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Supporting Information

Copper-Catalyzed Aerobic Oxidative Domino Cyclization of Methyl Azaarenes with 6-Amino-pyrimidine-2,4-diones and Pyrazol-5-amines: Access to Dipyrimidine/dipyrazolo-Fused Pyridines

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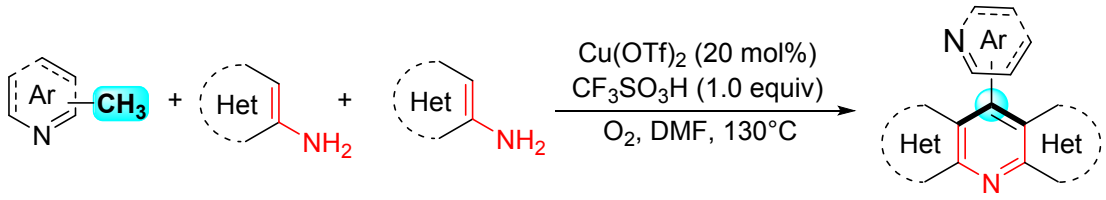
1. General Information

Materials and General Experimental: Methyl quinolines were purchased from Beijing Innochem Science & Technology Co. Ltd. 6-Amino-1,3-dimethylpyrimidine-2,4-dione and aminopyrazoles, were purchased from Shanghai Shaoyuan Co. Ltd. Copper catalysts and acids were purchased from Aladdin. Unless stated otherwise, all solvents and commercially available reagents were obtained from commercial suppliers and used without further purification. In addition, petroleumether (b.p. 60-90 ^{o}C), which was used for Column chromatography, was distilled prior to use. Non-commercial starting materials were prepared as described below or according to literature procedures. Analytical thin layer chromatography (TLC) was performed using pre-coated silica gel HF254 glass plates. Column chromatography was performed using silica gel (200-300 mesh).

Instrumentation: Nuclear magnetic resonance (NMR) spectra were recorded on a Bruker Advance 400 MHz spectrometer at ambient temperature using the non or partly deuterated solvent as internal standard (^{1}H: δ 7.26 ppm and ^{13}C{1H}: δ 77.0 ppm for $CDCl_3$). Chemical shifts (δ) are reported in ppm, relative to the internal standard of tetramethylsilane (TMS). The coupling constants (J) are quoted in hertz (Hz). Resonances are described as s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), br (broad) or combinations thereof. High resolution mass spectra were obtained on Thermo Scientific Q-Exactive (ESI mode) Melting points were determined using SGW X-4 apparatus and not corrected.

2. General Procedure for the Cyclization Process



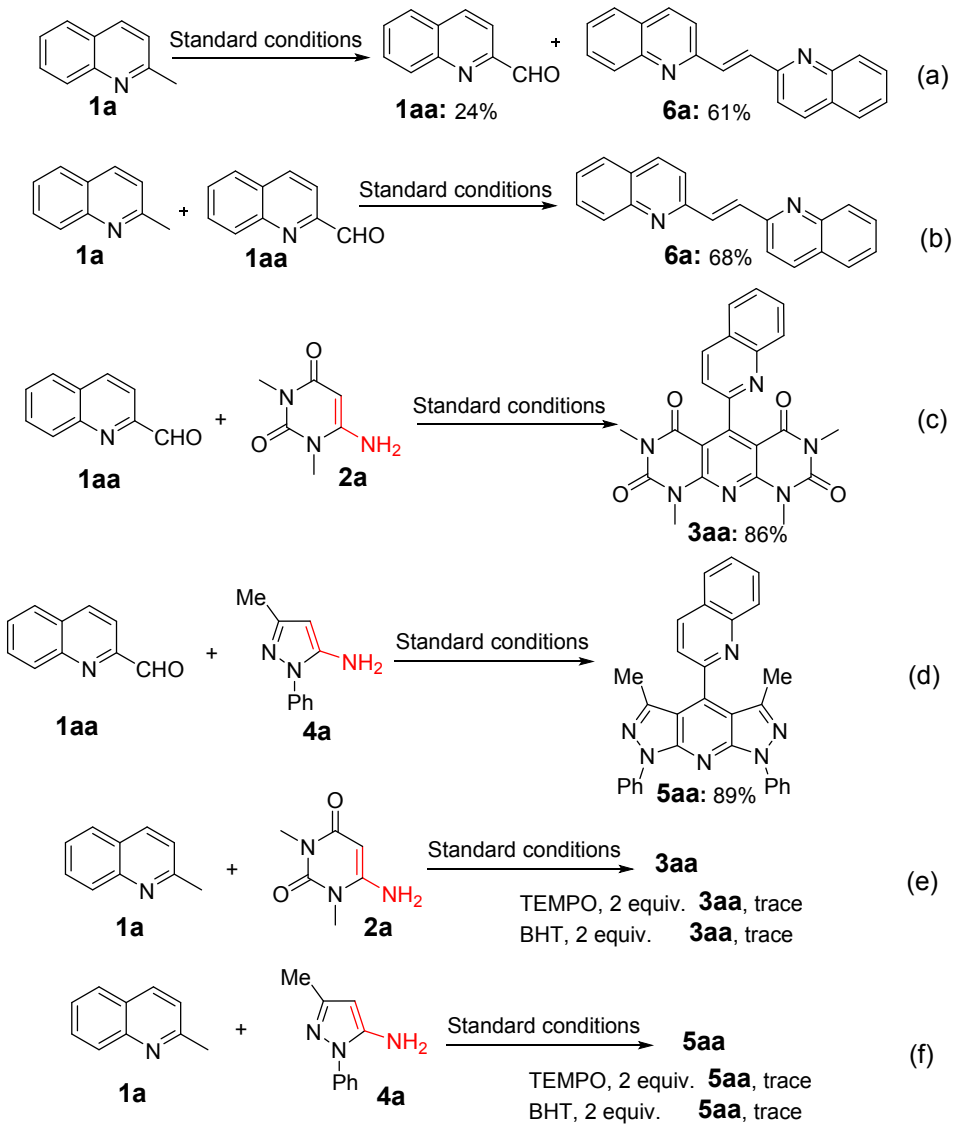
A 25 mL pressure vial was charged with 2-methylquinoline (**1a**) (42.9 mg, 0.30 mmol, 1.0 equiv.), 6-amino-1,3-dimethylpyrimidine-2,4-dione (**2a**) (102.5 mg, 0.66 mmol, 2.2 equiv.), $Cu(OTf)_2$ (21.7 mg, 0.06 mmol, 0.2 equiv.), CF_3SO_3H (45.1 mg, 0.30 mmol, 1.0 equiv.), and DMF (3.0 mL). The vial was sealed and the resulting mixture was stirred at 130 °C for 10-12 h under an O_2 atmosphere. After the reaction completed (monitored by TLC), solvent was then removed under reduced pressure and 50 mL water to the mixture, then extracted with EtOAc 3 times (3 × 50 mL). The combined organic phase was washed with 20% NaOH solution, dried over anhydrous Na_2SO_4 and concentrated in vacuum. The residue was purified by flash column chromatography on silica gel to yield the corresponding product **3aa**.

3. Control Experiments

To gain further insight into the reaction mechanism, some control experiments were conducted and the results were presented in Scheme S1. 2-Methyl quinoline **1a** could be oxidized under the standard conditions to generate quinoline-2-carbaldehyde **1aa** and 1,2-di(quinolin-2-yl)ethene **6a** in 24% and 61% yields, respectively (Scheme S1a). The reaction of 2-methyl quinoline **1a** with quinoline-2-carbaldehyde **1aa** under the standard conditions could also afford 1,2-di(quinolin-2-yl)ethane **6a** in 68% yield (Scheme S1b). The reaction of quinoline-2-carbaldehyde **1aa** with 6-amino-1,3-dimethylpyrimidine-2,4-dione **2a** could also proceed smoothly to generate product **3aa** in good yield under the standard conditions (Scheme S1c). Moreover, the reaction of quinoline-2-carbaldehyde **1aa** with 3-methyl-1-phenyl-1*H*-pyrazol-5-amine **4a** performed smoothly to afford product **5aa**

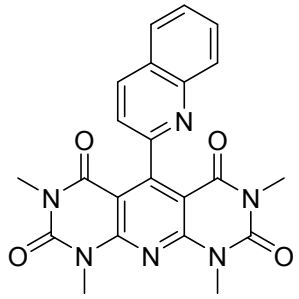
in good yield under the standard conditions (Scheme S1d). These results confirmed that quinoline-2-carbaldehyde **1aa** is the potential intermediate for this reaction process.

Notably, some radical inhibition experiments for **1a** and **2a** were performed with a stoichiometric amount of three radical inhibitors, TEMPO, 1,1-diphenyle-thene or BHT. A trace amount of target product **3aa** was observed for these reactions (Scheme S1e). What is more, radical inhibition experiments were also conducted using **1a** and **4a** with radical inhibitors (TEMPO, 1,1-diphenyle-thene or BHT) under the standard conditions (Scheme S1f). The product **5aa** was detected in a trace amount. These results discovered that the reaction proceeds through a radical process.



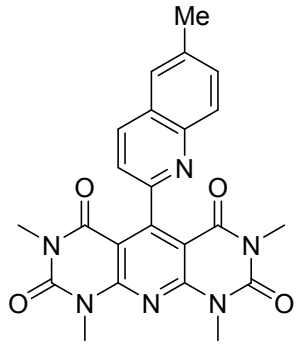
Scheme S1: Control experiments.

4. Characterization Data for Products



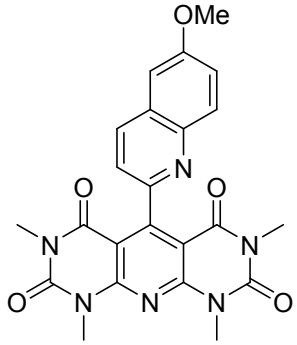
3aa

1,3,7,9-Tetramethyl-5-(quinolin-2-yl)pyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1*H*,3*H*,7*H*,9*H*)-tetraone (3aa), 106 mg, 83%, white solid, m.p. >300℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.3 Hz, 1H), 8.00 (d, *J* = 8.4 Hz, 1H), 7.91 (dd, *J* = 8.2, 1.1 Hz, 1H), 7.69 (ddd, *J* = 8.4, 7.0, 1.4 Hz, 1H), 7.55 (ddd, *J* = 8.1, 7.0, 1.2 Hz, 1H), 7.42 (d, *J* = 8.5 Hz, 1H), 3.78 (s, 6H), 3.25 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.0, 156.9, 156.7, 153.6, 150.8, 147.5, 135.1, 129.5, 128.9, 128.1, 127.2, 126.5, 120.2, 105.1, 30.3, 28.4. HRMS (ESI) m/z calculated for $[C_{22}H_{18}N_6O_4+H]^+$ 431.1462, found 431.1450.



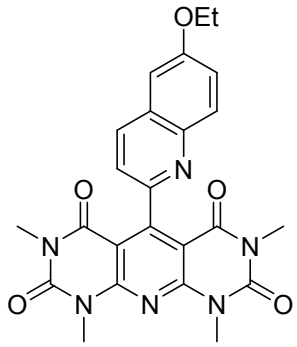
3ba

1,3,7,9-Tetramethyl-5-(6-methylquinolin-2-yl)pyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1*H*,3*H*,7*H*,9*H*)-tetraone (3ba), 124 mg, 92%, brown solid, m.p. >300℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, *J* = 8.5 Hz, 1H), 7.90 (d, *J* = 8.5 Hz, 1H), 7.67 (s, 1H), 7.52 (d, *J* = 8.6 Hz, 1H), 7.37 (d, *J* = 8.5 Hz, 1H), 3.78 (s, 6H), 3.24 (s, 6H), 2.54 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.0, 157.1, 155.7, 153.5, 150.8, 146.0, 136.3, 134.6, 131.8, 128.6, 127.2, 127.0, 120.1, 105.1, 30.3, 28.4, 21.5. HRMS (ESI) m/z calculated for $[C_{23}H_{20}N_6O_4+H]^+$ 445.1619, found 445.1611.



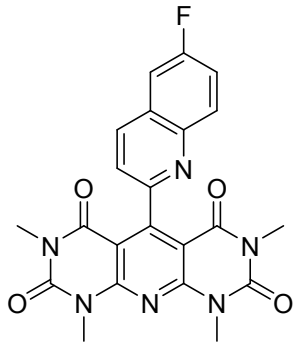
3ca

5-(6-Methoxyquinolin-2-yl)-1,3,7,9-tetramethylpyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1*H*,3*H*,7*H*,9*H*)-tetraone (3ca), 120 mg, 86%, white solid, m.p. >300℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.5 Hz, 1H), 7.90 (d, *J* = 9.2 Hz, 1H), 7.39 – 7.32 (m, 2H), 7.18 (d, *J* = 2.8 Hz, 1H), 3.93 (s, 3H), 3.78 (s, 6H), 3.25 (s, 6H).^{13}C NMR (101 MHz, $CDCl_3$) δ 159.1, 157.8, 157.1, 154.1, 153.6, 150.8, 143.5, 134.1, 130.4, 128.2, 122.1, 120.4, 106.0, 105.20, 55.6, 30.4, 28.5. HRMS (ESI) m/z calculated for $[C_{23}H_{20}N_6O_5+H]^+$ 461.1568, found 461.1569.



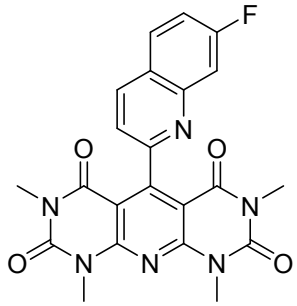
3da

5-(6-Ethoxyquinolin-2-yl)-1,3,7,9-tetramethylpyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1*H*,3*H*,7*H*,9*H*)-tetraone (3da), 99 mg, 69%, pink solid, m.p. >300℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, *J* = 8.5 Hz, 1H), 7.90 (d, *J* = 9.1 Hz, 1H), 7.38 – 7.32 (m, 2H), 7.17 (d, *J* = 2.7 Hz, 1H), 4.17 (q, *J* = 7.0 Hz, 2H), 3.78 (s, 6H), 3.25 (s, 6H), 1.49 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.1, 157.2, 157.2, 153.9, 153.6, 150.9, 143.4, 134.1, 130.3, 128.3, 122.5, 120.4, 106.8, 105.3, 63.8, 30.4, 28.5, 14.7. HRMS (ESI) m/z calculated for $[C_{24}H_{22}N_6O_5+H]^+$ 475.1724, found 475.1718.



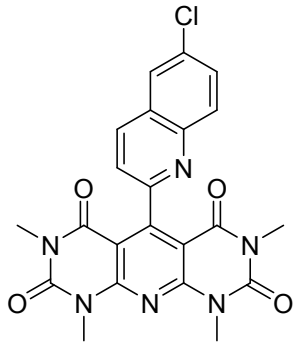
3ea

5-(6-Fluoroquinolin-2-yl)-1,3,7,9-tetramethylpyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1*H*,3*H*,7*H*,9*H*)-tetraone (3ea), 87 mg, 64%, yellow solid, m.p. >300℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, *J* = 8.5 Hz, 1H), 8.00 (dd, *J* = 9.2, 5.3 Hz, 1H), 7.53 (dd, *J* = 8.9, 2.8 Hz, 1H), 7.50 – 7.44 (m, 1H), 7.43 (d, *J* = 8.3 Hz, 1H), 3.79 (s, 6H), 3.26 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.3, 159.1, 156.7, 156.1, 153.7, 150.8, 144.6, 134.6, 131.5, 127.9, 121.1, 119.8, 111.4, 105.1, 30.4, 28.5. HRMS (ESI) m/z calculated for $[C_{22}H_{17}FN_6O_4+H]^+$ 449.1368, found 449.1359.



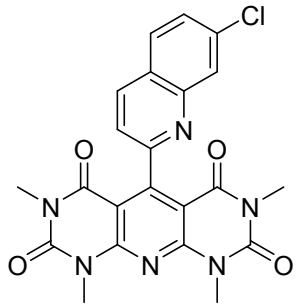
3fa

5-(7-Fluoroquinolin-2-yl)-1,3,7,9-tetramethylpyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1*H*,3*H*,7*H*,9*H*)-tetraone (3fa), 81 mg, 60%, white solid, m.p. >300℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 8.5 Hz, 1H), 7.90 (dd, *J* = 9.0, 6.0 Hz, 1H), 7.63 (dd, *J* = 10.2, 2.5 Hz, 1H), 7.42 – 7.31 (m, 2H), 3.78 (s, 6H), 3.25 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.1, 157.9, 153.7, 150.8, 135.3, 130.3, 130.2, 124.2, 119.7, 117.1, 116.9, 113.0, 112.7, 105.0, 30.4, 28.5. HRMS (ESI) m/z calculated for $[C_{22}H_{17}FN_6O_4+H]^+$ 449.1368, found 449.1358.



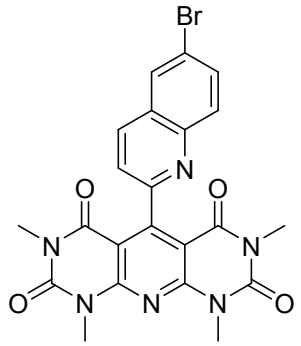
3ga

5-(6-Chloroquinolin-2-yl)-1,3,7,9-tetramethylpyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1*H*,3*H*,7*H*,9*H*)-tetraone (3ga), 86 mg, 61%, brown solid, m.p. >300℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.5 Hz, 1H), 7.93 (d, *J* = 8.9 Hz, 1H), 7.89 (d, *J* = 2.0 Hz, 1H), 7.62 (dd, *J* = 8.9, 2.0 Hz, 1H), 7.43 (d, *J* = 8.5 Hz, 1H), 3.79 (s, 6H), 3.25 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.1, 157.2, 156.5, 153.6, 150.7, 145.9, 134.2, 132.2, 130.6, 130.4, 127.8, 126.8, 121.2, 105.0, 30.4, 28.5. HRMS (ESI) m/z calculated for $[C_{22}H_{17}ClN_6O_4+H]^+$ 465.1073, found 465.1066.



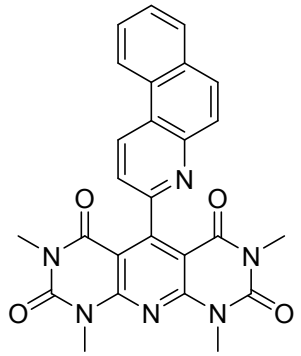
3ha

5-(7-Chloroquinolin-2-yl)-1,3,7,9-tetramethylpyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1*H*,3*H*,7*H*,9*H*)-tetraone (3ha), 98 mg, 70%, white solid, m.p. >300℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 8.5 Hz, 1H), 8.03 (s, 1H), 7.86 (d, *J* = 8.7 Hz, 1H), 7.53 (dd, *J* = 8.7, 2.1 Hz, 1H), 7.42 (d, *J* = 8.5 Hz, 1H), 3.79 (s, 6H), 3.26 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.2, 158.0, 156.6, 153.7, 150.8, 147.9, 135.4, 135.0, 129.4, 128.3, 127.6, 125.6, 120.6, 105.1, 30.5, 28.6. HRMS (ESI) m/z calculated for $[C_{22}H_{17}ClN_6O_4+H]^+$ 465.1073, found 465.1064.



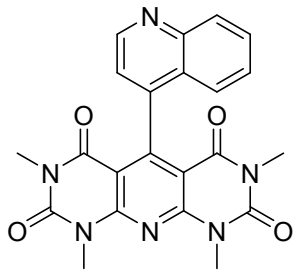
3ia

5-(6-Bromoquinolin-2-yl)-1,3,7,9-tetramethylpyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1*H*,3*H*,7*H*,9*H*)-tetraone (3ia), 118 mg, 77%, white solid, m.p. >300℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.5 Hz, 1H), 8.07 (d, *J* = 2.1 Hz, 1H), 7.87 (d, *J* = 9.0 Hz, 1H), 7.76 (dd, *J* = 8.9, 2.2 Hz, 1H), 7.43 (d, *J* = 8.5 Hz, 1H), 3.79 (s, 6H), 3.25 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.1, 157.3, 156.4, 153.6, 150.8, 146.0, 134.2, 133.0, 130.7, 130.1, 128.4, 121.2, 120.4, 105.0, 30.4, 28.5. HRMS (ESI) m/z calculated for $[C_{22}H_{17}BrN_6O_4+H]^+$ 509.0567, found 509.0564.



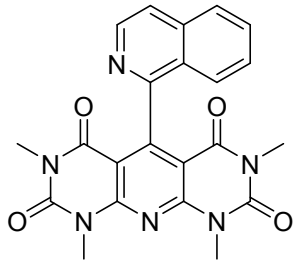
3ja

5-(Benzo[f]quinolin-3-yl)-1,3,7,9-tetramethylpyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1*H*,3*H*,7*H*,9*H*)-tetraone (3ia), 94 mg, 65%, white solid, m.p. >300℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.10 (d, *J* = 8.6 Hz, 1H), 8.68 (d, *J* = 8.5 Hz, 1H), 8.00 (d, *J* = 9.1 Hz, 1H), 7.98 – 7.91 (m, 2H), 7.74 – 7.63 (m, 2H), 7.60 (d, *J* = 8.6 Hz, 1H), 3.80 (s, 6H), 3.25 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.1, 157.1, 156.2, 153.7, 150.9, 147.6, 131.8, 131.1, 130.2, 130.0, 128.6, 127.9, 127.1, 127.0, 124.4, 122.8, 120.2, 105.2, 30.5, 28.5. HRMS (ESI) m/z calculated for $[C_{26}H_{20}N_6O_4+H]^+$ 481.1619, found 481.1609.



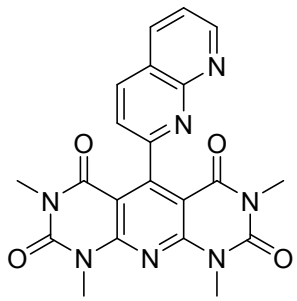
3ka

1,3,7,9-Tetramethyl-5-(quinolin-4-yl)pyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1*H*,3*H*,7*H*,9*H*)-tetraone (3ka), 41 mg, 31%, orange solid, m.p. >300℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.97 (d, *J* = 4.4 Hz, 1H), 8.21 (d, *J* = 8.4 Hz, 1H), 7.68 (ddd, *J* = 8.4, 6.8, 1.4 Hz, 1H), 7.37 (ddd, *J* = 8.1, 6.9, 1.2 Hz, 1H), 7.26 – 7.21 (m, 1H), 7.09 (d, *J* = 4.5 Hz, 1H), 3.82 (s, 6H), 3.19 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.3, 155.1, 153.6, 150.7, 149.5, 147.2, 145.6, 130.2, 129.3, 126.7, 126.2, 123.7, 117.6, 105.1, 30.5, 28.5. HRMS (ESI) m/z calculated for $[C_{22}H_{18}N_6O_4+H]^+$ 431.1462, found 431.1454.



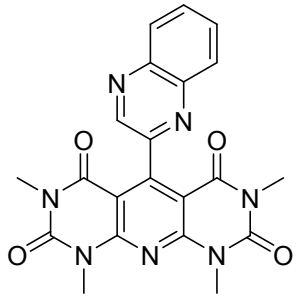
3la

5-(Isoquinolin-1-yl)-1,3,7,9-tetramethylpyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1*H*,3*H*,7H**,9H)-tetraone (3la)**, 85 mg, 65%, brown solid, m.p. >300℃, ^{1}H NMR (400 MHz, CDCl3) δ 8.56 (d, *J* = 5.7 Hz, 1H), 7.94 (d, *J* = 8.3 Hz, 1H), 7.78 (d, *J* = 5.7 Hz, 1H), 7.66 (ddd, *J* = 8.2, 6.3, 1.7 Hz, 1H), 7.46-7.34 (m, 2H), 3.82 (s, 6H), 3.20 (s, 6H). ^{13}C NMR (101 MHz, CDCl3) δ 158.6, 157.7, 155.9, 153.8, 150.9, 141.9, 135.2, 130.0, 127.5, 127.3, 127.1, 124.5, 120.5, 105.6, 30.4, 28.5. HRMS (ESI) m/z calculated for [C22H18N6O4+H]+ 431.1462, found 431.1454.



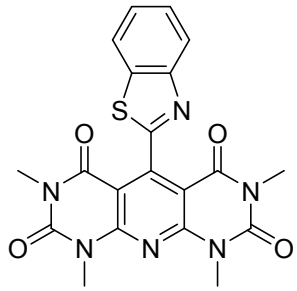
3ma

1,3,7,9-Tetramethyl-5-(1,8-naphthyridin-2-yl)pyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1*H*,3*H*,7*H*,9*H*)-tetraone (3ma), 102 mg, 78%, brown solid, m.p. >300℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.08 (dd, *J* = 3.9, 1.5 Hz, 1H), 8.30 (d, *J* = 8.4 Hz, 2H), 7.57 (d, *J* = 8.4 Hz, 1H), 7.53 (dd, *J* = 8.0, 4.2 Hz, 1H), 3.80 (s, 6H), 3.24 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.6, 159.2, 156.1, 155.6, 153.6, 153.2, 150.8, 137.6, 135.7, 122.2, 121.9, 121.8, 105.2, 30.5, 28.5. HRMS (ESI) m/z calculated for $[C_{21}H_{17}N_7O_4+H]^+$ 432.1415, found 432.1408.



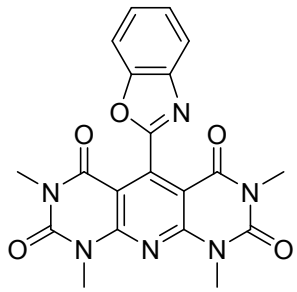
3na

1,3,7,9-Tetramethyl-5-(quinoxalin-2-yl)pyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1*H*,3*H*,7*H*,9*H*)-tetraone (3ma), 50 mg, 39%, red solid, m.p. >300℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.80 (s, 1H), 8.24-8.17 (m, 1H), 8.01-7.95 (m, 1H), 7.80-7.71 (m, 2H), 3.79 (s, 6H), 3.25 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.3, 154.0, 153.6, 152.6, 150.7, 143.7, 141.5, 141.1, 130.0, 129.7, 129.6, 128.9, 122.8, 105.5, 30.7, 28.6. HRMS (ESI) m/z calculated for $[C_{21}H_{17}N_7O4+H]^+$ 432.1415, found 432.1430.



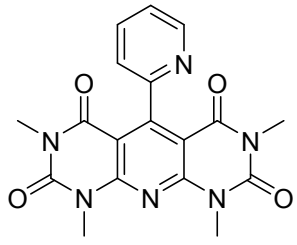
3oa

5-(Benzo[d]thiazol-2-yl)-1,3,7,9-tetramethylpyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1*H*,3*H*,7*H*,9*H*)-tetraone (3oa), 31 mg, 24%, brown solid, m.p. >300℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.1 Hz, 1H), 7.97 (ddd, *J* = 7.9, 1.2, 0.5 Hz, 1H), 7.52 (td, *J* = 8.2, 7.8, 1.3 Hz, 1H), 7.48 – 7.42 (m, 1H), 3.79 (s, 6H), 3.31 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.2, 158.5, 153.5, 152.8, 150.6, 150.1, 136.0, 126.2, 125.5, 123.5, 122.0, 105.6, 30.6, 28.7. HRMS (ESI) m/z calculated for $[C_{20}H_{16}N_6O_4S+H]^+$ 437.1026, found 437.1021.



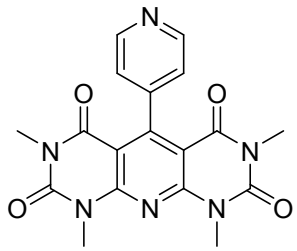
3pa

5-(Benzo[d]oxazol-2-yl)-1,3,7,9-tetramethylpyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1*H*,3*H*,7*H*,9*H*)-tetraone (3pa), 32 mg, 25%, brown solid, m.p. >300℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85-7.78 (m, 1H), 7.70-7.63 (m, 1H), 7.45-7.40 (m, 2H), 3.80 (s, 6H), 3.33 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.6, 157.5, 153.5, 150.8, 150.6, 143.3, 141.5, 125.4, 124.7, 120.4, 111.1, 106.2, 30.5, 28.7. HRMS (ESI) m/z calculated for $[C_{20}H_{16}N_6O_5+H]^+$ 421.1255, found 421.1247.



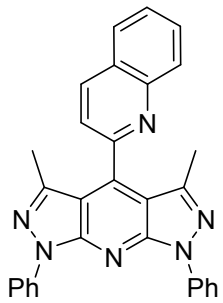
3qa

1,3,7,9-Tetramethyl-5-(pyridin-2-yl)pyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1*H*,3*H*,7*H*,9*H*)-tetraone (3qa), 67 mg, 59%, white solid, m.p. >300℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 4.9 Hz, 1H), 7.83 (td, *J* = 7.8, 1.7 Hz, 1H), 7.42 (ddd, *J* = 7.6, 5.0, 1.1 Hz, 1H), 7.28 (t, *J* = 1.0 Hz, 1H), 3.78 (s, 6H), 3.30 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.2, 156.8, 156.2, 153.6, 150.9, 149.0, 135.6, 122.7, 121.9, 104.9, 30.4, 28.6. HRMS (ESI) m/z calculated for $[C_{18}H_{16}N_6O_4+H]^+$ 381.1306, found 381.1300.



3ra

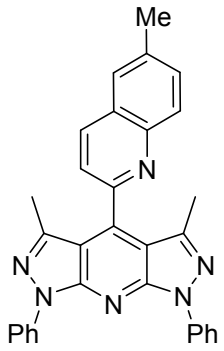
1,3,7,9-Tetramethyl-5-(pyridin-4-yl)pyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1*H*,3*H*,7*H*,9*H*)-tetraone (3ra), 80 mg, 71%, white solid, m.p. >300℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.72 (d, *J* = 5.9 Hz, 2H), 7.07 (dd, *J* = 4.4, 1.6 Hz, 2H), 3.78 (s, 6H), 3.30 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.9, 156.2, 153.5, 150.7, 149.2, 146.6, 120.9, 104.3, 30.5, 28.6. HRMS (ESI) m/z calculated for $[C_{18}H_{16}N_6O_4+H]^+$ 381.1306, found 381.1296.



5aa

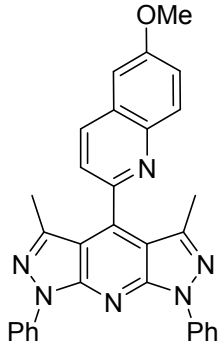
3,5-Dimethyl-1,7-diphenyl-4-(quinolin-2-yl)-1,7-dihydrodipyrazolo[3,4-b:4',3'-e]pyridine (5aa), 124 mg, 89%, green solid, m.p. 228-230℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 – 8.35 (m, 5H), 8.24 (d, *J* = 8.4 Hz, 1H), 8.01 (d, *J* = 8.1 Hz, 1H), 7.87 (t, *J* = 7.5 Hz, 1H), 7.71 (t, *J* = 7.2 Hz, 2H), 7.55 (t, *J* = 7.6 Hz, 4H), 7.35 – 7.27 (m, 2H), 2.05 (d, *J* = 3.8 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.4, 150.7, 147.4, 144.0, 139.6, 139.1, 136.3, 130.7, 129.7, 128.9, 127.9, 127.7, 127.4, 125.2, 122.1, 120.3, 113.1, 14.9. HRMS (ESI) m/z

calculated for $[C_{30}H_{22}N_6+H]^+$ 467.1979, found 467.1969.



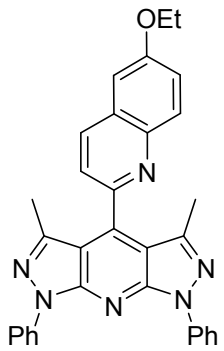
5ba

3,5-Dimethyl-4-(6-methylquinolin-2-yl)-1,7-diphenyl-1,7-dihydrodipyrazolo[3,4-b:4',3'-e]pyridine (5ba), 102 mg, 71%, brown solid, m.p. 213-215℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 (dd, *J* = 8.7, 1.0 Hz, 4H), 8.31 (d, *J* = 8.3 Hz, 1H), 8.14 (d, *J* = 8.6 Hz, 1H), 7.77 (s, 1H), 7.70 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.66 (d, *J* = 8.3 Hz, 1H), 7.55 (td, *J* = 7.5, 1.9 Hz, 4H), 7.33 – 7.27 (m, 2H), 2.64 (s, 3H), 2.06 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.7, 150.8, 150.6, 144.1, 143.5, 139.6, 139.3, 134.9, 131.1, 128.9, 128.7, 125.1, 123.7, 122.4, 120.3, 113.2, 105.1, 55.7, 14.9. HRMS (ESI) m/z calculated for $[C_{31}H_{24}N_6+H]^+$ 481.2135, found 481.2130.



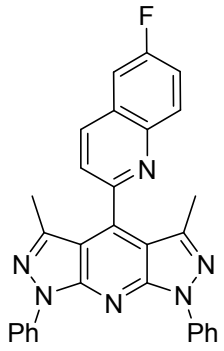
5ca

4-(6-Methoxyquinolin-2-yl)-3,5-dimethyl-1,7-diphenyl-1,7-dihydrodipyrazolo[3,4-b:4',3'-e]pyridine (5ca), 126 mg, 85%, white solid, m.p. 262-263℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 – 8.41 (m, 4H), 8.28 (d, *J* = 8.3 Hz, 1H), 8.13 (d, *J* = 9.2 Hz, 1H), 7.65 (d, *J* = 8.3 Hz, 1H), 7.57 – 7.50 (m, 5H), 7.29 (t, *J* = 7.4 Hz, 2H), 7.24 (d, *J* = 2.6 Hz, 1H), 4.01 (s, 3H), 2.06 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.1, 150.8, 150.6, 144.1, 143.5, 139.7, 139.5, 134.9, 131.1, 128.9, 128.7, 125.2, 123.9, 122.3, 120.4, 113.3, 105.8, 64.0, 14.9. HRMS (ESI) m/z calculated for $[C_{31}H_{24}N_6O+H]^+$ 497.2084, found 497.2075.



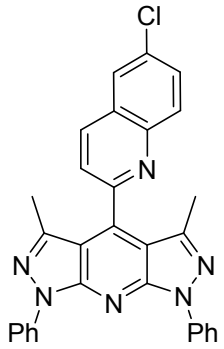
5da

4-(6-Ethoxyquinolin-2-yl)-3,5-dimethyl-1,7-diphenyl-1,7-dihydrodipyrazolo[3,4-b:4',3'-e]pyridine (5da), 106 mg, 69%, green solid, m.p. 279-281℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 (dd, *J* = 8.7, 1.1 Hz, 4H), 8.27 (d, *J* = 8.3 Hz, 1H), 8.11 (d, *J* = 9.2 Hz, 1H), 7.63 (d, *J* = 8.3 Hz, 1H), 7.57 – 7.49 (m, 5H), 7.32–7.27 (m, 2H), 7.23 (d, *J* = 2.7 Hz, 1H), 4.24 (q, *J* = 7.0 Hz, 2H), 2.07 (s, 6H), 1.55 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.1, 150.8, 150.6, 144.1, 143.4, 139.6, 139.4, 134.9, 131.1, 129.0, 128.7, 125.2, 124.0, 122.3, 120.4, 113.2, 105.8, 64.0, 14.9, 14.7. HRMS (ESI) m/z calculated for $[C_{32}H_{26}N_6O+H]^+$ 511.2241, found 511.2233.



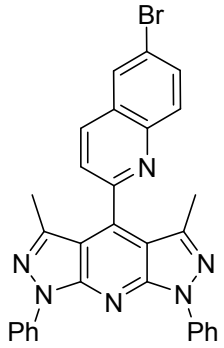
5ea

4-(6-Fluoroquinolin-2-yl)-3,5-dimethyl-1,7-diphenyl-1,7-dihydrodipyrazolo[3,4-b:4',3'-e]pyridine (5ea), 101 mg, 70%, green solid, m.p. 236-237℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44-8.39 (m, 4H), 8.34 (d, *J* = 8.4 Hz, 1H), 8.25 (dd, *J* = 9.1, 5.3 Hz, 1H), 7.72 (d, *J* = 8.3 Hz, 1H), 7.67-7.60 (m, 2H), 7.57-7.52 (m, 4H), 7.33-7.27 (m, 2H), 2.04 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.9, 152.7, 150.7, 144.4, 143.8, 139.5, 138.5, 135.8, 132.3, 129.0, 128.3, 125.3, 122.9, 121.4, 120.4, 113.0, 111.1, 14.9. HRMS (ESI) m/z calculated for $[C_{30}H_{21}FN_6+H]^+$ 485.1884, found 485.1876.



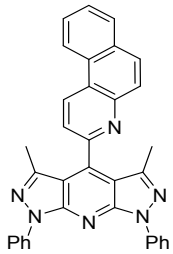
5ga

4-(6-Chloroquinolin-2-yl)-3,5-dimethyl-1,7-diphenyl-1,7-dihydrodipyrazolo[3,4-b:4',3'-e]pyridine (5ga), 108 mg, 72%, yellow solid, m.p. 227-229℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43-8.39 (m, 4H), 8.26 (d, *J* = 8.3 Hz, 1H), 8.16 (d, *J* = 9.0 Hz, 1H), 7.98 (d, *J* = 2.3 Hz, 1H), 7.79 (dd, *J* = 9.0, 2.3 Hz, 1H), 7.72 (d, *J* = 8.4 Hz, 1H), 7.57-7.51 (m, 4H), 7.32-7.27 (m, 2H), 2.01 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.7, 150.6, 145.8, 143.7, 139.5, 138.6, 135.3, 133.6, 131.7, 131.3, 128.9, 128.0, 126.5, 125.2, 123.0, 120.3, 112.9, 14.9. HRMS (ESI) m/z calculated for $[C_{30}H_{21}ClN_6+H]^+$ 501.1589, found 501.1585.



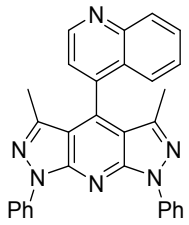
5ia

4-(6-Bromoquinolin-2-yl)-3,5-dimethyl-1,7-diphenyl-1,7-dihydrodipyrazolo[3,4-b:4',3'-e]pyridine (5ia), 115 mg, 70%, yellow solid, m.p. 213-215℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (dd, *J* = 8.6, 1.0 Hz, 4H), 8.27 (d, *J* = 8.4 Hz, 1H), 8.16 (d, *J* = 2.1 Hz, 1H), 8.09 (d, *J* = 9.0 Hz, 1H), 7.93 (dd, *J* = 8.9, 2.2 Hz, 1H), 7.72 (d, *J* = 8.4 Hz, 1H), 7.54 (td, *J* = 7.5, 1.8 Hz, 4H), 7.33 – 7.26 (m, 2H), 2.02 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.9, 150.7, 146.0, 143.7, 139.5, 138.6, 135.2, 134.3, 131.4, 129.9, 128.9, 128.5, 125.3, 123.0, 121.9, 120.3, 112.9, 14.9. HRMS (ESI) m/z calculated for $[C_{30}H_{21}BrN_6+H]^+$ 545.1084, found 545.1076.



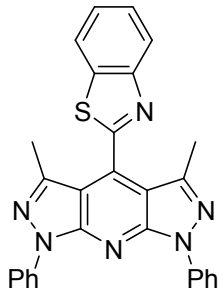
5ja

3-(3,5-Dimethyl-1,7-diphenyl-1,7-dihydrodipyrazolo[3,4-b:4',3'-e]pyridin-4-yl)benzo[f]quinoline (5ja), 127 mg, 82%, white solid, m.p. 279-280℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.20 (d, *J* = 8.4 Hz, 1H), 8.77 (d, *J* = 8.0 Hz, 1H), 8.46 – 8.42 (m, 4H), 8.17 – 8.10 (m, 2H), 8.05 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.85 – 7.74 (m, 2H), 7.59 – 7.52 (m, 4H), 7.34 – 7.28 (m, 2H), 2.08 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.8, 150.8, 147.6, 144.1, 139.6, 139.0, 132.4, 132.1, 131.0, 129.3, 129.0, 128.1, 127.9, 127.7, 125.2, 125.1, 122.9, 122.3, 120.4, 113.2, 15.0. HRMS (ESI) m/z calculated for $[C_{34}H_{24}N_6+H]^+$ 517.2135, found 517.2125.



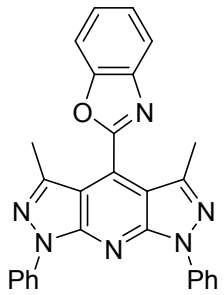
5ka

3,5-Dimethyl-1,7-diphenyl-4-(quinolin-4-yl)-1,7-dihydrodipyrazolo[3,4-b:4',3'-e]pyridine (5ka), 88 mg, 63%, brown solid, m.p. 264-266℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.13 (d, *J* = 4.3 Hz, 1H), 8.45 – 8.39 (m, 4H), 8.32 (d, *J* = 8.5 Hz, 1H), 7.83 (ddd, *J* = 8.4, 6.8, 1.4 Hz, 1H), 7.56 (td, *J* = 7.5, 2.0 Hz, 5H), 7.51 (ddd, *J* = 8.1, 6.8, 1.2 Hz, 1H), 7.42 – 7.38 (m, 1H), 7.34 – 7.29 (m, 2H), 1.82 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.5, 149.2, 147.7, 143.9, 141.3, 139.4, 135.8, 130.5, 130.0, 129.0, 128.0, 127.0, 125.5, 125.4, 121.4, 120.3, 113.4, 14.2. HRMS (ESI) m/z calculated for $[C_{30}H_{22}N_6+H]^+$ 467.1979, found 467.1976.



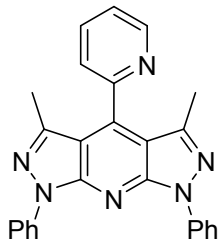
5oa

2-(3,5-Dimethyl-1,7-diphenyl-1,7-dihydrodipyrazolo[3,4-b:4',3'-e]pyridin-4-yl)benzo[d]thiazole (5oa), 77 mg, 55%, green solid, m.p. 214-216℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 – 8.38 (m, 4H), 8.27 (d, *J* = 8.2 Hz, 1H), 8.08 (d, *J* = 7.5 Hz, 1H), 7.68 (ddd, *J* = 8.3, 7.3, 1.3 Hz, 1H), 7.62 – 7.52 (m, 5H), 7.34 – 7.29 (m, 2H), 2.25 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.6, 152.9, 150.4, 143.6, 139.4, 135.8, 131.1, 129.0, 127.1, 126.4, 125.4, 124.2, 121.7, 120.4, 113.3, 14.6. HRMS (ESI) m/z calculated for $[C_{28}H_{20}N_6S+H]^+$ 473.1543, found 473.1538.



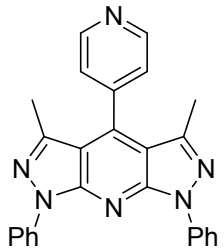
5pa

2-(3,5-Dimethyl-1,7-diphenyl-1,7-dihydrodipyrazolo[3,4-b:4',3'-e]pyridin-4-yl)benzo[d]oxazole (5pa), 68 mg, 50%, yellow solid, m.p. 214-216℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 – 8.37 (m, 4H), 7.99 – 7.96 (m, 1H), 7.76 – 7.72 (m, 1H), 7.58 – 7.52 (m, 6H), 7.34 – 7.28 (m, 2H), 2.45 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.7, 150.8, 150.5, 143.5, 141.2, 139.3, 129.0, 126.6, 125.5, 125.4, 124.2, 121.1, 120.5, 113.1, 111.1, 14.8. HRMS (ESI) m/z calculated for $[C_{28}H_{20}N_6O+H]^+$ 457.1771, found 457.1762.



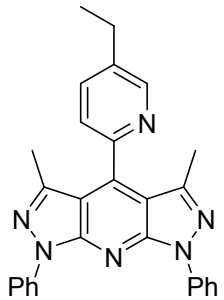
5qa

3,5-Dimethyl-1,7-diphenyl-4-(pyridin-2-yl)-1,7-dihydrodipyrazolo[3,4-b:4',3'-e]pyridine (5qa), 57 mg, 45%, green solid, m.p. 246-248℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.86 (s, 1H), 8.45-8.37 (m, 4H), 7.92 (t, *J* = 7.4 Hz, 1H), 7.59 (d, *J* = 7.7 Hz, 1H), 7.54 (t, *J* = 8.0 Hz, 5H), 7.29 (t, *J* = 7.4 Hz, 2H), 2.09 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.3, 150.7, 149.5, 143.9, 139.6, 138.7, 136.2, 128.9, 125.2, 124.8, 123.9, 120.3, 113.0, 14.7. HRMS (ESI) m/z calculated for $[C_{26}H_{20}N_6+H]^+$ 417.1822, found 417.1808.



5ra

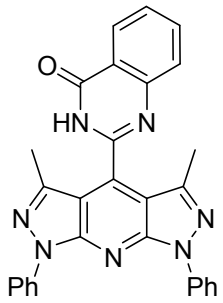
3,5-Dimethyl-1,7-diphenyl-4-(pyridin-4-yl)-1,7-dihydrodipyrazolo[3,4-b:4',3'-e]pyridine (5ra), 67 mg, 53%, yellow solid, m.p. 250-252℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.80 (d, *J* = 4.4 Hz, 2H), 8.34 (d, *J* = 7.7 Hz, 4H), 7.50 (t, *J* = 8.0 Hz, 4H), 7.43 (d, *J* = 5.3 Hz, 2H), 7.27 (t, *J* = 7.4 Hz, 2H), 2.01 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.1, 149.5, 143.5, 142.7, 139.3, 137.3, 128.9, 125.3, 123.7, 120.1, 112.4, 14.8. HRMS (ESI) m/z calculated for $[C_{26}H_{20}N_6+H]^+$ 417.1822, found 417.1808.



5sa

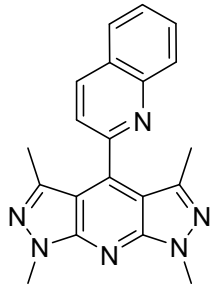
4-(5-Ethylpyridin-2-yl)-3,5-dimethyl-1,7-diphenyl-1,7-dihydrodipyrazolo[3,4-b:4',3'-

e]pyridine (5sa), 26 mg, 19%, white solid, m.p. 228-230℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (d, *J* = 1.6 Hz, 1H), 8.43 – 8.38 (m, 4H), 7.75 (dd, *J* = 7.9, 2.1 Hz, 1H), 7.56 – 7.49 (m, 5H), 7.29 (tt, *J* = 7.8, 1.2 Hz, 2H), 2.84 (q, *J* = 7.6 Hz, 2H), 2.10 (s, 6H), 1.40 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.7, 150.4, 149.1, 144.1, 139.8, 139.6, 139.1, 135.4, 128.9, 125.1, 124.4, 120.3, 113.2, 26.0, 15.1, 14.8. HRMS (ESI) m/z calculated for $[C_{28}H_{24}N_6+H]^+$ 445.2135, found 445.2121.



5ta

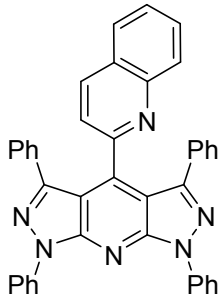
2-(3,5-Dimethyl-1,7-diphenyl-1,7-dihydrodipyrazolo[3,4-b:4',3'-e]pyridin-4-yl)quinazolin-4(3H)-one (5ta), 43 mg, 29%, yellow solid, m.p. 100-100℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (dd, J = 8.0, 0.9 Hz, 1H), 8.27 (d, J = 7.6 Hz, 4H), 7.94 – 7.87 (m, 1H), 7.83 (d, J = 8.1 Hz, 1H), 7.70 – 7.62 (m, 1H), 7.45 (t, J = 8.0 Hz, 4H), 7.30 (d, J = 7.4 Hz, 3H), 2.36 (s, 6H).^{13}C NMR (101 MHz, $CDCl_3$) δ 181.6, 150.3, 143.1, 138.9, 135.5, 129.1, 128.1, 126.9, 125.6, 119.7, 111.9, 14.4. (Some signals of the carbon were missing in the spectrum because of the poor solubility of the compound **5ta**). HRMS (ESI) m/z calculated for $[C_{29}H_{21}N_7O+H]^+$ 484.1880, found 484.1868.



5ab

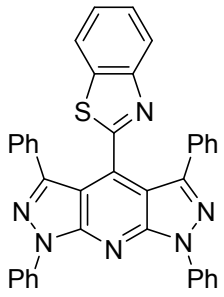
1,3,5,7-Tetramethyl-4-(quinolin-2-yl)-1,7-dihydrodipyrazolo[3,4-b:4',3'-e]pyridine (5ab), 36 mg, 36%, yellow liquid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (d, *J* = 7.9 Hz, 1H), 8.24 – 8.19 (m, 1H), 7.98 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.84 (ddd, *J* = 8.4, 6.9, 1.5 Hz, 1H), 7.69 (ddd, *J* = 8.1, 6.9, 1.2 Hz, 1H), 7.62 (d, *J* = 8.3 Hz, 1H), 4.09 (s, 6H), 1.98 (s, 6H). ^{13}C

NMR (101 MHz, $CDCl_3$) δ 154.1, 152.2, 147.4, 141.7, 138.6, 136.1, 130.6, 129.7, 127.8, 127.6, 127.4, 122.2, 111.1, 33.5, 14.8. HRMS (ESI) m/z calculated for $[C_{20}H_{18}N_6+H]^+$ 343.1666, found 343.1654.



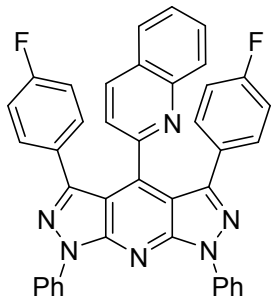
5ac

1,3,5,7-Tetraphenyl-4-(quinolin-2-yl)-1,7-dihydrodipyrazolo[3,4-b:4',3'-e]pyridine (5ac), 75 mg, 43%, yellow solid, m.p. 242-244℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 (dd, *J* = 8.7, 1.1 Hz, 4H), 7.69 – 7.50 (m, 10H), 7.41 – 7.33 (m, 2H), 7.12 – 7.03 (m, 5H), 6.90 – 6.82 (m, 2H), 6.75 (t, *J* = 7.6 Hz, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.3, 150.9, 147.5, 146.9, 139.6, 139.6, 135.0, 132.8, 129.6, 129.3, 129.0, 128.8, 127.6, 127.3, 127.2, 127.0, 126.8, 125.8, 122.7, 121.0, 112.6. HRMS (ESI) m/z calculated for $[C_{40}H_{26}N_6+H]^+$ 591.2292, found 591.2280.



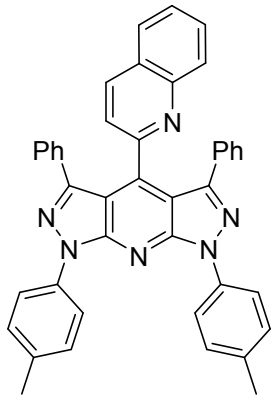
5oc

2-(1,3,5,7-Tetraphenyl-1,7-dihydrodipyrazolo[3,4-b:4',3'-e]pyridin-4-yl)benzo[d]thiazole (5oc), 85 mg, 47%, green solid, m.p. 239-240℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56-8.51 (m, 4H), 7.72-7.57 (m, 6H), 7.46-7.34 (m, 4H), 7.30-7.27 (m, 2H), 7.26-7.25 (m, 2H), 7.01-6.96 (m, 2H), 6.91-6.85 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.3, 152.3, 150.4, 147.2, 139.4, 136.3, 132.6, 131.9, 129.1, 128.6, 128.0, 127.5, 126.1, 126.0, 125.7, 123.7, 121.0, 120.7, 112.8. HRMS (ESI) m/z calculated for $[C_{38}H_{24}N_6S+H]^+$ 597.1856, found 597.1843.



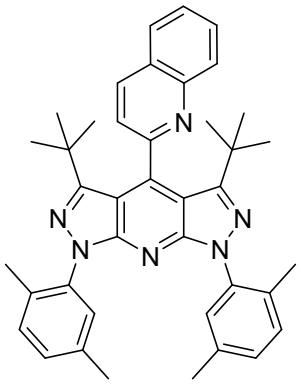
5ad

3,5-Bis(4-fluorophenyl)-1,7-diphenyl-4-(quinolin-2-yl)-1,7-dihydrodipyrazolo[3,4-b:4',3'-e]pyridine (5ad), 110 mg, 66%, yellow solid, m.p. 269-270℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56 – 8.50 (m, 4H), 7.74 (d, *J* = 8.3 Hz, 2H), 7.67 – 7.56 (m, 7H), 7.41 – 7.34 (m, 2H), 7.09 – 7.01 (m, 5H), 6.52 – 6.40 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.5, 161.0, 152.1, 150.8, 146.9, 146.4, 139.4, 135.1, 130.6, 130.0, 129.1, 129.0, 128.9, 127.6, 127.2, 126.8, 125.9, 122.6, 120.9, 114.5, 112.4. HRMS (ESI) m/z calculated for $[C_{40}H_{24}F_2N_6+H]^+$ 627.2103, found 627.2091.



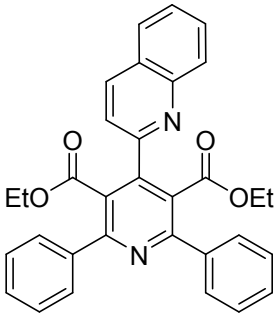
5ae

3,5-Diphenyl-4-(quinolin-2-yl)-1,7-di-p-tolyl-1,7-dihydrodipyrazolo[3,4-b:4',3'-e]pyridine (5ae), 96 mg, 53%, green solid, m.p. >300℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44-8.37 (m, 4H), 7.65 (t, *J* = 8.5 Hz, 2H), 7.61-7.54 (m, 2H), 7.52 (ddd, *J* = 8.1, 6.0, 2.3 Hz, 1H), 7.40 (d, *J* = 8.3 Hz, 4H), 7.12-7.01 (m, 5H), 6.89-6.82 (m, 2H), 6.74 (t, *J* = 7.5 Hz, 4H), 2.48 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.5, 150.7, 147.1, 146.9, 139.5, 137.2, 135.4, 134.8, 132.9, 129.6, 129.5, 129.3, 128.8, 127.5, 127.3, 127.1, 127.0, 126.8, 122.7, 120.9, 112.4, 21.1. HRMS (ESI) m/z calculated for $[C_{42}H_{30}N_6+H]^+$ 619.2605, found 619.2593.



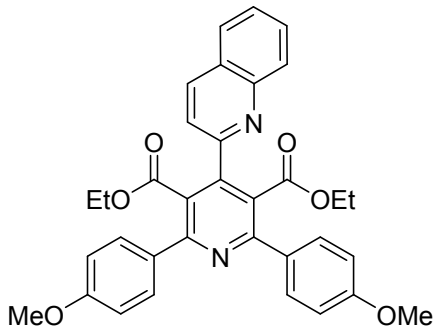
5af

3,5-Di-tert-butyl-1,7-bis(2,5-dimethylphenyl)-4-(quinolin-2-yl)-1,7-dihydrodipyrazolo[3,4-b:4',3'-e]pyridine (5af), 72 mg, 40%, yellow solid, m.p. 266-267℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, *J* = 8.3 Hz, 1H), 8.25 (d, *J* = 8.3 Hz, 1H), 8.02 – 7.98 (m, 1H), 7.88 (ddd, *J* = 8.4, 6.9, 1.4 Hz, 1H), 7.78 (d, *J* = 8.4 Hz, 1H), 7.73 (ddd, *J* = 8.1, 6.9, 1.2 Hz, 1H), 7.35 – 7.31 (m, 2H), 7.19 (d, *J* = 7.8 Hz, 2H), 7.08 (dd, *J* = 7.8, 1.4 Hz, 2H), 2.36 (s, 6H), 2.22 (s, 6H), 0.95 (s, 18H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.2, 153.9, 151.9, 146.8, 139.2, 137.3, 135.8, 135.6, 132.0, 131.0, 130.7, 129.8, 128.5, 128.0, 127.9, 127.8, 127.7, 125.4, 111.4, 34.5, 30.2, 20.9, 18.5. HRMS (ESI) m/z calculated for $[C_{40}H_{42}N_6+H]^+$ 607.3544, found 607.3530.



5ag

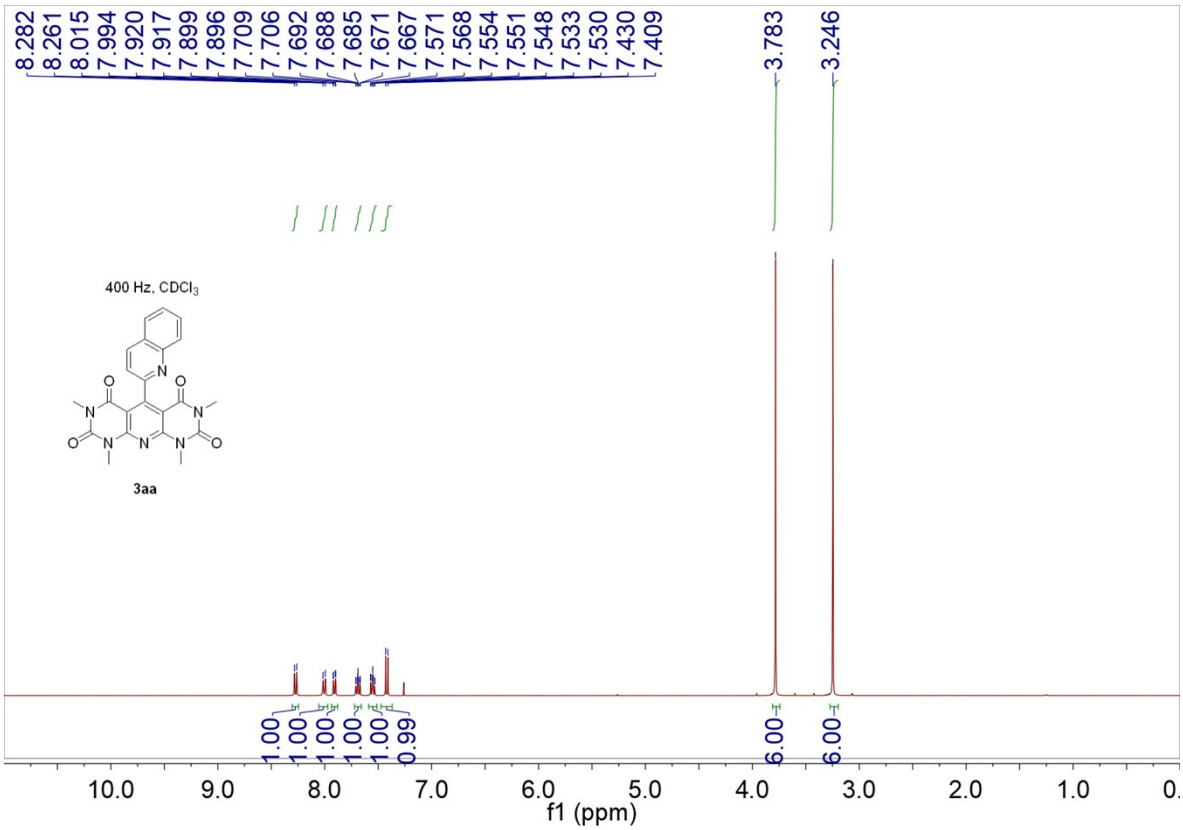
Diethyl 2,6-diphenyl-4-(quinolin-2-yl)pyridine-3,5-dicarboxylate (5ag), 37 mg, 25%, brown solid, m.p. 160-162℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 8.1 Hz, 1H), 8.08 (d, *J* = 8.1 Hz, 1H), 7.90 – 7.86 (m, 1H), 7.78 – 7.68 (m, 5H), 7.64 – 7.57 (m, 2H), 7.46 – 7.41 (m, 6H), 3.87 (q, *J* = 7.1 Hz, 4H), 0.77 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.7, 157.3, 155.0, 147.7, 146.8, 139.3, 136.5, 130.1, 129.4, 129.1, 128.7, 128.3, 127.7, 127.3, 127.2, 127.1, 61.5, 13.4. HRMS (ESI) m/z calculated for $[C_{32}H_{26}N_2O_4+H]^+$ 503.1965, found 503.1957.

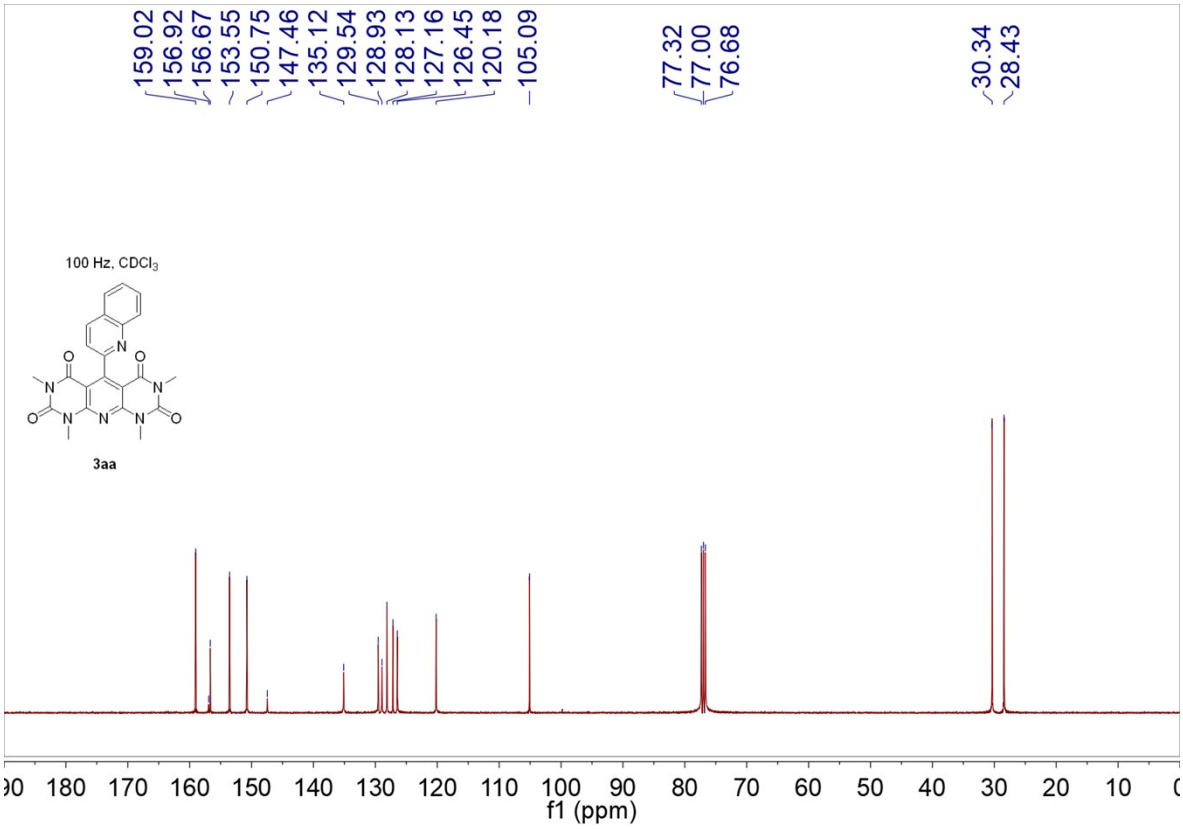


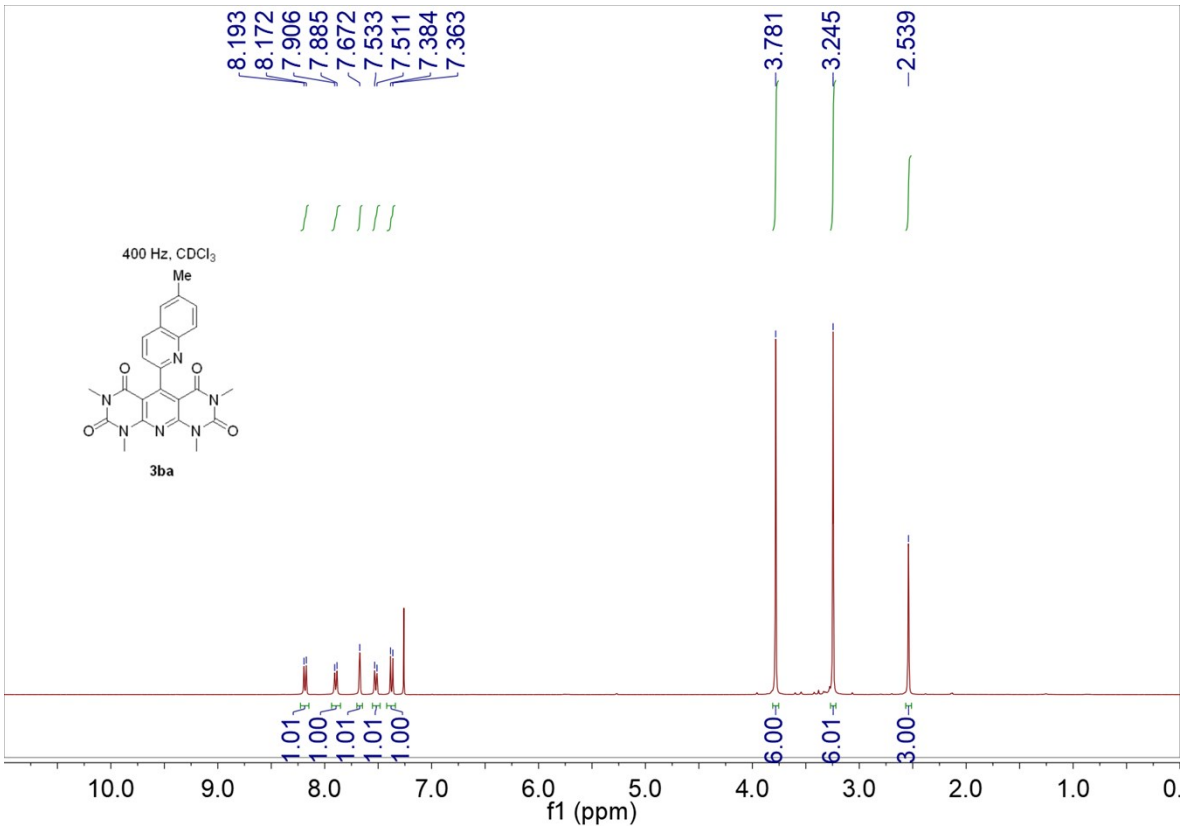
5ah

Diethyl 2,6-bis(4-methoxyphenyl)-4-(quinolin-2-yl)pyridine-3,5-dicarboxylate (5ah), 66 mg, 42%, yellow solid, m.p. 183-185℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 8.5 Hz, 1H), 8.09 (d, *J* = 8.6 Hz, 1H), 7.87 (d, *J* = 8.1 Hz, 1H), 7.76 – 7.72 (m, 1H), 7.71 – 7.67 (m, 4H), 7.62 – 7.55 (m, 2H), 6.99 – 6.94 (m, 4H), 3.90 (q, *J* = 7.1 Hz, 4H), 3.83 (s, 6H), 0.80 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.0, 160.4, 156.4, 155.2, 147.6, 146.8, 136.3, 131.7, 130.0, 130.0, 129.3, 127.6, 127.1, 127.1, 125.9, 120.8, 113.7, 61.3, 55.2, 13.4. HRMS (ESI) m/z calculated for $[C_{34}H_{30}N_2O_6+H]^+$ 563.2177, found 563.2164.

5. ^{1}H-NMR and ^{13}C-NMR Spectra of Products



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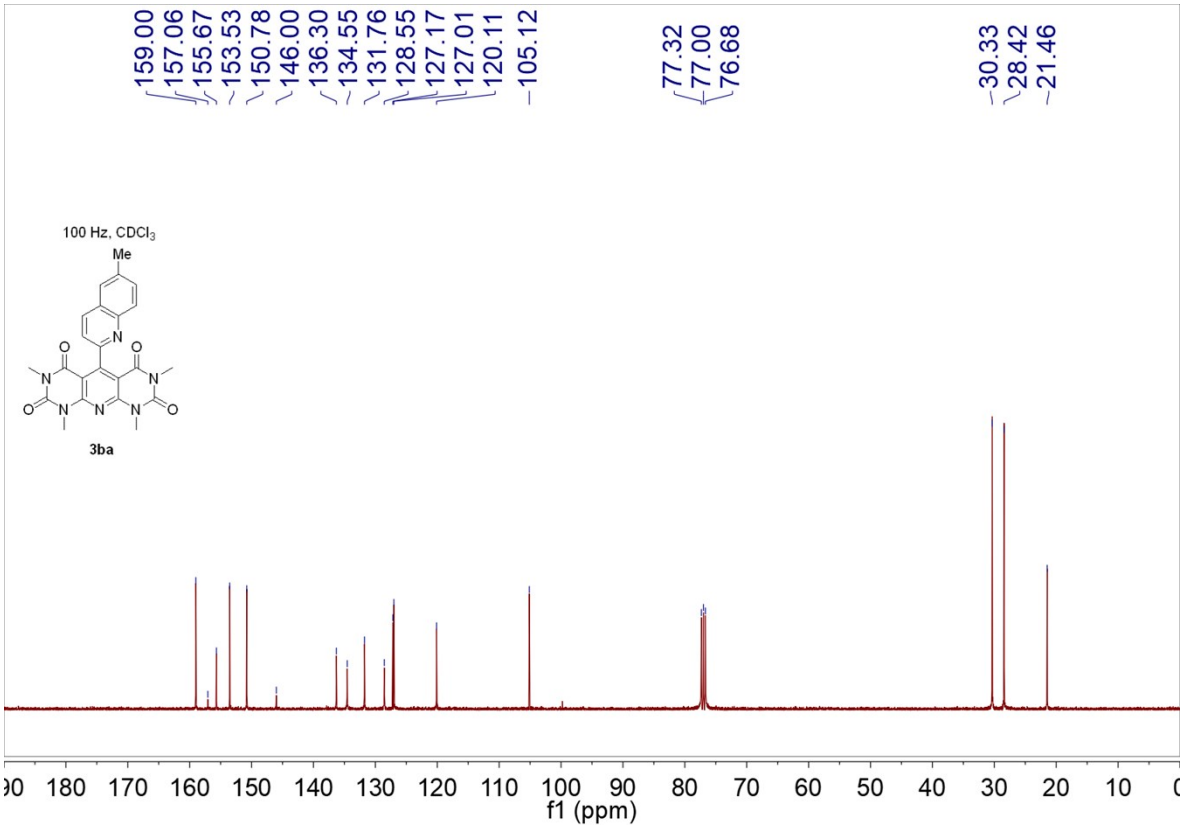
8.172
7.906
7.885
7.672
7.533
7.511
7.384
7.363
3.781
3.245
2.539
400 Hz, CDCl3
Me
3ba
1.01
1.00
1.01
1.01
1.00
6.00
6.01
3.00
f1 (ppm)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155.67
153.53
150.78
146.00
136.30
134.55
131.76
128.55
127.17
127.01
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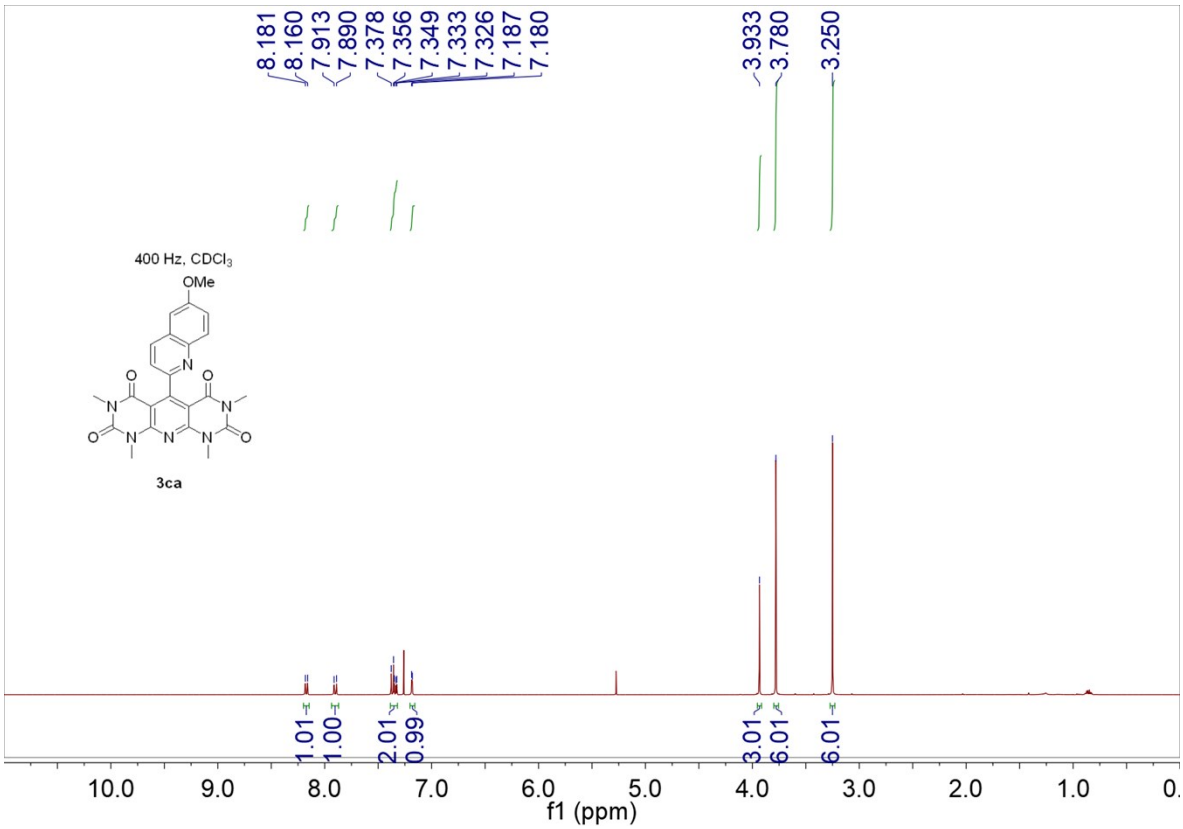
21.46
100 Hz, CDCl3
Me
3ba
f1 (ppm)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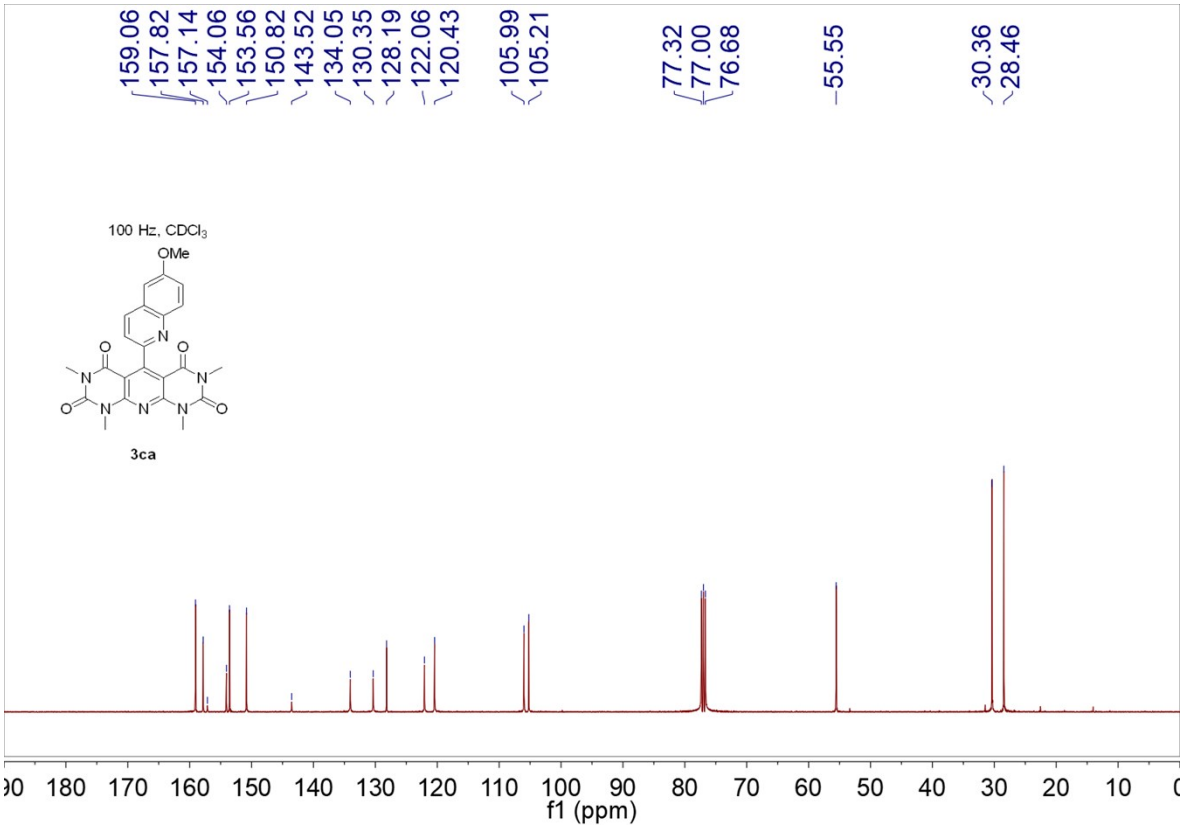
8.160
7.913
7.890
7.378
7.356
7.349
7.333
7.326
7.187
7.180
3.933
3.780
3.250
400 Hz, CDCl3
OMe
3ca
1.01
1.00
2.01
0.99
3.01
6.01
6.01
f1 (ppm)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157.82
157.14
154.06
153.56
150.82
143.52
134.05
130.35
128.19
122.06
120.43
105.99
105.21
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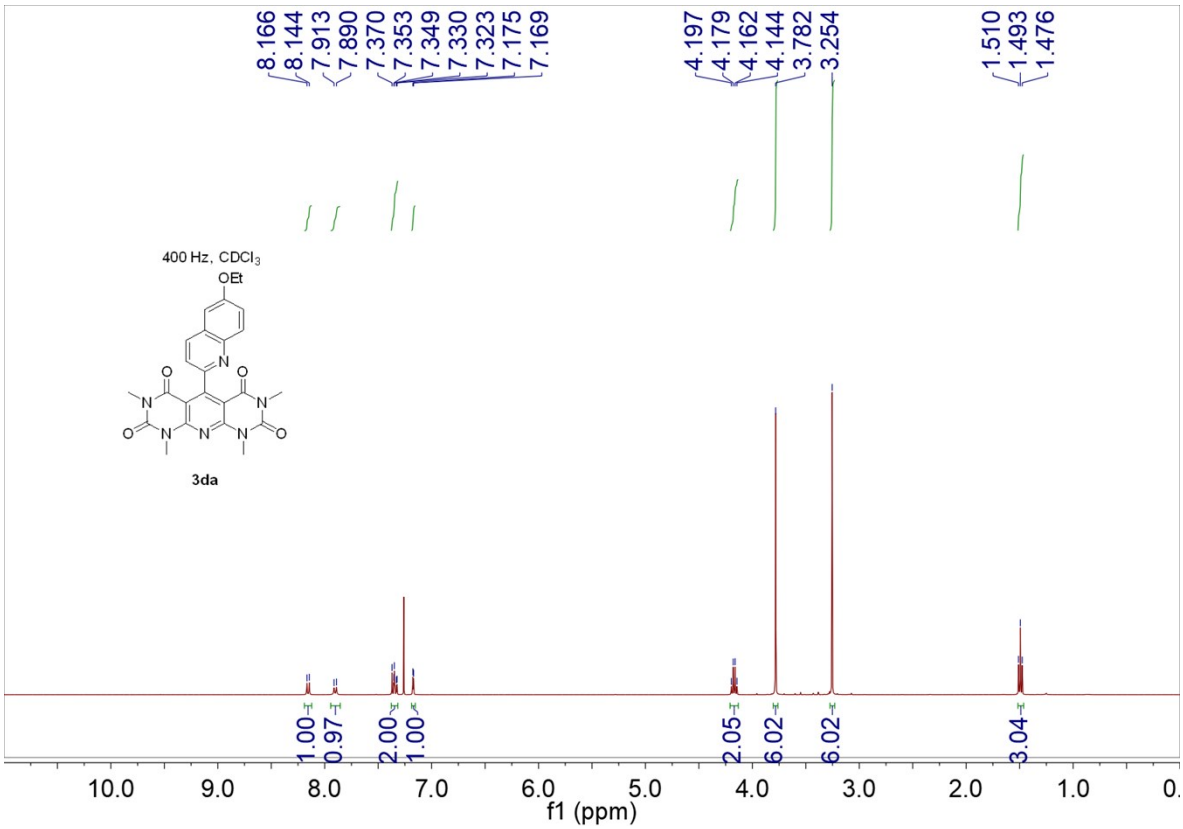
77.00
76.68
55.55
30.36
28.46
100 Hz, CDCl3
OMe
3ca
f1 (ppm)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8.144
7.913
7.890
7.370
7.353
7.349
7.330
7.323
7.175
7.169
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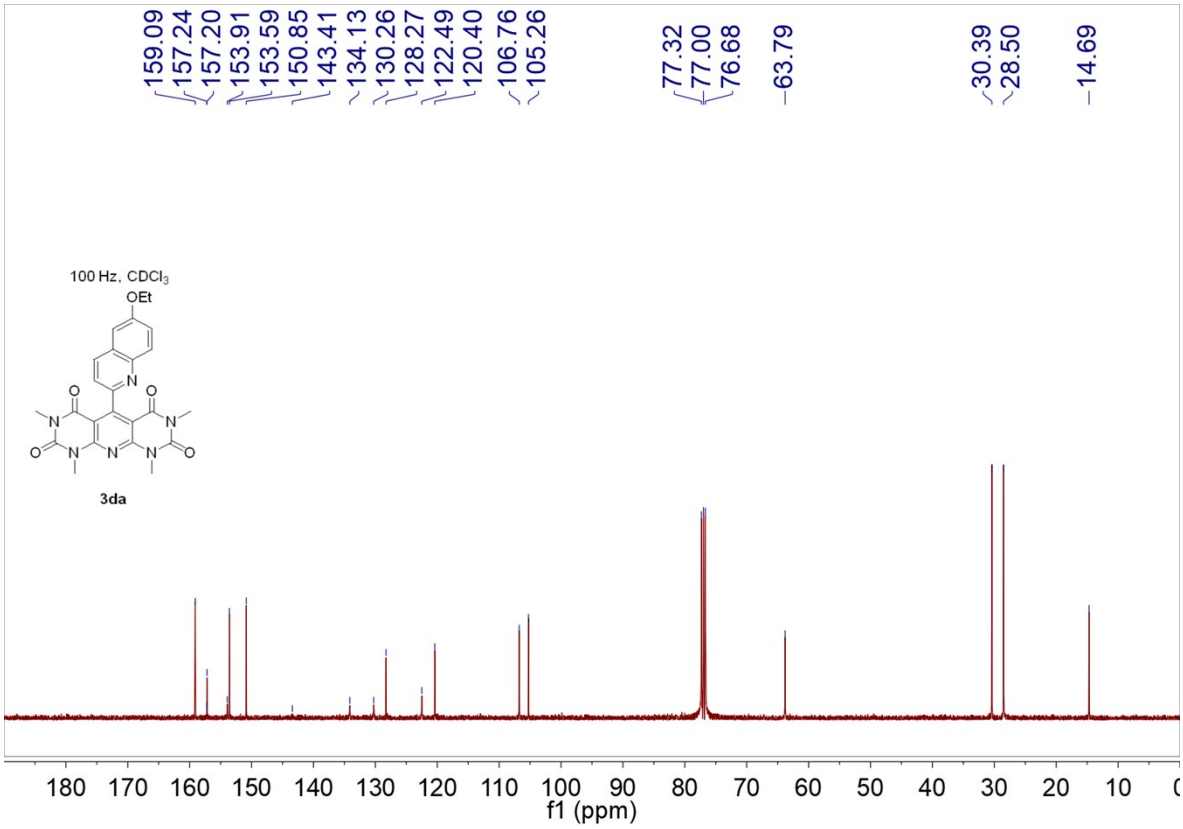
4.179
4.162
4.144
3.782
3.254
1.510
1.493
1.476
400 Hz, CDCl3
OEt
3da
1.00
0.97
2.00
1.00
2.05
6.02
6.02
3.04
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)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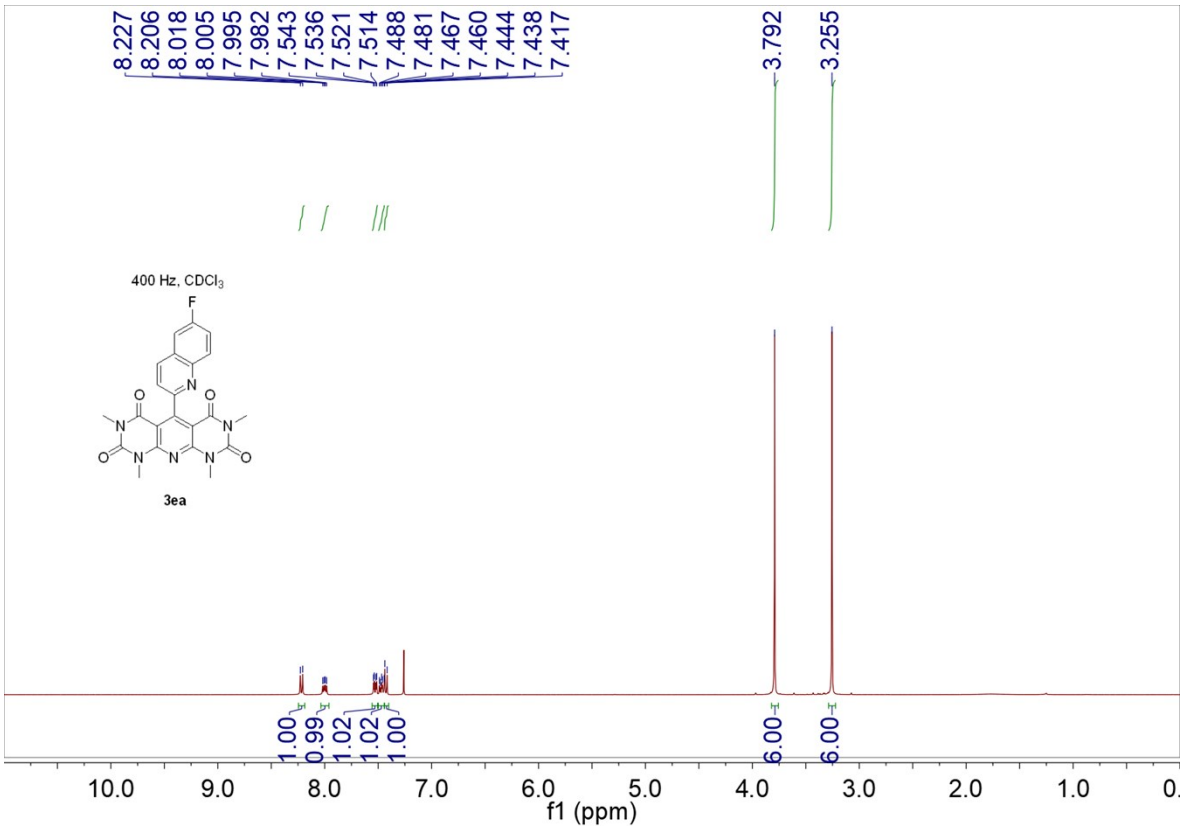
157.24
157.20
153.91
153.59
150.85
143.41
134.13
130.26
128.27
122.49
120.40
106.76
105.26
77.32
77.00
76.68
63.79
30.39
28.50
14.69
100 Hz, CDCl3
OEt
3da
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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8.005
7.995
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7.543
7.536
7.521
7.514
7.488
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7.467
7.460
7.444
7.438
7.417
3.792
3.255
400 Hz, CDCl3
F
N
O
O
N
N
N
N
N
O
O
3ea
1.00
0.99
1.02
1.02
1.00
6.00
6.00
10.0
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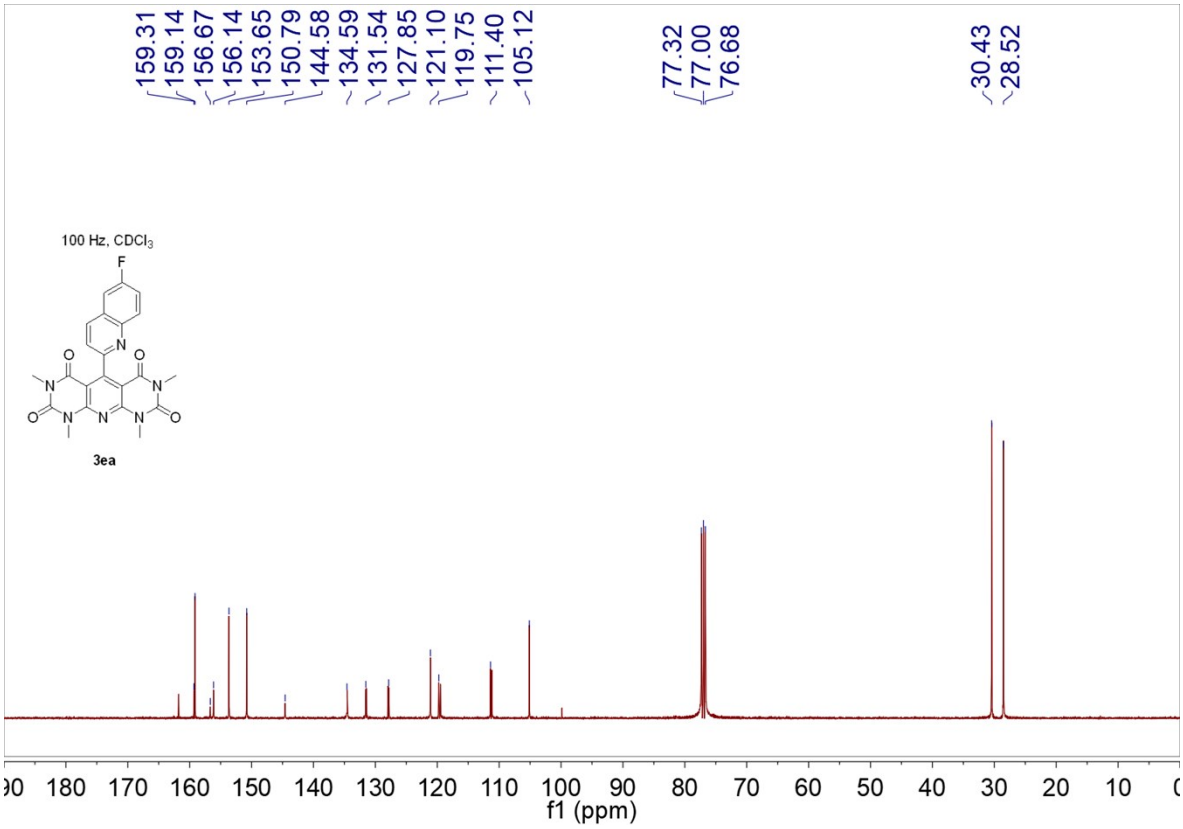
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)


159.31
159.14
156.67
156.14
153.65
150.79
144.58
134.59
131.54
127.85
121.10
119.75
111.40
105.12
77.32
77.00
76.68
30.43
28.52
100 Hz, CDCl3
F
N
O
O
N
N
N
N
N
O
O
3ea
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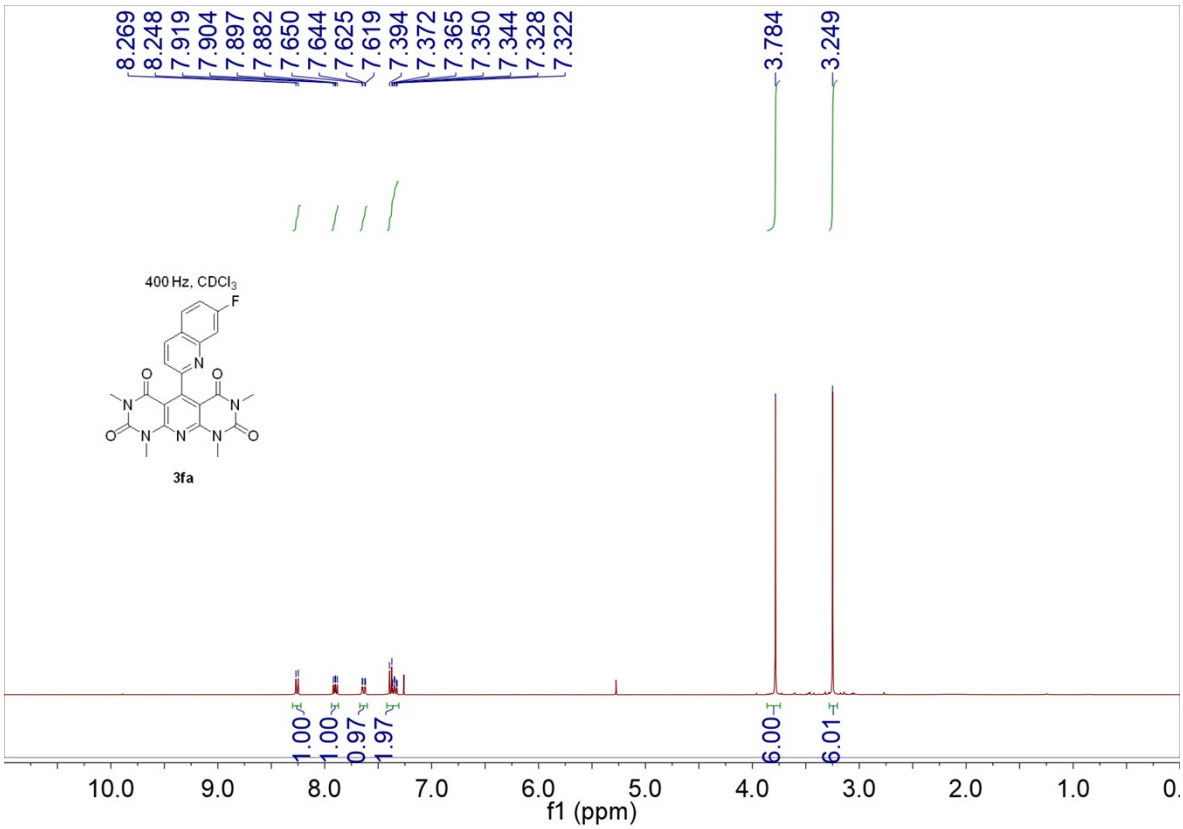
70
60
50
40
30
20
10
f1 (ppm)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7.882
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7.644
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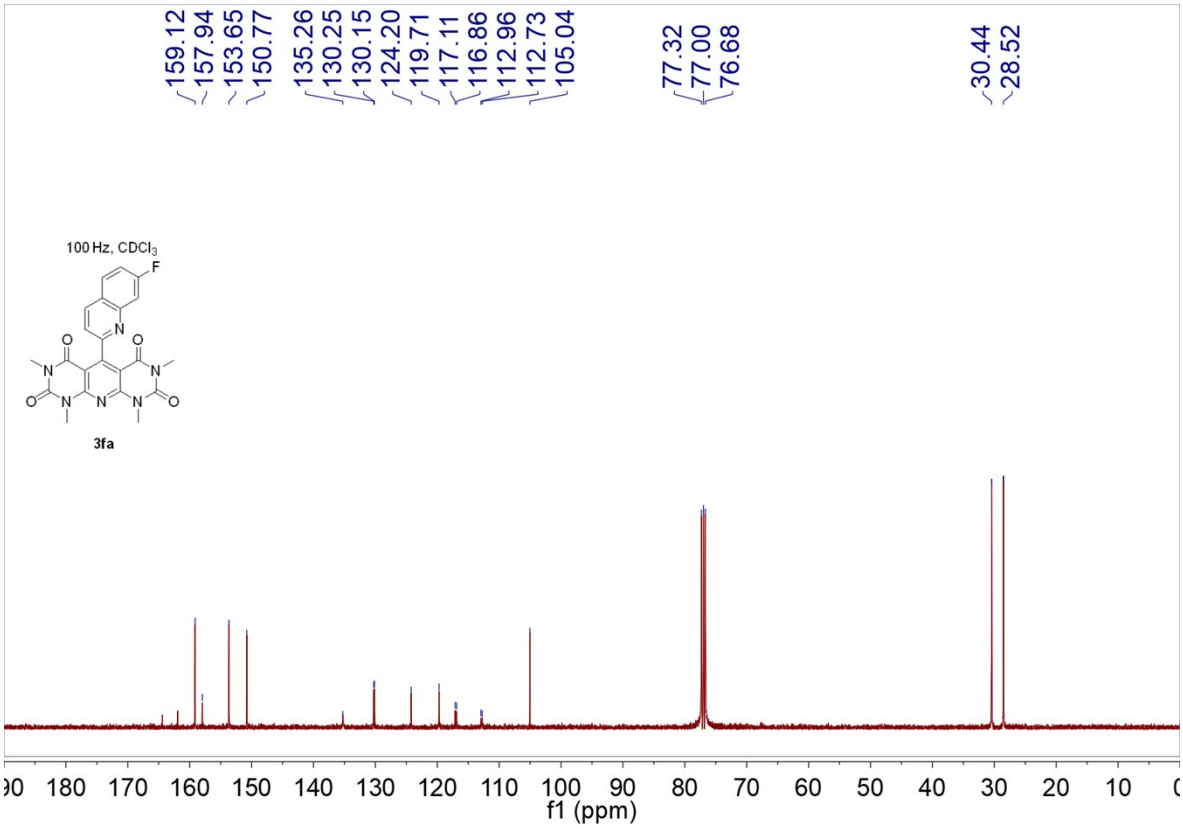
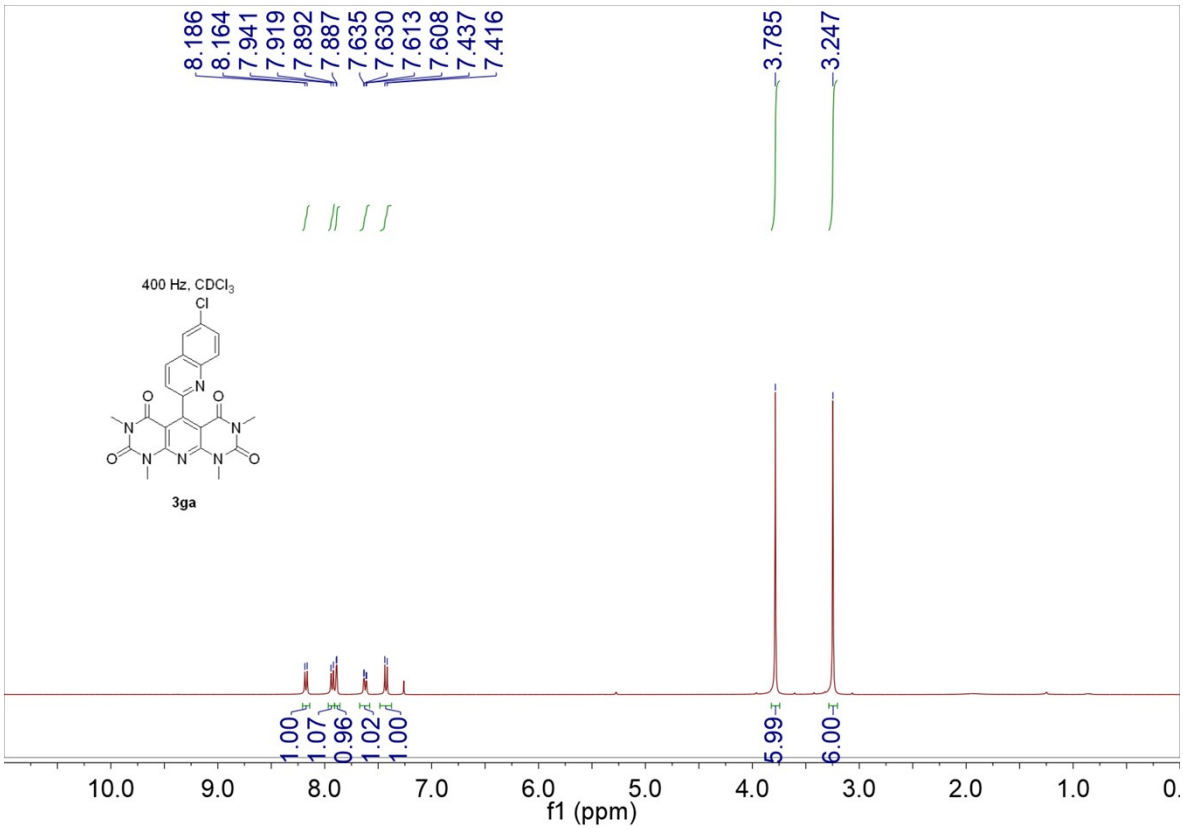
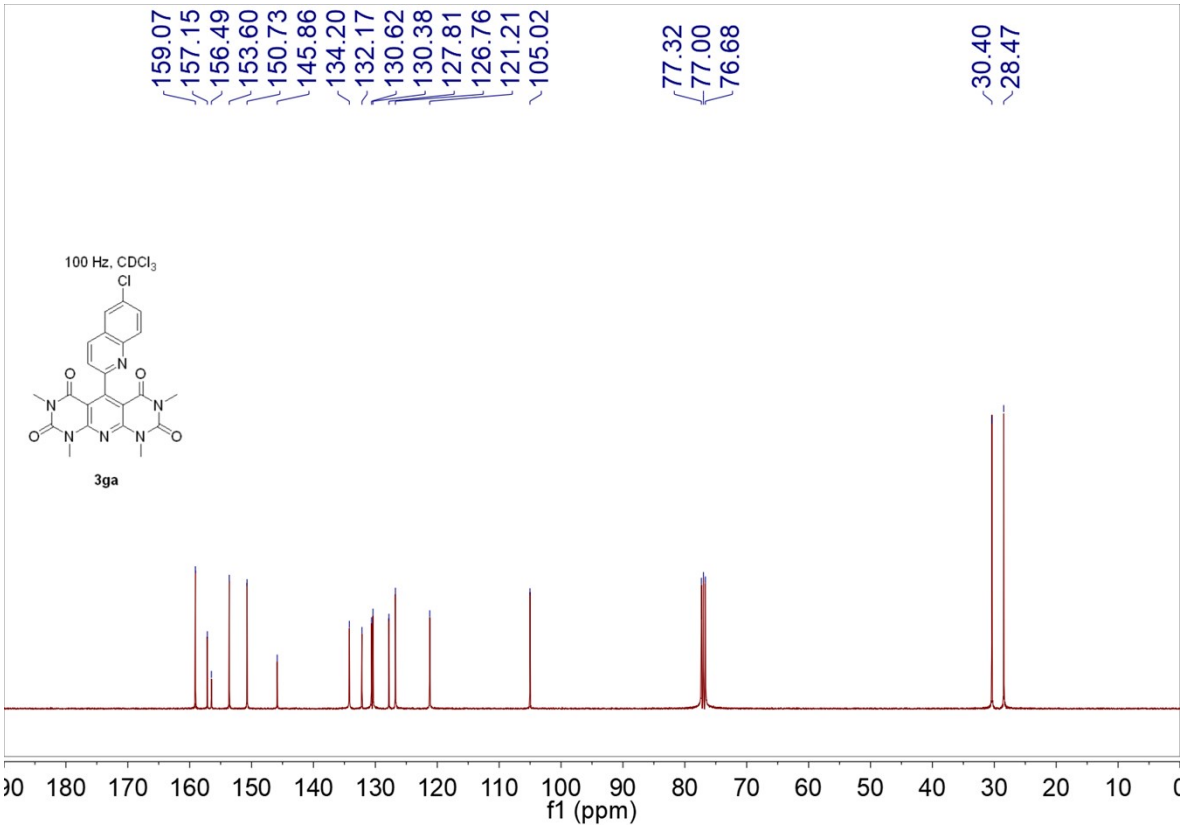
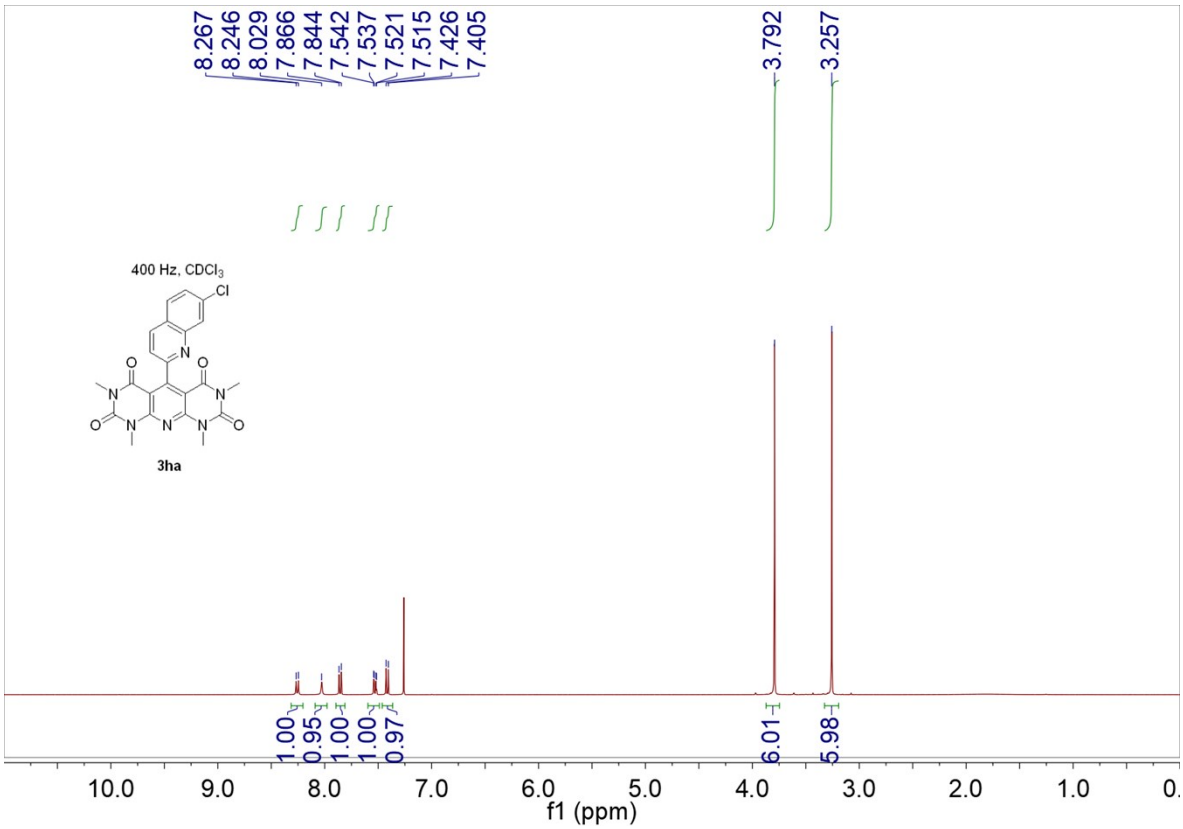
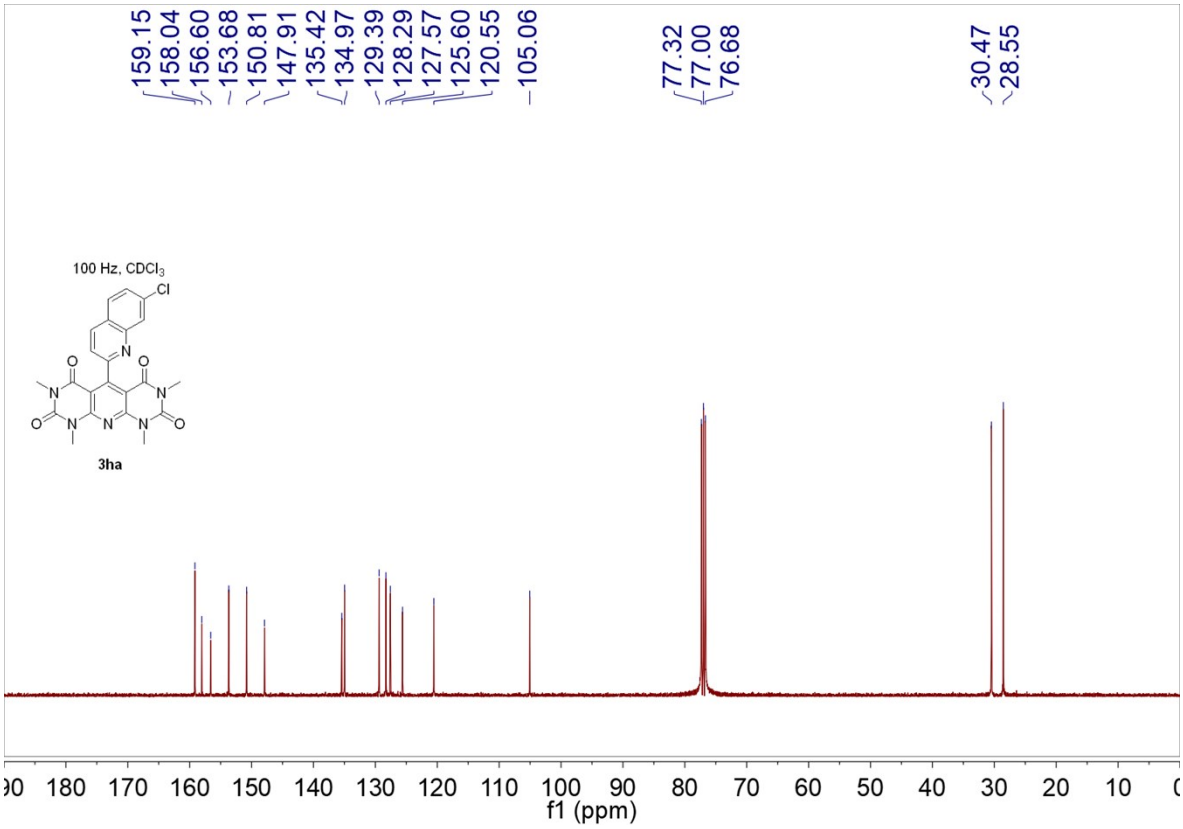
7.619
7.394
7.372
7.365
7.350
7.344
7.328
7.322
3.784
3.249
400 Hz, CDCl3
3fa
1.00
1.00
0.97
1.97
6.00
6.01
f1 (ppm)

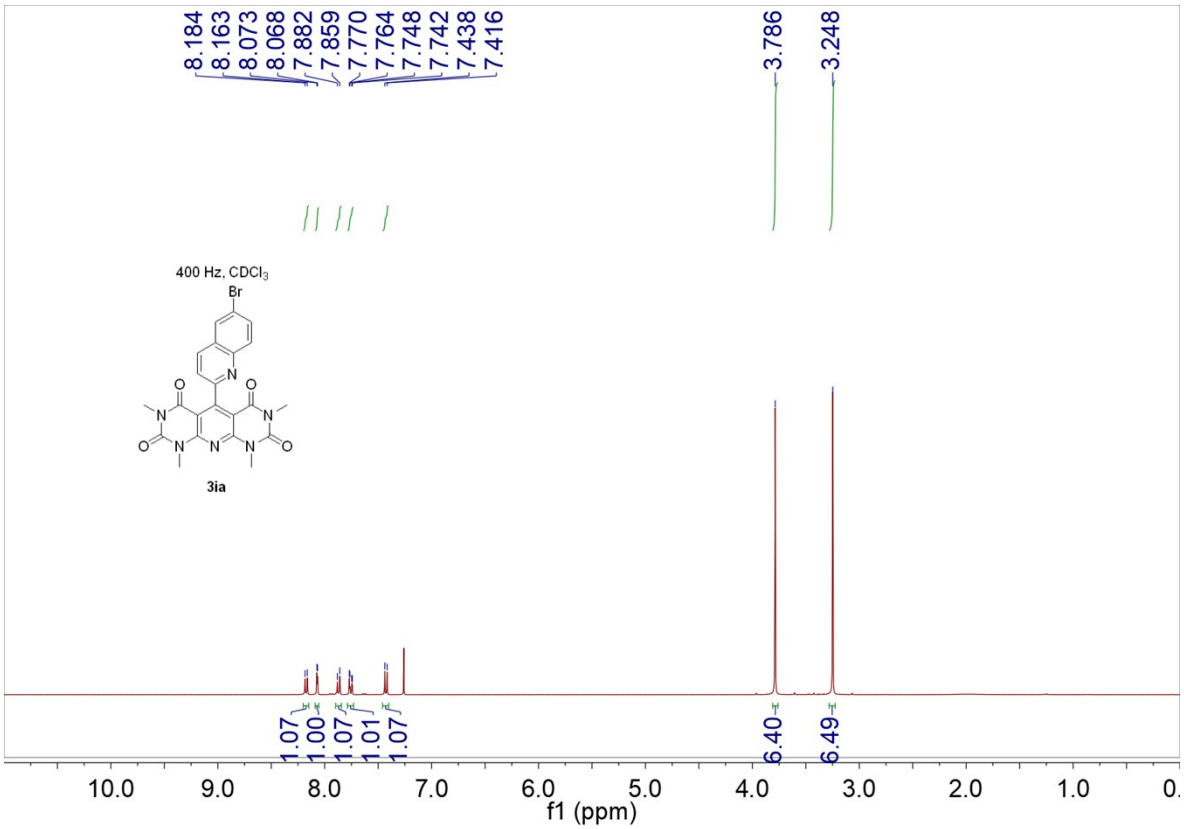

159.12
157.94
153.65
150.77
135.26
130.25
130.15
124.20
119.71
117.11
116.86
112.96
112.73
105.04
77.32
77.00
76.68
30.44
28.52
100 Hz, CDCl3
3fa
f1 (ppm)

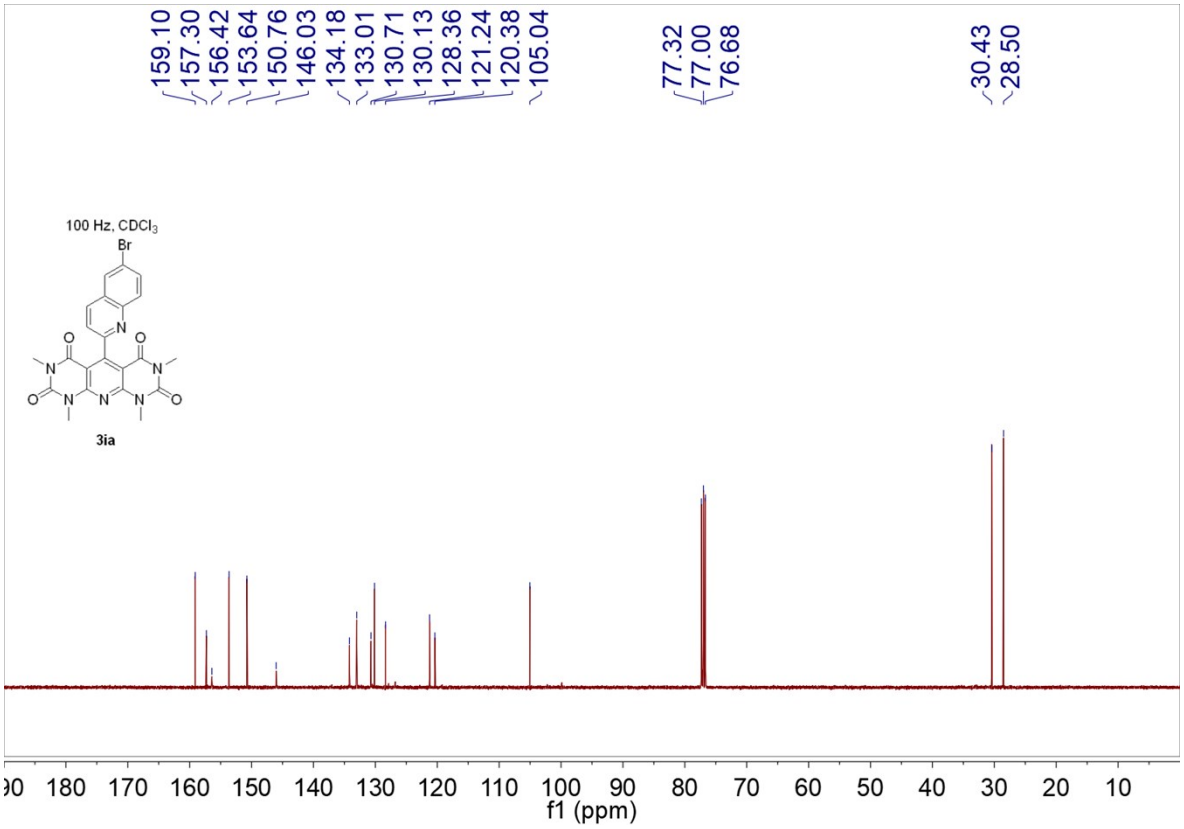

8.186
8.164
7.941
7.919
7.892
7.887
7.635
7.630
7.613
7.608
7.437
7.416
3.785
3.247
400 Hz, CDCl3
Cl
3ga
1.00
1.07
0.96
1.02
1.00
5.99
6.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)


159.07
157.15
156.49
153.60
150.73
145.86
134.20
132.17
130.62
130.38
127.81
126.76
121.21
105.02
77.32
77.00
76.68
30.40
28.47
100 Hz, CDCl3
Cl
3ga
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.267
8.246
8.029
7.866
7.844
7.542
7.537
7.521
7.515
7.426
7.405
3.792
3.257
400 Hz, CDCl3
Cl
N
O
O
N
N
N
N
O
O
3ha
1.00
0.95
1.00
1.00
0.97
6.01
5.98
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)


159.15
158.04
156.60
153.68
150.81
147.91
135.42
134.97
129.39
128.29
127.57
125.60
120.55
105.06
77.32
77.00
76.68
30.47
28.55
100 Hz, CDCl3
Cl
N
O
O
N
N
N
N
O
O
3ha
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.184
8.163
8.073
8.068
7.882
7.859
7.770
7.764
7.748
7.742
7.438
7.416
3.786
3.248
400 Hz, CDCl3
Br
3ia
1.07
1.00
1.07
1.01
1.07
6.40
6.49
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)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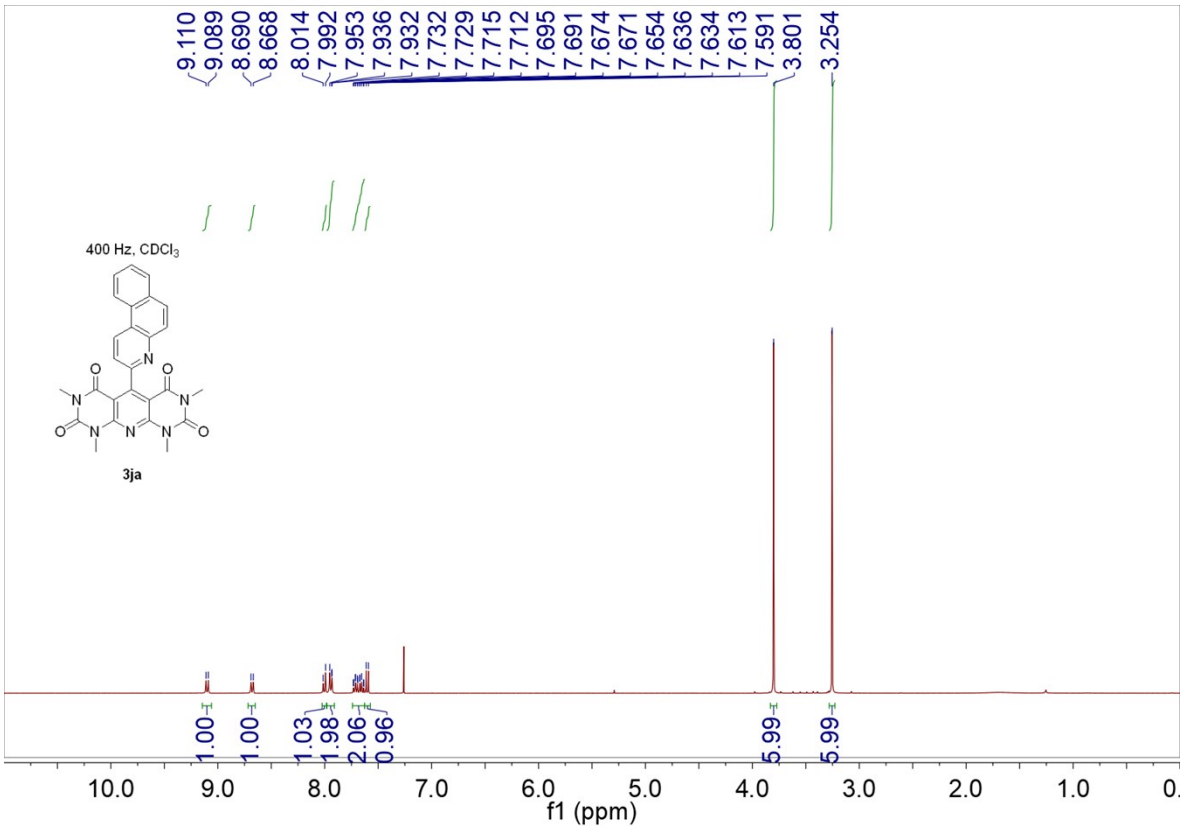
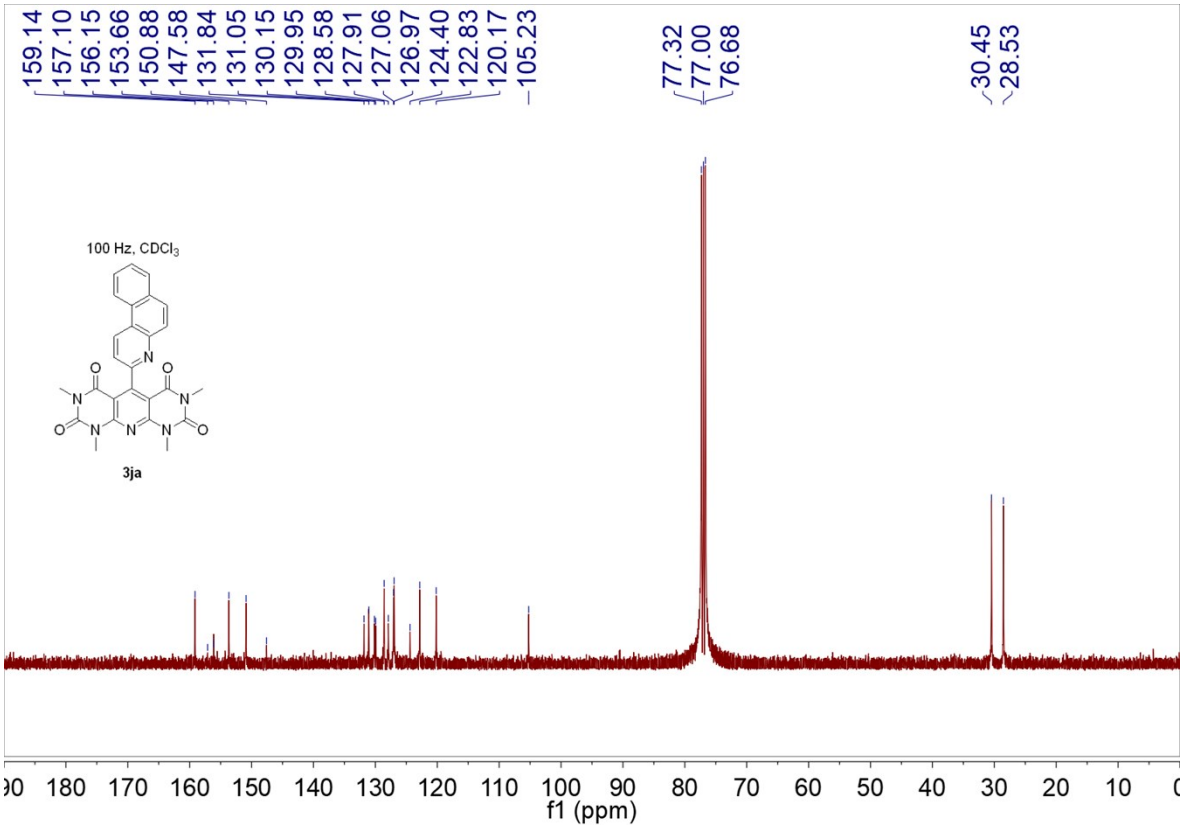
157.30
156.42
153.64
150.76
146.03
134.18
133.01
130.71
130.13
128.36
121.24
120.38
105.04
77.32
77.00
76.68
30.43
28.50
100 Hz, CDCl3
Br
3ia
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


9.110
9.089
8.690
8.668
8.014
7.992
7.953
7.936
7.932
7.732
7.729
7.715
7.712
7.695
7.691
7.674
7.671
7.654
7.636
7.634
7.613
7.591
3.801
3.254
400 Hz, CDCl3
3ja
1.00
1.00
1.03
1.98
2.06
0.96
5.99
5.99
f1 (ppm)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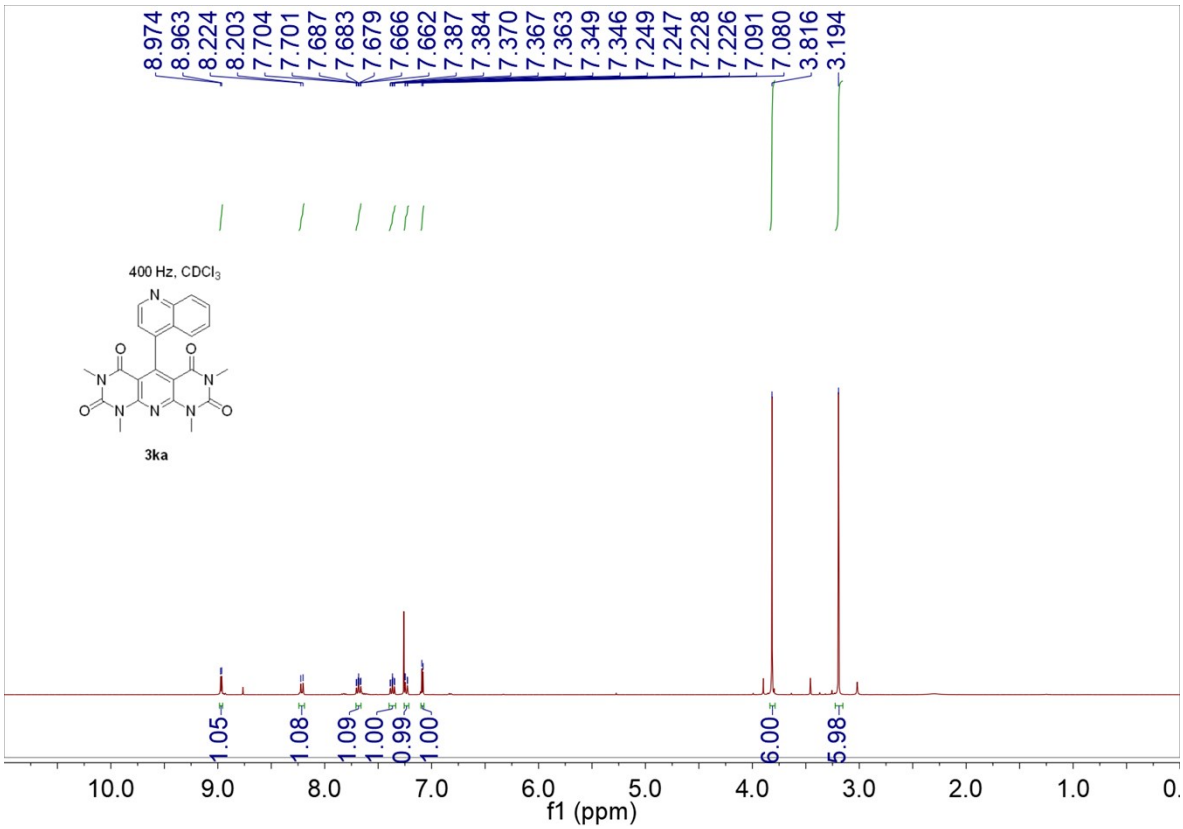
157.10
156.15
153.66
150.88
147.58
131.84
131.05
130.15
129.95
128.58
127.91
127.06
126.97
124.40
122.83
120.17
105.23
77.32
77.00
76.68
30.45
28.53
100 Hz, CDCl3
3ja
f1 (ppm)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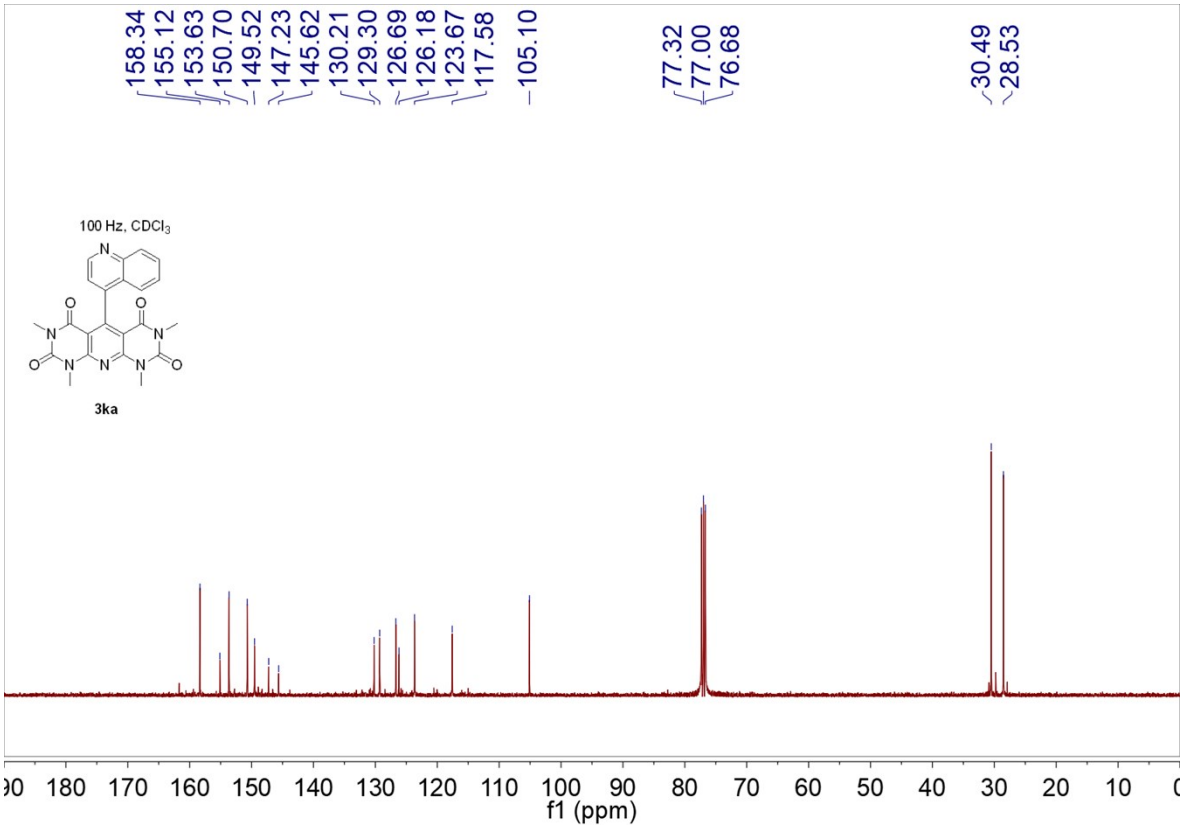
8.963
8.224
8.203
7.704
7.701
7.687
7.683
7.679
7.666
7.662
7.387
7.384
7.370
7.367
7.363
7.349
7.346
7.249
7.247
7.228
7.226
7.091
7.080
3.816
3.194
400 Hz, CDCl3
3ka
1.05
1.08
1.09
1.00
0.99
1.00
6.00
5.98
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)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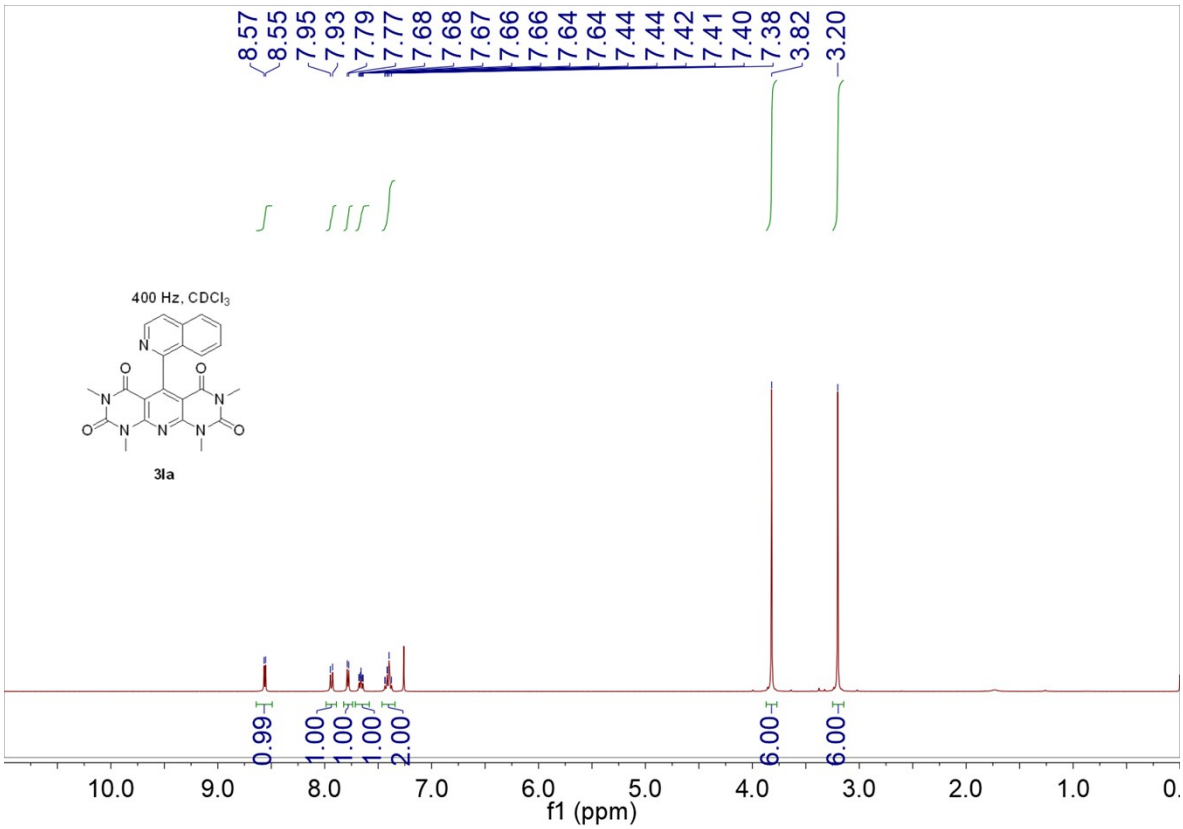
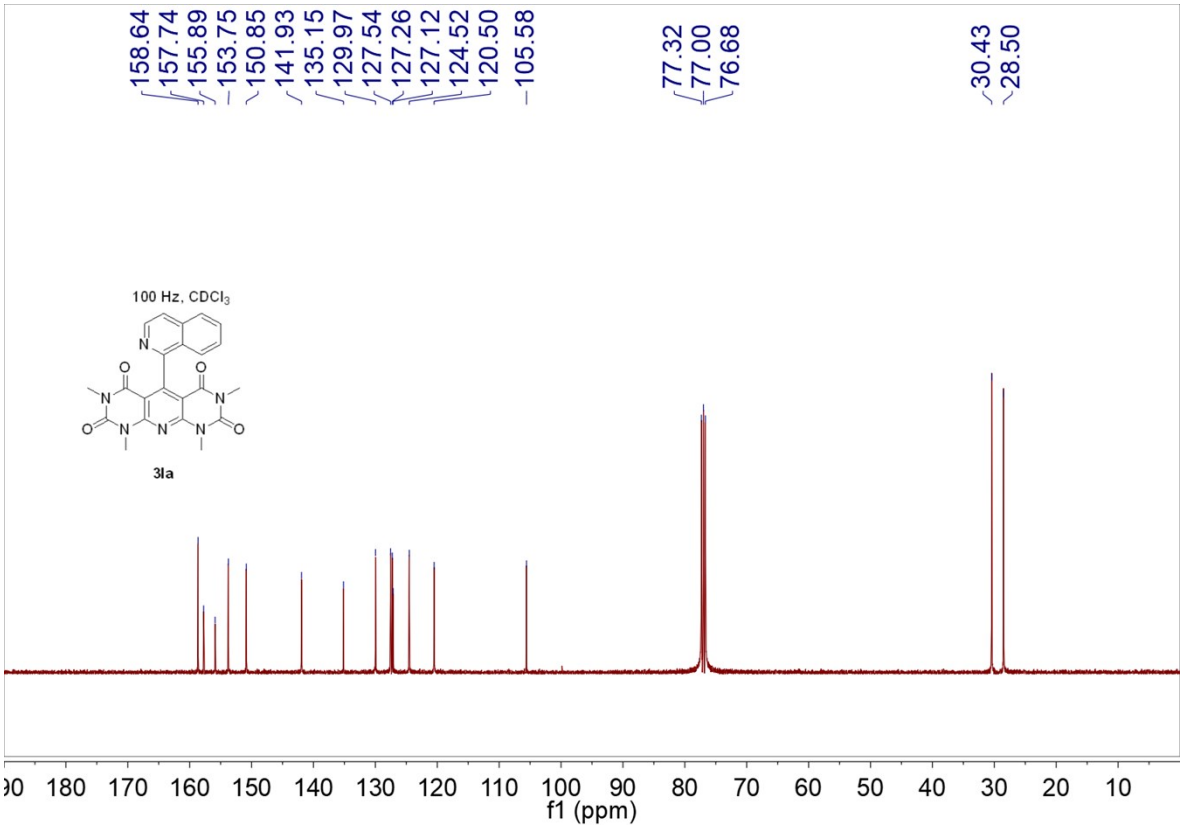
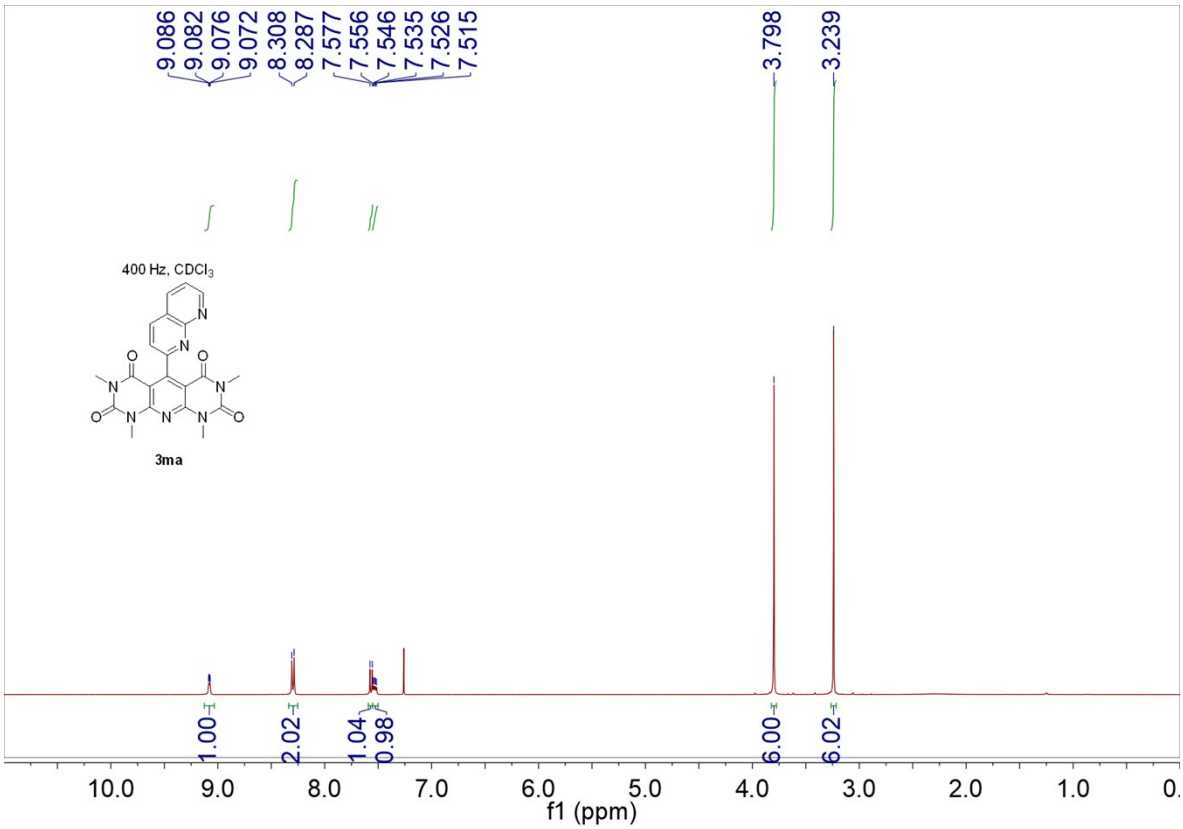
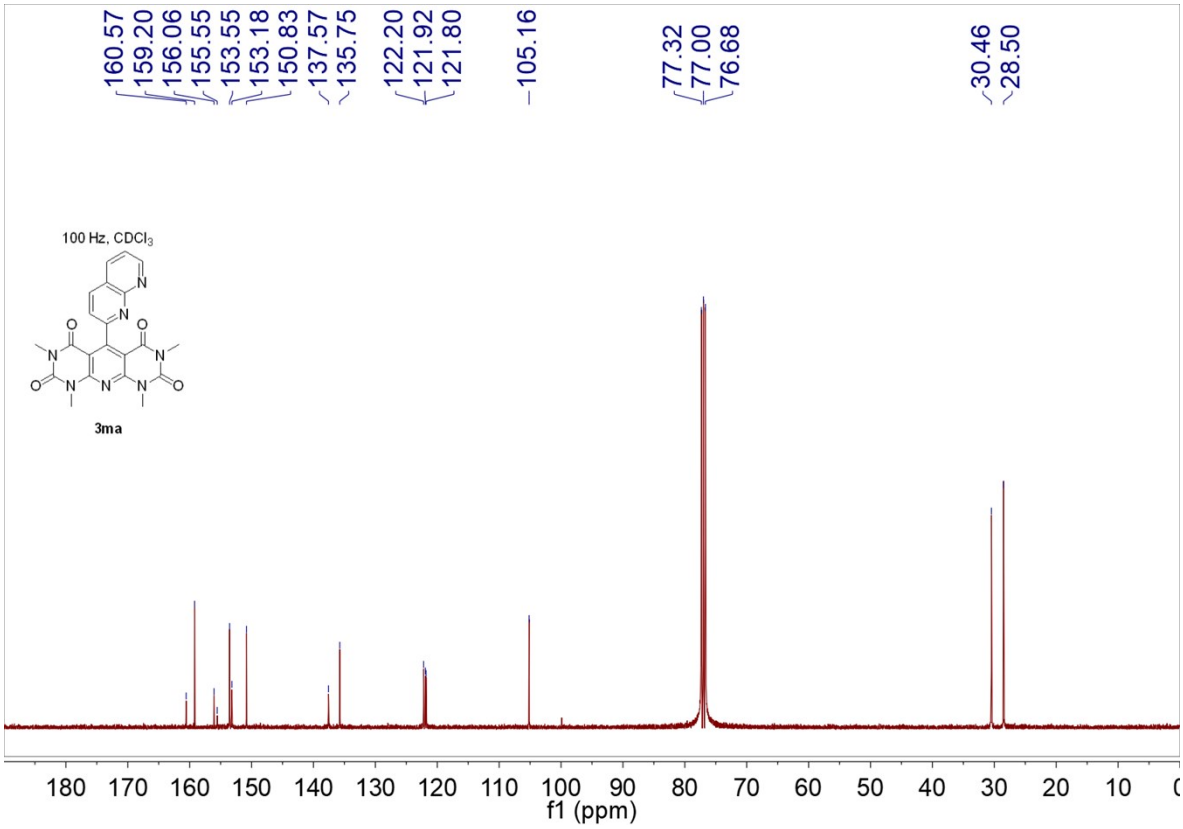
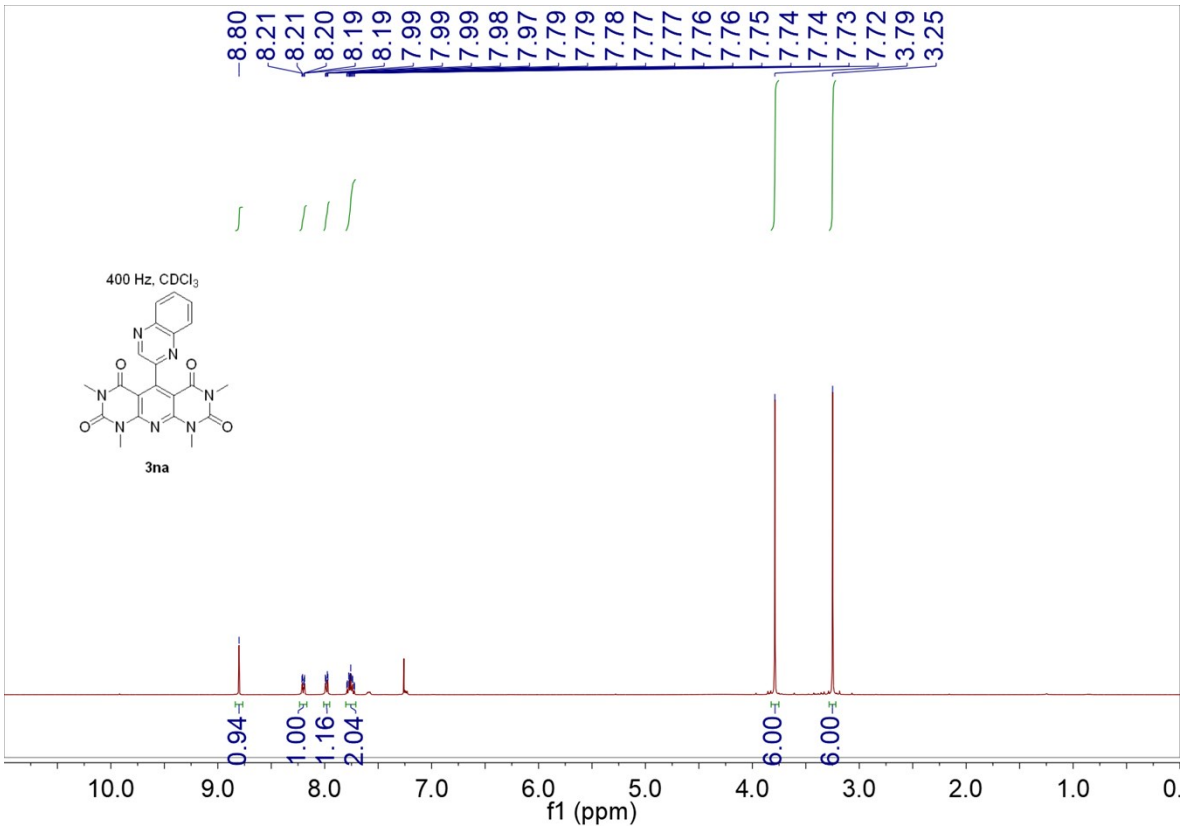
155.12
153.63
150.70
149.52
147.23
145.62
130.21
129.30
126.69
126.18
123.67
117.58
105.10
77.32
77.00
76.68
30.49
28.53
100 Hz, CDCl3
3ka
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

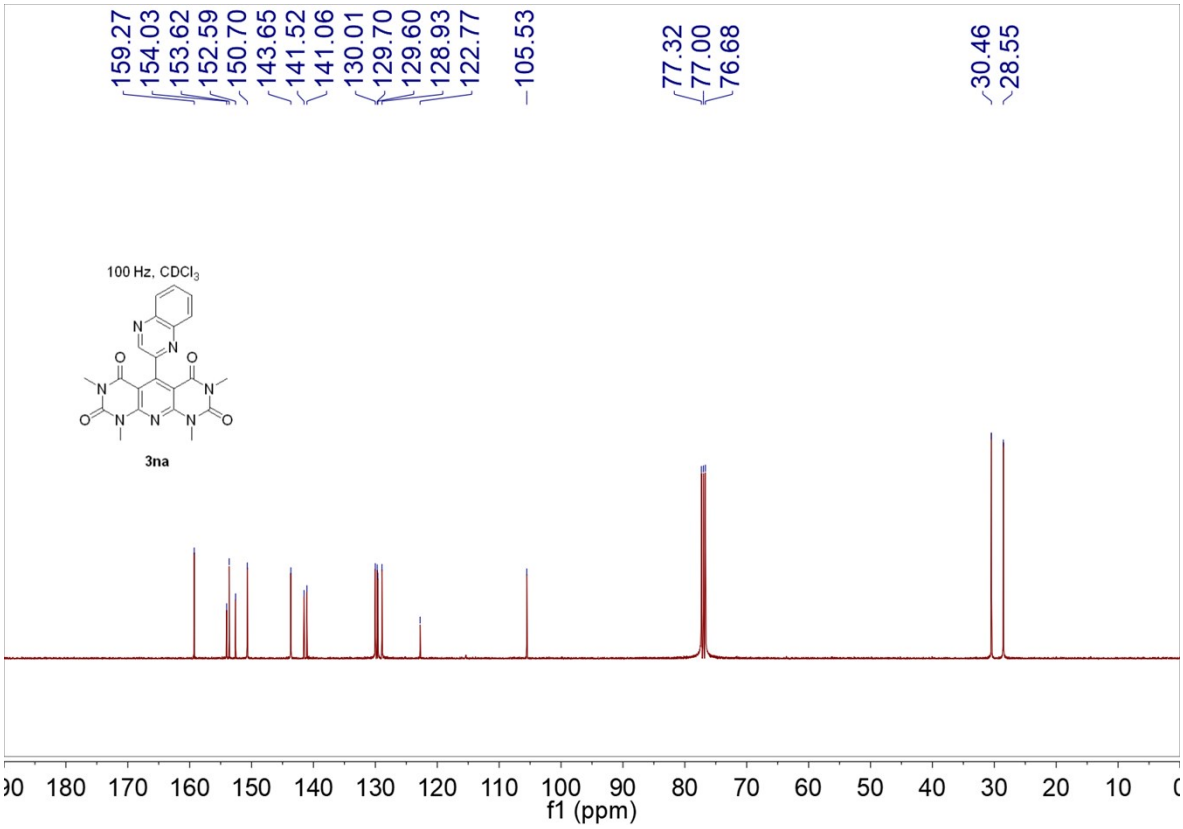

8.57
8.55
7.95
7.93
7.79
7.77
7.68
7.68
7.67
7.66
7.66
7.64
7.64
7.44
7.44
7.42
7.41
7.40
7.38
3.82
3.20
400 Hz, CDCl3
3la
0.99
1.00
1.00
1.00
2.00
6.00
6.00
f1 (ppm)


158.64
157.74
155.89
153.75
150.85
141.93
135.15
129.97
127.54
127.26
127.12
124.52
120.50
105.58
77.32
77.00
76.68
30.43
28.50
100 Hz, CDCl3
3la
f1 (ppm)


9.086
9.082
9.076
9.072
8.308
8.287
7.577
7.556
7.546
7.535
7.526
7.515
3.798
3.239
400 Hz, CDCl3
3ma
1.00
2.02
1.04
0.98
6.00
6.02
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)


160.57
159.20
156.06
155.55
153.55
153.18
150.83
137.57
135.75
122.20
121.92
121.80
105.16
77.32
77.00
76.68
30.46
28.50
100 Hz, CDCl3
3ma
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.80
8.21
8.21
8.20
8.19
8.19
7.99
7.99
7.99
7.98
7.97
7.79
7.79
7.78
7.77
7.77
7.76
7.76
7.75
7.74
7.74
7.73
7.72
3.79
3.25
400 Hz, CDCl3
3na
0.94
1.00
1.16
2.04
6.00
6.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)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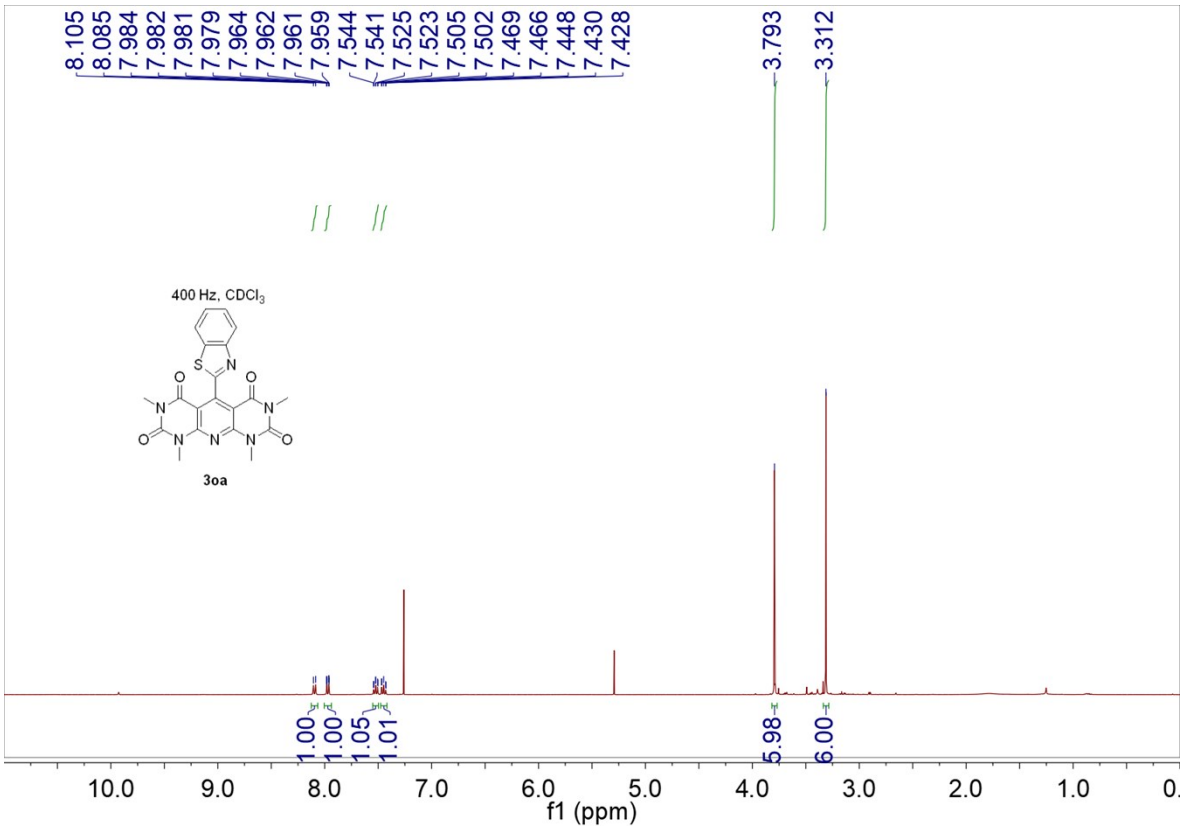
154.03
153.62
152.59
150.70
143.65
141.52
141.06
130.01
129.70
129.60
128.93
122.77
105.53
77.32
77.00
76.68
30.46
28.55
100 Hz, CDCl3
3na
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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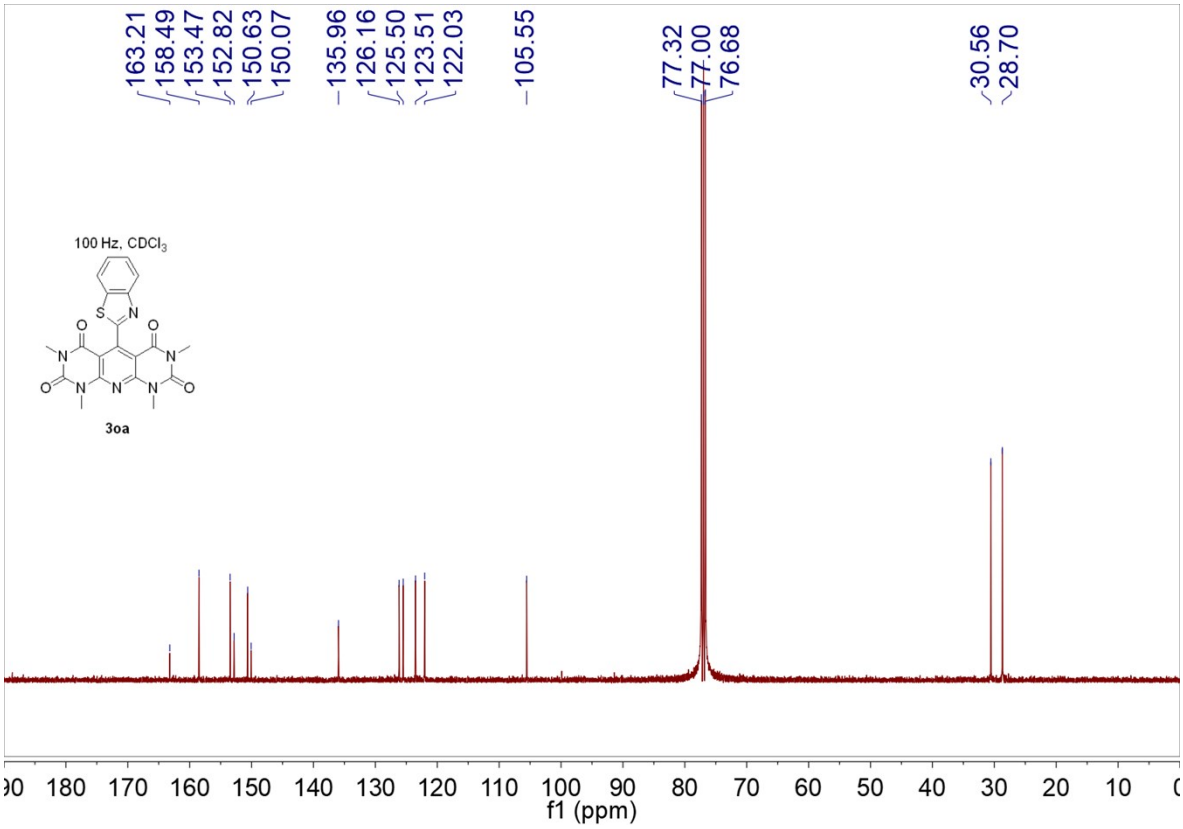
7.982
7.981
7.979
7.964
7.962
7.961
7.959
7.544
7.541
7.525
7.523
7.505
7.502
7.469
7.466
7.448
7.430
7.428
3.793
3.312
400 Hz, CDCl3
3oa
1.00
1.00
1.05
1.01
5.98
6.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)


163.21
158.49
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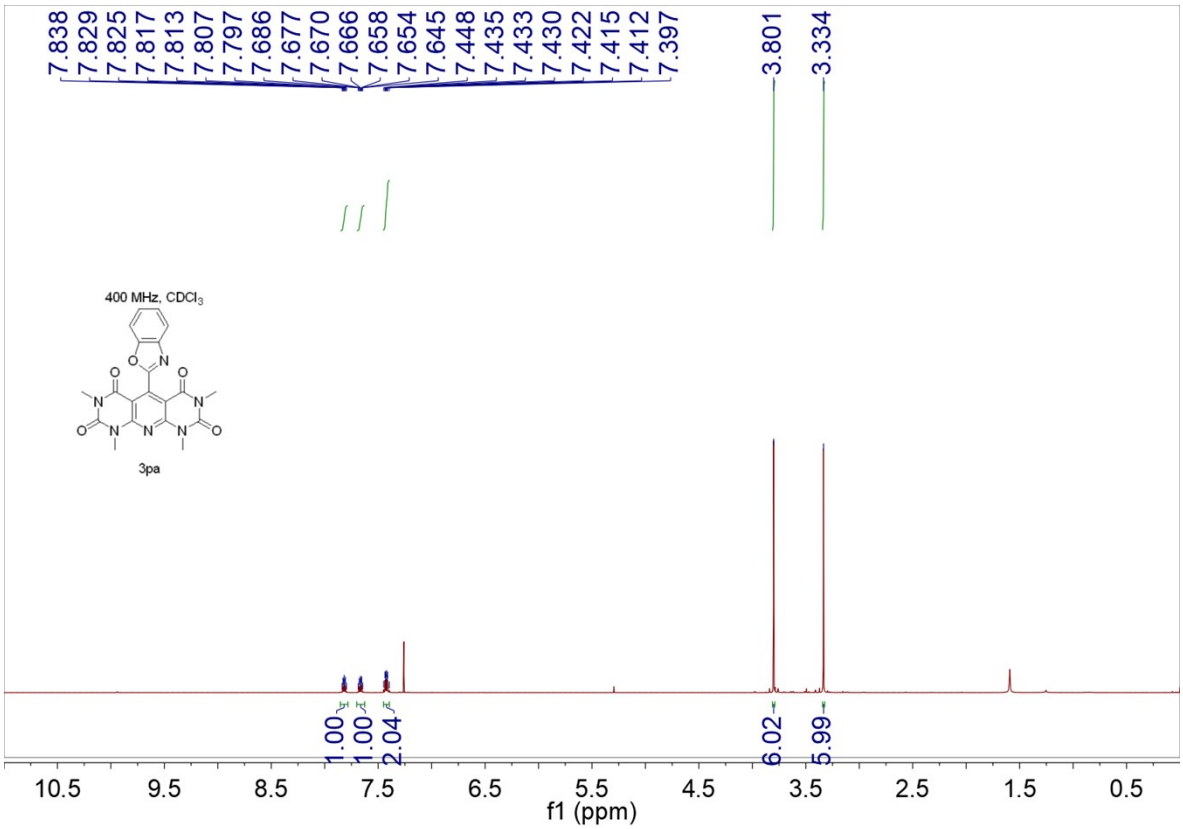
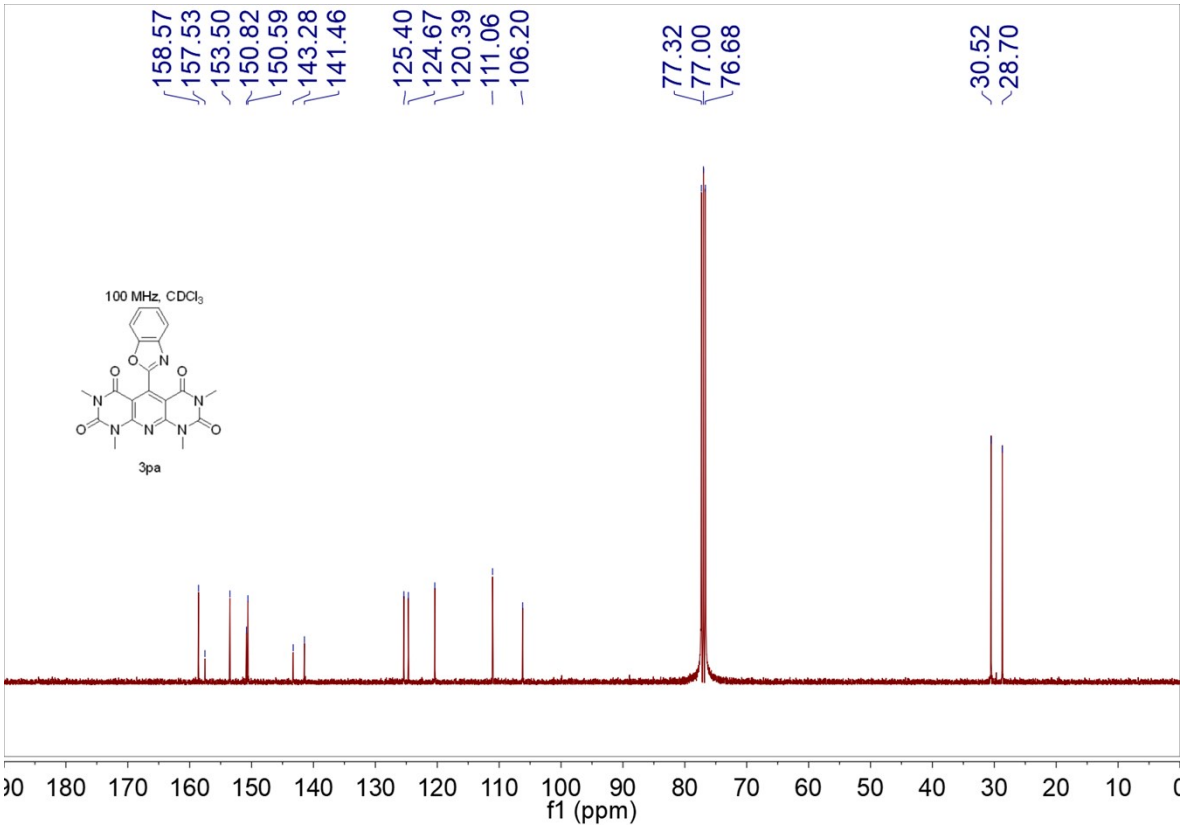
152.82
150.63
150.07
135.96
126.16
125.50
123.51
122.03
105.55
77.32
77.00
76.68
30.56
28.70
100 Hz, CDCl3
3oa
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.838
7.829
7.825
7.817
7.813
7.807
7.797
7.686
7.677
7.670
7.666
7.658
7.654
7.645
7.448
7.435
7.433
7.430
7.422
7.415
7.412
7.397
3.801
3.334
400 MHz, CDCl3
3pa
1.00
1.00
2.04
6.02
5.99
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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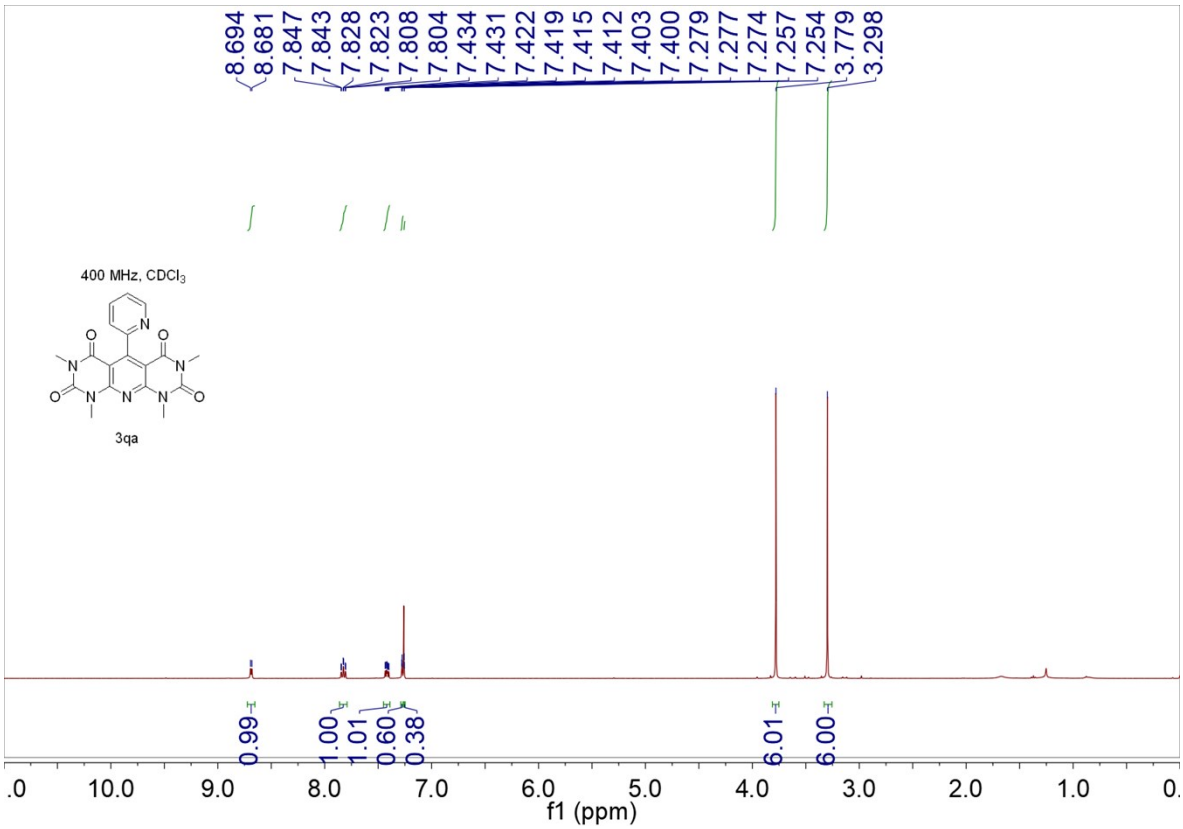
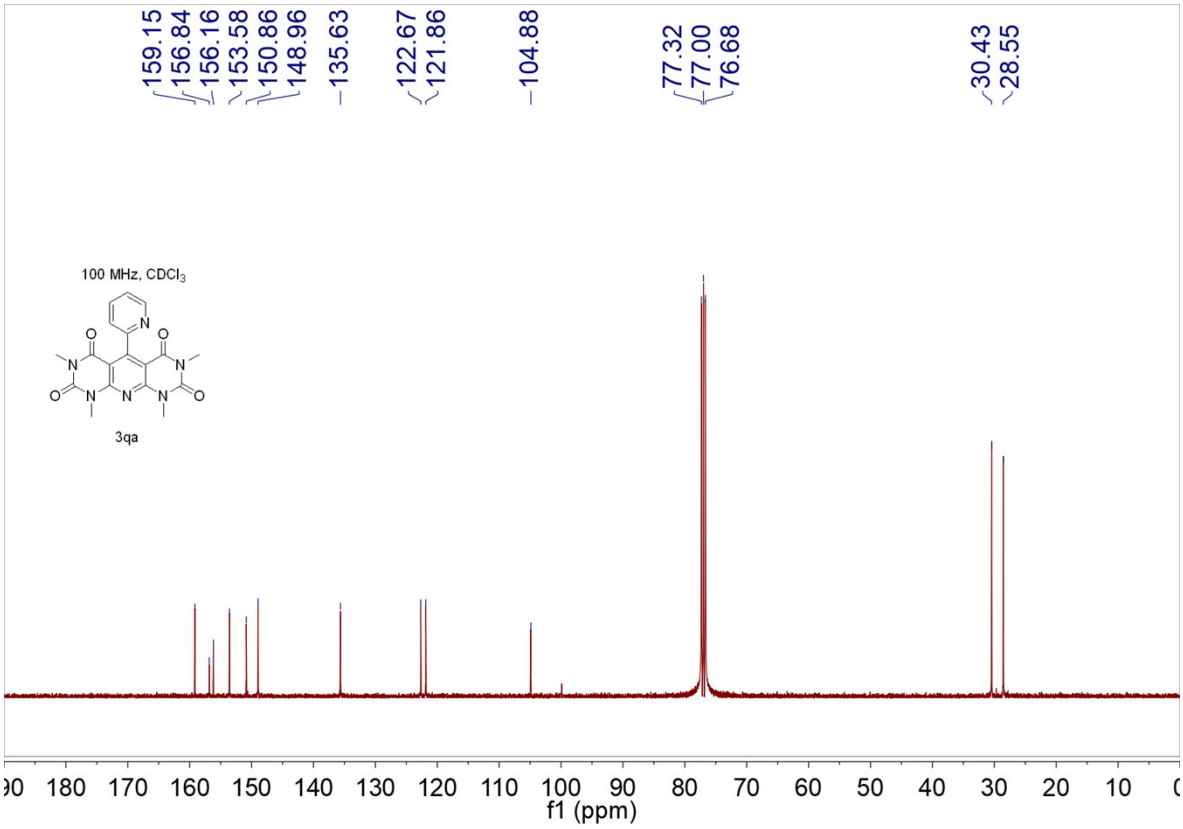
150.82
150.59
143.28
141.46
125.40
124.67
120.39
111.06
106.20
77.32
77.00
76.68
30.52
28.70
100 MHz, CDCl3
3pa
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.694
8.681
7.847
7.843
7.828
7.823
7.808
7.804
7.434
7.431
7.422
7.419
7.415
7.412
7.403
7.400
7.279
7.277
7.274
7.257
7.254
3.779
3.298
400 MHz, CDCl3
3qa
0.99
1.00
1.01
0.60
0.38
6.01
6.00
f1 (ppm)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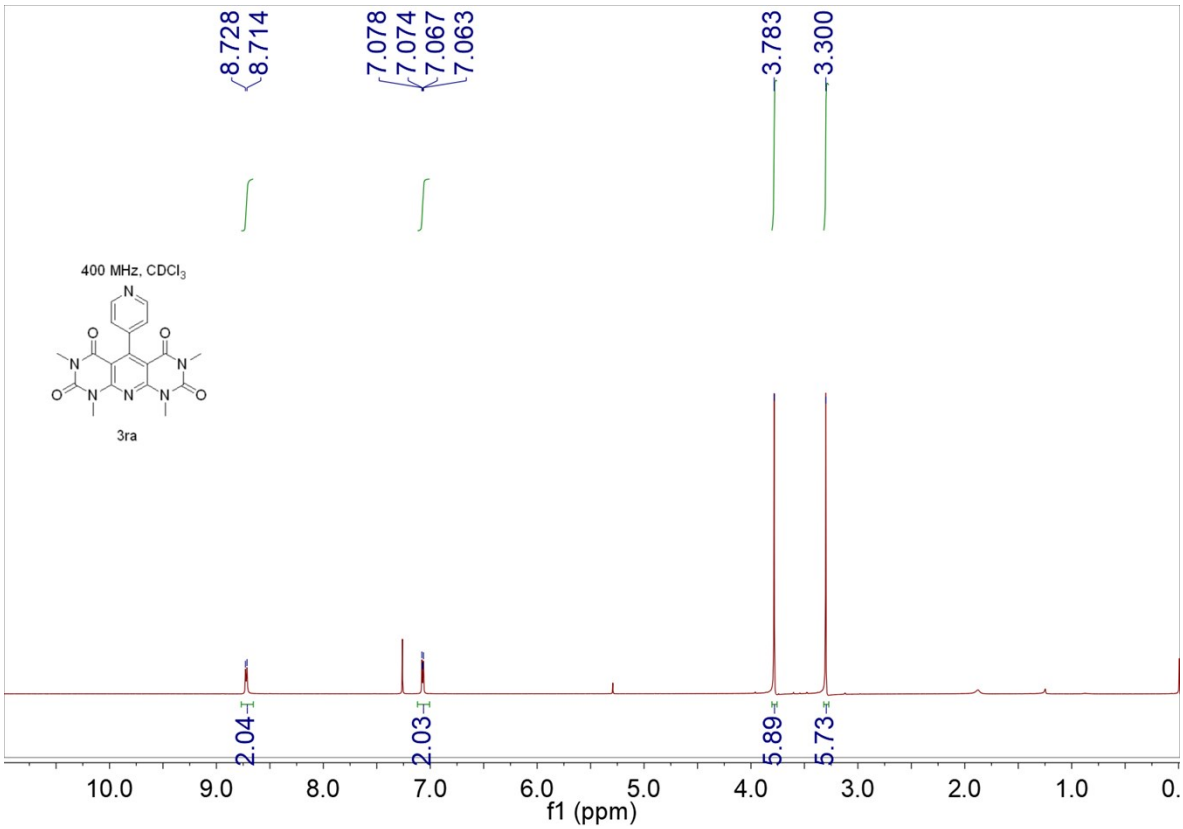
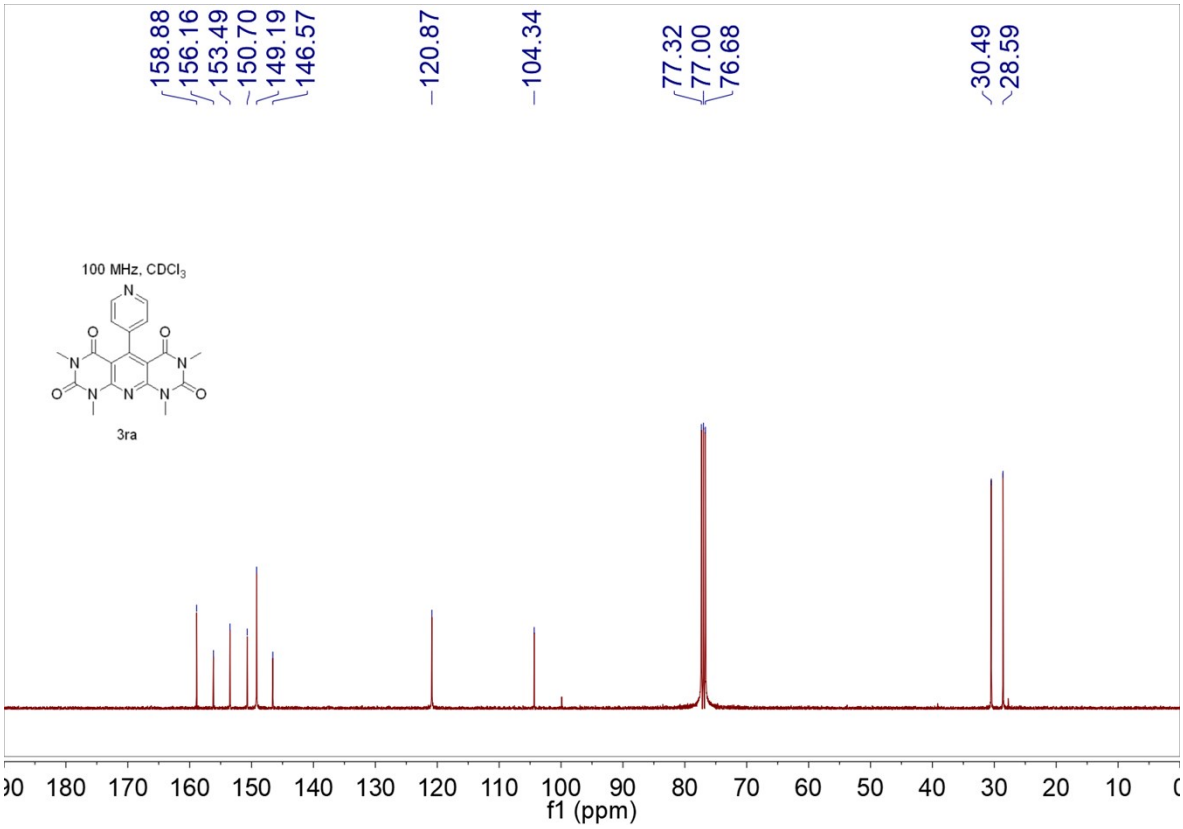
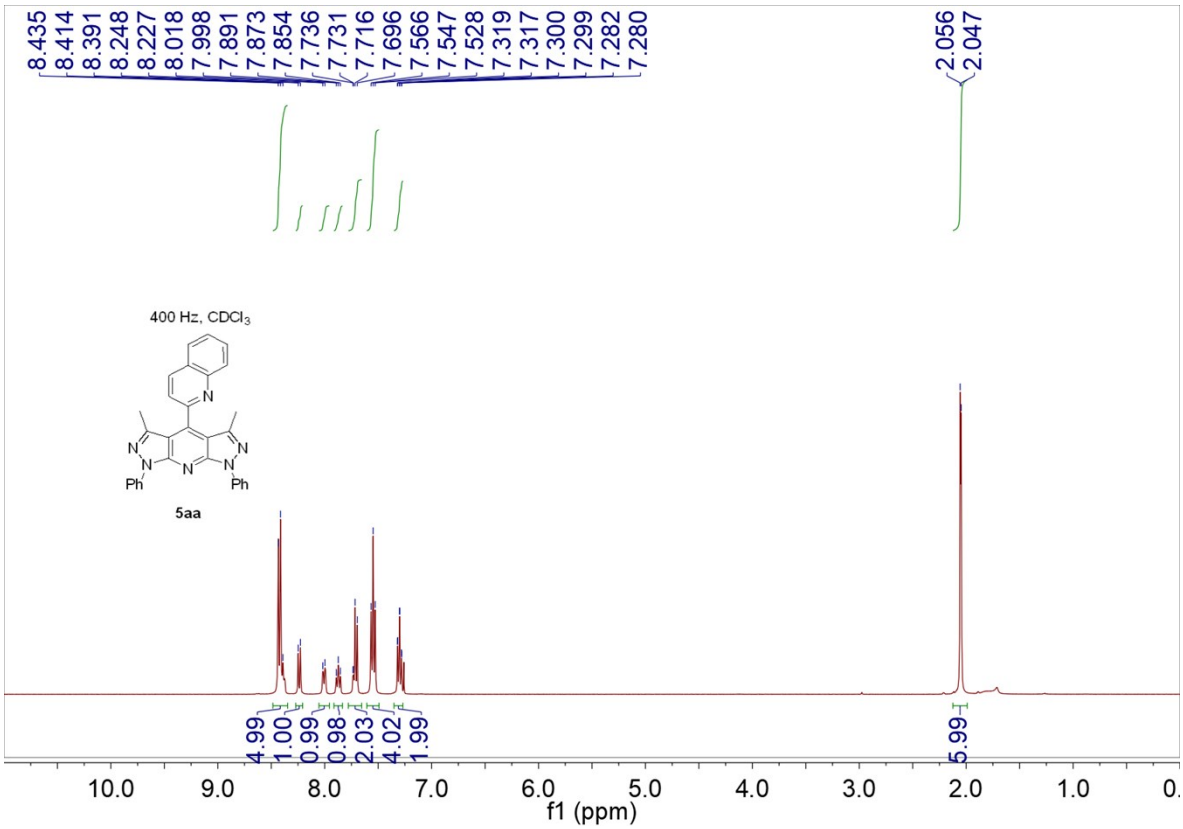
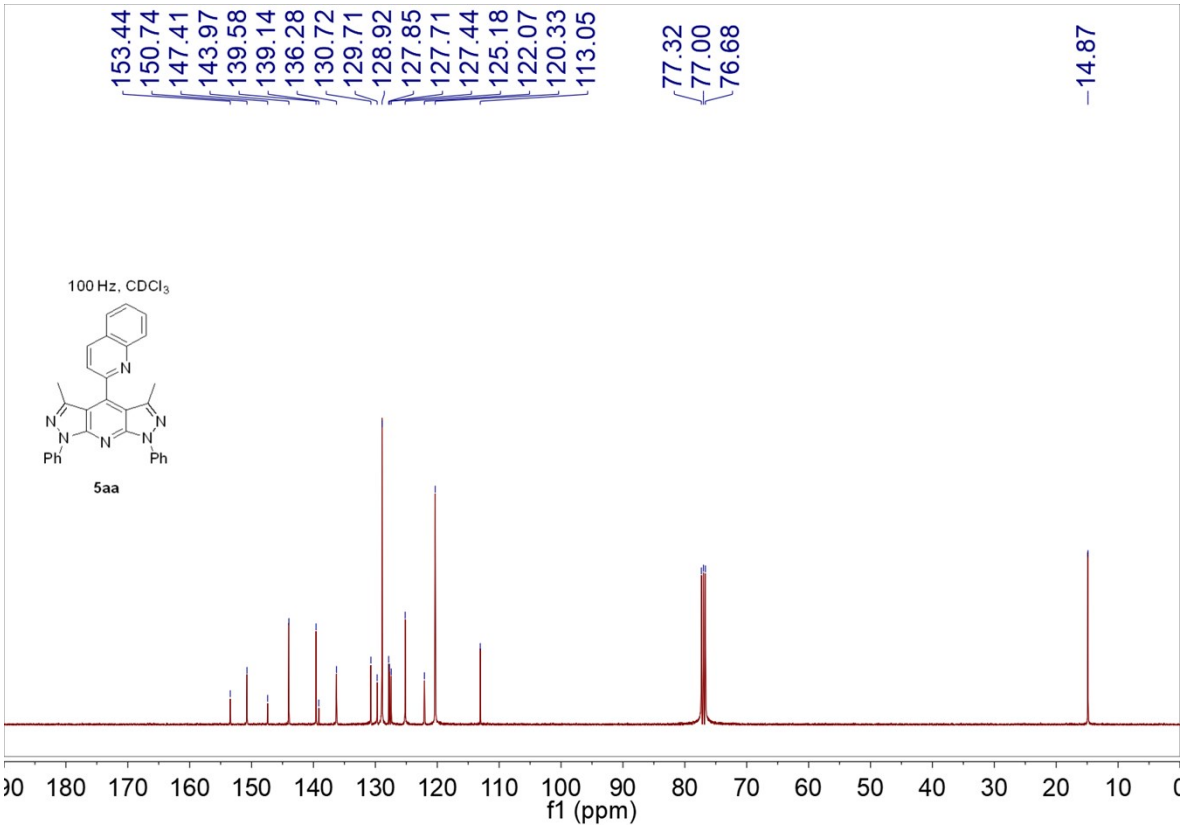
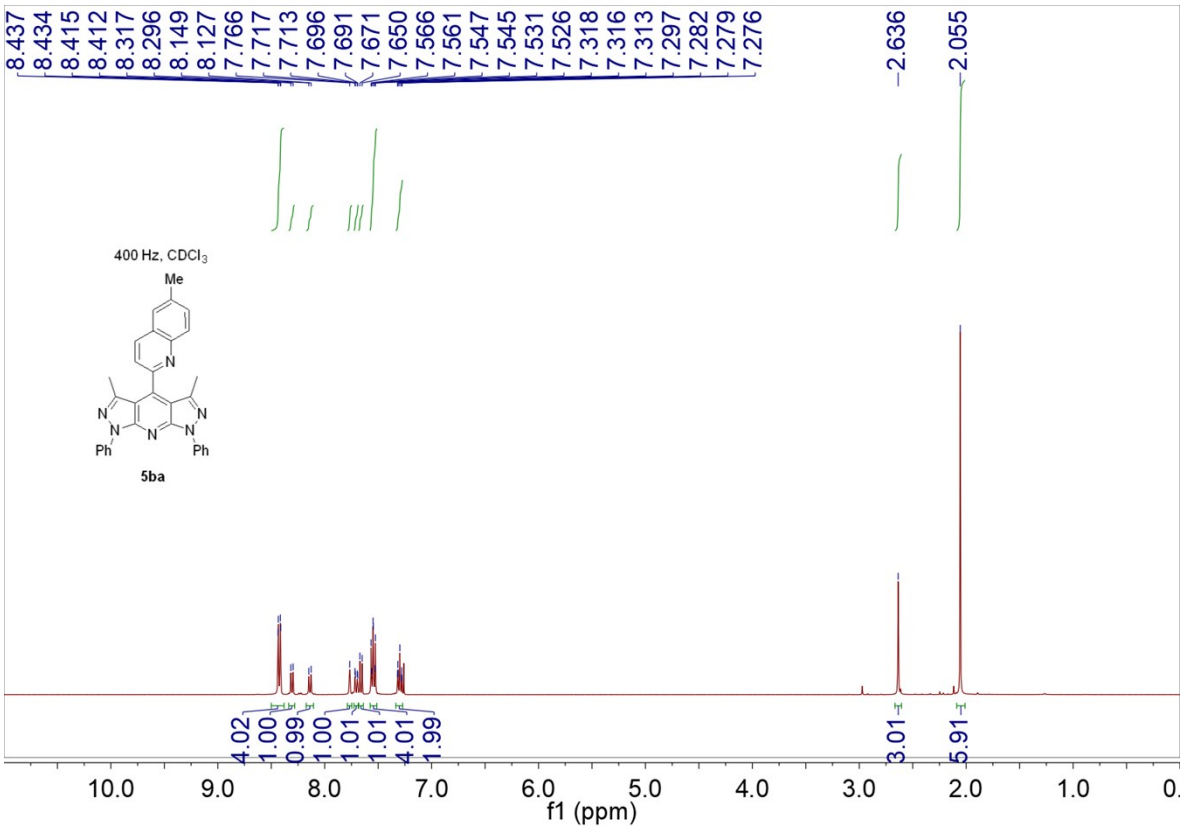
156.84
156.16
153.58
150.86
148.96
135.63
122.67
121.86
104.88
77.32
77.00
76.68
30.43
28.55
100 MHz, CDCl3
3qa
f1 (ppm)


8.728
8.714
7.078
7.074
7.067
7.063
3.783
3.300
400 MHz, CDCl3
3ra
2.04
2.03
5.89
5.73
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)


158.88
156.16
153.49
150.70
149.19
146.57
120.87
104.34
77.32
77.00
76.68
30.49
28.59
100 MHz, CDCl3
3ra
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.435
8.414
8.391
8.248
8.227
8.018
7.998
7.891
7.873
7.854
7.736
7.731
7.716
7.696
7.566
7.547
7.528
7.319
7.317
7.300
7.299
7.282
7.280
2.056
2.047
400 Hz, CDCl3
5aa
4.99
1.00
0.99
0.98
2.03
4.02
1.99
5.99
f1 (ppm)


153.44
150.74
147.41
143.97
139.58
139.14
136.28
130.72
129.71
128.92
127.85
127.71
127.44
125.18
122.07
120.33
113.05
77.32
77.00
76.68
14.87
100 Hz, CDCl3
5aa
f1 (ppm)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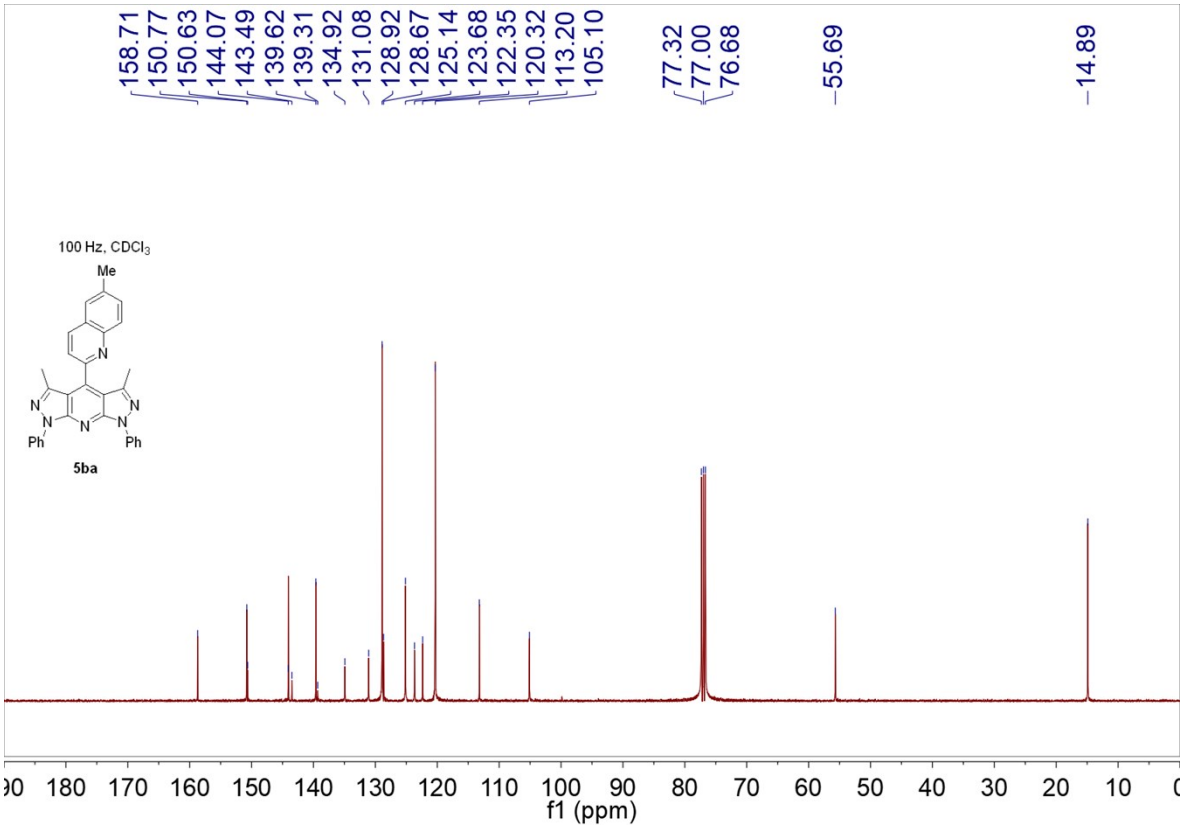
8.434
8.415
8.412
8.317
8.296
8.149
8.127
7.766
7.717
7.713
7.696
7.691
7.671
7.650
7.566
7.561
7.547
7.545
7.531
7.526
7.318
7.316
7.313
7.297
7.282
7.279
7.276
2.636
2.055
400 Hz, CDCl3
Me
N
N
N
N
N
Ph
Ph
5ba
4.02
1.00
0.99
1.00
1.01
1.01
4.01
1.99
3.01
5.91
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)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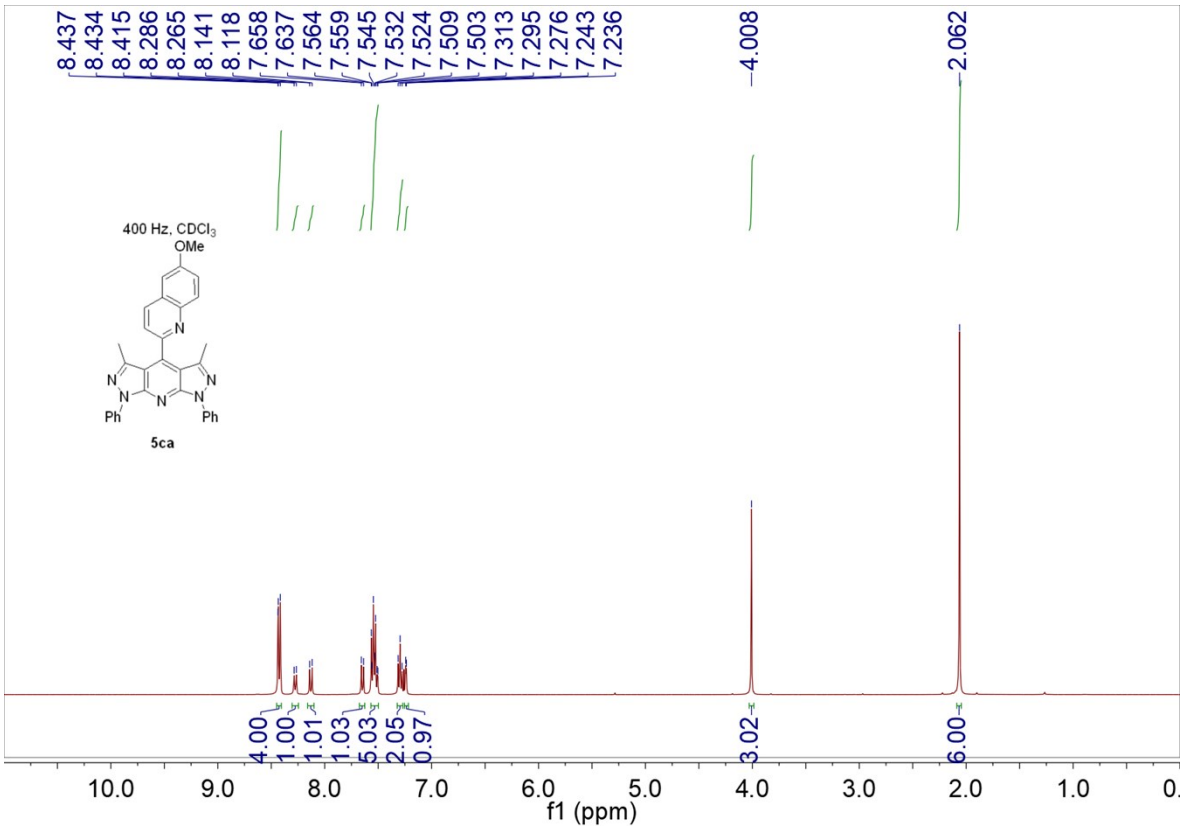
150.77
150.63
144.07
143.49
139.62
139.31
134.92
131.08
128.92
128.67
125.14
123.68
122.35
120.32
113.20
105.10
77.32
77.00
76.68
55.69
14.89
100 Hz, CDCl3
Me
N
N
N
N
N
Ph
Ph
5ba
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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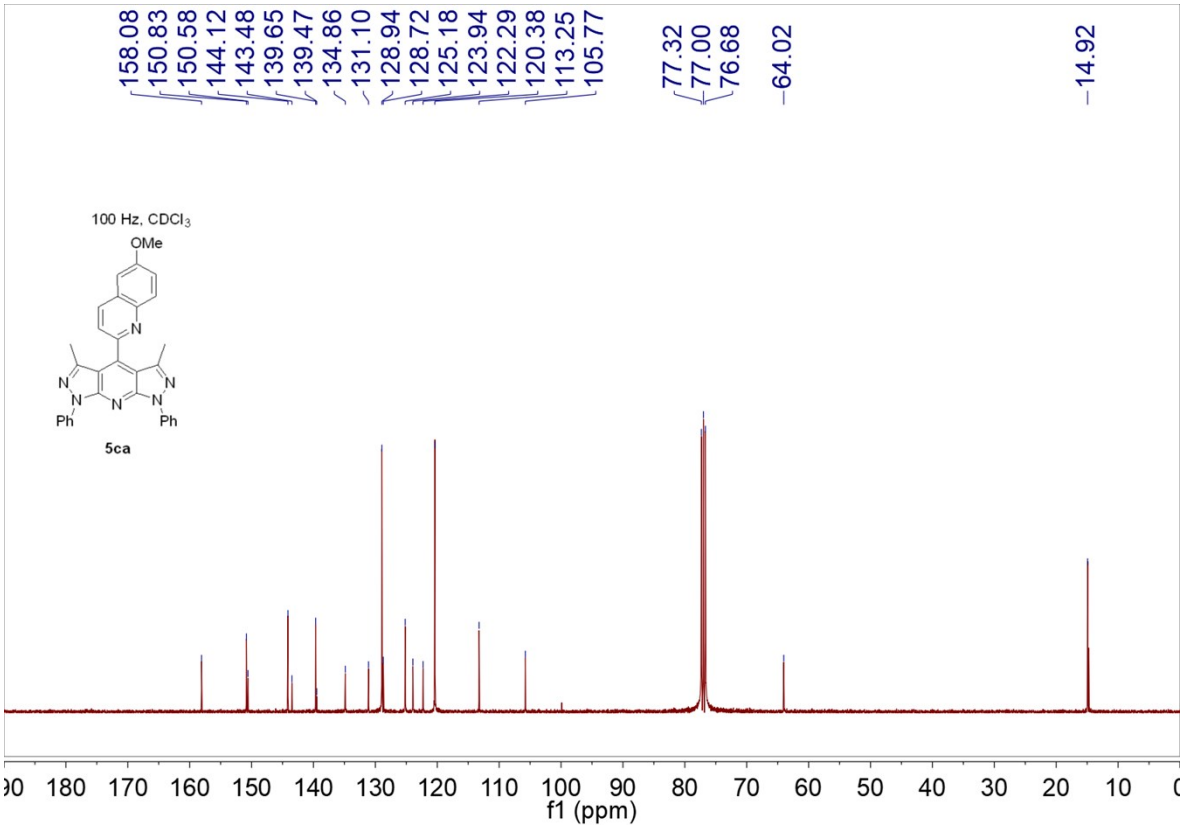
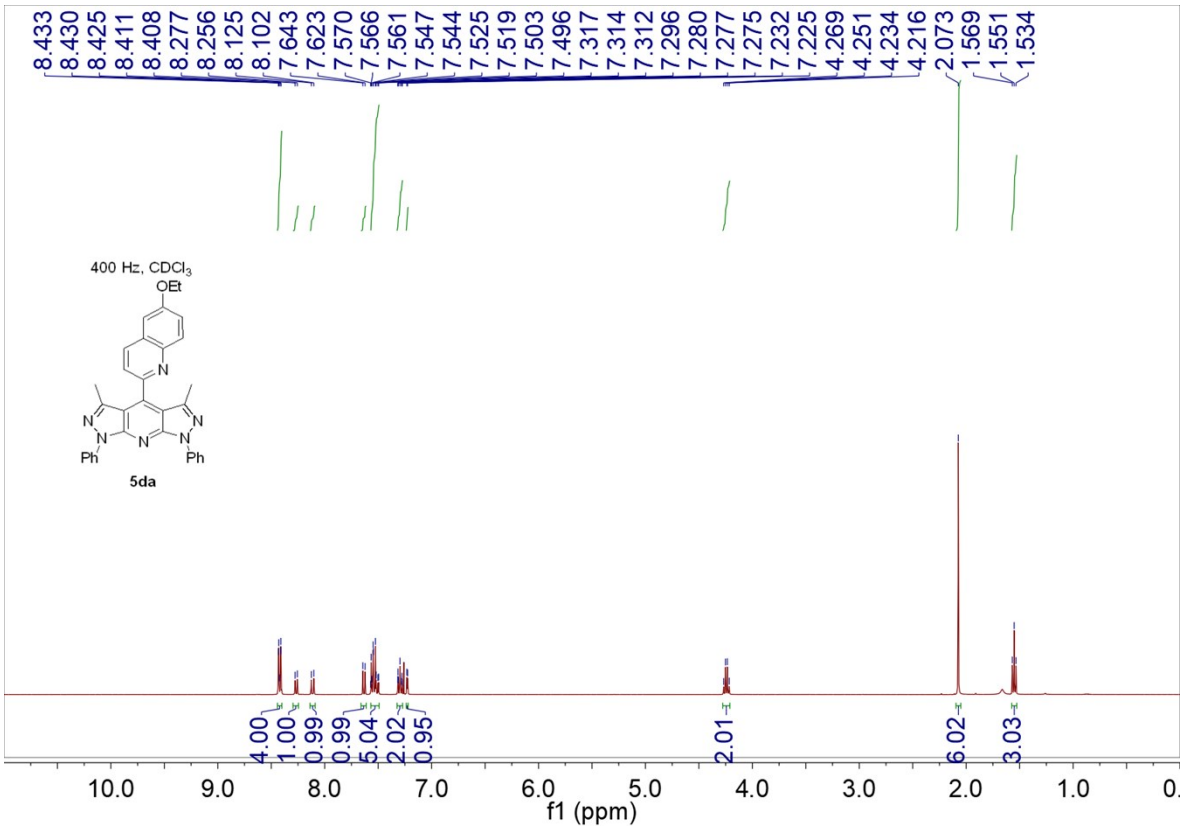
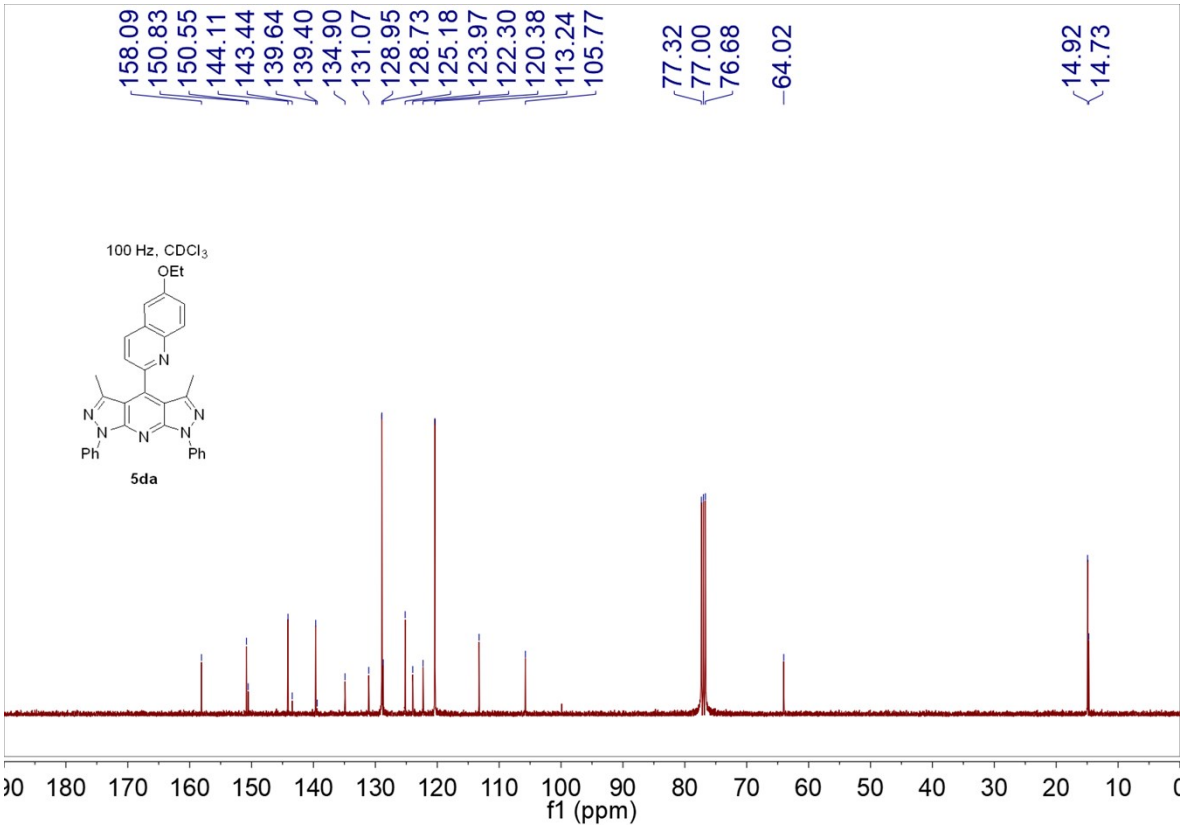
8.415
8.286
8.265
8.141
8.118
7.658
7.637
7.564
7.559
7.545
7.532
7.524
7.509
7.503
7.313
7.295
7.276
7.243
7.236
4.008
2.062
400 Hz, CDCl3
OMe
N
N
N
N
N
Ph
Ph
5ca
4.00
1.00
1.01
1.03
5.03
2.05
0.97
3.02
6.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)


158.08
150.83
150.58
144.12
143.48
139.65
139.47
134.86
131.10
128.94
128.72
125.18
123.94
122.29
120.38
113.25
105.77
77.32
77.00
76.68
64.02
14.92
100 Hz, CDCl3
OMe
N
N
N
N
N
Ph
Ph
5ca
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.433
8.430
8.425
8.411
8.408
8.277
8.256
8.125
8.102
7.643
7.623
7.570
7.566
7.561
7.547
7.544
7.525
7.519
7.503
7.496
7.317
7.314
7.312
7.296
7.280
7.277
7.275
7.232
7.225
4.269
4.251
4.234
4.216
2.073
1.569
1.551
1.534
400 Hz, CDCl3
OEt
N
N
N
N
N
Ph
Ph
5da
4.00
1.00
0.99
0.99
5.04
2.02
0.95
2.01
6.02
3.03
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)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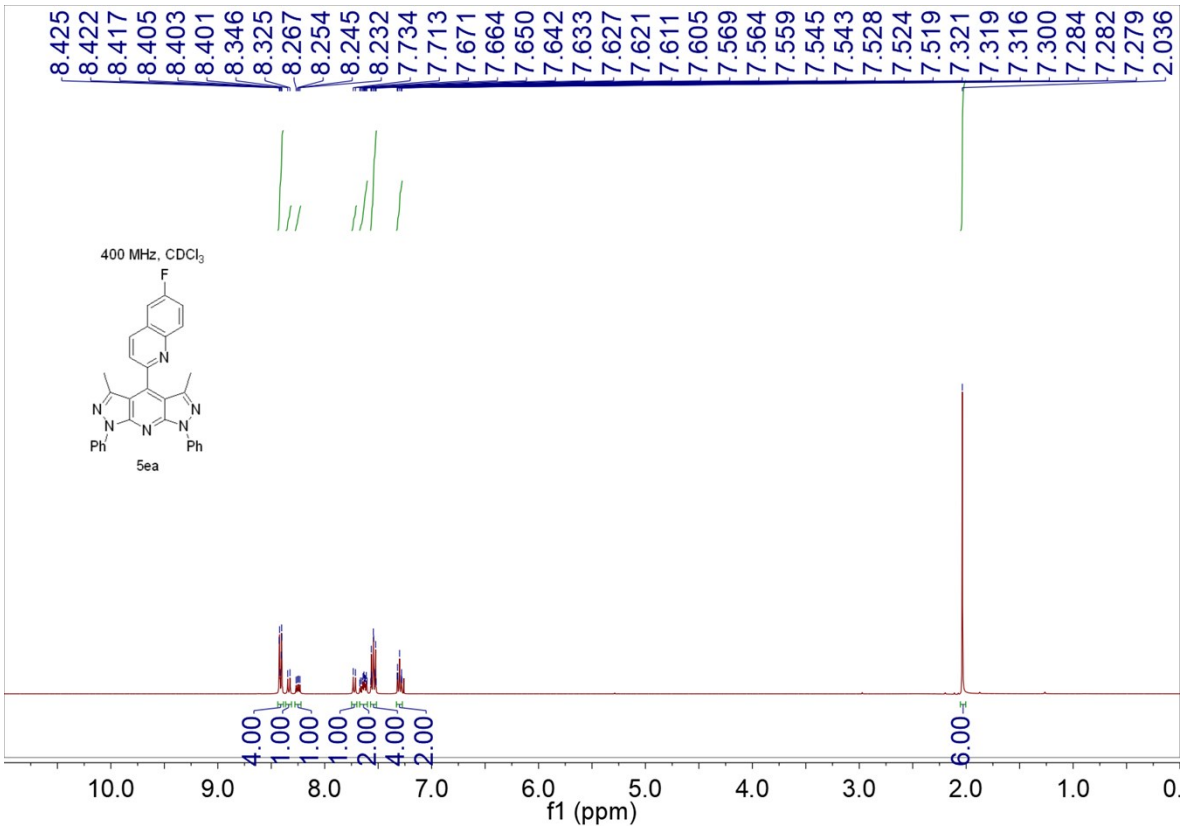
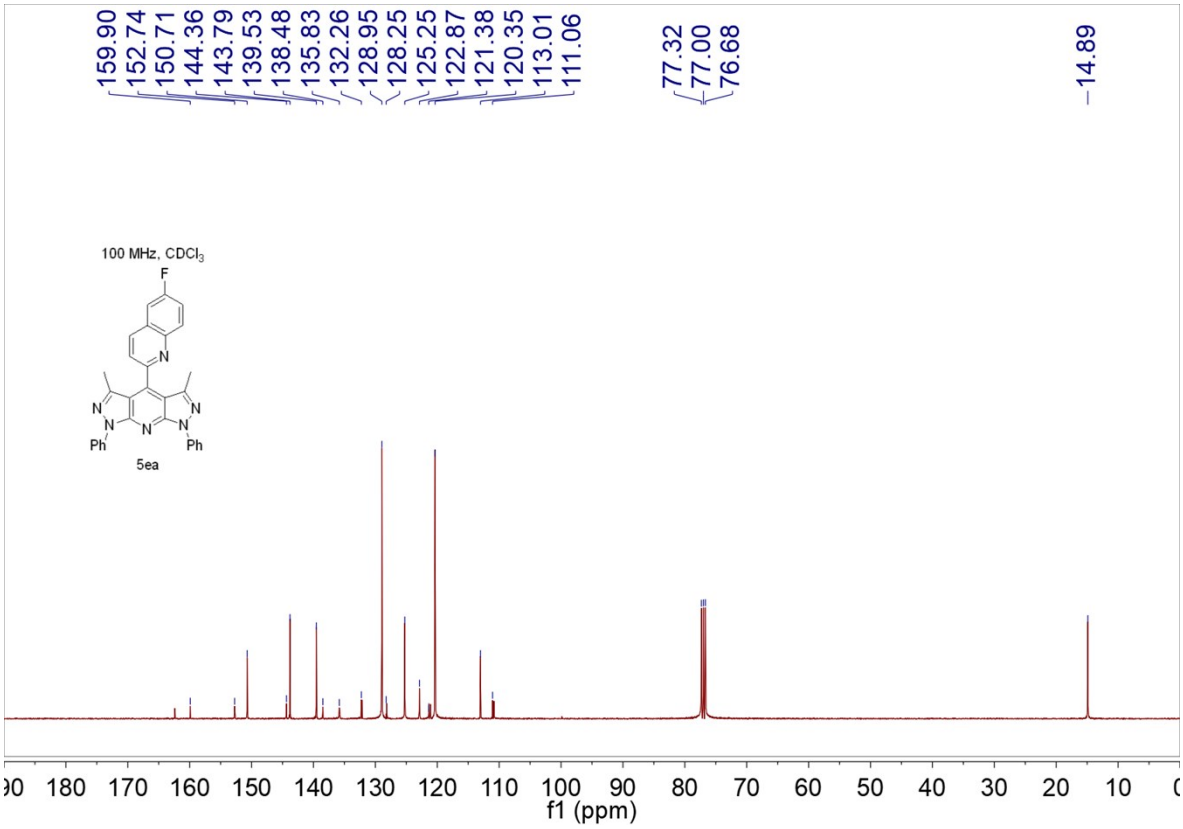
150.55
144.11
143.44
139.64
139.40
134.90
131.07
128.95
128.73
125.18
123.97
122.30
120.38
113.24
105.77
77.32
77.00
76.68
64.02
14.92
14.73
100 Hz, CDCl3
OEt
N
N
N
N
N
Ph
Ph
5da
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.425
8.422
8.417
8.405
8.403
8.401
8.346
8.325
8.267
8.254
8.245
8.232
7.734
7.713
7.671
7.664
7.650
7.642
7.633
7.627
7.621
7.611
7.605
7.569
7.564
7.559
7.545
7.543
7.528
7.524
7.519
7.321
7.319
7.316
7.300
7.284
7.282
7.279
2.036
400 MHz, CDCl3
5ea
4.00
1.00
1.00
1.00
2.00
4.00
2.00
6.00
f1 (ppm)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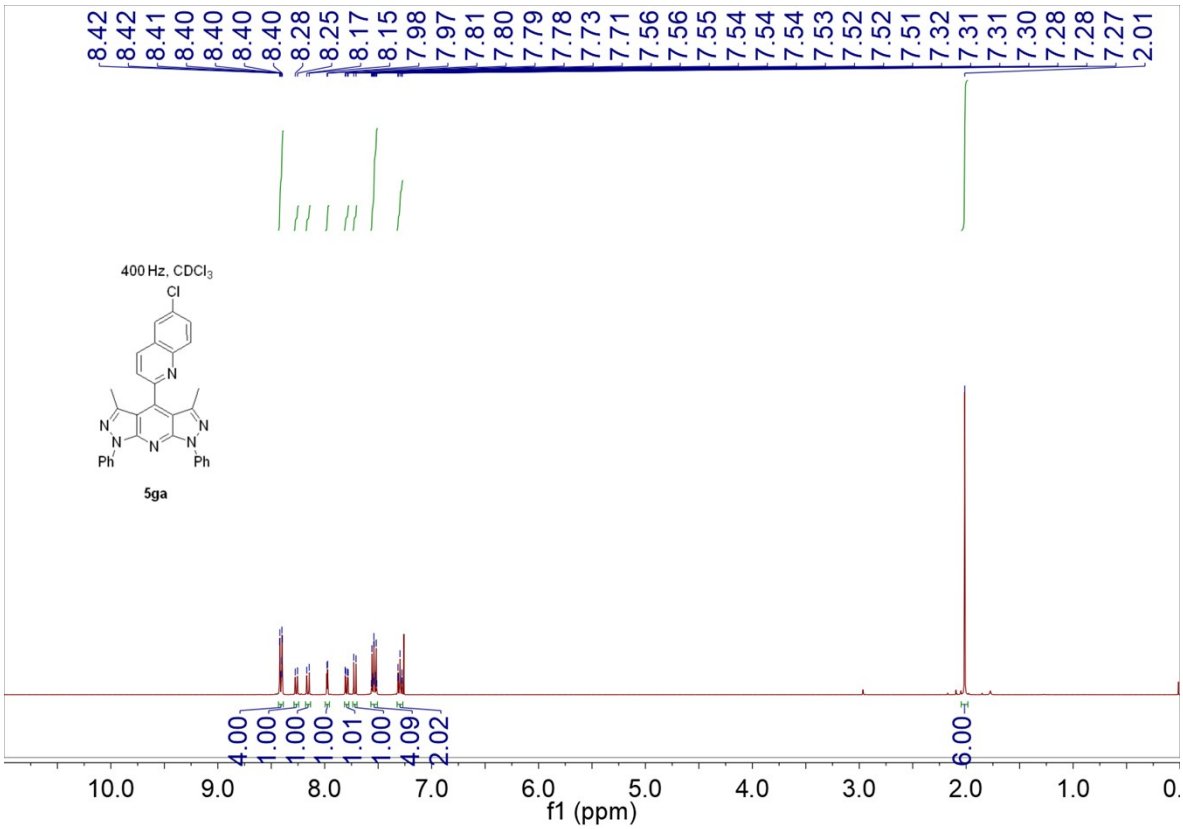
152.74
150.71
144.36
143.79
139.53
138.48
135.83
132.26
128.95
128.25
125.25
122.87
121.38
120.35
113.01
111.06
77.32
77.00
76.68
14.89
100 MHz, CDCl3
5ea
f1 (ppm)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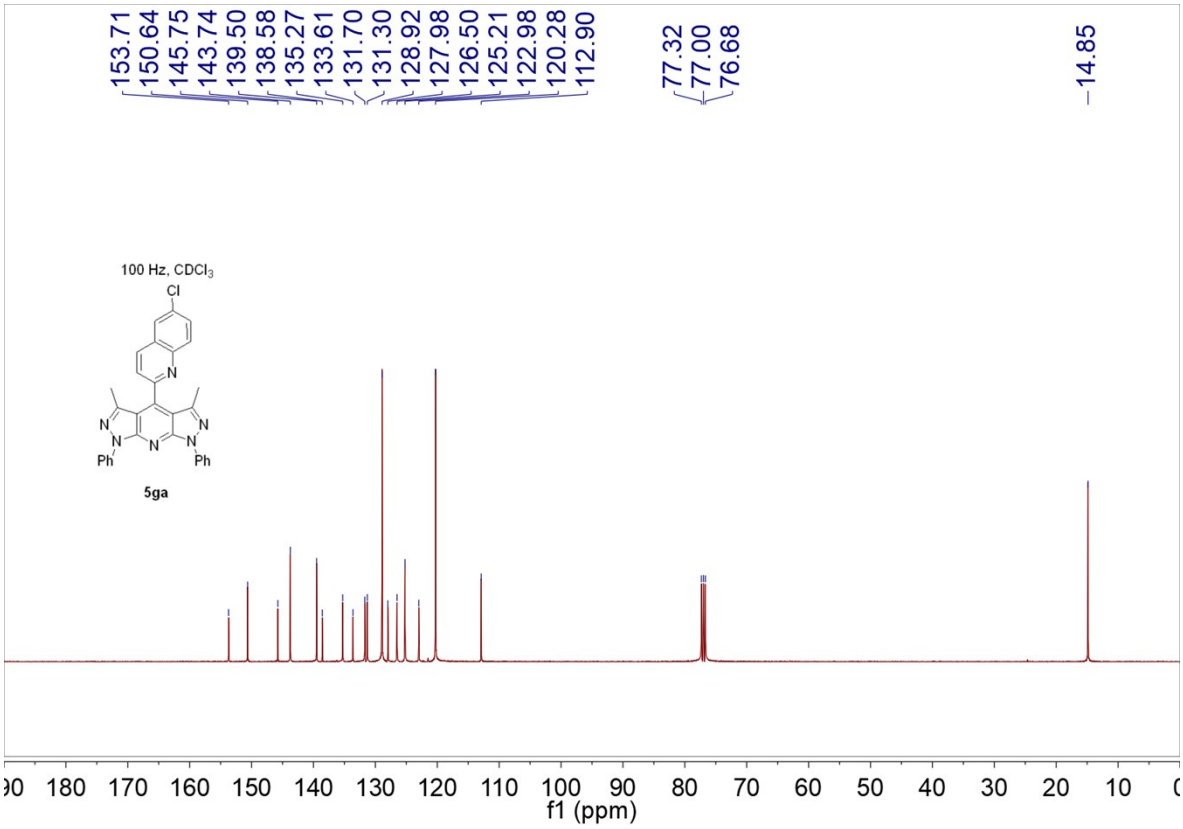
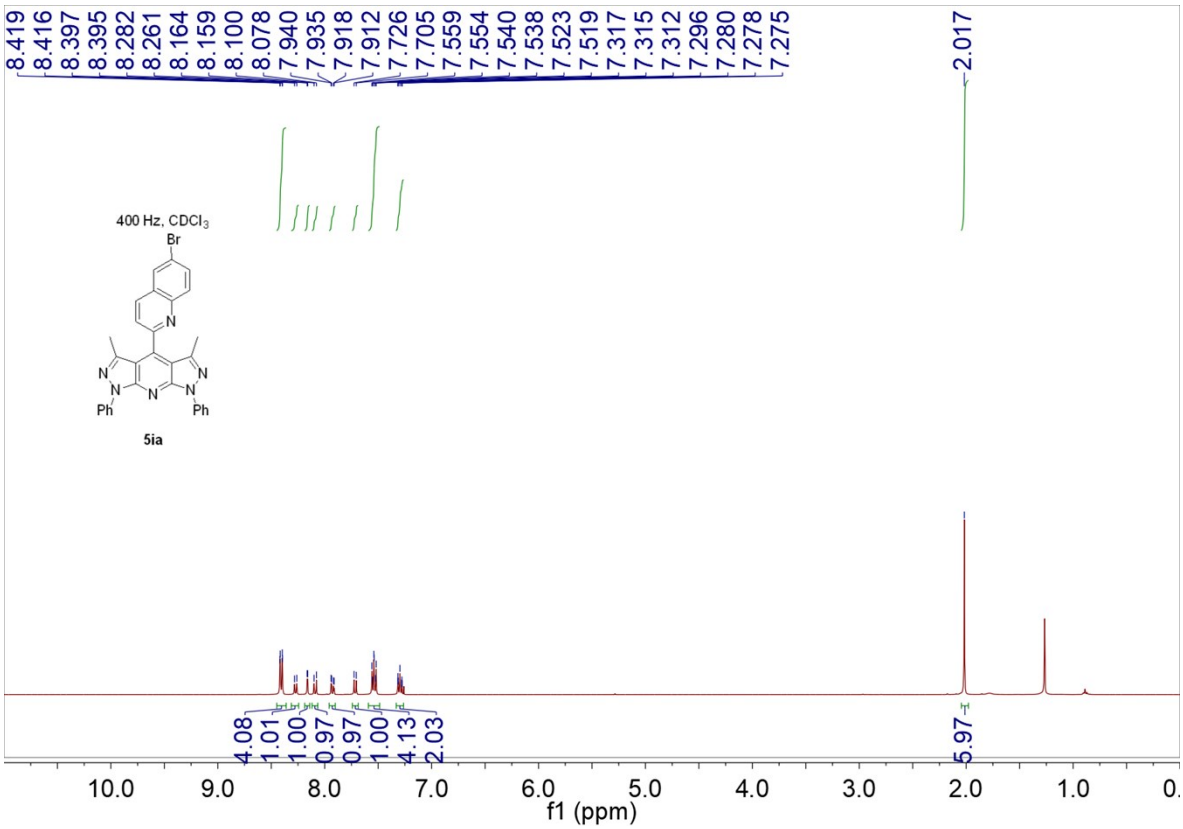
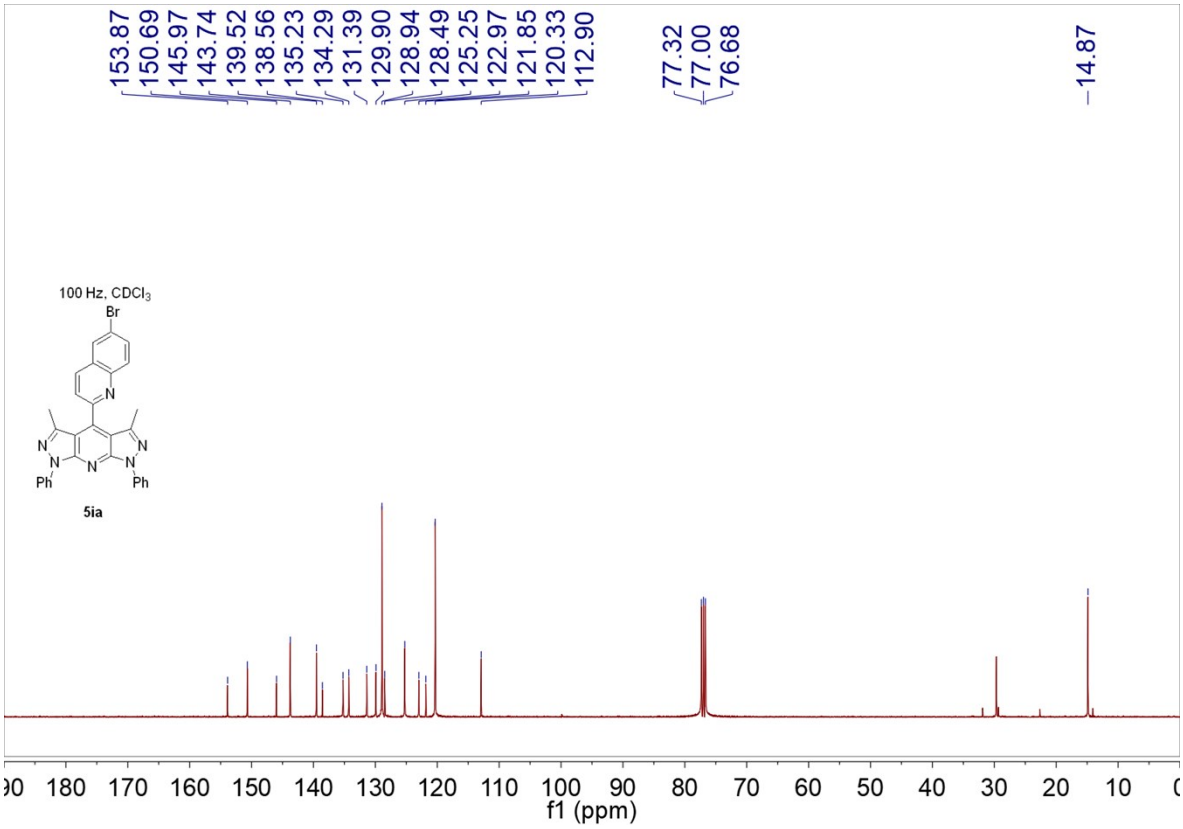
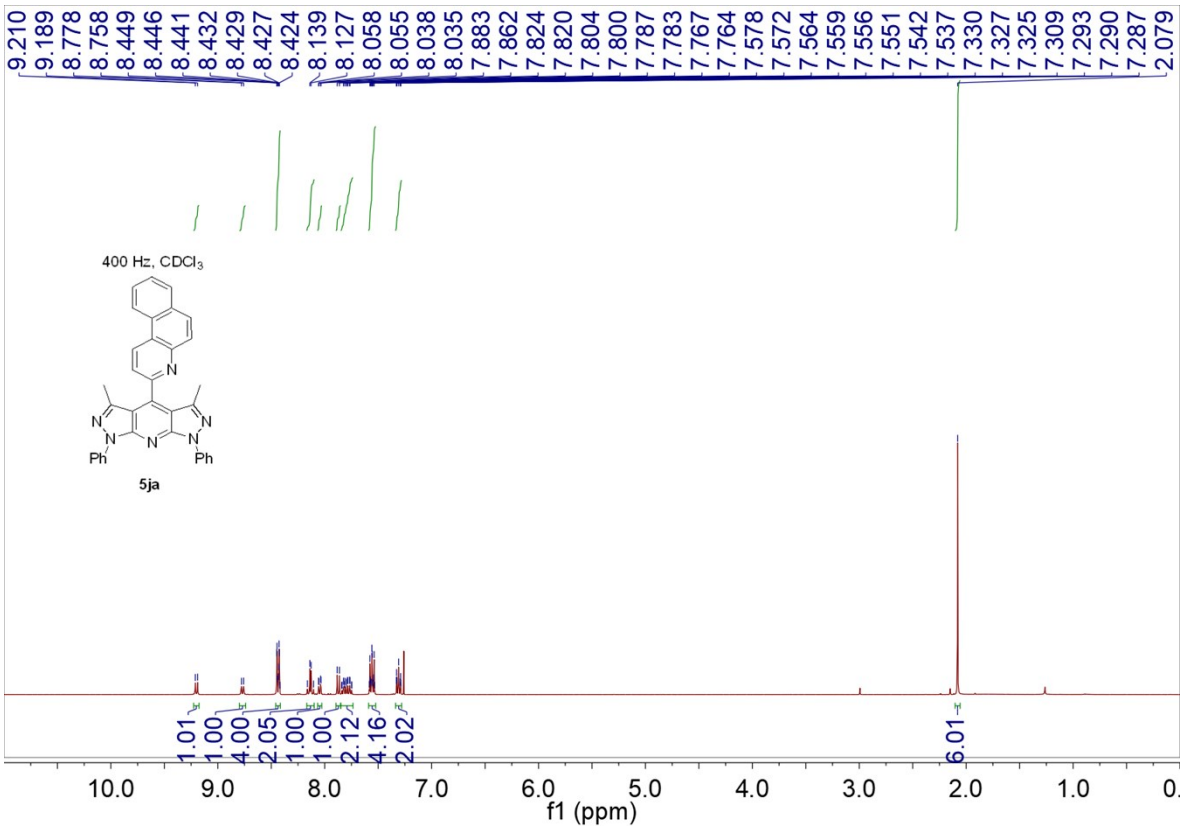
8.42
8.41
8.40
8.40
8.40
8.40
8.28
8.25
8.17
8.15
7.98
7.97
7.81
7.80
7.79
7.78
7.73
7.71
7.56
7.56
7.55
7.54
7.54
7.54
7.53
7.52
7.52
7.51
7.32
7.31
7.31
7.30
7.28
7.28
7.27
2.01
400 Hz, CDCl3
Cl
N
N
N
N
N
Ph
Ph
5ga
4.00
1.00
1.00
1.00
1.01
1.00
4.09
2.02
6.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)


153.71
150.64
145.75
143.74
139.50
138.58
135.27
133.61
131.70
131.30
128.92
127.98
126.50
125.21
122.98
120.28
112.90
77.32
77.00
76.68
14.85
100 Hz, CDCl3
Cl
N
N
N
N
N
Ph
Ph
5ga
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.419
8.416
8.397
8.395
8.282
8.261
8.164
8.159
8.100
8.078
7.940
7.935
7.918
7.912
7.726
7.705
7.559
7.554
7.540
7.538
7.523
7.519
7.317
7.315
7.312
7.296
7.280
7.278
7.275
2.017
400 Hz, CDCl3
Br
N
N
N
N
N
Ph
Ph
5ia
4.08
1.01
1.00
0.97
0.97
1.00
4.13
2.03
5.97
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)


153.87
150.69
145.97
143.74
139.52
138.56
135.23
134.29
131.39
129.90
128.94
128.49
125.25
122.97
121.85
120.33
112.90
77.32
77.00
76.68
14.87
100 Hz, CDCl3
Br
N
N
N
N
N
Ph
Ph
5ia
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


9.210
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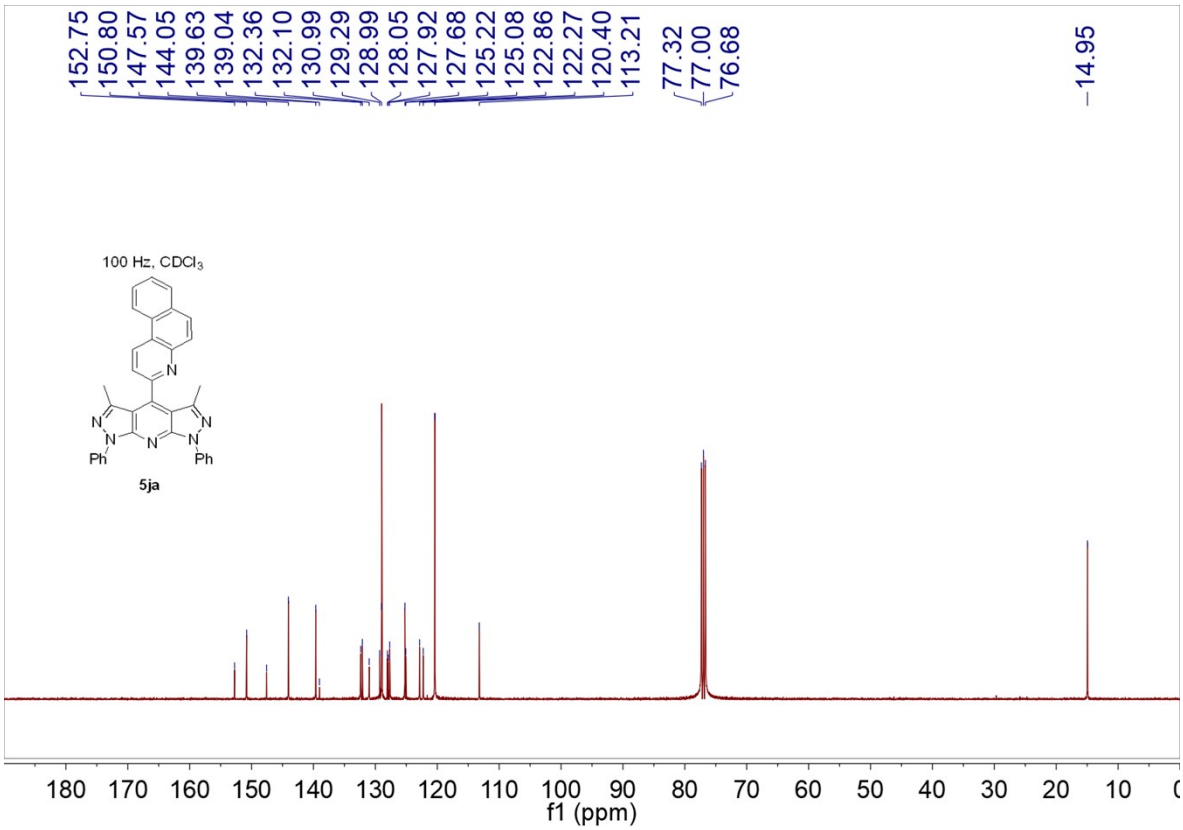
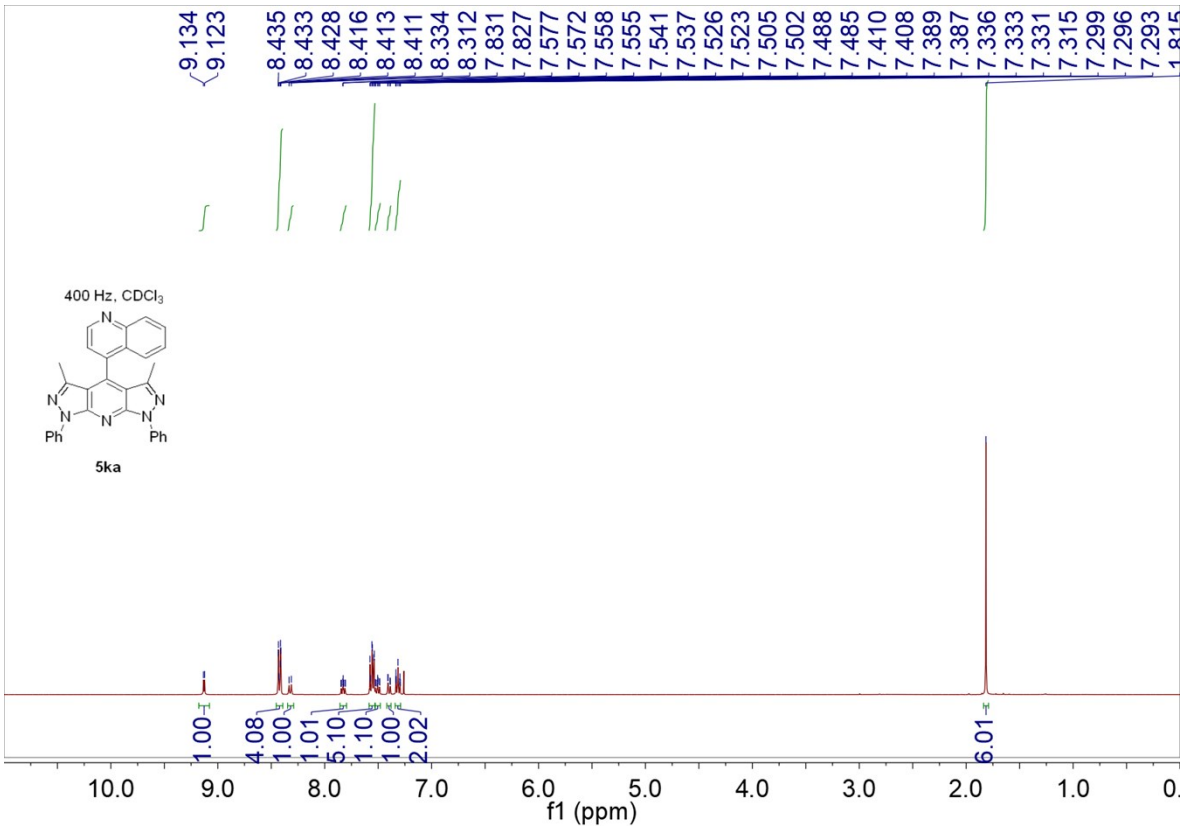
8.778
8.758
8.449
8.446
8.441
8.432
8.429
8.427
8.424
8.139
8.127
8.058
8.055
8.038
8.035
7.883
7.862
7.824
7.820
7.804
7.800
7.787
7.783
7.767
7.764
7.578
7.572
7.564
7.559
7.556
7.551
7.542
7.537
7.330
7.327
7.325
7.309
7.293
7.290
7.287
2.079
400 Hz, CDCl3
5ja
1.01
1.00
4.00
2.05
1.00
1.00
2.12
4.16
2.02
6.01
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)


152.75
150.80
147.57
144.05
139.63
139.04
132.36
132.10
130.99
129.29
128.99
128.05
127.92
127.68
125.22
125.08
122.86
122.27
120.40
113.21
77.32
77.00
76.68
14.95
100 Hz, CDCl3
5ja
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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9.123
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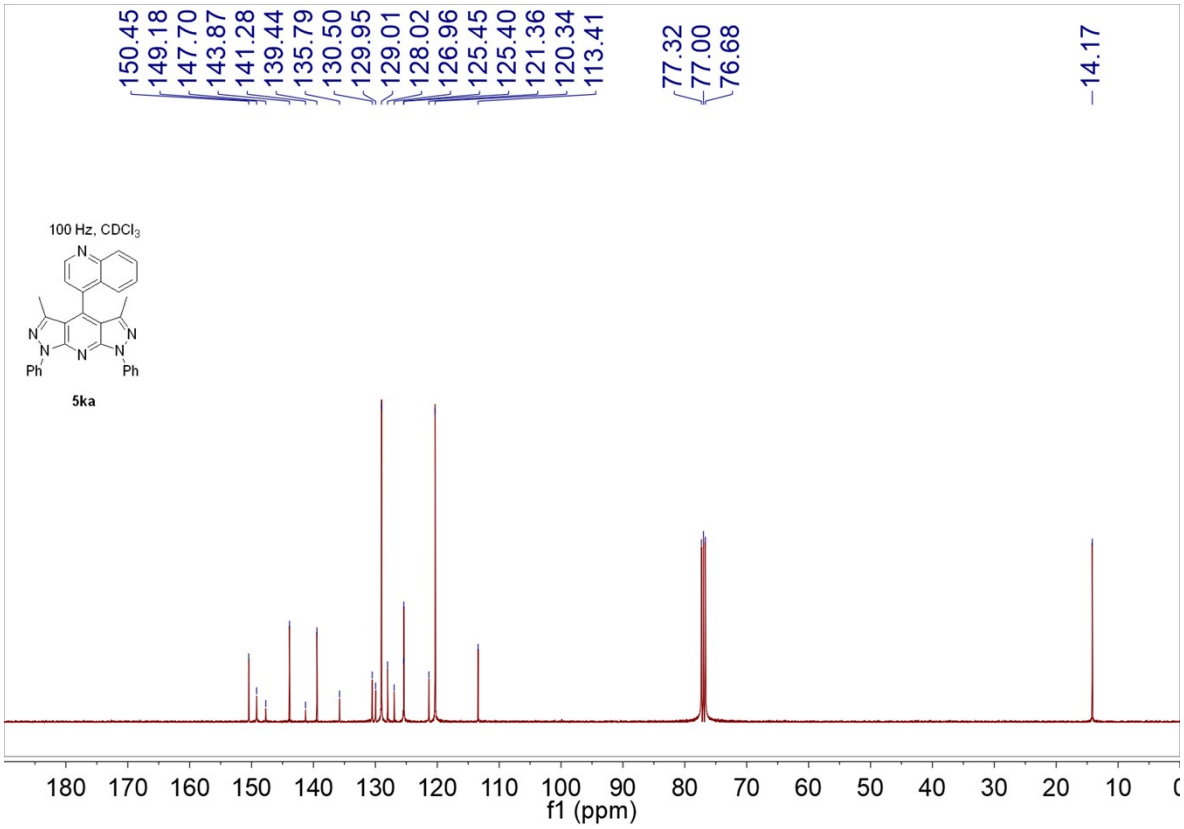
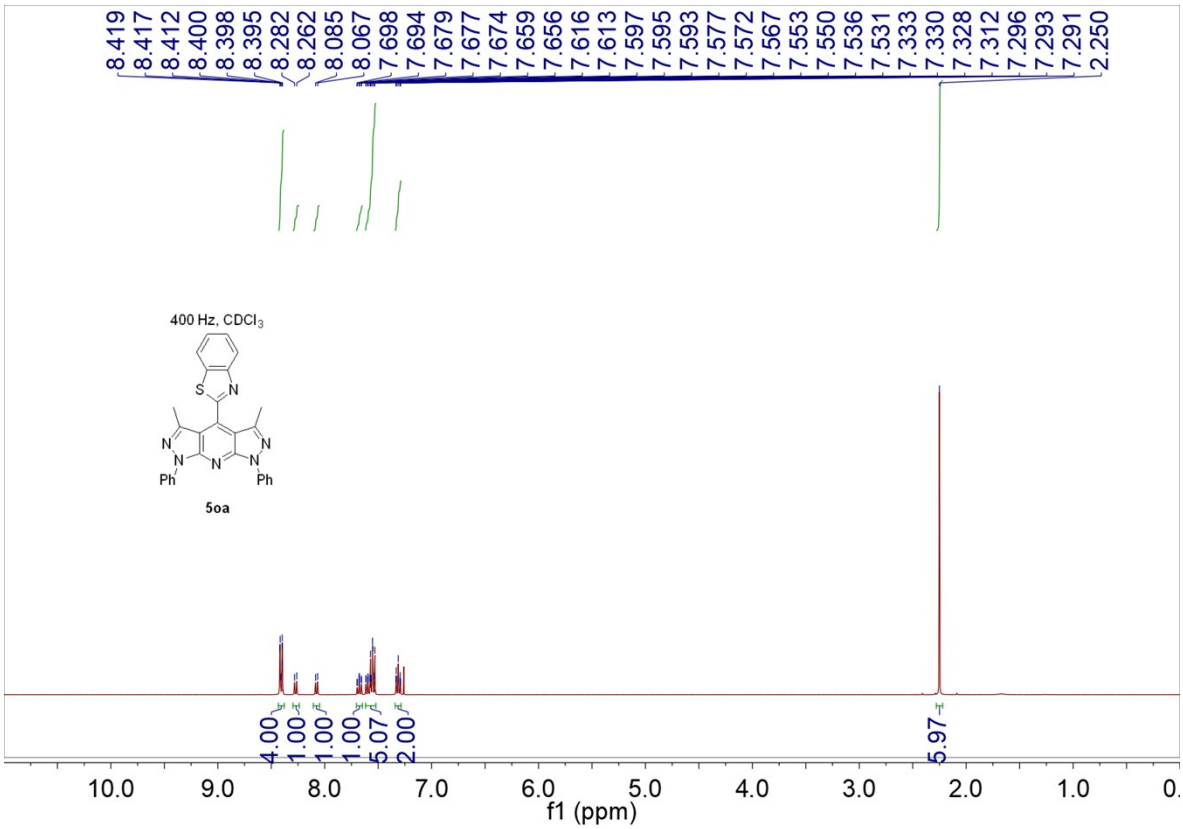
8.433
8.428
8.416
8.413
8.411
8.334
8.312
7.831
7.827
7.577
7.572
7.558
7.555
7.541
7.537
7.526
7.523
7.505
7.502
7.488
7.485
7.410
7.408
7.389
7.387
7.336
7.333
7.331
7.315
7.299
7.296
7.293
400 Hz, CDCl3
5ka
1.00
4.08
1.00
1.01
5.10
1.10
1.00
2.02
6.01
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)


150.45
149.18
147.70
143.87
141.28
139.44
135.79
130.50
129.95
129.01
128.02
126.96
125.45
125.40
121.36
120.34
113.41
77.32
77.00
76.68
14.17
100 Hz, CDCl3
5ka
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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8.400
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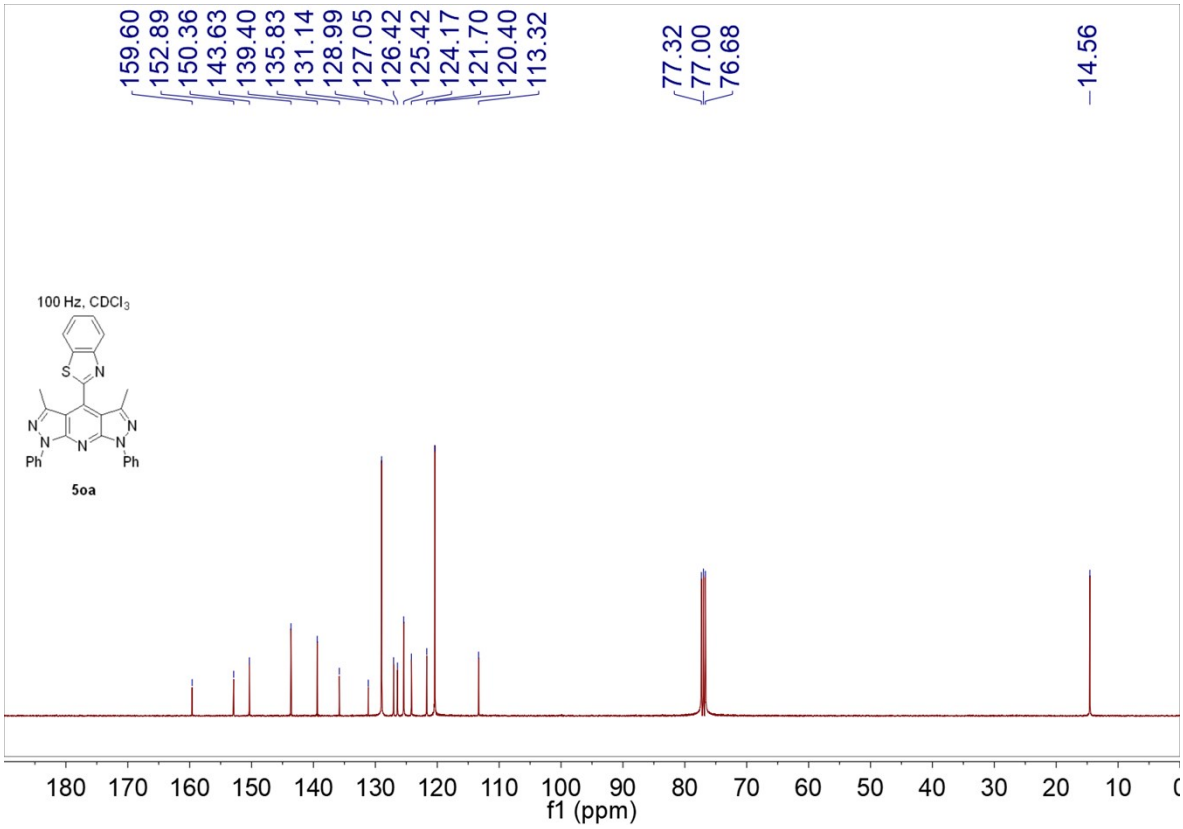
8.395
8.282
8.262
8.085
8.067
7.698
7.694
7.679
7.677
7.674
7.659
7.656
7.616
7.613
7.597
7.595
7.593
7.577
7.572
7.567
7.553
7.550
7.536
7.531
7.333
7.330
7.328
7.312
7.296
7.293
7.291
2.250
400 Hz, CDCl3
5oa
4.00
1.00
1.00
1.00
5.07
2.00
5.97
f1 (ppm)


159.60
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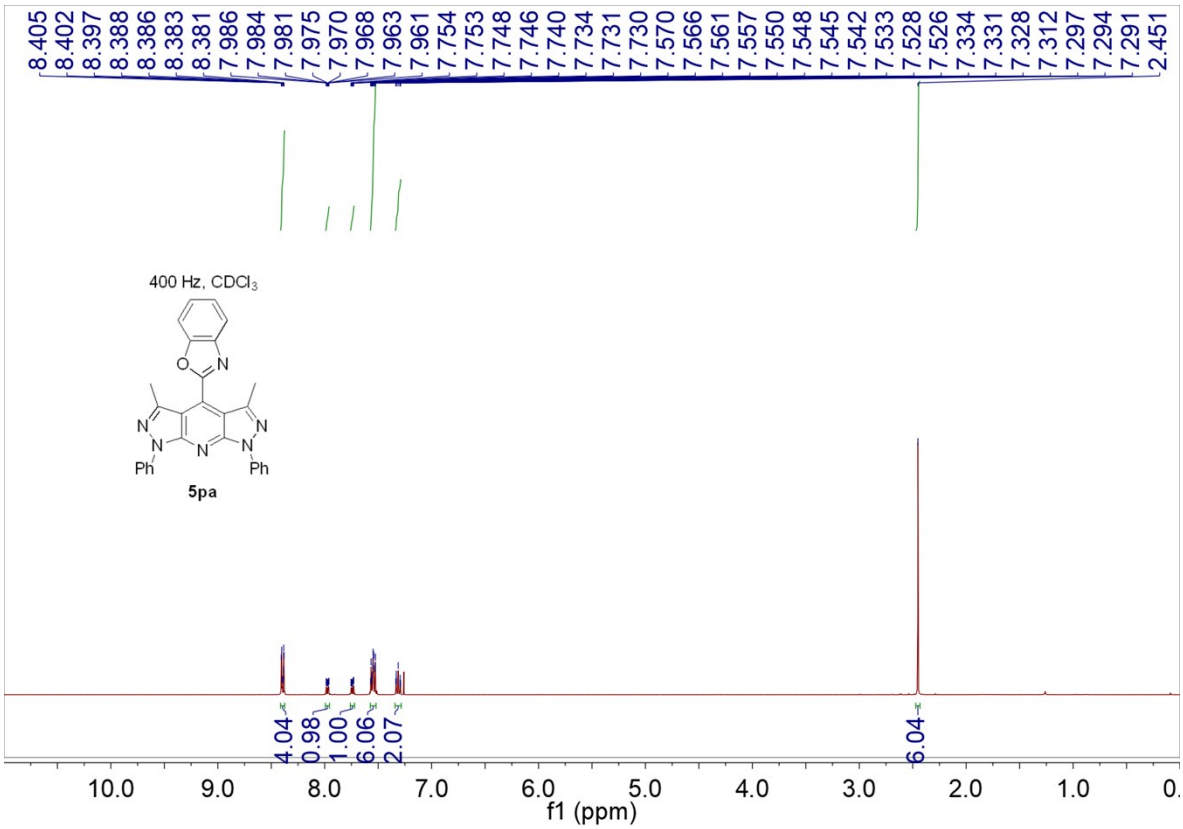
143.63
139.40
135.83
131.14
128.99
127.05
126.42
125.42
124.17
121.70
120.40
113.32
77.32
77.00
76.68
14.56
100 Hz, CDCl3
5oa
f1 (ppm)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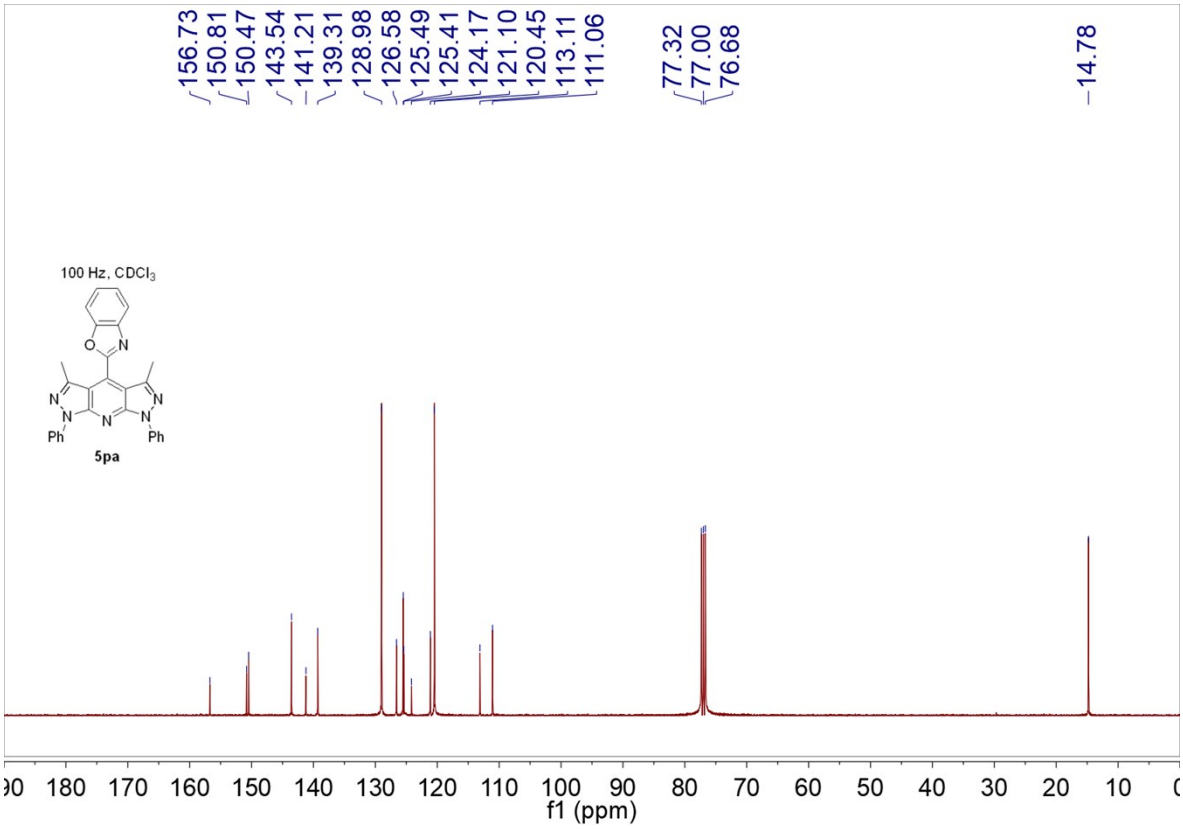
8.388
8.386
8.383
8.381
7.986
7.984
7.981
7.975
7.970
7.968
7.963
7.961
7.754
7.753
7.748
7.746
7.740
7.734
7.731
7.730
7.570
7.566
7.561
7.557
7.550
7.548
7.545
7.542
7.533
7.528
7.526
7.334
7.331
7.328
7.312
7.297
7.294
7.291
2.451
400 Hz, CDCl3
Ph
Ph
5pa
4.04
0.98
1.00
6.06
2.07
6.04
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)


156.73
150.81
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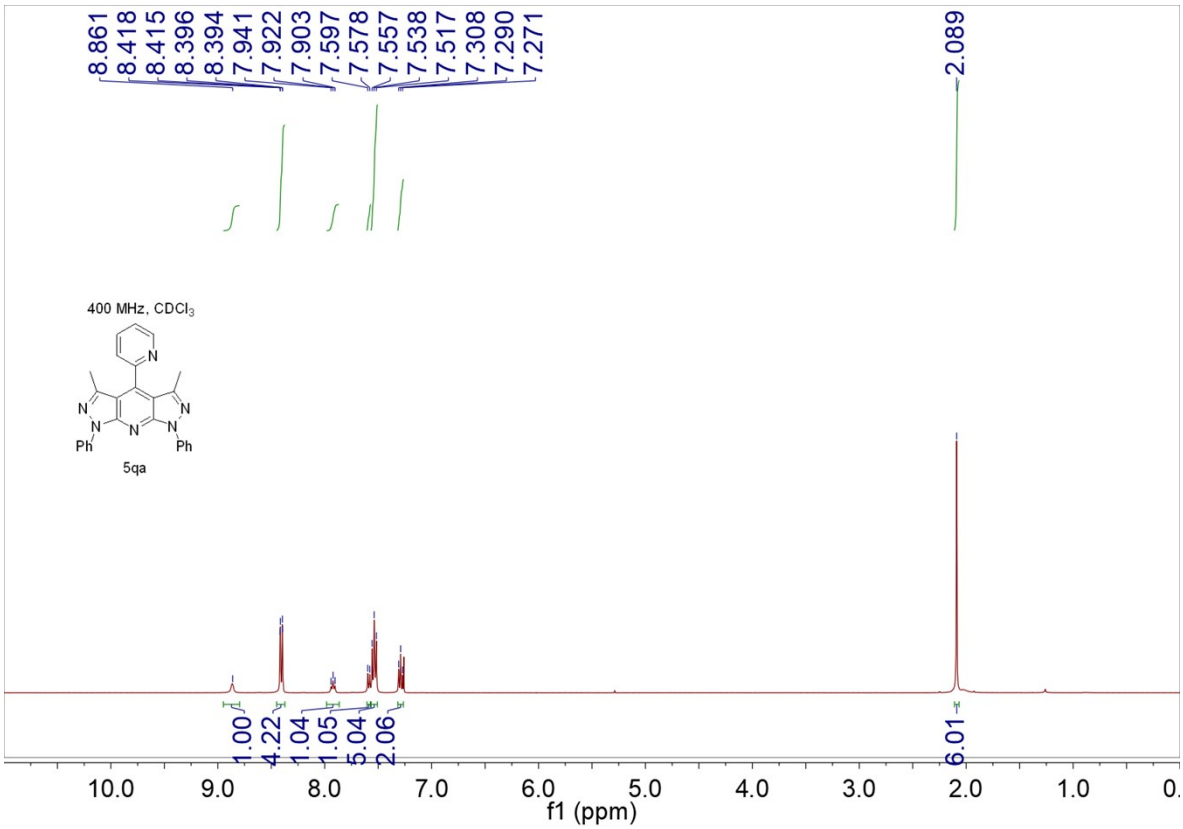
143.54
141.21
139.31
128.98
126.58
125.49
125.41
124.17
121.10
120.45
113.11
111.06
77.32
77.00
76.68
14.78
100 Hz, CDCl3
Ph
Ph
5pa
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.861
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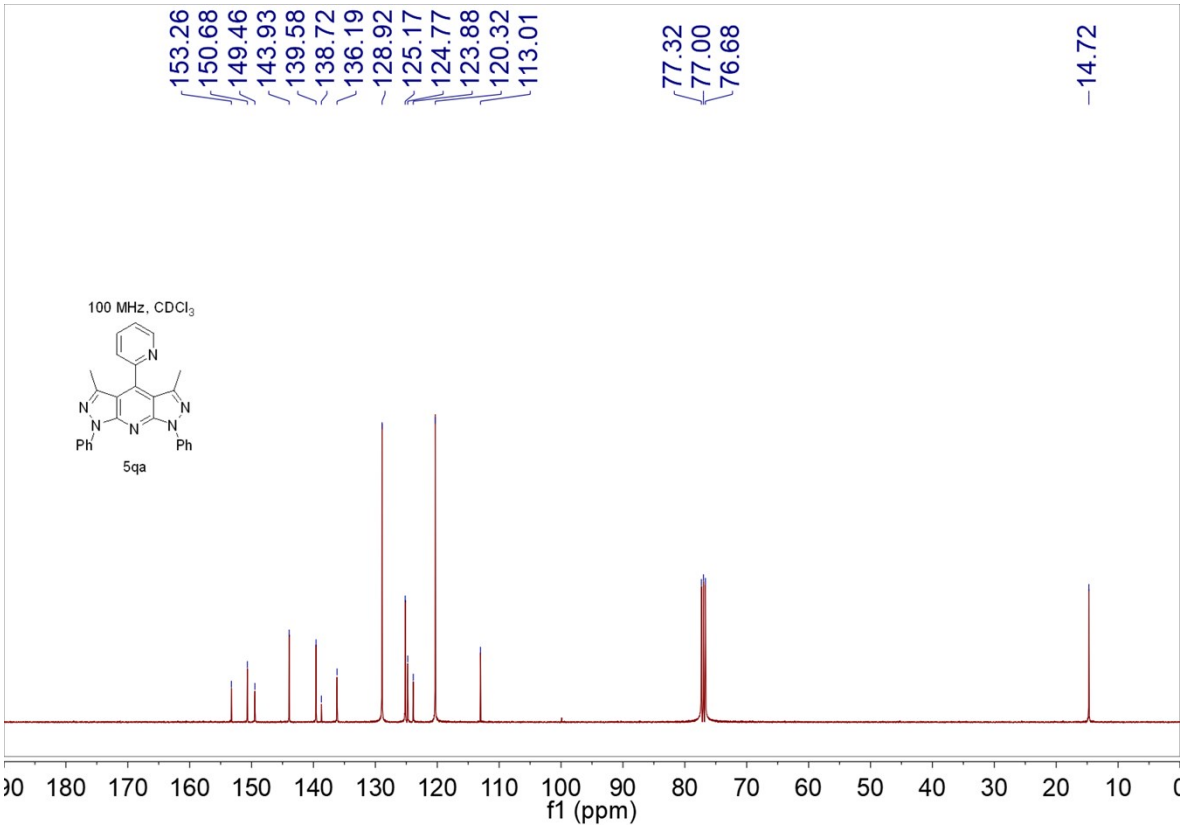
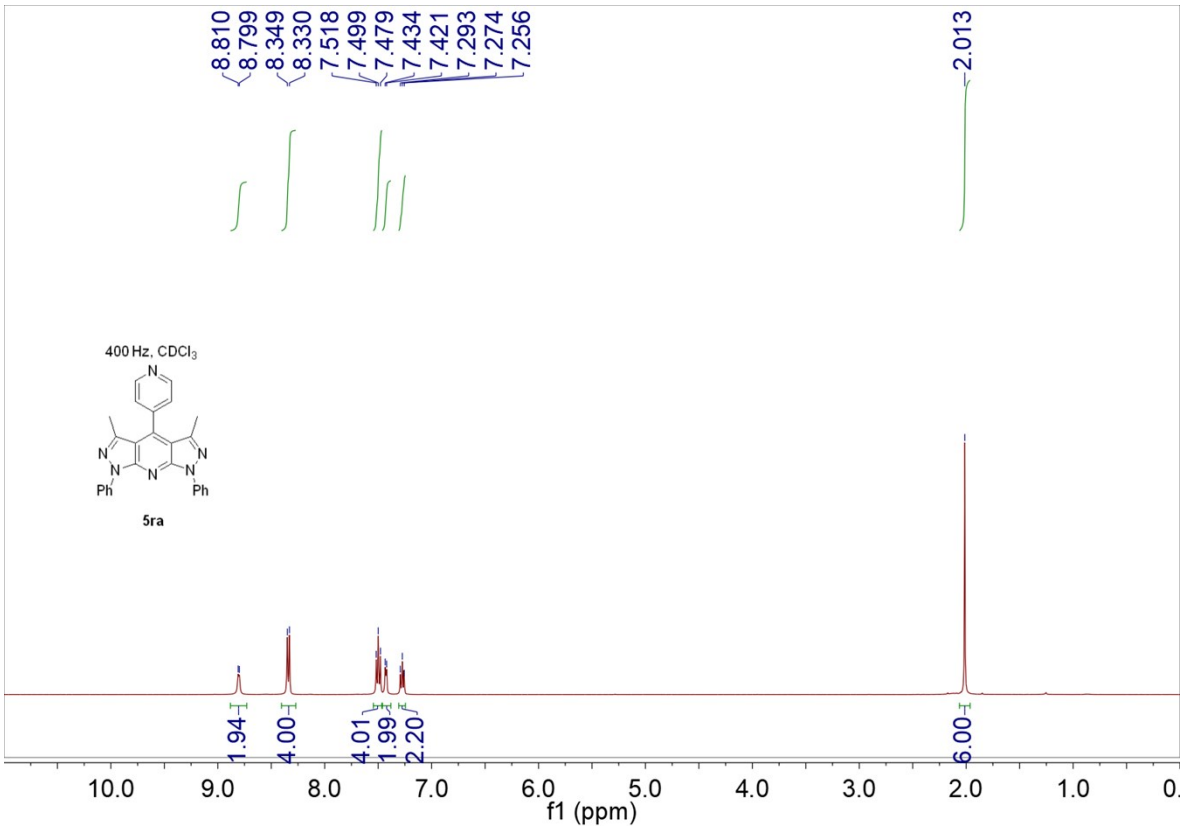
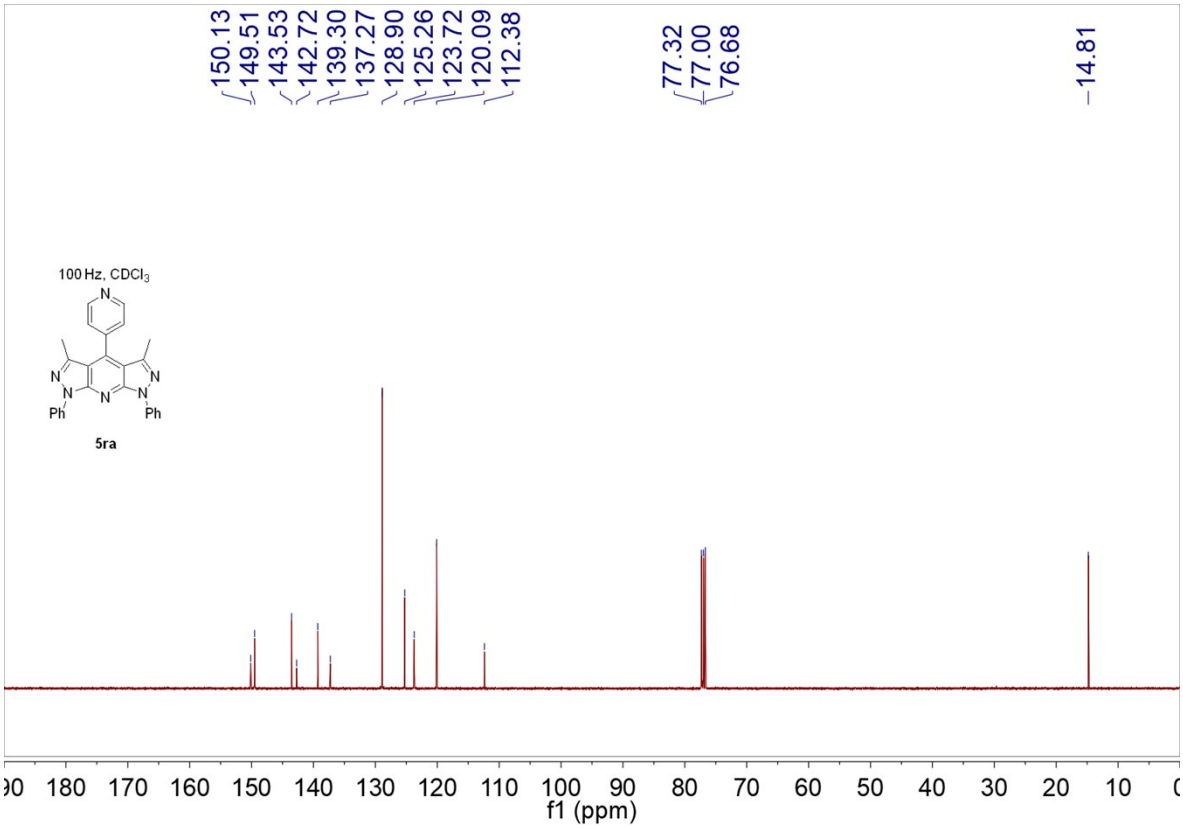
8.415
8.396
8.394
7.941
7.922
7.903
7.597
7.578
7.557
7.538
7.517
7.308
7.290
7.271
2.089
400 MHz, CDCl3
5qa
1.00
4.22
1.04
1.05
5.04
2.06
6.01
f1 (ppm)


153.26
150.68
149.46
143.93
139.58
138.72
136.19
128.92
125.17
124.77
123.88
120.32
113.01
77.32
77.00
76.68
14.72
100 MHz, CDCl3
5qa
f1 (ppm)


8.810
8.799
8.349
8.330
7.518
7.499
7.479
7.434
7.421
7.293
7.274
7.256
2.013
400 Hz, CDCl3
5ra
1.94
4.00
4.01
1.99
2.20
6.00
f1 (ppm)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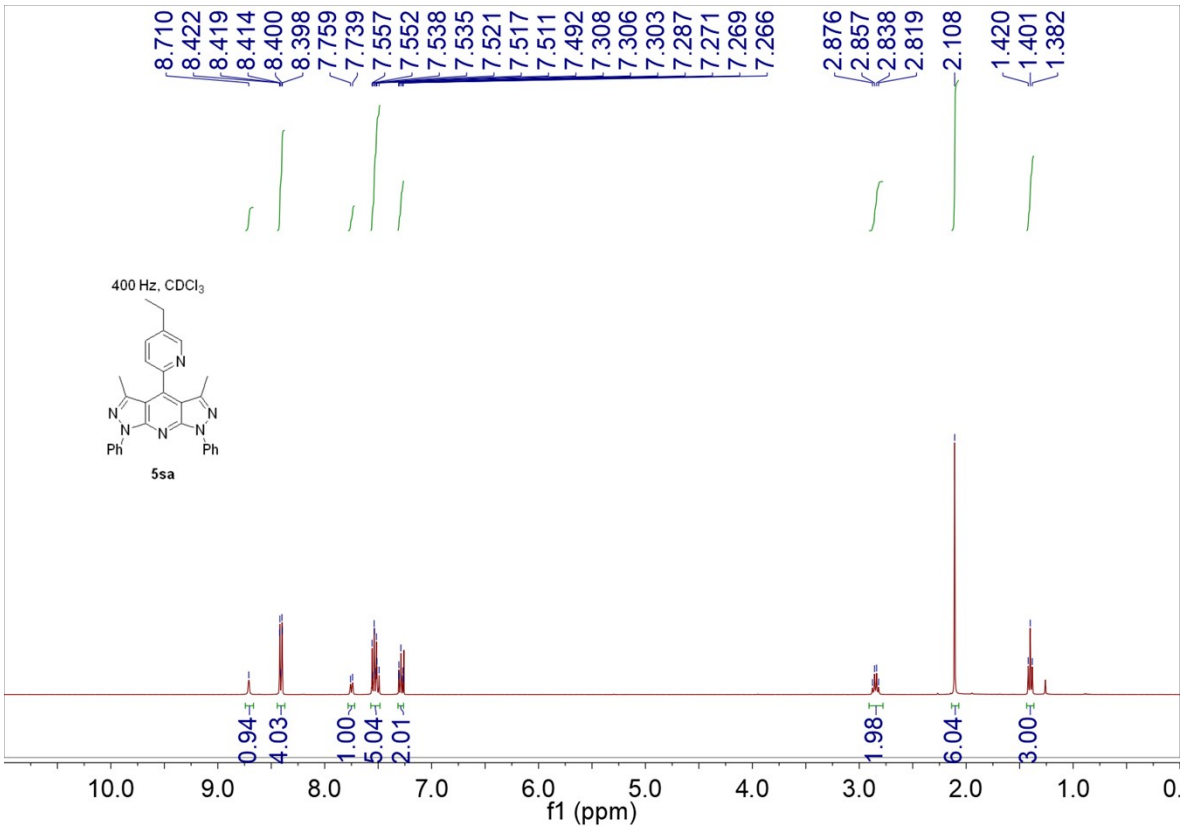
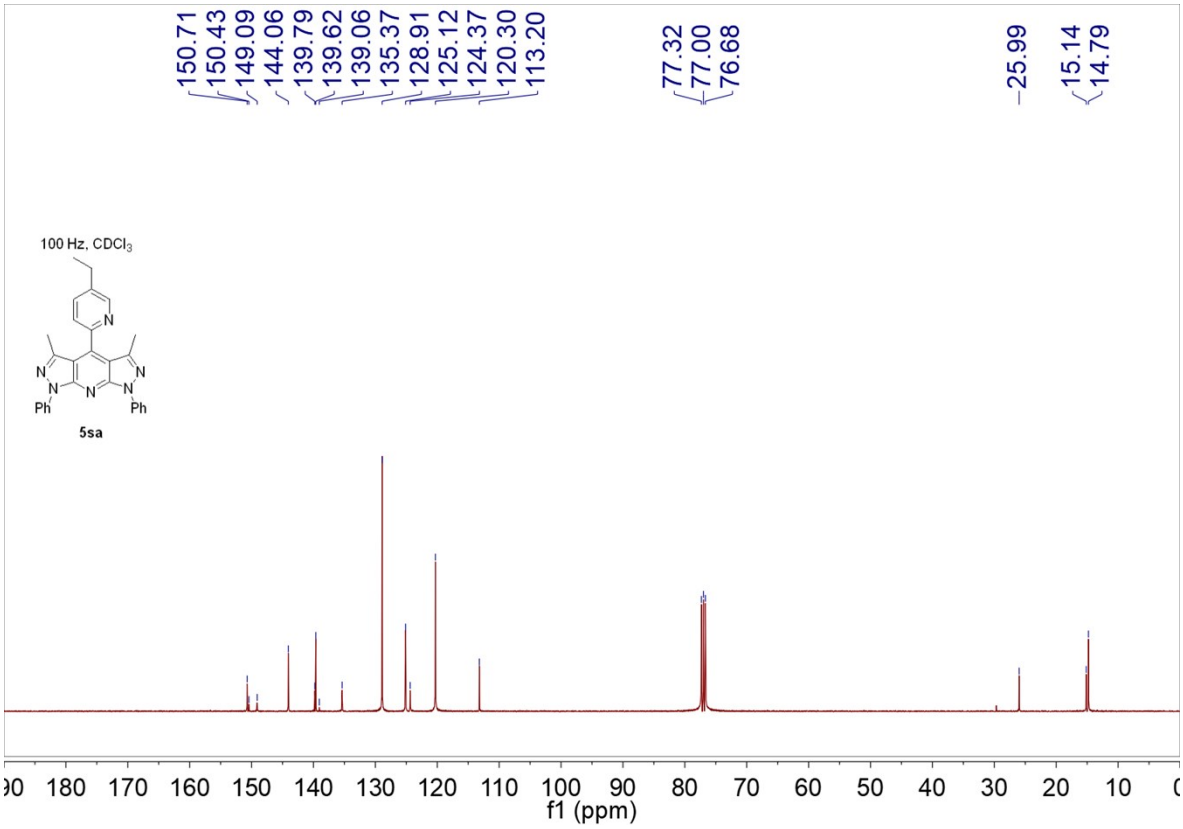
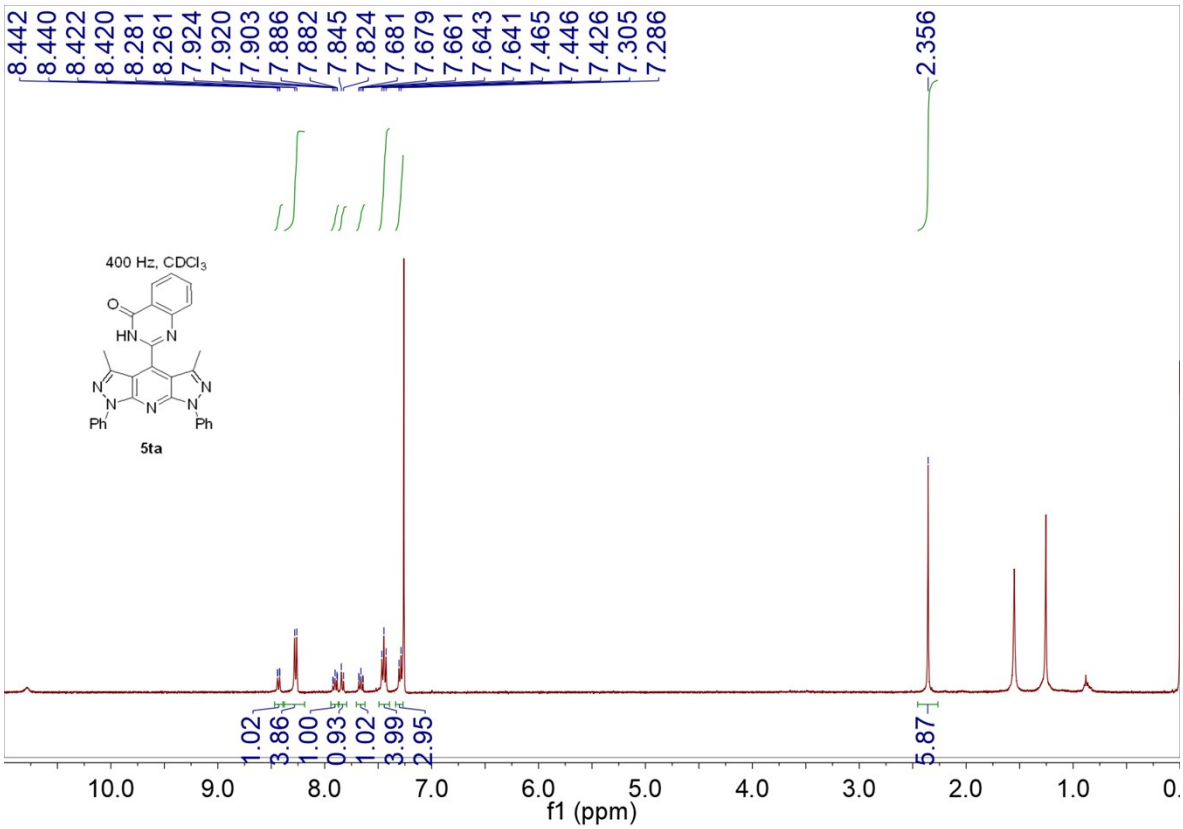
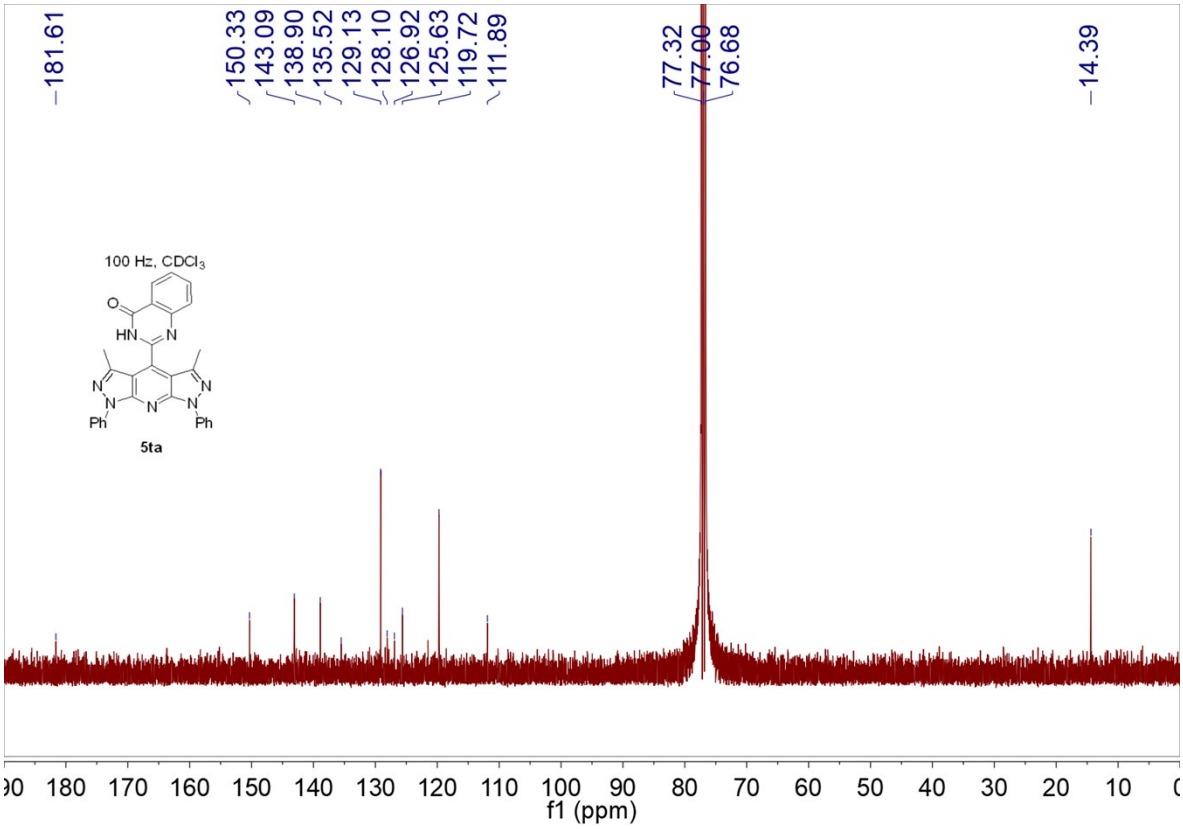
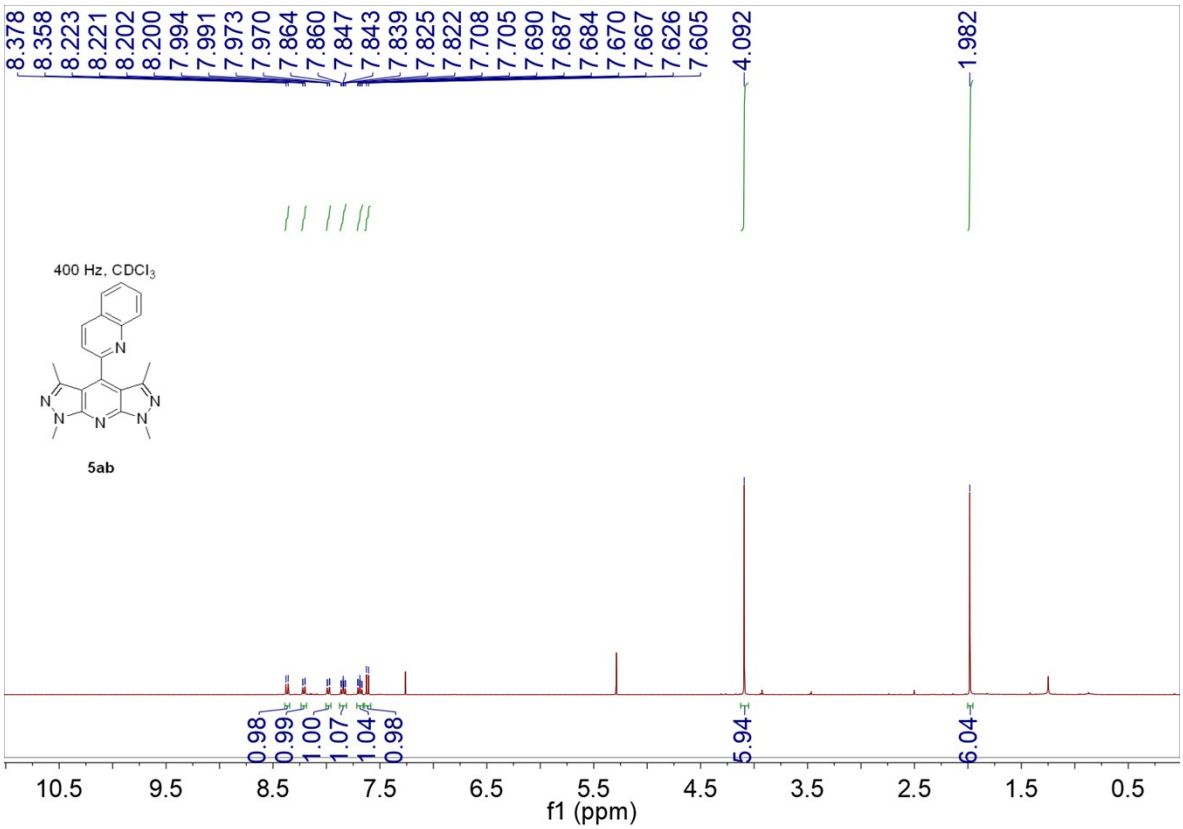
149.51
143.53
142.72
139.30
137.27
128.90
125.26
123.72
120.09
112.38
77.32
77.00
76.68
14.81
100 Hz, CDCl3
5ra
f1 (ppm)

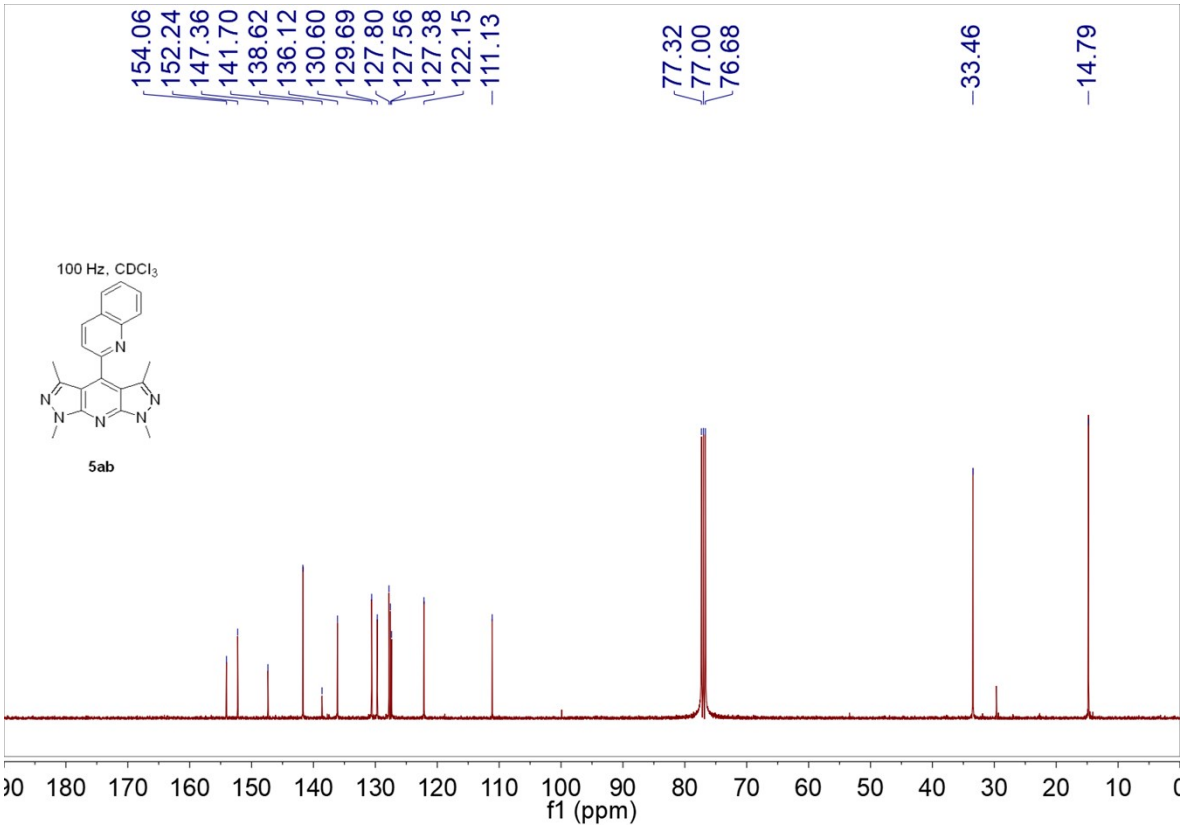

8.710
8.422
8.419
8.414
8.400
8.398
7.759
7.739
7.557
7.552
7.538
7.535
7.521
7.517
7.511
7.492
7.308
7.306
7.303
7.287
7.271
7.269
7.266
2.876
2.857
2.838
2.819
2.108
1.420
1.401
1.382
400 Hz, CDCl3
5sa
0.94
4.03
1.00
5.04
2.01
1.98
6.04
3.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)

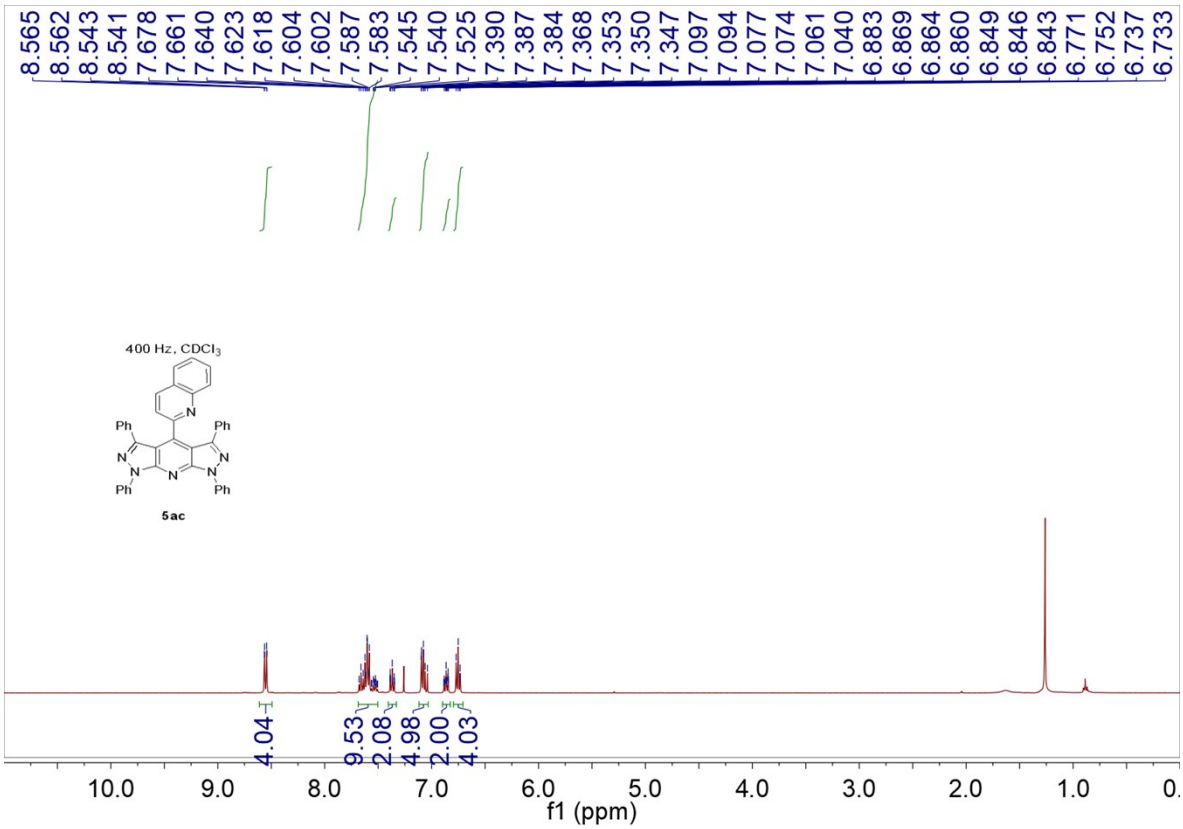

150.71
150.43
149.09
144.06
139.79
139.62
139.06
135.37
128.91
125.12
124.37
120.30
113.20
77.32
77.00
76.68
25.99
15.14
14.79
100 Hz, CDCl3
5sa
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

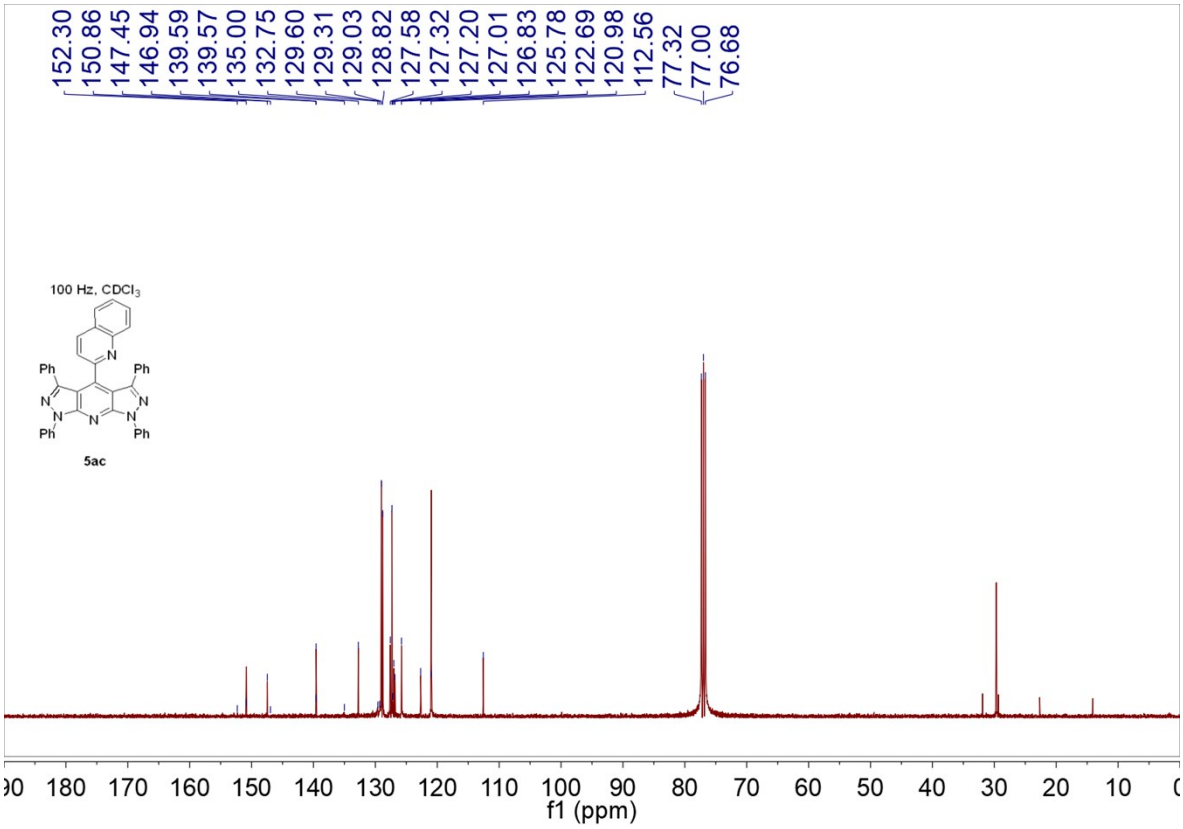

8.442
8.440
8.422
8.420
8.281
8.261
7.924
7.920
7.903
7.886
7.882
7.845
7.824
7.681
7.679
7.661
7.643
7.641
7.465
7.446
7.426
7.305
7.286
2.356
400 Hz, CDCl3
5ta
1.02
3.86
1.00
0.93
1.02
3.99
2.95
5.87
f1 (ppm)

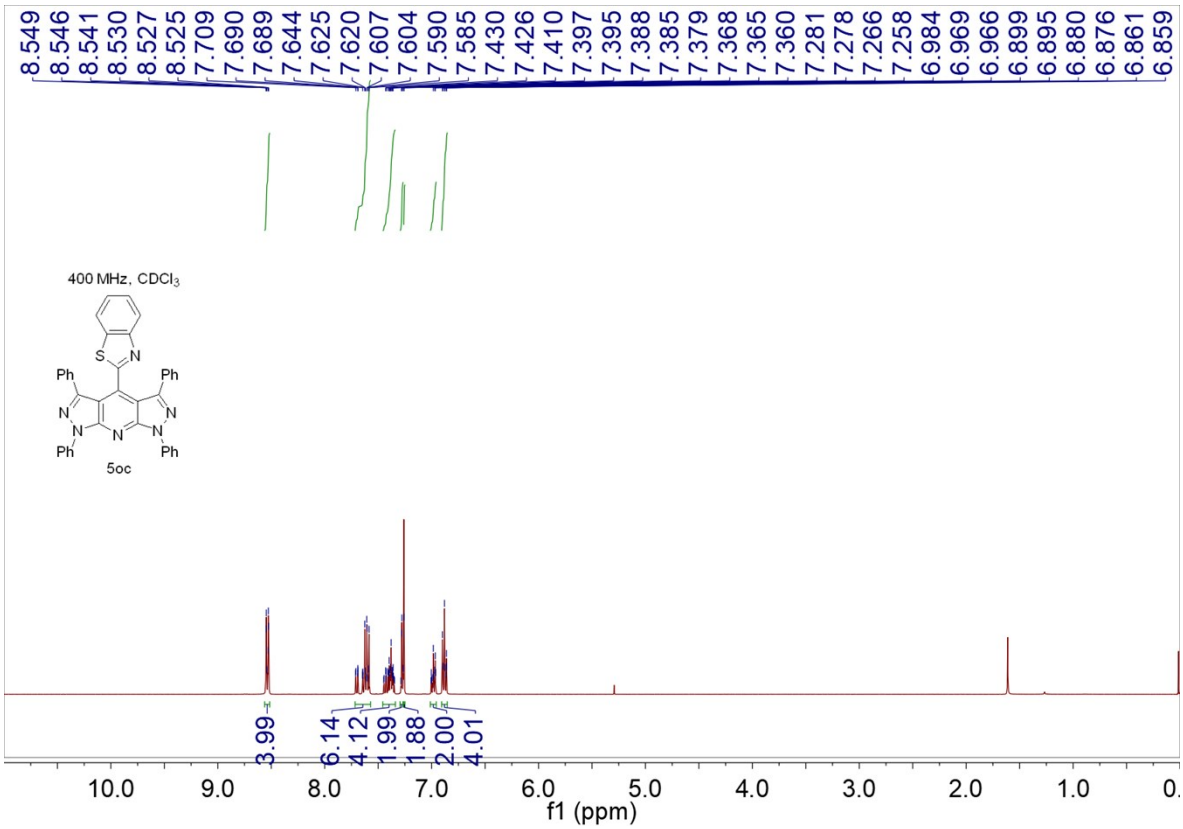

181.61
150.33
143.09
138.90
135.52
129.13
128.10
126.92
125.63
119.72
111.89
77.32
77.00
76.68
14.39
100 Hz, CDCl3
5ta
f1 (ppm)

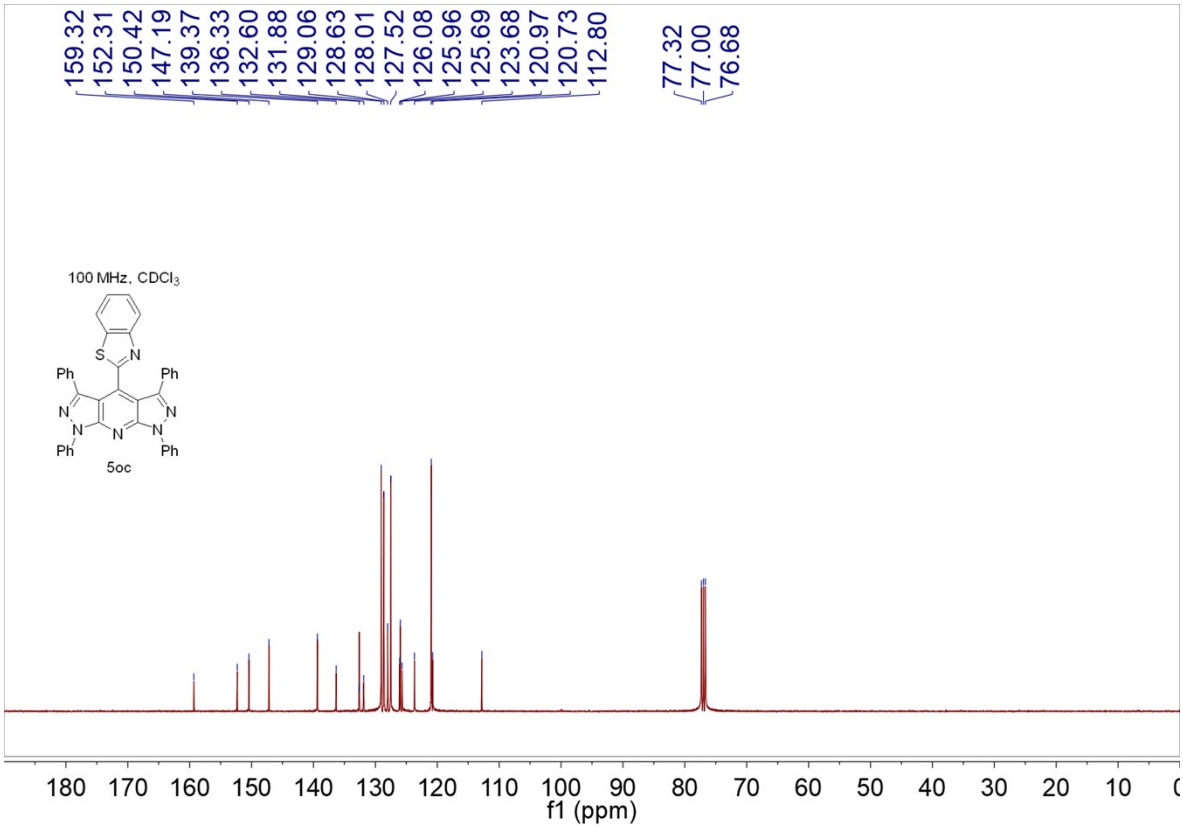

8.378
8.358
8.223
8.221
8.202
8.200
7.994
7.991
7.973
7.970
7.864
7.860
7.847
7.843
7.839
7.825
7.822
7.708
7.705
7.690
7.687
7.684
7.670
7.667
7.626
7.605
4.092
1.982
400 Hz, CDCl3
5ab
0.98
0.99
1.00
1.07
1.04
0.98
5.94
6.04
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

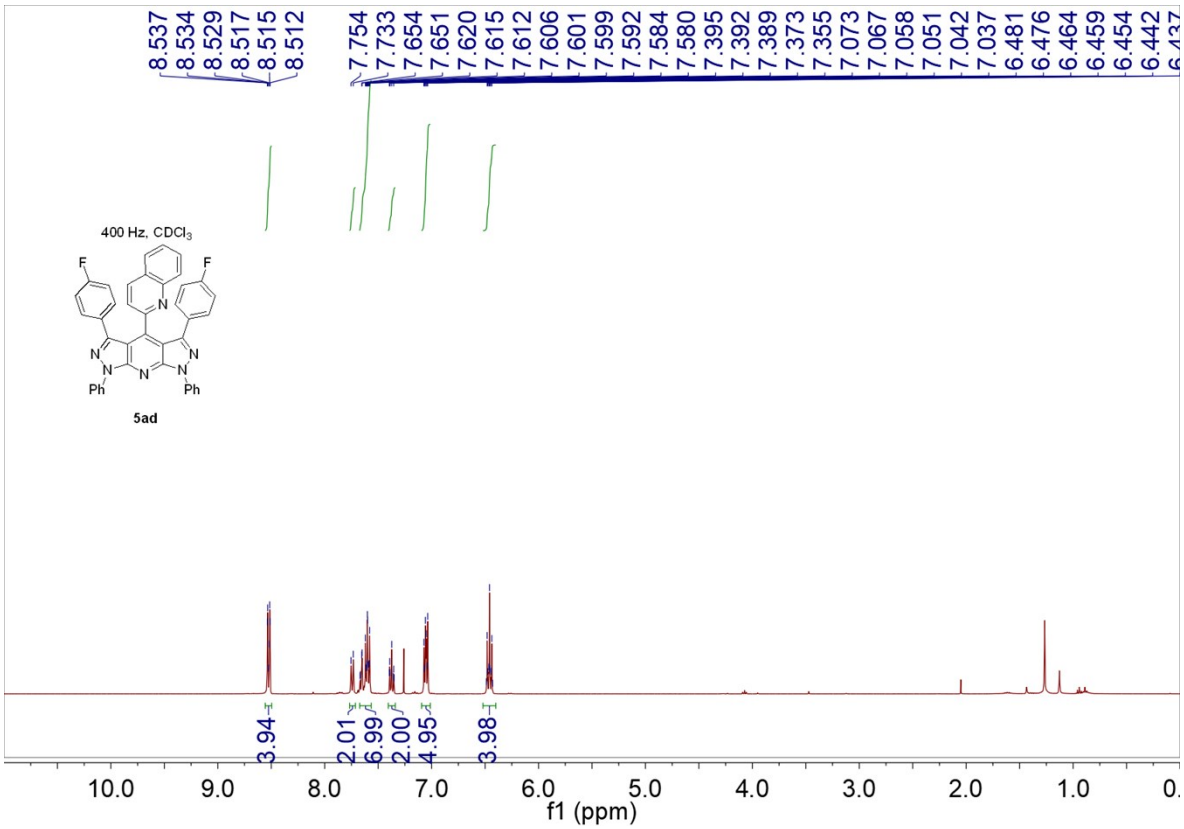

154.06
152.24
147.36
141.70
138.62
136.12
130.60
129.69
127.80
127.56
127.38
122.15
111.13
77.32
77.00
76.68
33.46
14.79
100 Hz, CDCl3
5ab
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

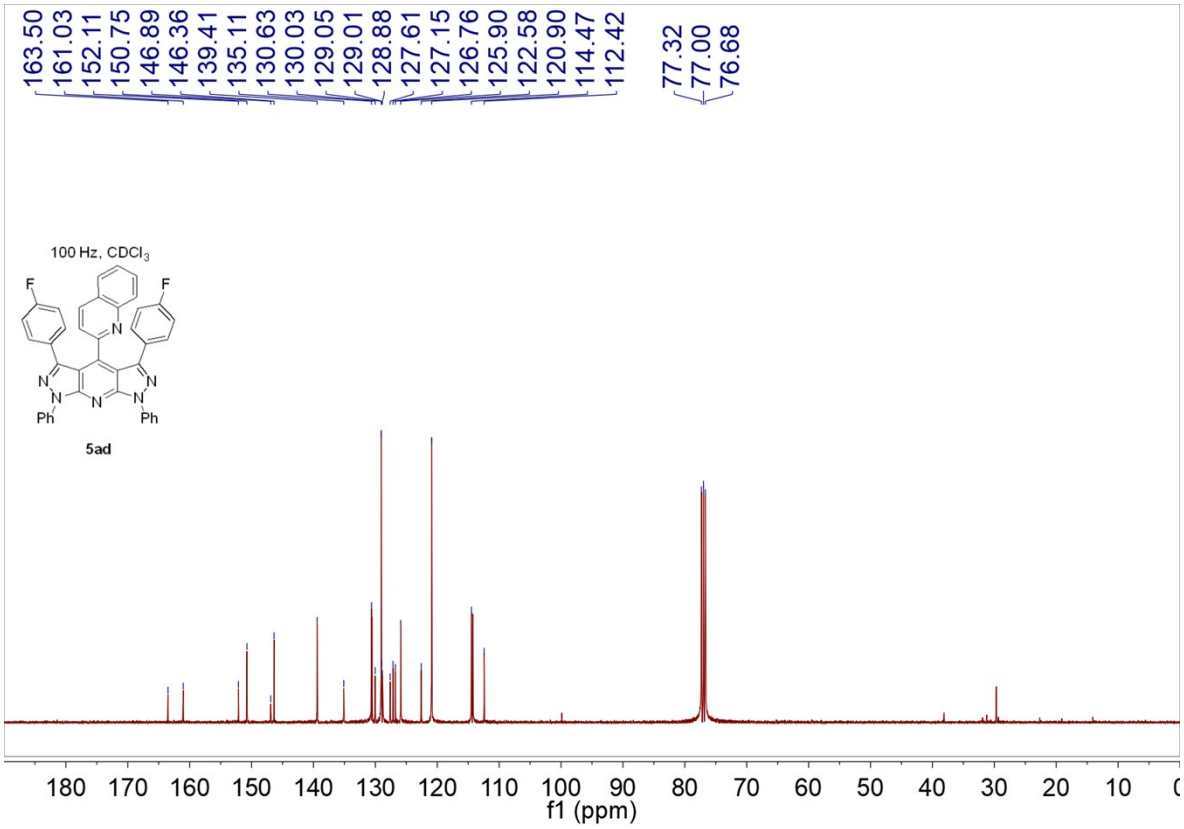

8.565
8.562
8.543
8.541
7.678
7.661
7.640
7.623
7.618
7.604
7.602
7.587
7.583
7.545
7.540
7.525
7.390
7.387
7.384
7.368
7.353
7.350
7.347
7.097
7.094
7.077
7.074
7.061
7.040
6.883
6.869
6.864
6.860
6.849
6.846
6.843
6.771
6.752
6.737
6.733
400 Hz, CDCl3
5ac
4.04
9.53
2.08
4.98
2.00
4.03
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)

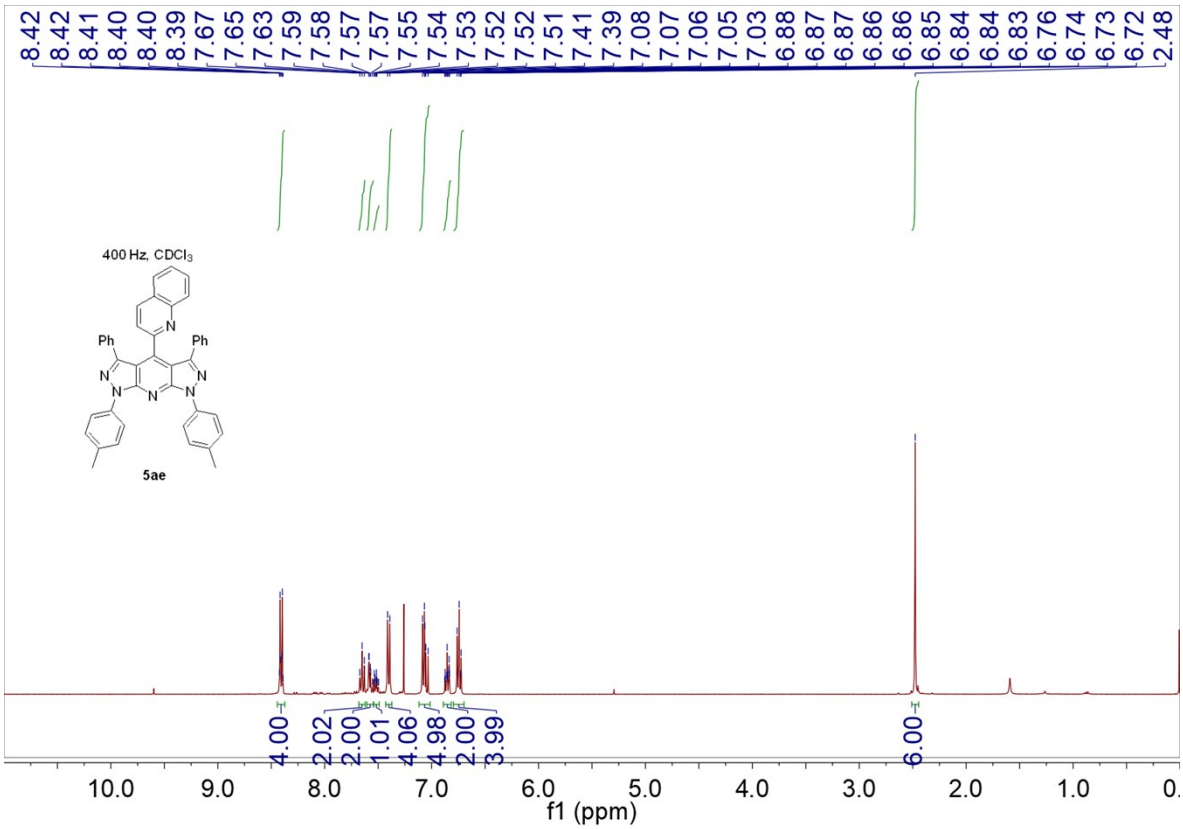

152.30
150.86
147.45
146.94
139.59
139.57
135.00
132.75
129.60
129.31
129.03
128.82
127.58
127.32
127.20
127.01
126.83
125.78
122.69
120.98
112.56
77.32
77.00
76.68
100 Hz, CDCl3
5ac
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

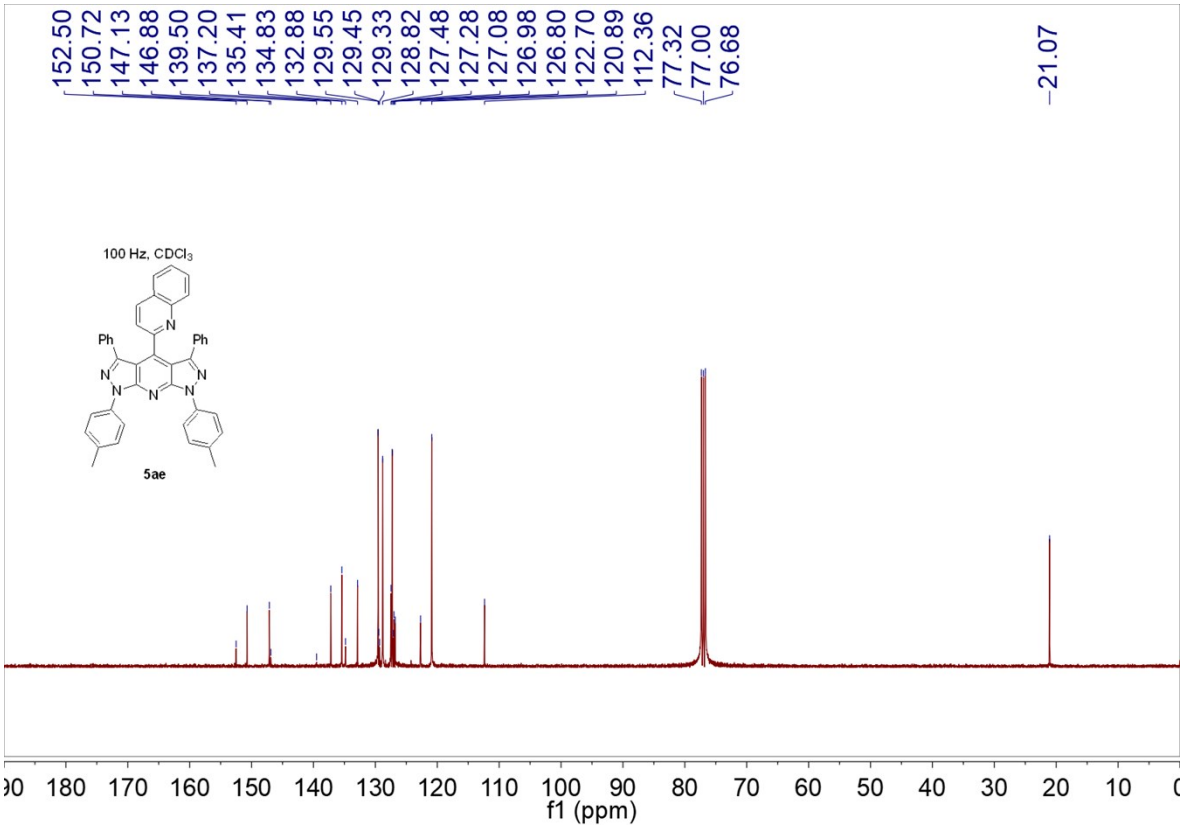

8.549
8.546
8.541
8.530
8.527
8.525
7.709
7.690
7.689
7.644
7.625
7.620
7.607
7.604
7.590
7.585
7.430
7.426
7.410
7.397
7.395
7.388
7.385
7.379
7.368
7.365
7.360
7.281
7.278
7.266
7.258
6.984
6.969
6.966
6.899
6.895
6.880
6.876
6.861
6.859
400 MHz, CDCl3
5oc
3.99
6.14
4.12
1.99
1.88
2.00
4.01
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)

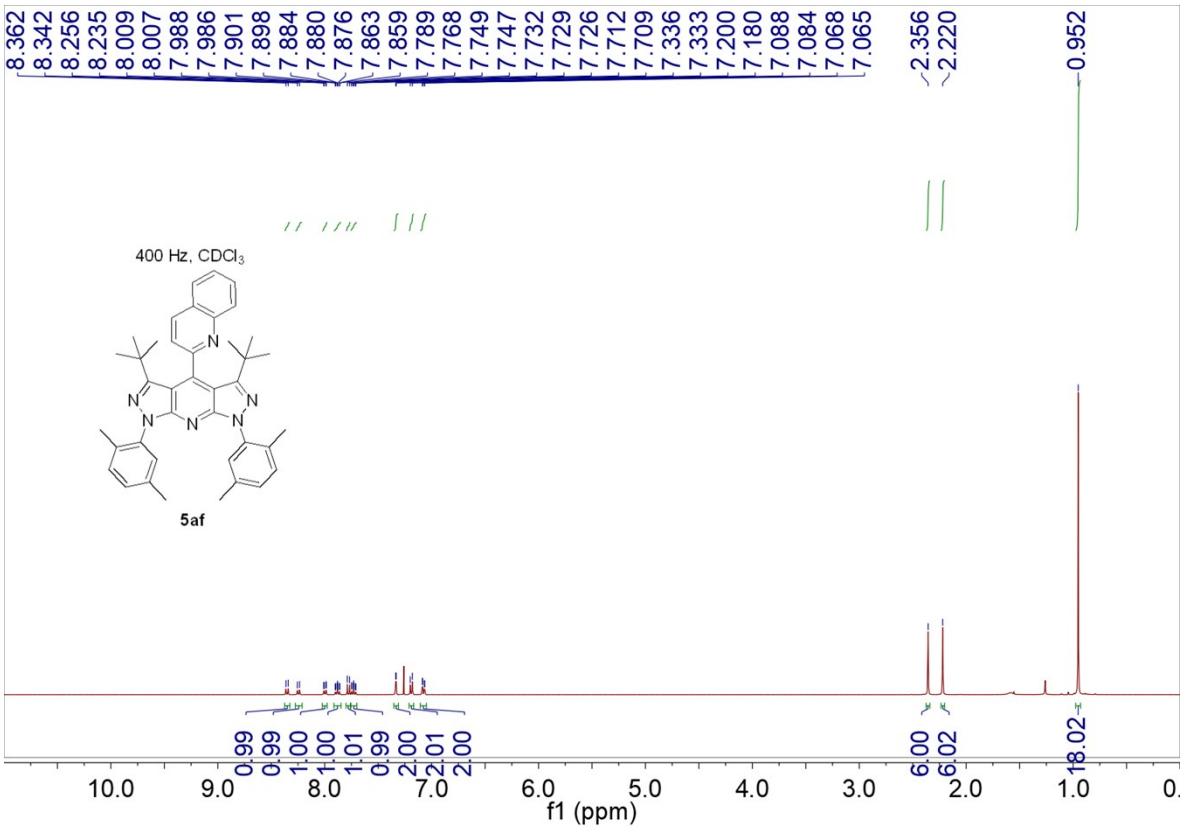

159.32
152.31
150.42
147.19
139.37
136.33
132.60
131.88
129.06
128.63
128.01
127.52
126.08
125.96
125.69
123.68
120.97
120.73
112.80
77.32
77.00
76.68
100 MHz, CDCl3
5oc
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

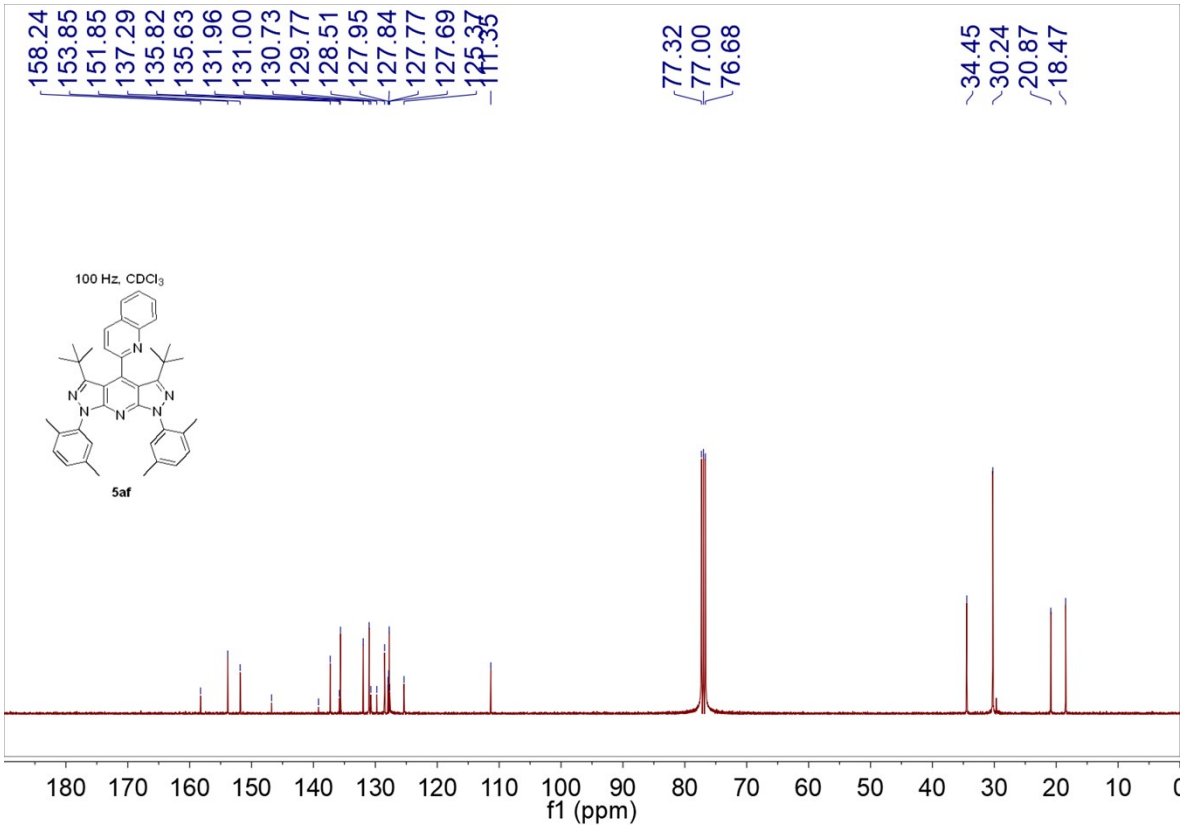

8.537
8.534
8.529
8.517
8.515
8.512
7.754
7.733
7.654
7.651
7.620
7.615
7.612
7.606
7.601
7.599
7.592
7.584
7.580
7.395
7.392
7.389
7.373
7.355
7.073
7.067
7.058
7.051
7.042
7.037
6.481
6.476
6.464
6.459
6.454
6.442
400 Hz, CDCl3
F
F
N
N
N
N
N
Ph
Ph
5ad
3.94
2.01
6.99
2.00
4.95
3.98
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)

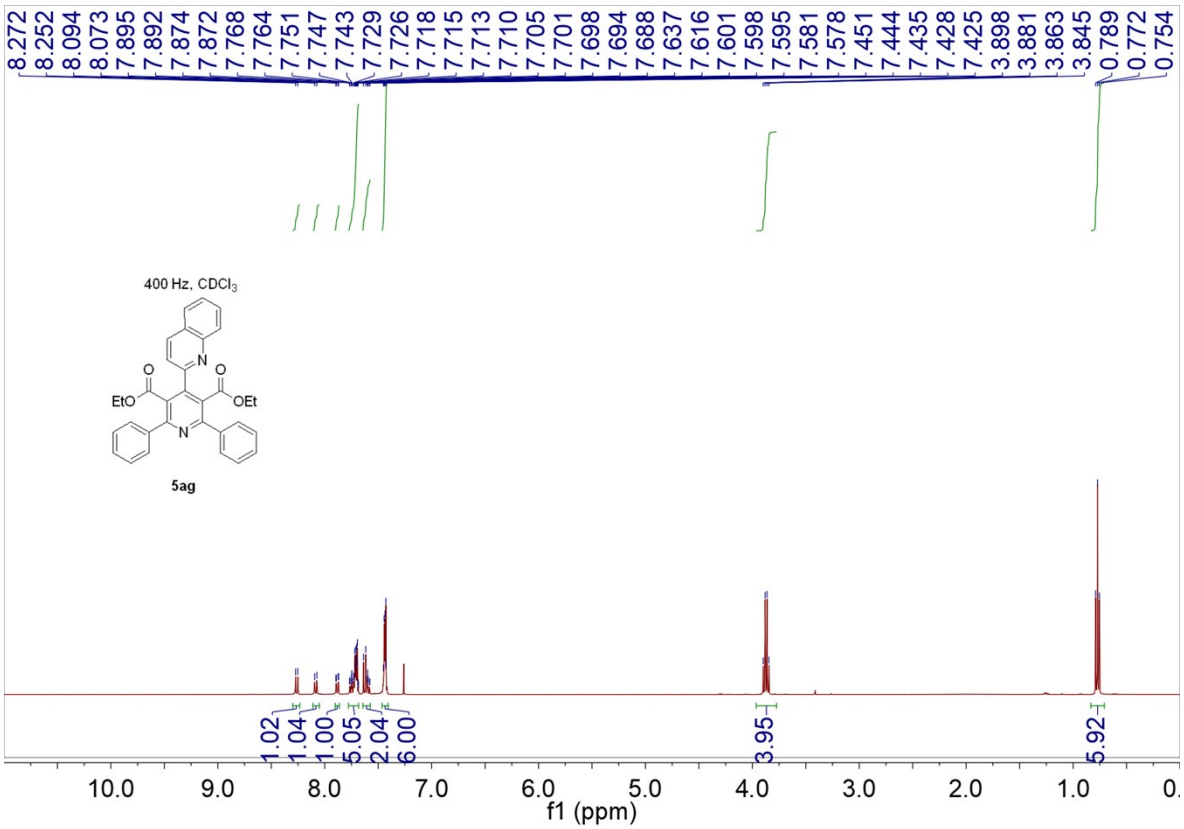

163.50
161.03
152.11
150.75
146.89
146.36
139.41
135.11
130.63
130.03
129.05
129.01
128.88
127.61
127.15
126.76
125.90
122.58
120.90
114.47
112.42
77.32
77.00
76.68
100 Hz, CDCl3
F
F
N
N
N
N
N
Ph
Ph
5ad
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.42 8.42 8.41 8.40 8.40 8.39 7.67 7.65 7.63 7.59 7.58 7.57 7.57 7.55 7.54 7.53 7.52 7.52 7.51 7.41 7.39 7.08 7.07 7.06 7.05 7.03 6.88 6.87 6.87 6.86 6.86 6.85 6.84 6.84 6.83 6.76 6.74 6.73 6.72 2.48
400 Hz, CDCl3
Ph
Ph
5ae
4.00 2.02 2.00 1.01 4.06 4.98 2.00 3.99 6.00
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0
f1 (ppm)


152.50 150.72 147.13 146.88 139.50 137.20 135.41 134.83 132.88 129.55 129.45 129.33 128.82 127.48 127.28 127.08 126.98 126.80 122.70 120.89 112.36 77.32 77.00 76.68
21.07
100 Hz, CDCl3
Ph
Ph
5ae
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


8.362
8.342
8.256
8.235
8.009
8.007
7.988
7.986
7.901
7.898
7.884
7.880
7.876
7.863
7.859
7.789
7.768
7.749
7.747
7.732
7.729
7.726
7.712
7.709
7.336
7.333
7.200
7.180
7.088
7.084
7.068
7.065
2.356
2.220
0.952
400 Hz, CDCl3
5af
0.99
0.99
1.00
1.00
1.01
0.99
2.00
2.01
2.00
6.00
6.02
18.02
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)


158.24
153.85
151.85
137.29
135.82
135.63
131.96
131.00
130.73
129.77
128.51
127.95
127.84
127.77
127.69
77.32
77.00
76.68
34.45
30.24
20.87
18.47
100 Hz, CDCl3
5af
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.272
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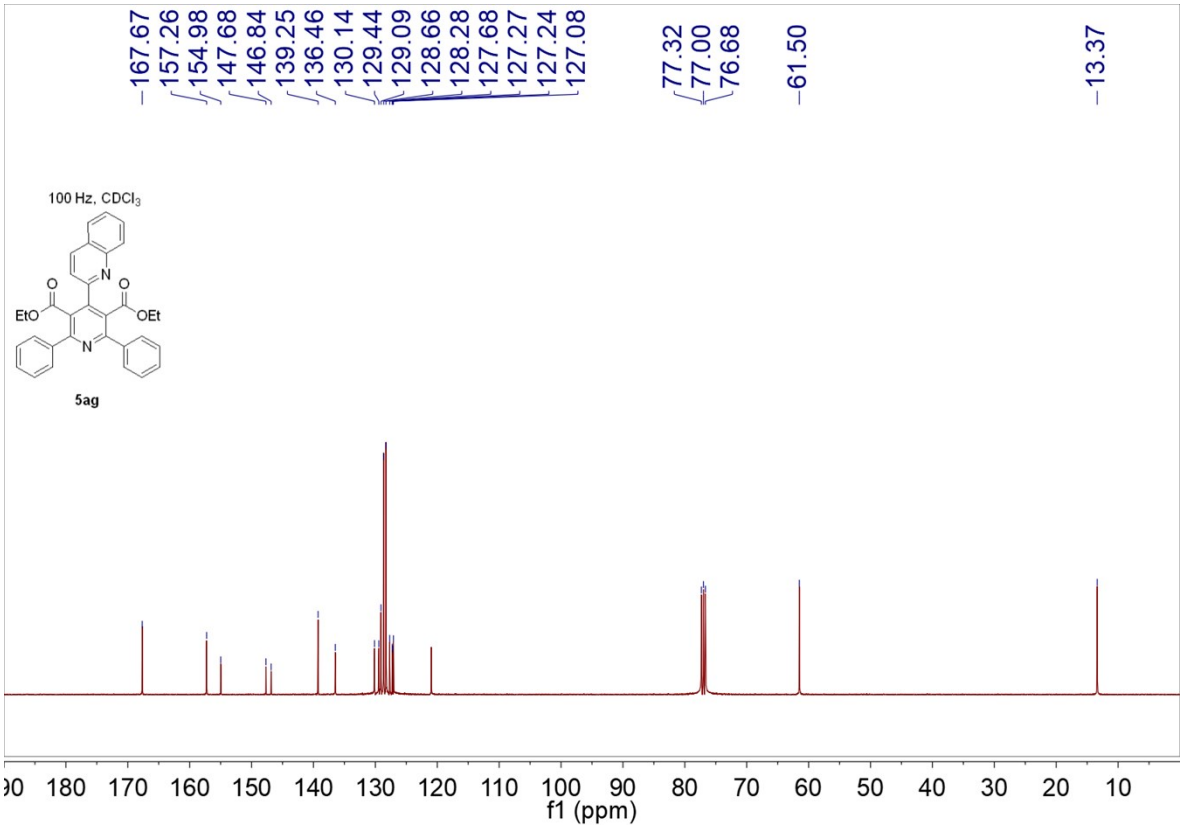
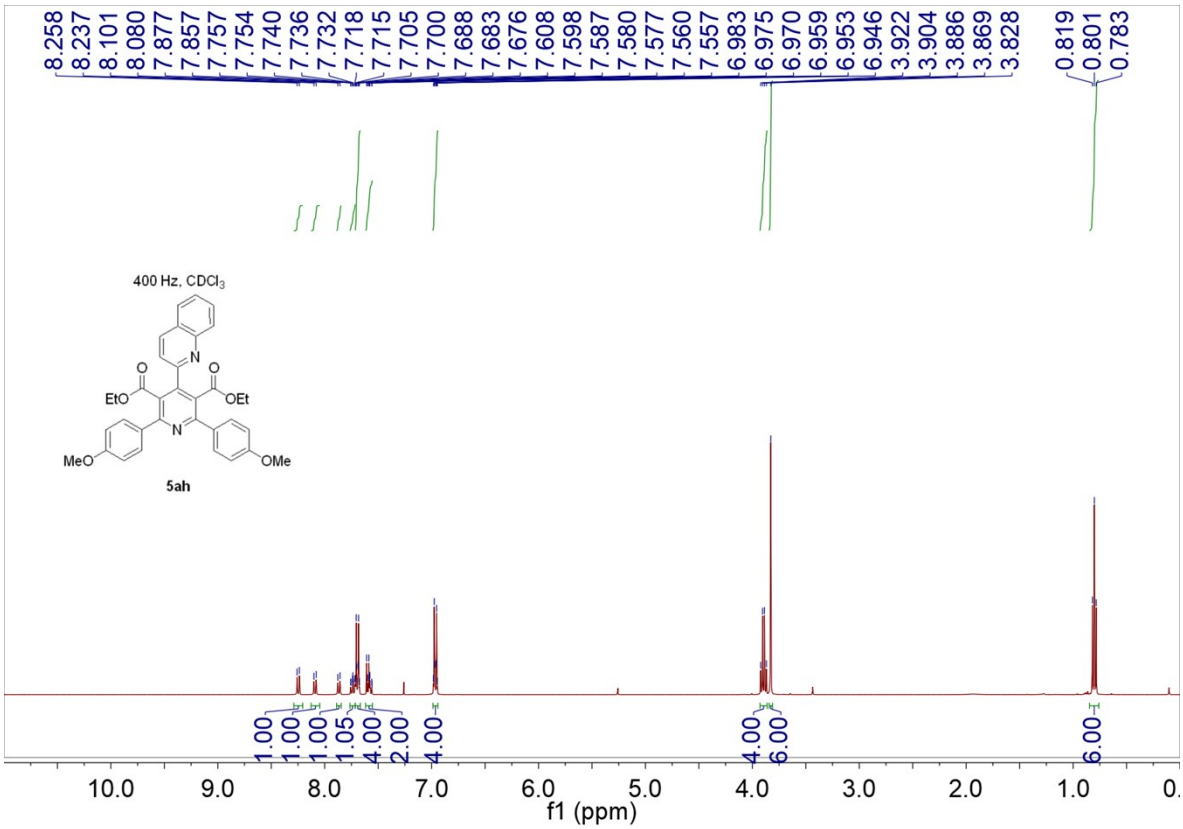
8.094
8.073
7.895
7.892
7.874
7.872
7.768
7.764
7.751
7.747
7.743
7.729
7.726
7.718
7.715
7.713
7.710
7.705
7.701
7.698
7.694
7.688
7.637
7.616
7.601
7.598
7.595
7.581
7.578
7.451
7.444
7.435
7.428
7.425
3.898
3.881
3.863
3.845
0.789
0.772
0.754
400 Hz, CDCl3
EtO
OEt
5ag
1.02
1.04
1.00
5.05
2.04
6.00
3.95
5.92
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)


167.67
157.26
154.98
147.68
146.84
139.25
136.46
130.14
129.44
129.09
128.66
128.28
127.68
127.27
127.24
127.08
77.32
77.00
76.68
61.50
13.37
100 Hz, CDCl3
EtO
OEt
5ag
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.258
8.237
8.101
8.080
7.877
7.857
7.757
7.754
7.740
7.736
7.732
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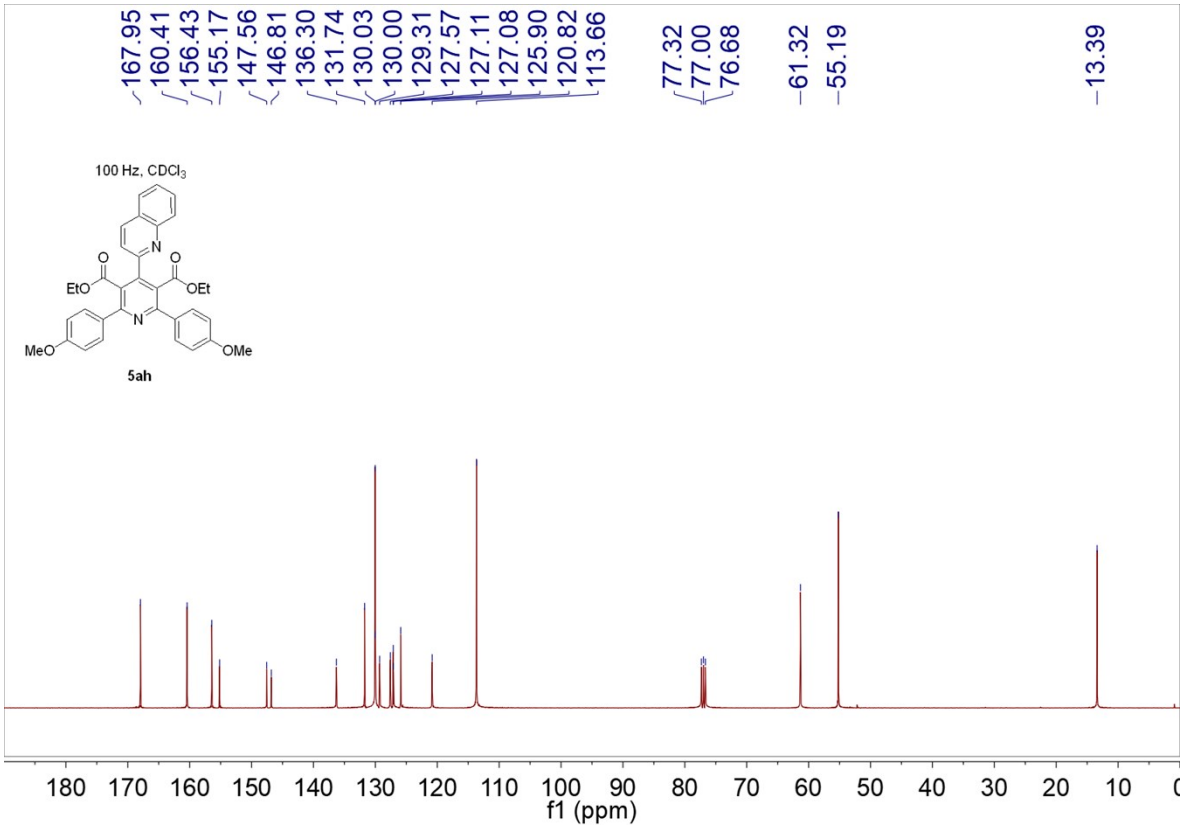
7.705
7.700
7.688
7.683
7.676
7.608
7.598
7.587
7.580
7.577
7.560
7.557
6.983
6.975
6.970
6.959
6.953
6.946
3.922
3.904
3.886
3.869
3.828
0.819
0.801
0.783
400 Hz, CDCl3
EtO
OEt
MeO
OMe
5ah
1.00
1.00
1.00
1.05
4.00
2.00
4.00
4.00
6.00
6.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)


167.95
160.41
156.43
155.17
147.56
146.81
136.30
131.74
130.03
130.00
129.31
127.57
127.11
127.08
125.90
120.82
113.66
77.32
77.00
76.68
61.32
55.19
13.39
100 Hz, CDCl3
EtO
OEt
MeO
OMe
5ah
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)