Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supporting Information

Radical-Based Regioselective Cross-Coupling of Indoles and Cycloalkanes

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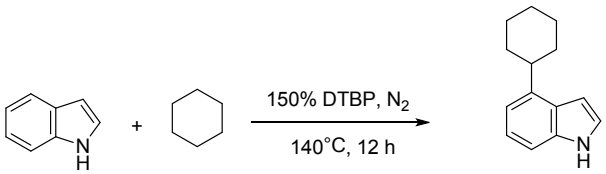
1. General Information

All reactions were run using flame-dried glassware and magnetic stirring. Chemicals and solvents were purchased from commercial suppliers and used as received. ^{1}H and ^{13}C NMR spectra were recorded on a 500 MHz Bruker DRX 500 and tetramethylsilane (TMS) was used as a reference. Chemical shifts were reported in parts per million (ppm), and the residual solvent peak was used as an internal reference: proton (chloroform δ 7.26, acetone δ 2.09, DMSO δ 2.50), carbon (chloroform δ 77.0, acetone *δ* 205.87, 30.60, DMSO δ 40.45). GC-MS were performed on an ISQ Trace 1300 (electrospray ionization: EI). For thin-layer chromatography (TLC), Sorbent silica gel XHL TLC plates (130815) were used, and compounds were visualized with a UV light at 254 nm.

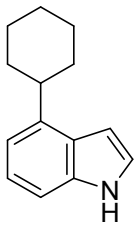
2. Representative Procedure and Analytical Data

Typical Procedure for the synthesis of 3a



A screw-capped test tube equipped with a magnetic stir bar was added indole **1a** (0.117 g, 1 mmol), DTBP (0.276 mL, 1.5 mmol), cyclohexane (4 mL). After being stirred at 140°C for 12 h under a nitrogen atmosphere, the reaction mixture was cooled to room temperature and diluted with ethyl acetate, washed with water, dried over anhydrous Na_2SO_4. The solvents were removed by rotary evaporation to provide raw products. The residue was then chromatographied on silica gel (eluent: petroleum) to give corresponding **3a** (0.14 g, yield 74%) as light brown needled solid.

4-cyclohexyl-1*H*-indole (3a)



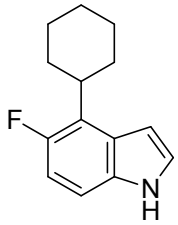
Chemical Formula: $C_{14}H_{17}N$
Calculated Exact Mass: 199.14

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.06 (bs, 1H), 7.18 (d,1H, J = 8.1 Hz), 7.12 (t, 1H, J = 2.8Hz), 7.09 (t, 1H, J = 7.4 Hz), 6.91 (d, 1H, J = 7.2 Hz), 6.57 (m, 1H), 2.90 (tt, 1H, J1 = 11.9 Hz, J2 = 3.2 Hz), 1.96 - 1.94 (m, 2H), 1.83 - 1.80 (m, 2H), 1.74 - 1.71 (m, 1H), 1.56 - 1.38 (m, 4H), 1.29 - 1.21 (m, 1H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 140.45 (s), 135.87 (s), 126.69 (s), 123.42 (s), 122.35 (s), 116.04 (s), 108.78 (s), 101.12 (s), 41.96 (s), 33.74 (s), 27.29 (s), 26.61 (s);

MS (EI): 199.20 (M^+).

4-cyclohexyl-5-fluoro-1*H*-indole (3b)

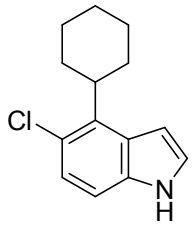


Chemical Formula: $C_{14}H_{16}FN$
Calculated Exact Mass: 217.13

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.03 (bs, 1H), 7.13 (t, 1H, J = 2.8Hz), 7.07 - 7.04 (dd, 1H, J1 = 5.3 Hz, J2 = 3.5 Hz), 6.85 - 6.81 (dd, 1H, J1 = 8.8 Hz, J2 = 2.5 Hz), 6.61 (s, 1H), 3.05 (tt, 1H, J1 = 12.2 Hz, J2 = 3.5 Hz), 1.95 - 1.87 (m, 2H), 1.81 - 1.71 (m, 5H), 1.41 - 1.28 (m, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 156.32 (d, J = 233.1 Hz), 132.58 (s), 127.25 (s), 124.74 (s), 124.40 (d, J = 13.9 Hz), 111.47 (d, J = 29.0 Hz), 109.23 (d, J = 10.1 Hz), 102.47 (s), 38.62 (s), 31.71 (s), 27.31 (s), 26.39 (s);
MS (EI): 217.16 (M^+).

5-chloro-4-cyclohexyl-1*H*-indole (3c)

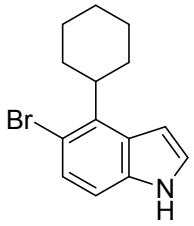


Chemical Formula: $C_{14}H_{16}ClN$
Calculated Exact Mass: 233.10

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04 (bs, 1H), 7.11 - 7.05 (m, 3H), 6.72 (s, 1H), 3.41 (s, 1H), 2.01 (s, 2H),1.83 - 1.73 (dd, 5H, J1 = 39 Hz, J2 = 13 Hz), 1.44 - 1.27 (m, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 136.25 (s), 136.10 (s), 124.16 (s), 124.00 (s), 110.02 (s), 103.18 (s), 41.88 (s), 31.20 (s), 27.27 (s), 26.48 (s);
MS (EI): 233.12 (M^+).

5-bromo-4-cyclohexyl-1*H*-indole (3d)



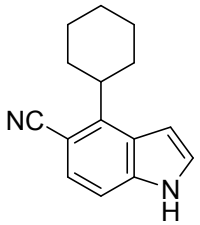
Chemical Formula: $C_{14}H_{16}BrN$
Calculated Exact Mass: 277.05

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 (bs, 1H), 7.36 (d, 1H, J = 8.6 Hz), 7.17 (t, 1H, J

= 2.8Hz), 7.09 (d, 1H, J = 8.6 Hz), 6.82 (s, 1H), 3.49 (s, 1H), 2.07 (s, 1H),1.91 - 1.82 (dd, 5H, J1 = 34.2 Hz, J2 = 13 Hz), 1.53 - 1.35 (m, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 138.00 (s), 135.69 (s), 126.71 (s),123.77 (s), 114.90 (s), 110.54 (s), 103.22 (s), 45.13 (s), 31.31 (s), 27.23 (s), 26.47 (s);
MS (EI): 277.09 (M^+).

4-cyclohexyl-1*H*-indole-5-carbonitrile (3e)

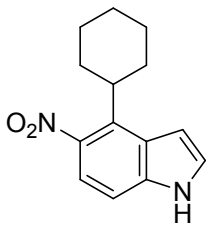


Chemical Formula: $C_{15}H_{16}N_2$
Calculated Exact Mass: 224.13

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.64 (bs, 1H), 7.38 (d, 1H, J = 8.4 Hz),7.31 - 7.29 (m,2H, J = 8.1 Hz), 6.84 (s, 1H), 2.92 (tt, 1H, J1 = 12.4 Hz, J2 = 3.4 Hz), 2.15 - 2.07 (m, 2H), 1.91 - 1.81 (m, 5H), 1.53 - 1.37 (m, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 145.76 (s), 138.10 (s), 126.45 (s), 125.97 (s), 125.05 (s), 120.85 (s), 110.20 (s), 103.50 (s), 101.50 (s), 44.23 (s), 31.91 (s), 26.99 (s), 26.16 (s);
MS (EI): 224.17 (M^+).

4-cyclohexyl-5-nitro-1*H*-indole (3f)

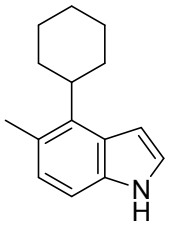


Chemical Formula: $C_{14}H_{16}N_2O_2$
Calculated Exact Mass: 244.12

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.47 (bs, 1H), 7.44 (d, 1H, J = 8.7 Hz), 7.25 (t, 1H, J = 2.8Hz), 7.19 (d, 1H, J = 7.7 Hz),, 6.87 (s, 1H), 2.92 (tt, 1H, J1 = 12.3 Hz, J2 = 3.4 Hz), 2.06 - 1.98 (m, 2H), 1.84 - 1.74 (m, 5H), 1.41 - 1.28 (m, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 144.16 (s), 137.42 (s), 134.82 (s)， 126.03 (s), 125.49 (s), 118.54 (s), 109.39 (s), 105.29 (s), 40.45 (s), 31.69 (s), 26.98 (s), 26.31 (s);
MS (EI): 244.17 (M^+).

4-cyclohexyl-5-methyl-1*H*-indole (3g)

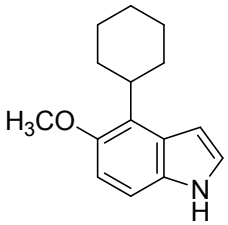


Chemical Formula: $C_{15}H_{19}N$
Calculated Exact Mass: 213.15

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00 (bs, 1H), 7.14 - 7.12 (m, 2H), 7.00 (d, 1H, J = 8.3 Hz), 6.75 (s, 1H), 3.10 (tt, 1H, J1 = 14.9 Hz, J2 = 3.5 Hz), 2.43 (s, 3H), 2.13 - 2.05 (m, 2H), 1.81 - 1.77 (m, 5H), 1.48 - 1.38 (m, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 137.24 (s), 135.61 (s), 125.61 (s), 125.37 (s), 123.00 (s), 108.65 (s), 103.01 (s), 41.32 (s), 31.55 (s), 27.59 (s), 26.64 (s), 20.38 (s);
MS (EI): 213.22 (M^+).

4-cyclohexyl-5-methoxy-1*H*-indole (3h)

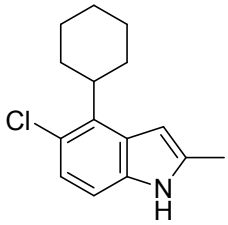


Chemical Formula: $C_{15}H_{19}NO$
Calculated Exact Mass: 229.15

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00 (bs, 1H), 7.16 - 7.15 (m, 2H),6.93 (d, 1H, J = 8.8 Hz), 6.69 (s, 1H), 3.83 (s, 3H), 3.32 - 3.28 (m, 1H), 2.11 - 2.03 (m, 2H), 1.87 - 1.75 (m, 5H), 1.49 - 1.35 (m, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 150.94 (s), 132.33 (s), 127.79 (s)，127.30 (s), 124.26 (s), 111.46 (s), 109.02 (s), 102.55 (s), 58.92 (s), 38.23 (s), 31.68 (s), 27.53 (s), 26.64 (s);
MS (EI): 229.21 (M^+).

5-chloro-4-cyclohexyl-2-methyl-1*H*-indole (3i)

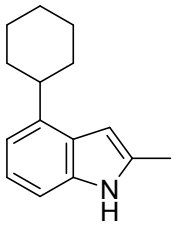


Chemical Formula: $C_{15}H_{18}ClN$
Calculated Exact Mass: 247.11

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82 (bs, 1H), 7.08 (d, 1H, J = 8.5 Hz), 7.02 (d, 1H, J = 8.5 Hz), 6.45 (s, 1H), 3.43 (s, 1H), 2.43 (s, 3H), 2.05 (s, 2H), 1.89 - 1.77 (m, 5H), 1.50 - 1.35 (m, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 135.26 (s), 134.95 (s), 124.03 (s), 122.74 (s), 109.27 (s), 101.15 (s), 41.76 (s), 31.10 (s), 27.29 (s), 26.50 (s), 13.82 (s);
MS (EI): 247.19 (M^+).

4-cyclohexyl-2-methyl-1*H*-indole (3k)

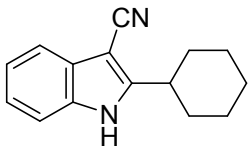


Chemical Formula: $C_{15}H_{19}N$
Calculated Exact Mass: 213.15

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (bs, 1H), 7.13 (d, 1H, J = 8.0 Hz), 7.06 (t, 1H, J = 7.4Hz), 6.92 (d, 1H, J = 7.2 Hz), 6.30 (s, 1H), 2.89 (tt, 1H, J1 = 11.9 Hz, J2 = 3.2 Hz), 2.44(s, 3H), 2.00 - 1.98 (m, 2H), 1.89 - 1.86 (m, 2H), 1.80 - 1.77 (m, 1H), 1.61 - 1.42 (m, 4H), 1.35 - 1.32 (m, 1H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 139.40 (s), 136.15 (s), 134.31 (s), 127.75 (s), 121.32 (s), 115.97 (s), 108.05 (s), 99.00 (s), 42.04 (s), 33.69 (s), 27.34 (s), 26.64 (s), 13.88 (s);
MS (EI): 213.21 (M^+).

2-cyclohexyl-1*H*-indole-3-carbonitrile (3l)

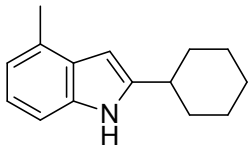


Chemical Formula: $C_{15}H_{16}N_2$
Calculated Exact Mass: 224.13

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.52 (bs, 1H), 7.67 (m, 1H), 7.37 (m, 1H), 7.24 (m, 2H), 6.29 (s, 1H), 3.05 (tt, 1H, J1 = 12.2 Hz, J2 = 3.5 Hz), 2.09 - 2.07 (m, 2H), 1.92 - 1.90 (m, 2H), 1.82 - 1.80 (m, 1H), 1.64 - 1.42 (m, 4H), 1.34 - 1.26 (m, 1H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 153.54 (s), 134.21 (s), 127.93 (s), 123.44 (s), 122.13 (s), 119.16 (s), 116.54 (s), 111.45 (s), 83.52 (s) 37.70 (s), 32.52 (s), 26.24 (s), 25.78 (s); **MS (EI)**: 224.17 (M^+).

2-cyclohexyl-4-methyl-1*H*-indole (3m)



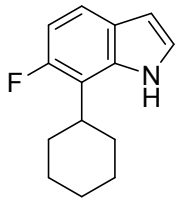
Chemical Formula: $C_{15}H_{19}N$
Calculated Exact Mass: 213.15

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.92 (bs, 1H), 7.16 (d, 1H, J = 8.1 Hz), 7.03 (t, 1H, J = 7.3 Hz), 6.88 (d, 1H, J = 7.2 Hz), 6.25 (m, 1H), 2.74 (tt, 1H, J1 = 11.3 Hz, J2 = 3.3

Hz), 2.12 - 2.09 (m, 2H), 1.89 - 1.86 (m, 2H), 1.78 - 1.76 (m, 1H), 1.52 - 1.39 (m, 4H), 1.34 - 1.28 (m, 1H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 144.57 (s), 135.28 (s), 129.48 (s), 128.51 (s), 121.19 (s), 119.84 (s), 108.04 (s), 96.10 (s), 37.52 (s), 33.19 (s), 26.41 (s), 26.26 (s), 18.98 (s);
MS (EI): 213.23 (M^+).

7-cyclohexyl-6-fluoro-1*H*-indole (3n-1)

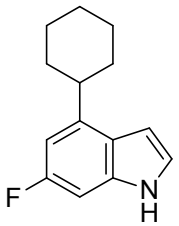


Chemical Formula: $C_{14}H_{16}FN$
Calculated Exact Mass: 217.13

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.22 (bs, 1H), 7.40 - 7.37 (m, 1H), 7.18 (t, 1H, J = 2.8 Hz) 6.88 - 6.84 (m, 1H), 6.53 - 6.52 (m, 1H), 3.01 - 2.95 (m, 1H), 1.92 - 1.89 (m, 6H), 1.83 - 1.80 (m, 1H), 1.49 - 1.35 (m, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 158.51 (d, J = 236.9Hz), 134.68 (d, J = 10.1 Hz), 124.59 (s), 124.05 (s), 118.87 (d, J = 10.1 Hz), 116.08 (d, J = 18.9 Hz), 109.74 (d, J = 27.7 Hz), 103.09 (s), 37.54 (s), 31.80 (s), 27.29 (s), 26.30 (s);
MS (EI): 217.14 (M^+).

4-cyclohexyl-6-fluoro-1*H*-indole (3n-2)



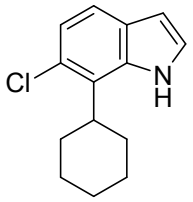
Chemical Formula: $C_{14}H_{16}FN$
Calculated Exact Mass: 217.13

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04 (bs, 1H), 7.10 (m, 1H), 6.87 - 6.85 (dd, 1H, J1 = 9.3 Hz, J2 = 1.5 Hz), 6.76 - 6.74 (dd, 1H, J1 = 11.3 Hz, J2 = 2.1 Hz), 6.58 (t, 1H, J = 2.1Hz), 2.94 (tt, 1H, J1 = 14.4 Hz, J2 = 2.9 Hz), 2.00 (d, 2H, J = 11.9 Hz), 1.88 (d, 2H, J = 12.3 Hz), 1.80 (d, 1H, J = 13.0 Hz), 1.56 - 1.42 (m, 4H), 1.34 - 1.26 (m, 1H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 161.46 (d, J = 238.1Hz), 142.04 (d, J = 7.6 Hz), 135.65 (d, J = 12.6 Hz), 123.69 (s), 123.18 (s), 105.37 (d, J = 25.2 Hz), 101.17 (s), 95.04 (d, J = 26.5 Hz), 41.80 (s), 33.66 (s), 27.16 (s), 26.53 (s);

MS (EI): 217.18 (M^+).

6-chloro-7-cyclohexyl-1*H*-indole (3o-1)

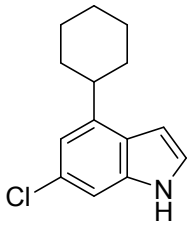


Chemical Formula: $C_{14}H_{16}ClN$
Calculated Exact Mass: 233.10

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.29 (bs, 1H), 7.31 (d, 1H, J = 8.4 Hz), 7.11 (t, 1H, J = 3.0 Hz), 7.04 (d, 1H, J = 8.4 Hz), 6.44 (s, 1H), 3.38 (s, 1H), 1.86 - 1.77 (m, 7H), 1.45 - 1.25 (m, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 134.80 (s), 130.38 (s), 129.04 (s), 126.91 (s), 124.17 (s), 122.24 (s), 119.32 (s), 102.88 (s), 40.73 (s), 31.38 (s), 27.18 (s), 26.43 (s);
MS (EI): 233.13 (M^+).

6-chloro-4-cyclohexyl-1*H*-indole (3o-2)

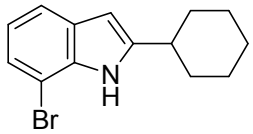


Chemical Formula: $C_{14}H_{16}ClN$
Calculated Exact Mass: 233.10

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05 (bs, 1H), 7.17 (s, 1H), 7.12 (t, 1H, J = 2.8 Hz), 6.94 (d, 1H, J = 1.5 Hz), 6.57 (s, 1H), 2.92 (tt, 1H, J1 = 11.7 Hz, J2 = 3.1 Hz), 1.98 - 1.96 (m, 2H), 1.88 - 1.86 (m, 2H), 1.79 - 1.77 (m, 1H), 1.57 - 1.41 (m, 4H), 1.33 - 1.26 (m, 1H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 141.81 (s), 136.16 (s), 128.30 (s)，125.40 (s), 124.12 (s), 117.20 (s), 108.76 (s), 101.28 (s), 41.87 (s), 33.64 (s), 27.18 (s), 26.52 (s);
MS (EI): 233.06 (M^+).

7-bromo-2-cyclohexyl-1*H*-indole (3p-1)

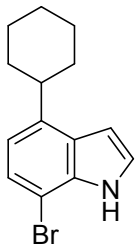


Chemical Formula: $C_{14}H_{16}BrN$
Calculated Exact Mass: 277.05

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04 (bs, 1H), 7.46 (d, 1H, J = 7.9 Hz), 7.25 (d, 1H, J = 7.5 Hz), 6.94 (t, 1H, J = 7.8Hz), 6.30 (d, 1H, J = 1.9 Hz), 2.74 (tt, 1H, J1 = 11.4 Hz, J2 = 3.3 Hz), 2.11 (d, 2H, J = 12.7 Hz), 1.88 (d, 2H, J = 12.9 Hz), 1.77 (d, 1H, J = 12.9 Hz), 1.53 - 1.39 (m, 4H), 1.34 - 1.27 (m, 1H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 145.98 (s), 134.32 (s), 129.93 (s), 123.36 (s), 120.86 (s), 119.18 (s), 104.12 (s), 98.88 (s), 37.47 (s), 33.04 (s), 26.34 (s), 26.17 (s);
MS (EI): 277.09 (M^+).

7-bromo-4-cyclohexyl-1*H*-indole (3p-2)

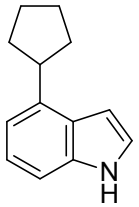


Chemical Formula: $C_{14}H_{16}BrN$
Calculated Exact Mass: 277.05

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.34 (bs, 1H), 7.30 (d, 1H, J = 7.9 Hz), 7.25 (t, 1H, J = 2.8 Hz), 6.86 (d, 1H, J = 7.9 Hz),6.70 (t, 1H, J = 2.3 Hz), 2.93 (tt, 1H, J1 = 11.7 Hz, J2 = 3.1 Hz), 1.99 (d, 2H, J = 12.8 Hz), 1.90 (d, 1H, J = 12.8 Hz), 1.81 (d, 1H, J = 13.0 Hz), 1.60 - 1.43 (m, 4H), 1.35 - 1.29 (m, 1H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 140.02 (s), 134.45 (s), 130.04 (s), 127.91 (s), 124.57 (s), 124.01(s), 117.56 (s), 102.43 (s), 41.73 (s), 33.77 (s), 27.21 (s), 26.52 (s);
MS (EI): 277.07 (M^+).

4-cyclopentyl-1*H*-indole (3q)

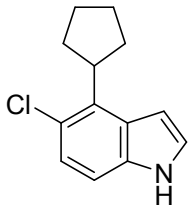


Chemical Formula: $C_{13}H_{15}N$
Calculated Exact Mass: 185.12

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 (bs, 1H), 7.25 （d, 1H, J = 8.2 Hz）, 7.19 (t, 1H, J = 2.7 Hz), 7.14 (t, 1H, J = 7.4 Hz), 7.01 (d, 1H, J = 7.2 Hz), 6.63 (t, 1H, J = 2.1 Hz); 3.48 - 3.41(m, 1H), 2.15 - 2.12 (m, 2H), 1.87 - 1.71 (m, 6H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 138.74 (s), 135.86 (s), 127.05 (s), 123.29 (s), 122.17 (s), 116.27 (s), 108.75 (s), 101.49 (s), 43.53 (s), 33.47 (s), 25.75 (s);
MS (EI): 185.19 (M+).

5-chloro-4-cyclopentyl-1*H*-indole (3r)

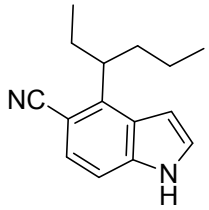


Chemical Formula: $C_{13}H_{14}ClN$
Calculated Exact Mass: 219.08

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.10 (bs, 1H), 7.14 - 7.08 (m, 3H), 6.57 - 6.06 (m, 1H), 3.87 - 3.80 (m, 1H), 2.06 - 1.89 (m, 6H), 1.75 - 1.72 (m, 2H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 135.06 (d, J = 16.4 Hz), 126.87 (s), 124.71 (s), 124.14 (d, J = 46.6 Hz), 109.97 (s), 102.36 (s), 41.83 (s), 31.93 (s), 27.12 (s);
MS (EI): 219.14 (M^+).

4-(hexan-3-yl)-1*H*-indole-5-carbonitrile (3s)

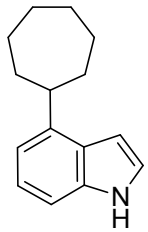


Chemical Formula: $C_{15}H_{18}N_2$
Calculated Exact Mass: 226.15

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.48 (bs, 1H), 7.39（d, 1H, J = 8.4 Hz）, 7.31-7.28(m, 2H), 6.78-6.76 (m, 1H), 3.57-3.50(m, 1H), 2.04-1.98 (m, 1H), 1.88 - 1.81 (m, 1H), 1.52 (d, 2H, J =7.1 Hz), 1.34 - 1.25 (m, 3H), 1.08 - 1.02 (m, 1H), 0.89 - 0.78 (m, 4H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 145.87 (s), 137.89 (s), 126.22 (s), 125.72 (s), 124.95 (s), 120.57 (s), 110.04 (s), 103.22 (s), 38.98 (s), 36.25 (s), 30.35 (s), 22.72 (s), 20.66 (s), 13.98(s);
MS (EI): 226.20 (M+).

4-cycloheptyl-1*H*-indole (3t)

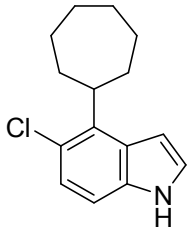


Chemical Formula: $C_{15}H_{19}N$
Calculated Exact Mass: 213.15

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 (bs, 1H), 7.23 （d, 1H, J = 8.1 Hz）, 7.18 (t, 1H, J = 2.8 Hz), 7.14 (t, 1H, J = 7.4 Hz), 6.97 (d, 1H, J = 7.2 Hz), 6.61 (t, 1H, J = 2.1 Hz); 3.12 (tt, 1H, J1 = 10.4 Hz, J2 = 3.5 Hz), 2.07 - 2.02 (m, 2H), 1.87 - 1.73 (m, 6H), 1.68 - 1.60 (m, 4H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 141.95 (s), 135.77 (s), 126.22 (s), 123.40 (s), 122.37 (s), 116.30 (s), 108.61 (s), 101.30 (s), 44.24 (s), 35.89 (s), 28.22 (s), 27.77 (s);
MS (EI): 213.22 (M+).

5-chloro-4-cycloheptyl-1*H*-indole (3u)

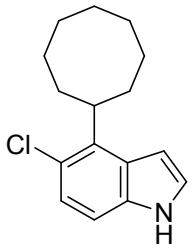


Chemical Formula: $C_{15}H_{18}ClN$
Calculated Exact Mass: 247.11

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 (bs, 1H), 7.18 (t, 1H, J = 2.7 Hz), 7.17 (d, 1H, J = 8.5 Hz), 7.13 (d, 1H, J = 8.5 Hz), 6.68 (s, 1H), 3.63 (s, 1H)，2.13 (s, 2H), 1.90 - 1.77 (m, 6H), 1.70 - 1.64 (m, 4H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 138.20 (s), 135.03 (s), 123.96 (s), 123.34 (s), 109.69 (s), 103.17 (s), 43.28 (s), 33.59 (s), 28.65(s), 28.16 (s);
MS (EI): 247.18 (M^+).

5-chloro-4-cyclooctyl-1*H*-indole (3v)

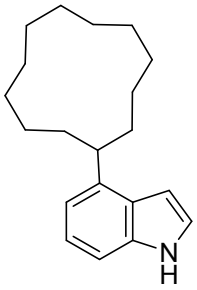


Chemical Formula: $C_{16}H_{20}ClN$
Calculated Exact Mass: 261.13

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.15 (bs, 1H), 7.19 - 7.11 （m, 3H）, 6.61(s, 1H), 3.80 (s, 1H), 2.11 (s, 2H), 1.87 - 1.62 (m, 12H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 139.50 (s), 135.20 (s), 126.57 (s), 124.01 (d, J = 86.9 Hz), 109.71(s), 103.43 (s), 40.34 (s), 33.79 (s), 29.82 (s)，27.10 (s)，26.53 (s);
MS (EI): 261.16 (M^+).

4-cyclododecyl-1*H*-indole (3w)

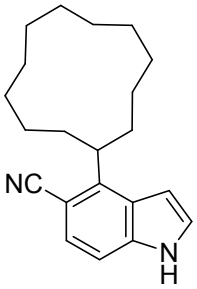


Chemical Formula: $C_{20}H_{29}N$
Calculated Exact Mass: 283.23

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 (bs, 1H), 7.25 （d, 1H, J = 8.1 Hz）, 7.19 (t, 1H, J = 2.9 Hz), 7.15 (t, 1H, J = 7.6 Hz), 6.99 (d, 1H, J = 7.2 Hz), 6.65 (t, 1H, J = 2.0 Hz); 3.28 - 3.23(m, 1H), 1.95 - 1.90 (m, 2H), 1.70 - 1.62 (m, 2H), 1.48 - 1.26 (m, 18H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 140.07 (s), 135.95 (s), 127.29 (s), 123.37 (s), 122.25 (s), 117.36 (s), 108.63 (s), 101.39 (s), 37.10 (s), 30.82 (s), 24.10 (s), 24.06 (s), 23.74 (s), 23.45(s), 23.18 (s);
MS (EI): 283.29 (M+).

4-cyclododecyl-1*H*-indole-5-carbonitrile （3x）

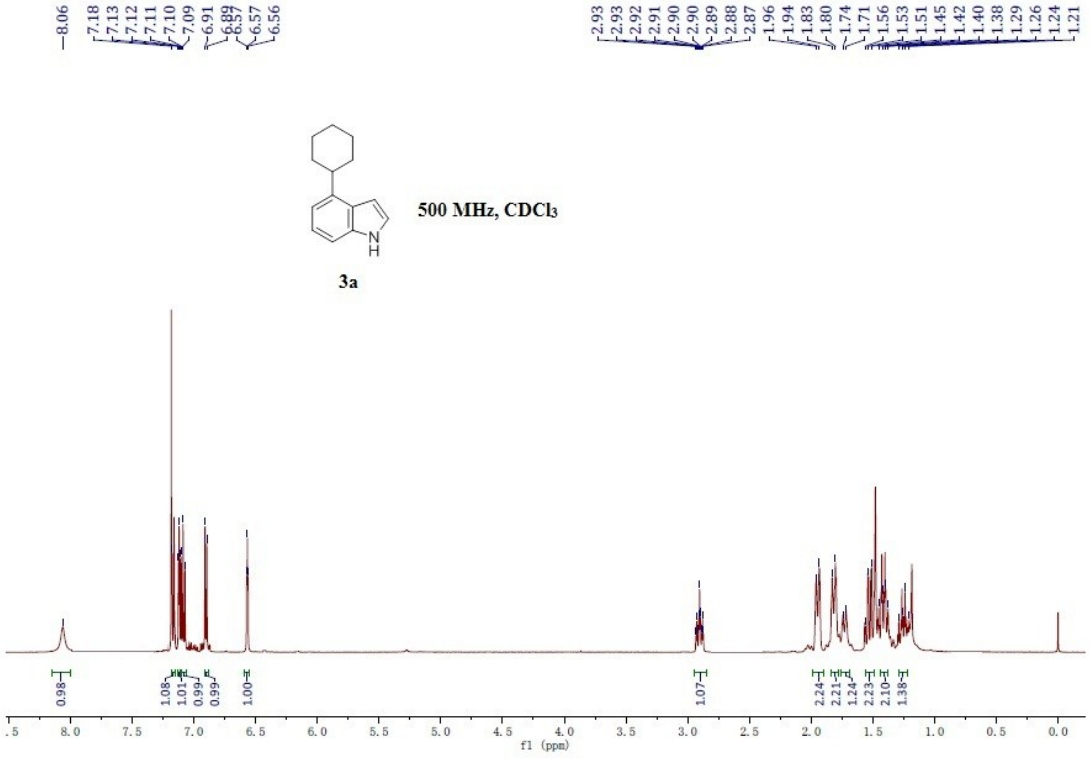


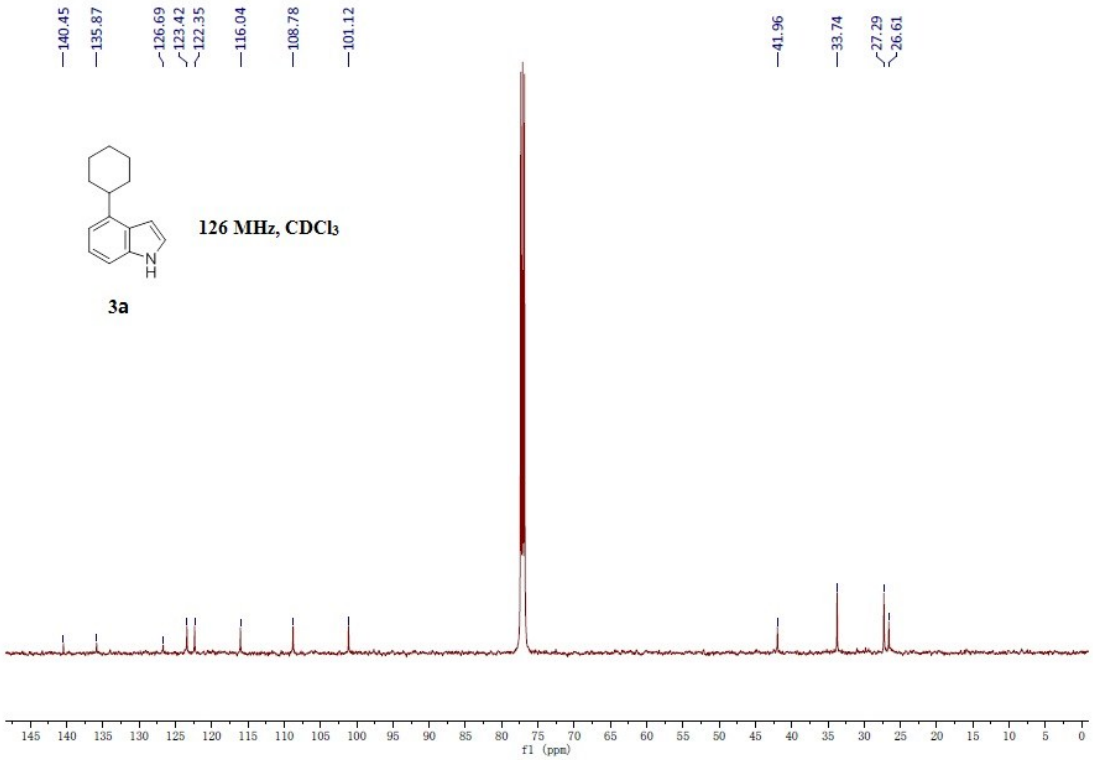
Chemical Formula: $C_{21}H_{28}N_2$
Calculated Exact Mass: 308.23

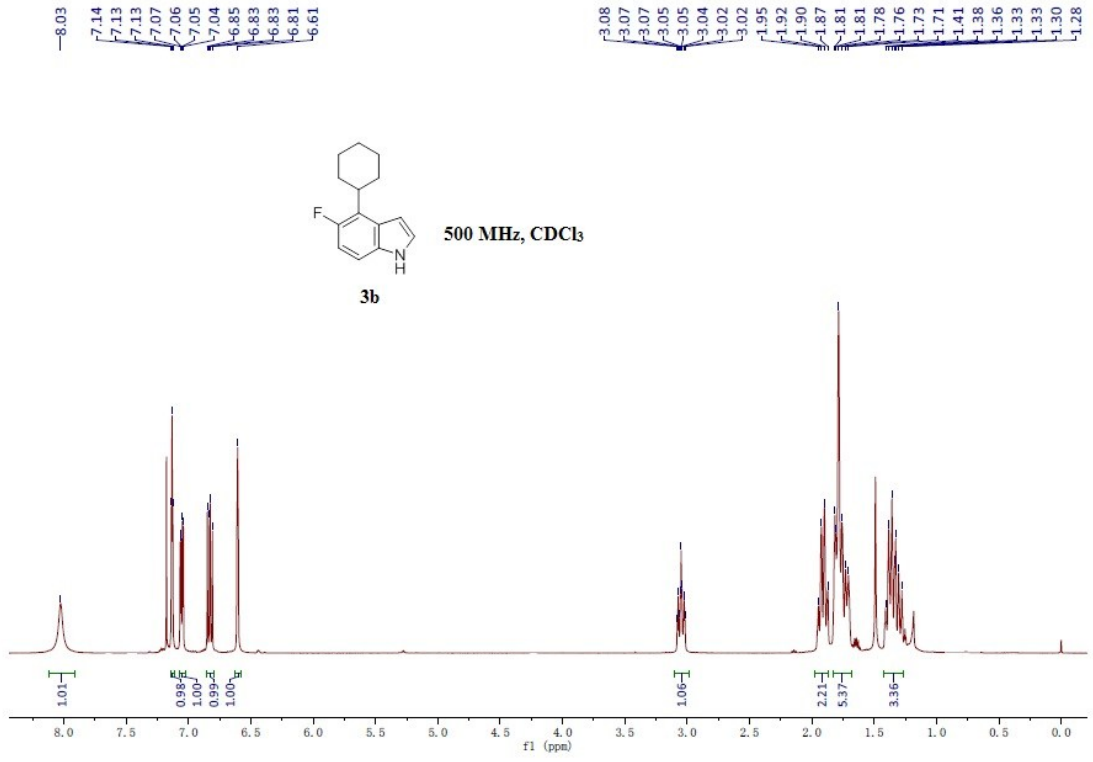
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.59 (bs, 1H), 7.41（d, 1H, J = 8.4 Hz）, 7.34 - 7.29(m, 2H), 6.79 (t, 1H, J = 2.2 Hz), 3.63 - 3.60 (m, 1H), 2.25 - 2.19(m, 2H), 1.84 - 1.78 (m, 4H), 1.66 - 1.63 (m, 2H), 1.52 - 1.35 (m, 14H);

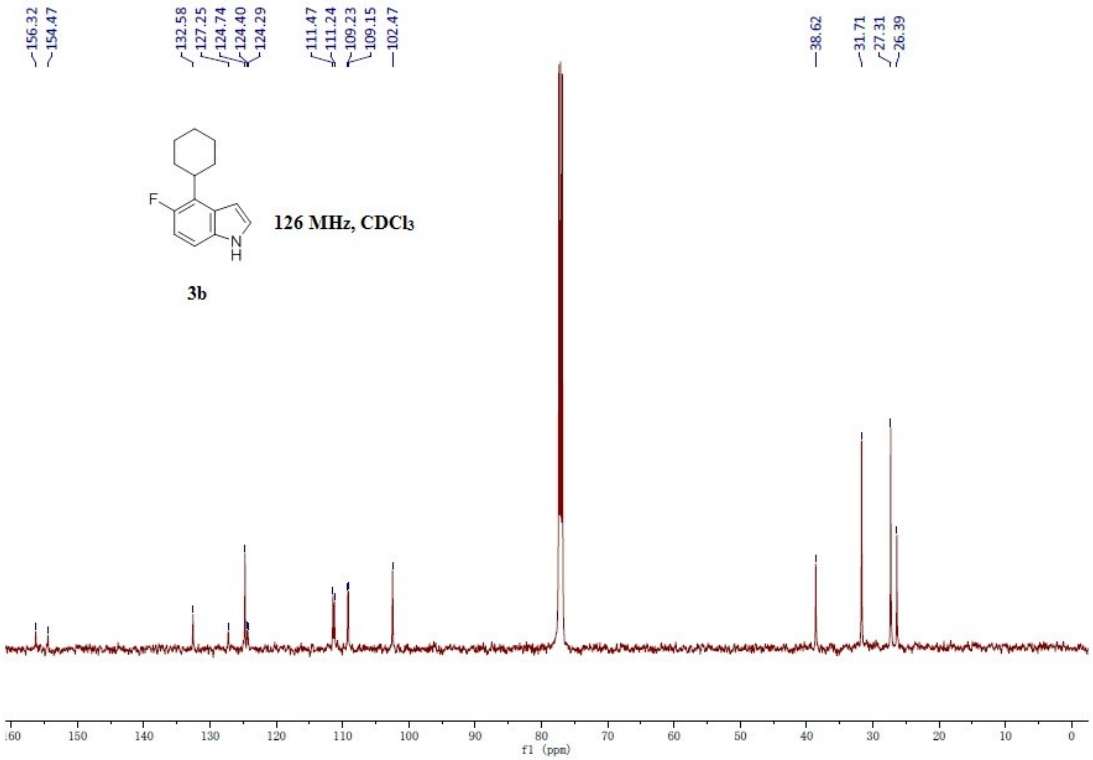
^{13}C NMR (126 MHz, $CDCl_3$) δ 146.17 (s), 138.06 (s), 126.00 (s), 124.99 (s), 120.81 (s), 110.21 (s), 103.62 (s), 38.33 (s), 30.63 (s), 24.54 (s), 24.44 (s), 23.92 (s), 22.89(s), 22.41 (s);
MS (EI): 308.21 (M^+).

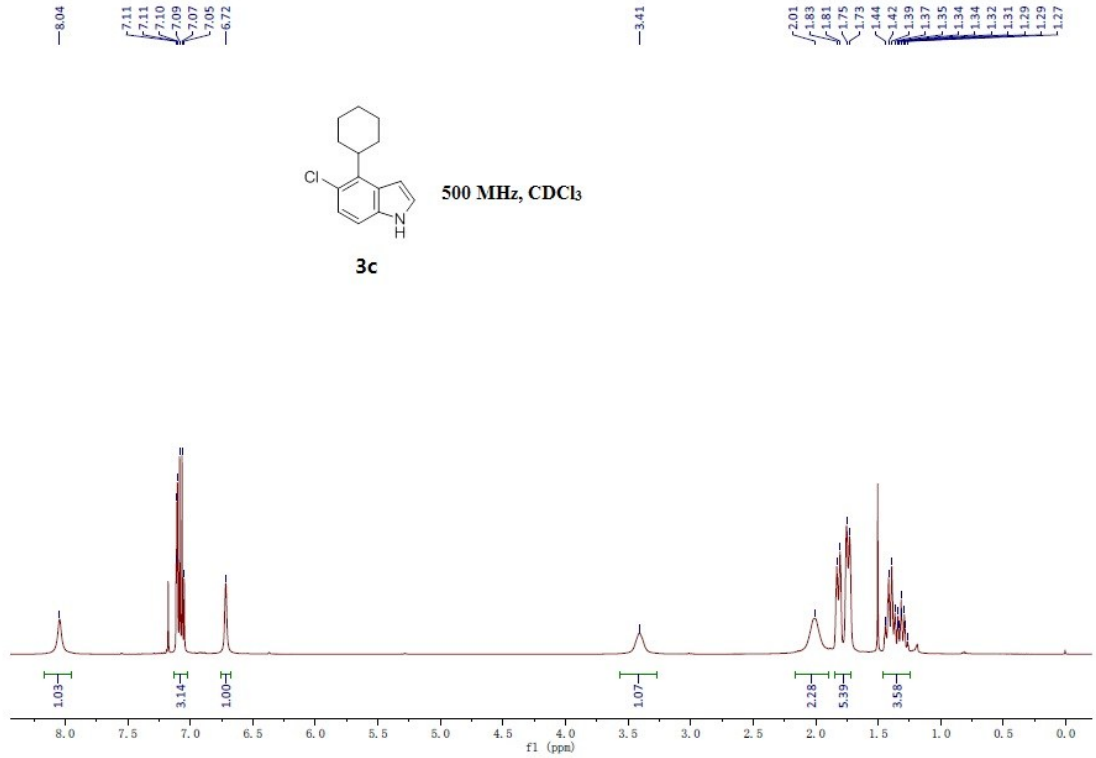
3. NMR Spectra

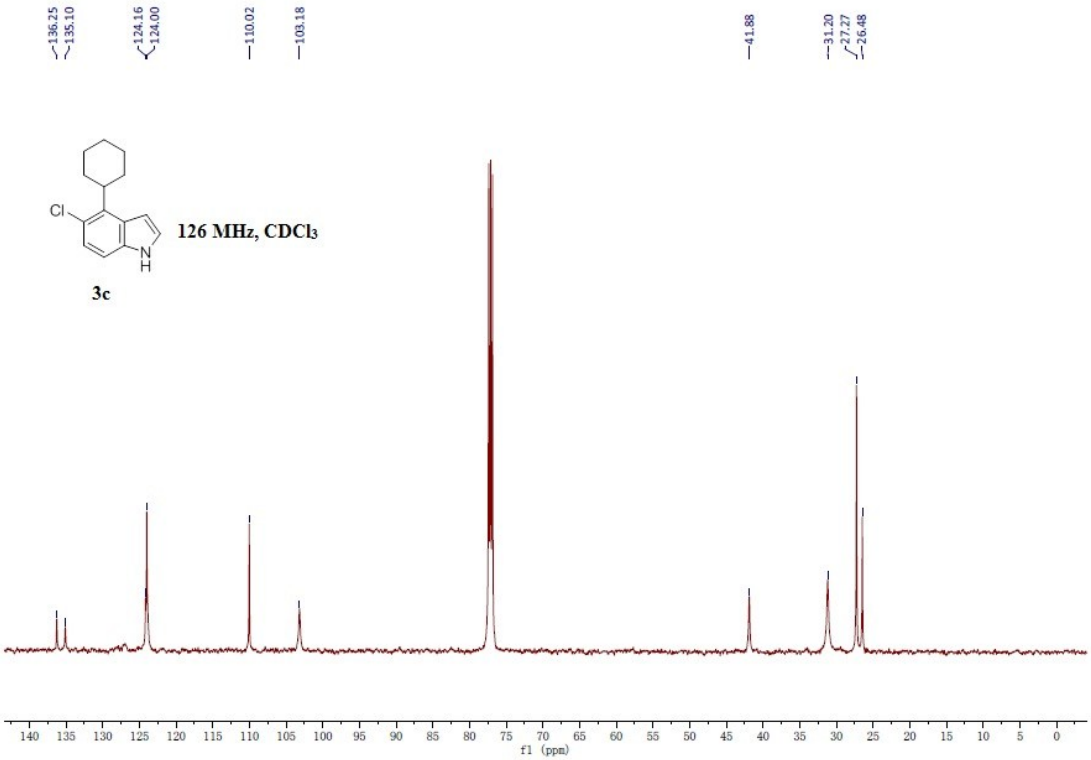


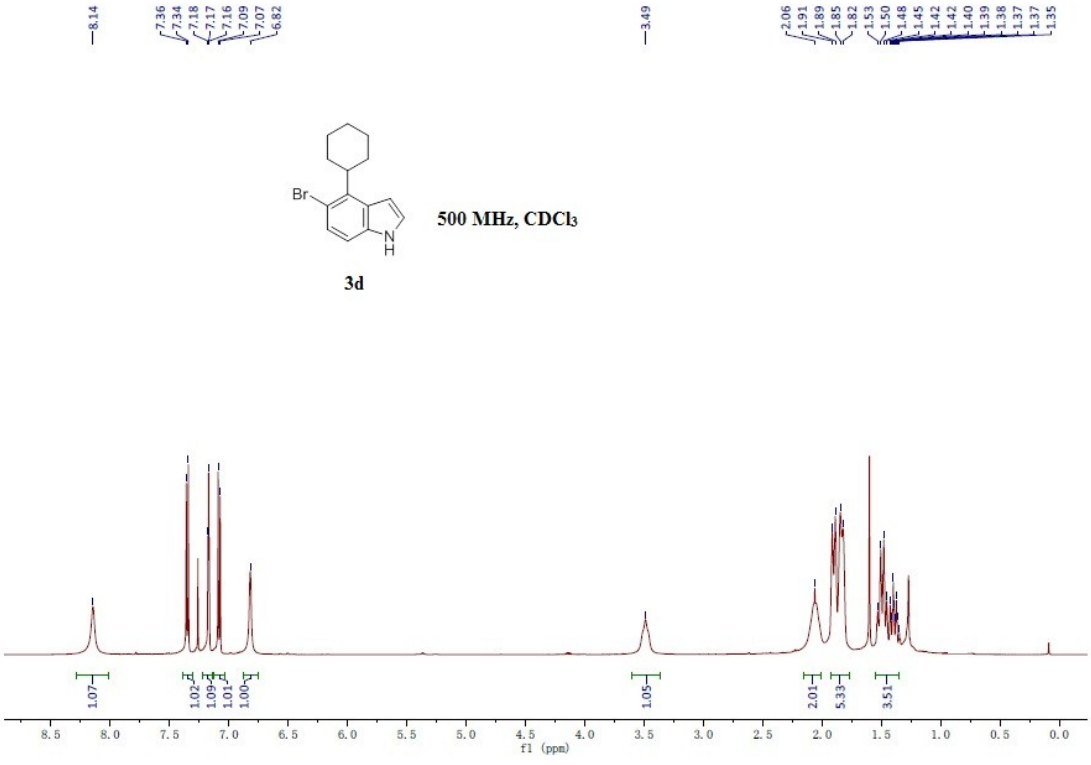

140.45
135.87
126.69
123.42
122.35
116.04
108.78
101.12
41.96
33.74
27.29
26.61
126 MHz, CDCl3
3a
f1 (ppm)

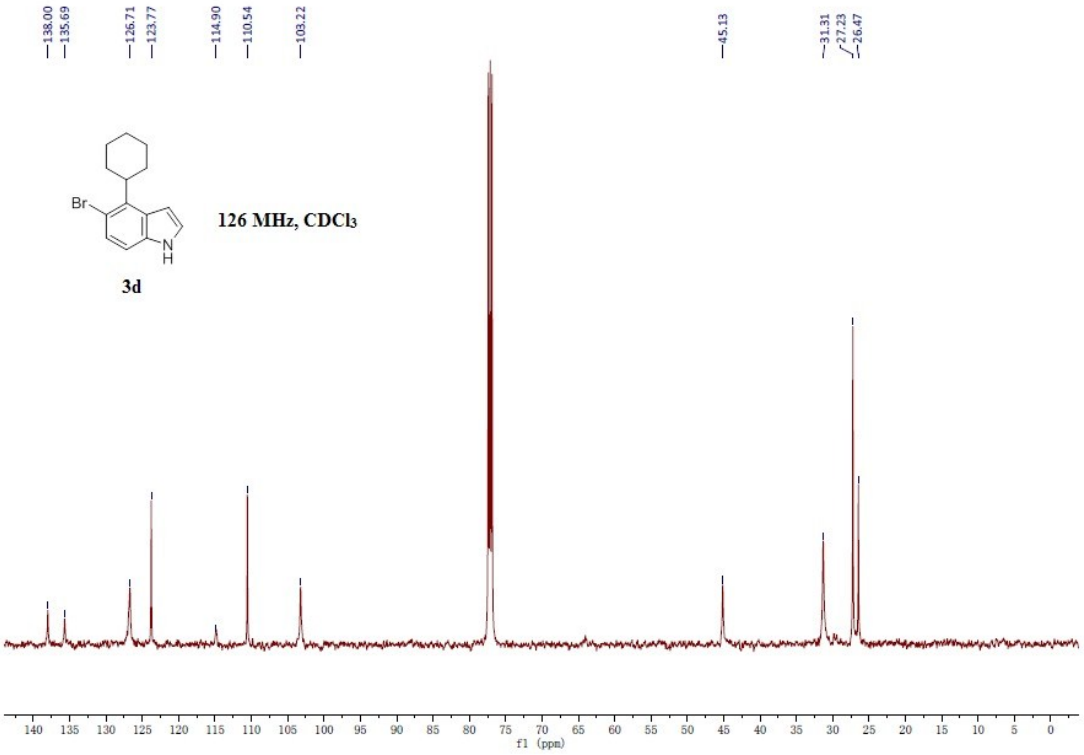

8.03
7.14
7.13
7.13
7.07
7.06
7.05
7.04
6.85
6.83
6.83
6.81
6.61
3.08
3.07
3.07
3.05
3.05
3.04
3.02
3.02
1.95
1.92
1.90
1.87
1.81
1.81
1.78
1.76
1.73
1.71
1.41
1.38
1.36
1.33
1.33
1.30
1.28
F
500 MHz, CDCl3
3b
1.01
0.98
1.00
0.99
1.00
1.06
2.21
5.37
3.36
f1 (ppm)

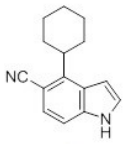

156.32
154.47
132.58
127.25
124.74
124.40
124.29
111.47
111.24
109.23
109.15
102.47
38.62
31.71
27.31
26.39
F
N
H
126 MHz, CDCl3
3b
f1 (ppm)


8.04
7.11
7.11
7.10
7.09
7.07
7.05
6.72
3.41
2.01
1.83
1.81
1.75
1.73
1.44
1.42
1.39
1.37
1.35
1.34
1.34
1.32
1.31
1.29
1.29
1.27
Cl
N
H
500 MHz, CDCl3
3c
1.03
3.14
1.00
1.07
2.28
5.39
3.58
f1 (ppm)


136.25
135.10
124.16
124.00
110.02
103.18
41.88
31.20
27.27
26.48
Cl
N
H
126 MHz, CDCl3
3c
140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)

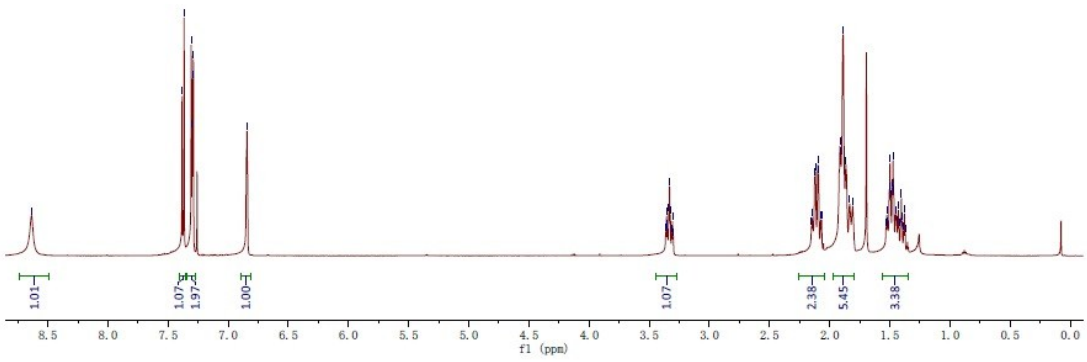

8.14
7.36
7.34
7.18
7.17
7.16
7.09
7.07
6.82
3.49
2.06
1.91
1.89
1.85
1.82
1.53
1.50
1.48
1.45
1.42
1.42
1.40
1.39
1.38
1.37
1.37
1.35
Br
N
H
500 MHz, CDCl3
3d
1.07
1.02
1.09
1.01
1.00
1.05
2.01
5.33
3.51
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

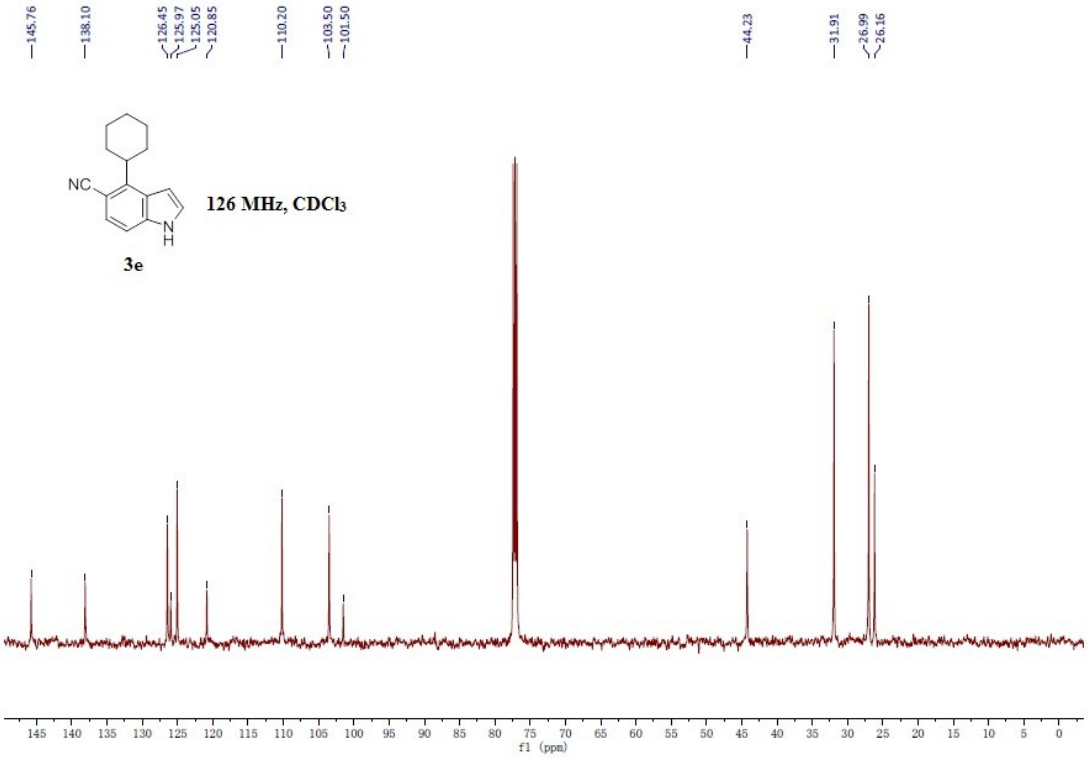


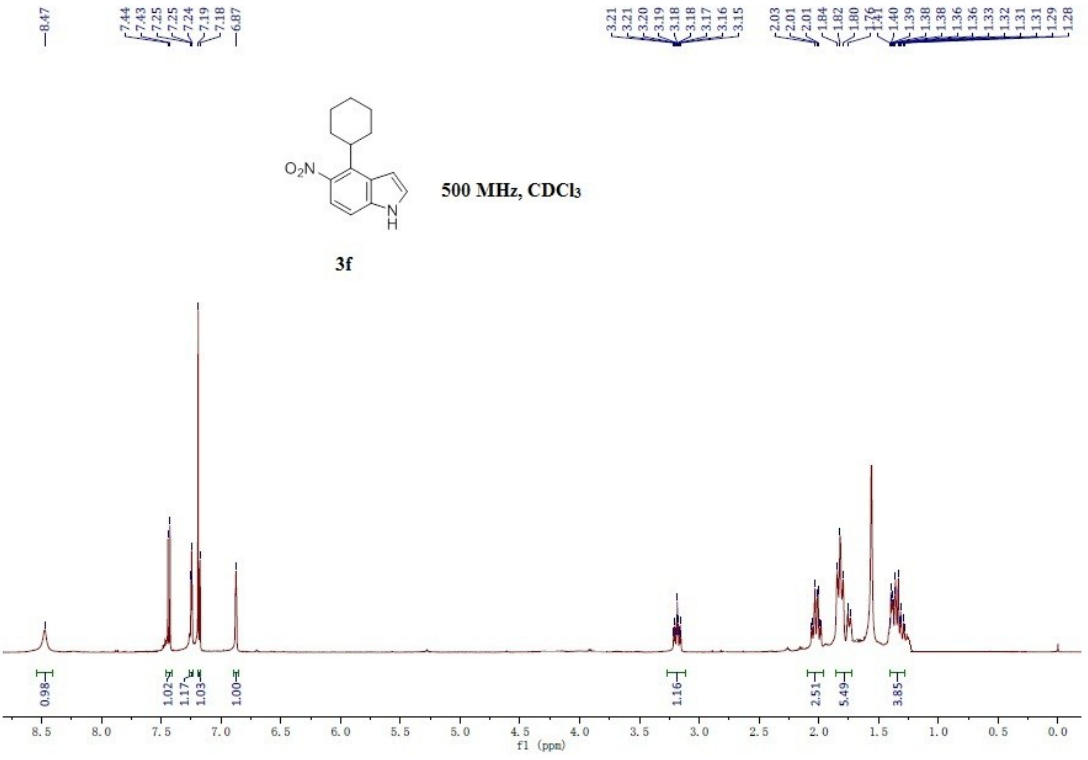


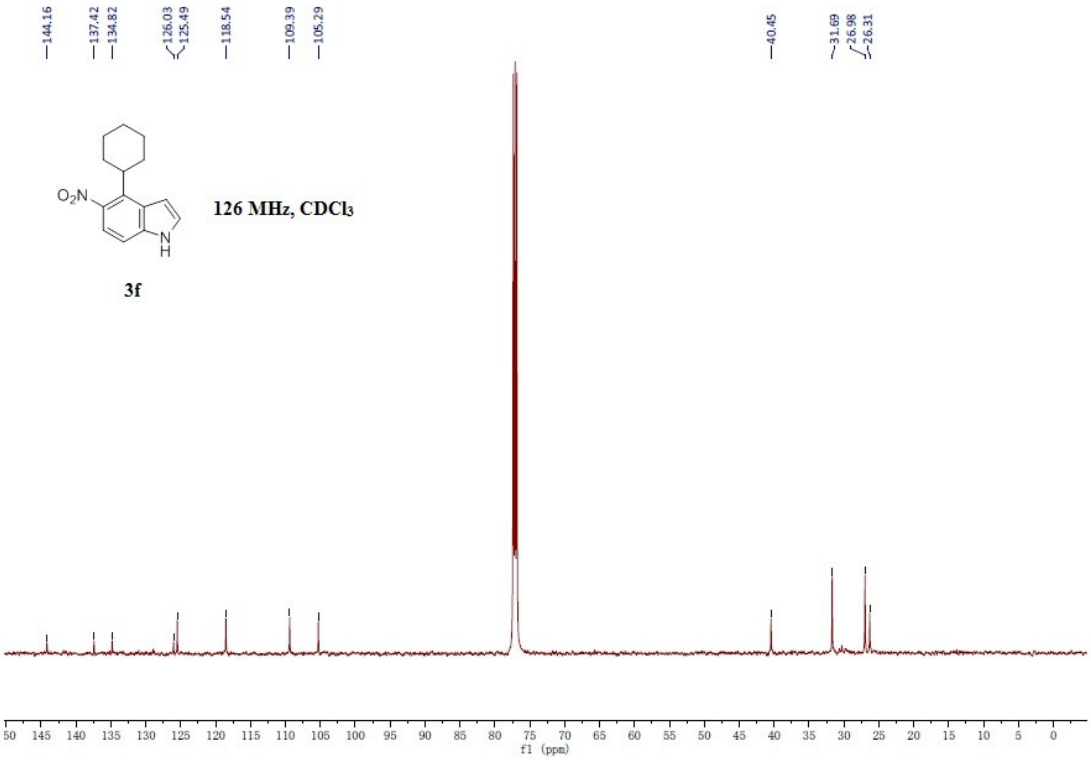
500 MHz, CDCl3

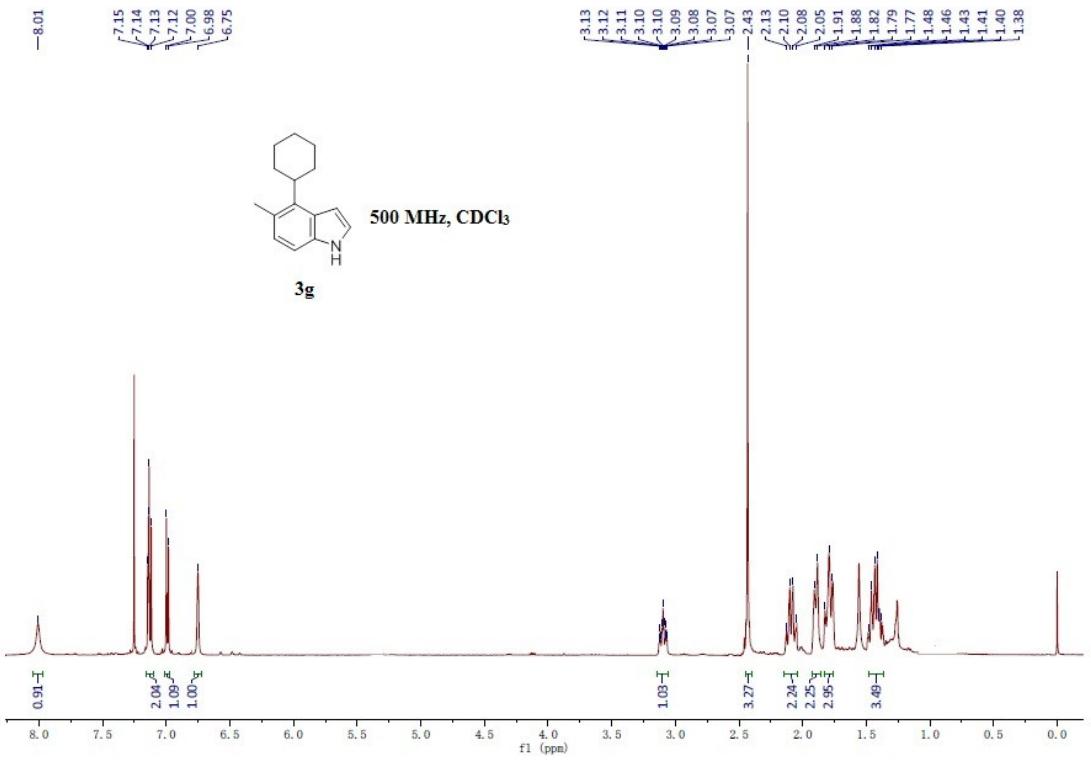
3e

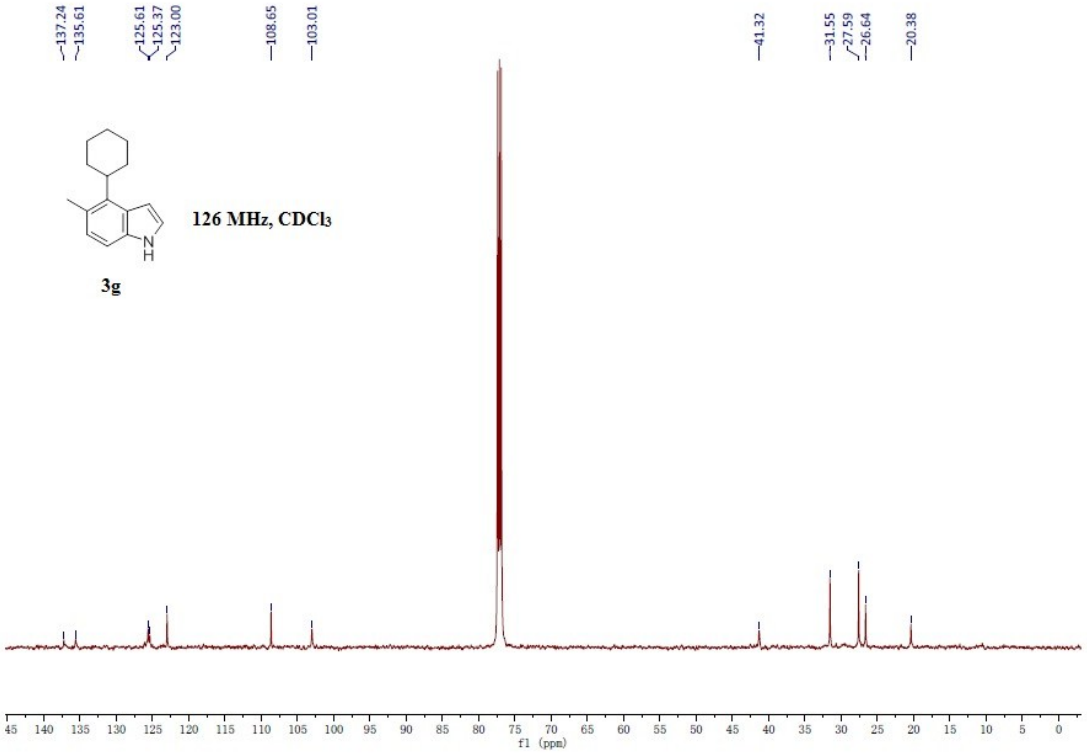


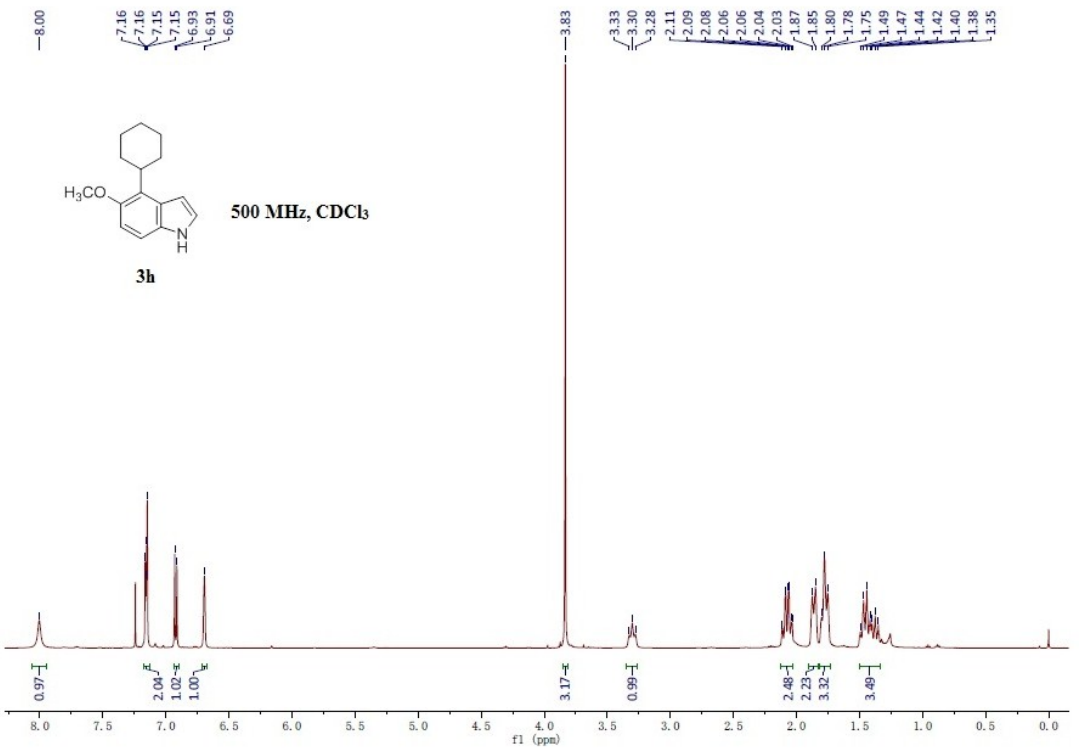

145.76
138.10
126.45
125.97
125.05
120.85
110.20
103.50
101.50
44.23
31.91
26.99
26.16
NC
N
H
126 MHz, CDCl3
3e
f1 (ppm)

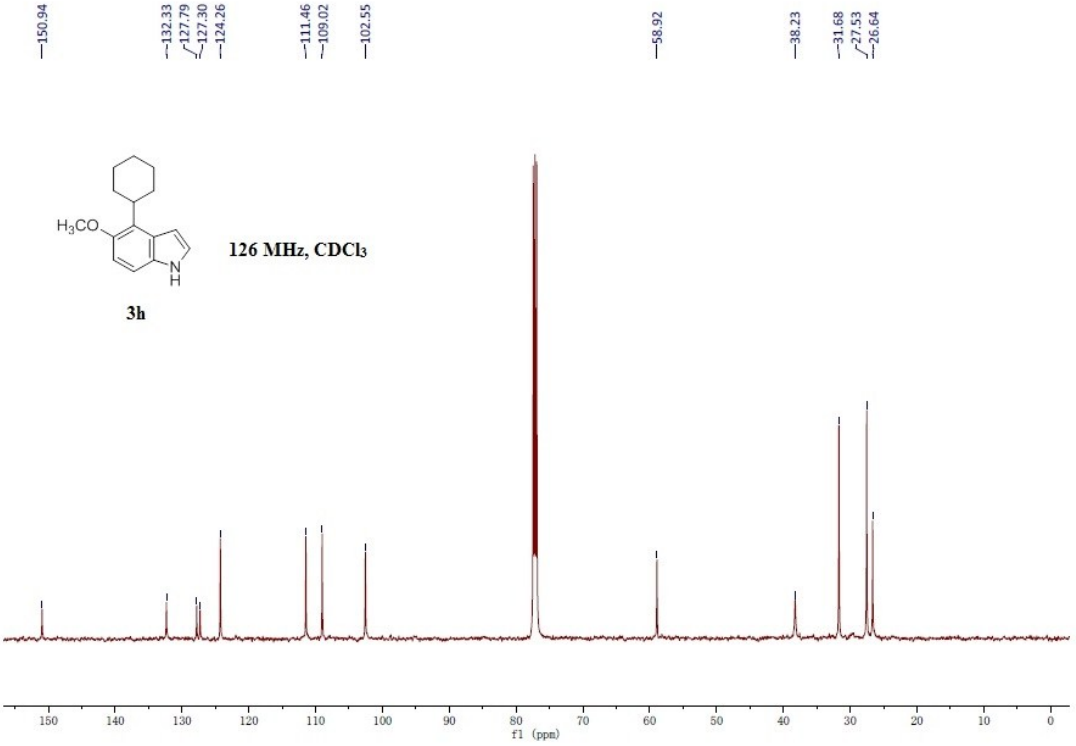

8.47
7.44
7.43
7.25
7.25
7.24
7.19
7.18
6.87
3.21
3.21
3.20
3.19
3.18
3.18
3.17
3.16
3.15
2.03
2.01
2.01
1.84
1.82
1.80
1.40
1.40
1.39
1.38
1.38
1.36
1.36
1.33
1.32
1.31
1.31
1.29
1.28
O2N
N
H
500 MHz, CDCl3
3f
0.98
1.02
1.17
1.03
1.00
1.16
2.51
5.49
3.85
f1 (ppm)


144.16
137.42
134.82
126.03
125.49
118.54
109.39
105.29
40.45
31.69
26.98
26.31
O2N
N
H
126 MHz, CDCl3
3f
f1 (ppm)


8.01
7.15
7.14
7.13
7.12
7.00
6.98
6.75
3.13
3.12
3.11
3.10
3.10
3.09
3.08
3.07
3.07
2.43
2.13
2.10
2.08
2.05
1.91
1.88
1.82
1.79
1.77
1.48
1.46
1.43
1.41
1.40
1.38
N
H
500 MHz, CDCl3
3g
0.91
2.04
1.09
1.00
1.03
3.27
2.24
2.25
2.95
3.49
f1 (ppm)


137.24
135.61
125.61
125.37
123.00
108.65
103.01
41.32
31.55
27.59
26.64
20.38
126 MHz, CDCl3
3g
f1 (ppm)


8.00
7.16
7.16
7.15
7.15
6.93
6.91
6.69
3.83
3.33
3.30
3.28
2.11
2.09
2.08
2.06
2.06
2.04
2.03
1.87
1.85
1.80
1.78
1.75
1.49
1.47
1.44
1.42
1.40
1.38
1.35
H3CO
500 MHz, CDCl3
3h
0.97
2.04
1.02
1.00
3.17
0.99
2.48
2.23
3.32
3.49
f1 (ppm)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132.33
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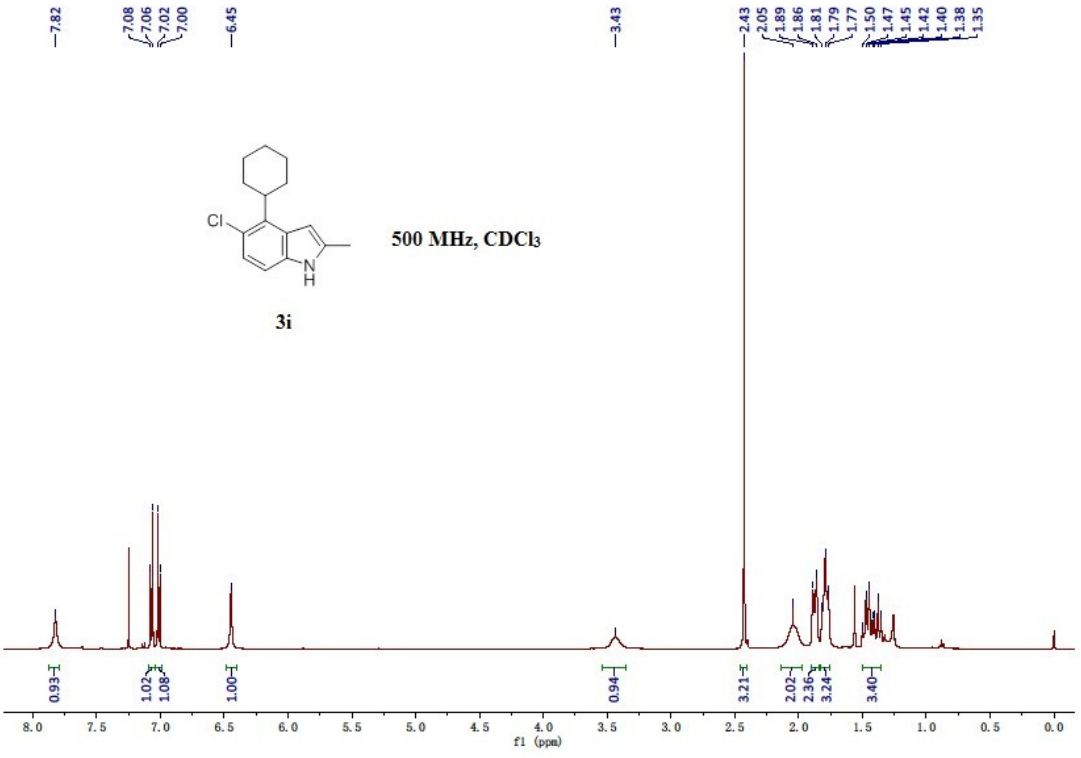
127.30
124.26
111.46
109.02
102.55
58.92
38.23
31.68
27.53
26.64
H3CO
N
H
126 MHz, CDCl3
3h
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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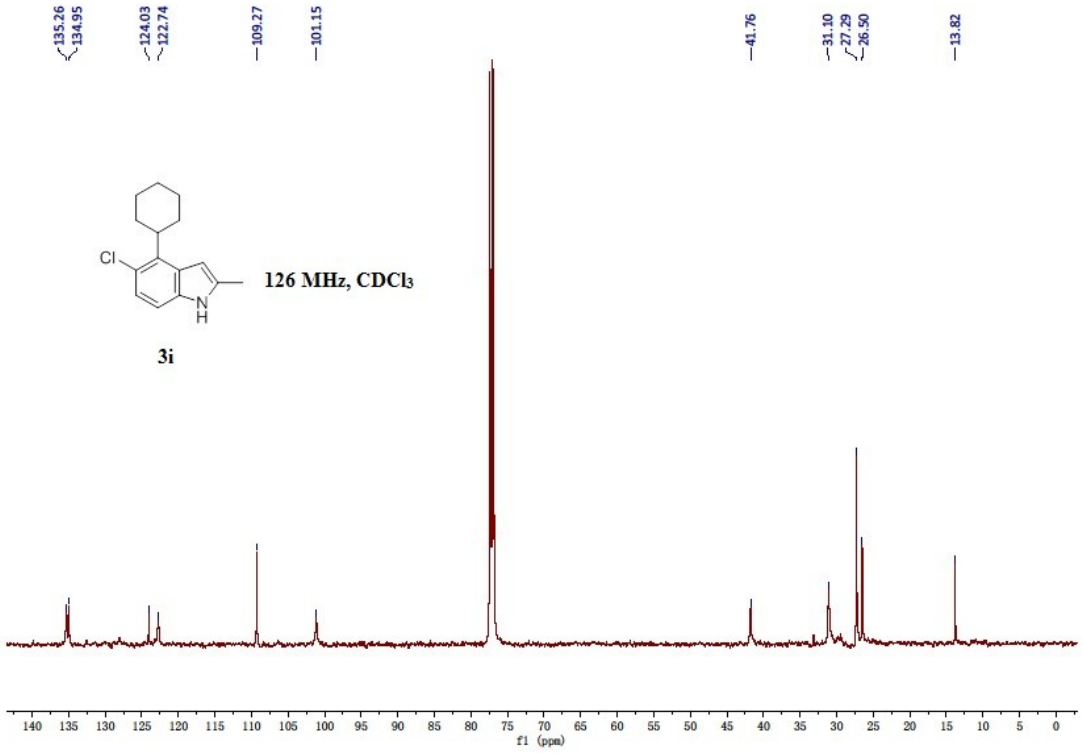
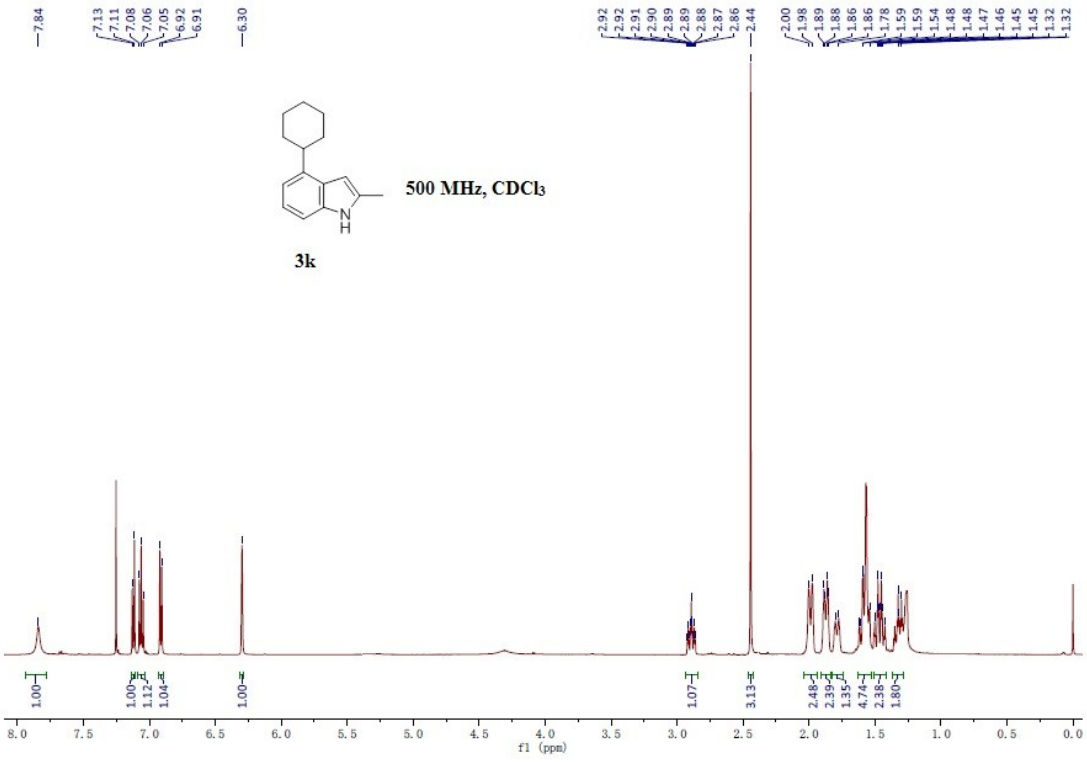
7.08
7.06
7.02
7.00
6.45
3.43
2.43
2.05
1.89
1.86
1.81
1.79
1.77
1.50
1.47
1.45
1.42
1.40
1.38
1.35
Cl
N
H
500 MHz, CDCl3
3i
0.93
1.02
1.08
1.00
0.94
3.21
2.02
2.36
3.24
3.40
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


135.26
134.95
124.03
122.74
109.27
101.15
41.76
31.10
27.29
26.50
13.82
Cl
N
H
126 MHz, CDCl3
3i
f1 (ppm)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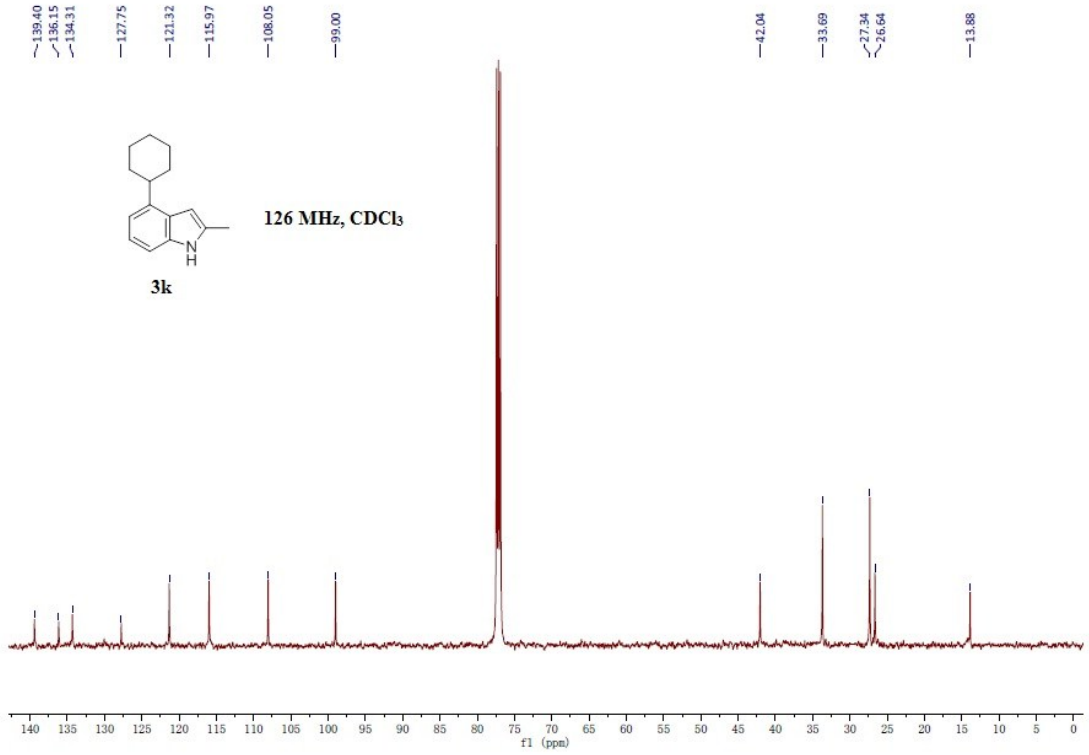
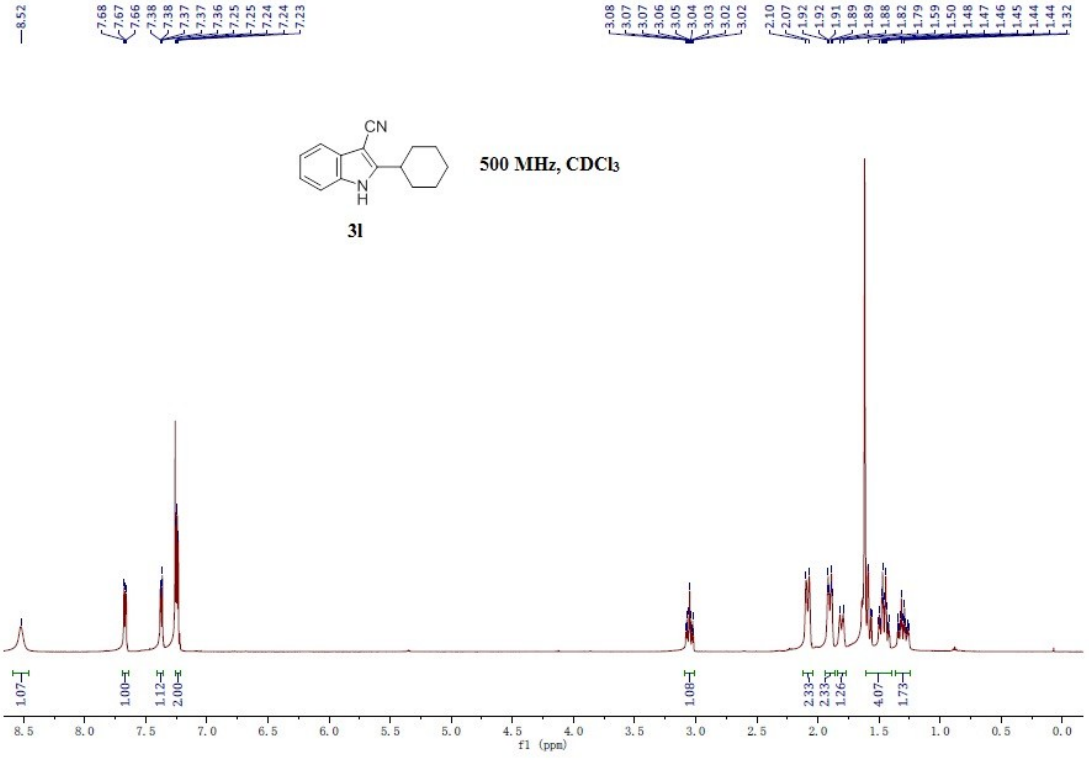
7.11
7.08
7.06
7.05
6.92
6.91
6.30
2.92
2.92
2.91
2.90
2.89
2.89
2.88
2.87
2.86
2.44
2.00
1.98
1.89
1.88
1.86
1.86
1.78
1.59
1.59
1.54
1.48
1.48
1.47
1.46
1.45
1.45
1.32
1.32
N
H
500 MHz, CDCl3
3k
1.00
1.00
1.12
1.04
1.00
1.07
3.13
2.48
2.39
1.35
4.74
2.38
1.80
f1 (ppm)


139.40
136.15
134.31
127.75
121.32
115.97
108.05
99.00
42.04
33.69
27.34
26.64
13.88
126 MHz, CDCl3
3k
f1 (ppm)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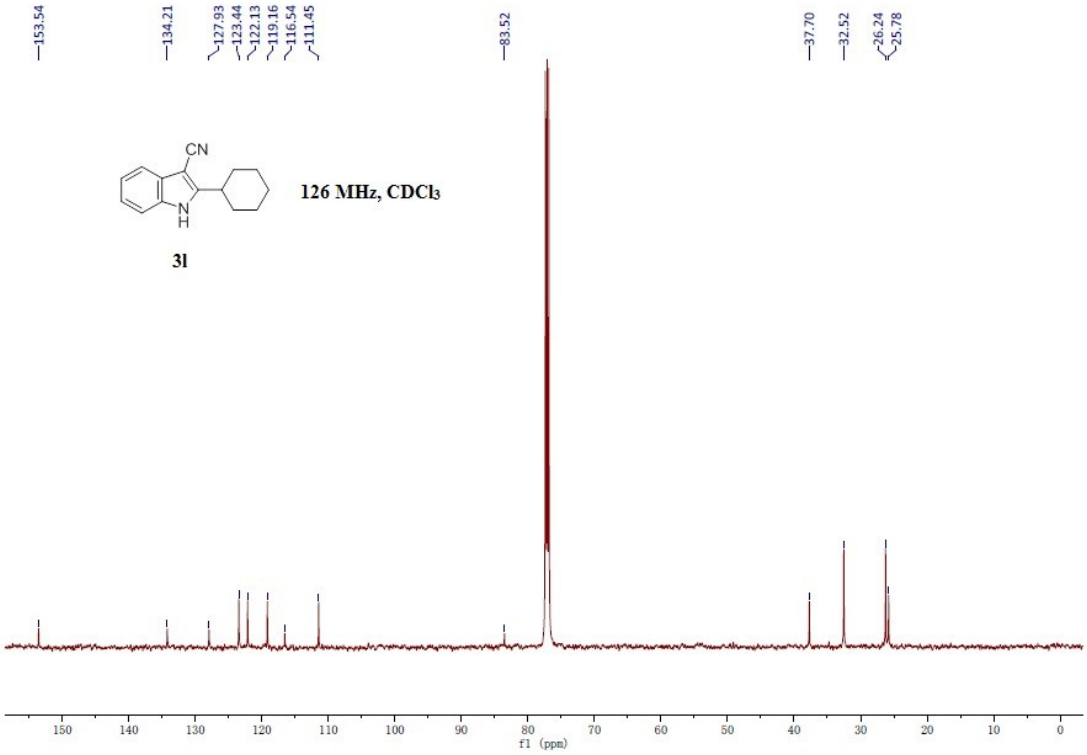
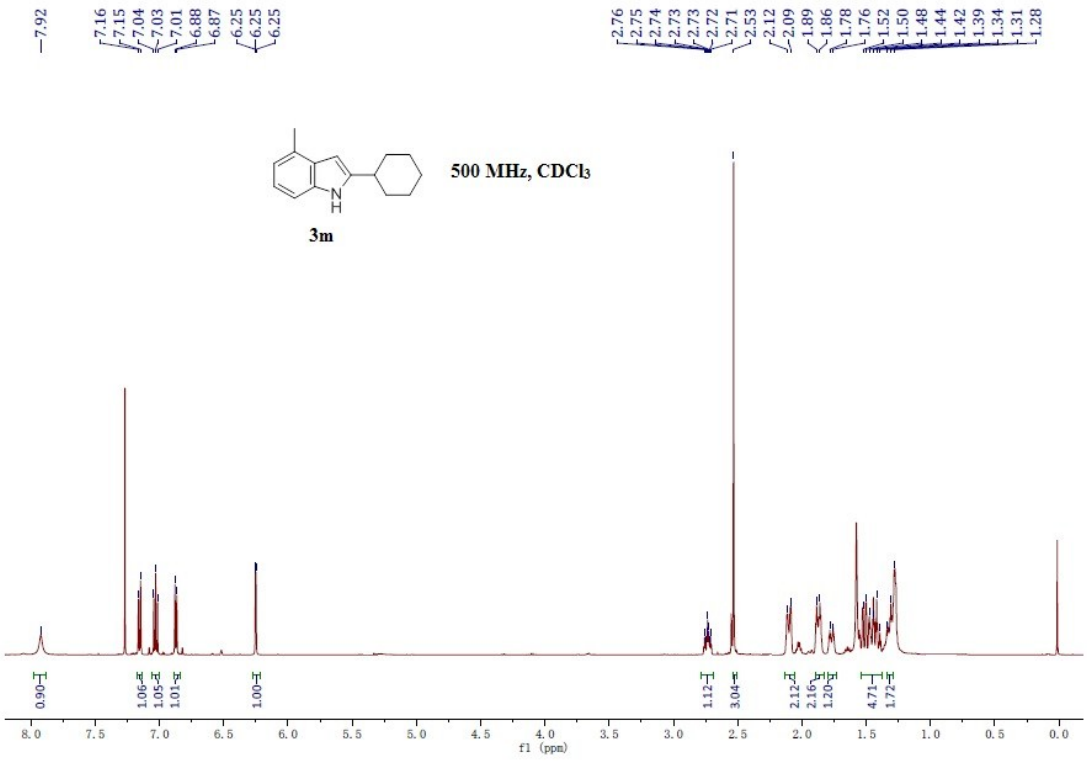
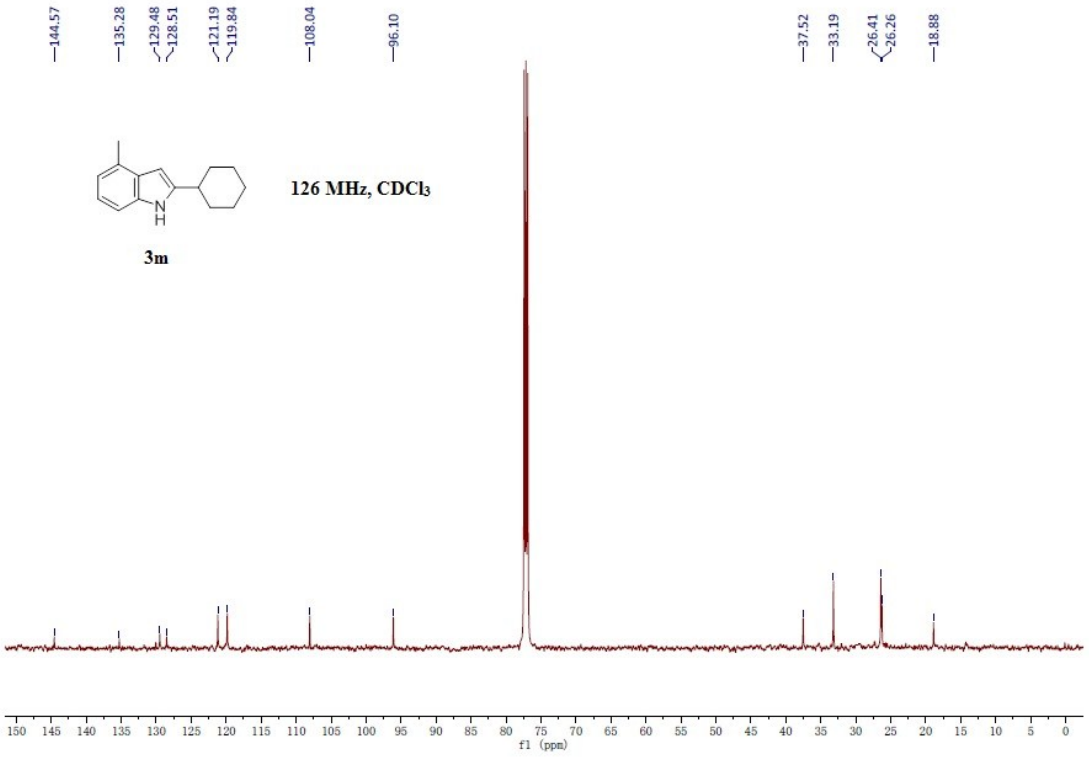
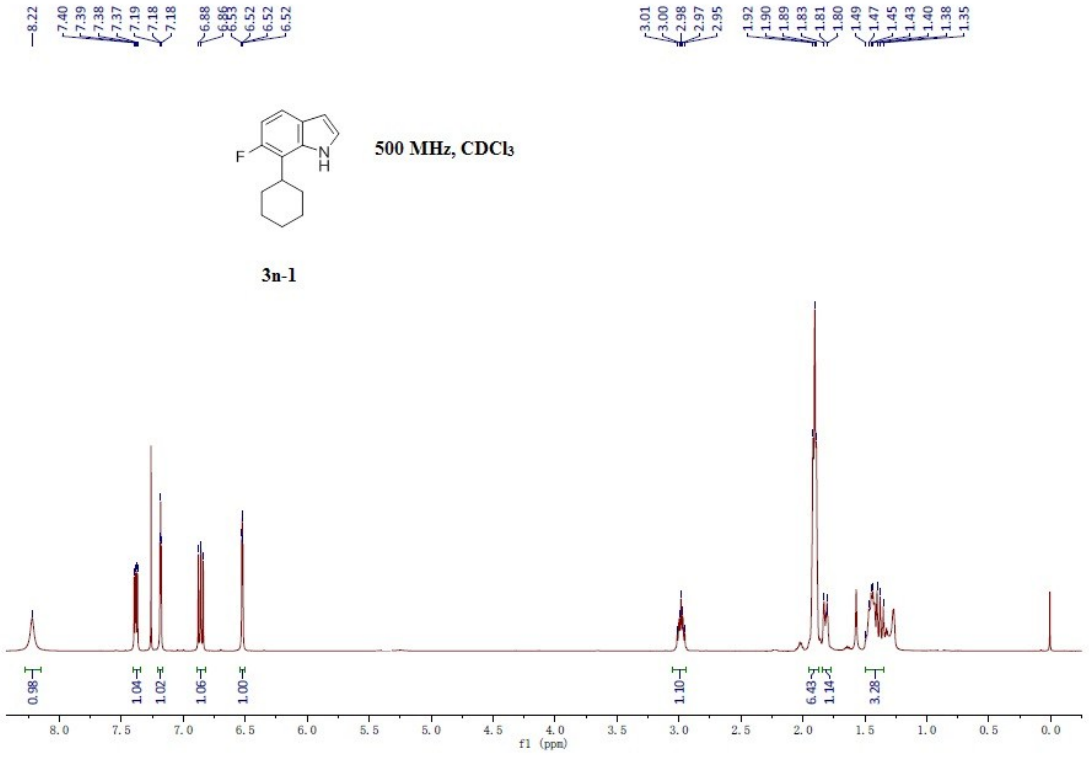
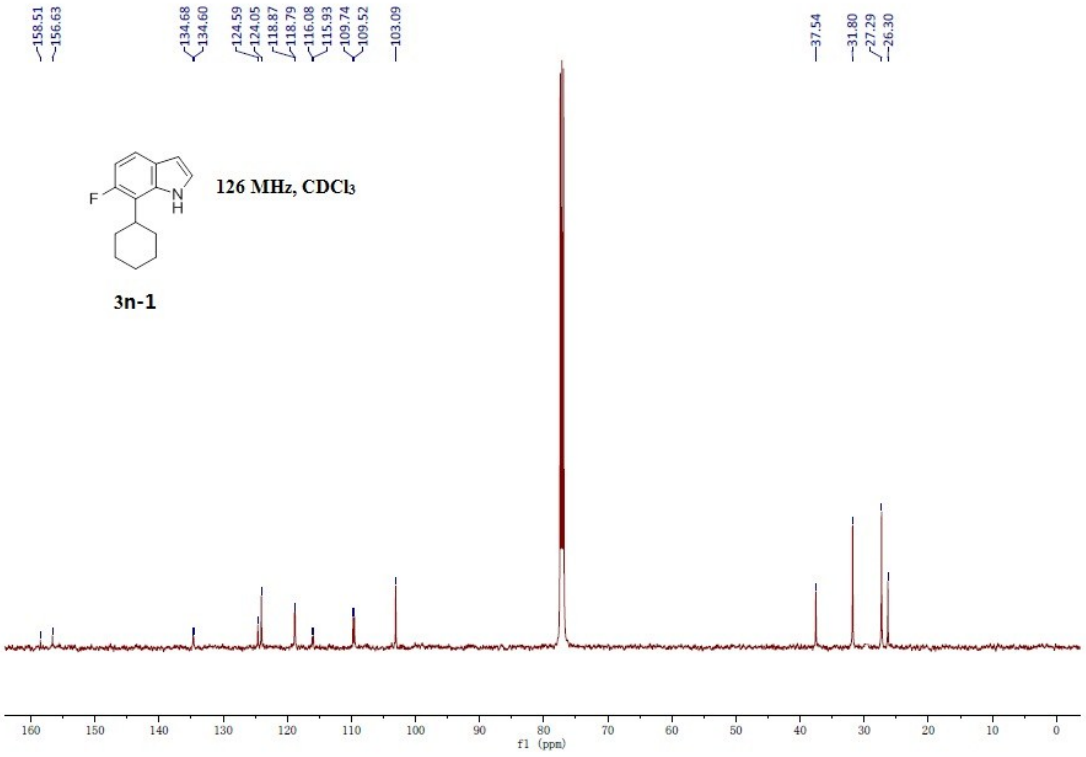
7.68
7.67
7.66
7.38
7.38
7.37
7.37
7.36
7.25
7.25
7.24
7.24
7.23
3.08
3.07
3.07
3.06
3.05
3.04
3.03
3.02
3.02
2.10
2.07
1.92
1.92
1.91
1.89
1.89
1.88
1.82
1.79
1.59
1.50
1.48
1.47
1.46
1.45
1.44
1.44
1.32
CN
500 MHz, CDCl3
3l
1.07
1.00
1.12
2.00
1.08
2.33
2.33
1.26
4.07
1.73
f1 (ppm)

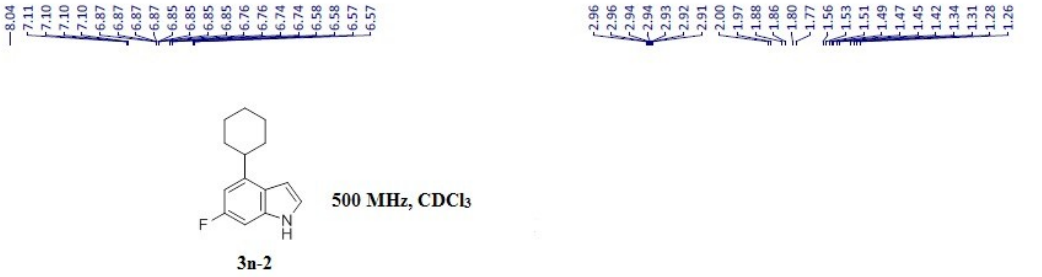

153.54
134.21
127.93
123.44
122.13
119.16
116.54
111.45
83.52
37.70
32.52
26.24
25.78
CN
N
H
126 MHz, CDCl3
31
f1 (ppm)


7.92
7.16
7.15
7.04
7.03
7.01
6.88
6.87
6.25
6.25
6.25
2.76
2.75
2.74
2.73
2.73
2.72
2.71
2.53
2.12
2.09
1.89
1.86
1.78
1.76
1.52
1.50
1.48
1.44
1.42
1.39
1.34
1.31
1.28
N
H
500 MHz, CDCl3
3m
0.90
1.06
1.05
1.01
1.00
1.12
3.04
2.12
2.16
1.20
4.71
1.72
f1 (ppm)

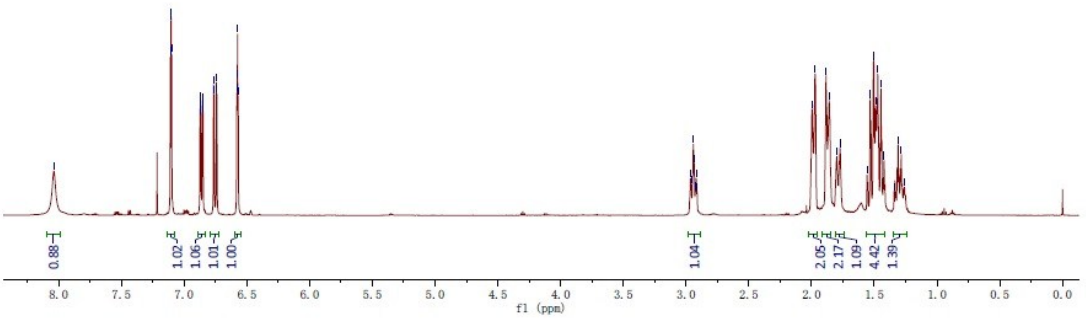

144.57
135.28
129.48
128.51
121.19
119.84
108.04
96.10
37.52
33.19
26.41
26.26
18.88
126 MHz, CDCl3
3m
f1 (ppm)

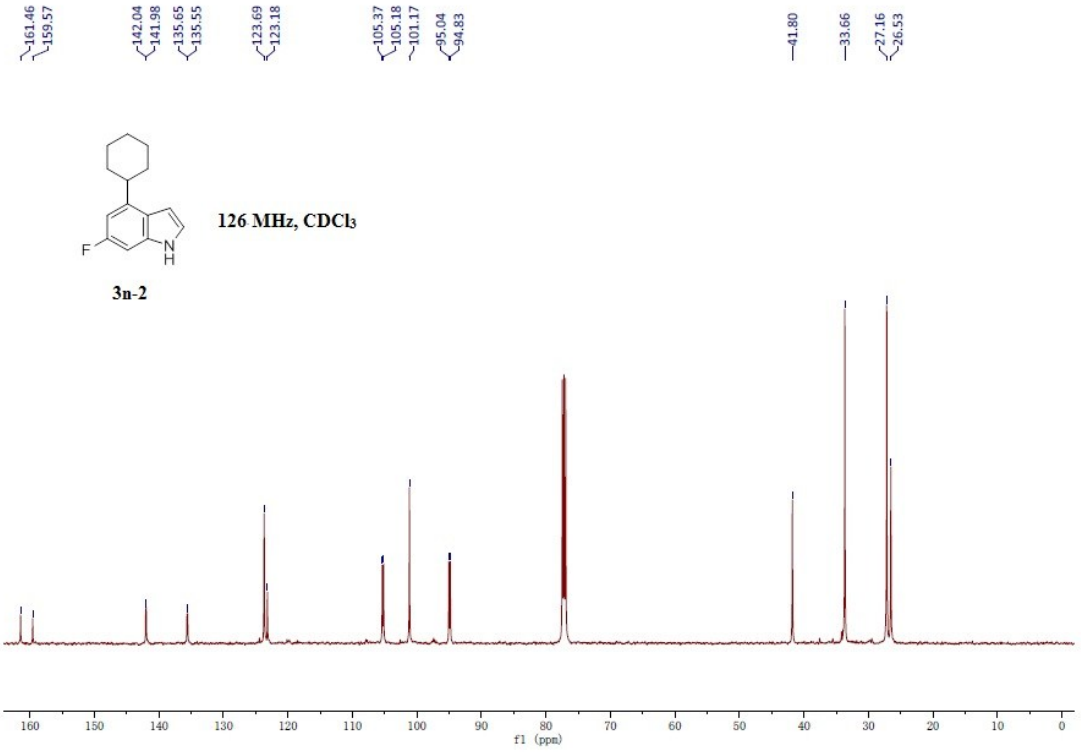

8.22
7.40
7.39
7.38
7.37
7.19
7.18
7.18
6.88
6.86
6.53
6.52
6.52
6.52
3.01
3.00
2.98
2.97
2.95
1.92
1.90
1.89
1.83
1.81
1.80
1.49
1.47
1.45
1.43
1.40
1.38
1.35
500 MHz, CDCl3
3n-1
0.98
1.04
1.02
1.06
1.00
1.10
6.43
1.14
3.28
f1 (ppm)

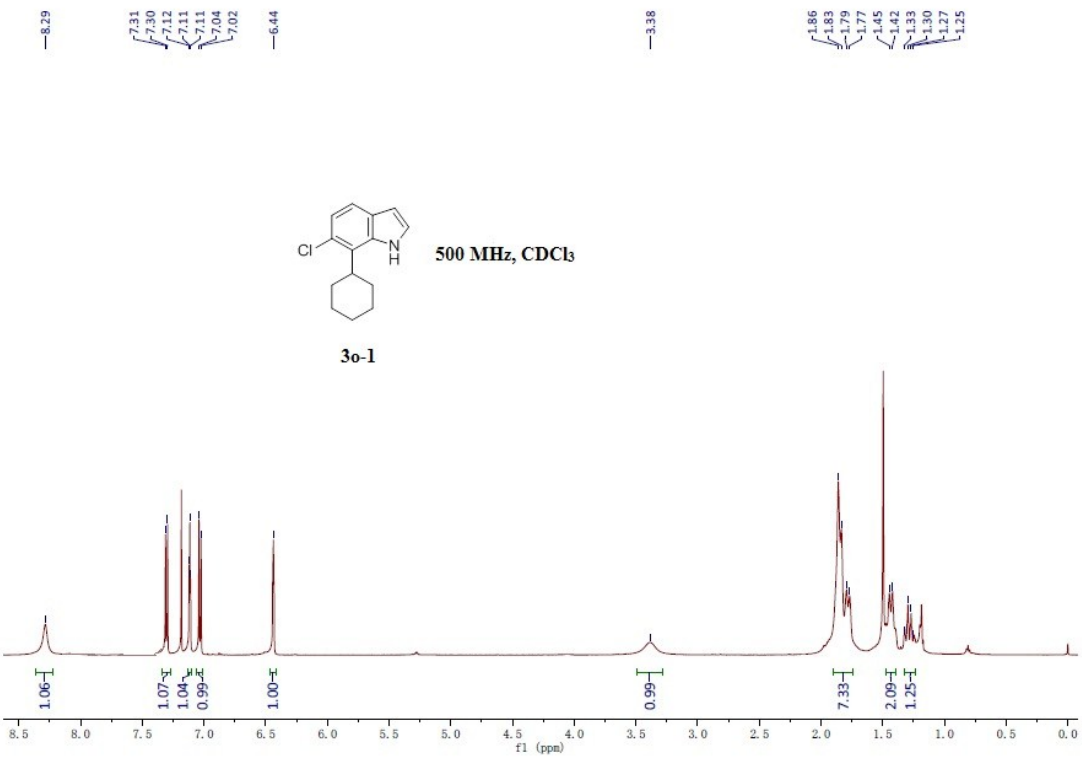

158.51
156.63
134.68
134.60
124.59
124.05
118.87
118.79
116.08
115.93
109.74
109.52
103.09
37.54
31.80
27.29
26.30
F
N
H
126 MHz, CDCl3
3n-1
f1 (ppm)

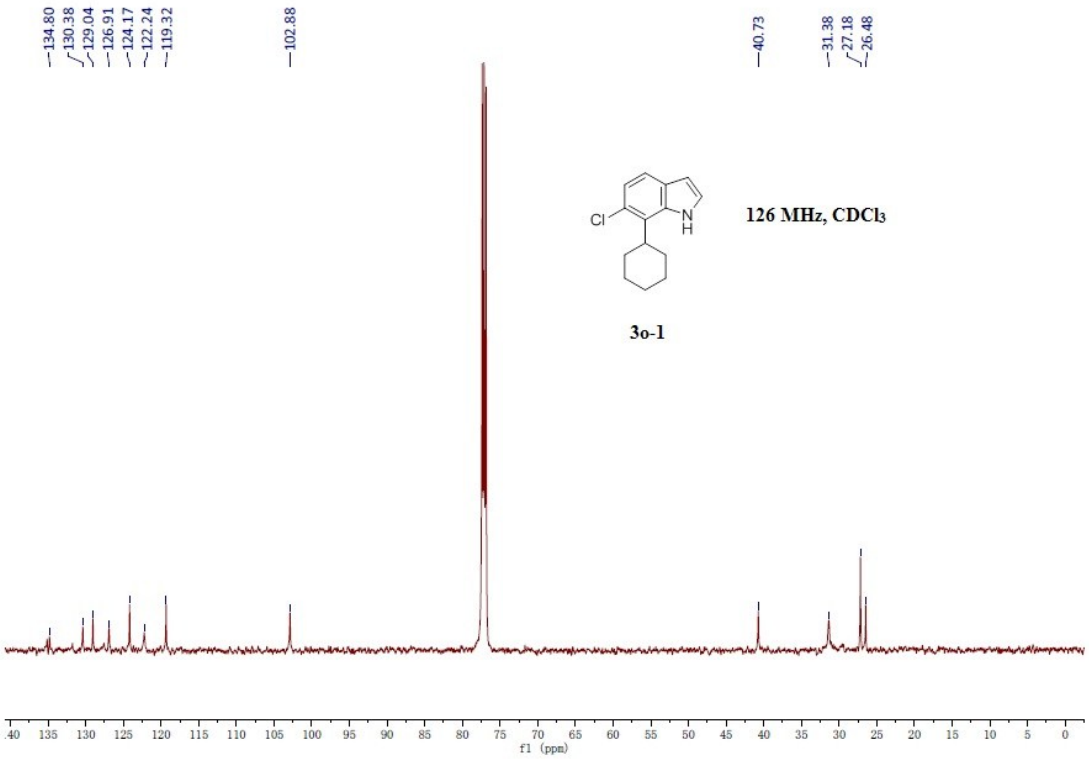

8.04
7.11
7.10
7.10
7.10
6.87
6.87
6.87
6.87
6.85
6.85
6.85
6.85
6.76
6.76
6.74
6.74
6.58
6.58
6.57
6.57
2.96
2.96
2.94
2.94
2.93
2.92
2.91
2.00
1.97
1.88
1.86
1.80
1.77
1.56
1.53
1.51
1.49
1.47
1.45
1.42
1.34
1.31
1.28
1.26

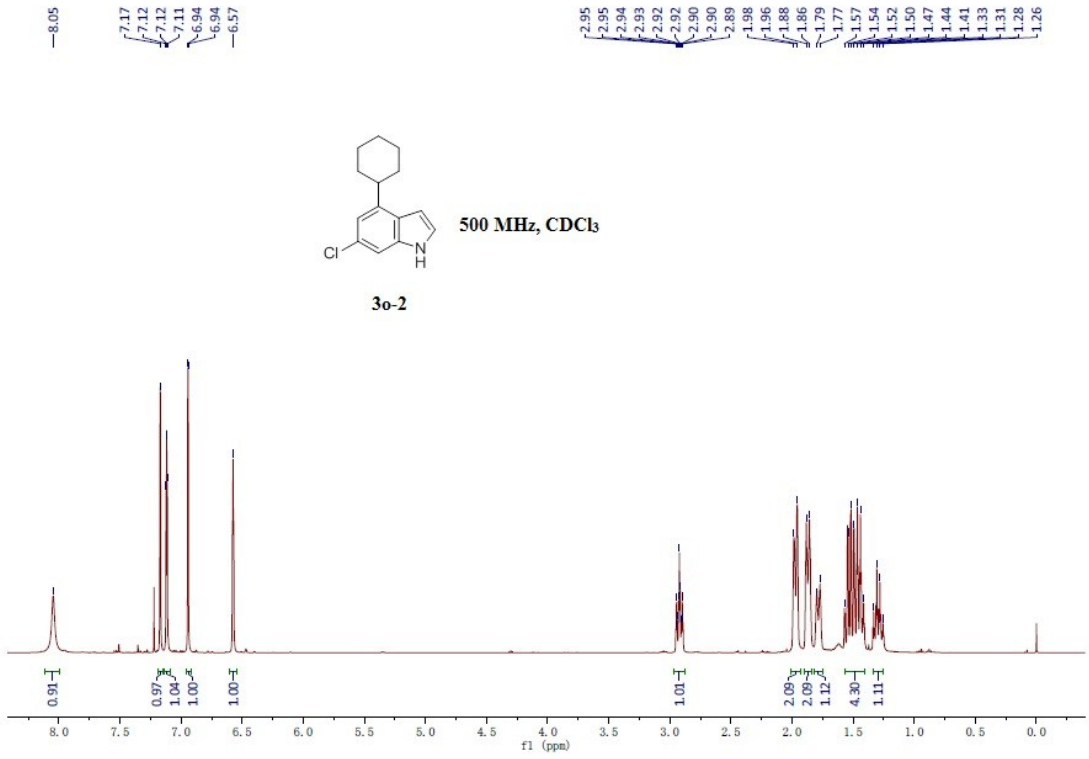
F
N
H
500 MHz, CDCl3
3n-2

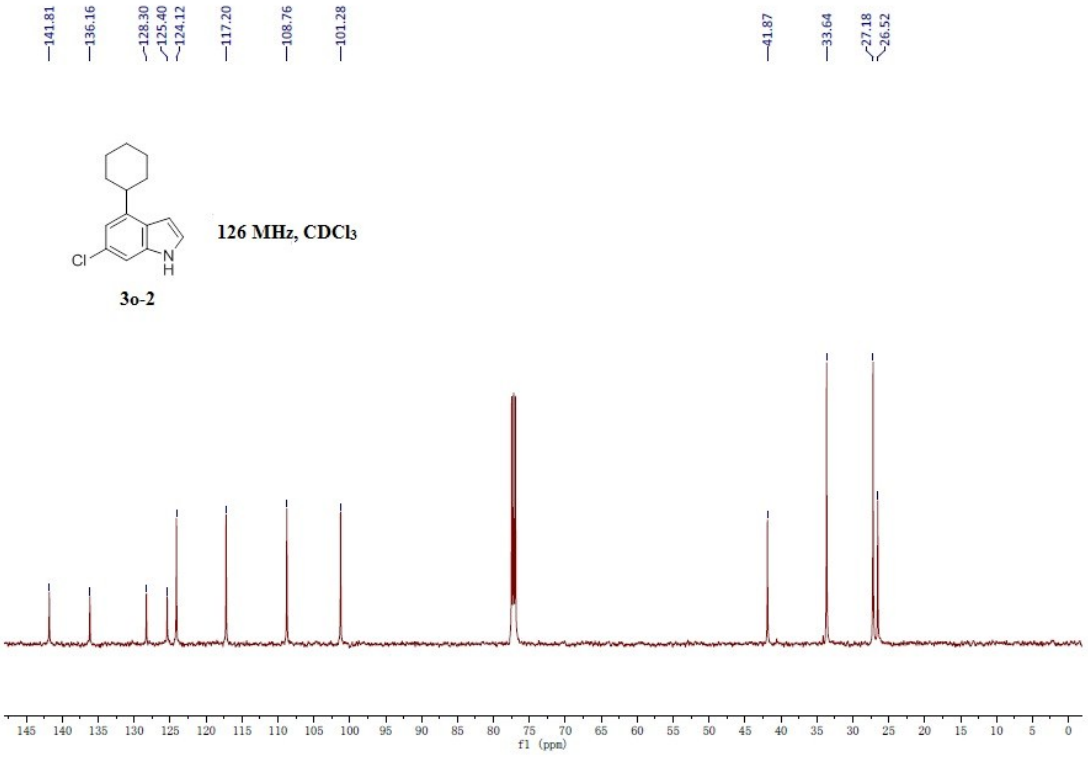

0.88
1.02
1.06
1.01
1.00
1.04
2.05
2.17
1.09
4.42
1.39
f1 (ppm)

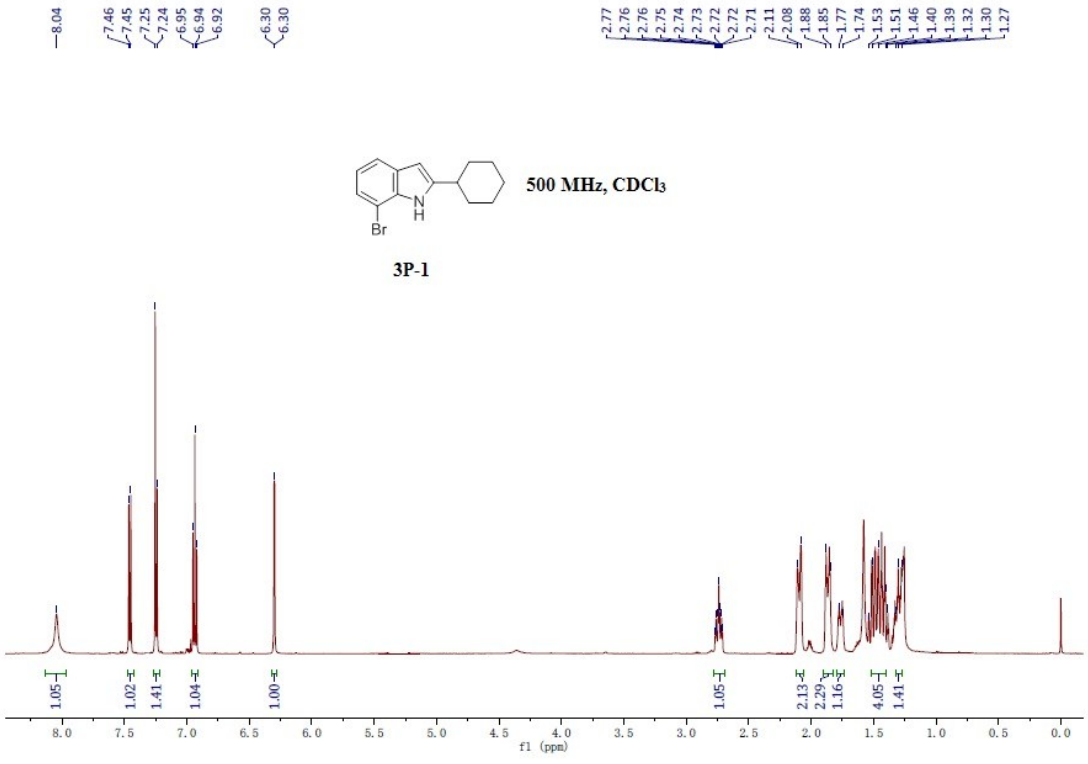

161.46
159.57
142.04
141.98
135.65
135.55
123.69
123.18
105.37
105.18
101.17
95.04
94.83
41.80
33.66
27.16
26.53
F
N
H
126 MHz, CDCl3
3n-2
f1 (ppm)

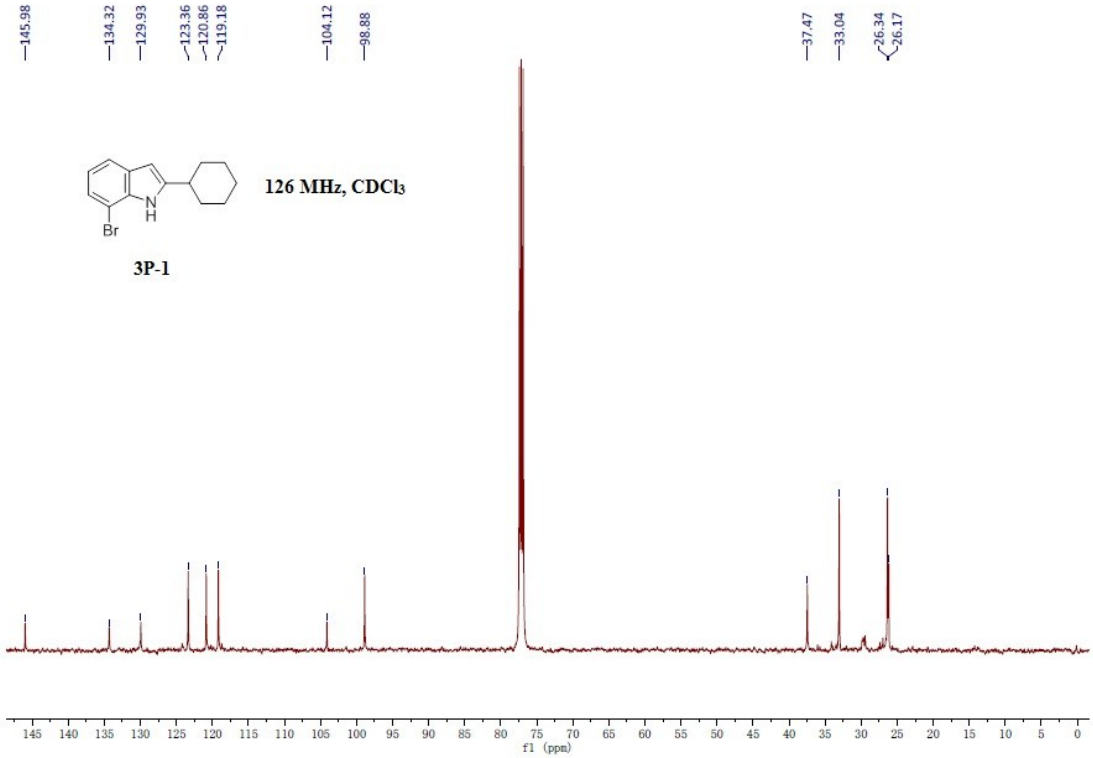

8.29
7.31
7.30
7.12
7.11
7.11
7.04
7.02
6.44
3.38
1.86
1.83
1.79
1.77
1.45
1.42
1.33
1.30
1.27
1.25
Cl
N
H
500 MHz, CDCl3
3o-1
1.06
1.07
1.04
0.99
1.00
0.99
7.33
2.09
1.25
f1 (ppm)

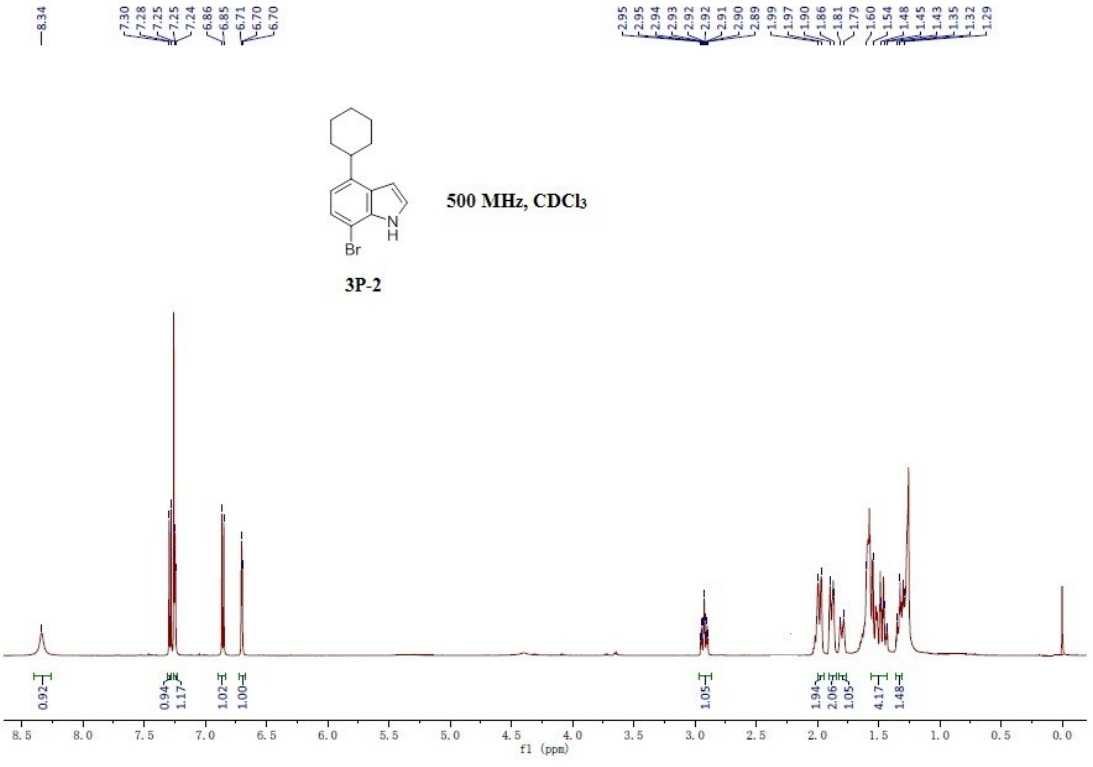

134.80
130.38
129.04
126.91
124.17
122.24
119.32
102.88
40.73
31.38
27.18
26.48
Cl
N
H
126 MHz, CDCl3
3o-1
f1 (ppm)

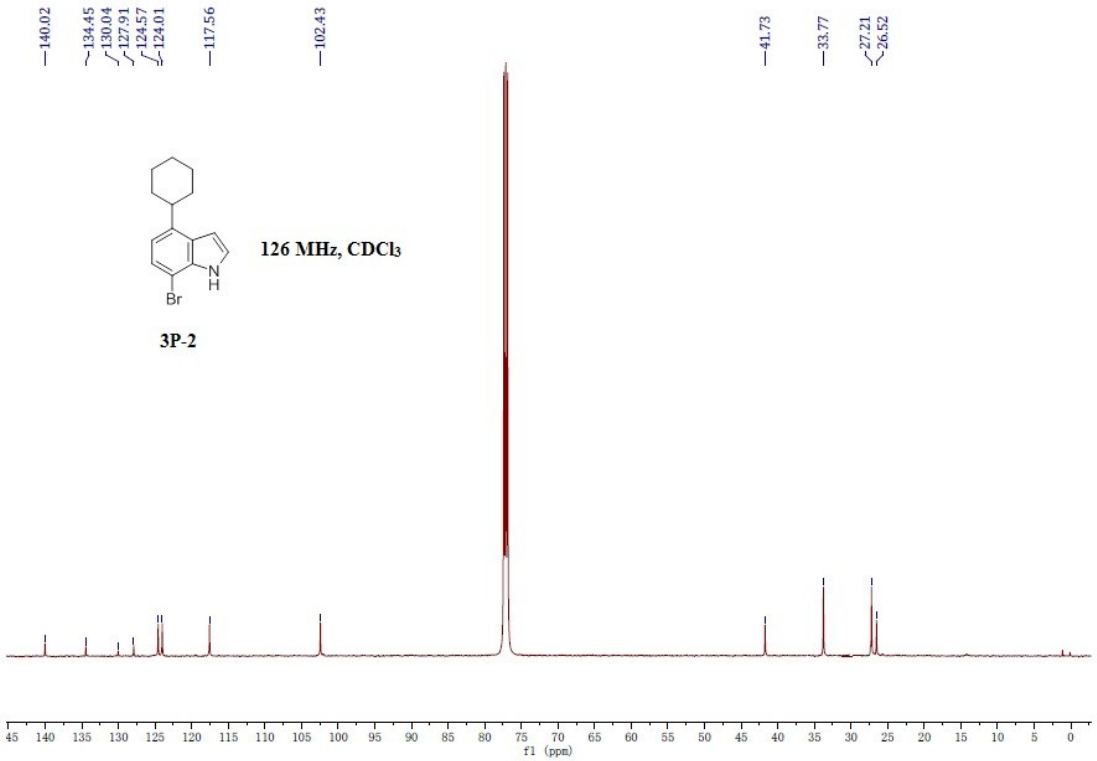

8.05
7.17
7.12
7.12
7.11
6.94
6.94
6.57
2.95
2.95
2.94
2.93
2.92
2.92
2.90
2.90
2.89
1.98
1.96
1.88
1.86
1.79
1.77
1.57
1.54
1.52
1.50
1.47
1.44
1.41
1.33
1.31
1.28
1.26
Cl
N
H
500 MHz, CDCl3
3o-2
0.91
0.97
1.04
1.00
1.00
1.01
2.09
2.09
1.12
4.30
1.11
f1 (ppm)

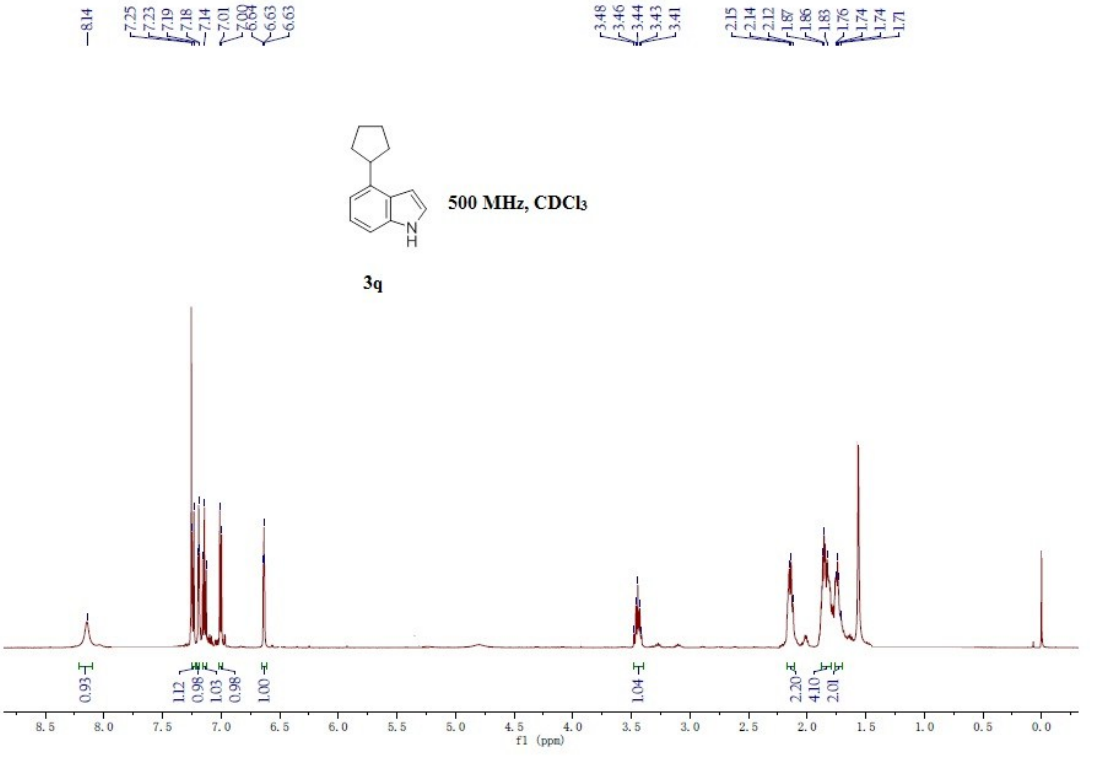

141.81
136.16
128.30
125.40
124.12
117.20
108.76
101.28
41.87
33.64
27.18
26.52
Cl
N
H
126 MHz, CDCl3
3o-2
f1 (ppm)

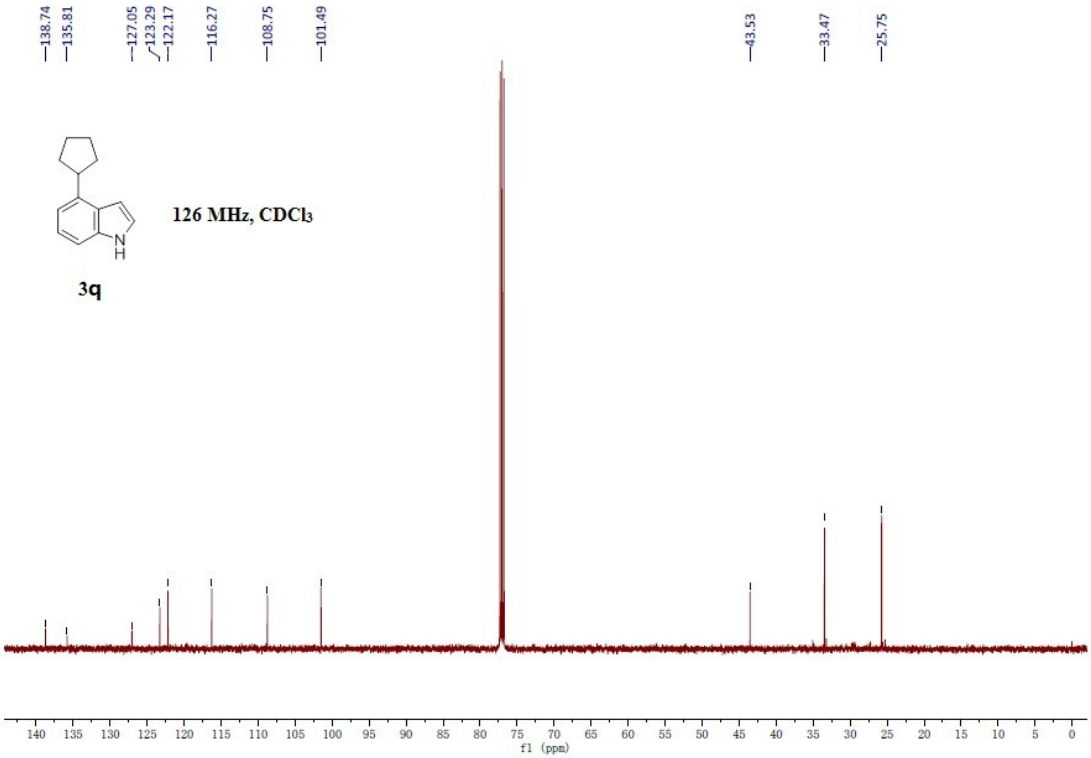

8.04
7.46
7.45
7.25
7.24
6.95
6.94
6.92
6.30
6.30
2.77
2.76
2.76
2.75
2.74
2.73
2.72
2.72
2.71
2.11
2.08
1.88
1.85
1.77
1.74
1.53
1.51
1.46
1.40
1.39
1.32
1.30
1.27
N
H
Br
500 MHz, CDCl3
3P-1
1.05
1.02
1.41
1.04
1.00
1.05
2.13
2.29
1.16
4.05
1.41
f1 (ppm)

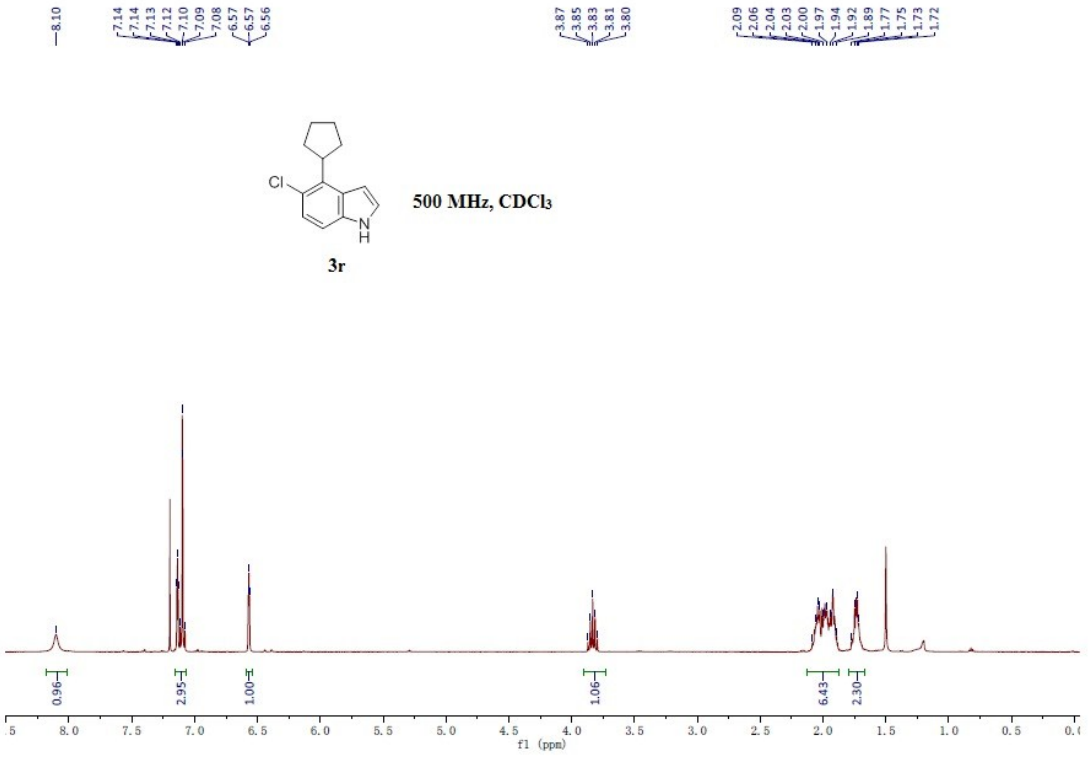

145.98
134.32
129.93
123.36
120.86
119.18
104.12
98.88
37.47
33.04
26.34
26.17
126 MHz, CDCl3
3P-1
f1 (ppm)

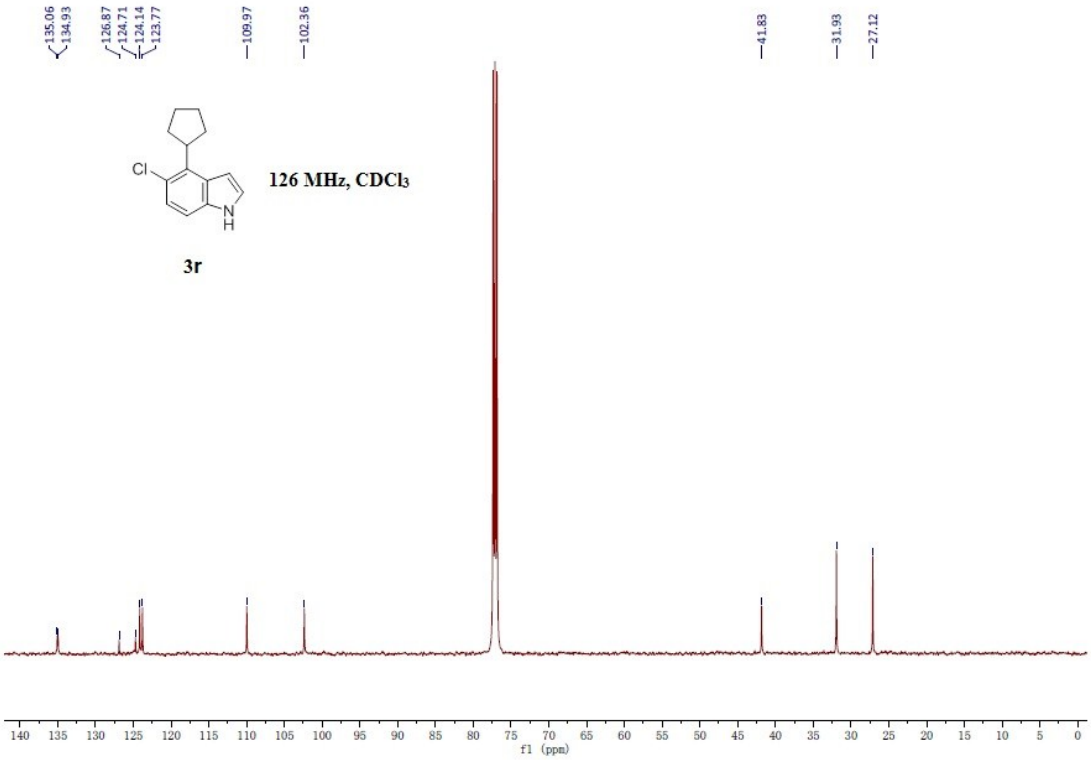

8.34
7.30
7.28
7.25
7.25
7.24
6.86
6.85
6.71
6.70
6.70
2.95
2.95
2.94
2.93
2.92
2.92
2.91
2.90
2.89
1.99
1.97
1.90
1.86
1.81
1.79
1.60
1.54
1.48
1.45
1.43
1.35
1.32
1.29
500 MHz, CDCl3
3P-2
0.92
0.94
1.17
1.02
1.00
1.05
1.94
2.06
1.05
4.17
1.48
f1 (ppm)


140.02
134.45
130.04
127.91
124.57
124.01
117.56
102.43
41.73
33.77
27.21
26.52
126 MHz, CDCl3
3P-2
f1 (ppm)


8.14
7.25
7.23
7.19
7.18
7.14
7.01
7.00
6.64
6.63
6.63
3.48
3.46
3.44
3.43
3.41
2.15
2.14
2.12
1.87
1.86
1.83
1.76
1.74
1.74
1.71
500 MHz, CDCl3
3q
0.93
1.12
0.98
1.03
0.98
1.00
1.04
2.20
4.10
2.01
f1 (ppm)


138.74
135.81
127.05
123.29
122.17
116.27
108.75
101.49
43.53
33.47
25.75
126 MHz, CDCl3
3q
f1 (ppm)


8.10
7.14
7.14
7.13
7.12
7.10
7.09
7.08
6.57
6.57
6.56
3.87
3.85
3.83
3.81
3.80
2.09
2.06
2.04
2.03
2.00
1.97
1.94
1.92
1.89
1.77
1.75
1.73
1.72
Cl
500 MHz, CDCl3
3r
0.96
2.95
1.00
1.06
6.43
2.30
f1 (ppm)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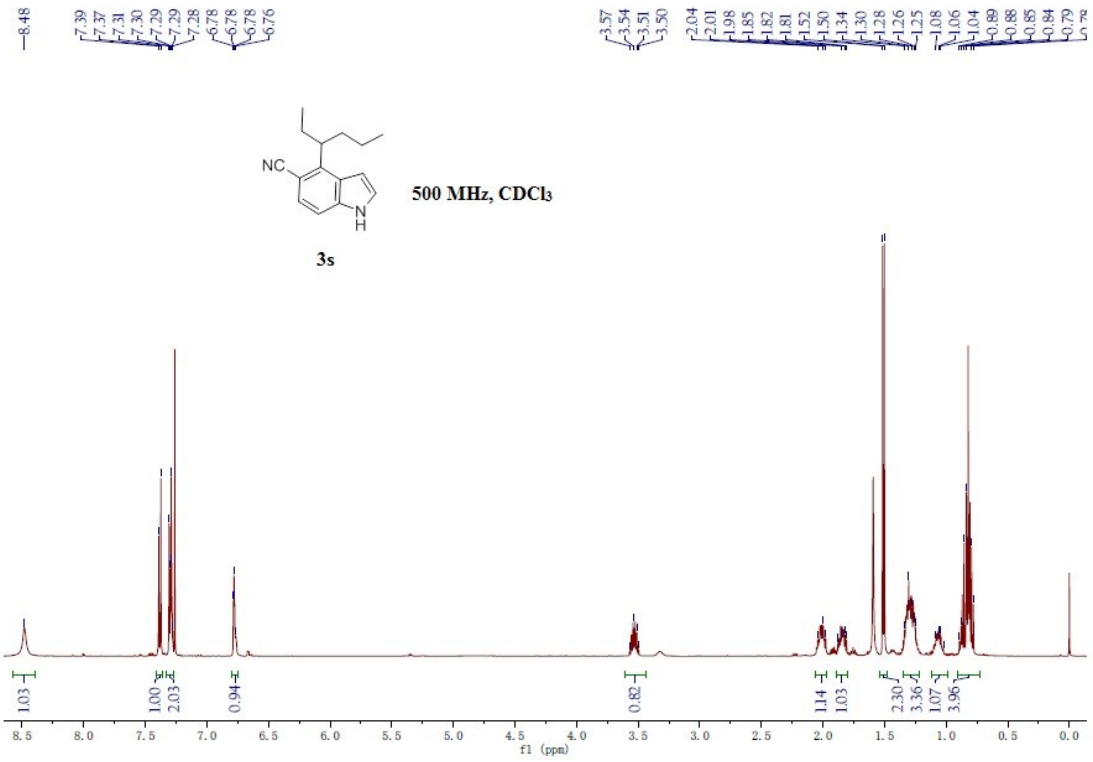
134.93
126.87
124.71
124.14
123.77
109.97
102.36
41.83
31.93
27.12
Cl
N
H
126 MHz, CDCl3
3r
140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)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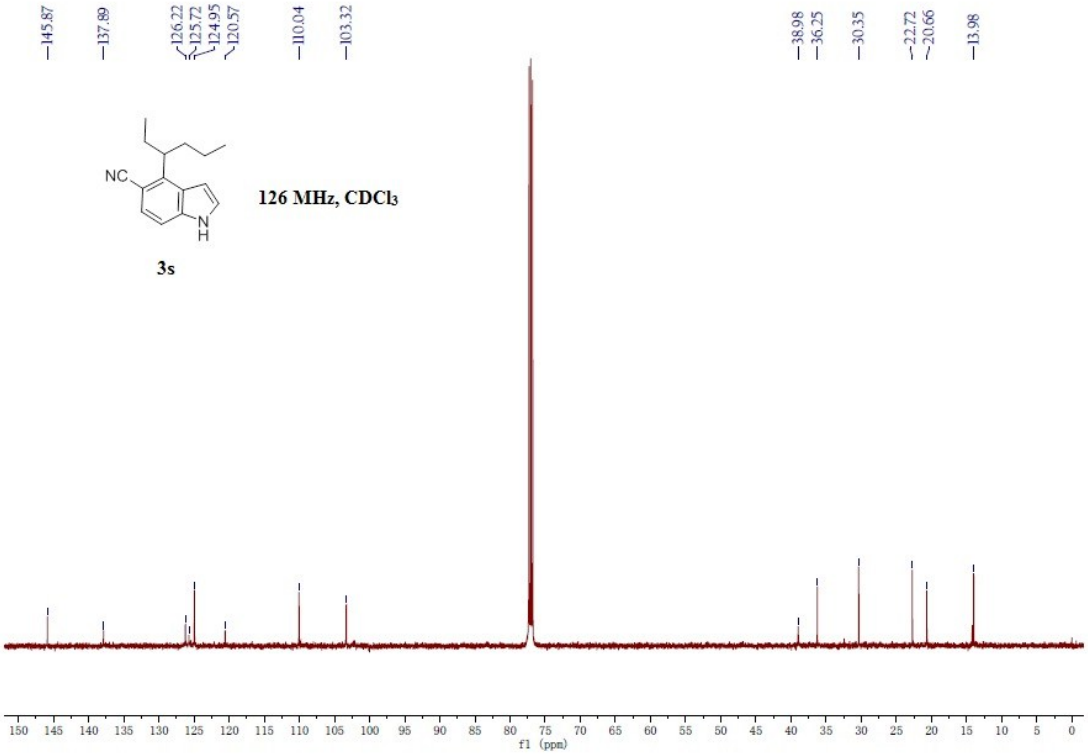
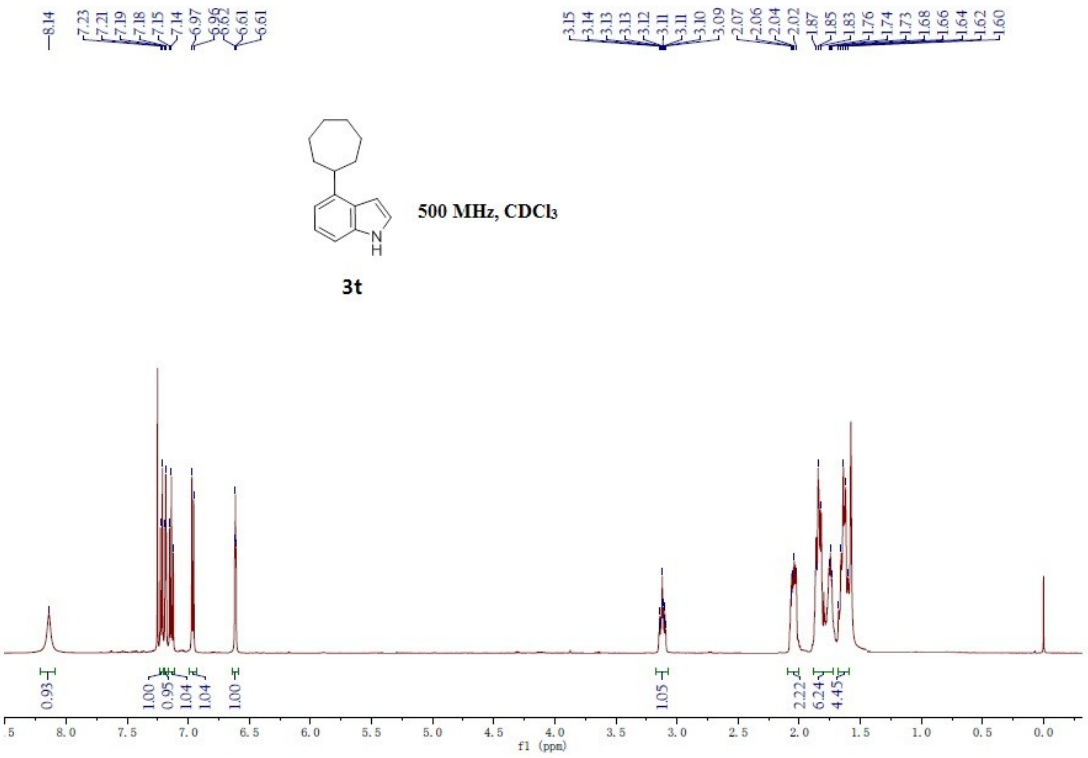
7.29
7.29
7.28
6.78
6.78
6.78
6.76
3.57
3.54
3.51
3.50
2.04
2.01
1.98
1.85
1.82
1.81
1.52
1.50
1.34
1.30
1.28
1.26
1.25
1.08
1.06
1.04
0.89
0.88
0.85
0.84
0.79
NC
N
H
500 MHz, CDCl3
3s
1.03
1.00
2.03
0.94
0.82
1.14
1.03
2.30
3.36
1.07
3.96
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


145.87
137.89
126.22
125.72
124.95
120.57
110.04
103.32
38.98
36.25
30.35
22.72
20.66
13.98
NC
N
H
126 MHz, CDCl3
3s
f1 (ppm)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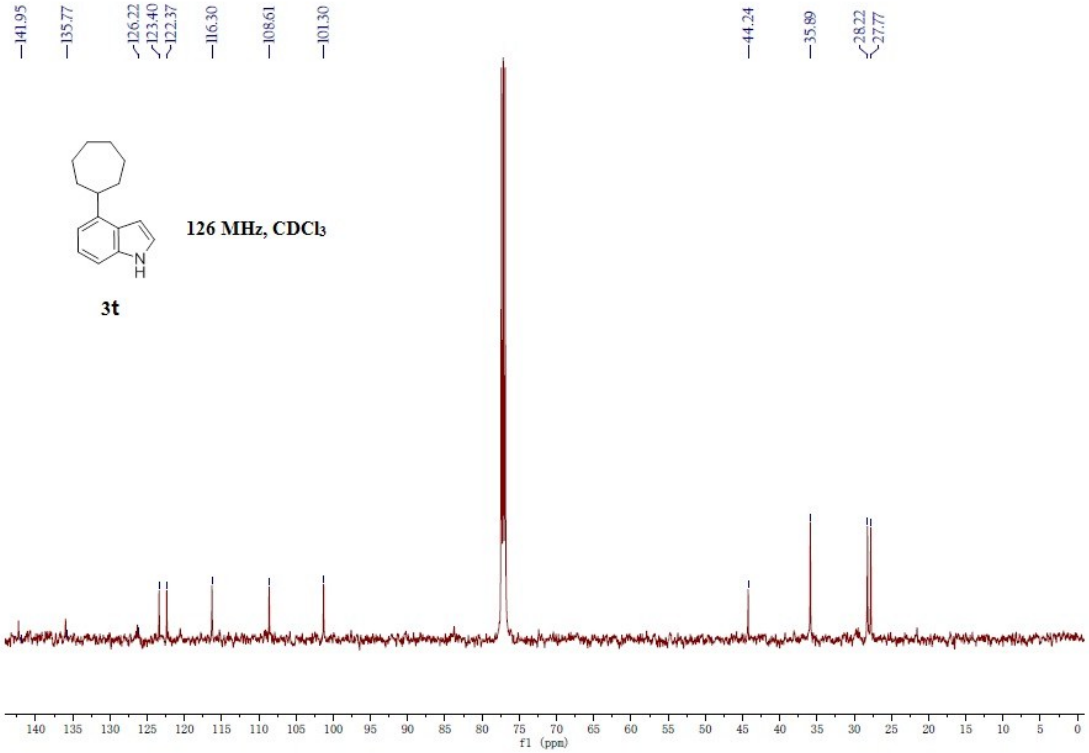
7.23
7.21
7.19
7.18
7.15
7.14
6.97
6.96
6.82
6.61
6.61
3.15
3.14
3.13
3.13
3.12
3.11
3.11
3.10
3.09
2.07
2.06
2.04
2.02
1.87
1.85
1.83
1.76
1.74
1.73
1.68
1.66
1.64
1.62
1.60
N
H
500 MHz, CDCl3
3t
0.93
1.00
0.95
1.04
1.04
1.00
1.05
2.22
6.24
4.45
f1 (ppm)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135.77
126.22
123.40
122.37
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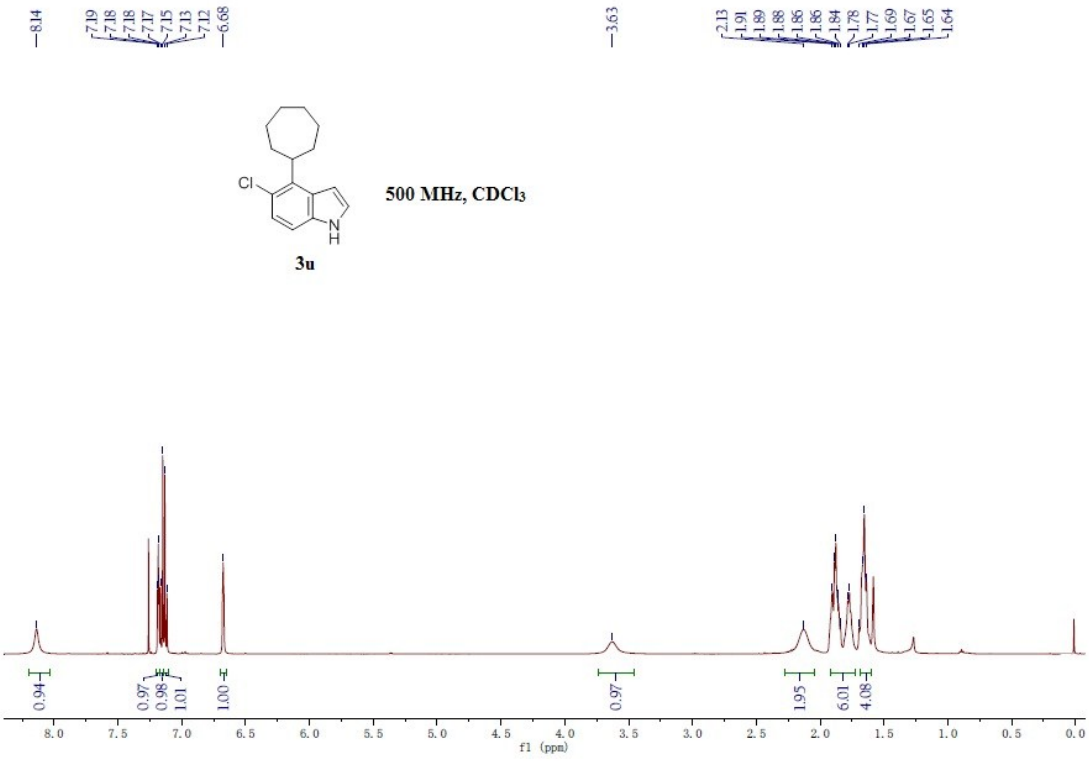
108.61
101.30
44.24
35.89
28.22
27.77
126 MHz, CDCl3
3t
f1 (ppm)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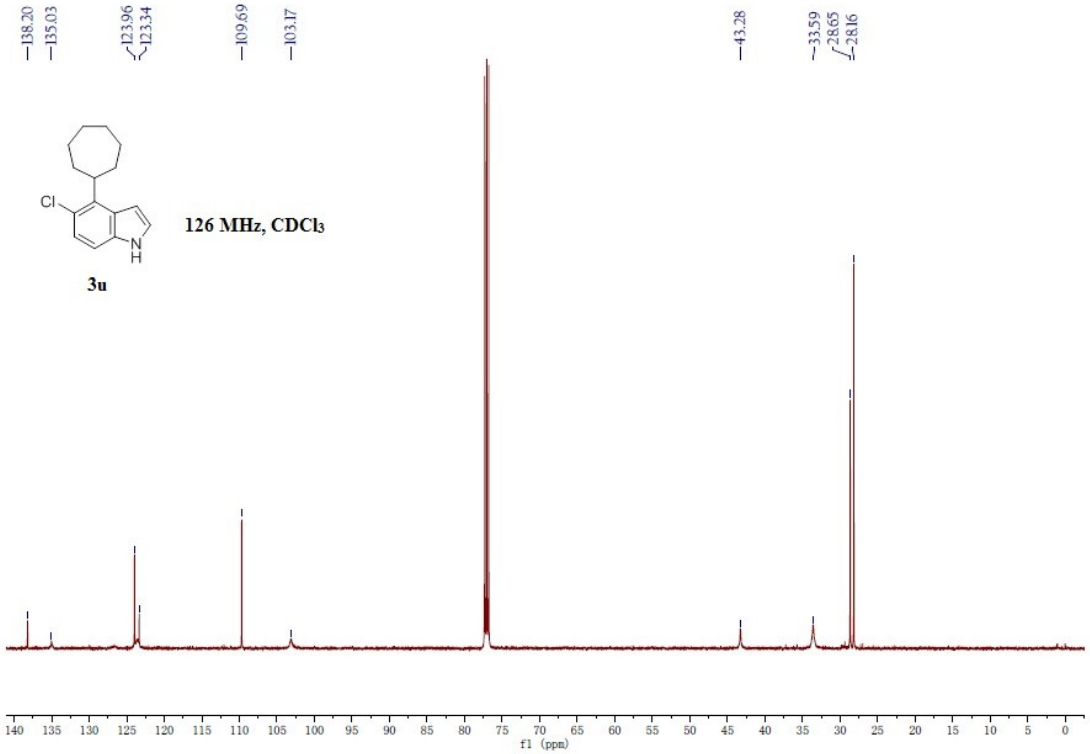
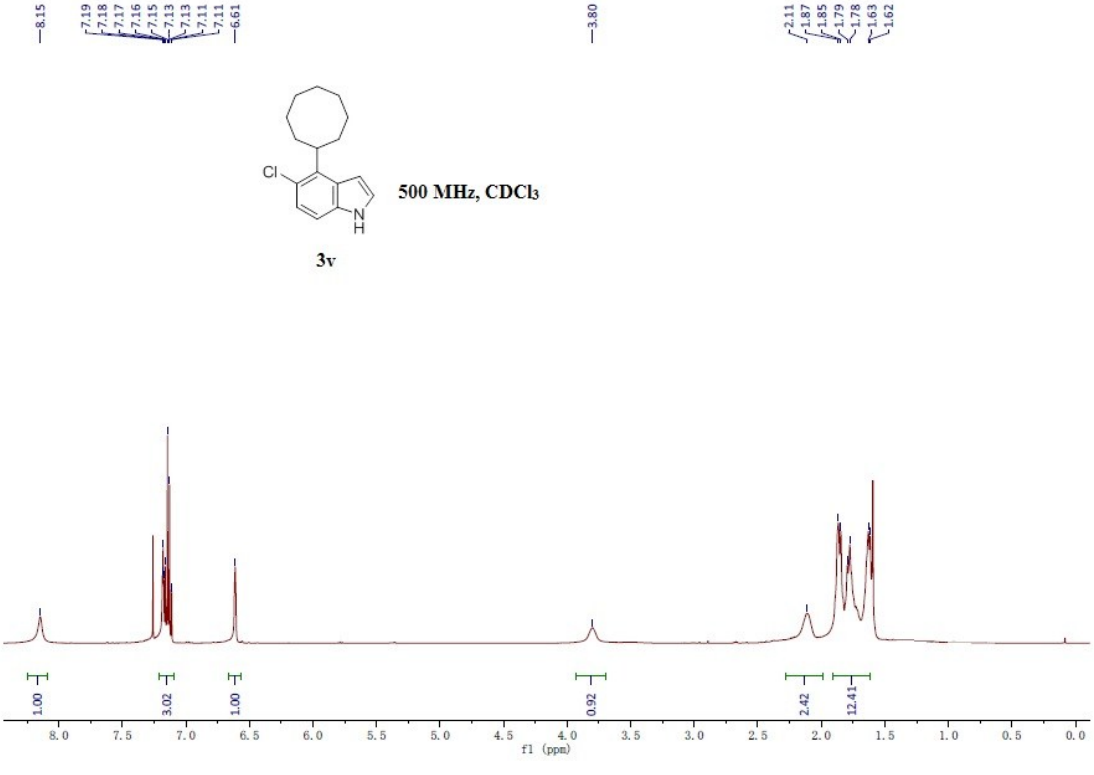
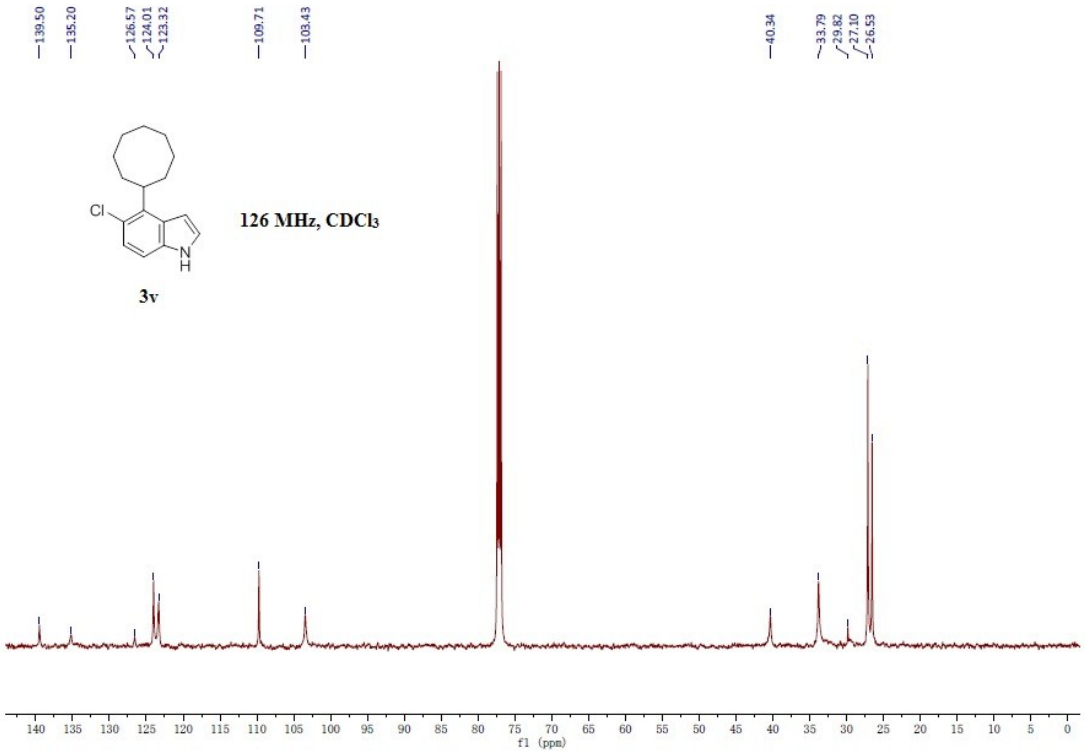
7.19
7.18
7.18
7.17
7.15
7.13
7.12
6.68
3.63
2.13
1.91
1.89
1.88
1.86
1.86
1.84
1.78
1.77
1.69
1.67
1.65
1.64
Cl
500 MHz, CDCl3
3u
0.94
0.97
0.98
1.01
1.00
0.97
1.95
6.01
4.08
f1 (ppm)


138.20
135.03
123.96
123.34
109.69
103.17
43.28
33.59
28.65
28.16
Cl
N
H
126 MHz, CDCl3
3u
f1 (ppm)


8.15
7.19
7.18
7.17
7.16
7.15
7.13
7.13
7.11
7.11
6.61
3.80
2.11
1.87
1.85
1.79
1.78
1.63
1.62
Cl
N
H
500 MHz, CDCl3
3v
1.00
3.02
1.00
0.92
2.42
12.41
f1 (ppm)


139.50
135.20
126.57
124.01
123.32
109.71
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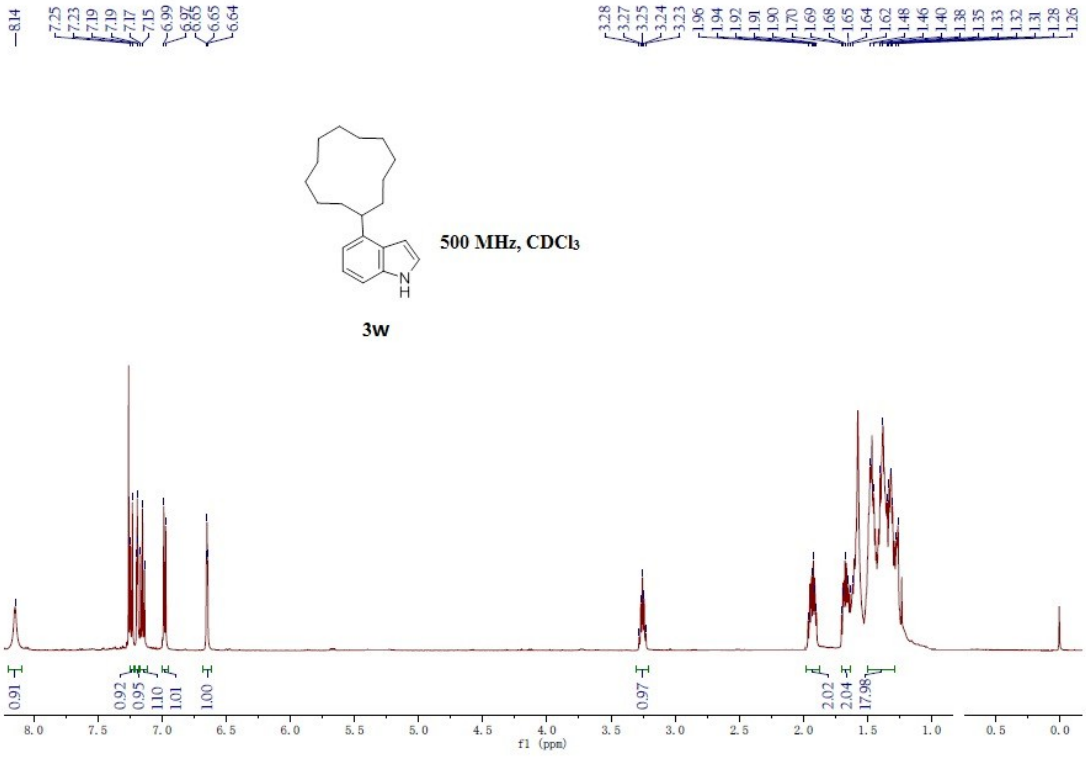
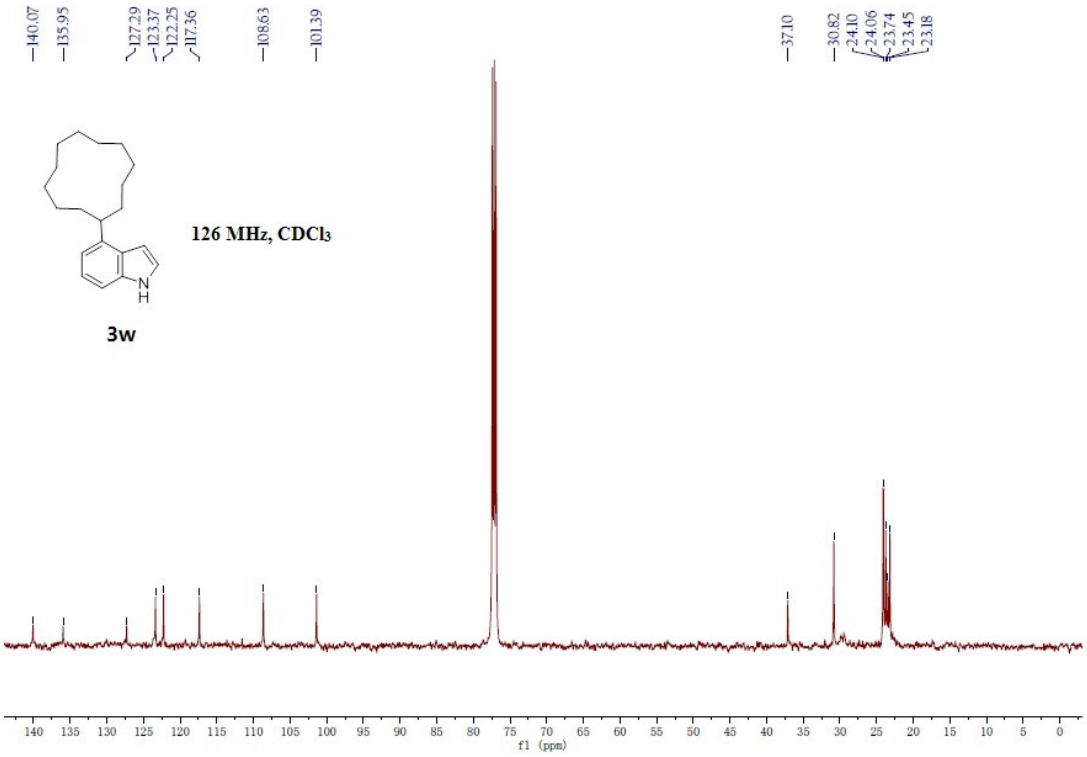
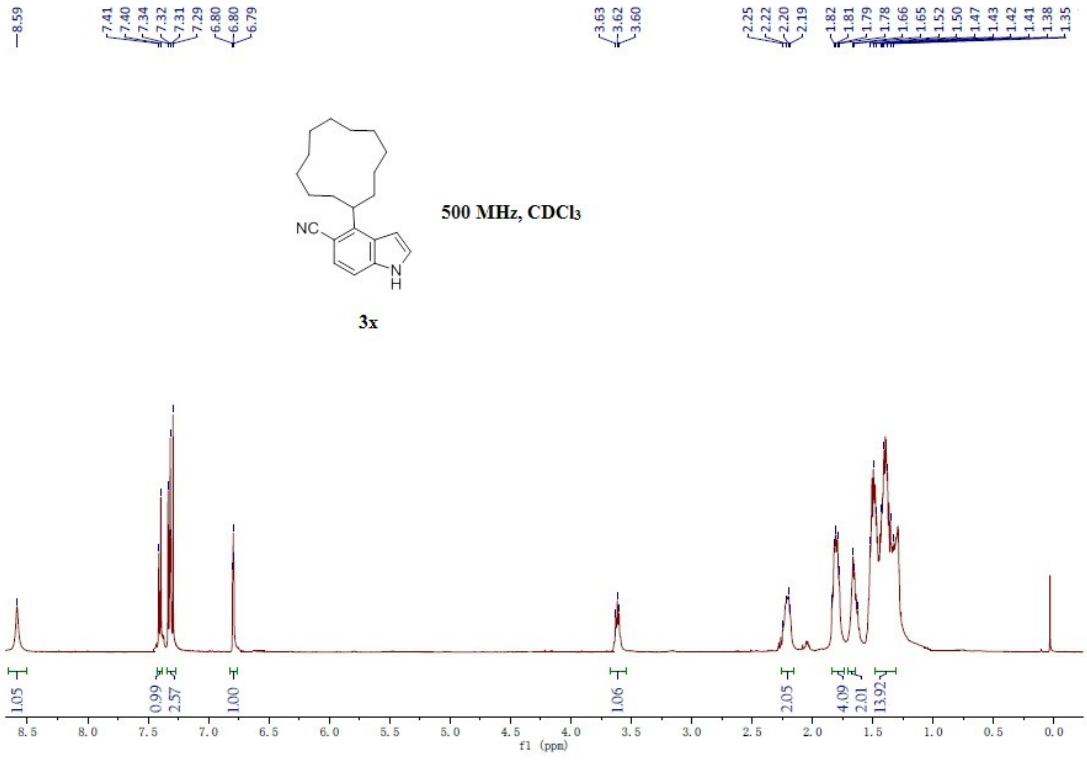
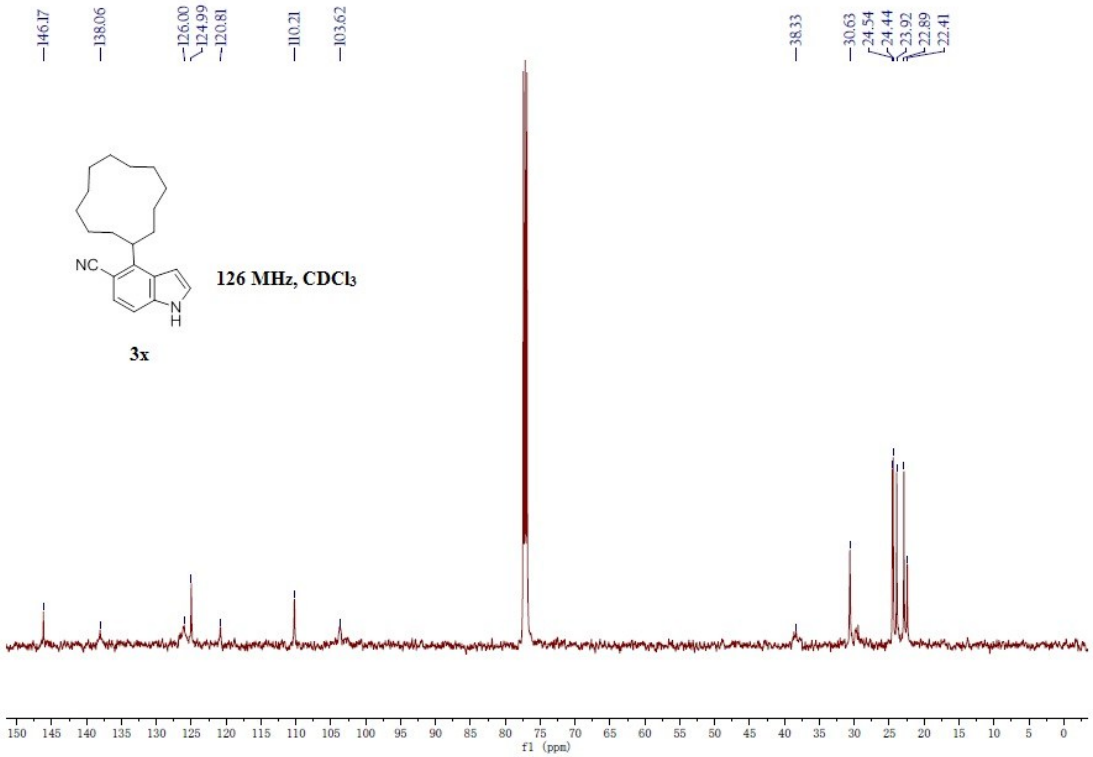
33.79
29.82
27.10
26.53
Cl
N
H
126 MHz, CDCl3
3v
f1 (ppm)


8.14
7.25
7.23
7.19
7.19
7.17
7.15
6.99
6.97
6.65
6.64
3.28
3.27
3.25
3.24
3.23
1.96
1.94
1.92
1.91
1.90
1.70
1.69
1.68
1.65
1.64
1.62
1.48
1.46
1.40
1.38
1.35
1.33
1.32
1.31
1.28
1.26
N
H
500 MHz, CDCl3
3w
0.91
0.92
0.95
1.10
1.01
1.00
0.97
2.02
2.04
17.98
f1 (ppm)


140.07
135.95
127.29
123.37
122.25
117.36
108.63
101.39
37.10
30.82
24.10
24.06
23.74
23.45
23.18
126 MHz, CDCl3
3w
f1 (ppm)


8.59
7.41
7.40
7.34
7.32
7.31
7.29
6.80
6.80
6.79
3.63
3.62
3.60
2.25
2.22
2.20
2.19
1.82
1.81
1.79
1.78
1.66
1.65
1.52
1.50
1.47
1.43
1.42
1.41
1.38
1.35
NC
500 MHz, CDCl3
3x
1.05
0.99
2.57
1.00
1.06
2.05
4.09
2.01
13.92
f1 (ppm)



4. Crystallographic Data

X-ray crystal structure of compound **3e**

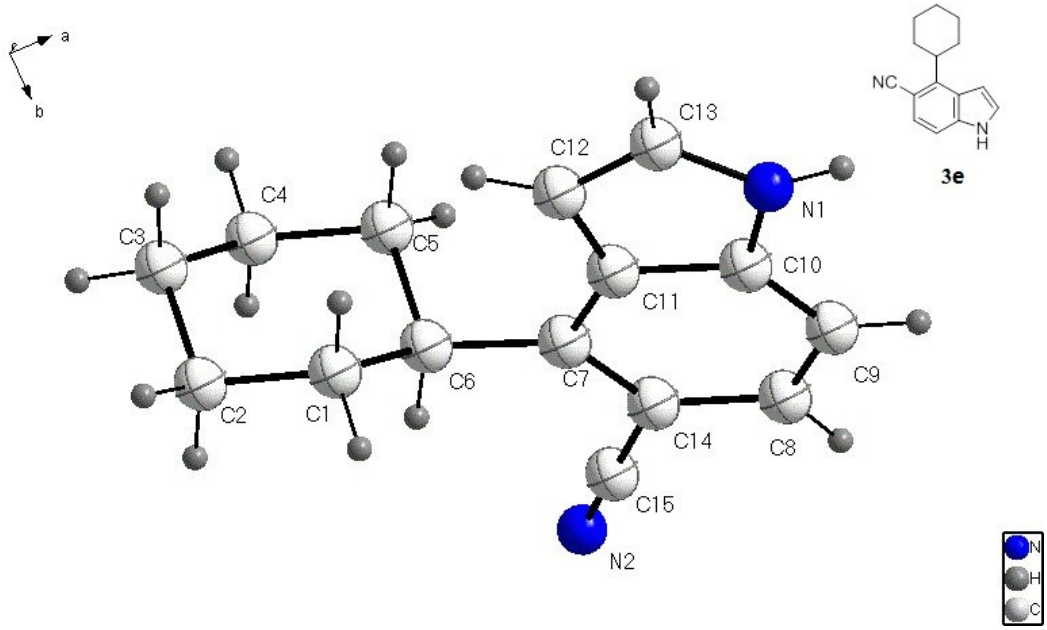


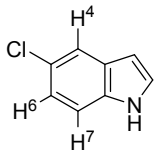
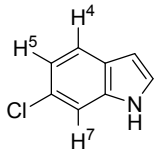
Table 1. Crystal data and structure refinement for compound **3e**.

complex	**3e**
Formula	$C_{15}H_{16}N_2$
Formula weight	224.30
Crystal system	Monoclinic
space group	*P*2(1)/c
a (Å)	15.783(3)
b (Å)	12.467(2)
c (Å)	12.928(2)
α (º)	90.00
β (º)	102.277(3)
γ (º)	90
Volume(Å^3)	2485.6(7)
Z	8
T (K)	293(2)
D_{calcd} (g/m^3)	1.199
F(000)	960
Reflections collected	4370
Unique reflections	3137
Goof	1.042
R_1[I> 2σ(I)]	0.0430
wR_2[I>2σ(I)]	0.1028[a]
CCDC NO.	1402249

[a] $w = 1/[\sigma^2(F_0)^2+(0.0532P)^2 +0.2324P]$, where $P = (F_0^2 + 2F_c^2)/3$;

5. Theoretic calculation results of 1c and 1o.

Compounds	Breaking	TS energy	Zero point	c-hexane	Zero point	Indole	Zero point	Active

	bonds	(hartree)	energies (hartree)	energies (hartree)	energies (hartree)	energies (hartree)	energies (hartree)	energies (kJ/mol)
 **1c**	C-H^4	-1058.6131	0.2785	-235.2139	0.1562	-823.4131	0.1203	41.75
	C-H^6	-1058.6105	0.2785	-235.2139	0.1562	-823.4131	0.1203	48.57
	C-H^7	-1058.6107	0.2785	-235.2139	0.1562	-823.4131	0.1203	48.05
 **1o**	C-H^4	-1058.6117	0.2785	-235.2139	0.1562	-823.4131	0.1203	45.42
	C-H^5	-1058.6083	0.2785	-235.2139	0.1562	-823.4131	0.1203	54.35
	C-H^7	-1058.6121	0.2786	-235.2139	0.1562	-823.4131	0.1203	44.63