1, 129.6, 128.6, 128.4, 128.3, 126.3, 124.6, 121.5, 17.50.

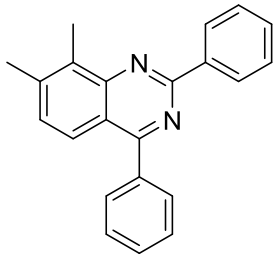
**8-Chloro-2,4-diphenylquinazoline (3na)**




The reaction was conducted with 2-chloroaniline (21.0 μL, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to give **3na** as white solid; yield: 31.3 mg (50%), mp 159-161 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.77 (d, *J* = 5.5 Hz, 2H), 8.04 (d, *J* = 8.4 Hz, 1H), 7.99 (d, *J* = 7.4 Hz, 1H), 7.86 (d, *J* = 4.0 Hz, 2H), 7.59-7.52 (m, 6H), 7.45 (t, *J* = 7.9 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 168.8, 160.5, 148.5, 137.7, 137.3, 133.7, 133.4, 130.9, 130.2, 130.1, 128.9, 128.6, 128.5, 126.5, 126.0, 122.9. HRMS (m/z): calcd for $C_{20}H_{14}ClN_2$ $[M+H]^+$ 317.0840, found 317.0846.

**7,8-Dimethyl-2,4-diphenylquinazoline (3oa)**

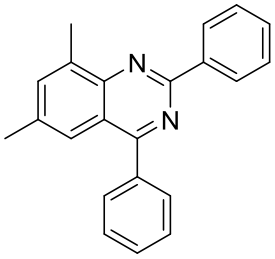



The reaction was conducted with 2,3-dimethylaniline (24.4 μL, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3oa** as white solid; yield: 53.2 mg (86%), mp 176-178 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.76 (d, *J* = 6.7 Hz, 2H), 7.86 (d, *J* = 7.7 Hz, 3H), 7.64-7.46 (m, 6H), 7.35 (d, *J* = 8.6 Hz, 1H), 2.88 (s, 3H), 2.55 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ

168.0, 158.9, 150.6, 141.6, 138.7, 138.1, 134.5, 130.1, 129.6, 129.5, 128.5, 128.4, 128.3, 123.7, 119.9, 20.8, 12.9; HRMS (m/z): calcd for $C_{22}H_{19}N_2$ $[M+H]^+$ 311.1543, found 311.1544.

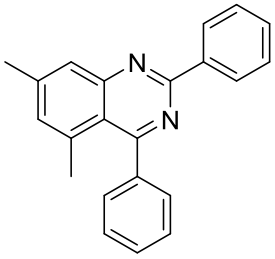
**6,8-Dimethyl-2,4-diphenylquinazoline (3pa)[5]**



The reaction was conducted with 2,4-dimethylaniline (24.8 μL, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3pa** as white solid; yield: 55.4 mg (89%), mp 150-152 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.73 (d, *J* = 7.0 Hz, 2H), 7.87 (d, *J* = 7.6 Hz, 2H), 7.70 (s, 1H), 7.59 (d, *J* = 7.0 Hz, 4H), 7.56-7.46 (m, 3H), 2.89 (s, 3H), 2.47 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 167.5, 158.3, 149.5, 138.6, 138.2, 137.0, 136.3, 135.6, 130.1, 130.1, 129.5, 128.4, 128.4, 128.4, 123.2, 121.5, 21.9, 17.4.

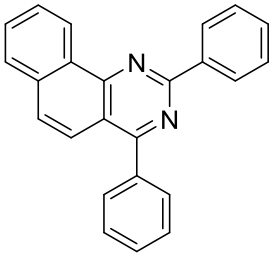
**5,7-Dimethyl-2,4-diphenylquinazoline (3qa)[4]**



The reaction was conducted with 3,5-dimethylaniline (24.9 μL, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3qa** as white solid; yield: 38.3 mg (62%), mp 153-156 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.63 (d, *J* = 8.0 Hz, 2H), 7.83 (s, 1H), 7.60-7.42 (m, 8H), 7.18 (s, 1H), 2.55 (s, 3H), 2.06 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 168.0, 158.6, 153.3, 143.8, 142.0, 137.9, 135.6, 132.4, 130.2, 128.9, 128.9, 128.5, 128.4, 128.1, 126.4, 120.2, 23.7, 21.8.

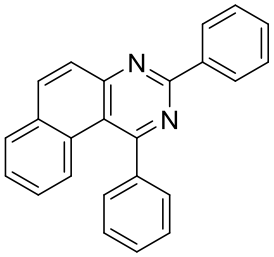
**2,4-Diphenylbenzo[*h*]quinazoline (3ra, CAS: 36547-38-3)[1]**



The reaction was conducted with 1-naphthalenamine (28.6 mg, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to give **3ra** as white solid; yield: 46.4 mg (70%), mp 155-157 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 9.56 (d, *J* = 9.6 Hz, 1H), 8.85 (d, *J* = 6.7 Hz, 2H), 8.01-7.89 (m, 4H), 7.87-7.75 (m, 3H), 7.65-7.53 (m, 6H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 166.6, 160.0, 151.8, 138.4, 138.0, 134.9, 130.6, 130.4, 130.3, 129.9, 129.6, 128.6, 128.5, 128.4, 127.7, 127.7, 127.2, 125.2, 122.7, 119.1.

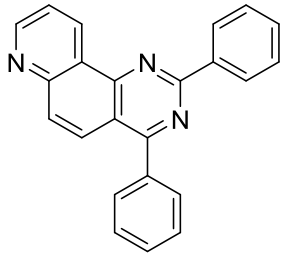
**1,3-Diphenylbenzo[*f*]quinazoline (3sa, CAS: 60708-99-8)[6]**



The reaction was conducted with 2-naphthalenamine (28.6 mg, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3sa** as white solid; yield: 52.1 mg (78%), mp 154-157 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.70 (d, *J* = 6.6 Hz, 2H), 8.16 (d, *J* = 9.0 Hz, 1H), 8.04 (d, *J* = 9.0 Hz, 1H), 7.89 (d, *J* = 7.9 Hz, 1H), 7.80 (d, *J* = 8.5 Hz, 1H), 7.73 (d, *J* = 7.8 Hz, 2H), 7.58-7.51 (m, 7H), 7.26 (t, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 166.1, 159.7, 154.2, 141.8, 137.6, 135.6, 132.7, 130.5, 129.5, 129.1, 129.0, 128.9, 128.7, 128.6, 128.5, 127.7, 127.2, 127.0, 126.4, 119.3.

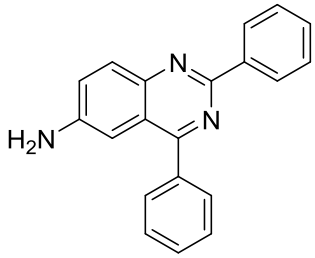
**2,4-Diphenylpyrido[2,3-*h*]quinazoline (3ta)**



The reaction was conducted with 5-aminoquinoline (28.8 mg, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to give **3ta** as white solid; yield: 26.6 mg (40%), mp 199-202 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 9.83 (d, *J* = 8.2 Hz, 1H), 9.16 (d, *J* = 2.9 Hz, 1H), 8.83 (d, *J* = 6.3 Hz, 2H), 8.27 (d, *J* = 9.3 Hz, 1H), 8.11 (d, *J* = 9.3 Hz, 1H), 7.93 (d, *J* = 7.7 Hz, 2H), 7.76 (q, 4.5 Hz, 1H), 7.66-7.52 (m, 6H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 167.1, 160.7, 152.5, 151.4, 150.3, 137.9, 137.4, 134.0, 130.8, 130.3, 130.0, 128.7, 128.6, 128.6, 128.3, 127.0, 126.3, 122.2, 119.0; HRMS (m/z): calcd for $C_{23}H_{16}N_3$ $[M+H]^+$ 334.1339, found 334.1340.

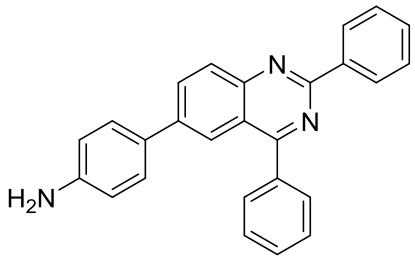
**2,4-Diphenylquinazolin-6-amine (3ua)**



The reaction was conducted with benzene-1,4-diamine (21.6 mg, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to give **3ua** as yellow solid; yield: 36.2 mg (61%), mp 159-162 ℃.

$^1$H NMR (400 MHz, DMSO-$d_6$, ppm) δ 8.49 (d, *J* = 7.6 Hz, 2H), 7.86-7.81 (m, 3H), 7.62 (d, *J* = 5.8 Hz, 3H), 7.53-7.46 (m, 3H), 7.41 (d, *J* = 9.0 Hz, 1H), 7.02 (s, 1H), 5.97 (s, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 165.6, 157.4, 146.6, 145.2, 138.5, 138.1, 130.2, 129.8, 129.7, 129.5, 128.4, 128.3, 128.1, 125.3, 122.9, 106.1; HRMS (m/z): calcd for $C_{20}H_{16}N_3$ $[M+H]^+$ 298.1339, found 298.1340.

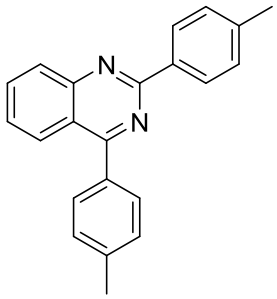
**4-(2,4-Diphenylquinazolin-6-yl)aniline (3va)**



The reaction was conducted with benzidine (36,8 mg, 0.2 mmol), benzaldehyde (61.2 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to give **3ua** as yellow solid; yield: 31.8 mg (43%), mp 202-204 ℃.

$^1$H NMR (400 MHz, DMSO-$d_6$, ppm) δ 8.60 (d, *J* = 7.9 Hz, 2H), 8.27 (d, *J* = 8.8 Hz, 1H), 8.13 (d, *J* = 8.8 Hz, 1H), 8.09 (s, 1H), 7.95 (d, *J* = 7.6 Hz, 2H), 7.68 (d, *J* = 4.8 Hz, 3H), 7.57 (d, *J* = 6.7 Hz, 3H), 7.43 (d, *J* = 8.5 Hz, 2H), 6.68 (d, *J* = 8.5 Hz, 2H), 5.42 (s, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 168.0, 159.6, 150.8, 146.4, 139.8, 138.2, 137.8, 132.8, 130.3, 130.1, 130.0, 129.9, 129.8, 129.3, 128.5, 128.5, 128.2, 122.8, 121.9, 115.4; HRMS (m/z): calcd for $C_{26}H_{20}N_3$ $[M+H]^+$ 374.1652, found 374.1653.

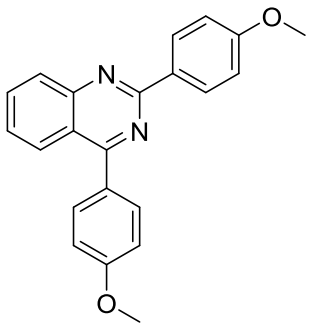
**2,4-Di-*p*-tolylquinazoline (3ab, CAS: 1446786-00-0)[6]**



The reaction was conducted with aniline (18.2 μL, 0.2 mmol), 4-methylbenzaldehyde (71.0 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3ab** as white solid; yield: 45.1 mg (73%), mp 132-134 ℃.

1H NMR (400 MHz, $CDCl_3$, ppm) δ 8.59 (d, *J* = 8.0 Hz, 2H), 8.14 (d, *J* = 8.9 Hz, 2H), 7.87 (t, *J* = 8.2 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 2H), 7.52 (t, *J* = 7.6 Hz, 1H), 7.41 (d, *J* = 7.9 Hz, 2H), 7.33 (d, *J* = 8.1 Hz, 2H), 2.50 (s, 3H), 2.44 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 168.3, 158.9, 150.8, 138.5, 138.0, 137.3, 133.2, 130.3, 130.1, 129.6, 128.6, 128.4, 128.3, 126.3, 124.6, 121.5, 17.50.

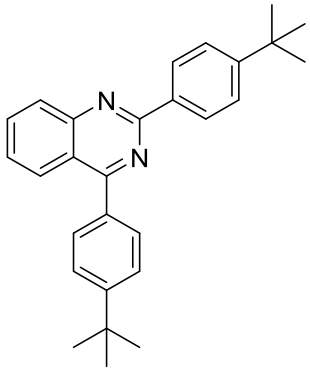
**2,4-Bis(4-methoxyphenyl)quinazoline (3ac, CAS: 1446785-99-4)[5]**



The reaction was conducted with aniline (18.2 μL, 0.2 mmol), 4-methoxybenzaldehyde (72.9 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 20:1) to give **3ac** as white solid; yield: 27.3 mg (40%), mp 134-137 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.66 (d, *J* = 8.8 Hz, 2H), 8.12 (q, 8.4 Hz, 2H), 7.90-7.83 (m, 3H), 7.51 (t, *J* = 8.0 Hz, 1H), 7.12 (d, *J* = 8.7 Hz, 2H), 7.04 (d, *J* = 8.9 Hz, 2H), 3.93 (s, 3H), 3.90 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 167.5, 161.6, 161.1, 159.8, 152.0, 133.2, 131.8, 130.9, 130.2, 130.2, 128.8, 127.0, 126.3, 121.2, 113.9, 113.7, 55.4, 55.3.

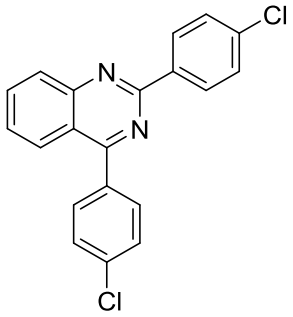
**2,4-Bis(4-(*tert*-butyl)phenyl)quinazoline (3ad)**



The reaction was conducted with aniline (18.2 μL, 0.2 mmol), 4-(*tert*-butyl)benzaldehyde (100.2 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to give **3ad** as yellow solid; yield: 56.9 mg (72%), mp 124-126 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.62 (d, *J* = 8.3 Hz, 2H), 8.19 (d, *J* = 8.3 Hz, 2H), 7.90-7.84 (m, 3H), 7.62 (d, *J* = 8.3 Hz, 2H), 7.55 (d, *J* = 8.4 Hz, 3H), 1.43 (s, 9H), 1.39 (s, 9H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 168.1, 160.3, 153.7, 153.1, 151.9, 135.5, 134.9, 133.3, 130.0, 129.0, 128.4, 127.1, 126.6, 125.5, 125.4, 121.5, 34.8, 31.3; HRMS (m/z): calcd for $C_{28}H_{31}N_2$ $[M+H]^+$395.2482, found 395.2484.

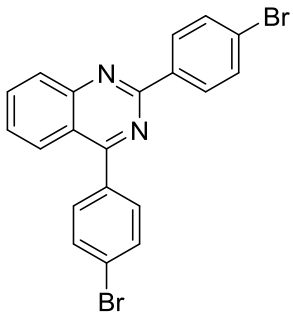
**2,4-Bis(4-chlorophenyl)quinazoline (3ae, CAS: 1520087-48-2)[7]**




The reaction was conducted with aniline (18.2 μL, 0.2 mmol), 4-chlorobenzaldehyde (84.3 mg, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30:1) to give **3ae** as white solid; yield: 63.6 mg (90%), mp 194-196 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.63 (d, *J* = 8.5 Hz, 2H), 8.15 (d, *J* = 8.5 Hz, 1H), 8.08 (d, *J* = 8.4 Hz, 1H), 7.91 (t, *J* = 8.2 Hz, 1H), 7.83 (d, *J* = 8.4 Hz, 2H), 7.59 (d, *J* = 8.3 Hz, 3H), 7.49 (d, *J* = 8.5 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 167.1, 159.1, 151.9, 136.8, 136.4, 136.4, 135.9, 133.8, 131.4, 129.9, 129.2, 128.8, 128.7, 127.4, 126.5, 121.4.

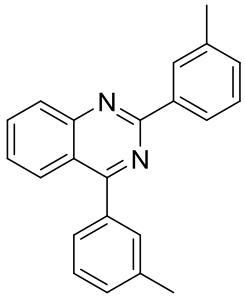
**2,4-Bis(4-bromophenyl)quinazoline (3af, CAS: 1446785-97-2)[5]**




The reaction was conducted with aniline (18.2 μL, 0.2 mmol), 4-bromobenzaldehyde (111.0 mg, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30:1) to give **3af** as white solid; yield: 71.8 mg (82%), mp 218-221 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.56 (d, *J* = 8.6 Hz, 2H), 8.16 (d, *J* = 8.4 Hz, 1H), 8.07 (d, *J* = 8.4 Hz, 1H), 7.91 (t, *J* = 8.3 Hz, 1H), 7.75 (s, 4H), 7.65 (d, *J* = 8.6 Hz, 2H), 7.58 (t, *J* = 8.1 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 167.2, 159.2, 151.9, 136.9, 136.3, 133.8, 131.8, 131.7, 130.2, 129.2, 127.4, 126.5, 125.4, 124.7, 121.4.

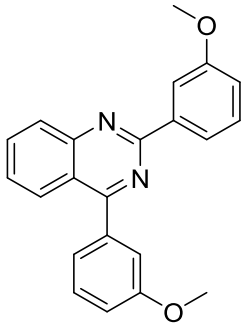
**2,4-Di-*m*-tolylquinazoline (3ag)**



The reaction was conducted with aniline (18.2 μL, 0.2 mmol), 3-methylbenzaldehyde (70.7 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to give **3ag** as white solid; yield: 40.4 mg (65%), mp 88-91 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.50 (s, 2H), 8.17 (d, *J* = 8.4 Hz, 1H), 8.12 (d, *J* = 8.4 Hz, 1H), 7.89 (t, *J* = 8.0 Hz, 1H), 7.70 (s, 1H), 7.66 (d, *J* = 7.9 Hz, 1H), 7.55 (t, *J* = 7.6 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 1H), 7.42 (q, *J* = 7.0 Hz, 2H), 7.32 (d, *J* = 7.4 Hz, 1H), 2.51 (s, 3H), 2.49 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 168.5, 160.3, 151.8, 138.3, 138.1, 138.0, 137.5, 133.4, 131.2, 130.6, 130.6, 129.1, 129.0, 128.4, 128.3, 127.3, 127.0, 126.8, 125.9, 121.7, 21.5, 21.5; HRMS (m/z): calcd for $C_{22}H_{19}N_2$ $[M+H]^+$ 311.1543, found 311.1545.

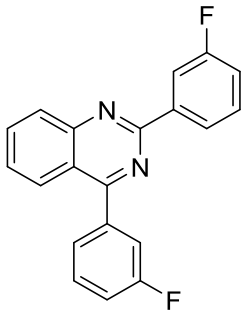
**2,4-Bis(3-methoxyphenyl)quinazoline (3ah)[6]**



The reaction was conducted with aniline (18.2 μL, 0.2 mmol), 3-methoxybenzaldehyde (73.0 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30:1) to give **3ah** as yellow solid; yield: 52.6 mg (77%), mp 96-98 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.31 (d, *J* = 7.8 Hz, 1H), 8.27 (s, 1H), 8.20 (d, *J* = 8.3 Hz, 1H), 8.16 (d, *J* = 8.4 Hz, 1H), 7.90 (t, *J* = 7.7 Hz, 1H), 7.56 (t, *J* = 7.6 Hz, 1H), 7.51 (t, *J* = 8.0 Hz, 1H), 7.47-7.41 (m, 3H), 7.14 (d, *J* = 9.0 Hz, 1H), 7.07 (d, *J* = 8.2 Hz, 1H), 3.96 (s, 3H), 3.92 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 168.0, 159.9, 159.9, 159.6, 151.8, 139.5, 138.8, 133.5, 129.5, 129.5, 129.0, 127.0, 126.9, 122.6, 121.6, 121.3, 116.8, 115.5, 115.5, 113.3, 55.4, 55.4.

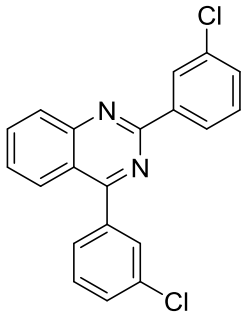
**2,4-Bis(3-fluorophenyl)quinazoline (3ai)**




The reaction was conducted with aniline (18.2 μL, 0.2 mmol), 3-fluorobenzaldehyde (63.0 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to give **3ai** as yellow solid; yield: 53.0 mg (83%), mp 158-160 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.50 (d, *J* = 7.8 Hz, 1H), 8.40 (d, *J* = 10.3 Hz, 1H), 8.22 (d, *J* = 8.4 Hz, 1H), 8.13 (d, *J* = 8.3 Hz, 1H), 7.94 (t, *J* = 7.7 Hz, 1H), 7.66 (d, *J* = 7.7 Hz, 1H), 7.64-7.55 (m, 3H), 7.51 (q, *J* = 6.7 Hz, 1H), 7.31 (t, *J* = 8.4 Hz, 1H), 7.21 (t, *J* = 8.2 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 166.9 (d, *J* = 2.4 Hz), 163.2 (d, *J* = 243.2 Hz), 162.7 (d, *J* = 245.7 Hz), 158.9 (d, *J* = 3.3 Hz), 151.9, 140.3 (d, *J* = 7.8 Hz), 139.5 (d, *J* = 7.4 Hz), 133.9, 130.1 (d, *J* = 8.1 Hz), 130.0 (d, *J* = 7.9 Hz), 129.3, 127.6, 126. 6, 125.9 (d, *J* = 3.1 Hz), 124.2 (d, *J* = 2.9 Hz), 121.5, 117.4 (d, *J* = 21.4 Hz), 117.1 (d, *J* = 22.6 Hz), 117.0 (d, *J* = 21.0 Hz), 115.4 (d, *J* = 23.0 Hz); HRMS (m/z): calcd for $C_{20}H_{13}F_2N_2$ $[M+H]^+$ 319.1041, found 319.1044.

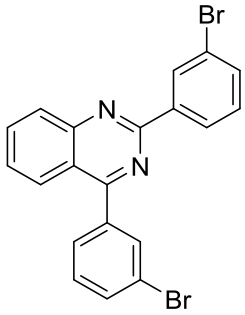
**2,4-Bis(3-chlorophenyl)quinazoline (3aj)**




The reaction was conducted with aniline (18.2 μL, 0.2 mmol), 3-chlorobenzaldehyde (68.0 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to give **3aj** as white solid; yield: 61.6 mg (88%), mp 143-145 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.69 (s, 1H), 8.59 (d, *J* = 6.5 Hz, 1H), 8.20 (d, *J* = 8.4 Hz, 1H), 8.09 (d, *J* = 8.4 Hz, 1H), 7.94 (t, *J* = 8.3 Hz, 1H), 7.87 (s, 1H), 7.75 (d, *J* = 7.3 Hz, 1H), 7.64-7.53 (m, 3H), 7.48-7.47 (m, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 166.8, 158.7, 151.8, 139.7, 139.0, 134.6, 133.9, 130.5, 130.0, 130.0, 129.8, 129.7, 129.2, 128.6, 128.3, 127.6, 126.7, 126.5, 121.5; HRMS (m/z): calcd for $C_{20}H_{13}Cl_2N_2$ $[M+H]^+$ 351.0450, found 351.0455.

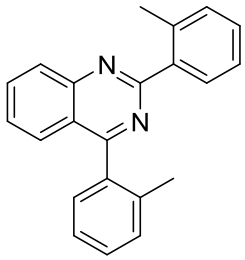
**2,4-Bis(3-bromophenyl)quinazoline (3ak)[6]**




The reaction was conducted with aniline (18.2 μL, 0.2 mmol), 3-bromobenzaldehyde (70.0 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to give **3ak** as white solid; yield: 81.3 mg (92%), mp 142-145 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.84 (s, 1H), 8.64 (d, *J* = 7.9 Hz, 1H), 8.20 (d, *J* = 8.4 Hz, 1H), 8.08 (d, *J* = 8.1 Hz, 1H), 8.02 (s, 1H), 7.94 (t, *J* = 7.7 Hz, 1H), 7.79 (d, *J* = 7.7 Hz, 1H), 7.74 (d, *J* = 8.1 Hz, 1H), 7.62 (q, *J* = 7.8 Hz, 2H), 7.49 (t, *J* = 7.9 Hz, 1H), 7.41 (t, *J* = 7.9 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 166.7, 158.6, 151.8, 139.9, 139.2, 133.9, 133.4, 132.9, 132.8, 131.5, 130.0, 129.2, 128.7, 127.6, 127.1, 126.5, 122.8, 122.7, 121.5.

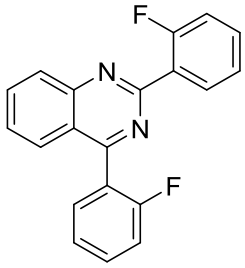
**2,4-Di-*o*-tolylquinazoline (3al, CAS: 1446786-01-1)[5]**




The reaction was conducted with aniline (18.2 μL, 0.2 mmol), 2-methylbenzaldehyde (69.4 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30:1) to give **3al** as white solid; yield: 31.9 mg (51%), mp 108-111 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.18 (d, *J* = 8.5 Hz, 1H), 7.91 (t, *J* = 8.4 Hz, 2H), 7.71 (d, *J* = 8.3 Hz, 1H), 7.54 (t, *J* = 7.6 Hz, 1H), 7.46-7.30 (m, 7H), 2.63 (s, 3H), 2.22 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 169.6, 163.4, 150.9, 138.8, 137.2, 136.7, 136.1, 133.8, 131.1, 130.6, 130.5, 129.4, 129.1, 128.8, 127.3, 127.0, 125.9, 125.6, 121.9, 21.1, 19.9.

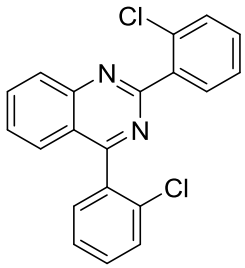
**2,4-Bis(2-fluorophenyl)quinazoline (3am)**




The reaction was conducted with aniline (18.2 μL, 0.2 mmol), 2-fluorobenzaldehyde (63.0 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30:1) to give **3am** as white solid; yield: 42.3 mg (66%), mp 97-99 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.24-8.16 (m, 2H), 7.94 (t, *J* = 7.7 Hz, 1H), 7.87 (dd, *J* = 8.3, 3.6 Hz, 1H), 7.71 (t, *J* = 7.3 Hz, 1H), 7.62 (t, *J* = 8.0 Hz,1H), 7.59-7.52 (m, 1H), 7.50-7.42 (m, 1H), 7.38 (t, *J* = 7.5 Hz, 1H), 7.33-7.20 (m, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 164.6, 161.2 (d, *J* = 253.1 Hz), 159.8 (d, *J* = 248.4 Hz), 159.2 (d, *J* = 4.3 Hz), 151.1, 134.0, 132.2 (d, *J* = 1.9 Hz), 131.8 (d, *J* = 3.0 Hz), 131.7 (d, *J* = 8.1 Hz), 131.5(d, *J* = 8.5 Hz), 128.9, 127.8, 127.1 (d, *J* = 10.1 Hz), 126.7 (d, *J* = 3.2 Hz), 125.2 (d, *J* = 15.0 Hz), 124.6 (d, *J* = 3.5 Hz), 124.1 (d, *J* = 3.8 Hz), 122.0, 116.8 (d, *J* = 22.0 Hz), 116.0 (d, *J* = 21.4 Hz); HRMS (m/z): calcd for $C_{20}H_{13}F_2N_2$ $[M+H]^+$ 319.1041, found 319.1044.

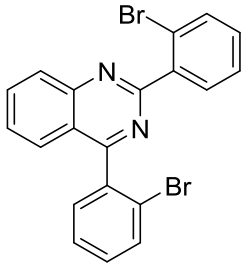
**2,4-Bis(2-chlorophenyl)quinazoline (3an)**




The reaction was conducted with aniline (18.2 μL, 0.2 mmol), 2-chlorobenzaldehyde (67.5 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 20:1) to give **3an** as yellow liquid; yield: 56.7 mg (80%).

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.22 (d, *J* = 8.5 Hz, 1H), 7.96 (t, *J* = 7.7 Hz, 1H), 7.88 (dd, *J* = 7.0, 2.3 Hz, 1H), 7.73 (d, *J* = 7.8 Hz, 1H), 7.64-7.35 (m, 8H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 167.0, 161.3, 150.8, 138.2, 135.9, 134.1, 132.9, 132.8, 131.7, 131.0, 130.6, 130.4, 130.2, 129.8, 128.9, 127.9, 126.9, 126.8, 126.8, 121.9; HRMS (m/z): calcd for $C_{20}H_{13}Cl_2N_2$ $[M+H]^+$ 351.0450, found 351.0455.

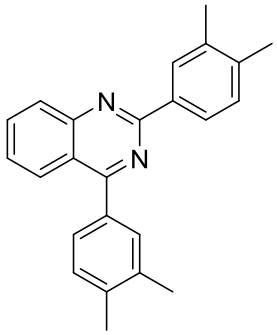
**2,4-Bis(2-bromophenyl)quinazoline (3ao)[6]**




The reaction was conducted with aniline (18.2 μL, 0.2 mmol), 2-bromobenzaldehyde (70.0 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 20:1) to give **3ao** as yellow liquid; yield: 50.1 mg (58%).

$^{1}$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.24 (d, *J* = 8.5 Hz, 1H), 7.97 (t, *J* = 8.3 Hz, 1H), 7.86 (d, *J* = 7.6 Hz, 1H), 7.74 (dd, *J* = 15.4, 8.1 Hz, 3H), 7.63 (t, *J* = 7.6 Hz, 1H), 7.56-7.39 (m, 4H), 7.31 (t, *J* = 8.5 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 168.2, 162.1, 150.8, 140.1, 137.9, 134.2, 133.5, 133.0, 131.6, 130.9, 130.7, 130.3, 128.9, 128.0, 127.5, 127.4, 126.9, 122.0, 121.8.

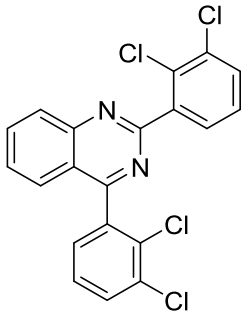
**2,4-Bis(3,4-dimethylphenyl)quinazoline (3ap)**




The reaction was conducted with aniline (18.2 μL, 0.2 mmol), 3,4-dimethylbenzaldehyde (79.6 μL, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3ap** as yellow solid; yield: 36.9 mg (55%), mp 158-160 ℃.

$^{1}$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.46 (s, 1H), 8.43 (d, *J* = 7.9 Hz, 1H), 8.14 (d, *J* = 8.5 Hz, 2H), 7.86 (t, *J* = 8.1 Hz, 1H), 7.68 (s, 1H), 7.61 (d, *J* = 7.7 Hz, 1H), 7.52 (t, *J* = 7.5 Hz, 1H), 7.36 (d, *J* = 7.7 Hz, 1H), 7.29 (d, *J* = 7.9 Hz, 1H), 2.42 (s, 3H), 2.40 (d, *J* = 3.4 Hz, 6H), 2.35 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 168.3, 160.4, 151.9, 139.3, 138.7, 136.9, 136.6, 135.9, 135.3, 133.3, 131.2, 129.8, 129.7, 129.6, 128.9, 127.7, 127.2, 126.5, 126.3, 121.6, 19.9, 19.9, 19.9, 19.8; HRMS (m/z): calcd for $C_{24}H_{23}N_2^+$ $[M+H]^+$ 339.1856, found 339.1854.

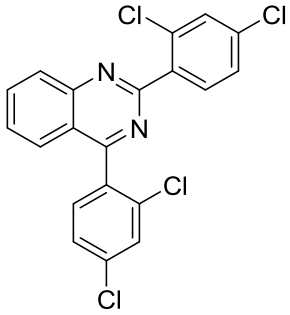
**2,4-Bis(2,3-dichlorophenyl)quinazoline (3aq)**



The reaction was conducted with aniline (18.2 μL, 0.2 mmol), 2,3-dichlorobenzaldehyde (105.0 mg, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 20:1) to give **3aq** as yellow solid; yield: 64.1 mg (76%), mp 188-191 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.22 (d, *J* = 8.5 Hz, 1H), 7.99 (t, *J* = 7.6 Hz, 1H), 7.75-7.63 (m, 4H), 7.58 (d, *J* = 6.5 Hz, 1H), 7.45-7.38 (m, 2H), 7.36 (t, *J* = 7.9 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 166.7, 161.0, 150.9, 140.3, 137.9, 134.6, 134.0, 133.9, 131.5, 131.5, 131.4, 131.1, 129.7, 129.1, 129.0, 128.5, 127.7, 127.4, 126.6, 121.8; HRMS (m/z): calcd for $C_{20}H_{13}Cl_4N_2$ $[M+H]^+$ 420.9827, found 420.9823.

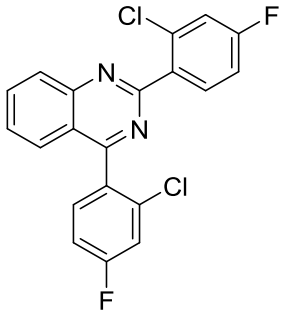
**2,4-Bis(2,4-dichlorophenyl)quinazoline (3ar)**



The reaction was conducted with aniline (18.2 μL, 0.2 mmol), 2,4-dichlorobenzaldehyde (105.0 mg, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3ar** as yellow liquid; yield: 75.1 mg (89%).

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.20 (d, *J* = 8.5 Hz, 1H), 7.97 (t, *J* = 7.6 Hz, 1H), 7.87 (d, *J* = 8.3 Hz, 1H), 7.71 (d, *J* = 7.7 Hz, 1H), 7.67-7.59 (m, 2H), 7.56 (s, 1H), 7.50-7.45 (m, 2H), 7.40 (d, *J* = 8.3 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 166.1, 160.3, 150.9, 136.4, 136.2, 135.7, 134.4, 134.4, 133.9, 133.8, 132.8, 131.9, 130.3, 129.8, 129.0, 128.3, 127.4, 127.2, 126.6, 121.8; HRMS (m/z): calcd for $C_{20}H_{13}Cl_4N_2$ $[M+H]^+$ 420.9827, found 420.9823.

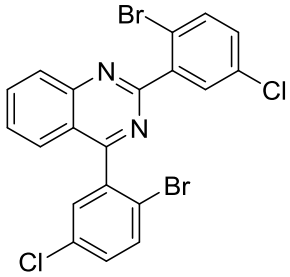
**2,4-Bis(2-chloro-4-fluorophenyl)quinazoline (3as)**




The reaction was conducted with aniline (18.2 μL, 0.2 mmol), 2-chloro-4-fluorobenzaldehyde (95.1 mg, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to give **3as** as yellow solid; yield: 55.1 mg (72%), mp 82-85 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.25 (d, *J* = 8.5 Hz, 1H), 7.99 (t, *J* = 7.7 Hz, 1H), 7.93 (t, *J* = 7.7 Hz, 1H), 7.72 (d, *J* = 8.4 Hz, 1H), 7.65 (t, *J* = 8.1 Hz, 1H), 7.54 (t, *J* = 8.0 Hz, 1H), 7.34 (d, *J* = 8.5 Hz, 1H), 7.29 (d, *J* = 8.6 Hz, 1H), 7.21 (t, *J* = 8.9 Hz, 1H), 7.15 (t, *J* = 8.3 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 166.3, 163.1 (d, *J* = 251.2 Hz), 162.8 (d, *J* = 250.6 Hz), 160.4, 150.9, 134.4, 134.4, 134.2 (d, *J* = 10.5 Hz), 134.0 (d, *J* = 10.4 Hz), 133.3 (d, *J* = 9.1 Hz), 132.4 (d, *J* = 9.0 Hz), 132.2 (d, *J* = 3,7 Hz), 129.0, 128.12, 126.6, 121.9, 117.8 (d, *J* = 24.6 Hz), 117.4 (d, *J* = 24.7 Hz), 114.5(d, *J* = 21.4 Hz), 114.2(d, *J* = 21.2 Hz); HRMS (m/z): calcd for $C_{20}H_{11}Cl_2F_2N_2$ $[M+H]^+$ 387.0262, found 387.0263.

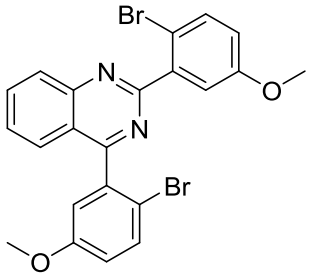
**2,4-Bis(2-bromo-5-chlorophenyl)quinazoline (3at)**




The reaction was conducted with aniline (18.2 μL, 0.2 mmol), 2-bromo-5-chlorobenzaldehyde (131.7 mg, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give **3at** as yellow solid; yield: 88.8 mg (87%), mp 133-136 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.25 (d, *J* = 8.5 Hz, 1H), 8.01 (t, *J* = 8.4 Hz, 1H), 7.85 (s, 1H), 7.72-7.65 (m, 4H), 7.50 (s, 1H), 7.41 (d, *J* = 8.6 Hz, 1H), 7.31 (d, *J* = 8.6 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 167.1, 160.9, 150.8, 141.3, 141.1, 139.2, 134.8, 134.7, 134.2, 133.8, 133.5, 131.6, 130.94, 130.7, 130.4, 129.0, 128.6, 126.6, 121.6, 120.0; HRMS (m/z): calcd for $C_{20}H_{11}Br_2Cl_2N_2$ $[M+H]^+$ 506.8661, found 506.8666.

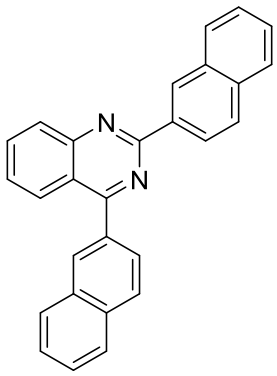
**2,4-Bis(2-bromo-5-methoxyphenyl)quinazoline (3au)**




The reaction was conducted with aniline (18.2 μL, 0.2 mmol), 2-bromo-5-methoxybenzaldehyde (129.0 mg, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 10:1) to give **3au** as yellow solid; yield: 63.9 mg (64%), mp 151-154 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 8.25 (d, *J* = 8.5 Hz, 1H), 7.97 (t, *J* = 7.1 Hz, 1H), 7.76 (d, *J* = 7.7 Hz, 1H), 7.66-7.58 (m, 3H), 7.40 (s, 1H), 7.07 (s, 1H), 6.97 (d, *J* = 8.9 Hz, 1H), 6.89 (d, *J* = 8.8 Hz, 1H), 3.86 (s, 3H), 3.83 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 168.1, 162.0, 158.8, 150.7, 140.7, 138.6, 134.3, 133.7, 128.9, 128.0, 127.0, 121.7, 117.1, 116.9, 116.6, 116.2, 112.5, 112.3, 55.6, 55.6; HRMS (m/z): calcd for $C_{22}H_{17}Br_2N_2O_2^+$ $[M+H]^+$ 498.9651, found 498.9659.

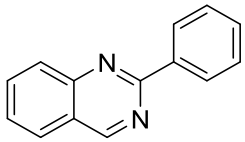
**2,4-Di(naphthalen-2-yl)quinazoline (3av)[6]**




The reaction was conducted with aniline (18.2 μL, 0.2 mmol), 2-naphthaldehyde (93.7 mg, 0.6 mmol) and ammonium iodide (34.8 mg, 0.24 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to give **3av** as yellow solid; yield: 54.2 mg (71%), mp 187-189 ℃.

$^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 9.29 (s, 1H), 8.85 (d, *J* = 8.8 Hz, 1H), 8.41 (s, 1H), 8.27 (d, *J* = 8.4 Hz, 1H), 8.22 (d, *J* = 8.3 Hz, 1H), 8.13-7.97 (m, 6H), 7.96-7.90 (m, 2H), 7.66-7.49 (m, 5H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 168.2, 160.1, 152.0, 135.5, 134.9, 134.6, 133.9, 133.5, 133.3, 132.9, 130.3, 129.2, 129.1, 129.0, 128.7, 128.3, 128.1, 127.8, 127.7, 127.2, 127.0, 127.0, 126.9, 126.6, 126.1, 125.6, 121.8.

**2-Phenylquinazoline (6 CAS: 25855-20-3)[8]**



A 10 mL oven-dried reaction vessel was charged with 2-aminobenzaldehyde (24.2 mg, 0.2 mmol) ammonium iodide (34.8 mg, 0.24 mmol). The reaction vessel was purged with oxygen for three times and then was added benzaldehyde (40.8 μL, 0.4 mmol), chlorobenzene (0.5 mL) and DMSO (0.1 mL) by syringe. The reaction vessel was stirred at 150 $^{o}$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 (petroleum ether/ethyl acetate = 20:1) to give **6** as yellow solid; yield: 23.1 mg (56 %).

$^{1}$H NMR (400 MHz, $CDCl_3$, ppm) δ 9.48 (s, 1H), 8.63 (d, *J* = 8.2 Hz, 2H), 8.11 (d, *J* = 8.4 Hz, 1H), 7.95-7.90 (m, 2H), 7.62 (t, *J* = 8.0 Hz, 1H), 7.57-7.48 (m, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 161.0, 160.5, 150.7, 137.9, 134.1, 130.6, 128.6, 128.6, 128.6, 127.3, 127.1, 123.6.

**5. Reference**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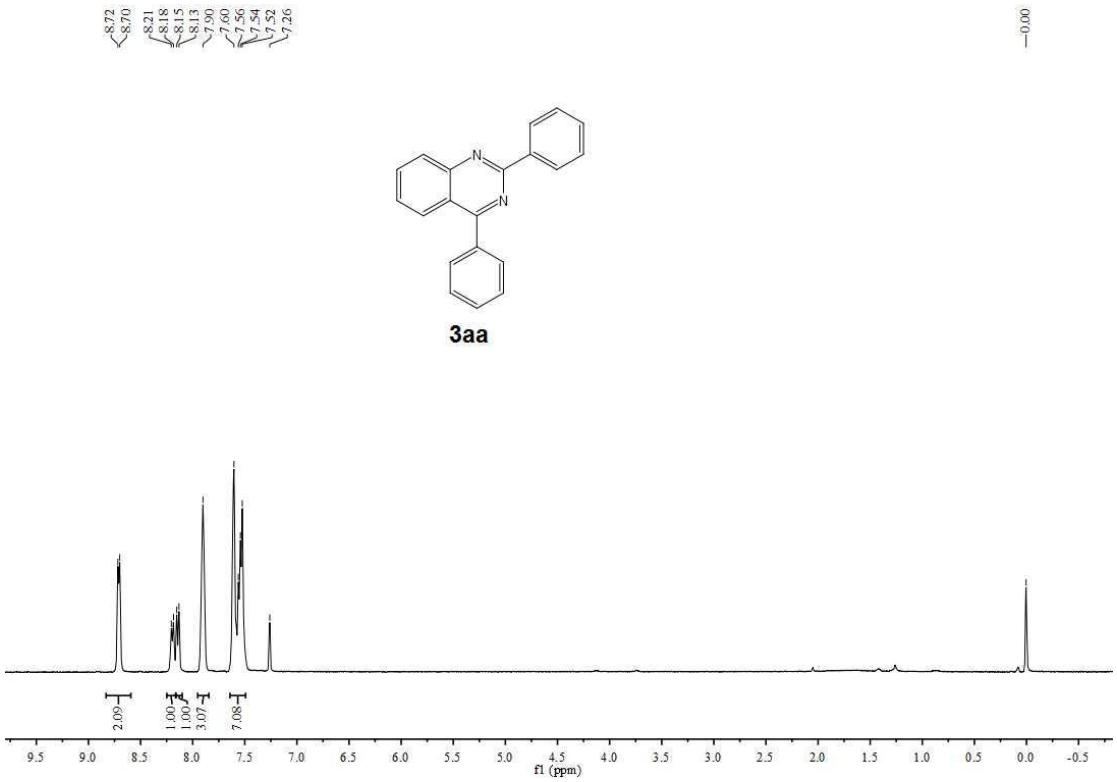
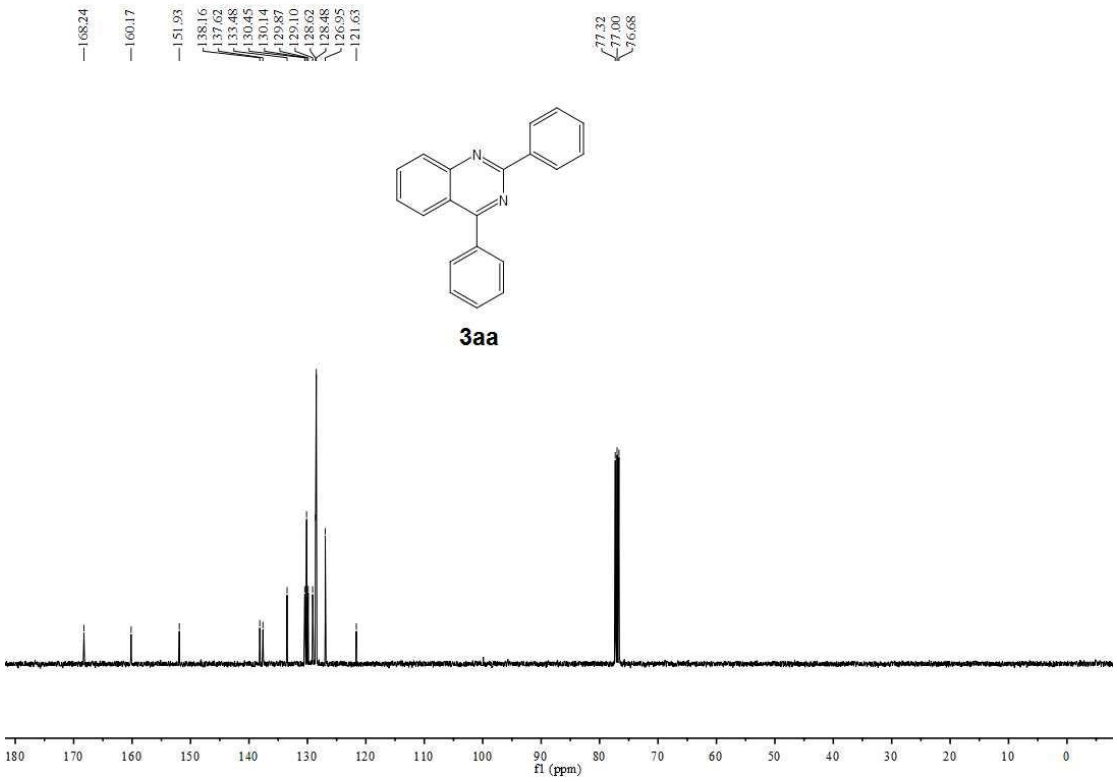
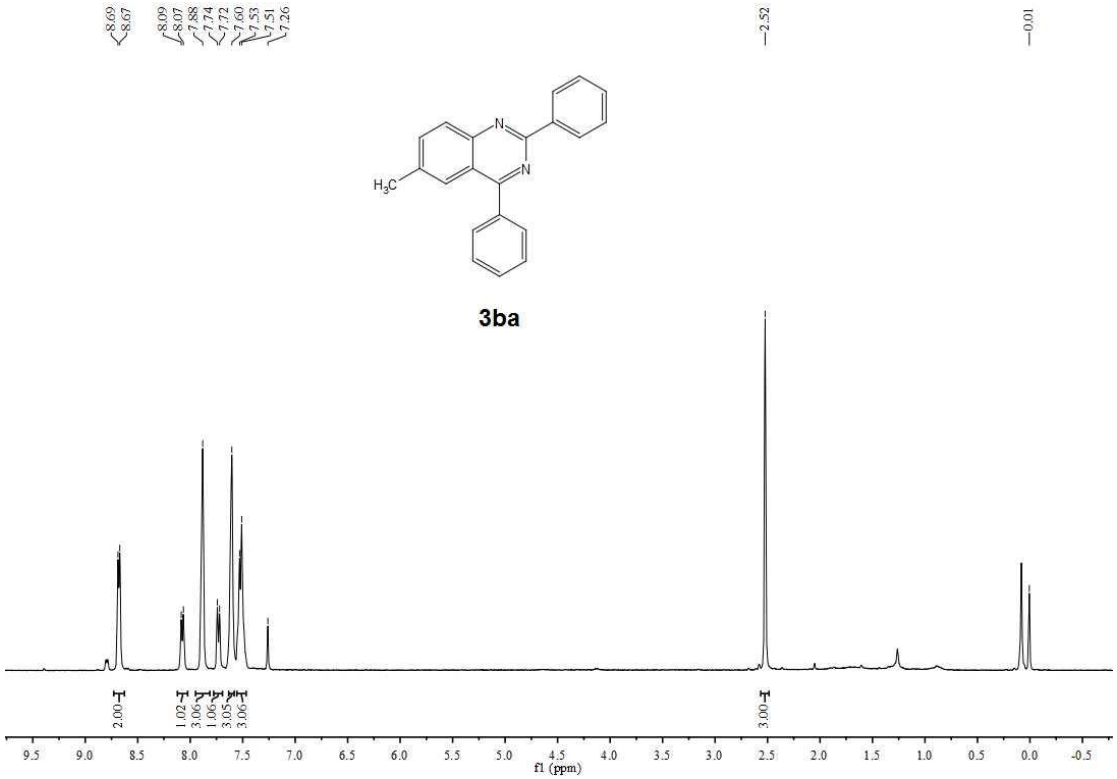
8. X. F. Cheng, H. M. Wang, F. H. Xiao, G. J. Deng, *Green Chem.*, 2016**, 18**, 5773.

## 6. $^{1}$H NMR and $^{13}$C NMR spectra for all products

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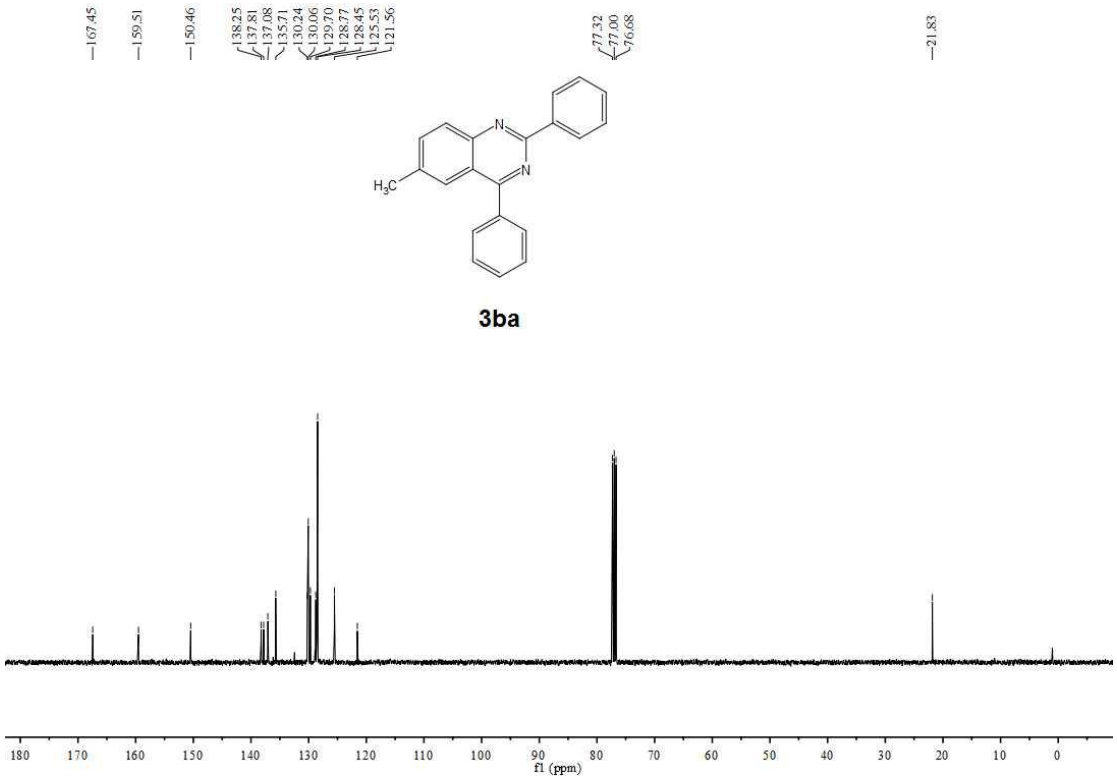
8.67
8.09
8.07
7.88
7.74
7.72
7.60
7.53
7.51
7.26
2.52
0.01
N
N
H3C
2.00
1.02
3.06
1.06
3.05
3.06
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

**3ba**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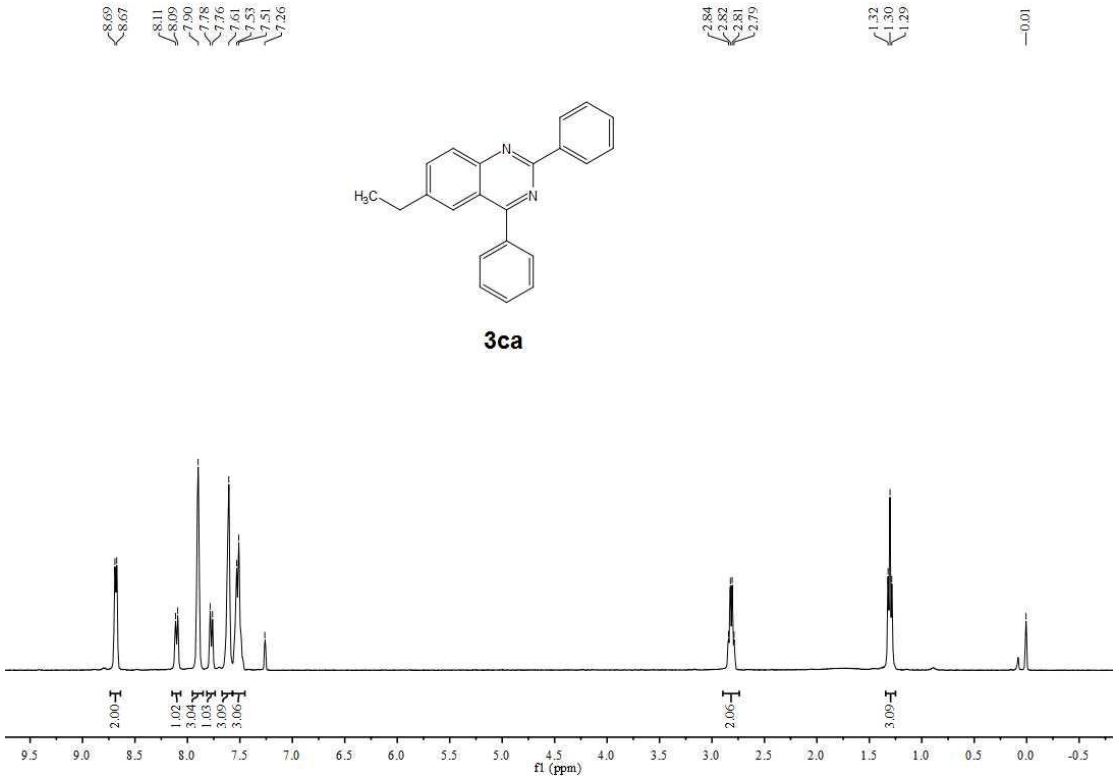
159.51
150.46
138.25
137.81
137.08
135.71
130.24
130.06
129.70
128.77
128.45
125.53
121.56
77.32
77.00
76.68
21.83
N
N
H3C
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

**3ba**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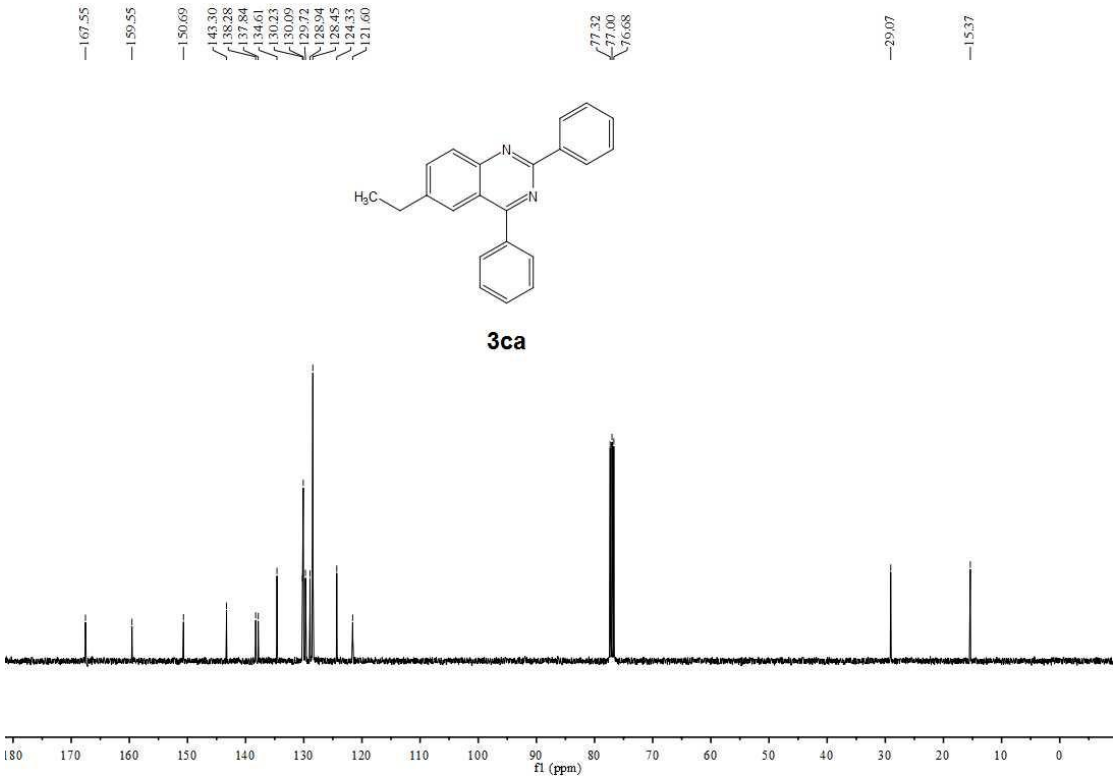
8.67
8.11
8.09
7.90
7.78
7.76
7.61
7.53
7.51
7.26
2.84
2.82
2.81
2.79
1.32
1.30
1.29
0.01
N
N
H3C
2.00
1.02
3.04
1.03
3.09
3.06
2.06
3.09
f1 (ppm)

**3ca**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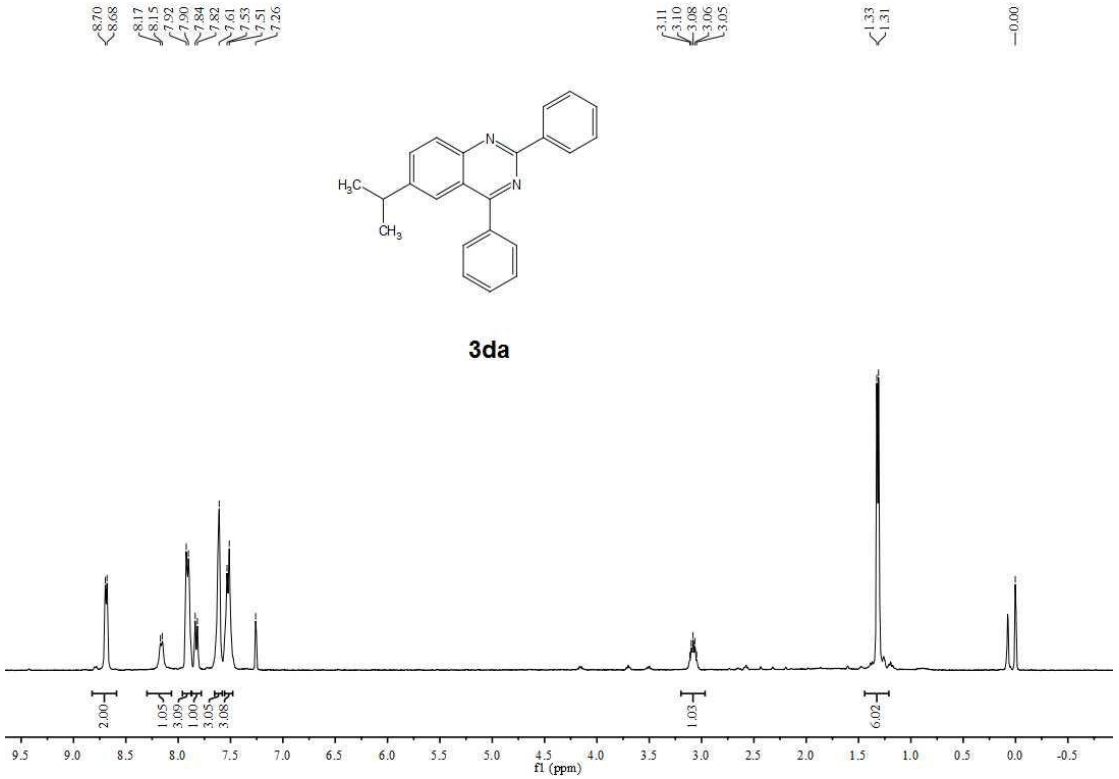
150.69
143.30
138.28
137.84
134.61
130.23
130.09
129.72
128.94
128.45
124.33
121.60
77.32
77.00
76.68
29.07
15.37
N
N
H3C
f1 (ppm)

**3ca**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8.68
8.17
8.15
7.92
7.90
7.84
7.82
7.61
7.53
7.51
7.26
3.11
3.10
3.08
3.06
3.05
1.33
1.31
0.00
N
N
H3C
CH3
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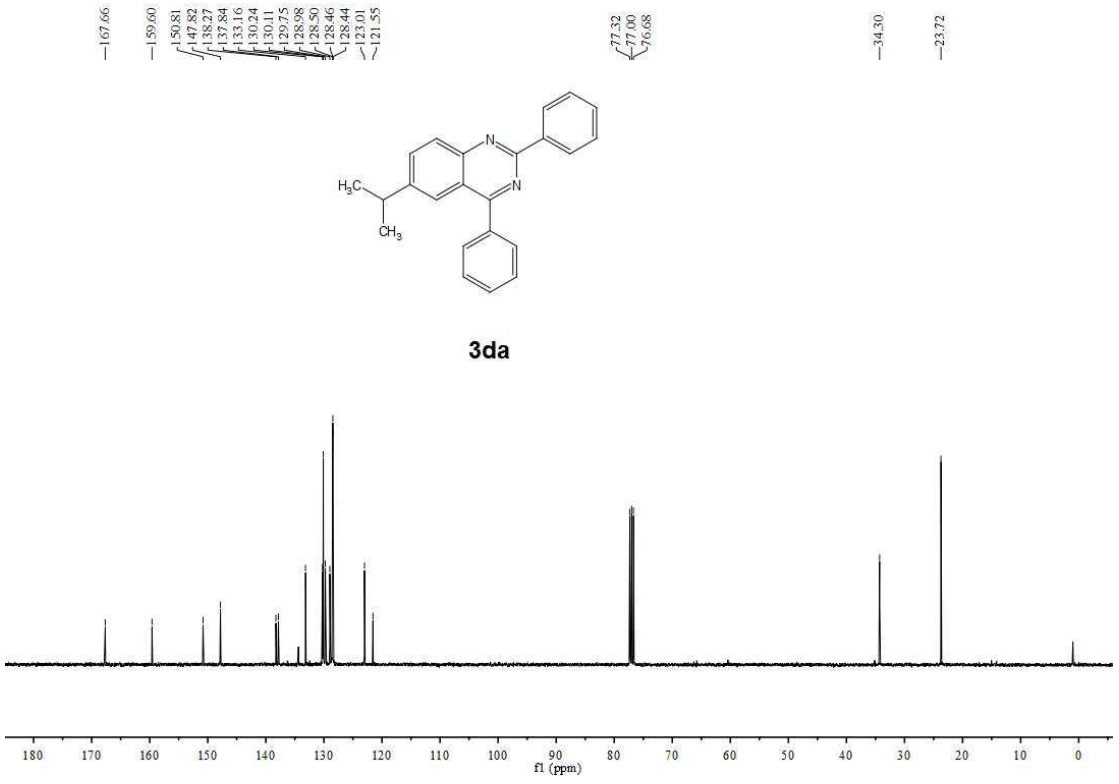
1.05
3.09
1.00
3.05
3.08
1.03
6.02
f1 (ppm)

**3da**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130.24
130.11
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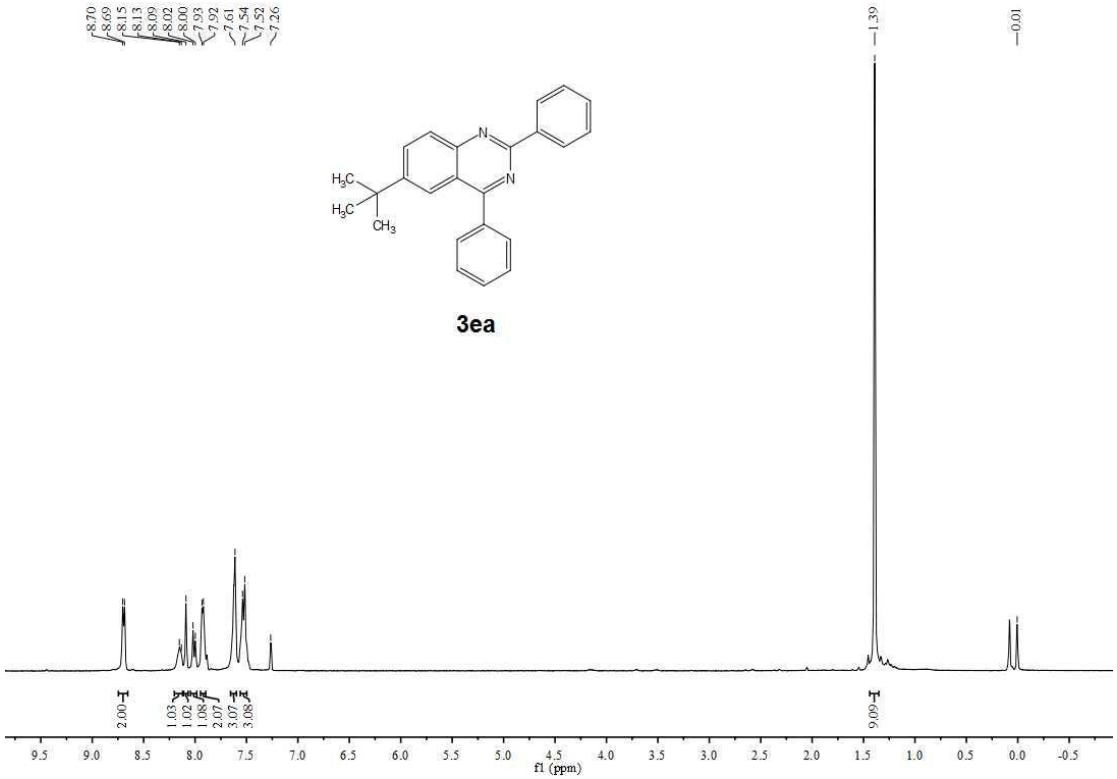
128.98
128.50
128.46
128.44
123.01
121.55
77.32
77.00
76.68
34.30
23.72
N
N
H3C
CH3
f1 (ppm)

**3da**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8.09
8.02
8.00
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7.92
7.61
7.54
7.52
7.26
1.39
0.01
N
N
H3C
H3C
CH3
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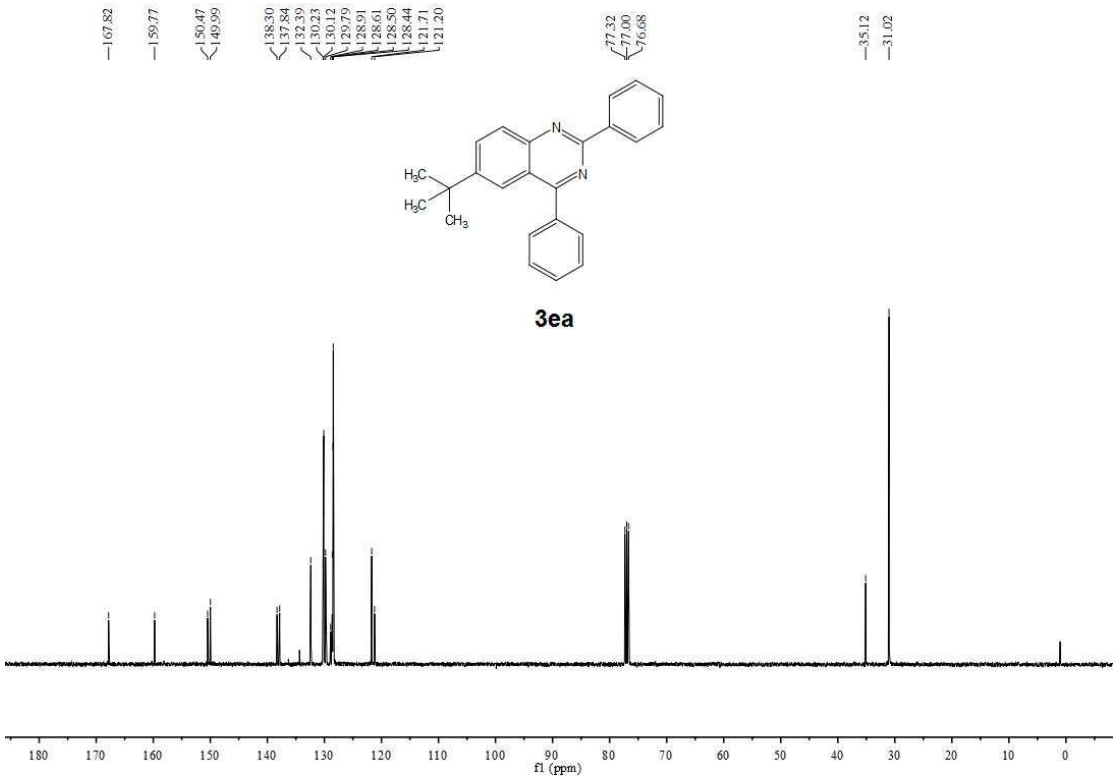
1.03
1.02
1.08
2.07
3.07
3.08
9.09
f1 (ppm)

**3ea**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137.84
132.39
130.23
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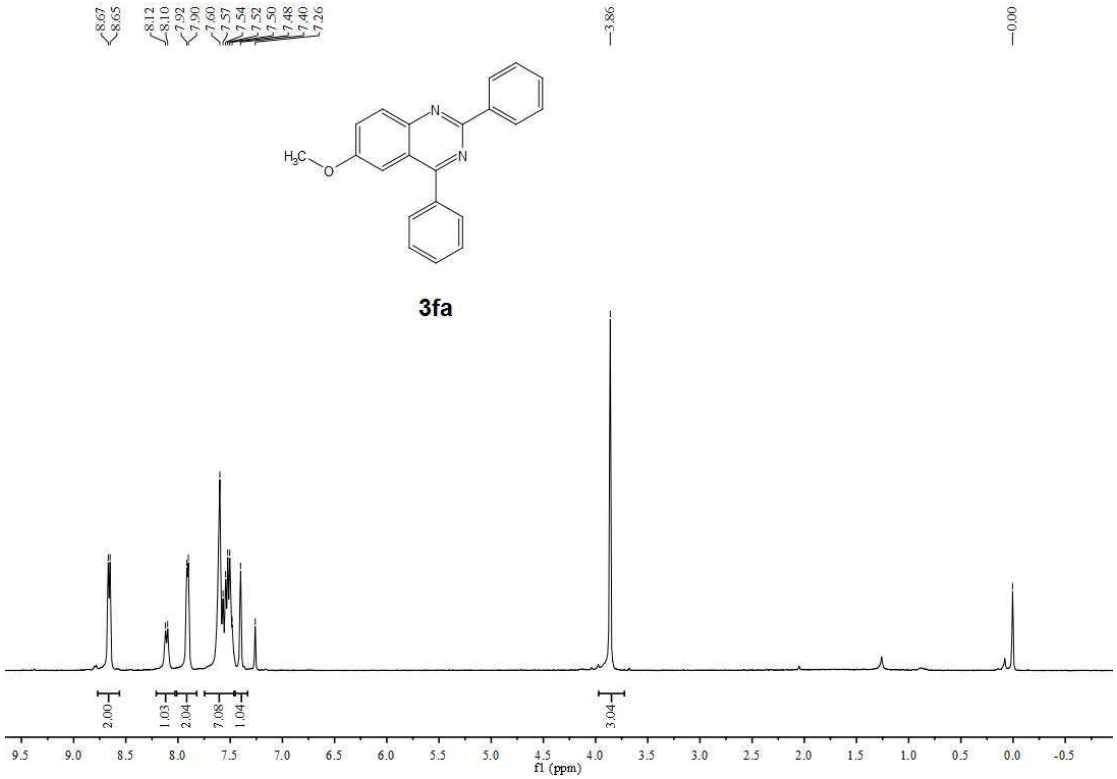
129.79
128.91
128.61
128.50
128.44
121.71
121.20
77.32
77.00
76.68
35.12
31.02
N
N
H3C
H3C
CH3
f1 (ppm)

**3ea**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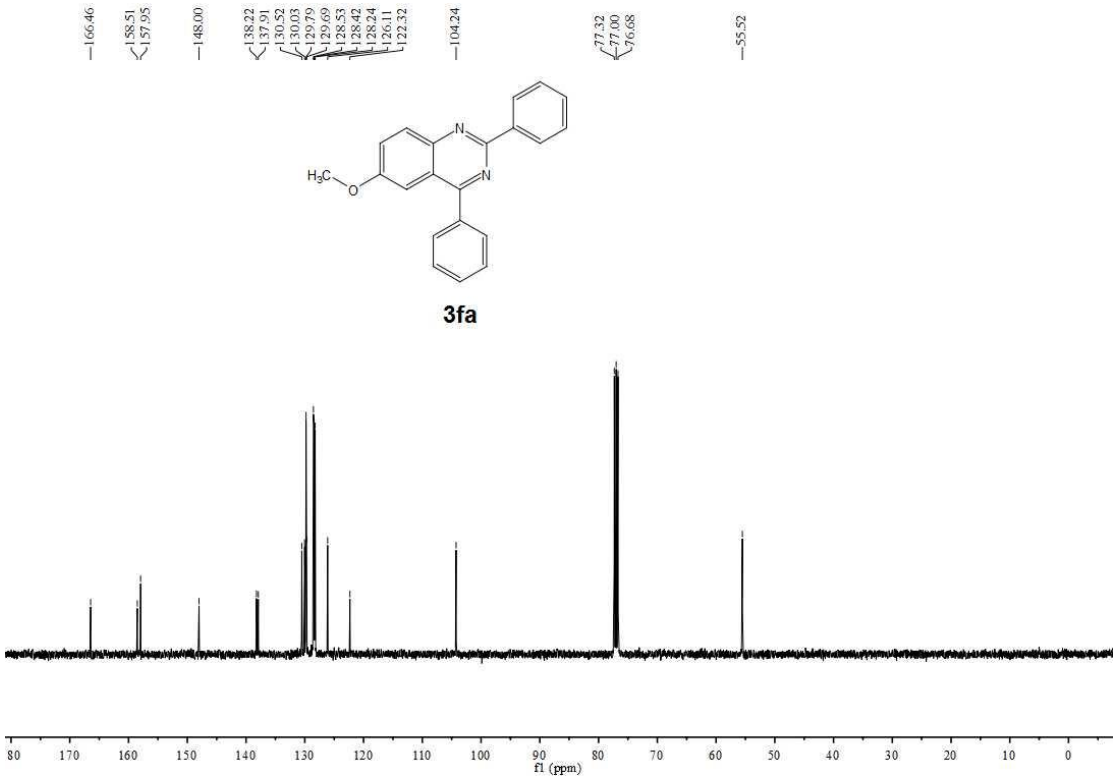
7.90
7.60
7.57
7.54
7.52
7.50
7.48
7.40
7.26
3.86
0.00
N
N
H3C
O
2.00
1.03
2.04
7.08
1.04
3.04
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

**3fa**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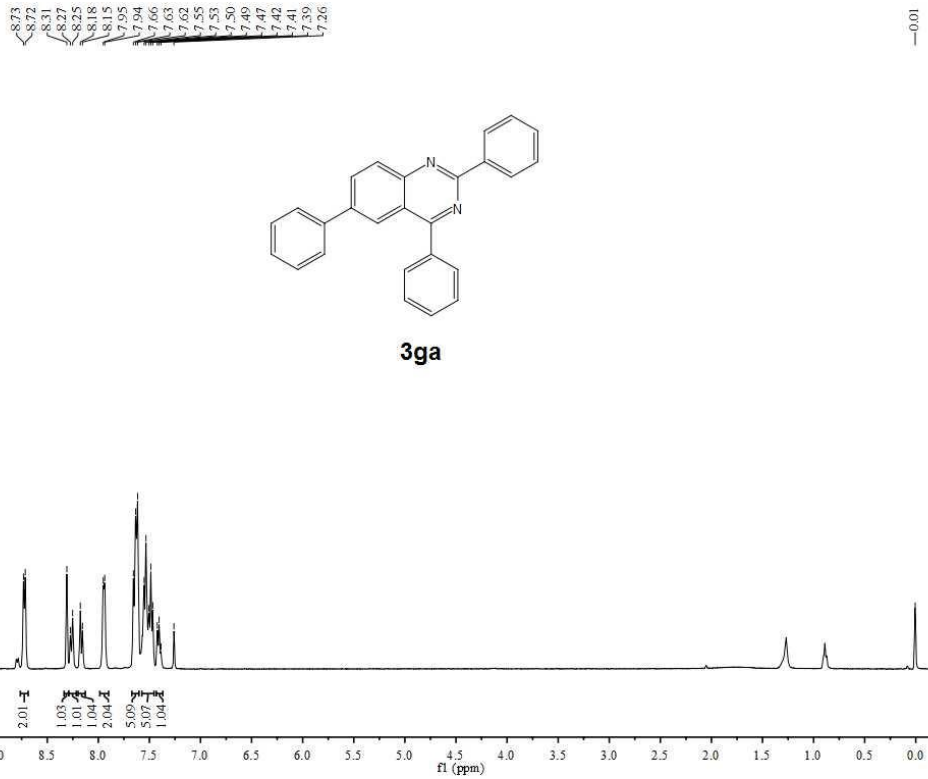
158.51
157.95
148.00
138.22
137.91
130.52
130.03
129.79
129.69
128.53
128.42
128.24
126.11
122.32
104.24
77.32
77.00
76.68
55.52
N
N
H3C
O
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

**3fa**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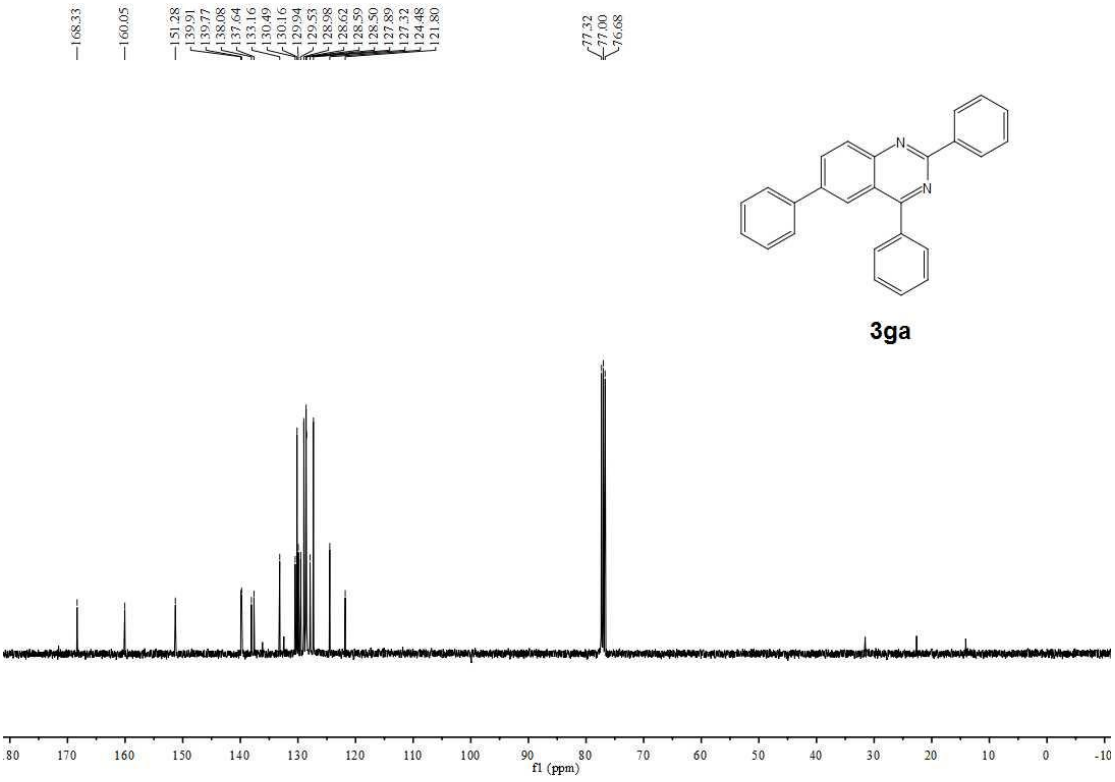
8.72
8.31
8.27
8.25
8.18
8.15
7.95
7.94
7.66
7.63
7.62
7.55
7.53
7.50
7.49
7.47
7.42
7.41
7.39
7.26
0.01
N
N
3ga
2.01
1.03
1.01
1.04
2.04
5.09
5.07
1.04
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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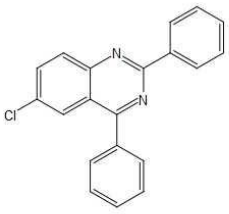
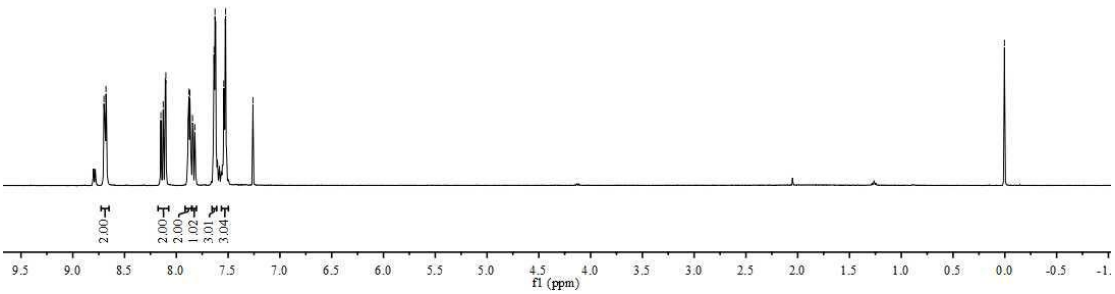
151.28
139.91
139.77
138.08
137.64
133.16
130.49
130.16
129.94
129.53
128.98
128.62
128.59
128.50
127.89
127.32
124.48
121.80
77.32
77.00
76.68
N
N
3ga
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

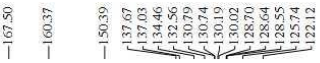

8.70
8.68
8.15
8.13
8.11
8.10
7.88
7.87
7.84
7.82
7.64
7.63
7.62
7.54
7.53
7.52
7.26


0.00


N
N
Cl

**3ha**


2.00
2.00
2.00
1.02
3.01
3.04
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)


167.50
160.37
150.39
137.67
137.03
134.46
132.56
130.79
130.74
130.19
130.02
128.70
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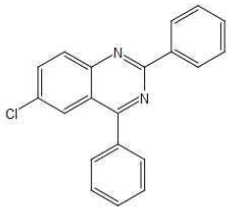
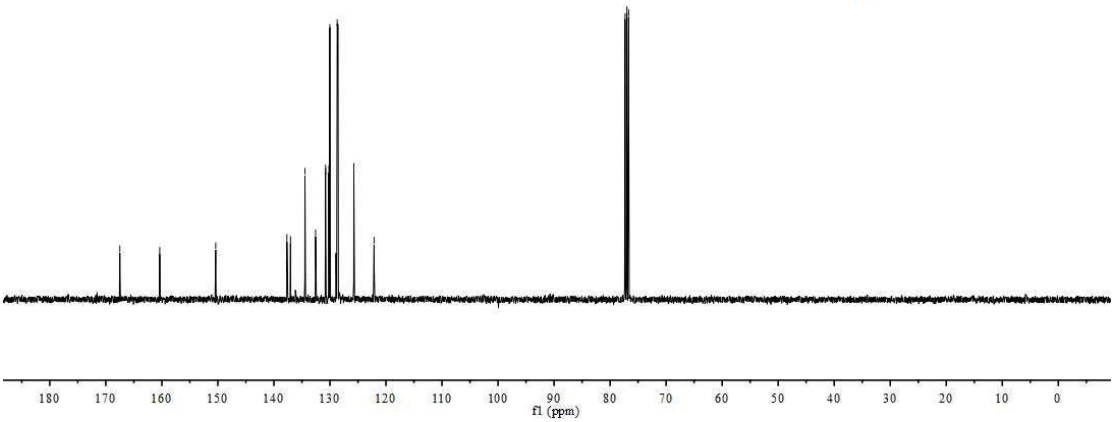
128.55
125.74
122.12

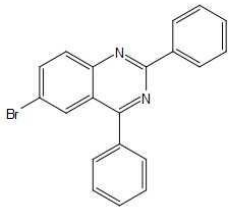

77.32
77.00
76.68


N
N
Cl

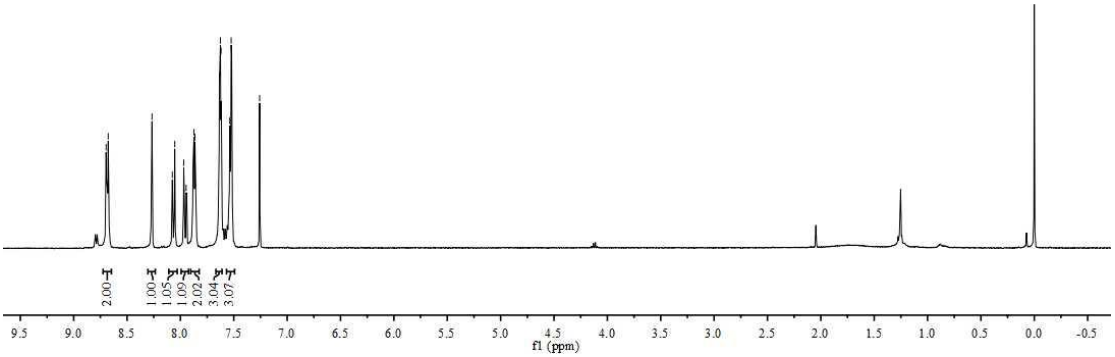
**3ha**


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


8.70
8.68
8.27
8.08
8.05
7.97
7.95
7.87
7.86
7.63
7.62
7.54
7.52
7.52
7.26


N
N
Br

**3ia**


2.00
1.00
1.05
1.09
2.02
3.04
3.07
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)


167.41
160.44
150.62
137.70
137.04
137.02
130.89
130.78
130.21
130.04
129.07
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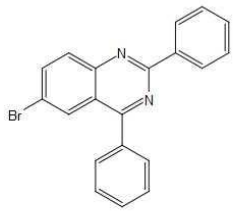
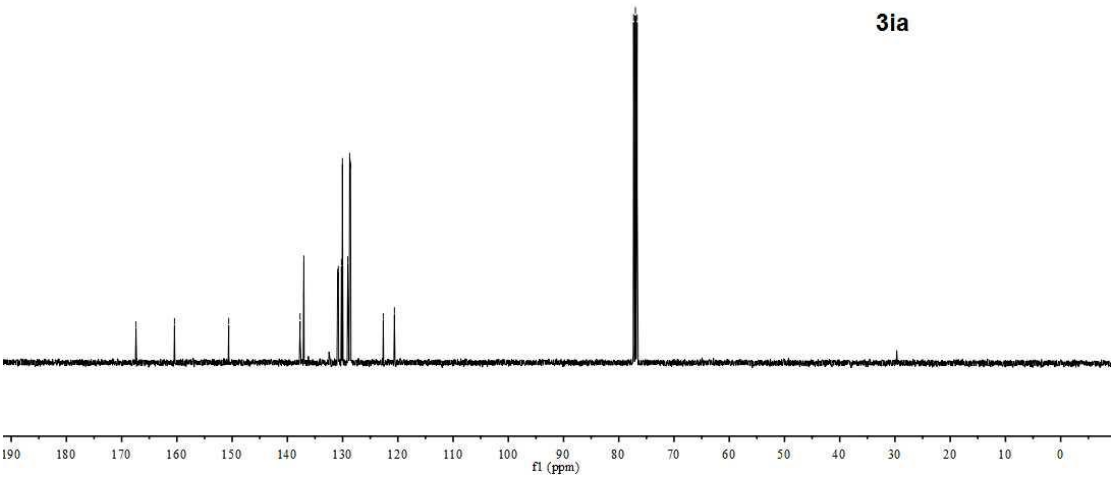
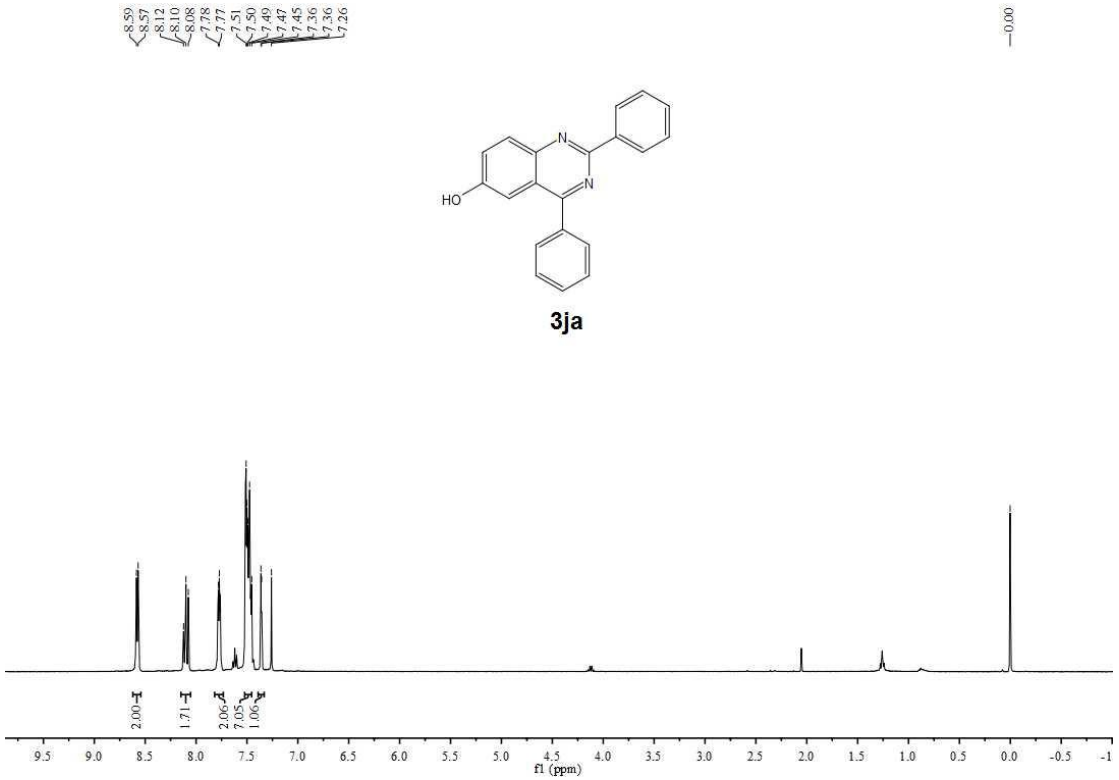
128.56
122.64
120.63


77.32
77.00
76.68

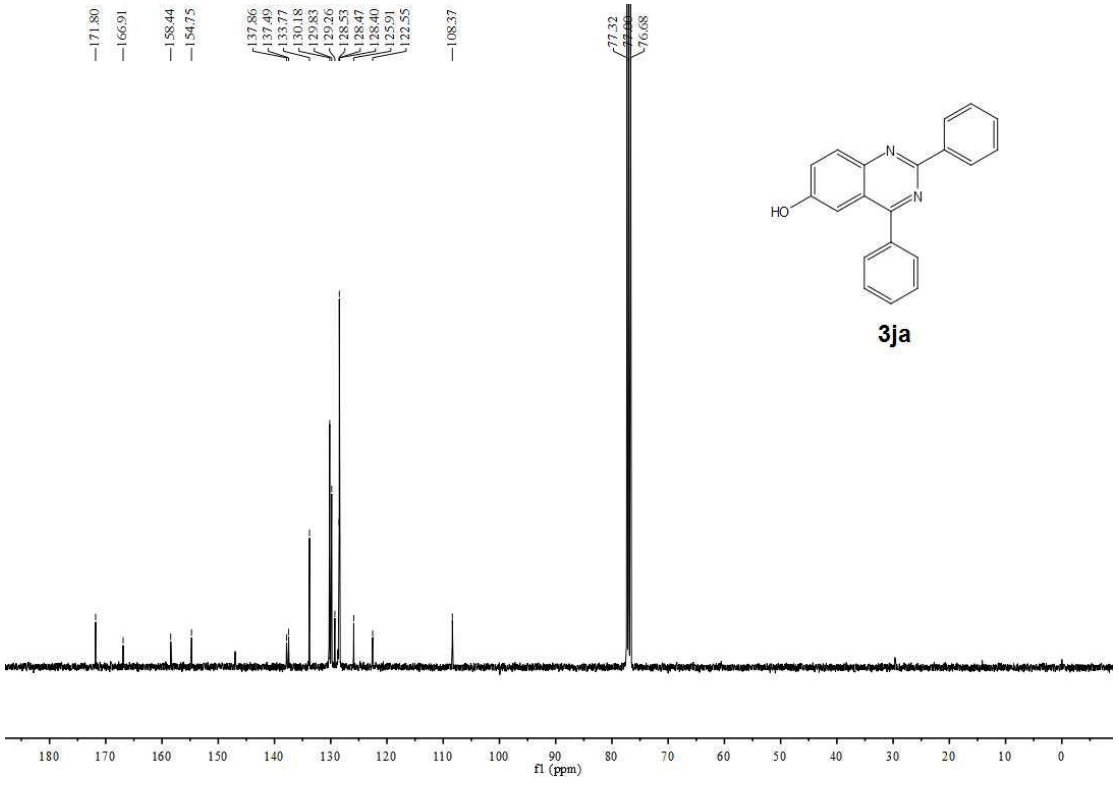

N
N
Br

**3ia**


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


8.59
8.57
8.12
8.10
8.08
7.78
7.77
7.51
7.50
7.49
7.47
7.45
7.36
7.26
0.00
N
N
HO
2.00
1.71
2.06
7.05
1.06
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)

**3ja**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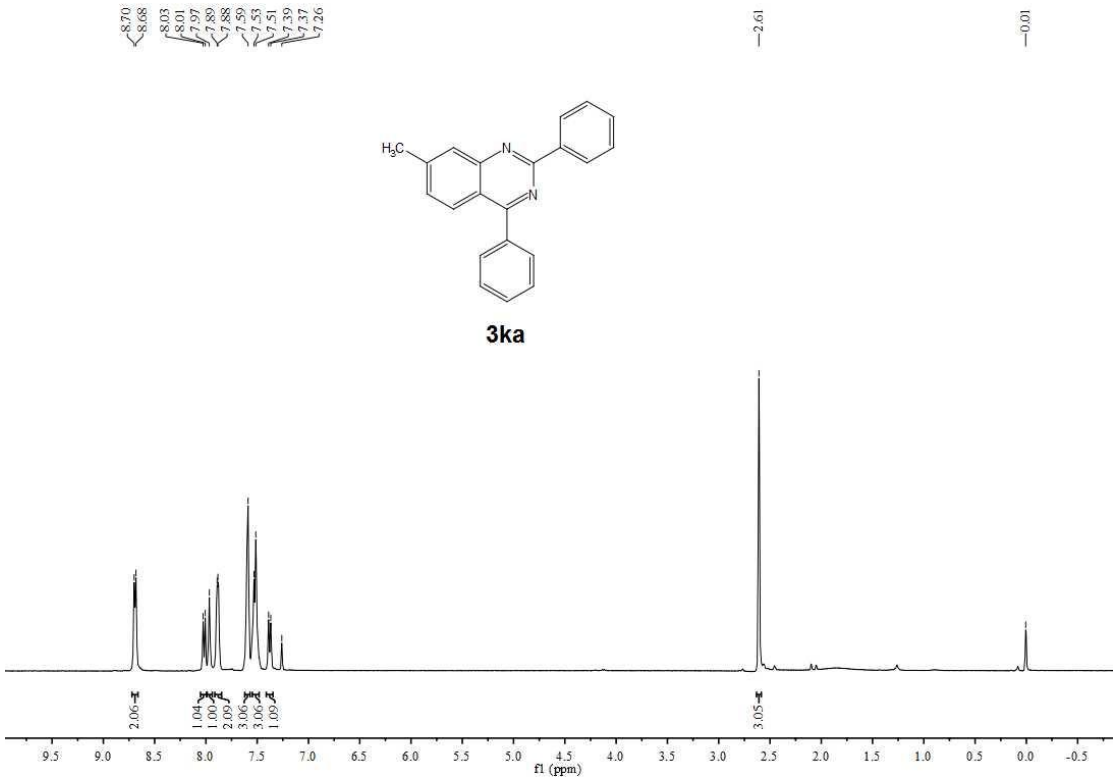
154.75
137.86
137.49
133.77
130.18
129.83
129.26
128.53
128.47
128.40
125.91
122.55
108.37
77.32
77.00
76.68
N
N
HO
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

**3ja**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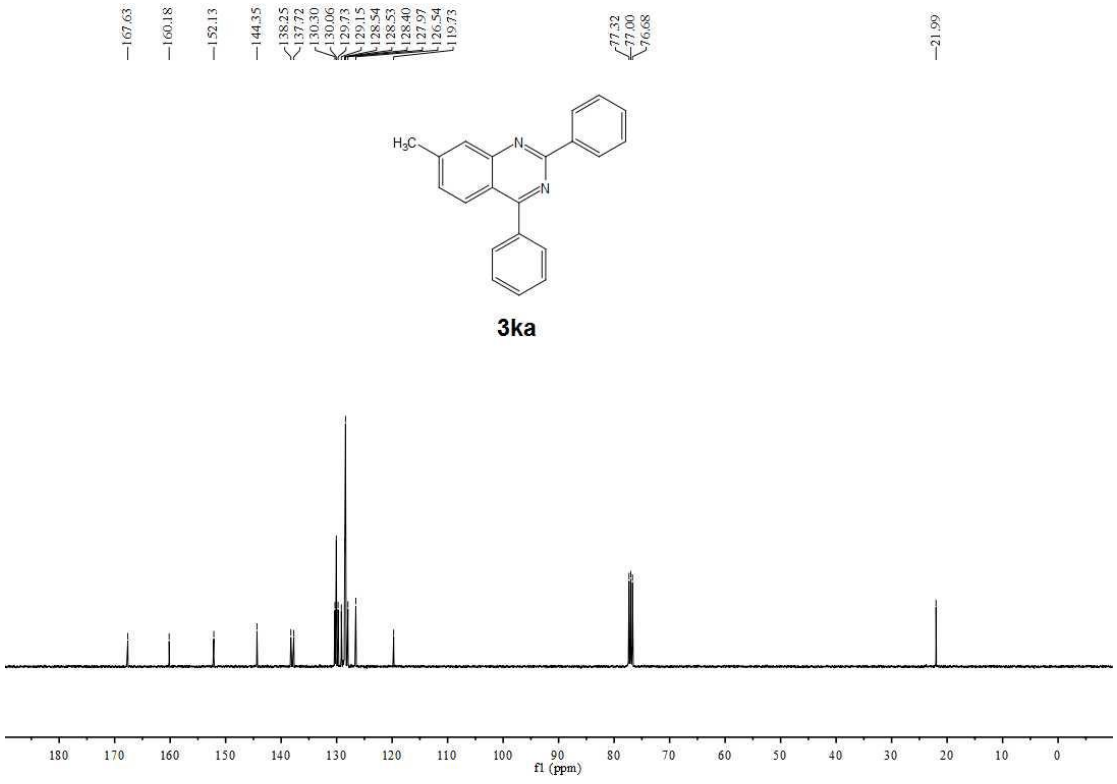
8.68
8.03
8.01
7.97
7.89
7.88
7.59
7.53
7.51
7.39
7.37
7.26
2.61
0.01
H3C
N
N
2.06
1.04
1.00
2.09
3.06
3.06
1.09
3.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

**3ka**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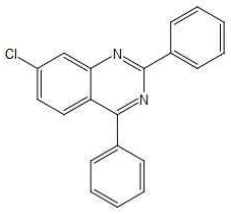
152.13
144.35
138.25
137.72
130.30
130.06
129.73
129.15
128.54
128.53
128.40
127.97
126.54
119.73
77.32
77.00
76.68
21.99
H3C
N
N
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

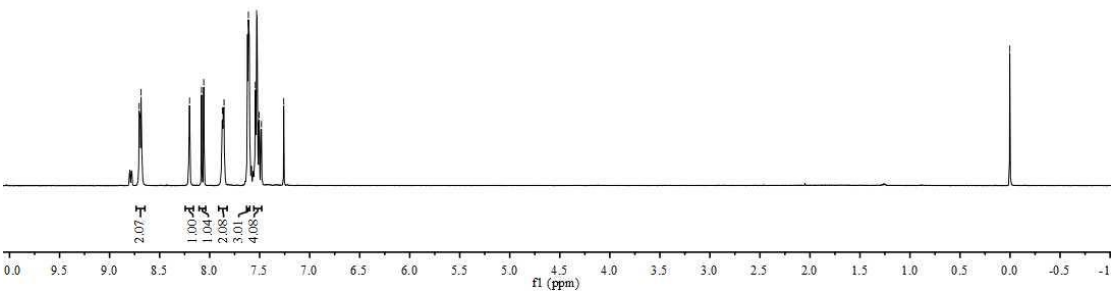
**3ka**


8.70
8.69
8.20
8.08
8.06
7.87
7.86
7.61
7.54
7.53
7.50
7.48
7.26


0.00


Cl
N
N

**3la**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1.04
2.08
3.01
4.08
0.0
9.5
9.0
8.5
8.0
7.5
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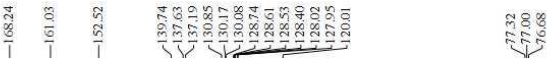
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)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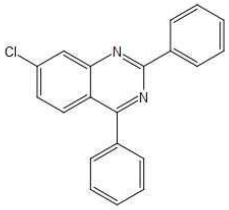
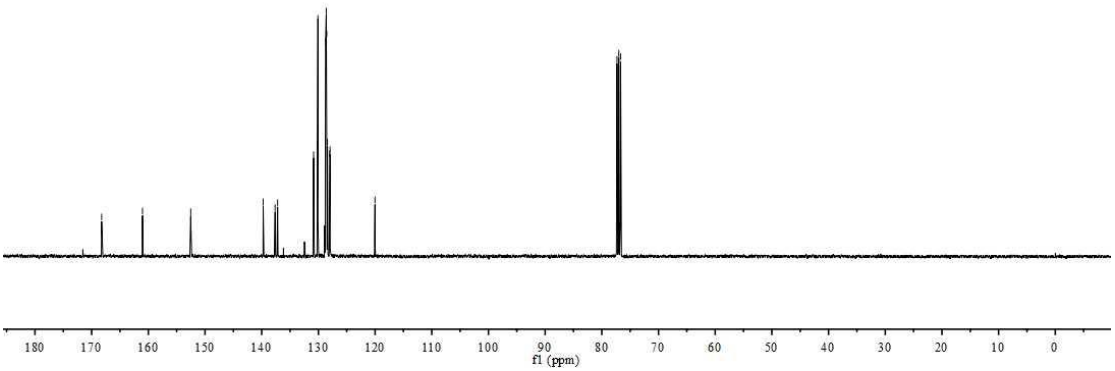
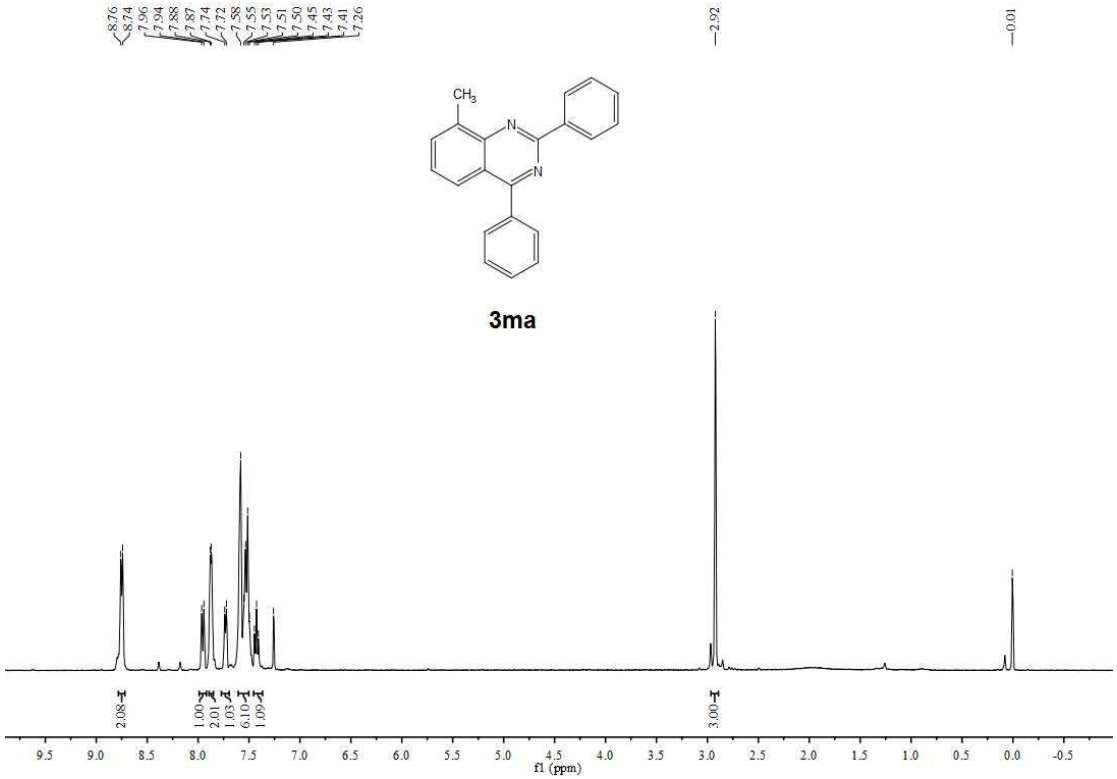
139.74
137.63
137.19
130.85
130.17
130.08
128.74
128.61
128.53
128.40
128.02
127.95
120.01


77.32
77.00
76.68

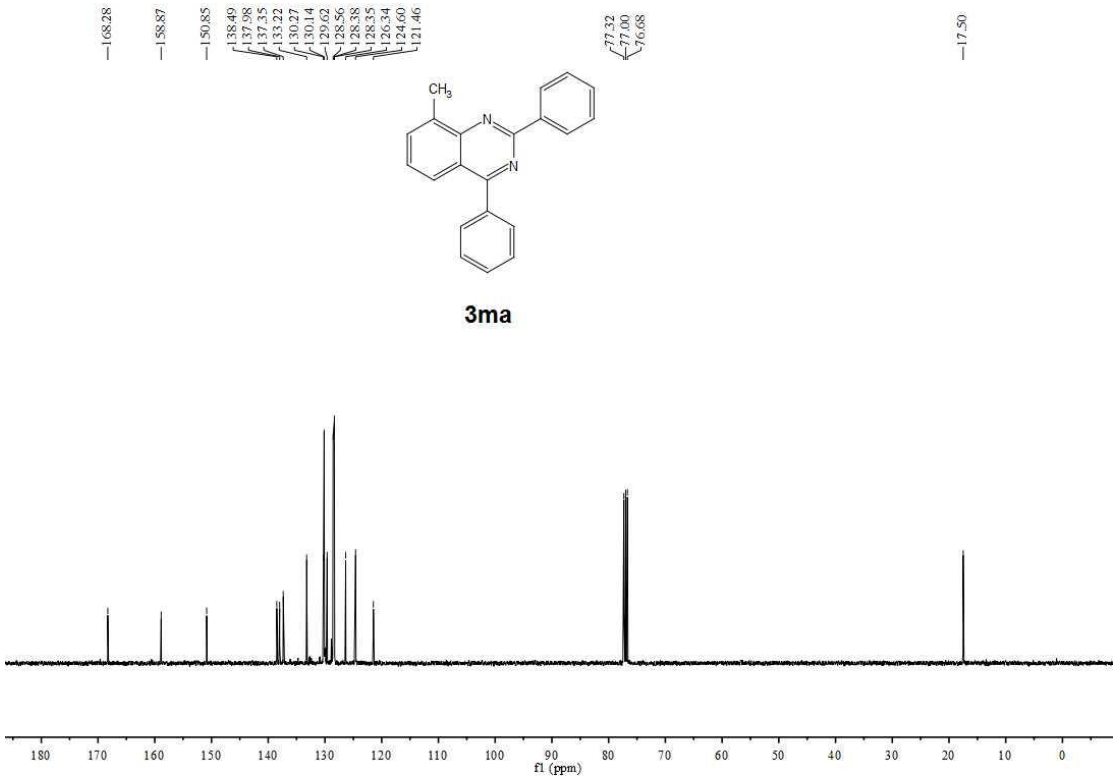

Cl
N
N

**3la**

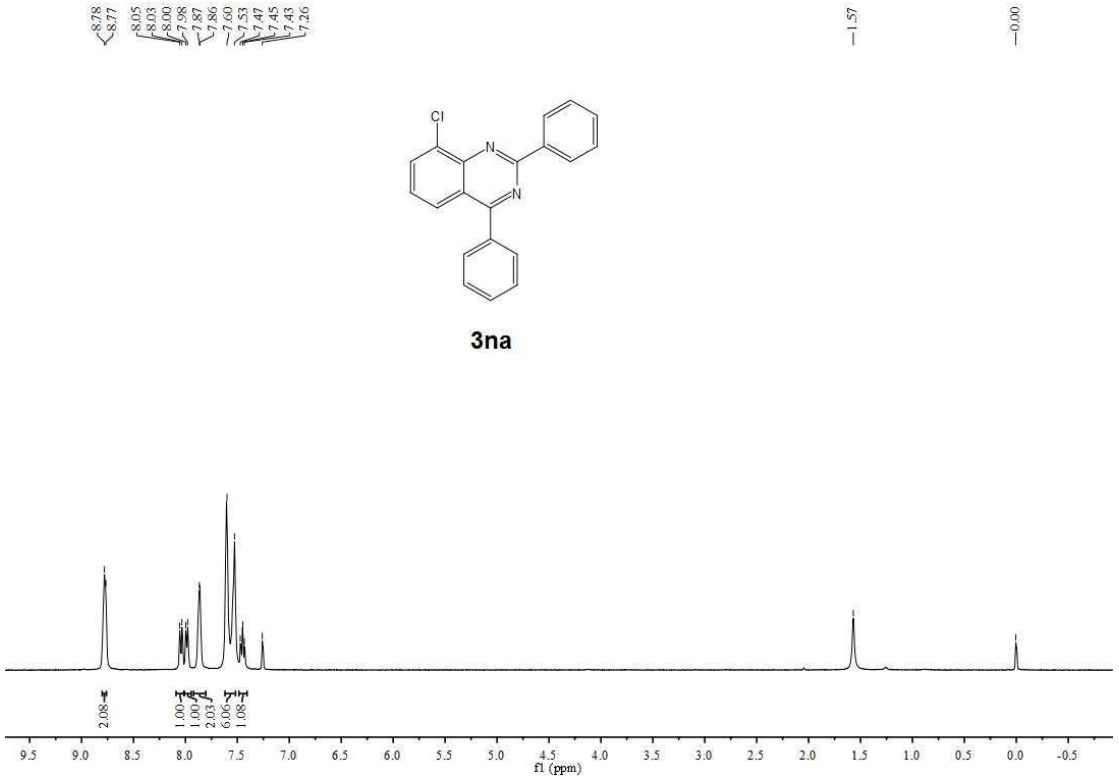

180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.76
8.74
7.96
7.94
7.88
7.87
7.74
7.72
7.58
7.55
7.53
7.51
7.50
7.45
7.43
7.41
7.26
2.92
0.01
CH3
N
N
2.08
1.00
2.01
1.03
6.10
1.09
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)

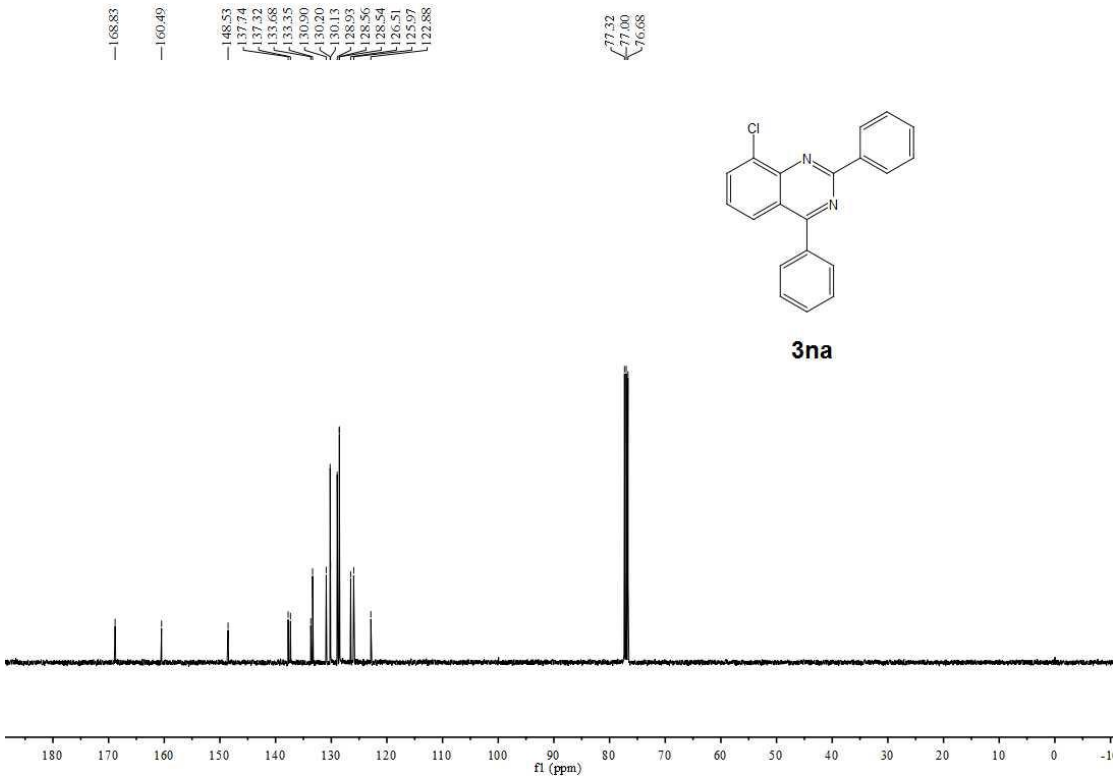
**3ma**


168.28
158.87
150.85
138.49
137.98
137.35
133.22
130.27
130.14
129.62
128.56
128.38
128.35
126.34
124.60
121.46
77.32
77.00
76.68
17.50
CH3
N
N
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

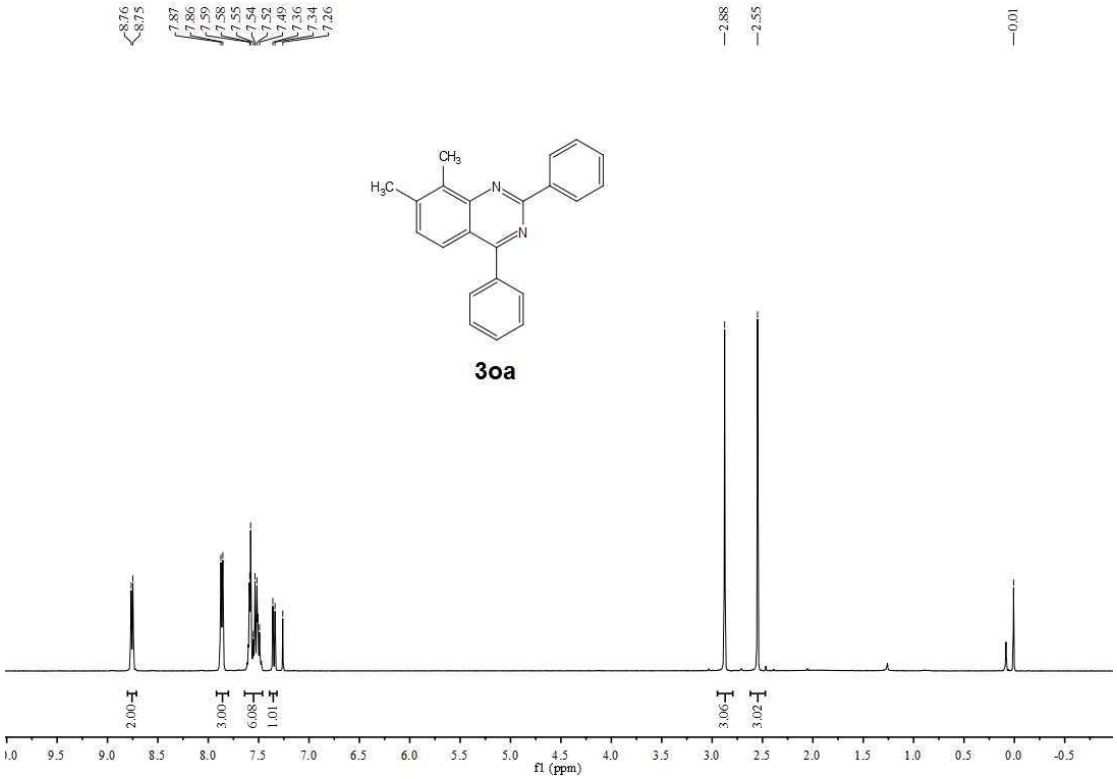
**3ma**


8.78
8.77
8.05
8.03
8.00
7.98
7.87
7.86
7.60
7.53
7.47
7.45
7.43
7.26
1.57
0.00
Cl
N
N
2.08
1.00
1.00
2.03
6.06
1.08
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
f1 (ppm)

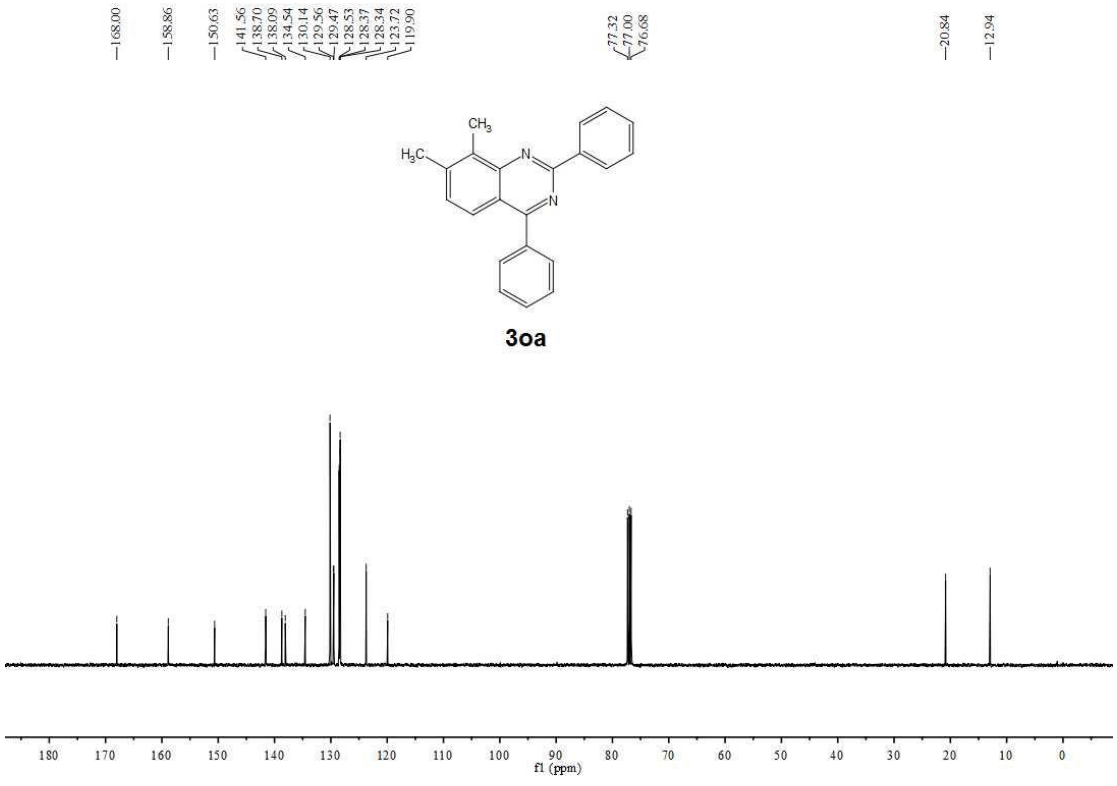
**3na**


168.83
160.49
148.53
137.74
137.32
133.68
133.35
130.90
130.20
130.13
128.93
128.56
128.54
126.51
125.97
122.88
77.32
77.00
76.68
Cl
N
N
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

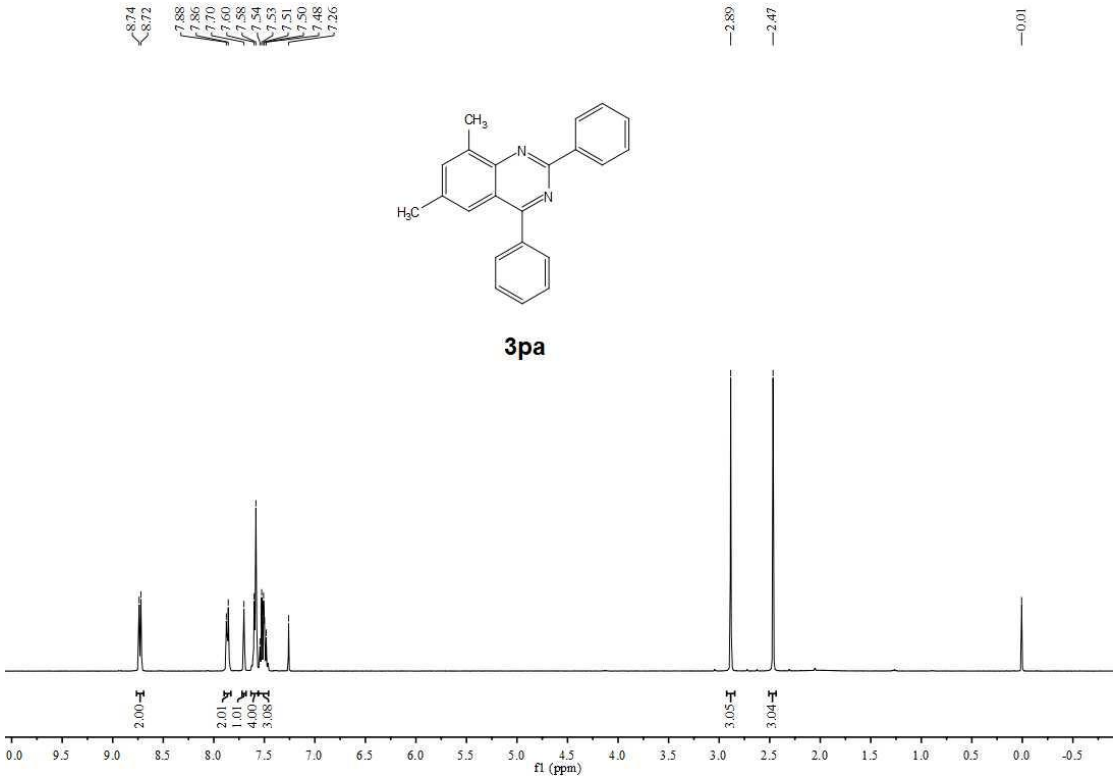
**3na**


8.76
8.75
7.87
7.86
7.59
7.58
7.55
7.54
7.52
7.49
7.36
7.34
7.26
2.88
2.55
0.01
CH3
H3C
N
N
2.00
3.00
6.08
1.01
3.06
3.02
f1 (ppm)

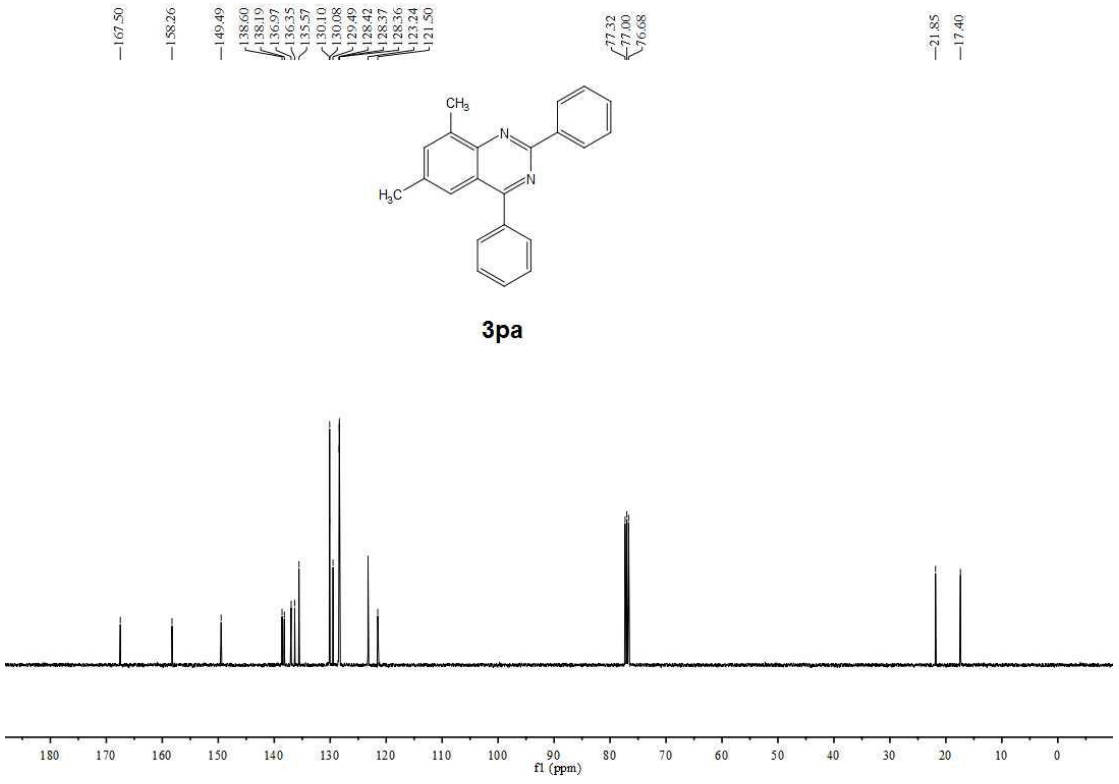
**3oa**


168.00
158.86
150.63
141.56
138.70
138.09
134.54
130.14
129.56
129.47
128.53
128.37
128.34
123.72
119.90
77.32
77.00
76.68
20.84
12.94
CH3
H3C
N
N
f1 (ppm)

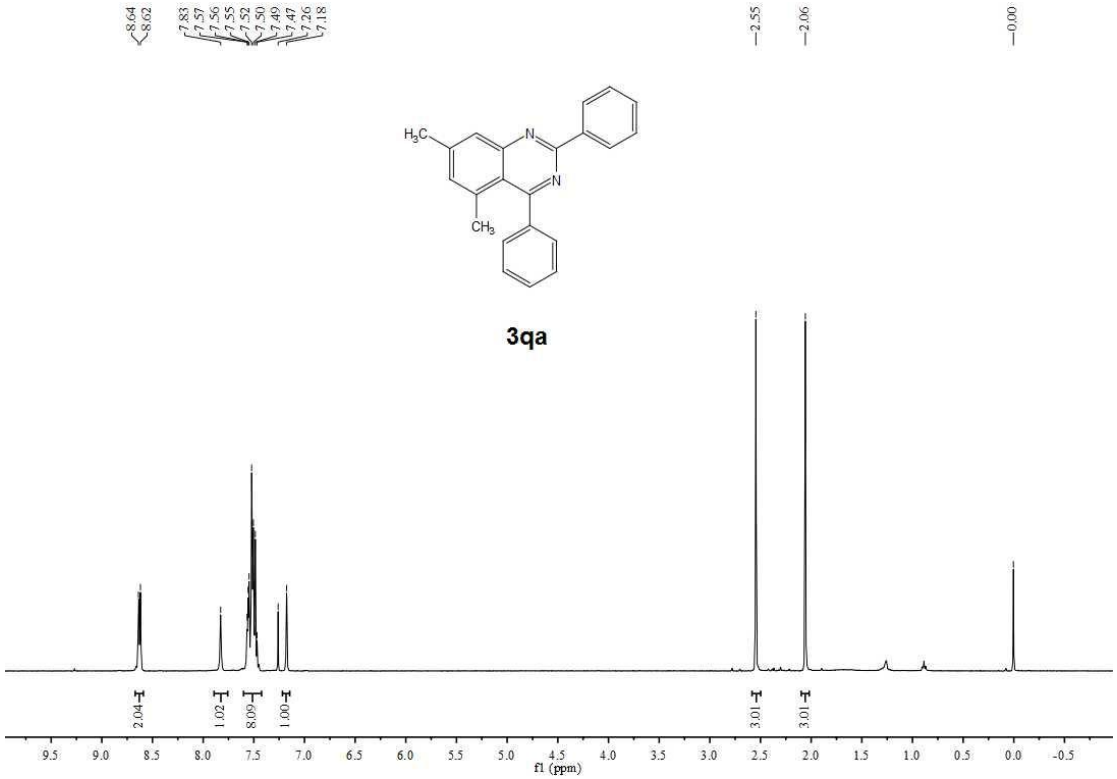
**3oa**


8.74
8.72
7.88
7.86
7.70
7.60
7.58
7.54
7.53
7.51
7.50
7.48
7.26
2.89
2.47
0.01
CH3
N
N
H3C
2.00
2.01
1.01
4.00
3.08
3.05
3.04
f1 (ppm)

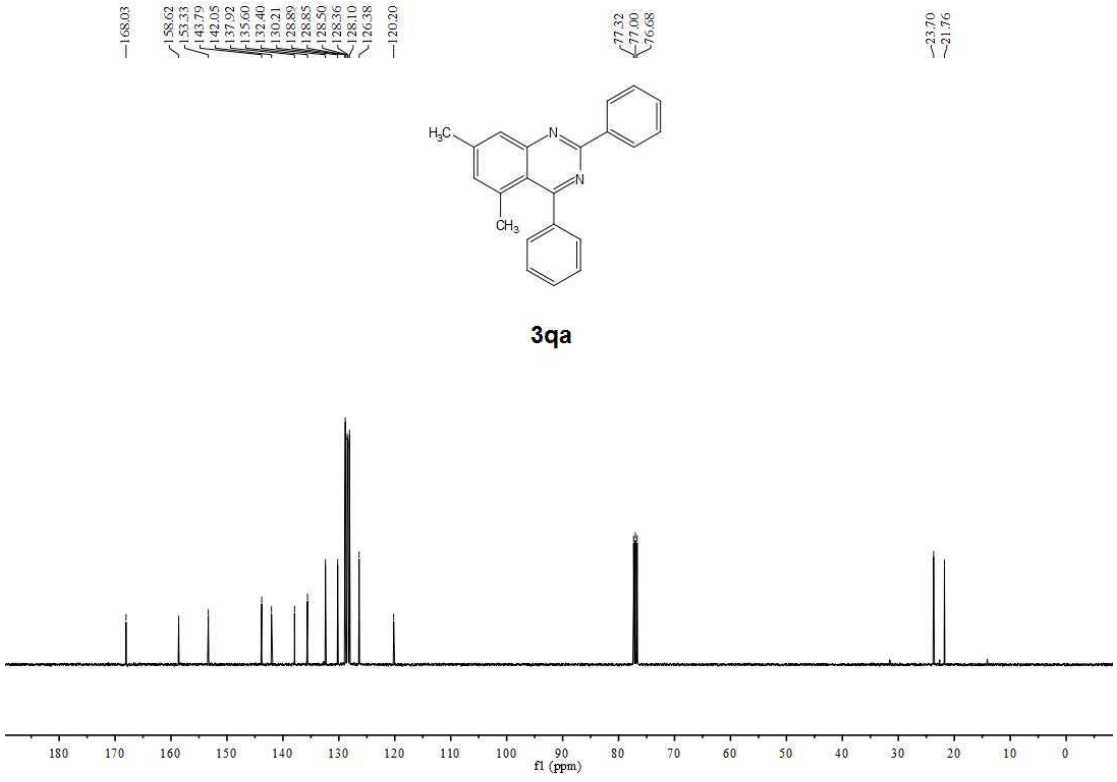
**3pa**


167.50
158.26
149.49
138.60
138.19
136.97
136.35
135.57
130.10
130.08
129.49
128.42
128.37
128.36
123.24
121.50
77.32
77.00
76.68
21.85
17.40
CH3
N
N
H3C
f1 (ppm)

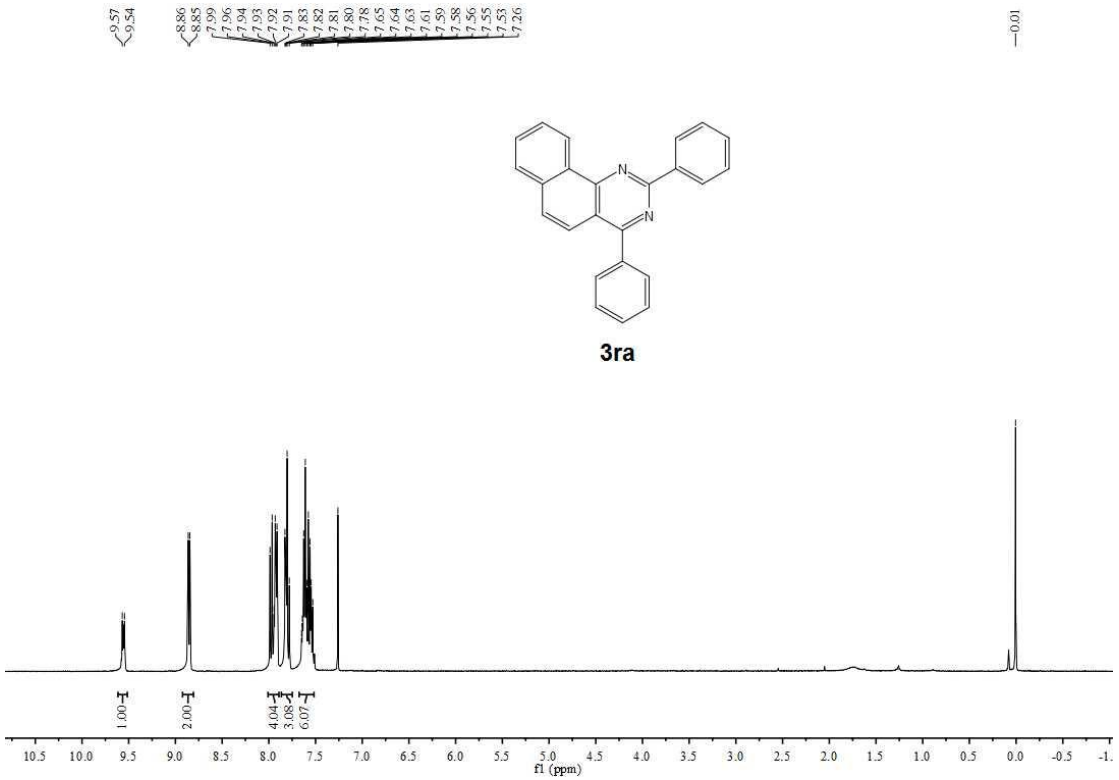
**3pa**


8.64
8.62
7.83
7.57
7.56
7.55
7.52
7.50
7.49
7.47
7.26
7.18
2.55
2.06
0.00
H3C
N
N
CH3
2.04
1.02
8.09
1.00
3.01
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
f1 (ppm)

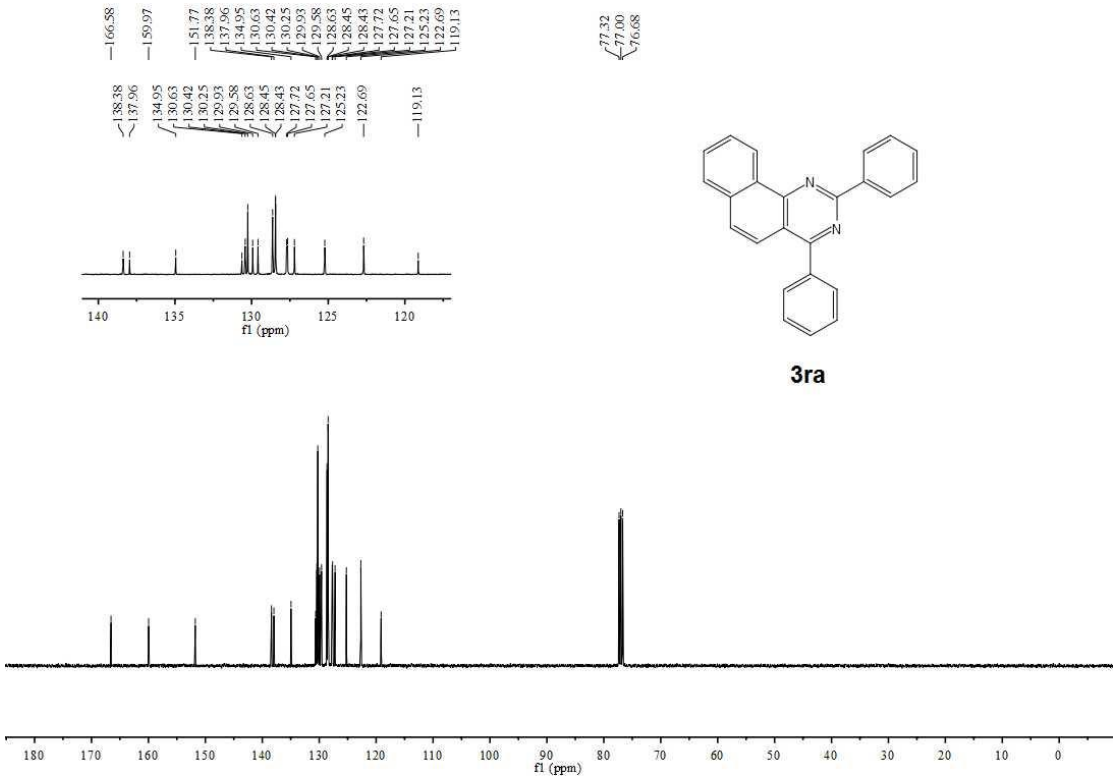
**3qa**


168.03
158.62
153.33
143.79
142.05
137.92
135.60
132.40
130.21
128.89
128.85
128.50
128.36
128.10
126.38
120.20
77.32
77.00
76.68
23.70
21.76
H3C
N
N
CH3
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

**3qa**


9.57
9.54
8.86
8.85
7.99
7.96
7.94
7.93
7.92
7.91
7.83
7.82
7.81
7.80
7.78
7.65
7.64
7.63
7.61
7.59
7.58
7.56
7.55
7.53
7.26
0.01
N
N
1.00
2.00
4.04
3.08
6.07
f1 (ppm)

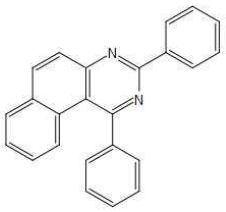
**3ra**


166.58
159.97
151.77
138.38
137.96
134.95
130.63
130.42
130.25
129.93
129.58
128.63
128.45
128.43
127.72
127.65
127.21
125.23
122.69
119.13
77.32
77.00
76.68
N
N
f1 (ppm)

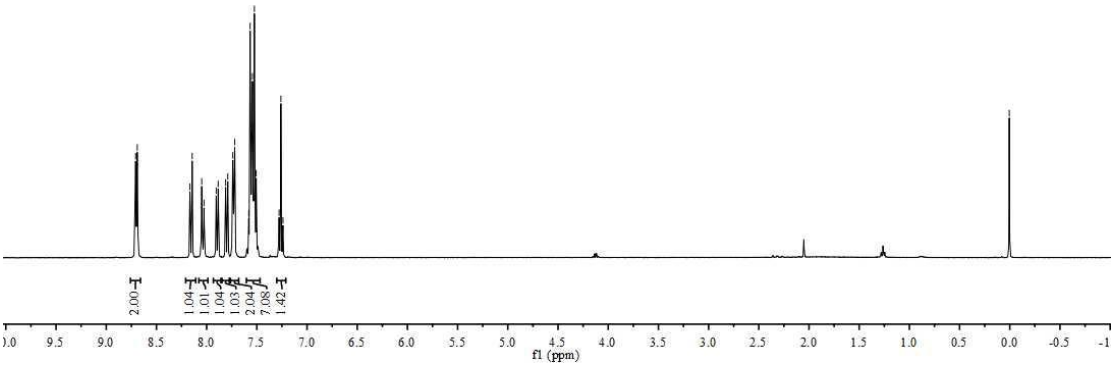
**3ra**

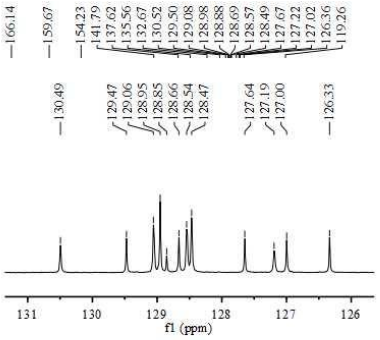

8.71
8.69
8.17
8.14
8.05
8.03
7.90
7.88
7.81
7.79
7.74
7.72
7.58
7.57
7.54
7.52
7.51
7.28
7.26
7.24


0.00

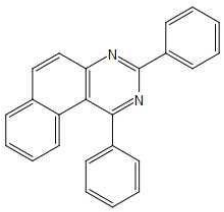

N
N

**3sa**

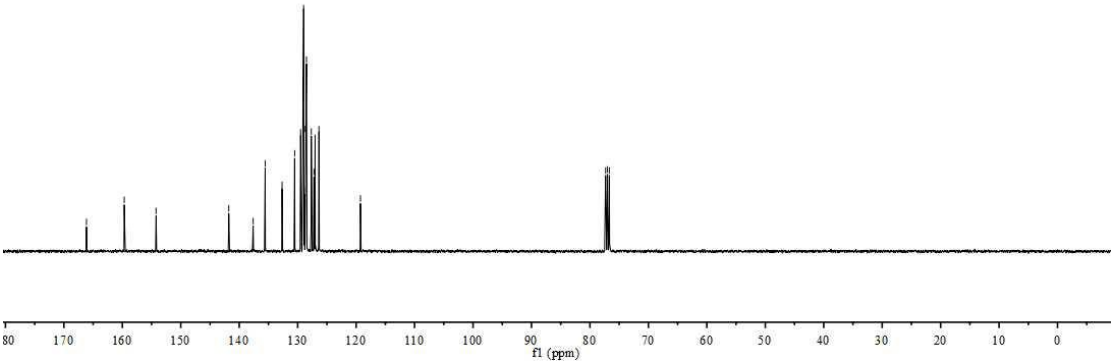

2.00
1.04
1.01
1.04
1.03
2.04
7.08
1.42
f1 (ppm)

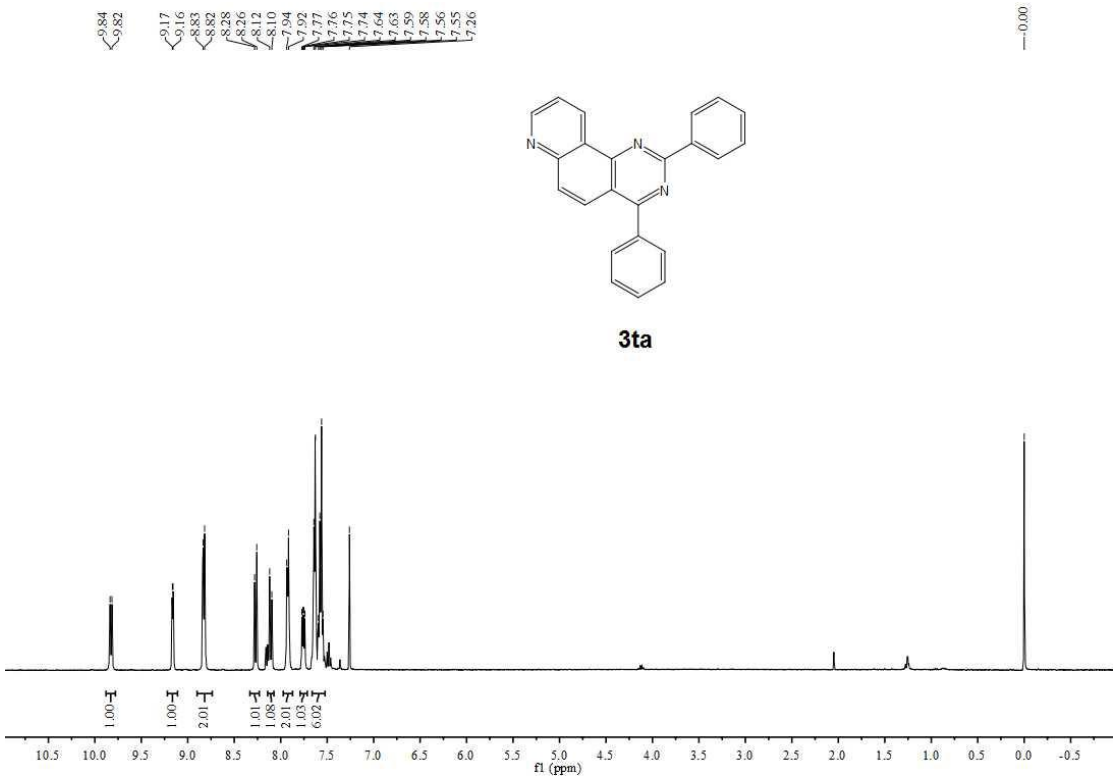

166.14
159.67
154.23
141.79
137.62
135.56
132.67
130.52
129.50
129.08
128.98
128.88
128.69
128.57
128.49
127.67
127.22
127.02
126.36
119.26
130.49
129.47
129.06
128.95
128.85
128.66
128.54
128.47
127.64
127.19
127.00
126.33
131
130
129
128
127
126
f1 (ppm)


77.32
77.00
76.68

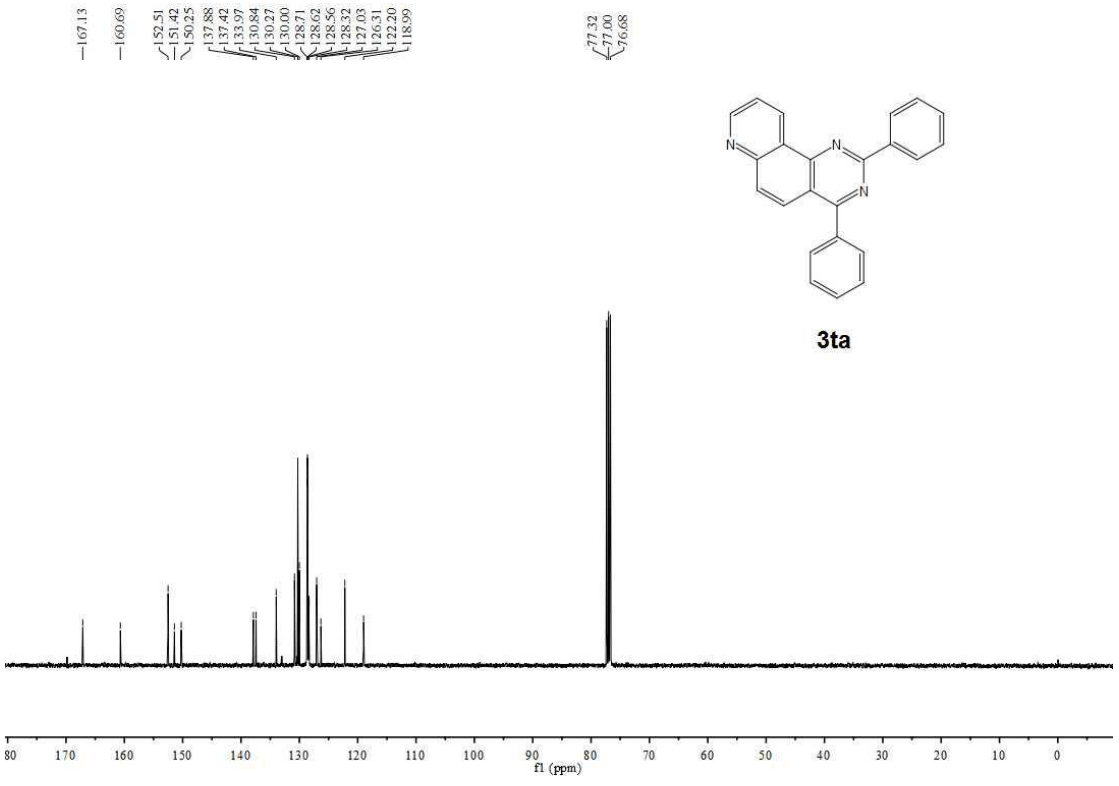

N
N

**3sa**

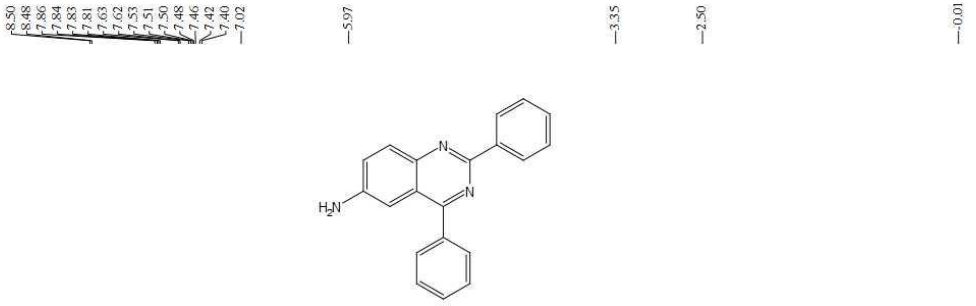

80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


9.84
9.82
9.17
9.16
8.83
8.82
8.28
8.26
8.12
8.10
7.94
7.92
7.77
7.76
7.75
7.74
7.64
7.63
7.59
7.58
7.56
7.55
7.26
0.00
N
N
N
1.00
1.00
2.01
1.01
1.08
2.01
1.03
6.02
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
f1 (ppm)

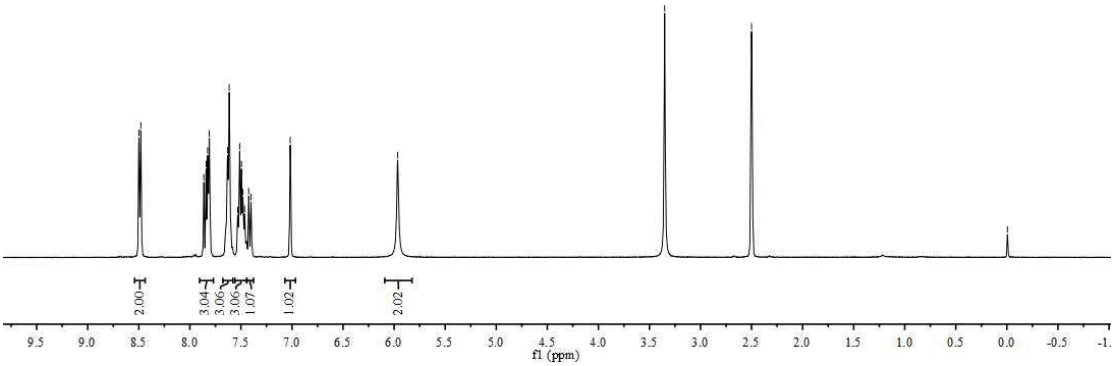
**3ta**

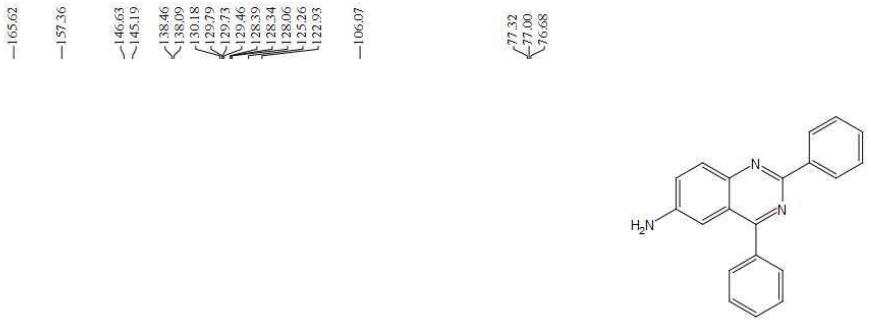

167.13
160.69
152.51
151.42
150.25
137.88
137.42
133.97
130.84
130.27
130.00
128.71
128.62
128.56
128.32
127.03
126.31
122.20
118.99
77.32
77.00
76.68
N
N
N
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

**3ta**

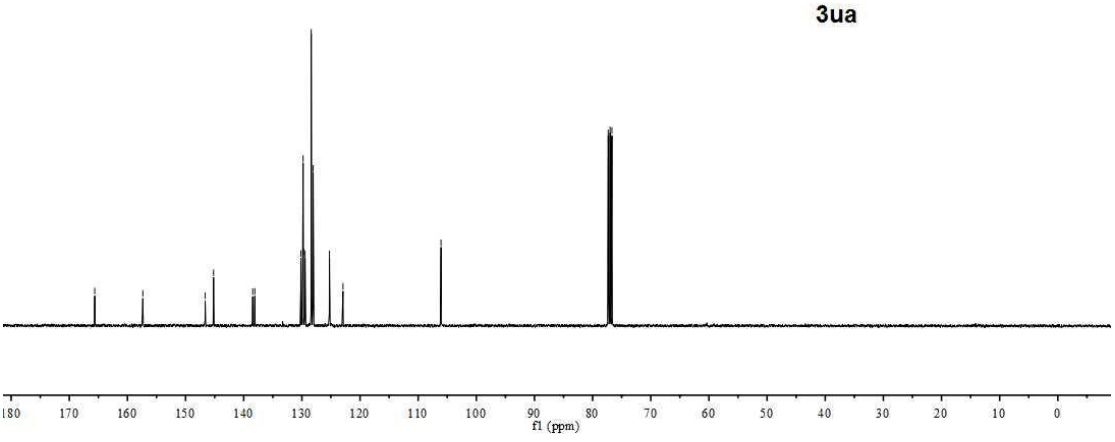

8.50
8.48
7.86
7.84
7.83
7.81
7.63
7.62
7.53
7.51
7.50
7.48
7.46
7.42
7.40
7.02
5.97
3.35
2.50
0.01
N
N
H2N

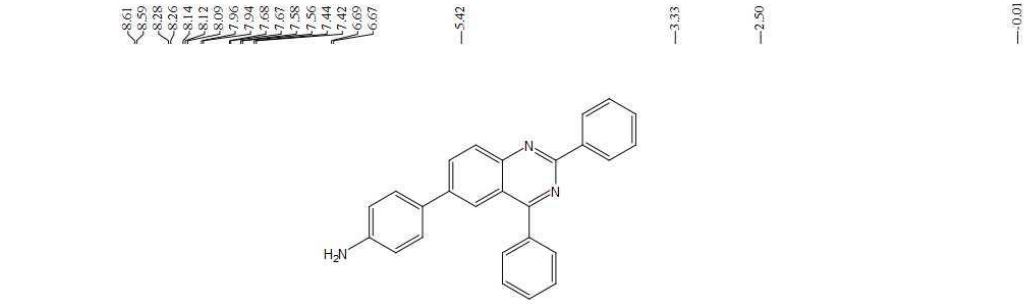
**3ua**


2.00
3.04
3.06
3.06
1.07
1.02
2.02
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)

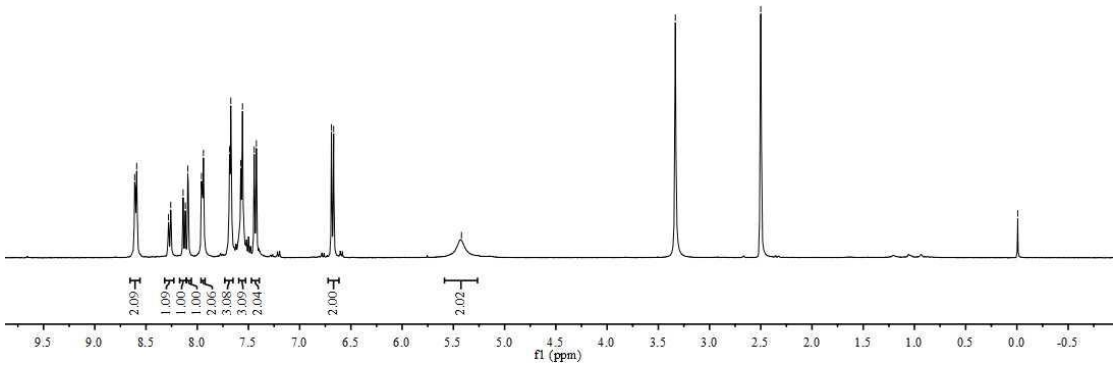

165.62
157.36
146.63
145.19
138.46
138.09
130.18
129.79
129.73
129.46
128.39
128.34
128.06
125.26
122.93
106.07
77.32
77.00
76.68
N
N
H2N

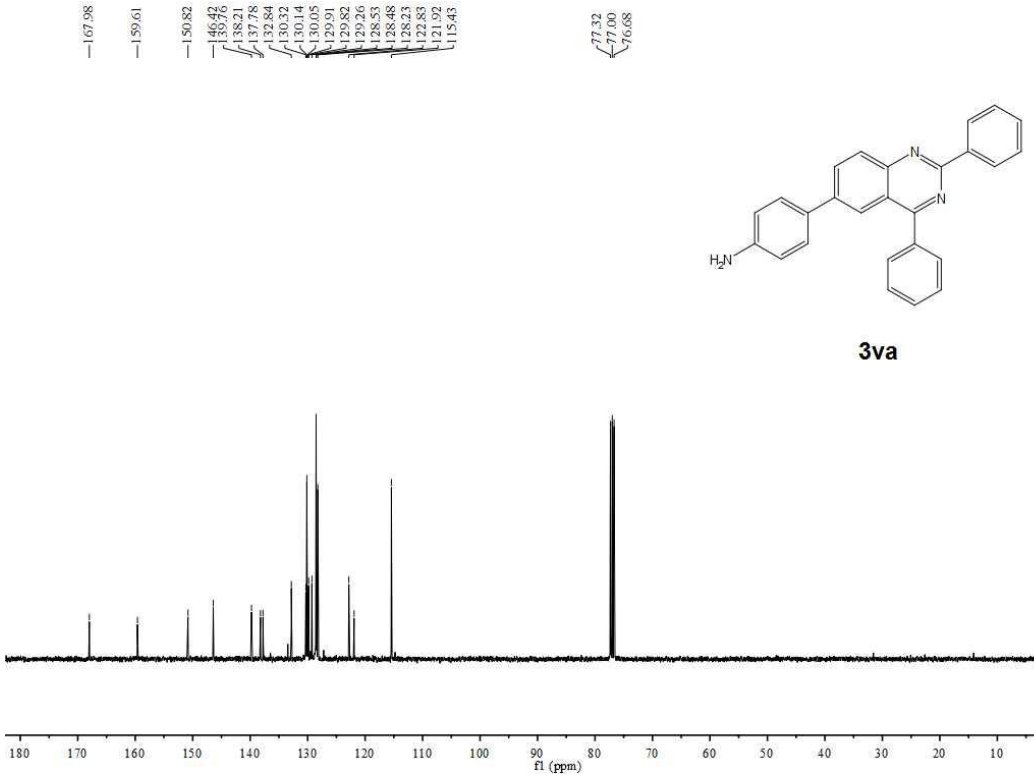
**3ua**


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

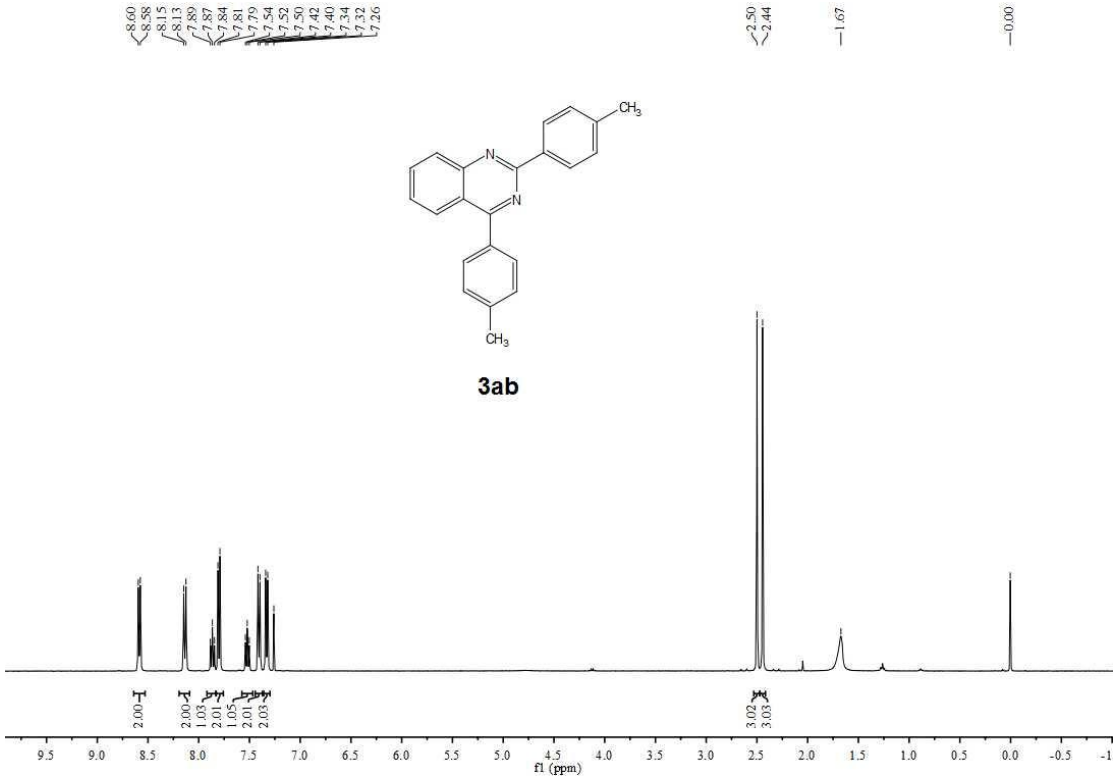

8.61
8.59
8.28
8.26
8.14
8.12
8.09
7.96
7.94
7.68
7.67
7.58
7.56
7.44
7.42
6.69
6.67
5.42
3.33
2.50
0.01
N
N
H2N

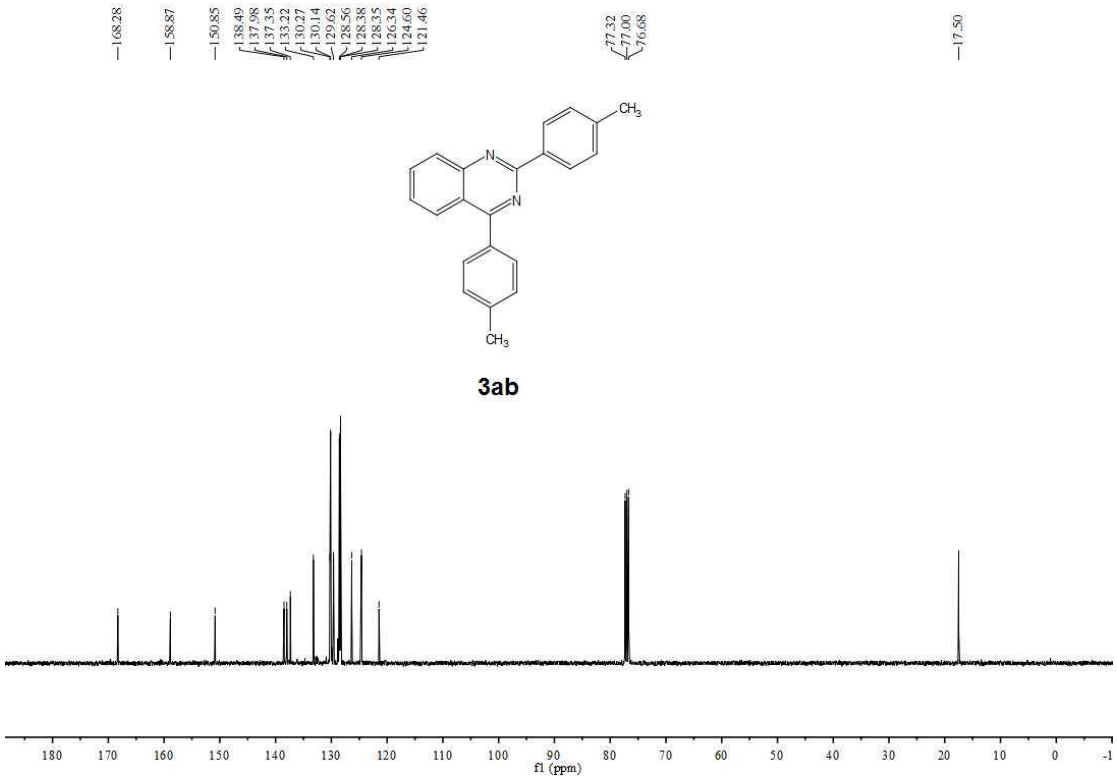
**3va**

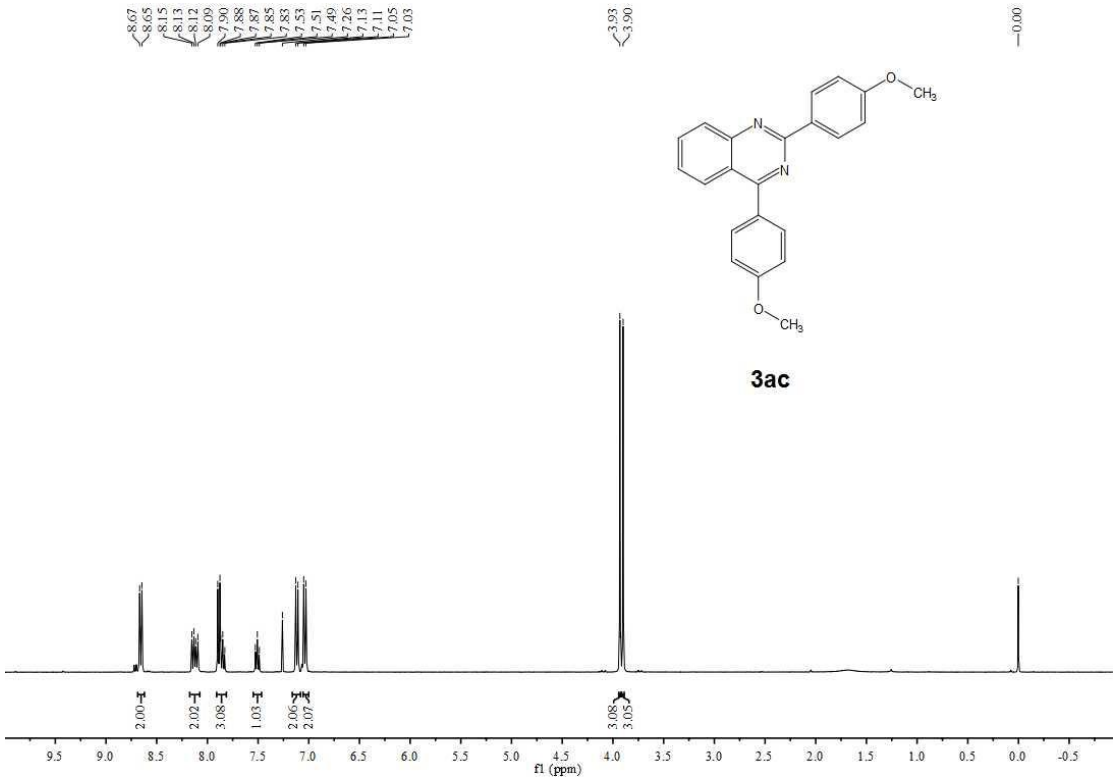

2.09
1.09
1.00
1.00
2.06
3.08
3.09
2.04
2.00
2.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


167.98
159.61
150.82
146.42
139.76
138.21
137.78
132.84
130.32
130.14
130.05
129.91
129.82
129.26
128.53
128.48
128.23
122.83
121.92
115.43
77.32
77.00
76.68
N
N
H2N
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

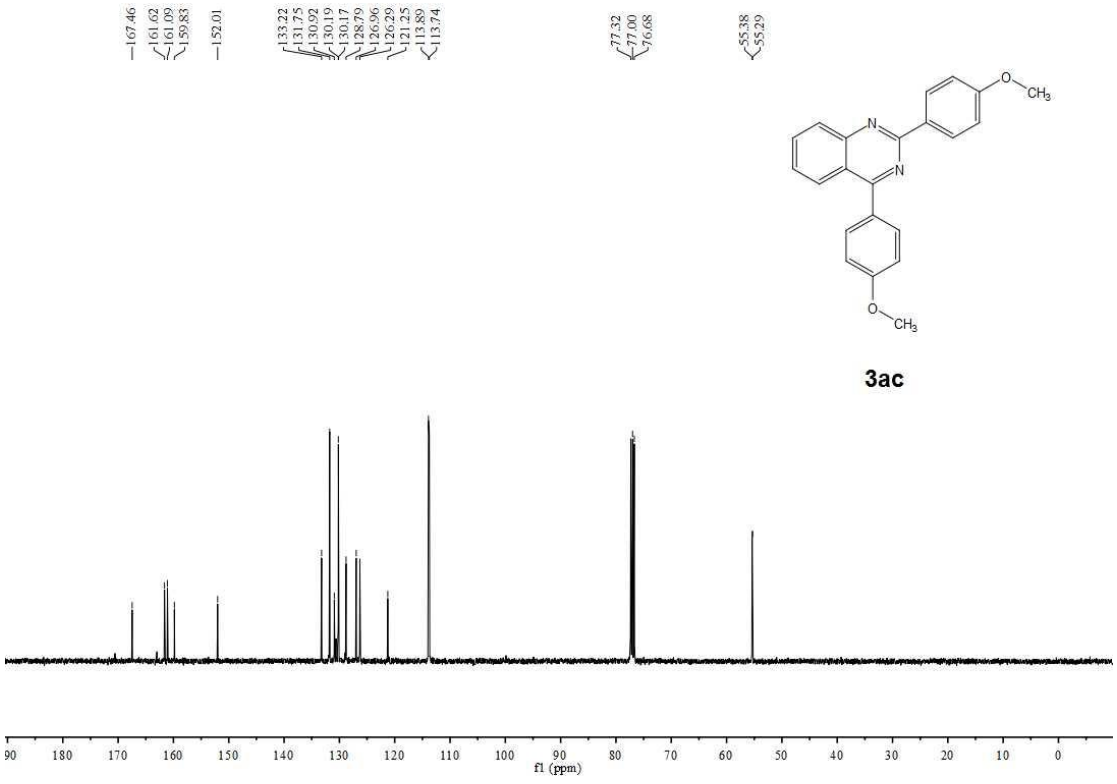
**3va**


8.60
8.58
8.15
8.13
7.89
7.87
7.84
7.81
7.79
7.54
7.52
7.50
7.42
7.40
7.34
7.32
7.26
2.50
2.44
1.67
0.00
CH3
N
N
CH3
3ab
2.00
2.00
1.03
2.01
1.05
2.01
2.03
3.02
3.03
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)

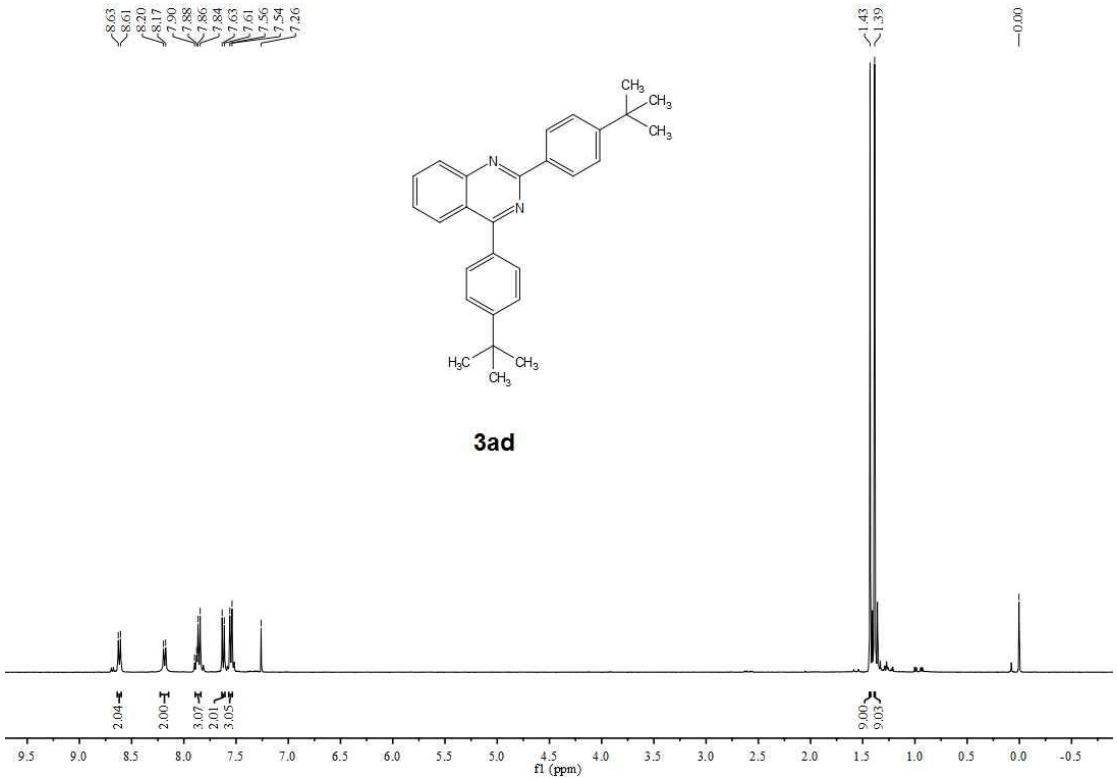

168.28
158.87
150.85
138.49
137.98
137.35
133.22
130.27
130.14
129.62
128.56
128.38
128.35
126.34
124.60
121.46
77.32
77.00
76.68
17.50
CH3
N
N
CH3
3ab
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)


8.67
8.65
8.15
8.13
8.12
8.09
7.90
7.88
7.87
7.85
7.83
7.53
7.51
7.49
7.26
7.13
7.11
7.05
7.03
3.93
3.90
0.00
O
CH3
N
N
O
CH3
2.00
2.02
3.08
1.03
2.06
2.07
3.08
3.05
f1 (ppm)

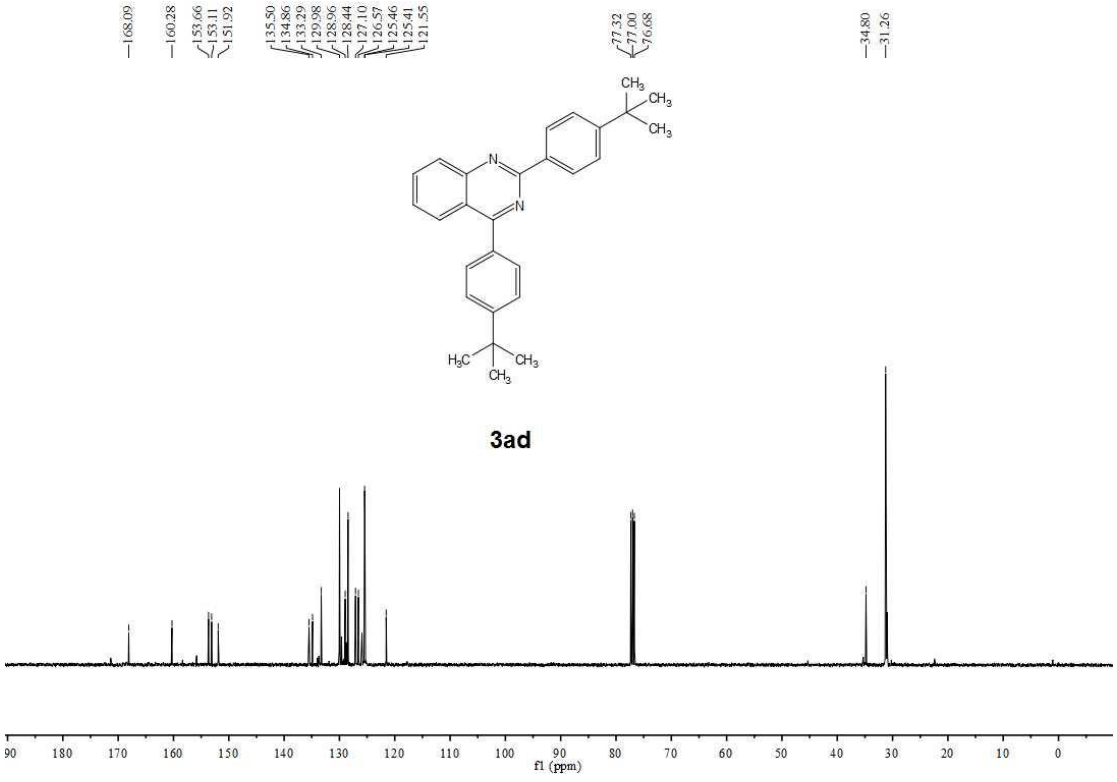
**3ac**


167.46
161.62
161.09
159.83
152.01
133.22
131.75
130.92
130.19
130.17
128.79
126.96
126.29
121.25
113.89
113.74
77.32
77.00
76.68
55.38
55.29
O
CH3
N
N
O
CH3
f1 (ppm)

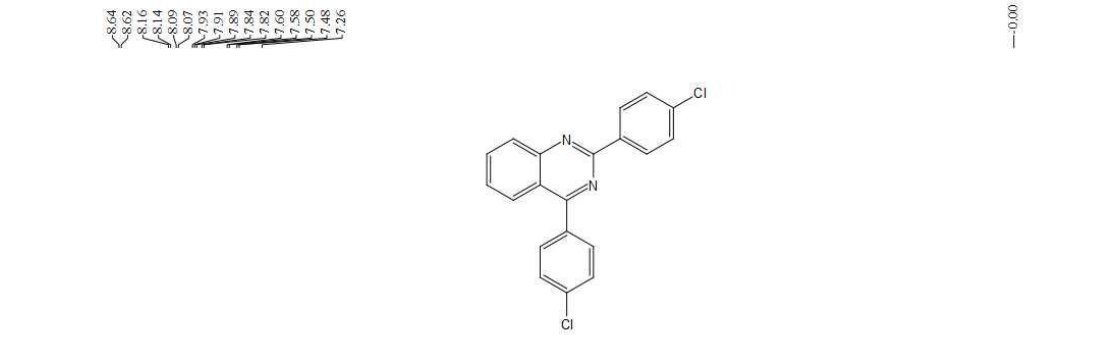
**3ac**


8.63
8.61
8.20
8.17
7.90
7.88
7.86
7.84
7.63
7.61
7.56
7.54
7.26
1.43
1.39
0.00
2.04
2.00
3.07
2.01
3.05
9.00
9.03
f1 (ppm)

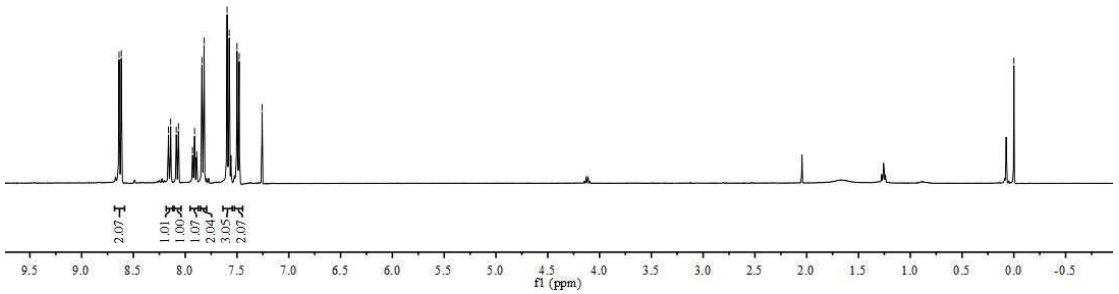
**3ad**

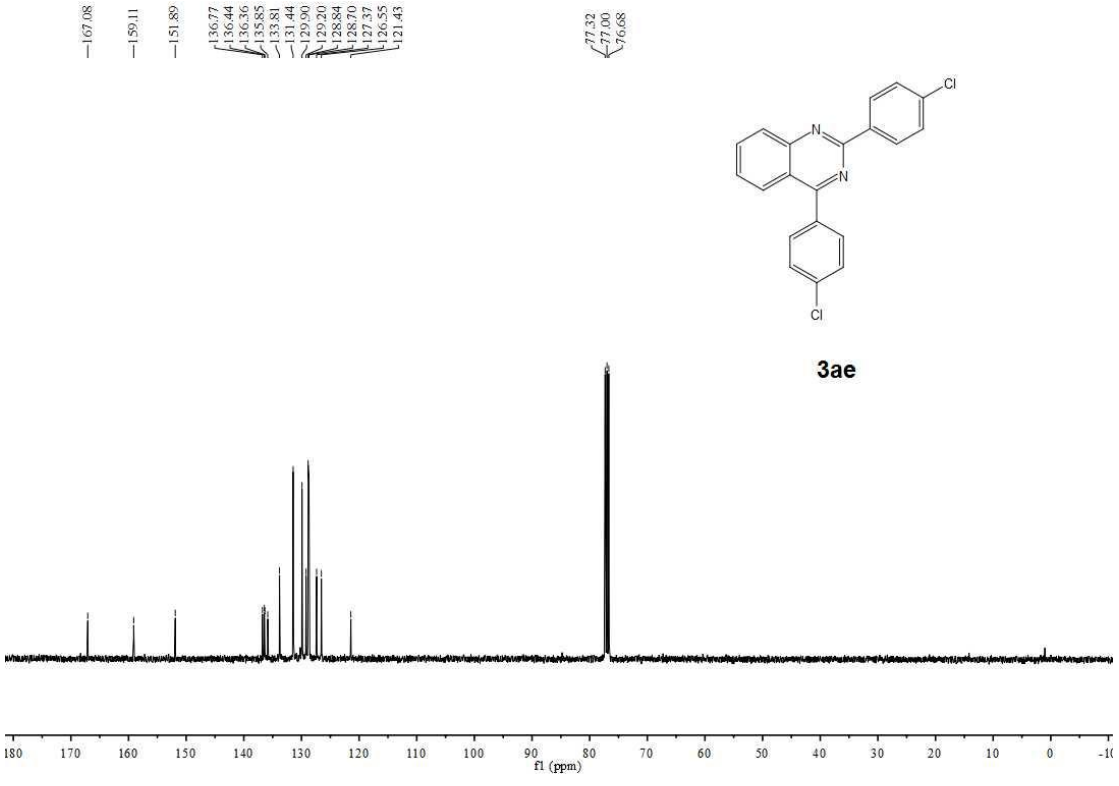

168.09
160.28
153.66
153.11
151.92
135.50
134.86
133.29
129.98
128.96
128.44
127.10
126.57
125.46
125.41
121.55
77.32
77.00
76.68
34.80
31.26
f1 (ppm)

**3ad**

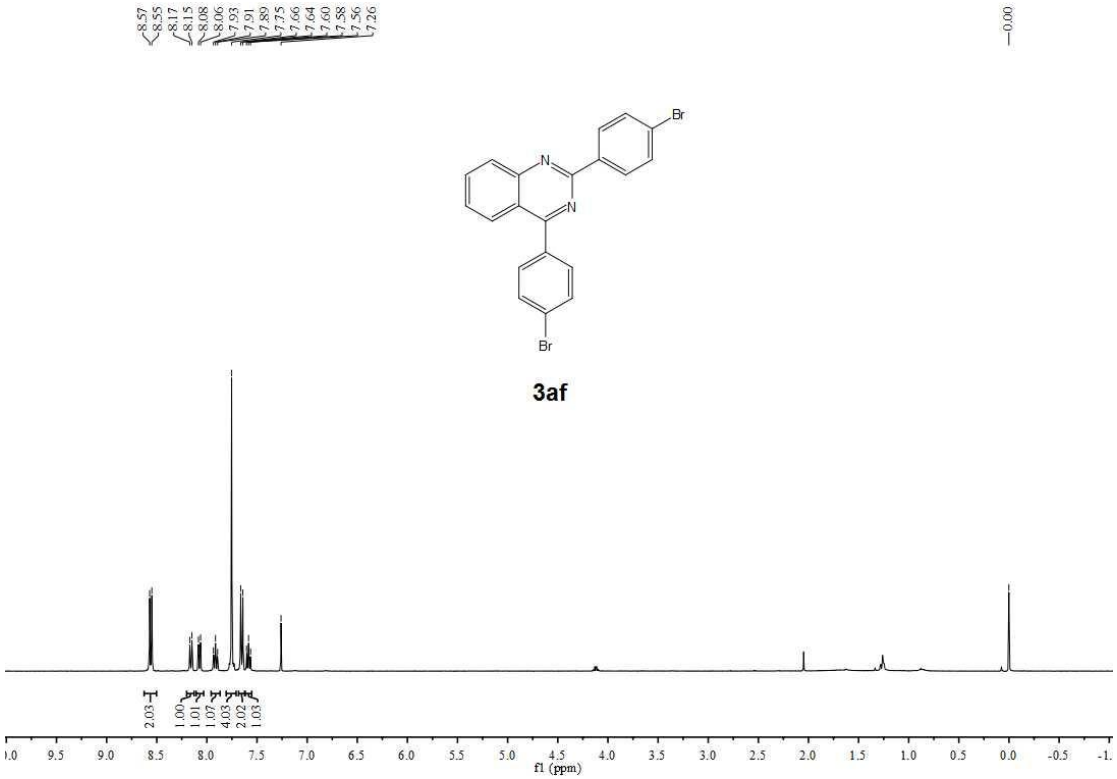

8.64
8.62
8.16
8.14
8.09
8.07
7.93
7.91
7.89
7.84
7.82
7.60
7.58
7.50
7.48
7.26
0.00
Cl
N
N
Cl

**3ae**

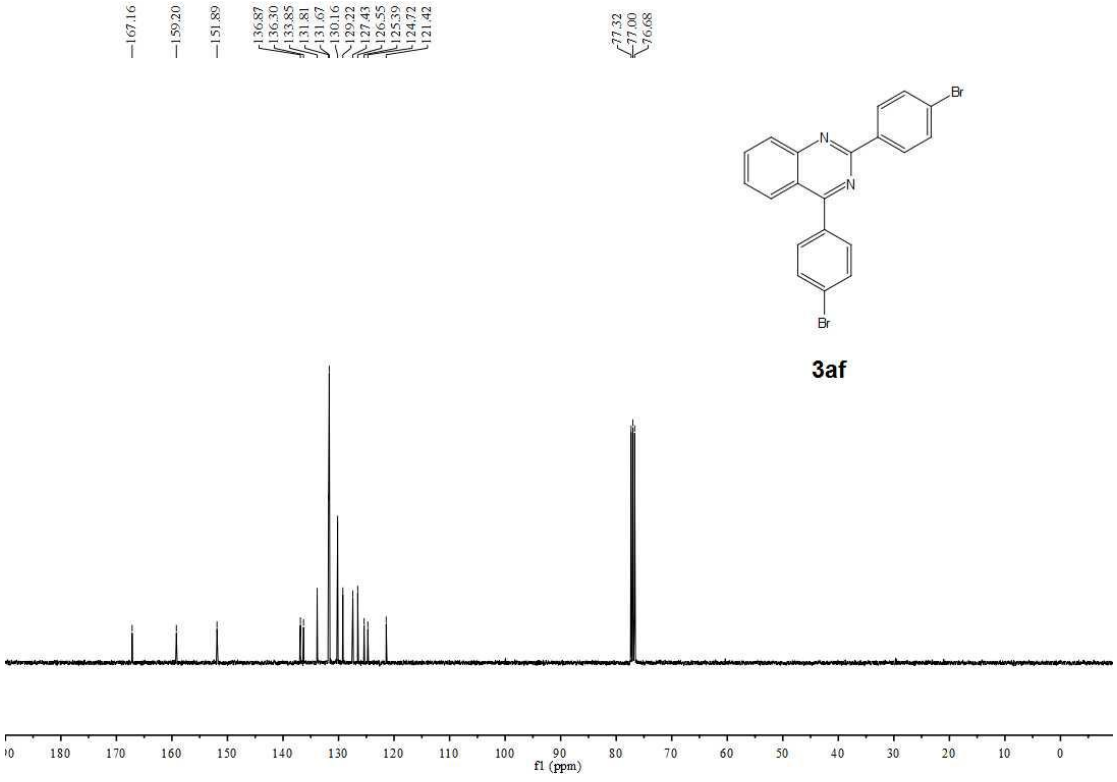

2.07
1.01
1.00
1.07
2.04
3.05
2.07
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


167.08
159.11
151.89
136.77
136.44
136.36
135.85
133.81
131.44
129.90
129.20
128.84
128.70
127.37
126.55
121.43
77.32
77.00
76.68
Cl
N
N
Cl
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

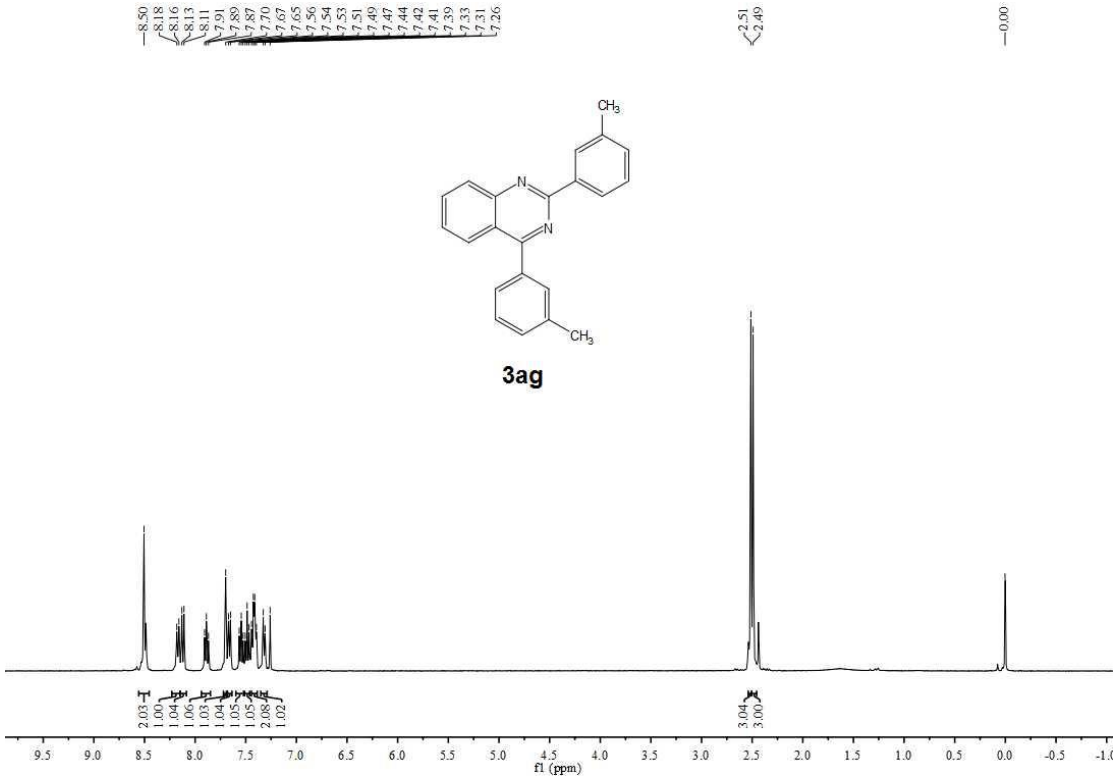
**3ae**

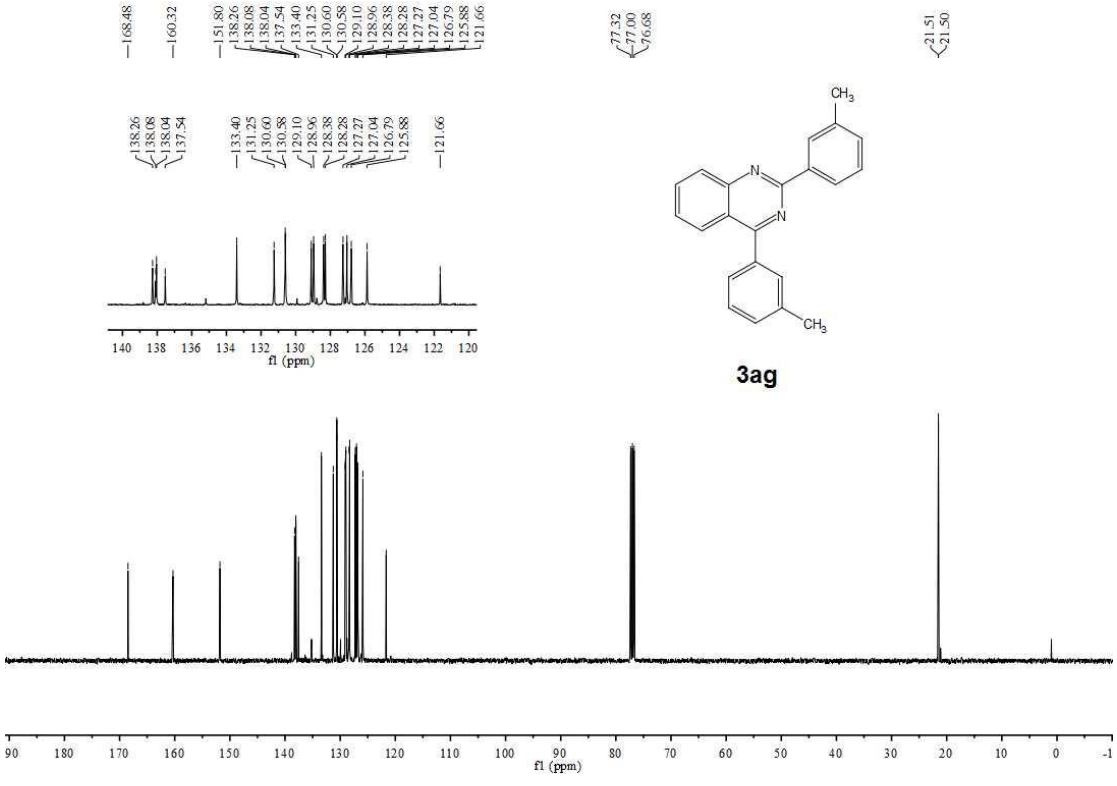

8.57
8.55
8.17
8.15
8.08
8.06
7.93
7.91
7.80
7.75
7.66
7.64
7.60
7.58
7.56
7.26
0.00
Br
N
N
Br
2.03
1.00
1.01
1.07
4.03
2.02
1.03
f1 (ppm)

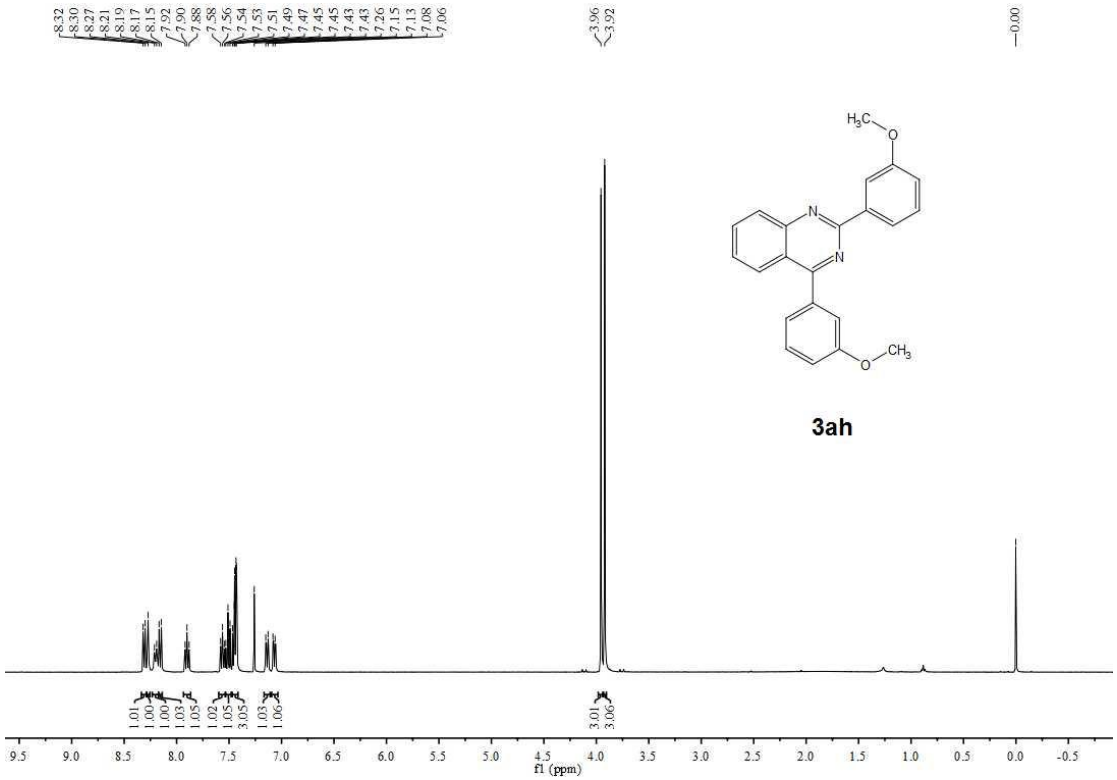
**3af**

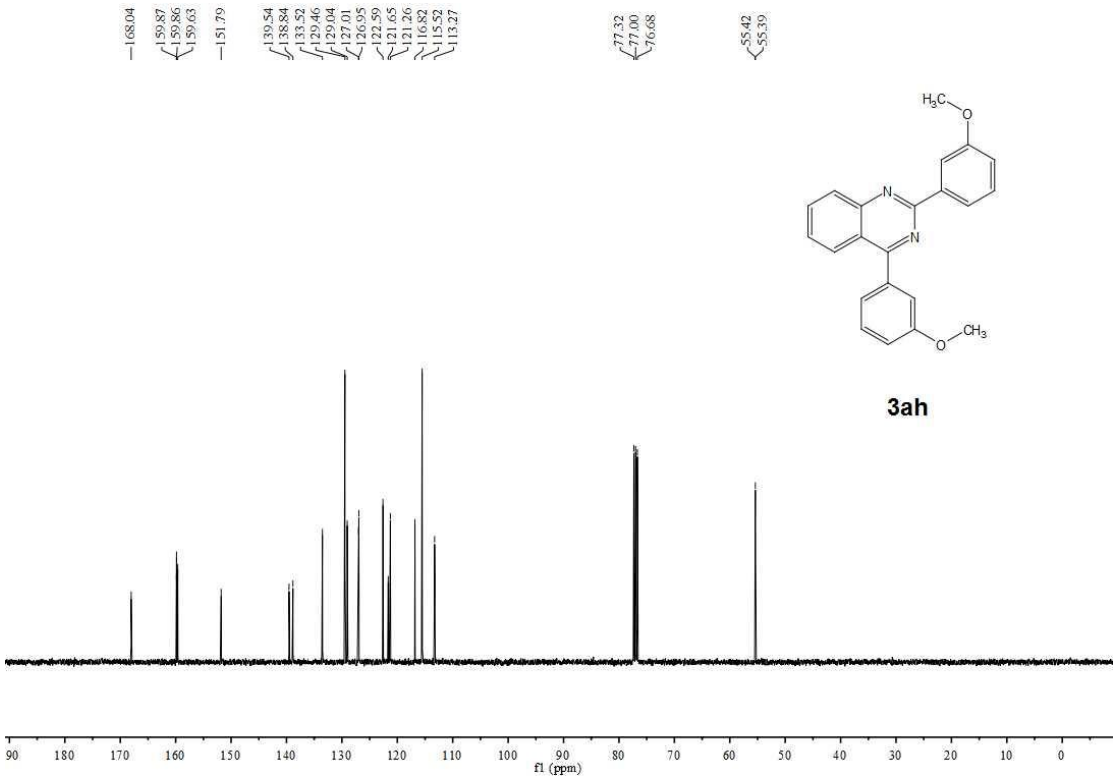

167.16
159.20
151.89
136.87
136.30
133.85
131.81
131.67
130.16
129.22
127.43
126.55
125.39
124.72
121.42
77.32
77.00
76.68
Br
N
N
Br
f1 (ppm)

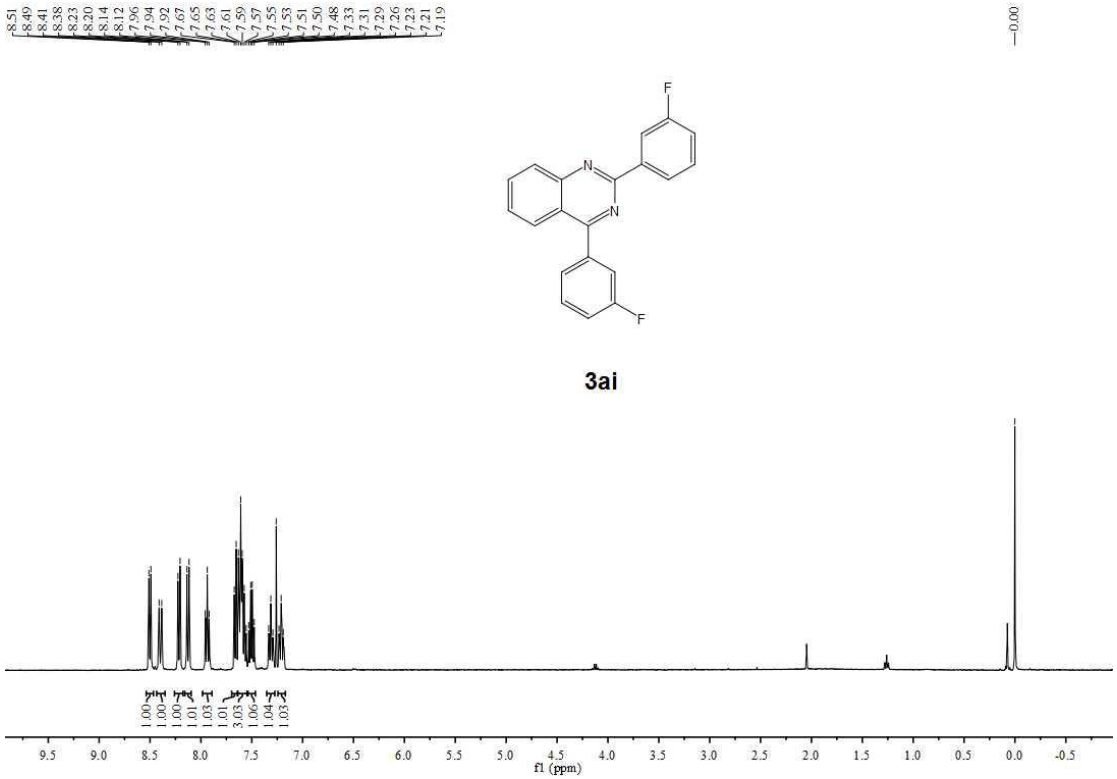
**3af**

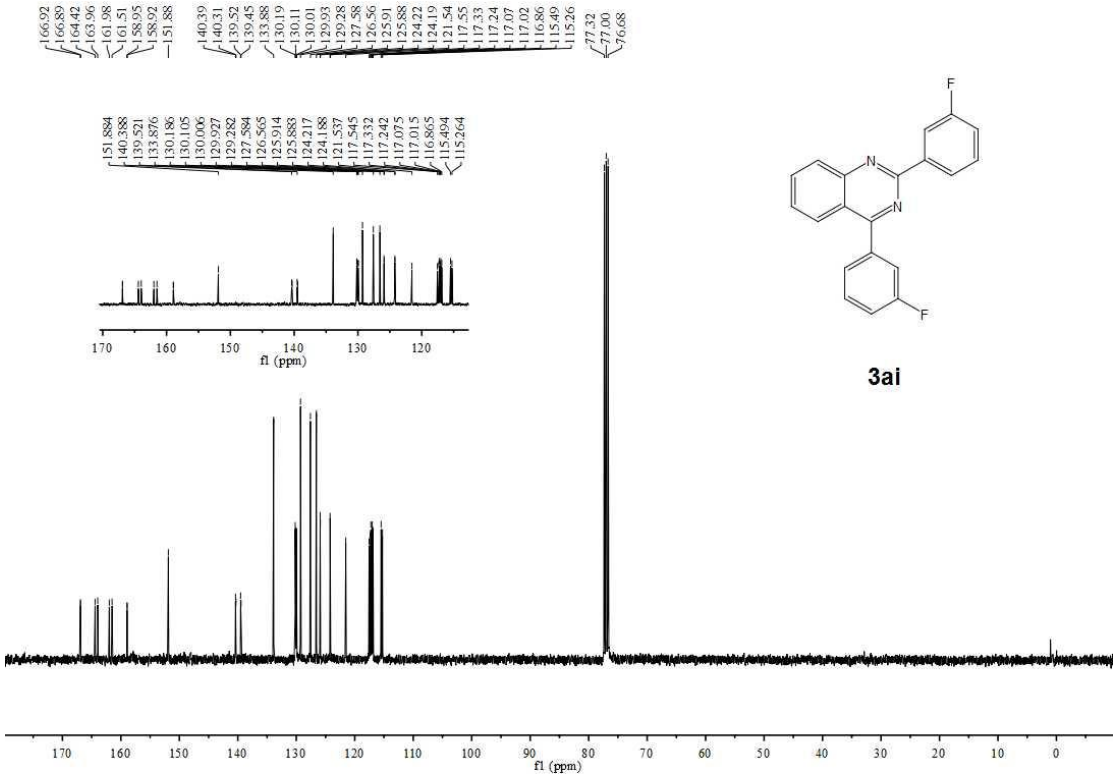

8.50
8.18
8.16
8.13
8.11
7.91
7.89
7.87
7.70
7.67
7.65
7.56
7.54
7.53
7.51
7.49
7.47
7.44
7.42
7.41
7.39
7.33
7.31
7.26
2.51
2.49
0.00
CH3
N
N
CH3
3ag
2.03
1.00
1.04
1.06
1.03
1.04
1.05
1.05
2.08
1.02
3.04
3.00
f1 (ppm)

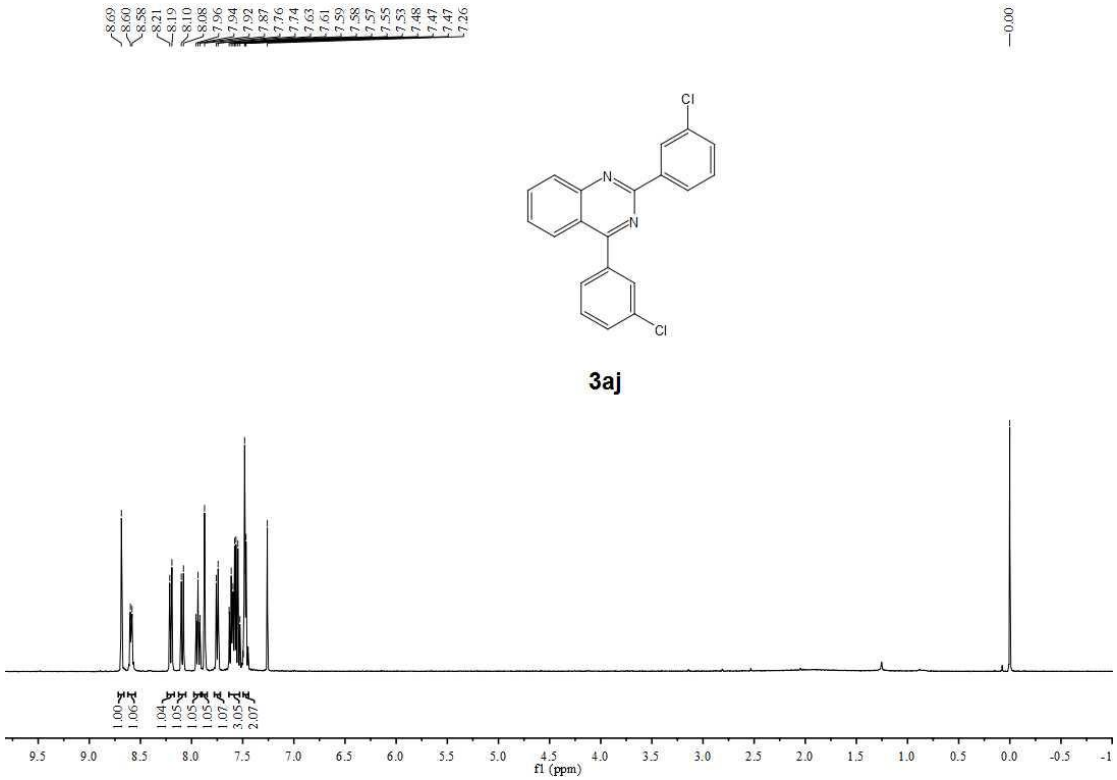

168.48
160.32
151.80
138.26
138.08
138.04
137.54
133.40
131.25
130.60
130.58
129.10
128.96
128.38
128.28
127.27
127.04
126.79
125.88
121.66
77.32
77.00
76.68
21.51
21.50
CH3
N
N
CH3
3ag
f1 (ppm)


8.32
8.30
8.27
8.21
8.19
8.17
8.15
7.92
7.90
7.88
7.58
7.56
7.54
7.53
7.51
7.49
7.47
7.45
7.45
7.43
7.43
7.26
7.15
7.13
7.08
7.06
3.96
3.92
0.00
1.01
1.00
1.00
1.03
1.05
1.02
1.05
3.05
1.03
1.06
3.01
3.06
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)
3ah

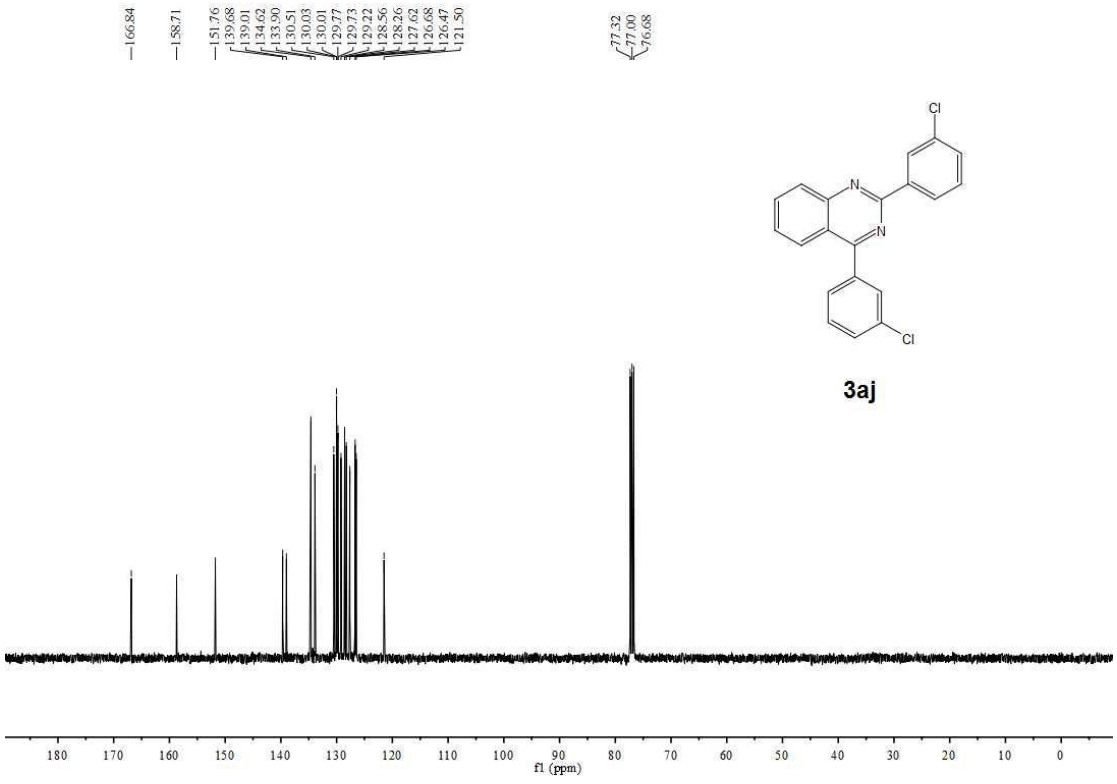

168.04
159.87
159.86
159.63
151.79
139.54
138.84
133.52
129.46
129.04
127.01
126.95
122.59
121.65
121.26
116.82
115.52
113.27
77.32
77.00
76.68
55.42
55.39
90 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
3ah


8.51
8.49
8.41
8.38
8.23
8.20
8.14
8.12
7.96
7.94
7.92
7.67
7.65
7.63
7.61
7.59
7.57
7.55
7.53
7.51
7.50
7.48
7.33
7.31
7.29
7.26
7.23
7.21
7.19
0.00
F
N
N
F
3ai
1.00
1.00
1.00
1.01
1.03
1.01
3.03
1.06
1.04
1.03
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)

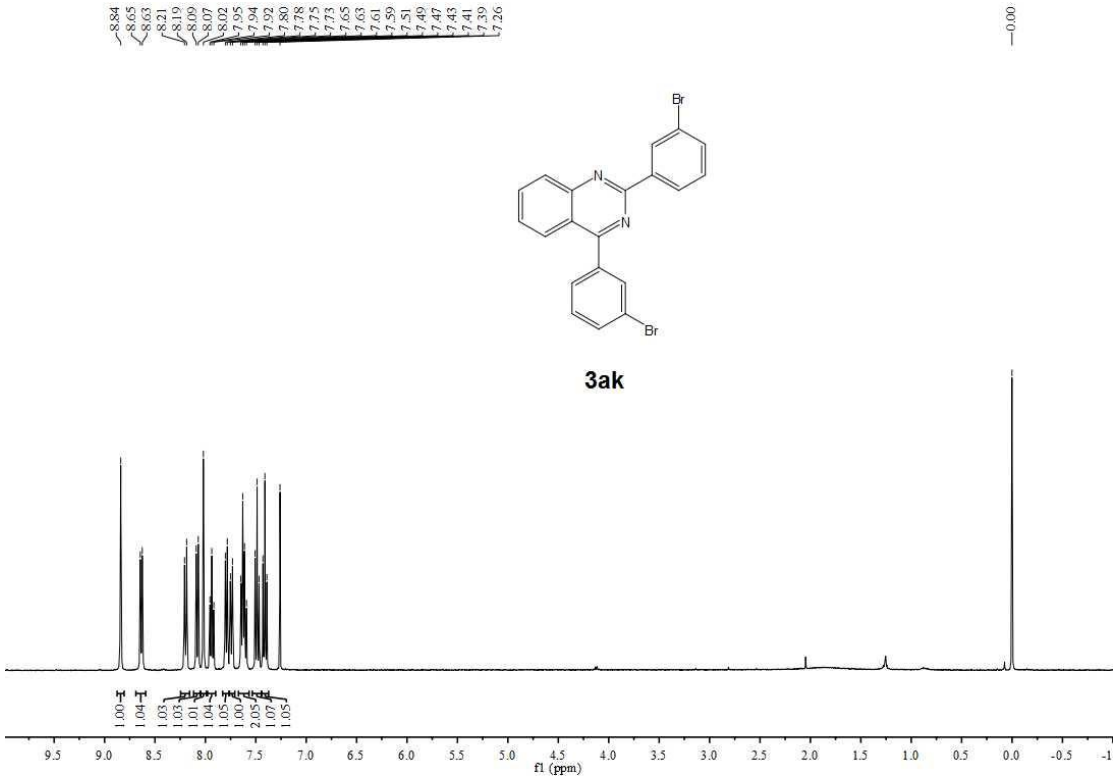

166.92
166.89
164.42
163.96
161.98
161.51
158.95
158.92
151.88
140.39
140.31
139.52
139.45
133.88
130.19
130.11
130.01
129.93
129.28
127.58
126.56
125.91
125.88
124.22
124.19
121.54
117.55
117.33
117.24
117.07
117.02
116.86
115.49
115.26
77.32
77.00
76.68
151.8884
140.388
139.521
133.876
130.186
130.105
130.006
129.927
129.282
127.584
126.565
125.914
125.883
124.217
124.188
121.537
117.545
117.332
117.242
117.075
117.015
116.865
115.494
115.264
170
160
150
140
130
120
f1 (ppm)
F
N
N
F
3ai
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.69
8.60
8.58
8.21
8.19
8.10
8.08
7.96
7.94
7.92
7.87
7.76
7.74
7.63
7.61
7.59
7.58
7.57
7.55
7.53
7.48
7.47
7.47
7.26
0.00
Cl
N
N
Cl
1.00
1.06
1.04
1.05
1.05
1.05
1.07
3.05
2.07
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)

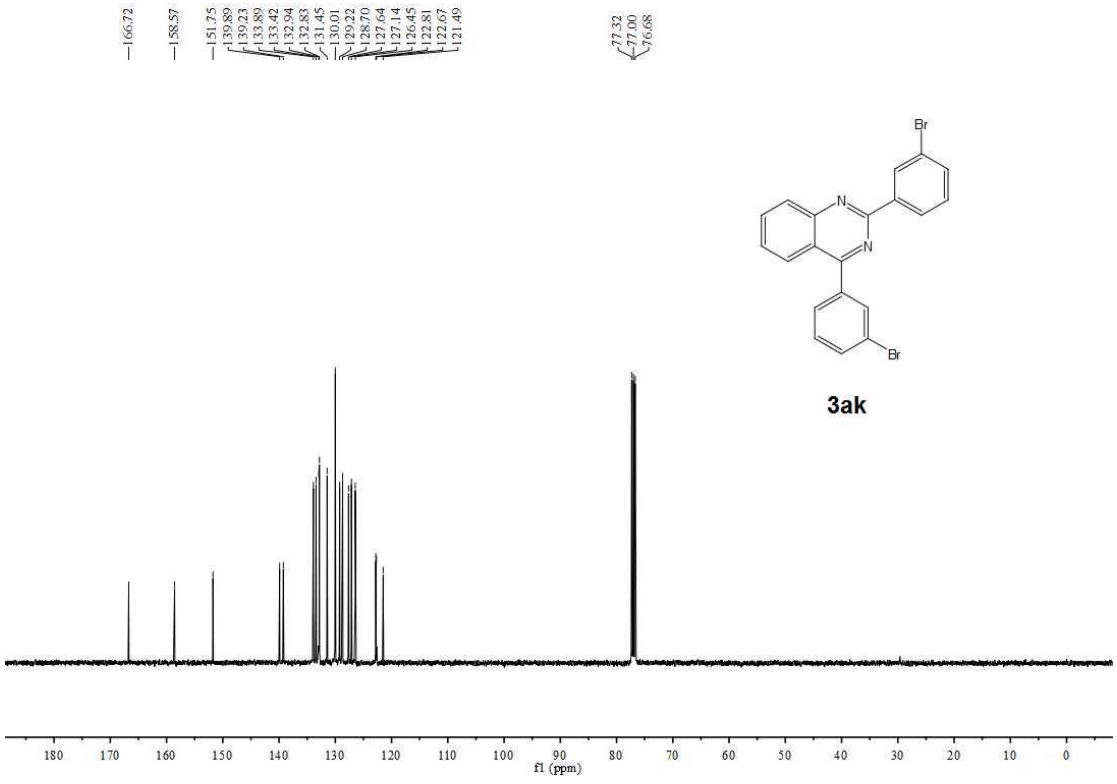
**3aj**


166.84
158.71
151.76
139.68
139.01
134.62
133.96
130.51
130.03
130.01
129.77
129.73
129.22
128.56
128.26
127.62
126.68
126.47
121.50
77.32
77.00
76.68
Cl
N
N
Cl
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

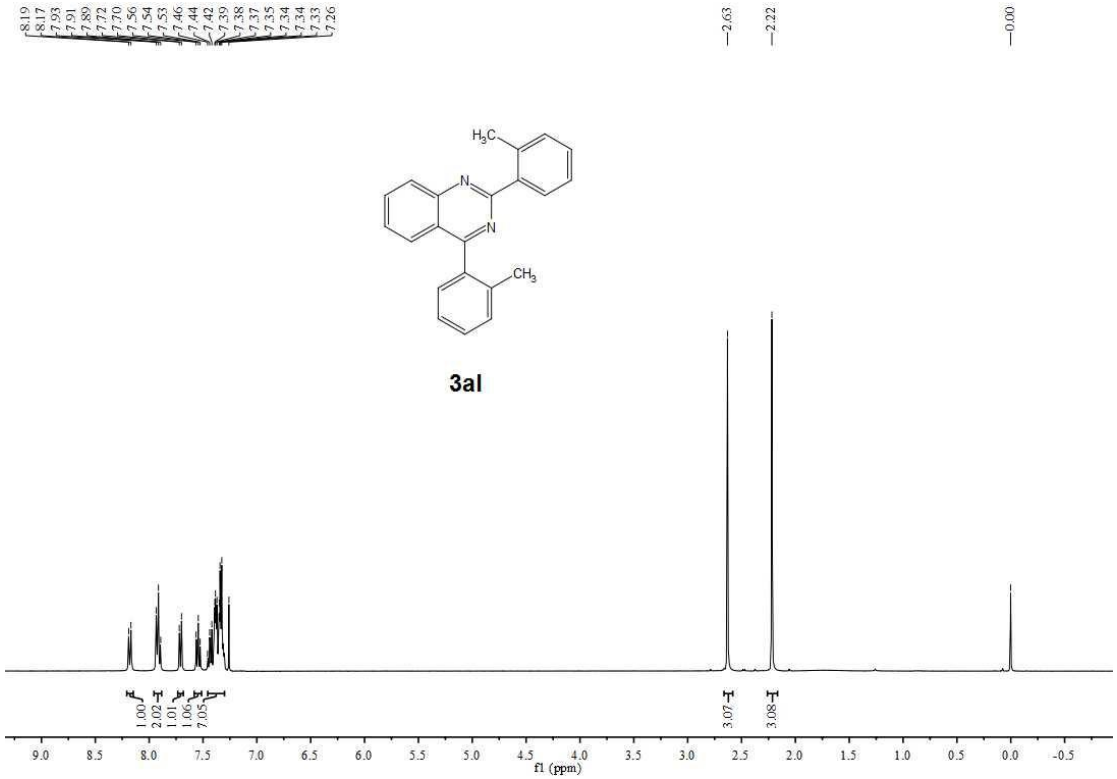
**3aj**


8.84
8.65
8.63
8.21
8.19
8.09
8.07
8.02
7.95
7.94
7.92
7.80
7.78
7.75
7.73
7.65
7.63
7.61
7.59
7.51
7.49
7.47
7.43
7.41
7.39
7.26
0.00
Br
N
N
Br
1.00
1.04
1.03
1.03
1.01
1.04
1.05
1.00
2.05
1.07
1.05
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
f1 (ppm)

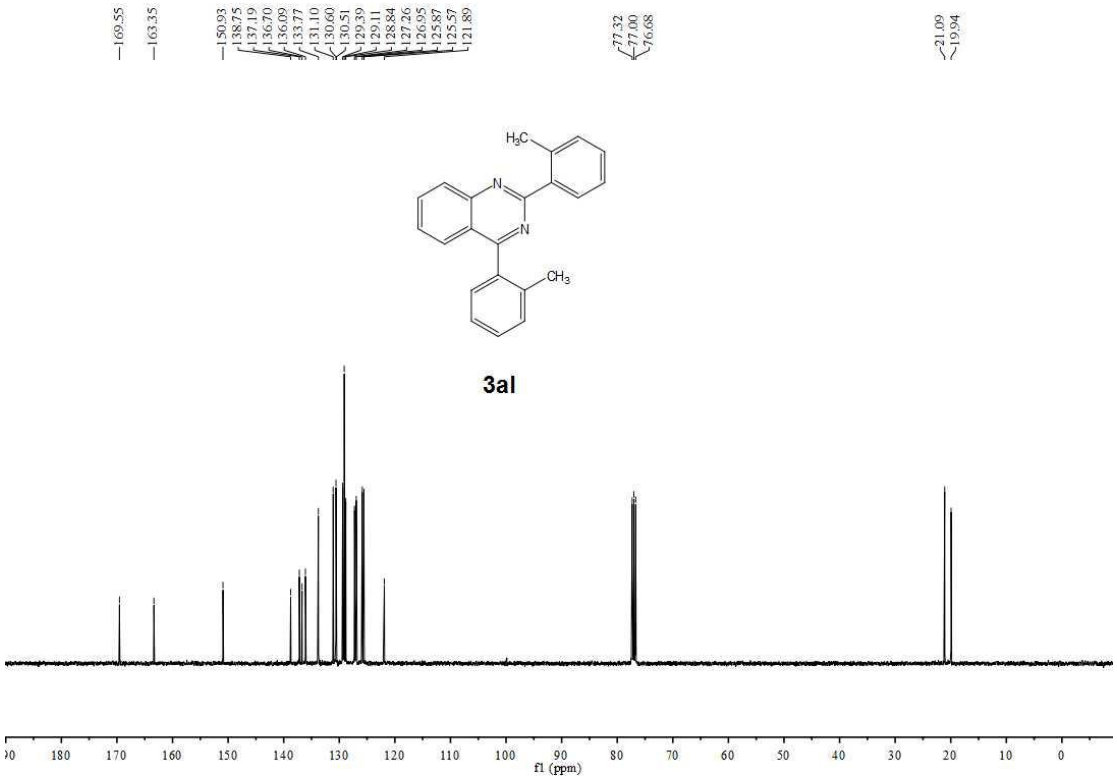
**3ak**


166.72
158.57
151.75
139.89
139.23
133.89
133.42
132.94
132.83
131.45
130.01
129.22
128.70
127.64
127.14
126.45
122.81
122.67
121.49
77.32
77.00
76.68
Br
N
N
Br
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

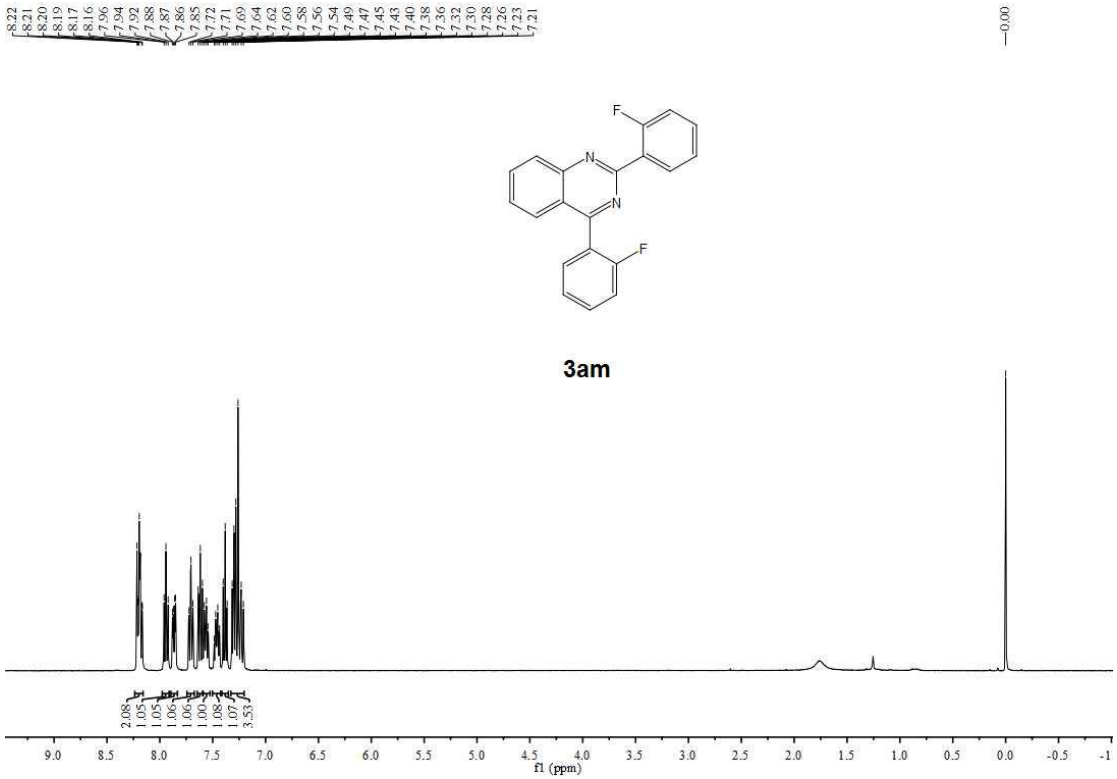
**3ak**

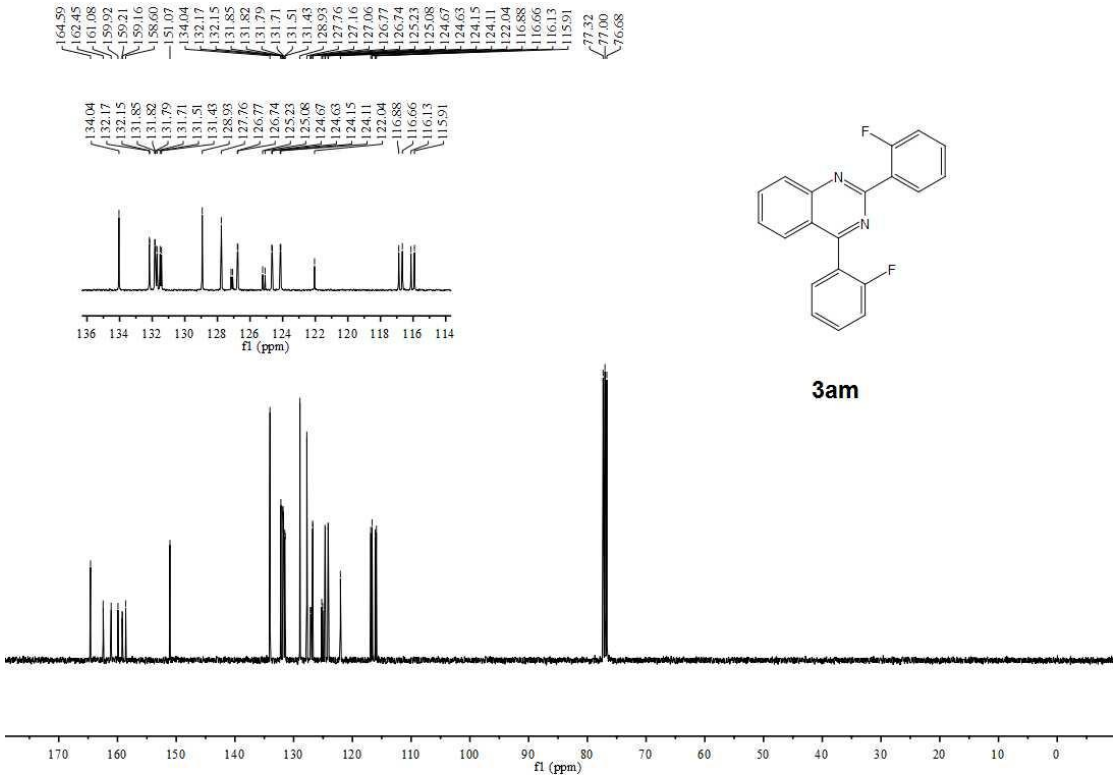

8.19
8.17
7.93
7.91
7.89
7.72
7.70
7.56
7.54
7.53
7.46
7.44
7.42
7.39
7.38
7.37
7.35
7.34
7.33
7.26
2.63
2.22
0.00
H3C
N
N
CH3
1.00
2.02
1.01
1.06
7.05
3.07
3.08
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

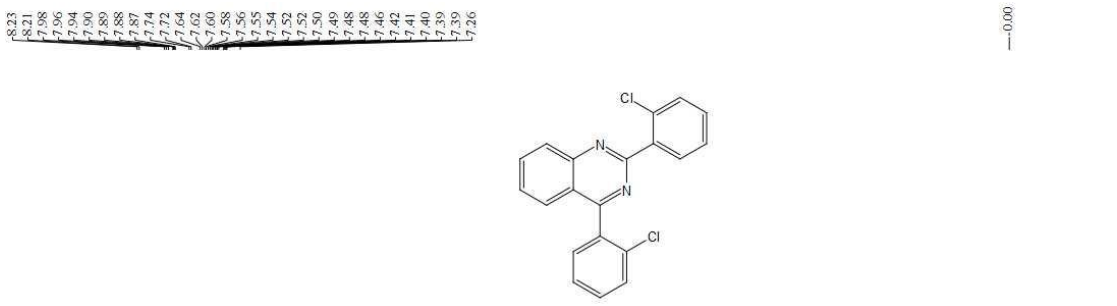
**3al**


169.55
163.35
150.93
138.75
137.19
136.70
136.09
133.77
131.10
130.60
130.51
129.39
129.11
128.84
127.26
126.95
125.87
125.57
121.89
77.32
77.00
76.68
21.09
19.94
H3C
N
N
CH3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

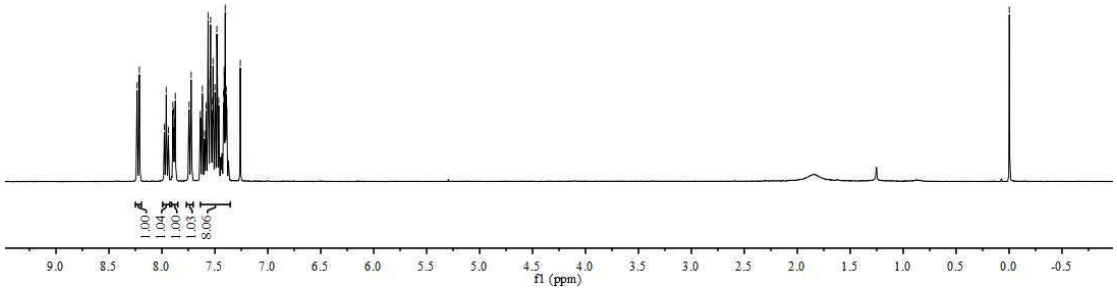
**3al**

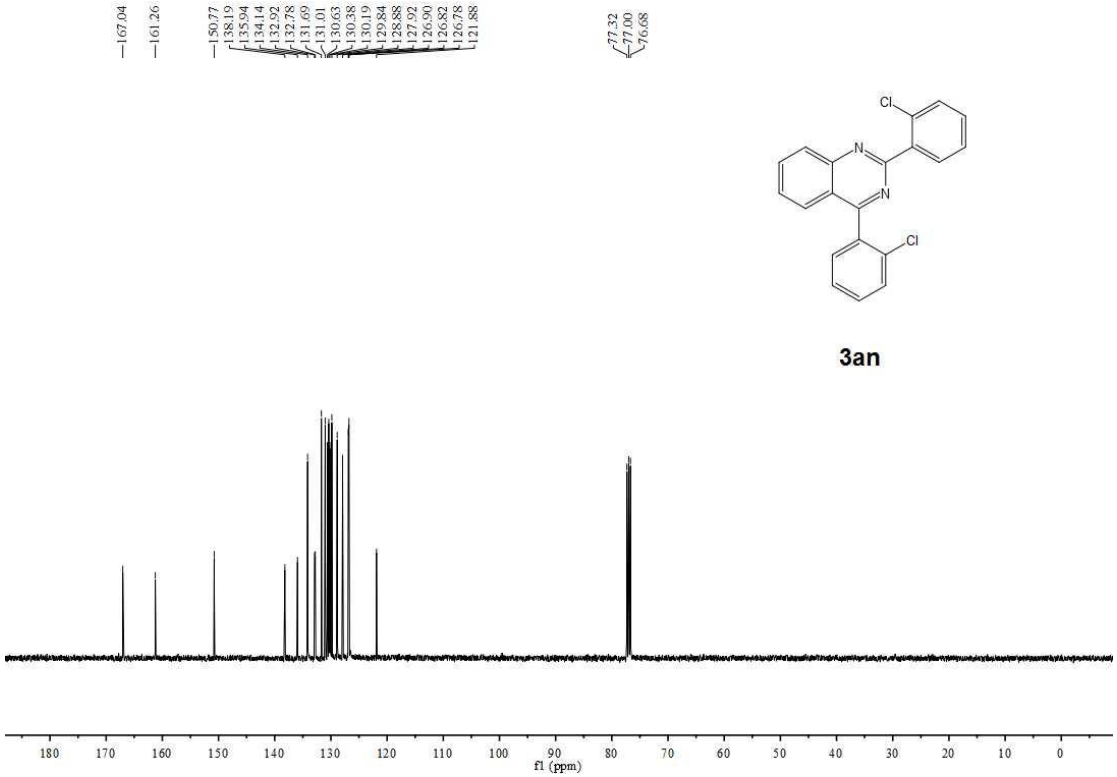

8.22
8.21
8.20
8.19
8.17
8.16
7.96
7.94
7.92
7.88
7.87
7.86
7.85
7.72
7.71
7.69
7.64
7.62
7.60
7.58
7.56
7.54
7.49
7.47
7.45
7.43
7.40
7.38
7.36
7.32
7.30
7.28
7.26
7.23
7.21
0.00
F
N
N
F
3am
2.08
1.05
1.05
1.06
1.06
1.00
1.08
1.07
3.53
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)


164.59
162.45
161.08
159.92
159.21
159.16
158.60
151.07
134.04
132.17
132.15
131.85
131.82
131.79
131.71
131.51
131.43
128.93
127.76
127.16
127.06
126.77
126.74
125.23
125.08
124.67
124.63
124.15
124.11
122.04
116.88
116.66
116.13
115.91
77.32
77.00
76.68
136 134 132 130 128 126 124 122 120 118 116 114
f1 (ppm)
F
N
N
F
3am
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

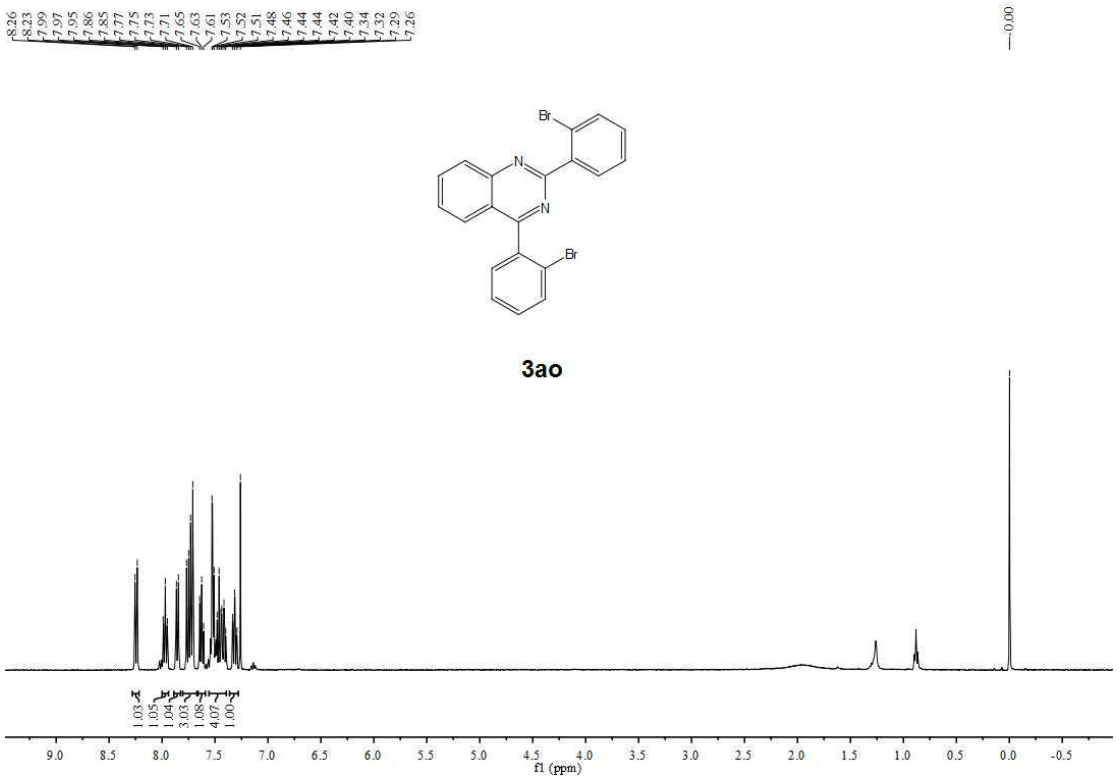

8.23
8.21
7.98
7.96
7.94
7.90
7.89
7.88
7.87
7.74
7.72
7.64
7.62
7.60
7.58
7.56
7.55
7.54
7.52
7.52
7.50
7.49
7.48
7.48
7.46
7.42
7.41
7.40
7.39
7.39
7.26
0.00
Cl
N
N
Cl

**3an**

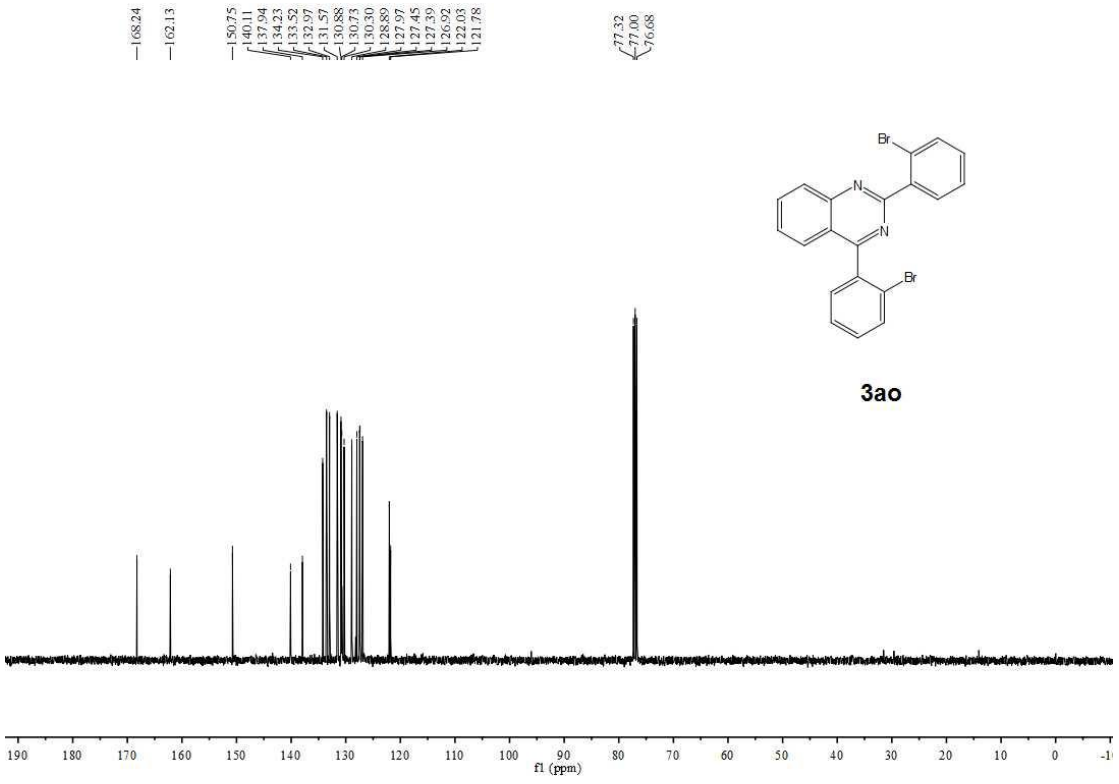

1.00
1.04
1.00
1.03
8.06
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


167.04
161.26
150.77
138.19
135.94
134.14
132.92
132.78
131.69
131.01
130.63
130.38
130.19
129.84
128.88
127.92
126.90
126.82
126.78
121.88
77.32
77.00
76.68
Cl
N
N
Cl
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

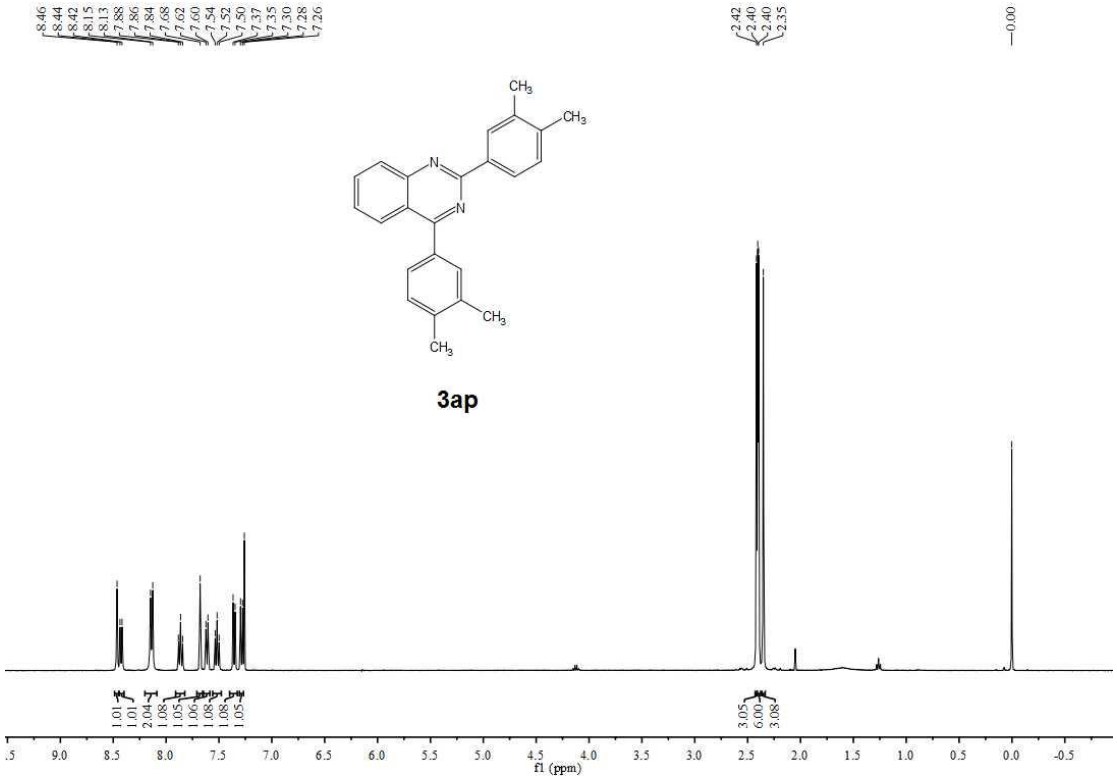
**3an**


8.26
8.23
7.99
7.97
7.95
7.86
7.85
7.77
7.75
7.73
7.71
7.65
7.63
7.61
7.53
7.52
7.51
7.48
7.46
7.44
7.44
7.42
7.40
7.34
7.32
7.29
7.26
0.00
Br
N
N
Br
1.03
1.05
1.04
3.03
1.08
4.07
1.00
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)

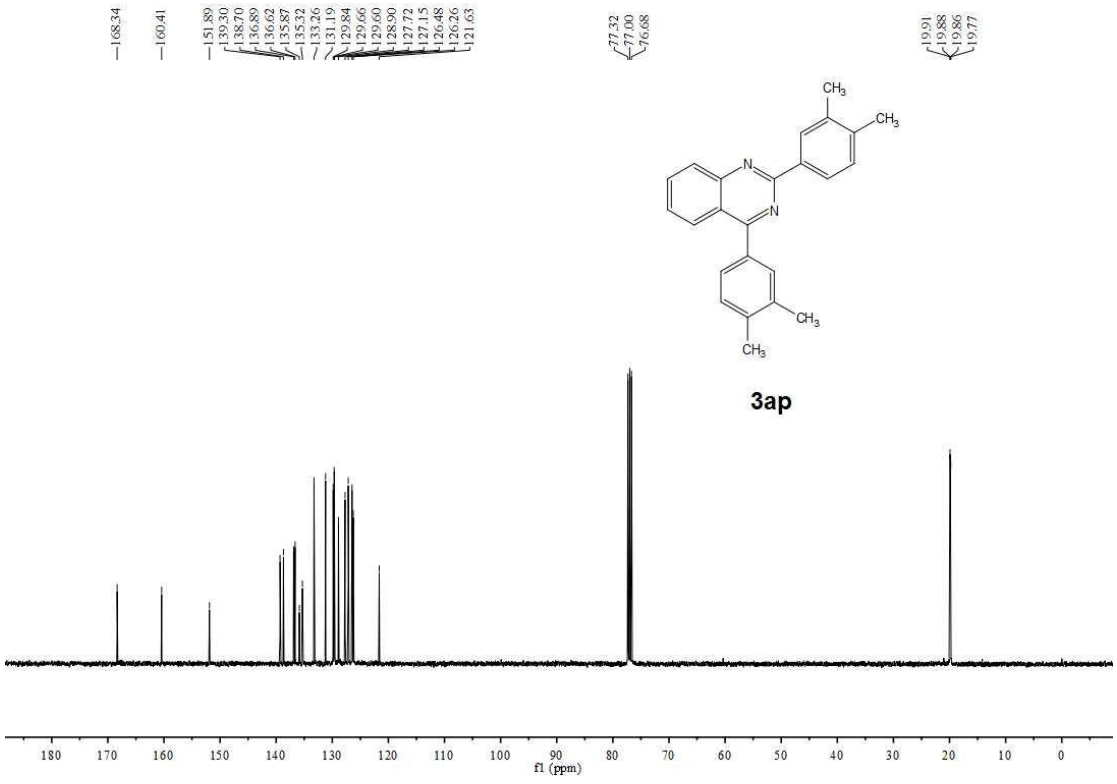
**3ao**


168.24
162.13
150.75
140.11
137.94
134.23
133.52
132.97
131.57
130.88
130.73
130.30
128.89
127.97
127.45
127.39
126.92
122.03
121.78
77.32
77.00
76.68
Br
N
N
Br
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

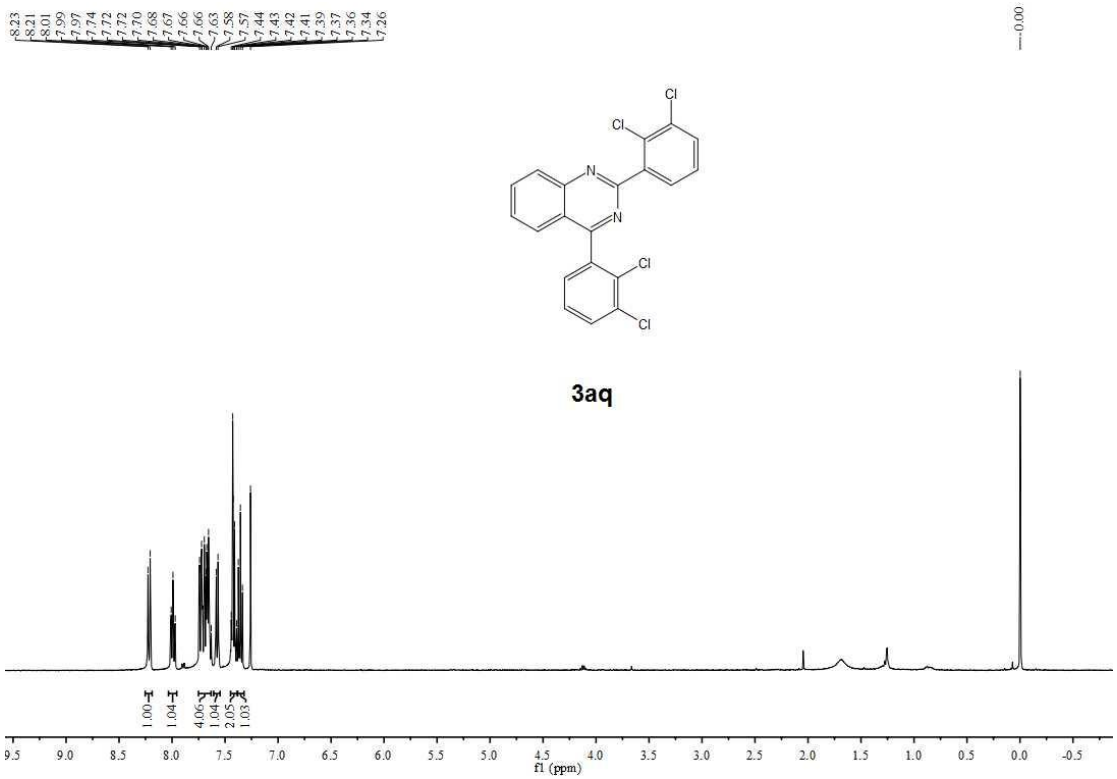
**3ao**

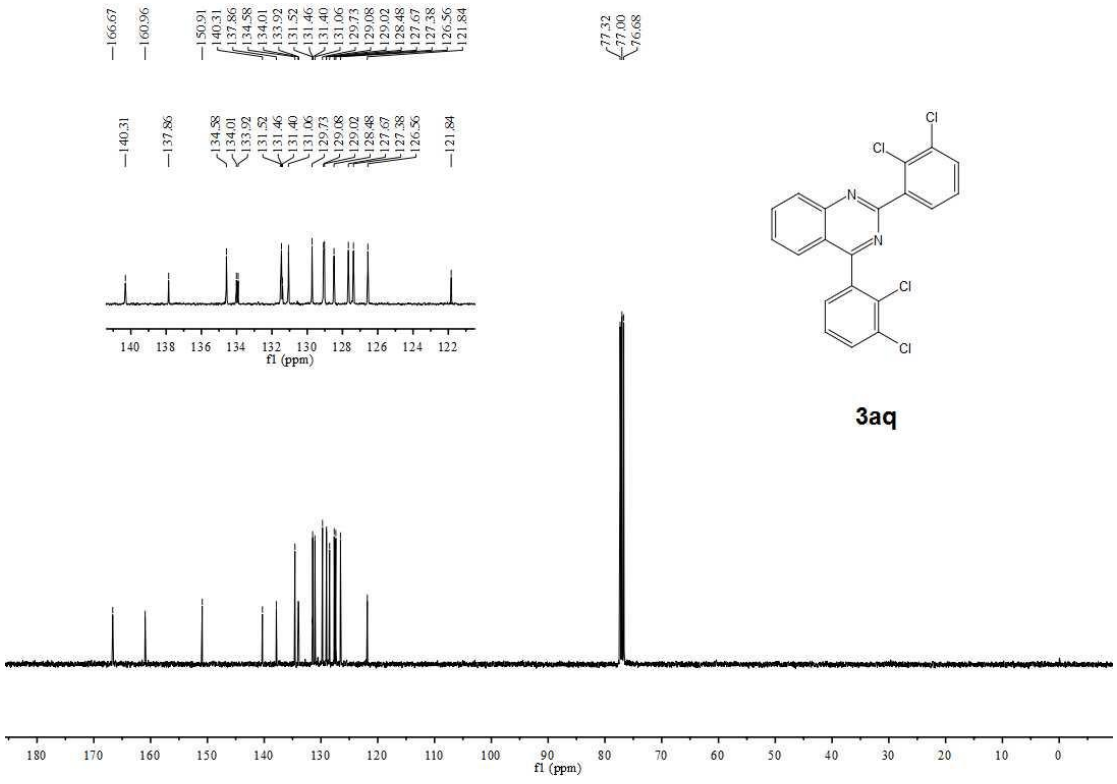

8.46
8.44
8.42
8.15
8.13
7.88
7.86
7.84
7.68
7.62
7.60
7.54
7.52
7.50
7.37
7.35
7.30
7.28
7.26
2.42
2.40
2.40
2.35
0.00
CH3
CH3
N
N
CH3
CH3
1.01
1.01
2.04
1.08
1.05
1.06
1.08
1.08
1.05
3.05
6.00
3.08
f1 (ppm)

**3ap**


168.34
160.41
151.89
139.30
138.70
136.89
136.62
135.87
135.32
133.26
131.19
129.84
129.66
129.60
128.90
127.72
127.15
126.48
126.26
121.63
77.32
77.00
76.68
19.91
19.88
19.86
19.77
CH3
CH3
N
N
CH3
CH3
f1 (ppm)

**3ap**


8.23
8.21
8.01
7.99
7.97
7.74
7.72
7.72
7.70
7.68
7.67
7.66
7.66
7.63
7.58
7.57
7.44
7.43
7.42
7.41
7.39
7.37
7.36
7.34
7.26
0.00
Cl
Cl
N
N
Cl
Cl
3aq
1.00
1.04
4.06
1.04
2.05
1.03
f1 (ppm)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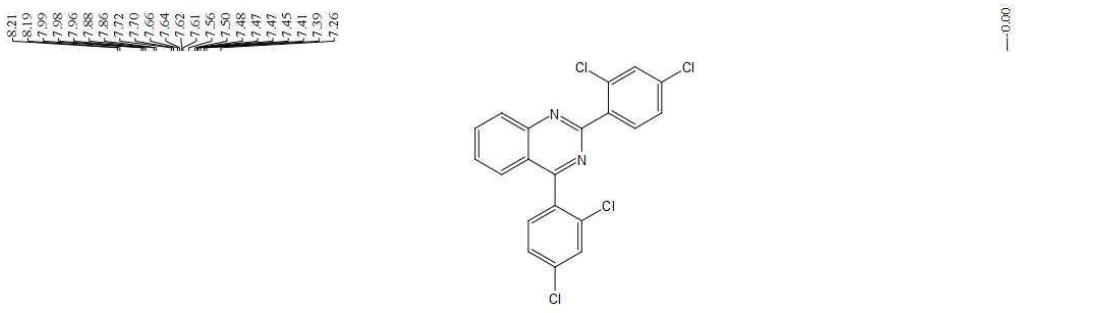
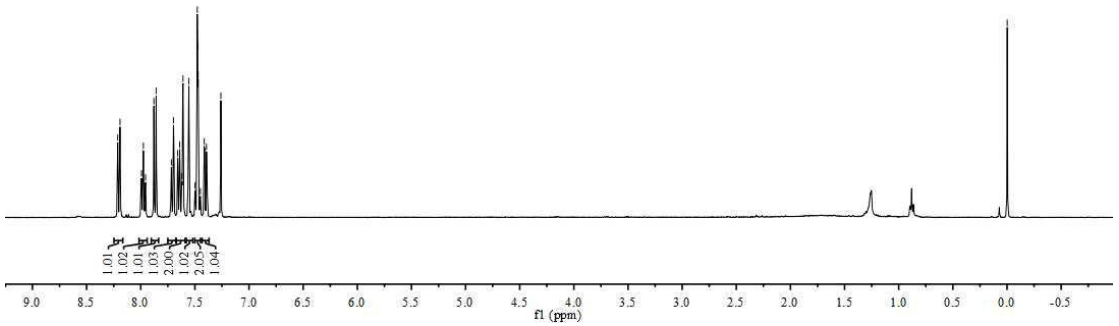
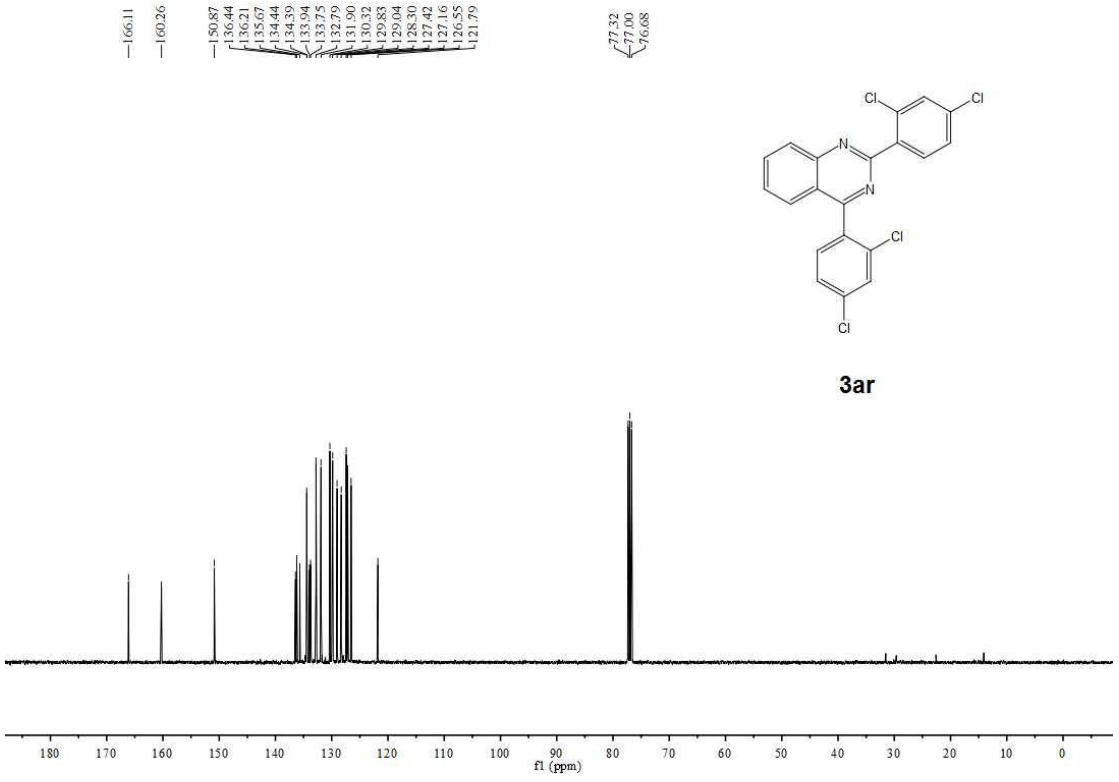
150.91
140.31
137.86
134.58
134.01
133.92
131.52
131.46
131.40
131.06
129.73
129.08
129.02
128.48
127.67
127.38
126.56
121.84
77.32
77.00
76.68
Cl
Cl
N
N
Cl
Cl
3aq
f1 (ppm)

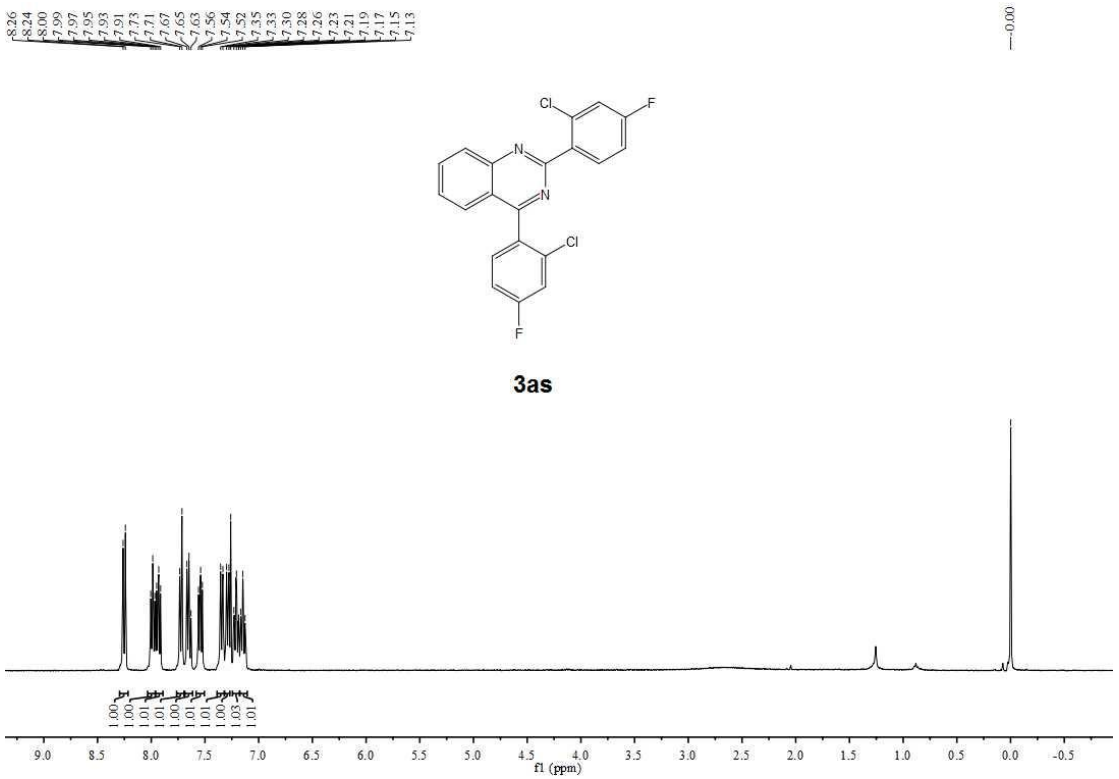

8.21
8.19
7.99
7.98
7.96
7.88
7.86
7.72
7.70
7.66
7.64
7.62
7.61
7.56
7.50
7.48
7.47
7.47
7.45
7.41
7.39
7.26
0.00
Cl
Cl
N
N
Cl
Cl

**3ar**

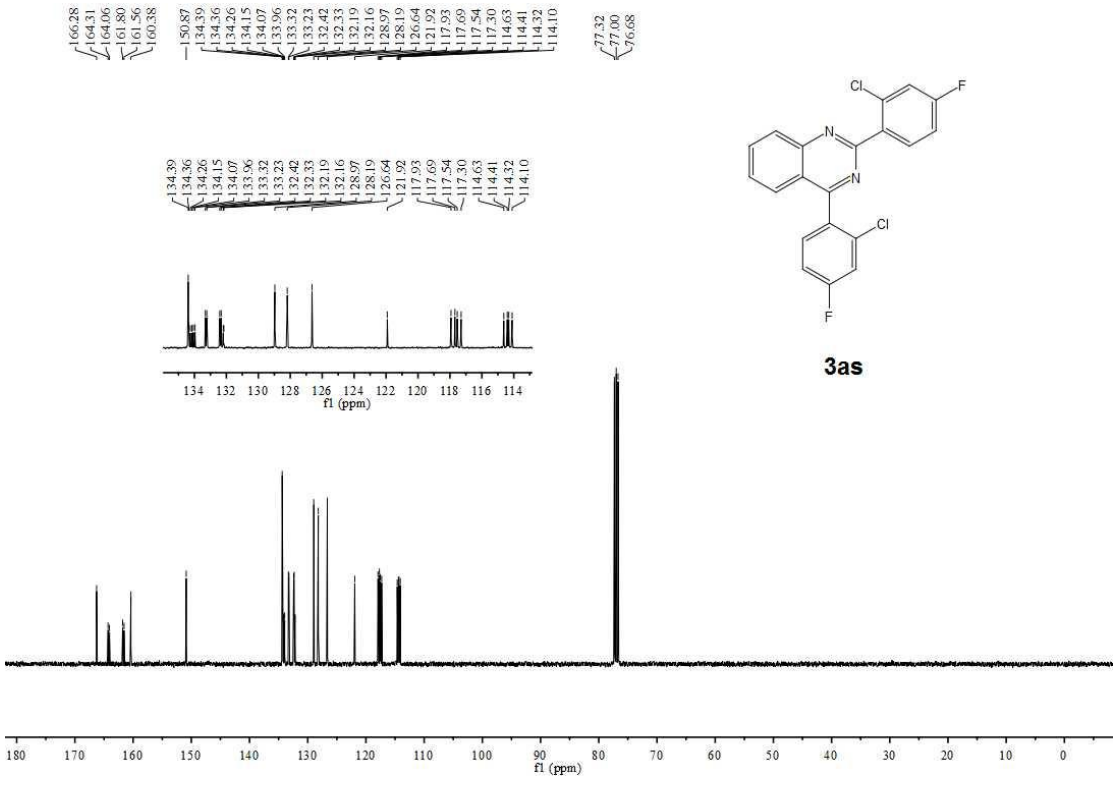

1.01
1.02
1.01
1.03
2.00
1.02
2.05
1.04
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


166.11
160.26
150.87
136.44
136.21
135.67
134.44
134.39
133.94
133.75
132.79
131.90
130.32
129.83
129.04
128.30
127.42
127.16
126.55
121.79
77.32
77.00
76.68
Cl
Cl
N
N
Cl
Cl
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

**3ar**

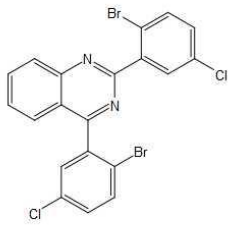

8.26
8.24
8.00
7.99
7.97
7.95
7.93
7.91
7.73
7.71
7.67
7.65
7.63
7.56
7.54
7.52
7.35
7.33
7.30
7.28
7.26
7.23
7.21
7.19
7.17
7.15
7.13
0.00
Cl
F
N
N
Cl
F
1.00
1.00
1.01
1.01
1.01
1.00
1.01
1.01
1.00
1.03
1.01
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

**3as**

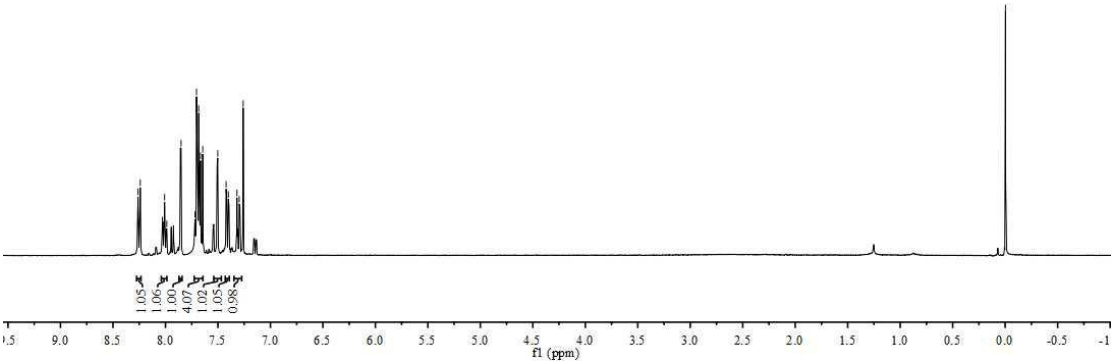

166.28
164.31
164.06
161.80
161.56
160.38
150.87
134.39
134.36
134.26
134.15
134.07
133.96
133.32
133.23
132.42
132.33
132.19
132.16
128.97
128.19
126.64
121.92
117.93
117.69
117.54
117.30
114.63
114.41
114.32
114.10
77.32
77.00
76.68
Cl
F
N
N
Cl
F
134 132 130 128 126 124 122 120 118 116 114
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

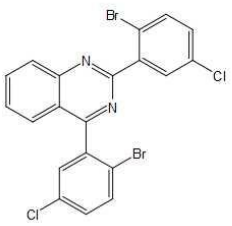
**3as**



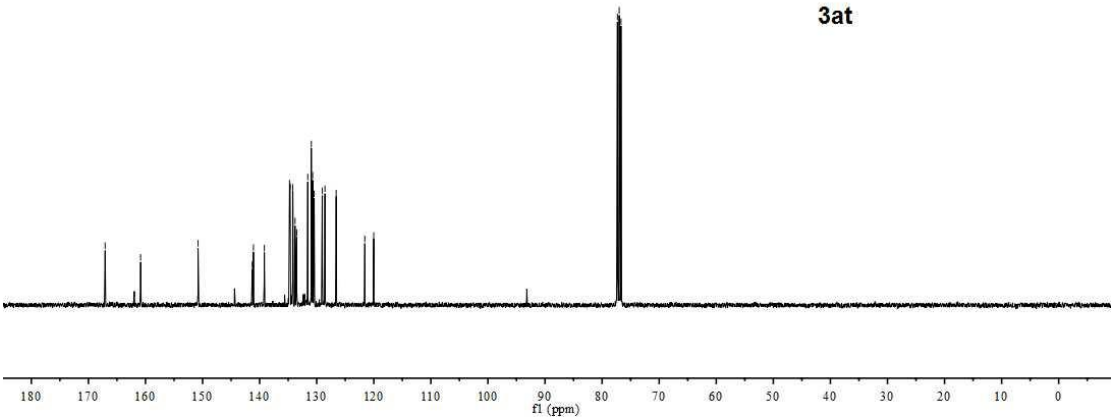

Br
N
Cl
N
Br
Cl

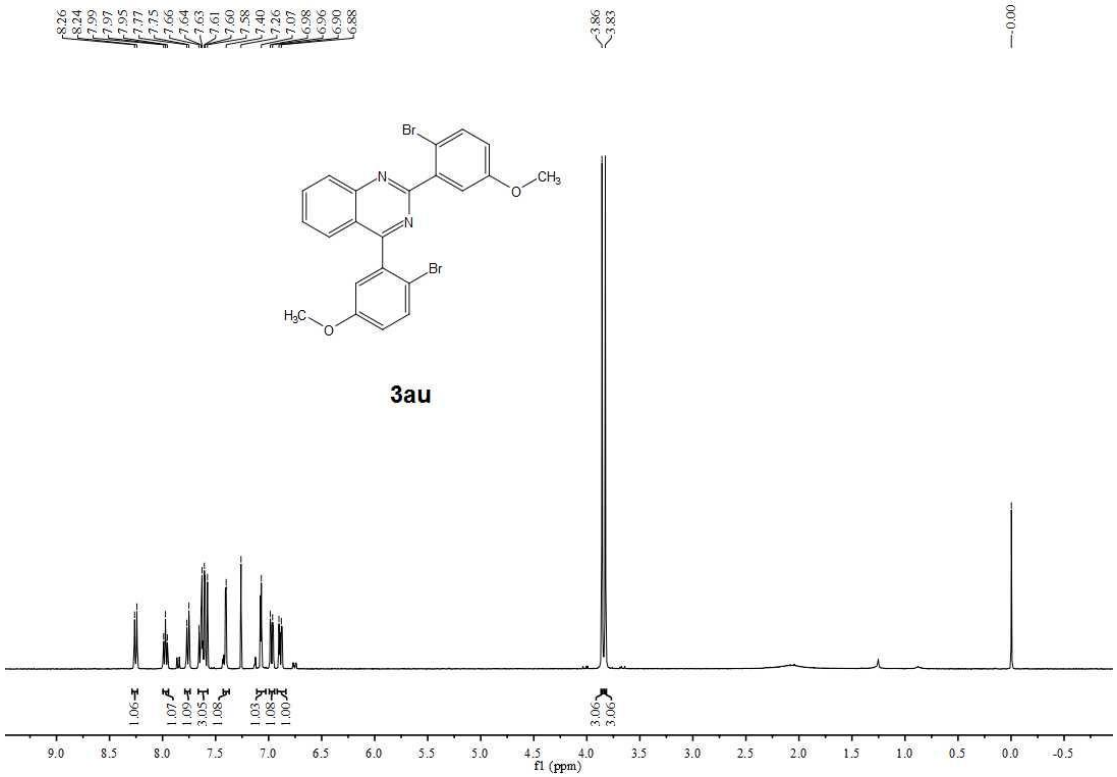
**3at**


1.05
1.06
1.00
4.07
1.02
1.05
0.98
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)

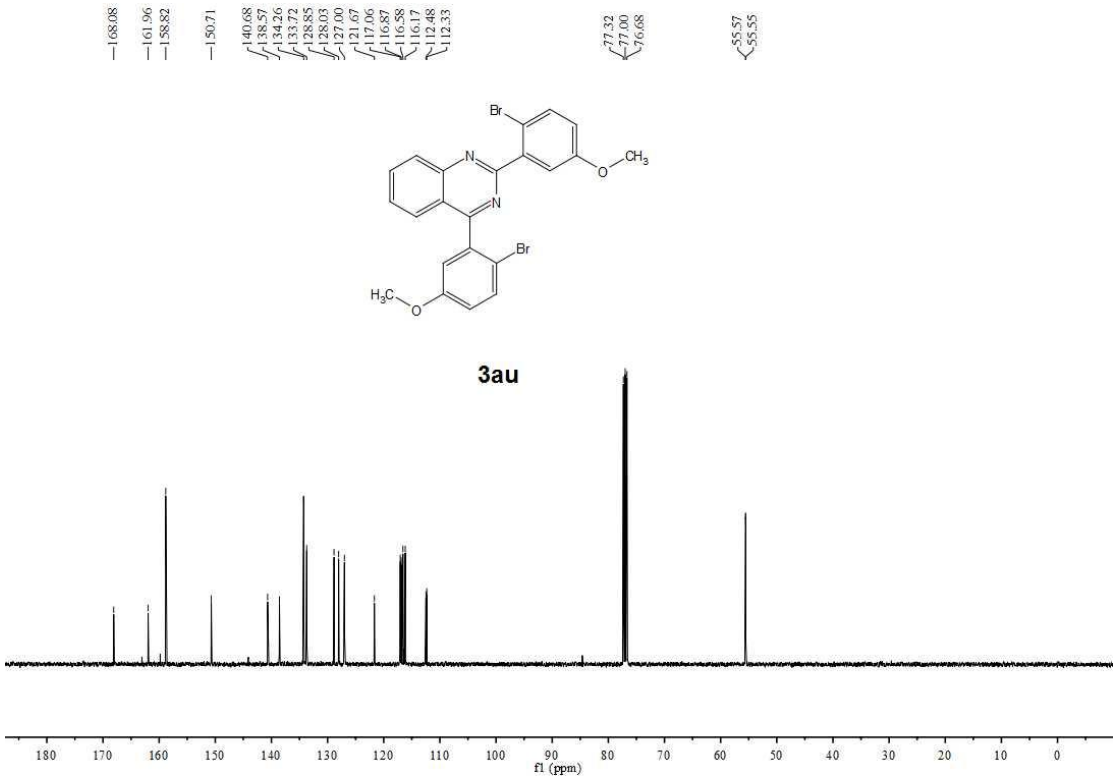

Br
N
Cl
N
Br
Cl

**3at**

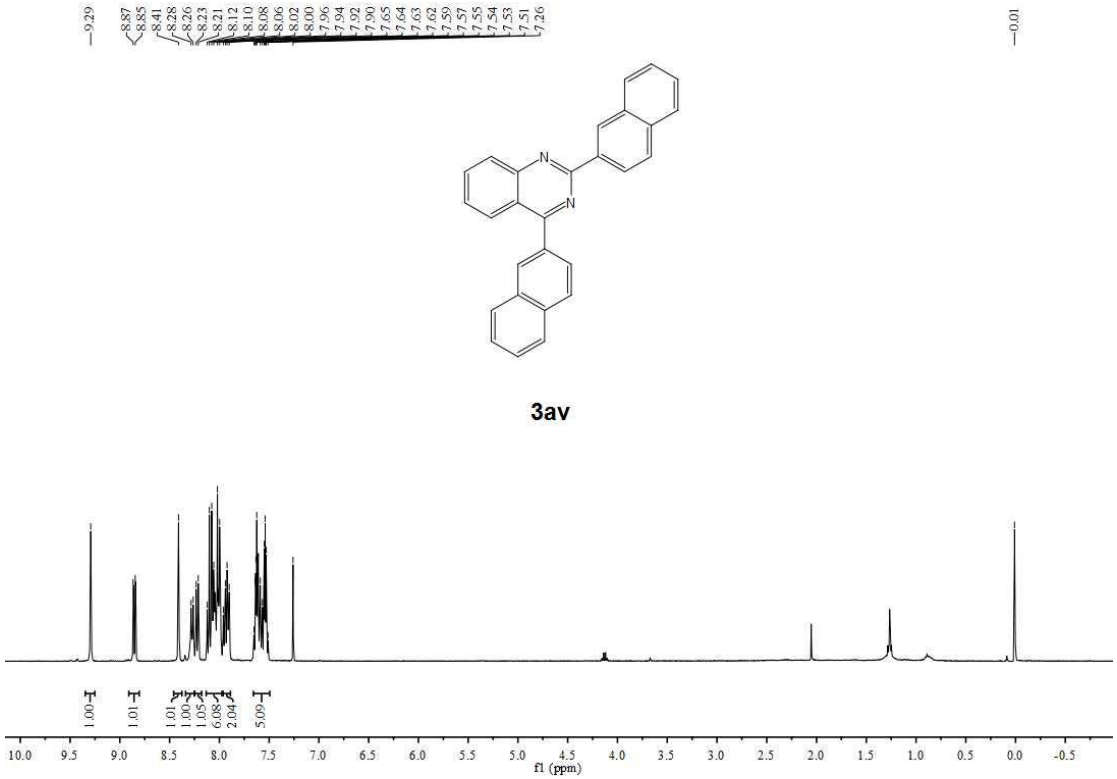

180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

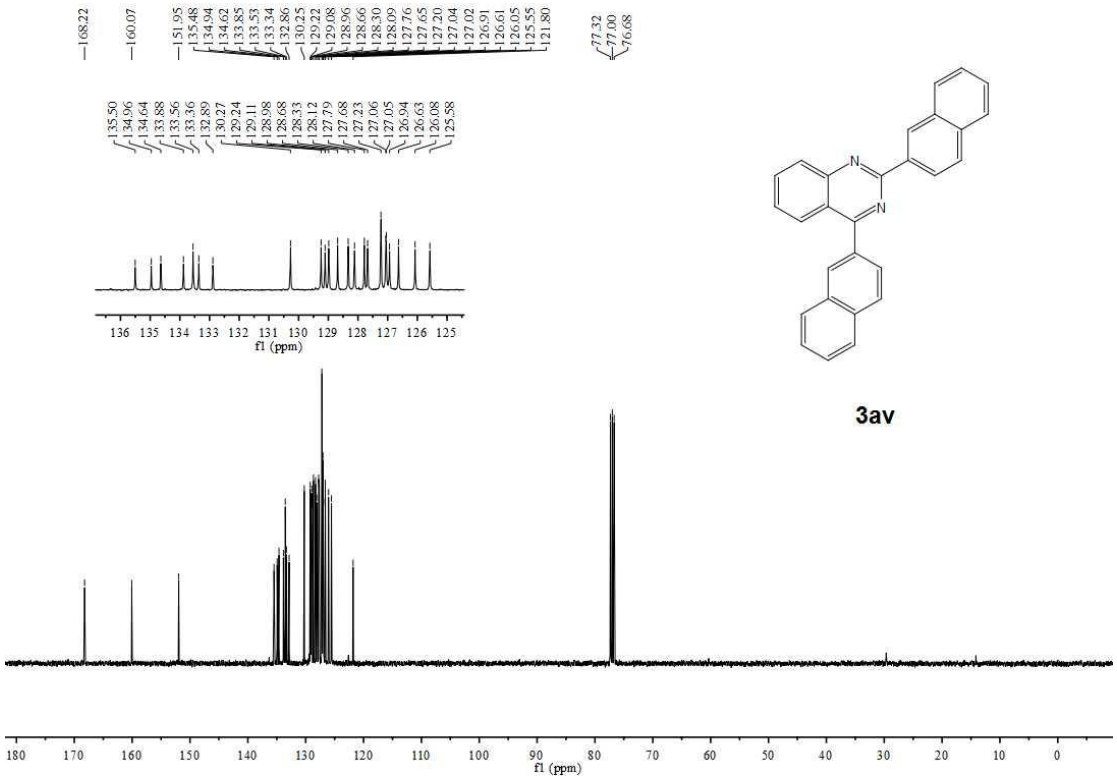

8.26
8.24
7.99
7.97
7.95
7.77
7.75
7.66
7.64
7.63
7.61
7.60
7.58
7.40
7.26
7.07
6.98
6.96
6.90
6.88
3.86
3.83
0.00
Br
N
O
CH3
N
Br
H3C
O
1.06
1.07
1.09
3.05
1.08
1.03
1.08
1.00
3.06
3.06
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

**3au**

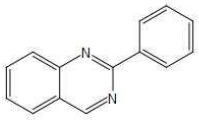

168.08
161.96
158.82
150.71
140.68
138.57
134.26
133.72
128.85
128.03
127.00
121.67
117.06
116.87
116.58
116.17
112.48
112.33
77.32
77.00
76.68
55.57
55.55
Br
N
O
CH3
N
Br
H3C
O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

**3au**

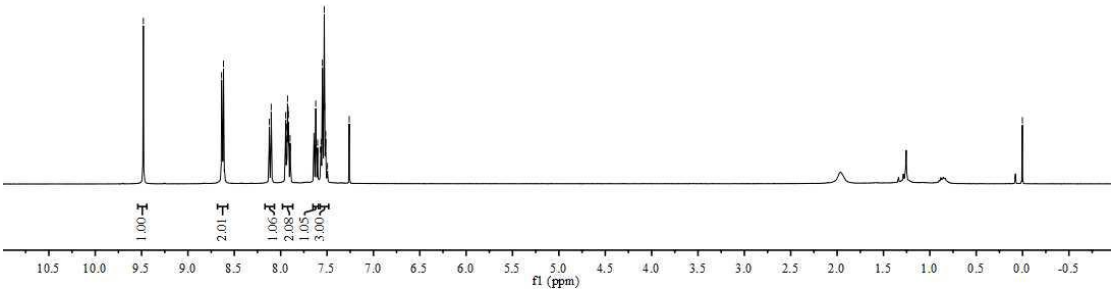

9.29
8.87
8.85
8.41
8.28
8.26
8.23
8.21
8.12
8.10
8.08
8.06
8.02
8.00
7.96
7.94
7.92
7.90
7.65
7.64
7.63
7.62
7.59
7.57
7.55
7.54
7.53
7.51
7.26
0.01
N
N
3av
1.00
1.01
1.01
1.00
1.05
6.08
2.04
5.09
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


168.22
160.07
151.95
135.48
134.94
134.62
133.85
133.53
133.34
132.86
130.25
129.22
129.08
128.96
128.66
128.30
128.09
127.76
127.65
127.20
127.04
127.02
126.91
126.61
126.05
125.55
121.80
77.32
77.00
76.68
135.50
134.96
134.64
133.88
133.56
133.36
132.89
130.27
129.24
129.11
128.98
128.68
128.33
128.12
127.79
127.68
127.23
127.06
127.05
126.94
126.63
126.08
125.58
136 135 134 133 132 131 130 129 128 127 126 125
f1 (ppm)
N
N
3av
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

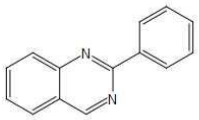

9.48
8.64
8.62
8.12
8.10
7.95
7.94
7.93
7.93
7.92
7.92
7.91
7.90
7.90
7.64
7.62
7.60
7.57
7.56
7.55
7.54
7.53
7.53
7.51
7.50
7.26
0.00



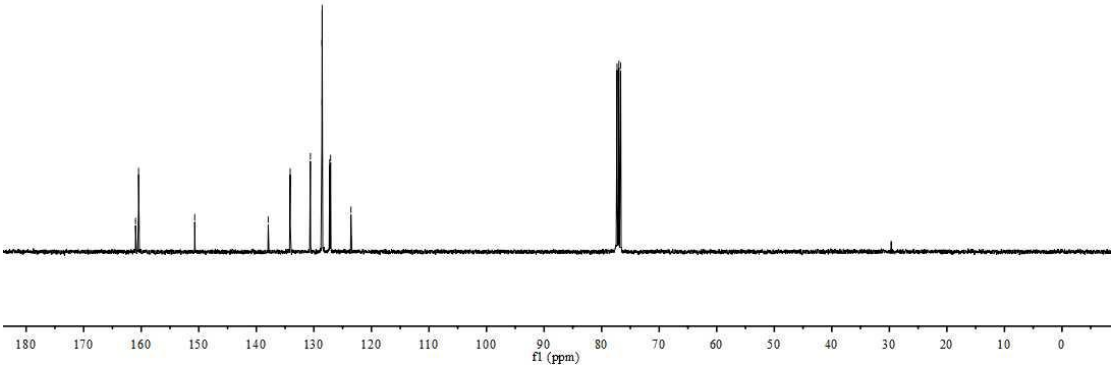
**6**


1.00
2.01
1.06
2.08
1.05
3.00
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
f1 (ppm)


160.99
160.46
150.70
137.93
134.11
130.60
128.61
128.58
128.56
127.25
127.09
123.56
77.32
77.00
76.68



**6**


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