Electronic Supplementary Material (ESI) for Chemical Communications.

Supporting Information

for

Cobalt-Catalyzed Cross-Dehydrogenative Coupling between N-(2-pyridyl) and Free Indoles for the Synthesis of Unsymmetrical 2,2'-Biindoles

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Table of Contents

1. General Information S2

2. Synthesis of Unsymmetrical 2,2'-Biindoles S3

*3. X-ray of Compound **3kf** S17*

4. Removal of the Pyridine Directing Group S19

5. Mechanistic studies. S21

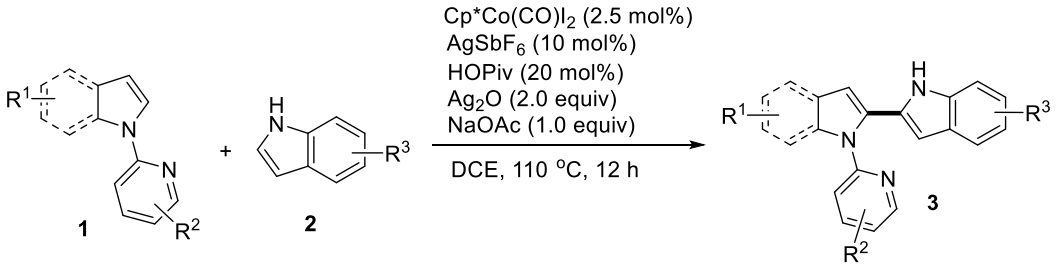
6. NMR Spectra for New Compounds S23

1. General Information

Ethyl acetate (ACS grade), hexanes (ACS grade) and diethyl ether (ACS grade) were purchased from Fisher Scientific and used without further purification. Anhydrous dichloromethane (HPLC grade) was purified by distillation over calcium hydride. Anhydrous tetrahydrofuran from Aldrich was used directly without further purification. Commercially available reagents were used without further purification. Reactions were monitored by thin layer chromatography(TLC) using whatman precoated silica gel plates. Flash column chromatography was performed over silacycle silica gel (230-400 mesh). ^{1}H NMR and ^{13}C NMR spectra were recorded on a Varian 400 MHz Unity plus spectrometer using residue solvent peaks as internal standards. Infrared spectra were recorded with a Perkin Elmer FT-IR spectrum 2000 spectrometer and are reported in reciprocal centimeter (cm-1). Mass spectra were recorded with Waters micromass ZQ detector using electron spray method. *N*-(2-pyridyl) indoles were prepared following literatures reports.

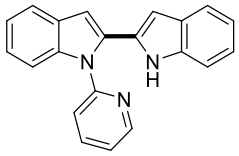
2. Synthesis of Unsymmetrical 2,2'-Biindoles

***General Procedure A*：**



A suspension of **1** (0.20 mmol), **2** (0.40 mmol), [Cp*Co(CO)I_2] (2.5 mol %), $AgSbF_6$ (10 mol %)，HOPiv (20 mol %), Ag_2O (2.0 equiv) and NaOAc (1.0 equiv) in DCE (2 mL) was stirred at 110 ℃ for 12 h. Then the solvent was removed in vacuo and the remaining residue was purified by column chromatography on silica gel to afford the desired product **3**.

1-(pyridin-2-yl)-1*H*,1'*H*-2,2'-biindole (3aa)



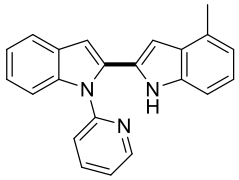
Compound **3aa** was obtained as purple solid in 86% yield according to general procedure **A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.95 (br, 1H), 8.73 (d, *J* = 3.6 Hz, 1H), 7.78 (td, *J* = 7.8, 1.7 Hz, 1H), 7.71 – 7.64 (m, 1H), 7.53 (d, J = 7.8 Hz, 1H), 7.48 – 7.41 (m, 1H), 7.36 (dd, *J* = 7.0, 5.2 Hz, 1H), 7.32 (d, *J* = 8.1 Hz, 1H), 7.27 (d, *J* = 8.1 Hz, 1H), 7.24 – 7.19 (m, 2H), 7.17 (t, *J* = 7.4 Hz, 1H), 7.08 (t, *J* = 7.4 Hz, 1H), 6.94 (s, 1H), 6.37 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.88, 149.24, 138.81, 138.49, 136.38, 132.61, 129.85, 128.53, 128.46, 123.27, 122.74, 122.45, 122.38, 121.53, 120.70, 120.60, 120.11, 111.10, 110.89, 105.25, 103.28.

HRMS m/z (ESI) Calcd for $C_{21}H_{15}N_3Na$ [M+Na^+] 332.1158, found: 332.1161.

4'-methyl-1-(pyridin-2-yl)-1*H*,1'*H*-2,2'-biindole (3ab)



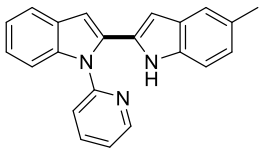
Compound **3ab** was obtained as purple solid in 71% yield according to general procedure **A**.

^{1}H NMR (400 MHz, CD_2Cl_2) δ 8.81 (br, 1H), 8.68 (d, *J* = 3.5 Hz, 1H), 7.78 (td, *J* = 7.8, 1.8 Hz, 1H), 7.66 – 7.59 (m, 1H), 7.36 (dd, *J* = 6.4, 5.3 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 1H), 7.26 (d, *J* = 8.0 Hz, 1H), 7.18 – 7.13 (m, 2H), 7.09 (s, 1H), 6.88 (s, 1H), 6.85 (d, *J* = 8.1 Hz, 1H), 6.19 (s, 1H), 2.38 (s, 3H).

^{13}C NMR (101 MHz, CD_2Cl_2) δ 151.73, 149.29, 138.79, 138.48, 136.81, 132.82, 132.39, 129.06, 128.46, 126.23, 122.93, 122.86, 122.34, 121.83, 121.29, 120.43, 119.98, 110.93, 110.66, 104.28, 102.75, 21.34.

HRMS m/z (ESI) Calcd for $C_{22}H_{17}N_3Na$ [M+Na^+] 346.1315, found: 346.1312.

5'-methyl-1-(pyridin-2-yl)-1*H*,1'*H*-2,2'-biindole (3ac)



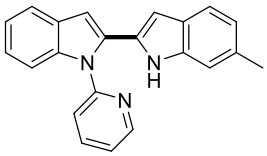
Compound **3ac** was obtained as purple solid in 85% yield according to general procedure **A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.79 (br, 1H), 8.72 (d, *J* = 3.7 Hz, 1H), 7.75 (td, *J* = 7.8, 1.7 Hz, 1H), 7.71 – 7.61 (m, 1H), 7.49 – 7.44 (m, 1H), 7.34 (dd, *J* = 6.9, 5.3 Hz, 1H), 7.32 (s, 1H), 7.25 – 7.17 (m, 4H), 6.99 (d, *J* = 8.1 Hz, 1H), 6.91 (s, 1H), 6.27 (d, *J* = 0.8 Hz, 1H), 2.42 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.92, 149.20, 138.77, 138.42, 134.75, 132.73, 129.87, 129.34, 128.75, 128.56, 124.11, 123.20, 122.65, 122.34, 121.49, 120.65, 120.18, 111.12, 110.55, 105.05, 102.83, 21.37.

HRMS m/z (ESI) Calcd for $C_{22}H_{17}N_3Na$ [M+Na^+] 346.1315, found: 346.1312.

6'-methyl-1-(pyridin-2-yl)-1*H*,1'*H*-2,2'-biindole (3ad)



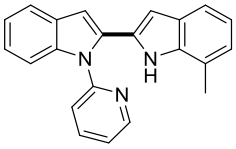
Compound **3ad** was obtained as purple solid as purple solid in 72% yield according to general procedure **A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.93 (br, 1H), 8.68 – 8.58 (m, 1H), 7.66 (td, *J* = 7.8, 1.9 Hz, 1H), 7.59 (dd, *J* = 6.3, 2.6 Hz, 1H), 7.45 – 7.37 (m, 1H), 7.25 (dd, *J* = 6.7, 5.0 Hz, 1H), 7.17 – 7.13 (m, 3H), 7.06 (d, *J* = 8.1 Hz, 1H), 6.99 (d, *J* = 8.0 Hz, 1H), 6.84 (s, 1H), 6.81 (d, *J* = 7.0 Hz, 1H), 6.34 (d, *J* = 1.2 Hz, 1H), 2.41 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.85, 149.10, 138.68, 138.45, 136.08, 132.72, 130.09, 129.22, 128.56, 128.37, 123.18, 122.63, 122.55, 122.31, 121.49, 120.65, 120.15, 111.10, 108.50, 105.28, 101.86, 18.63.

HRMS m/z (ESI) Calcd for $C_{22}H_{17}N_3Na$ [M+Na^+] 346.1315, found: 346.1312.

7'-methyl-1-(pyridin-2-yl)-1*H*,1'*H*-2,2'-biindole (3ae)



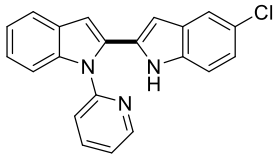
Compound **3ae** was obtained as purple solid in 77% yield according to general procedure **A**.

^{1}H NMR (400 MHz, DMSO) δ 11.27 (br, 1H), 8.83 – 8.71 (m, 1H), 8.04 (td, *J* = 7.7, 1.9 Hz, 1H), 7.82 – 7.72 (m, 1H), 7.60 (ddd, *J* = 7.5, 4.9, 0.9 Hz, 1H), 7.43 (d, *J* = 7.9 Hz, 1H), 7.37 – 7.32 (m, 1H), 7.31 (s, 1H), 7.27 – 7.19 (m, 3H), 6.95 – 6.87 (m, 2H), 5.71 (d, *J* = 2.0 Hz, 1H).

^{13}C NMR (101 MHz, DMSO) δ 151.72, 149.95, 139.47, 139.04, 136.48, 133.14, 130.00, 128.34, 128.22, 123.93, 123.32, 123.07, 122.99, 121.55, 121.04, 120.91, 120.07, 118.13, 111.29, 104.57, 102.23, 17.50.

HRMS m/z (ESI) Calcd for $C_{22}H_{17}N_3Na$ [M+Na^+] 346.1315, found: 346.1312.

5'-chloro-1-(pyridin-2-yl)-1*H*,1'*H*-2,2'-biindole (3ag)



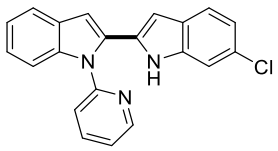
Compound **3ag** was obtained as purple solid in 82% yield according to general procedure **A**.

^{1}H NMR (400 MHz, DMSO) δ 11.76 (br, 1H), 8.71 (d, *J* = 3.6 Hz, 1H), 8.02 (td, *J* = 7.7, 1.8 Hz, 1H), 7.72 (dd, *J* = 5.4, 3.2 Hz, 1H), 7.58 (dd, *J* = 6.9, 5.1 Hz, 1H), 7.46 – 7.40 (m, 2H), 7.38 (d, *J* = 8.6 Hz, 1H), 7.30 (dd, *J* = 5.8, 2.8 Hz, 1H), 7.24 – 7.12 (m, 3H), 7.09 (dd, *J* = 8.6, 1.9 Hz, 1H), 5.66 (d, *J* = 1.1 Hz, 1H).

^{13}C NMR (101 MHz, DMSO) δ 151.42, 150.05, 139.61, 139.14, 135.41, 132.53, 131.71, 129.62, 128.21, 124.39, 124.09, 123.65, 123.00, 122.28, 121.68, 121.12, 119.66, 113.06, 111.32, 104.59, 101.01.

HRMS m/z (ESI) Calcd for $C_{21}H_{14}ClN_3Na$ [M+Na$^+$] 366.0768, found: 366.0772.

6'-chloro-1-(pyridin-2-yl)-1*H*,1'*H*-2,2'-biindole (3ah)



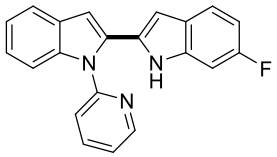
Compound **3ah** was obtained as purple solid in 88% yield according to general procedure **A**.

^{1}H NMR (400 MHz, DMSO) δ 11.71 (br, 1H), 8.71 (d, *J* = 4.7 Hz, 1H), 8.03 (t, *J* = 7.7 Hz, 1H), 7.74 – 7.65 (m, 1H), 7.58 (dd, *J* = 6.9, 5.4 Hz, 1H), 7.43 (d, *J* = 7.9 Hz, 1H), 7.38 (d, *J* = 8.5 Hz, 2H), 7.32 – 7.23 (m, 1H), 7.23 – 7.14 (m, 3H), 6.96 (d, *J* = 8.4 Hz, 1H), 5.69 (d, *J* = 0.9 Hz, 1H).

^{13}C NMR (101 MHz, DMSO) δ 151.44, 150.07, 139.63, 139.15, 137.35, 132.57, 131.16, 128.22, 127.29, 126.94, 124.12, 123.61, 123.03, 121.92, 121.66, 121.08, 120.21, 111.29, 111.10, 104.42, 101.42.

HRMS m/z (ESI) Calcd for $C_{21}H_{14}ClN_3Na$ [M+Na$^+$] 366.0768, found: 366.0772.

6'- fluoro -1-(pyridin-2-yl)-1*H*,1'*H*-2,2'-biindole (3ai)



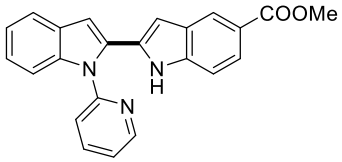
Compound **3ai** was obtained as purple solid in 81% yield according to general procedure **A**.

^{1}H NMR (400 MHz, DMSO) δ 11.58 (br, 1H), 8.72 (d, *J* = 3.2 Hz, 1H), 8.02 (t, *J* = 7.5 Hz, 1H), 7.67 – 7.55 (m, 1H), 7.51 (d, *J* = 9.2 Hz, 1H), 7.47 – 7.32 (m, 3H), 7.27 (dd, *J* = 8.5, 4.1 Hz, 1H), 7.19 – 7.07 (m, 2H), 7.02 (t, *J* = 9.0 Hz, 1H), 6.95 (t, *J* = 7.2 Hz, 1H), 5.67 (s, 1H).

^{13}C NMR (101 MHz, DMSO) δ 151.40, 150.06, 139.66, 137.03, 135.76, 134.80, 129.60, 128.80 (d, *J* = 8.6 Hz), 128.40, 124.22, 123.05, 122.57, 120.67, 119.90, 112.45 (d, *J* = 9.5 Hz), 111.67, 111.32 (d, *J* = 26.4 Hz), 105.82, 105.62, 103.90 (d, *J* = 5.1 Hz), 101.71.

HRMS m/z (ESI) Calcd for $C_{21}H_{14}FN_3Na$ [M+Na^+] 350.1064, found: 350.1063.

methyl 1'-(pyridin-2-yl)-1*H*,1'*H*-[2,2'-biindole]-5-carboxylate (3aj)



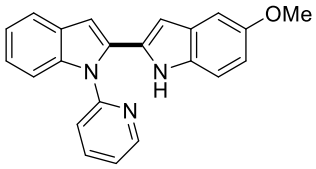
Compound **3aj** was obtained as purple solid in 50% yield according to general procedure **A**.

^{1}H NMR (400 MHz, DMSO) δ 11.95 (br, 1H), 8.71 (d, *J* = 3.6 Hz, 1H), 8.07 (s, 1H), 8.03 (td, *J* = 7.8, 1.8 Hz, 1H), 7.77 – 7.70 (m, 2H), 7.59 (dd, *J* = 7.1, 5.1 Hz, 1H), 7.45 (dd, *J* = 8.2, 3.9 Hz, 2H), 7.30 (d, *J* = 6.8 Hz, 1H), 7.24 – 7.17 (m, 3H), 5.81 (s, 1H), 3.82 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ 167.51, 151.37, 150.07, 139.63, 139.53, 139.17, 132.38, 131.86, 128.19, 128.12, 124.13, 123.71, 123.31, 123.13, 123.02, 121.69, 121.43, 121.16, 111.52, 111.32, 104.67, 102.49, 52.08.

HRMS m/z (ESI) Calcd for $C_{23}H_{17}O_2N_3H$ [M+H$^+$] 368.1394, found: 368.1389.

5'-methoxy-1-(pyridin-2-yl)-1*H*,1'*H*-2,2'-biindole (3ak)



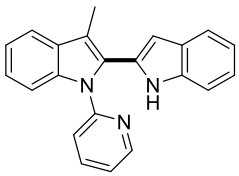
Compound **3ak** was obtained as purple solid in 76% yield according to general procedure **A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.84 (s, 1H), 8.70 (d, *J* = 3.7 Hz, 1H), 7.76 (t, *J* = 6.9 Hz, 1H), 7.68 – 7.63 (m, 1H), 7.46 – 7.39 (m, 1H), 7.34 (dd, *J* = 6.8, 5.3 Hz, 1H), 7.24 – 7.16 (m, 3H), 6.96 (s, 1H), 6.89 (s, 1H), 6.81 (dd, *J* = 8.7, 2.1 Hz, 1H), 6.27 (s, 1H), 3.81 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 154.47, 151.90, 149.20, 138.77, 138.48, 132.67, 131.64, 130.49, 128.89, 128.55, 123.22, 122.71, 122.37, 121.52, 120.67, 112.92, 111.62, 111.09, 105.08, 103.05, 102.18, 55.84.

HRMS m/z (ESI) Calcd for $C_{22}H_{17}ON_3Na$ [M+Na$^+$] 362.1264, found: 362.1262.

3-methyl-1-(pyridin-2-yl)-1*H*,1'*H*-2,2'-biindole (3ba)



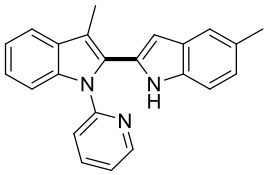
Compound **3ba** was obtained as purple solid in 71% yield according to general procedure **A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.97 (br, 1H), 8.60 (d, *J* = 3.7 Hz, 1H), 7.65 – 7.56 (m, 4H), 7.29 (d, *J* = 8.1 Hz, 1H), 7.24 – 7.15 (m, 4H), 7.13 – 7.09 (m, 1H), 7.03 (d, *J* = 8.0 Hz, 1H), 6.60 (d, *J* = 1.2 Hz, 1H), 2.46 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 152.22, 148.68, 138.32, 137.64, 136.37, 129.53, 128.94, 128.44, 128.33, 123.63, 122.20, 121.81, 121.26, 121.07, 120.53, 119.93, 119.12, 114.92, 111.30, 110.91, 104.99, 9.82.

HRMS m/z (ESI) Calcd for $C_{22}H_{17}N_3Na$ [M+Na$^+$] 346.1315, found: 346.1312.

3,5'-dimethyl-1-(pyridin-2-yl)-1*H*,1'*H*-2,2'-biindole (3bc)



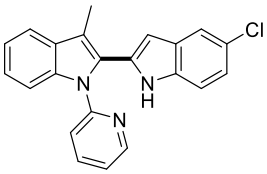
Compound **3bc** was obtained as purple solid in 71% yield according to general procedure **A**.

^{1}H NMR (400 MHz, DMSO) δ 11.01 (br, 1H), 8.59 (d, *J* = 4.8 Hz, 1H), 7.78 – 7.71 (m, 1H), 7.68 (dd, *J* = 10.4, 4.3 Hz, 2H), 7.37 (d, *J* = 8.0 Hz, 1H), 7.31 (dd, *J* = 6.9, 5.4 Hz, 1H), 7.26 – 7.19 (m, 2H), 7.12 (s, 1H), 6.96 (d, *J* = 8.1 Hz, 1H), 6.83 (d, *J* = 8.1 Hz, 1H), 6.25 (s, 1H), 2.43 (s, 3H), 2.38 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ 151.98, 149.19, 138.73, 137.60, 137.43, 131.10, 129.43, 129.30, 128.47, 126.24, 123.74, 122.23, 121.48, 121.30, 120.69, 120.21, 119.35, 113.70, 112.09, 111.68, 103.90, 21.87, 9.92.

HRMS m/z (ESI) Calcd for $C_{23}H_{19}N_3H$ [M+H$^+$] 338.1652, found: 338.1657

5'-chloro-3-methyl-1-(pyridin-2-yl)-1*H*,1'*H*-2,2'-biindole (3bf)



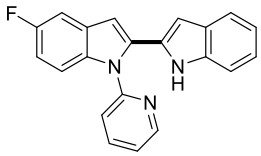
Compound **3bf** was obtained as purple solid in 71% yield according to general procedure **A**.

^{1}H NMR (400 MHz, DMSO) δ 11.34 (br, 1H), 8.62 – 8.56 (m, 1H), 7.76 (td, *J* = 7.8, 1.9 Hz, 1H), 7.71 – 7.66 (m, 2H), 7.51 (d, *J* = 8.4 Hz, 1H), 7.36 – 7.31 (m, 2H), 7.27 – 7.21 (m, 2H), 7.02 – 6.98 (m, 2H), 6.41 – 6.33 (m, 1H), 2.44 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ 151.78, 149.31, 138.88, 137.53, 137.48, 130.39, 129.34, 128.57, 127.10, 126.62, 124.04, 122.39, 121.87, 121.40, 120.75, 120.08, 119.53, 114.30, 112.05, 111.41, 104.11, 9.91.

HRMS m/z (ESI) Calcd for $C_{22}H_{16}N_3ClNa$ [M+Na$^+$]380.0925, found: 380.0930.

5-fluoro-1-(pyridin-2-yl)-1*H*,1'*H*-2,2'-biindole (3ca)



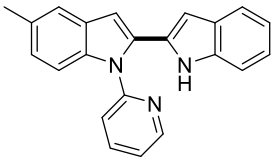
Compound **3ca** was obtained as purple solid in 71% yield according to general procedure **A**.

1H NMR (400 MHz, CDCl3) δ 9.08 (br, 1H), 8.72 (d, *J* = 3.4 Hz, 1H), 7.82 (dd, *J* = 10.8, 4.5 Hz, 1H), 7.67 (dd, *J* = 6.1, 2.5 Hz, 1H), 7.43 (d, *J* = 7.1 Hz, 1H), 7.41 – 7.36 (m, 1H), 7.30 (d, *J* = 7.9 Hz, 1H), 7.22 (dt, *J* = 8.1, 7.1 Hz, 3H), 7.16 (dd, *J* = 9.5, 2.0 Hz, 1H), 6.98 – 6.78 (m, 2H), 6.33 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 157.2, 151.8, 149.3, 138.8, 138.6, 132.9, 132.3, 131.7, 128.8 (d, $J_{C\text{-}F}$ = 10.0 Hz), 128.5, 123.4, 122.9, 122.4, 121.6, 120.8, 111.5 (d, $J_{C\text{-}F}$ = 9.0 Hz), 111.1, 110.8 (d, $J_{C\text{-}F}$ = 26.4 Hz), 105.6, 105.2 (d, $J_{C\text{-}F}$ = 23.7 Hz), 103.2, 103.1.

HRMS m/z (ESI) Calcd for $C_{21}H_{14}FN_3Na$ [M+Na^+] 350.1064, found: 350.1063.

5-methyl-1-(pyridin-2-yl)-1*H*,1'*H*-2,2'-biindole (3da)



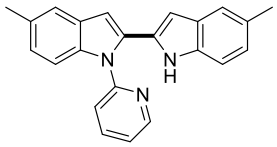
Compound **3da** was obtained as purple solid in 71% yield according to general procedure **A**.

^{1}H NMR (400 MHz, DMSO) δ 11.52 (br, 1H), 8.70 (d, *J* = 3.5 Hz, 1H), 8.00 (td, *J* = 7.7, 1.7 Hz, 1H), 7.55 (dd, *J* = 7.0, 5.2 Hz, 1H), 7.49 (s, 1H), 7.36 (t, *J* = 9.3 Hz, 3H), 7.19 (d, *J* = 8.4 Hz, 1H), 7.09 (t, *J* = 7.5 Hz, 1H), 7.05 (s, 1H), 7.01 (d, *J* = 8.3 Hz, 1H), 6.94 (t, *J* = 7.4 Hz, 1H), 5.65 (s, 1H), 2.42 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ 151.77, 149.94, 139.46, 137.60, 136.94, 133.07, 130.31, 130.16, 128.57, 128.50, 124.90, 123.85, 122.90, 122.30, 120.52, 119.78, 111.57, 111.04, 103.77, 101.24, 21.50.

HRMS m/z (ESI) Calcd for $C_{22}H_{17}N_3Na$ [M+Na^+] 346.1315, found: 346.1312.

5,5'-dimethyl-1-(pyridin-2-yl)-1*H*,1'*H*-2,2'-biindole (3dc)



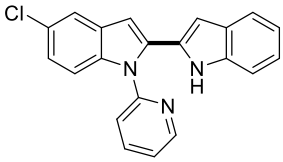
Compound **3dc** was obtained as purple solid in 71% yield according to general procedure **A**.

^{1}H NMR (400 MHz, DMSO) δ 11.38 (br, 1H), 8.70 (d, *J* = 4.2 Hz, 1H), 8.03 – 7.91 (m, 1H), 7.54 (dd, *J* = 7.3, 5.0 Hz, 1H), 7.47 (s, 1H), 7.35 (d, *J* = 7.9 Hz, 1H), 7.26 (d, *J* = 8.2 Hz, 1H), 7.19 (d, *J* = 8.4 Hz, 1H), 7.12 (s, 1H), 7.03 (s, 1H), 7.00 (d, *J* = 8.4 Hz, 1H), 6.91 (d, *J* = 8.2 Hz, 1H), 5.55 (s, 1H), 2.41 (s, 3H), 2.31 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ 151.81, 149.90, 139.41, 137.54, 135.32, 133.24, 130.28, 130.14, 128.76, 128.60, 128.27, 124.81, 123.93, 123.79, 122.89, 120.48, 120.06, 111.28, 111.02, 103.57, 100.86, 21.55, 21.50.

HRMS m/z (ESI) Calcd for $C_{23}H_{19}N_3Na$ [M+Na$^+$] 360.1471, found: 360.1478.

5-chloro-1-(pyridin-2-yl)-1*H*,1'*H*-2,2'-biindole (3ea)



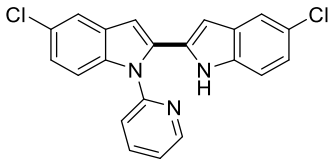
Compound **3ea** was obtained as purple solid in 71% yield according to general procedure **A**.

^{1}H NMR (400 MHz, DMSO) δ 11.76 (s, 1H), 8.71 (d, *J* = 3.6 Hz, 1H), 8.02 (td, *J* = 7.7, 1.8 Hz, 1H), 7.72 (dd, *J* = 5.4, 3.2 Hz, 1H), 7.58 (dd, *J* = 6.9, 5.1 Hz, 1H), 7.48 – 7.40 (m, 2H), 7.38 (d, *J* = 8.6 Hz, 1H), 7.30 (dd, *J* = 5.8, 2.8 Hz, 1H), 7.23 – 7.13 (m, 3H), 7.09 (dd, *J* = 8.6, 1.9 Hz, 1H), 5.66 (d, *J* = 1.1 Hz, 1H).

^{13}C NMR (101 MHz, DMSO) δ 151.42, 150.05, 139.61, 139.14, 135.41, 132.53, 131.71, 129.62, 128.21, 124.39, 124.09, 123.65, 123.00, 122.28, 121.68, 121.12, 119.66, 113.06, 111.32, 104.59, 101.01.

HRMS m/z (ESI) Calcd for $C_{21}H_{14}ClN_3Na$ [M+Na$^+$] 366.0768, found: 366.0772.

5,5'-dichloro-1-(pyridin-2-yl)-1*H*,1'*H*-2,2'-biindole (3ee)



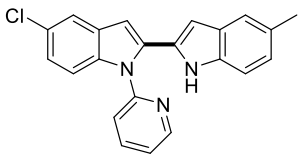
Compound **3ee** was obtained as purple solid in 78% yield according to general procedure **A**.

^{1}H NMR (400 MHz, DMSO) δ 11.83 (br, 1H), 8.71 (s, 1H), 8.03 (s, 1H), 7.81 (s, 1H), 7.59 (s, 1H), 7.42 (d, *J* = 20.5 Hz, 2H), 7.39 (d, *J* = 8.3 Hz, 1H), 7.29 (d, *J* = 8.3 Hz, 1H), 7.26 – 7.07 (m, 3H), 5.68 (s, 1H).

^{13}C NMR (101 MHz, DMSO) δ 150.99, 150.13, 139.77, 137.56, 135.50, 134.01, 131.09, 129.51, 129.40, 126.18, 124.50, 124.39, 123.51, 122.98, 122.55, 120.27, 119.81, 113.17, 112.92, 103.97, 101.47.

HRMS m/z (ESI) Calcd for $C_{21}H_{13}N_3Cl_2Na$ [M+Na^+] 400.0378, found: 400.0384.

5-chloro-5'-methyl-1-(pyridin-2-yl)-1*H*,1'*H*-2,2'-biindole (3ec)



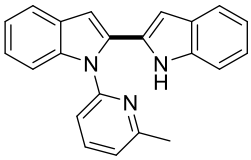
Compound **3ec** was obtained as purple solid in 66% yield according to general procedure **A**.

^{1}H NMR (400 MHz, DMSO) δ 11.47 (s, 1H), 8.72 (d, *J* = 3.7 Hz, 1H), 8.02 (td, *J* = 7.8, 1.7 Hz, 1H), 7.78 (d, *J* = 1.6 Hz, 1H), 7.60 (dd, *J* = 7.0, 5.0 Hz, 1H), 7.41 (d, *J* = 7.9 Hz, 1H), 7.27 (d, *J* = 8.3 Hz, 2H), 7.20 – 7.13 (m, 2H), 7.10 (s, 1H), 6.93 (d, *J* = 8.1 Hz, 1H), 5.55 (s, 1H), 2.31 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ 151.21, 150.08, 139.68, 137.49, 135.44, 134.79, 129.54, 129.36, 128.63, 128.45, 126.04, 124.34, 124.30, 123.13, 123.11, 120.21, 120.04, 112.79, 111.38, 103.12, 101.43, 21.53.

HRMS m/z (ESI) Calcd for $C_{22}H_{16}N_3ClNa$ [M+Na^+]380.0925, found: 380.0930.

1-(6-methylpyridin-2-yl)-1*H*,1'*H*-2,2'-biindole (3ga)



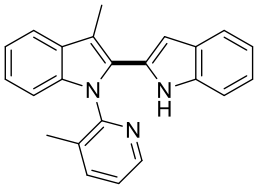
Compound **3ga** was obtained as purple solid in 52% yield according to general procedure **A**.

^{1}H NMR (400 MHz, DMSO) δ 11.52 (br, 1H), 7.89 (t, *J* = 7.7 Hz, 1H), 7.73 – 7.67 (m, 1H), 7.44 (d, *J* = 7.6 Hz, 1H), 7.40 – 7.35 (m, 2H), 7.30 – 7.25 (m, 1H), 7.17 (ddd, *J* = 10.2, 6.4, 5.1 Hz, 3H), 7.12 (s, 1H), 7.11 – 7.00 (m, 1H), 6.98 – 6.92 (m, 1H), 5.68 (d, *J* = 1.8 Hz, 1H), 2.57 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ 158.84, 150.90, 139.61, 139.15, 136.95, 133.06, 130.06, 128.48, 128.25, 123.31, 122.35, 121.47, 120.87, 120.57, 119.96, 119.80, 111.57, 111.41, 103.77, 101.33, 24.34.

HRMS m/z (ESI) Calcd for $C_{22}H_{17}N_3Na$ [M+Na$^+$] 346.1315, found: 346.1312.

3-methyl-1-(3-methylpyridin-2-yl)-1*H*,1'*H*-2,2'-biindole (3ha)



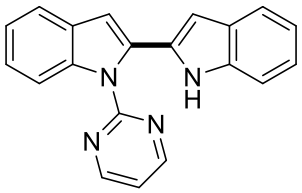
Compound **3ha** was obtained as purple solid in 62% yield according to general procedure **A**.

^{1}H NMR (400 MHz, DMSO) δ 11.18 (s, 1H), 8.41 (s, 1H), 7.68 (dd, *J* = 6.3, 1.9 Hz, 1H), 7.58 (dd, *J* = 7.1, 4.6 Hz, 2H), 7.49 (d, *J* = 7.8 Hz, 1H), 7.34 (d, *J* = 8.1 Hz, 1H), 7.24 – 7.18 (m, 2H), 7.08 (dd, *J* = 11.1, 4.0 Hz, 1H), 6.99 (t, *J* = 7.5 Hz, 1H), 6.92 (dd, *J* = 8.2, 2.5 Hz, 1H), 6.28 (s, 1H), 2.43 (s, 3H), 2.31 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ 149.68, 149.27, 139.20, 137.63, 137.11, 131.69, 129.29, 129.26, 129.25, 128.32, 123.67, 121.91, 121.12, 120.50, 120.42, 119.65, 119.36, 113.47, 111.91, 103.96, 100.00, 17.83, 9.91.

HRMS m/z (ESI) Calcd for $C_{23}H_{19}N_3Na$ [M+Na$^+$] 360.1471, found: 360.1478.

1-(pyrimidin-2-yl)-1*H*,1'*H*-2,2'-biindole (3ia)



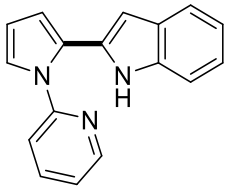
Compound **3ia** was obtained as purple solid in 71% yield according to general procedure **A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.27 (s, 1H), 8.78 (d, *J* = 4.6 Hz, 2H), 8.12 (d, *J* = 8.2 Hz, 1H), 7.67 (d, *J* = 7.6 Hz, 1H), 7.61 (d, *J* = 7.8 Hz, 1H), 7.35 (dd, *J* = 19.8, 8.1 Hz, 2H), 7.29 (t, *J* = 7.3 Hz, 1H), 7.21 (dd, *J* = 10.0, 5.7 Hz, 2H), 7.13 (t, *J* = 7.4 Hz, 1H), 6.98 (s, 1H), 6.56 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.37, 157.97, 138.13, 136.40, 132.53, 130.58, 129.09, 128.43, 123.96, 122.40, 122.33, 120.73, 120.60, 120.01, 118.10, 113.30, 110.95, 109.31, 104.06.

HRMS m/z (ESI) Calcd for $C_{20}H_{14}N_4Na$ [M+Na+] 333.1110, found: 333.1109.

2-(1-(pyridin-2-yl)-1*H*-pyrrol-2-yl)-1*H*-indole (3ja)



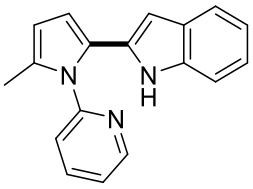
Compound **3ja** was obtained as purple solid in 46% yield according to general procedure **A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.04 (br, 1H), 8.47 (s, 1H), 7.57 (t, *J* = 6.9 Hz, 1H), 7.47 (d, *J* = 7.8 Hz, 1H), 7.24 (dd, *J* = 8.1, 0.7 Hz, 1H), 7.18 – 7.10 (m, 2H), 7.09 – 6.97 (m, 3H), 6.53 (d, *J* = 3.3 Hz, 1H), 6.32 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.40, 138.46, 136.05, 130.51, 128.58, 125.91, 123.85, 121.98, 121.85, 120.31, 119.89, 119.00, 113.32, 110.82, 110.51, 102.05.

HRMS m/z (ESI) Calcd for $C_{17}H_{13}N_3Na[M+Na^+]$ 282.1002, found: 282.1001.

2-(5-methyl-1-(pyridin-2-yl)-1*H*-pyrrol-2-yl)-1*H*-indole (3ka)



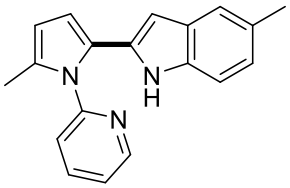
Compound **3ka** was obtained as purple solid in 76% yield according to general procedure **A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 – 8.65 (m, 1H), 8.34 (s, 1H), 7.74 (td, *J* = 7.7, 1.9 Hz, 1H), 7.42 (d, *J* = 7.8 Hz, 1H), 7.38 – 7.33 (m, 1H), 7.23 (d, *J* = 8.1 Hz, 1H), 7.18 (d, *J* = 7.9 Hz, 1H), 7.08 (dd, *J* = 11.1, 4.0 Hz, 1H), 7.02 (t, *J* = 7.4 Hz, 1H), 6.46 (d, *J* = 3.5 Hz, 1H), 6.13 (d, *J* = 3.4 Hz, 1H), 5.86 (d, *J* = 1.3 Hz, 1H), 2.20 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 152.21, 149.20, 138.28, 135.75, 132.26, 130.96, 128.72, 126.29, 123.27, 121.49, 120.02, 119.71, 110.43, 109.30, 108.48, 100.08, 13.02.

HRMS m/z (ESI) Calcd for $C_{18}H_{15}N_3Na$ [M+Na^+] 296.1158, found: 296.1154.

5-methyl-2-(5-methyl-1-(pyridin-2-yl)-1*H*-pyrrol-2-yl)-1*H*-indole (3kc)



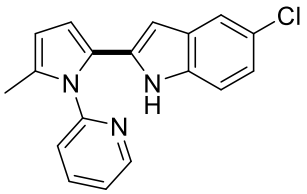
Compound **3kc** was obtained as purple solid in 72% yield according to general procedure **A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 – 8.64 (m, 1H), 8.19 (br, 1H), 7.73 (td, *J* = 7.7, 1.9 Hz, 1H), 7.35 (ddd, *J* = 7.5, 4.9, 1.0 Hz, 1H), 7.20 (s, 1H), 7.18 – 7.15 (m, 1H), 7.12 (d, *J* = 8.2 Hz, 1H), 6.92 (dd, *J* = 8.2, 1.1 Hz, 1H), 6.44 (d, *J* = 3.5 Hz, 1H), 6.12 (dd, *J* = 3.5, 0.8 Hz, 1H), 5.83 – 5.70 (m, 1H), 2.39 (s, 3H), 2.19 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 152.25, 149.17, 138.23, 134.09, 132.16, 131.03, 129.00, 128.89, 126.44, 123.26, 123.20, 123.07, 119.71, 110.09, 109.11, 108.42, 99.71, 21.33, 13.01.

HRMS m/z (ESI) Calcd for $C_{19}H_{17}N_3Na$ [M+Na^+] 310.1315, found: 310.1319.

5-chloro-2-(5-methyl-1-(pyridin-2-yl)-1*H*-pyrrol-2-yl)-1*H*-indole (3kf)



Compound **3kf** was obtained as purple solid in 62% yield according to general procedure **A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (d, *J* = 3.8 Hz, 1H), 8.43 (s, 1H), 7.77 (dd, *J* = 10.8, 4.6 Hz, 1H), 7.38 (dd, *J* = 6.8, 5.5 Hz, 1H), 7.35 (s, 1H), 7.18 (d, *J* = 7.9 Hz, 1H), 7.10 (d, *J* = 8.5 Hz, 1H), 7.01 (dd, *J* = 8.5, 1.6 Hz, 1H), 6.45 (d, *J* = 3.3 Hz, 1H), 6.11 (d, *J* = 2.5 Hz, 1H), 5.74 (s, 1H), 2.18 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 152.08, 149.27, 138.40, 134.08, 132.61, 132.44, 129.84, 125.79, 125.33, 123.44, 123.25, 121.63, 119.31, 111.33, 109.68, 108.65, 99.44, 13.00.

HRMS m/z (ESI) Calcd for $C_{18}H_{14}ClN_3Na$ [M+Na^+] 330.0768, found: 330.0771.

3. X-ray of Compound 3kf

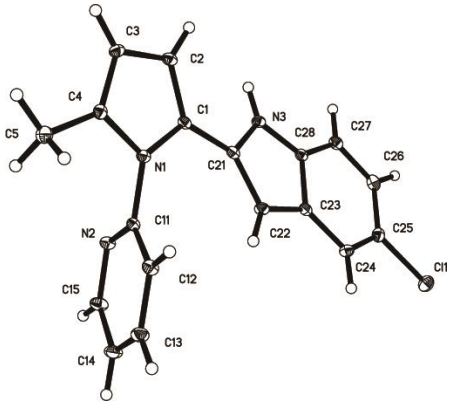


Figure S1. Ortep drawing of compound **3kf.**

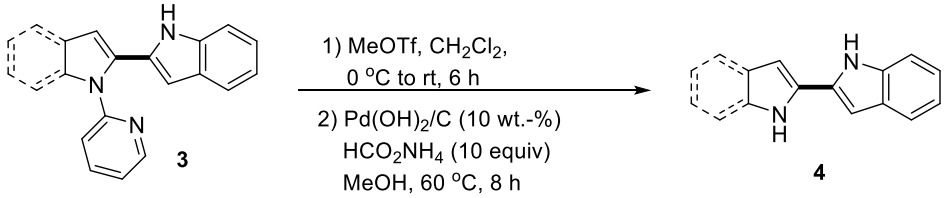
Table S1: Crystallographic Details for **3kf**

Complex.	**3kf**
empirical formula	$C_{18}\ H_{14}\ Cl_1\ N_3$
formula weight	307.77
temperature, K	103(2)
radiation (Mo Kα), Å	0.71073
crystal system	Triclinic
space group	P-1
a, Å	9.2962(7)
b, Å	9.3721(8)
c, Å	9.4578(7)
α, °	90.096(6)
β, °	109.097(7)
γ, °	101.608(7)
V, Å^3	760.70(10)
Z	2
F(000)	320
crystal size, mm	0.25x 0.21 x 0.15
θ range, °	3.26 to 25.99
indep reflns	13551 / 2613 [R(int) = 0.1266]
data-restraints-params	2613/ 0 / 199

GOF on F^2	0.636
final R ($I > 2\sigma(I)$)	R_1 = 0.0590, wR_2 = 0.1623
R indices (all data)	R_1 = 0.1454, wR_2 = 0.2243
peak and hole, e.Å^{-3}	0.184 and -0.288

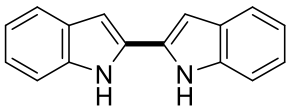
4. Removal of the Pyridine Directing Group

***General Procedure B*:**



Methyl trifluoromethanesulfonate (0.24 mmol) was added dropwise to a solution of **3** (0.20 mmol) in dry CH_2Cl_2 (5.0 mL) at 0 °C, and the resulting solution was stirred for 6 h at room temperature. Then the solvent was removed under vacuum, and $Pd(OH)_2$/C (8 mg, 10 wt.-%) and ammonium formate (126mg, 2.00 mmol, 10.0 equiv) were added. The mixture was diluted with MeOH (2.0 mL, 0.1 M) and stirred at 60 ℃ for 6 h. The solvents were removed, and the resulting residue was extracted with CH_2Cl_2 (2 × 10 mL). The combined organic layers were washed with brine, dried over Na_2SO_4, and concentrated in vacuo. The residue was purified by flash chromatography, affording the desired product **4**.

1*H*,1'*H*-2,2'-biindole (4a)



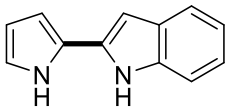
Compound **4a** was obtained as purple solid in 71% yield according to general procedure **B**.

^{1}H NMR (400 MHz, DMSO): δ 11.54 (br, 1H), 7.56 (d, *J* = 8.5 Hz, 1H), 7.40 (d, *J* = 8.5 Hz, 1H), 7.11 (t, *J* = 8.1 Hz, 1H), 7.02 (d, *J* = 7.6 Hz, 1H), 6.92 (d, *J* = 0.2 Hz, 1H);

^{13}C NMR (101 MHz, DMSO): δ 136.88, 131.37, 128.41, 121.66, 120.00, 119.38, 111.03, 98.38.

HRMS m/z (ESI) Calcd for $C_{16}H_{12}N_2Na$ [M+Na^+] 255.0893, found: 255.0891.

2-(1*H*-pyrrol-2-yl)-1*H*-indole (4b)



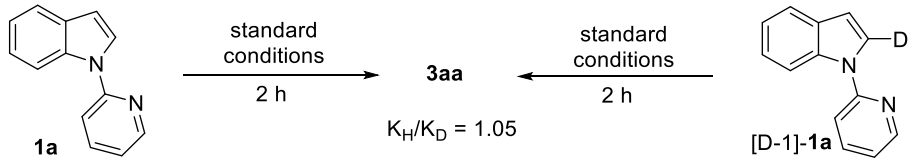
Compound **4b** was obtained as purple solid in 74% yield according to general procedure **B**.

^{1}H NMR (400 MHz, DMSO) δ 11.03 (br, 1H), 10.90 (br, 1H), 7.17 (s, 1H), 7.04 (s, 1H), 6.94 – 6.50 (m, 3H), 6.38 – 6.19 (m, 2H), 5.85 (s, 1H).

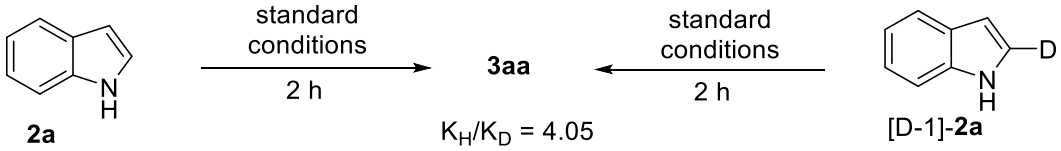
^{13}C NMR (101 MHz, DMSO) δ 136.49, 132.83, 129.04, 125.26, 120.76, 119.51, 119.40, 119.30, 110.89, 108.97, 105.88, 95.28.

HRMS m/z (ESI) Calcd for $C_{12}H_{10}N_2Na$ [M+Na^+] 205.0736, found: 205.07367.

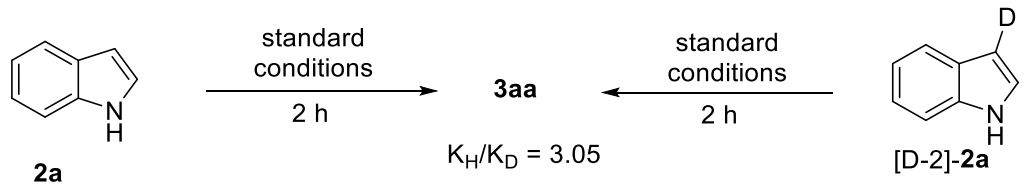
5. Mechanistic studies.



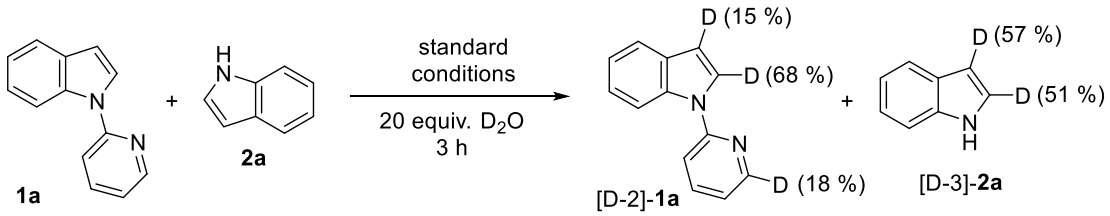
1a (0.2 mmol) or [D-1]-**1a** (0.2 mmol) was allowed to react with **2a** in two paralleled dried Schlenk tube under standard conditions for 2 h. After cooling to room temperature, the mixture was diluted with ethyl acetate, filtrated through ceilt. After concentration, the yield of the resulting product of **3aa** was collected to calculate the KIE.



2a (0.2 mmol) or [D-1]-**2a** (0.2 mmol) was allowed to react with **1a** in two paralleled dried Schlenk tube under standard conditions for 2 h. After cooling to room temperature, the mixture was diluted with ethyl acetate, filtrated through ceilt. After concentration, the yield of the resulting product of **3aa** was collected to calculate the KIE.

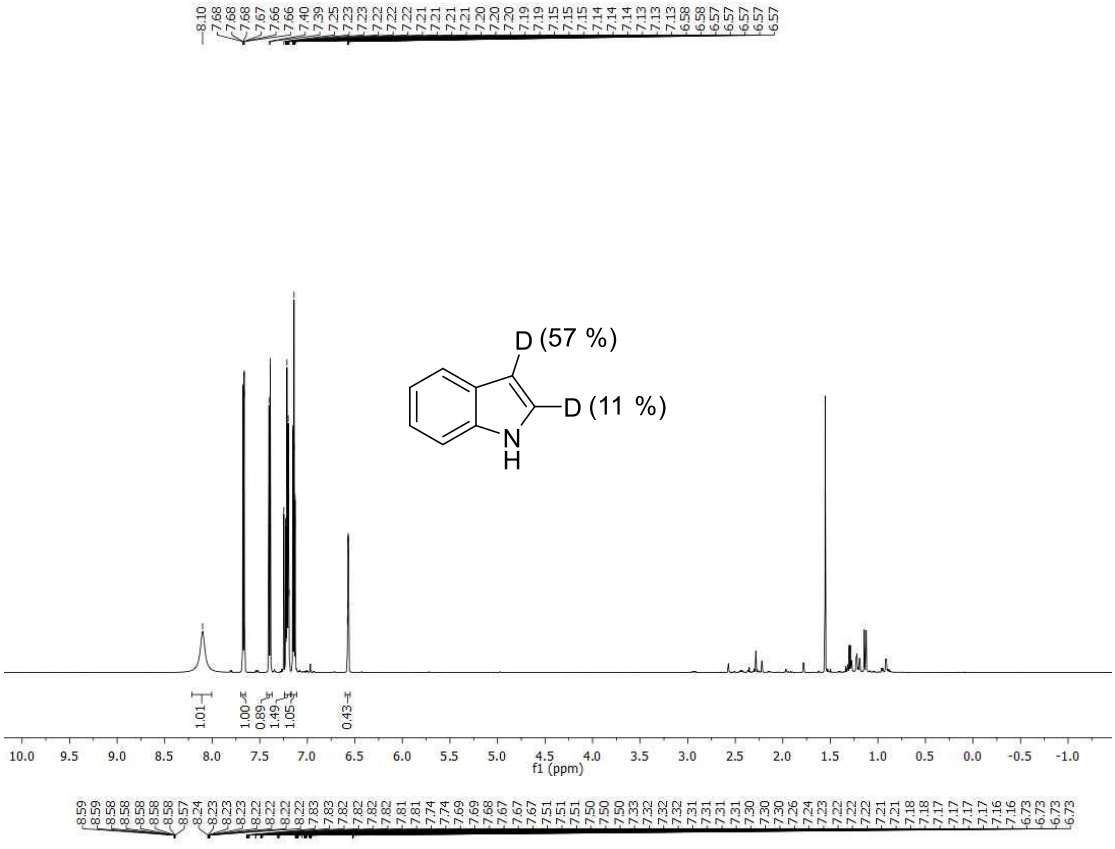


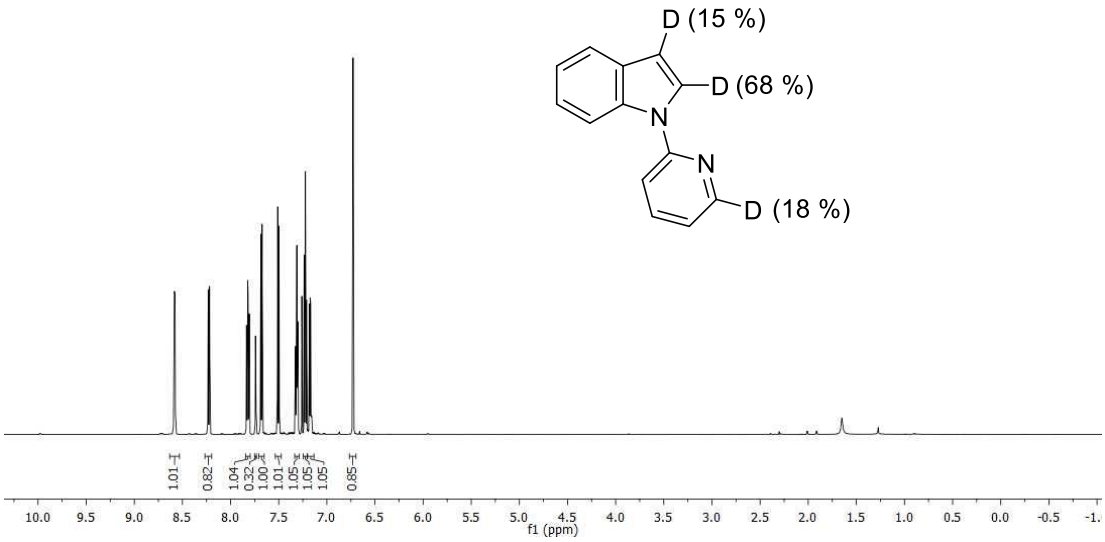
2a (0.2 mmol) or [D-2]-**2a** (0.2 mmol) was allowed to react with **1a** in two paralleled dried Schlenk tube under standard conditions for 2 h. After cooling to room temperature, the mixture was diluted with ethyl acetate, filtrated through ceilt. After concentration, the yield of the resulting product of **3aa** was collected to calculate the KIE.

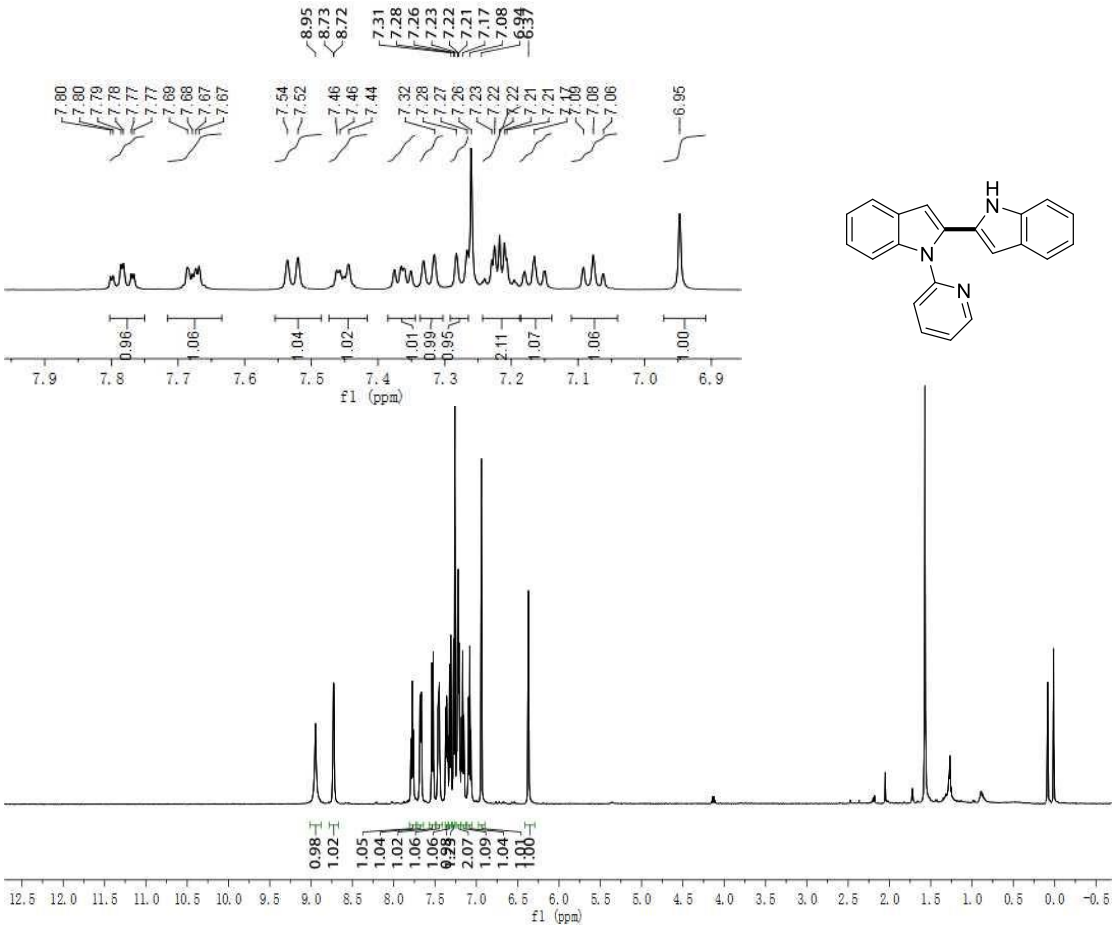


1a (0.2 mmol) was allowed to react with **2a** in one dried Schlenk tube in the presense

of 20 equiv D_2O under standard conditions for 2 h. After cooling to room temperature, the mixture was diluted with ethyl acetate, filtrated through ceilt. After purification, the NMR of [D-2]-**1a** and [D-3]-**2a** was collected.



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7.28
7.26
7.23
7.22
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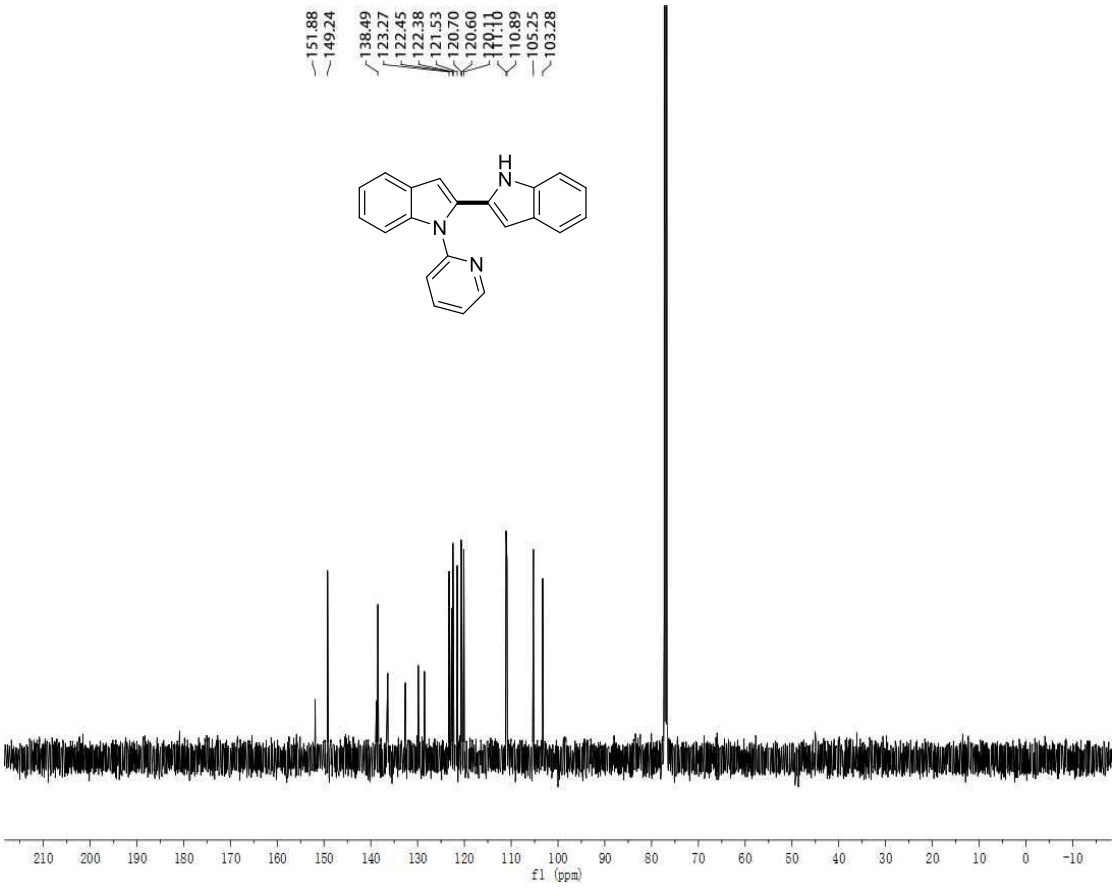
7.17
7.08
6.94
6.93
7.80
7.80
7.79
7.78
7.77
7.77
7.69
7.68
7.67
7.67
7.54
7.52
7.46
7.46
7.44
7.32
7.28
7.27
7.26
7.23
7.22
7.22
7.21
7.21
7.17
7.08
7.08
7.06
6.95
0.96
1.06
1.04
1.02
1.01
0.99
0.95
2.11
1.07
1.06
1.00
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
f1 (ppm)
H
N
N
N
0.98
1.02
1.05
1.04
1.02
1.06
2.07
1.09
1.04
1.01
1.00
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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120.11
111.10
110.89
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103.28
H
N
N
N
210
200
190
180
170
160
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140
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120
110
100
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80
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60
50
40
30
20
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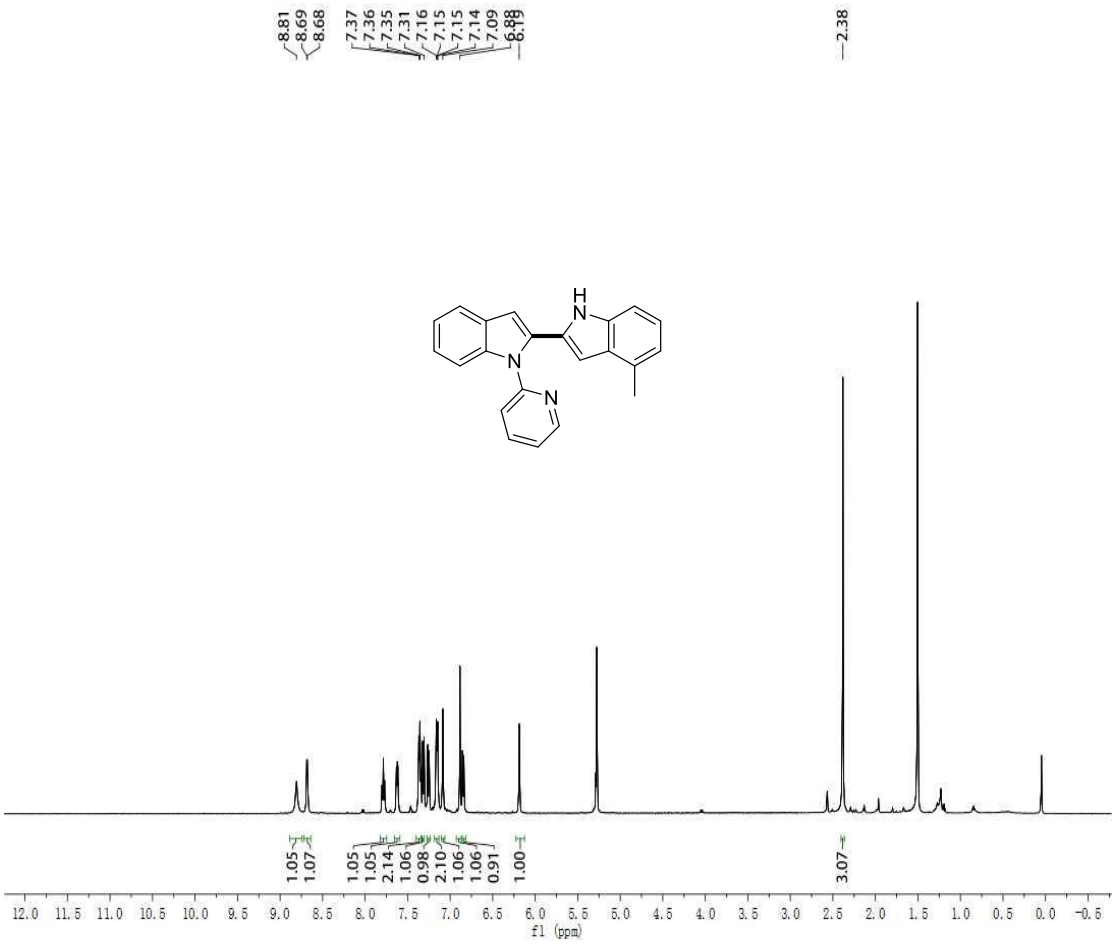
-10
f1 (ppm)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8.69
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7.31
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7.15
7.14
7.09
6.88
6.87
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H
N
N
1.05
1.07
1.05
1.05
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2.10
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1.06
0.91
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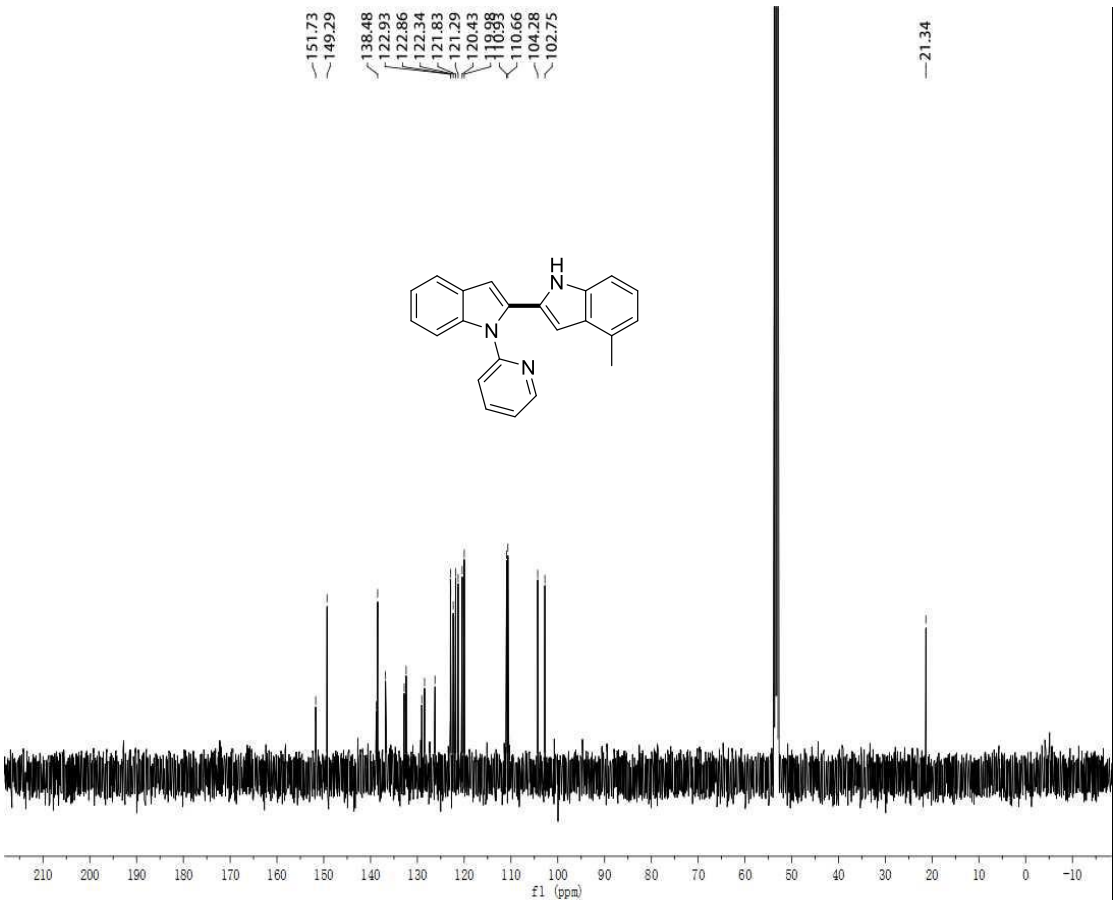
f1 (ppm)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149.29
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21.34
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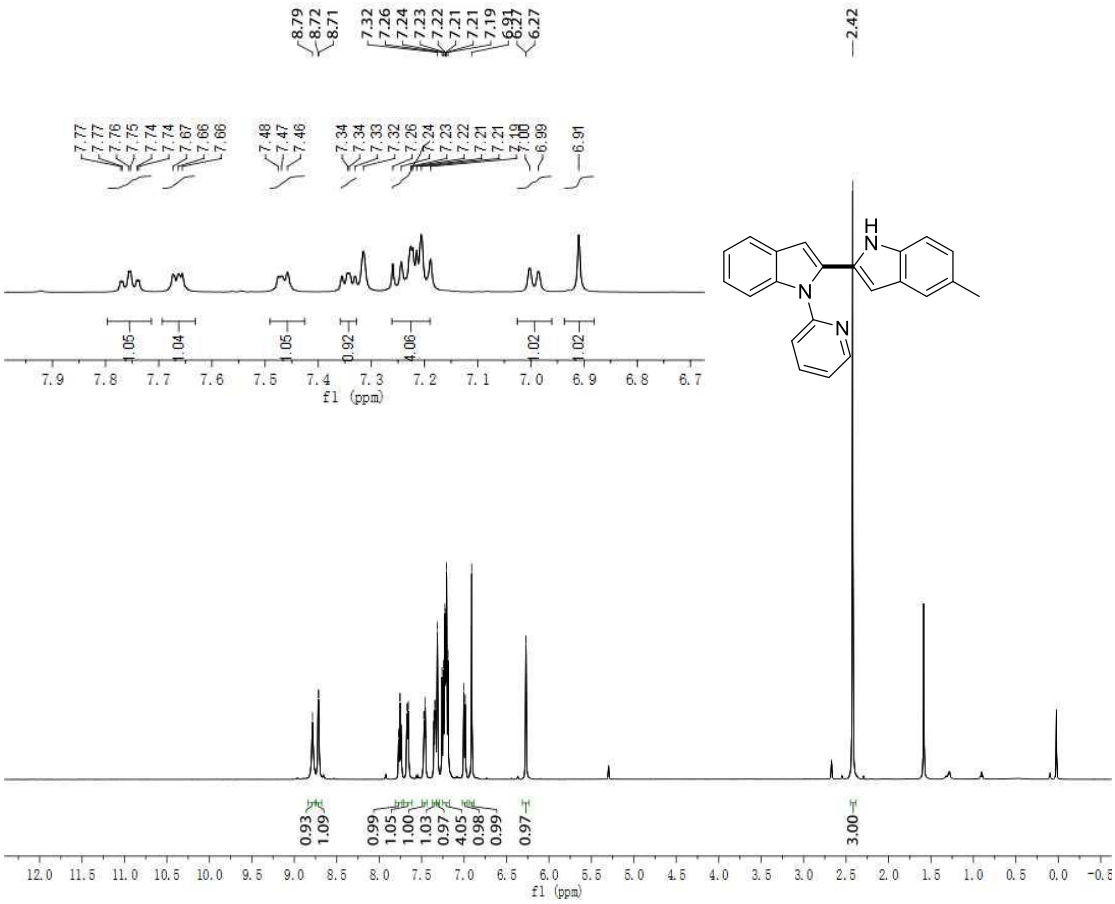
N
N
f1 (ppm)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7.24
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7.22
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7.21
7.19
6.91
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7.76
7.75
7.74
7.74
7.67
7.66
7.66
7.48
7.47
7.46
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7.34
7.33
7.32
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7.24
7.23
7.22
7.21
7.21
7.19
7.00
6.99
6.91
1.05
1.04
1.05
0.92
4.06
1.02
1.02
f1 (ppm)
H
N
N
N
0.93
1.09
0.99
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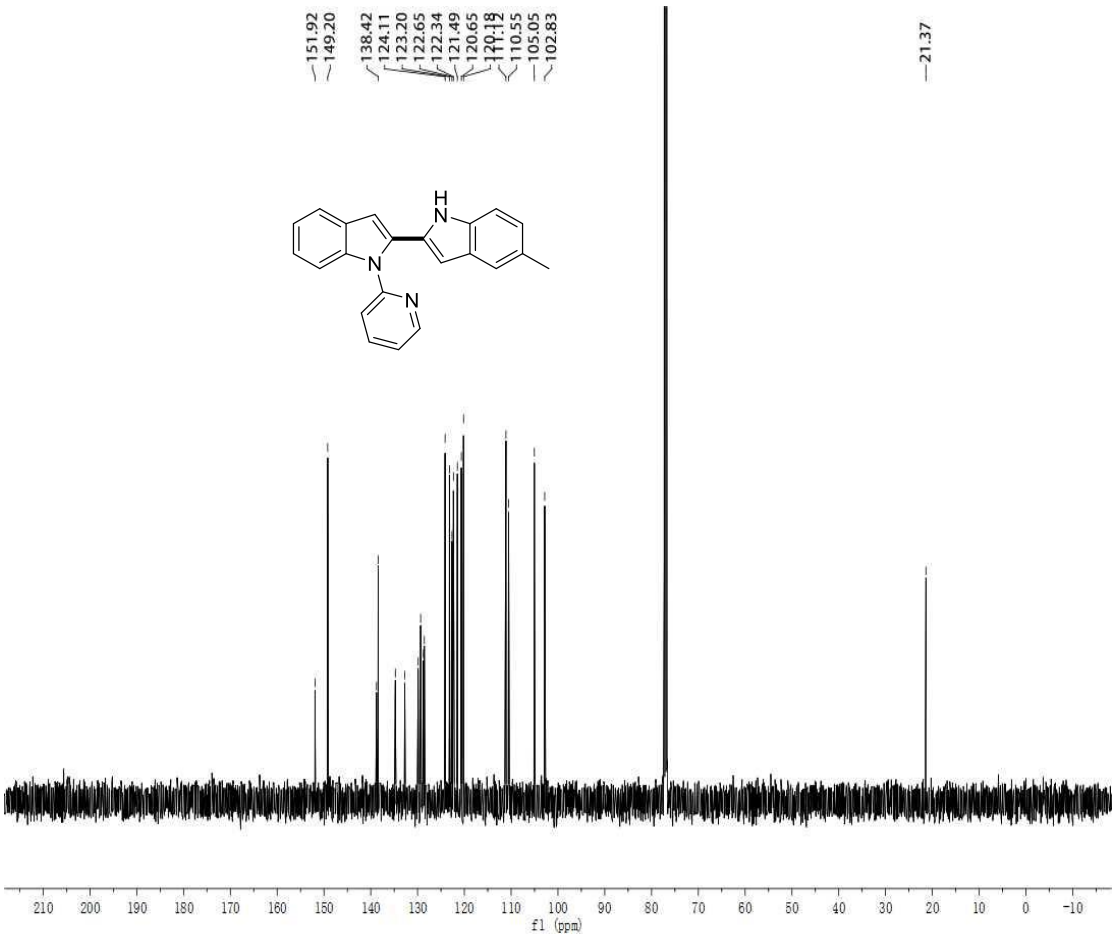
1.00
1.03
0.97
4.05
0.98
0.99
0.97
3.00
f1 (ppm)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122.34
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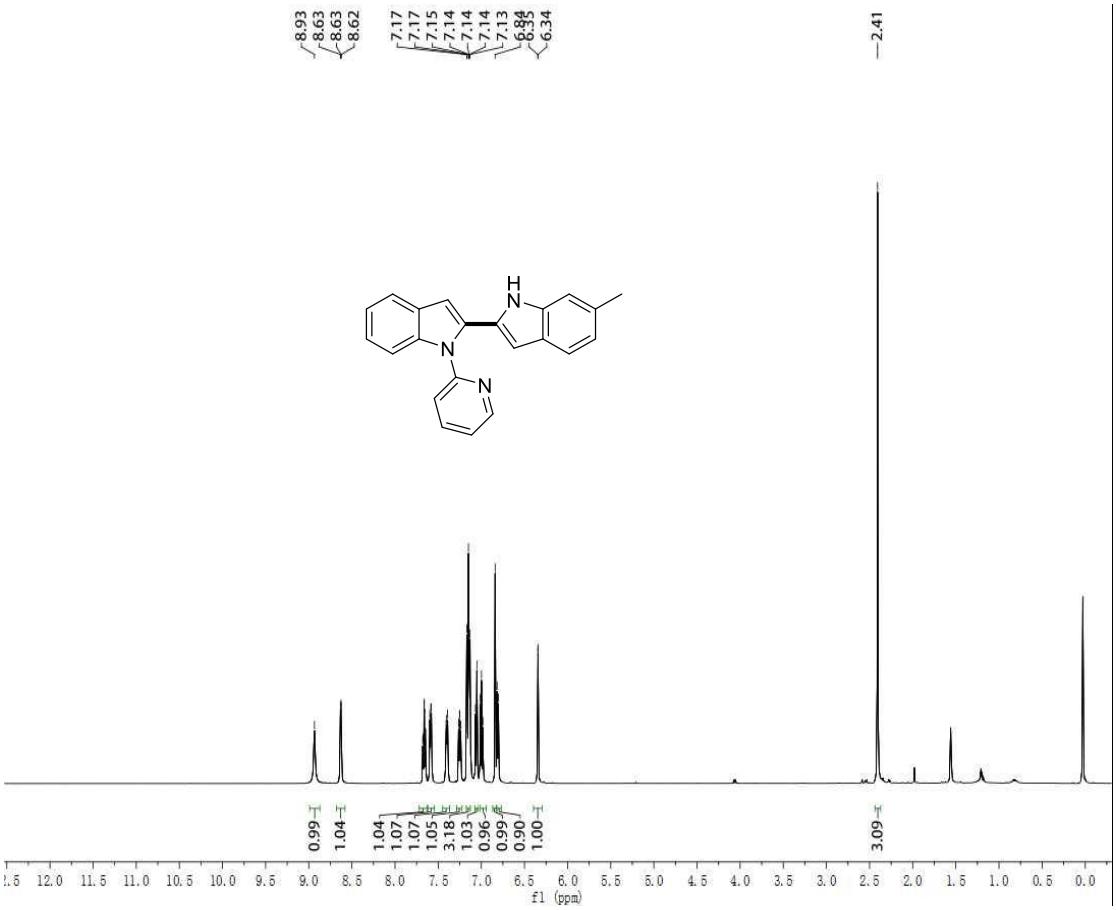
111.12
110.55
105.05
102.83
21.37
H
N
N
N
f1 (ppm)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7.17
7.15
7.14
7.14
7.14
7.13
6.34
2.41
H
N
N
N
0.99
1.04
1.04
1.07
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1.05
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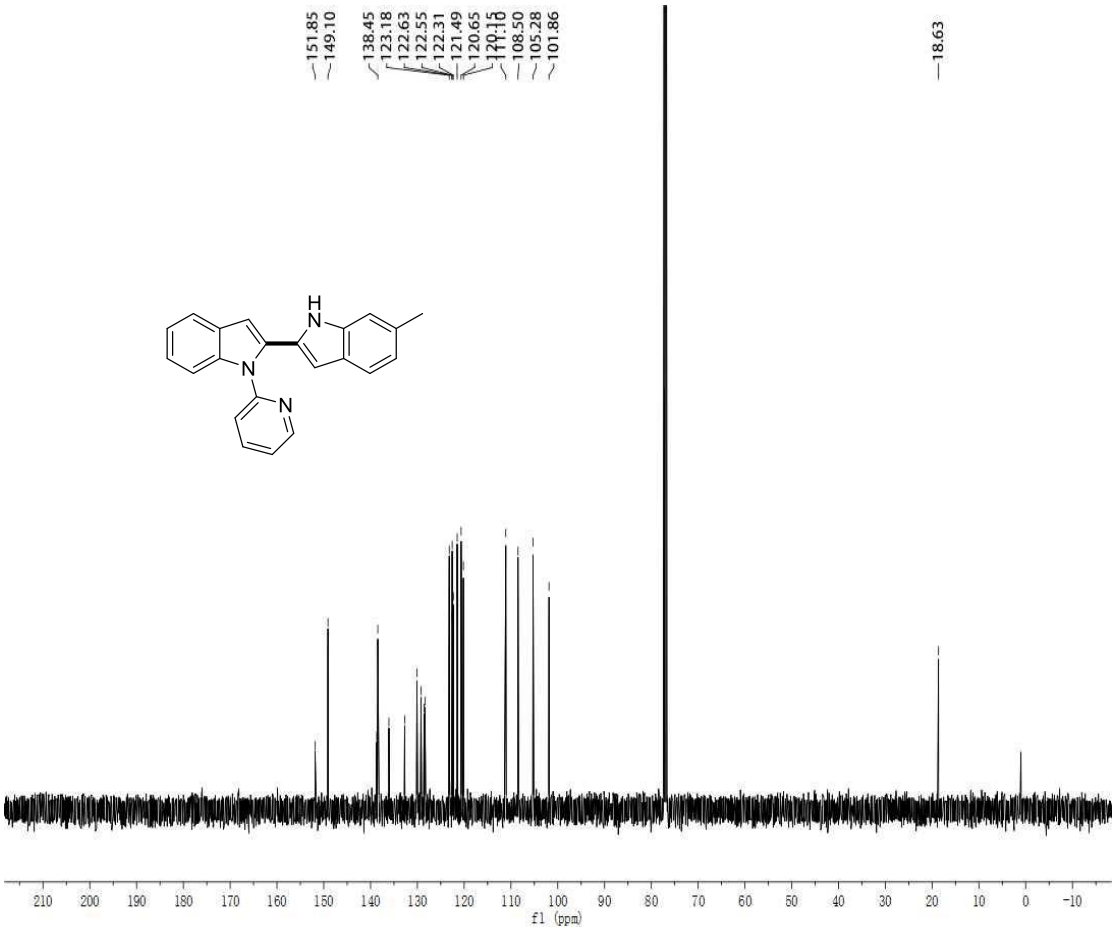
3.09
f1 (ppm)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108.50
105.28
101.86
18.63
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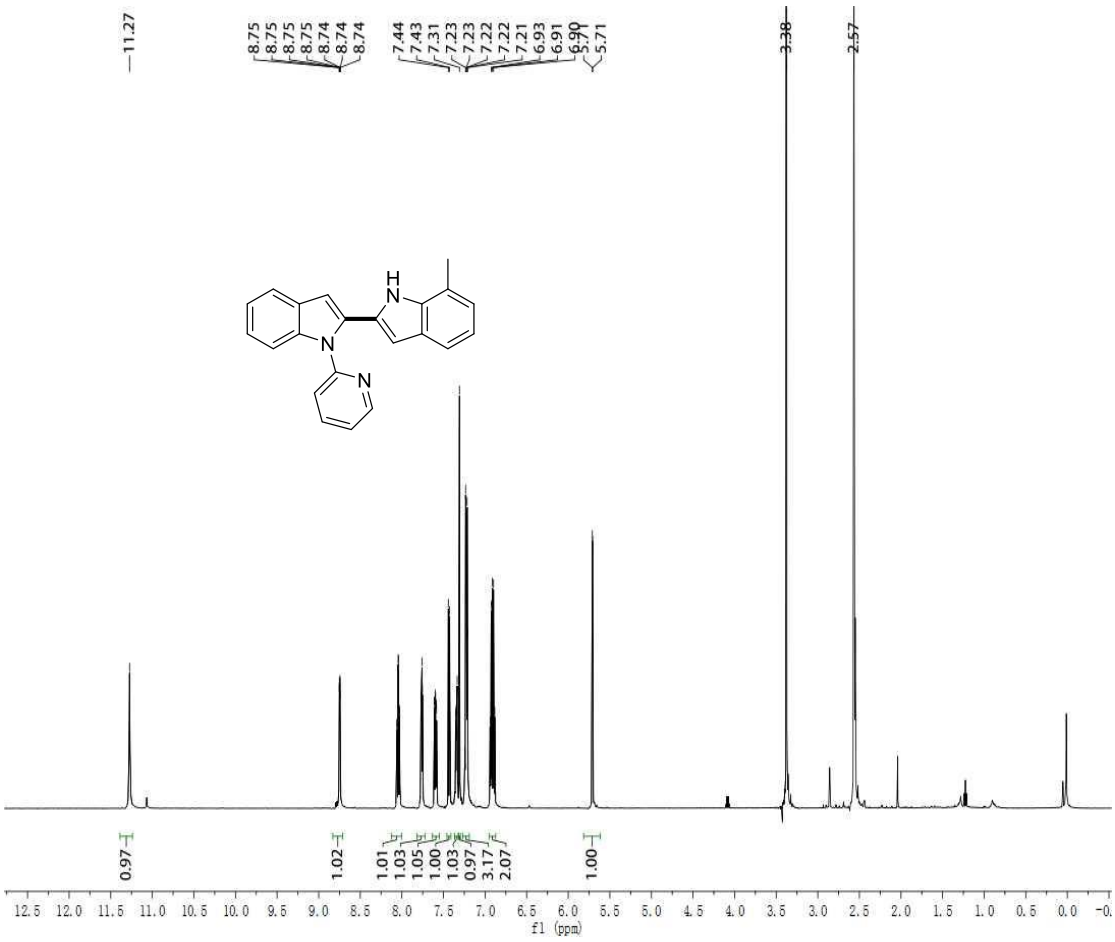
N
N
f1 (ppm)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8.74
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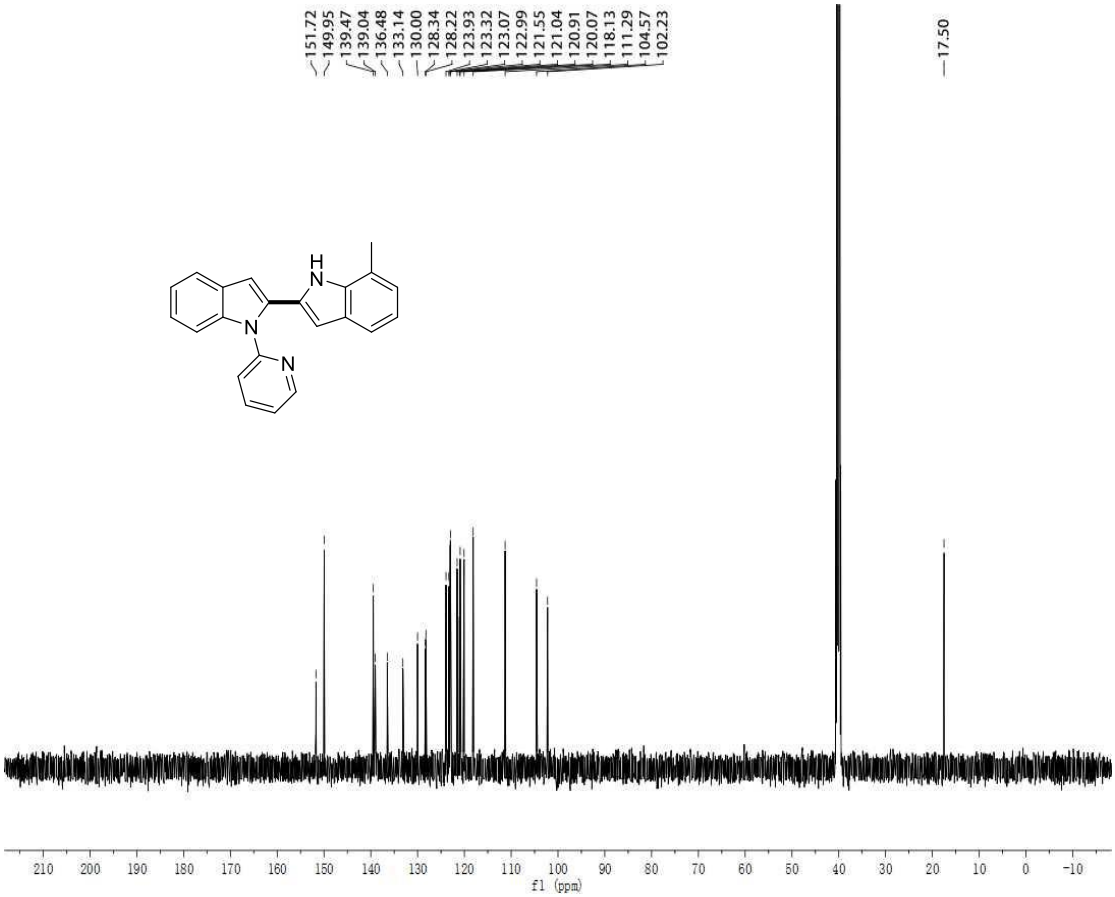
7.43
7.31
7.23
7.23
7.22
7.22
7.21
6.93
6.91
6.90
5.71
3.38
2.57
0.97
1.02
1.01
1.03
1.05
1.00
1.03
0.97
3.17
2.07
1.00
H
N
N
f1 (ppm)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111.29
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102.23
17.50
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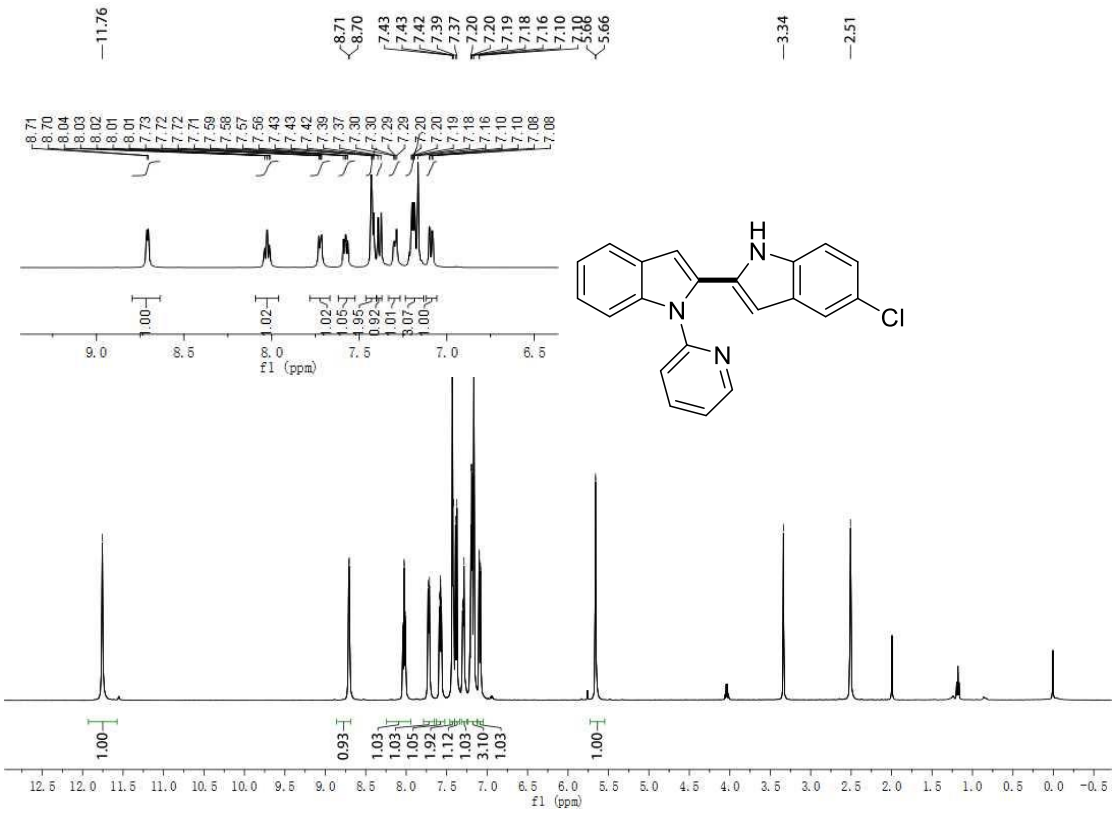
N
N
f1 (ppm)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7.39
7.37
7.20
7.19
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7.16
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5.66
3.34
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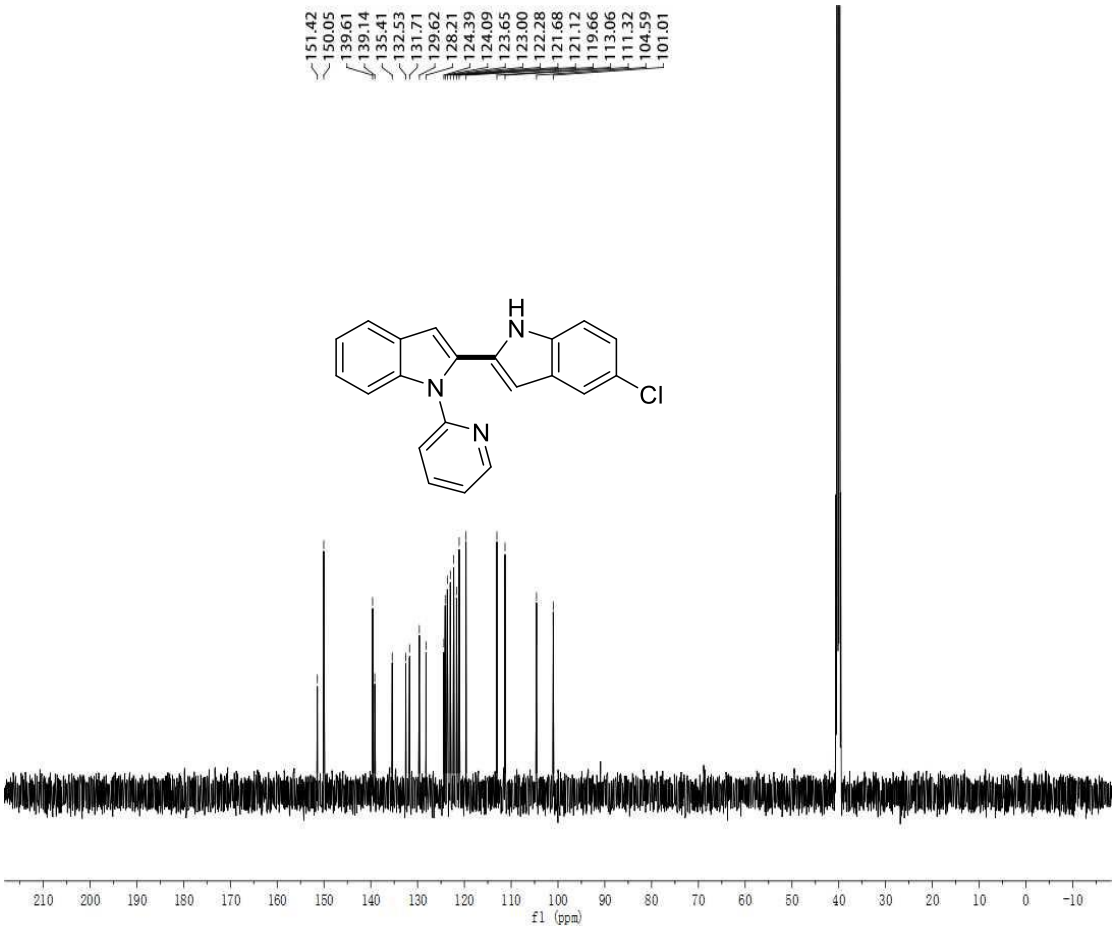
N
N
Cl
f1 (ppm)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131.71
129.62
128.21
124.39
124.09
123.65
123.00
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111.32
104.59
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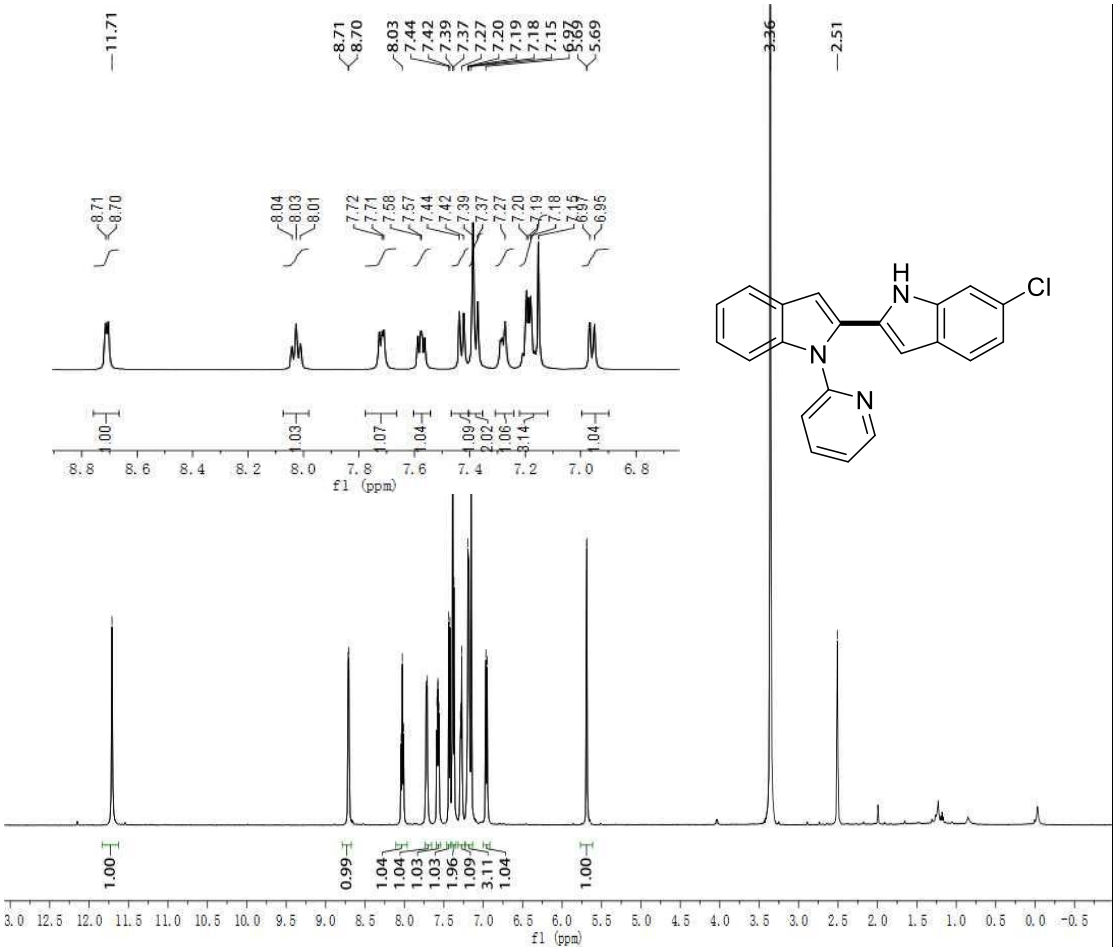
N
N
Cl
f1 (ppm)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6.95
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2.51
f1 (ppm)
Cl
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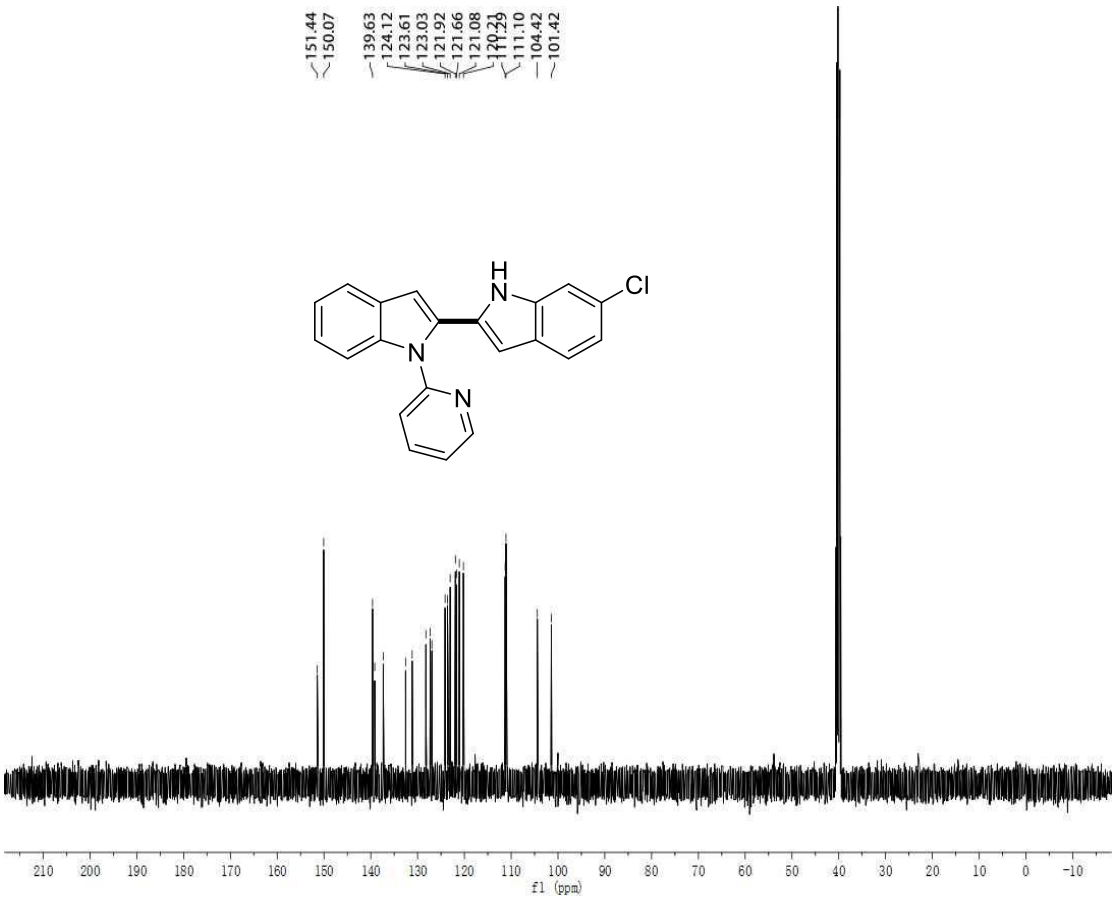
N
N
N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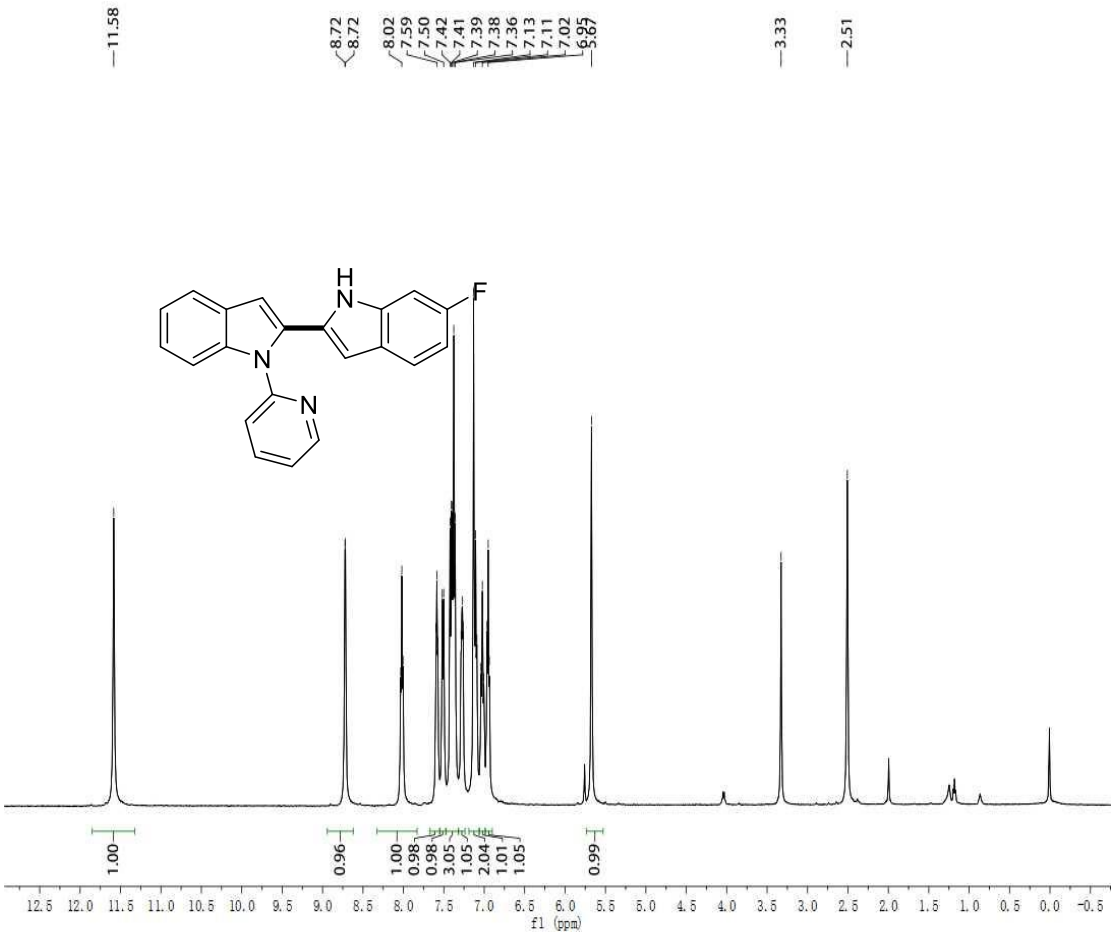
121.66
121.08
111.10
104.42
101.42
f1 (ppm)
Cl
H
N
N
N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7.02
6.95
5.87
3.33
2.51
H
N
F
N
N
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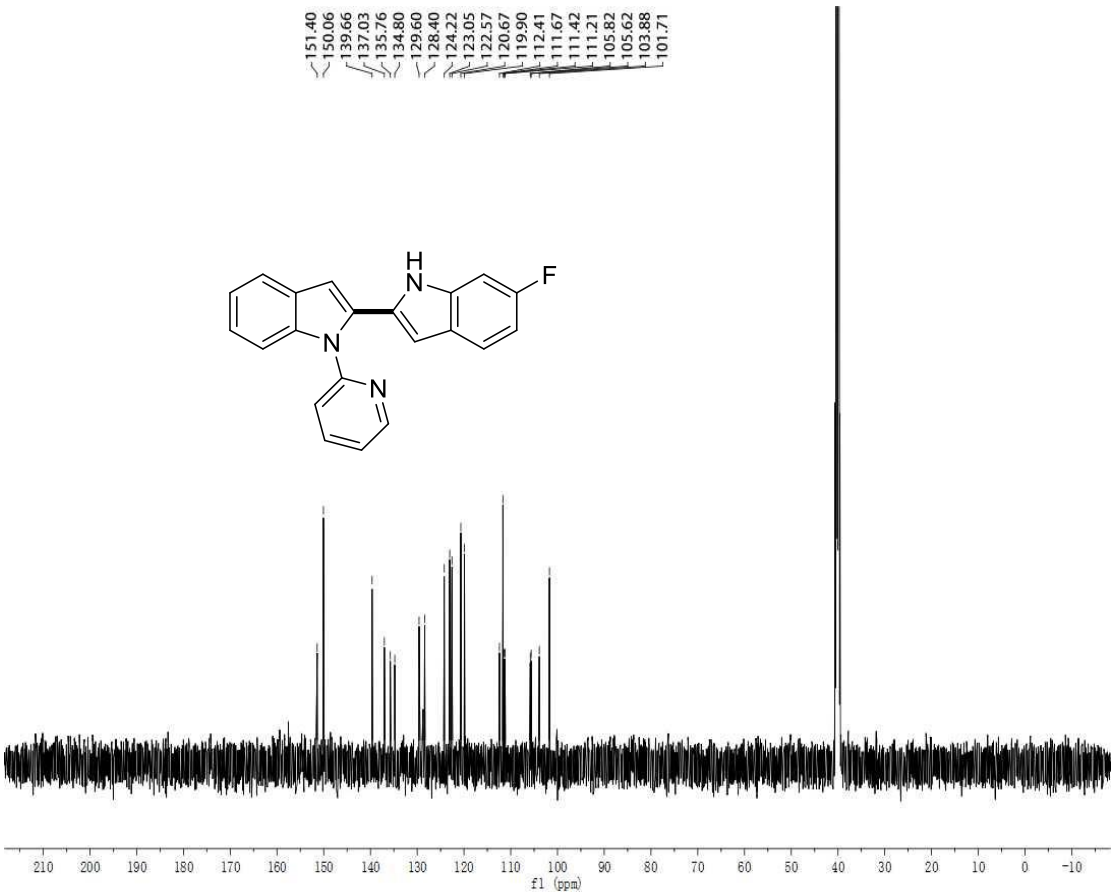
0.98
0.98
3.05
1.05
2.04
1.01
1.05
0.99
f1 (ppm)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119.90
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105.62
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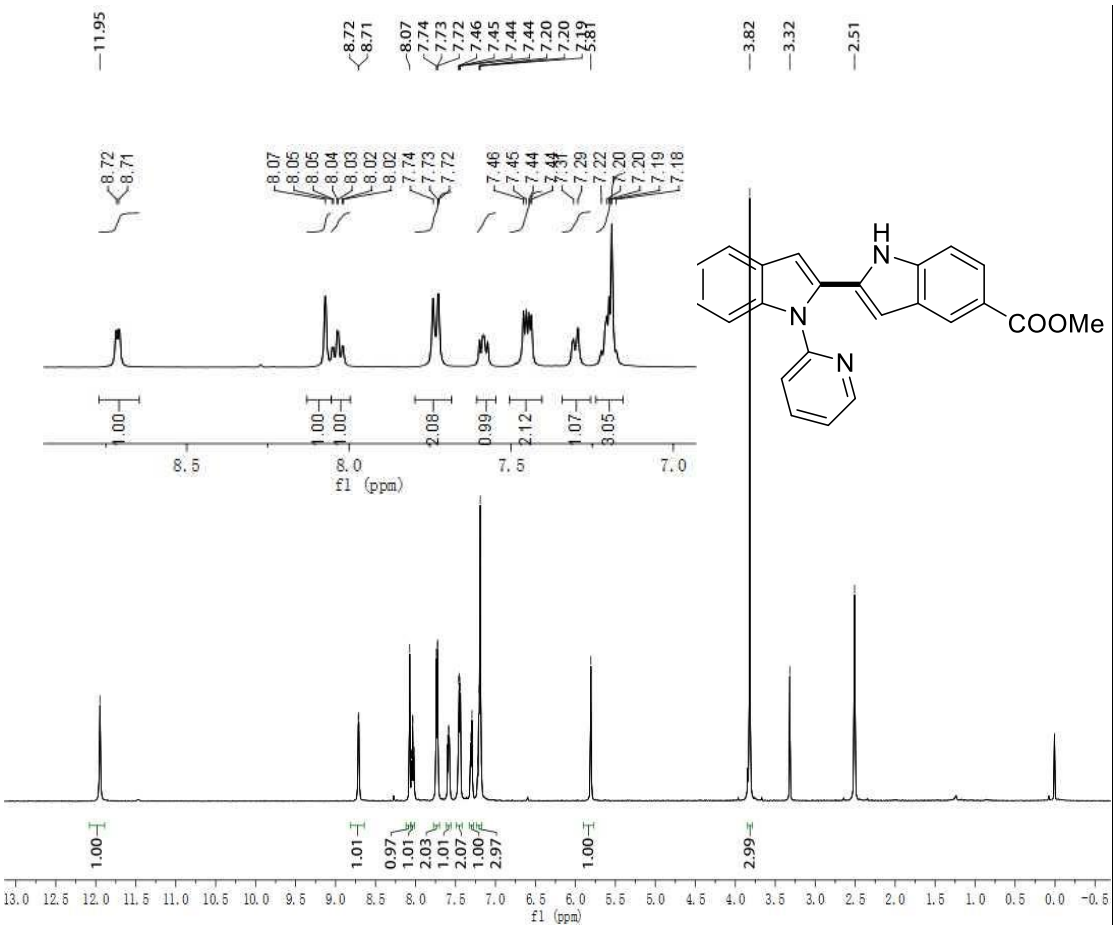
N
f1 (ppm)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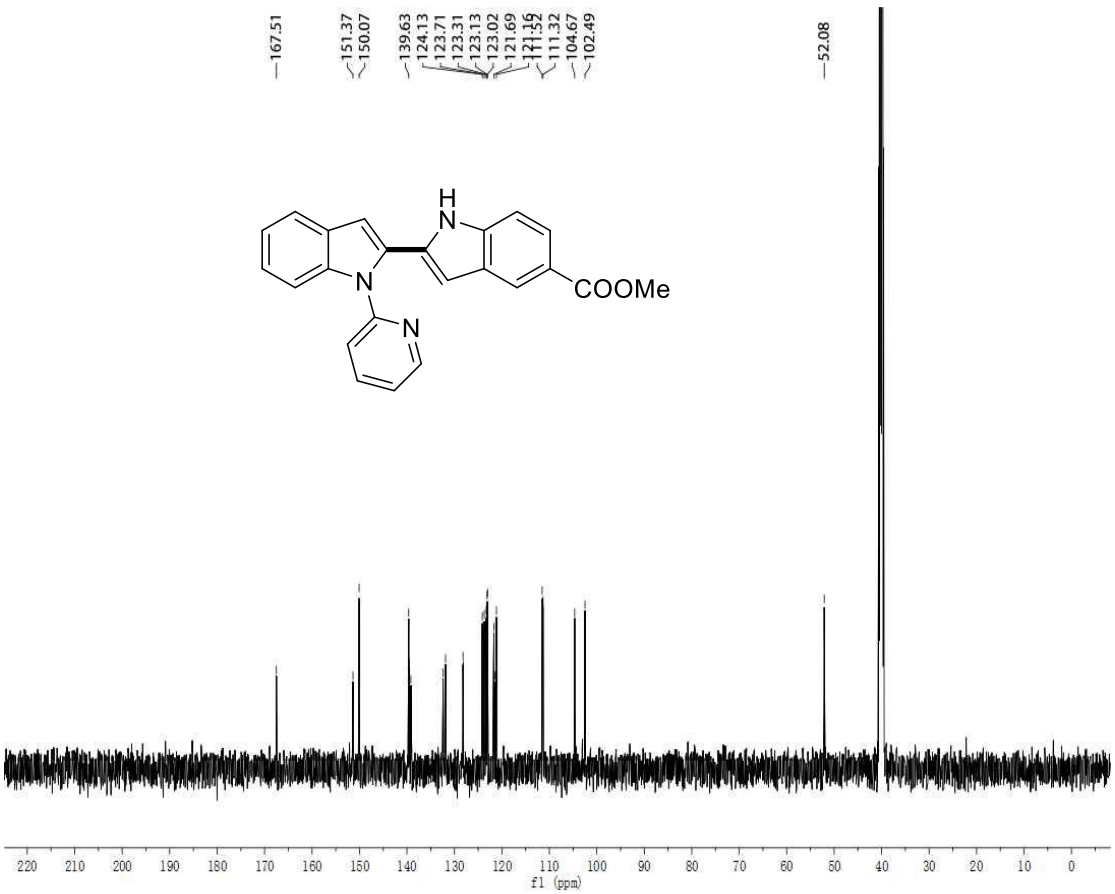
7.19
5.81
3.82
3.32
2.51
COOMe
f1 (ppm)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150.07
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123.13
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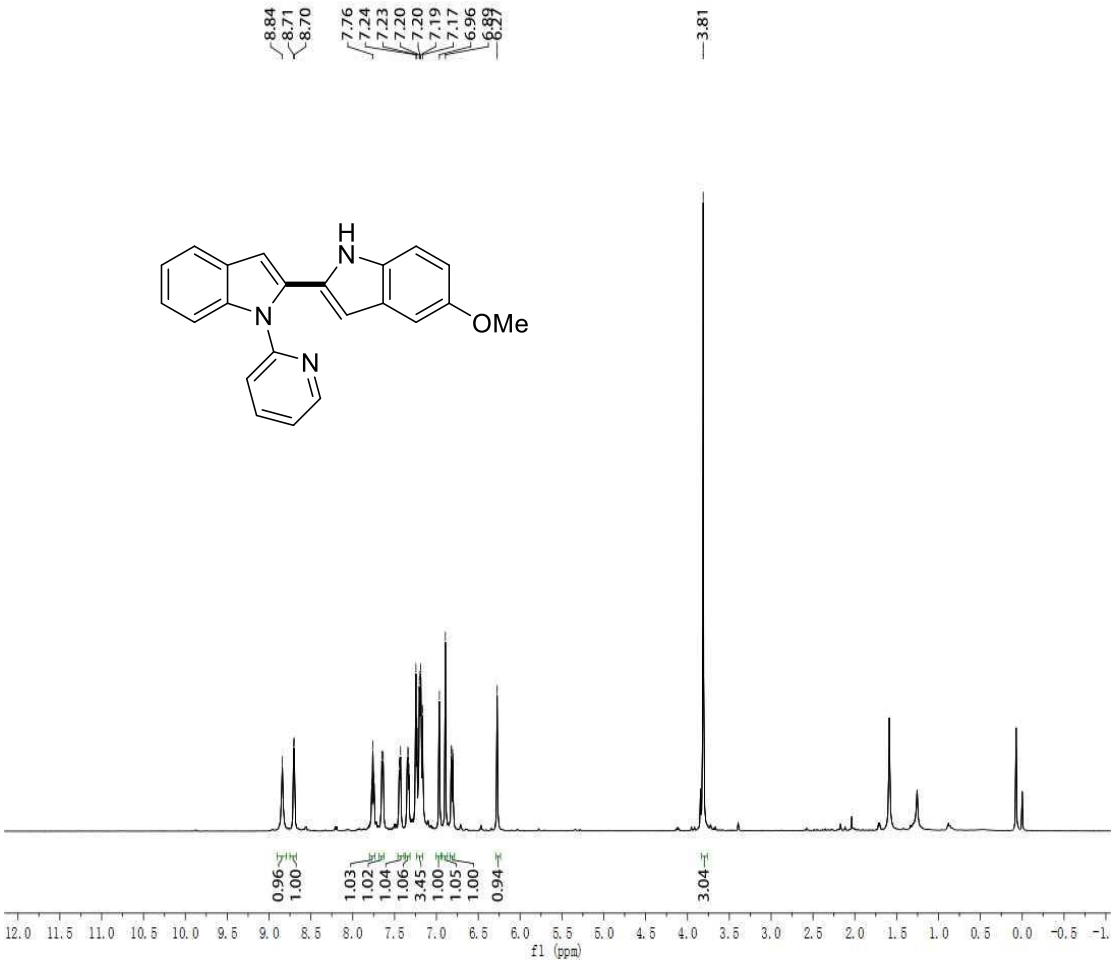
111.32
104.67
102.49
52.08
COOMe
f1 (ppm)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7.23
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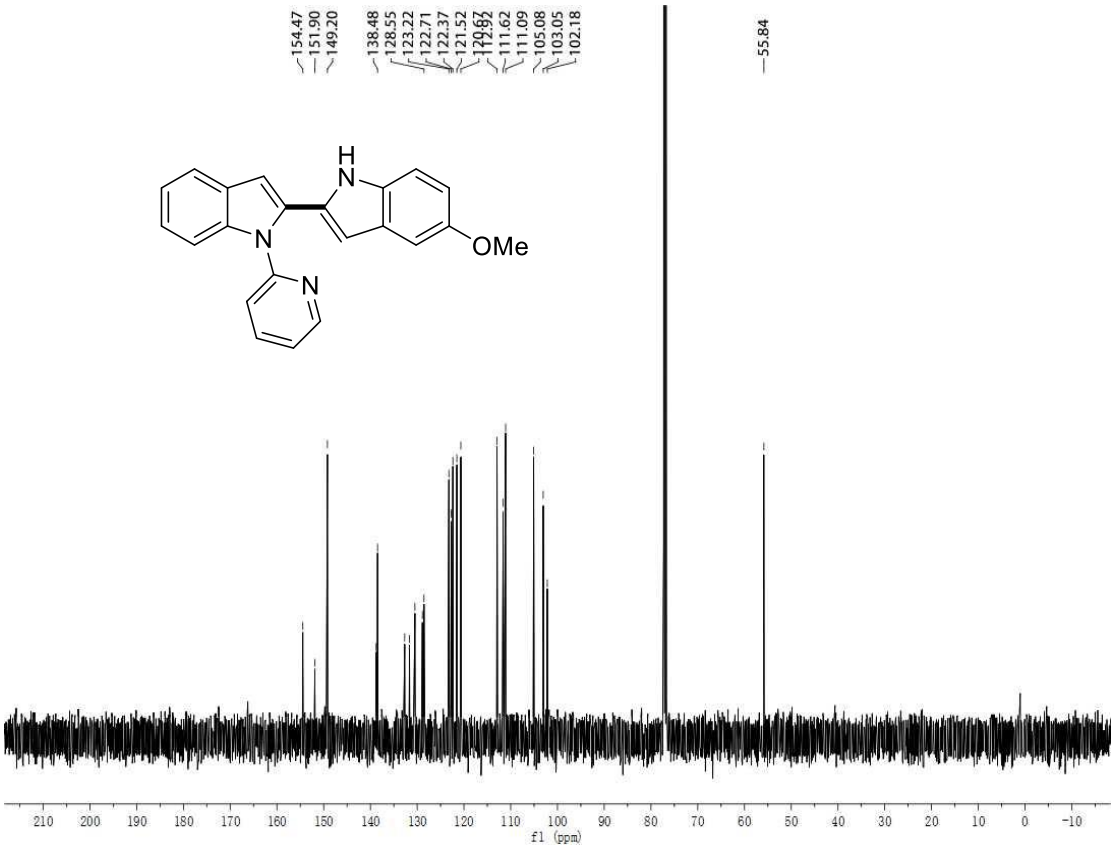
7.20
7.19
7.17
6.96
6.89
6.87
3.81
H
N
N
N
OMe
0.96
1.00
1.03
1.02
1.04
1.06
3.45
1.00
1.05
1.00
0.94
3.04
f1 (ppm)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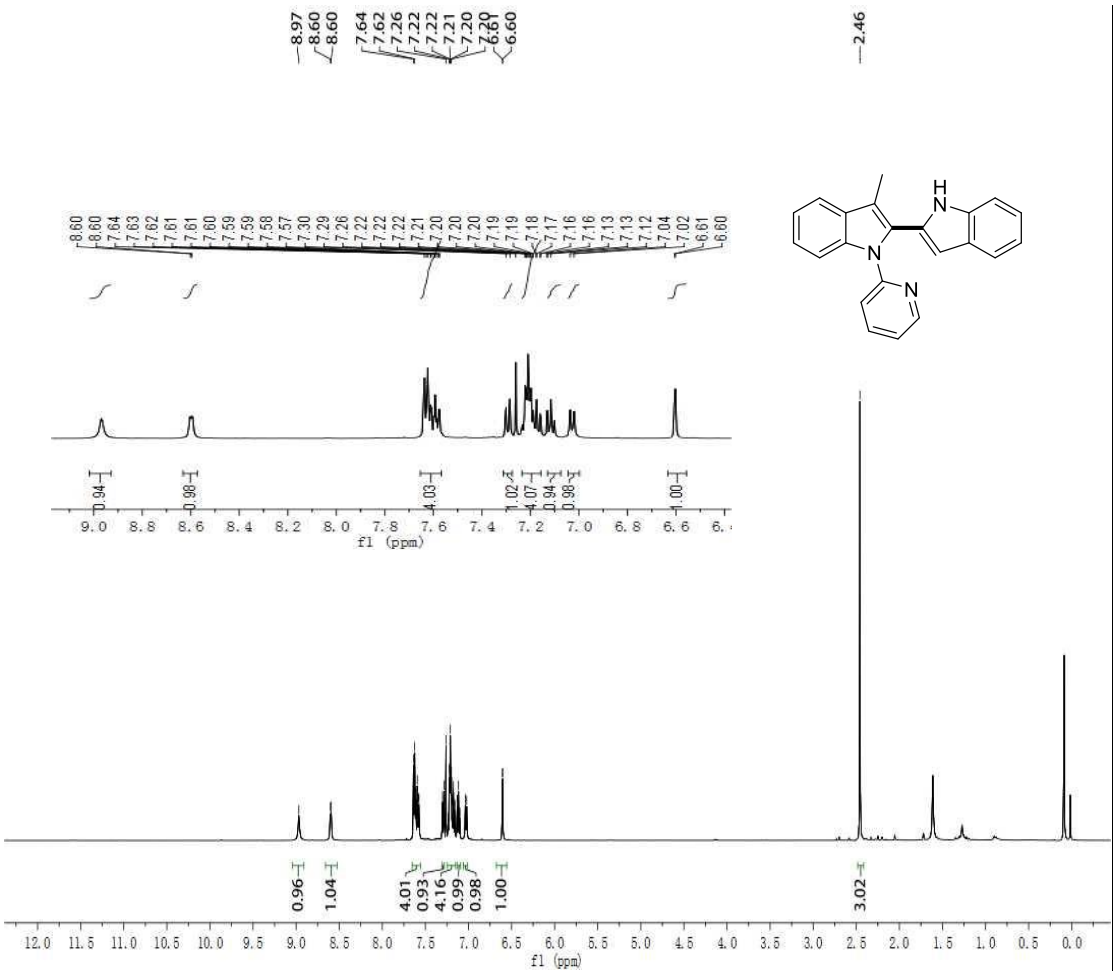
111.09
105.08
103.05
102.18
55.84
H
N
N
N
OMe
f1 (ppm)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7.22
7.21
7.20
6.61
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4.16
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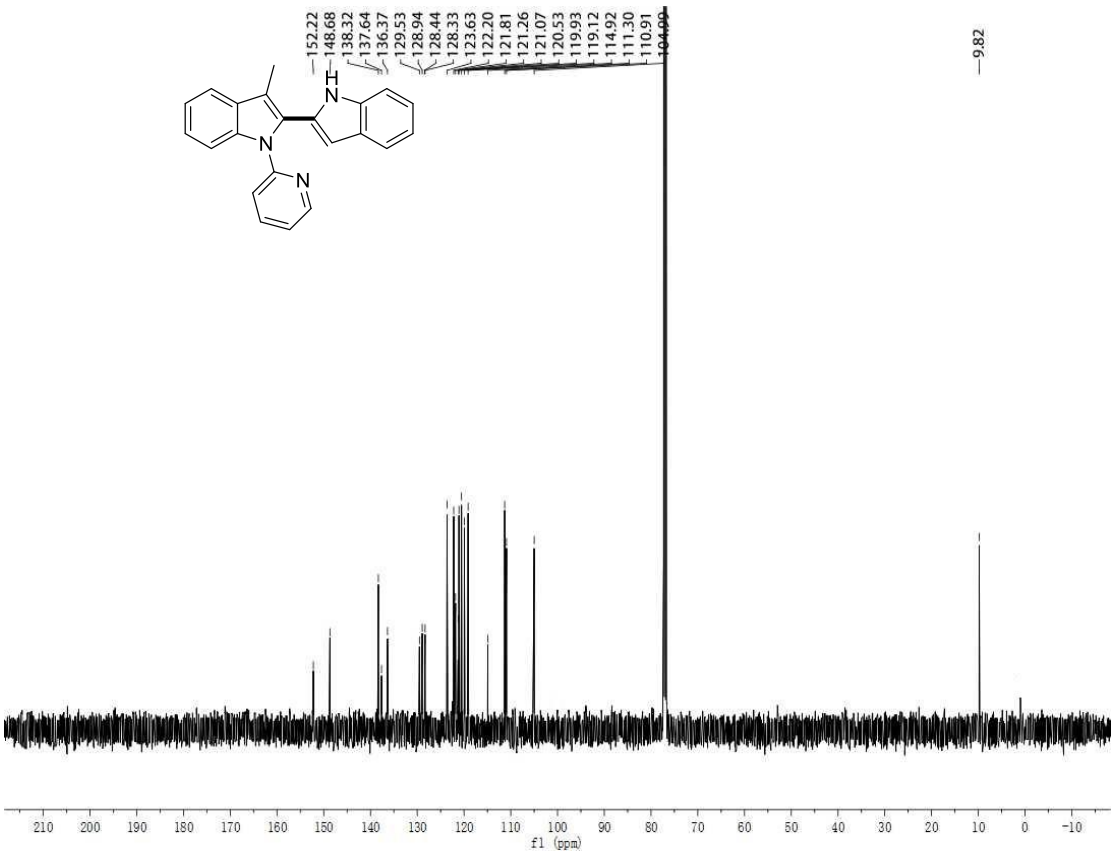
0.98
1.00
3.02
f1 (ppm)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128.33
123.63
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121.07
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119.93
119.12
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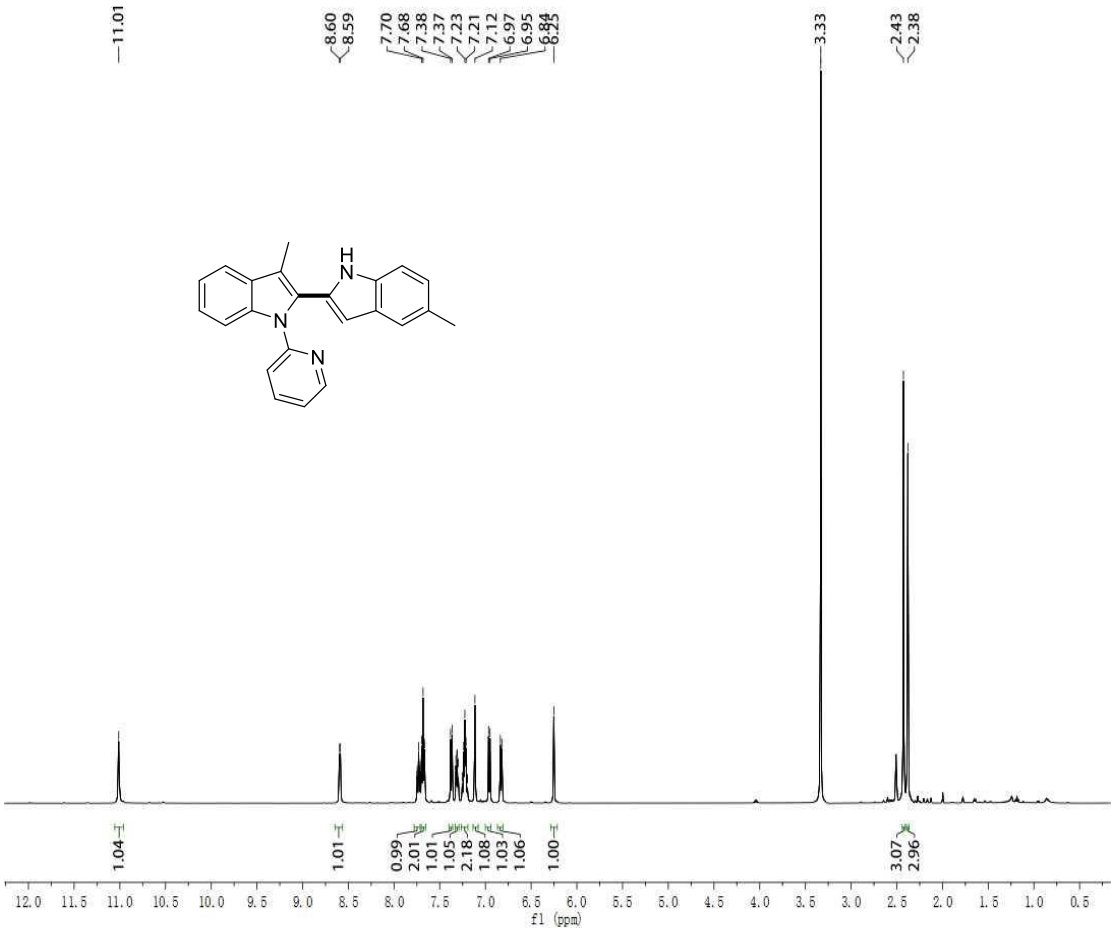
111.30
110.91
9.82
f1 (ppm)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7.68
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7.37
7.23
7.21
7.12
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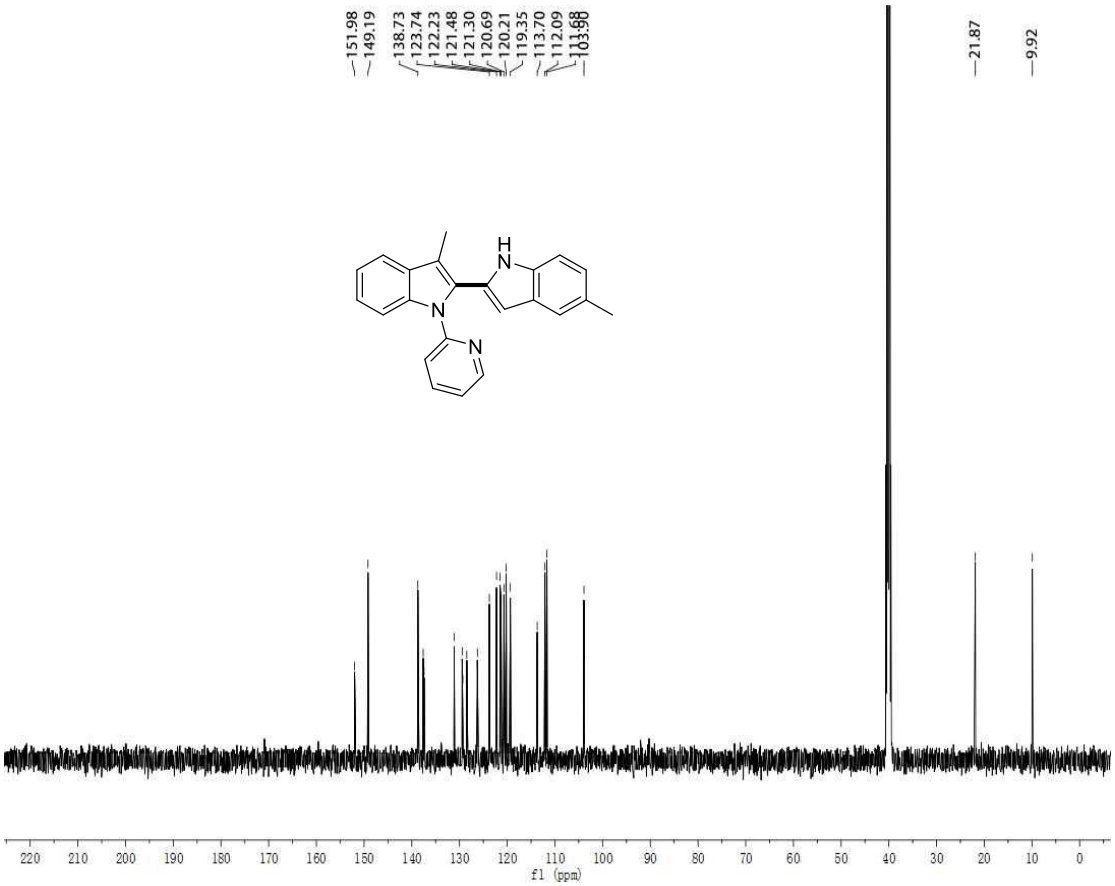
6.84
6.25
3.33
2.43
2.38
1.04
1.01
0.99
2.01
1.01
1.05
2.18
1.08
1.03
1.06
1.00
3.07
2.96
f1 (ppm)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149.19
138.73
123.74
122.23
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113.70
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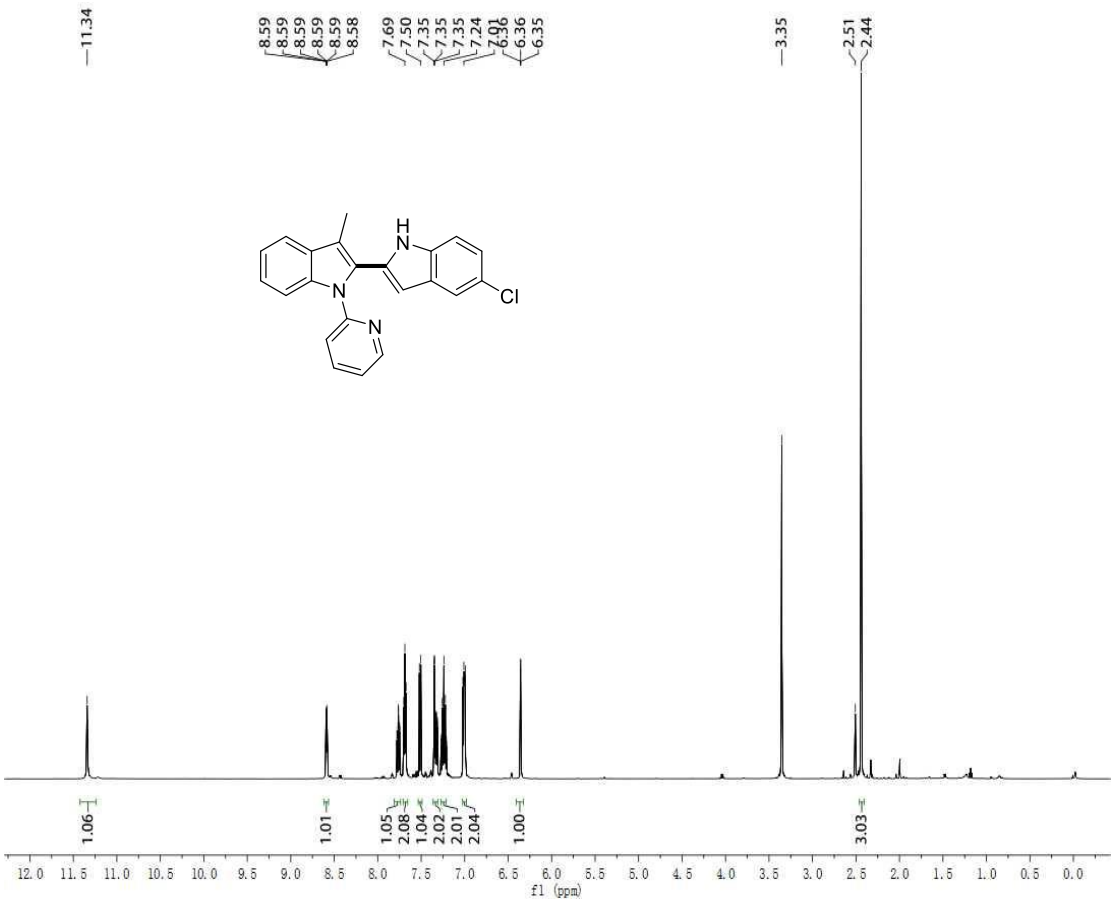
111.68
103.98
21.87
9.92
f1 (ppm)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8.59
8.59
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7.69
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7.35
7.35
7.35
7.24
6.36
6.35
3.35
2.51
2.44
H
N
N
N
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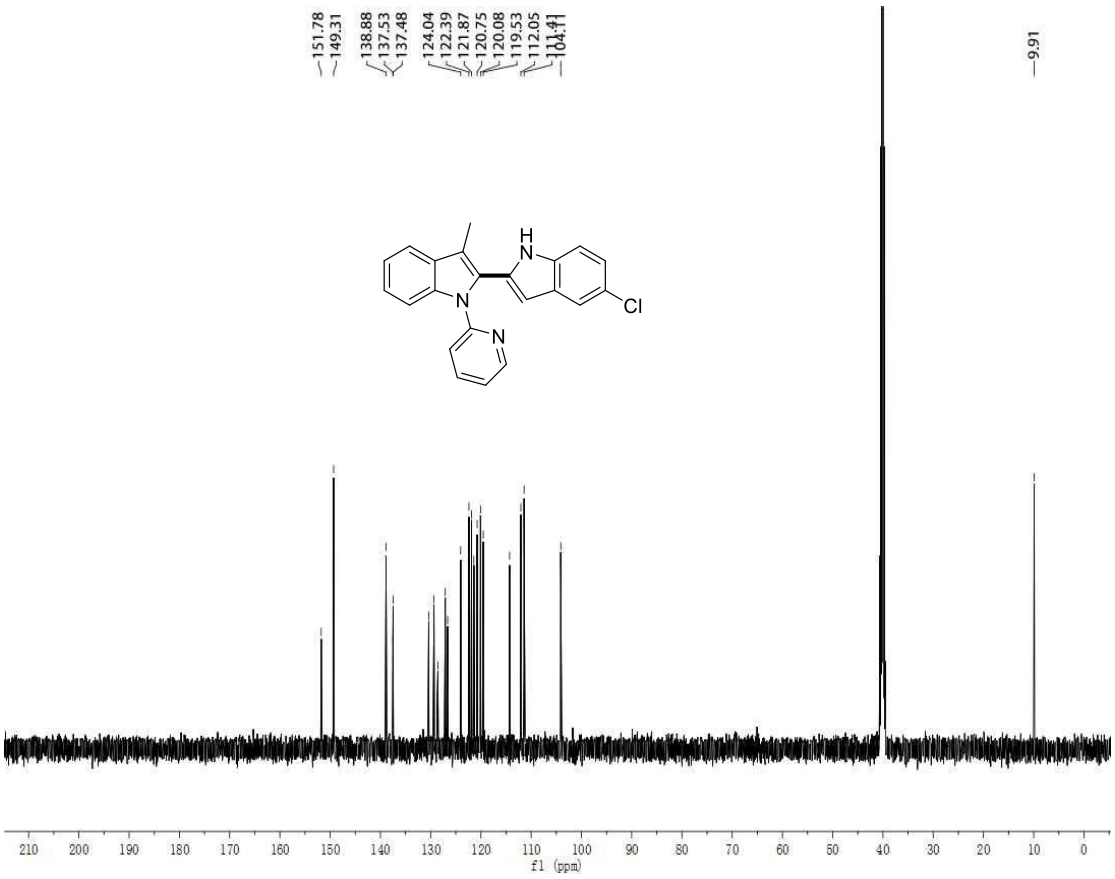
1.05
2.08
1.04
2.02
2.01
2.04
1.00
3.03
f1 (ppm)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112.05
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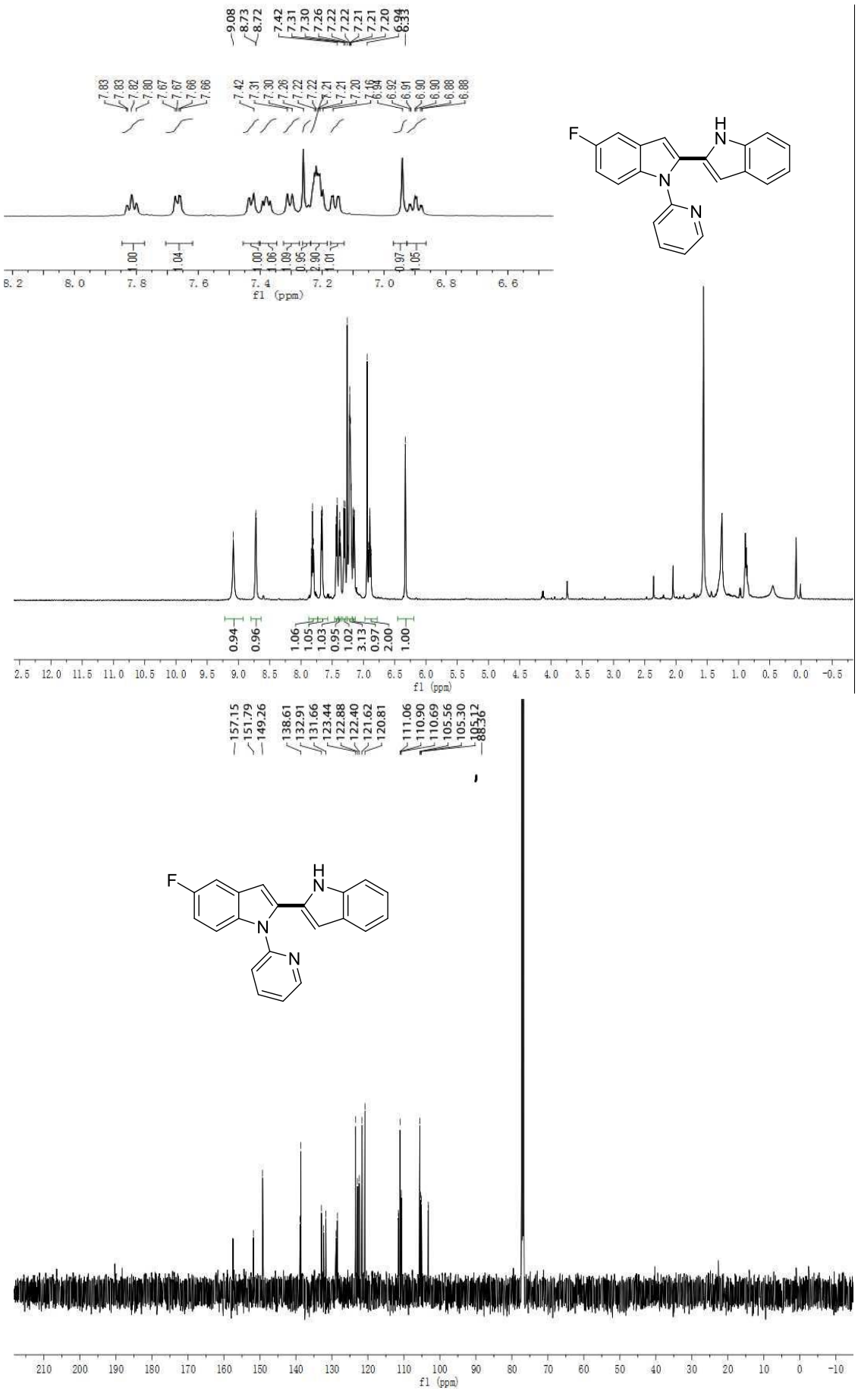
N
N
Cl
f1 (ppm)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7.30
7.26
7.22
7.22
7.21
7.21
7.20
6.94
6.93
F
H
N
N
N
f1 (ppm)
0.94
0.96
1.06
1.05
1.03
0.95
1.02
3.13
0.97
2.00
1.00
157.15
151.79
149.26
138.61
132.91
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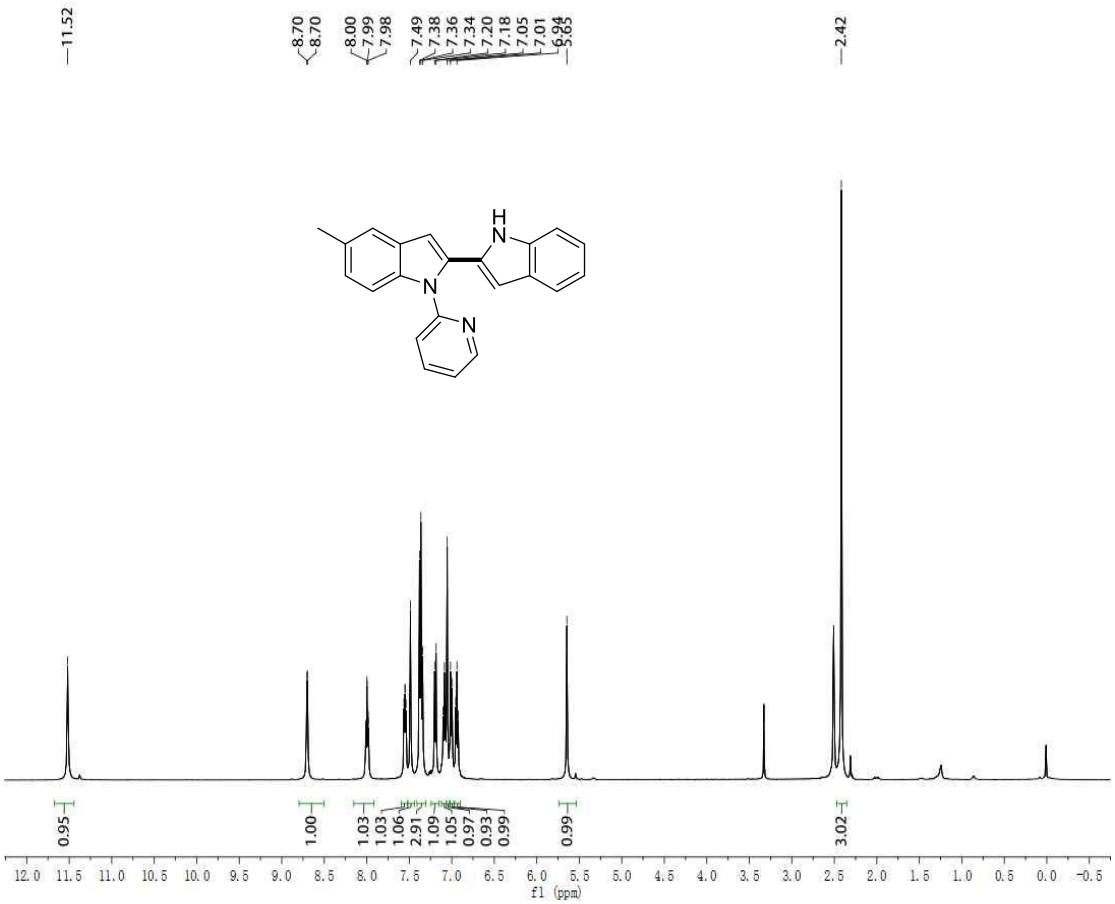
105.30
88.36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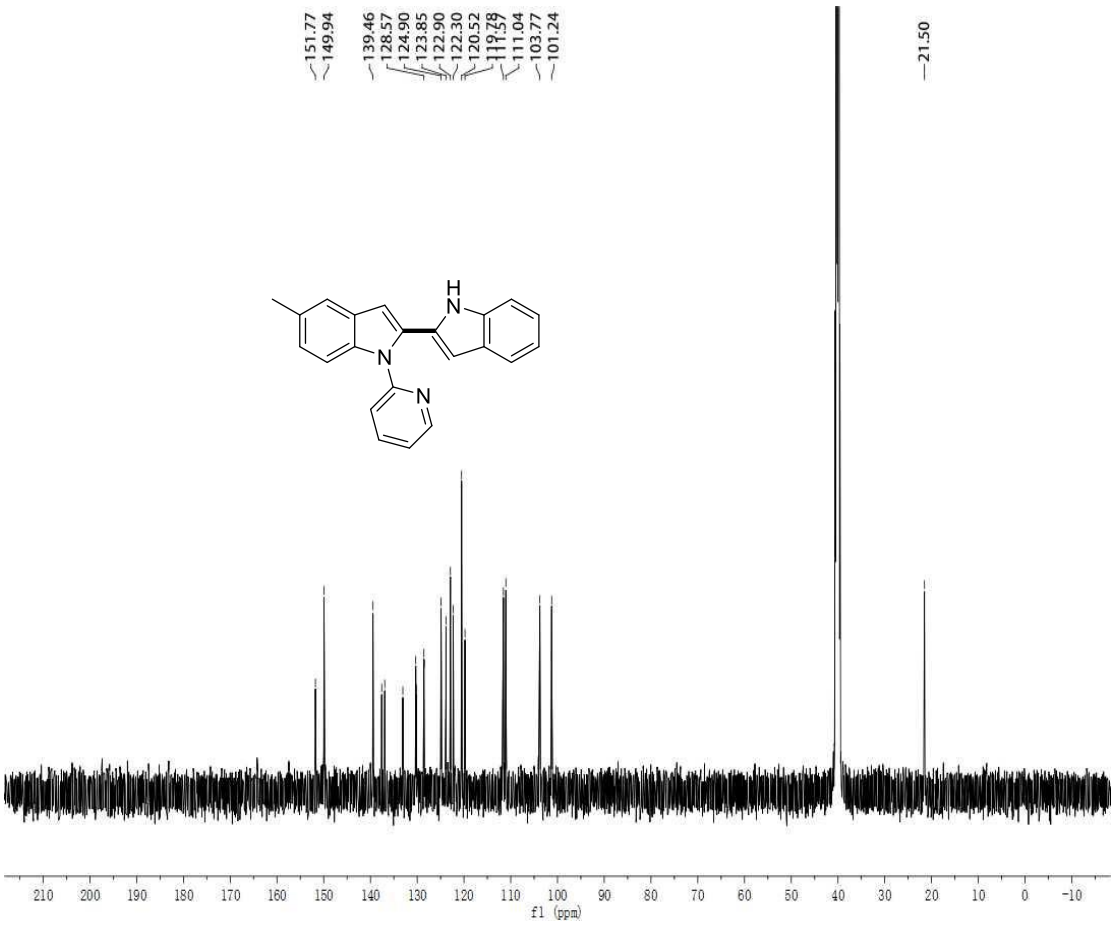
7.20
7.18
7.05
7.01
6.94
6.93
5.65
2.42
H
N
N
N
0.95
1.00
1.03
1.03
1.06
2.91
1.09
1.05
0.97
0.93
0.99
0.99
3.02
f1 (ppm)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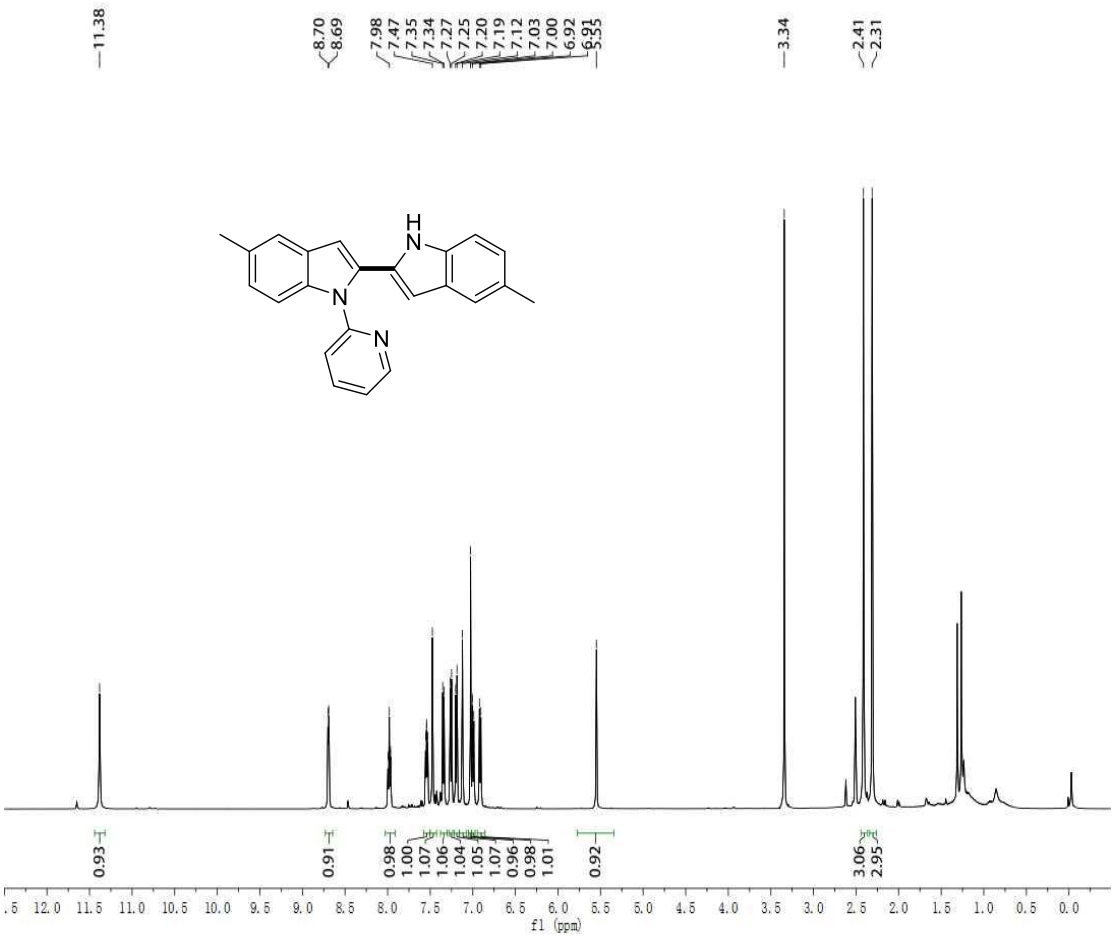
N
N
f1 (ppm)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7.34
7.27
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7.20
7.19
7.12
7.03
7.00
6.92
6.91
5.55
3.34
2.41
2.31
H
N
N
N
0.93
0.91
0.98
1.00
1.07
1.06
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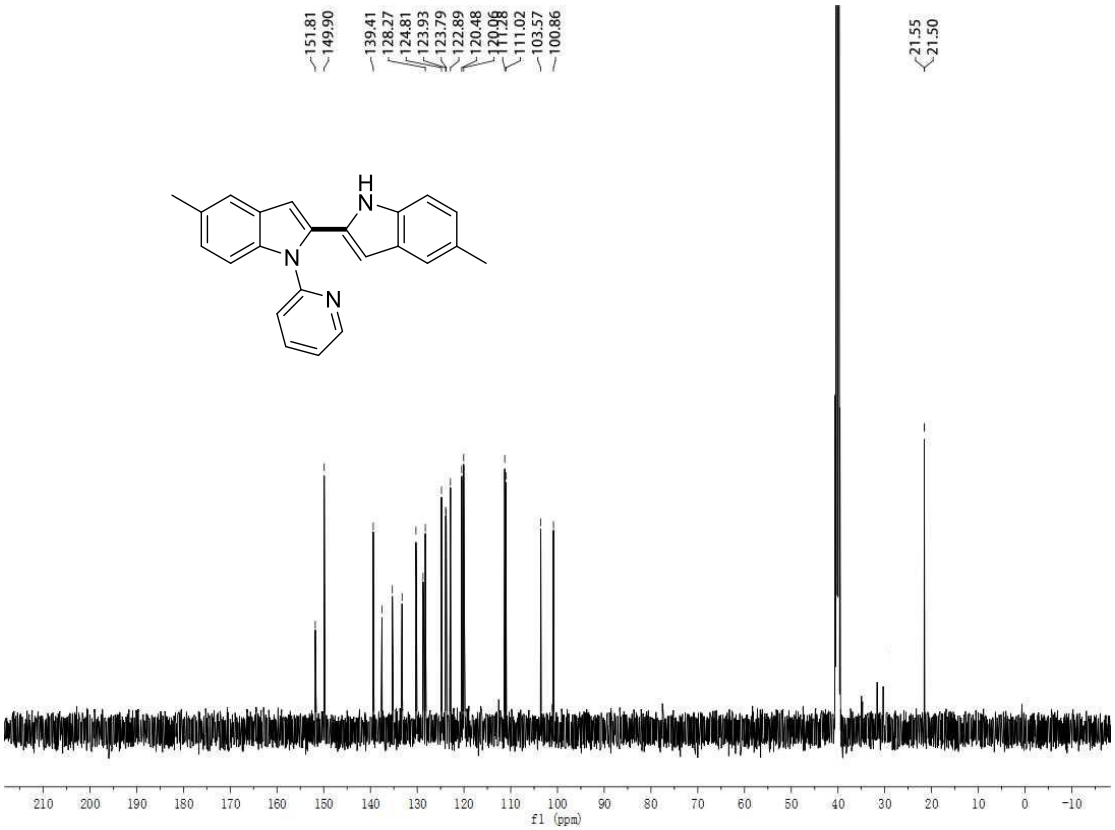
1.05
1.07
0.96
0.98
1.01
0.92
3.06
2.95
f1 (ppm)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21.50
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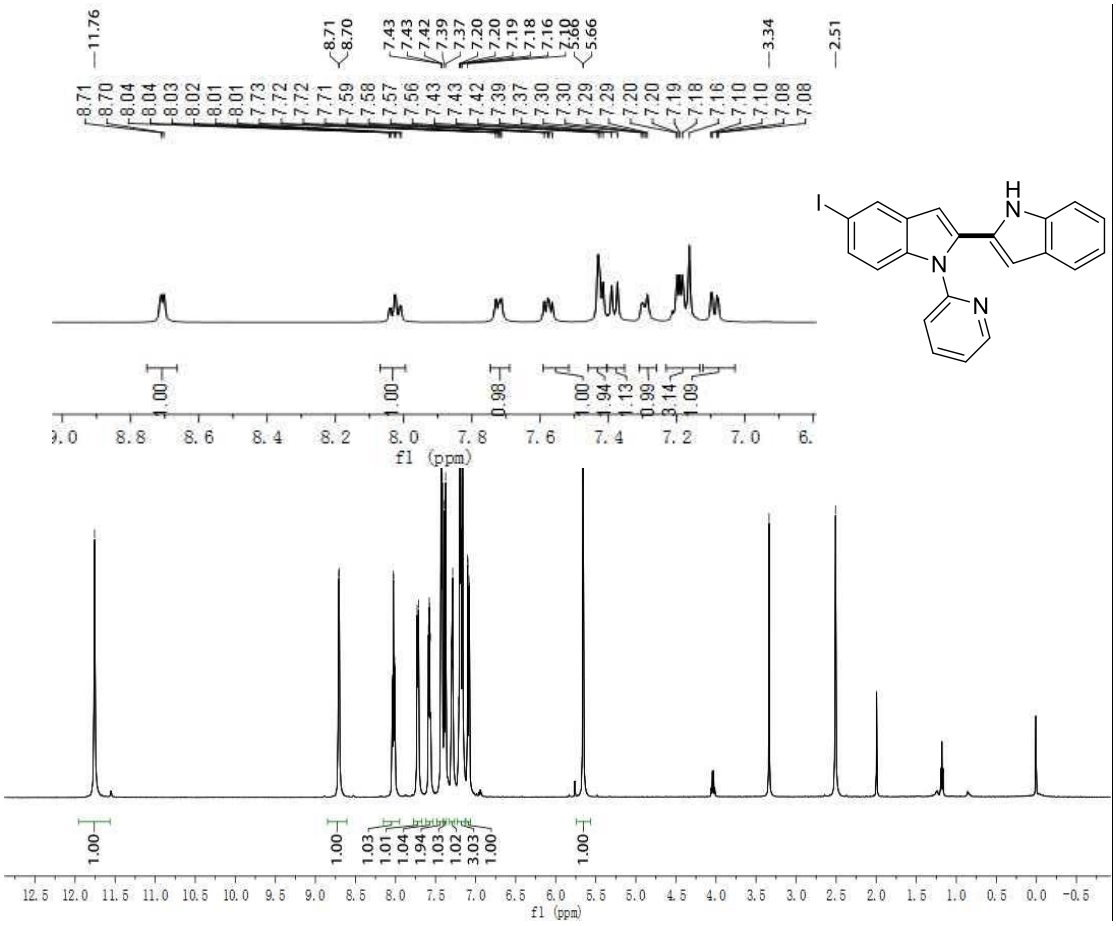
N
N
f1 (ppm)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8.01
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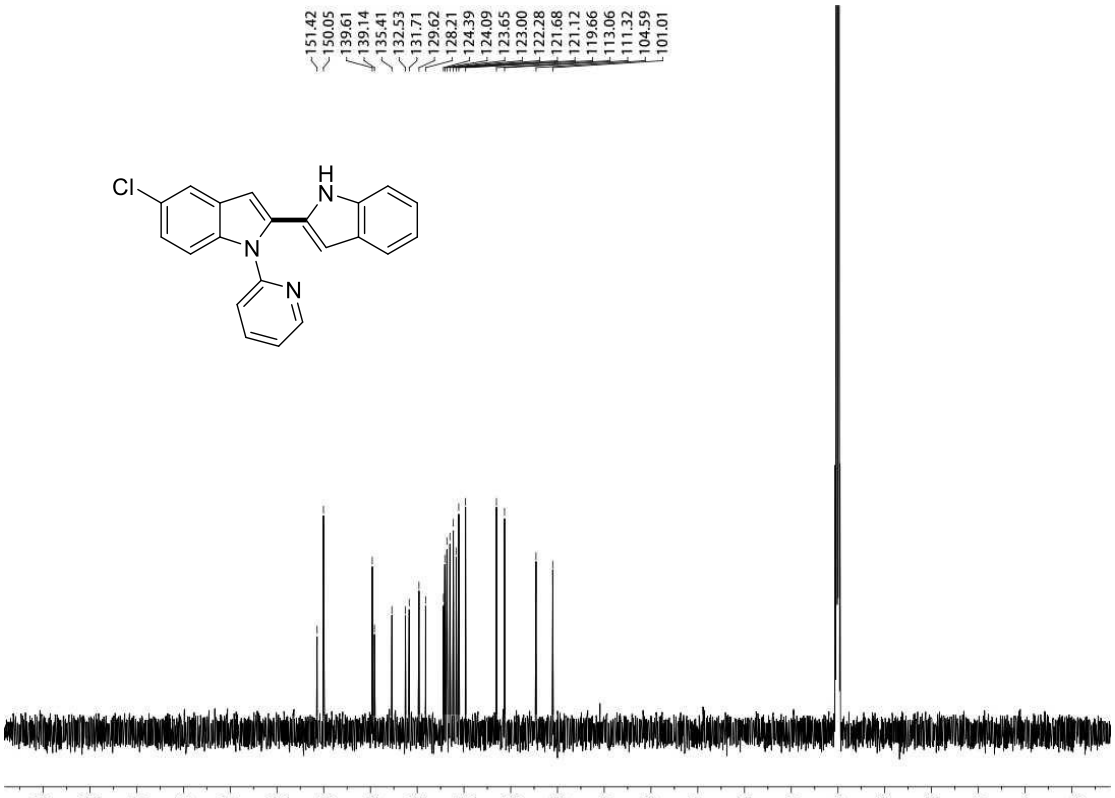
7.58
7.57
7.56
7.43
7.43
7.42
7.39
7.37
7.30
7.30
7.29
7.20
7.20
7.19
7.18
7.16
7.10
7.10
7.08
7.08
3.34
2.51
I
H
N
N
f1 (ppm)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124.09
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123.00
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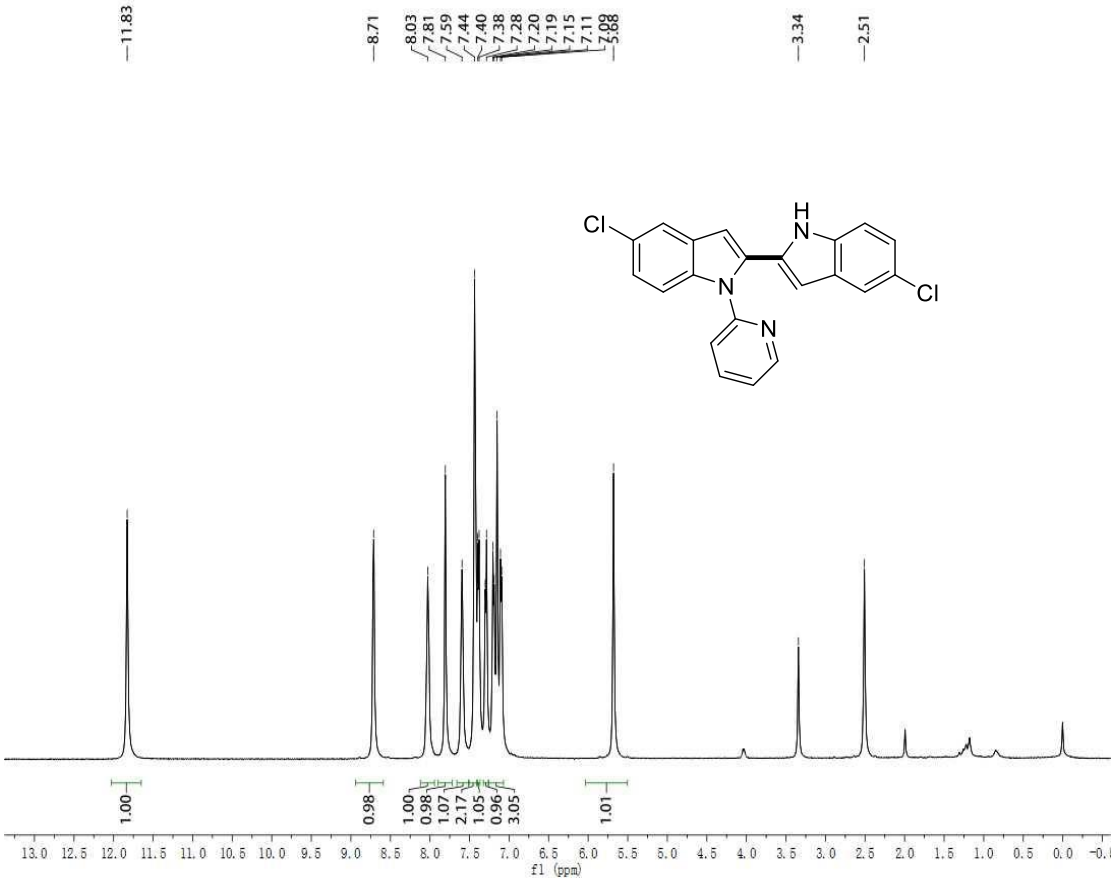
119.66
113.06
111.32
104.59
101.01
Cl
H
N
N
N
f1 (ppm)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7.20
7.19
7.15
7.11
7.09
5.88
3.34
2.51
Cl
H
N
N
N
Cl
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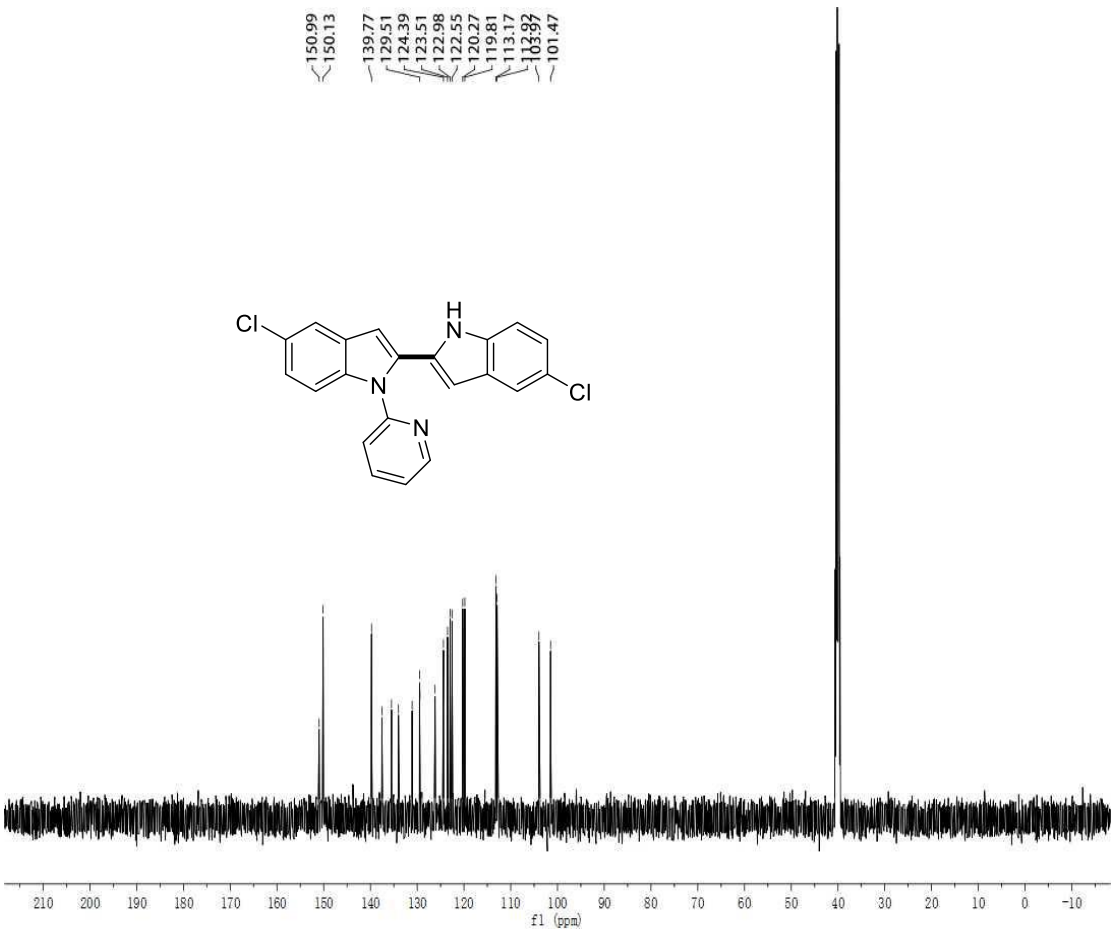
1.00
0.98
1.07
2.17
1.05
0.96
3.05
1.01
f1 (ppm)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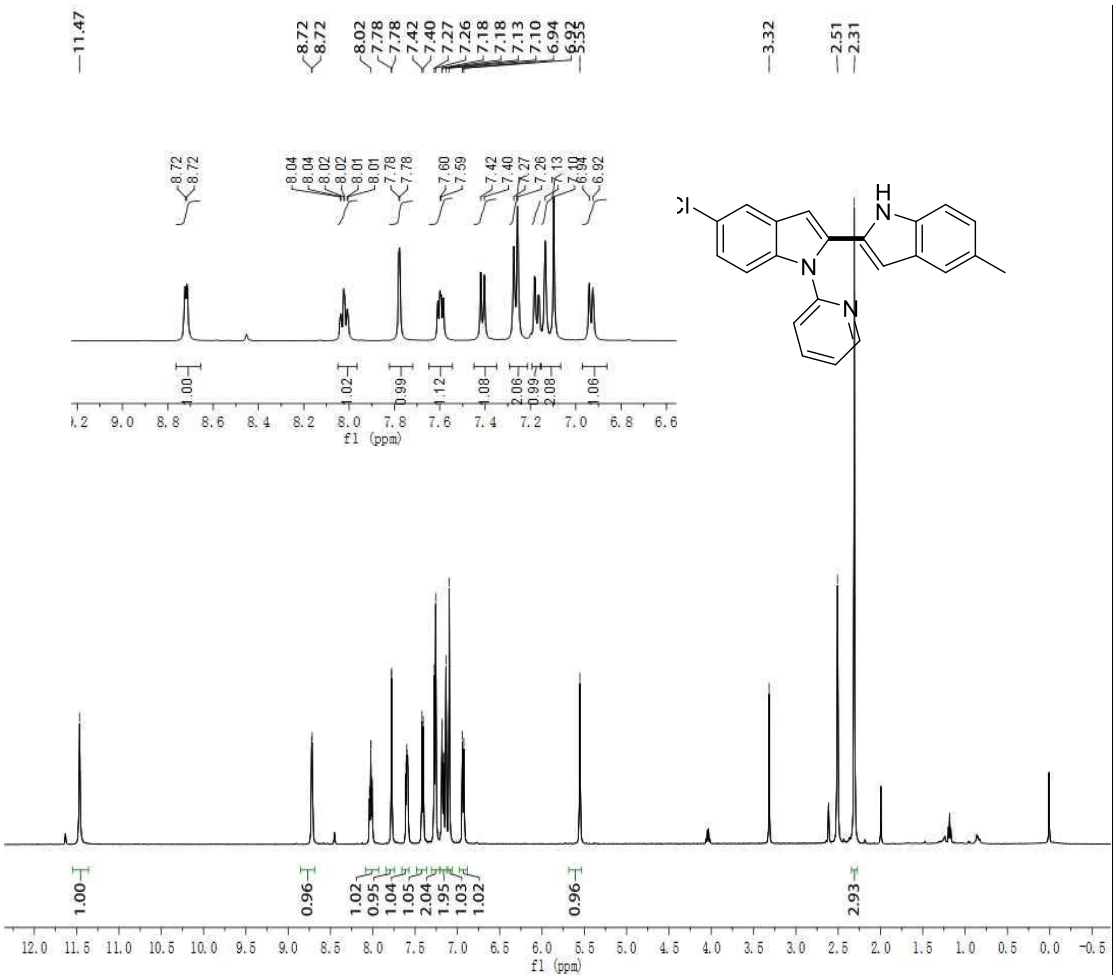
113.17
101.47
Cl
H
N
N
N
Cl
f1 (ppm)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8.72
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7.27
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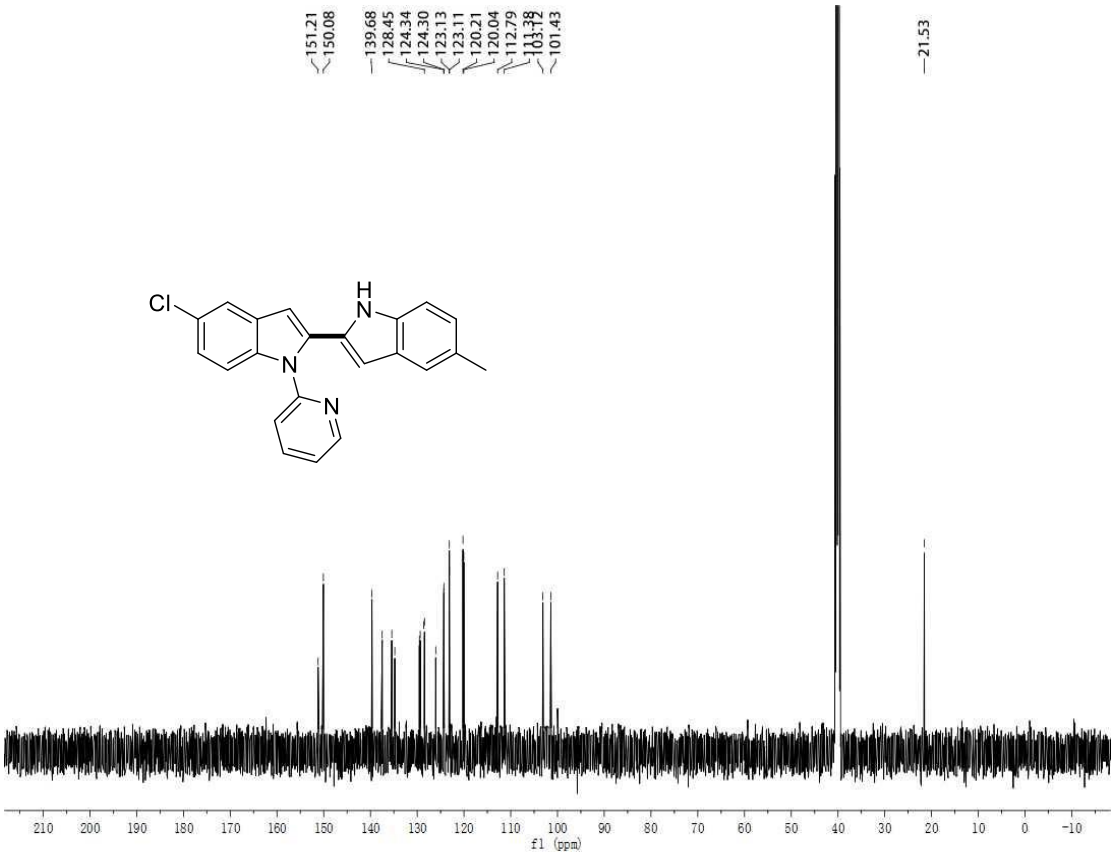
7.13
7.10
6.94
6.92
5.35
3.32
2.51
2.31
f1 (ppm)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112.79
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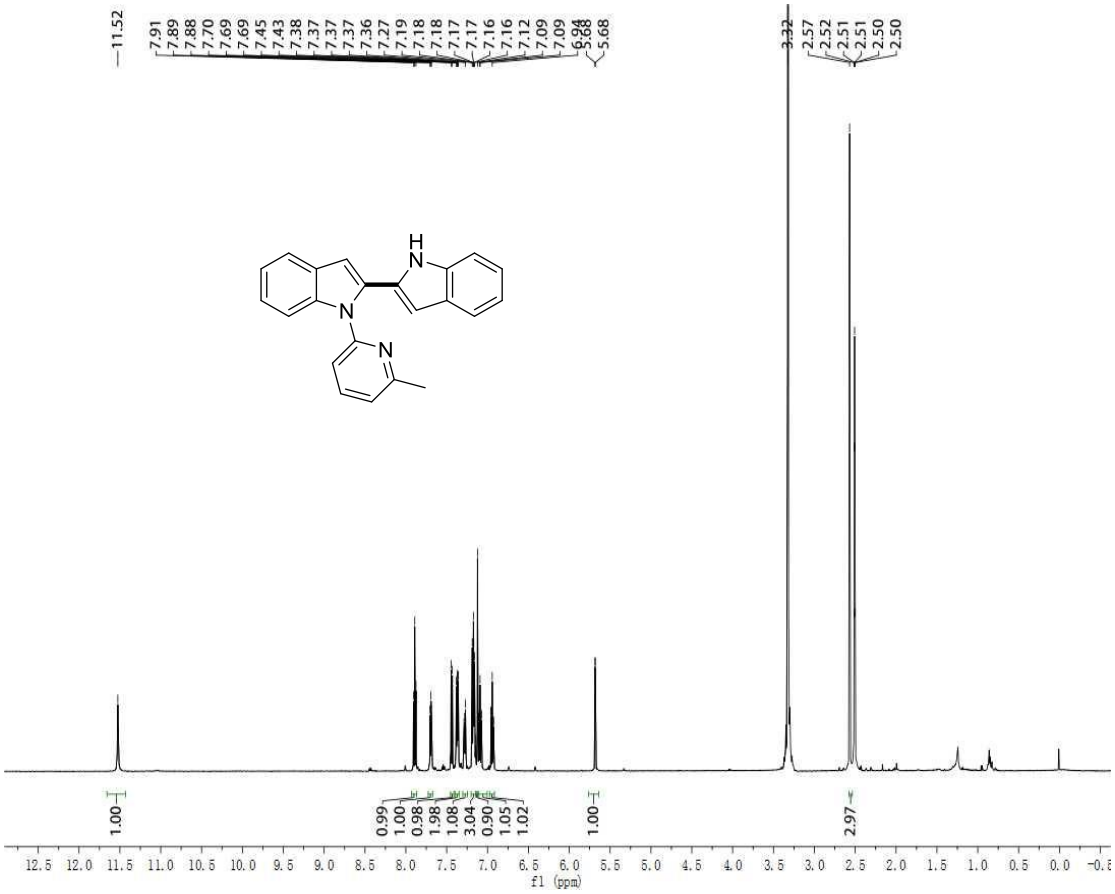
103.12
101.43
21.53
f1 (ppm)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7.45
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7.38
7.37
7.37
7.37
7.36
7.27
7.19
7.18
7.18
7.17
7.17
7.16
7.16
7.12
7.09
7.09
6.94
5.68
5.68
3.32
2.57
2.52
2.51
2.51
2.50
2.50
H
N
N
N
1.00
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1.00
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1.98
1.08
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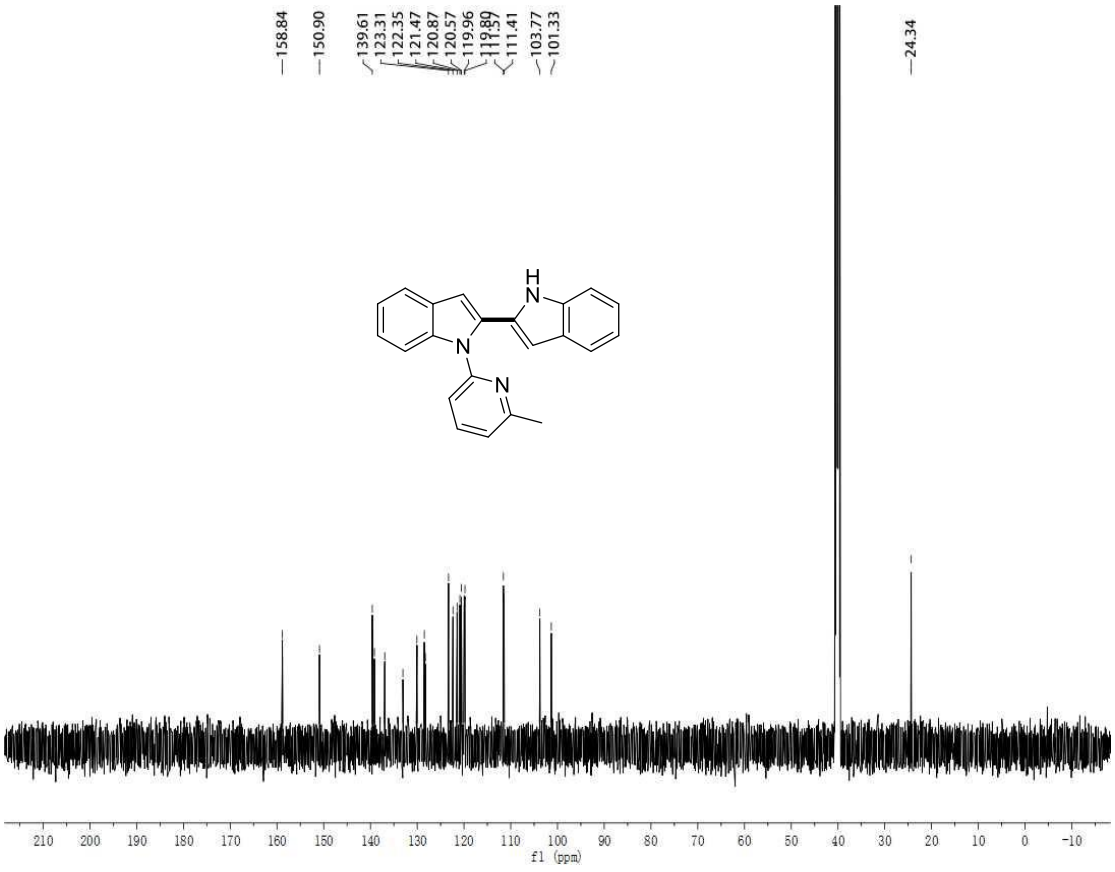
1.02
1.00
2.97
f1 (ppm)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24.34
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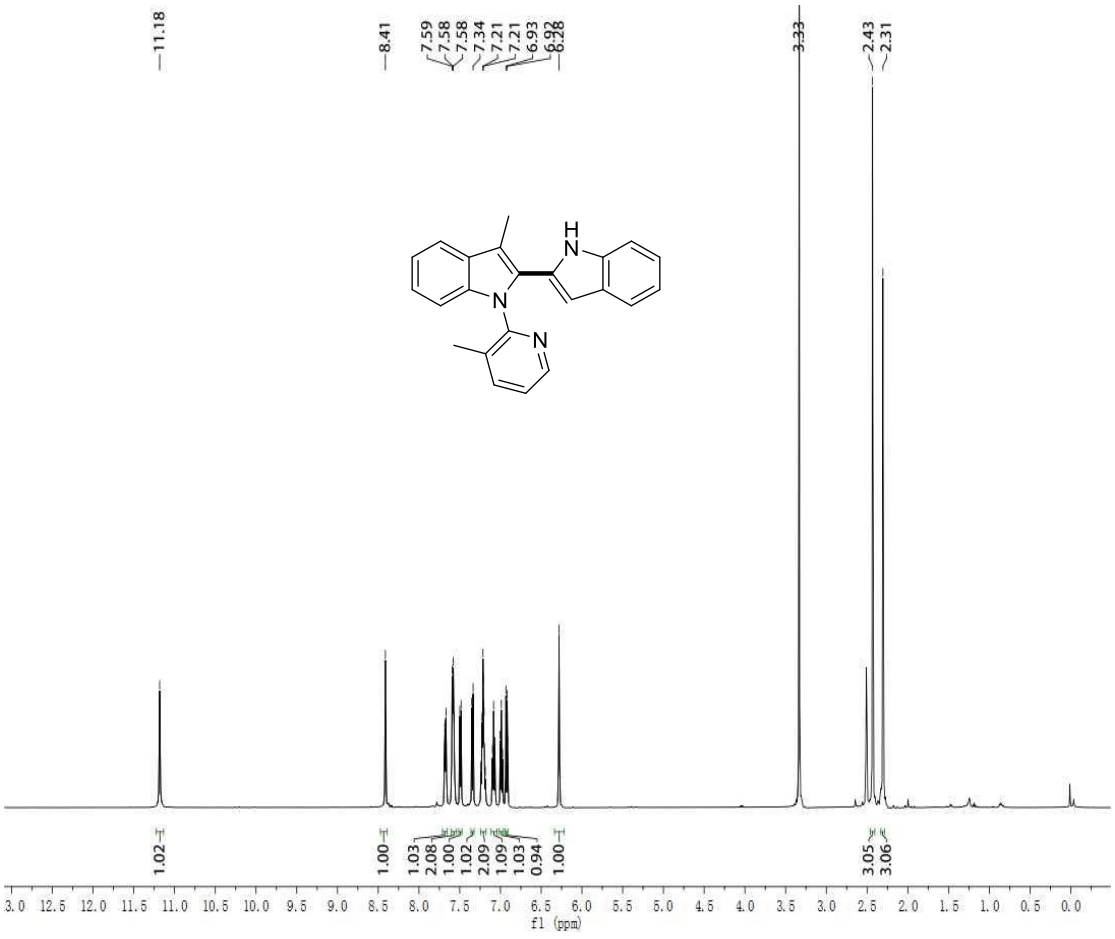
N
N
f1 (ppm)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6.92
6.88
3.33
2.43
2.31
1.02
1.00
1.03
2.08
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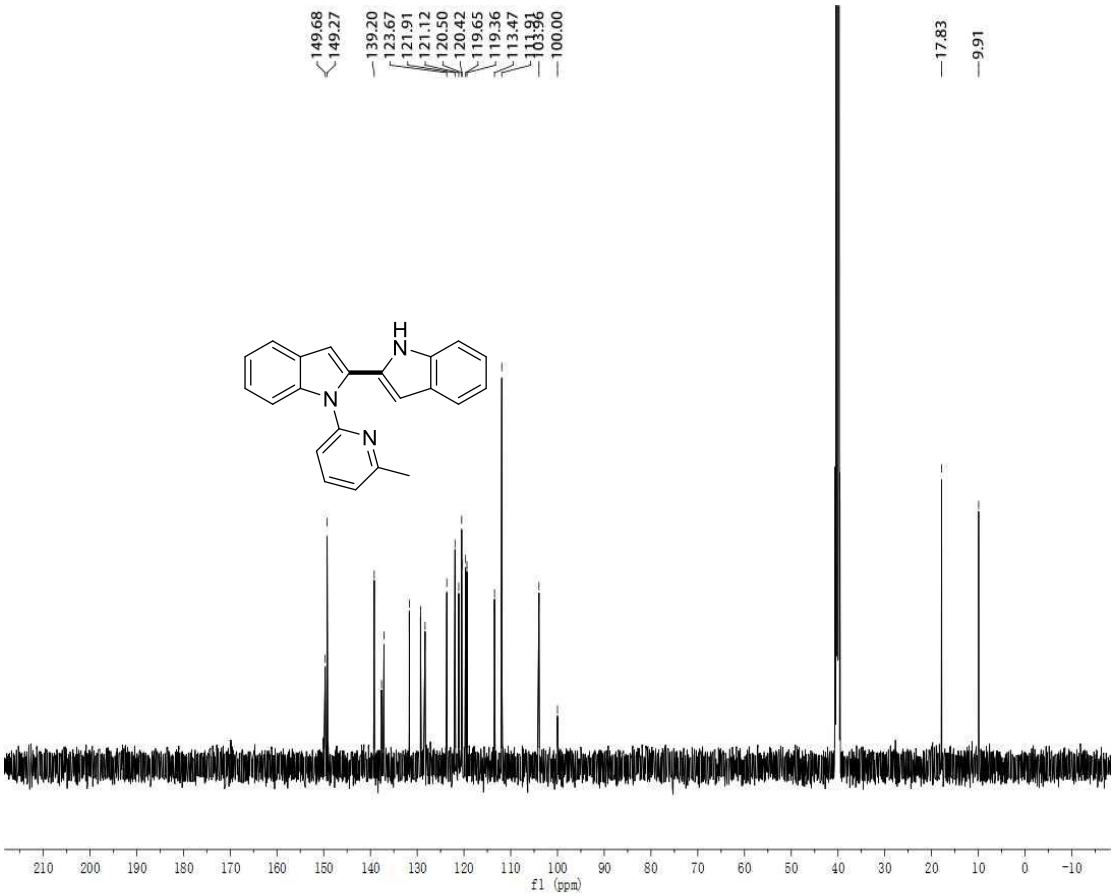
1.02
2.09
1.09
1.03
0.94
1.00
3.05
3.06
f1 (ppm)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111.91
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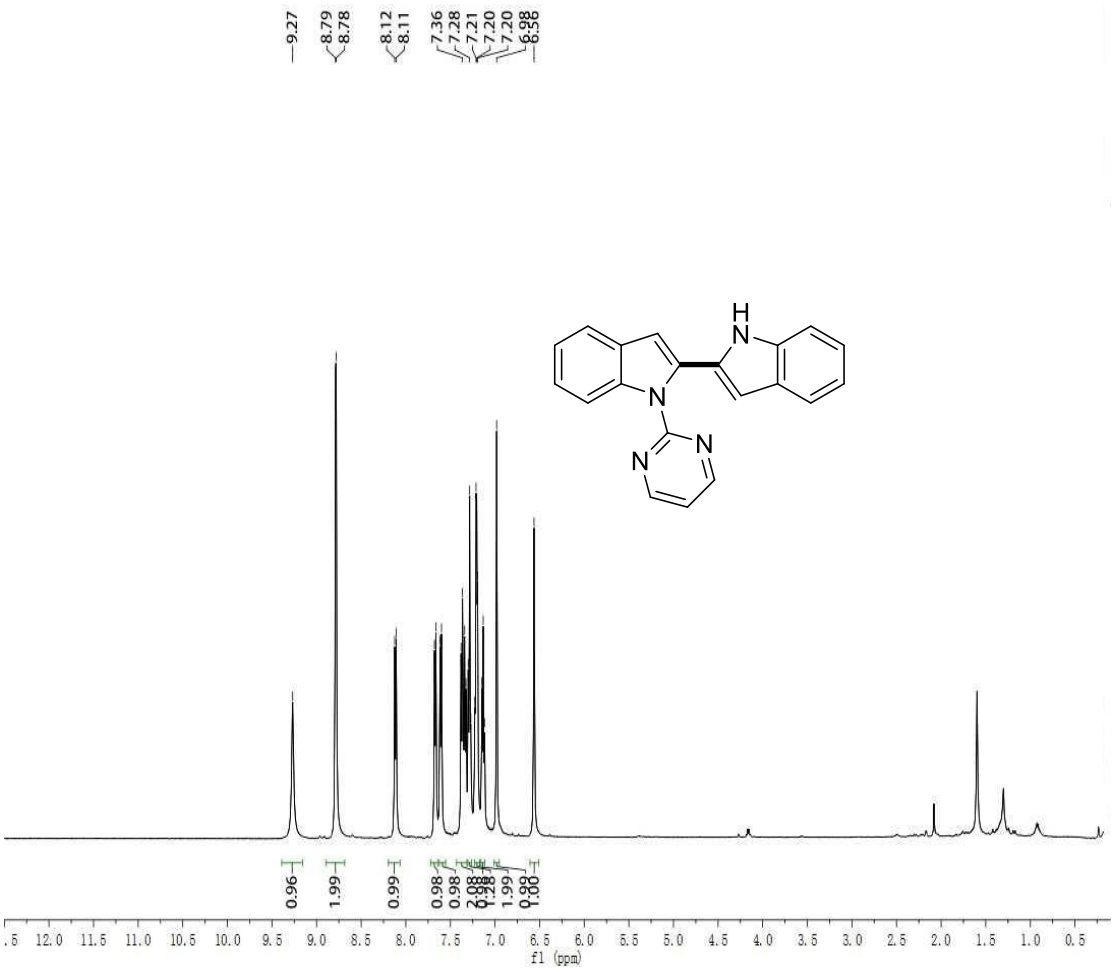
9.91
f1 (ppm)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7.28
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7.20
6.98
6.98
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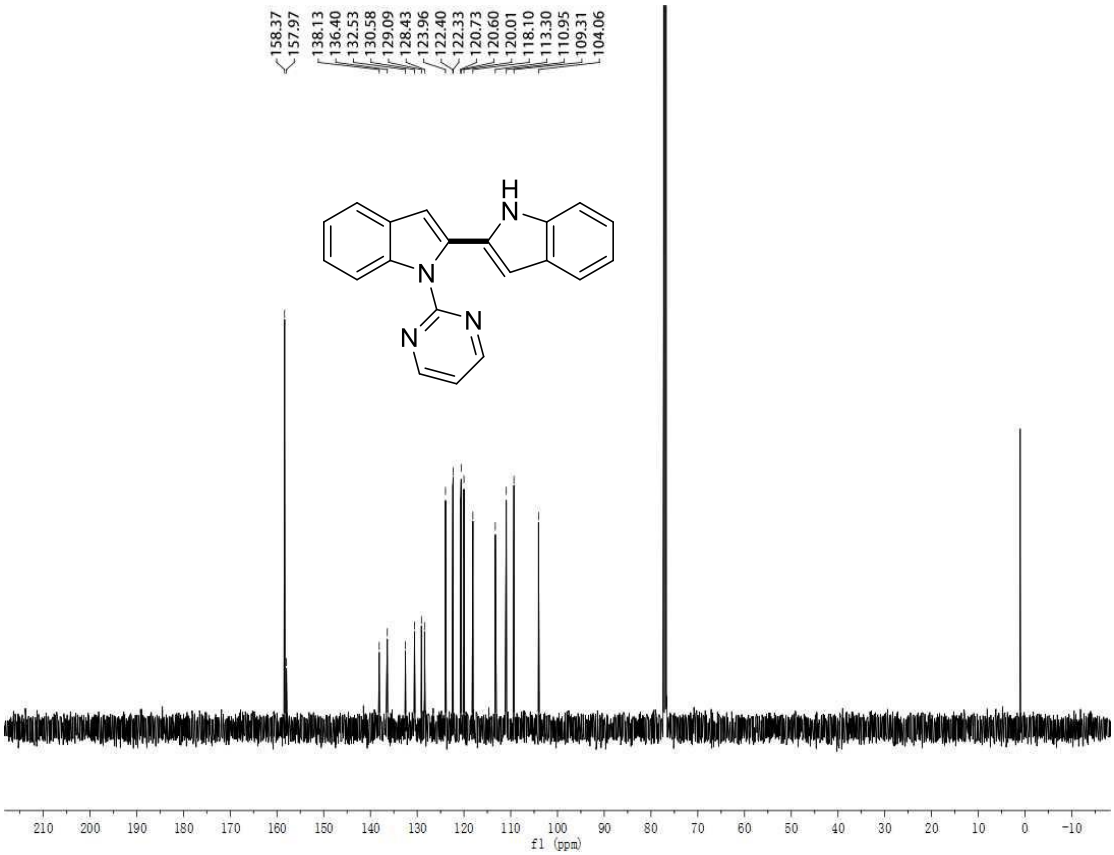
1.99
0.99
0.98
0.98
2.08
1.99
1.00
f1 (ppm)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122.33
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118.10
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110.95
109.31
104.06
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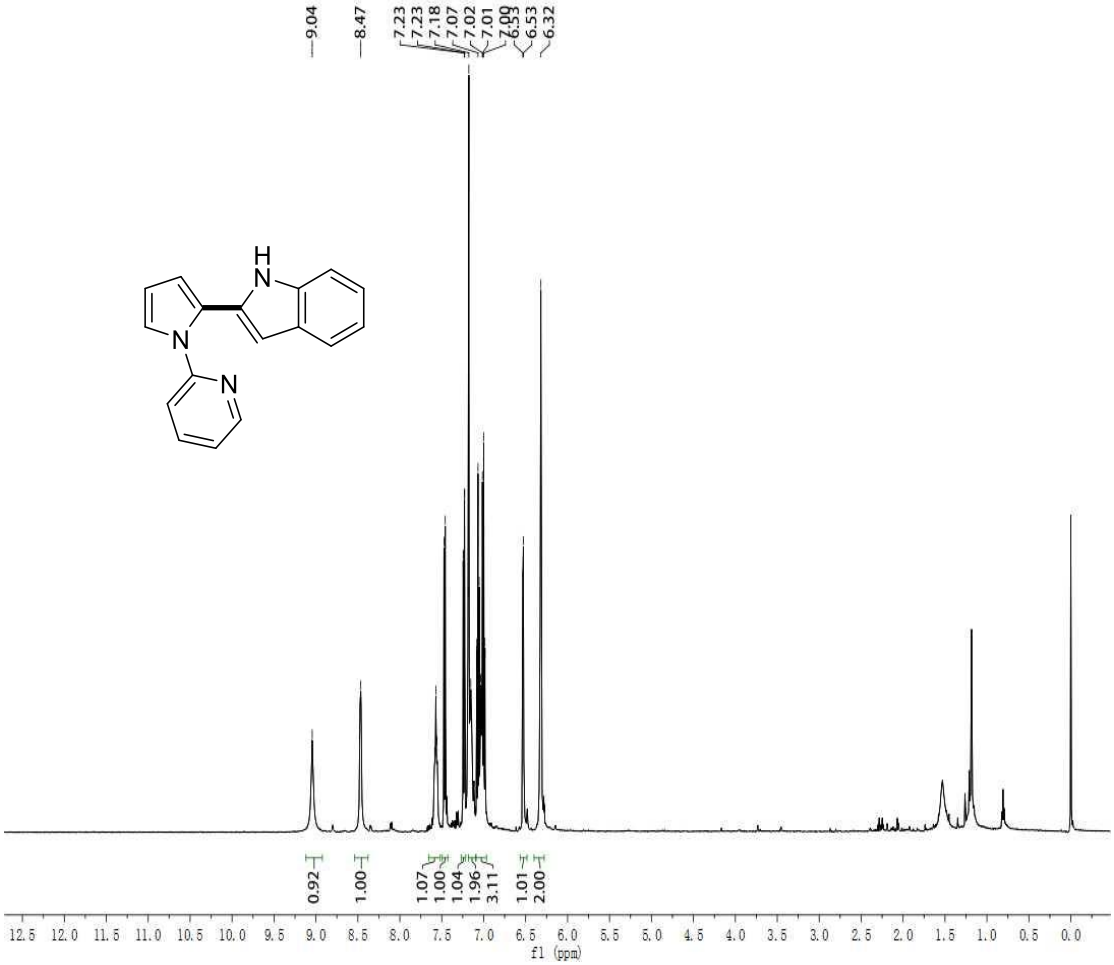
N
N
N
N
f1 (ppm)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7.07
7.02
7.01
7.00
6.53
6.32
H
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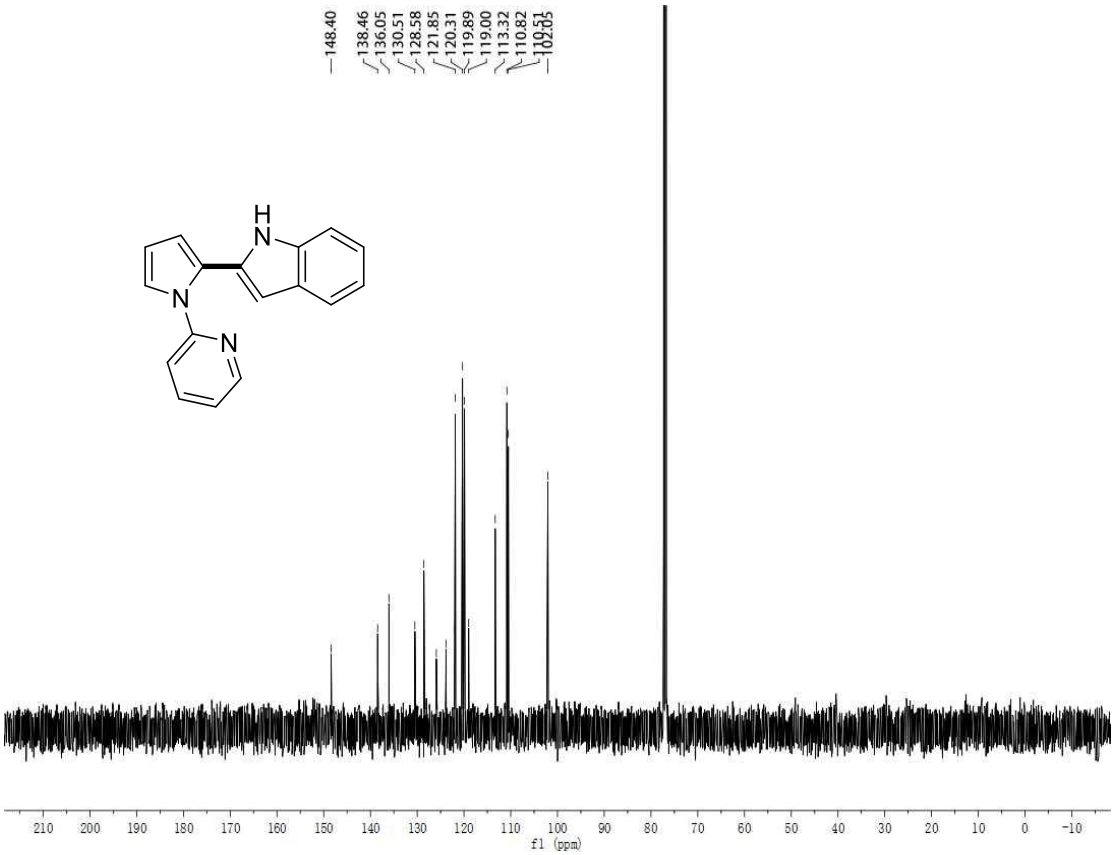
1.07
1.00
1.04
1.96
3.11
1.01
2.00
f1 (ppm)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102.05
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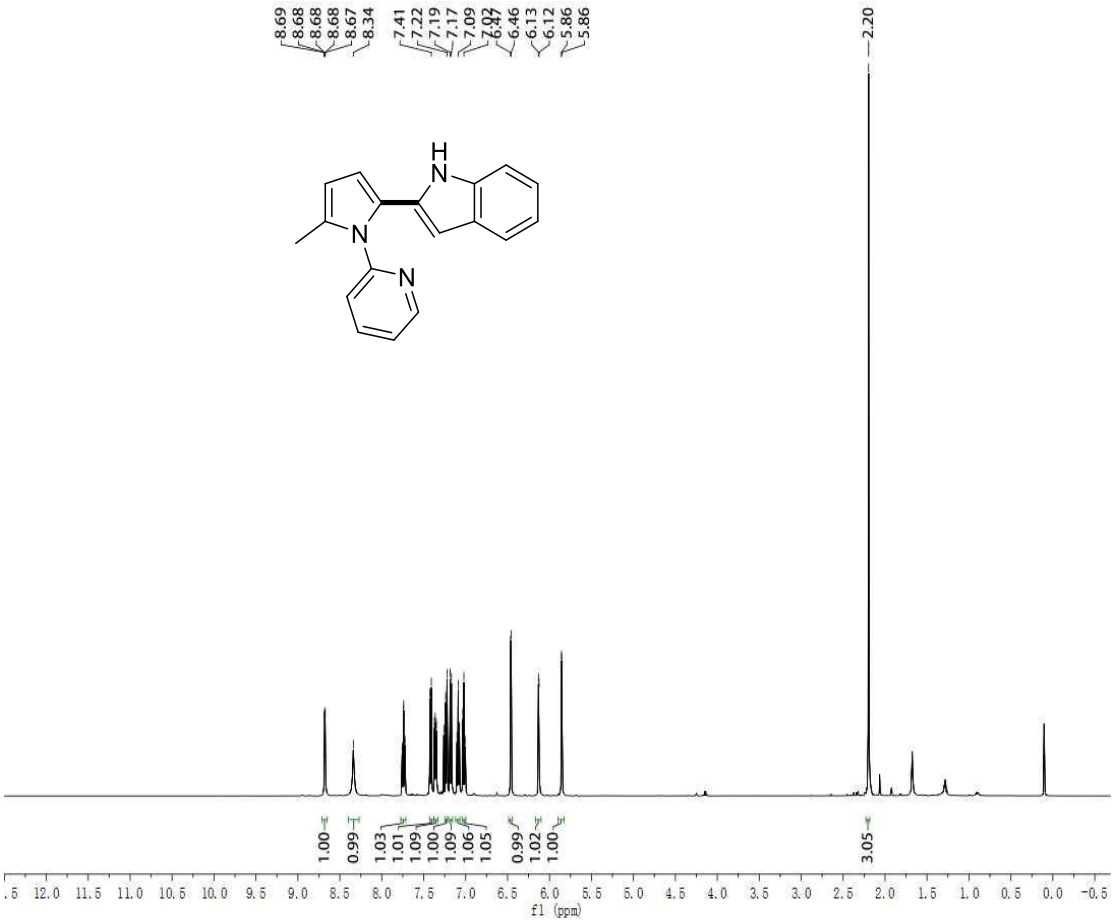
N
f1 (ppm)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7.22
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7.17
7.09
7.02
6.47
6.46
6.13
6.12
5.86
5.86
2.20
H
N
N
N
1.00
0.99
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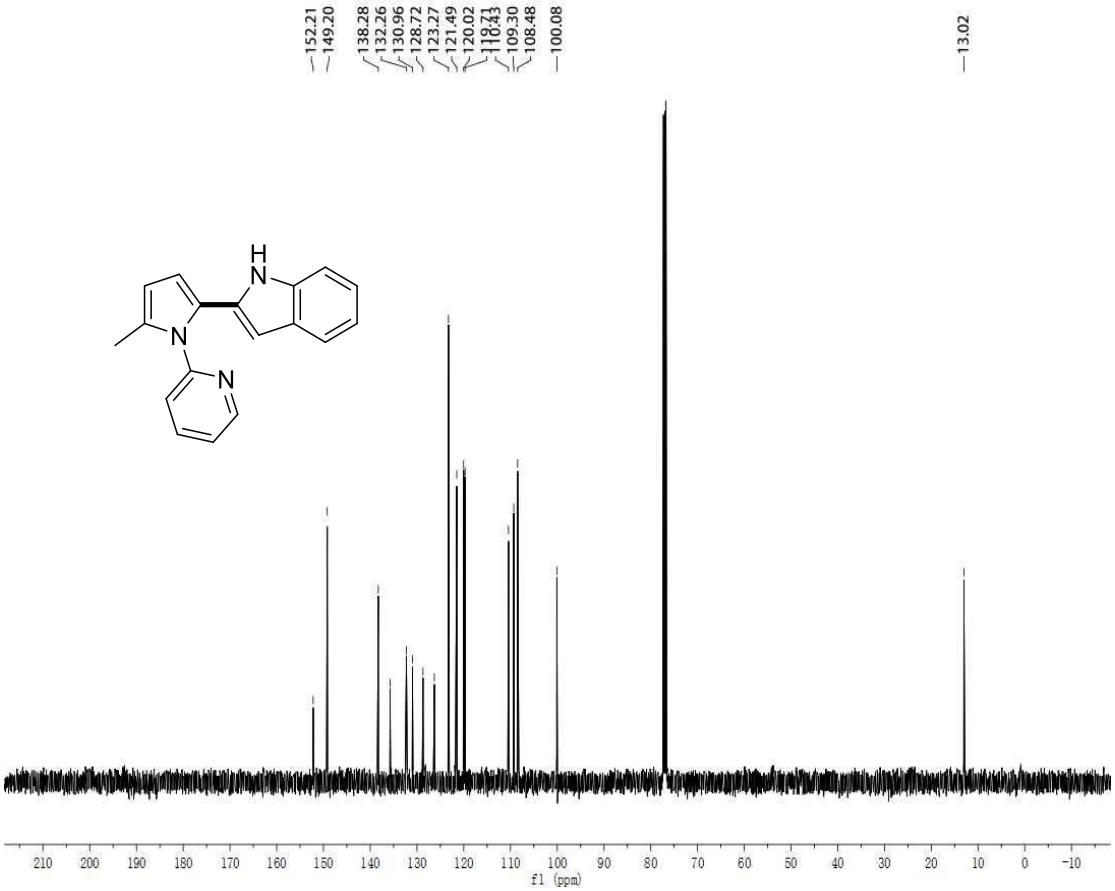
1.01
1.09
1.00
1.09
1.06
1.05
0.99
1.02
1.00
3.05
f1 (ppm)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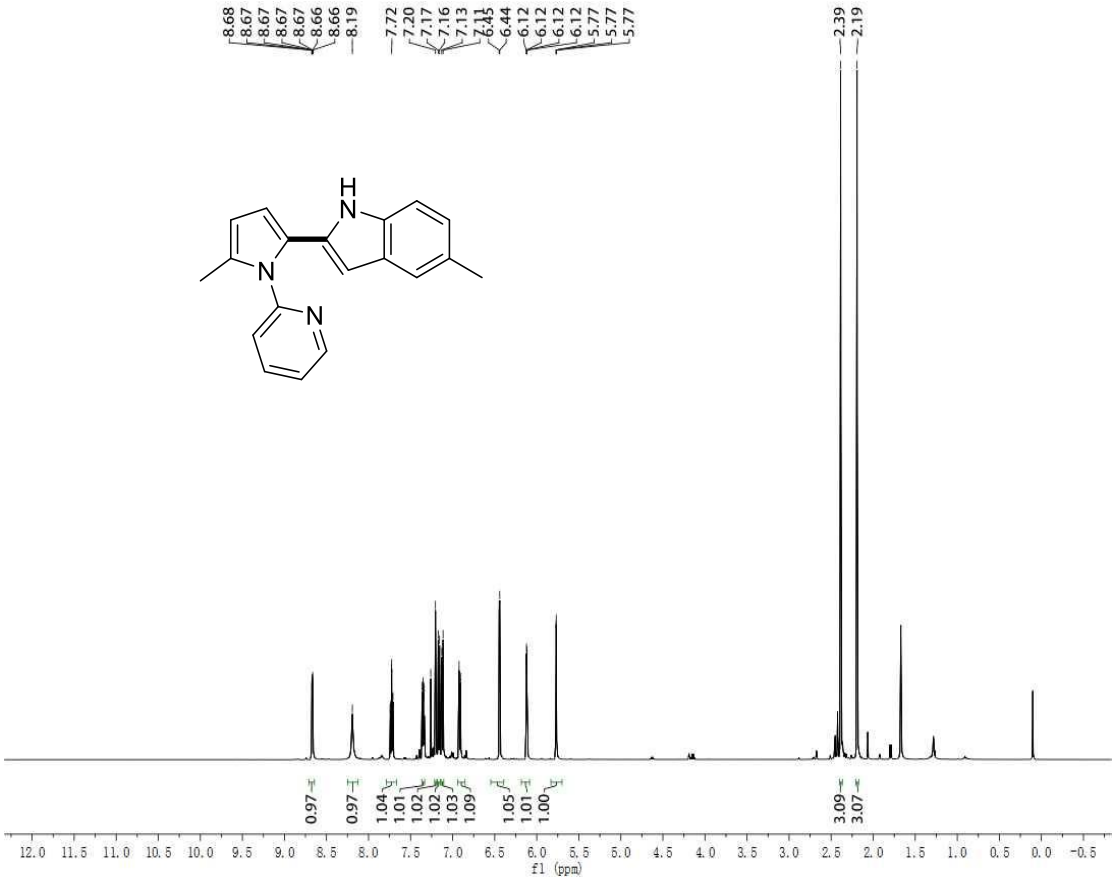
118.43
109.30
108.48
100.08
13.02
H
N
N
N
f1 (ppm)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7.16
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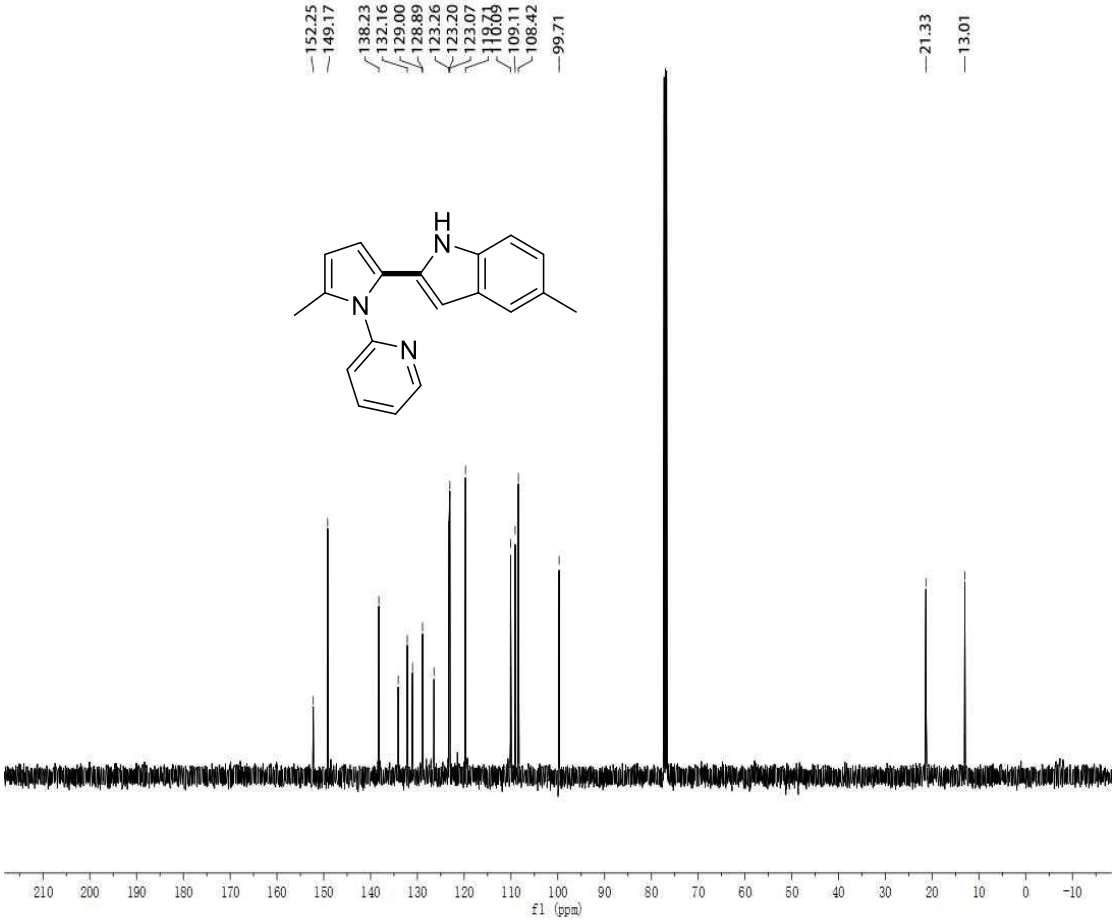
7.11
6.45
6.44
6.12
6.12
6.12
6.12
5.77
5.77
5.77
5.77
2.39
2.19
H
N
N
N
0.97
0.97
1.04
1.01
1.02
1.02
1.03
1.09
1.05
1.01
1.00
3.09
3.07
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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123.20
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110.05
109.11
108.42
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13.01
H
N
N
N
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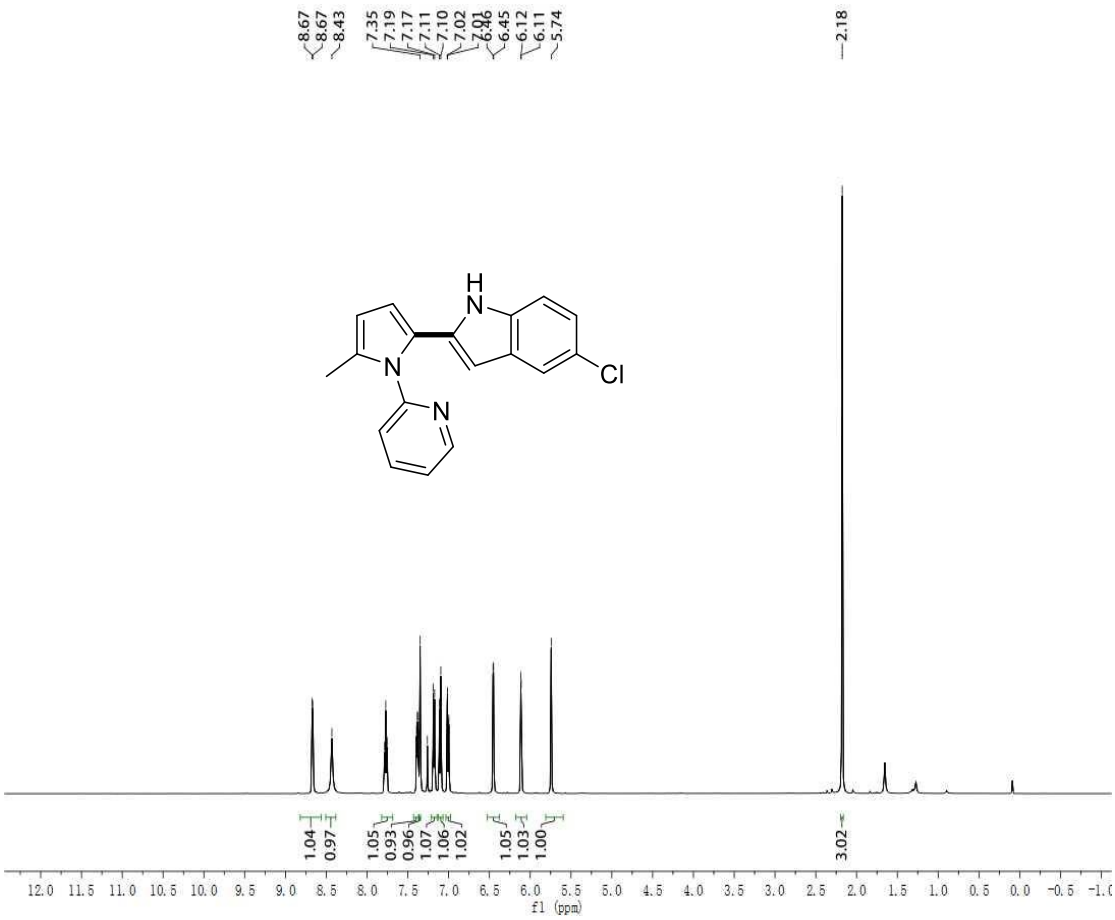
f1 (ppm)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7.10
7.02
7.01
6.46
6.45
6.12
6.11
5.74
2.18
H
N
N
N
Cl
1.04
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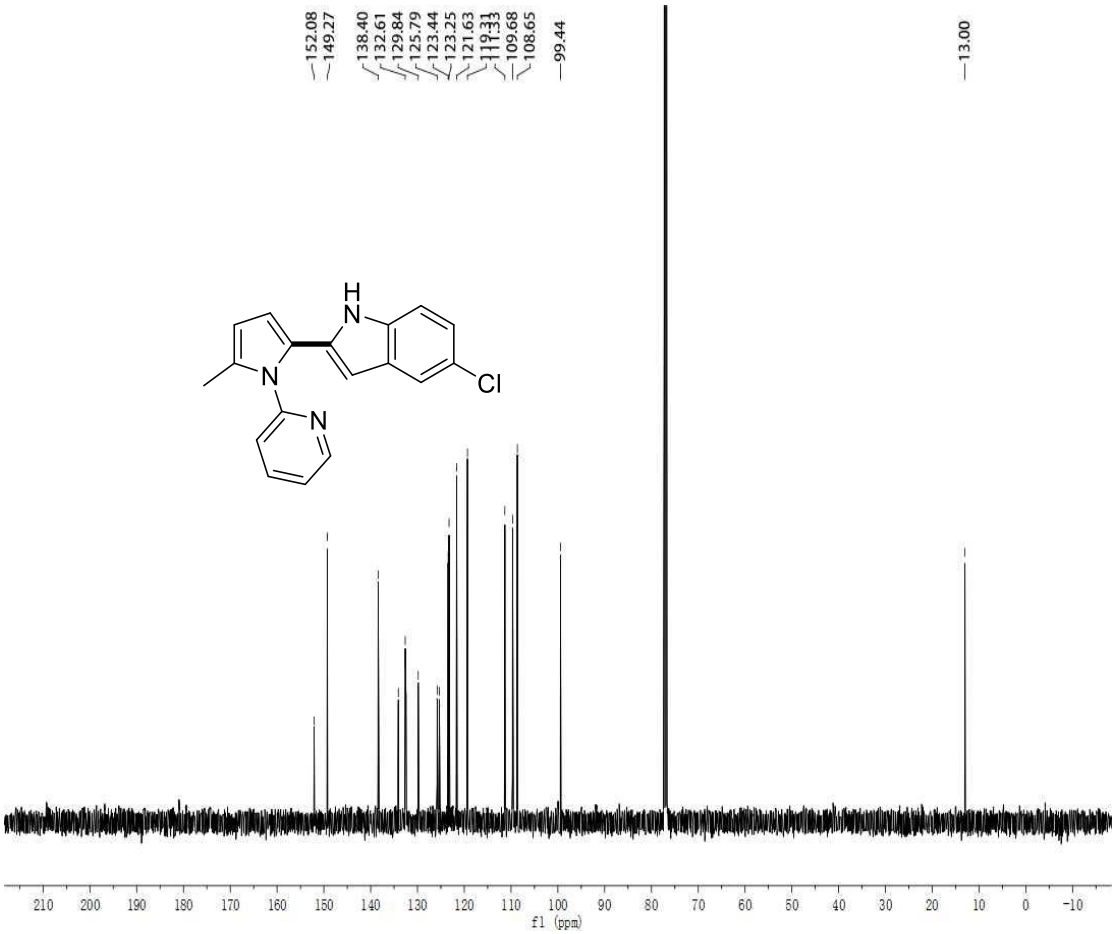
0.96
1.07
1.06
1.02
1.05
1.03
1.00
3.02
f1 (ppm)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132.61
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125.79
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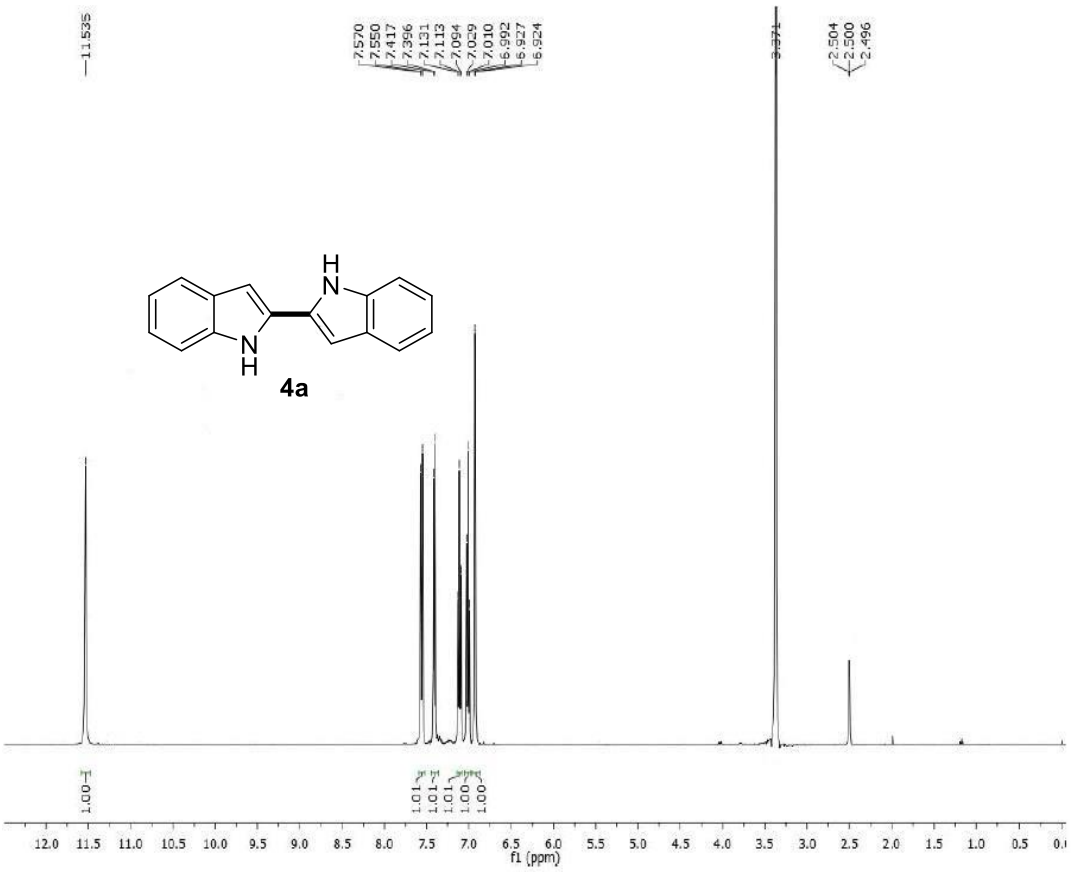
111.33
109.68
108.65
99.44
13.00
H
N
N
N
Cl
f1 (ppm)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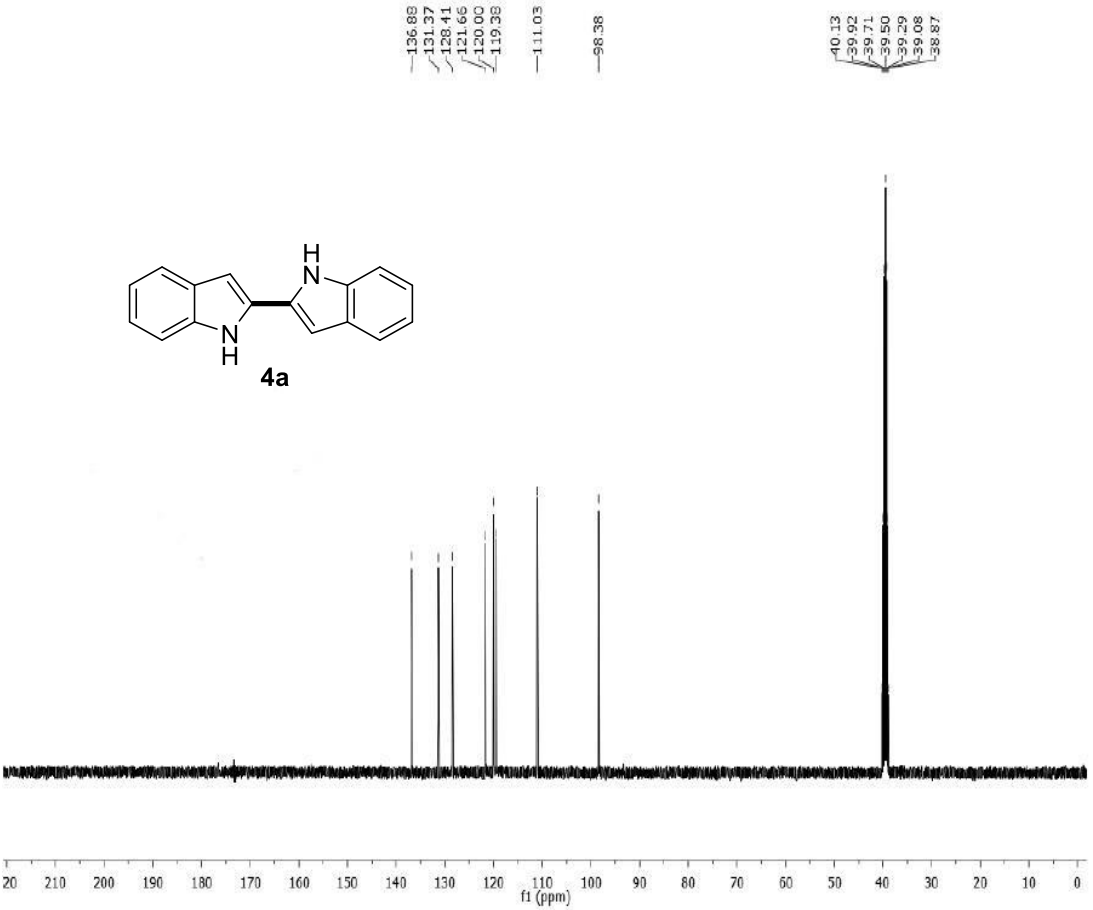
7.131
7.113
7.094
7.029
7.010
6.992
6.927
6.924
3.371
2.504
2.500
2.496
1.00
1.01
1.01
1.01
1.00
1.00
f1 (ppm)

4a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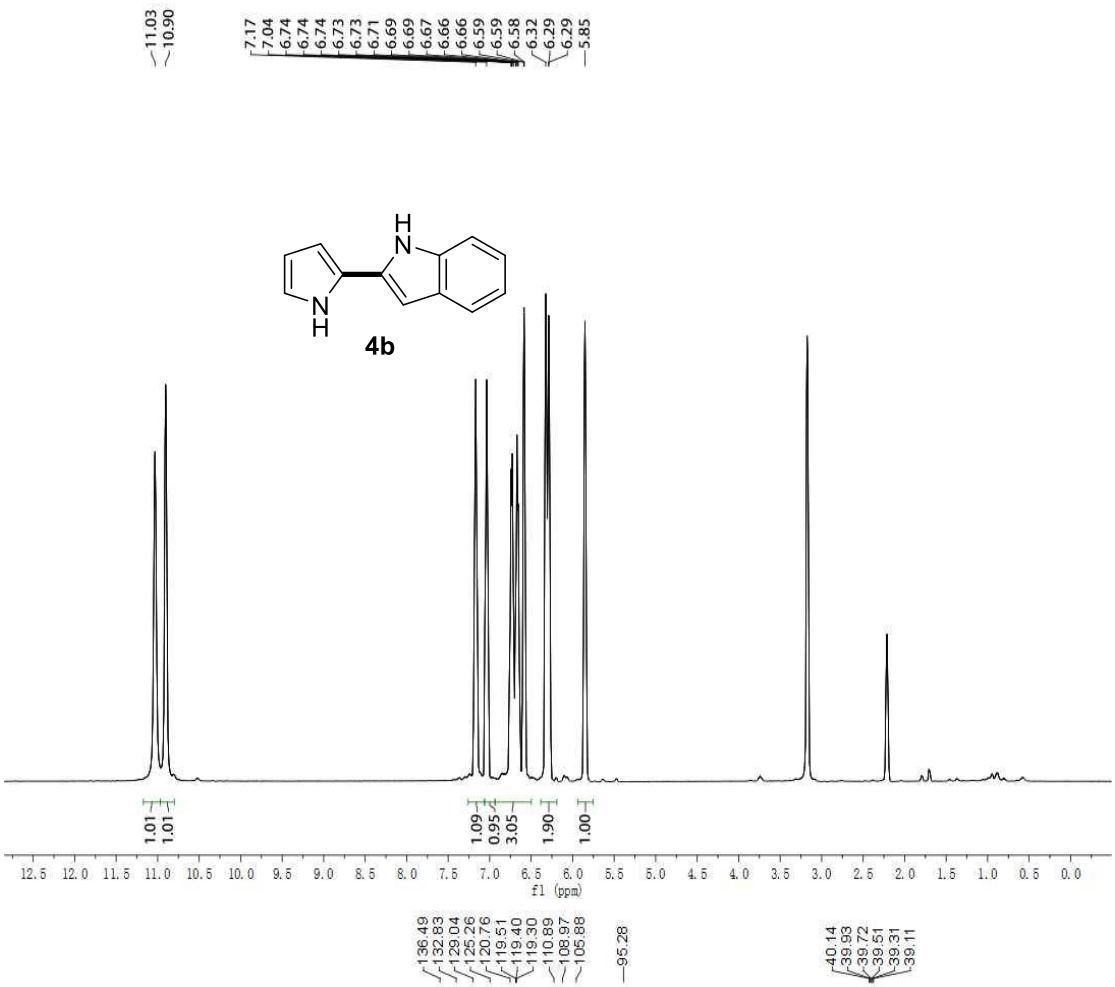
121.66
120.00
119.38
111.03
98.38
40.13
39.92
39.71
39.50
39.29
39.08
38.87
f1 (ppm)

4a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6.71
6.69
6.69
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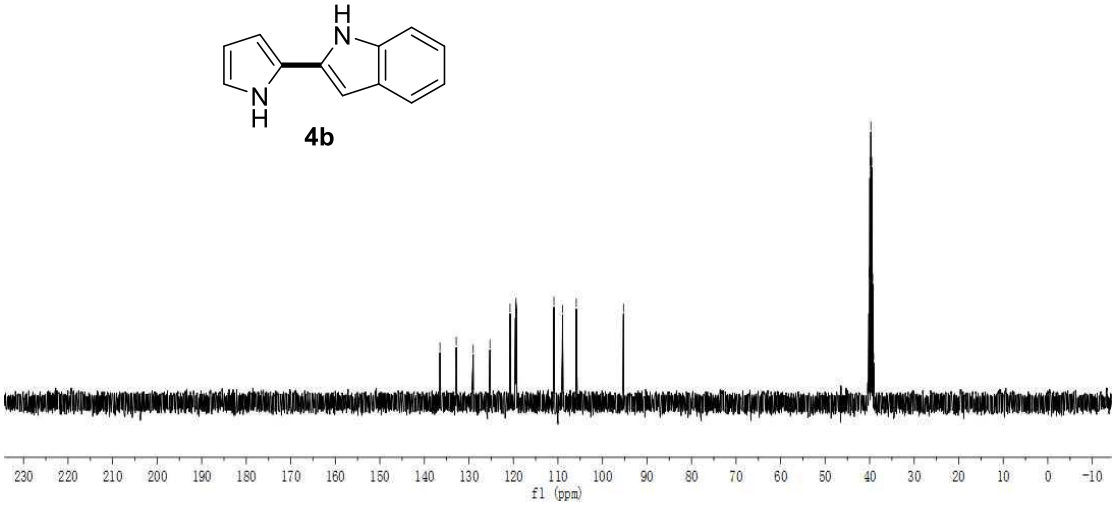
6.66
6.66
6.59
6.59
6.58
6.32
6.29
6.29
5.85
4b
1.01
1.01
1.09
0.95
3.05
1.90
1.00
f1 (ppm)
136.49
132.83
129.04
125.26
120.76
119.51
119.40
119.30
110.89
108.97
105.88
95.28
40.14
39.93
39.72
39.51
39.31
39.11


4b
f1 (ppm)