Supporting Information

Access to Structurally Diverse Quinoline-Fused Heterocycles via Rhodium(III)-Catalyzed C-C/C-N Coupling of Bifunctional Substrates

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Contents

I. General Remarks

All commercially available chemicals were used as received without further purification, unless otherwise stated. All reactions were performed in a nitrogen-filled dry box. ^{1}H, ^{13}C, and ^{19}F NMR spectra were recorded on Bruker 400 MHz NMR spectrometer in the solvents indicated. HRMS were obtained on an Agilent Q-TOF 6540. Column chromatography was performed on silica gel (300-400 mesh) using ethyl acetate/petroleum ether as eluents. The indole substrates,[1] pyridone substrates,[2]and anthranils[3] were prepared according to literature reports.

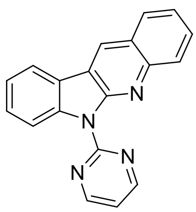
II. Experimental Information and Characterization Data

Representative procedures for the synthesis of product 3

N-pyrimidinylindole (0.2 mmol), $[Cp^*RhCl_2]_2$ (0.006 mmol), $AgSbF_6$ (0.04 mmol), and PivOH (0.4 mmol) were dissolved in MeOH (3 mL) in a pressure tube. The resulting mixture was stirred for seconds under N_2 atmosphere, to which was added anthranil (0.4 mmol). The mixture was stirred at 120 ^{o}C for 20 hours. After that, the solvent was removed under vacuum and the residue was purified by silica gel chromatography using ethyl acetate/petroleum ether/Et_3N (30:60:1) to afford product **3aa** as a yellow solid (92%).

Representative procedures for the synthesis of product 5

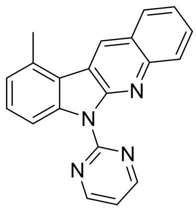
Pyridone (0.2 mmol), $[Cp^*RhCl_2]_2$ (0.006 mmol), $AgSbF_6$ (0.04 mmol), and PivOH (0.6 mmol) were dissolved in DCE (3 mL) in a pressure tube. The resulting mixture was stirred for seconds under N_2 atmosphere, to which was added anthranil (0.4 mmol). The mixture was stirred at 120 ^{o}C for 20 hours. After that, the solvent was removed under vacuum and the residue was purified by silica gel chromatography using ethyl acetate/petroleum ether (1:2) to afford product **5ag** as a white solid (95%).



3aa, 92%

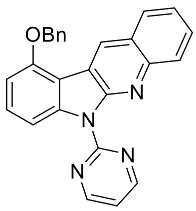
Product **3aa** was obtained as a yellow solid in 92% yield (54.5 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.06 (d, J = 4.8 Hz, 2H), 8.81 (s, 1H), 8.40 (d, J = 8.4 Hz, 1H), 8.29 (d, J = 8.5 Hz, 1H), 8.21 (d, J = 7.7 Hz, 1H), 8.06 (dd, J = 8.2, 1.4 Hz, 1H), 7.79 (ddd, J = 8.5, 6.8, 1.5 Hz, 1H), 7.63 (ddd, J = 8.5, 7.3, 1.3 Hz, 1H), 7.57 (ddd, J = 8.0, 6.8, 1.2 Hz, 1H), 7.46 (td, J = 7.5, 1.0

Hz, 1H), 7.34 (t, *J* = 4.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 158.6, 157.4, 152.0, 146.7, 140.6, 128.89, 128.85, 128.4, 128.1, 127.3, 125.4, 124.4, 122.5, 122.0, 120.9, 119.3, 118.1, 113.8.HRMS: m/z: $[M+H]^+$ calculated for $C_{19}H_{13}N_4$: 297.1140, found 297.1144.



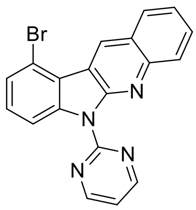
3ba, 84%

Product **3ba** was obtained as a yellow solid in 84% yield (52.1 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) *δ* 9.00 (d, *J* = 4.9 Hz, 2H), 8.81 (s, 1H), 8.18 (d, *J* = 8.5 Hz, 1H), 8.12 (d, *J* = 8.3 Hz, 1H), 8.01 (d, *J* = 8.1 Hz, 1H), 7.71 (ddd, *J* = 8.4, 6.8, 1.5 Hz, 1H), 7.50 (ddd, *J* = 8.0, 6.8, 1.2 Hz, 1H), 7.45 (t, *J* = 7.9 Hz, 1H), 7.30 (t, *J* = 4.8 Hz, 1H), 7.18 (d, *J* = 7.4 Hz, 1H), 2.94 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 158.7, 157.4, 152.0, 146.0, 140.7, 134.4, 129.7, 128.8, 128.7, 128.3, 128.1, 125.4, 124.3, 124.2, 120.3, 119.9, 118.3, 110.9, 21.0. HRMS: m/z: $[M+H]^+$ calculated for $C_{20}H_{15}N_4$: 311.1297, found 311.1293.



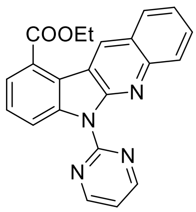
3ca, 94%

Product **3ca** was obtained as a yellow solid in 94% yield (75.6 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) *δ* 8.97 (s, 2H), 8.95 (s, 1H), 8.19 (d, *J* = 8.5 Hz, 1H), 7.92 (d, *J* = 7.2 Hz, 1H), 7.90 (d, *J* = 8.3 Hz, 1H), 7.68 (ddd, *J* = 8.4, 6.7, 1.5 Hz, 1H), 7.62 – 7.55 (m, 2H), 7.51 – 7.33 (m, 5H), 7.24 (t, *J* = 4.8 Hz, 1H), 6.90 (d, *J* = 8.2 Hz, 1H), 5.37 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 157.5, 155.6, 151.7, 146.1, 141.9, 136.9, 130.2, 129.2, 128.82, 128.77, 128.6, 128.3, 128.2, 127.5, 125.7, 124.2, 118.5, 118.2, 111.2, 106.7, 105.2, 70.4. HRMS: m/z: $[M+H]^+$ calculated for $C_{26}H_{19}N_4O$: 403.1559, found 403.1563.



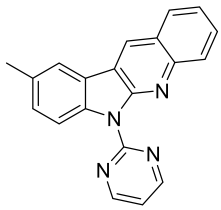
3da, 79%

Product **3da** was obtained as a yellow solid in 79% yield (59.3 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.57 (s, 1H), 9.08 (d, J = 4.8 Hz, 2H), 8.29 (d, J = 8.3 Hz, 1H), 8.24 (d, J = 8.5 Hz, 1H), 8.13 (d, J = 8.2 Hz, 1H), 7.81 (ddd, J = 8.4, 6.8, 1.5 Hz, 1H), 7.65 – 7.56 (m, 2H), 7.45 (t, J = 8.1 Hz, 1H), 7.40 (t, J = 4.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 157.0, 151.5, 146.6, 141.8, 130.6, 129.4, 128.7, 128.62, 128.60, 126.5, 125.0, 124.5, 120.8, 118.6, 117.5, 112.2. One signal is missing due to overlap. HRMS: m/z: $[M+H]^+$ calculated for $C_{19}H_{12}N_4Br$: 375.0245, found 375.0245.



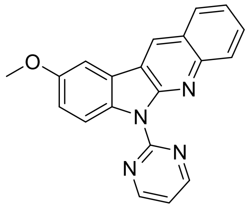
3ea, 74%

Product **3ea** was obtained as a yellow solid in 74% yield (54.5 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.85 (s, 1H), 9.02 (d, J = 4.8 Hz, 2H), 8.41 (dd, J = 8.3, 1.1 Hz, 1H), 8.14 (d, J = 8.6 Hz, 1H), 8.11 (d, J = 8.3 Hz, 1H), 8.04 (d, J = 7.7 Hz, 1H), 7.73 (ddd, J = 8.4, 6.7, 1.5 Hz, 1H), 7.58 (t, J = 8.0 Hz, 1H), 7.51 (ddd, J = 8.1, 6.8, 1.2 Hz, 1H), 7.35 (t, J = 4.8 Hz, 1H), 4.11 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.7, 158.8, 157.0, 151.9, 146.8, 141.4, 135.1, 129.7, 129.3, 128.3, 127.2, 126.0, 125.5, 125.3, 124.2, 121.5, 118.8, 117.5, 117.1, 52.5. HRMS: m/z: $[M+H]^+$ calculated for $C_{21}H_{15}N_4O_2$: 355.1195, found 355.1196.



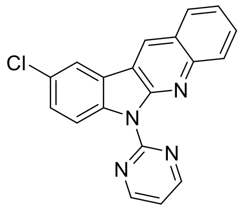
3fa, 81%

Product **3fa** was obtained as a yellow solid in 81% yield (50.2 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.81 (s, 2H), 8.75 (s, 1H), 8.20 (t, J = 8.4 Hz, 2H), 8.15 (d, J = 7.6 Hz, 1H), 7.98 (d, J = 8.0 Hz, 1H), 7.70 (ddd, J = 8.3, 6.7, 1.5 Hz, 1H), 7.54 (t, J = 7.7 Hz, 1H), 7.49 (t, J = 7.4 Hz, 1H), 7.38 (t, J = 7.5 Hz, 1H), 2.40 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 155.4, 152.1, 146.80, 140.76, 128.9, 128.8, 128.4, 128.1, 127.7, 127.4, 125.2, 124.2, 122.3, 121.8, 121.0, 119.2, 113.4, 15.4. HRMS: m/z: $[M+H]^+$ calculated for $C_{20}H_{15}N_4$: 311.1297, found 311.1295.



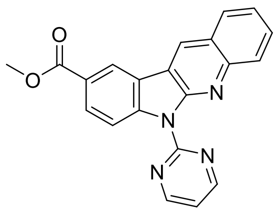
3ga, 85%

Product **3ga** was obtained as a yellow solid in 85% yield (55.4 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.97 (d, J = 4.8 Hz, 2H), 8.72 (s, 1H), 8.33 (d, J = 9.1 Hz, 1H), 8.21 (d, J = 8.6 Hz, 1H), 7.98 (d, J = 8.2 Hz, 1H), 7.71 (ddd, J = 8.4, 6.7, 1.5 Hz, 1H), 7.63 (d, J = 2.6 Hz, 1H), 7.50 (ddd, J = 8.0, 6.8, 1.2 Hz, 1H), 7.25 (t, J = 4.9 Hz, 1H), 7.16 (dd, J = 9.0, 2.7 Hz, 1H), 3.94 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.6, 157.5, 155.8, 152.3, 146.8, 134.9, 129.0, 128.9, 128.1, 127.3, 125.1, 124.4, 122.9, 119.5, 117.7, 116.2, 115.3, 104.4, 56.0. HRMS: m/z: $[M+H]^+$ calculated for $C_{20}H_{15}N_4O$: 327.1246, found 327.1246.



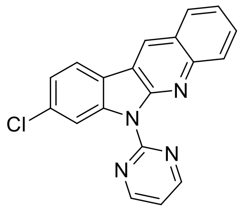
3ha, 80%

Product **3ha** was obtained as a yellow solid in 80% yield (52.8 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.98 (d, J = 4.8 Hz, 2H), 8.67 (s, 1H), 8.27 (d, J = 8.8 Hz, 1H), 8.19 (d, J = 8.5 Hz, 1H), 8.06 (s, 1H), 7.95 (d, J = 8.2 Hz, 1H), 7.72 (t, J = 7.7 Hz, 1H), 7.58 – 7.40 (m, 2H), 7.29 (t, J = 4.8 Hz, 1H).^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 157.2, 151.9, 147.0, 138.8, 129.4, 128.9, 128.3, 128.2, 128.0, 127.9, 125.2, 124.7, 123.3, 120.7, 118.2, 115.3. One signal is missing due to overlap. HRMS: m/z: $[M+H]^+$ calculated for $C_{19}H_{12}N_4Cl$: 331.0750, found 331.0755.



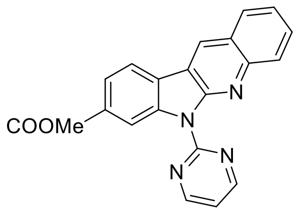
3ia, 86%

Product **3ia** was obtained as a yellow solid in 86% yield (60.9 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.01 (d, J = 4.8 Hz, 2H), 8.82 (d, J = 15.0 Hz, 2H), 8.29 (d, J = 8.7 Hz, 1H), 8.23 (d, J = 8.8 Hz, 1H), 8.19 (d, J = 8.5 Hz, 1H), 8.00 (d, J = 8.1 Hz, 1H), 7.73 (t, J = 7.7 Hz, 1H), 7.52 (t, J = 7.5 Hz, 1H), 7.35 (t, J = 4.8 Hz, 1H), 3.98 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.0, 158.8, 157.0, 152.3, 146.9, 143.5, 129.9, 129.3, 128.9, 128.3, 128.1, 125.4, 124.8, 124.3, 122.9, 121.9, 118.7, 118.6, 113.4, 52.2. HRMS: m/z: $[M+H]^+$ calculated for $C_{21}H_{15}N_4O_2$: 355.1195, found 355.1200.



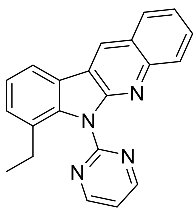
3ja, 73%

Product **3ja** was obtained as a yellow solid in 73% yield (48.2 mg). ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.30 – 8.96 (m, 3H), 8.34 (d, J = 8.0 Hz, 1H), 8.23 – 8.06 (m, 2H), 7.99 (d, J = 8.4 Hz, 1H), 7.84 – 7.69 (m, 1H), 7.68 – 7.51 (m, 2H), 7.46 (d, J = 8.1 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 159.8, 156.4, 151.8, 146.5, 141.2, 133.3, 130.0, 129.1, 128.9, 128.3, 125.4, 124.9, 123.5, 122.9, 120.4, 120.1, 117.8, 113.2. HRMS: m/z: $[M+H]^+$ calculated for $C_{19}H_{12}N_4Cl$: 331.0750, found 331.0751.



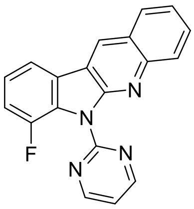
3ka, 90%

Product **3ka** was obtained as a yellow solid in 90% yield (63.7 mg). ^{1}H NMR (400 MHz, Chloroform-d) δ 9.04 (d, J = 4.9 Hz, 2H), 8.9 (s, 1H), 8.76 (s, 1H), 8.20 (d, J = 8.5 Hz, 1H), 8.14 (d, J = 8.0 Hz, 1H), 8.06 (dd, J = 8.0, 1.4 Hz, 1H), 7.96 (d, J = 8.2 Hz, 1H), 7.73 (ddd, J = 8.4, 6.8, 1.4 Hz, 1H), 7.49 (t, J = 7.0 Hz, 1H), 7.34 (t, J = 4.9 Hz, 1H), 3.97 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.1, 158.8, 157.1, 152.4, 147.3, 140.1, 129.7, 129.6, 128.9, 128.8, 128.3, 125.8, 125.2, 124.7, 123.8, 120.6, 118.4, 118.2, 115.2, 52.3. HRMS: m/z: $[M+H]^+$ calculated for $C_{21}H_{15}N_4O_2$: 355.1195, found 355.1193.



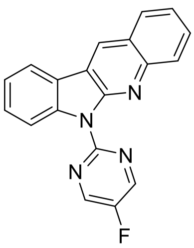
3la, 86%

Product **3la** was obtained as a yellow solid in 86% yield (55.7 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.97 (dd, J = 4.9, 2.2 Hz, 2H), 8.71 (s, 1H), 8.08 – 7.99 (m, 2H), 7.95 (d, J = 8.2 Hz, 1H), 7.63 (ddd, J = 8.5, 6.7, 1.5 Hz, 1H), 7.43 (ddd, J = 8.0, 6.7, 1.2 Hz, 1H), 7.40 – 7.29 (m, 3H), 2.35 (q, J = 7.5 Hz, 2H), 1.06 (t, J = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0, 158.5, 154.2, 146.9, 139.9, 129.1, 128.7, 128.7, 128.6, 128.2, 127.4, 125.3, 123.9, 122.7, 122.4, 119.9, 119.2, 119.1, 25.7, 13.9. HRMS: m/z: $[M+H]^+$ calculated for $C_{21}H_{17}N_4$: 325.1453, found 325.1457.



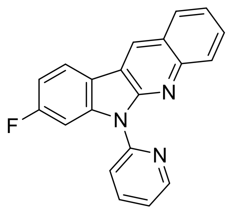
3ma, 88%

Product **3ma** was obtained as a yellow solid in 88% yield (55.3 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.99 (d, J = 4.9 Hz, 2H), 8.74 (s, 1H), 8.12 (d, J = 8.5 Hz, 1H), 7.97 (d, J = 8.2 Hz, 1H), 7.92 (d, J = 7.1 Hz, 1H), 7.68 (t, J = 7.7 Hz, 1H), 7.47 (t, J = 7.5 Hz, 1H), 7.37 (t, J = 4.9 Hz, 1H), 7.33 – 7.20 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 156.7, 152.6, 149.5 (J = 246.6 Hz), 147.1, 129.2, 128.7, 128.5 (J = 9.2 Hz), 128.4, 128.3, 125.22, 125.19, 124.4, 122.6(J = 6.6 Hz), 119.6, 118.6 (J = 2.3 Hz), 117.0 (J = 3.6 Hz), 115.5 (J = 19.0 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -122.1. HRMS: m/z: $[M+H]^+$ calculated for $C_{19}H_{12}N_4F$: 315.1046, found 315.1046.



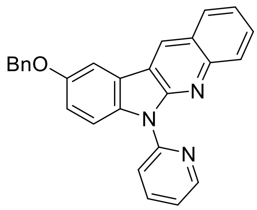
3na, 90%

Product **3na** was obtained as a yellow solid in 90% yield (56.5 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.85 (s, 2H), 8.73 (s, 1H), 8.21 – 8.15 (m, 2H), 8.13 (d, J = 7.6 Hz, 1H), 7.98 (d, J = 8.2 Hz, 1H), 7.71 (ddd, J = 8.4, 6.8, 1.5 Hz, 1H), 7.54 (ddd, J = 8.4, 7.3, 1.3 Hz, 1H), 7.49 (ddd, J = 8.1, 6.8, 1.2 Hz, 1H), 7.38 (td, J = 7.5, 1.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.3 (J = 260.9 Hz), 153.2 (J = 3.4 Hz), 151.9, 146.6 (J = 21.6 Hz), 146.3, 140.5, 129.0, 128.9, 128.5, 128.2, 127.5, 125.3, 124.5, 122.7, 121.9, 121.1, 119.2, 113.3. ^{19}F NMR (376 MHz, $CDCl_3$) δ -141.5. HRMS: m/z: $[M+H]^+$ calculated for $C_{19}H_{12}N_4F$: 315.1046, found 315.1042.



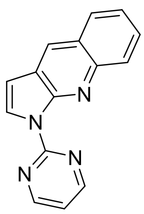
3oa, 71%

Product **3oa** was obtained as a yellow solid in 71% yield (44.6 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.65 (dd, J = 5.0, 1.9 Hz, 1H), 8.58 (d, J = 8.1 Hz, 2H), 8.15 (dd, J = 10.6, 2.4 Hz, 1H), 8.07 (d, J = 8.5 Hz, 1H), 8.01 (dd, J = 8.5, 5.5 Hz, 1H), 7.98 – 7.91 (m, 2H), 7.68 (ddd, J = 8.4, 6.7, 1.5 Hz, 1H), 7.47 (ddd, J = 8.1, 6.7, 1.2 Hz, 1H), 7.28 (dd, J = 6.8, 5.0 Hz, 1H), 7.06 (td, J = 8.8, 2.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.1(J = 244.0 Hz), 152.1, 151.0, 148.2, 145.9, 142.0 (J = 12.9 Hz), 138.1, 128.9, 128.22, 128.15, 126.7 (J = 1.8 Hz), 125.0, 124.2, 121.9(J = 10.2 Hz), 121.2, 119.8, 118.5 (J = 0.7 Hz), 117.7 (J = 2.1 Hz), 109.6 (J = 24.0 Hz), 101.8 (J = 28.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -110.3. HRMS: m/z: $[M+H]^+$ calculated for $C_{20}H_{14}N_3F$: 314.1094, found 314.1096.



3pa, 95%

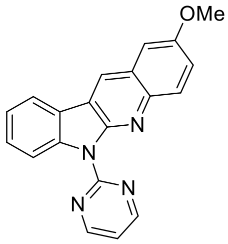
Product **3pa** was obtained as a yellow solid in 95% yield (76.2 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.92 (s, 1H), 8.65 (dd, J = 4.9, 1.9 Hz, 1H), 8.49 (d, J = 8.2 Hz, 1H), 8.07 (d, J = 8.4 Hz, 1H), 7.99 – 7.88 (m, 3H), 7.65 (ddd, J = 8.4, 6.8, 1.5 Hz, 1H), 7.61 – 7.55 (m, 2H), 7.49 – 7.35 (m, 5H), 7.26 (dd, J = 7.3, 4.9 Hz, 1H), 6.85 (d, J = 8.1 Hz, 1H), 5.37 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.6, 151.5, 151.2, 148.4, 145.7, 142.5, 138.0, 137.1, 130.0, 129.2, 128.8, 128.6, 128.5, 128.2, 128.1, 127.5, 125.4, 123.7, 121.2, 120.4, 118.3, 110.7, 106.6, 104.6, 70.3. HRMS: m/z: $[M+H]^+$ calculated for $C_{27}H_{20}N_3O$: 402.1606, found 402.1603.



3qa, 71%

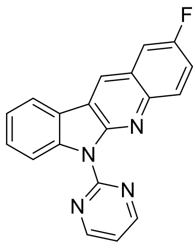
Product **3qa** was obtained as a yellow solid in 71% yield (34.9 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.87 (d, J = 4.8 Hz, 2H), 8.47 (d, J = 4.2 Hz, 1H), 8.39 (s, 1H), 8.29 (d, J = 8.6

Hz, 1H), 7.93 (d, J = 8.1 Hz, 1H), 7.69 (ddd, J = 8.4, 6.7, 1.5 Hz, 1H), 7.49 (ddd, J = 8.1, 6.8, 1.2 Hz, 1H), 7.17 (t, J = 4.8 Hz, 1H), 6.79 (d, J = 4.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.8, 156.9, 149.0, 145.6, 130.7, 129.5, 128.10, 128.05, 127.8, 125.4, 124.4, 117.1, 104.2.One signal is missing due to overlap. HRMS: m/z: $[M+H]^+$ calculated for $C_{15}H_{11}N_4$: 247.0984, found 247.0989.



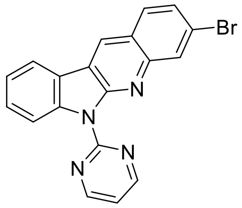
3ab, 89%

Product **3ab** was obtained as a yellow solid in 89% yield (58.0 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.97 (d, J = 4.8 Hz, 2H), 8.64 (s, 1H), 8.36 (d, J = 8.3 Hz, 1H), 8.12 (s, 1H), 8.10 (d, J = 2.1 Hz, 1H), 7.54 (t, J = 7.4 Hz, 1H), 7.41 – 7.35 (m, 2H), 7.25 (t, J = 3.9 Hz, 2H), 3.93 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.6, 157.5, 156.3, 150.8, 142.7, 140.5, 130.3, 128.4, 126.1, 122.5, 122.0, 121.6, 120.9, 119.5, 117.9, 114.0, 105.6, 55.5. One signal is missing due to overlap. HRMS: m/z: $[M+H]^+$ calculated for $C_{20}H_{15}N_4O$: 327.1246, found 327.1243.



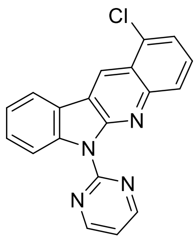
3ac, 95%

Product **3ac** was obtained as a yellow solid in 95% yield (59.7 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.98 (d, J = 4.9 Hz, 2H), 8.65 (s, 1H), 8.33 (d, J = 8.3 Hz, 1H), 8.18 (dd, J = 9.3, 5.3 Hz, 1H), 8.11 (d, J = 7.6 Hz, 1H), 7.62 – 7.53 (m, 2H), 7.52 – 7.44 (m, 1H), 7.38 (t, J = 7.4 Hz, 1H), 7.28 (t, J = 4.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.2 (J = 243.5 Hz), 158.7, 157.3, 151.7 (J = 2.2 Hz), 143.6, 140.7, 131.0 (J = 9.0 Hz), 128.8, 126.5 (J = 5.3 Hz), 125.6 (J = 9.7 Hz), 122.7, 121.5, 121.2, 120.0, 119.0 (J = 25.5 Hz), 118.1, 114.0, 110.9 (J = 21.7 Hz). HRMS: m/z: $[M+H]^+$ calculated for $C_{19}H_{12}N_4F$: 315.1046, found 315.1042.



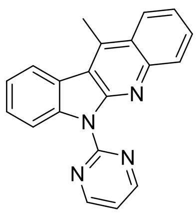
3ad, 79%

Product **3ad** was obtained as a yellow solid in 79% yield (59.3 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.01 (d, J = 4.8 Hz, 2H), 8.70 (s, 1H), 8.39 (s, 1H), 8.30 (d, J = 8.4 Hz, 1H), 8.13 (d, J = 7.7 Hz, 1H), 7.84 (d, J = 8.7 Hz, 1H), 7.68 – 7.52 (m, 2H), 7.40 (t, J = 7.6 Hz, 1H), 7.33 (t, J = 4.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.6, 157.2, 152.3, 147.2, 140.7, 131.1, 129.1, 128.7, 127.8, 127.1, 123.8, 122.9, 122.7, 121.6, 121.0, 119.6, 118.3, 113.8. HRMS: m/z: $[M+H]^+$ calculated for $C_{19}H_{12}N_4Br$: 375.0245, found 375.0250.



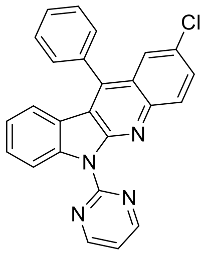
3ae, 62%

Product **3ae** was obtained as a yellow solid in 62% yield (40.9 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.20 (s, 1H), 9.07 – 8.95 (m, 2H), 8.34 (d, J = 8.3 Hz, 1H), 8.24 (d, J = 7.7 Hz, 1H), 8.13 (dd, J = 7.3, 2.3 Hz, 1H), 7.66 – 7.57 (m, 3H), 7.44 (t, J = 7.5 Hz, 1H), 7.33 (t, J = 4.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 157.3, 152.2, 147.4, 140.8, 131.5, 128.9, 128.4, 128.2, 124.6, 124.3, 123.4, 122.9, 121.8, 121.4, 120.2, 118.3, 114.0. HRMS: m/z: $[M+H]^+$ calculated for $C_{19}H_{12}N_4Cl$: 331.0750, found 331.0752.



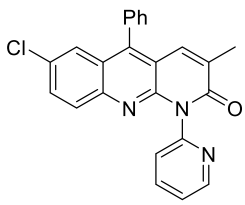
3af, 82%

Product **3af** was obtained as a yellow solid in 82% yield (50.8 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.00 (d, J = 4.8 Hz, 2H), 8.29 (d, J = 8.3 Hz, 1H), 8.27 (d, J = 8.6 Hz, 1H), 8.24 (d, J = 8.5 Hz, 1H), 8.17 (d, J = 8.5Hz, 1H), 7.70 (ddd, J = 8.3, 6.7, 1.4 Hz, 1H), 7.57 – 7.48 (m, 2H), 7.40 (t, J = 7.5 Hz, 1H), 7.29 (t, J = 4.8 Hz, 1H), 3.20 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 157.3, 151.6, 146.4, 140.5, 139.3, 129.4, 128.6, 127.6, 125.3, 124.0, 123.7, 123.5, 123.0, 122.4, 118.3, 117.2, 113.2, 15.2. HRMS: m/z: $[M+H]^+$ calculated for $C_{20}H_{15}N_4$: 311.1297, found 311.1296.



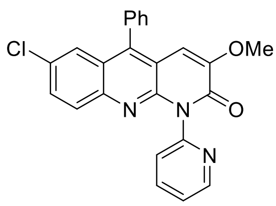
3ag, 97%

Product **3ag** was obtained as a yellow solid in 97% yield (78.8 mg). ^{1}H NMR (400 MHz, Methylene Chloride-d_2) δ 9.03 (d, J = 4.8 Hz, 2H), 8.14 (d, J = 8.3 Hz, 1H), 8.06 (d, J = 8.9 Hz, 1H), 7.75 – 7.67 (m, 4H), 7.64 (dd, J = 9.0, 2.4 Hz, 1H), 7.58 – 7.51 (m, 2H), 7.46 (ddd, J = 8.5, 7.2, 1.4 Hz, 1H), 7.39 (t, J = 4.8 Hz, 1H), 7.11 – 7.05 (m, 1H), 7.00 (d, J = 2.0 Hz, 1H). ^{13}C NMR (100 MHz, CD_2Cl_2) δ 158.8, 157.1, 151.7, 141.6, 141.1, 135.5, 129.8, 129.5, 129.3, 129.2, 128.9, 128.3, 125.7, 124.9, 123.0, 122.1, 121.6, 118.8, 117.5, 112.9. Two signals are missing due to overlap. HRMS: m/z: $[M+H]^+$ calculated for $C_{25}H_{16}N_4Cl$: 407.1063, found 407.1065.



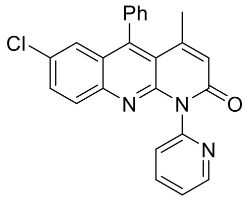
5ag, 95%

Product **5ag** was obtained as a white solid in 95% yield (75.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.78 (d, J = 3.8 Hz, 1H), 7.98 (t, J = 7.1 Hz, 1H), 7.66-7.61 (m, 4H), 7.50– 7.42 (m, 5H), 7.36 (br, 2H), 2.20 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.7, 151.6, 150.1, 149.5, 146.3, 145.1, 138.5, 134.2, 132.7, 132.5, 131.1, 130.8, 130.4, 130.1(br), 129.1, 129.0, 125.2, 125.1, 124.7, 123.7, 115.0, 17.4. HRMS: m/z: $[M+H]^+$ calculated for $C_{24}H_{17}ClN_3O$: 398.1055, found 398.1058.



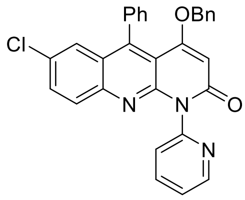
5bg, 95%

Product **5bg** was obtained as a white solid in 95% yield (78.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77 (dd, J = 4.7, 1.0 Hz, 1H), 7.99 (td, J = 7.7, 1.8 Hz, 1H), 7.65-7.60 (m, 4H), 7.50 – 7.42 (m, 4H), 7.38 (br, 2H), 6.68 (s, 1H), 3.75 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0, 151.0, 150.1, 149.1, 147.0, 144.6, 143.9, 138.6, 134.5, 130.9, 130.4, 130.3, 129.8 (br), 129.13, 129.1, 125.4, 124.7, 124.6, 123.9, 115.2, 106.7, 56.1. HRMS: m/z: $[M+H]^+$ calculated for $C_{24}H_{17}ClN_3O_2$: 414.1004, found 414.1008.



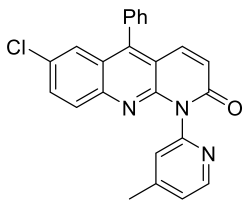
5cg, 92%

Product **5cg** was obtained as a white solid in 92% yield (73.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.76 (dd, J = 4.8, 1.3 Hz, 1H), 7.97 (td, J = 7.7, 1.9 Hz, 1H), 7.59 – 7.53 (m, 4H), 7.50 – 7.42 (m, 3H), 7.32 (br, 2H), 7.19 (d, J = 2.2 Hz, 1H), 6.60 (d, J = 1.0 Hz, 1H), 1.80 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ162.3, 151.6, 150.1, 150.0, 147.8, 147.7, 144.6, 138.5, 137.2, 131.6, 130.9, 129.9, 129.7 (br), 129.1, 128.5, 126.3, 125.6, 125.4, 124.7, 123.6, 115.4, 24.3. HRMS: m/z: $[M+H]^+$ calculated for $C_{24}H_{17}ClN_3O$: 398.1055, found 398.1053.



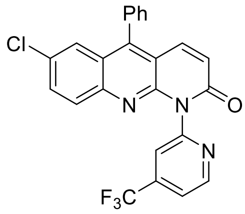
5dg, 61%

Product **5dg** was obtained as a white solid in 61% yield (68.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77 (d, J = 3.7 Hz, 1H), 7.98 (t, J = 7.4 Hz, 1H), 7.58 (d, J = 8.9 Hz, 1H), 7.49-7.43 (m, 3H), 7.34 – 7.21 (m, 5H), 7.17 – 7.08 (m, 4H), 6.92 (d, J = 6.8 Hz, 2H), 6.11 (s, 1H), 4.77 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.9, 162.6, 151.5, 150.0, 149.7, 147.6, 145.4, 138.5, 137.4, 133.8, 131.9, 130.8, 129.9, 128.4, 128.4, 128.3, 127.8, 127.6 (br), 126.3, 125.8, 125.0, 123.6, 110.5, 99.2, 71.4. HRMS: m/z: $[M+H]^+$ calculated for $C_{30}H_{21}ClN_3O_2$: 490.1317, found 490.1321.



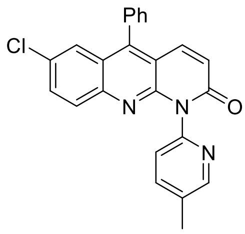
5eg, 72%

Product **5eg** was obtained as a white solid in 72% yield (57.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 (d, J = 5.0 Hz, 1H), 7.76 (d, J = 9.0 Hz, 1H), 7.71 – 7.65 (m, 4H), 7.61 (dd, J = 9.0, 2.3 Hz, 1H), 7.55 (d, J = 2.2 Hz, 1H), 7.43 (br, 2H), 7.36 (dd, J = 14.2, 4.9 Hz, 2H), 6.79 (d, J = 9.9 Hz, 1H), 2.58 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.1, 151.0, 150.1, 149.8, 149.6, 147.8, 145.7, 136.6, 133.8, 131.6, 131.0, 130.5, 130.0 (br), 129.2, 129.0 (br), 125.3, 125.2, 124.9, 124.91, 123.7, 114.6, 21.2. HRMS: m/z: $[M+H]^+$ calculated for $C_{24}H_{17}ClN_3O$: 398.1055, found 398.1055.



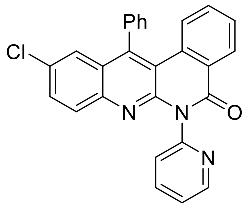
5fg, 63%

Product **5fg** was obtained as a white solid in 63% yield (57.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.97 (d, J = 5.0 Hz, 1H), 7.72-7.71 (m, 2H), 7.68 – 7.61 (m, 5H), 7.57 (dd, J = 9.0, 2.3 Hz, 1H), 7.50 (d, J = 2.2 Hz, 1H), 7.37 (dd, J = 1.8, 0.7 Hz, 2H), 6.72 (d, J = 10.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.8, 152.2, 151.1, 149.5, 148.3, 145.6, 140.9 (q, J = 34.2 Hz), 137.1, 133.6, 132.0, 131.4, 130.4, 129.9, 129.4, 129.0, 125.4, 125.2, 122.6 (q, J = 271.8 Hz), 123.5, 121.2 (q, J = 3.7 Hz), 119.7 (q, J = 3.4 Hz), 114.5. HRMS: m/z: $[M+H]^+$ calculated for $C_{24}H_{14}ClF_3N_3O$: 452.0772, found 452.0776.



5gg, 92%

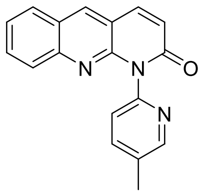
Product **5gg** was obtained as a white solid in 92% yield (72.7 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (s, 1H), 7.79 (dd, J = 7.9, 1.8 Hz, 1H), 7.68 (d, J = 9.0 Hz, 1H), 7.63 – 7.57 (m, 4H), 7.53 (dd, J = 9.0, 2.2 Hz, 1H), 7.47 (d, J = 2.1 Hz, 1H), 7.34 (m, 3H), 6.71 (d, J = 9.9 Hz, 1H), 2.49 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.2, 150.4, 149.9, 148.6, 147.9, 145.8, 139.2, 136.6, 133.8, 133.5, 131.7, 131.0, 130.5, 130.0 (br), 129.3, 129.0 (br), 125.3, 125.0, 123.9, 123.8, 114.7, 18.3. HRMS: m/z: $[M+H]^+$ calculated for $C_{24}H_{17}ClN_3O$: 398.1055, found 398.1050.



5hg, 72%

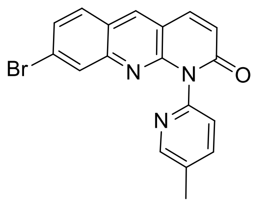
Product **5hg** was obtained as a white solid in 72% yield (93.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.79 (d, J = 4.2 Hz, 1H), 8.55 (d, J = 7.8, 1.0 Hz, 1H), 8.00 (td, J = 7.7, 1.8 Hz, 1H), 7.66 – 7.65

(m, 3H), 7.58 (d, J = 8.9 Hz, 1H), 7.50 – 7.45 (m, 4H), 7.41 – 7.33 (m, 3H), 7.30 – 7.25 (m, 1H), 7.09 (d, J = 8.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.6, 152.2, 150.0, 149.3, 146.4, 144.1, 138.5, 137.8, 132.7, 132.2, 131.0, 130.9, 130.1, 129.9, 129.2, 129.2, 128.6, 127.8, 127.3, 126.5, 125.3, 124.8, 123.6, 114.1. HRMS: m/z $[M+H]^+$ calculated for $C_{27}H_{17}ClN_3O$: 434.1055, found 434.1057.



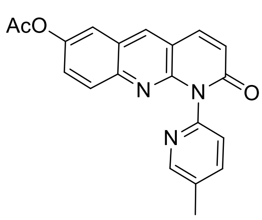
5ga, 82%

Product **5ga** was obtained as a white solid in 82% yield (46.9 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (s, 1H), 8.36 (s, 1H), 7.83 (d, J = 9.4 Hz, 2H), 7.74 (dd, J = 19.6, 8.3 Hz, 2H), 7.62 (t, J = 7.5 Hz, 1H), 7.43 (t, J = 7.4 Hz, 1H), 7.31 (d, J = 8.0 Hz, 1H), 6.79 (d, J = 9.6 Hz, 1H), 2.47 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.6, 150.4, 149.8, 148.6, 147.5, 139.2, 138.4, 136.8, 133.5, 131.1, 128.7, 127.9, 125.4, 124.9, 123.9, 123.6, 116.0 18.3. HRMS: m/z: $[M+H]^+$ calculated for $C_{18}H_{14}N_3O$: 288.1131, found 288.1128.



5gd, 86%

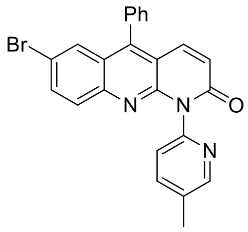
Product **5gd** was obtained as a white solid in 86% yield (63.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (s, 1H), 8.31 (s, 1H), 7.91 (s, 1H), 7.81 – 7.76 (m, 2H), 7.68 (d, J = 8.2 Hz, 1H), 7.49 (d, J = 7.8 Hz, 1H), 7.28 (d, J = 7.5 Hz, 1H), 6.79 (d, J = 9.1 Hz, 1H), 2.48 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.4, 150.4, 150.36, 148.3, 147.8, 139.2, 138.1, 136.6, 133.7, 130.9, 129.1, 129.0, 125.7, 123.9, 123.8, 123.4, 116.1, 18.3. HRMS: m/z: $[M+H]^+$ calculated for $C_{18}H_{13}BrN_3O^+$: 366.0237, found 366.0238.



5gh, 76%

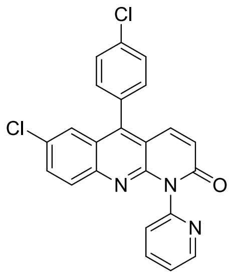
Product **5gh** was obtained as a white solid in 76% yield (52.5 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (s, 1H), 8.30 (s, 1H), 7.81 (d, J = 9.7 Hz, 1H), 7.76 (dd, J = 8.0, 1.8 Hz, 1H), 7.71 (d, J = 9.2

Hz, 1H), 7.59 (d, J = 2.4 Hz, 1H), 7.38 (dd, J = 9.2, 2.5 Hz, 1H), 7.29 (d, J = 8.0 Hz, 1H), 6.80 (d, J = 9.6 Hz, 1H), 2.46 (s, 3H), 2.33 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.3, 163.4, 150.4, 149.7, 148.4, 147.5, 145.4, 139.2, 138.1, 136.3, 133.5, 130.0, 126.4, 124.9, 124.1, 123.9, 118.2, 116.3, 21.2, 18.3. HRMS: m/z: $[M+H]^+$ calculated for $C_{20}H_{16}N_3O_3^+$: 346.1186, found 346.1184.



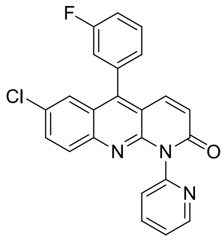
5gi, 76%

Product **5gi** was obtained as a white solid in 76% yield (67.5 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (s, 1H), 7.79 (d, J = 7.2 Hz, 1H), 7.64 - 7.57(m, 7H), 7.37 -7.33 (m, 3H), 6.71 (d, J = 9.9 Hz, 1H), 2.49 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.2, 150.4, 150.0, 148.6, 147.8, 146.0, 139.2, 136.6, 134.2, 133.8, 133.6, 130.6, 130.1, 129.9, 129.0, 128.7, 125.5, 123.9, 123.8, 119.1, 114.7, 18.3. HRMS: m/z: $[M+H]^+$ calculated for $C_{24}H_{17}BrN_3O^+$: 442.0550, found 442.0551.



5ij, 99%

Product **5ij** was obtained as a white solid in 99% yield (83.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77 (d, J = 4.0 Hz, 1H), 7.99 (t, J = 7.1 Hz, 1H), 7.66 (d, J = 9.0 Hz, 1H), 7.61 (d, J = 8.3 Hz, 2H), 7.58 - 7.53 (m, 2H), 7.50 – 7.43 (m, 3H), 7.32 (br, 2H), 6.73 (d, J = 9.9 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.9, 151.0, 150.1, 149.8, 146.4, 145.7, 138.6, 136.3, 135.6, 132.2, 131.9, 131.3, 130.6, 129.4, 125.0, 124.8, 124.7, 124.1, 123.9, 114.6. HRMS: m/z: $[M+H]^+$ calculated for $C_{23}H_{14}Cl_2N_3O^+$: 418.0508, found 418.0509.



5ik, 97%

Product **5ik** was obtained as a yellow solid in 97% yield (78.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.78 (d, J = 4.1 Hz, 1H), 8.00 (t, J = 7.3 Hz, 1H), 7.67 (d, J = 9.0 Hz, 1H), 7.64 – 7.52 (m, 3H), 7.52 – 7.41 (m, 3H), 7.32 (t, *J* = 7.7 Hz, 1H), 7.14 (br, 2H), 6.74 (d, *J* = 9.9 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.9, 162.8 (d, *J* = 248.0 Hz), 151.0, 150.1, 149.7, 146.1, 145.7, 138.6, 136.2, 135.9 (d, *J* = 7.7 Hz), 131.9, 131.3, 130.9 (d, *J* = 6.1 Hz), 130.6, 125.8, 125.0, 124.7, 124.6, 124.2, 123.9, 117.1, 116.4 (d, *J* = 20.8 Hz), 114.6. HRMS: m/z: $[M+H]^+$ calculated for $C_{23}H_{14}ClFN_3O^+$: 402.0804, found 402.0804.

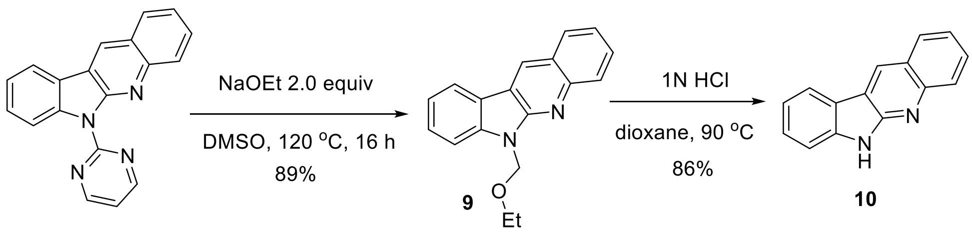
Reference

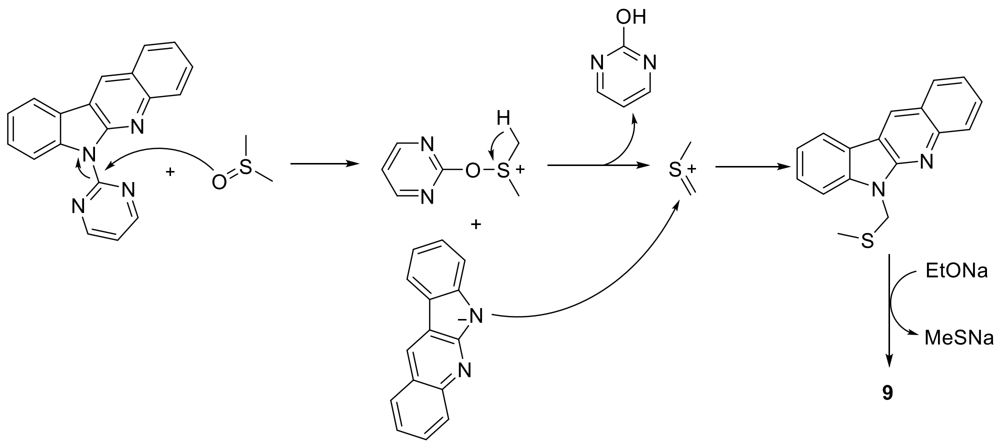
1. Ackermann, L.; Lygin, A. V. *Org. Lett.*, **2011**, *13*, 3332.

2. Modak, A.; Rana, S.; Maiti, D. *J. Org. Chem.* **2015**, *80*, 296.

3. Jin, H.; Huang, L.; Xie, J.; Rudolph, M.; Rominger, F.; Hashmi, A. S. K. *Angew. Chem. Int. Ed.* **2016**, *55*,794.

III. Derivatization of coupled products





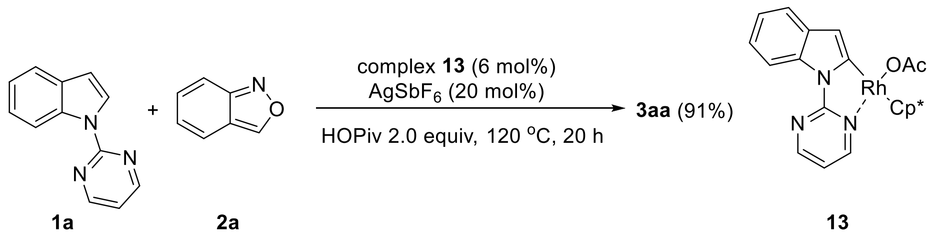
A mixture of **3aa** (0.4mmol) and sodium ethoxide (0.9 mmol) in DMSO (5 mL) was stirred at 120 °C under N_2 atmosphere for 16 h. After cooled to the ambient temperature, the reaction mixture was quenched with H_2O. The aqueous phase was extracted with DCM, and the combined organic phase was dried over anhydrous Na_2SO_4. After filtration and evaporation of the solvents under reduced pressure, the crude product was purified by column chromatography on silica gel to afford **9** as a light yellow solid (89%).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.77 (s, 1H), 8.22 (d, J = 3.3 Hz, 1H), 8.20 (d, J = 4.1 Hz, 1H), 8.08 (d, J = 8.2Hz, 1H), 7.80 (ddd, J = 8.4, 6.8, 1.5 Hz, 1H), 7.71 (d, J = 8.1 Hz, 1H), 7.65 (t, J = 7.8 Hz, 1H), 7.55 (ddd, J = 8.0, 6.6, 1.2 Hz, 1H), 7.42 (t, J = 7.5 Hz, 1H), 6.07 (s, 2H), 3.70 (q, J = 7.0 Hz, 2H), 1.26 (t, J = 7.0 Hz, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 152.8, 146.6, 141.8, 128.8, 128.4, 128.2, 127.8, 127.3, 124.6, 123.3, 121.3, 120.81, 120.79, 118.2, 110.2, 70.9, 64.2, 15.0.HRMS: m/z: $[M+H]^+$ calculated for $C_{18}H_{17}N_2O$: 277.1341, found 277.1340.

Compound **9** (0.4 mmol) was dissolved in 1, 4-dioxane (5 mL), to which was added 1N HCl (4 mL). The reaction mixture was stirred at 90 ^{o}C for 16 h. After that, the solution was neutralized with saturation aqueous $NaHCO_3$. The solution was extracted with dichloromethane. The combined organic layer was dried over Na_2SO_4, and the solvent was removed under reduced pressure. The crude product was purified by column chromatography on silica gel to afford **10** as a yellow solid (86%).

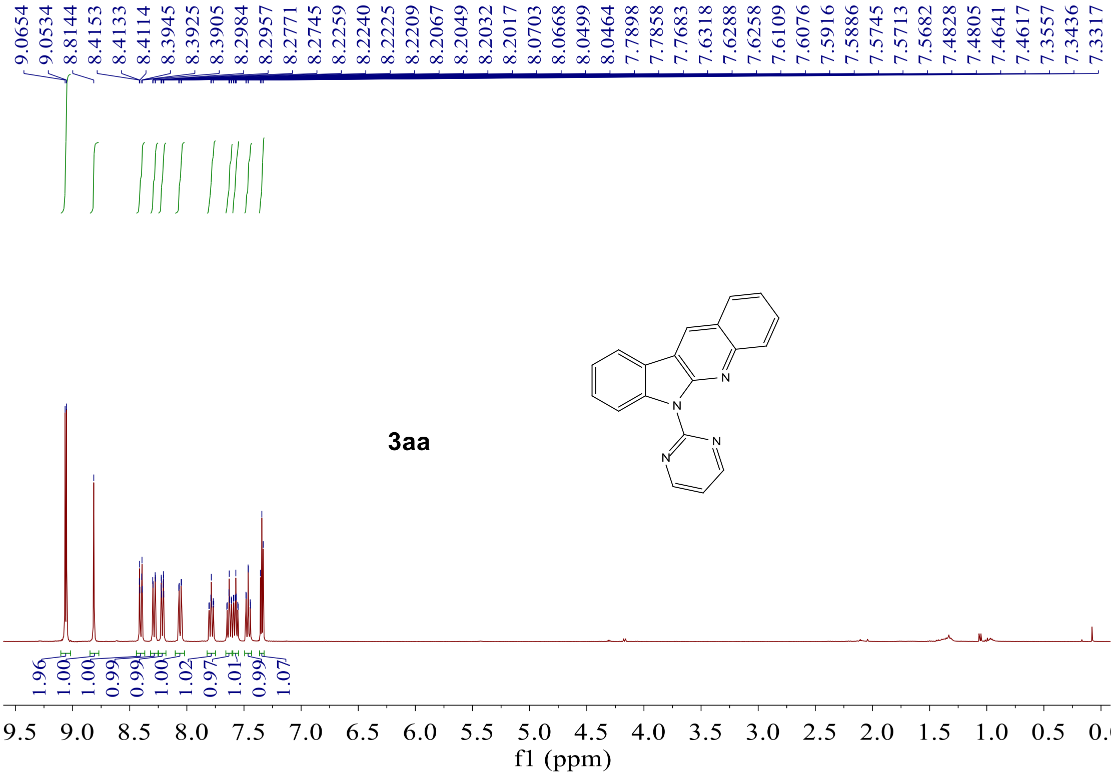
^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 9.05 (s, 1H), 8.27 (d, J = 7.6 Hz, 1H), 8.11 (d, J = 8.2 Hz, 1H), 7.98 (d, J = 8.5 Hz, 1H), 7.72 (ddd, J = 8.4, 6.8, 1.6 Hz, 1H), 7.57 – 7.46 (m, 3H), 7.27 (ddd, J = 8.0, 6.9, 1.4 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-*d*$_6$) δ 158.1, 151.6, 146.7, 133.9, 133.4, 132.7, 132.7, 132.2, 128.9, 127.9, 127.0, 125.5, 124.9, 123.1, 116.1.HRMS: m/z: $[M+H]^+$ calculated for $C_{15}H_{11}N_2$: 219.0922, found 219.0918.

IV. Mechanistic Studies

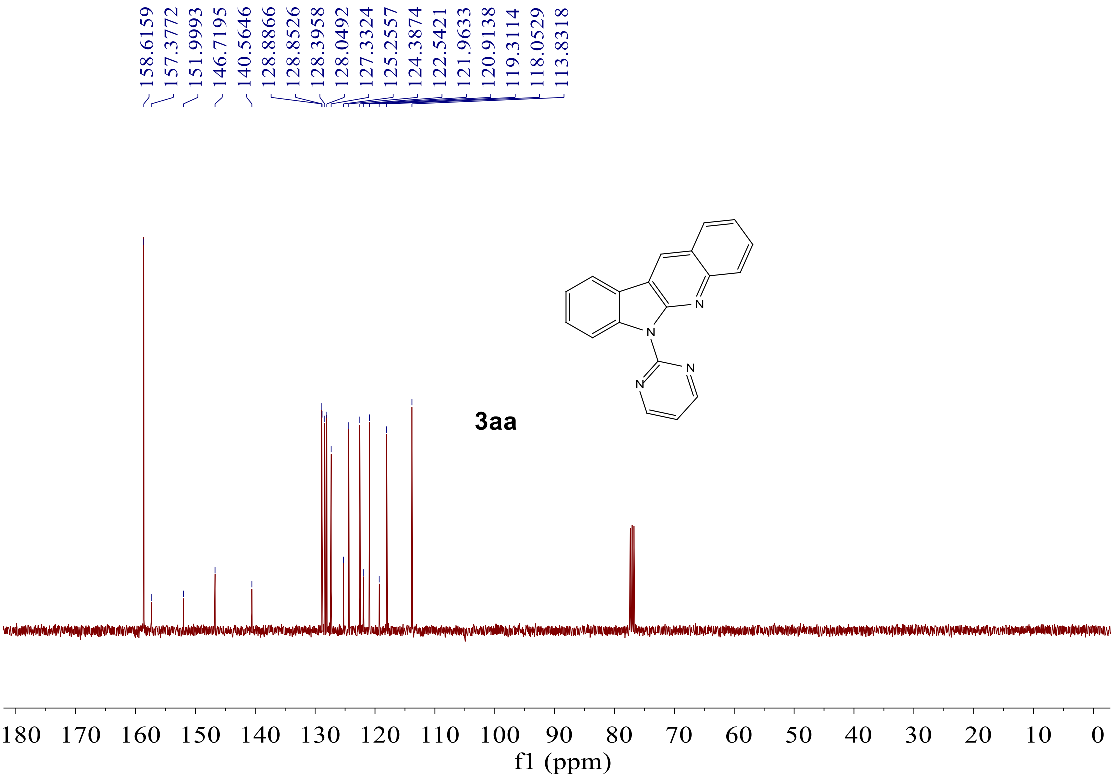


N-pyrimidinylindole (**1a**, 0.2 mmol), complex **13** (0.012 mmol), $AgSbF_6$ (0.04 mmol), and PivOH (0.4 mmol) were dissolved in MeOH (3 mL) in a pressure tube. The resulting mixture was stirred for seconds under N_2 atmosphere, to which was added anthranil (0.4 mmol). The mixture was stirred at 120 ^{o}C for 20 hours. After that, the solvent was removed under vacuum and the residue was purified by silica gel chromatography using ethyl acetate/petroleum ether/Et_3N (30:60:1) to afford product **3aa** as a yellow solid (91%).

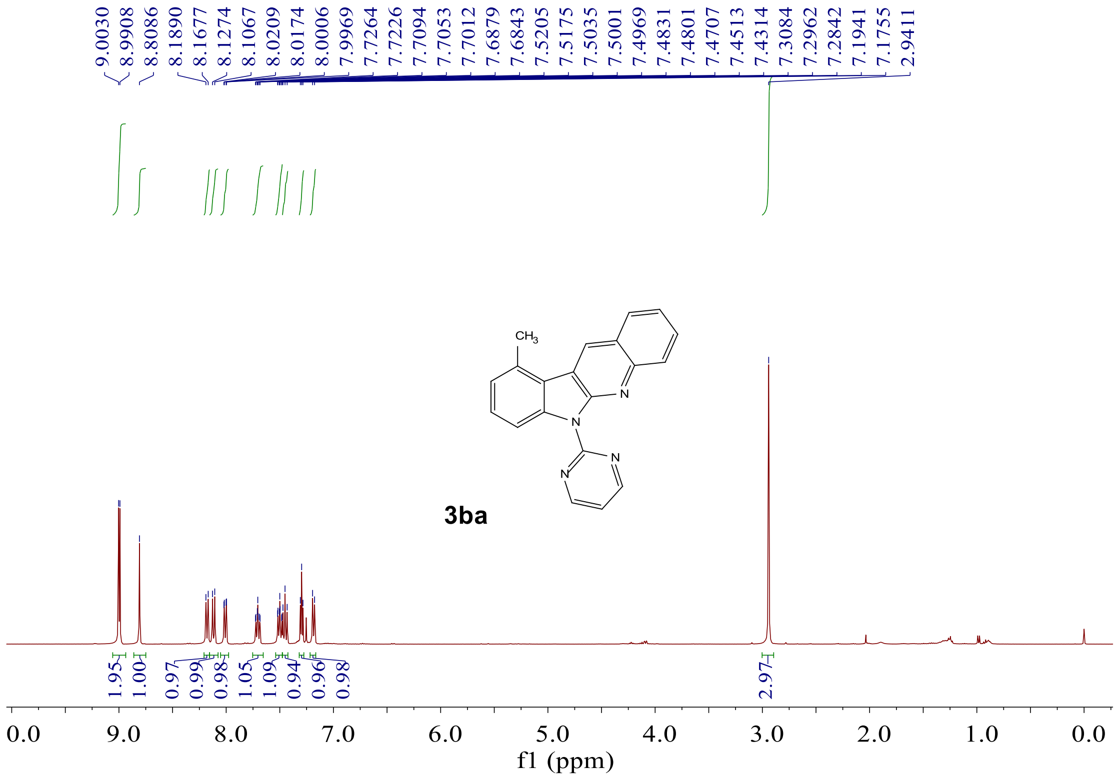
V. NMR Spectra



3aa



3aa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7.7012
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7.5175
7.5035
7.5001
7.4969
7.4831
7.4801
7.4707
7.4513
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7.3084
7.2962
7.2842
7.1941
7.1755
2.9411
CH_3
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N
N
N
3ba
1.95
1.00
0.97
0.99
0.98
1.05
1.09
0.94
0.96
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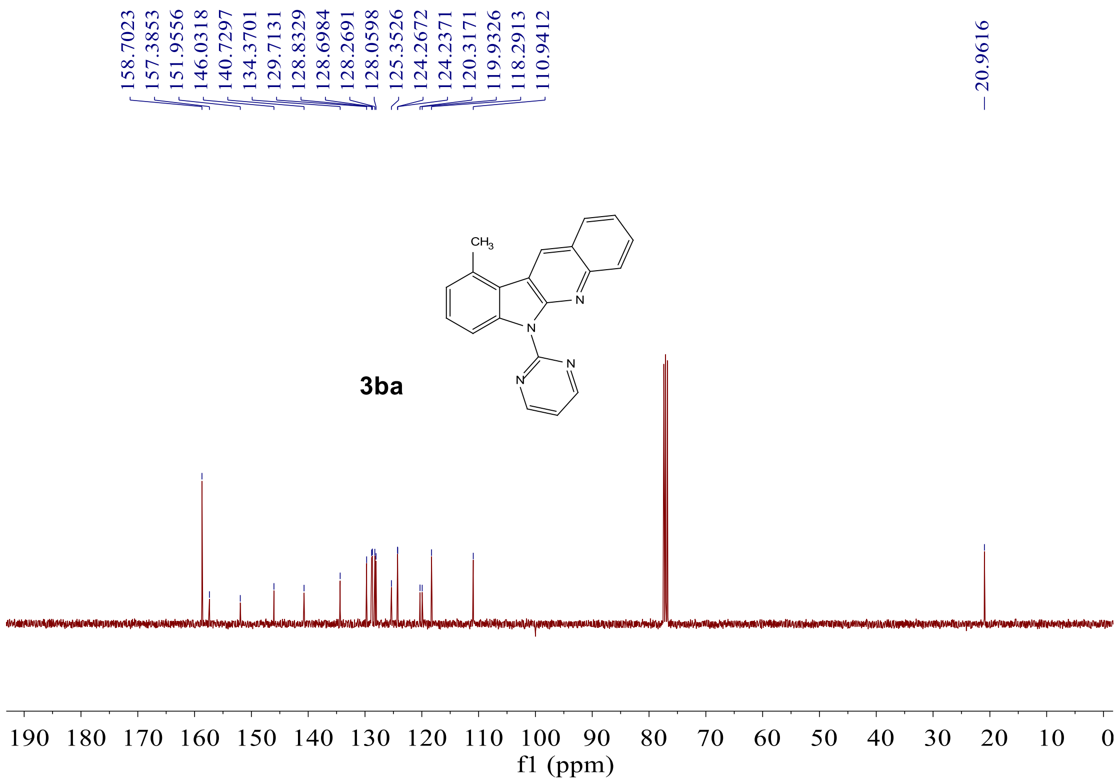
f1 (ppm)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129.7131
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128.6984
128.2691
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125.3526
124.2672
124.2371
120.3171
119.9326
118.2913
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20.9616
CH_3
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N
N
N
3ba
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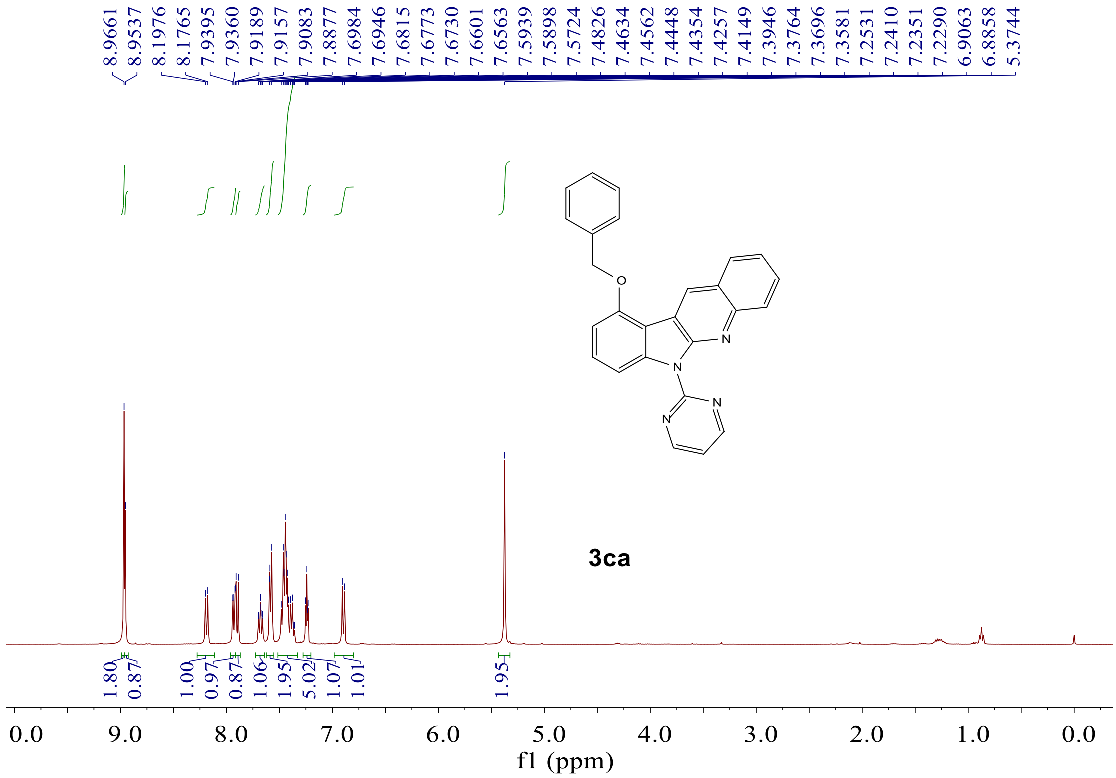
f1 (ppm)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7.3581
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7.2351
7.2290
6.9063
6.8858
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1.95
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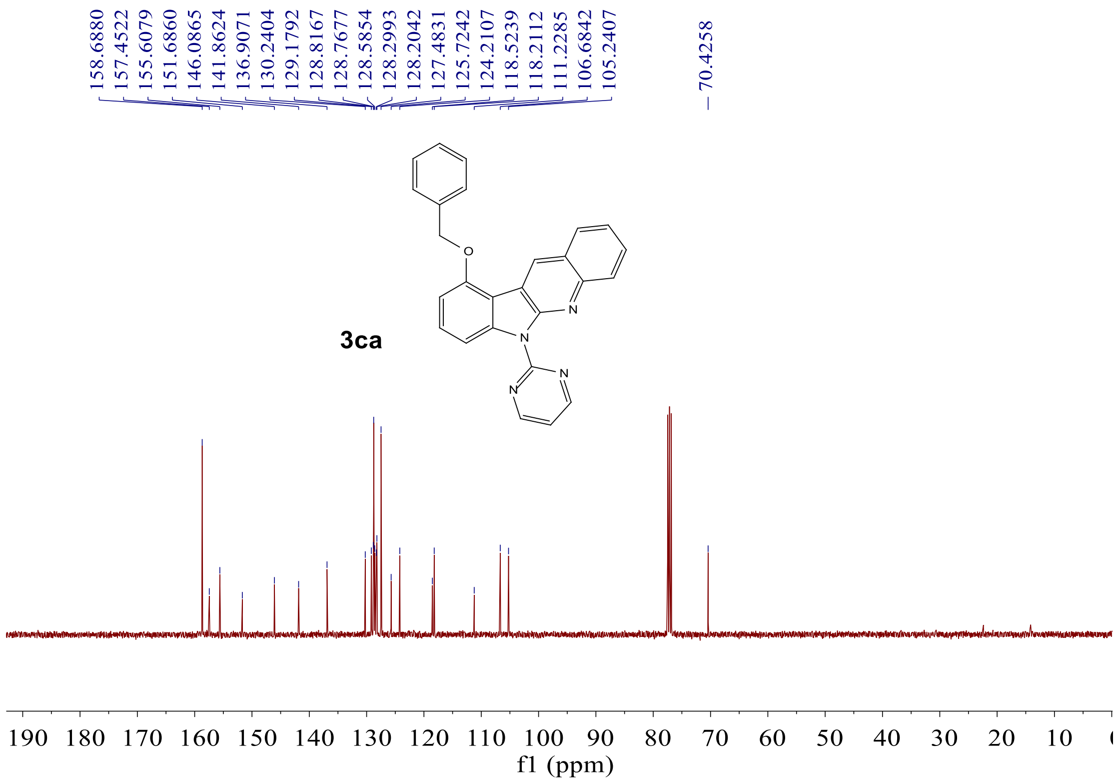
1.01
1.95
f1 (ppm)

3ca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151.6860
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129.1792
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128.7677
128.5854
128.2993
128.2042
127.4831
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105.2407
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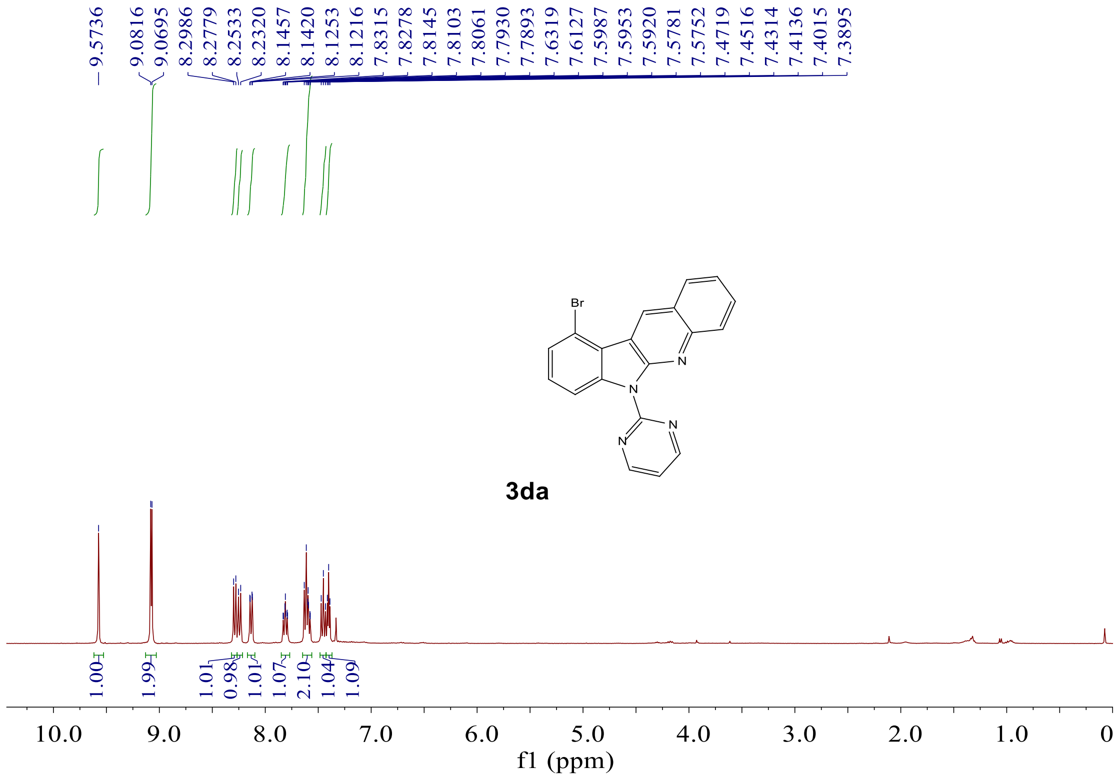
f1 (ppm)

3ca



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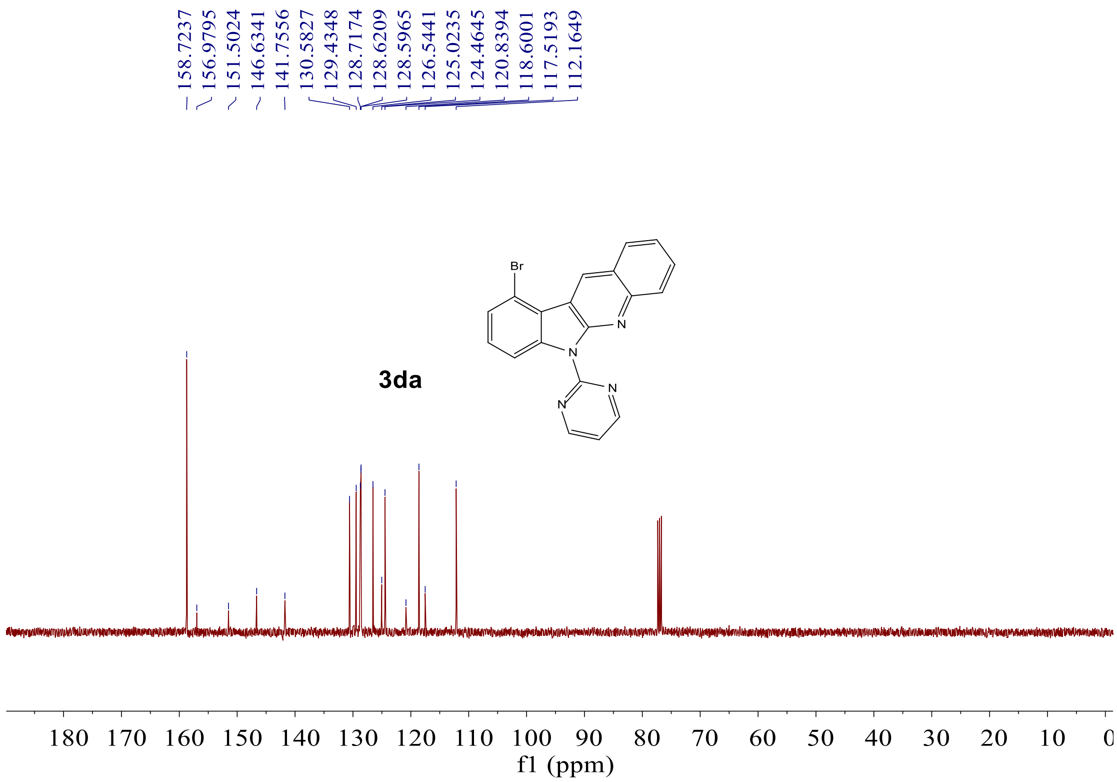

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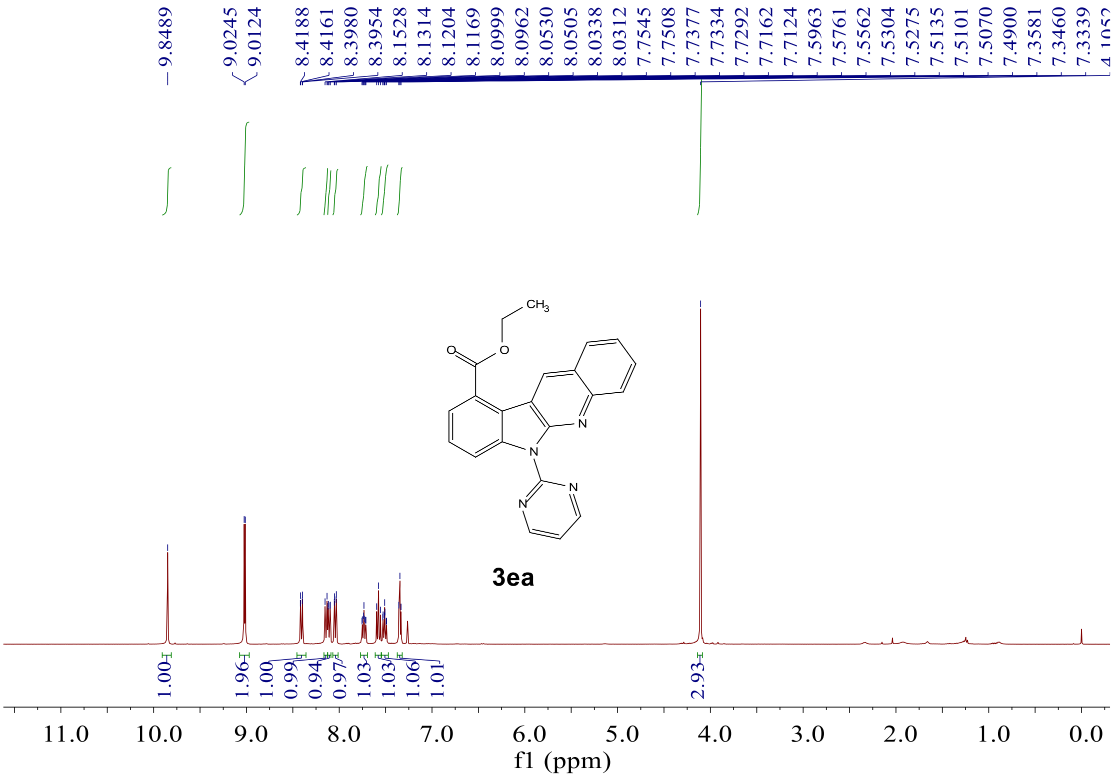
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1.00
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1.03
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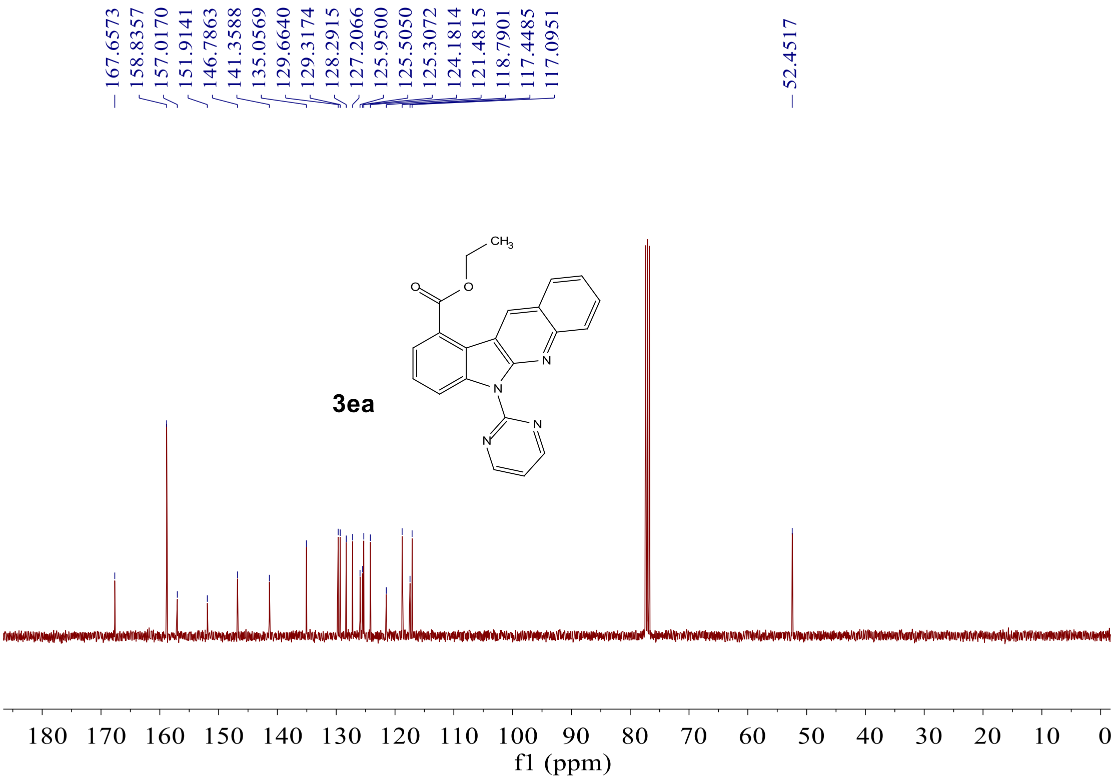
f1 (ppm)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124.1814
121.4815
118.7901
117.4485
117.0951
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O
N
N
N
N
3ea
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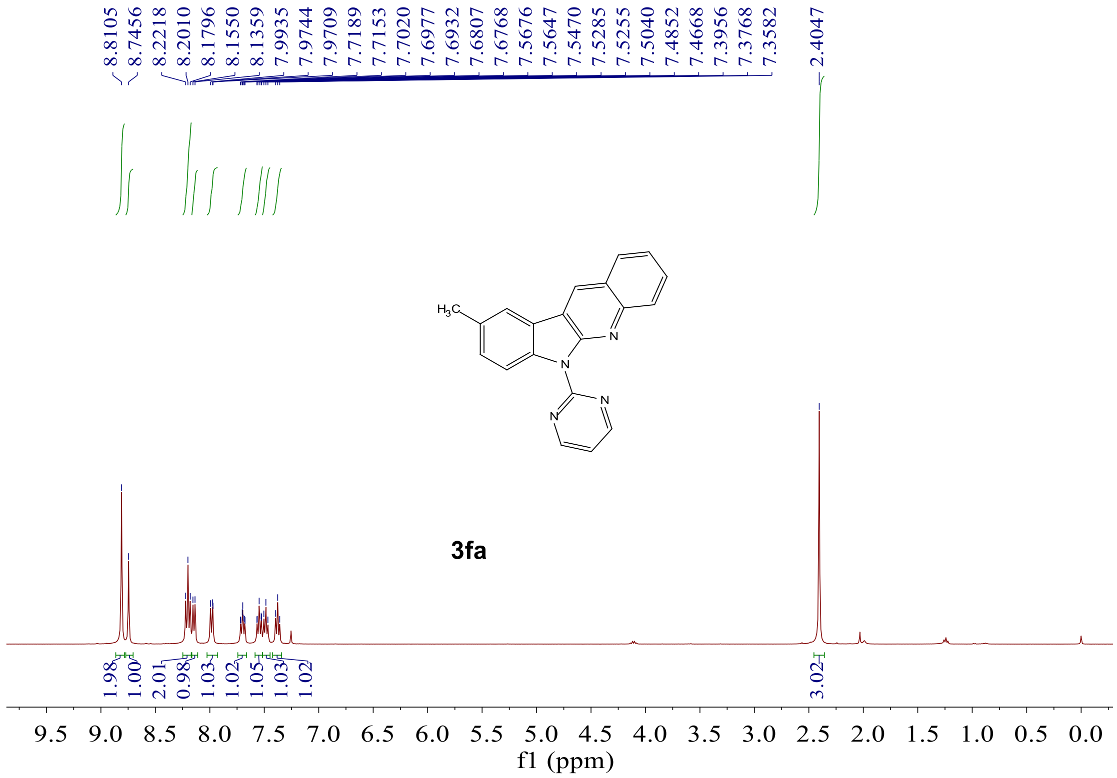
f1 (ppm)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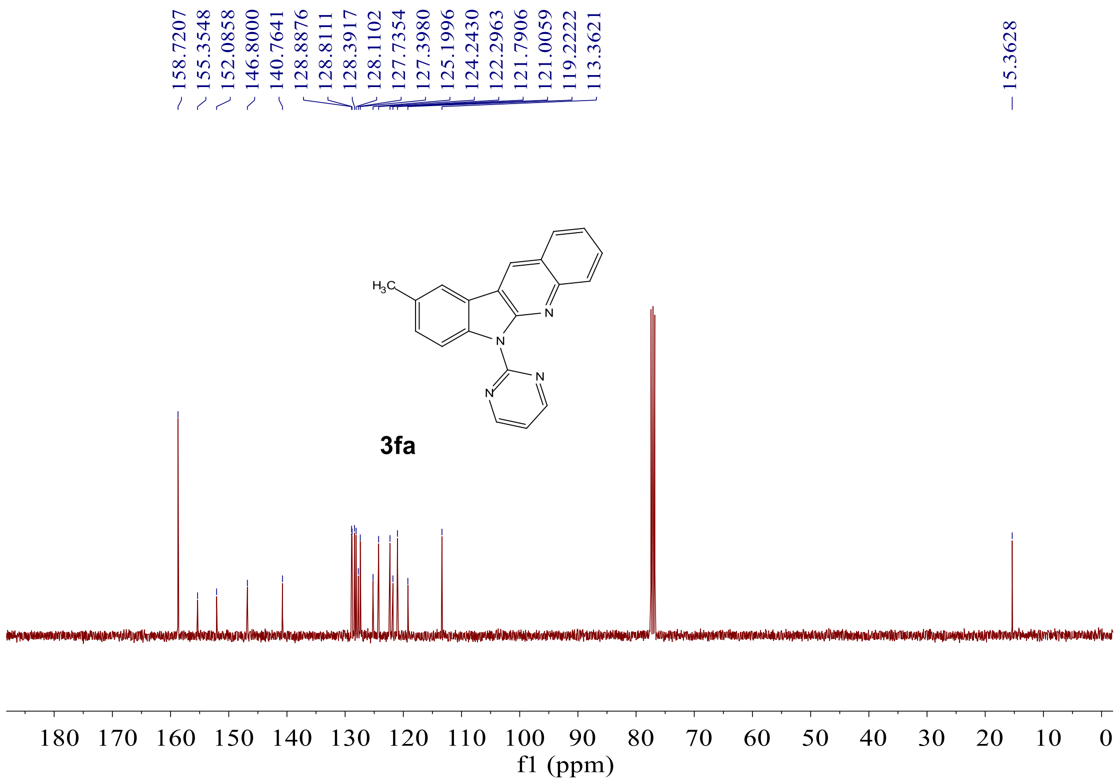
f1 (ppm)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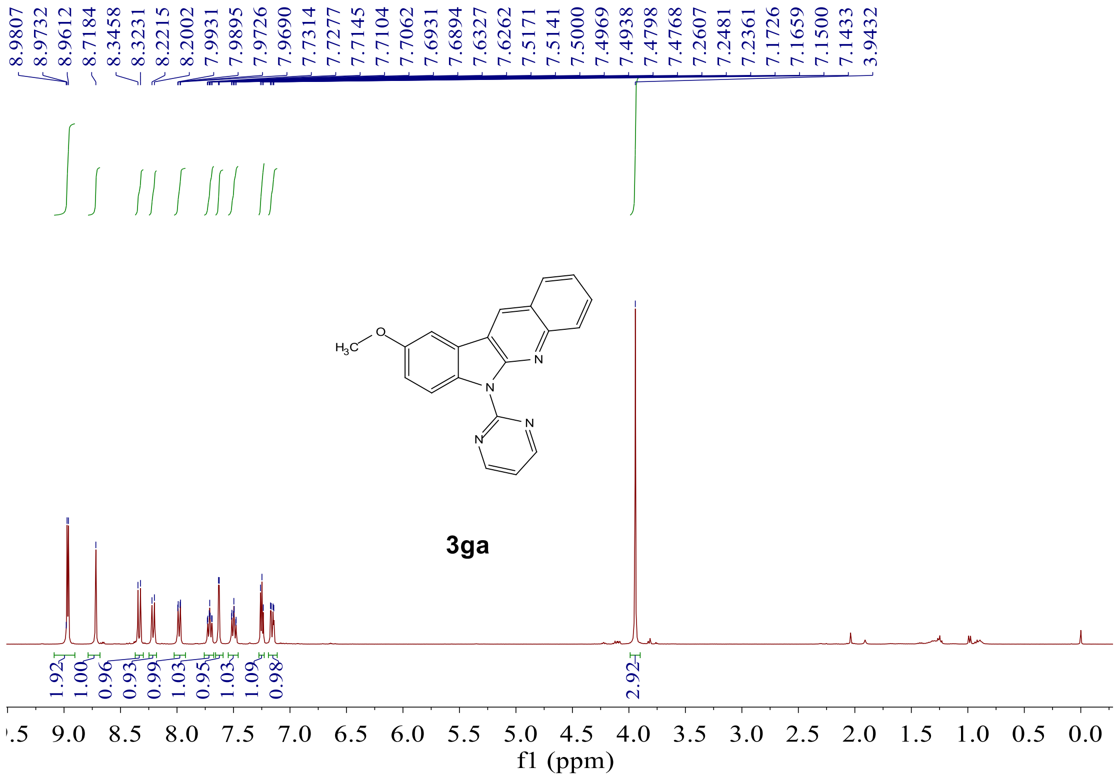
f1 (ppm)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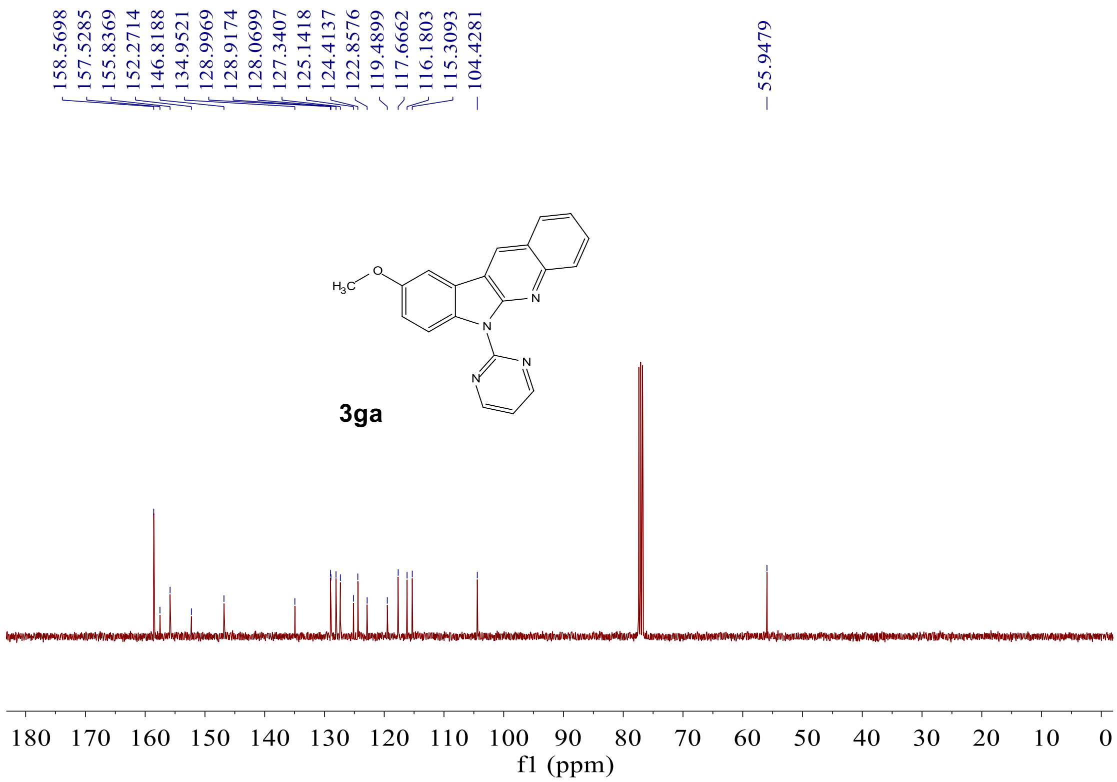
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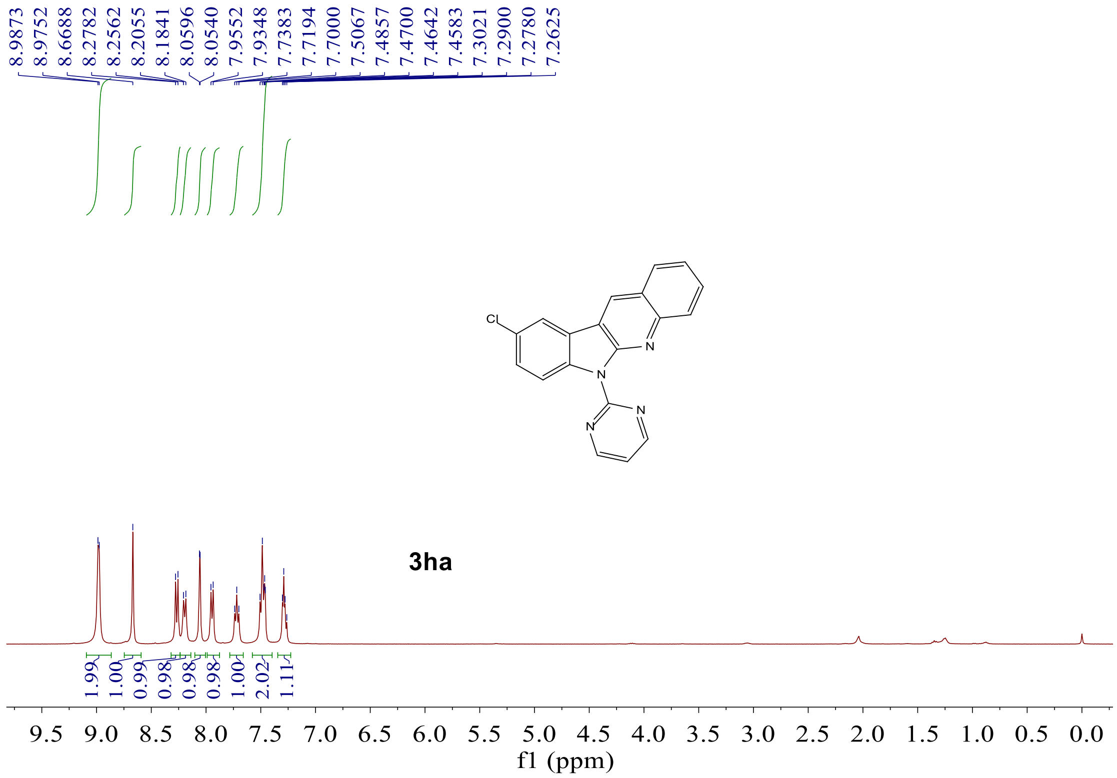

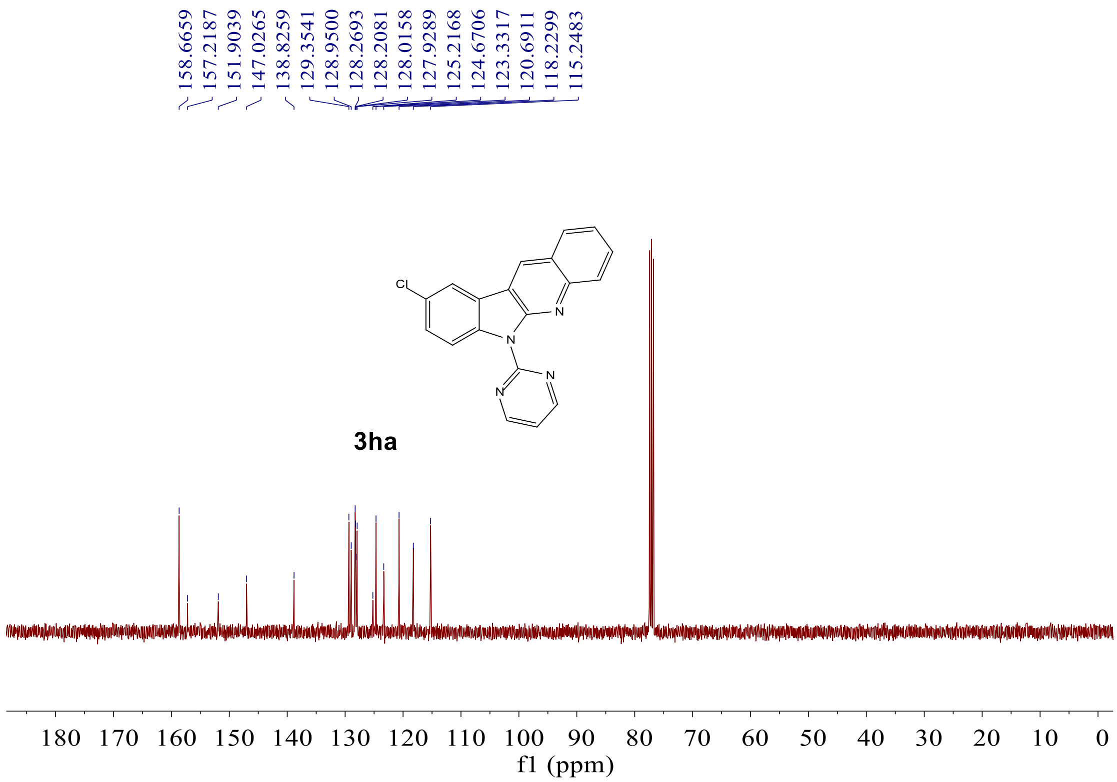

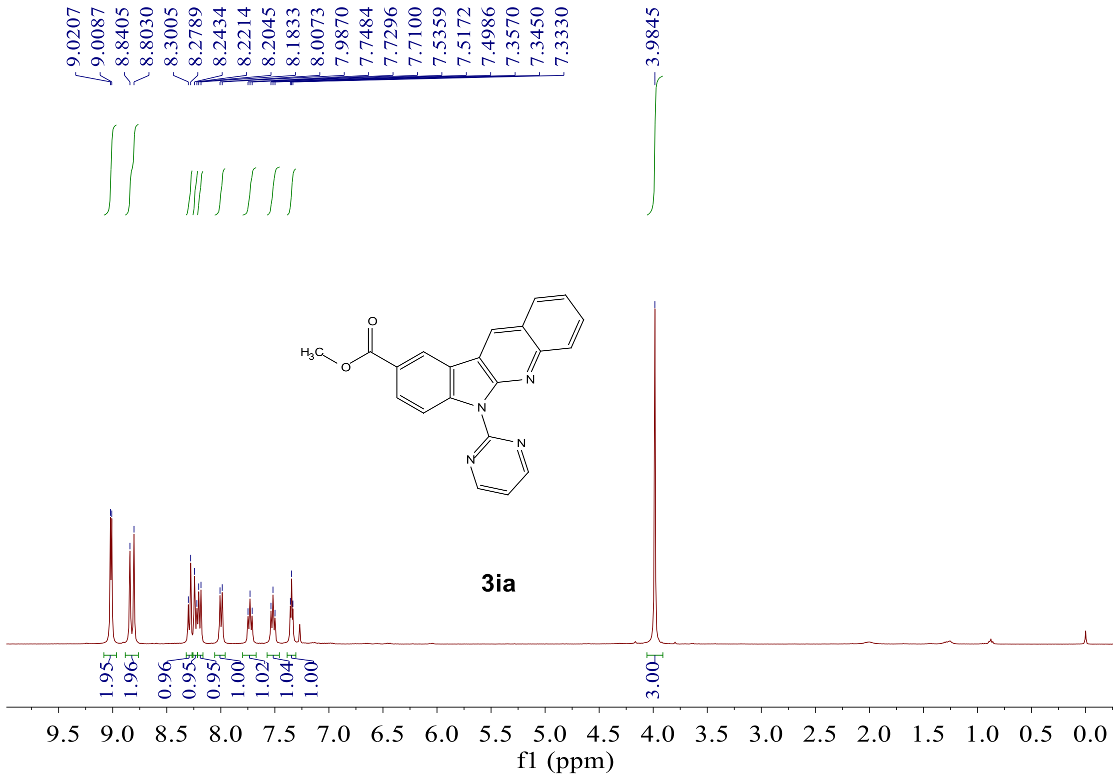
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7.3330
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1.96
0.96
0.95
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1.00
1.02
1.04
1.00
3.00
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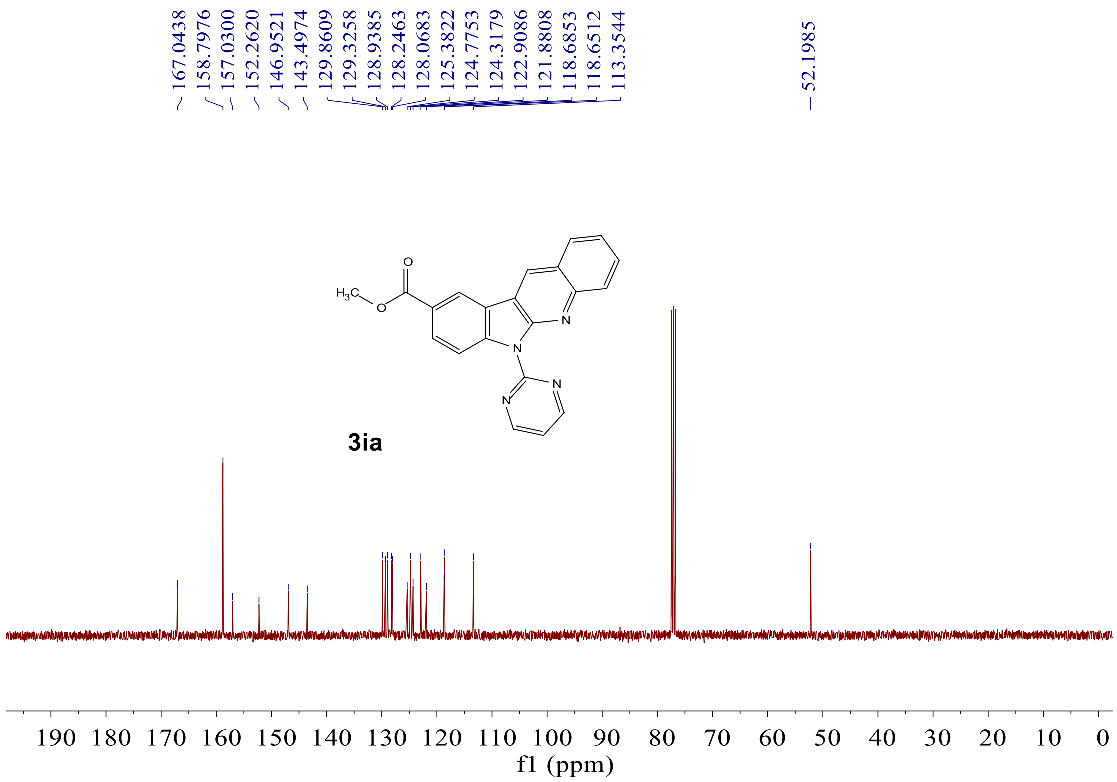
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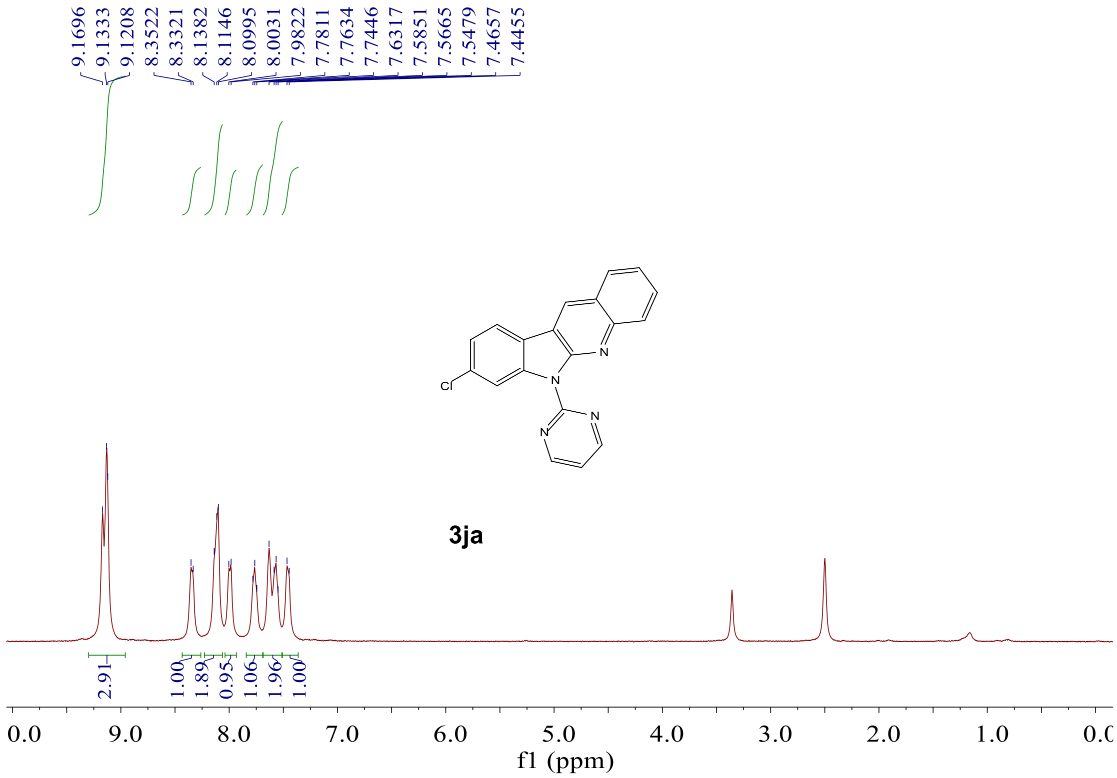
f1 (ppm)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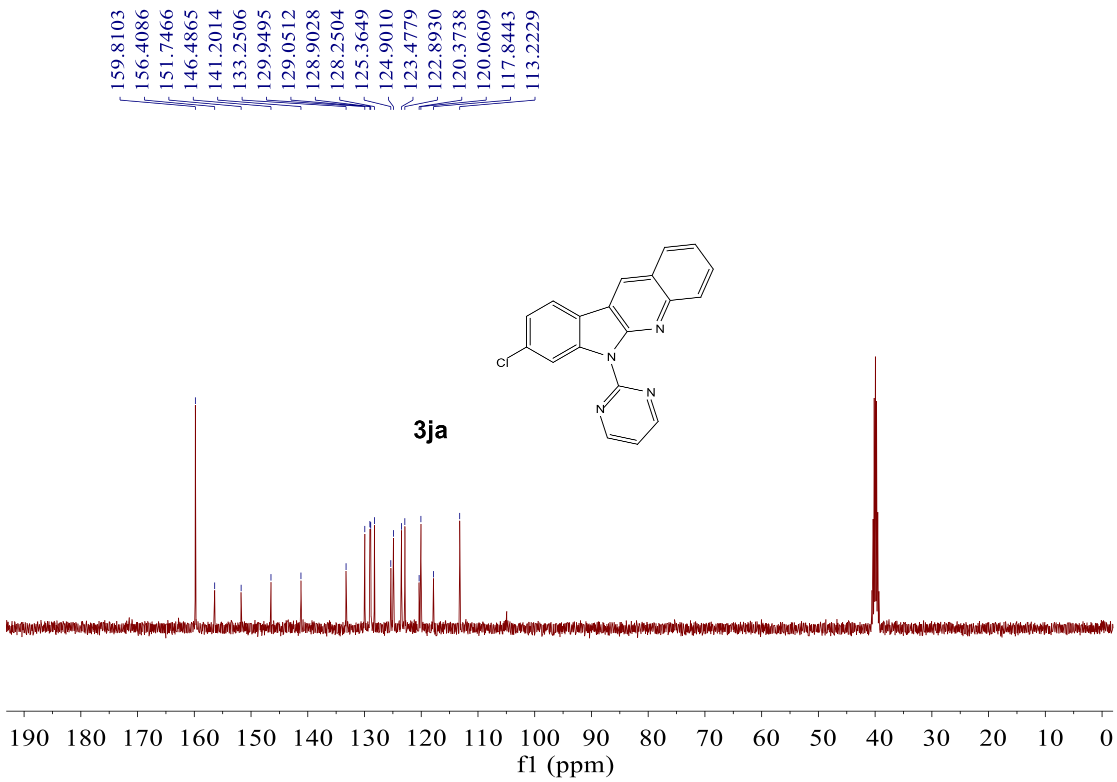
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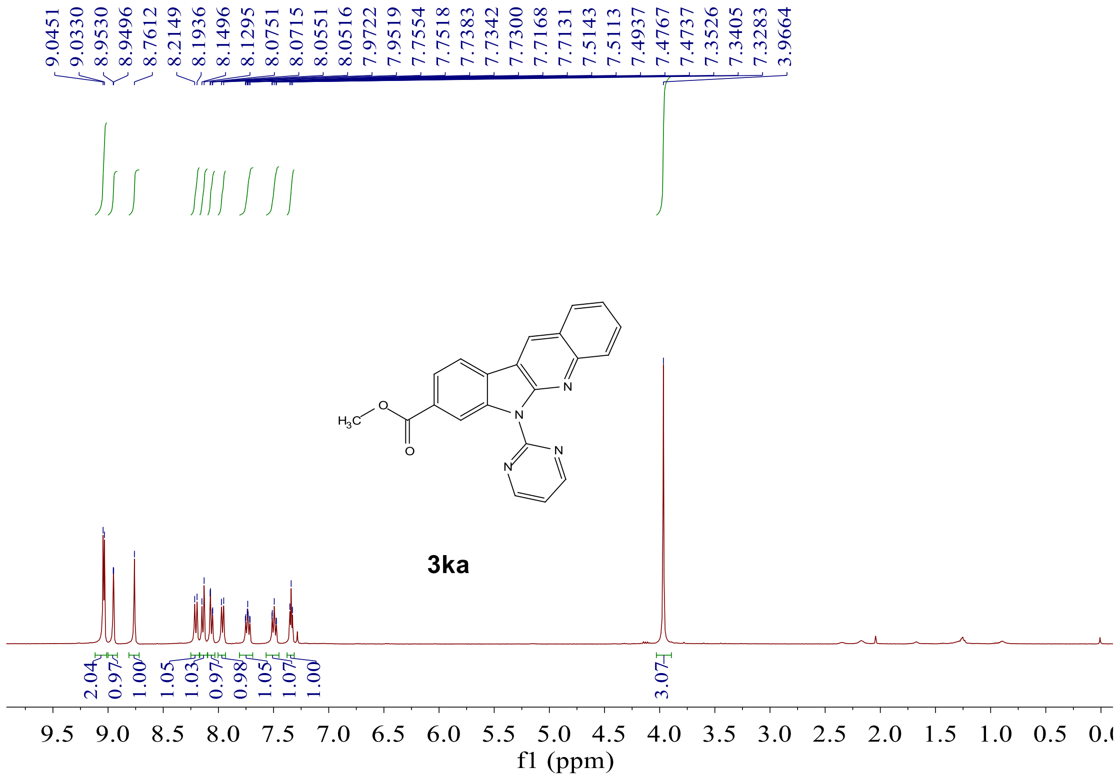
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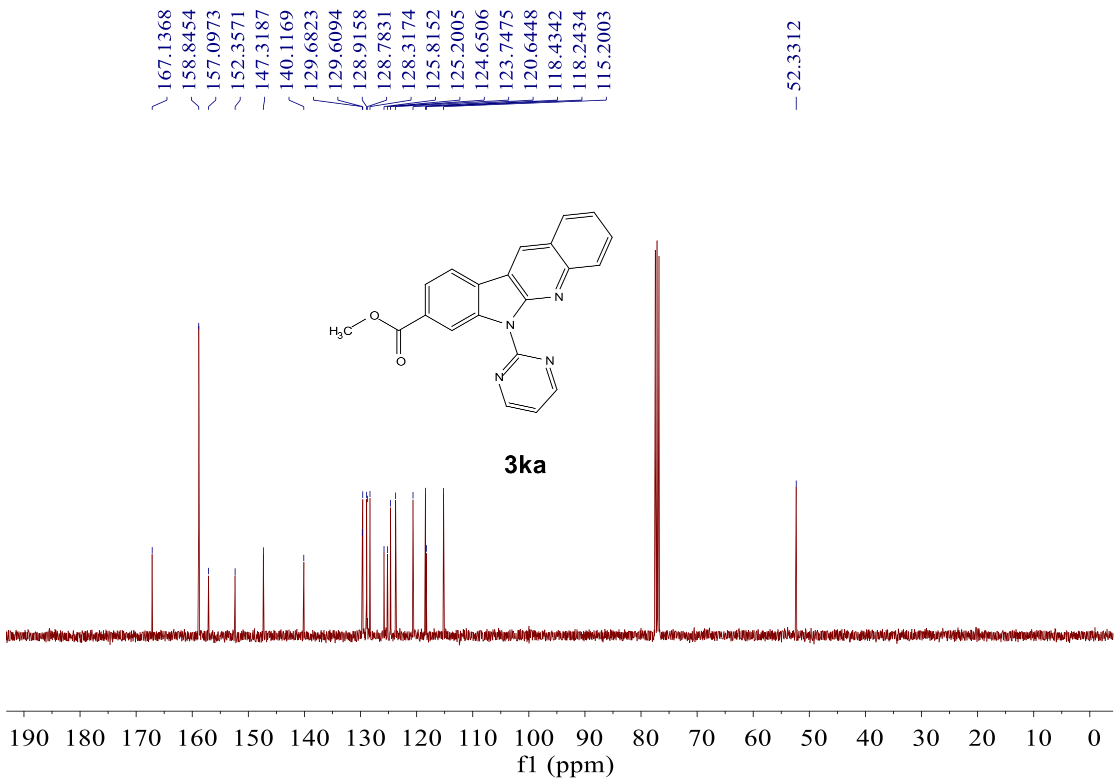
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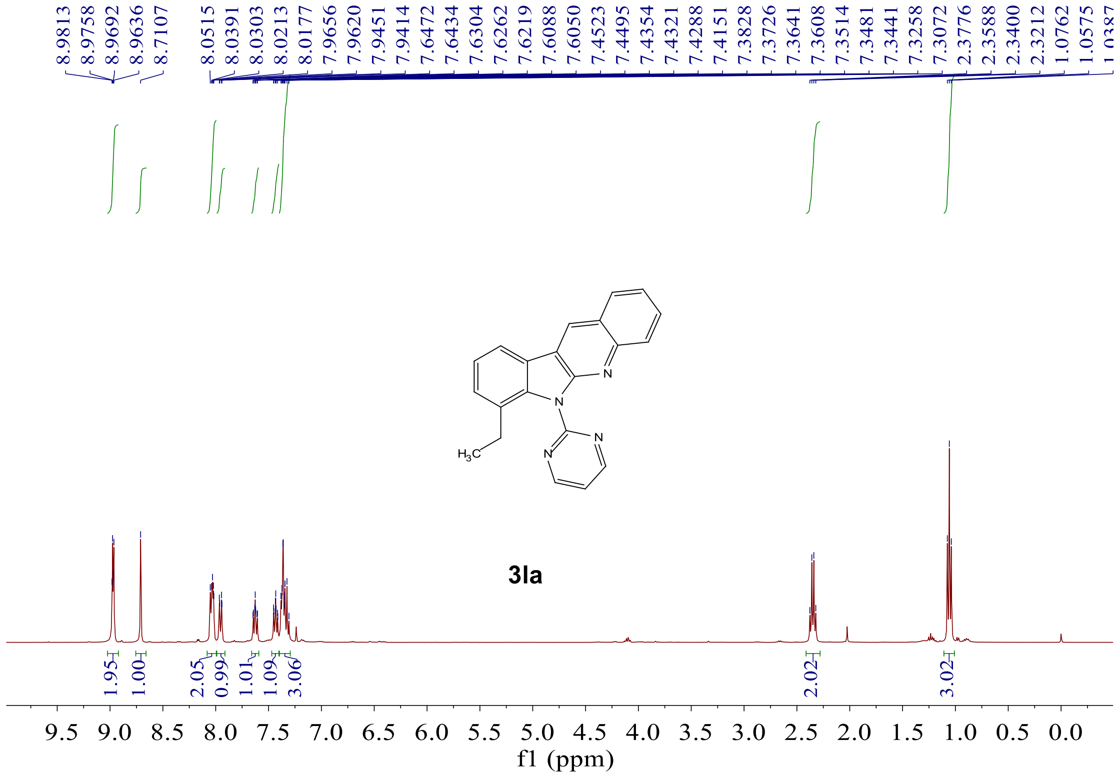
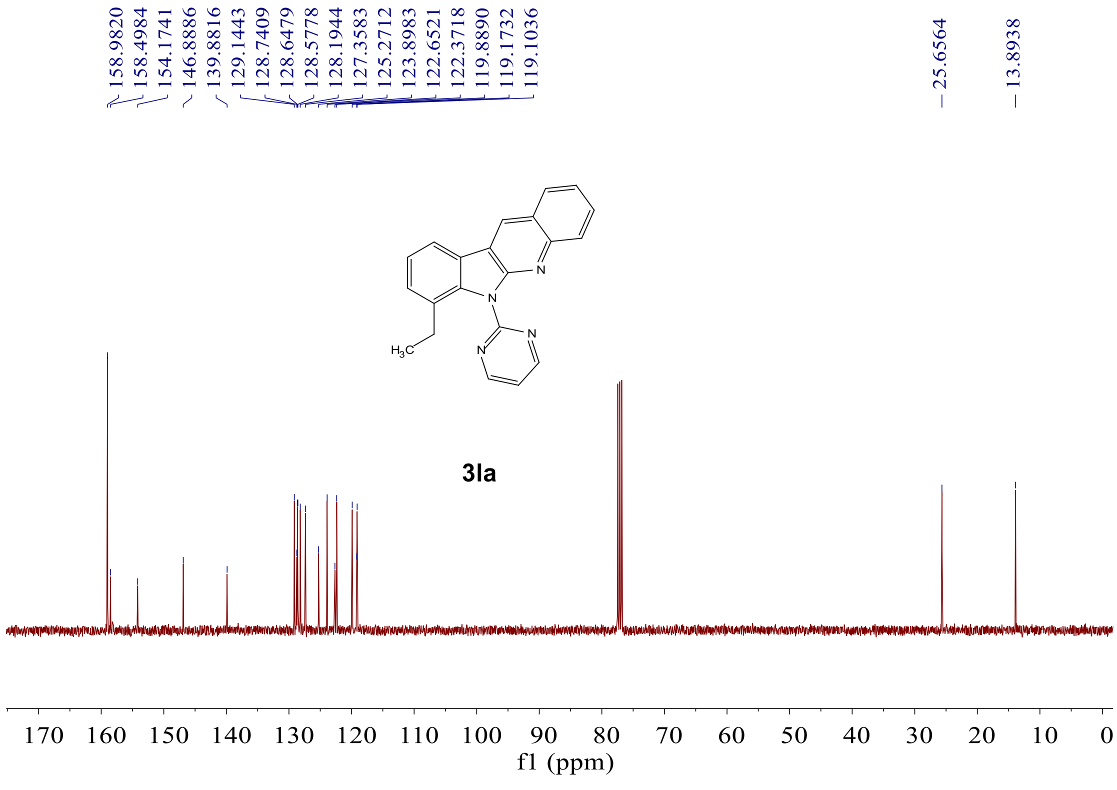
3ka
f1 (ppm)



3la



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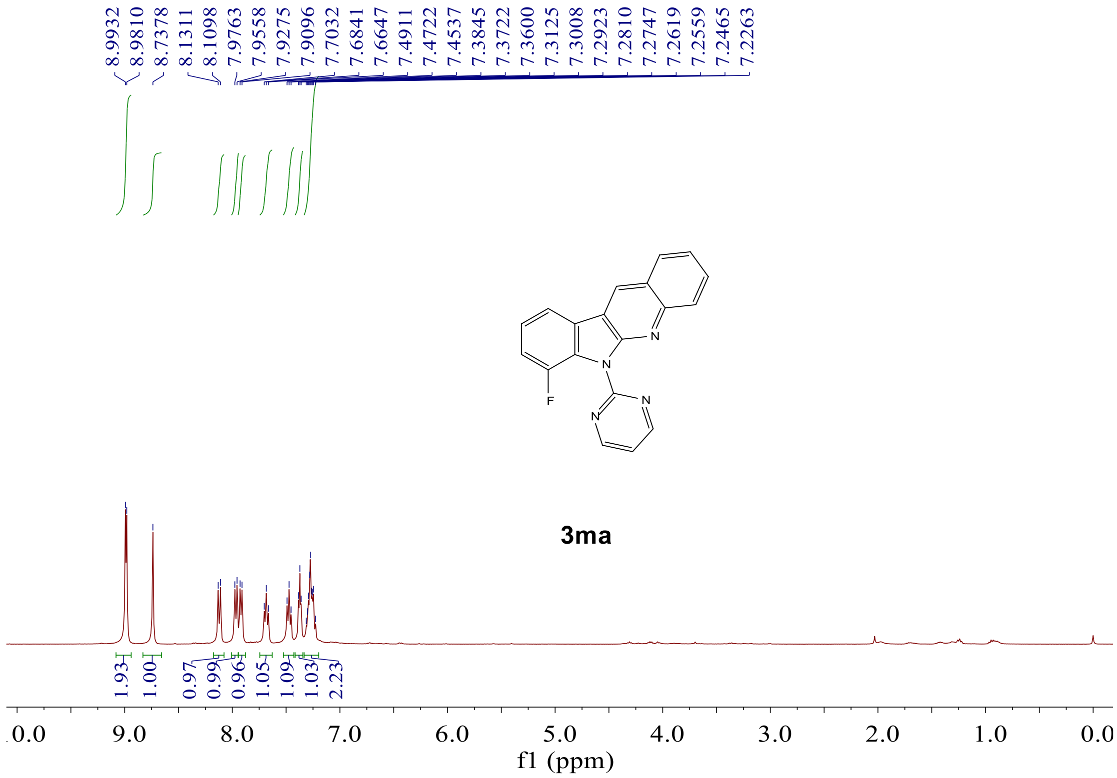
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7.6841
7.6647
7.4911
7.4722
7.4537
7.3845
7.3722
7.3600
7.3125
7.3008
7.2923
7.2810
7.2747
7.2619
7.2559
7.2465
7.2263
N
N
N
N
F
3ma
1.93
1.00
0.97
0.99
0.96
1.05
1.09
1.03
2.23
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7.0
6.0
5.0
4.0
3.0
2.0
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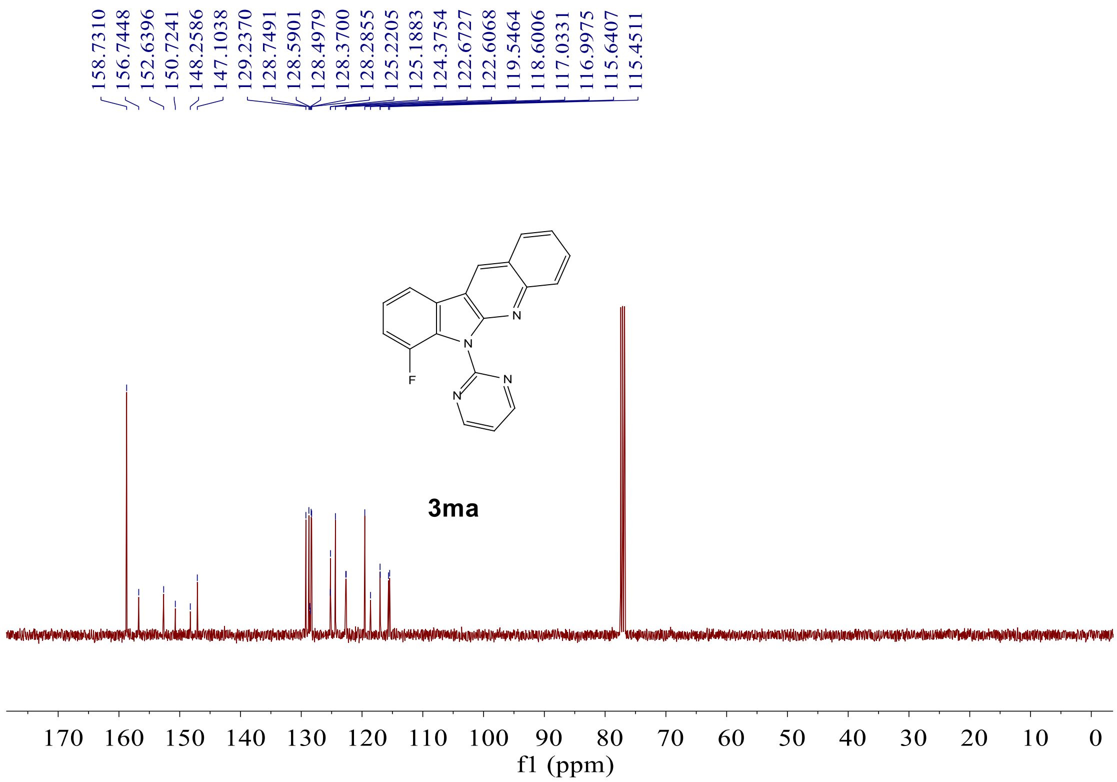
0.0
f1 (ppm)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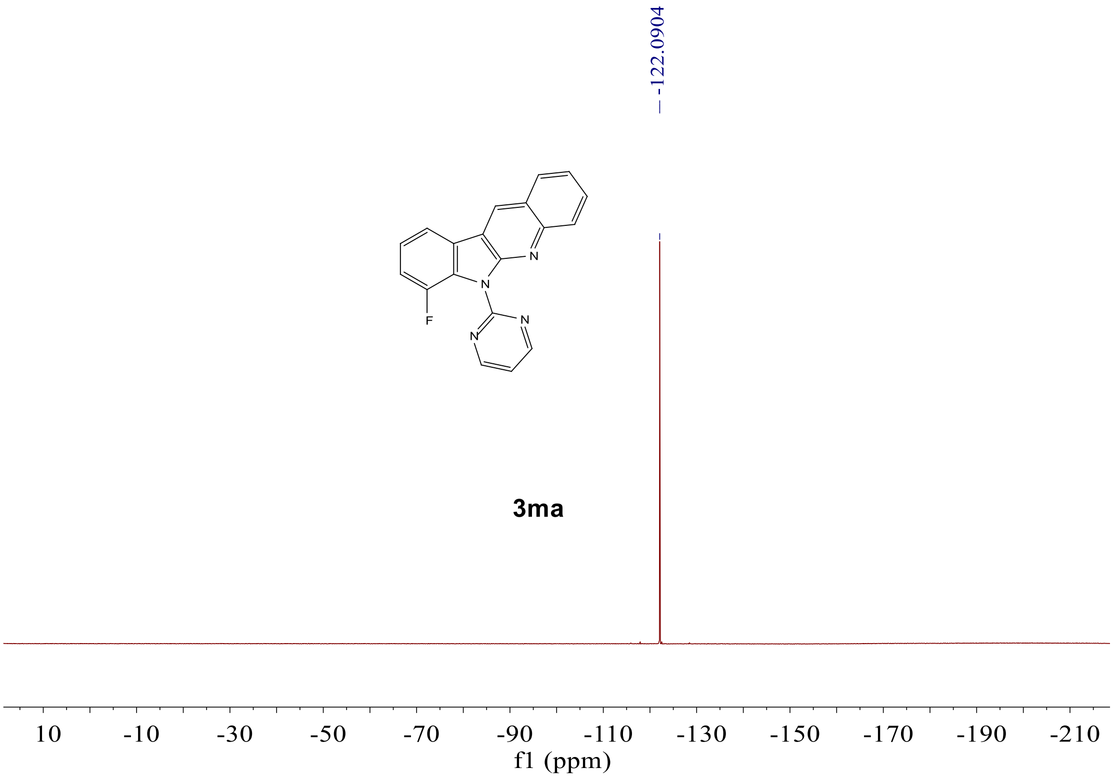
128.4979
128.3700
128.2855
125.2205
125.1883
124.3754
122.6727
122.6068
119.5464
118.6006
117.0331
116.9975
115.6407
115.4511
N
N
N
N
F
3ma
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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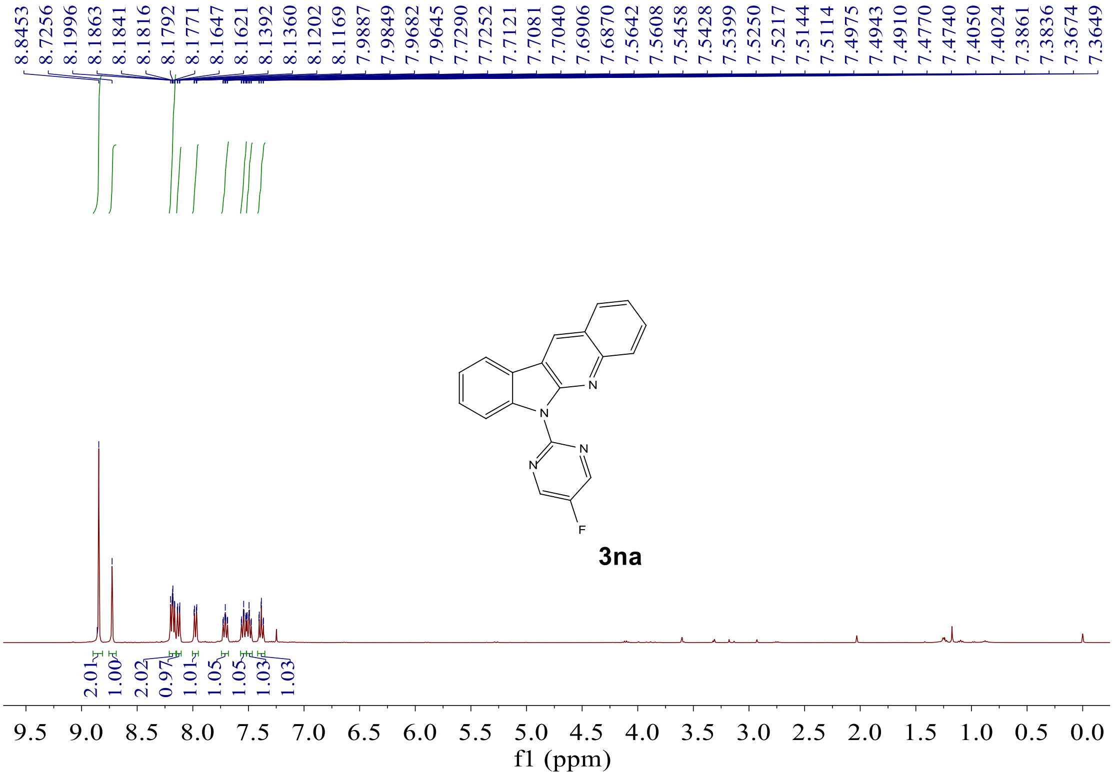
-190
-210
f1 (ppm)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8.1202
8.1169
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7.9849
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7.9645
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7.7252
7.7121
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7.7040
7.6906
7.6870
7.5642
7.5608
7.5458
7.5428
7.5399
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7.5217
7.5144
7.5114
7.4975
7.4943
7.4910
7.4770
7.4740
7.4050
7.4024
7.3861
7.3836
7.3674
7.3649
N
N
N
N
F
3na
2.01
1.00
2.02
0.97
1.01
1.05
1.05
1.03
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
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1.0
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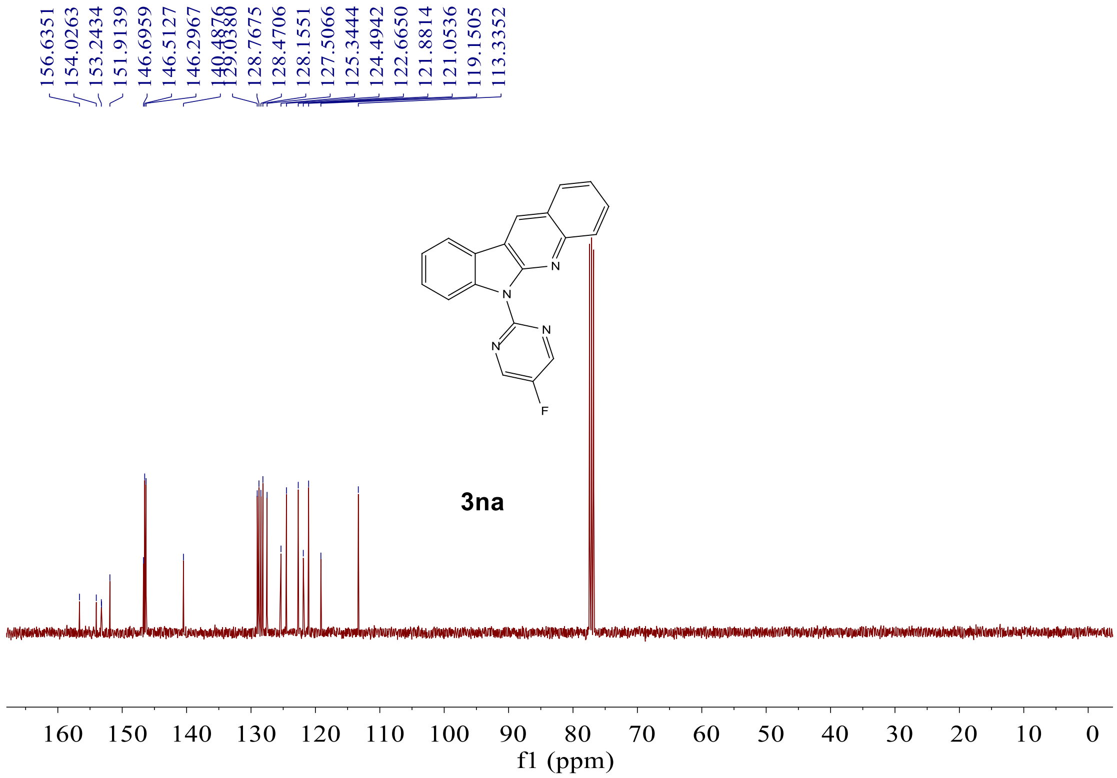
0.0
f1 (ppm)



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146.5127
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128.4706
128.1551
127.5066
125.3444
124.4942
122.6650
121.8814
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113.3352
N
N
N
N
F
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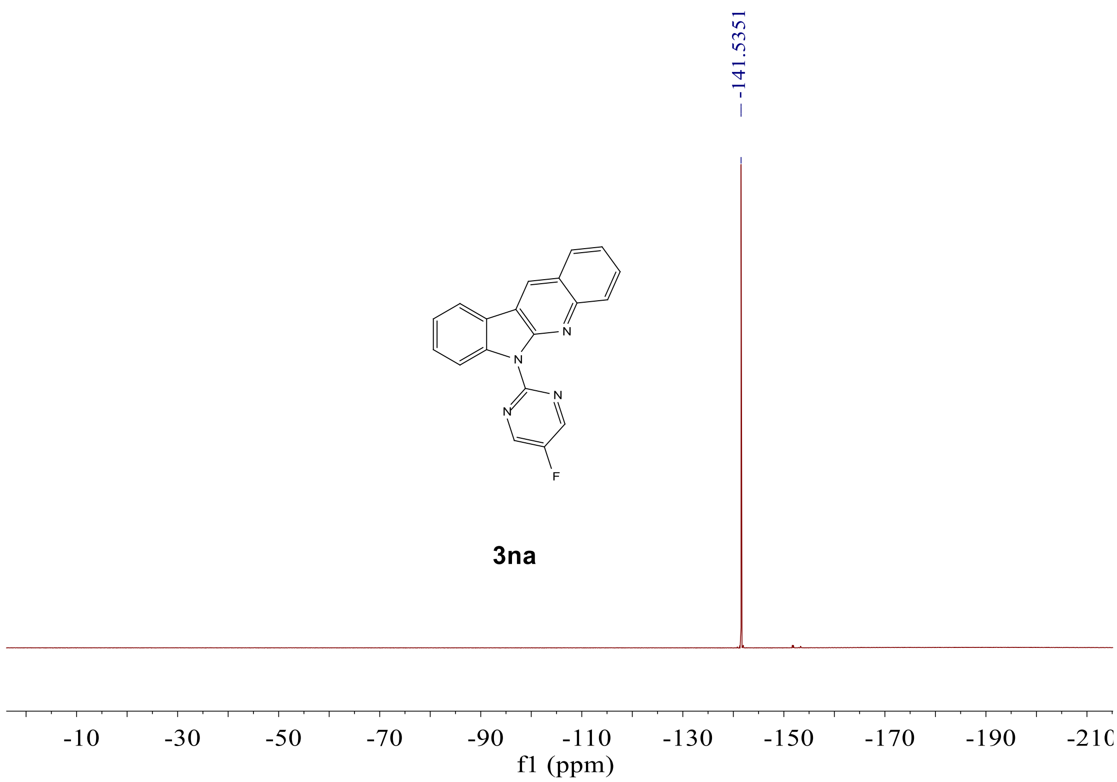
f1 (ppm)



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N
N
F
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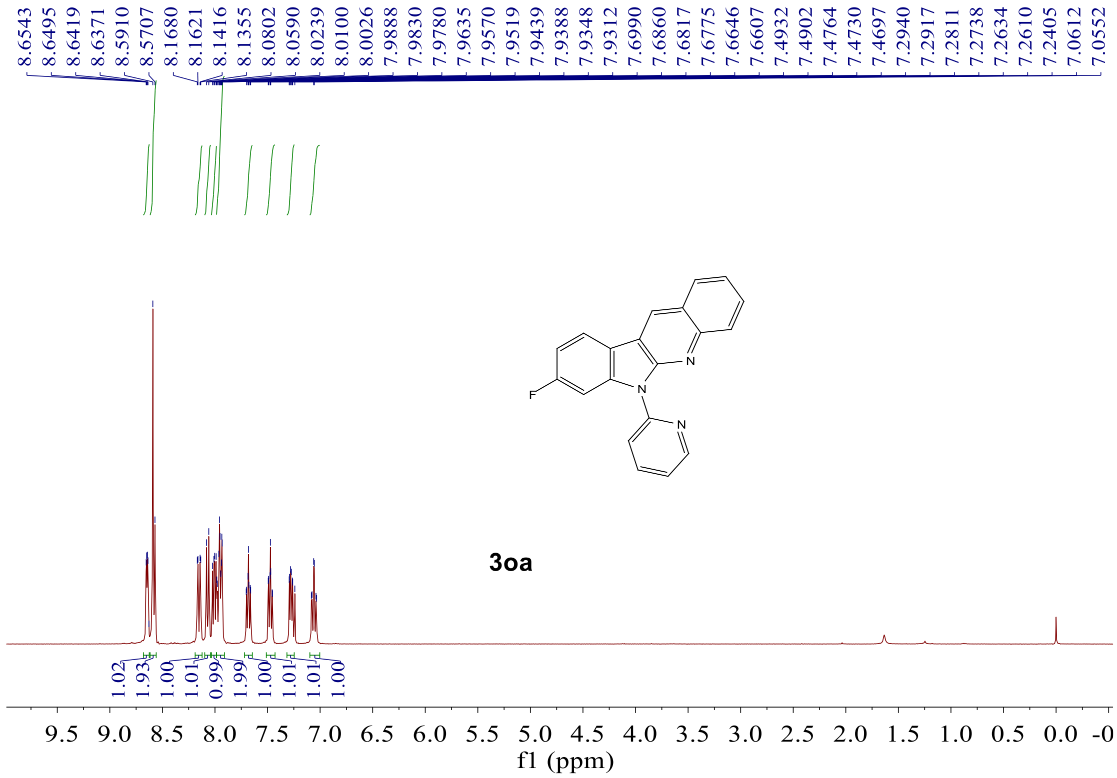
-10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)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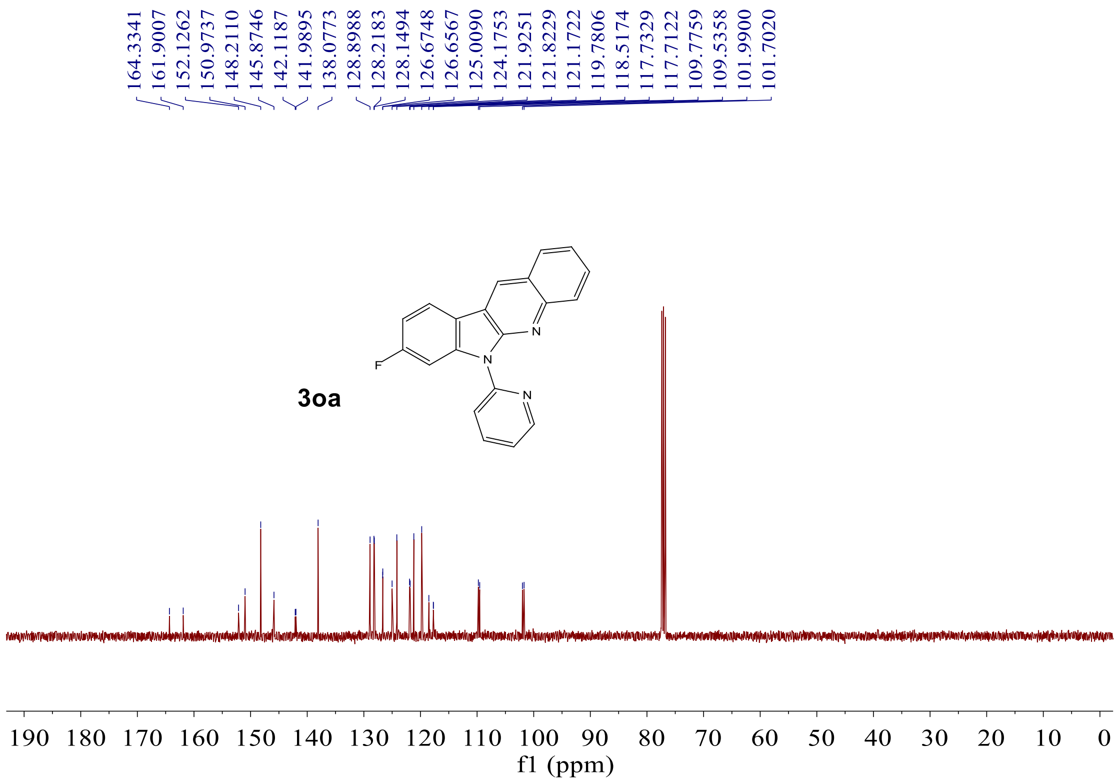
8.0590
8.0239
8.0100
8.0026
7.9888
7.9830
7.9780
7.9635
7.9570
7.9519
7.9439
7.9388
7.9348
7.9312
7.6990
7.6860
7.6817
7.6775
7.6646
7.6607
7.4932
7.4902
7.4764
7.4730
7.4697
7.2940
7.2917
7.2811
7.2738
7.2634
7.2610
7.2405
7.0612
7.0552
F
N
N
N
3oa
1.02
1.93
1.00
1.01
0.99
1.99
1.00
1.01
1.01
1.00
9.5 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
f1 (ppm)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128.1494
126.6748
126.6567
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124.1753
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121.8229
121.1722
119.7806
118.5174
117.7329
117.7122
109.7759
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F
N
N
N
3oa
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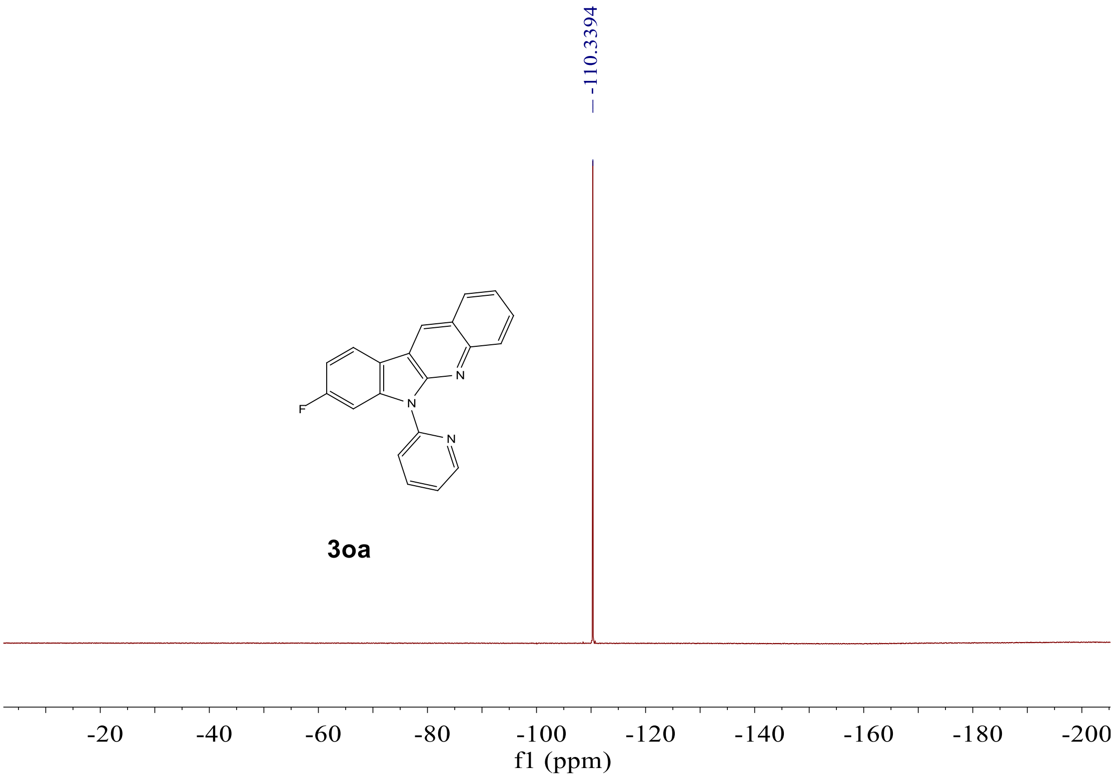
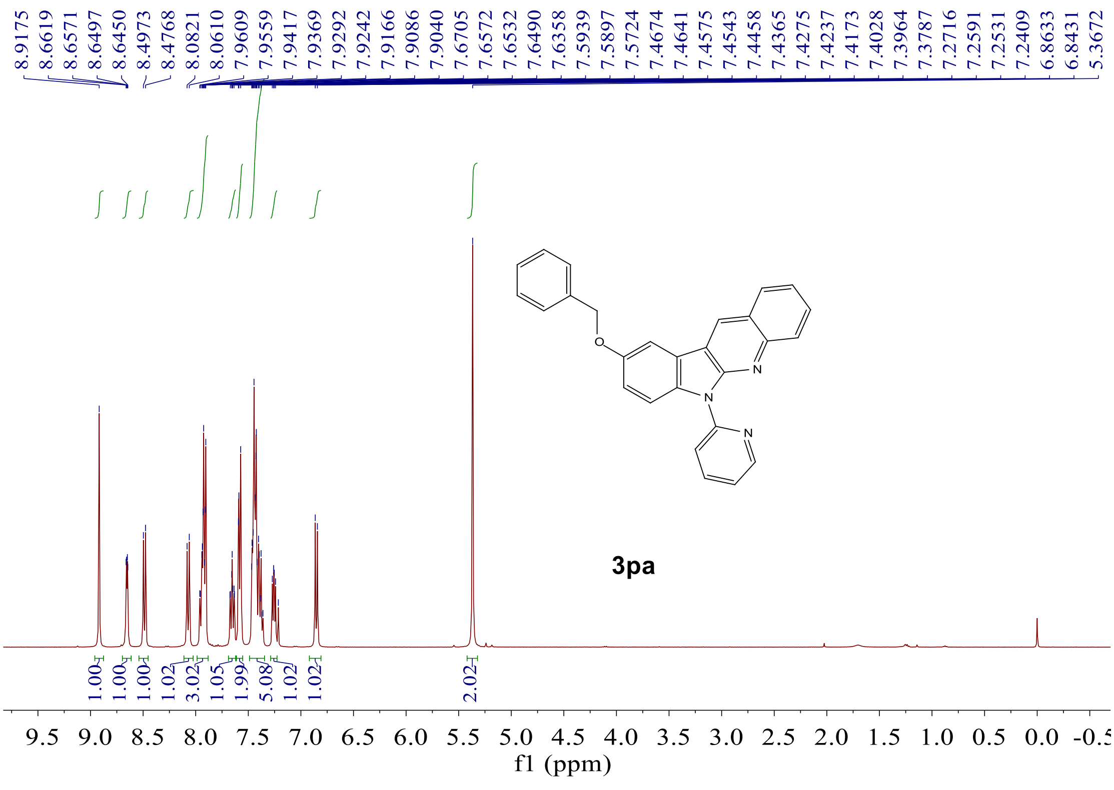
f1 (ppm)



3oa



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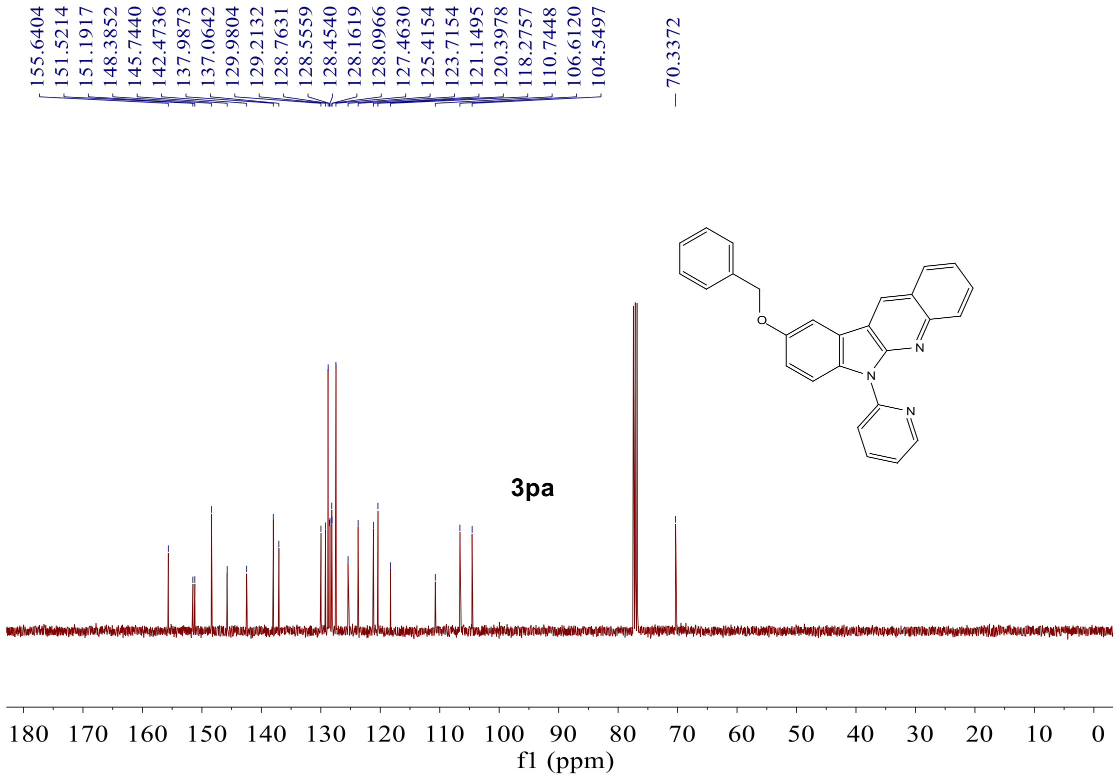
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128.4540
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125.4154
123.7154
121.1495
120.3978
118.2757
110.7448
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N
O
N
N
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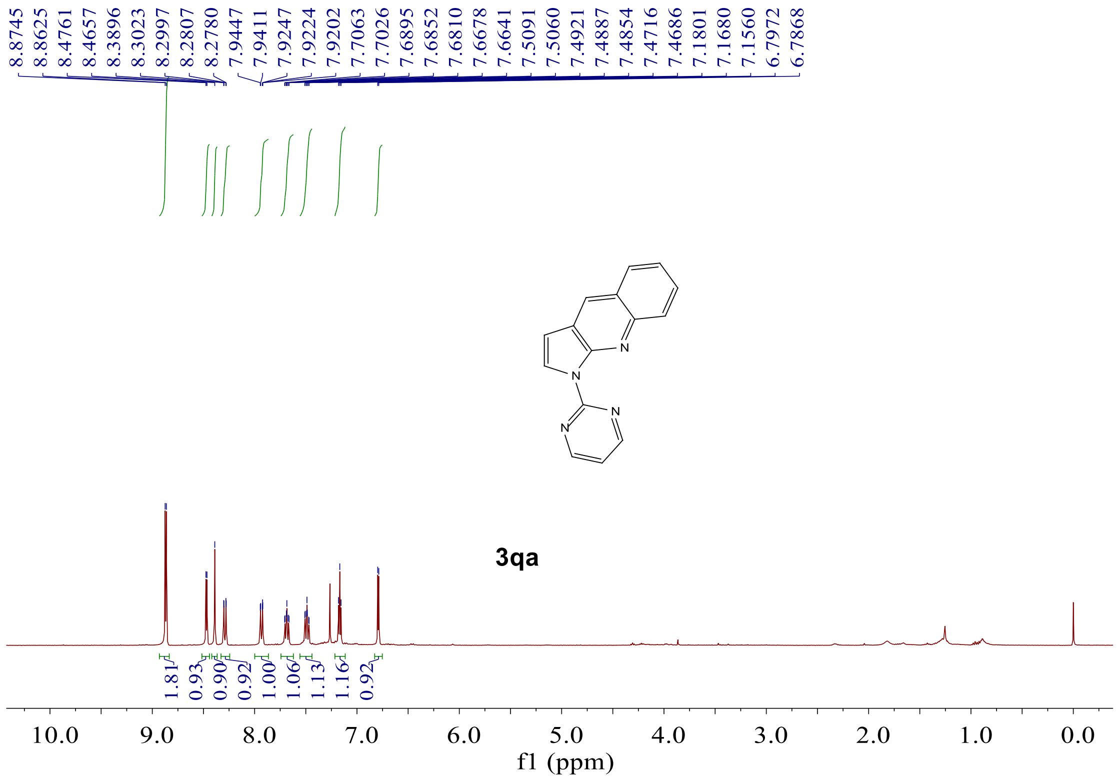
f1 (ppm)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7.9224
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7.7063
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7.6895
7.6852
7.6810
7.6678
7.6641
7.5091
7.5060
7.4921
7.4887
7.4854
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7.4686
7.1801
7.1680
7.1560
6.7972
6.7868
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N
N
N
3qa
1.81
0.93
0.90
0.92
1.00
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1.13
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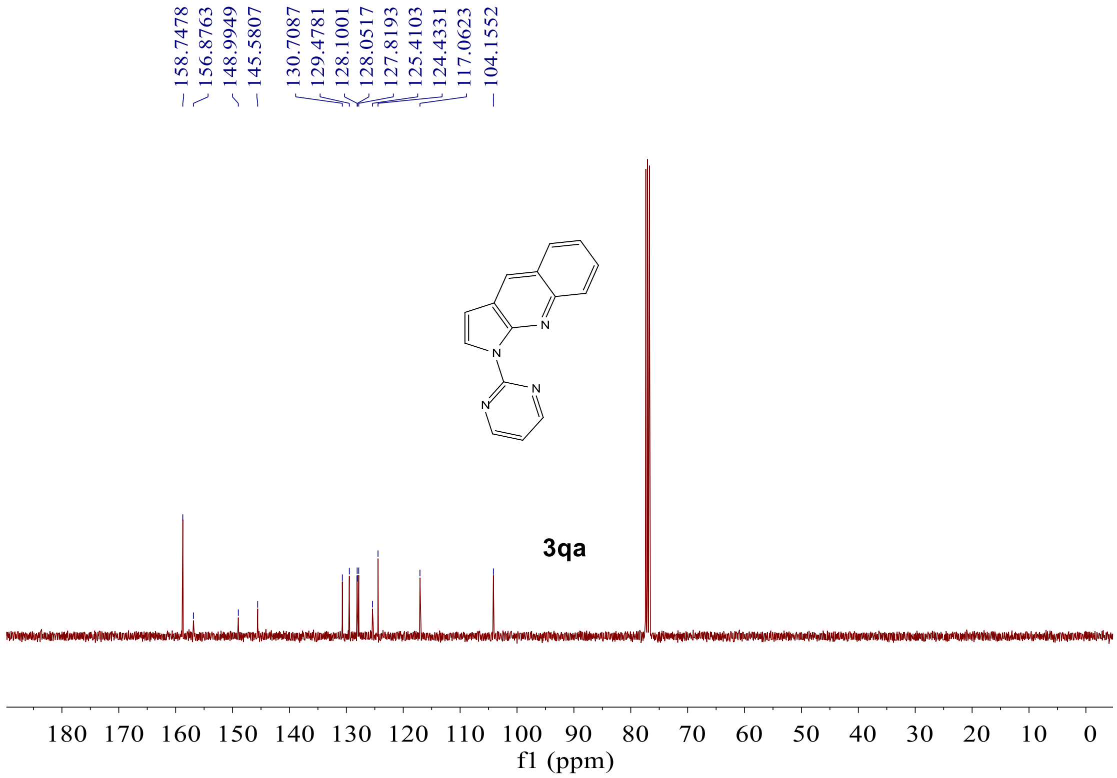
0.92
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)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f1 (ppm)

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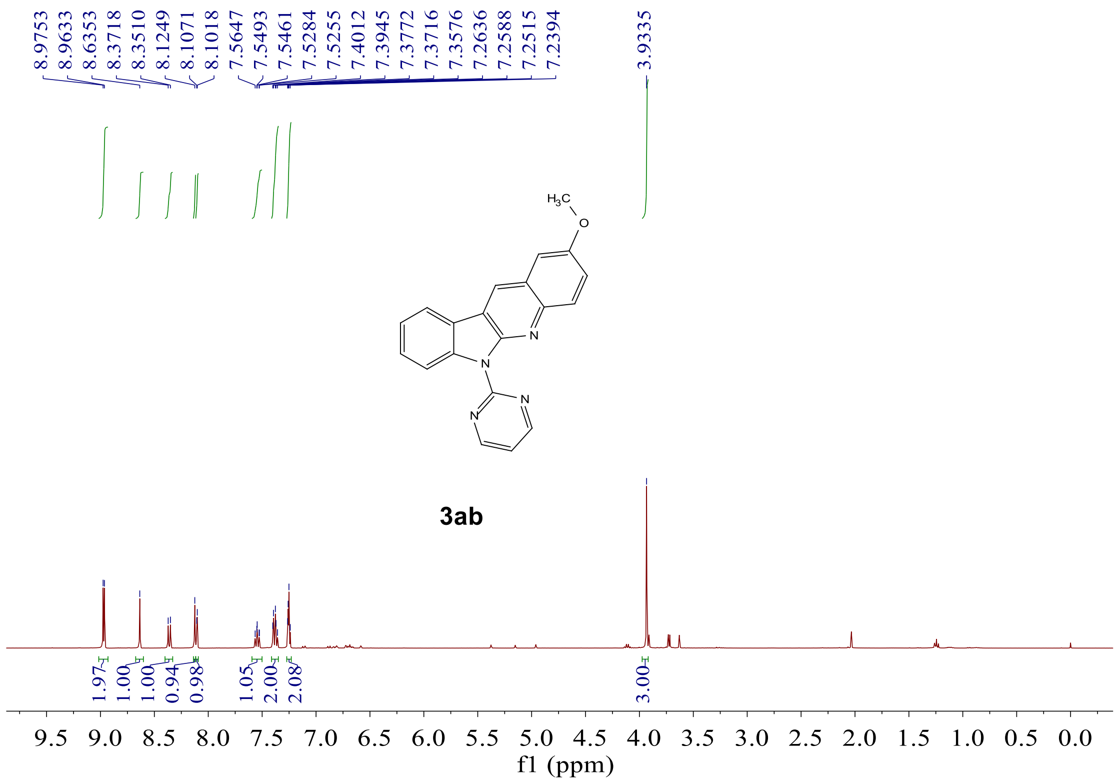
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7.5255
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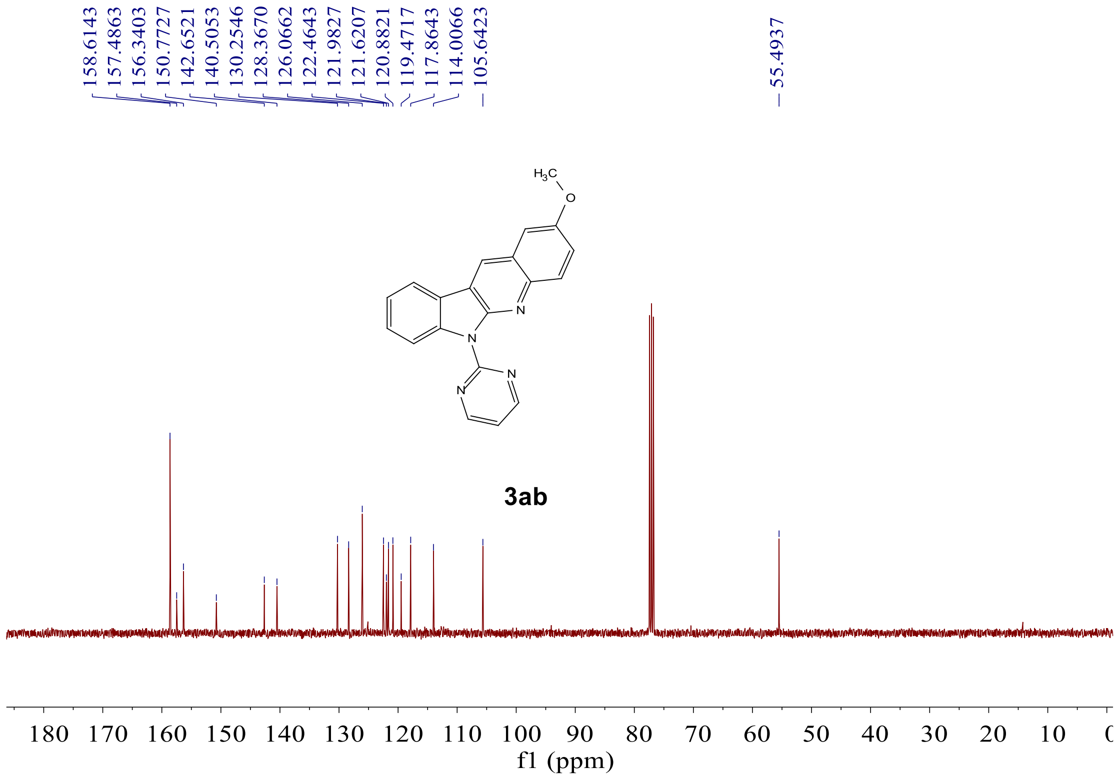
7.3716
7.3576
7.2636
7.2588
7.2515
7.2394
3.9335
H3C
O
N
N
N
N
1.97
1.00
1.00
0.94
0.98
1.05
2.00
2.08
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3ab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121.6207
120.8821
119.4717
117.8643
114.0066
105.6423
55.4937
H_3C
O
N
N
N
N
3ab
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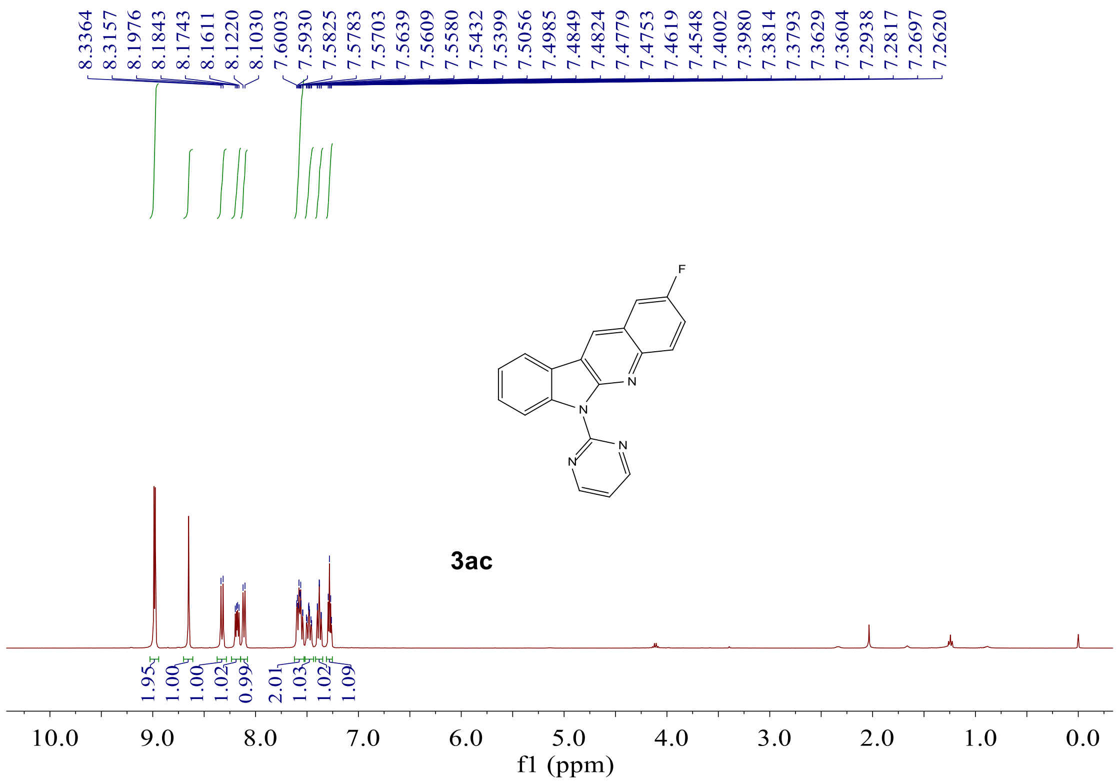
f1 (ppm)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8.1220
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7.5825
7.5783
7.5703
7.5639
7.5609
7.5580
7.5432
7.5399
7.5056
7.4985
7.4849
7.4824
7.4779
7.4753
7.4619
7.4548
7.4002
7.3980
7.3814
7.3793
7.3629
7.3604
7.2938
7.2817
7.2697
7.2620
F
N
N
N
N
3ac
1.95
1.00
1.00
1.02
0.99
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1.03
1.02
1.09
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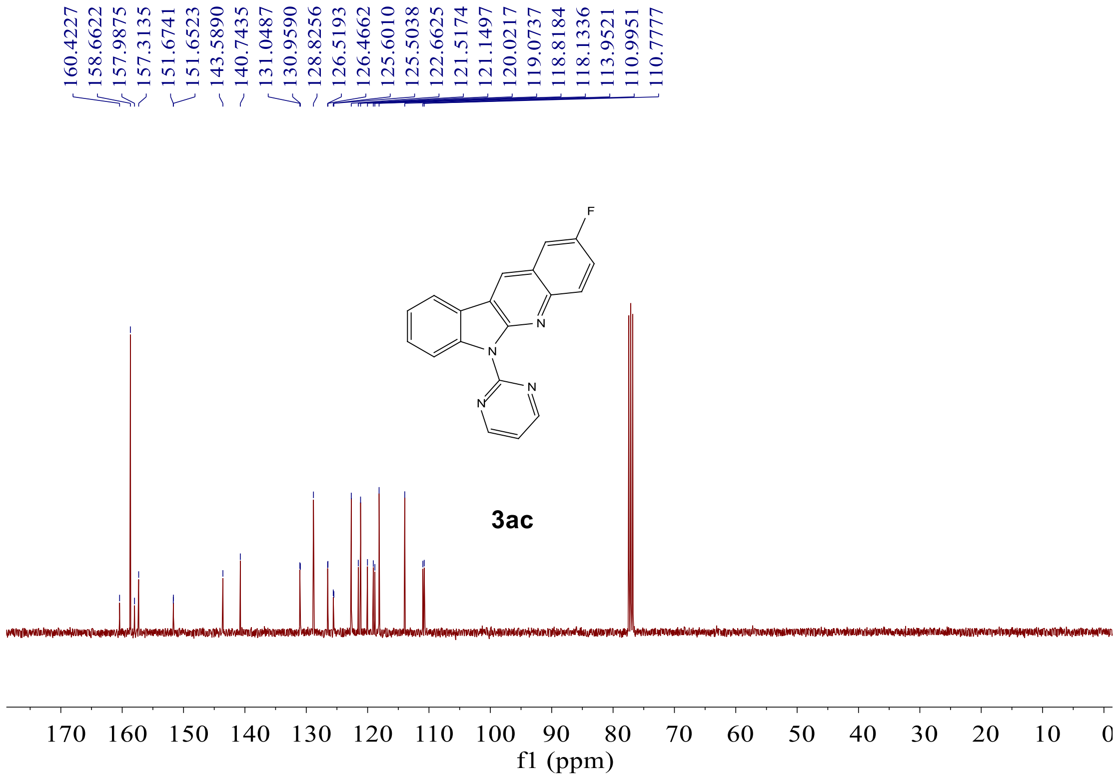
f1 (ppm)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121.1497
120.0217
119.0737
118.8184
118.1336
113.9521
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N
N
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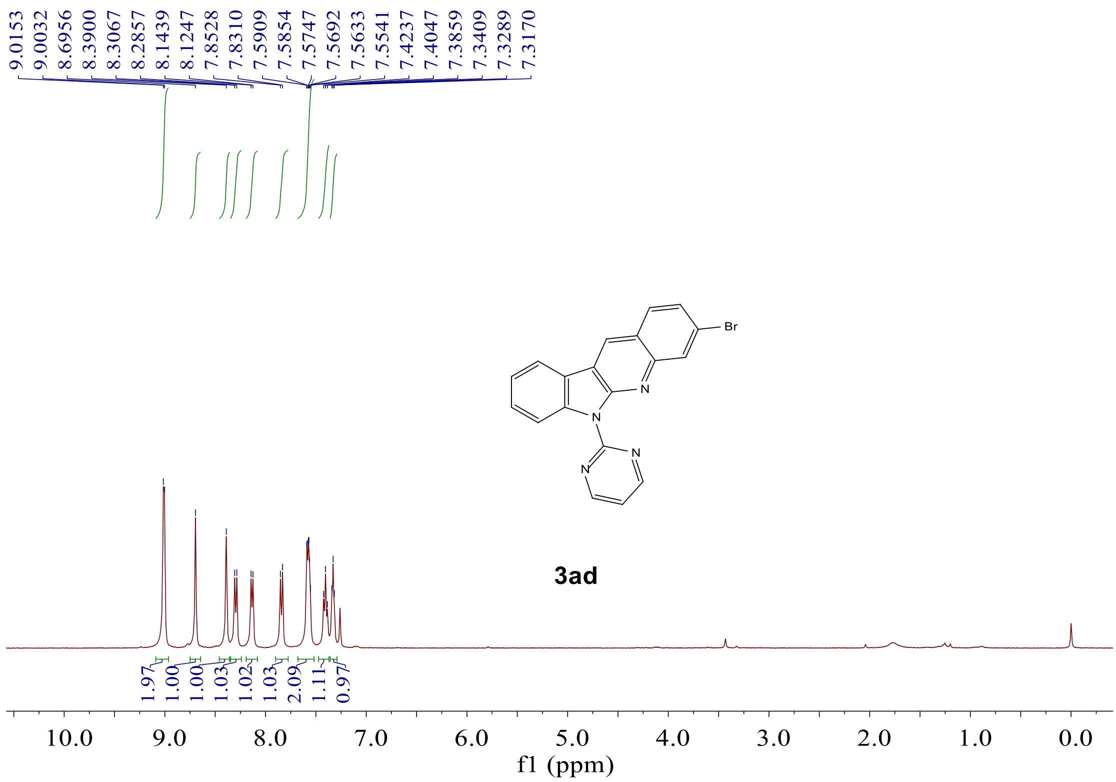
f1 (ppm)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7.5747
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7.5633
7.5541
7.4237
7.4047
7.3859
7.3409
7.3289
7.3170
Br
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N
N
N
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1.97
1.00
1.00
1.03
1.02
1.03
2.09
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0.97
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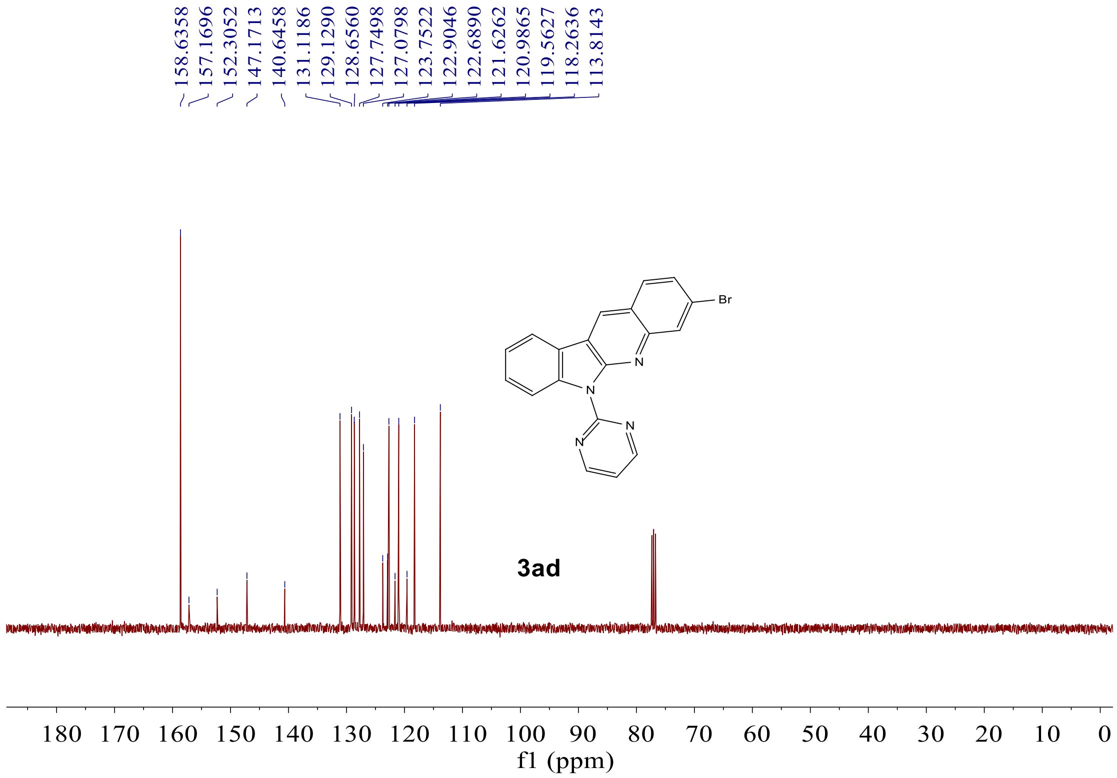
f1 (ppm)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120.9865
119.5627
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Br
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N
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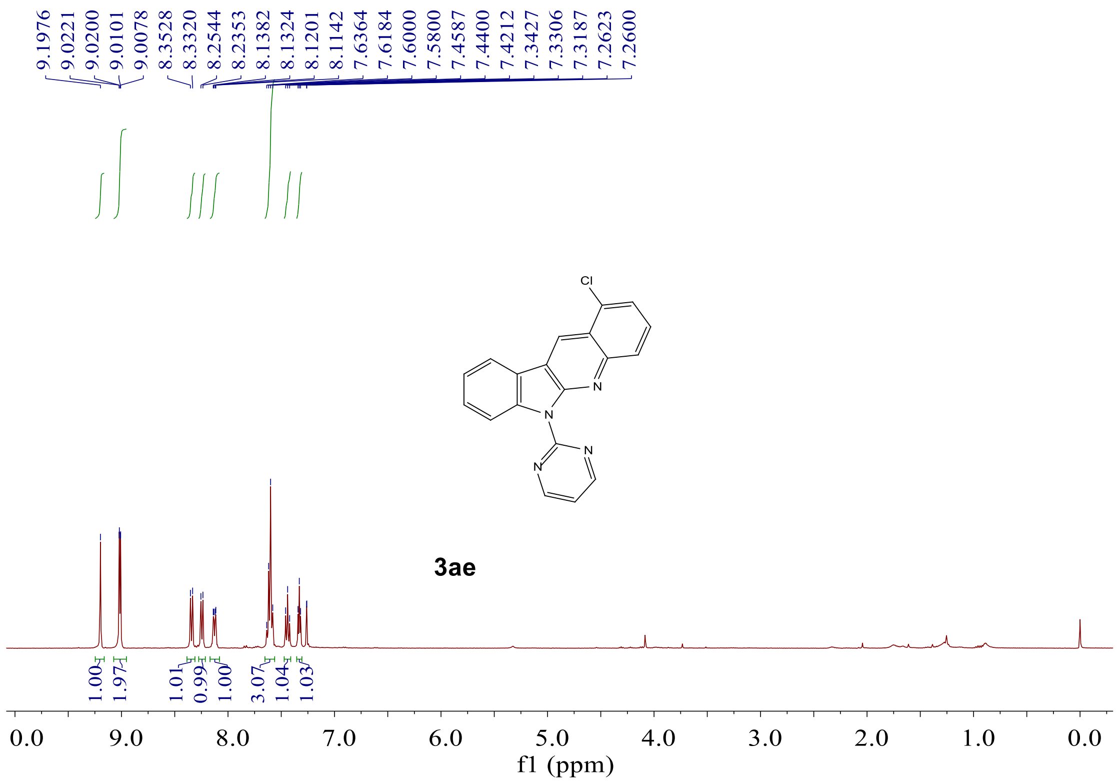
f1 (ppm)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8.1201
8.1142
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7.6184
7.6000
7.5800
7.4587
7.4400
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7.3187
7.2623
7.2600
Cl
N
N
N
N
3ae
1.00
1.97
1.01
0.99
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3.07
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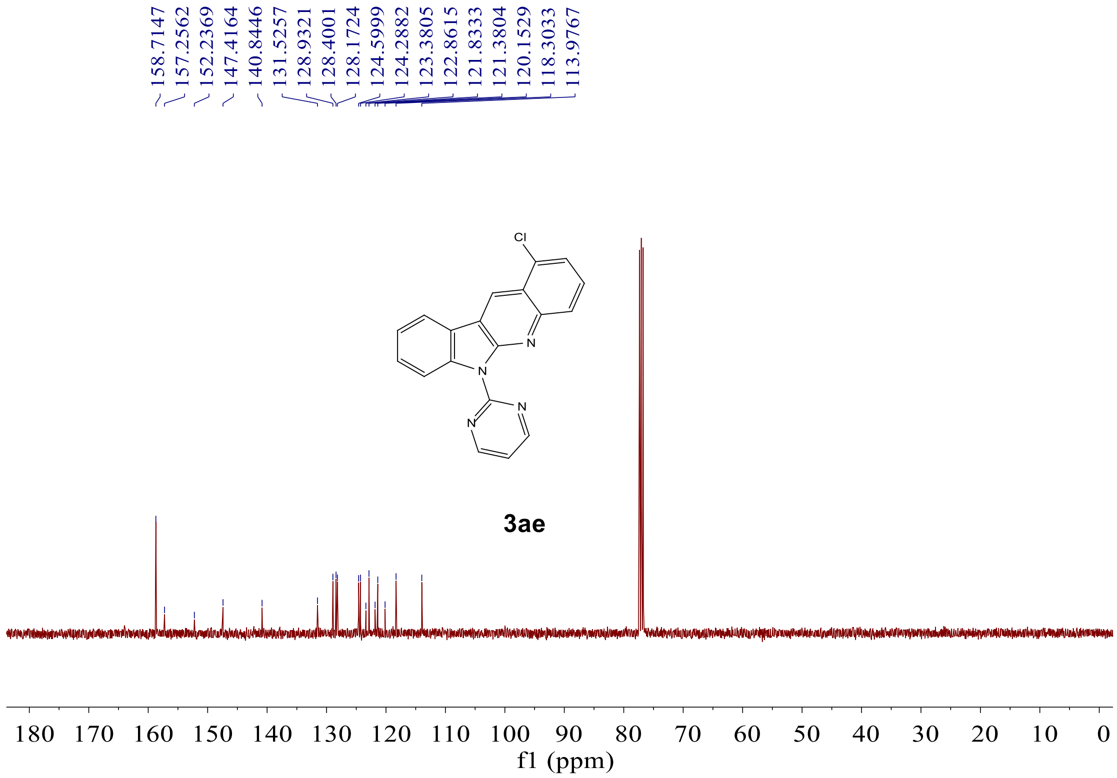
1.03
0.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)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121.8333
121.3804
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N
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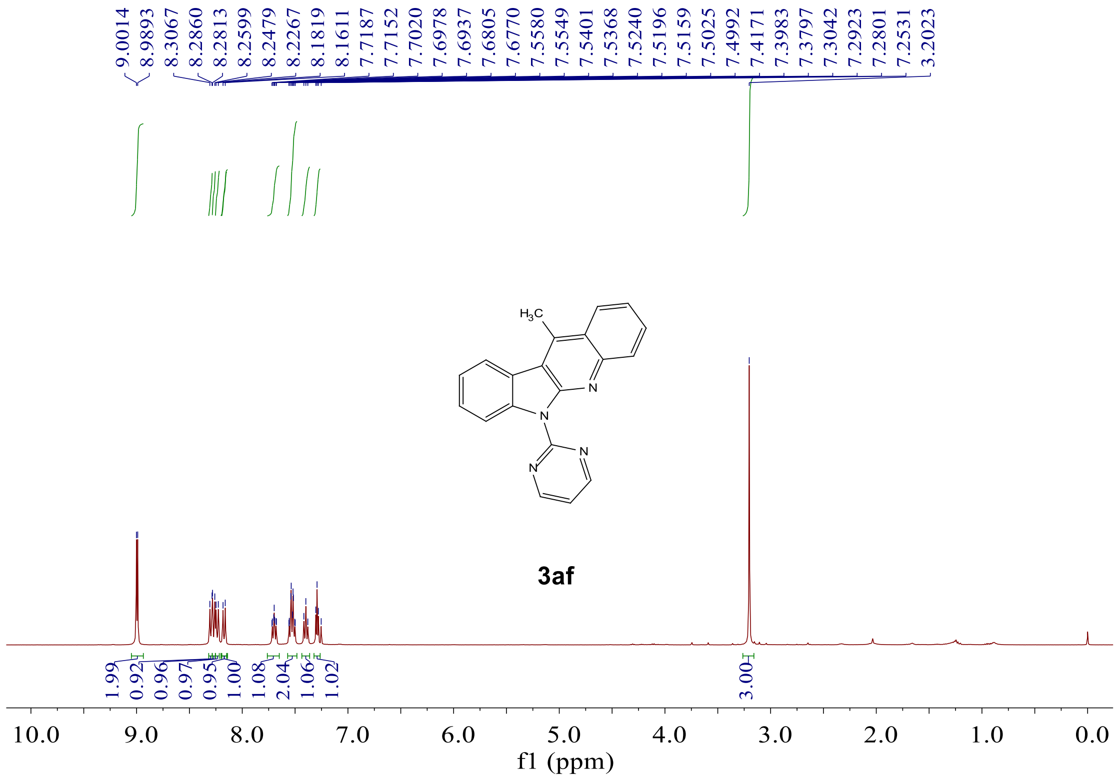
f1 (ppm)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0.96
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0.95
1.00
1.08
2.04
1.06
1.02
3.00
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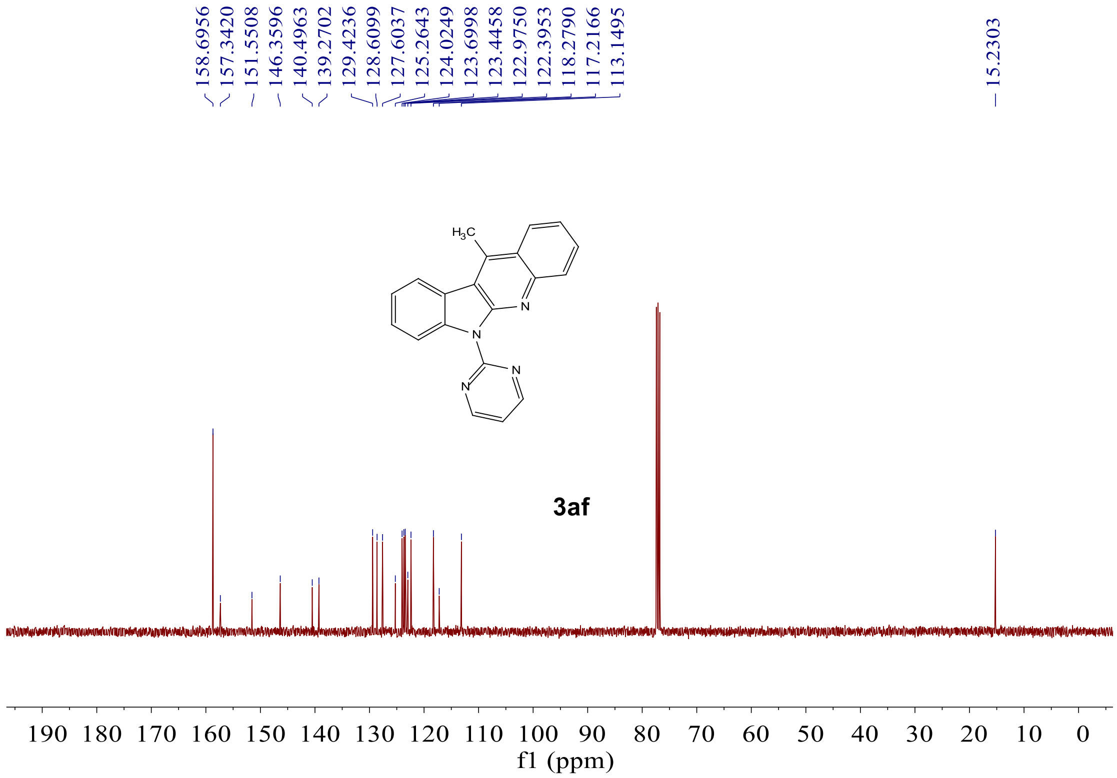
f1 (ppm)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122.9750
122.3953
118.2790
117.2166
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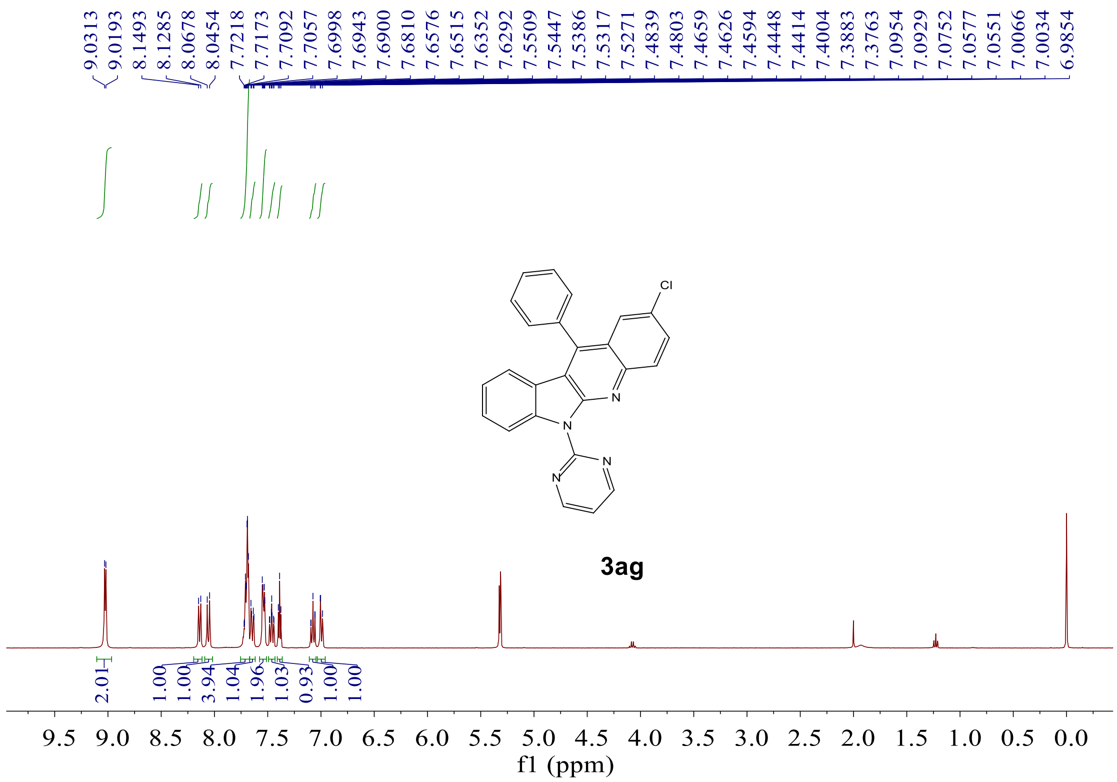
N
N
N
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3af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1.00
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1.96
1.03
0.93
1.00
1.00
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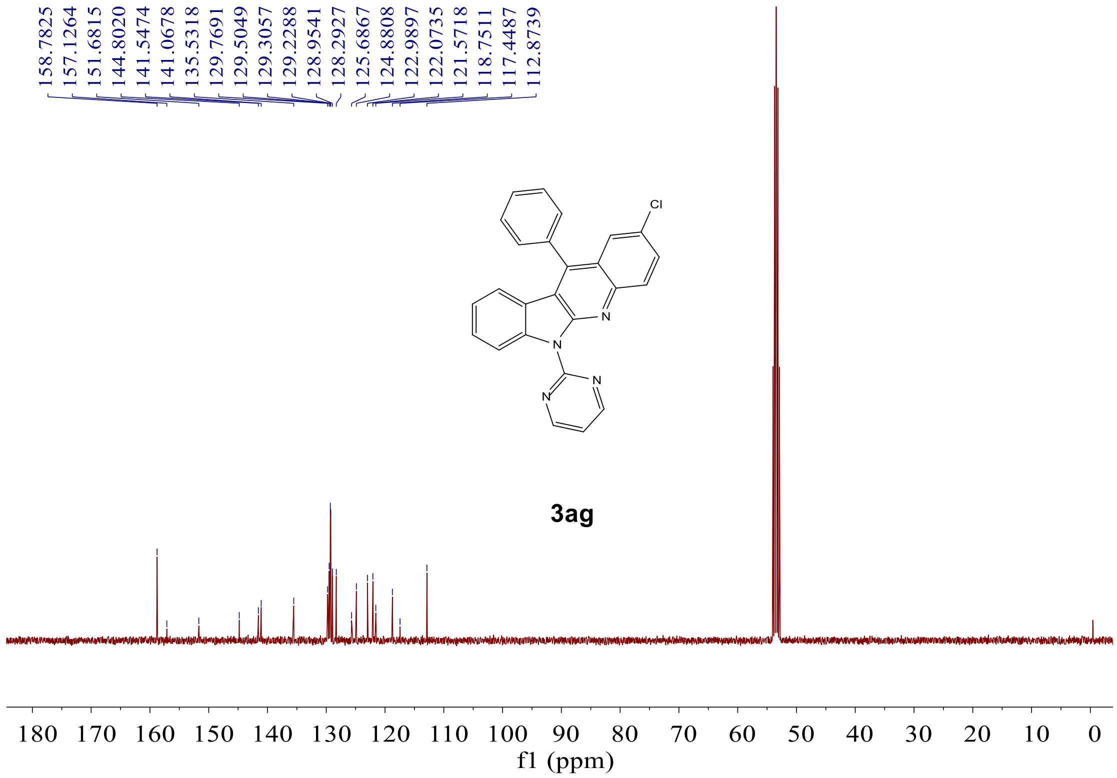
f1 (ppm)

3ag



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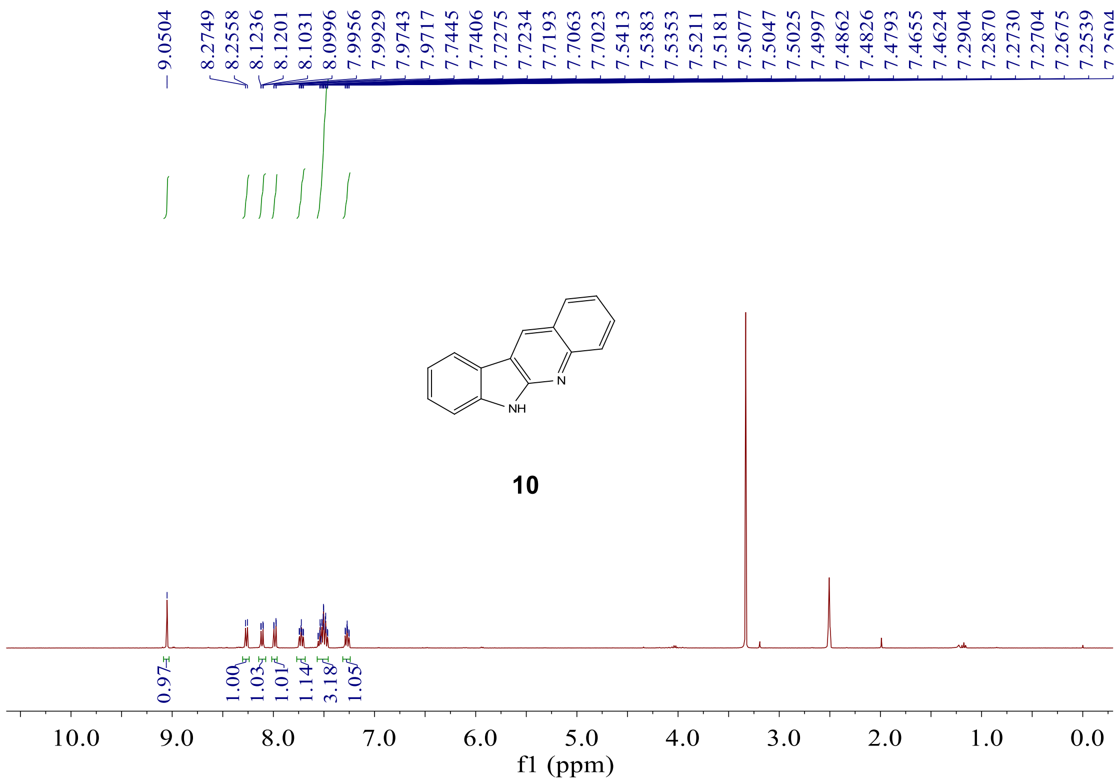
N
N
N
f1 (ppm)

3ag



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7.9956
7.9929
7.9743
7.9717
7.7445
7.7406
7.7275
7.7234
7.7193
7.7063
7.7023
7.5413
7.5383
7.5353
7.5211
7.5181
7.5077
7.5047
7.5025
7.4997
7.4862
7.4826
7.4793
7.4655
7.4624
7.2904
7.2870
7.2730
7.2704
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NH
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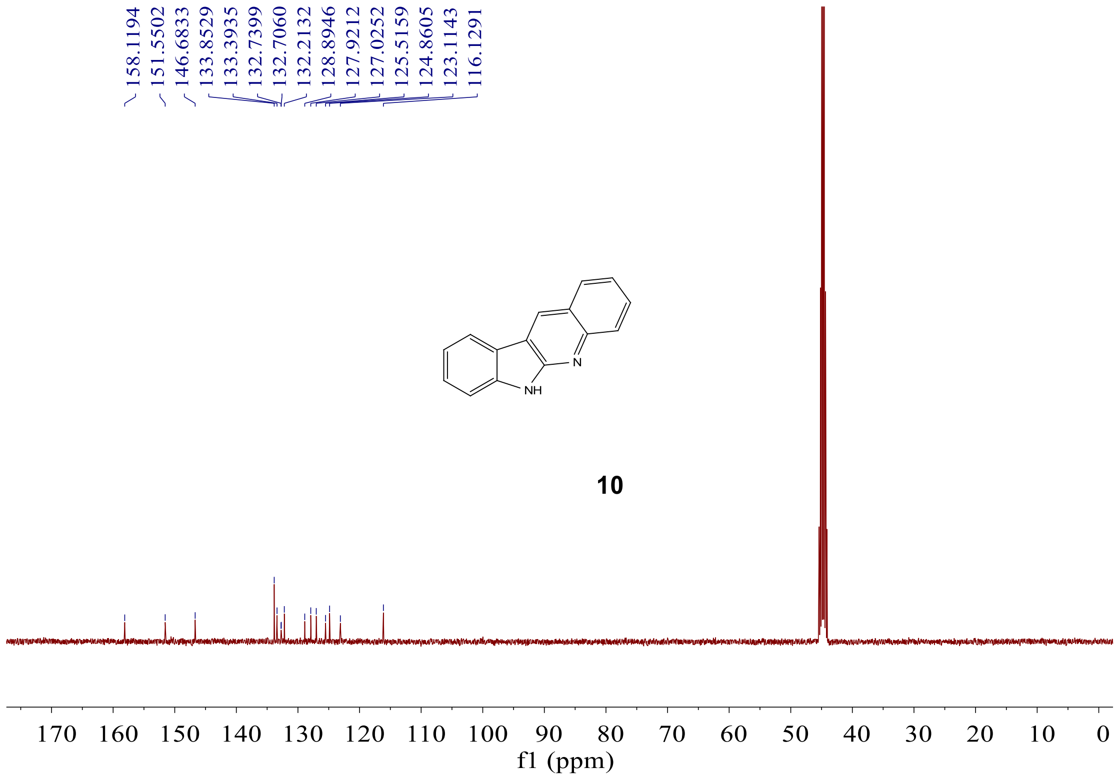
1.03
1.01
1.14
3.18
1.05
f1 (ppm)

10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127.0252
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123.1143
116.1291
NH
N
10
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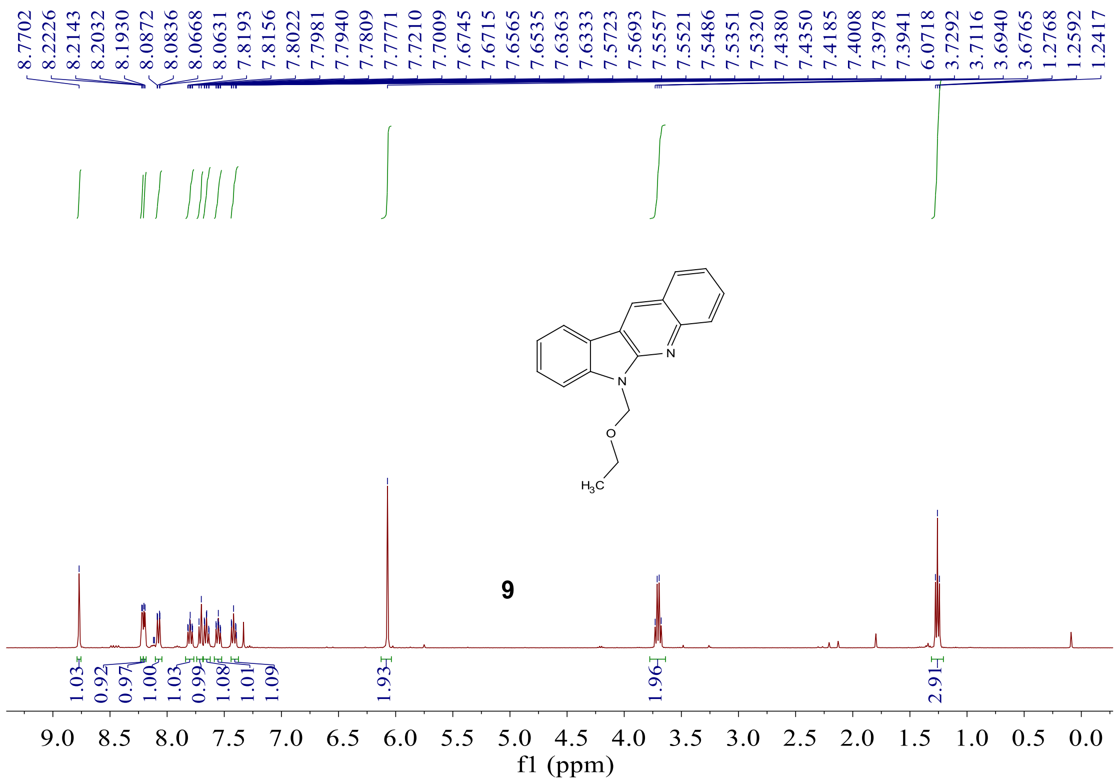
f1 (ppm)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8.2143
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8.1930
8.0872
8.0836
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8.0631
7.8193
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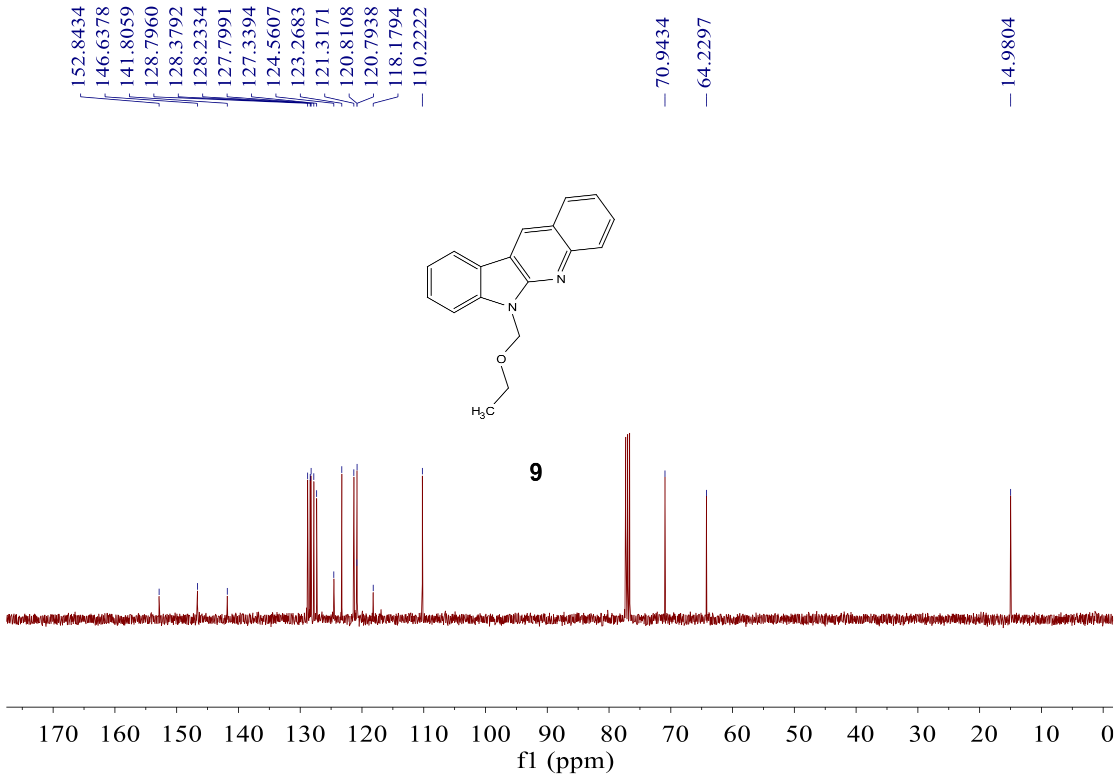
7.8022
7.7981
7.7940
7.7809
7.7771
7.7210
7.7009
7.6745
7.6715
7.6565
7.6535
7.6363
7.6333
7.5723
7.5693
7.5557
7.5521
7.5486
7.5351
7.5320
7.4380
7.4350
7.4185
7.4008
7.3978
7.3941
6.0718
3.7292
3.7116
3.6940
3.6765
1.2768
1.2592
1.2417
N
N
O
H_3C
9
1.03
0.92
0.97
1.00
1.03
0.99
1.08
1.01
1.09
1.93
1.96
2.91
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
f1 (ppm)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121.3171
120.8108
120.7938
118.1794
110.2222
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N
N
O
H_3C
9
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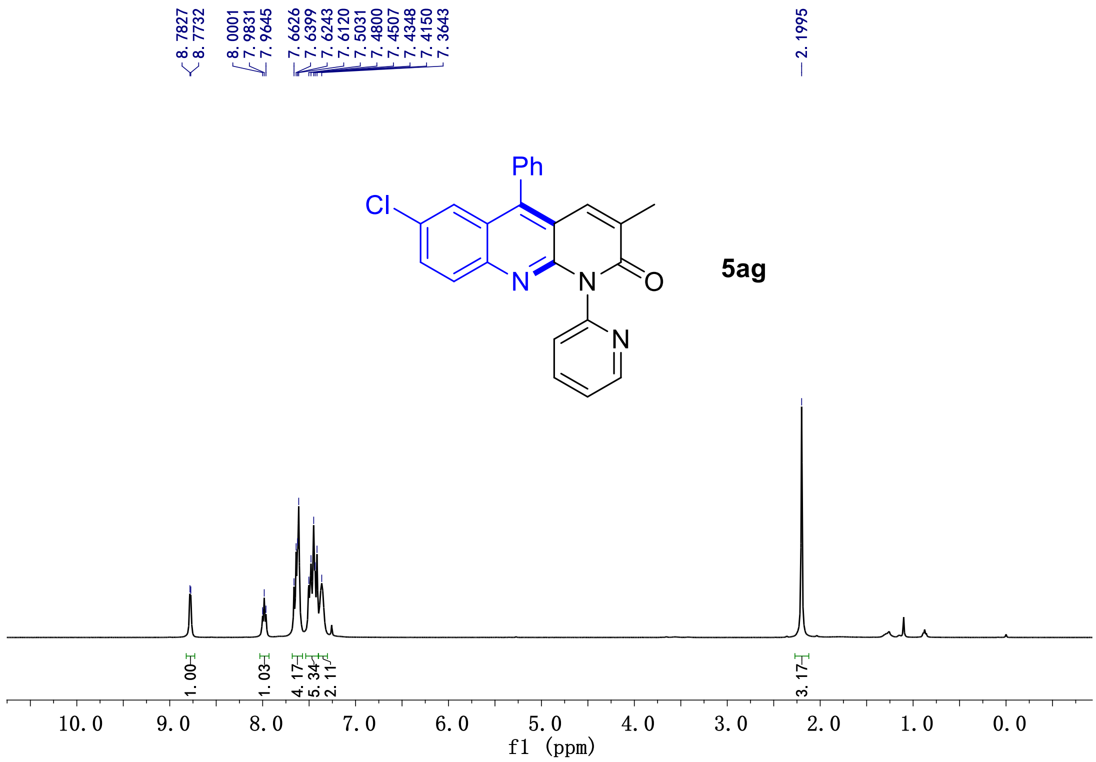
f1 (ppm)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8.7732
8.0001
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7.6399
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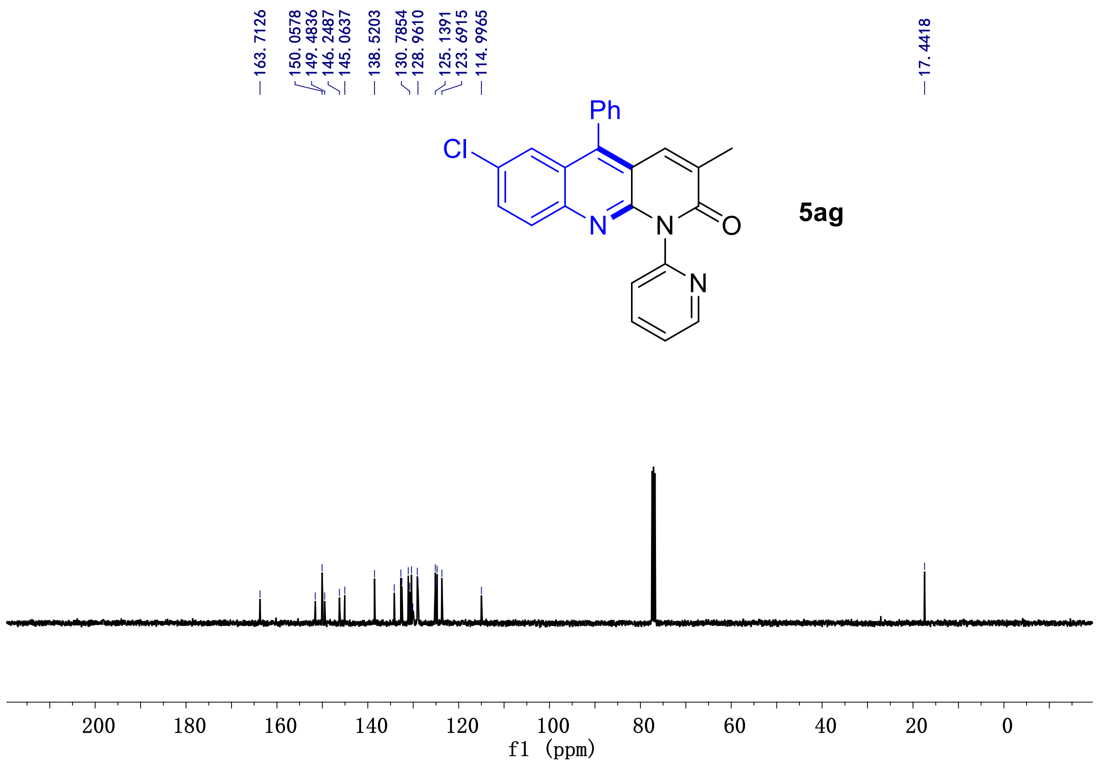
7.5031
7.4800
7.4507
7.4348
7.4150
7.3643
2.1995
Ph
Cl
N
N
O
N
5ag
1.00
1.03
4.17
5.34
2.11
3.17
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)



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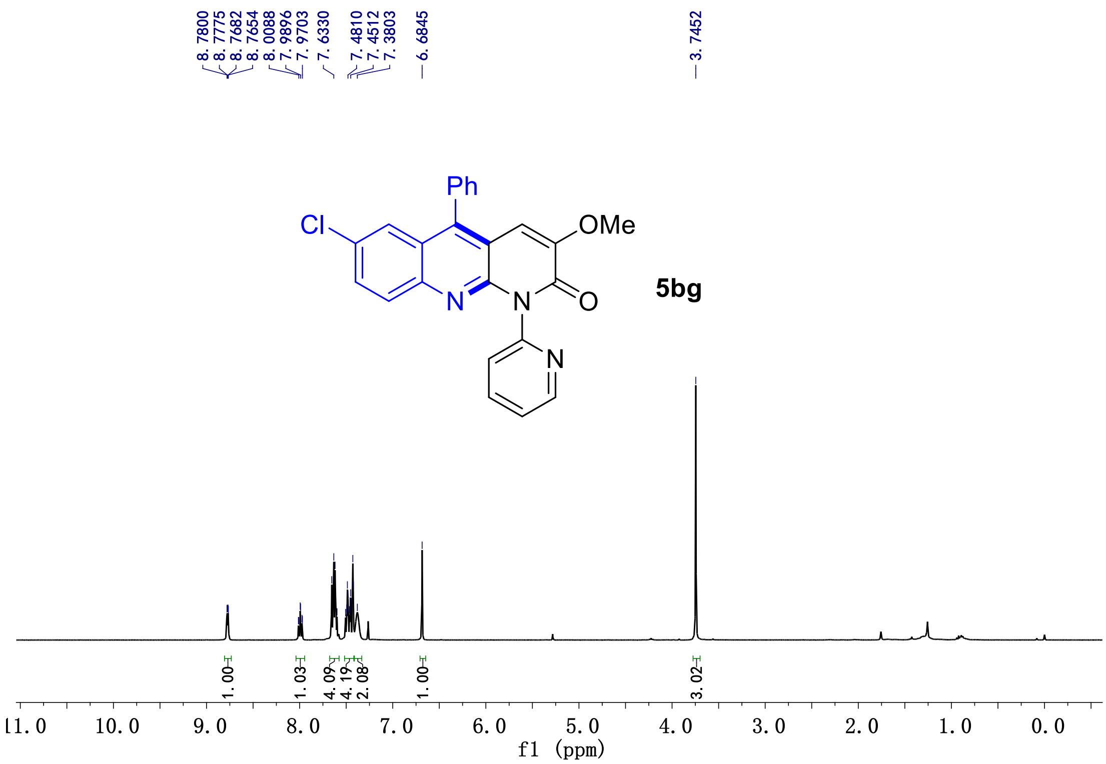
130.7854
128.9610
125.1391
123.6915
114.9965
17.4418
Ph
Cl
N
N
O
N
5ag
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)



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8.7682
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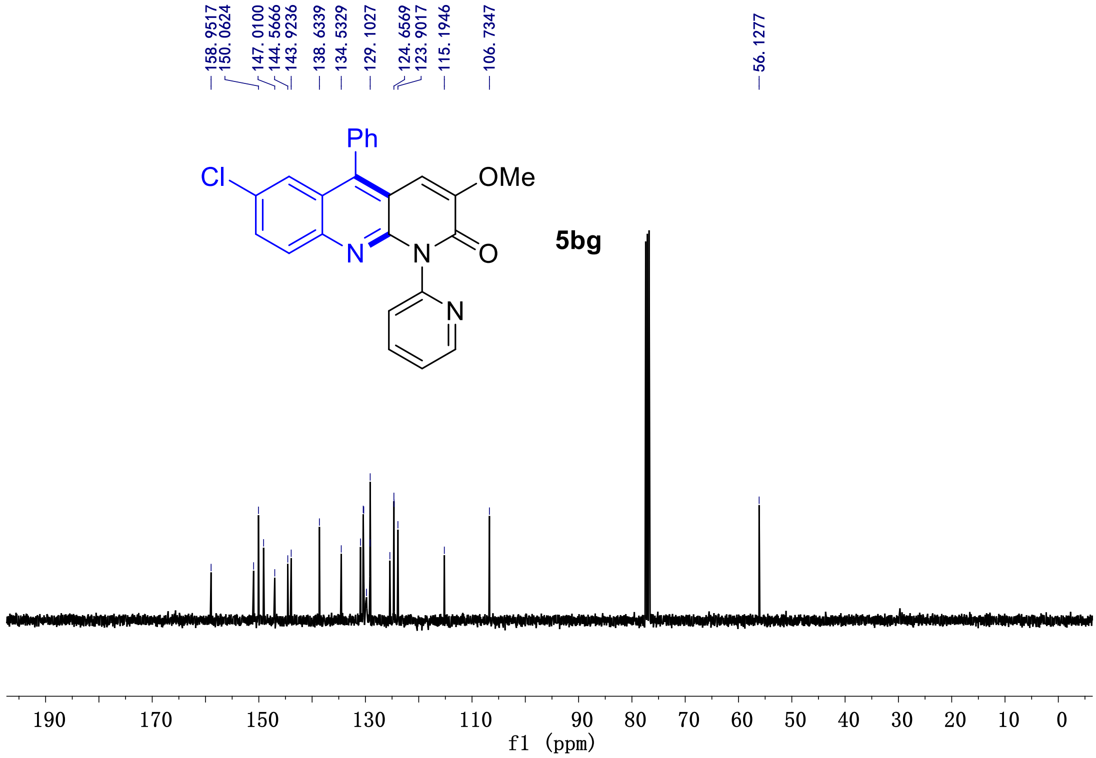
8.0088
7.9896
7.9703
7.6330
7.4810
7.4512
7.3803
6.6845
3.7452
Ph
Cl
OMe
N
N
O
N
5bg
1.00
1.03
4.09
4.19
2.08
1.00
3.02
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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115.1946
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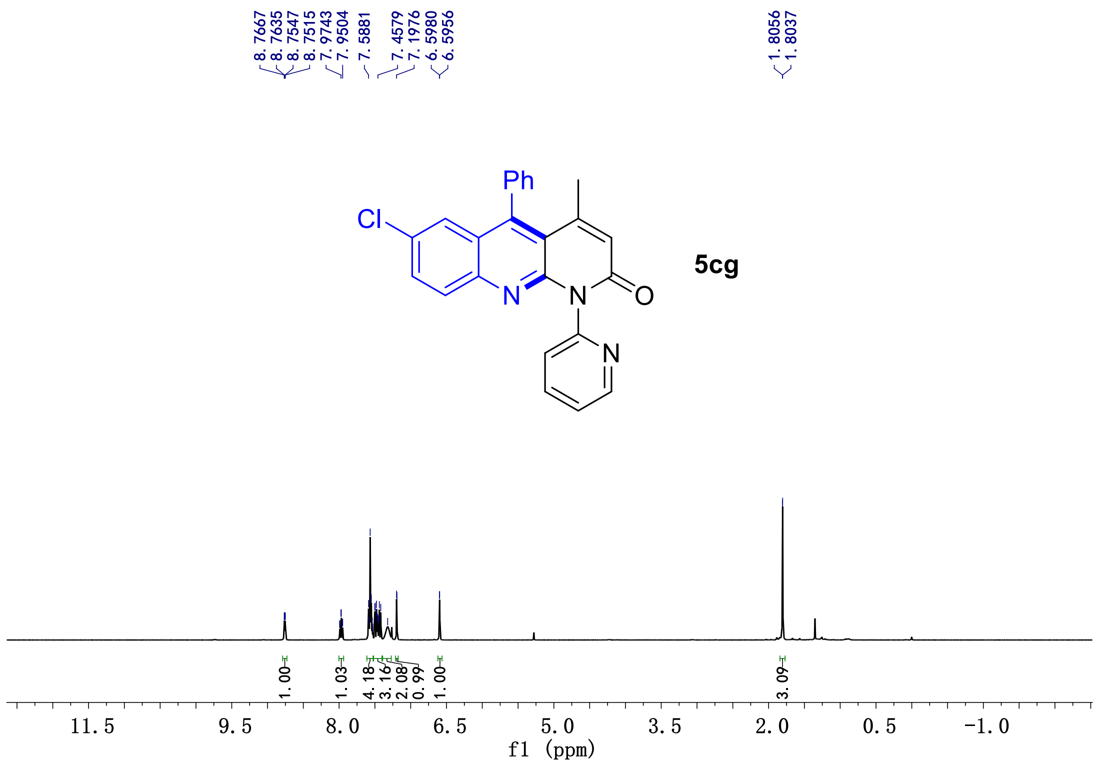
Ph
Cl
OMe
N
N
O
N
190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

5bg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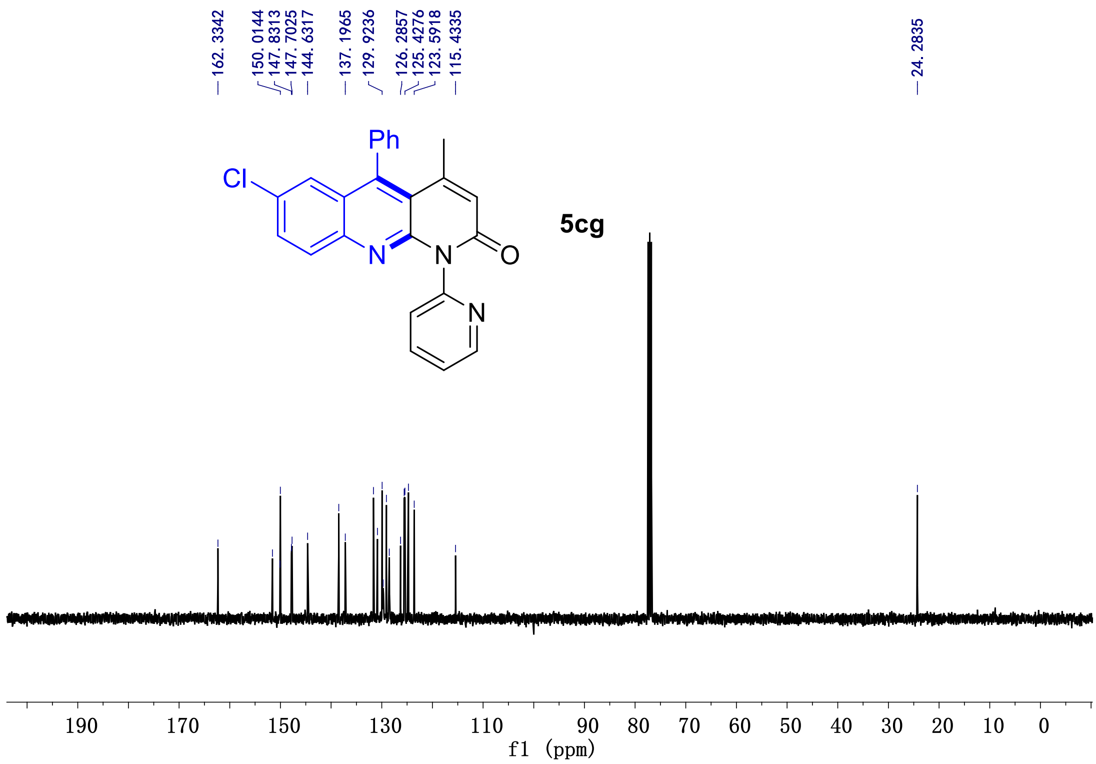
8.7635
8.7547
8.7515
7.9743
7.9504
7.5881
7.4579
7.1976
6.5980
6.5956
1.8056
1.8037
Ph
Cl
N
N
O
N
1.00
1.03
4.18
3.16
2.08
0.99
1.00
3.09
11.5 9.5 8.0 6.5 5.0 3.5 2.0 0.5 -1.0
f1 (ppm)

5cg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129.9236
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125.4276
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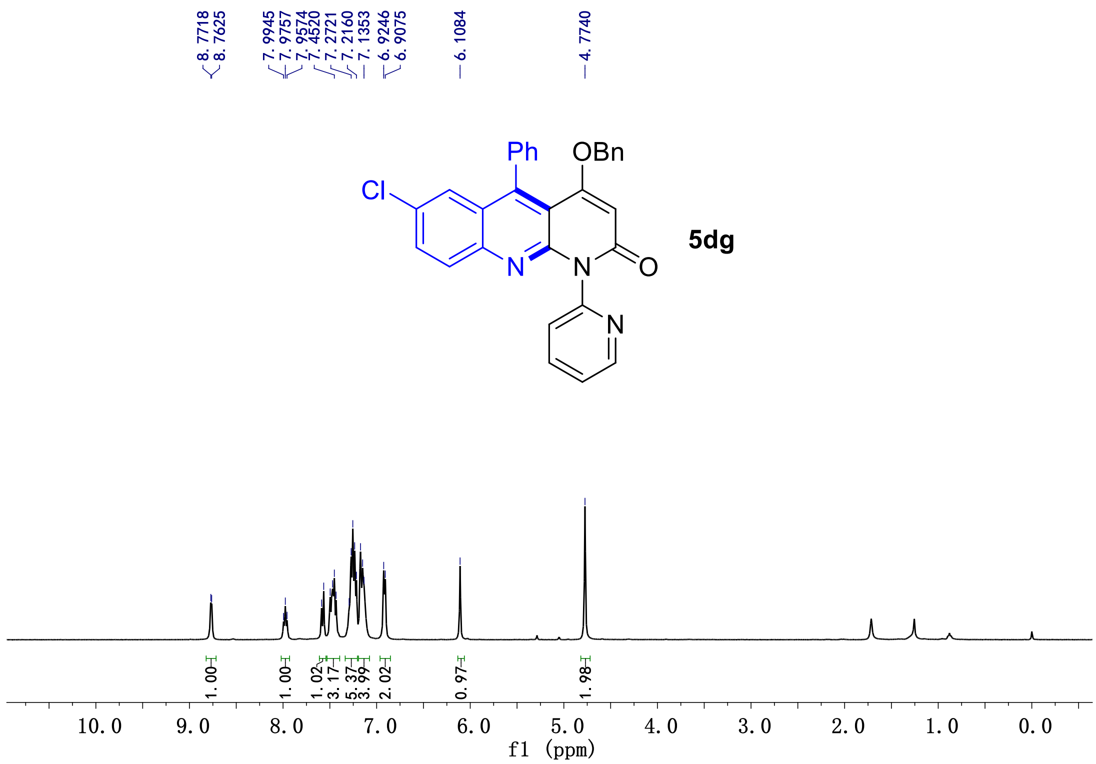
115.4335
24.2835
Ph
Cl
N
N
O
N
5cg
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.2721
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7.1353
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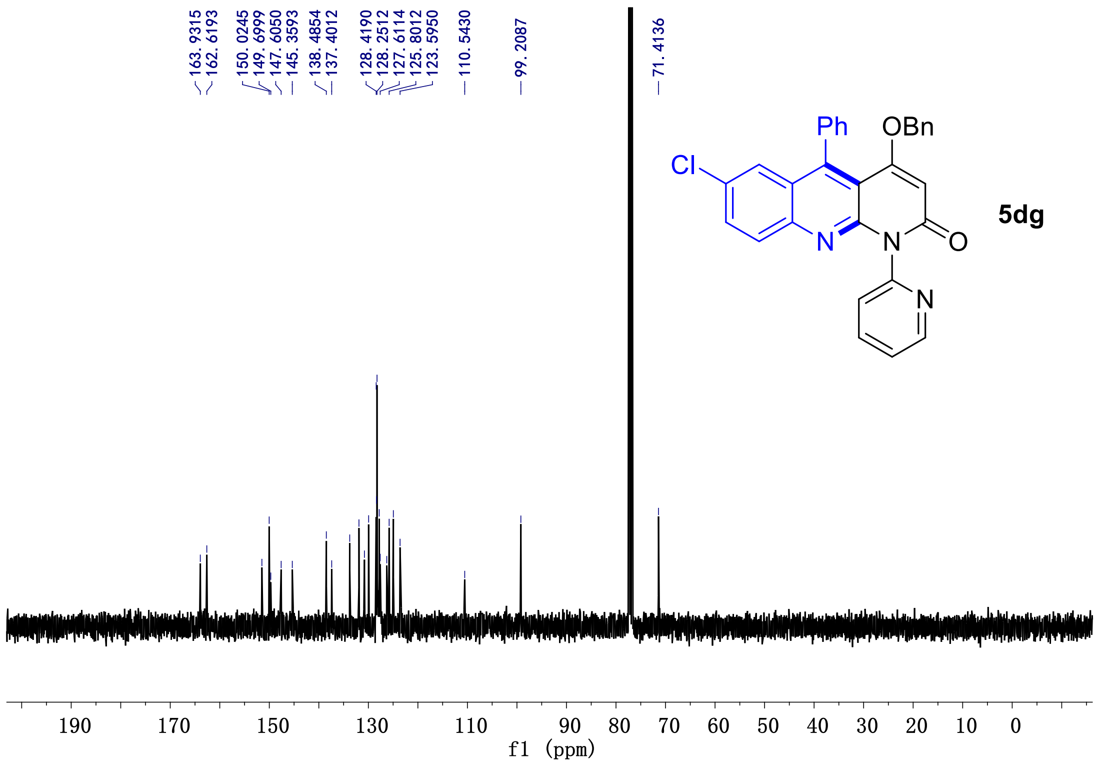
6.9075
6.1084
4.7740
Ph
OBn
Cl
N
N
O
N
5dg
1.00
1.00
1.02
3.17
5.37
3.99
2.02
0.97
1.98
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)



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138.4854
137.4012
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127.6114
125.8012
123.5950
110.5430
99.2087
71.4136
Ph
OBn
Cl
N
N
O
N
5dg
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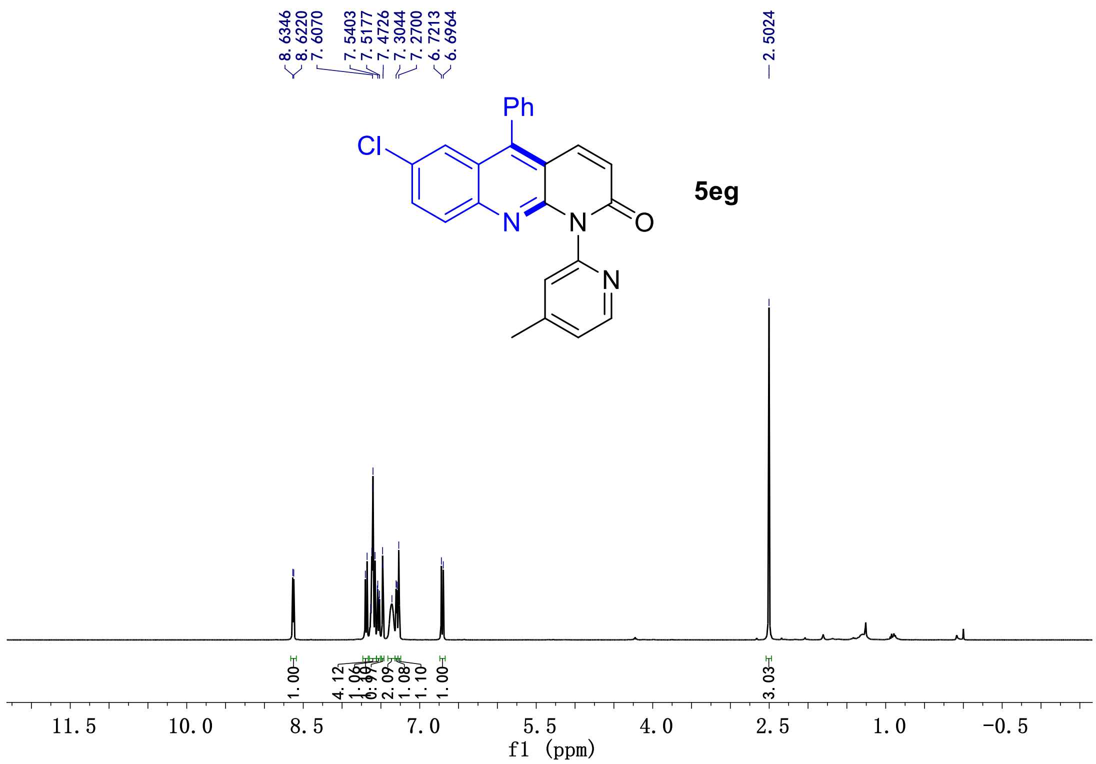
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



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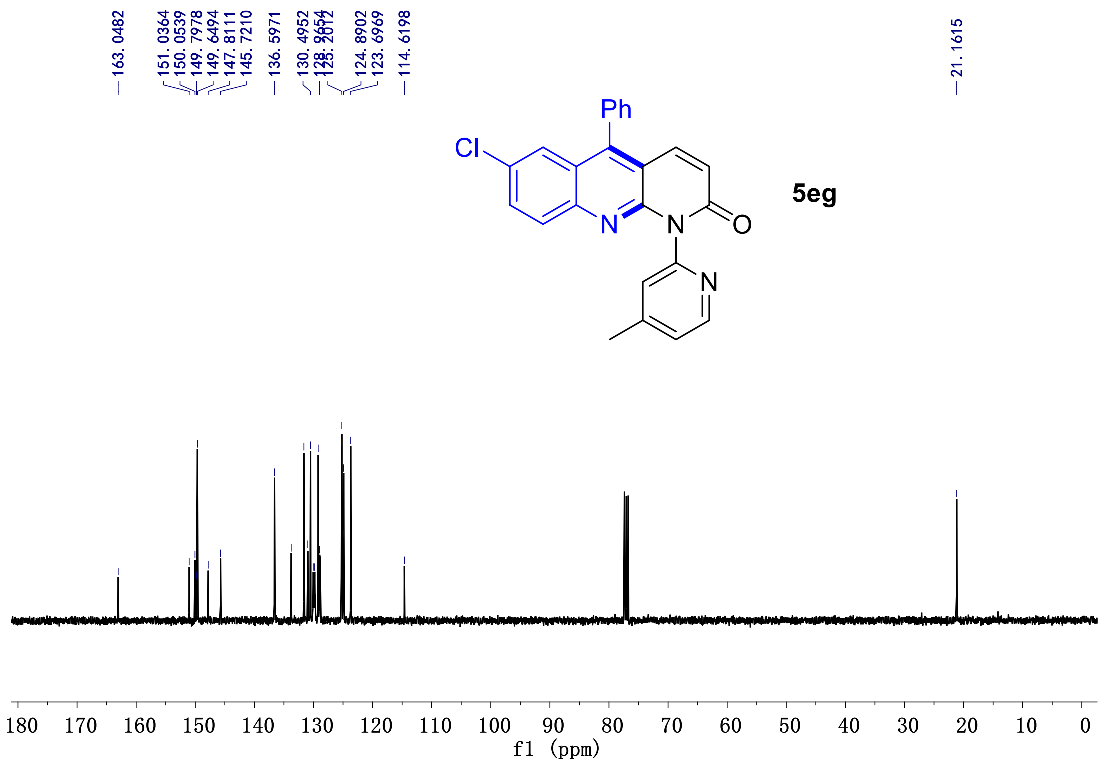
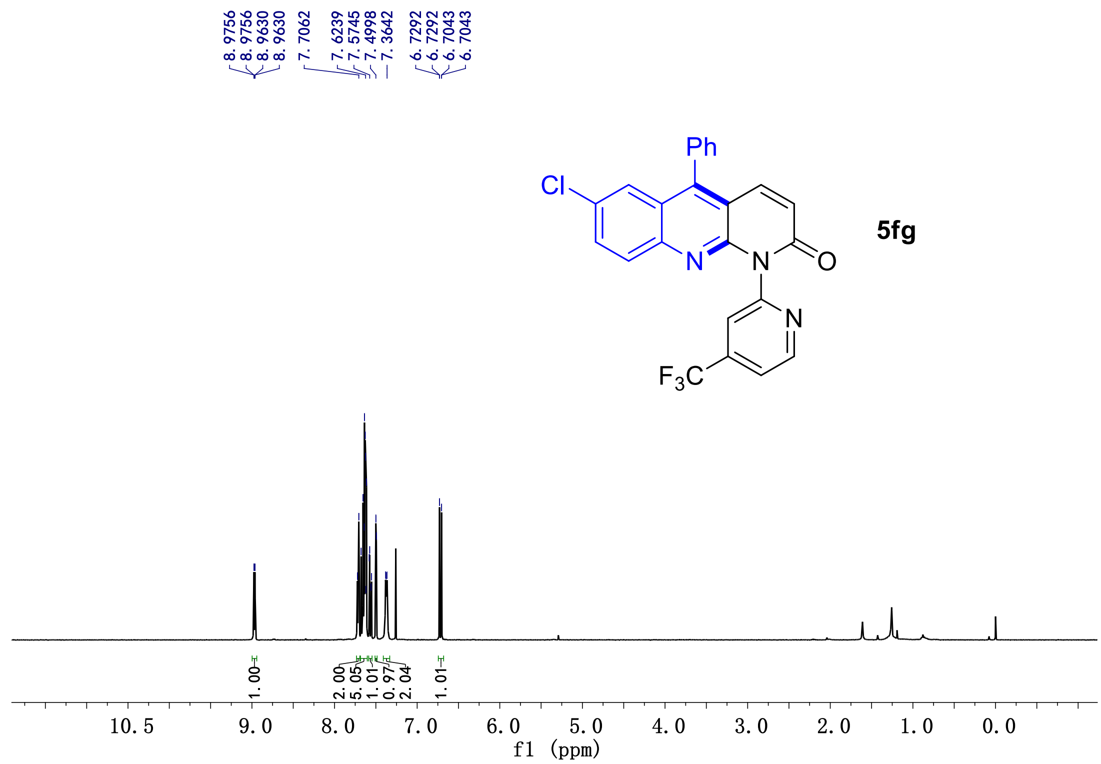
7.5177
7.4726
7.3044
7.2700
6.7213
6.6964
2.5024
Ph
Cl
N
N
O
N
5eg
1.00
4.12
1.06
0.97
2.09
1.08
1.10
1.00
3.03
11.5
10.0
8.5
7.0
5.5
4.0
2.5
1.0
-0.5
f1 (ppm)


5eg
Cl
Ph
N
O
f1 (ppm)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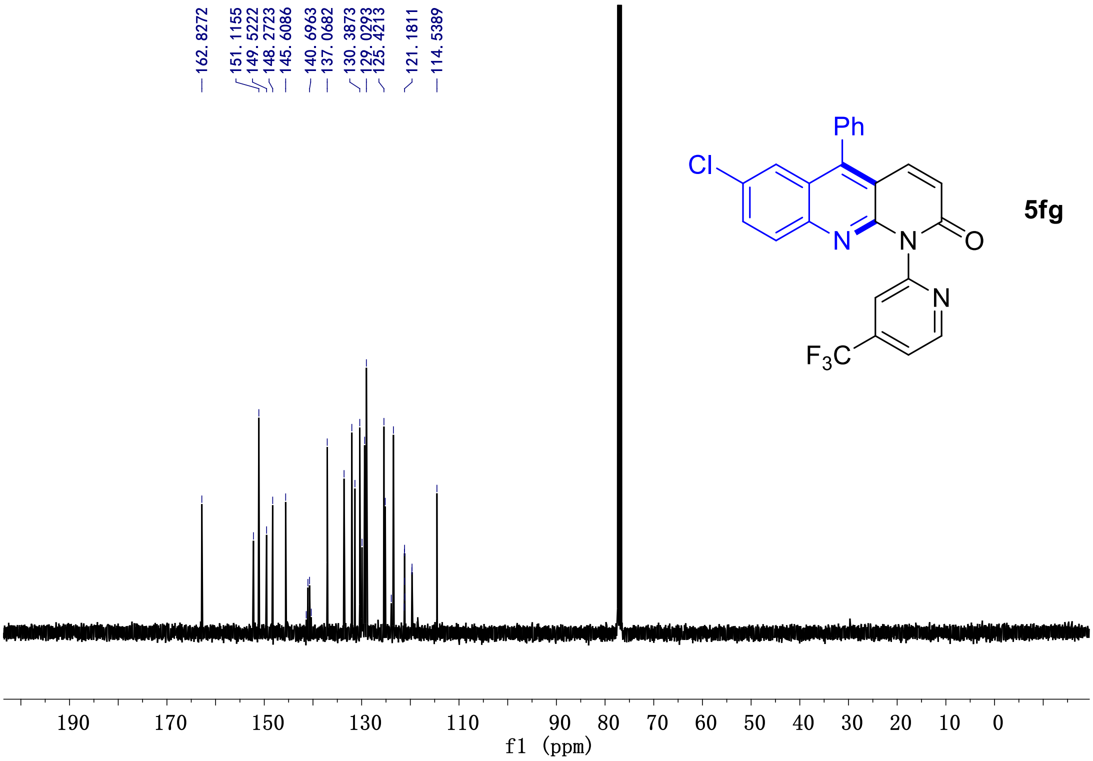
Cl
Ph
N
O
F_3C
f1 (ppm)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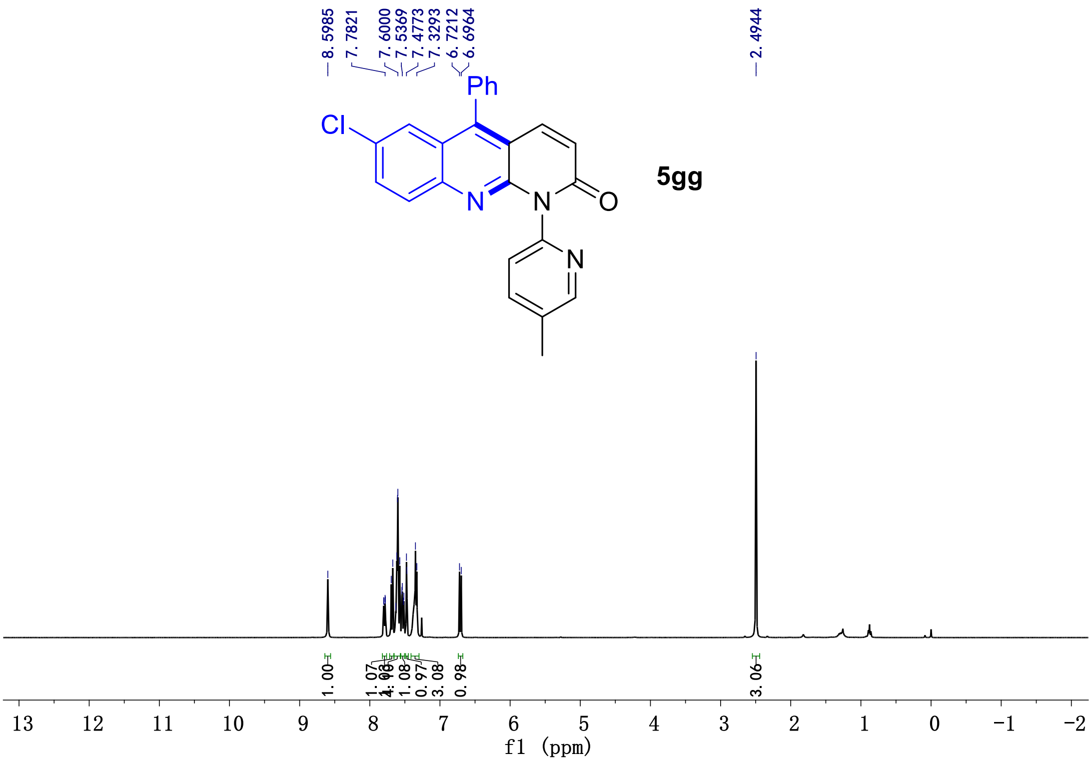
121.1811
114.5389
Ph
Cl
N
N
O
N
F3C
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

5fg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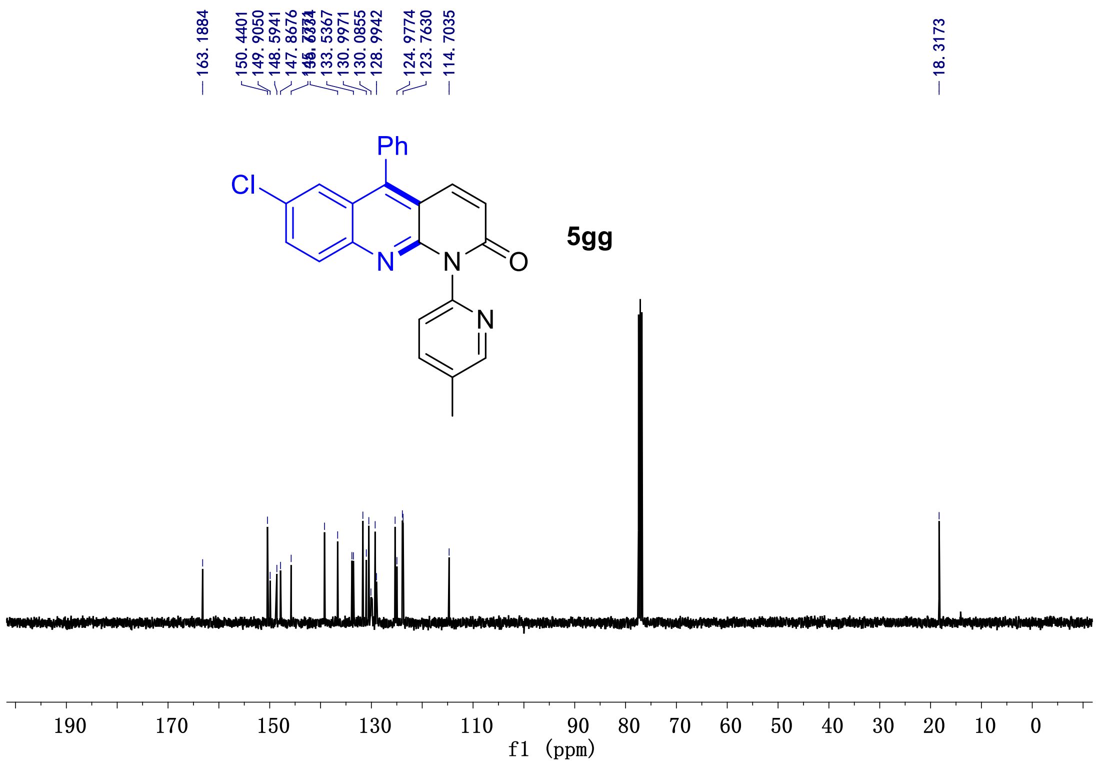
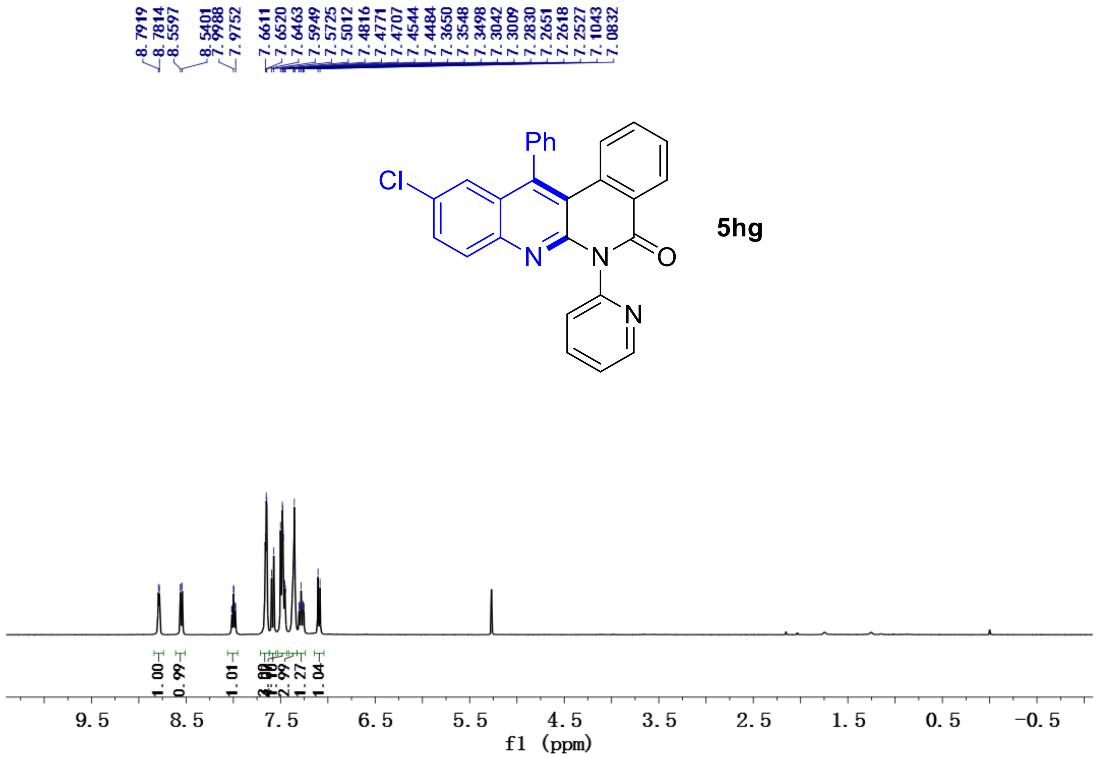
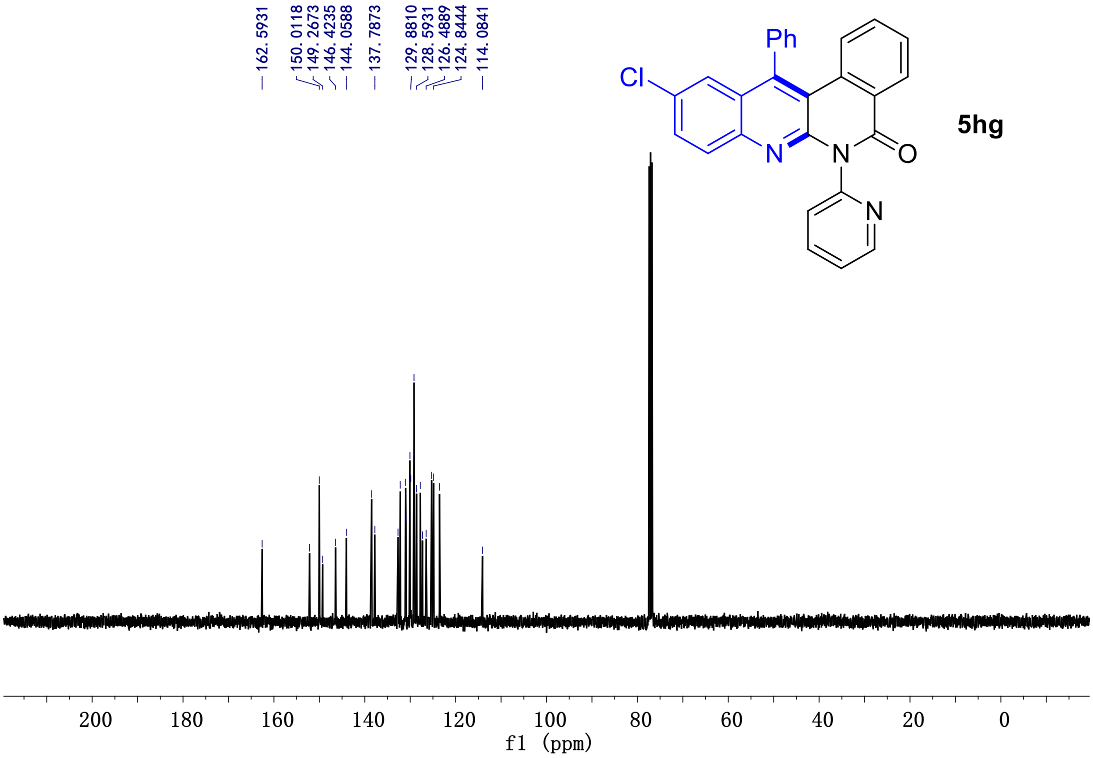
2.4944
Ph
Cl
N
N
O
N
1.00
1.07
1.00
1.08
0.97
3.08
0.98
3.06
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
−2
f1 (ppm)

5gg



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114.0841
Ph
Cl
N
N
O
N
5hg
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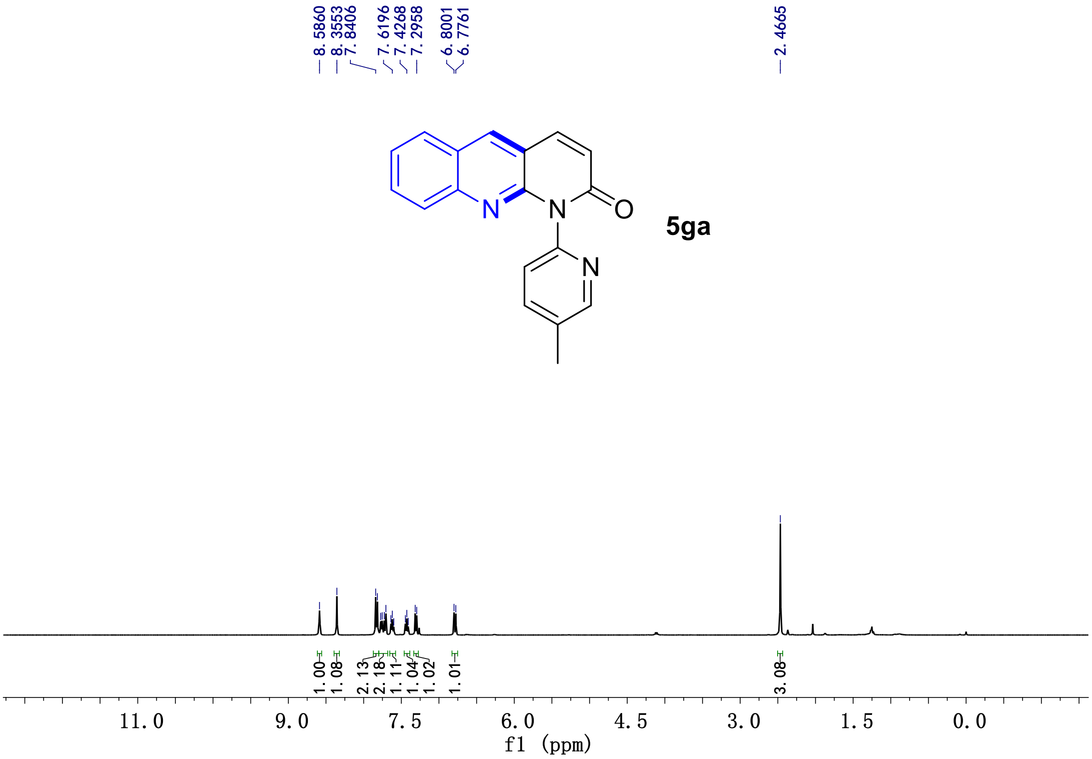
f1 (ppm)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7.6196
7.4268
7.2958
6.8001
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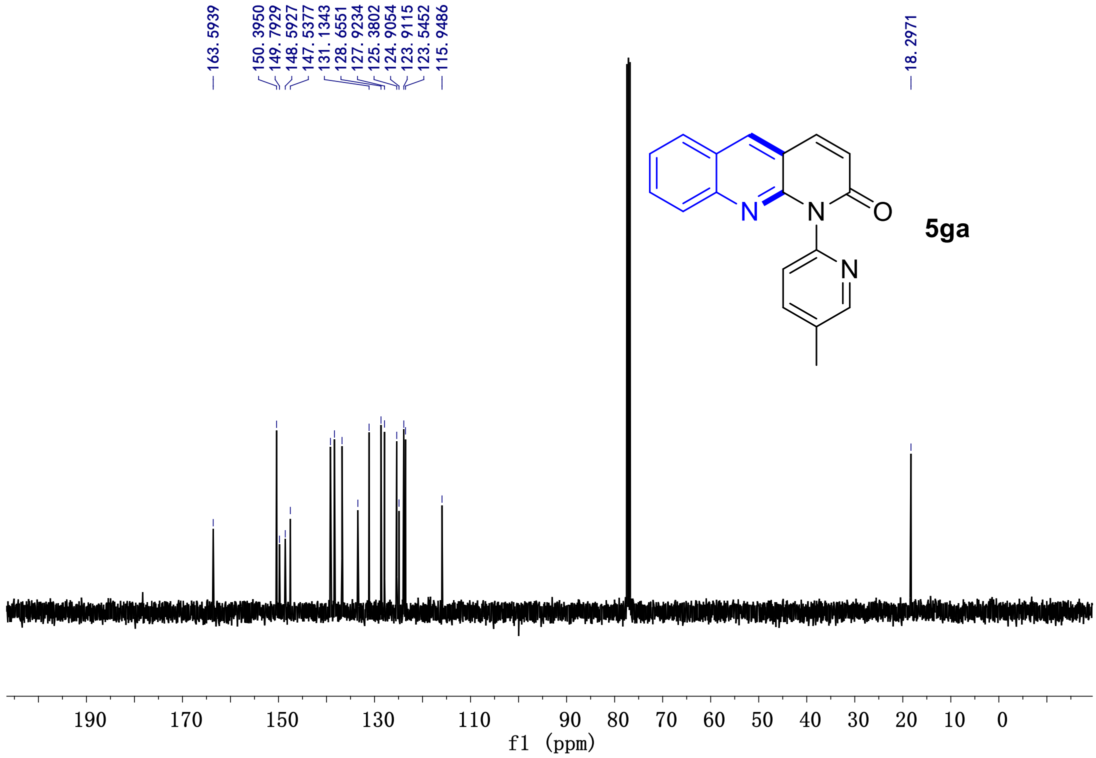
2.4665
N
N
O
N
5ga
1.00
1.08
2.13
2.18
1.11
1.04
1.02
1.01
3.08
11.0 9.0 7.5 6.0 4.5 3.0 1.5 0.0
f1 (ppm)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128.6551
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125.3802
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115.9486
18.2971
5ga
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170
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130
110
90
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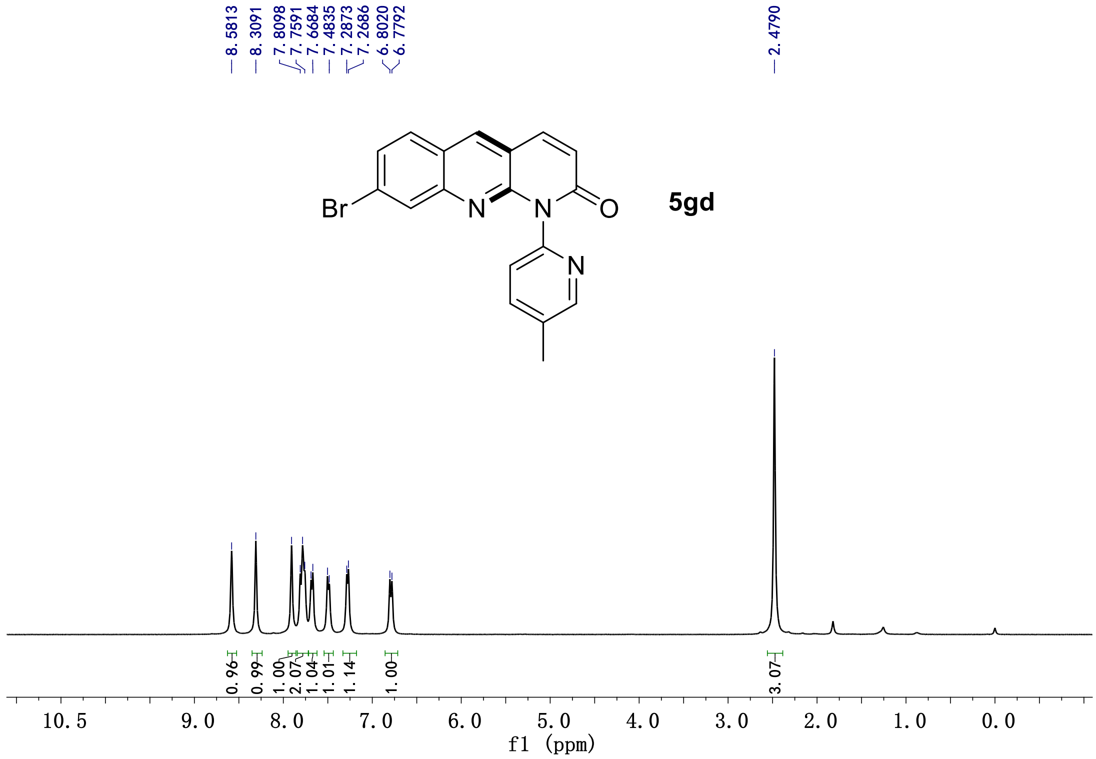
70
60
50
40
30
20
10
0
f1 (ppm)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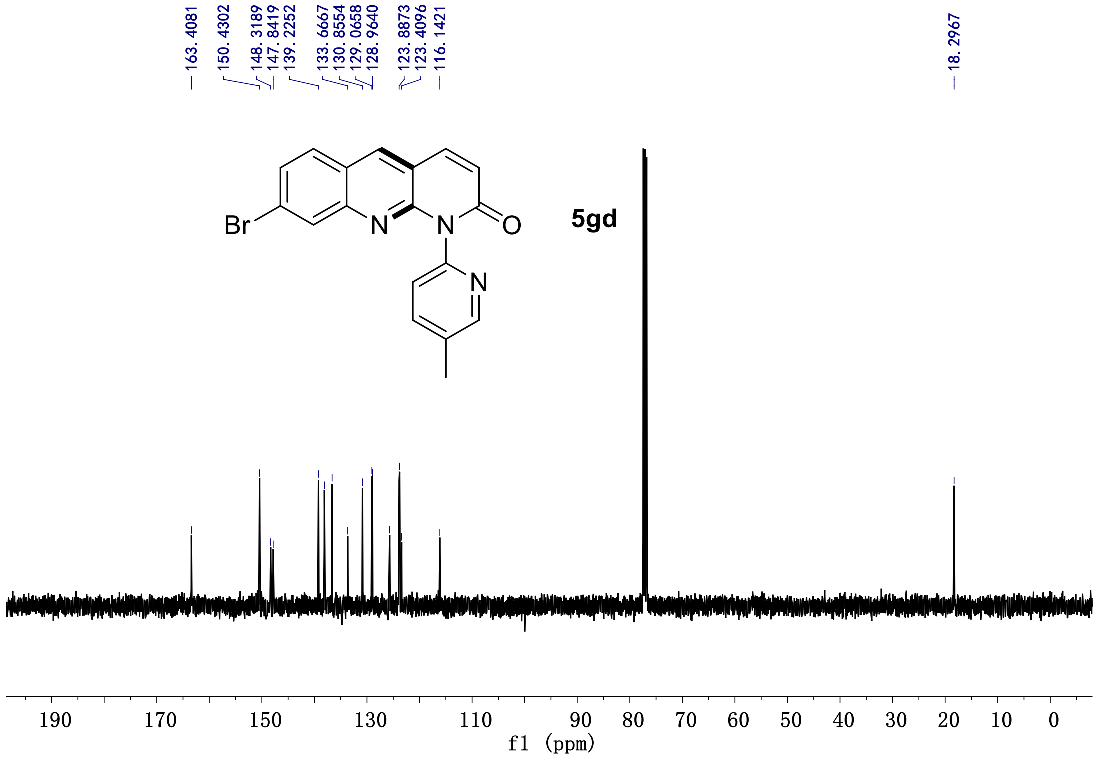
2.4790
Br
5gd
0.96
0.99
1.00
2.07
1.04
1.01
1.14
1.00
3.07
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)



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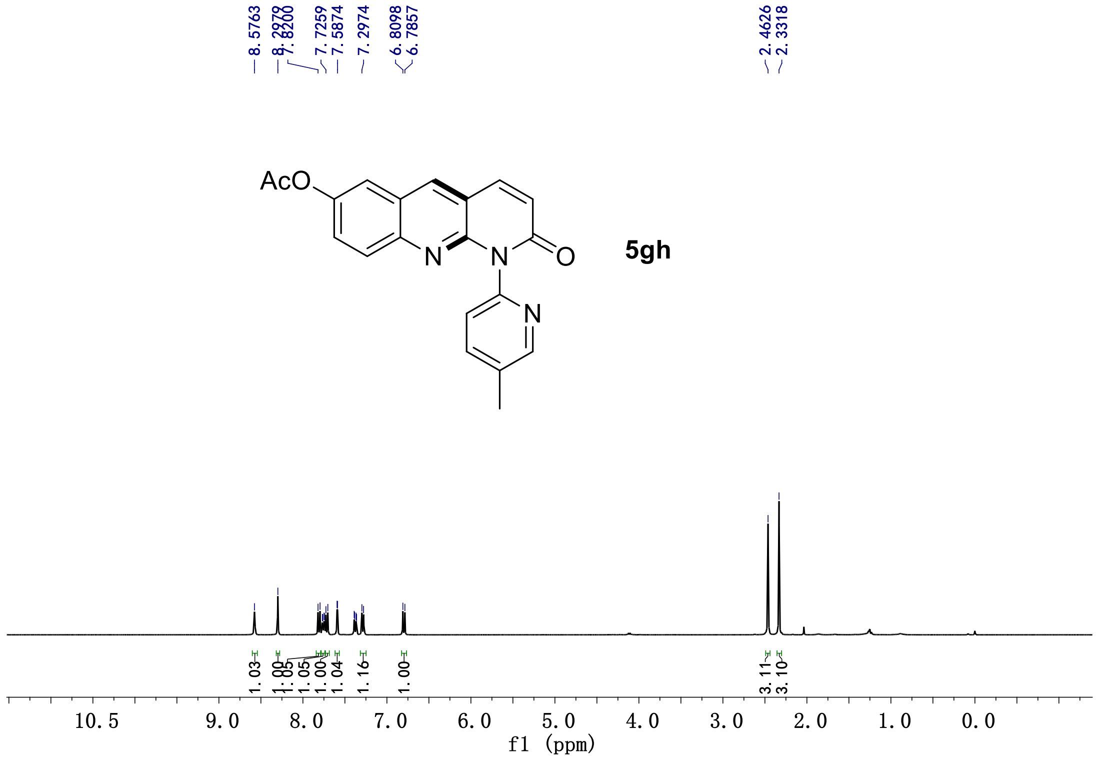

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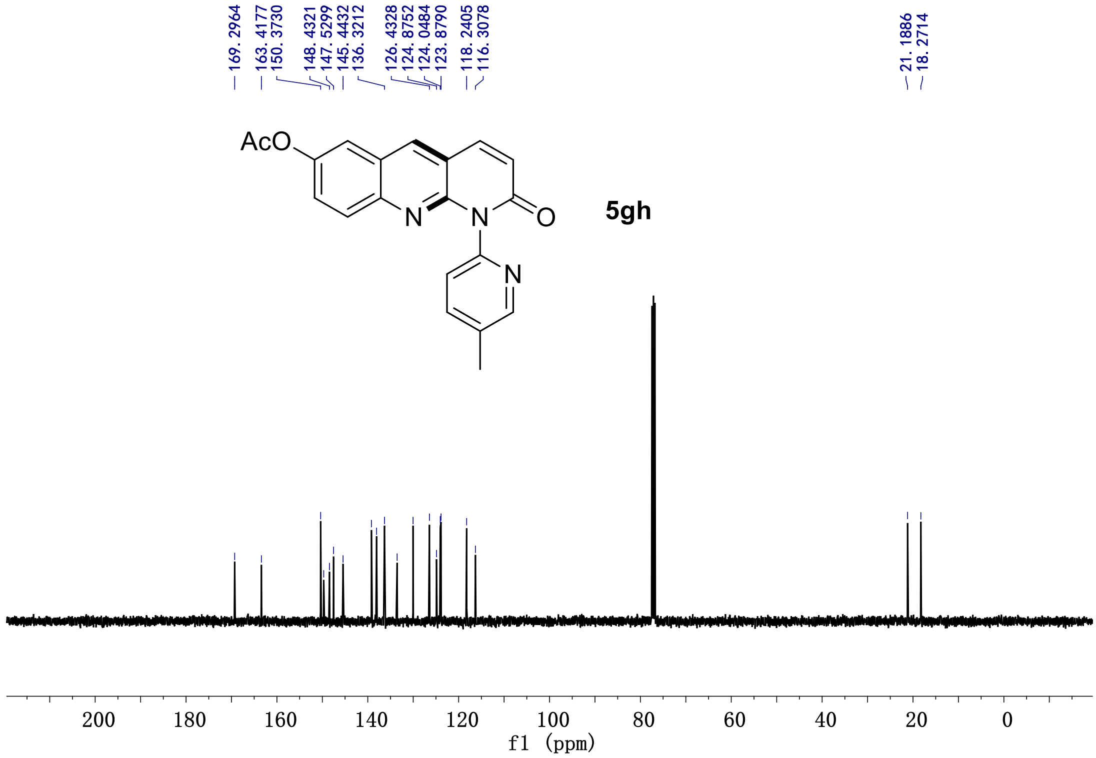
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123.8790
118.2405
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O
N
5gh
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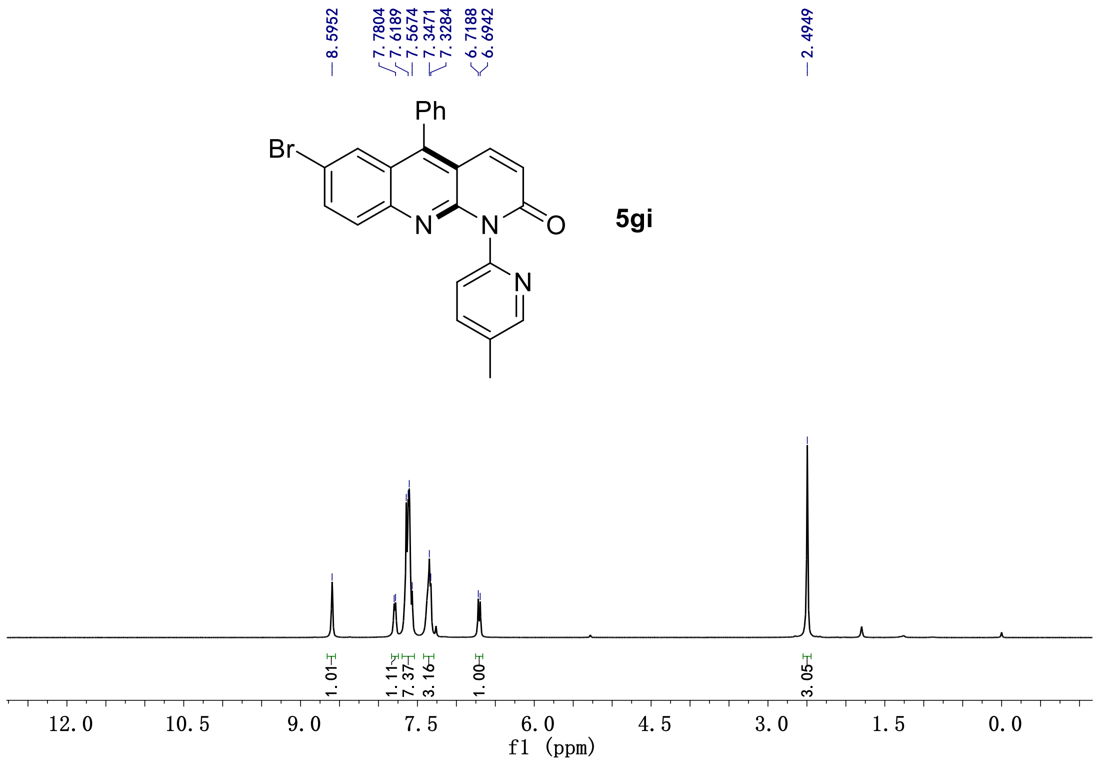
f1 (ppm)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2.4949
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N
O
N
5gi
1.01
1.11
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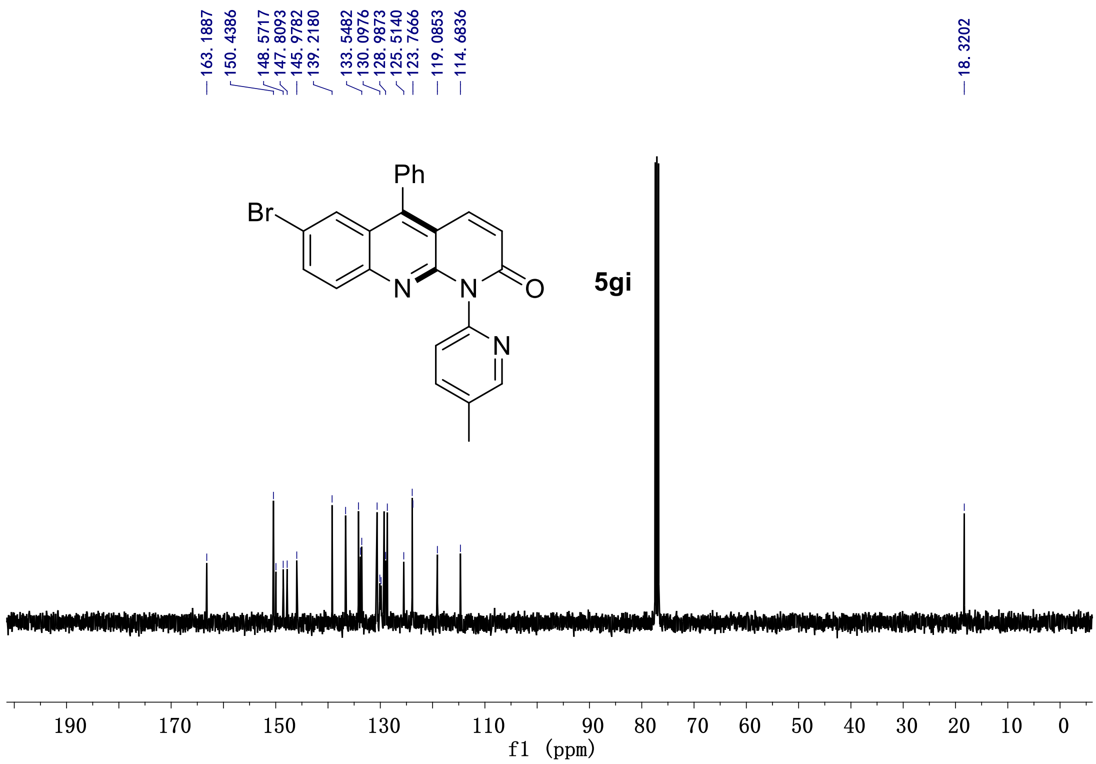
3.16
1.00
3.05
12.0 10.5 9.0 7.5 6.0 4.5 3.0 1.5 0.0
f1 (ppm)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123.7666
119.0853
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Ph
Br
N
N
O
N
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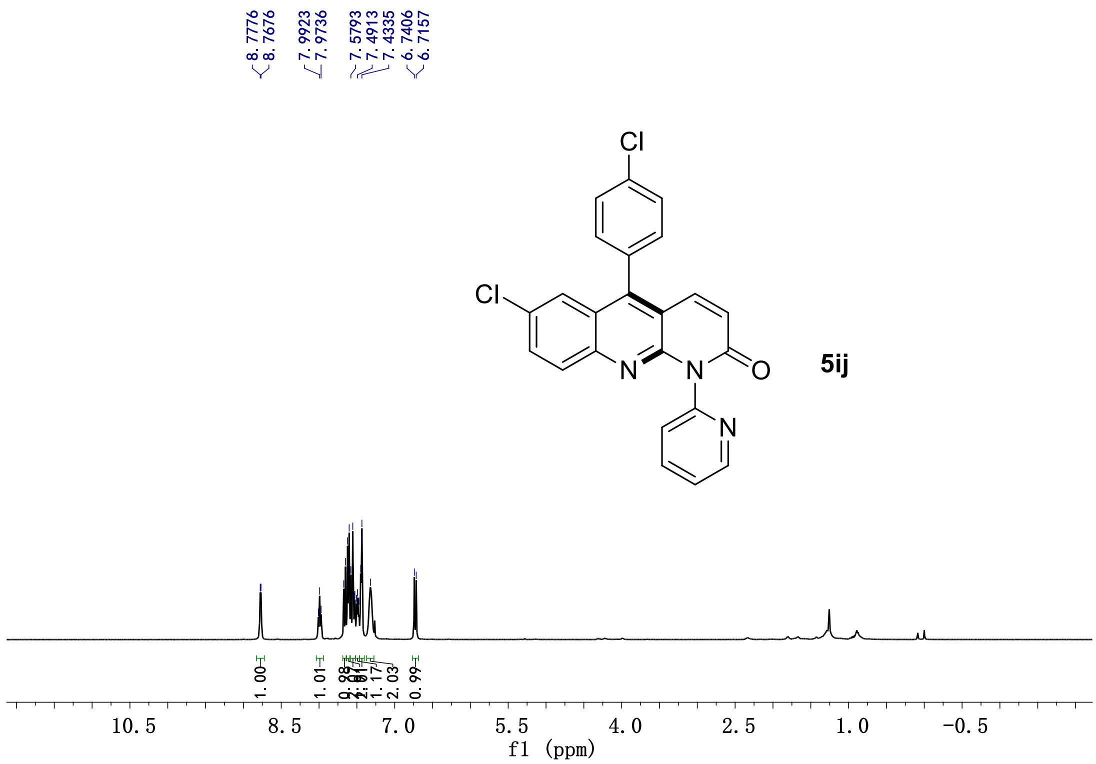
f1 (ppm)

5gi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6.7157
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N
O
N
1.00
1.01
0.98
2.07
2.01
1.17
2.03
0.99
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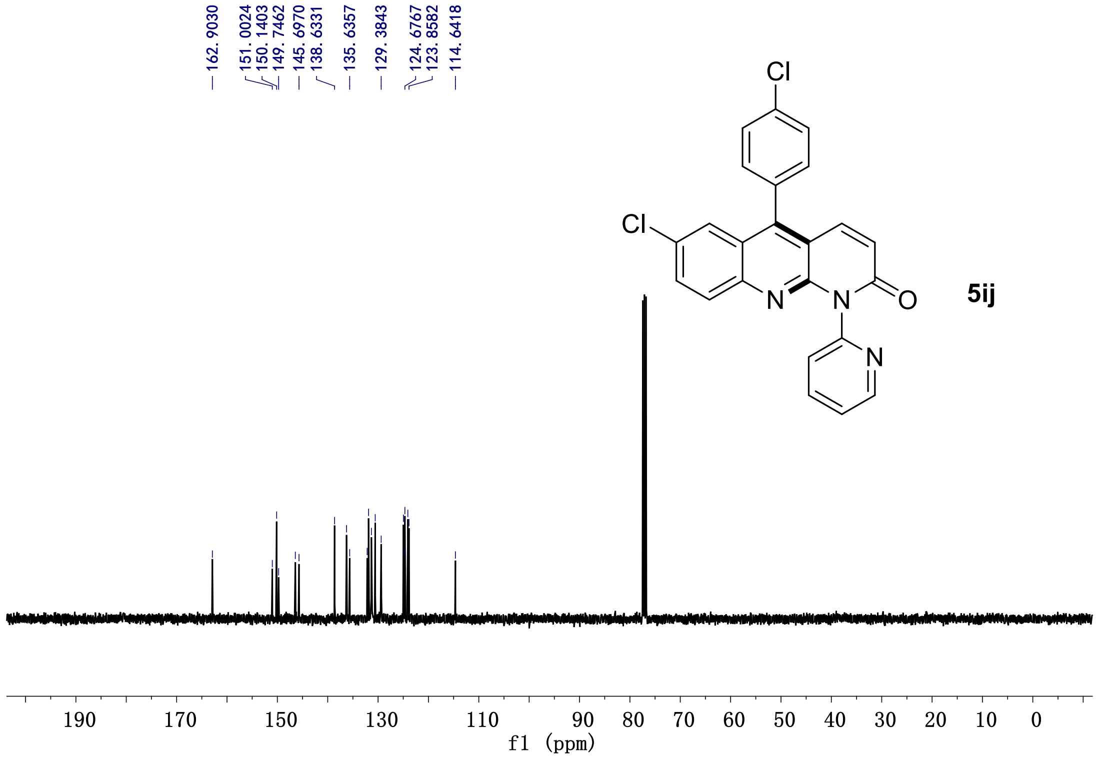
f1 (ppm)

5ij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Cl
Cl
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N
O
N
5ij
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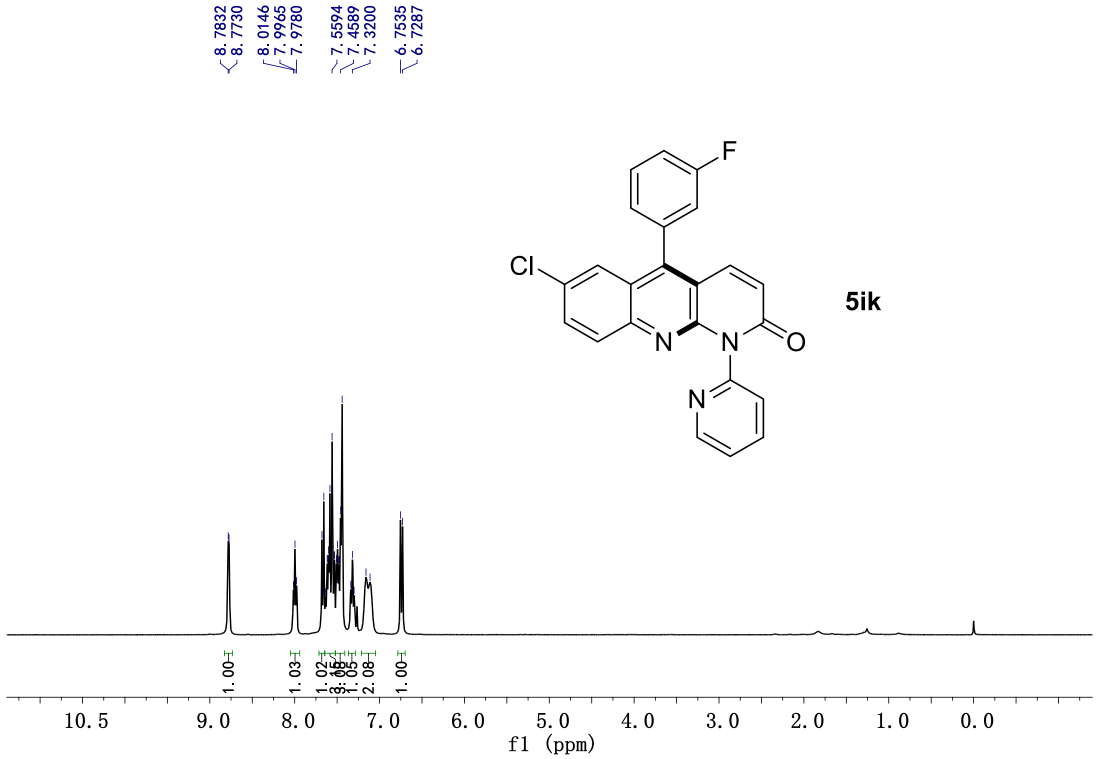
f1 (ppm)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F
Cl
N
N
O
N
5ik
1.00
1.03
1.02
2.08
1.00
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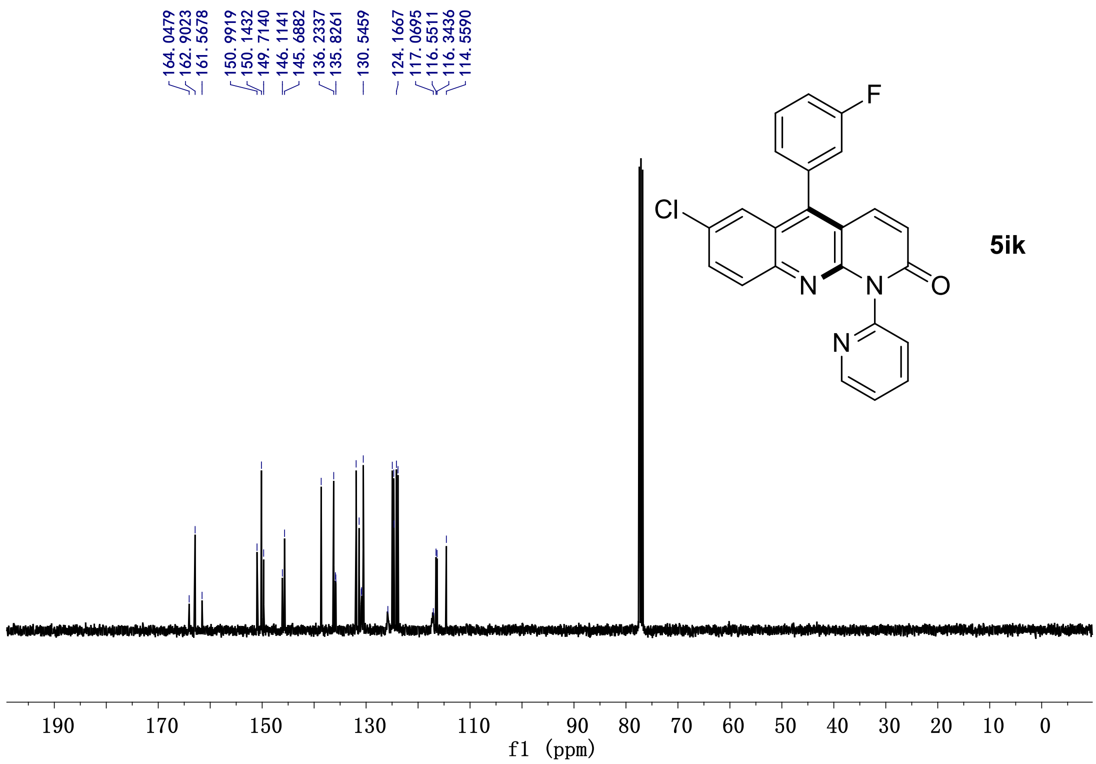
f1 (ppm)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124.1667
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116.3436
114.5590
F
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N
N
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N
5ik
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)