Supporting information

Oxidative C(sp3)–H functionalization of methyl-azaheteroarenes: a facile route to 1,2,4-triazolo[4,3-a]pyridines

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Contents

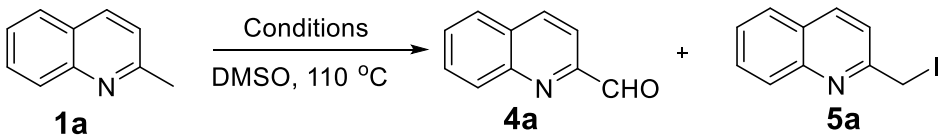
1. General information

Unless stated otherwise, all solvents and commercially available reagents were obtained from commercial suppliers and used without further purification. Aniline was distilled prior to use and stored under nitrogen. In addition petroleumether (b.p. 60-90 ºC), 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. TLC analysis was performed using pre-coated glass plates. Column chromatography was performed using silica gel (200-300 mesh). 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-spectrometric (HRMS) were obtained on an Apex-Ultra MS equipped with an electrospray source. Melting points were determined using SGW X-4 apparatus and not corrected.

2. Mechanism Investigation

Further experiments were conducted to understand the reaction mechanism of the transformation (Scheme S1-S3).

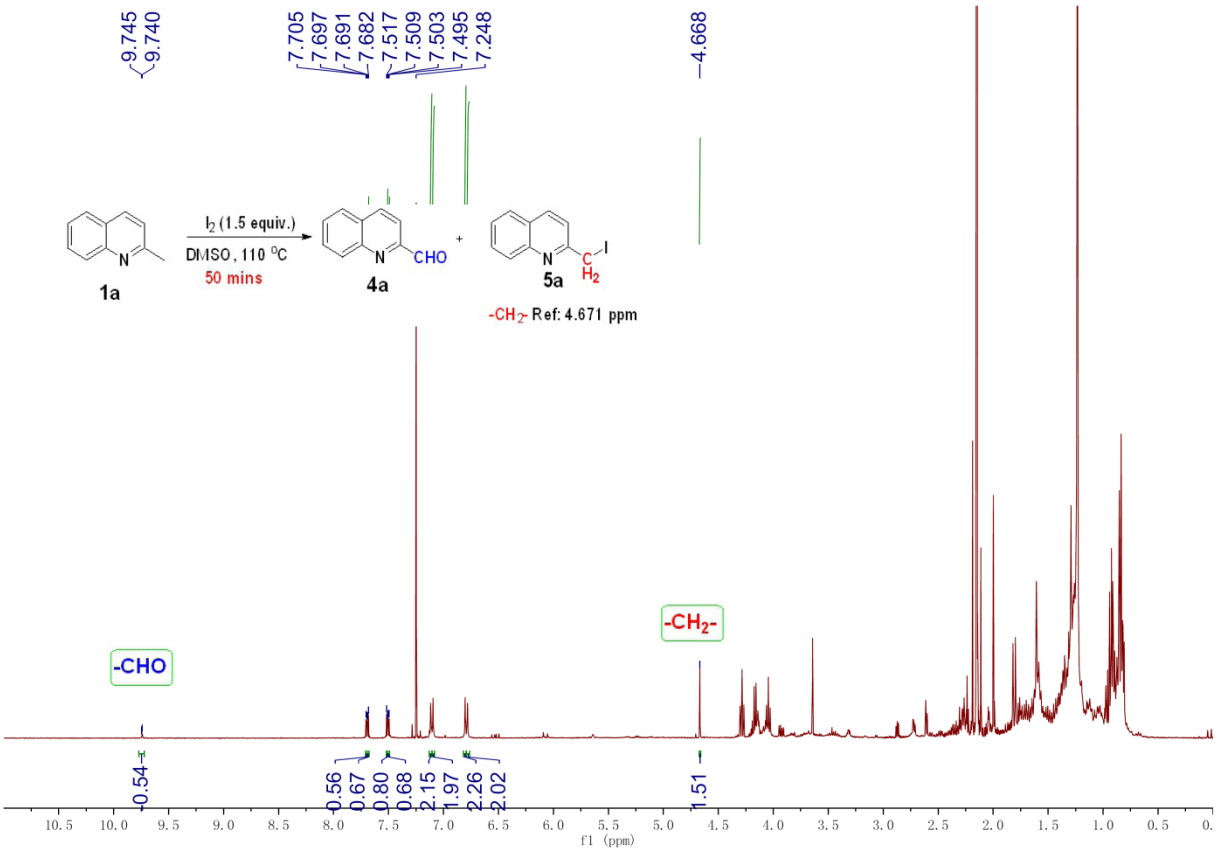
When 2-methylquinoline performed the reaction under standard conditions for 4 hours without 2-hydrazinylpyridine, it absolutely transferred to quinolin-2-carboxaldehyde in 86% isolated yield, whereas this reaction could not proceed any more without I_2 (Schme S1). If the reaction of 2-methylquinoline with iodine performed at 110 ºC in DMSO for only 50 mins, 2-(iodomethyl)quinoline and quinolin-2-carboxaldehyde could be detected in 52% and 38% yields, respectively (Scheme S1b). There results indicate that 2-(iodomethyl)quinoline and quinolin-2-carboxaldehyde are the potential intermediates in the reaction, and I_2 is very essential for this transformation. In addition, 2-(iodomethyl)quinoline could transfer to quinolin-2-carboxaldehyde with time under standard conditions.



standard conditions:
4 h, **4a**: 86% yield, **5a**: not detected (**1a** full conversion)
50 mins, **4a**: 38% yield, **5a**: 52% (**1a** full conversion)

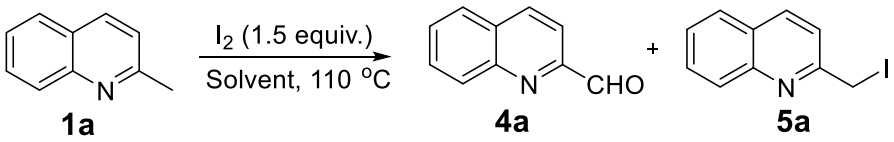
standard conditions, without I_2: **4a**: not detected, **5a**: not detected, (**1a** remain)

Scheme S1a 2-Methylquinoline **1a** reacted with iodine without 2-hydrazinylpyridine.



Scheme S1b The spectrum of products for the reaction of 2-methylquinoline **1a** with iodine without 2-hydrazinylpyridine for 50 mins.

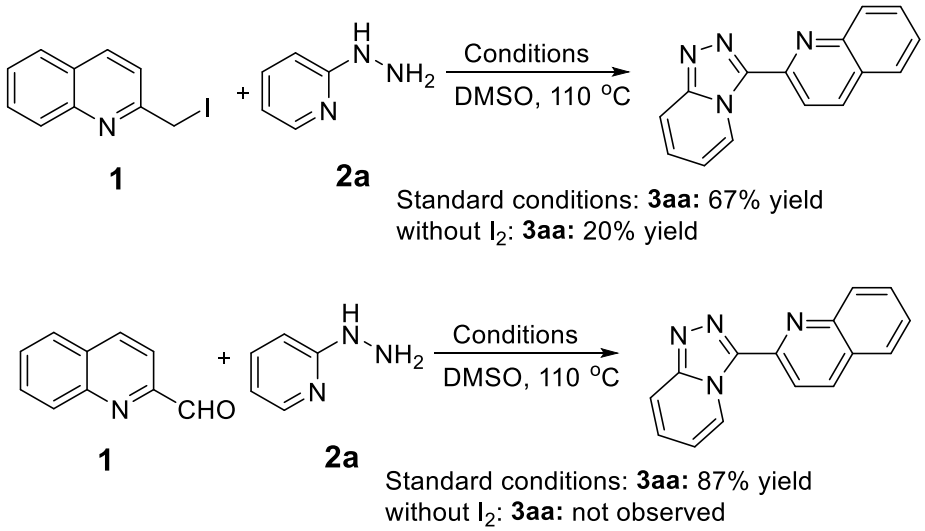
Giving the potential intermediate of 2-(iodomethyl)quinoline **5a**, the reactions of 2-methylquinoline **1a** with iodine were conducted in MeOH, Dioxane, MeCN and Toluene (Schme S2). Interestingly, 2-(iodomethyl)quinoline**4 a** could be observed, and quinolin-2-carboxaldehyde **5a** was not detected in these reactions. These results indicated that DMSO plays an important role in the transformation of 2-(iodomethyl)quinoline **5a** to quinolin-2-carboxaldehyde **4a**.



MeOH:	0	20%
Dioxane:	0	24%
MeCN:	0	54%
Toluene:	0	35%

Scheme S2 2-Methylquinoline **1a** reacted with iodine in different solvents.

2-(Iodomethyl)quinoline was also reacted with 2-hydrazinylpyridine under standard conditions, the desired product **3aa** was obtained in good yield (Schme S3). If no iodide was added, the reaction could generate **3aa** in 20% yield. Subsequently, the reaction of quinolin-2-carboxaldehyde with 2-hydrazinylpyridine was conducted under standard conditions, the product **3aa** could be generated in excellent yield. However, the reaction could not give the desired product without I_2. These results uncovered that I_2 may play an important role in the condensation steps of 2-(iodomethyl)quinoline and quinolin-2-carboxaldehyde with 2-hydrazinylpyridine.



Scheme S3. 2-(Iodomethyl)quinoline **5a** and quinolin-2-carboxaldehyde **4a** reacted with 2-hydrazinylpyridine **2a**.

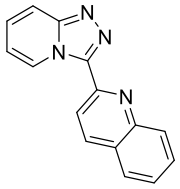
3. Triazolo[4,3-a]pyridin-3-yl)quinoline Synthesis and Characterization Date

3.1. General procedure for 2-([1,2,4]triazolo[4,3-a]pyridin-3-yl)quinoline synthesis

Standard procedure for the synthesis of 2-([1,2,4]triazolo[4,3-a]pyridin-3-yl)quinolines: A 25 mL pressure vial was charged with 2-methylquinoline (**1a**) (71.5 mg, 0.50 mmol, 1.0 equiv.), I_2 (190.4 mg, 0.75 mmol, 1.5 equiv.) and DMSO (3.0 mL). The vial was sealed and the resulting mixture was stirred at 110 °C for 4-6 h under an air atmosphere, after disappearance of the reactant (monitored by TLC), then added 2-hydrazinylpyridines (**2a**) (65.4 mg, 0.6 mmol, 1.2 equiv.) at 110 °C for another 4-6 h. After the reaction completed, cooled to room temperature, then added 50 mL water to the mixture, and extracted with EtOAc 3 times (3 × 50 mL). The extract was washed with 10% $Na_2S_2O_3$ solution (w/w), dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel to yield the corresponding product **3aa** as a brown solid (71% yield).

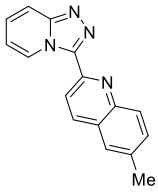
3.2. Characterization data for [1,2,4]triazolo[4,3-a]pyridin-3-yl)quinoline

2-([1,2,4]Triazolo[4,3-a]pyridin-3-yl)quinoline **(3aa)**



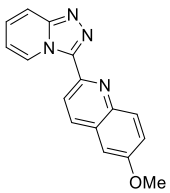
Brown solid, m.p.: 191-192 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 10.03 (d, J = 6.8 Hz, 1H), 8.55 (d, J = 8.4 Hz, 1H), 8.17 (d, J = 8.4 Hz, 1H), 8.03 (d, J = 8.4 Hz, 1H), 7.82 (d, J = 9.2 Hz, 1H), 7.75 (d, J = 8.0 Hz, 1H), 7.63 (t, J = 8.4 Hz, 1H), 7.46 (t, J = 7.6 Hz, 1H), 7.32 (t, J = 7.2 Hz, 1H), 6.95 (t, J = 6.8 Hz, 1H). ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 148.1, 147.0, 136.8, 129.9, 129.1, 128.1, 127.7, 127.6, 127.4, 127.1, 120.0, 116.0, 114.5. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{11}N_4$: 247.0978; found: 247.0991.

2-([1,2,4]Triazolo[4,3-a]pyridin-3-yl)-6-methylquinoline **(3ba)**



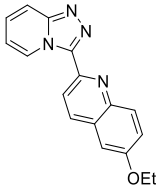
Brown solid, m.p.: 182-185 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 10.0 (dt, J = 1.2, 6.8 Hz, 1H), 8.50 (d, J = 8.8 Hz, 1H), 8.08 (t, J = 8.8 Hz, 1H), 7.93 (d, J = 8.0 Hz, 1H), 7.82 (dt, J = 1.2, 9.2 Hz, 1H), 7.49 (s, 1H), 7.47 (s, 1H), 7.25-7.33 (ddd, J = 1.2, 6.4, 9.2 Hz, 1H), 6.93-6.97 (dt, J = 1.2, 7.2 Hz, 1H), 2.48 (s, 3H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 147.2, 145.5, 137.2, 136.0, 132.1, 128.8, 127.9, 127.6, 127.3, 126.6, 119.9, 115.9, 114.3, 21.5, HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{13}N_4$: 261.1135; found: 261.1218.

2-([1,2,4]Triazolo[4,3-a]pyridin-3-yl)-6-methoxyquinoline **(3ca)**



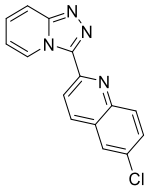
Brown solid, m.p.: 200-205 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 10.0 (dt, J = 1.2, 7.2 Hz, 1H), 8.50 (d, J = 8.8 Hz, 1H), 8.08 (d, J = 8.8 Hz, 1H), 7.94 (d, J = 9.2 Hz, 1H), 7.82 (dt, J = 1.2, 9.2 Hz, 1H), 7.30-7.34 (m, 2H), 7.01 (d, J = 2.8 Hz, 1H), 6.93-6.97 (dt, J = 1.2, 6.8 Hz, 1H), 3.90 (s, 3H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 158.2, 151.1, 145.7, 144.4, 143.0, 135.4, 130.5, 128.7, 127.9, 127.3, 122.6, 120.3, 115.9, 114.3, 105.3, 55.5, HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{13}N_4O$: 277.1084; found: 277.1099.

2-([1,2,4]Triazolo[4,3-a]pyridin-3-yl)-6-ethoxyquinoline **(3da)**



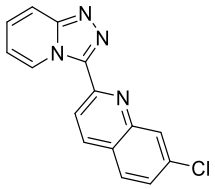
Offwhite solid, m.p.: 166-169 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 10.12 (dt, J = 1.2, 7.2 Hz, 1H), 8.58 (d, J = 8.4 Hz, 1H), 8.16 (d, J = 8.4 Hz, 1H), 8.05 (d, J = 9.6 Hz, 1H), 7.87 (dt, J = 1.2, 9.2 Hz, 1H), 7.35-7.41 (m, 2H), 7.09 (d, J = 2.8 Hz, 1H), 7.01 (dt, J = 1.2, 7.2 Hz, 1H), 4.18 (q, J = 7.2 Hz, 2H), 1.50 (t, J = 7.2 Hz, 3H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 157.9, 146.0, 143.2, 135.7, 130.8, 129.0, 128.0, 127.5, 123.1, 120.6, 116.2, 114.4, 106.2, 64.0, 14.8, HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{17}H_{15}N_4O$: 291.1240; found: 291.1255.

2-([1,2,4]Triazolo[4,3-a]pyridin-3-yl)-6-chloroquinoline **(3ea)**



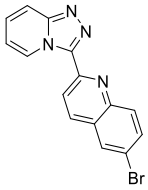
Brown solid, m.p.: 241-244 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 10.1 (dt, J = 1.2, 6.8 Hz, 1H), 8.68 (d, J = 8.8 Hz, 1H), 8.20 (d, J = 8.8 Hz, 1H), 8.10 (d, J = 9.2 Hz, 1H), 7.91 (dt, J = 1.2, 9.2 Hz, 1H), 7.84 (d, J = 2.0 Hz, 1H), 7.69 (dd, J = 2.4, 8.8 Hz, 1H), 7.40-7.44 (ddd, J = 1.2, 6.4, 9.2 Hz, 1H), 7.03-7.06 (dt, J = 1.2, 7.2 Hz, 1H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 151.5, 148.5, 145.5, 144.2, 135.9, 132.9, 131.0, 130.8, 128.2, 127.3, 126.6, 121.0, 116.2, 114.7. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{10}N_4Cl$: 281.0588; found: 281.0570.

2-([1,2,4]Triazolo[4,3-a]pyridin-3-yl)-7-chloroquinoline **(3fa)**



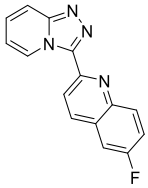
Brown solid, m.p.: 225-229 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 10.1 (dt, J = 1.2, 7.2 Hz, 1H), 8.63 (d, J = 8.4 Hz, 1H), 8.26 (d, J = 8.8 Hz, 1H), 8.17 (d, J = 3.2 Hz, 1H), 7.79 (d, J = 8.8 Hz, 2H), 7.52 (dd, J = 2.4, 8.8 Hz, 1H), 7.41-7.46 (dq, J = 1.2, 6.4 Hz, 1H), 7.06-7.09 (dt, J = 1.2, 6.8 Hz, 1H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 151.5, 147.6, 136.7, 136.0, 129.1, 129.0, 128.2, 127.4, 120.4, 116.2, 114.9, HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{10}N_4Cl$: 281.0588; found: 281.0577.

2-([1,2,4]Triazolo[4,3-a]pyridin-3-yl)-6-bromoquinoline **(3ga)**



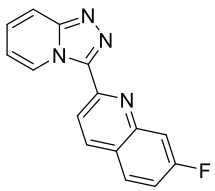
Yellow solid, m.p.: 236-237 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 10.8 (dt, J = 1.2, 6.8 Hz, 1H), 8.65 (d, J = 8.8 Hz, 1H), 8.17 (d, J = 8.8 Hz, 1H), 8.01 (s, 1H), 7.99 (s, 1H), 7.90 (dt, J = 1.2, 8.0 Hz, 1H), 7.80 (dt, J = 2.4, 8.8 Hz, 1H), 7.38-7.43 (ddd, J = 1.2, 6.8, 9.2 Hz, 1H), 7.03-7.06 (dt, J = 1.2, 6.8 Hz, 1H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 151.5, 148.6, 145.7, 135.8, 133.5, 130.8, 129.9, 128.7, 128.3, 127.3, 121.0, 116.2, 114.7. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{10}N_4Br$: 325.0083; found: 325.0091.

2-([1,2,4]Triazolo[4,3-a]pyridin-3-yl)-6-fluoroquinoline **(3ha)**



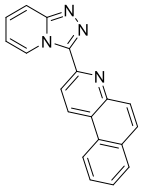
Brown solid, m.p.: 200-204 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 10.1 (dt, J = 1.2, 6.8 Hz, 1H), 8.64 (d, J = 8.8 Hz, 1H), 8.21 (d, J = 8.8 Hz, 1H), 8.12 (q, J = 5.2 Hz, 1H), 7.88 (dt, J = 1.2, 9.2 Hz, 1H), 7.48-7.53 (ddd, J = 1.2, 6.4, 9.2 Hz, 1H), 7.43-7.46 (dd, J = 2.8, 8.8 Hz, 1H), 7.37-7.41 (ddd, J = 1.2, 6.8, 9.2 Hz, 1H), 7.01-7.05 (dt, J = 1.2, 7.2 Hz, 1H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 162.0, 159.5, 151.4, 147.7, 144.2, 136.2 (d, J = 6.0 Hz, 2C), 131.6 (d, J = 9.0 Hz, 2C), 128.4 (d, J = 10.0 Hz, 2C), 128.2, 127.2, 120.9, 120.2 (d, J = 26.0 Hz, 2H), 115.4 (d, J = 150.0 Hz, 2C), 111.1 (d, J = 22 Hz, 2C), HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{10}N_4F$: 265.0884; found: 265.0897.

2-([1,2,4]Triazolo[4,3-a]pyridin-3-yl)-7-fluoroquinoline **(3ia)**



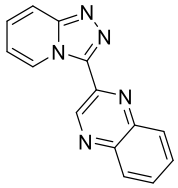
Yellow solid, m.p.: 213-216 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 10.10 (dt, J = 1.2, 7.2 Hz, 1H), 8.62 (d, J = 8.8 Hz, 1H), 8.27 (d, J = 8.8 Hz, 1H), 7.90 (dt, J = 1.2, 9.2 Hz, 1H), 7.76-7.86 (m, 2H), 7.33-7.43 (m, 2H), 7.06 (dt, J = 1.2, 7.2 Hz, 1H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 163.4 (d, J = 251 Hz, 2C), 151.5, 149.2, 148.1 (d, J = 12 Hz, 2C), 144.2, 136.8, 129.8 (d, J = 10 Hz, 2C), 128.3, 127.4, 124.7, 119.5, 117.5 (d, J = 25 Hz, 2C), 116.2, 114.7, 113.0 (d, J = 20 Hz, 2C), HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{10}N_4F$: 265.0884; found: 265.0890.

3-([1,2,4]Triazolo[4,3-a]pyridin-3-yl)benzo[f]quinoline **(3ja)**



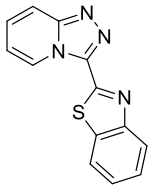
Gray solid, m.p.: 232-236 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 10.12 (dt, J = 1.2, 7.2 Hz, 1H), 9.01 (d, J = 9.2 Hz, 1H), 8.75 (d, J = 8.8 Hz, 1H), 8.60 (d, J = 8.4 Hz, 1H), 8.0 (br, 2H), 7.86-7.93 (m, 2H), 7.62-7.70 (m, 2H), 7.37 (dq, J = 1.2, 6.4 Hz, 1H), 7.01 (dt, J = 1.2, 6.8 Hz, 1H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 151.4, 147.1, 144.4, 131.6, 131.5, 129.4, 128.7, 128.0, 127.6, 127.4, 124.9, 122.8, 120.3, 116.1, 114.5, HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{19}H_{13}N_4$: 297.1135; found: 297.1146.

2-([1,2,4]Triazolo[4,3-a]pyridin-3-yl)quinoxaline **(3ka)**



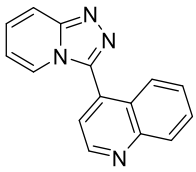
Yellow solid, m.p.: 181-185 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 8.66 (s, 1H), 8.64 (s, 1H), 8.52 (d, J = 8.4 Hz, 1H), 8.17 (q, J = 1.6 Hz, 1H), 8.15 (q, J = 1.6 Hz, 1H), 7.89 (dt, J = 2.0 Hz, 7.2 Hz, 1H), 7.78 (dt, J = 1.2, 8.4 Hz, 1H), 7.70 (dt, J = 1.2, 7.2 Hz, 1H), 7.22-7.25 (dd, J = 4.8, 7.2 Hz, 1H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 150.7, 148.7, 141.8, 141.2, 141.1, 138.3, 138.0, 136.5, 131.0, 129.9, 129.0, 128.4. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{14}H_{10}N_5$: 248.0931; found: 248.0952.

2-([1,2,4]Triazolo[4,3-a]pyridin-3-yl)benzo[d]thiazole **(3la)**



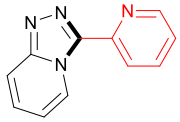
Yellow solid, m.p.: 93-95 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 9.73 (dt, J = 1.2, 7.2 Hz, 1H), 8.12 (dq, J = 0.8, 8.0 Hz, 1H), 7.98 (dq, J = 0.8, 8.4 Hz, 1H), 7.93 (dt, J = 1.2, 9.2 Hz, 1H), 7.52-7.57 (m, 1H), 7.43-7.49 (m, 2H), 7.12 (dt, J = 1.2, 6.8 Hz, 1H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 155.9, 153.5, 151.3, 134.3, 128.8, 126.6, 126.33, 126.26, 123.5, 121.9, 121.8, 116.3, 115.5, HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{13}H_9N_4S$: 253.0542; found: 253.0547.

4-([1,2,4]Triazolo[4,3-a]pyridin-3-yl)quinoline **(3ma)**



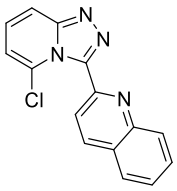
Yellow solid, m.p.: 182-185 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 9.11 (d, J = 4.8 Hz, 1H), 8.26 (d, J = 8.4 Hz, 1H), 7.91-7.95 (m, 3H), 7.82 (dt, J = 1.2, 8.4 Hz, 1H), 7.68 (d, J = 4.4 Hz, 1H), 7.59 (dt, J = 1.2, 8.4 Hz, 1H), 7.35-7.39 (m, 1H), 6.88 (dt, J = 1.2, 7.2 Hz, 1H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 149.9, 146.1, 132.1, 130.40, 130.34, 128.1, 127.8, 125.7, 125.3, 122.7, 121.8, 117.0, 114.7, HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{11}N_4$: 247.0978; found: 247.0985.

3-(pyridin-2-yl)-[1,2,4]triazolo[4,3-a]pyridine **(3pa)**



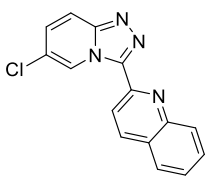
White solid, m.p.: 130-132 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 9.82 (dt, J = 1.2, 7.2 Hz, 1H), 8.69 (dq, J = 1.2, 4.8 Hz, 1H), 8.52 (dt, J = 1.2, 8.0 Hz, 1H), 7.84-7.88 (m, 2H), 7.32-7.37 (m, 2H), 6.95 (t, J = 7.2 Hz, 1H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 148.6, 148.3, 137.0, 127.9, 127.1, 123.6, 122.7, 116.0, 114.3, HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{11}H_9N_4$:197.0827; found: 197.0832.

2-(5-Chloro-[1,2,4]triazolo[4,3-a]pyridin-3-yl)quinoline **(3ab)**



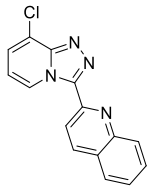
Green solid, m.p.: 158-161 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 8.33 (d, J = 8.4 Hz, 1H), 8.14 (d, J = 8.4 Hz, 1H), 7.96 (d, J = 8.4 Hz, 1H), 7.92 (d, J = 8.4 Hz, 1H), 7.84 (dd, J = 1.2, 9.2 Hz, 1H), 7.78 (dt, J = 1.2, 8.0 Hz, 1H), 7.63 (dt, J = 1.2, 8.0 Hz, 1H), 7.27 (q, J = 7.2 Hz, 1H), 6.92 (dd, J = 1.2, 8.8 Hz, 1H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 152.0, 147.7, 147.0, 146.7, 136.5, 130.3, 129.7, 128.1, 127.79, 127.77, 126.4, 123.1, 115.6, 115.2, HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{10}N_4Cl$: 281.0588; found: 281.0598.

2-(6-Chloro-[1,2,4]triazolo[4,3-a]pyridin-3-yl)quinoline **(3ac)**



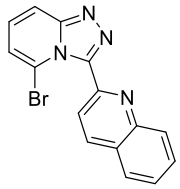
Brown solid, m.p.: 215-217 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 10.31 (q, J = 1.2 Hz, 1H), 8.63 (d, J = 8.8 Hz, 1H), 8.32 (d, J = 8.8 Hz, 1H), 8.21 (d, J = 8.4 Hz, 1H), 7.87 (t, J = 8.4 Hz, 2H), 7.79 (dt, J = 1.2, 8.4 Hz, 1H), 7.61 (dt, J = 1.2, 8.0 Hz, 1H), 7.37 (dd, J = 2.0, 9.6 Hz, 1H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 147.8, 147.1, 137.2, 130.2, 129.8, 129.3, 127.9, 127.8, 127.5, 125.2, 123.1, 120.0, 116.4, HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{10}N_4Cl$: 281.0588; found: 281.0596.

2-(8-Chloro-[1,2,4]triazolo[4,3-a]pyridin-3-yl)quinoline **(3ad)**



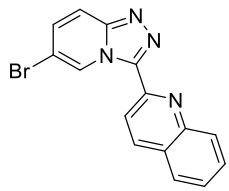
Brown solid, m.p.: 211-214 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 10.09 (dd, J = 1.2, 7.2 Hz, 1H), 8.62 (d, J = 8.4Hz, 1H), 8.27 (dd, J = 1.2, 8.8 Hz, 1H), 8.11 (dt, J = 1.2, 8.4 Hz, 1H), 7.83 (dd, J = 1.6, 8.4 Hz, 1H), 7.74 (dt, J = 1.2, 8.4 Hz, 1H), 7.56 (dt, J = 1.2, 8.4 Hz, 1H), 7.42 (dd, J = 1.2, 8.8 Hz, 1H), 6.96 (t, J = 7.2 Hz, 1H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 149.3, 147.7, 147.0, 145.7, 136.9, 130.1, 129.2, 127.8, 127.3, 126.9, 126.1, 122.1, 120.1, 114.3, HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{10}N_4Cl$: 281.0588; found: 281.0590.

2-(5-Bromo-[1,2,4]triazolo[4,3-a]pyridin-3-yl)quinoline **(3ae)**



Brown solid, m.p.: 203-206 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 8.31 (d, J = 8.4 Hz, 1H), 8.12 (dq, J = 0.8, 8.4 Hz, 1H), 7.92 (s, 1H), 7.90(s, 1H), 7.84 (dd, J = 1.2, 9.2 Hz, 1H), 7.75 (dt, J = 1.6, 8.8 Hz, 1H), 7.60 (dt, J = 1.2, 8.0 Hz, 1H), 7.16 (d, J = 7.2 Hz, 1H), 7.09 (dd, J = 1.2, 7.2 Hz, 1H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 151.8, 147.6, 147.2, 146.8, 136.4, 130.3, 129.6, 128.2, 127.8, 127.7, 123.2, 120.3, 115.6, 112.9, HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{10}N_4Br$: 325.0083; found: 325.0090.

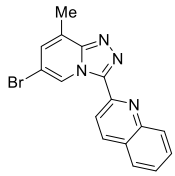
2-(6-Bromo-[1,2,4]triazolo[4,3-a]pyridin-3-yl)quinoline **(3af)**



Brown solid, m.p.: 218-220 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 10.40 (d, J = 2.8 Hz, 1H), 8.62 (d, J = 8.4 Hz, 1H), 8.31 (d, J = 9.2 Hz, 1H), 8.20 (d, J = 9.2 Hz, 1H), 7.87 (d, J = 8.4 Hz, 1H), 7.76-7.82 (m, 2H), 7.60 (t, J = 8.4 Hz, 1H), 7.46 (dd, J = 1.6, 9.6 Hz, 1H), ^{13}C-

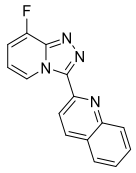
NMR (100 MHz, $CDCl_3$): δ (ppm) 147.8, 147.1, 137.1, 131.8, 130.2, 129.3, 127.87, 127.82, 127.5, 127.4, 120.0, 116.6, 109.8, HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{10}N_4Br$: 325.0083; found: 325.0095.

2-(6-Bromo-8-methyl-[1,2,4]triazolo[4,3-a]pyridin-3-yl)quinoline **(3ag)**



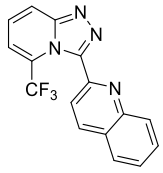
Brown solid, m.p.: 241-243 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 10.26 (q, J = 0.8 Hz, 1H), 8.63 (d, J = 8.8 Hz, 1H), 8.30 (d, J = 8.8 Hz, 1H), 8.20 (d, J = 8.4 Hz, 1H), 7.87 (dd, J = 1.2, 8.4 Hz, 1H), 7.78 (dt, J = 1.2, 8.4 Hz, 1H), 7.60 (dt, J = 1.2, 8.4 Hz, 1H), 7.26 (t, J = 1.2 Hz, 1H), 2.76 (s, 3H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 150.4, 147.8, 147.1, 137.1, 130.4, 130.2, 129.3, 127.9, 127.8, 127.5, 127.4, 125.0, 120.1, 110.0, 99.9, 16.8, HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{12}N_4Br$: 339.0240; found: 339.0251.

2-(8-Fluoro-[1,2,4]triazolo[4,3-a]pyridin-3-yl)quinoline **(3ah)**



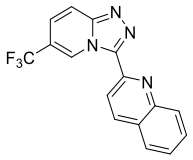
Yellow solid, m.p.: 198-201 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 10.03 (dd, J = 0.8, 7.2 Hz, 1H), 8.67 (d, J = 8.8 Hz, 1H), 8.32 (d, J = 8.8 Hz, 1H), 8.17 (d, J = 8.4 Hz, 1H), 7.88 (dd, J = 1.2, 8.4 Hz, 1H), 7.78 (dt, J = 1.2, 8.4 Hz, 1H), 7.61 (dt, J = 1.2, 8.4 Hz, 1H), 7.07-7.11 (m, 1H), 6.97-7.01 (dt, J = 4.4, 7.2 Hz, 1H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 151.3, 148.8, 147.5 (d, J = 248 Hz, 2C), 137.1, 130.2, 129.3, 127.9, 127.5, 123.9 (d, J = 24 Hz, 2C), 120.3, 113.9 (d, J = 24 Hz, 2C), 110.2 (d, J = 60 Hz, 2C), HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{10}N_4F$: 265.0884; found: 265.0896.

2-(5-(Trifluoromethyl)-[1,2,4]triazolo[4,3-a]pyridin-3-yl)quinoline **(3ai)**



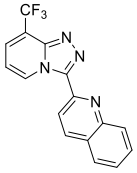
Yellow solid, m.p.: 189-191 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 8.38 (dd, J = 1.2, 8.8 Hz, 1H), 8.10 (t, J = 8.4 Hz, 2H), 7.94 (d, J = 8.4 Hz, 2H), 7.79 (dt, J = 2.4, 7.2 Hz, 1H), 7.65 (dt, J = 1.2, 8.4 Hz, 1H), 7.40-7.43 (m, 2H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 151.3, 147.2, 137.1, 130.3, 129.5, 128.0, 127.8, 126.4 (d, J = 37 Hz, 2C), 125.7, 121.7 (d, J = 202 Hz, 2C), 118.5, 117.0 (q, J = 6.0 Hz, 4C), HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{10}N_4F_3$: 315.0852; found: 315.0861.

2-(6-(Trifluoromethyl)-[1,2,4]triazolo[4,3-a]pyridin-3-yl)quinoline **(3aj)**



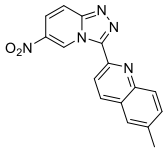
Brown solid, m.p.: 207-210 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 8.65 (s, 1H), 8.64 (d, J = 8.8 Hz, 1H), 8.34 (d, *J* = 8.8 Hz, 1H), 8.16 (d, *J* = 8.4 Hz, 1H), 8.00 (d, *J* = 9.2 Hz, 1H), 7.88 (dd, *J* = 1.2, 8.4 Hz, 1H), 7.79 (dt, *J* = 1.2, 8.4 Hz, 1H), 7.61 (dt, *J* = 1.2, 8.0 Hz, 1H), 7.53 (dd, *J* = 1.6, 9.2 Hz, 1H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 150.7, 147.3 (d, *J* = 176 Hz, 2C), 145.2, 137.3, 129.9 (d, *J* = 420 Hz, 2C), 127.9, 127.7, 127.3, 127.2, 124.5 (q, *J* = 12 Hz, 4C), 124.07, 124.04, 120.0, 119.0 (d, *J* = 136 Hz, 2C), 117.2, HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{10}N_4F_3$: 315.0852; found: 315.0864.

2-(8-(Trifluoromethyl)-[1,2,4]triazolo[4,3-a]pyridin-3-yl)quinoline **(3ak)**



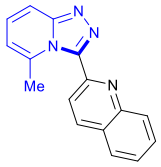
Yellow solid, m.p.: 74-77 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 10.40 (d, *J* = 7.2 Hz, 1H), 8.69 (d, *J* = 8.8 Hz, 2H), 8.33 (d, *J* = 8.8 Hz, 1H), 8.18 (dd, *J* = 0.8, 8.4 Hz, 1H), 7.89 (dd, *J* = 1.6, 8.4 Hz, 1H), 7.74-7.81 (m, 1H), 7.62 (dt, *J* = 1.2, 8.0 Hz, 1H), 7.14 (t, *J* = 7.2 Hz, 1H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 147.4 (d, *J* = 248 Hz, 2C), 145.1, 137.2, 130.9 , 130.2, 129.3, 127.8 (d, *J* = 152 Hz, 2C), 126.7 (q, *J* = 20 Hz, 4C), 123.5, 120.8, 120.4, 118.6 (d, *J* = 140 Hz, 2C), 113.0, HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{10}N_4F_3$: 315.0852; found: 315.0868.

6-Methyl-2-(6-nitro-[1,2,4]triazolo[4,3-a]pyridin-3-yl)quinoline **(3bl)**



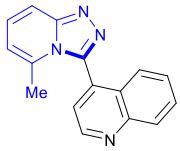
Yellow solid, m.p.: 56-67 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 7.80 (d, *J* = 8.8 Hz, 1H), 7.96 (s, 1H), 7.92 (d, *J* = 8.8 Hz, 1H), 7.90 (d, *J* = 8.8 Hz, 1H), 7.50-7.54 (m, 2H), 5.85 (s, 2H), 2.51 (s, 3H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 153.7, 153.2, 146.3, 143.1, 136.5, 135.5, 131.9, 128.7, 127.9, 126.59, 126.57, 121.5, 117.7, 21.6, HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{12}N_5O_2$: 306.0986; found:306.0995.

2-(5-Methyl-[1,2,4]triazolo[4,3-a]pyridin-3-yl)quinoline **(3am)**



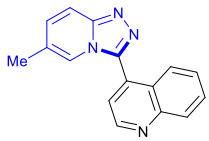
Yellow solid, m.p.: 182-184 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 8.30 (d, J = 8.4 Hz, 1H), 8.10 (t, J = 8.4 Hz, 1H), 8.08 (s, 1H), 7.89 (d, J = 8.4 Hz, 1H), 7.72-7.75 (m, 2H), 7.60 (dt, J = 1.2, 8.0 Hz, 1H), 7.23 (t, J = 6.8 Hz, 1H), 6.63 (dt, J = 0.4, 6.8 Hz, 1H)2.45 (s, 3H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 152.0, 148.5, 147.0, 146.8, 136.6, 136.2, 130.3, 129.3, 128.1, 127.8, 127.6, 127.5, 123.2, 115.0, 114.0, 21.9, HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{13}N_4$: 261.1135; found:261.1147.

4-(5-Methyl-[1,2,4]triazolo[4,3-a]pyridin-3-yl)quinoline **(3mm)**



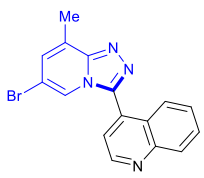
Yellow solid, m.p.: 175-177 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 9.06 (d, J = 8.0 Hz, 1H), 8.23 (d, J = 8.4 Hz, 1H), 7.75-7.82 (m, 2H), 7.61 (d, J = 4.4 Hz, 1H), 7.52 (dt, J = 1.2, 8.0 Hz, 1H), 7.24-7.32 (m, 2H), 6.56 (d, J = 6.8 Hz, 1H), 1.95 (s, 3H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 149.2, 147.9, 143.1, 136.1, 134.6, 130.3, 130.0, 128.4, 128.1, 125.4, 124.1, 114.84, 114.78, 19.7, HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{13}N_4$: 261.1135; found:261.1144.

4-(6-Methyl-[1,2,4]triazolo[4,3-a]pyridin-3-yl)quinoline **(3mn)**



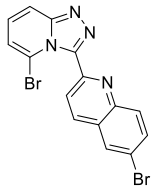
Yellow solid, m.p.: 168-170 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 8.91 (d, J = 4.8 Hz, 1H), 8.55 (d, J = 8.4 Hz, 1H), 8.33 (s, 1H), 8.13 (t, J = 8.4 Hz, 1H), 8.01 (s, 1H), 7.75 (d, J = 4.4 Hz, 1H), 7.61-7.64 (m, 1H), 7.52 (dd, J = 2.0, 8.4 Hz, 1H), 7.38 (d, J = 8.8 Hz, 1H), 2.28 (s, 3H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 150.0, 148.9, 146.9, 139.5, 138.4, 134.4, 130.2, 129.4, 127.0, 125.9, 125.1,123.7, 118.3, 107.6, 17.6, HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{13}N_4$: 261.1135; found:261.1138.

4-(6-Bromo-8-methyl-[1,2,4]triazolo[4,3-a]pyridin-3-yl)quinoline **(3mg)**



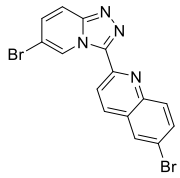
Brown solid, m.p.: 220-222 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 9.12 (d, J = 8.4 Hz, 1H), 8.27 (d, J = 8.4 Hz, 1H), 7.92 (t, J = 0.4 Hz, 1H), 7.90 (d, J = 0.4 Hz, 1H), 7.83 (dt, J = 1.2, 7.2 Hz, 1H), 7.65 (d, J = 4.4, 1H), 7.61 (dt, J = 1.2, 8.4 Hz, 1H), 7.20 (t, J = 1.2 Hz, 1H), 2.77 (s, 3H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 150.1, 149.7, 148.8, 143.7, 132.0, 130.6, 130.2, 129.7, 128.7, 128.3, 125.7, 125.2, 121.7, 120.2, 110.2, 16.7, HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{12}N_4Br$: 339.0240; found: 339.0248.

6-Bromo-2-(5-bromo-[1,2,4]triazolo[4,3-a]pyridin-3-yl)quinoline **(3ge)**



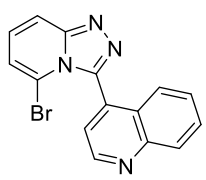
Brown solid, m.p.: 193-196 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 8.24 (dd, J = 1.2, 8.4 Hz, 1H), 8.08 (d, J = 2.8 Hz, 1H), 8.00 (d, J = 9.2 Hz, 1H), 7.96 (d, J = 8.4 Hz, 1H), 7.87 (dd, J = 0.8, 8.8 Hz, 1H), 7.84 (dd, J = 2.4, .2 Hz, 1H), 7.22 (q, J = 8.4 Hz, 1H), 7.13 (dd, J = 1.2, 7.2 Hz, 1H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 152.0, 148.0, 147.0, 145.4, 135.4, 133.9, 131.3, 129.8, 128.8, 128.3, 124.2, 121.9, 120.5, 115.7, 112.9, HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_9N_4Br_2$: 402.9188; found: 402.9199.

6-Bromo-2-(6-bromo-[1,2,4]triazolo[4,3-a]pyridin-3-yl)quinoline **(3gf)**



Yellow solid, m.p.: 290-293 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 10.33 (q, J = 0.8 Hz, 1H), 8.66 (d, J = 8.8 Hz, 1H), 8.24 (d, J = 8.4 Hz, 1H), 8.08 (d, J = 8.8 Hz, 1H), 8.04 (d, J = 2.0 Hz, 1H), 7.86 (dd, J = 2.4, 8.8 Hz, 1H), 7.82 (dd, J = 1.2, 9.6 Hz, 1H), 7.49 (dd, J = 1.6, 9.6 Hz, 1H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 148.2, 145.8, 136.2, 133.8, 132.0, 131.0, 128.9, 127.4, 121.5, 121.0, 116.8, 110.1, HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_9N_4Br_2$: 402.9188; found: 402.9196.

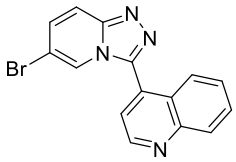
4-(5-Bromo-[1,2,4]triazolo[4,3-a]pyridin-3-yl)quinoline **(3me)**



Yellow solid, m.p.: 195-200 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 9.03 (d, J = 4.4 Hz, 1H), 8.20 (d, J = 8.4 Hz, 1H), 7.91 (dd, J = 0.8, 9.2 Hz, 1H), 7.75 (dt, J = 1.2, 6.8 Hz, 1H), 7.59 (d, J = 4.4 Hz, 1H), 7.50 (dt, J = 1.2, 8.4 Hz, 1H), 7.28 (dd, J = 0.8, 8.4 Hz, 1H), 7.20-

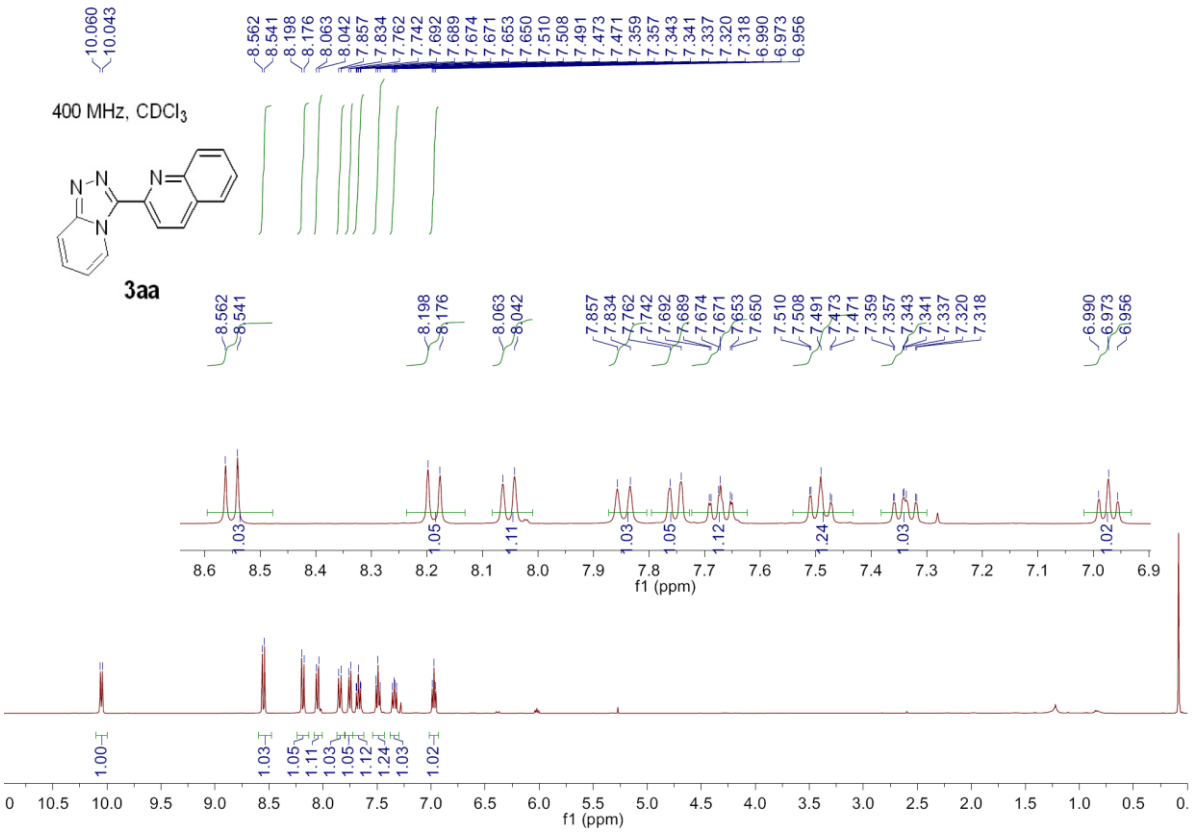
7.25 (m, 1H), 7.04 (dd, J = 1.2, 7.2 Hz, 1H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 151.7, 149.1, 147.8, 144.1, 134.9, 130.0, 129.9, 128.7, 128.3, 127.8, 125.4, 124.5, 120.1, 116.1, 112.2, HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{10}N_4Br$: 325.0083; found: 325.0095.

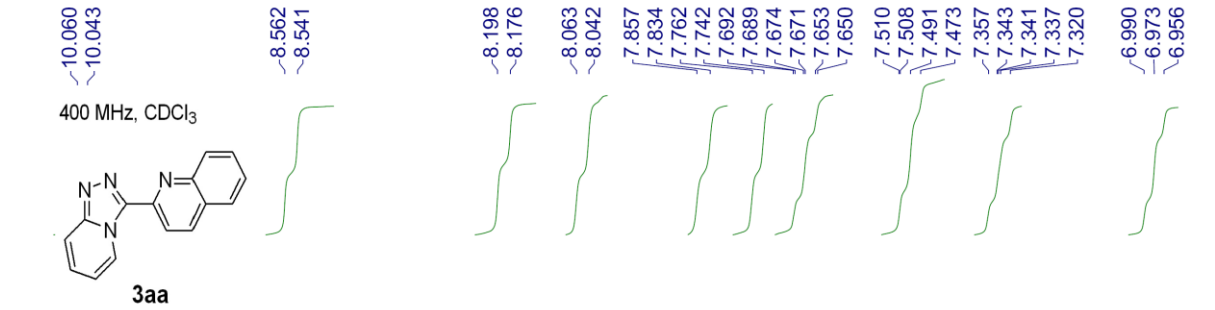
4-(6-Bromo-[1,2,4]triazolo[4,3-a]pyridin-3-yl)quinoline **(3mf)**



Brown solid, m.p.: 183-186 °C, ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 9.14 (d, J = 8.4 Hz, 1H), 8.27 (d, J = 8.4 Hz, 1H), 8.07 (q, J = 1.2 Hz, 1H), 7.90 (dq, J = 0.8, 8.4 Hz, 1H), 7.84-7.86 (m, 1H), 7.82 (q, J = 1.2 Hz, 1H), 7.66 (d, J = 4.4 Hz, 1H), 7.62 (dt, J = 1.6, 7.2 Hz, 1H), 7.42 (dd, J = 1.6, 9.6 Hz, 1H), ^{13}C-NMR (100 MHz, $CDCl_3$): δ (ppm) 149.9, 149.3, 149.08, 149.06, 132.6, 131.5, 130.6, 130.4, 128.4, 125.6, 125.0, 122.6, 121.7, 117.5, 110.1, HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{10}N_4Br$: 325.0083; found: 325.0092.

4. Copies of NMR Spectra

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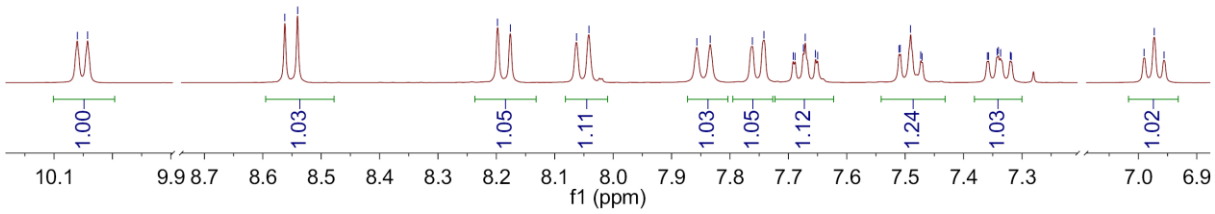
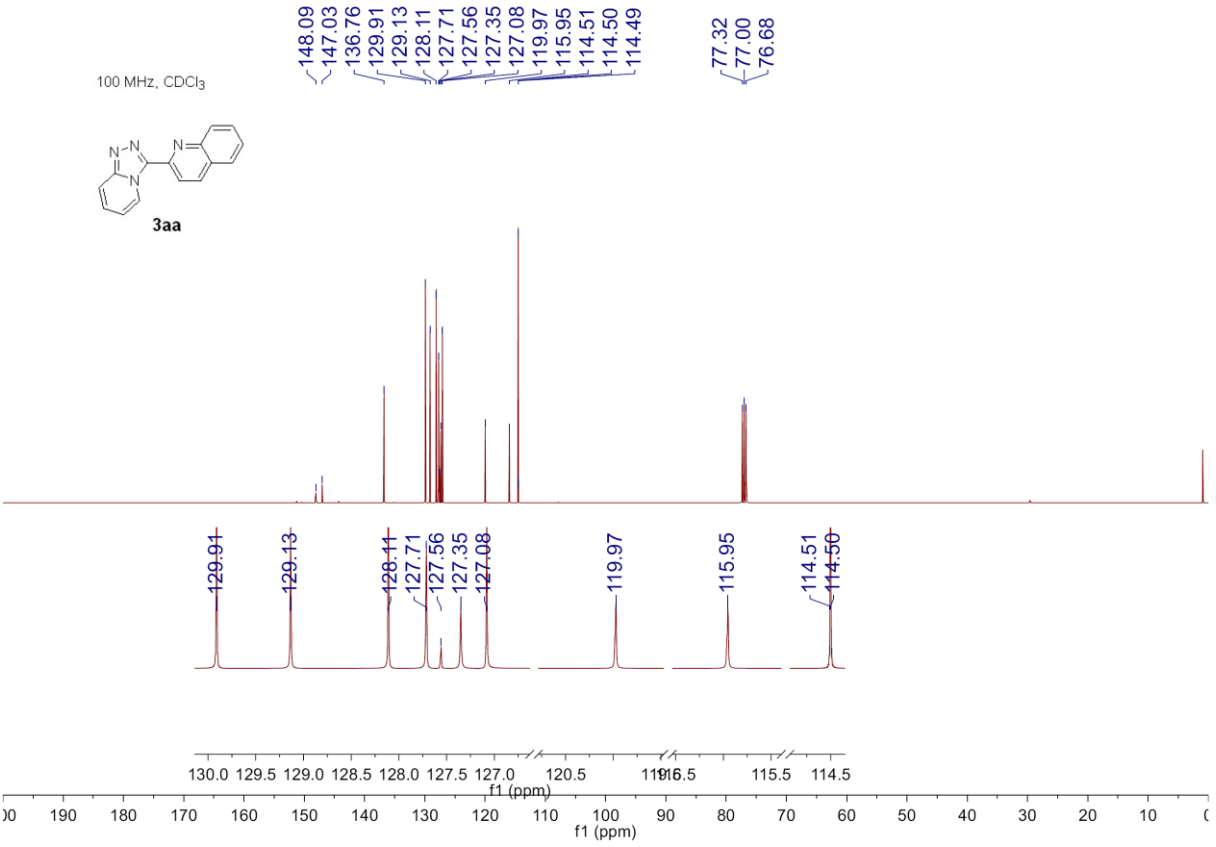
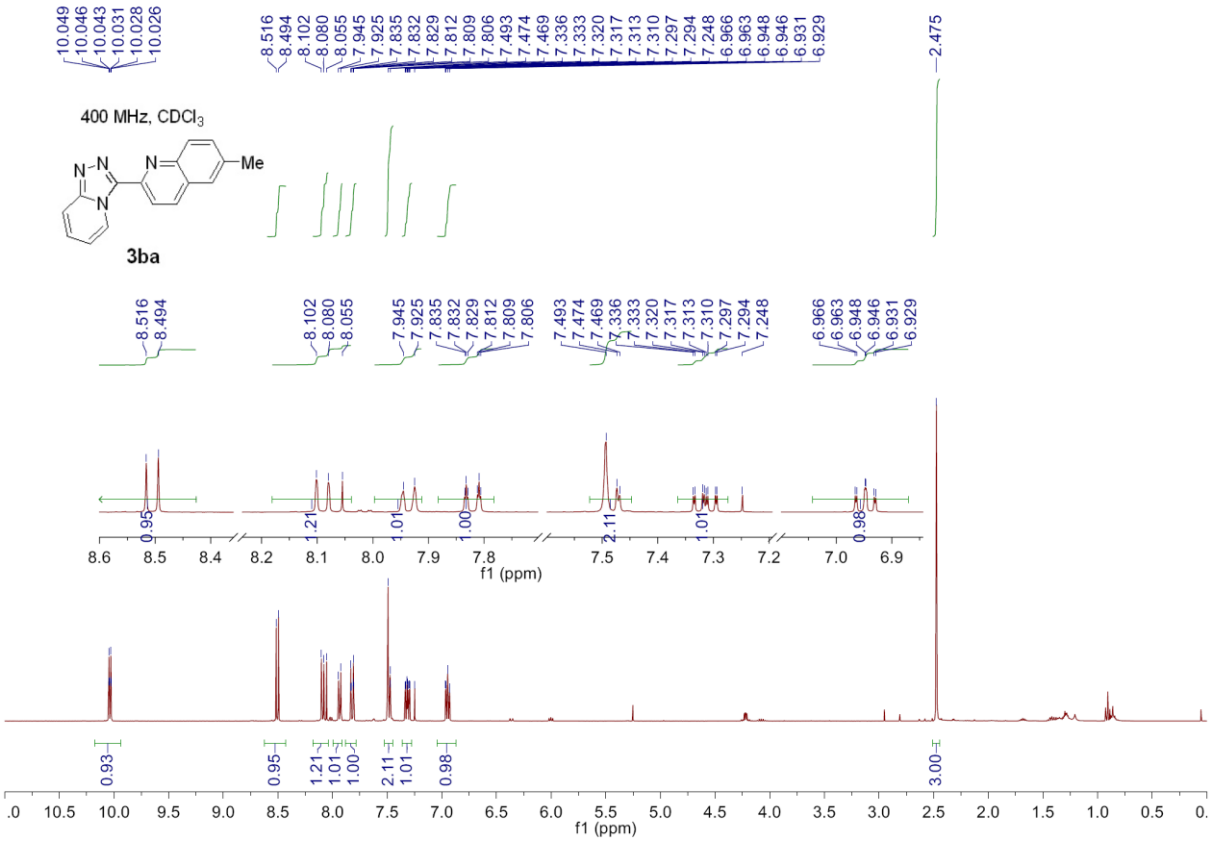
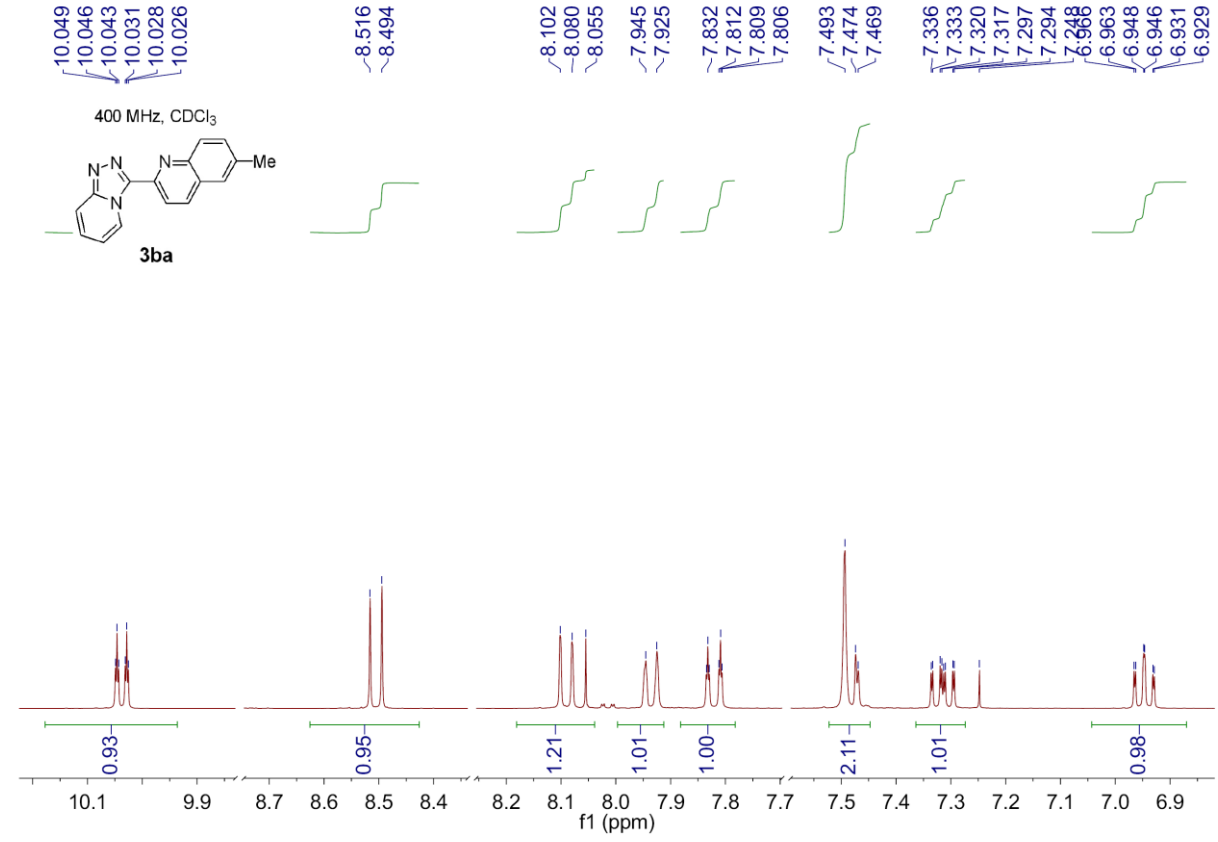
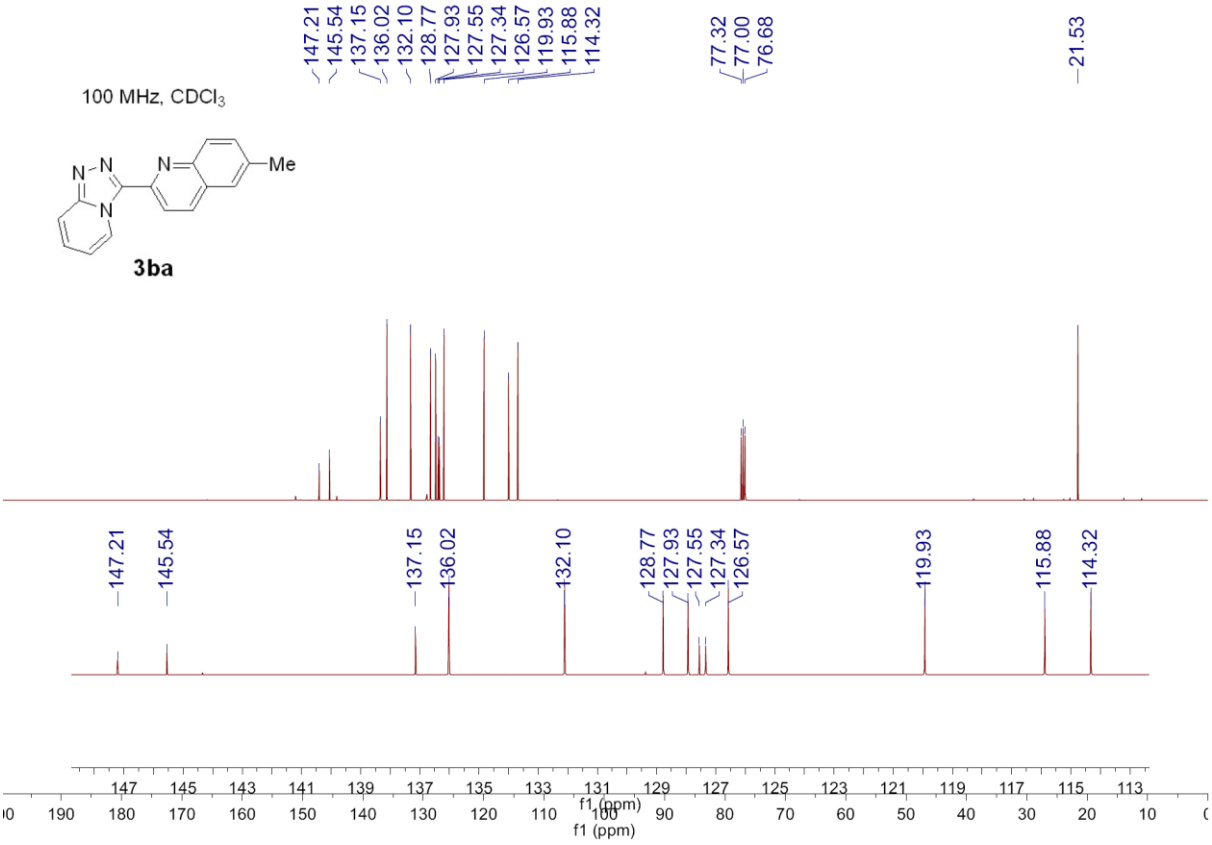
10.043
8.562
8.541
8.198
8.176
8.063
8.042
7.857
7.834
7.762
7.742
7.692
7.689
7.674
7.671
7.653
7.650
7.510
7.508
7.491
7.473
7.357
7.343
7.341
7.337
7.320
6.990
6.973
6.956
400 MHz, CDCl3
N
N
N
N
3aa


1.00
1.03
1.05
1.11
1.03
1.05
1.12
1.24
1.03
1.02
10.1
9.9
8.7
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.0
6.9
f1 (ppm)


148.09
147.03
136.76
129.91
129.13
128.11
127.71
127.56
127.35
127.08
119.97
115.95
114.51
114.50
114.49
77.32
77.00
76.68
100 MHz, CDCl3
N
N
N
N
3aa
129.91
129.13
128.11
127.71
127.56
127.35
127.08
119.97
115.95
114.51
114.50
130.0
129.5
129.0
128.5
128.0
127.5
127.0
120.5
116.5
115.5
114.5
f1 (ppm)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


400 MHz, CDCl3
Me
3ba
f1 (ppm)


400 MHz, CDCl3
Me
3ba
f1 (ppm)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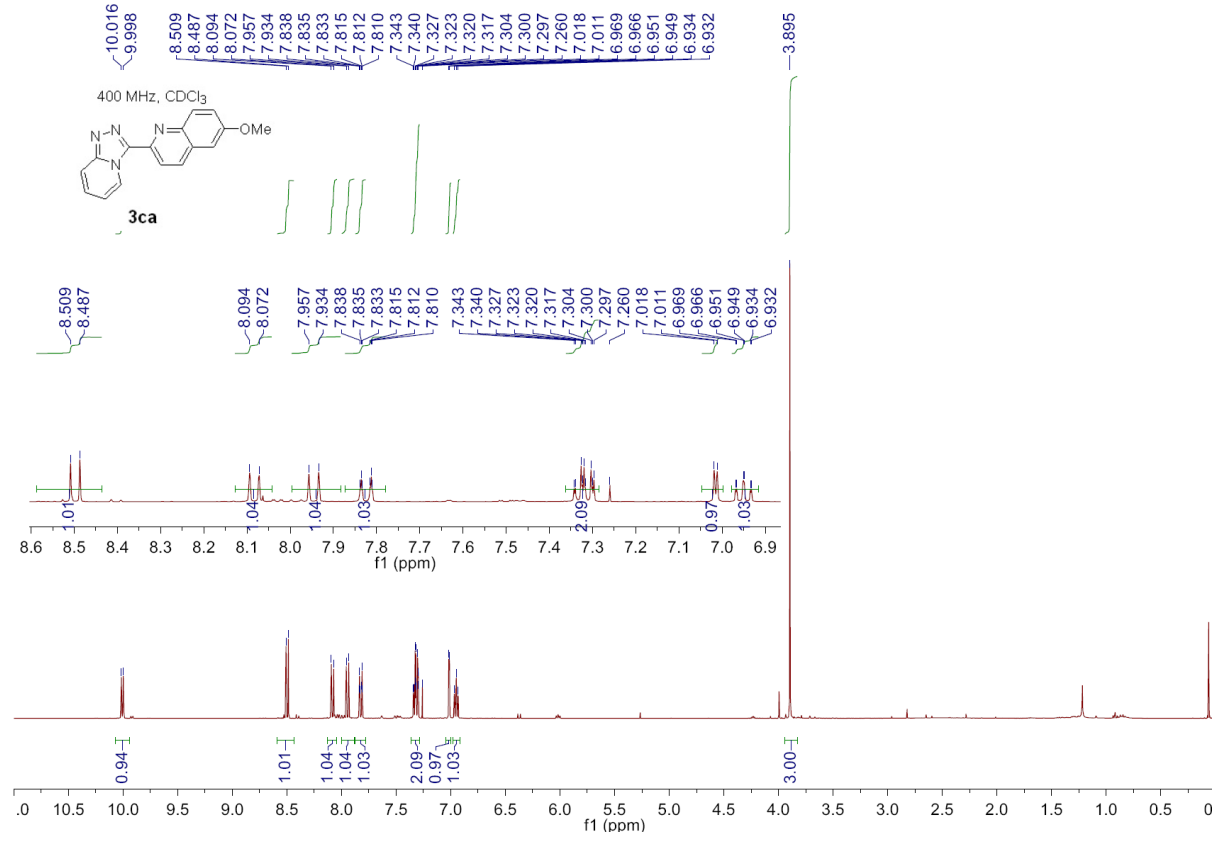
145.54
137.15
136.02
132.10
128.77
127.93
127.55
127.34
126.57
119.93
115.88
114.32
77.32
77.00
76.68
21.53
100 MHz, CDCl3
Me
3ba
f1 (ppm)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9.998
8.509
8.487
8.094
8.072
7.957
7.934
7.838
7.835
7.833
7.815
7.812
7.810
7.343
7.340
7.327
7.323
7.320
7.317
7.304
7.300
7.297
7.260
7.018
7.011
6.969
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6.949
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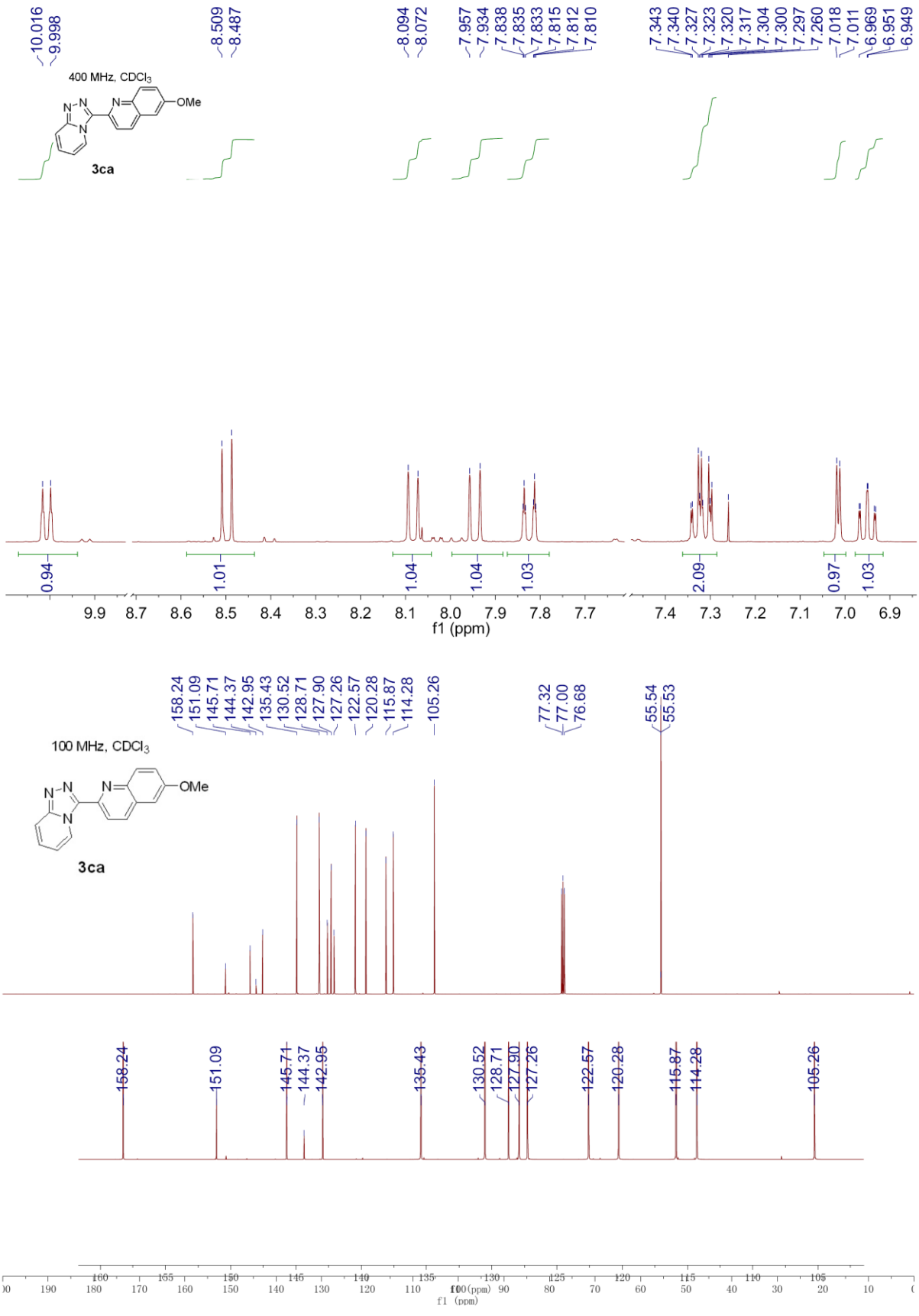
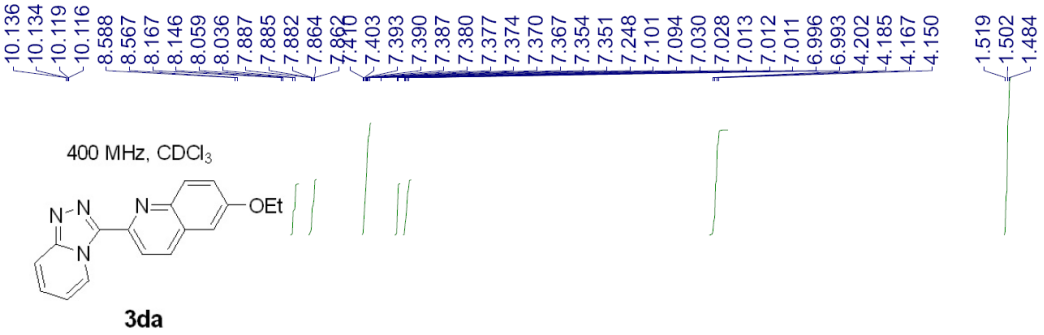
3.895
400 MHz, CDCl3
OMe
3ca
f1 (ppm)


10.016
9.998
8.509
8.487
8.094
8.072
7.957
7.934
7.838
7.835
7.833
7.815
7.812
7.810
7.343
7.340
7.327
7.323
7.320
7.317
7.304
7.300
7.297
7.260
7.018
7.011
6.969
6.951
6.949
400 MHz, CDCl3
OMe
3ca
0.94
1.01
1.04
1.04
1.03
2.09
0.97
1.03
9.9 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.4 7.3 7.2 7.1 7.0 6.9
f1 (ppm)
158.24
151.09
145.71
144.37
142.95
135.43
130.52
128.71
127.90
127.26
122.57
120.28
115.87
114.28
105.26
77.32
77.00
76.68
55.54
55.53
100 MHz, CDCl3
OMe
3ca
160 155 150 145 140 135 130 125 120 115 110 105
f1 (ppm)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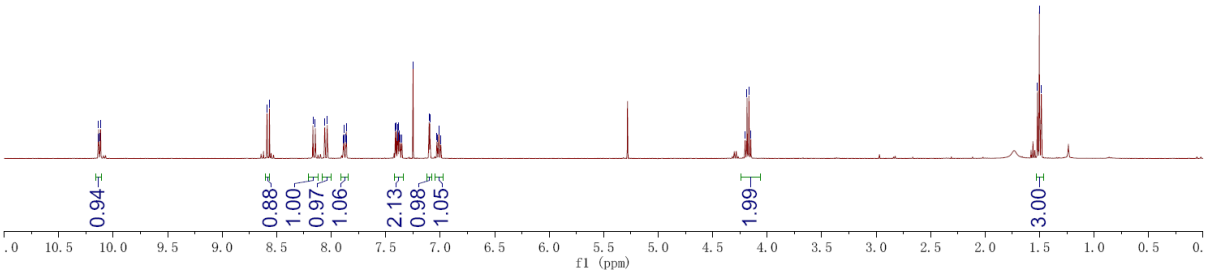
10.134
10.119
10.116
8.588
8.567
8.167
8.146
8.059
8.036
7.887
7.885
7.882
7.864
7.862
7.410
7.403
7.393
7.390
7.387
7.380
7.377
7.374
7.370
7.367
7.354
7.351
7.248
7.101
7.094
7.030
7.028
7.013
7.012
7.011
6.996
6.993
4.202
4.185
4.167
4.150
1.519
1.502
1.484
400 MHz, CDCl3
OEt
3da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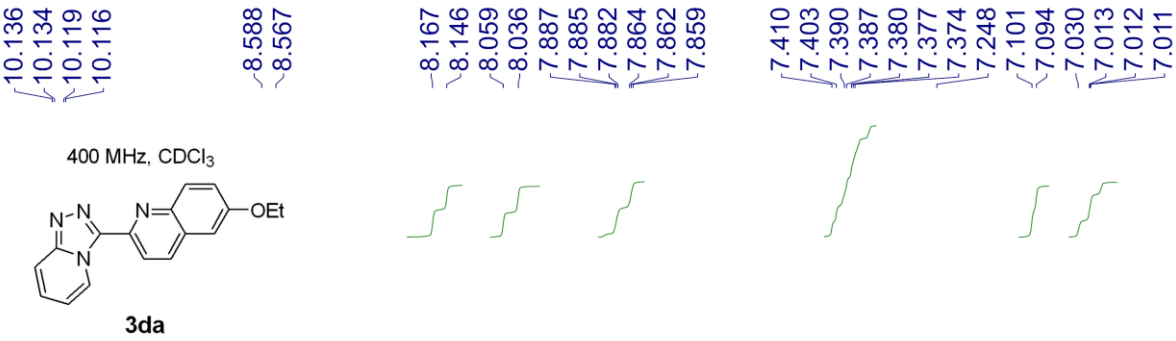
0.88
1.00
0.97
1.06
2.13
0.98
1.05
1.99
3.00
f1 (ppm)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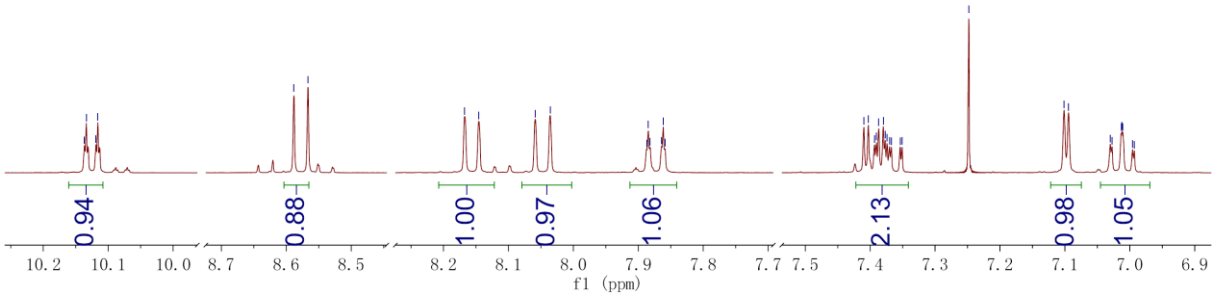
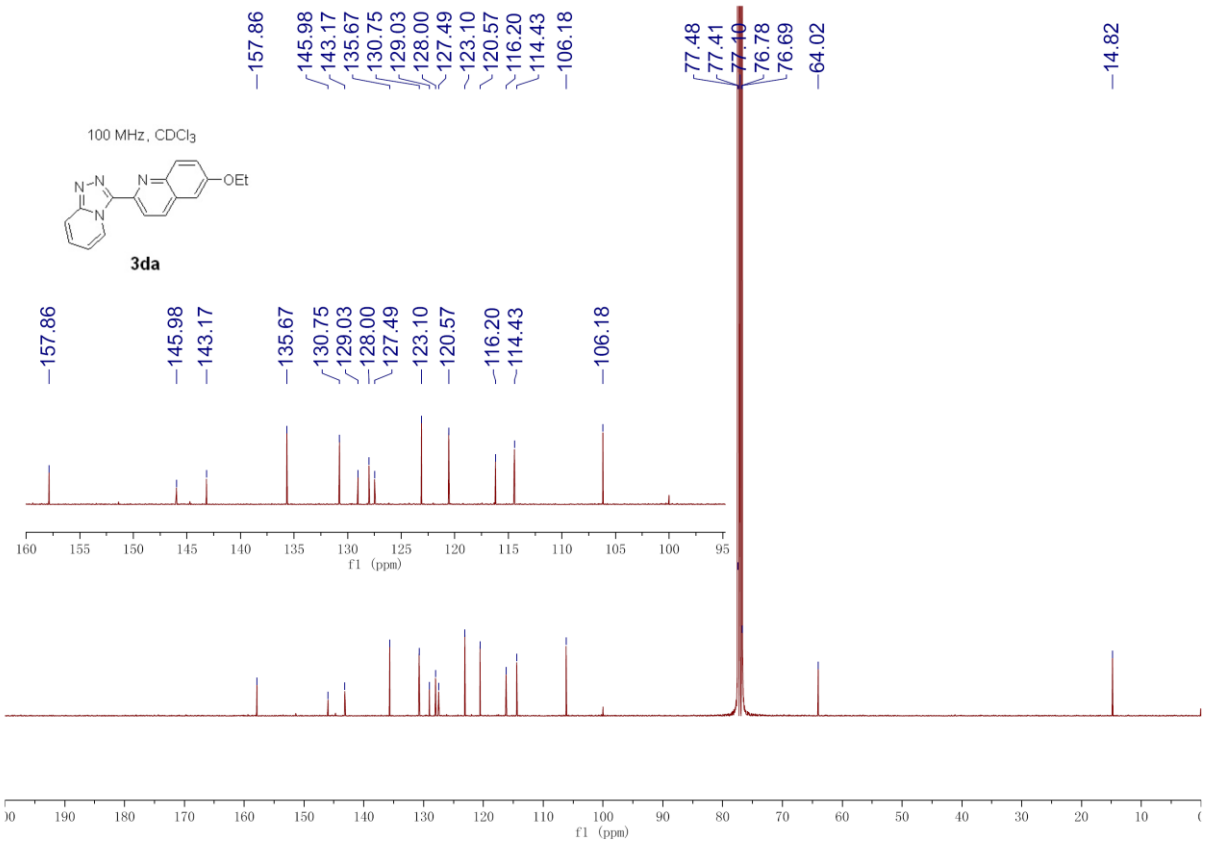
10.134
10.119
10.116
8.588
8.567
8.167
8.146
8.059
8.036
7.887
7.885
7.882
7.864
7.862
7.859
7.410
7.403
7.390
7.387
7.380
7.377
7.374
7.248
7.101
7.094
7.030
7.013
7.012
7.011
400 MHz, CDCl3
OEt
3da


0.94
0.88
1.00
0.97
1.06
2.13
0.98
1.05
f1 (ppm)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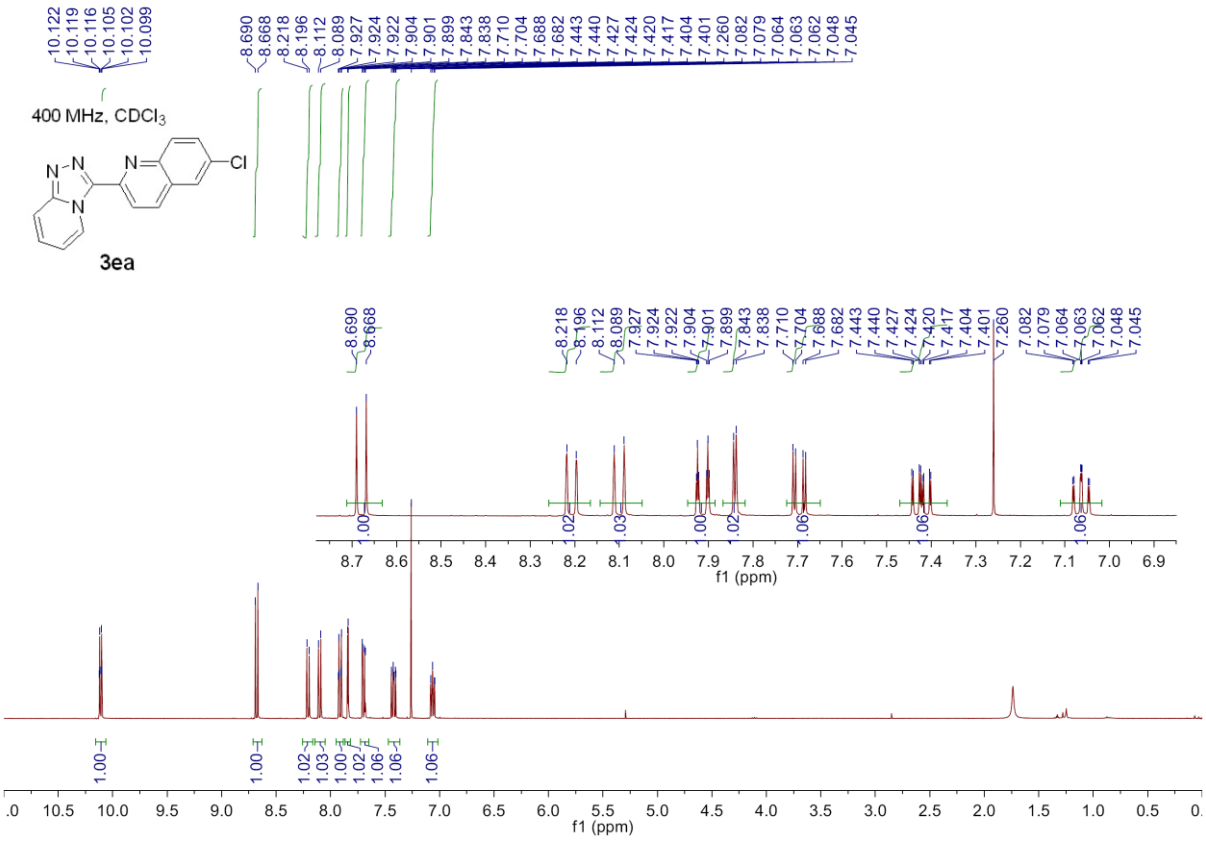
145.98
143.17
135.67
130.75
129.03
128.00
127.49
123.10
120.57
116.20
114.43
106.18
77.48
77.41
77.10
76.78
76.69
64.02
14.82
100 MHz, CDCl3
OEt
3da
f1 (ppm)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10.119
10.116
10.105
10.102
10.099
8.690
8.668
8.218
8.196
8.112
8.089
7.927
7.924
7.922
7.904
7.901
7.899
7.843
7.838
7.710
7.704
7.688
7.682
7.443
7.440
7.427
7.424
7.420
7.417
7.404
7.401
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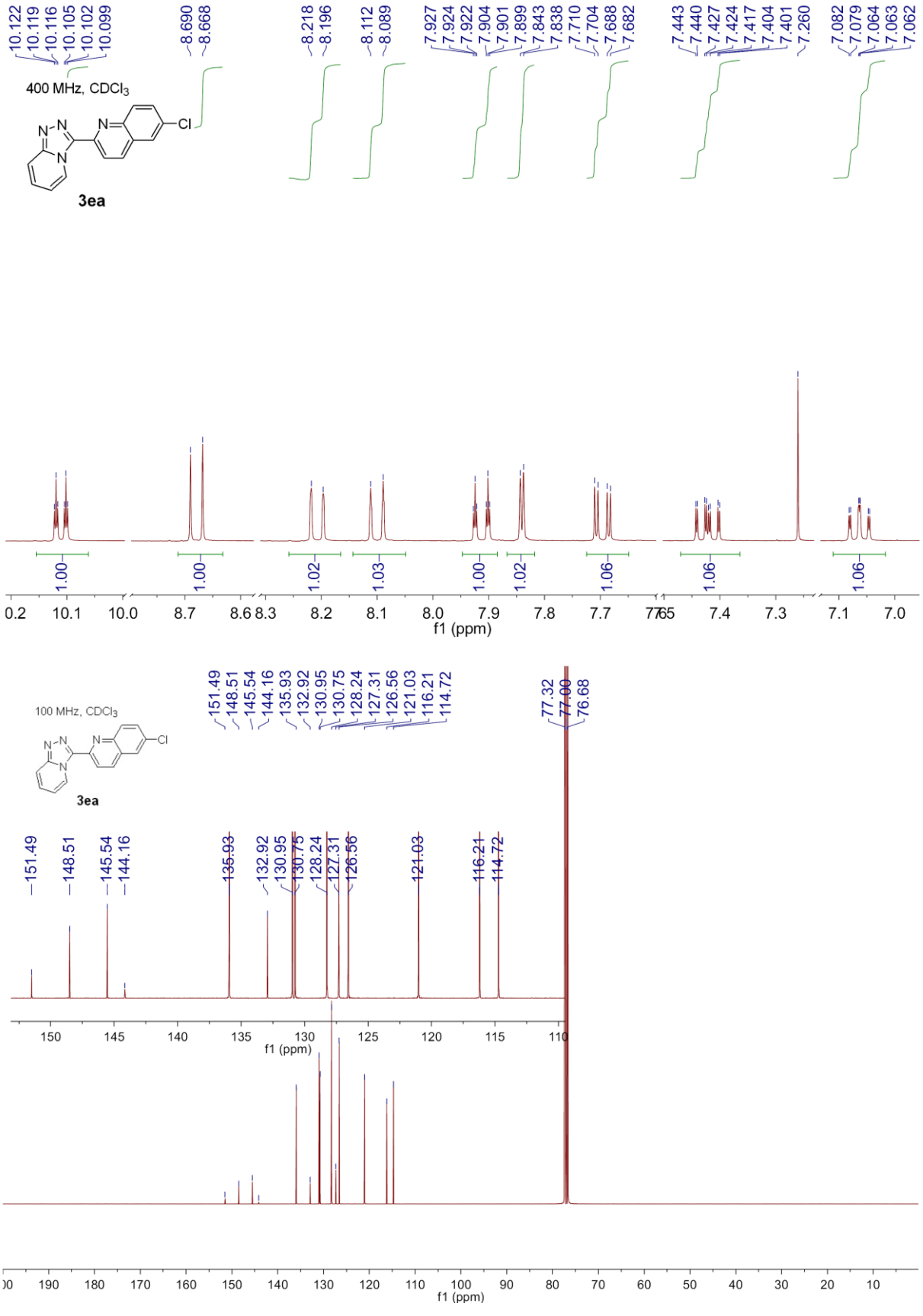
7.045
400 MHz, CDCl3
Cl
3ea
f1 (ppm)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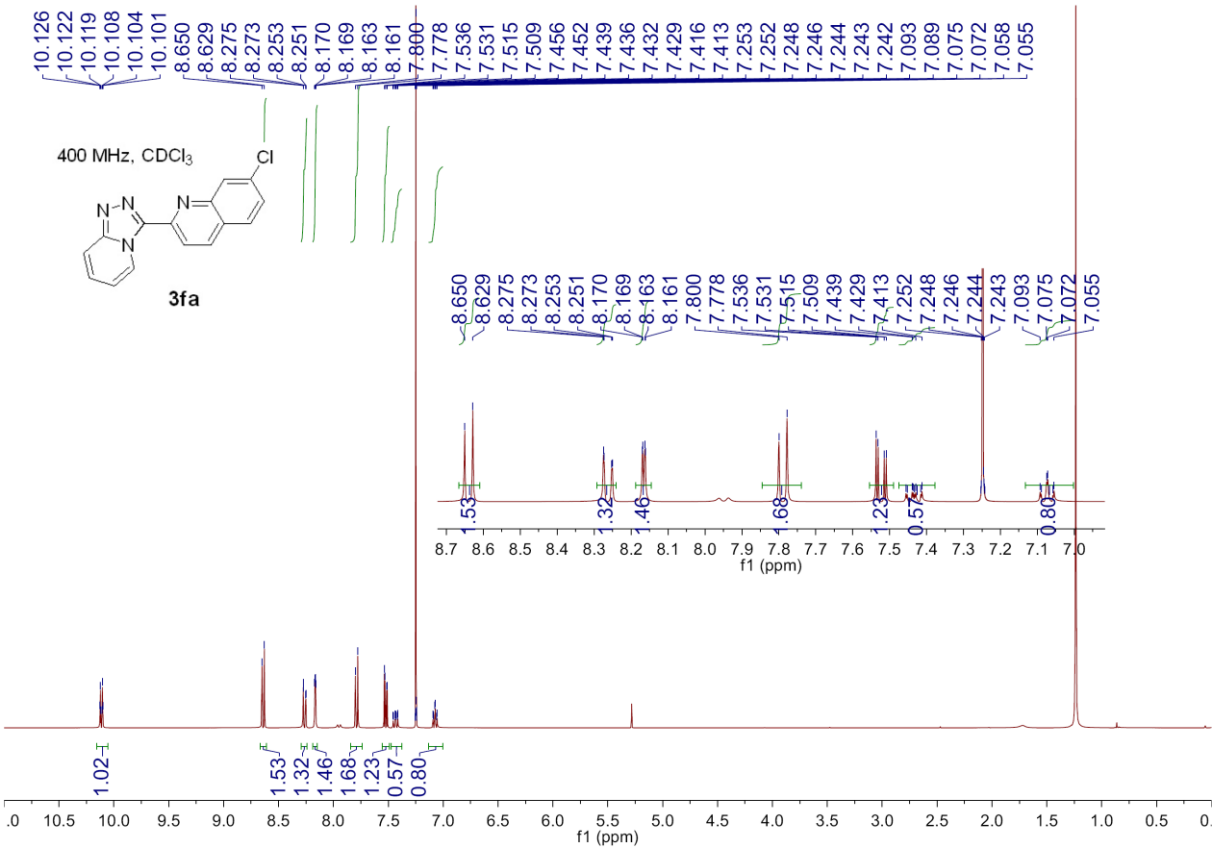
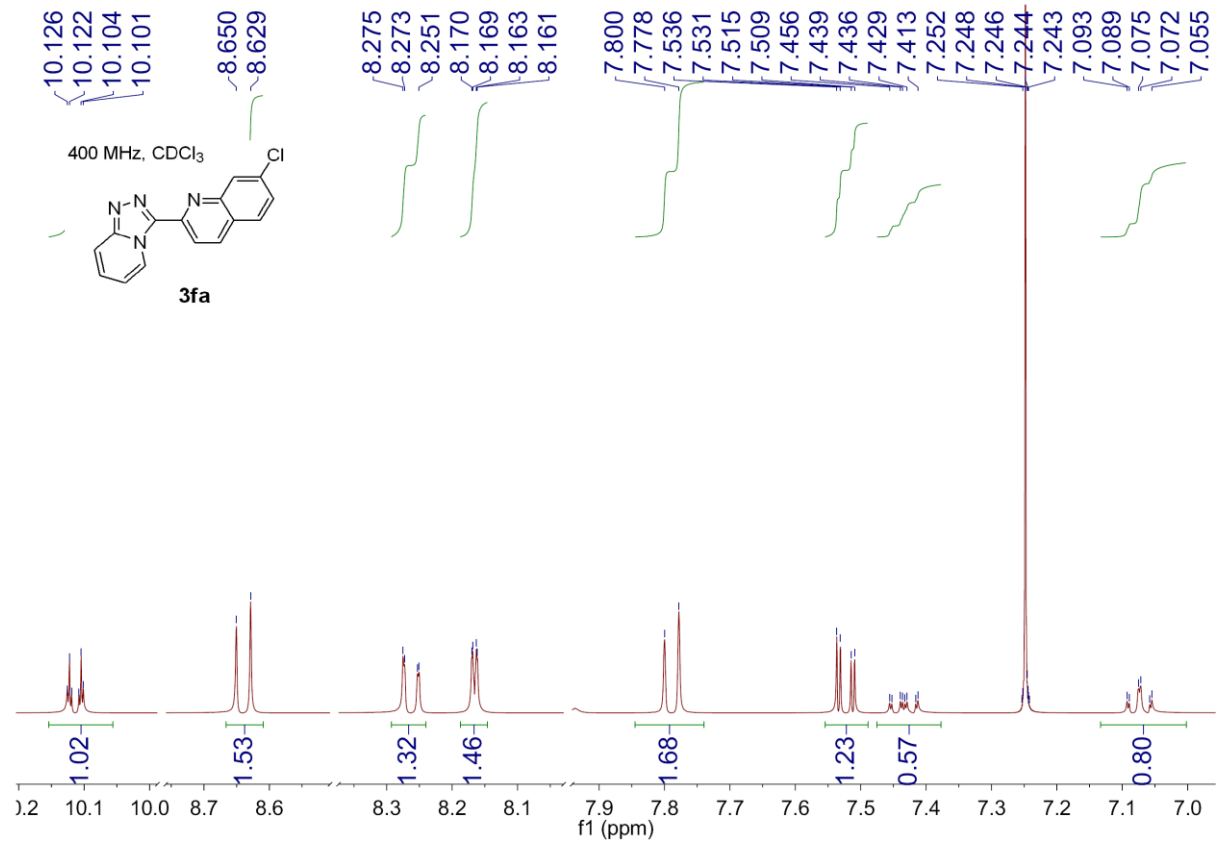
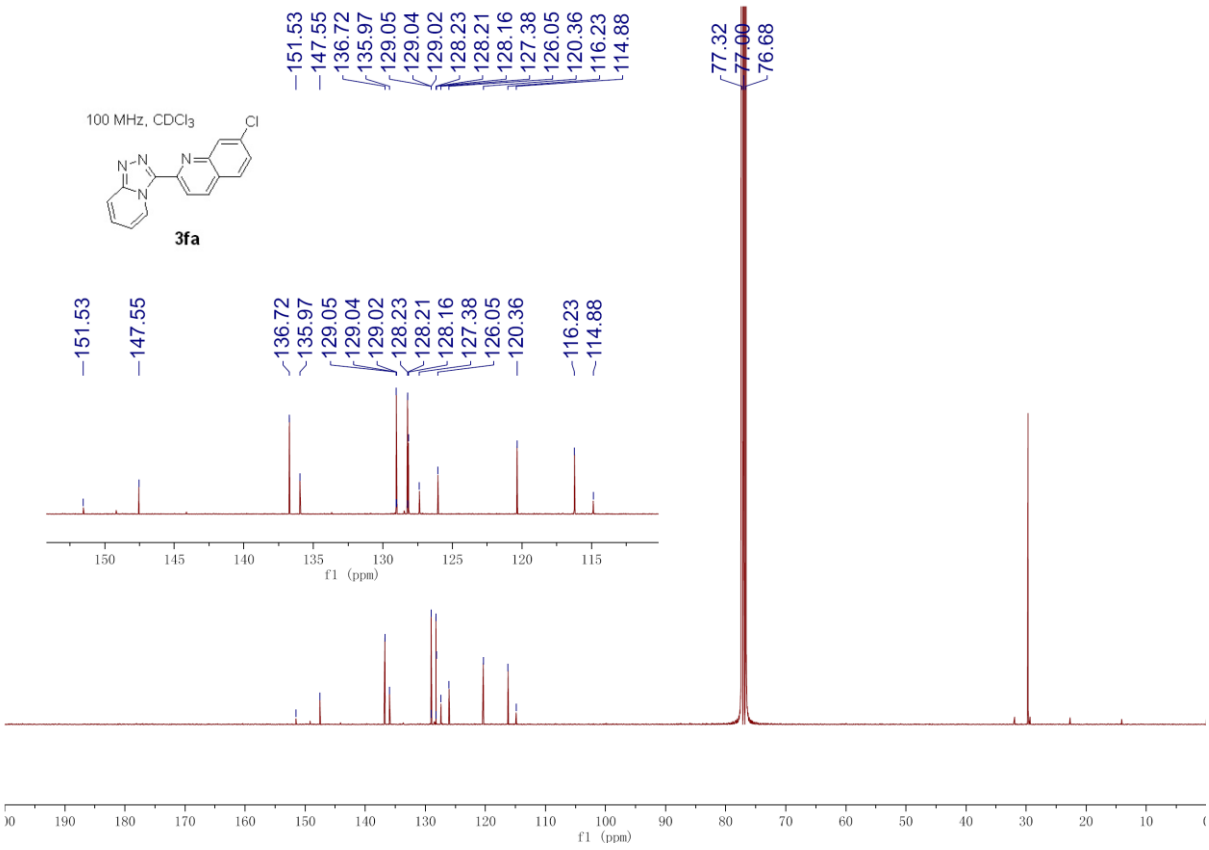
10.119
10.116
10.105
10.102
10.099
8.690
8.668
8.218
8.196
8.112
8.089
7.927
7.924
7.922
7.904
7.901
7.899
7.843
7.838
7.710
7.704
7.688
7.682
7.443
7.440
7.427
7.424
7.417
7.404
7.401
7.260
7.082
7.079
7.064
7.063
7.062
400 MHz, CDCl3
Cl
3ea
1.00
1.00
1.02
1.03
1.00
1.02
1.06
1.06
1.06
f1 (ppm)
151.49
148.51
145.54
144.16
135.93
132.92
130.95
130.75
128.24
127.31
126.56
121.03
116.21
114.72
77.32
77.00
76.68
100 MHz, CDCl3
Cl
3ea
f1 (ppm)


400 MHz, CDCl3
Cl
N
N
N
3fa
f1 (ppm)


400 MHz, CDCl3
Cl
N
N
N
3fa
f1 (ppm)


100 MHz, CDCl3
3fa
151.53
147.55
136.72
135.97
129.05
129.04
129.02
128.23
128.21
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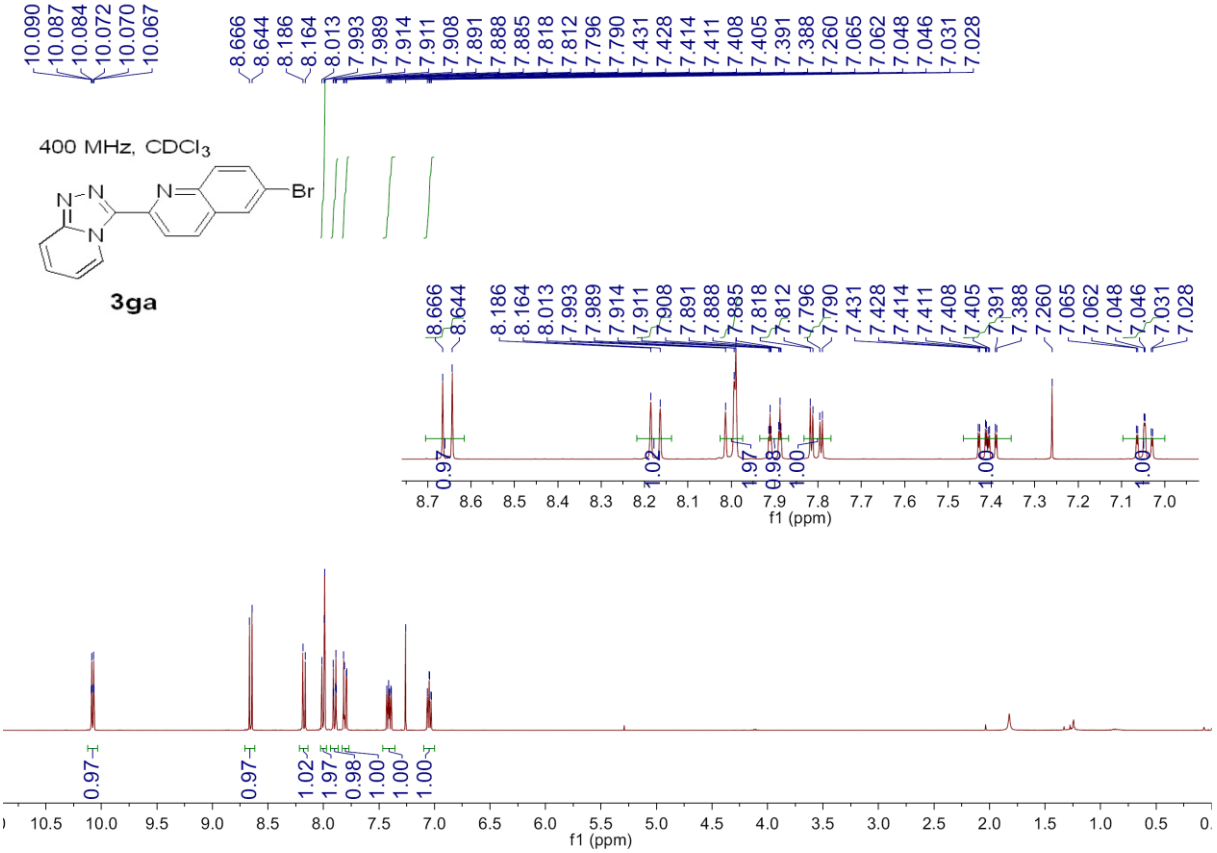
114.88
77.32
77.00
76.68
f1 (ppm)


400 MHz, CDCl3
3ga
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10.084
10.072
10.070
10.067
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8.644
8.186
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8.013
7.993
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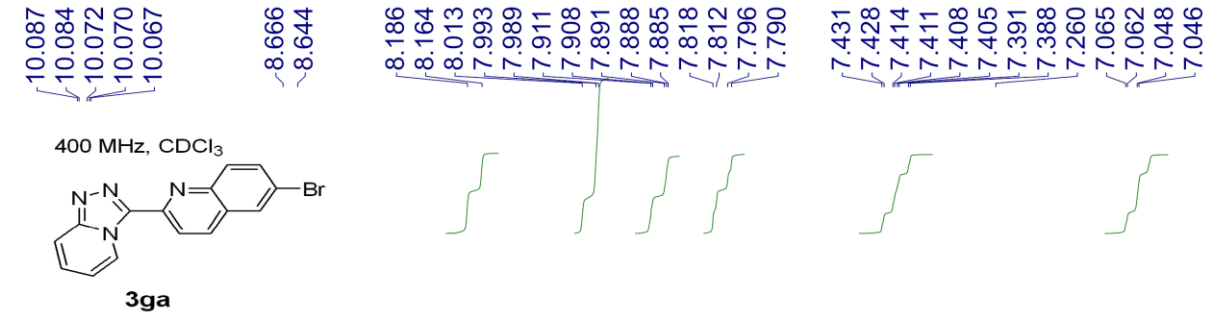
7.914
7.911
7.908
7.891
7.888
7.885
7.818
7.812
7.796
7.790
7.431
7.428
7.414
7.411
7.408
7.405
7.391
7.388
7.260
7.065
7.062
7.048
7.046
7.031
7.028
0.97
0.97
1.02
1.97
0.98
1.00
1.00
1.00
f1 (ppm)


10.087
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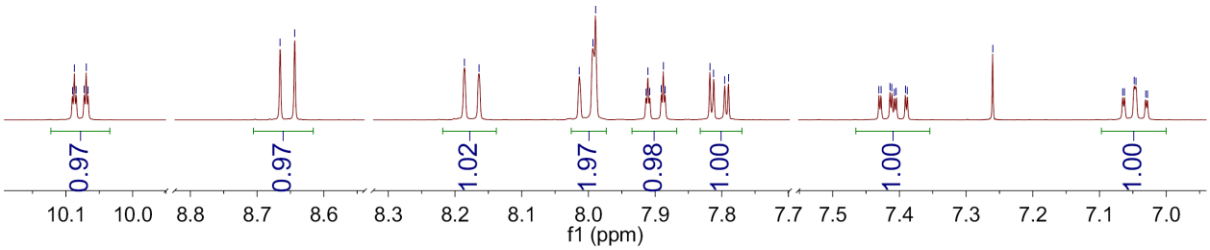
10.070
10.067
8.666
8.644
8.186
8.164
8.013
7.993
7.989
7.911
7.908
7.891
7.888
7.885
7.818
7.812
7.796
7.790
7.431
7.428
7.414
7.411
7.408
7.405
7.391
7.388
7.260
7.065
7.062
7.048
7.046
400 MHz, CDCl3
Br
3ga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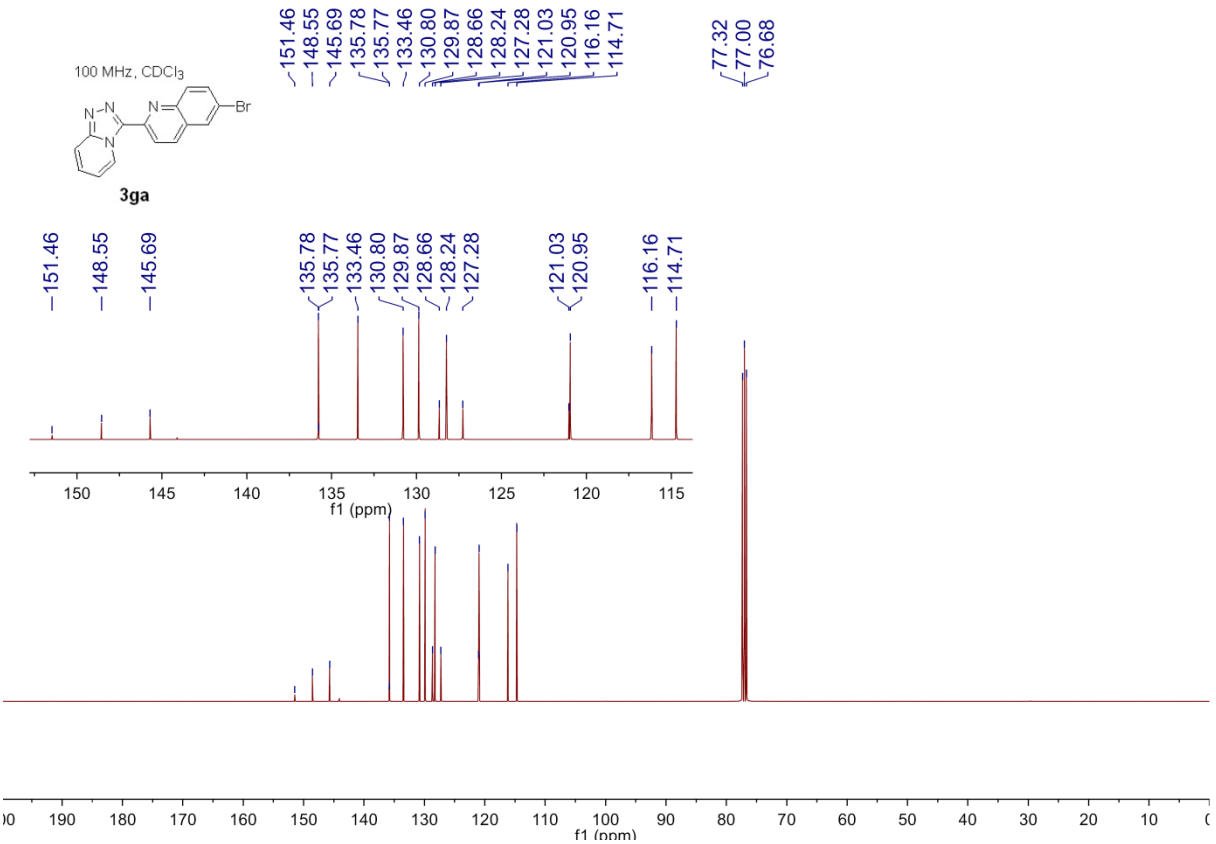
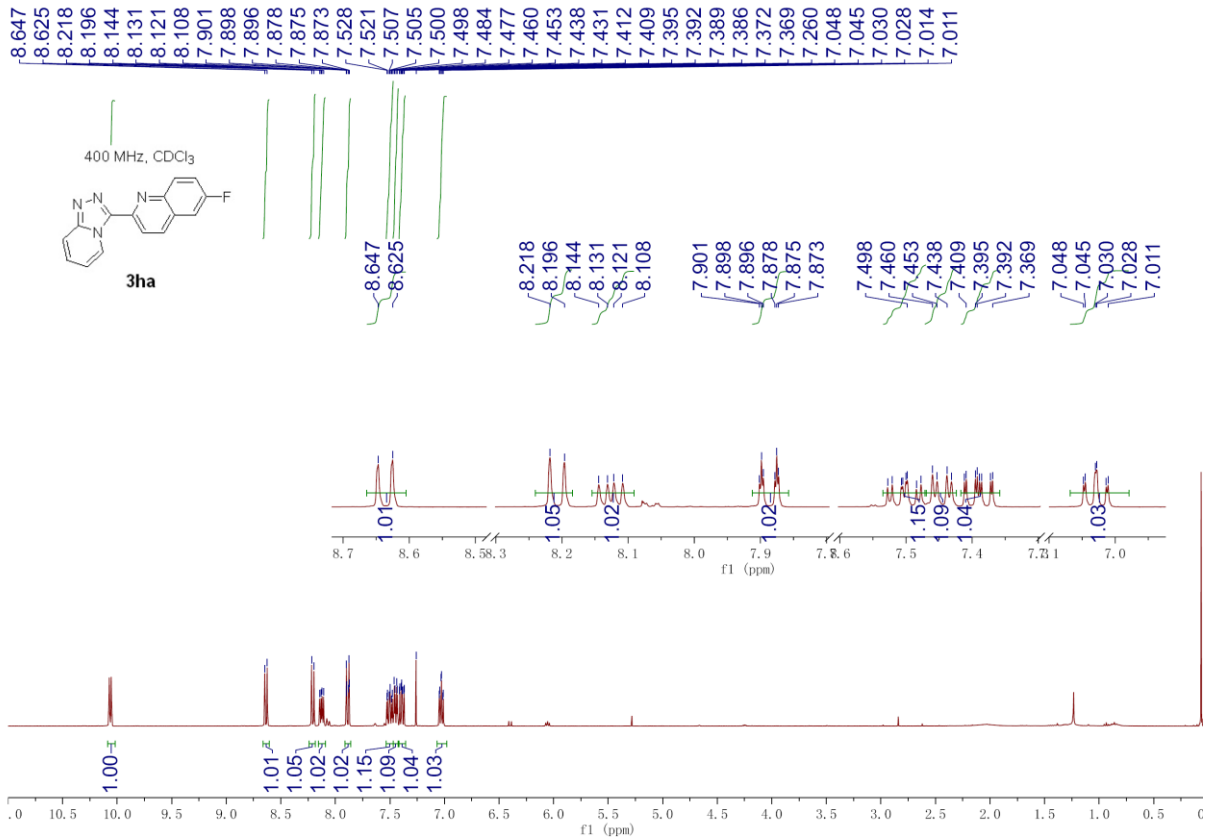
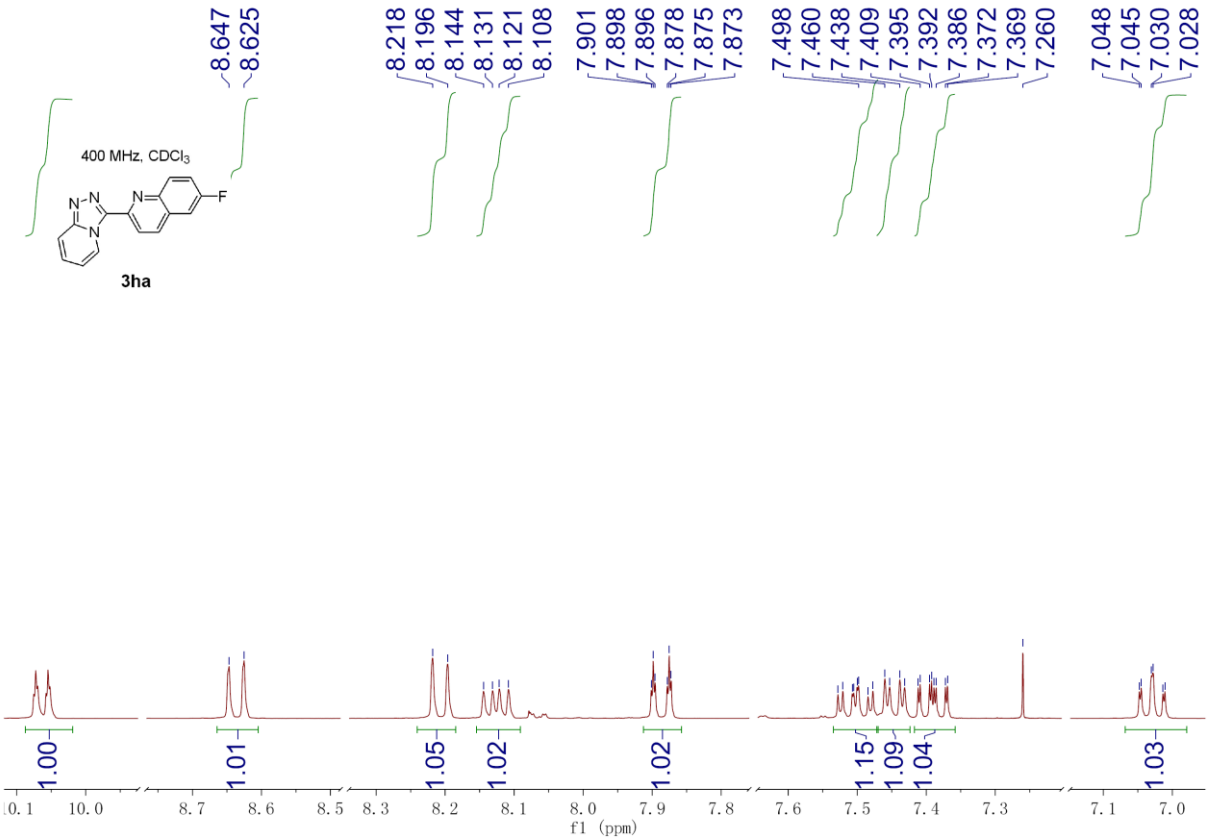
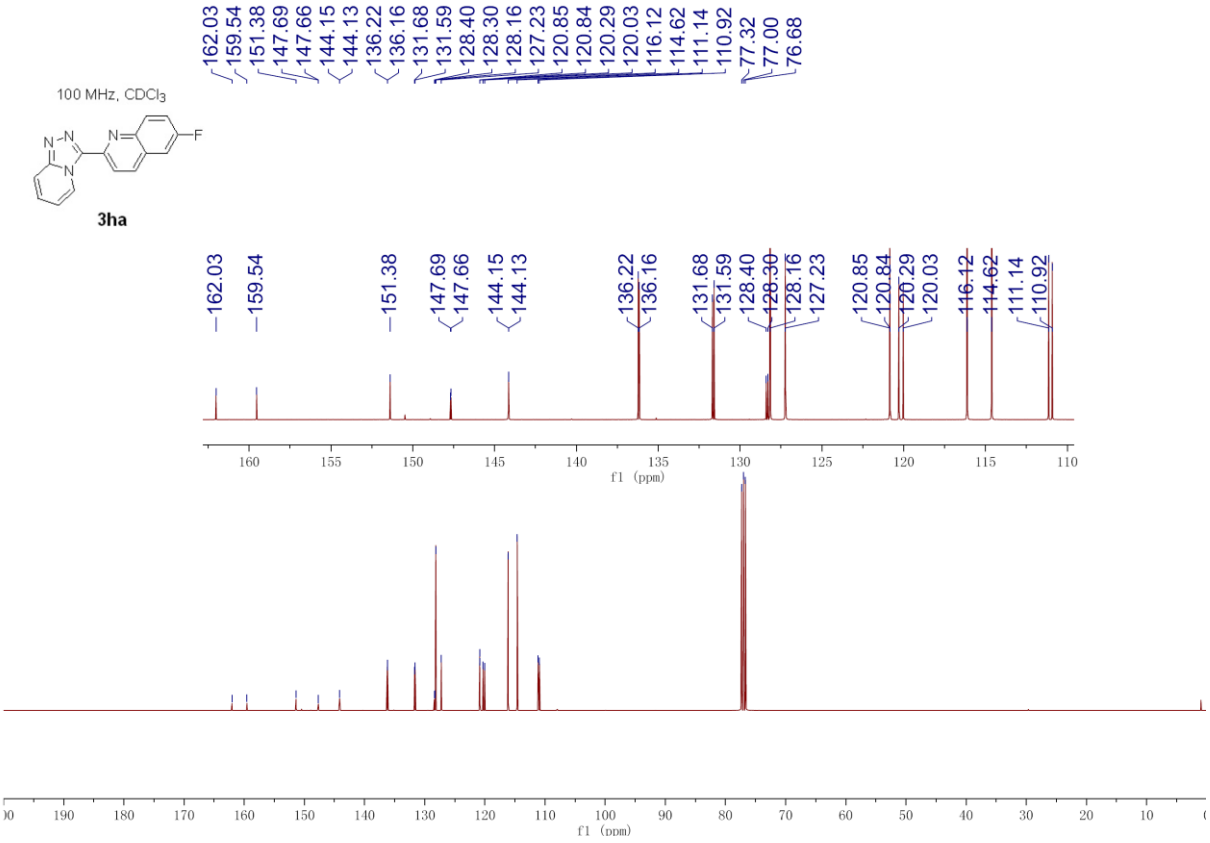
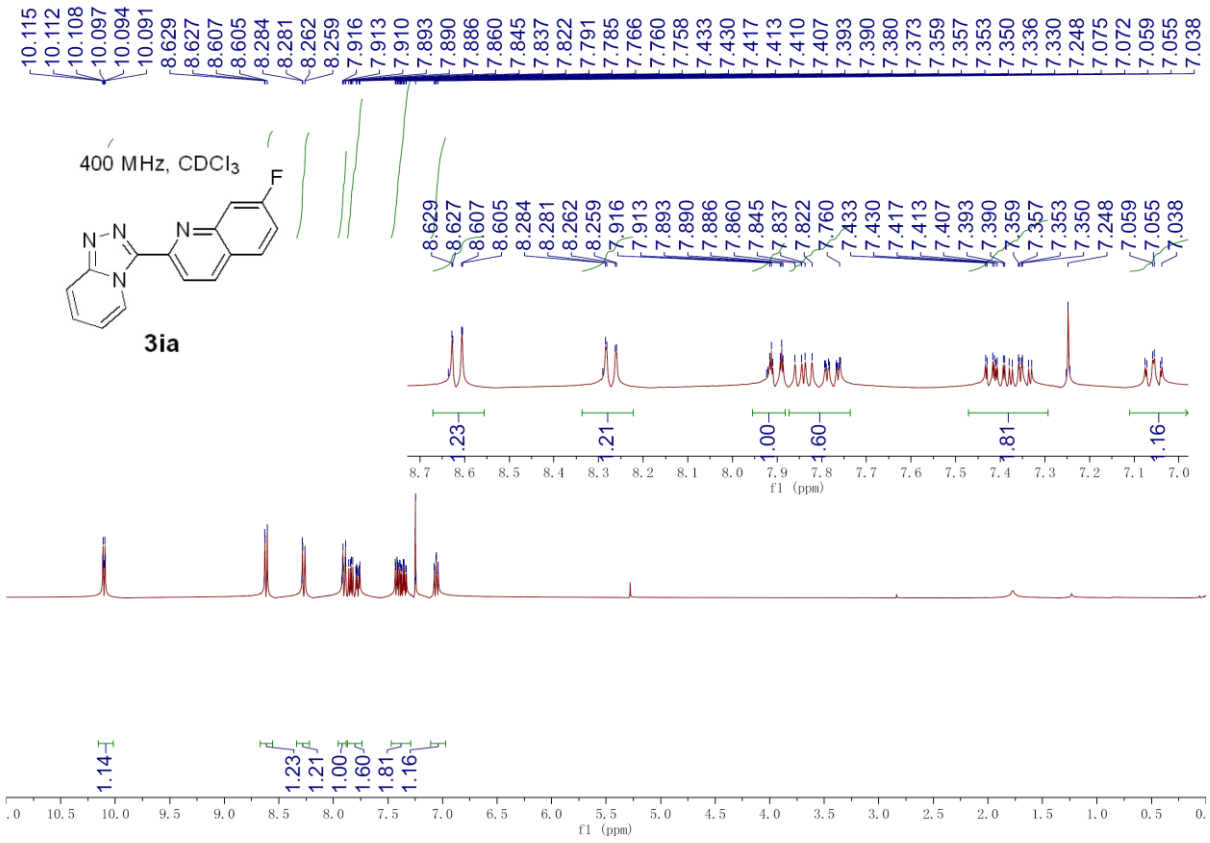
0.97
1.02
1.97
0.98
1.00
1.00
1.00
10.1
10.0
8.8
8.7
8.6
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.5
7.4
7.3
7.2
7.1
7.0
f1 (ppm)

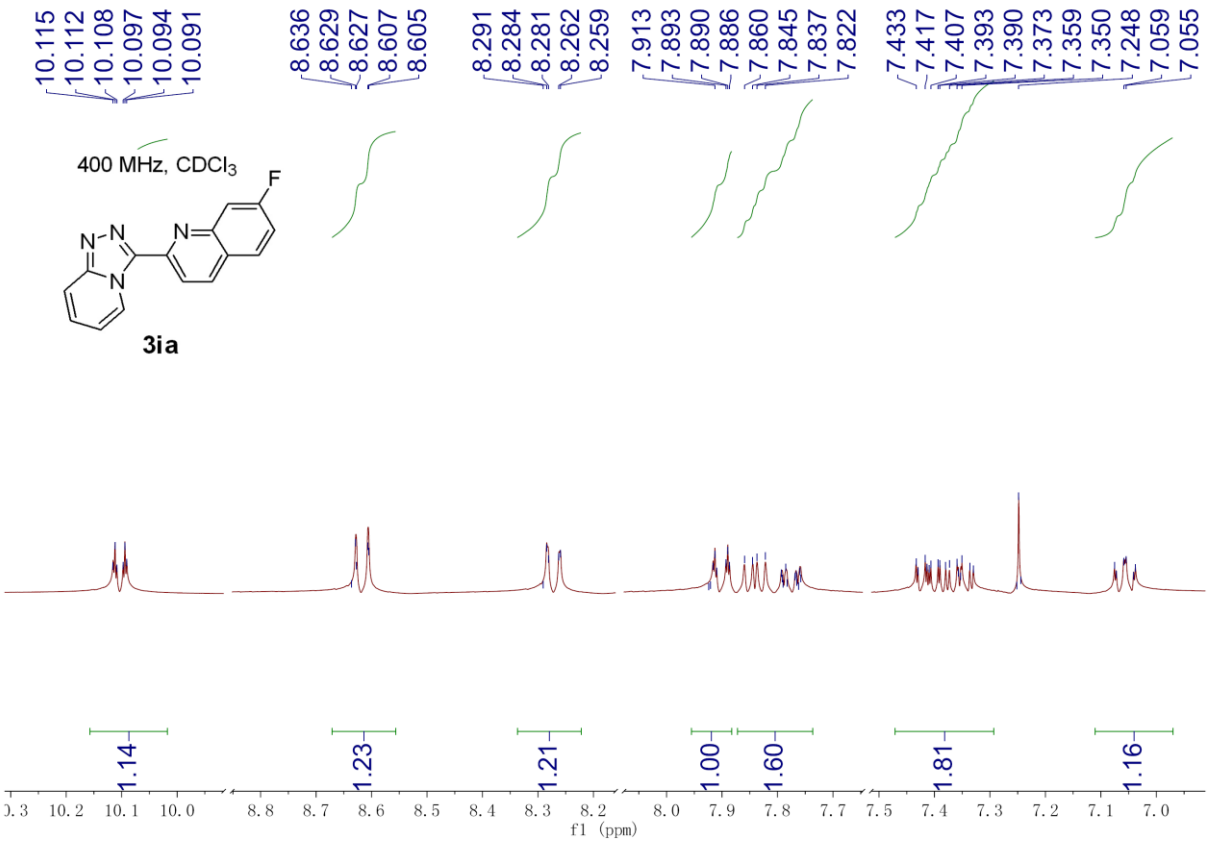

151.46
148.55
145.69
135.78
135.77
133.46
130.80
129.87
128.66
128.24
127.28
121.03
120.95
116.16
114.71
77.32
77.00
76.68
100 MHz, CDCl3
Br
3ga
f1 (ppm)

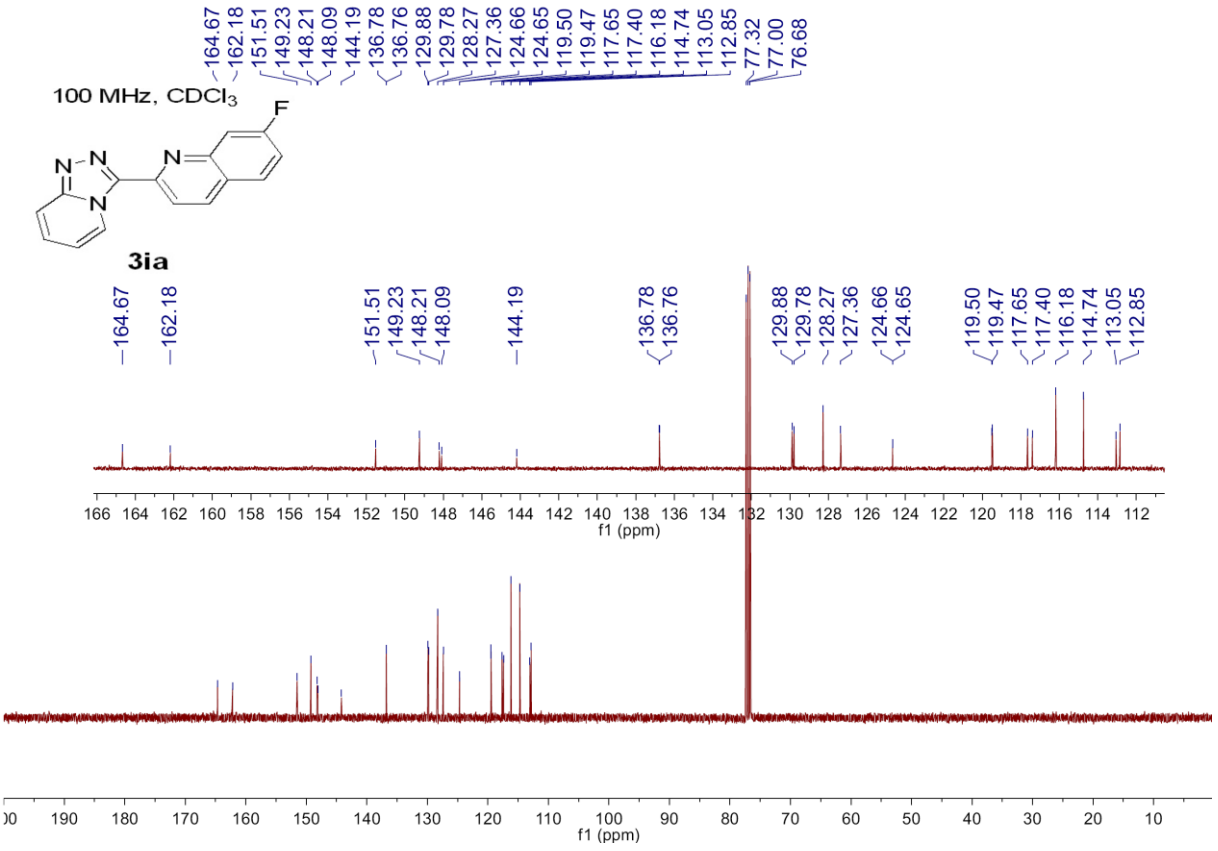

8.647
8.625
8.218
8.196
8.144
8.131
8.121
8.108
7.901
7.898
7.896
7.878
7.875
7.873
7.528
7.521
7.507
7.505
7.500
7.498
7.484
7.477
7.460
7.453
7.438
7.431
7.412
7.409
7.395
7.392
7.389
7.386
7.372
7.369
7.260
7.048
7.045
7.030
7.028
7.014
7.011
400 MHz, CDCl3
3ha
1.00
1.01
1.05
1.02
1.02
1.15
1.09
1.04
1.03
f1 (ppm)

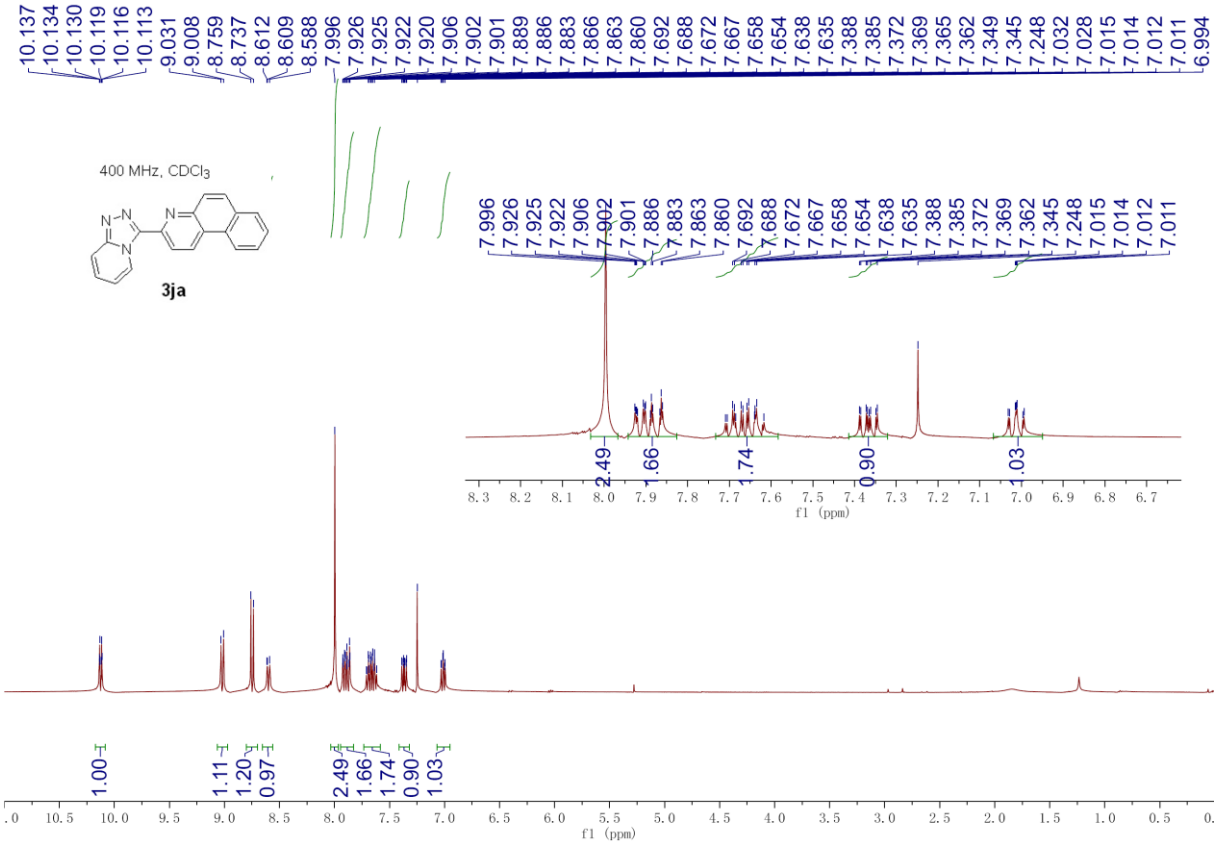

8.647
8.625
8.218
8.196
8.144
8.131
8.121
8.108
7.901
7.898
7.896
7.878
7.875
7.873
7.498
7.460
7.438
7.409
7.395
7.392
7.386
7.372
7.369
7.260
7.048
7.045
7.030
7.028
400 MHz, CDCl3
3ha
1.00
1.01
1.05
1.02
1.02
1.15
1.09
1.04
1.03
f1 (ppm)

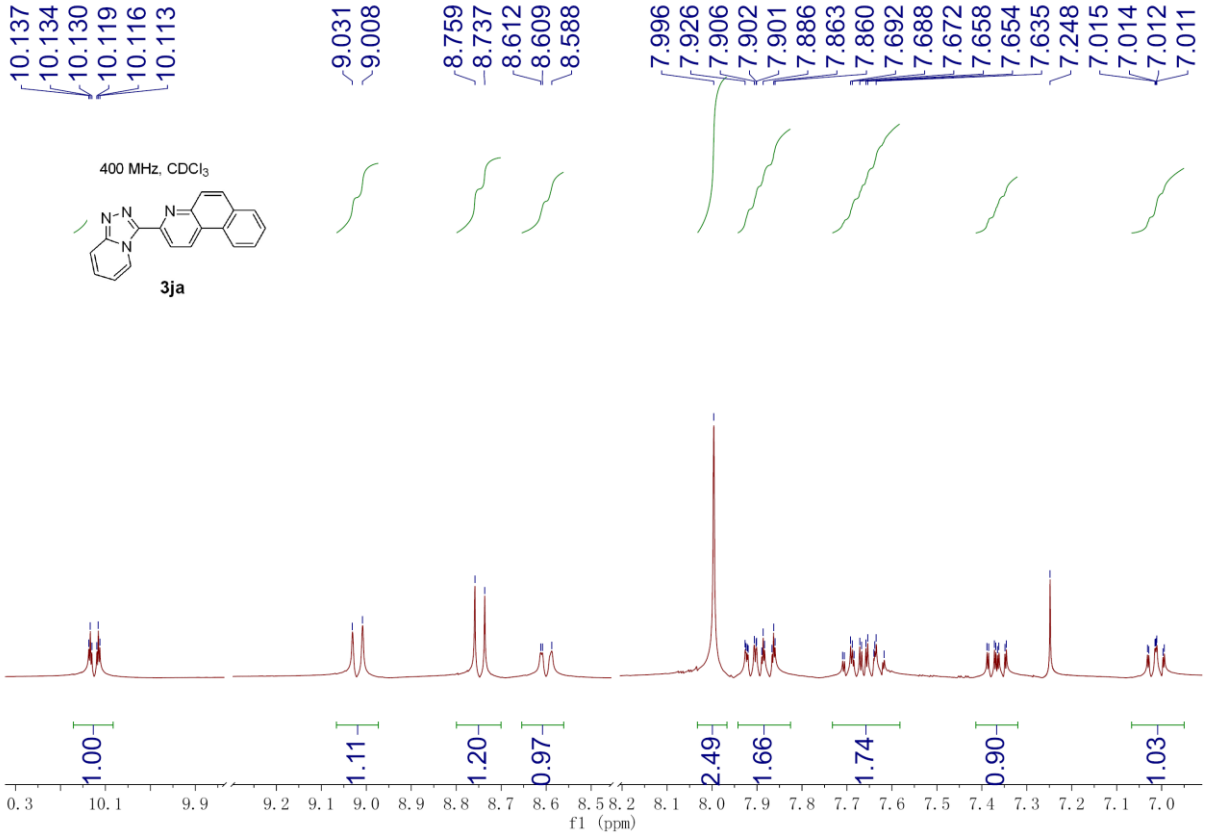

100 MHz, CDCl3
3ha
f1 (ppm)

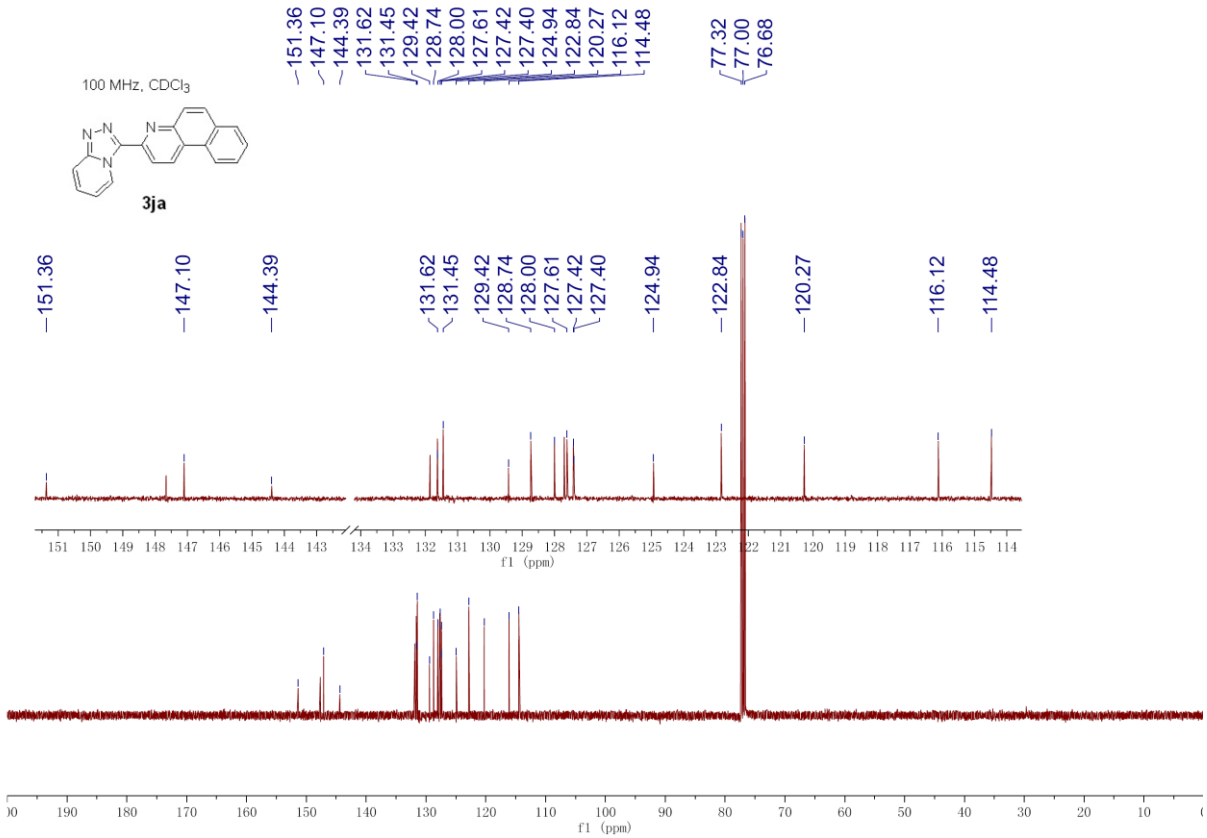

400 MHz, CDCl3
3ia
f1 (ppm)

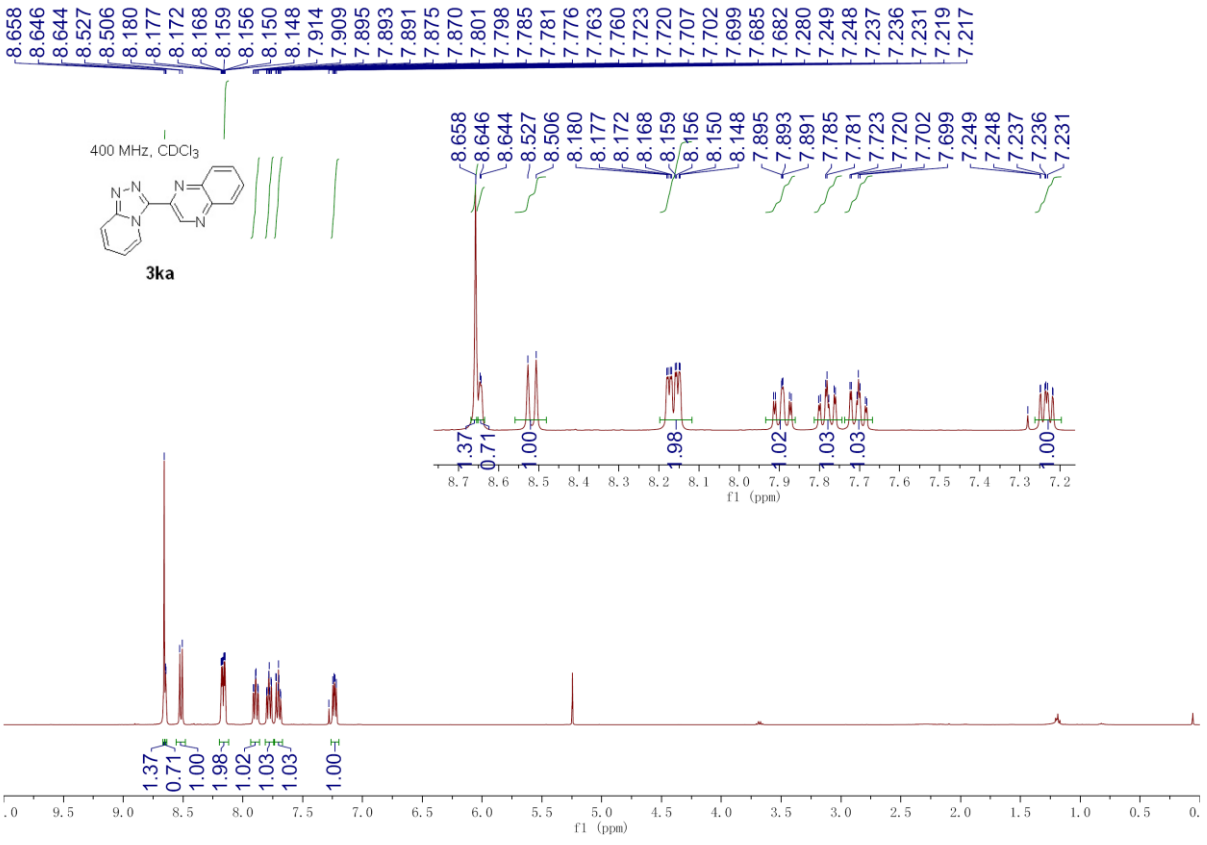

10.115
10.112
10.108
10.097
10.094
10.091
8.636
8.629
8.627
8.607
8.605
8.291
8.284
8.281
8.262
8.259
7.913
7.893
7.890
7.886
7.860
7.845
7.837
7.822
7.433
7.417
7.407
7.393
7.390
7.373
7.359
7.350
7.248
7.059
7.055
400 MHz, CDCl3
F
N
N
N
3ia
1.14
1.23
1.21
1.00
1.60
1.81
1.16
f1 (ppm)

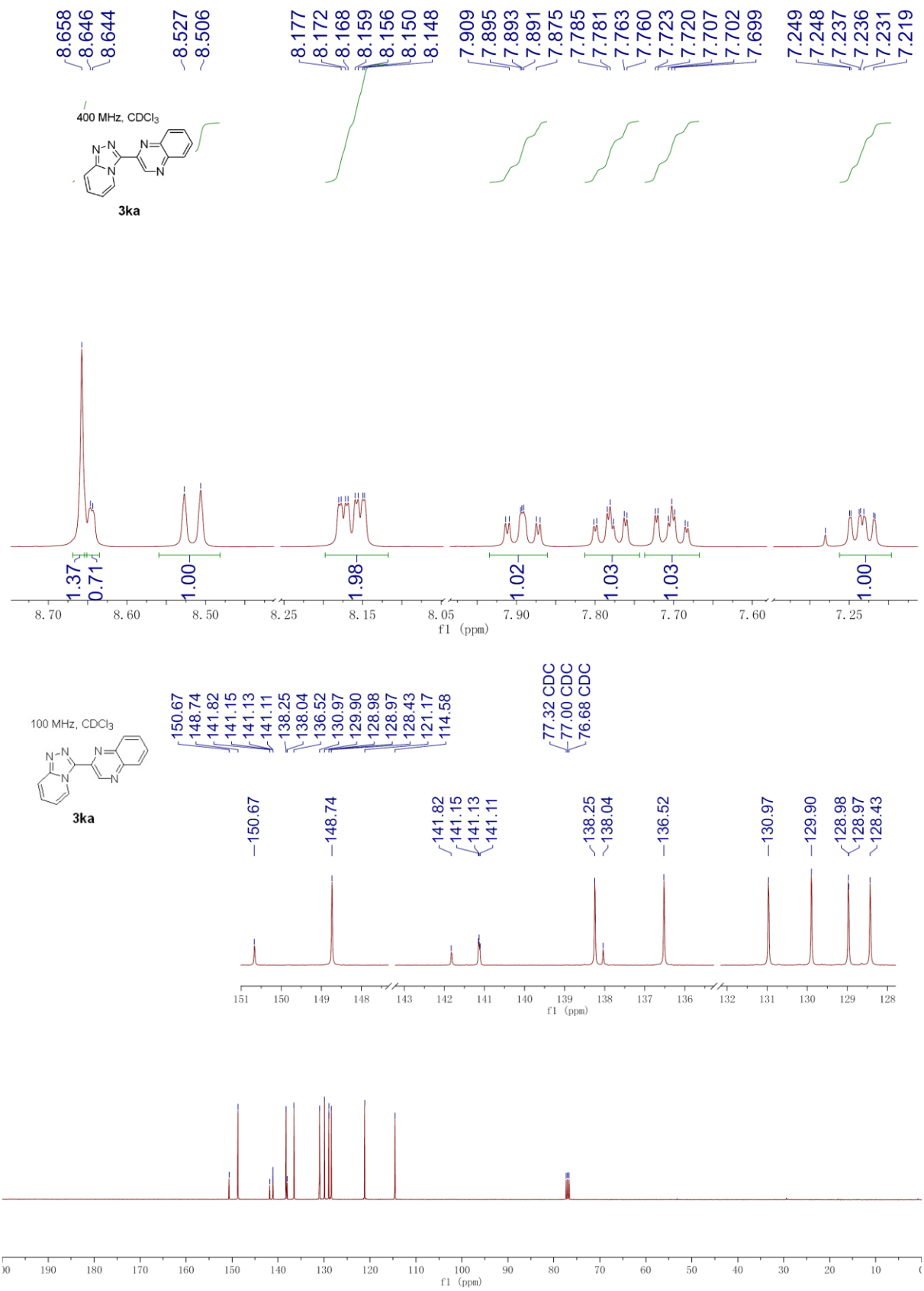

164.67
162.18
151.51
149.23
148.21
148.09
144.19
136.78
136.76
129.88
129.78
128.27
127.36
124.66
124.65
119.50
119.47
117.65
117.40
116.18
114.74
113.05
112.85
77.32
77.00
76.68
100 MHz, CDCl3
F
N
N
N
3ia
f1 (ppm)

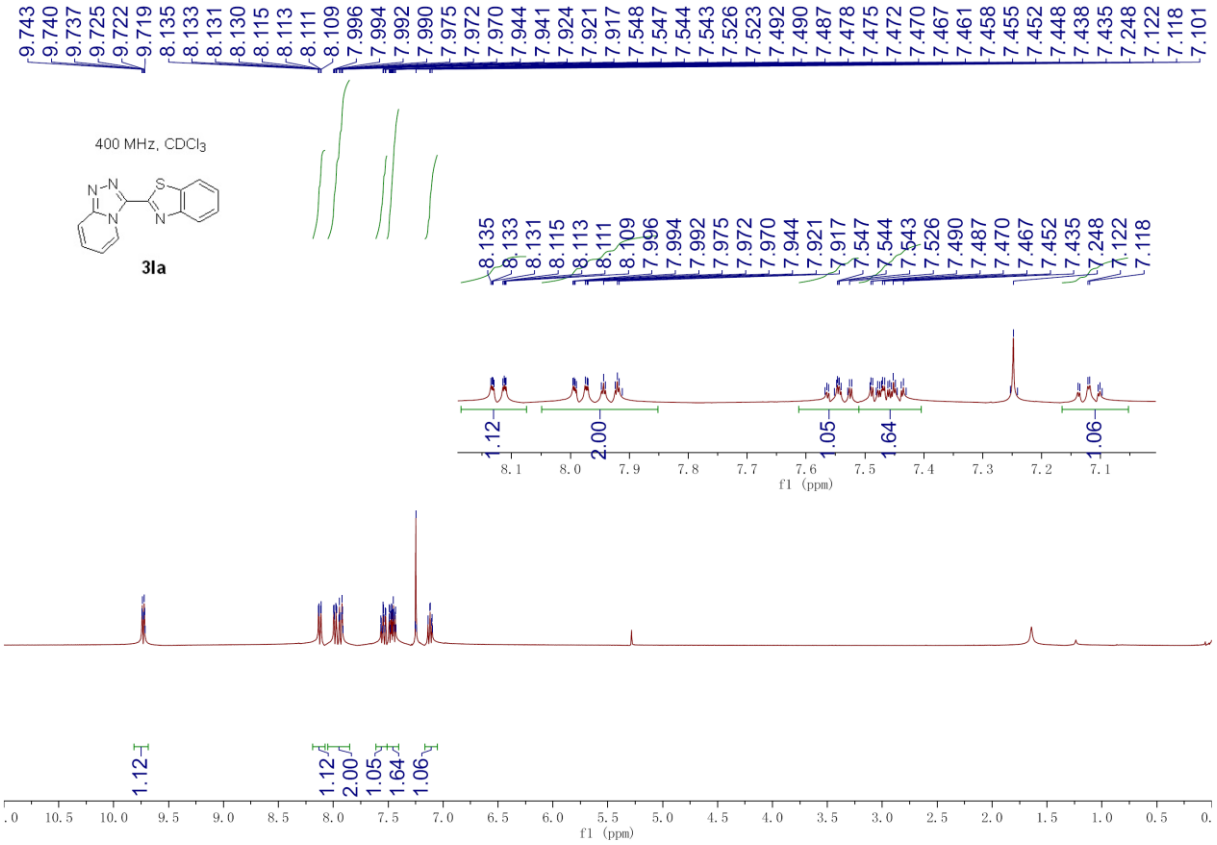

10.137
10.134
10.130
10.119
10.116
10.113
9.031
9.008
8.759
8.737
8.612
8.609
8.588
7.996
7.926
7.925
7.922
7.920
7.906
7.902
7.901
7.889
7.886
7.883
7.866
7.863
7.860
7.692
7.688
7.672
7.667
7.658
7.654
7.638
7.635
7.388
7.385
7.372
7.369
7.365
7.362
7.349
7.345
7.248
7.032
7.028
7.015
7.014
7.012
7.011
6.994
400 MHz, CDCl3
3ja
1.00
1.11
1.20
0.97
2.49
1.66
1.74
0.90
1.03
f1 (ppm)

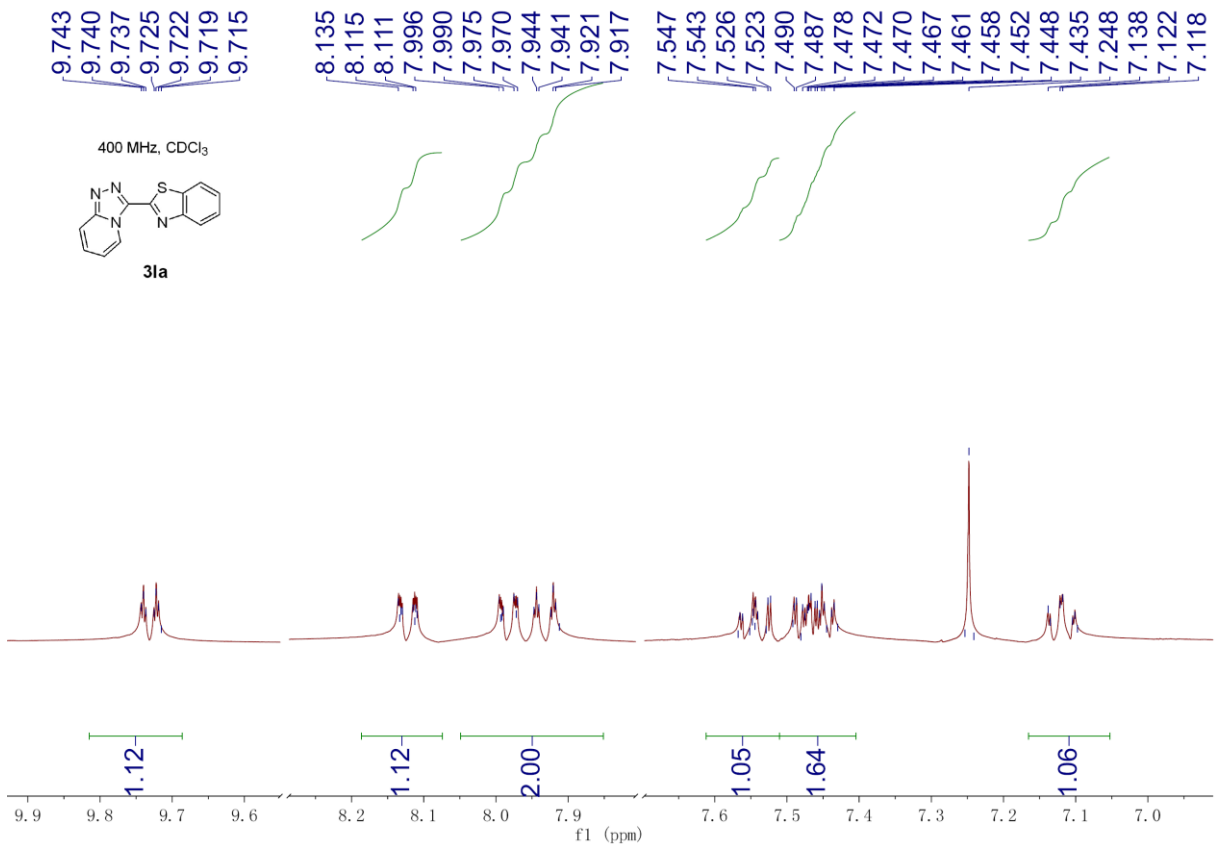

10.137
10.134
10.130
10.119
10.116
10.113
9.031
9.008
8.759
8.737
8.612
8.609
8.588
7.996
7.926
7.906
7.902
7.901
7.886
7.863
7.860
7.692
7.688
7.672
7.658
7.654
7.635
7.248
7.015
7.014
7.012
7.011
400 MHz, CDCl3
3ja
1.00
1.11
1.20
0.97
2.49
1.66
1.74
0.90
1.03
f1 (ppm)

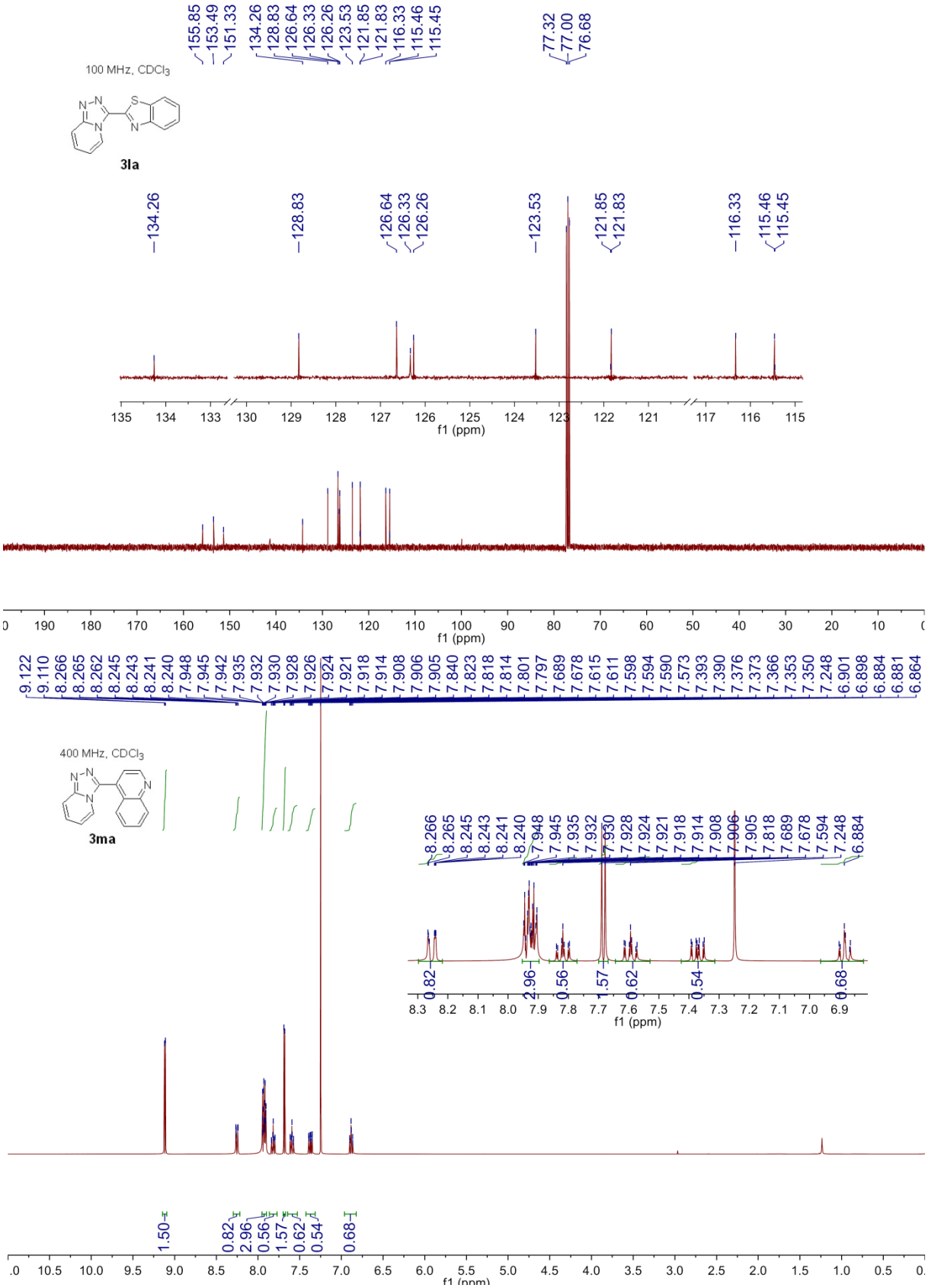

100 MHz, CDCl3
3ja
151.36
147.10
144.39
131.62
131.45
129.42
128.74
128.00
127.61
127.42
127.40
124.94
122.84
120.27
116.12
114.48
77.32
77.00
76.68
f1 (ppm)

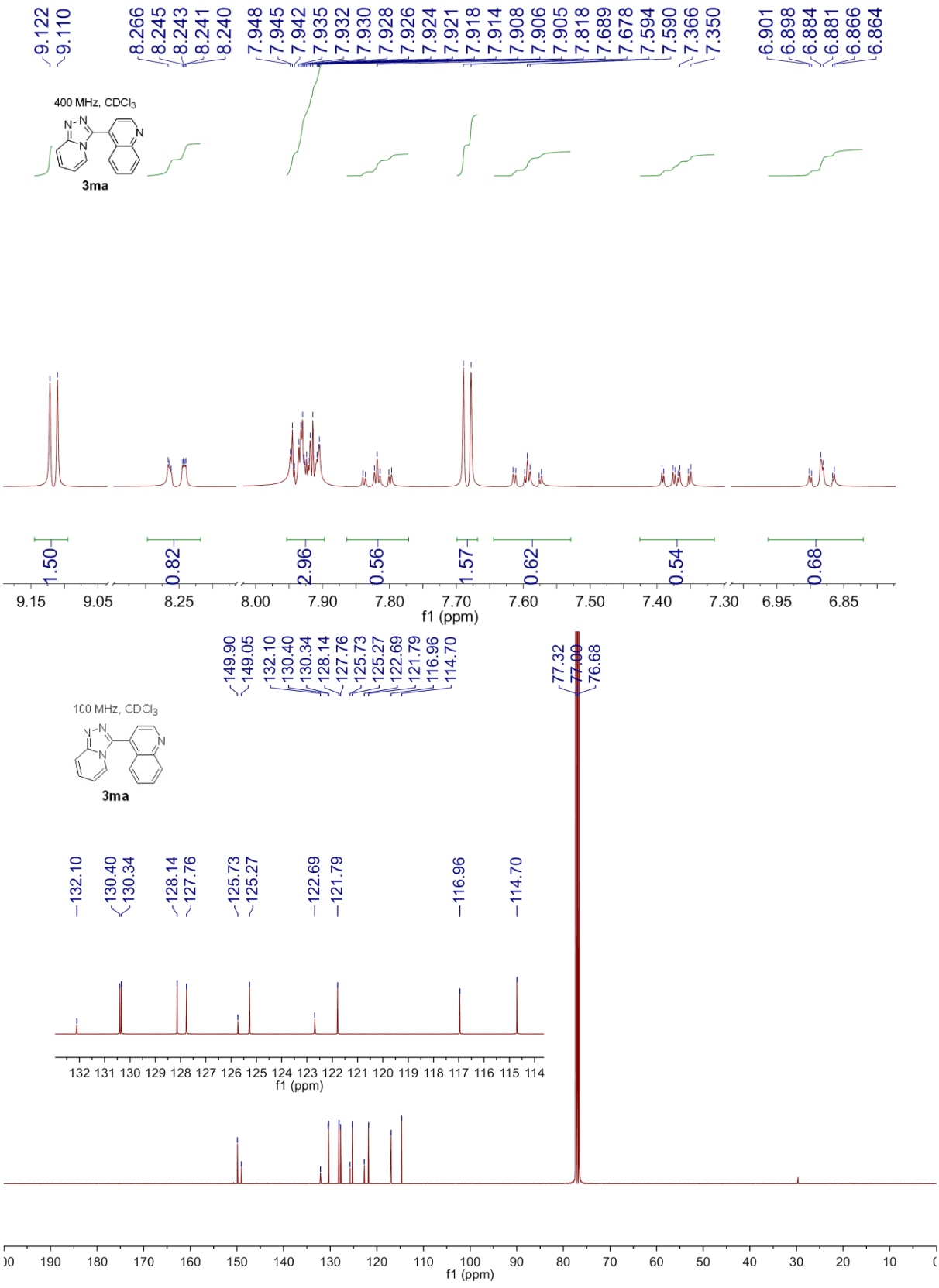

400 MHz, CDCl3
3ka
8.658
8.646
8.644
8.527
8.506
8.180
8.177
8.172
8.168
8.159
8.156
8.150
8.148
7.914
7.909
7.895
7.893
7.891
7.875
7.870
7.801
7.798
7.785
7.781
7.776
7.763
7.760
7.723
7.720
7.707
7.702
7.699
7.685
7.682
7.280
7.249
7.248
7.237
7.236
7.231
7.219
7.217
1.37
0.71
1.00
1.98
1.02
1.03
1.03
1.00
f1 (ppm)

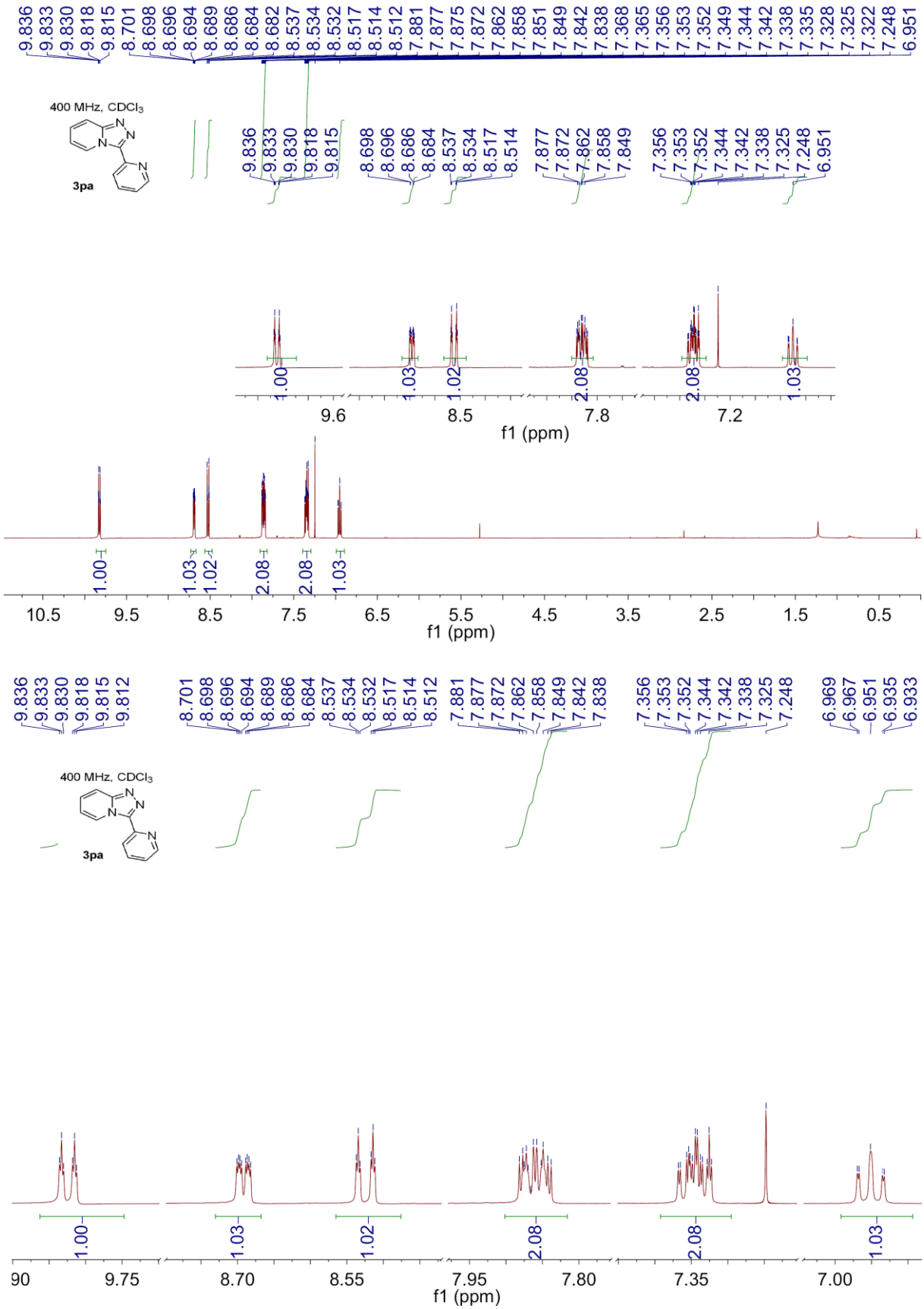

8.658
8.646
8.644
8.527
8.506
8.177
8.172
8.168
8.159
8.156
8.150
8.148
7.909
7.895
7.893
7.891
7.875
7.785
7.781
7.763
7.760
7.723
7.720
7.707
7.702
7.699
7.249
7.248
7.237
7.236
7.231
7.219
400 MHz, CDCl3
3ka
1.37
0.71
1.00
1.98
1.02
1.03
1.03
1.00
f1 (ppm)
100 MHz, CDCl3
3ka
150.67
148.74
141.82
141.15
141.13
141.11
138.25
138.04
136.52
130.97
129.90
128.98
128.97
128.43
121.17
114.58
77.32 CDC
77.00 CDC
76.68 CDC
f1 (ppm)
f1 (ppm)

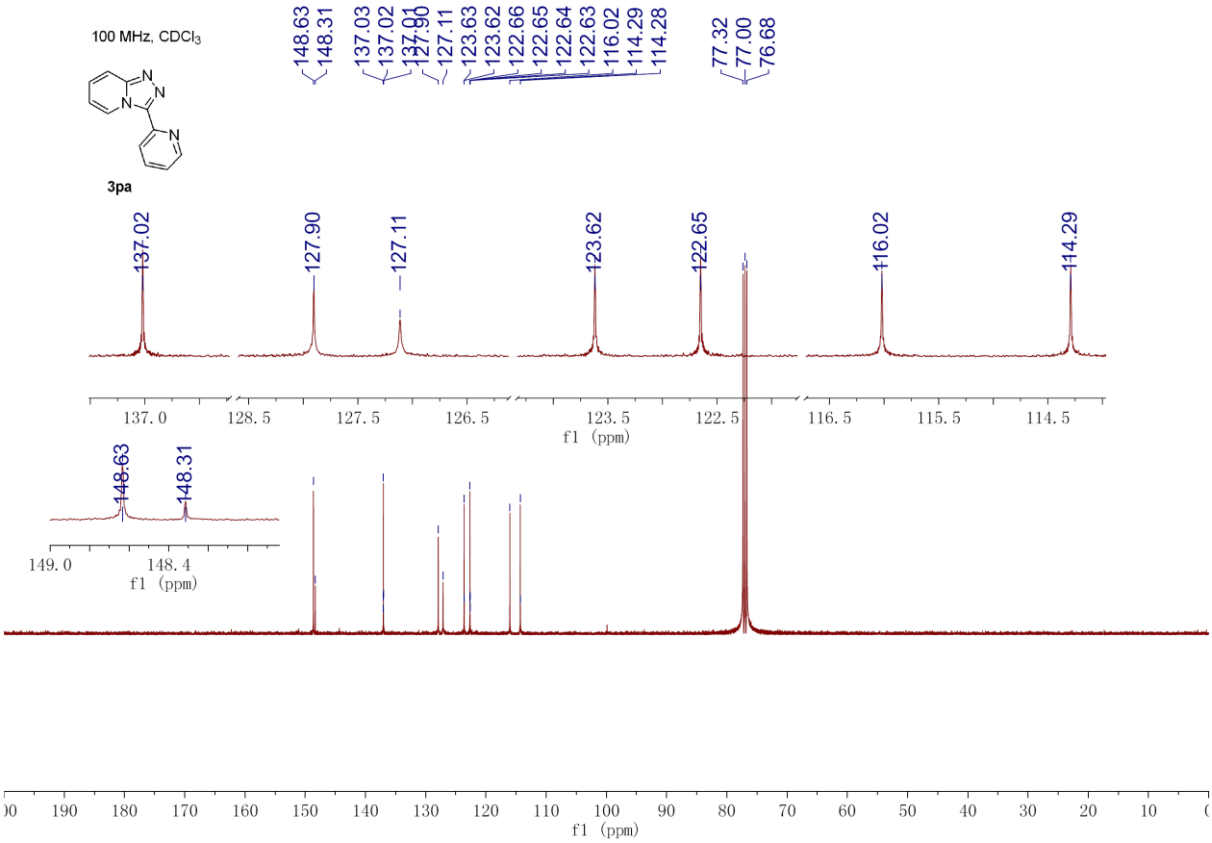

9.743
9.740
9.737
9.725
9.722
9.719
8.135
8.133
8.131
8.115
8.113
8.111
8.109
7.996
7.994
7.992
7.990
7.975
7.972
7.970
7.944
7.941
7.924
7.921
7.917
7.548
7.547
7.544
7.543
7.526
7.523
7.492
7.490
7.487
7.478
7.475
7.472
7.470
7.467
7.461
7.458
7.455
7.452
7.448
7.438
7.435
7.248
7.122
7.118
7.101
400 MHz, CDCl3
3la
1.12
2.00
1.05
1.64
1.06
f1 (ppm)

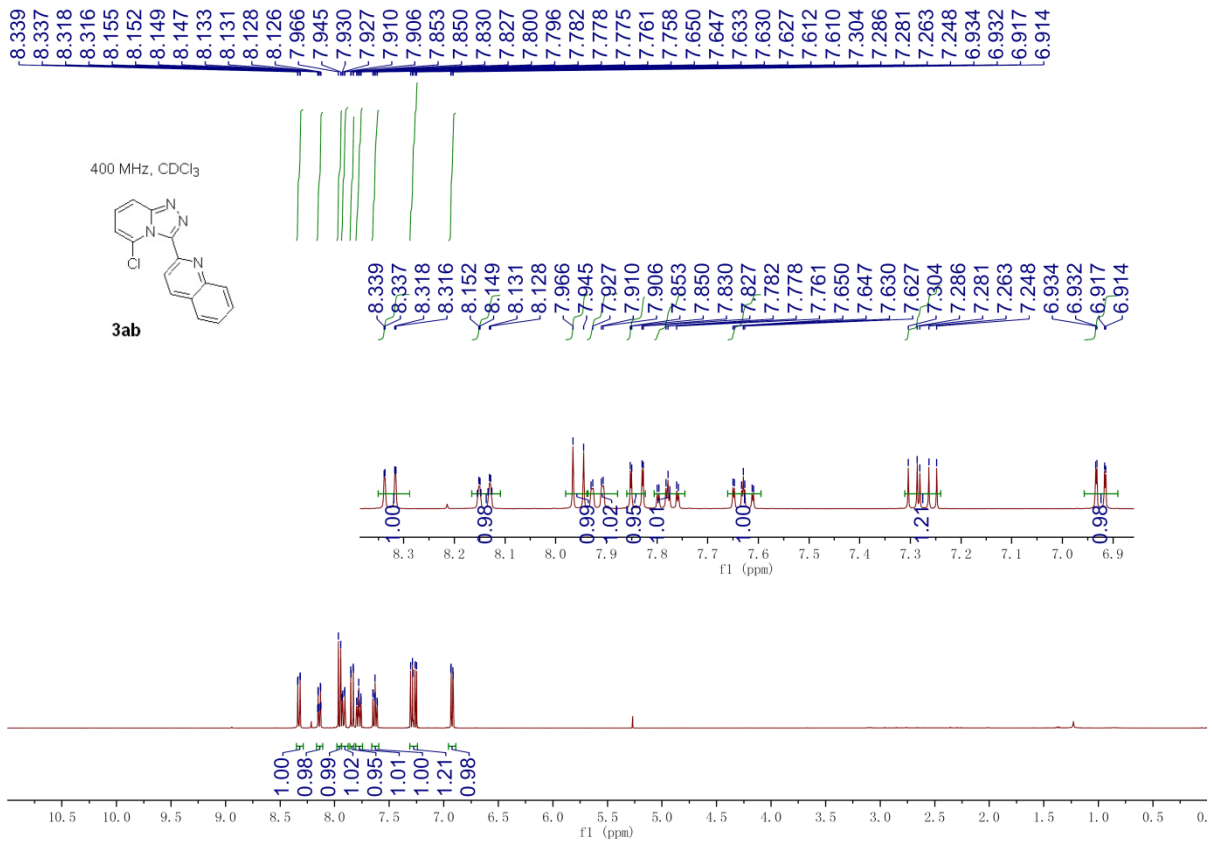

9.743
9.740
9.737
9.725
9.722
9.719
9.715
8.135
8.115
8.111
7.996
7.990
7.975
7.970
7.944
7.941
7.921
7.917
7.547
7.543
7.526
7.523
7.490
7.487
7.478
7.472
7.470
7.467
7.461
7.458
7.452
7.448
7.435
7.248
7.138
7.122
7.118
400 MHz, CDCl3
3la
1.12
1.12
2.00
1.05
1.64
1.06
f1 (ppm)


155.85
153.49
151.33
134.26
128.83
126.64
126.33
126.26
123.53
121.85
121.83
116.33
115.46
115.45
77.32
77.00
76.68
100 MHz, CDCl3
3la
f1 (ppm)
9.122
9.110
8.266
8.265
8.262
8.245
8.243
8.241
8.240
7.948
7.945
7.942
7.935
7.932
7.930
7.928
7.926
7.924
7.921
7.918
7.914
7.908
7.906
7.905
7.840
7.823
7.818
7.814
7.801
7.797
7.689
7.678
7.615
7.611
7.598
7.594
7.590
7.573
7.393
7.390
7.376
7.373
7.366
7.353
7.350
7.248
6.901
6.898
6.884
6.881
6.864
400 MHz, CDCl3
3ma
0.82
2.96
0.56
1.57
0.62
0.54
0.68
1.50
f1 (ppm)


9.122
9.110
8.266
8.245
8.243
8.241
8.240
7.948
7.945
7.942
7.935
7.932
7.930
7.928
7.926
7.924
7.921
7.918
7.914
7.908
7.906
7.905
7.818
7.689
7.678
7.594
7.590
7.366
7.350
6.901
6.898
6.884
6.881
6.866
6.864
400 MHz, CDCl3
3ma
1.50
0.82
2.96
0.56
1.57
0.62
0.54
0.68
f1 (ppm)
149.90
149.05
132.10
130.40
130.34
128.14
127.76
125.73
125.27
122.69
121.79
116.96
114.70
77.32
77.00
76.68
100 MHz, CDCl3
3ma
f1 (ppm)
f1 (ppm)


9.836
9.833
9.830
9.818
9.815
8.701
8.698
8.696
8.694
8.689
8.686
8.684
8.682
8.537
8.534
8.532
8.517
8.514
8.512
7.881
7.877
7.875
7.872
7.862
7.858
7.851
7.849
7.842
7.838
7.368
7.365
7.356
7.353
7.352
7.349
7.344
7.342
7.338
7.335
7.328
7.325
7.322
7.248
6.951
400 MHz, CDCl3
3pa
1.00
1.03
1.02
2.08
2.08
1.03
f1 (ppm)
9.812
6.969
6.967
6.935
6.933


100 MHz, CDCl3
3pa
148.63
148.31
137.03
137.02
137.01
127.90
127.11
123.63
123.62
122.66
122.65
122.64
122.63
116.02
114.29
114.28
77.32
77.00
76.68
137.02
127.90
127.11
123.62
122.65
116.02
114.29
137.0
128.5
127.5
126.5
123.5
122.5
116.5
115.5
114.5
f1 (ppm)
148.63
148.31
149.0
148.4
f1 (ppm)
f1 (ppm)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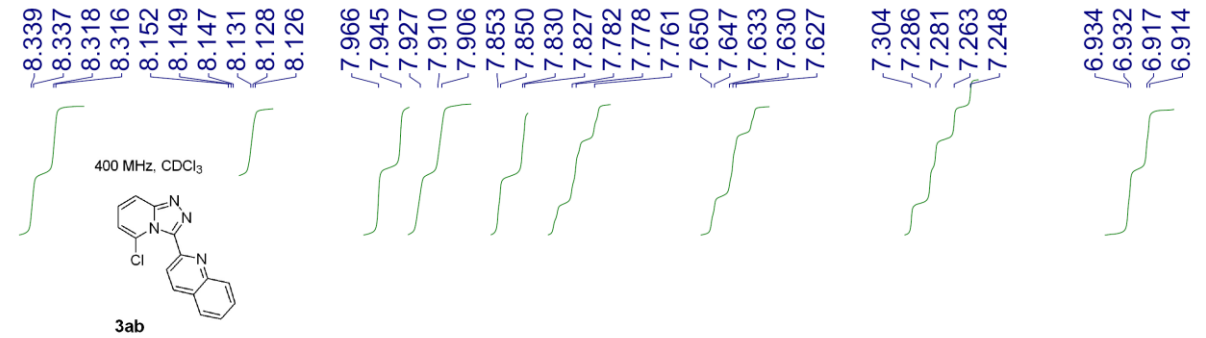
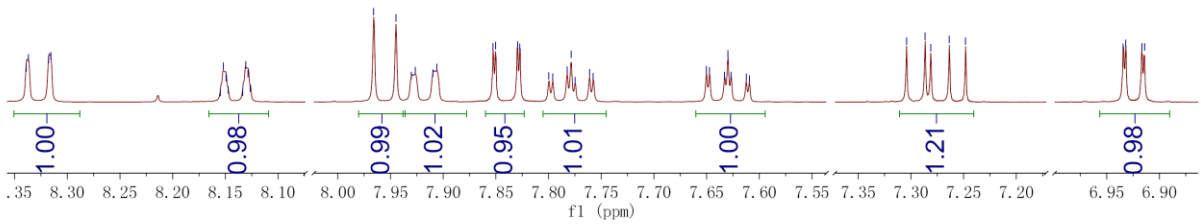
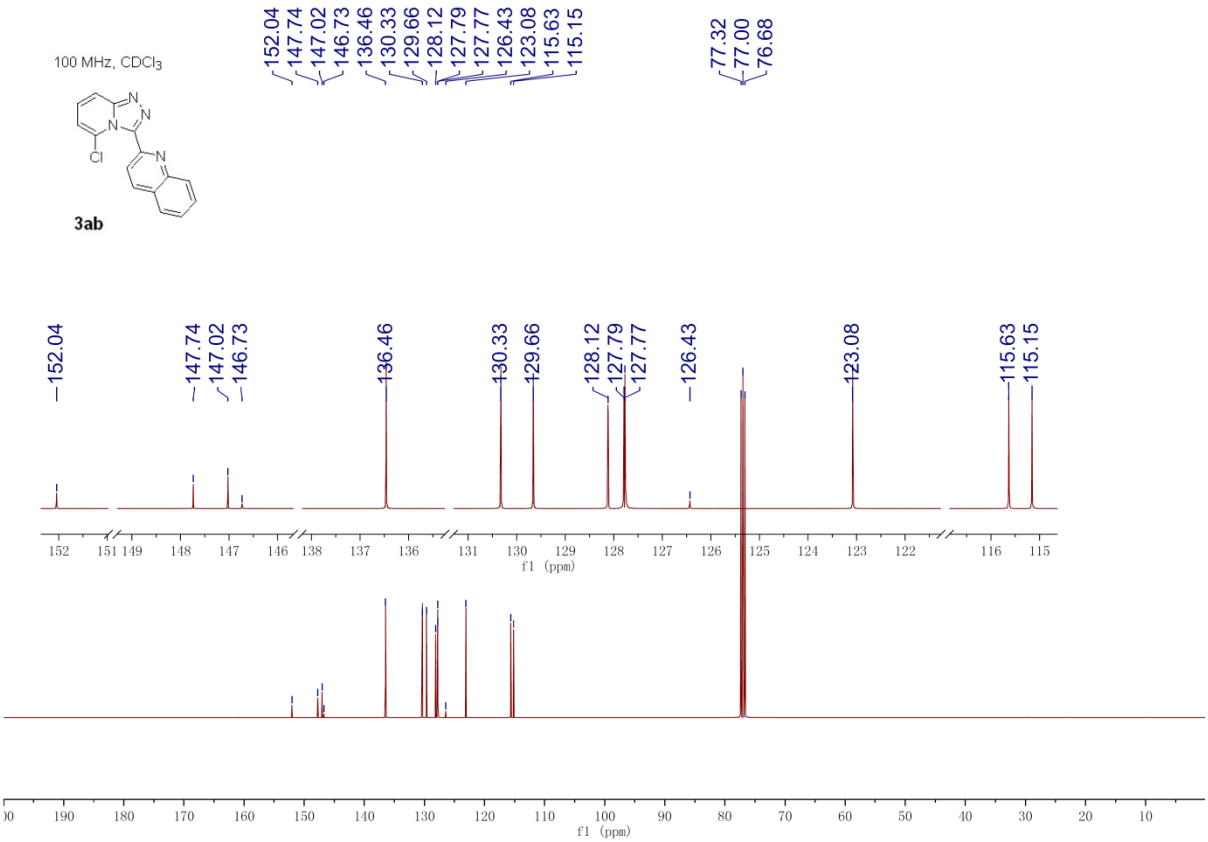
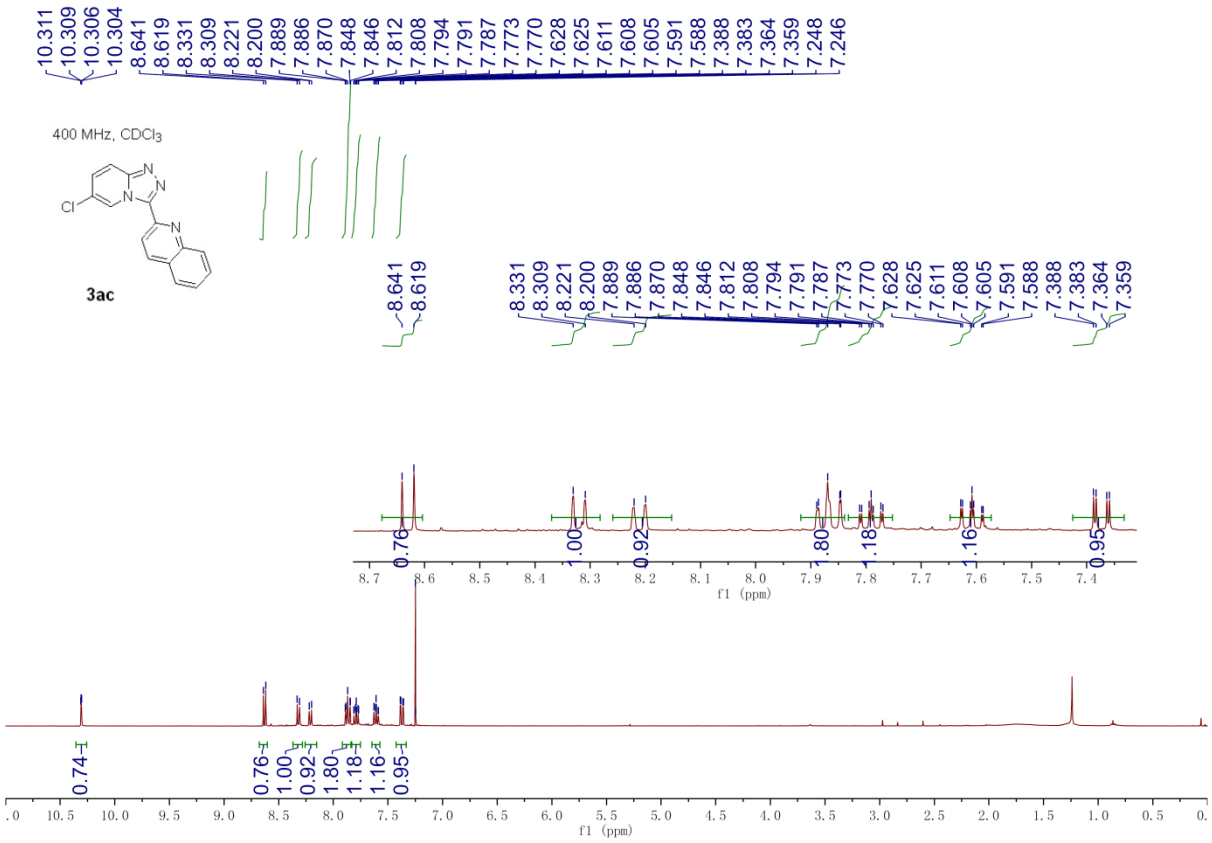
8.337
8.318
8.316
8.155
8.152
8.149
8.147
8.133
8.131
8.128
8.126
7.966
7.945
7.930
7.927
7.910
7.906
7.853
7.850
7.830
7.827
7.800
7.796
7.782
7.778
7.775
7.761
7.758
7.650
7.647
7.633
7.630
7.627
7.612
7.610
7.304
7.286
7.281
7.263
7.248
6.934
6.932
6.917
6.914
400 MHz, CDCl3
Cl
3ab
1.00
0.98
0.99
1.02
0.95
1.01
1.00
1.21
0.98
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
f1 (ppm)
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


8.339
8.337
8.318
8.316
8.152
8.149
8.147
8.131
8.128
8.126
7.966
7.945
7.927
7.910
7.906
7.853
7.850
7.830
7.827
7.782
7.778
7.761
7.650
7.647
7.633
7.630
7.627
7.304
7.286
7.281
7.263
7.248
6.934
6.932
6.917
6.914
400 MHz, CDCl3
Cl
3ab


1.00
0.98
0.99
1.02
0.95
1.01
1.00
1.21
0.98
f1 (ppm)


152.04
147.74
147.02
146.73
136.46
130.33
129.66
128.12
127.79
127.77
126.43
123.08
115.63
115.15
77.32
77.00
76.68
100 MHz, CDCl3
Cl
3ab
f1 (ppm)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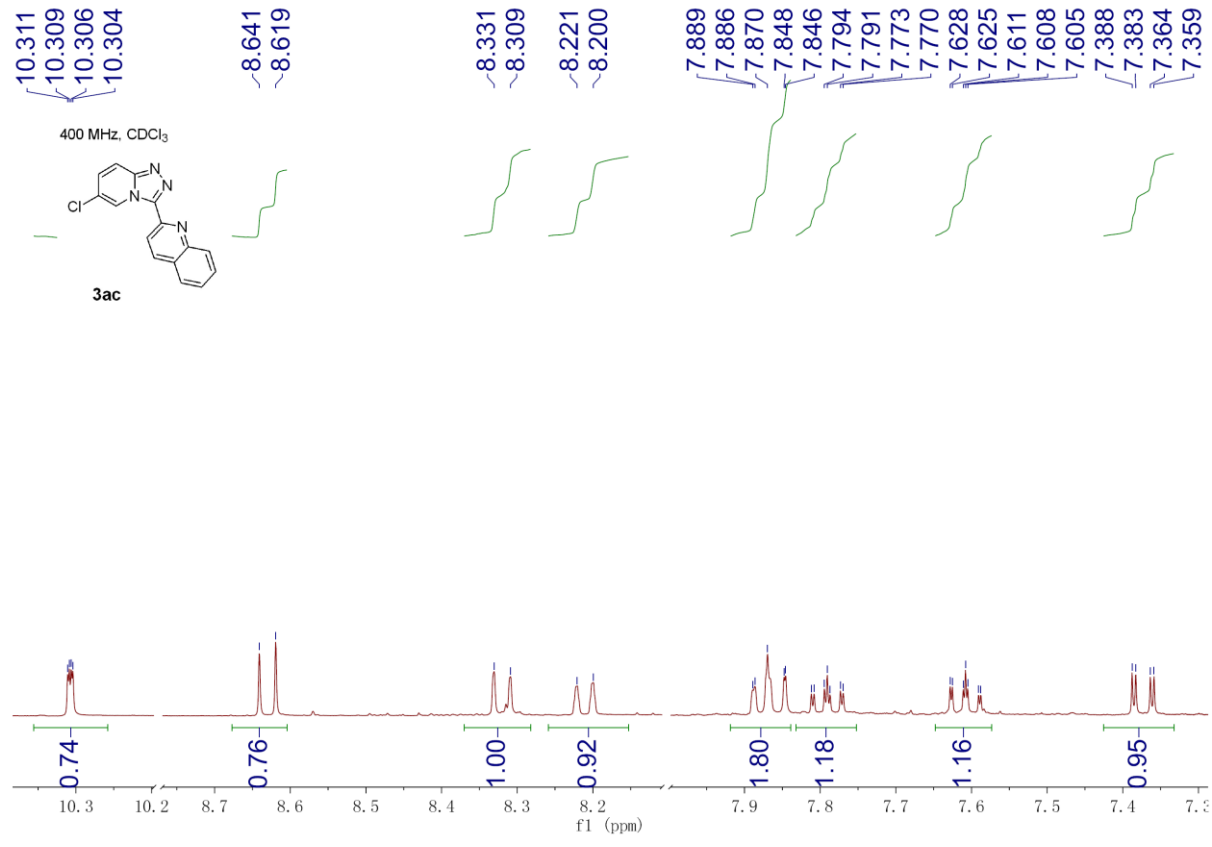
10.309
10.306
10.304
8.641
8.619
8.331
8.309
8.221
8.200
7.889
7.886
7.870
7.848
7.846
7.812
7.808
7.794
7.791
7.787
7.773
7.770
7.628
7.625
7.611
7.608
7.605
7.591
7.588
7.388
7.383
7.364
7.359
7.248
7.246
400 MHz, CDCl3
3ac
0.76
1.00
0.92
1.80
1.18
1.16
0.95
f1 (ppm)
0.74
0.76
1.00
0.92
1.80
1.18
1.16
0.95
f1 (ppm)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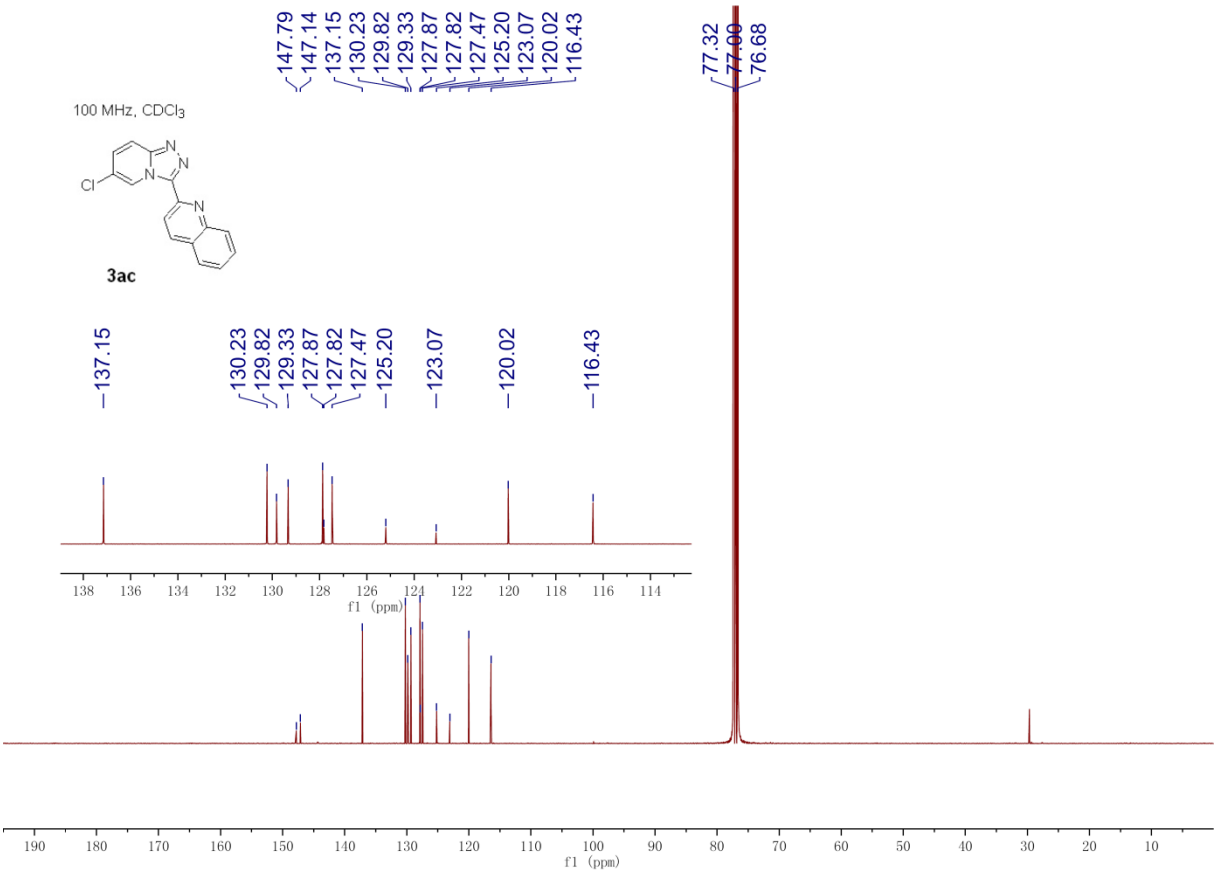
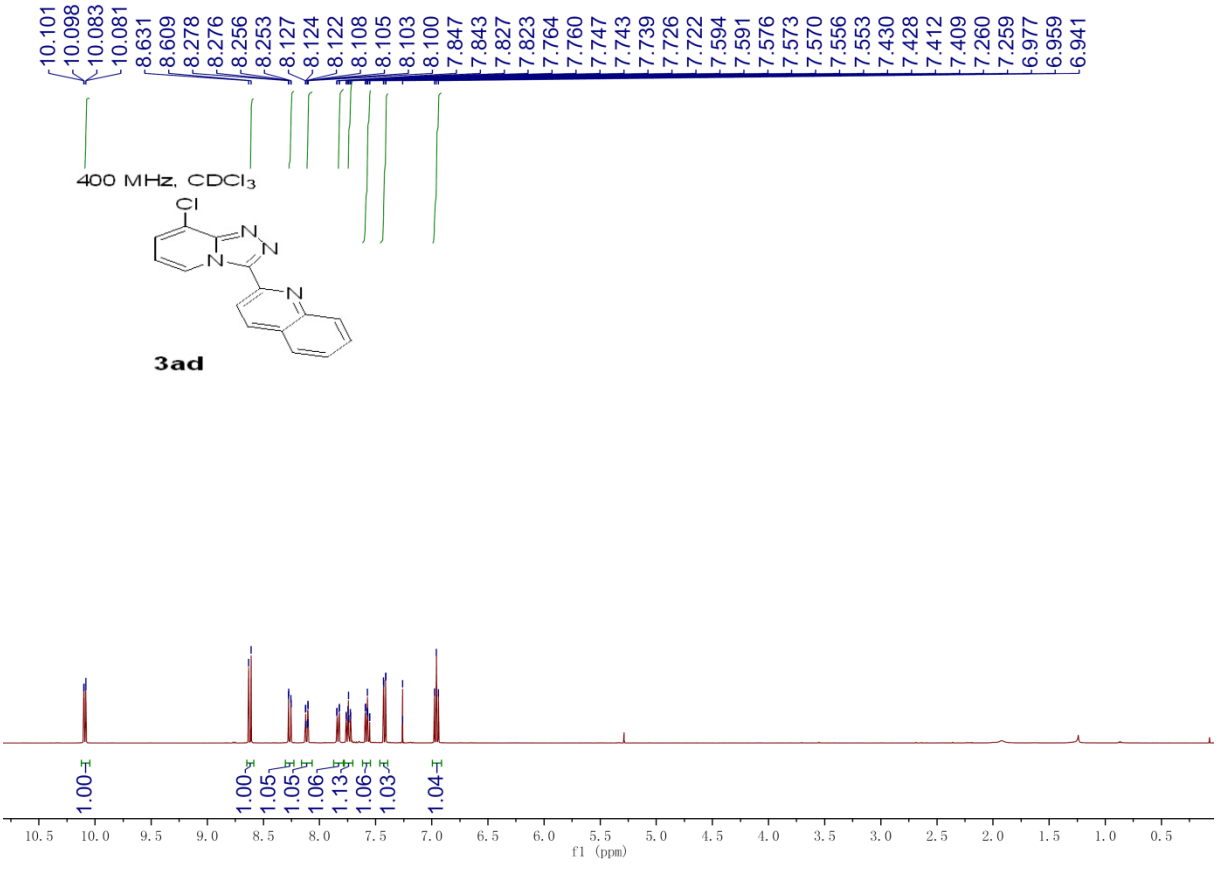
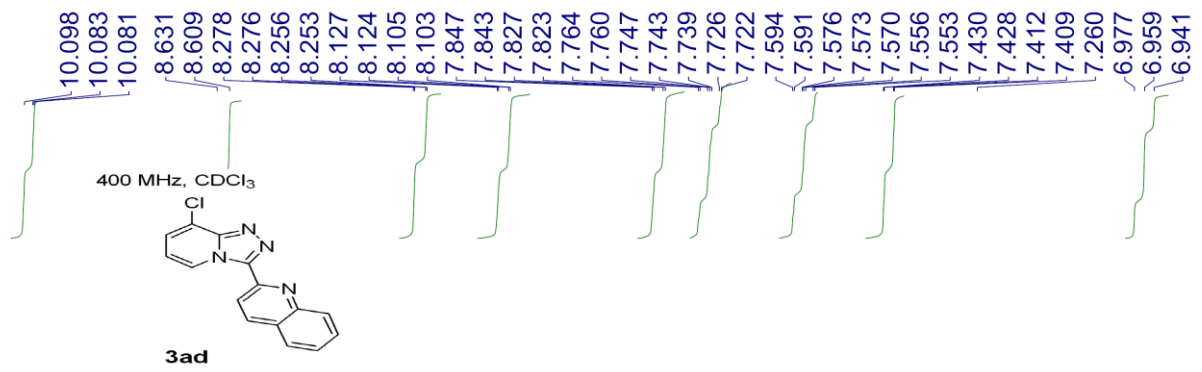
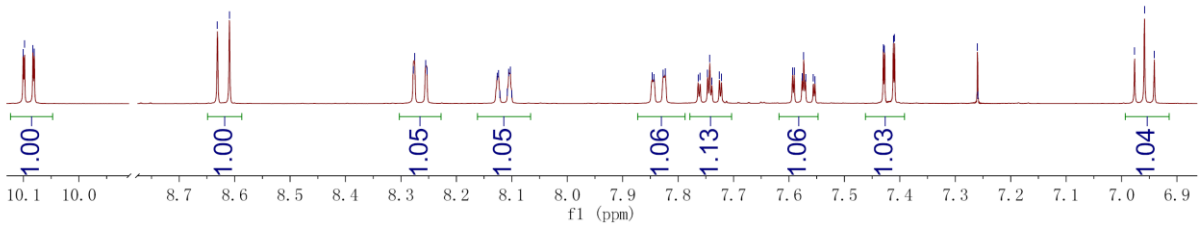
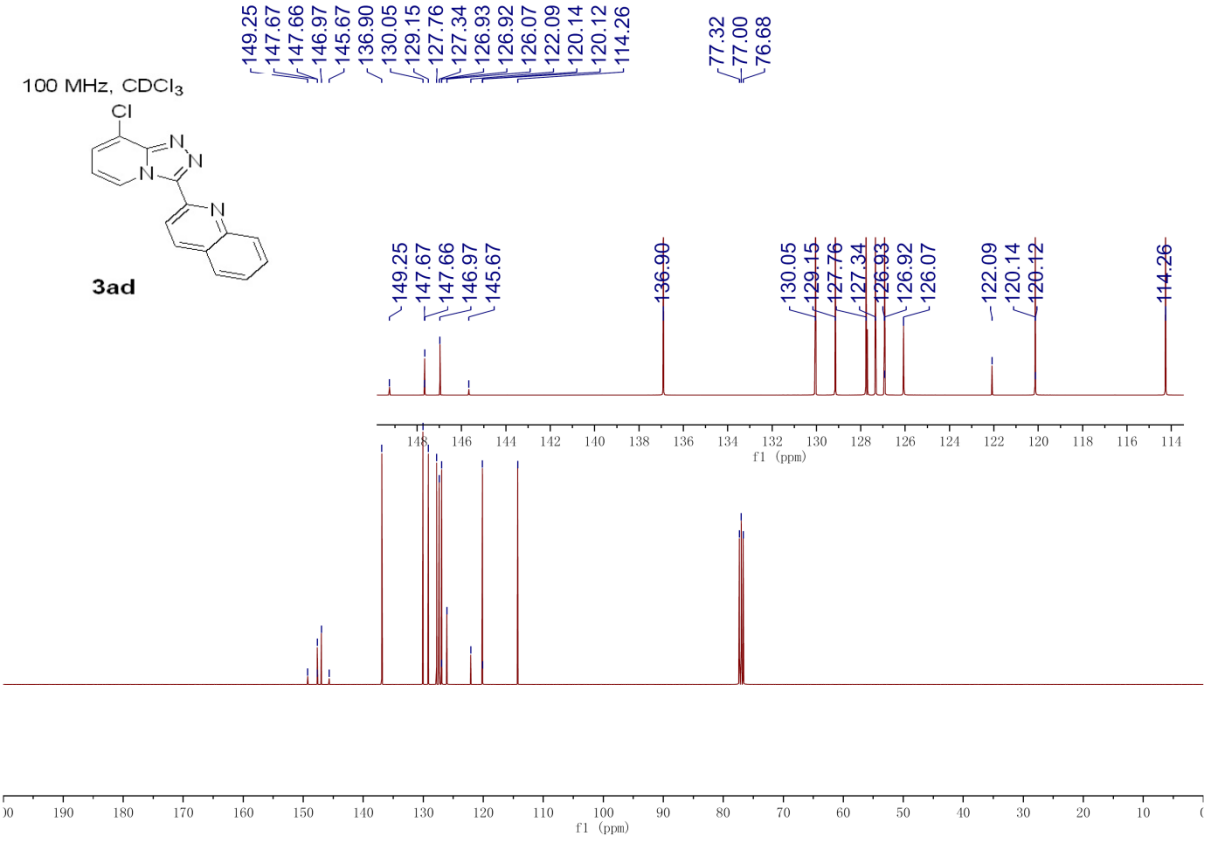
10.309
10.306
10.304
8.641
8.619
8.331
8.309
8.221
8.200
7.889
7.886
7.870
7.848
7.846
7.794
7.791
7.773
7.770
7.628
7.625
7.611
7.608
7.605
7.388
7.383
7.364
7.359
400 MHz, CDCl3
3ac
0.74
0.76
1.00
0.92
1.80
1.18
1.16
0.95
f1 (ppm)

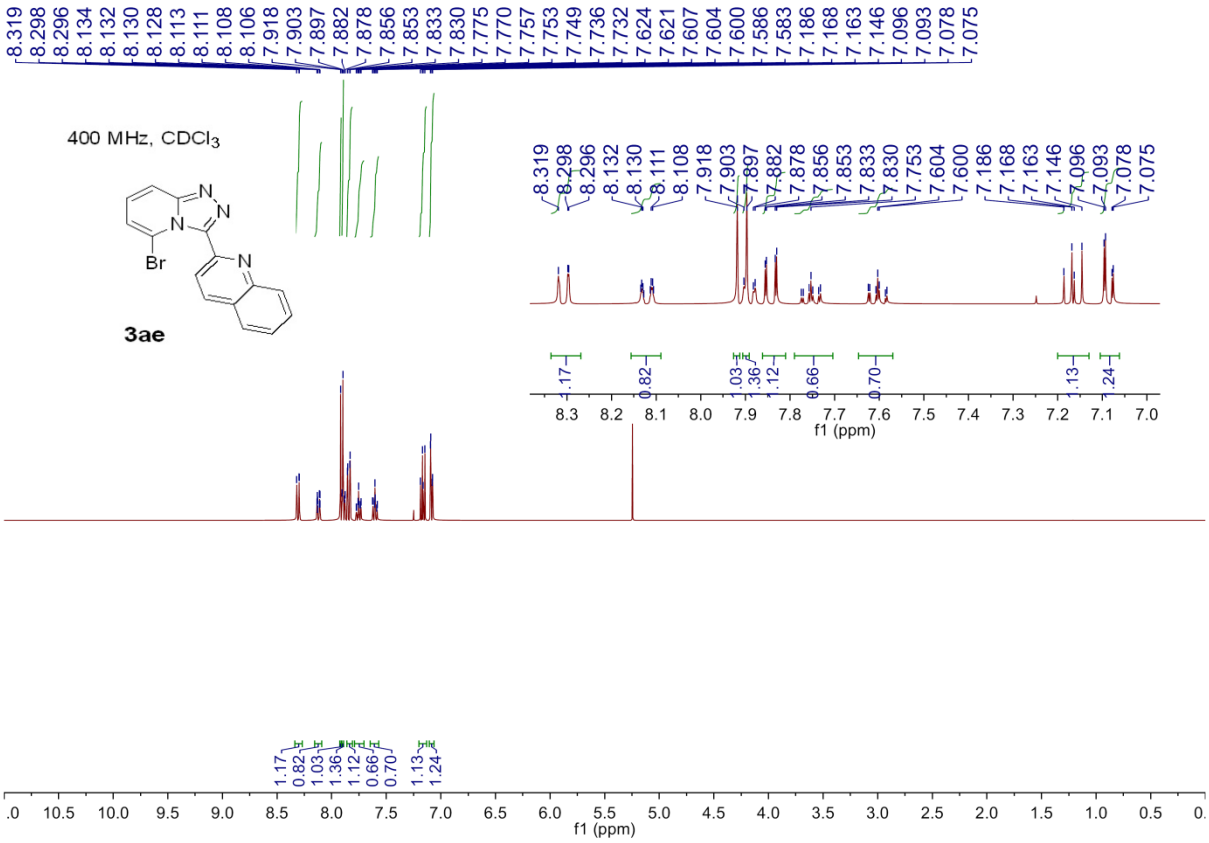

147.79
147.14
137.15
130.23
129.82
129.33
127.87
127.82
127.47
125.20
123.07
120.02
116.43
77.32
77.00
76.68
100 MHz, CDCl3
Cl
N
N
N
N
3ac
137.15
130.23
129.82
129.33
127.87
127.82
127.47
125.20
123.07
120.02
116.43
138 136 134 132 130 128 126 124 122 120 118 116 114
f1 (ppm)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

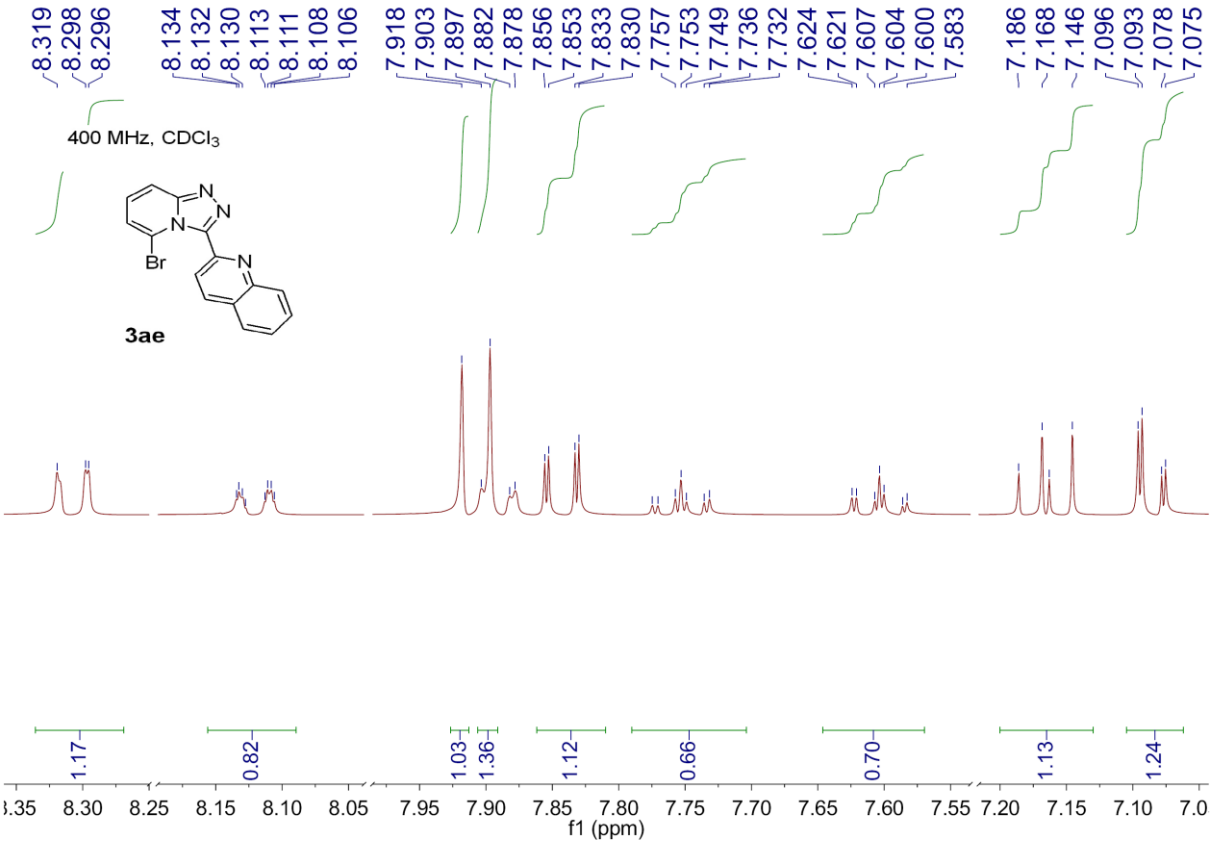

10.101
10.098
10.083
10.081
8.631
8.609
8.278
8.276
8.256
8.253
8.127
8.124
8.122
8.108
8.105
8.103
8.100
7.847
7.843
7.827
7.823
7.764
7.760
7.747
7.743
7.739
7.726
7.722
7.594
7.591
7.576
7.573
7.570
7.556
7.553
7.430
7.428
7.412
7.409
7.260
7.259
6.977
6.959
6.941
400 MHz, CDCl3
Cl
N
N
N
N
3ad
1.00
1.00
1.05
1.05
1.06
1.13
1.06
1.03
1.04
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

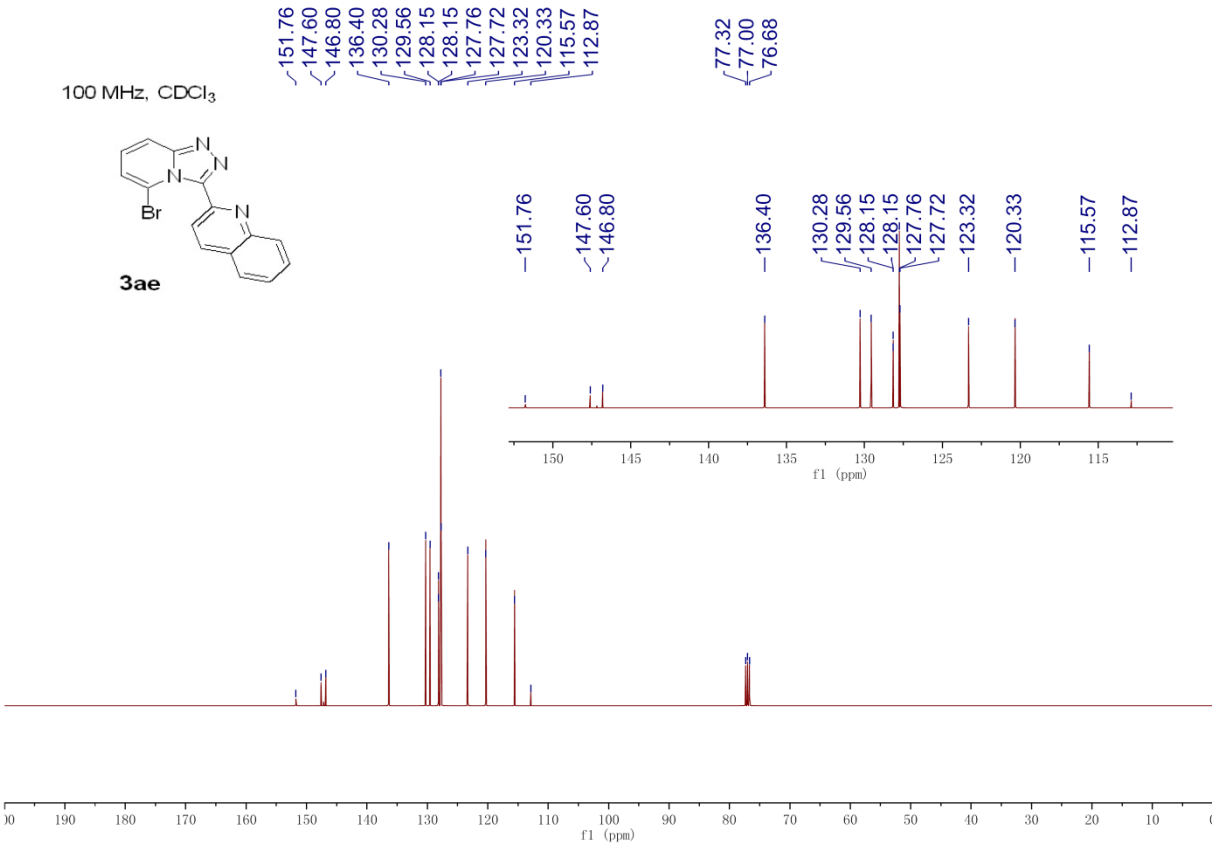

10.098
10.083
10.081
8.631
8.609
8.278
8.276
8.256
8.253
8.127
8.124
8.105
8.103
7.847
7.843
7.827
7.823
7.764
7.760
7.747
7.743
7.739
7.726
7.722
7.594
7.591
7.576
7.573
7.570
7.556
7.553
7.430
7.428
7.412
7.409
7.260
6.977
6.959
6.941
400 MHz, CDCl3
Cl
N
N
N
N
3ad

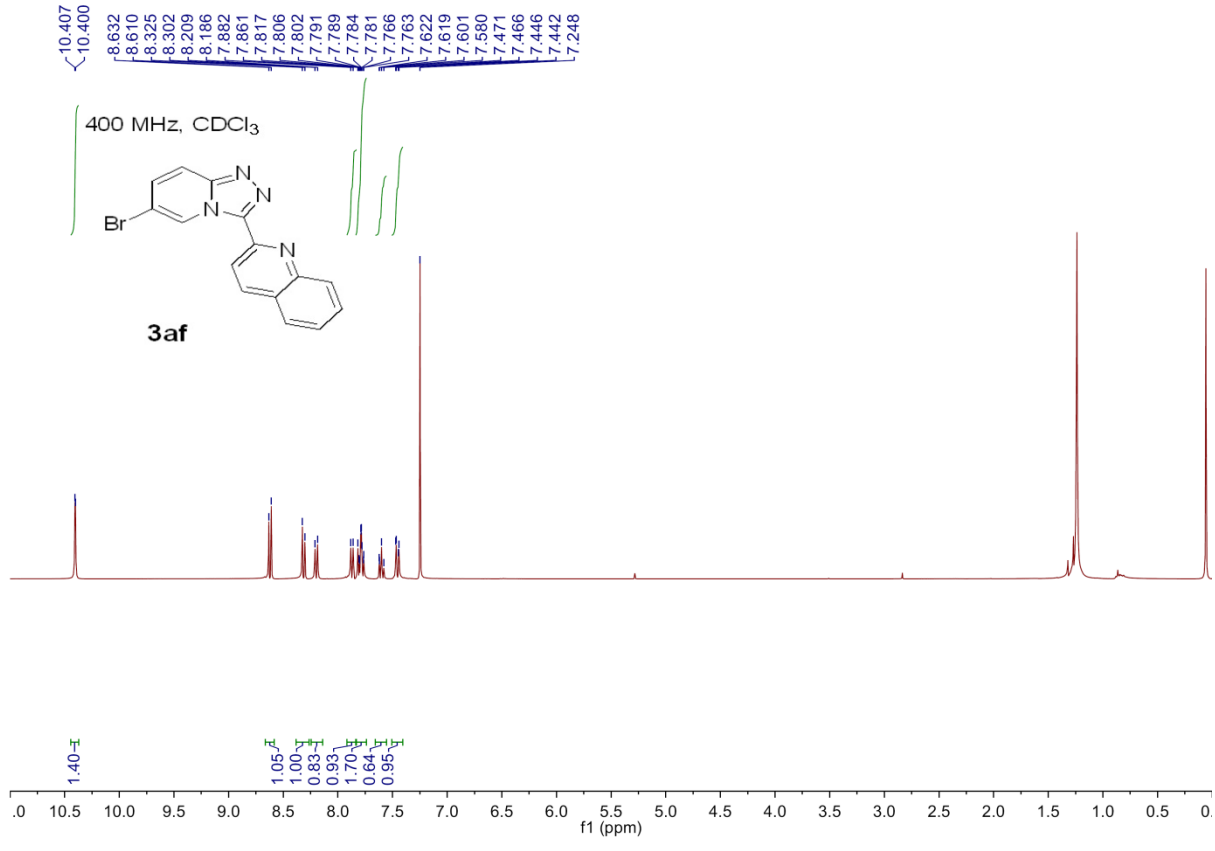

1.00
1.00
1.05
1.05
1.06
1.13
1.06
1.03
1.04
10.1 10.0 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9
f1 (ppm)

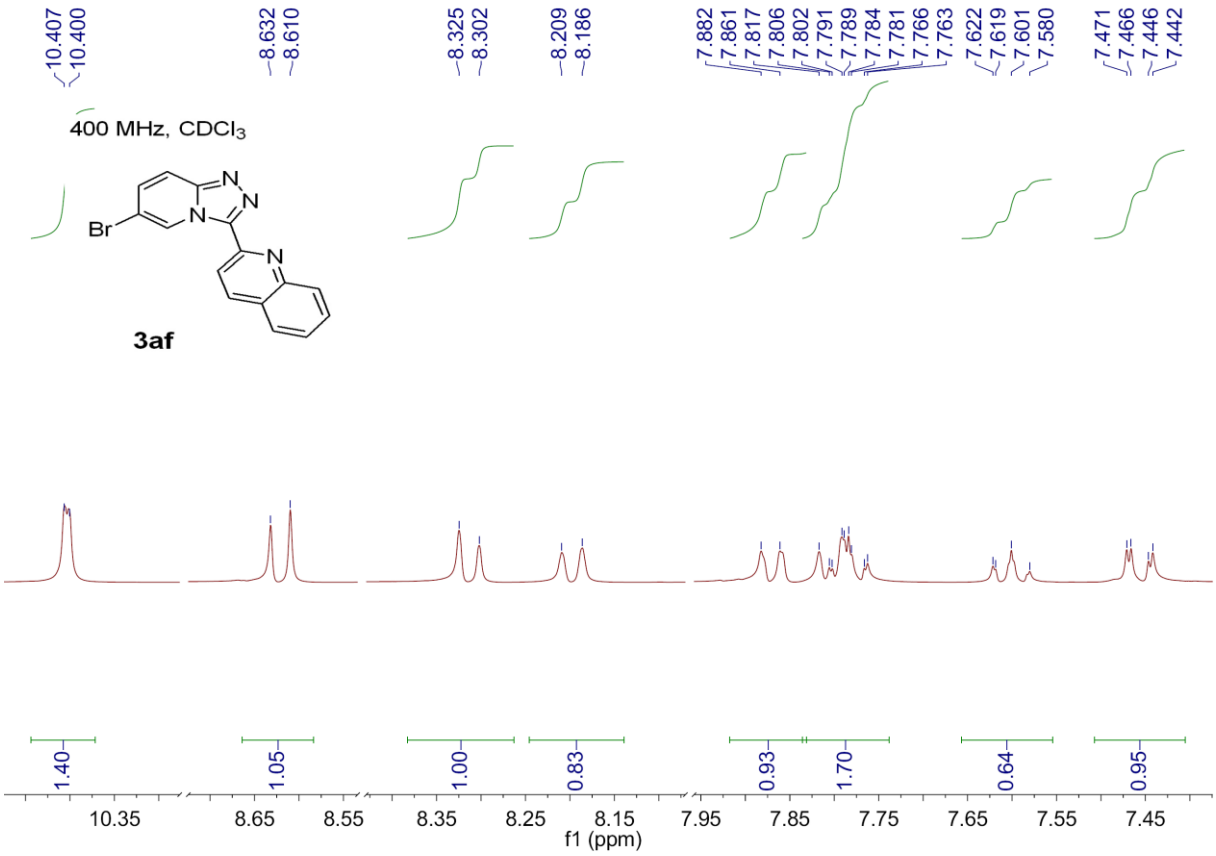

149.25
147.67
147.66
146.97
145.67
136.90
130.05
129.15
127.76
127.34
126.93
126.92
126.07
122.09
120.14
120.12
114.26
77.32
77.00
76.68
100 MHz, CDCl3
Cl
N
N
N
N
3ad
148 146 144 142 140 138 136 134 132 130 128 126 124 122 120 118 116 114
f1 (ppm)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

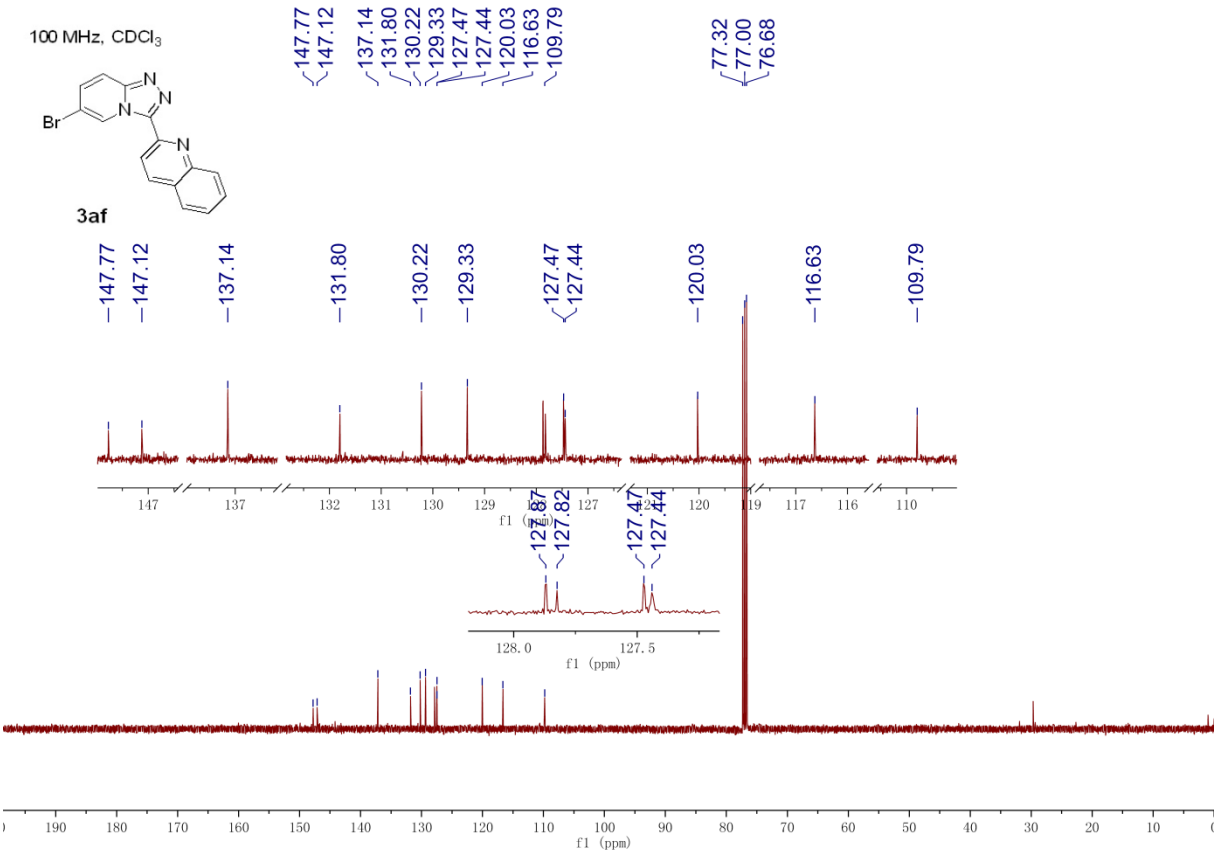

8.319
8.298
8.296
8.134
8.132
8.130
8.128
8.113
8.111
8.108
8.106
7.918
7.903
7.897
7.882
7.878
7.856
7.853
7.833
7.830
7.775
7.770
7.757
7.753
7.749
7.736
7.732
7.624
7.621
7.607
7.604
7.600
7.586
7.583
7.186
7.168
7.163
7.146
7.096
7.093
7.078
7.075
400 MHz, CDCl3
Br
N
3ae
1.17
0.82
1.03
1.36
1.12
0.66
0.70
1.13
1.24
f1 (ppm)

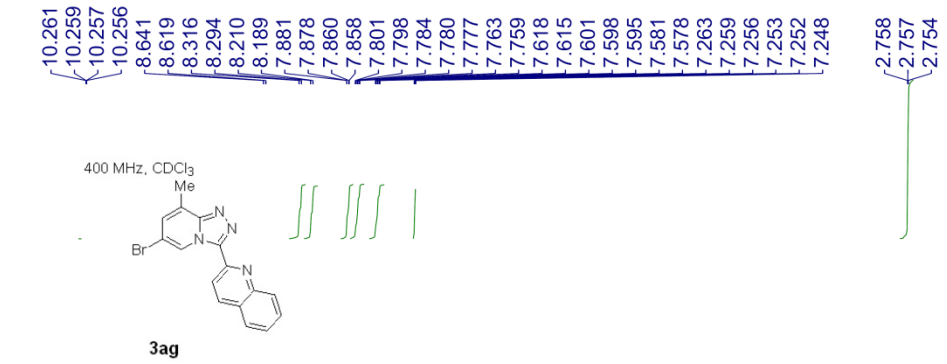

8.319
8.298
8.296
8.134
8.132
8.130
8.113
8.111
8.108
8.106
7.918
7.903
7.897
7.882
7.878
7.856
7.853
7.833
7.830
7.757
7.753
7.749
7.736
7.732
7.624
7.621
7.607
7.604
7.600
7.583
7.186
7.168
7.146
7.096
7.093
7.078
7.075
400 MHz, CDCl3
Br
N
3ae
1.17
0.82
1.03
1.36
1.12
0.66
0.70
1.13
1.24
f1 (ppm)


151.76
147.60
146.80
136.40
130.28
129.56
128.15
128.15
127.76
127.72
123.32
120.33
115.57
112.87
77.32
77.00
76.68
100 MHz, CDCl3
Br
N
N
N
N
3ae
f1 (ppm)
f1 (ppm)


10.407
10.400
8.632
8.610
8.325
8.302
8.209
8.186
7.882
7.861
7.817
7.806
7.802
7.791
7.789
7.784
7.781
7.766
7.763
7.622
7.619
7.601
7.580
7.471
7.466
7.446
7.442
7.248
400 MHz, CDCl3
Br
N
N
N
N
3af
1.40
1.05
1.00
0.83
0.93
1.70
0.64
0.95
f1 (ppm)

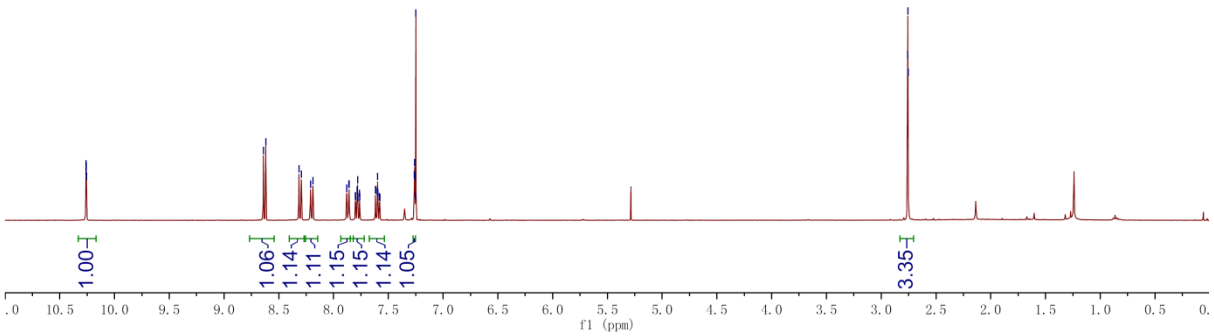

10.407
10.400
8.632
8.610
8.325
8.302
8.209
8.186
7.882
7.861
7.817
7.806
7.802
7.791
7.789
7.784
7.781
7.766
7.763
7.622
7.619
7.601
7.580
7.471
7.466
7.446
7.442
400 MHz, CDCl3
Br
N
N
N
3af
1.40
1.05
1.00
0.83
0.93
1.70
0.64
0.95
10.35
8.65
8.55
8.35
8.25
8.15
7.95
7.85
7.75
7.65
7.55
7.45
f1 (ppm)


100 MHz, CDCl3
147.77
147.12
137.14
131.80
130.22
129.33
127.47
127.44
120.03
116.63
109.79
77.32
77.00
76.68
Br
N
N
N
3af
147
137
132
131
130
129
127
120
119
117
116
110
f1 (ppm)
127.87
127.82
127.47
127.44
128.0
127.5
f1 (ppm)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


10.261
10.259
10.257
10.256
8.641
8.619
8.316
8.294
8.210
8.189
7.881
7.878
7.860
7.858
7.801
7.798
7.784
7.780
7.777
7.763
7.759
7.618
7.615
7.601
7.598
7.595
7.581
7.578
7.263
7.259
7.256
7.253
7.252
7.248
2.758
2.757
2.754

400 MHz, CDCl3
Me
Br
N
N
N

3ag


1.00
1.06
1.14
1.11
1.15
1.15
1.14
1.05
3.35
f1 (ppm)


10.261
10.259
10.257
10.256
8.641
8.619
8.316
8.294
8.210
8.189
7.881
7.878
7.860
7.858
7.801
7.784
7.780
7.763
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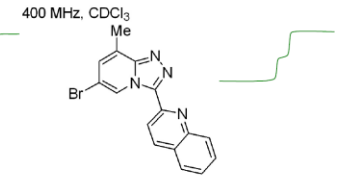
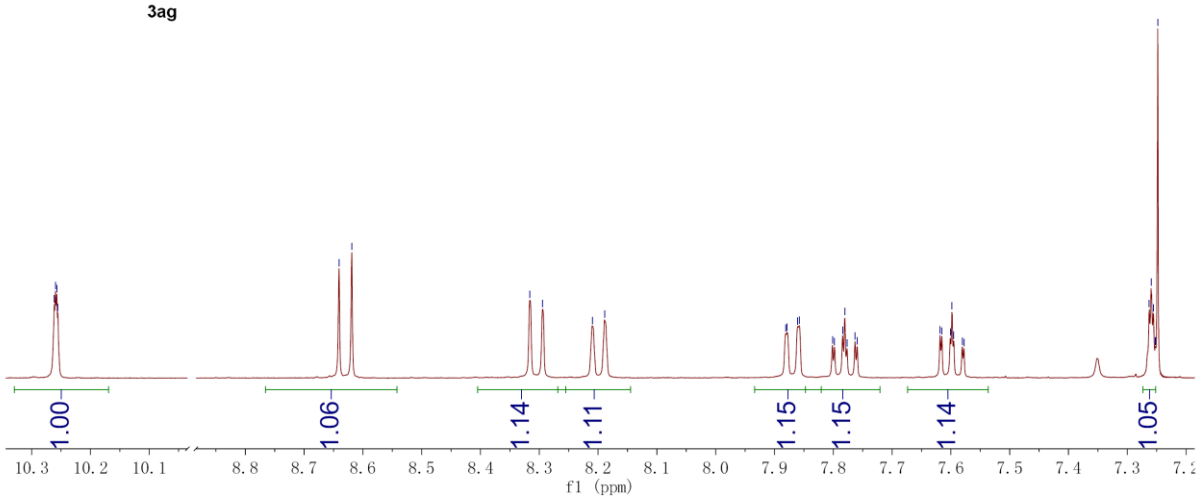
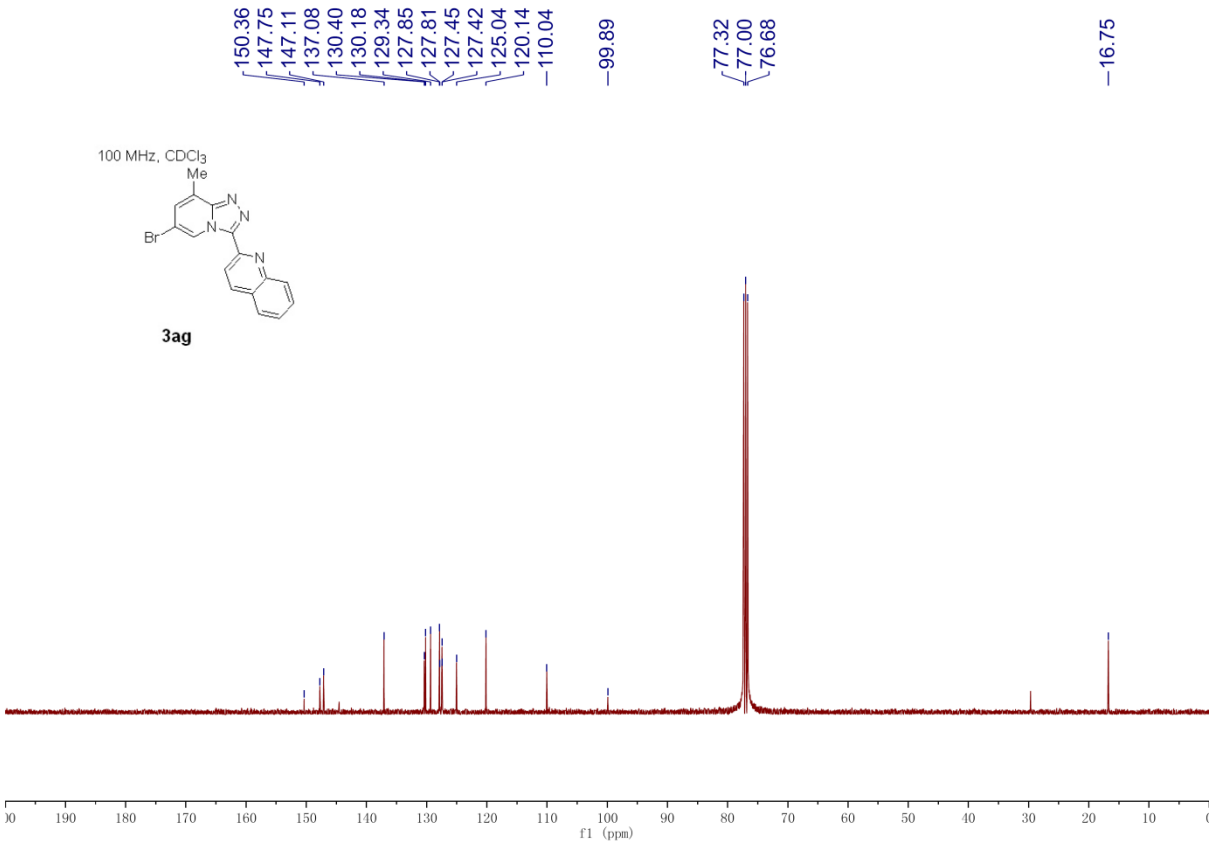
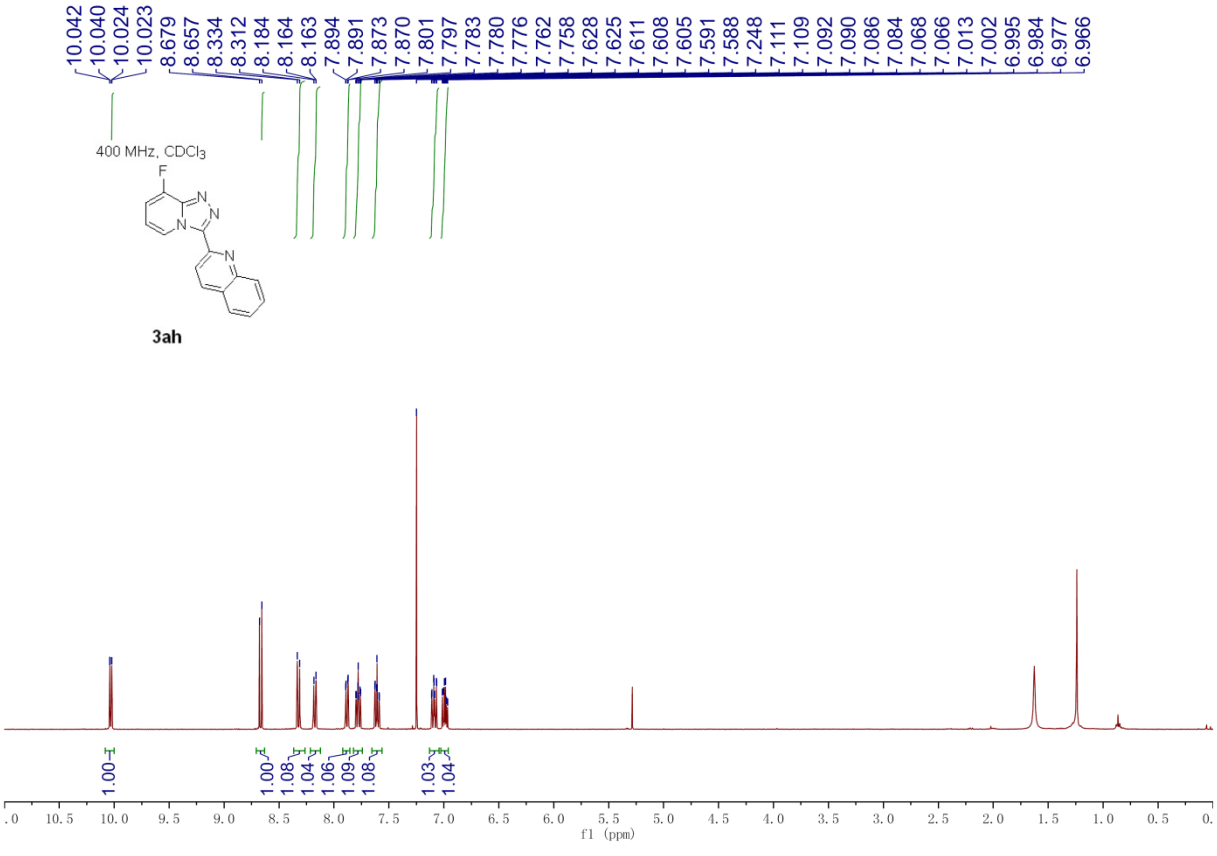
7.601
7.598
7.595
7.263
7.259
7.256


400 MHz, CDCl3
Me
Br
N
N
N

3ag


1.00
1.06
1.14
1.11
1.15
1.15
1.14
1.05
f1 (ppm)


150.36
147.75
147.11
137.08
130.40
130.18
129.34
127.85
127.81
127.45
127.42
125.04
120.14
110.04
99.89
77.32
77.00
76.68
16.75
100 MHz, CDCl3
Me
Br
N
N
N
N
3ag
f1 (ppm)


10.042
10.040
10.024
10.023
8.679
8.657
8.334
8.312
8.184
8.164
8.163
7.894
7.891
7.873
7.870
7.801
7.797
7.783
7.780
7.776
7.762
7.758
7.628
7.625
7.611
7.608
7.605
7.591
7.588
7.248
7.111
7.109
7.092
7.090
7.086
7.084
7.068
7.066
7.013
7.002
6.995
6.984
6.977
6.966
400 MHz, CDCl3
F
N
N
N
N
3ah
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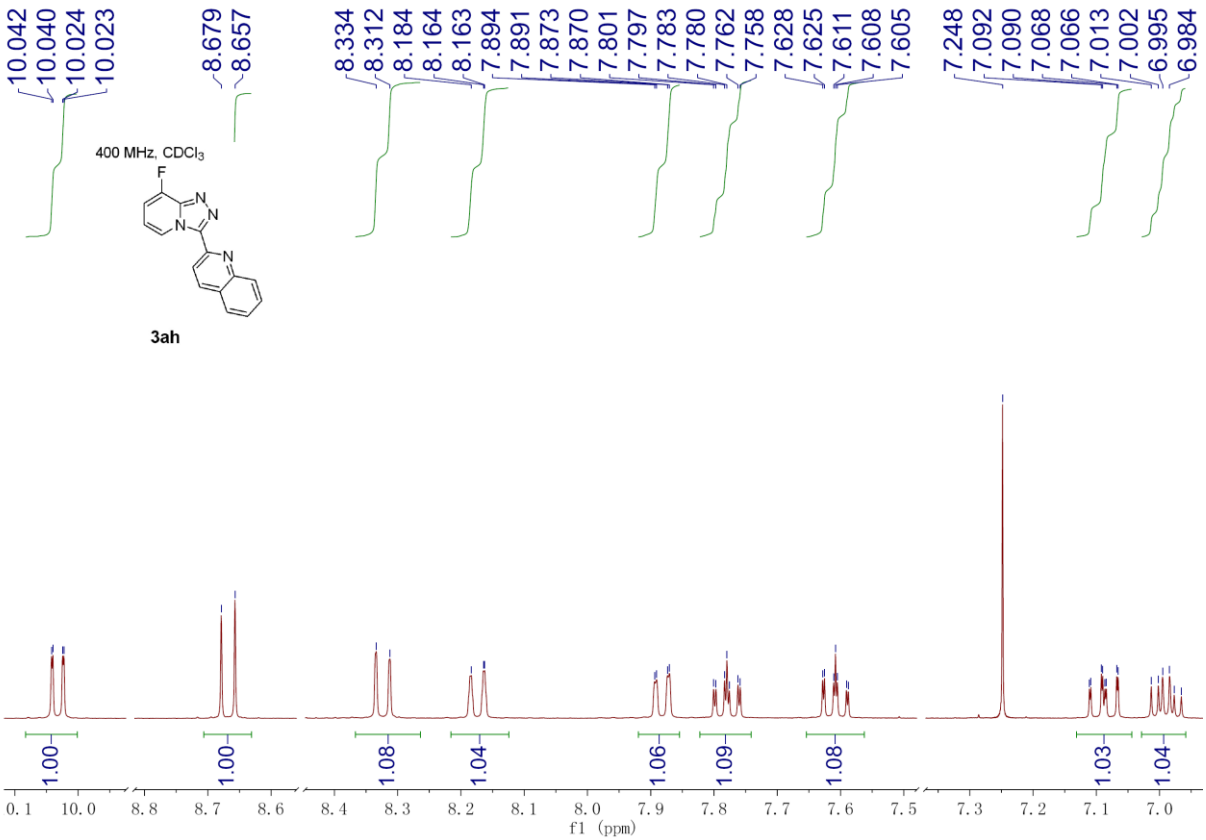
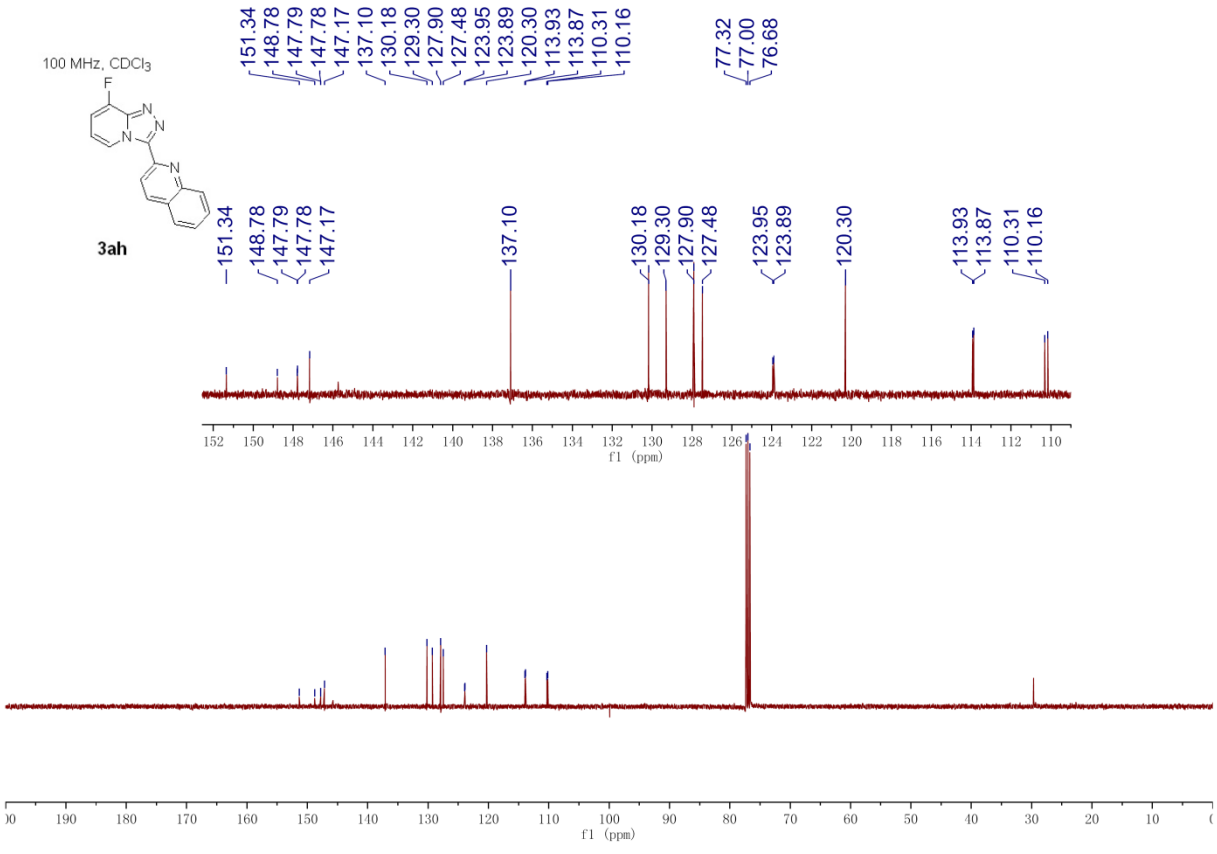
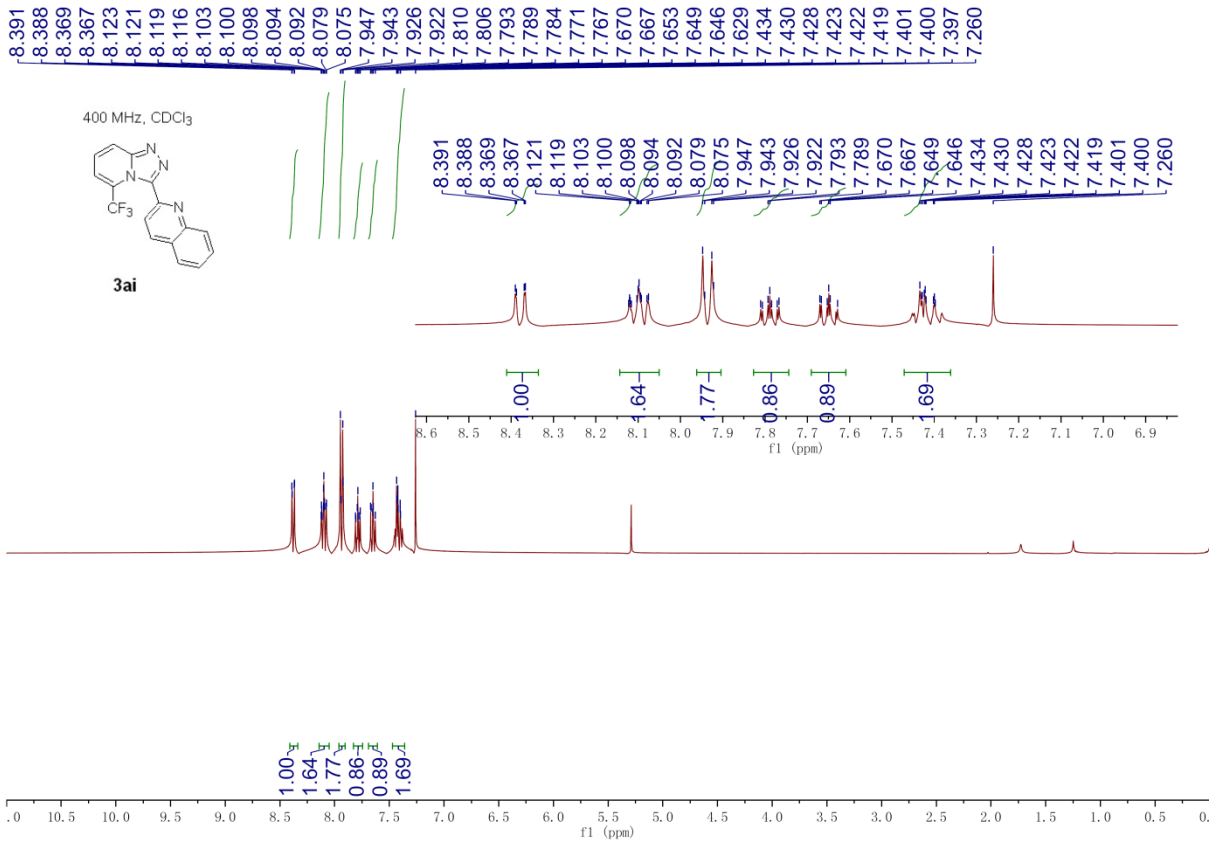
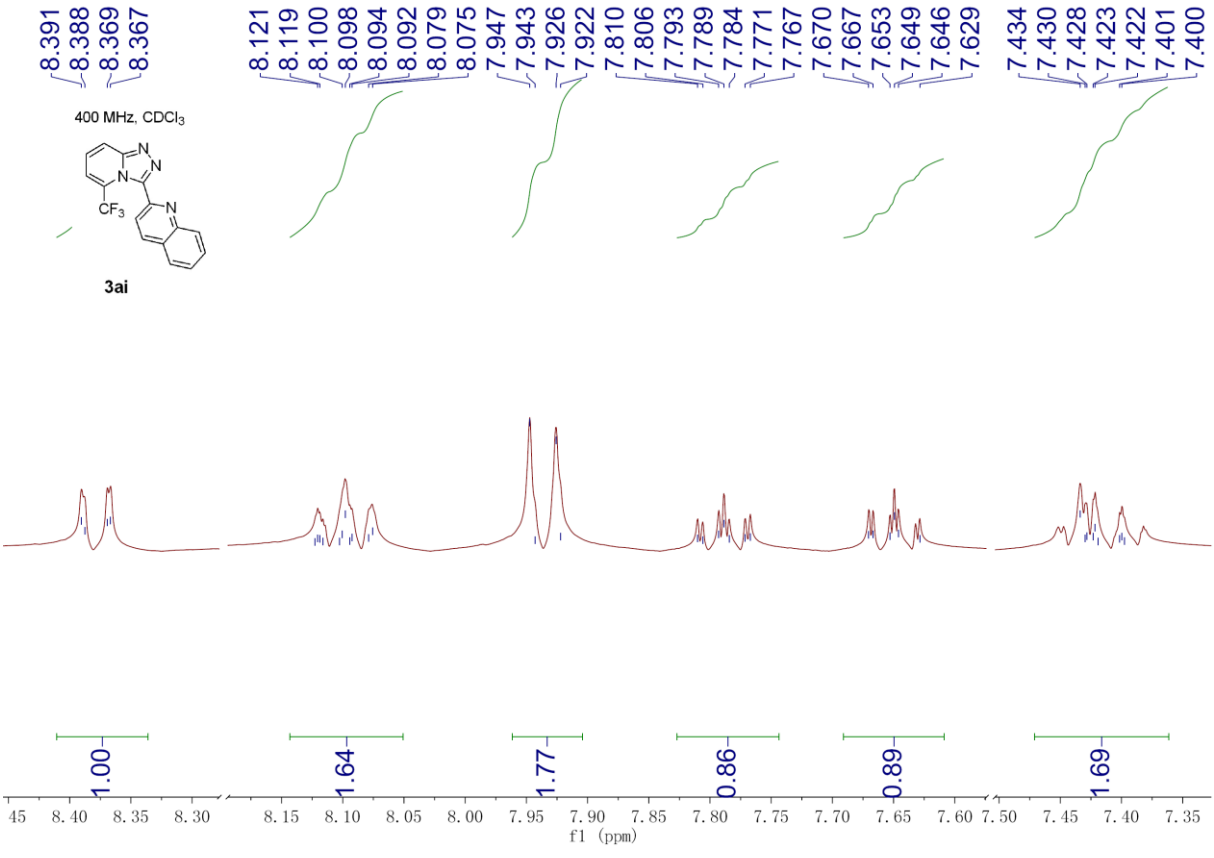
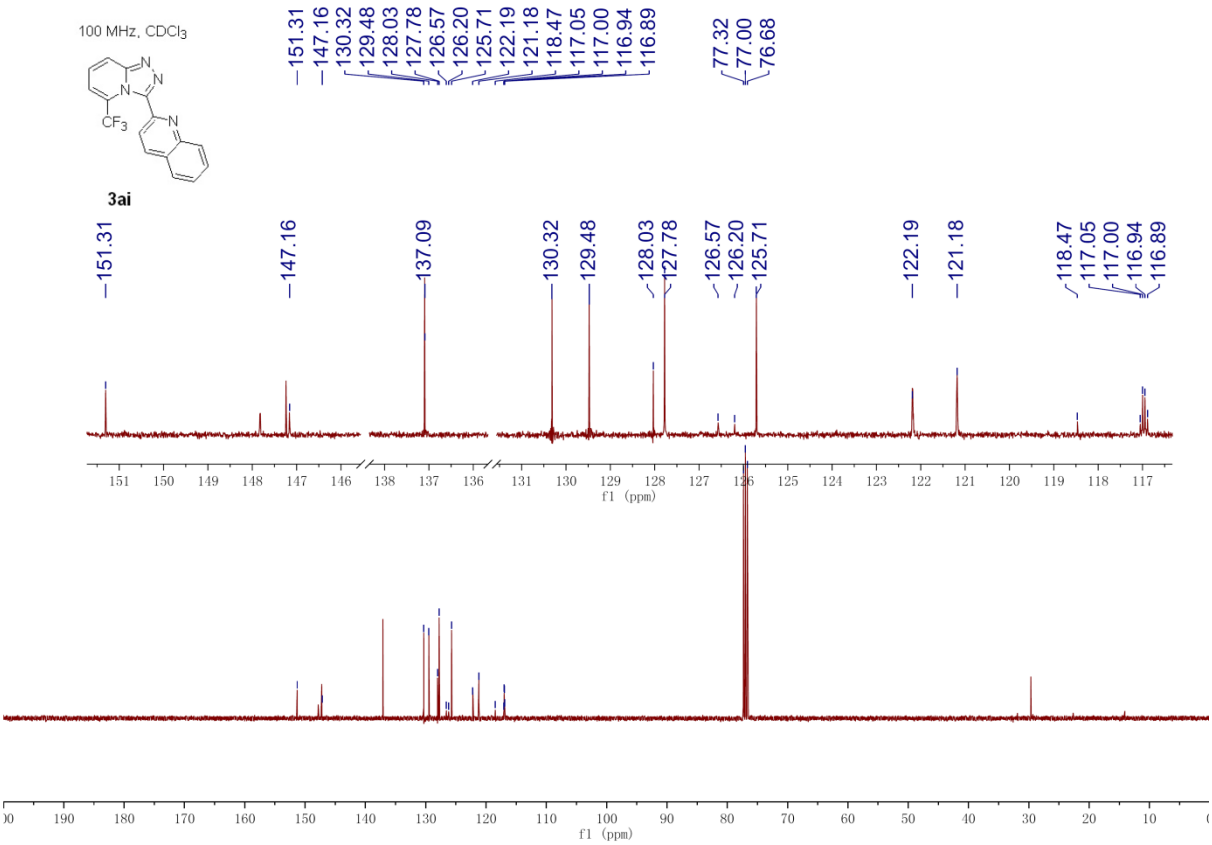
1.06
1.09
1.08
1.03
1.04
f1 (ppm)

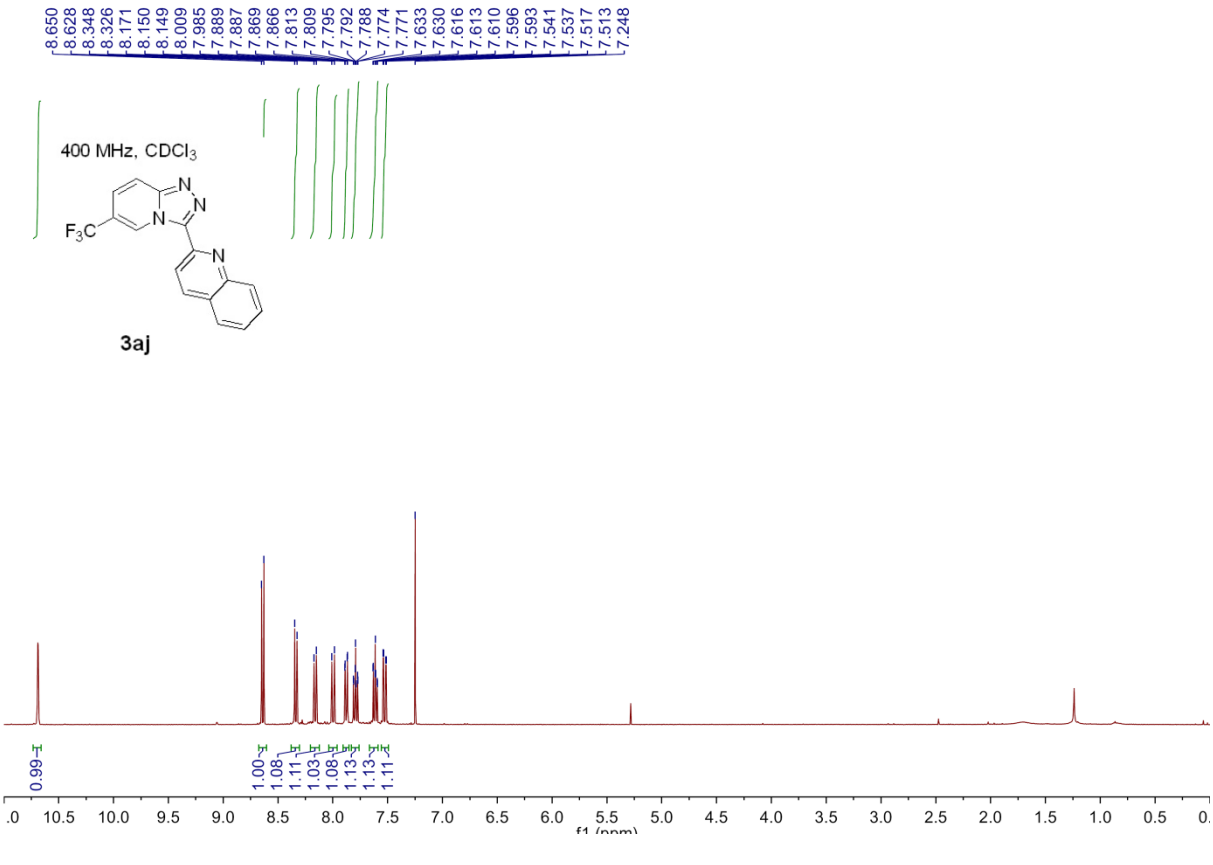

10.042
10.040
10.024
10.023
8.679
8.657
8.334
8.312
8.184
8.164
8.163
7.894
7.891
7.873
7.870
7.801
7.797
7.783
7.780
7.762
7.758
7.628
7.625
7.611
7.608
7.605
7.248
7.092
7.090
7.068
7.066
7.013
7.002
6.995
6.984
400 MHz, CDCl3
3ah
1.00
1.00
1.08
1.04
1.06
1.09
1.08
1.03
1.04
f1 (ppm)


151.34
148.78
147.79
147.78
147.17
137.10
130.18
129.30
127.90
127.48
123.95
123.89
120.30
113.93
113.87
110.31
110.16
77.32
77.00
76.68
100 MHz, CDCl3
3ah
f1 (ppm)


8.391
8.388
8.369
8.367
8.123
8.121
8.119
8.116
8.103
8.100
8.098
8.094
8.092
8.079
8.075
7.947
7.943
7.926
7.922
7.810
7.806
7.793
7.789
7.784
7.771
7.767
7.670
7.667
7.653
7.649
7.646
7.629
7.434
7.430
7.428
7.423
7.422
7.419
7.401
7.400
7.397
7.260
400 MHz, CDCl3
CF3
N
3ai
1.00
1.64
1.77
0.86
0.89
1.69
f1 (ppm)


8.391
8.388
8.369
8.367
8.121
8.119
8.100
8.098
8.094
8.092
8.079
8.075
7.947
7.943
7.926
7.922
7.810
7.806
7.793
7.789
7.784
7.771
7.767
7.670
7.667
7.653
7.649
7.646
7.629
7.434
7.430
7.428
7.423
7.422
7.401
7.400
400 MHz, CDCl3
CF3
N
3ai
1.00
1.64
1.77
0.86
0.89
1.69
f1 (ppm)


100 MHz, CDCl3
3ai
151.31
147.16
130.32
129.48
128.03
127.78
126.57
126.20
125.71
122.19
121.18
118.47
117.05
117.00
116.94
116.89
77.32
77.00
76.68
f1 (ppm)


400 MHz, CDCl3
3aj
8.650
8.628
8.348
8.326
8.171
8.150
8.149
8.009
7.985
7.889
7.887
7.869
7.866
7.813
7.809
7.795
7.792
7.788
7.774
7.771
7.633
7.630
7.616
7.613
7.610
7.596
7.593
7.541
7.537
7.517
7.513
7.248
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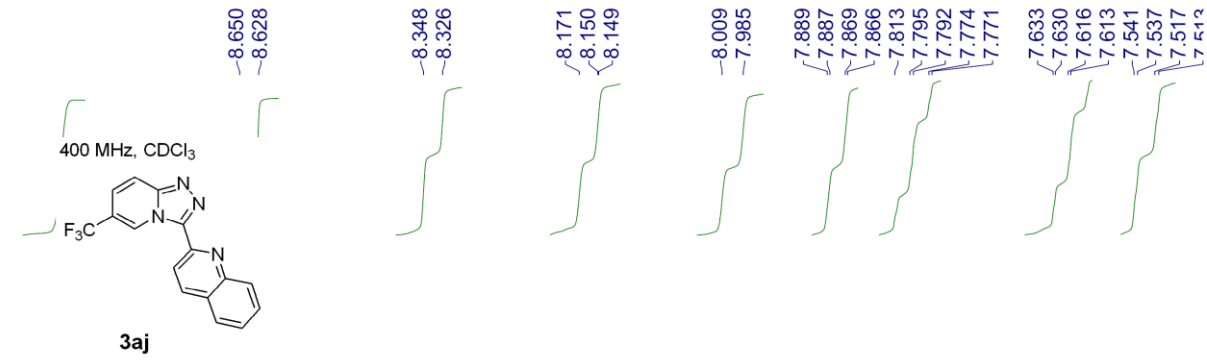
1.00
1.08
1.11
1.03
1.08
1.13
1.13
1.11
f1 (ppm)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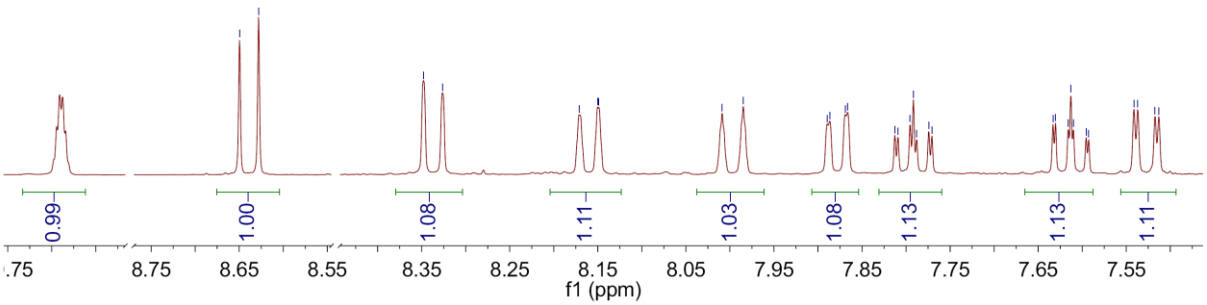
8.628
8.348
8.326
8.171
8.150
8.149
8.009
7.985
7.889
7.887
7.869
7.866
7.813
7.795
7.792
7.774
7.771
7.633
7.630
7.616
7.613
7.541
7.537
7.517
400 MHz, CDCl3
F3C
N
N
N
N
3aj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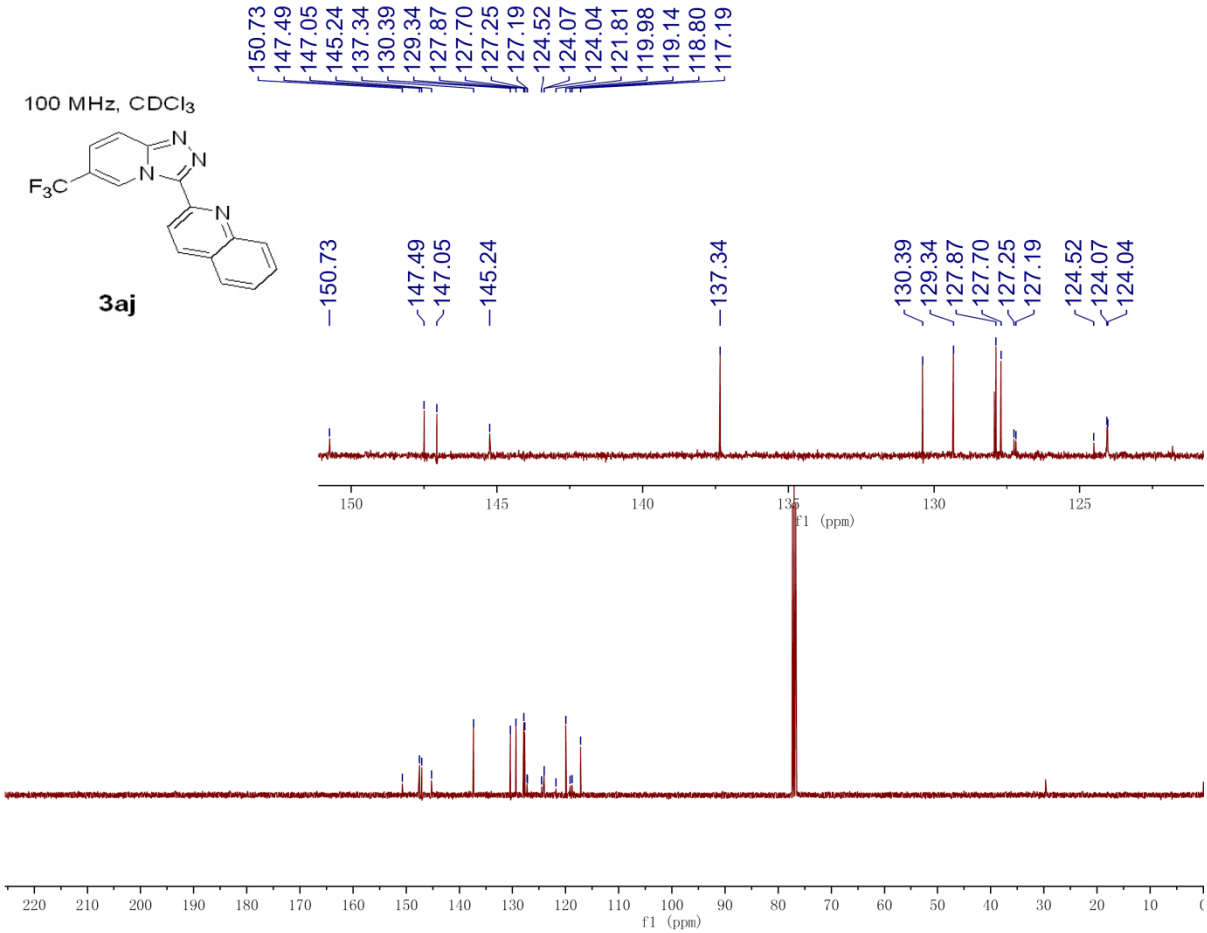
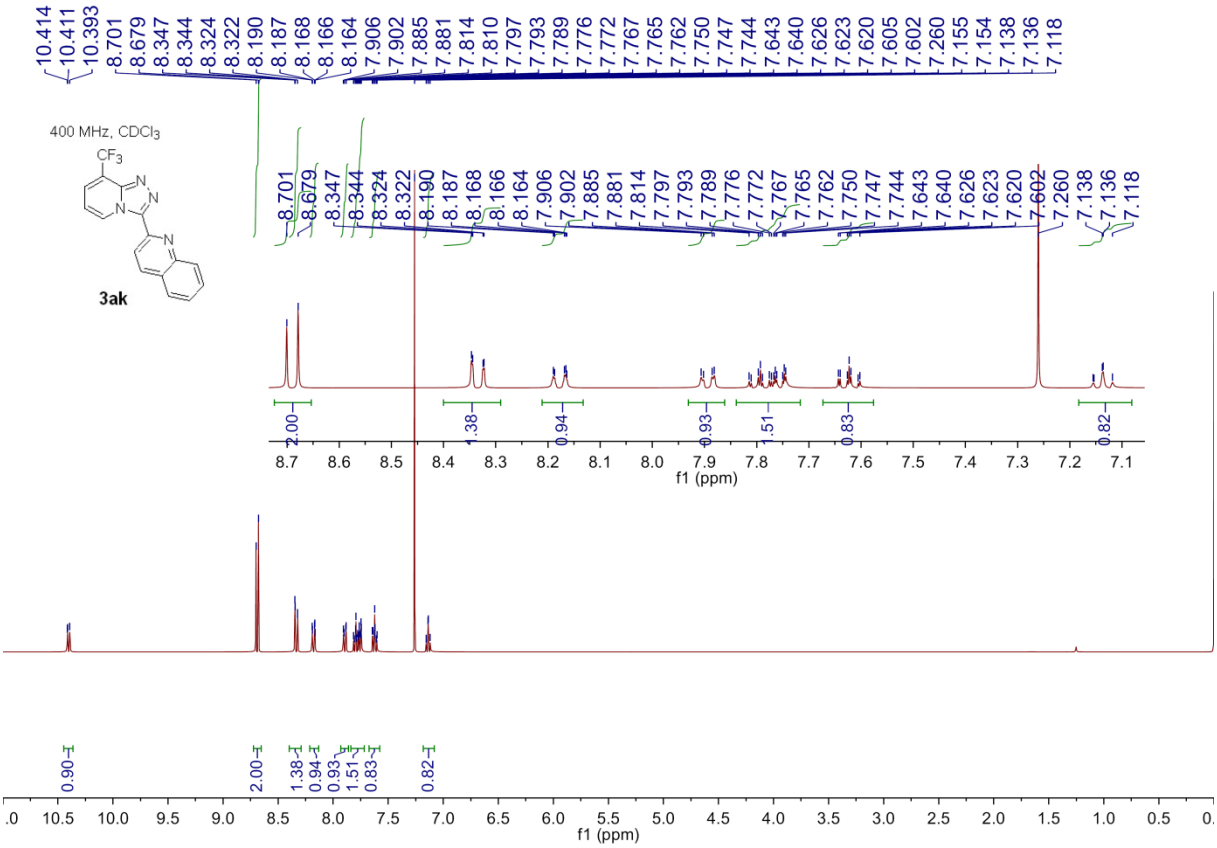
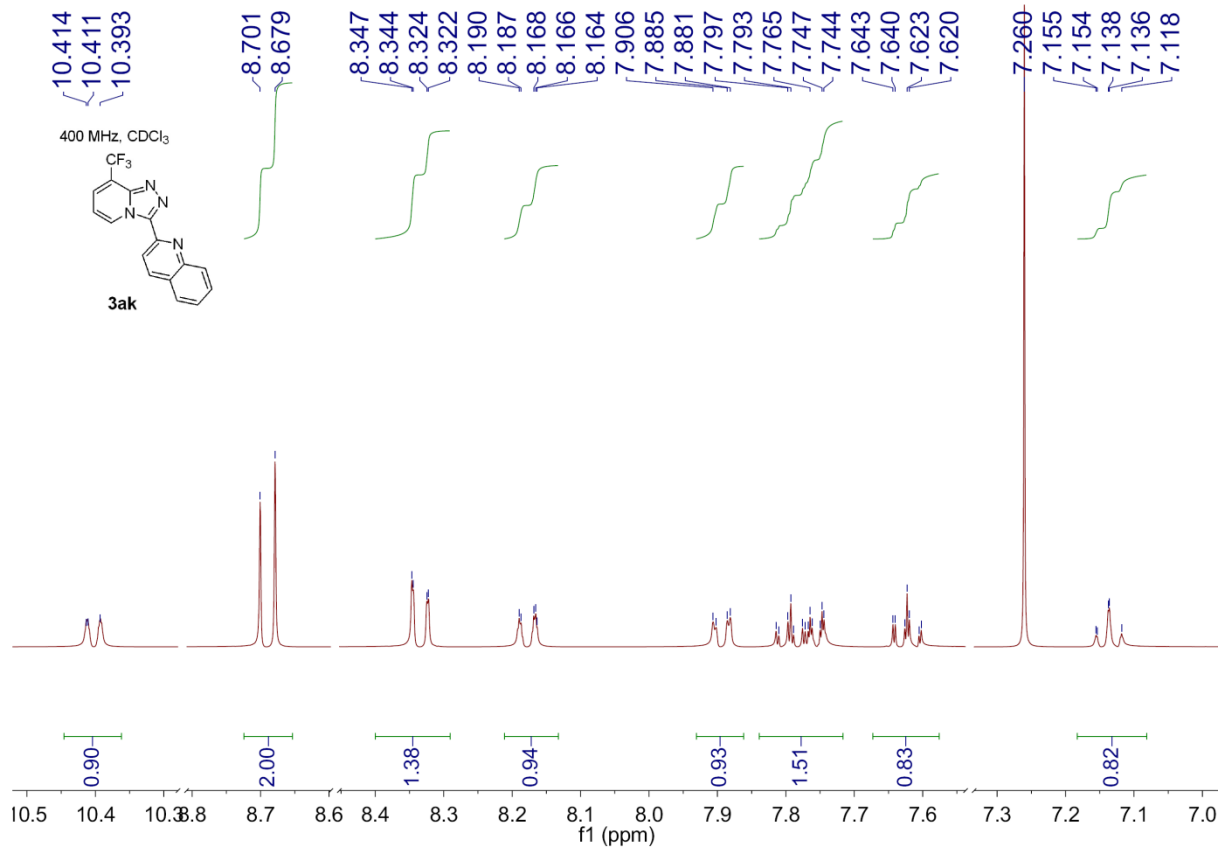
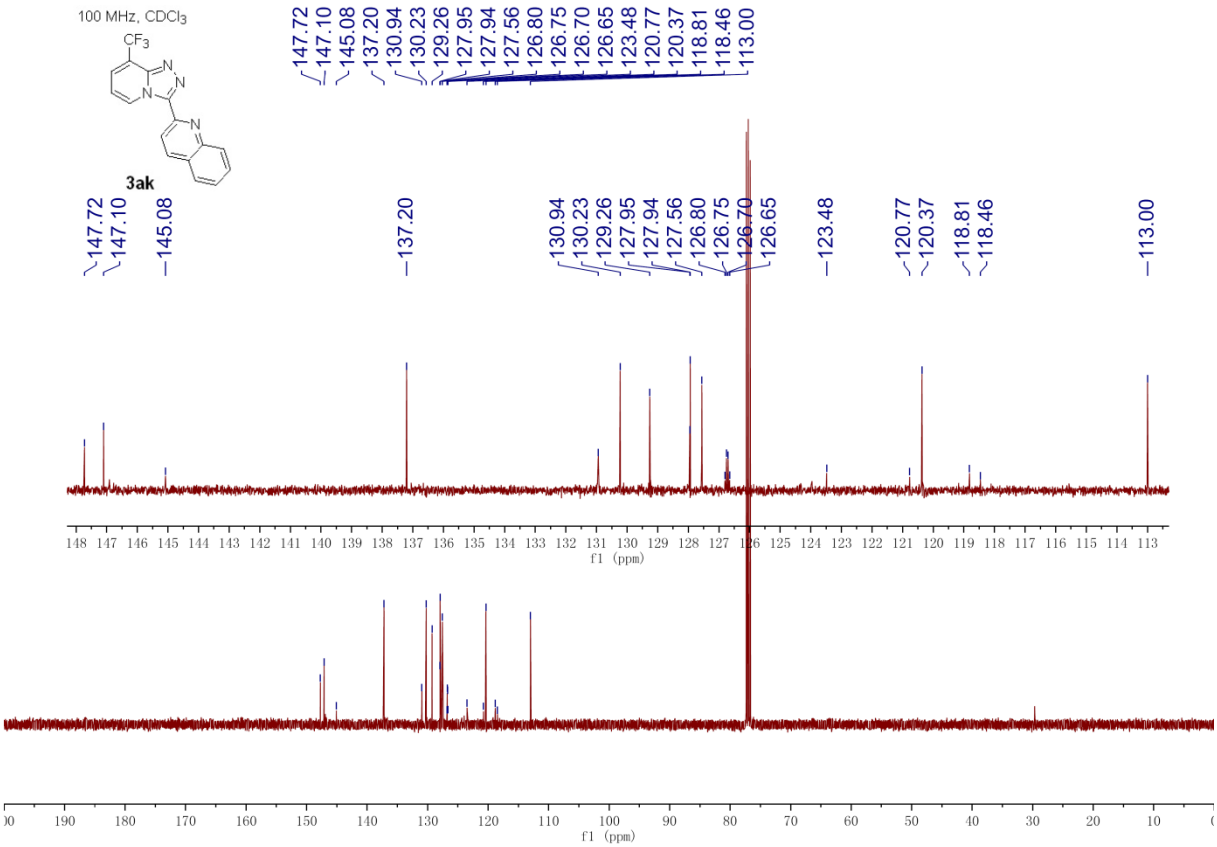
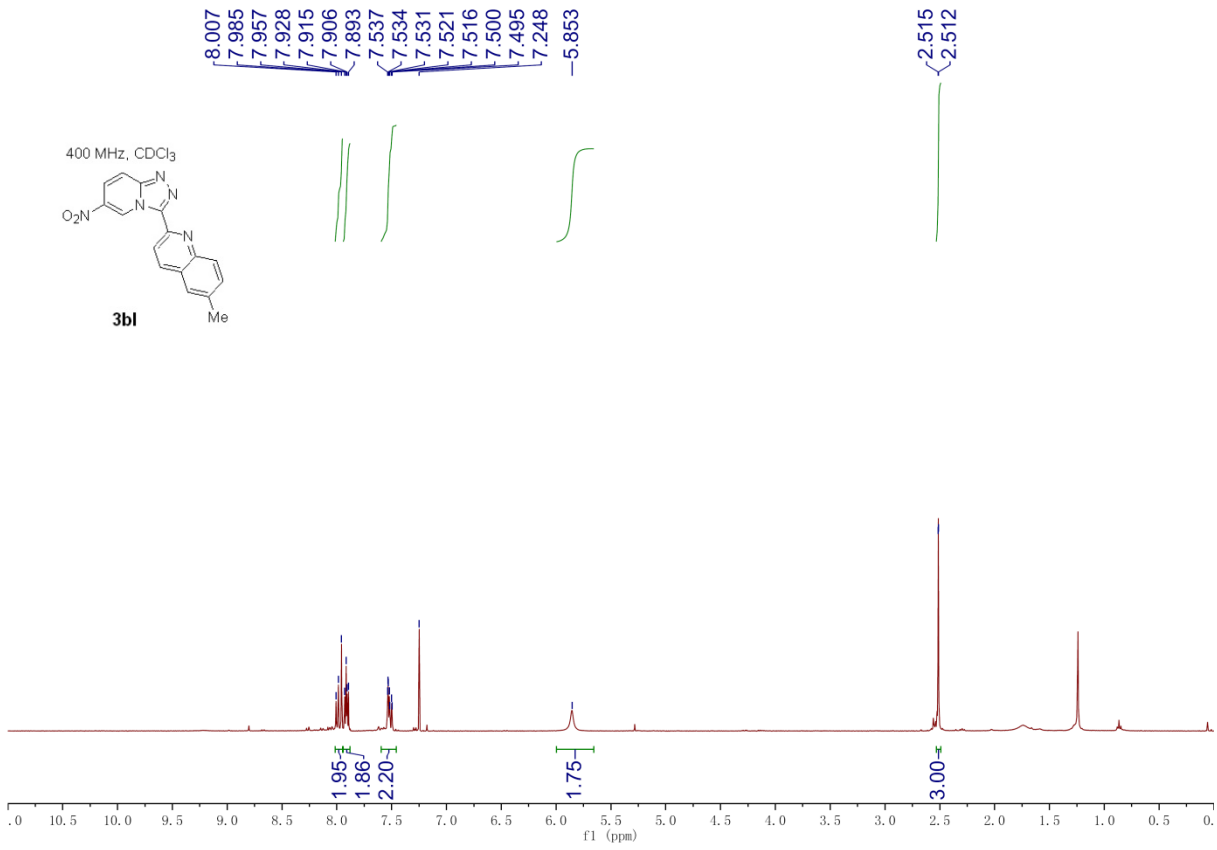
1.00
1.08
1.11
1.03
1.08
1.13
1.13
1.11
8.75
8.65
8.55
8.35
8.25
8.15
8.05
7.95
7.85
7.75
7.65
7.55
f1 (ppm)

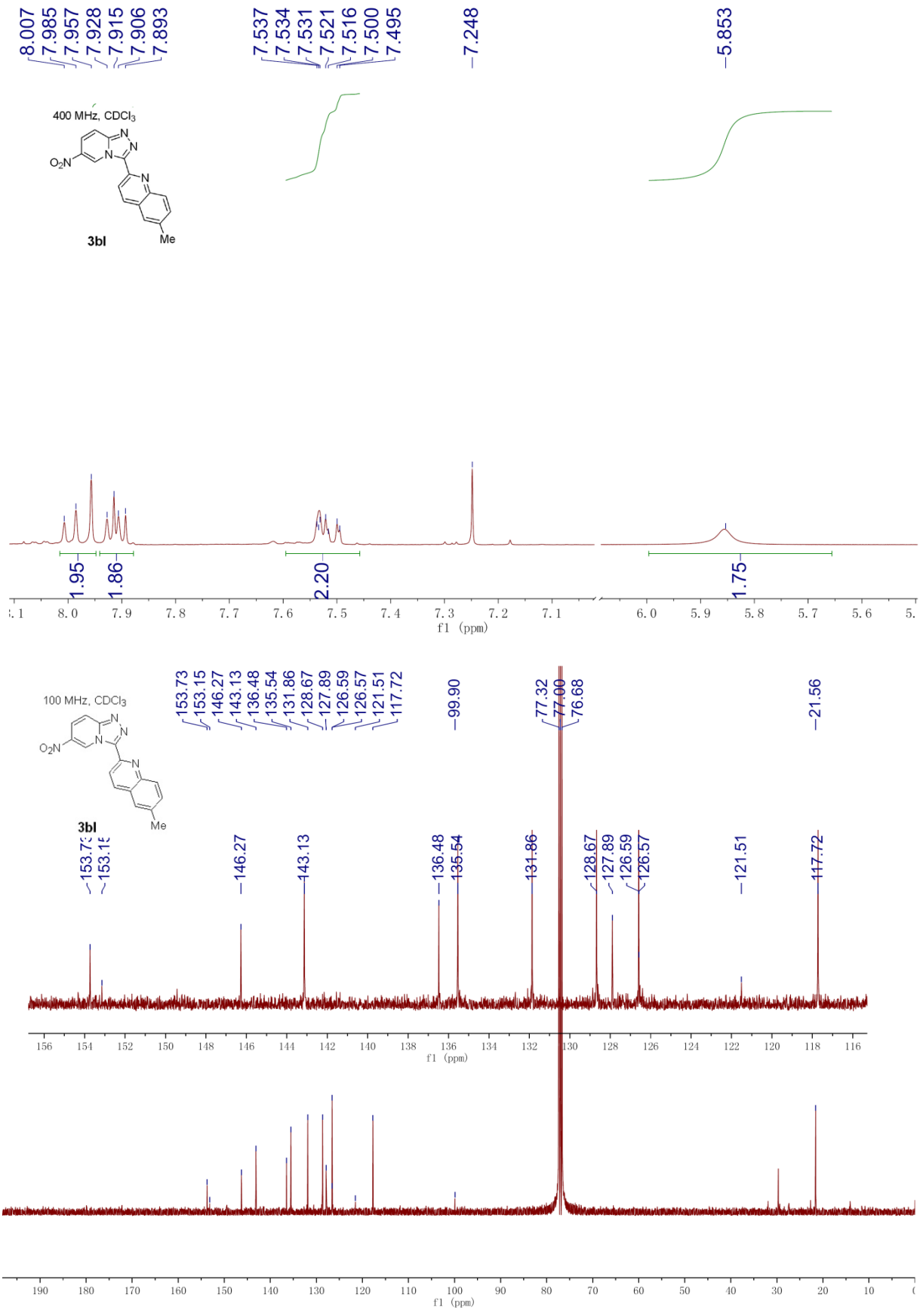

150.73
147.49
147.05
145.24
137.34
130.39
129.34
127.87
127.70
127.25
127.19
124.52
124.07
124.04
121.81
119.98
119.14
118.80
117.19
100 MHz, CDCl3
F3C
N
N
N
N
3aj
150
145
140
130
125
f1 (ppm)
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

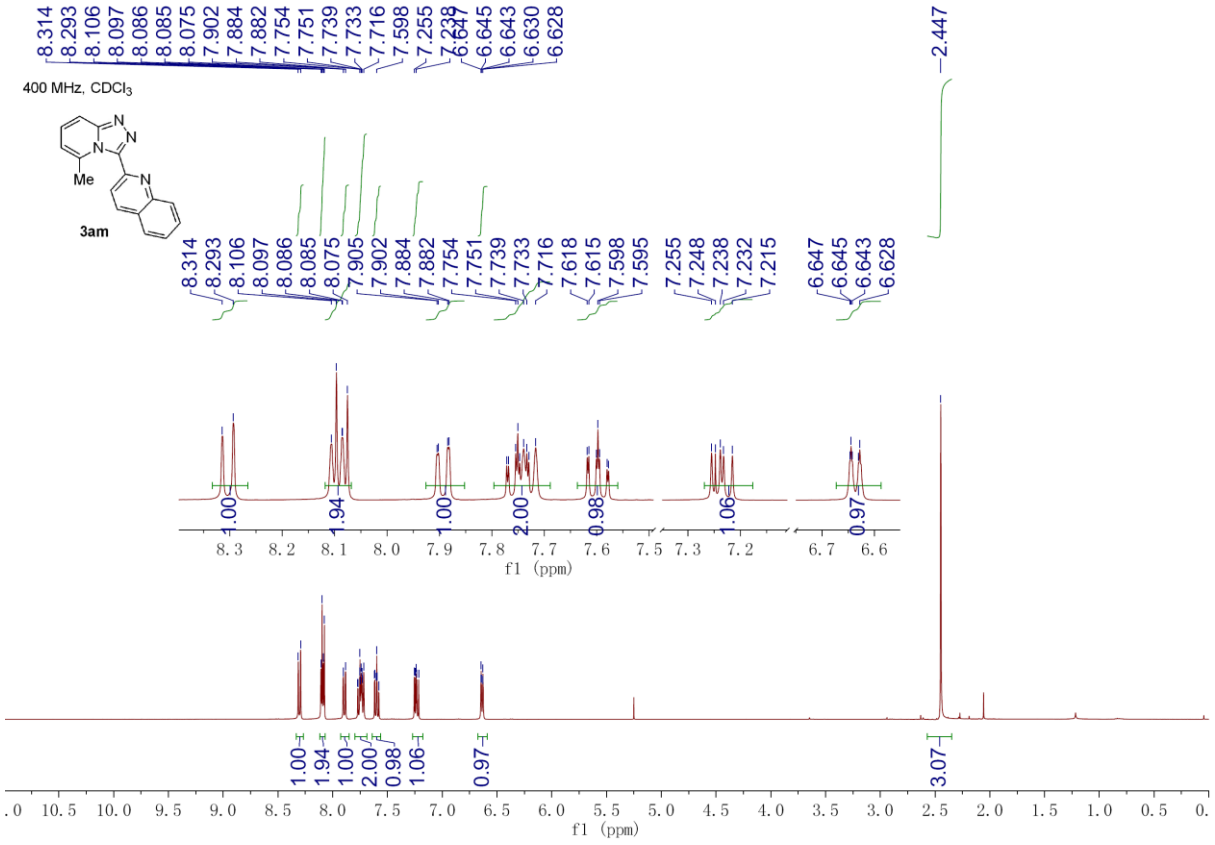

400 MHz, CDCl3
3ak
f1 (ppm)

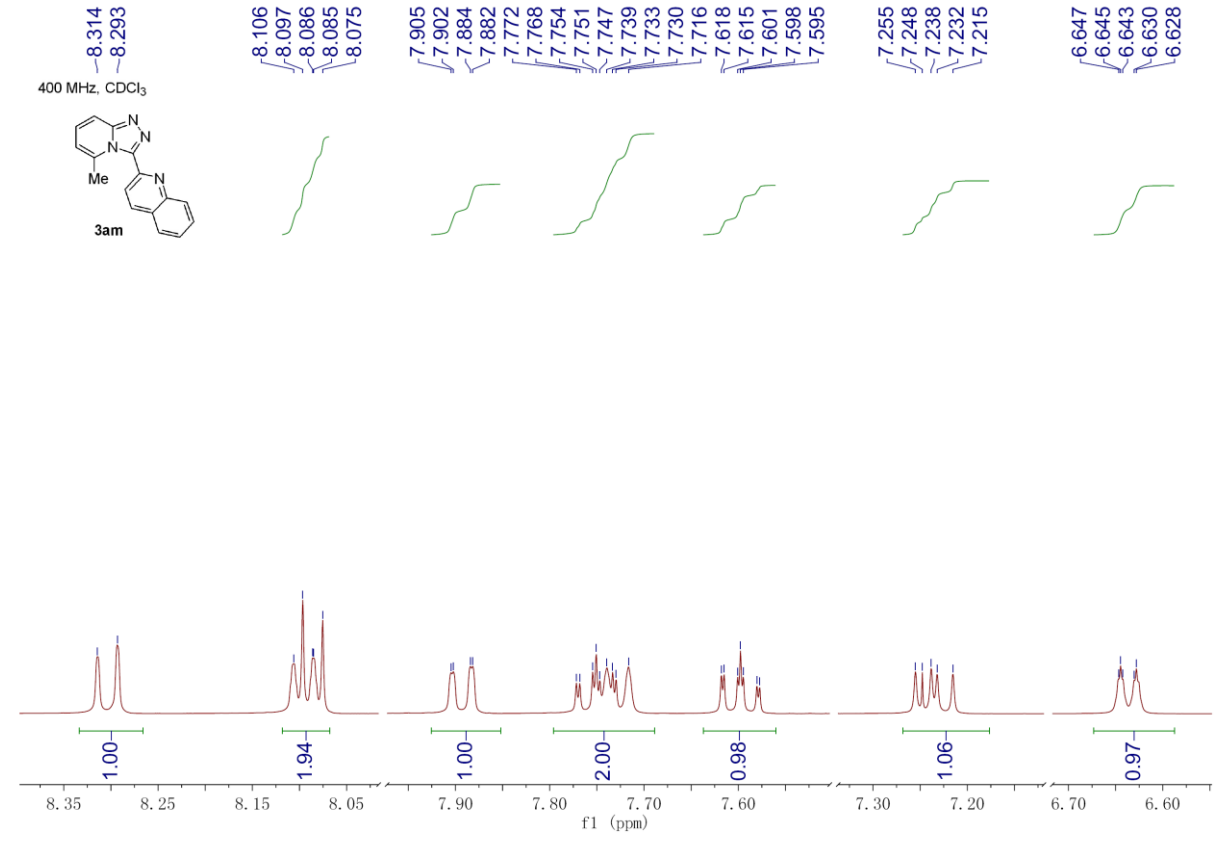

400 MHz, CDCl3
3ak
f1 (ppm)

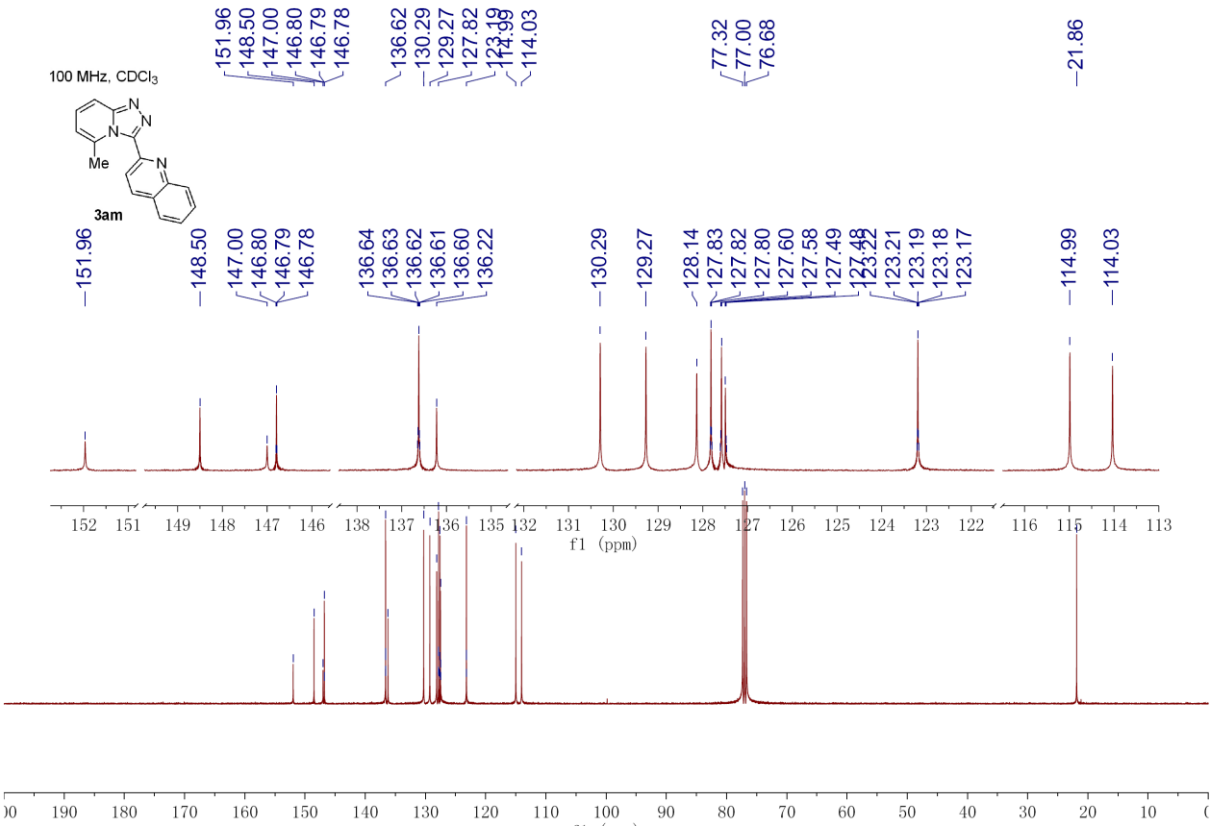

100 MHz, CDCl3
CF3
3ak
147.72
147.10
145.08
137.20
130.94
130.23
129.26
127.95
127.94
127.56
126.80
126.75
126.70
126.65
123.48
120.77
120.37
118.81
118.46
113.00
f1 (ppm)


400 MHz, CDCl3
O2N
Me
3bl
8.007
7.985
7.957
7.928
7.915
7.906
7.893
7.537
7.534
7.531
7.521
7.516
7.500
7.495
7.248
5.853
2.515
2.512
1.95
1.86
2.20
1.75
3.00
f1 (ppm)


8.007
7.985
7.957
7.928
7.915
7.906
7.893
7.537
7.534
7.531
7.521
7.516
7.500
7.495
7.248
5.853
400 MHz, CDCl3
3bl
Me
1.95
1.86
2.20
1.75
f1 (ppm)
100 MHz, CDCl3
153.73
153.15
146.27
143.13
136.48
135.54
131.86
128.67
127.89
126.59
126.57
121.51
117.72
99.90
77.32
77.00
76.68
21.56


8.314
8.293
8.106
8.097
8.086
8.085
8.075
7.902
7.884
7.882
7.754
7.751
7.739
7.733
7.716
7.598
7.255
6.645
6.643
6.630
6.628
2.447
400 MHz, CDCl3
Me
3am
7.905
7.902
7.884
7.882
7.754
7.751
7.739
7.733
7.716
7.618
7.615
7.598
7.595
7.248
7.238
7.232
7.215
6.647
6.645
6.643
6.628
1.00
1.94
1.00
2.00
0.98
1.06
0.97
3.07
f1 (ppm)


8.314
8.293
8.106
8.097
8.086
8.085
8.075
7.905
7.902
7.884
7.882
7.772
7.768
7.754
7.751
7.747
7.739
7.733
7.730
7.716
7.618
7.615
7.601
7.598
7.595
7.255
7.248
7.238
7.232
7.215
6.647
6.645
6.643
6.630
6.628
400 MHz, CDCl3
Me
3am
1.00
1.94
1.00
2.00
0.98
1.06
0.97
f1 (ppm)


100 MHz, CDCl3
Me
3am
151.96
148.50
147.00
146.80
146.79
146.78
136.64
136.63
136.62
136.61
136.60
136.22
130.29
129.27
128.14
127.83
127.82
127.80
127.60
127.58
127.49
123.21
123.19
123.18
123.17
114.99
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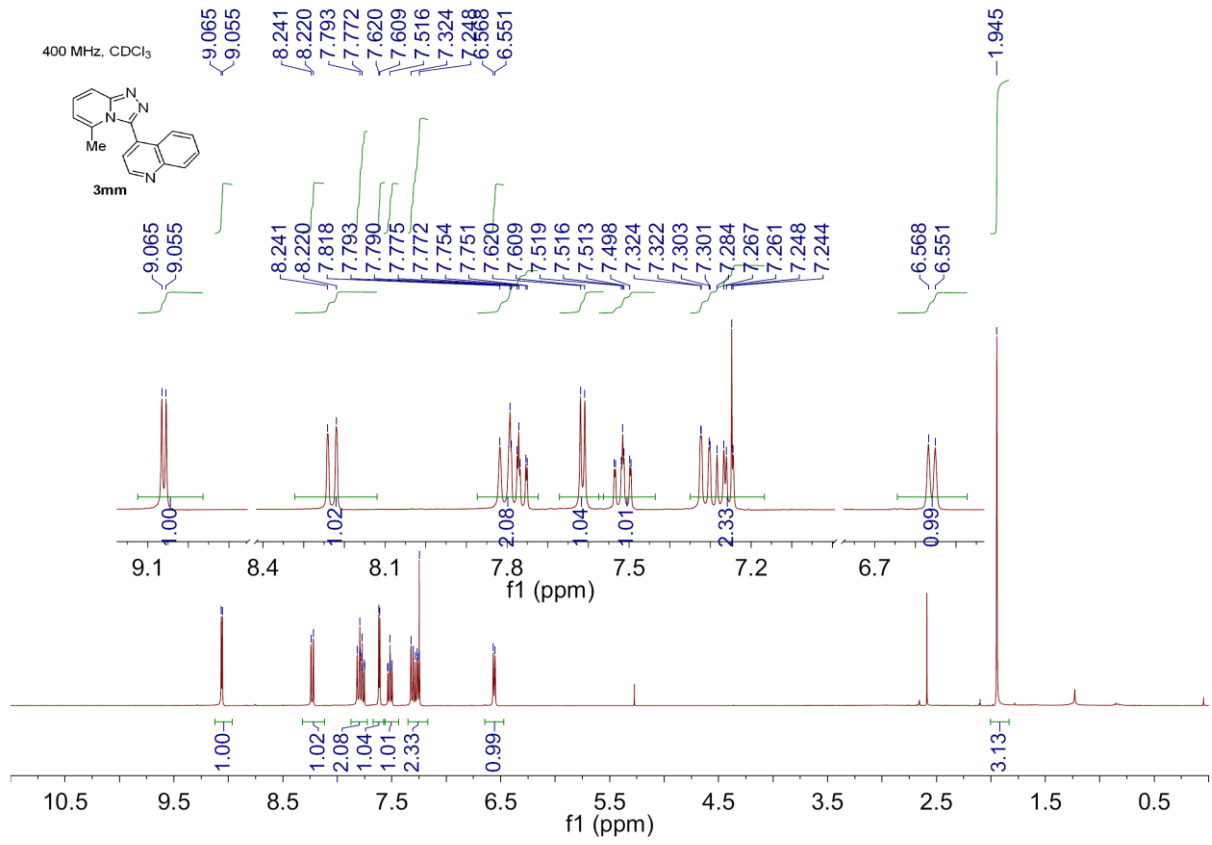
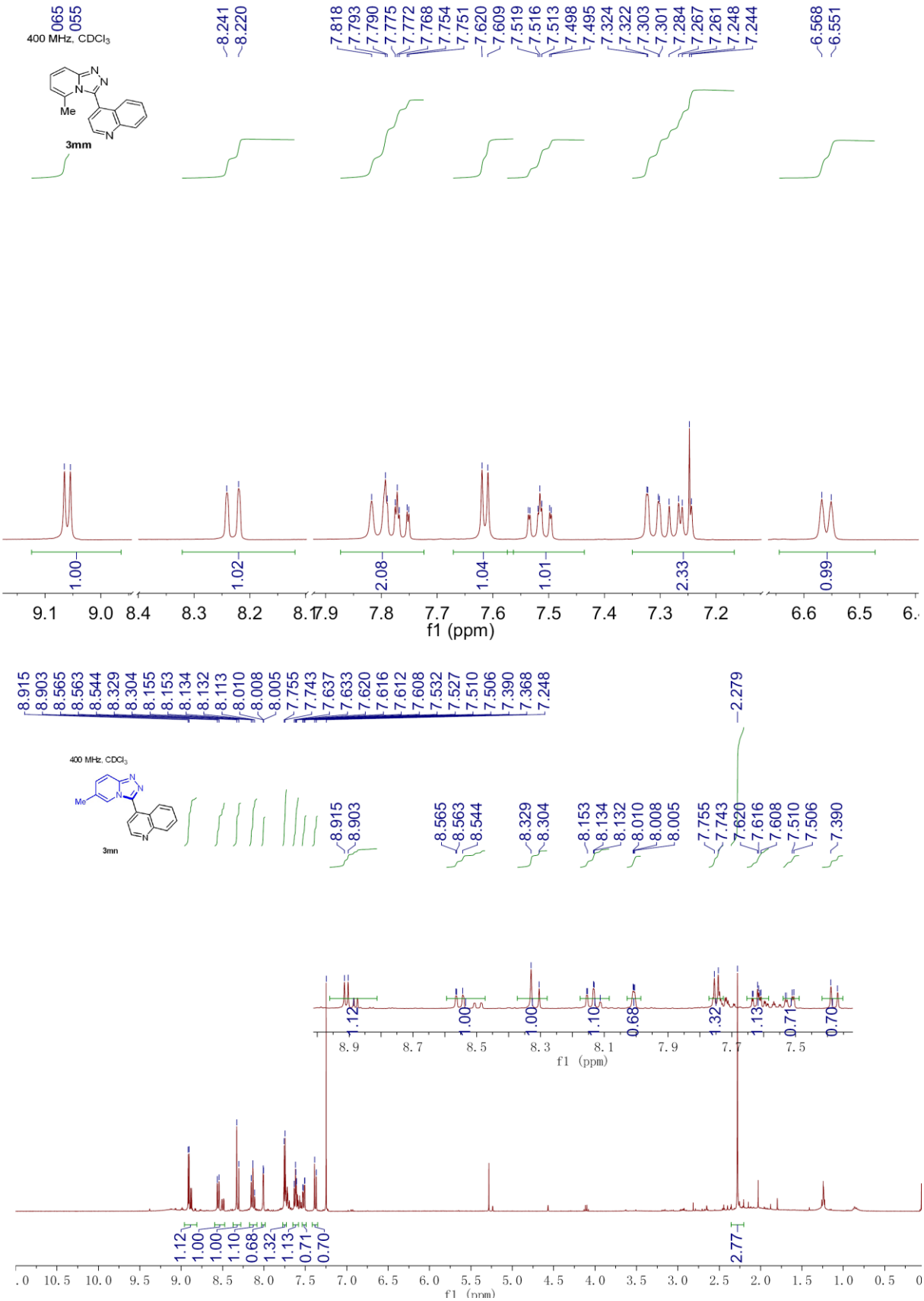
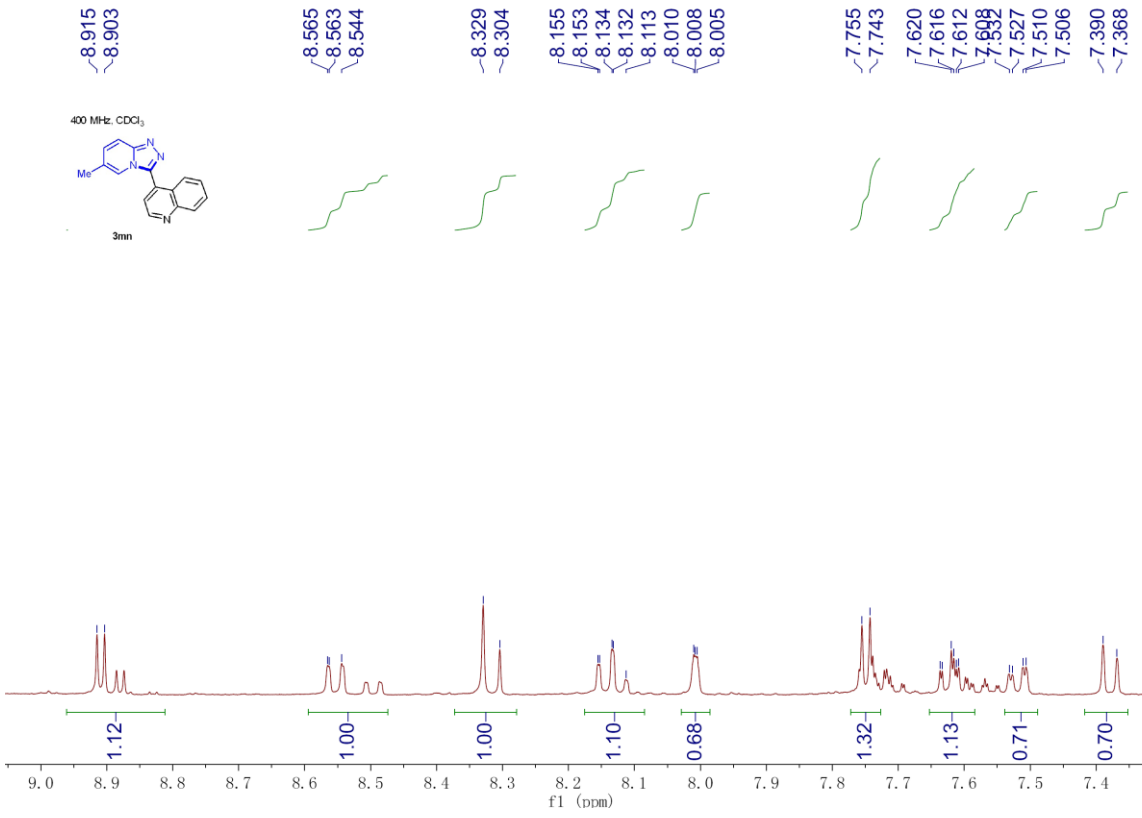
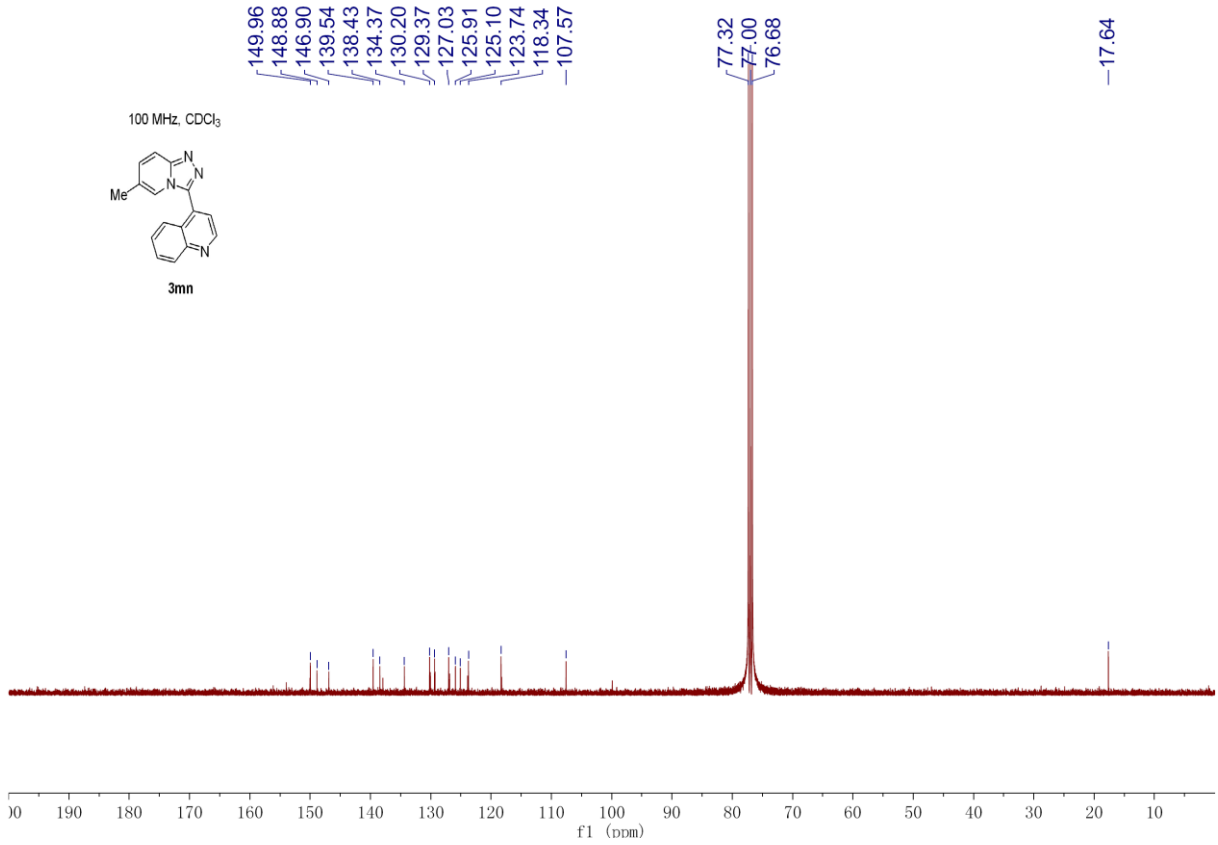
77.32
77.00
76.68
21.86
f1 (ppm)


400 MHz, CDCl3
Me
3mm
9.065
9.055
8.241
8.220
7.818
7.793
7.790
7.775
7.772
7.754
7.751
7.620
7.609
7.519
7.516
7.513
7.498
7.324
7.322
7.303
7.301
7.284
7.267
7.261
7.248
7.244
6.568
6.551
1.945
1.00
1.02
2.08
1.04
1.01
2.33
0.99
3.13
f1 (ppm)


400 MHz, CDCl3
Me
3mm
f1 (ppm)
400 MHz, CDCl3
Me
3mn
f1 (ppm)
f1 (ppm)


8.915
8.903
8.565
8.563
8.544
8.329
8.304
8.155
8.153
8.134
8.132
8.113
8.010
8.008
8.005
7.755
7.743
7.620
7.616
7.612
7.608
7.532
7.527
7.510
7.506
7.390
7.368
400 MHz, CDCl3
Me
3mn
1.12
1.00
1.00
1.10
0.68
1.32
1.13
0.71
0.70
f1 (ppm)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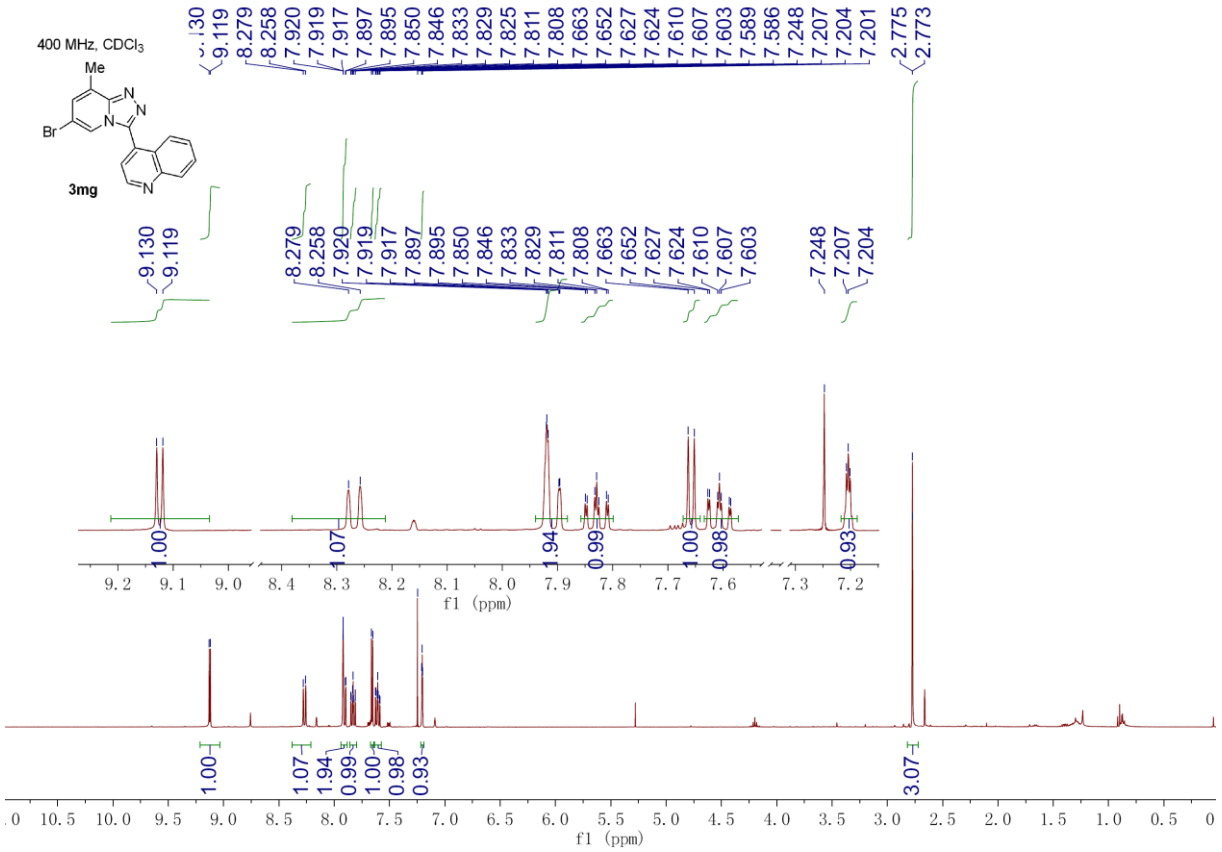
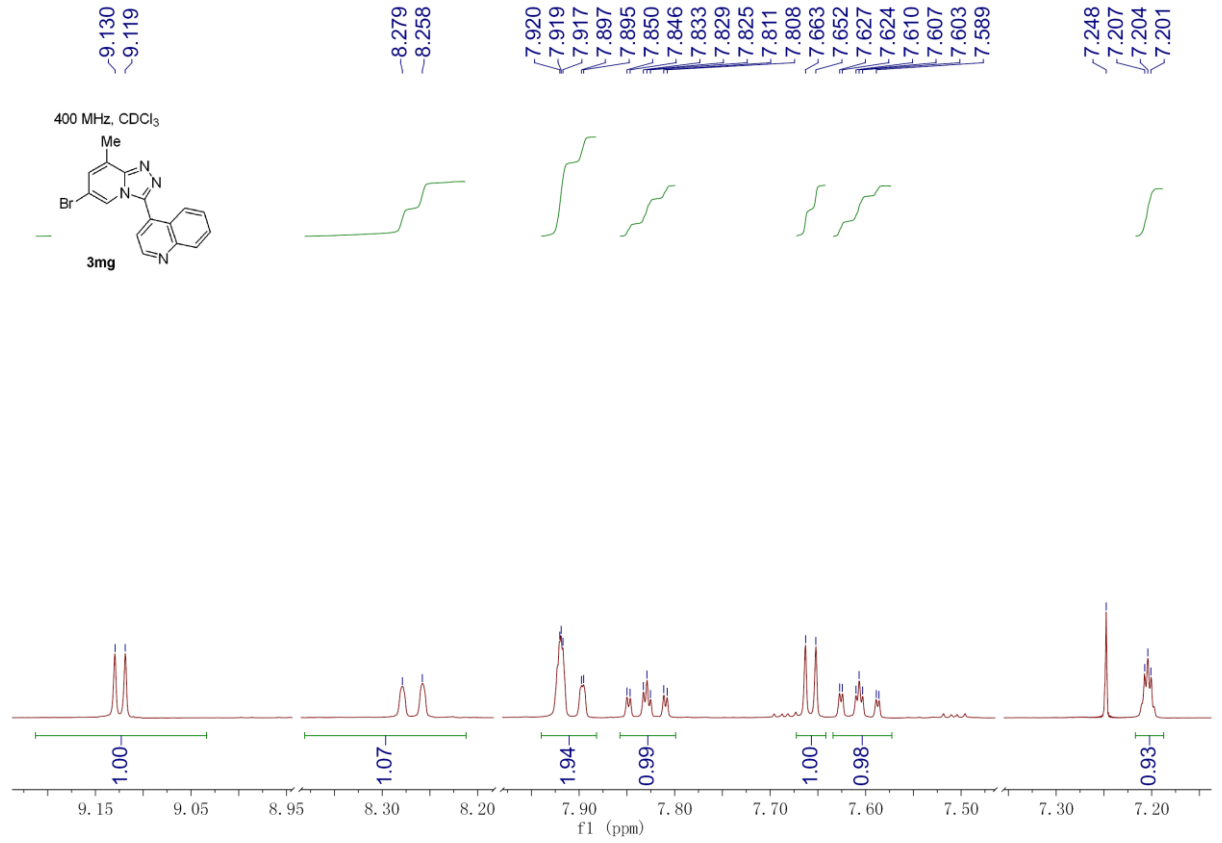
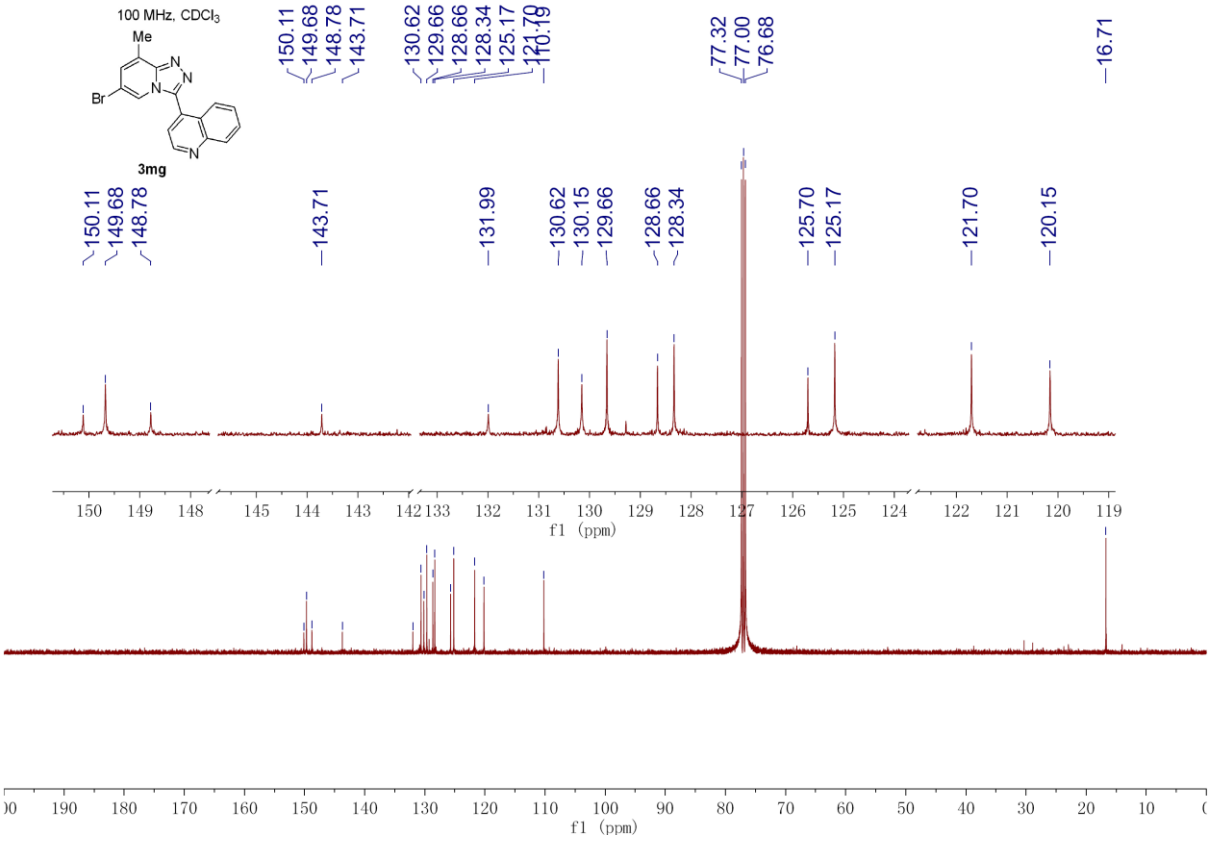
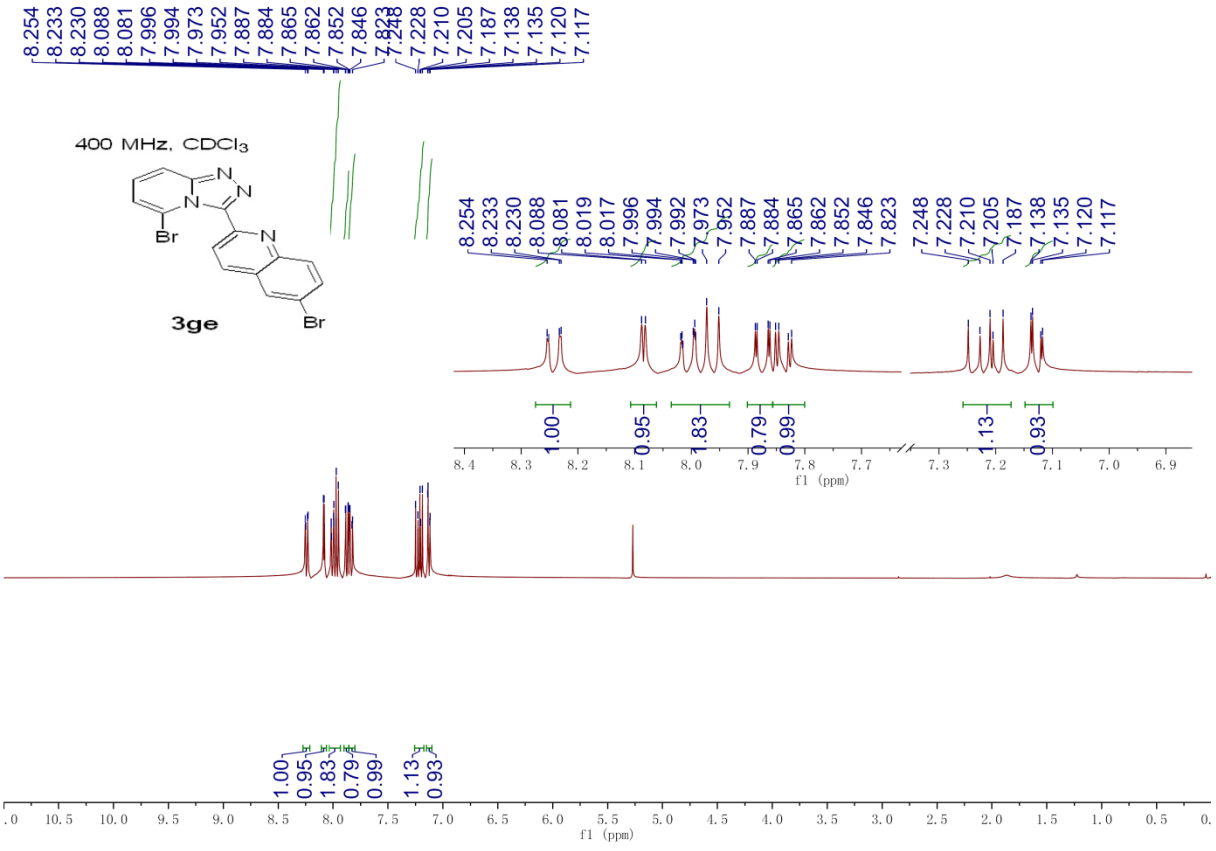
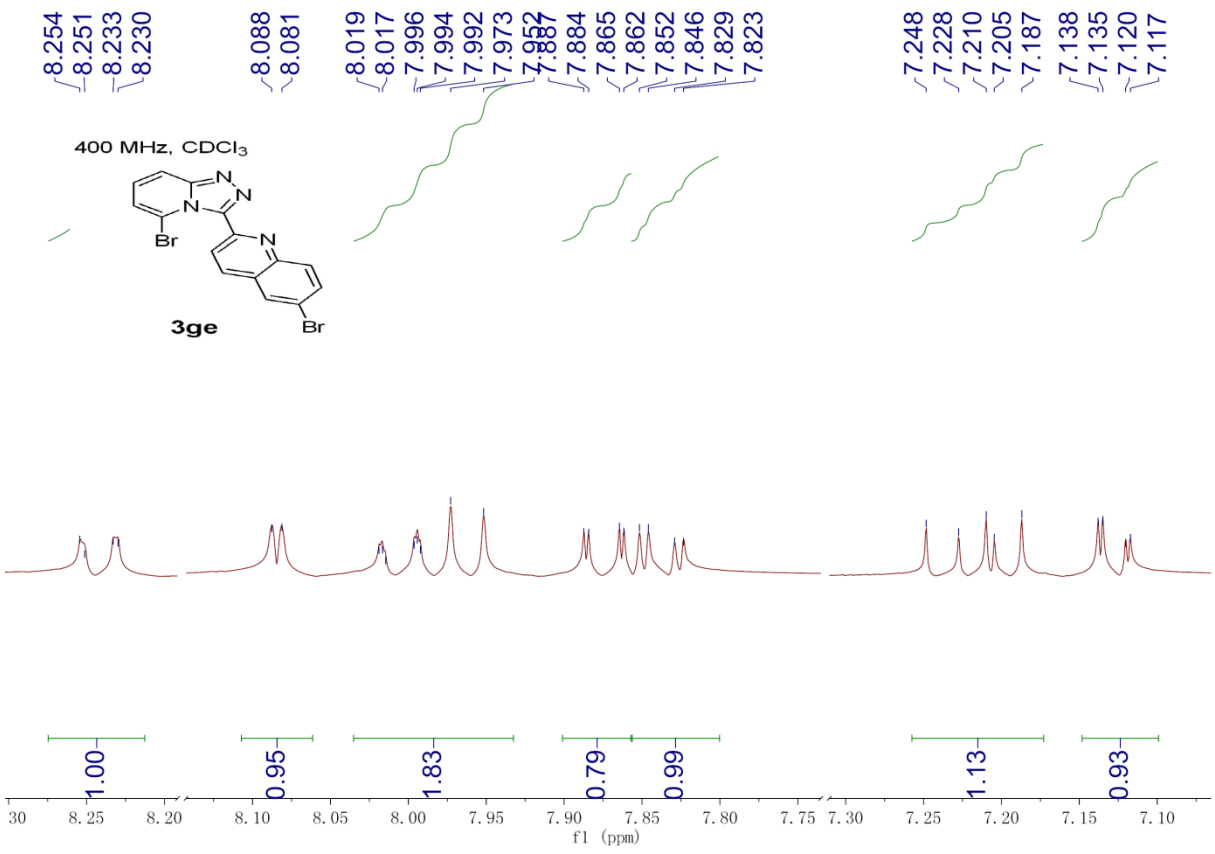
148.88
146.90
139.54
138.43
134.37
130.20
129.37
127.03
125.91
125.10
123.74
118.34
107.57
77.32
77.00
76.68
17.64
100 MHz, CDCl3
Me
3mn
f1 (ppm)

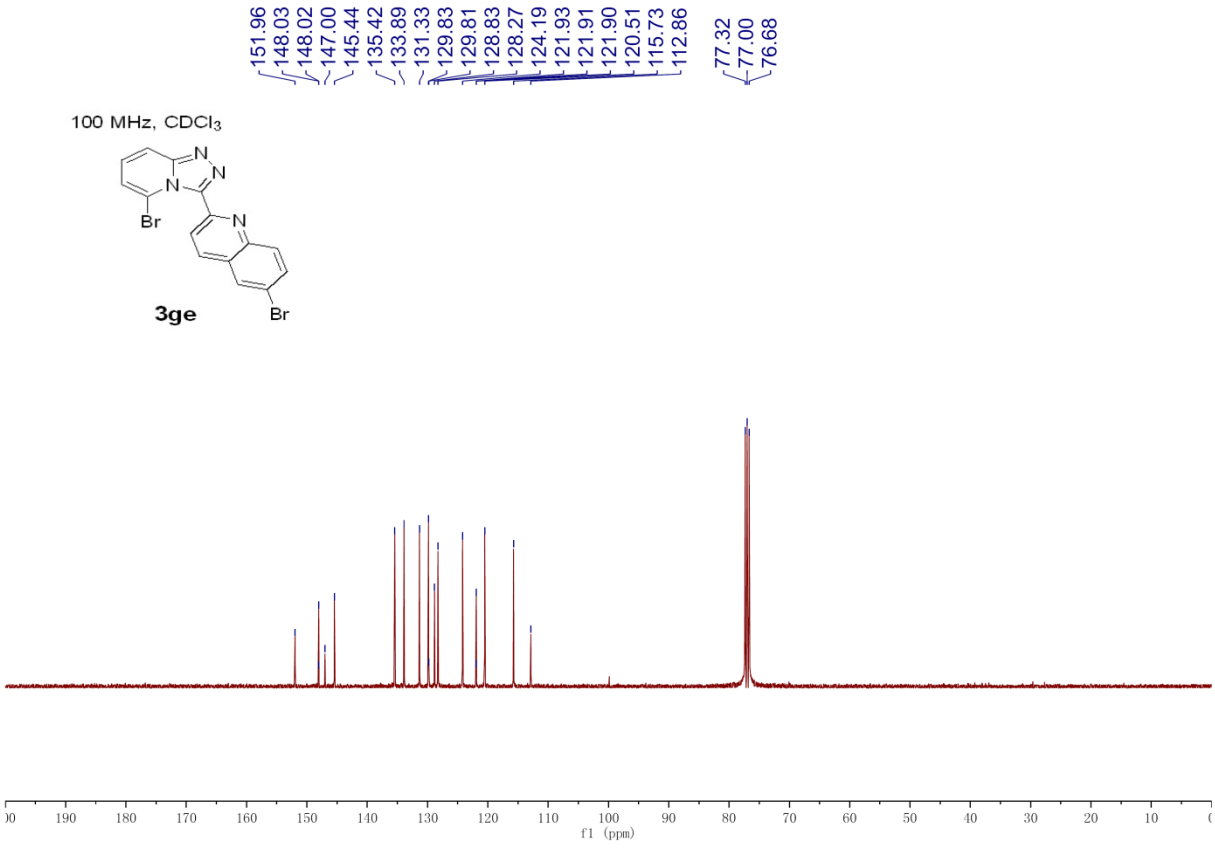

400 MHz, CDCl3
Me
Br
N
3mg
9.130
9.119
8.279
8.258
7.920
7.919
7.917
7.897
7.895
7.850
7.846
7.833
7.829
7.825
7.811
7.808
7.663
7.652
7.627
7.624
7.610
7.607
7.603
7.589
7.586
7.248
7.207
7.204
7.201
2.775
2.773
1.00
1.07
1.94
0.99
1.00
0.98
0.93
3.07
f1 (ppm)


400 MHz, CDCl3
Me
Br
N
3mg
9.130
9.119
8.279
8.258
7.920
7.919
7.917
7.897
7.895
7.850
7.846
7.833
7.829
7.825
7.811
7.808
7.663
7.652
7.627
7.624
7.610
7.607
7.603
7.589
7.248
7.207
7.204
7.201
1.00
1.07
1.94
0.99
1.00
0.98
0.93
f1 (ppm)


100 MHz, CDCl3
Me
Br
3mg
150.11
149.68
148.78
143.71
130.62
129.66
128.66
128.34
125.17
121.70
120.15
77.32
77.00
76.68
16.71
f1 (ppm)


400 MHz, CDCl3
Br
3ge
Br
8.254
8.233
8.230
8.088
8.081
8.019
8.017
7.996
7.994
7.992
7.973
7.952
7.887
7.884
7.865
7.862
7.852
7.846
7.823
7.248
7.228
7.210
7.205
7.187
7.138
7.135
7.120
7.117
1.00
0.95
1.83
0.79
0.99
1.13
0.93
f1 (ppm)


8.254
8.251
8.233
8.230
8.088
8.081
8.019
8.017
7.996
7.994
7.992
7.973
7.952
7.887
7.884
7.865
7.862
7.852
7.846
7.829
7.823
7.248
7.228
7.210
7.205
7.187
7.138
7.135
7.120
7.117
400 MHz, CDCl3
Br
N
N
N
N
Br
3ge
1.00
0.95
1.83
0.79
0.99
1.13
0.93
f1 (ppm)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148.02
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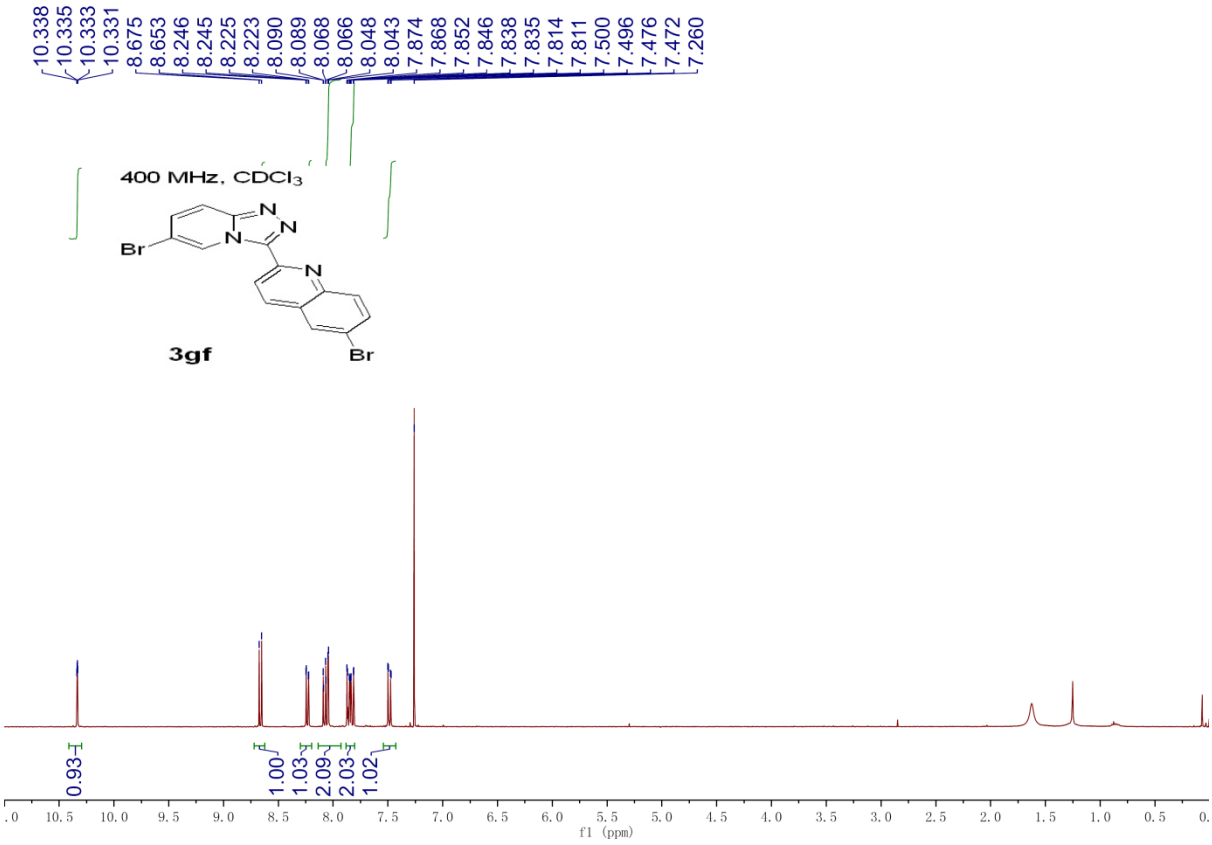
145.44
135.42
133.89
131.33
129.83
129.81
128.83
128.27
124.19
121.93
121.91
121.90
120.51
115.73
112.86
77.32
77.00
76.68
100 MHz, CDCl3
Br
N
N
N
N
Br
3ge
f1 (ppm)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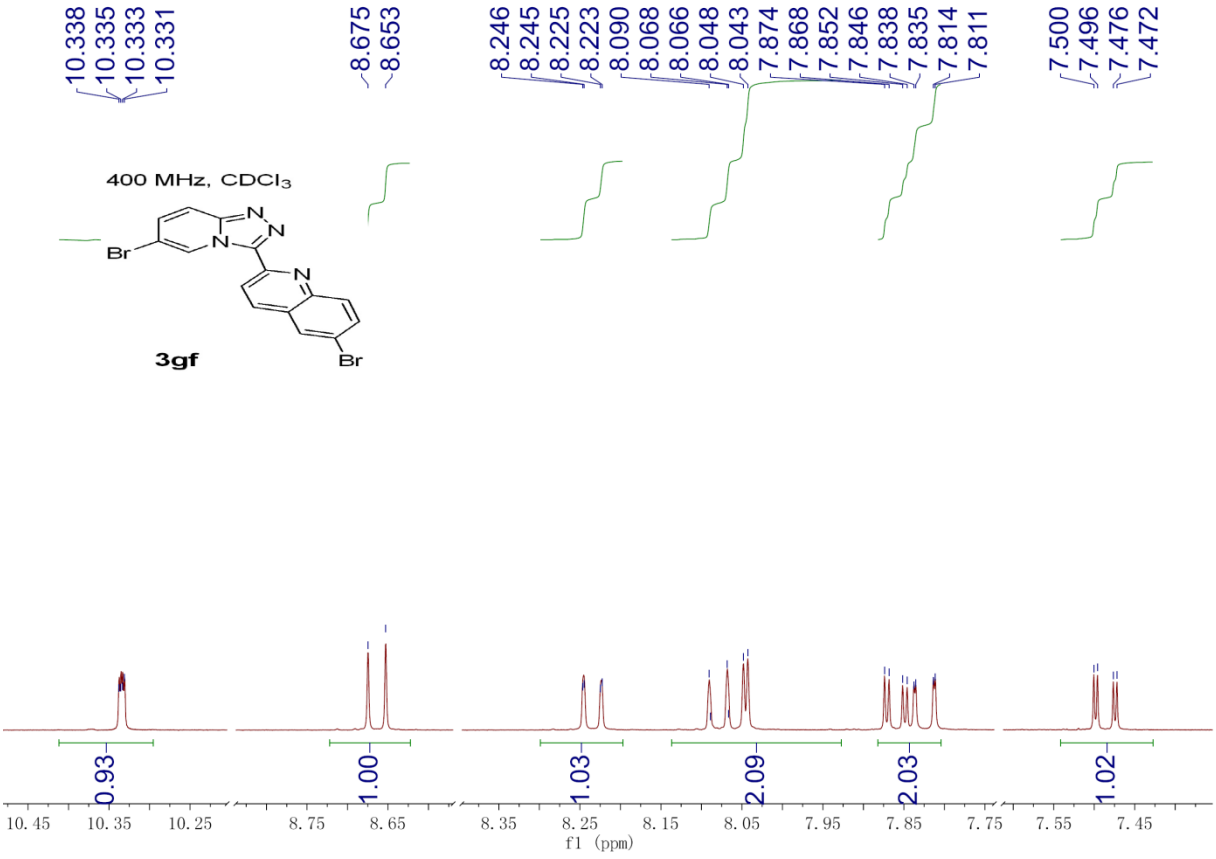
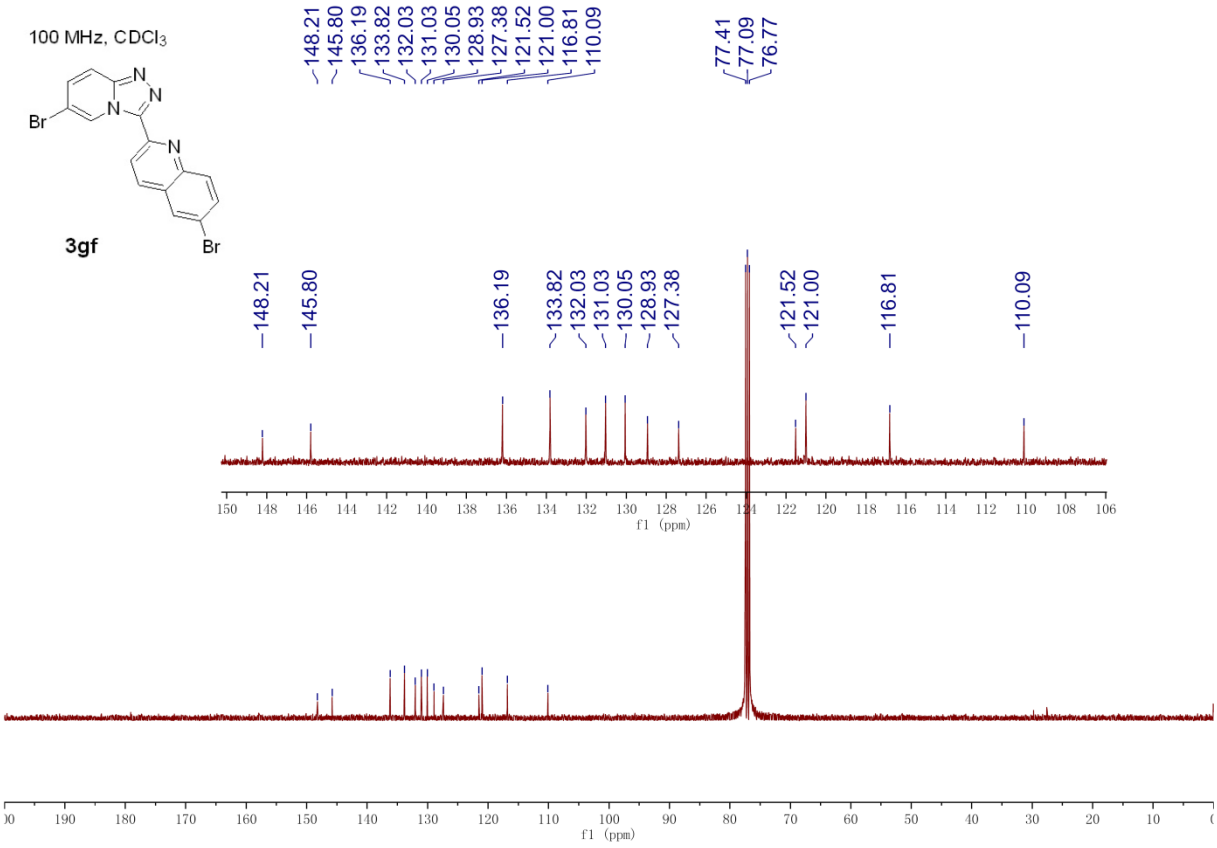
10.335
10.333
10.331
8.675
8.653
8.246
8.245
8.225
8.223
8.090
8.089
8.068
8.066
8.048
8.043
7.874
7.868
7.852
7.846
7.838
7.835
7.814
7.811
7.500
7.496
7.476
7.472
7.260
400 MHz, CDCl3
Br
N
N
N
Br
3gf
0.93
1.00
1.03
2.09
2.03
1.02
f1 (ppm)


10.338
10.335
10.333
10.331
8.675
8.653
8.246
8.245
8.225
8.223
8.090
8.068
8.066
8.048
8.043
7.874
7.868
7.852
7.846
7.838
7.835
7.814
7.811
7.500
7.496
7.476
7.472
400 MHz, CDCl3
Br
N
N
N
Br
3gf
0.93
1.00
1.03
2.09
2.03
1.02
f1 (ppm)


100 MHz, CDCl3
Br
N
N
N
Br
3gf
148.21
145.80
136.19
133.82
132.03
131.03
130.05
128.93
127.38
121.52
121.00
116.81
110.09
77.41
77.09
76.77
f1 (ppm)


400 MHz, CDCl3
Br
N
N
N
3me
9.043
9.032
8.211
8.208
8.205
8.190
8.187
8.184
7.927
7.925
7.904
7.901
7.766
7.749
7.745
7.741
7.728
7.724
7.601
7.590
7.519
7.502
7.498
7.494
7.480
7.477
7.296
7.294
7.292
7.290
7.275
7.273
7.271
7.269
7.248
7.237
7.219
7.214
7.196
7.053
7.050
7.035
7.032
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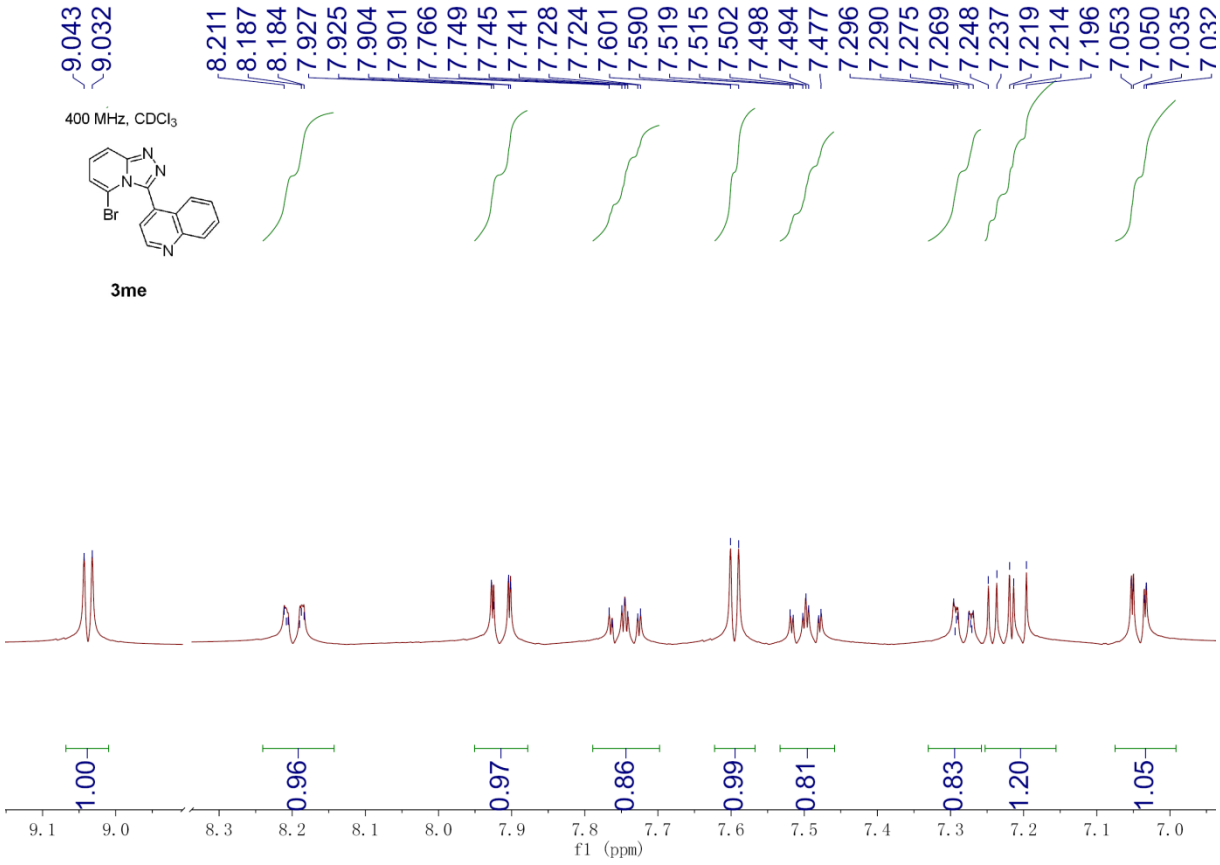
0.97
0.86
0.99
0.81
0.83
1.20
1.05
1.00
f1 (ppm)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9.032
8.211
8.187
8.184
7.927
7.925
7.904
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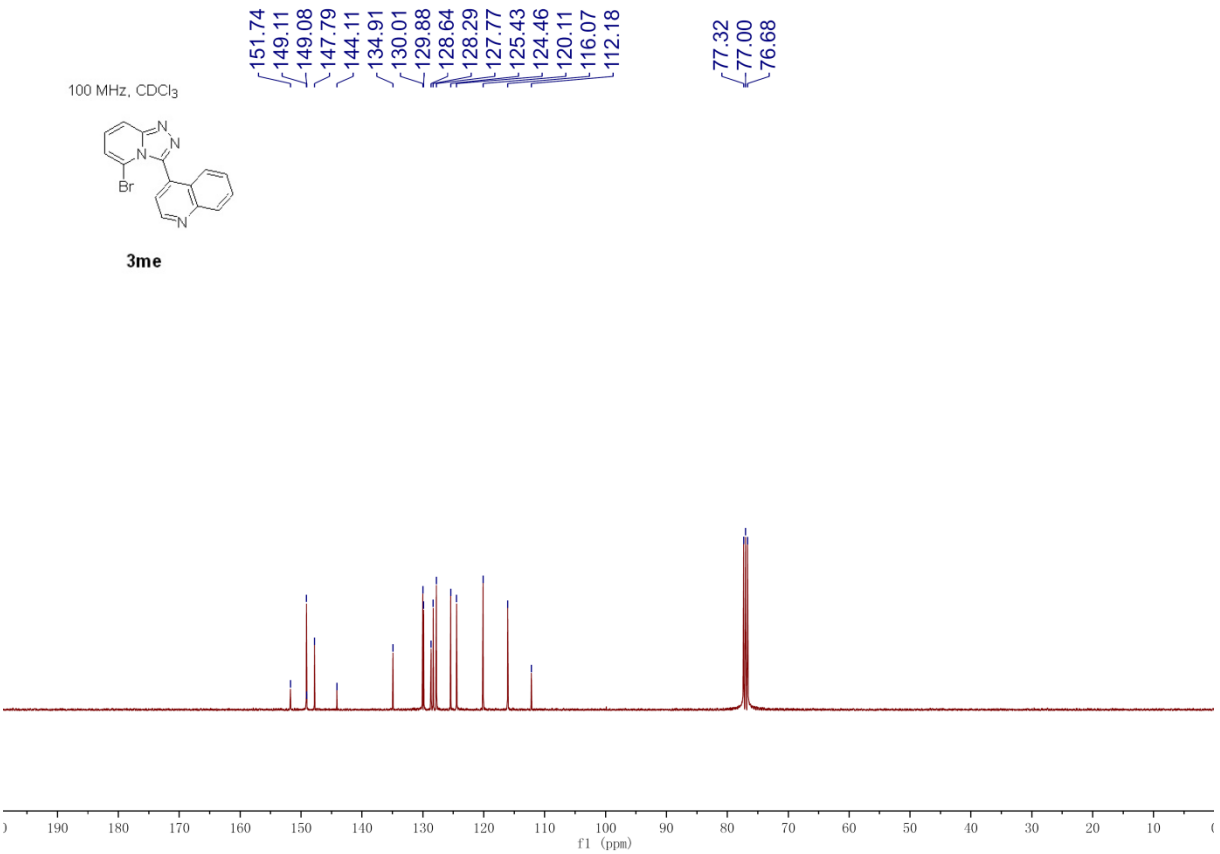
7.766
7.749
7.745
7.741
7.728
7.724
7.601
7.590
7.519
7.515
7.502
7.498
7.494
7.477
7.296
7.290
7.275
7.269
7.248
7.237
7.219
7.214
7.196
7.053
7.050
7.035
7.032
400 MHz, CDCl3
Br
N
N
N
N
3me
1.00
0.96
0.97
0.86
0.99
0.81
0.83
1.20
1.05
9.1
9.0
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
f1 (ppm)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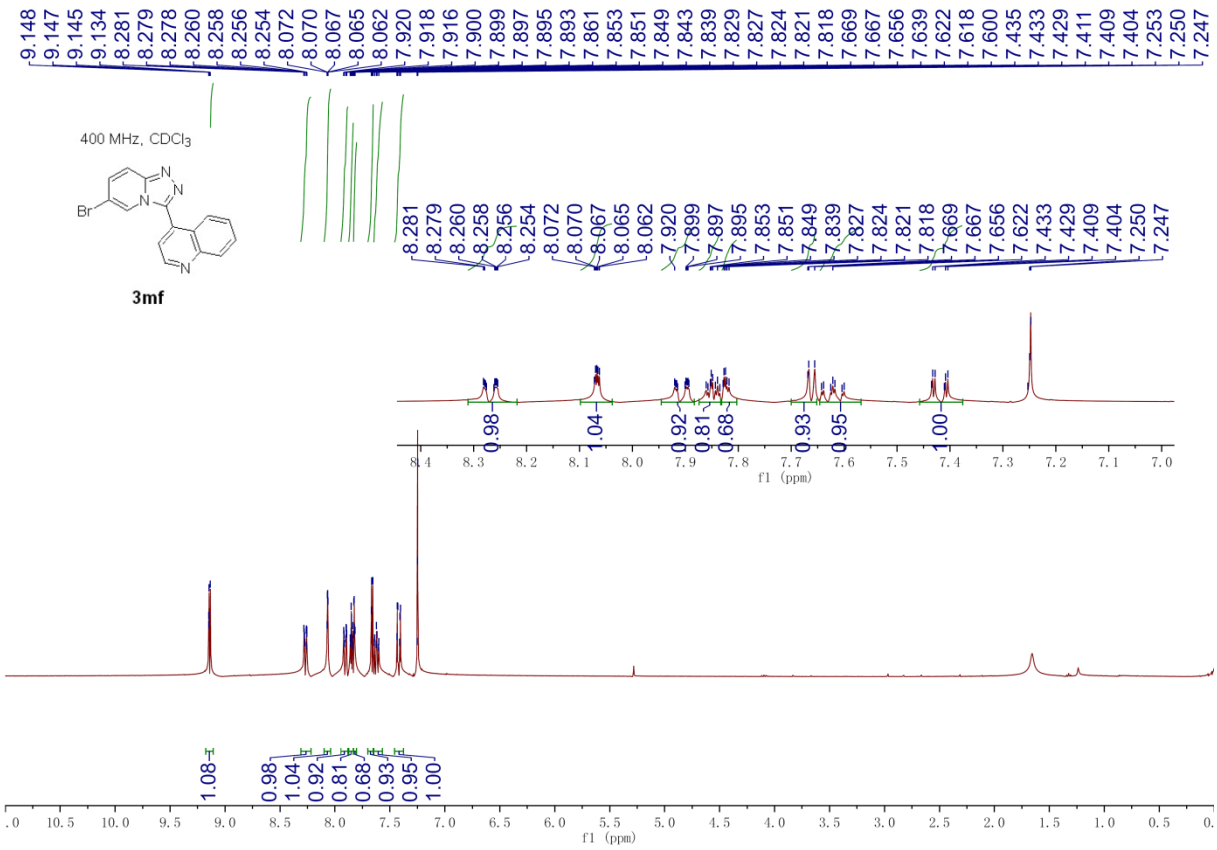
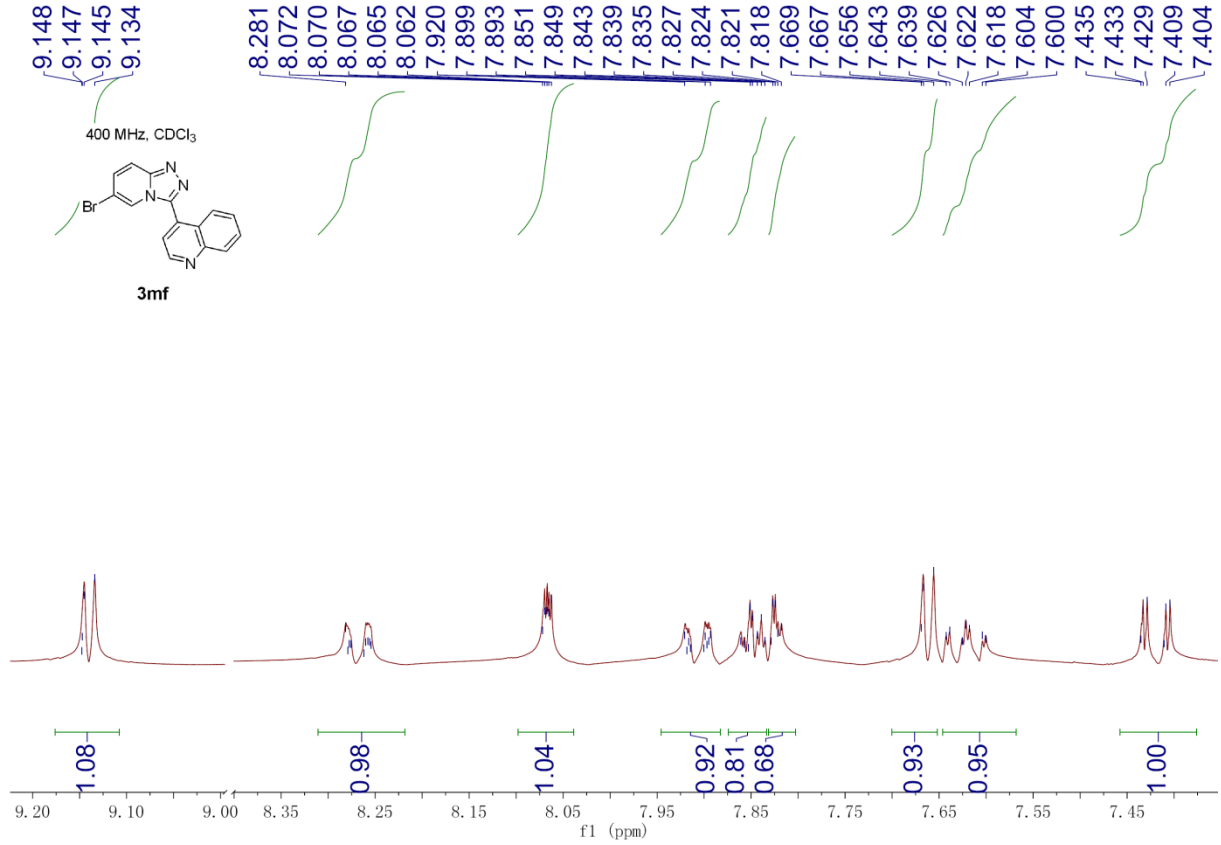
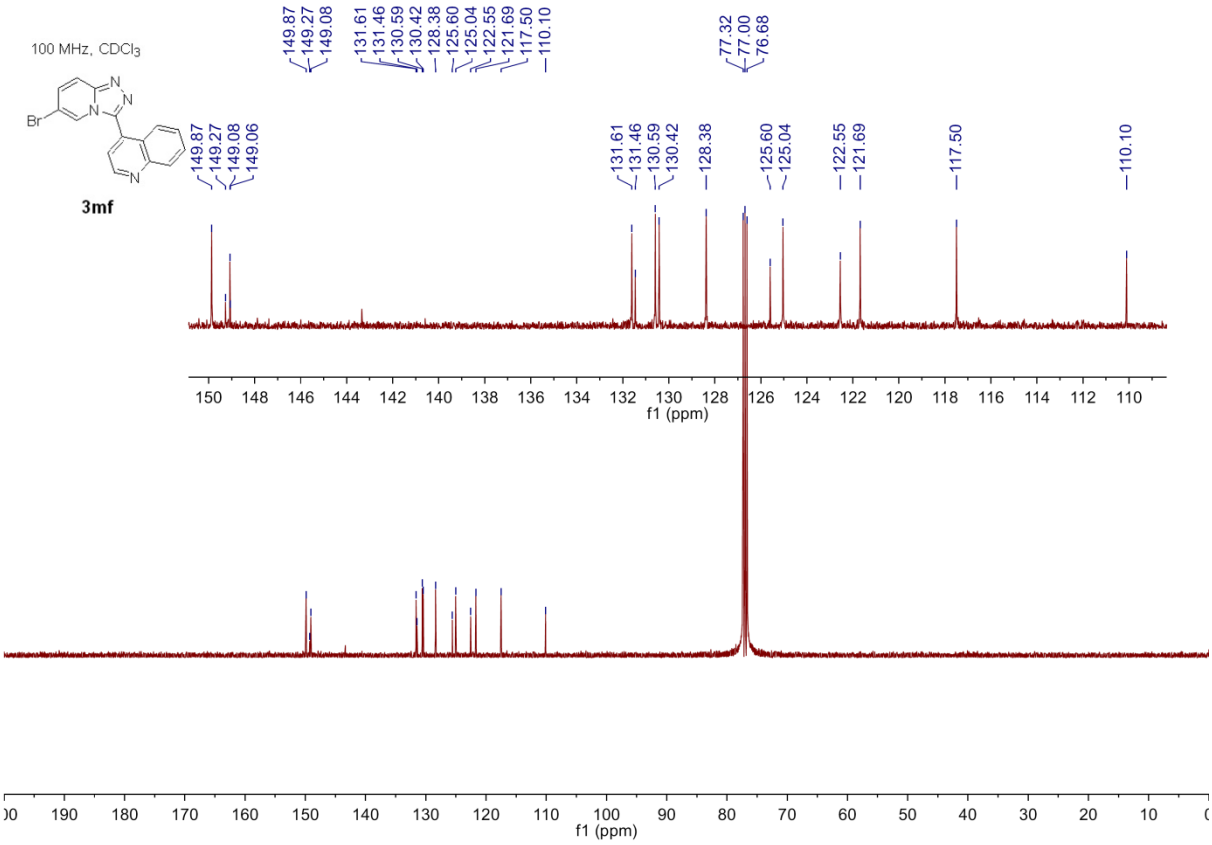
149.11
149.08
147.79
144.11
134.91
130.01
129.88
128.64
128.29
127.77
125.43
124.46
120.11
116.07
112.18
77.32
77.00
76.68
100 MHz, CDCl3
Br
N
N
N
N
3me
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


400 MHz, CDCl3
3mf
f1 (ppm)


400 MHz, CDCl3
3mf
f1 (ppm)


100 MHz, CDCl3
Br
N
N
N
N
3mf
149.87
149.27
149.08
149.06
131.61
131.46
130.59
130.42
128.38
125.60
125.04
122.55
121.69
117.50
110.10
77.32
77.00
76.68
150 148 146 144 142 140 138 136 134 132 130 128 126 124 122 120 118 116 114 112 110
f1 (ppm)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)