Supporting Information for

Direct C3-Arylations of 2-Indolylmethanols with Tryptamines and Tryptophols via An Umpolung Strategy

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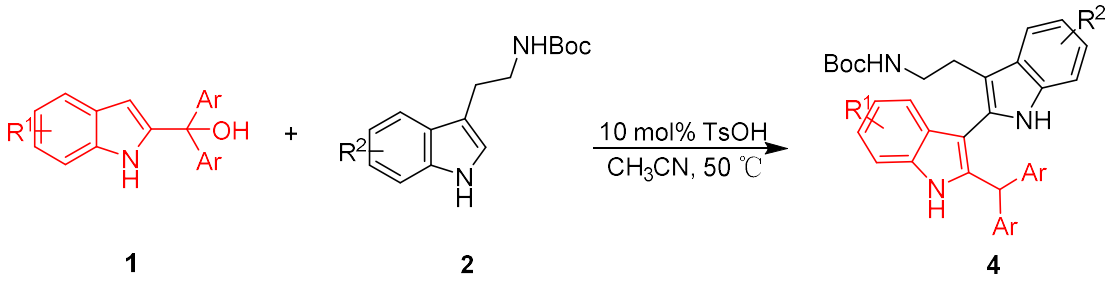
1. General information:

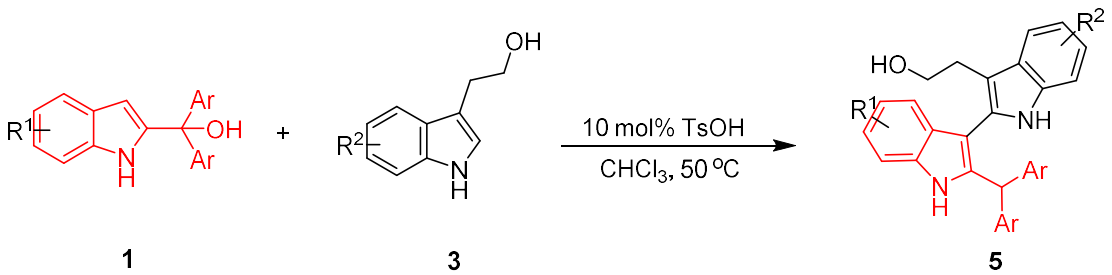
^{1}H and ^{13}C NMR spectra were measured at 400 and 100 MHz, respectively. The solvent used for NMR spectroscopy was $CDCl_3$ and acetone-d_6, using tetramethylsilane as the internal reference. HRMS (ESI) was determined by a HRMS/MS instrument. Analytical grade solvents for the column chromatography were used after distillation and commercially available reagents were used as received.

2. General procedure for the synthesis of products 4 and 5:



1 2 4

To the mixture of 2-indolylphenylmethanols **1** (0.1 mmol), tryptamines **2** (0.12 mmol), and TsOH (0.01 mmol) was added MeCN (1 mL), which was stirred at 50 °C for 12 h. After the completion of the reaction, which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography on silica gel to afford pure products **4**.

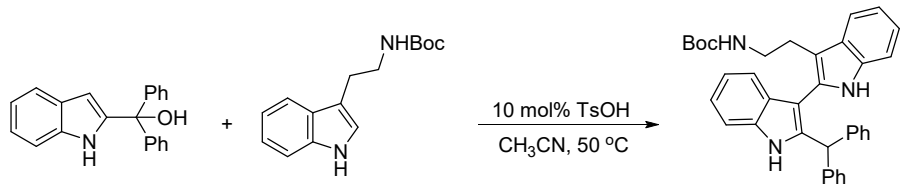


1 3 5

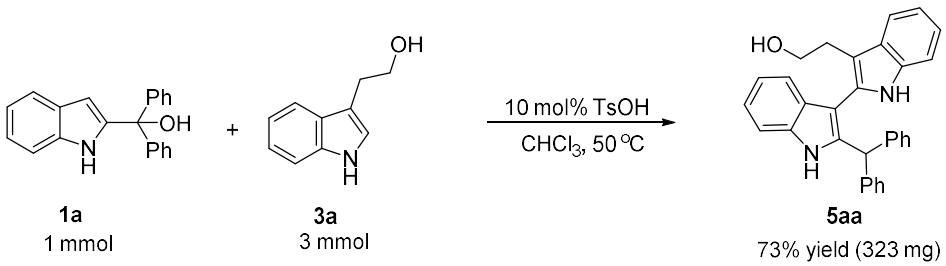
To the mixture of 2-indolylphenylmethanols **1** (0.1 mmol), tryptophols **3** (0.3 mmol), and TsOH (0.01 mmol) was added $CHCl_3$ (1 mL), which was stirred at 50 °C for 12 h. After the completion of the reaction, which was indicated by TLC, the

reaction mixture was directly purified through preparative thin layer chromatography on silica gel to afford pure products **5**.

3. Procedure for large scale synthesis of products 4aa and 5aa:



To the mixture of 2-indolylphenylmethanols **1a** (1 mmol), tryptamines **2a** (1.2 mmol), and TsOH (0.1 mmol) was added MeCN (10 mL), which was stirred at 50 °C for 12 h. After the completion of the reaction, which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel to afford pure product **4aa**.



To the mixture of 2-indolylphenylmethanols **1a** (1 mmol), tryptophols **3a** (3 mmol), and TsOH (0.1 mmol) was added $CHCl_3$ (10 mL), which was stirred at 50 °C for 12 h. After the completion of the reaction, which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel to afford pure product **5aa**.

4. Characterization of products 4 and 5:

***tert*-butyl (2-(2'-benzhydryl-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethyl)carbamate (4aa):** Preparative thin layer chromatography: petroleum ether/ethyl acetate = 10/1; reaction time = 12 h; yield: 84% (45.5 mg); yellow solid; m.p. 68-69 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.71 (d, *J* = 7.2 Hz, 1H), 7.64 (s, 1H), 7.44 (d, *J* = 7.8 Hz, 1H), 7.37 – 7.30 (m, 7H), 7.23 – 7.14 (m, 9H), 5.73 (s, 1H), 4.32 (s, 1H), 3.25 (s, 2H), 2.87 (t, *J* = 7.0 Hz, 2H), 1.37 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.8, 138.8, 136.0, 135.4, 128.9, 128.8, 128.5, 127.2, 122.3, 121.7, 120.6, 119.6, 119.3, 119.0, 112.1, 111.2, 110.7, 106.1, 78.8, 48.7, 40.9, 28.4, 25.4; IR (KBr): 3126, 1696, 1521, 1399, 1168, 745, 668, 649 cm^{-1}; ESI FTMS exact mass calcd for ($C_{36}H_{35}N_3O_2$+Na)$^+$ requires m/z 564.2627, found m/z 564.2623.

***tert*-butyl (2-(2'-benzhydryl-5'-methoxy-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethyl)carbamate (4ba):** Preparative thin layer chromatography: petroleum ether/ethyl acetate = 10/1; reaction time = 12 h; yield: 93% (53.1 mg); brown solid; m.p. 110-111 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (s, 1H), 7.70 (d, *J* = 7.3 Hz, 1H), 7.63 (s, 1H), 7.36 – 7.27 (m, 7H), 7.21 – 7.11 (m, 7H), 6.85 – 6.78 (m, 2H), 5.67 (s, 1H), 4.30 (s, 1H), 3.83 (s, 3H), 3.25 (s, 2H), 2.86 (t, *J* = 7.0 Hz, 2H), 1.37 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.6, 155.8, 137.3, 136.1, 135.9, 128.9, 128.8, 128.5, 127.1, 122.7, 121.6, 120.2, 119.3, 119.0, 111.9, 110.6, 110.3, 105.9, 94.9, 78.7, 55.7, 48.6, 40.9, 28.4, 25.4; IR (KBr): 3126, 1695, 1558, 1398, 1160, 744, 668, 654 cm^{-1}; ESI FTMS exact mass calcd for ($C_{37}H_{37}N_3O_3$+Na)$^+$ requires m/z 594.2733, found m/z 594.2735.

***tert*-butyl (2-(2'-benzhydryl-5'-chloro-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethyl)carbamate (4ca):** Preparative thin layer chromatography: petroleum ether/ethyl acetate = 10/1; reaction time = 12 h; yield: 70% (40.3 mg); yellow solid; m.p. 103-104 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.69 (d, *J* = 7.5 Hz, 1H), 7.59 (s, 1H), 7.39 – 7.28 (m, 7H), 7.25 – 7.05 (m, 9H), 5.70 (s, 1H), 4.29 (s, 1H), 3.22 (s, 2H), 2.83 (s, 2H), 1.35 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.7, 140.2, 136.0, 133.6, 129.7, 129.0, 128.7,

128.4, 128.2, 127.6, 127.3, 127.2, 126.4, 122.6, 121.9, 119.5, 119.1, 118.9, 112.3, 112.2, 110.7, 105.9, 78.8, 48.7, 40.9, 28.3, 25.4; IR (KBr): 3126, 1684, 1558, 1398, 1167, 745, 668, 648 cm^{-1}; ESI FTMS exact mass calcd for ($C_{36}H_{34}ClN_3O_2$+Na)$^+$ requires m/z 598.2238, found m/z 598.2235.

***tert*-butyl (2-(2'-benzhydryl-5'-bromo-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethyl)carbamate (4da):** Preparative thin layer chromatography: petroleum ether/ethyl acetate = 10/1; reaction time = 12 h; yield: 72% (44.6 mg); yellow solid; m.p. 68-69 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (s, 1H), 7.69 (d, *J* = 7.5 Hz, 1H), 7.60 (s, 1H), 7.54 (d, *J* = 1.4 Hz, 1H), 7.36 – 7.27 (m, 7H), 7.22 – 7.11 (m, 8H), 5.71 (s, 1H), 4.30 (s, 1H), 3.22 (s, 2H), 2.83 (s, 2H), 1.35 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.8, 145.1, 140.1, 136.0, 133.9, 129.0, 128.7, 128.4, 128.2, 127.6, 127.3, 127.2, 125.2, 122.0, 121.9, 119.5, 119.1, 113.9, 112.6, 110.7, 105.8, 78.8, 48.6, 40.9, 28.3, 25.4; IR (KBr): 3126, 1696, 1516, 1399, 1167, 745, 668, 472 cm^{-1}; ESI FTMS exact mass calcd for ($C_{36}H_{34}BrN_3O_2$+Na)$^+$ requires m/z 642.1732, found m/z 642.1733.

***tert*-butyl (2-(2'-benzhydryl-6'-methoxy-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethyl)carbamate (4ea):** Preparative thin layer chromatography: petroleum ether/ethyl acetate = 10/1; reaction time = 12 h; yield: 92% (52.6 mg); yellow solid; m.p. 118-119 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (s, 1H), 7.72 (d, *J* = 7.1 Hz, 1H), 7.58 (s, 1H), 7.38 – 7.28 (m, 6H), 7.24 – 7.13 (m, 8H), 6.89 – 6.81 (m, 2H), 5.69 (s, 1H), 4.32 (s, 1H), 3.75 (s, 3H), 3.26 (s, 2H), 2.88 (s, 2H), 1.37 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.8, 154.9, 139.4, 135.9, 130.3, 128.9, 128.8, 127.2, 121.7, 119.3, 119.0, 112.7, 111.9, 110.6, 105.9, 100.9, 78.8, 55.8, 48.8, 41.0, 28.3, 25.5; IR (KBr): 3126, 1696, 1521, 1399, 1168, 745, 668, 649 cm^{-1}; ESI FTMS exact mass calcd for ($C_{37}H_{37}N_3O_3$+Na)$^+$ requires m/z 594.2733, found m/z 594.2743

***tert*-butyl (2-(2'-benzhydryl-6'-chloro-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethyl)carbamate (4fa):** Preparative thin layer chromatography: petroleum ether/ethyl acetate = 10/1; reaction time = 12 h; yield: 76% (43.7 mg); yellow solid; m.p. 107-108 ºC; ^{1}H NMR (400

MHz, $CDCl_3$) δ 8.09 (s, 1H), 7.69 (d, *J* = 7.5 Hz, 1H), 7.63 (s, 1H), 7.36 – 7.29 (m, 8H), 7.21 – 7.08 (m, 8H), 5.70 (s, 1H), 4.30 (s, 1H), 3.22 (s, 2H), 2.83 (s, 2H), 1.36 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.7, 139.5, 136.0, 135.7, 129.0, 128.7, 128.4, 128.2, 128.1, 127.3, 127.2, 121.9, 121.3, 120.4, 119.4, 111.2, 110.7, 106.2, 78.9, 48.7, 40.9, 28.3, 25.4; IR (KBr): 3126, 1696, 1521, 1399, 1168, 745, 668, 649 cm^{-1}; ESI FTMS exact mass calcd for ($C_{36}H_{34}ClN_3O_2$+Na)$^+$ requires m/z 598.2238, found m/z 598.2240.

***tert*-butyl (2-(2'-benzhydryl-6'-bromo-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethyl)carbamate (4ga):** Preparative thin layer chromatography: petroleum ether/ethyl acetate = 10/1; reaction time = 12 h; yield: 71% (44.0 mg); yellow solid; m.p. 115-116 ºC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.08 (s, 1H), 7.69 (d, *J* = 7.5 Hz, 1H), 7.61 (s, 1H), 7.48 (d, *J* = 1.3 Hz, 1H), 7.36 – 7.28 (m, 7H), 7.24 – 7.12 (m, 8H), 5.69 (s, 1H), 4.30 (s, 1H), 3.22 (s, 2H), 2.82 (t, *J* = 6.5 Hz, 2H), 1.36 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.7, 139.4, 136.1, 136.0, 129.0, 128.7, 128.4, 127.8, 127.3, 123.9, 121.9, 120.8, 119.5, 119.1, 115.7, 114.1, 112.4, 110.7, 106.3, 78.1, 48.6, 40.9, 28.3, 25.4; IR (KBr): 3133, 1689, 1507, 1398, 1167, 744, 668, 490 cm^{-1}; ESI FTMS exact mass calcd for ($C_{36}H_{34}BrN_3O_2$+Na)$^+$ requires m/z 642.1732, found m/z 642.1740.

***tert*-butyl (2-(2'-benzhydryl-7'-bromo-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethyl)carbamate (4ha):** Preparative thin layer chromatography: petroleum ether/ethyl acetate = 10/1; reaction time = 12 h; yield: 60% (37.2 mg); brown solid; m.p. 92-93 ºC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.08 (s, 1H), 7.71 (d, *J* = 7.2 Hz, 1H), 7.60 (s, 1H), 7.39 – 7.30 (m, 8H), 7.22 – 7.11 (m, 7H), 7.02 (t, *J* = 7.8 Hz, 1H), 5.72 (s, 1H), 4.31 (s, 1H), 3.25 (s, 2H), 2.85 (t, *J* = 6.8 Hz, 2H), 1.35 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.7, 139.4, 136.0, 134.1, 129.6, 129.0, 128.7, 128.4, 127.8, 127.4, 124.7, 121.9, 121.8, 119.5, 119.1, 118.8, 112.5, 110.7, 107.4, 104.7, 78.8, 48.7, 40.9, 28.3, 25.5; IR (KBr): 3133, 1695, 1540, 1398, 1168, 740, 668, 658 cm^{-1}; ESI FTMS exact mass calcd for ($C_{36}H_{34}BrN_3O_2$+Na)$^+$ requires m/z 642.1732, found m/z 642.1736.

***tert*-butyl**

2-(2'-(di-m-tolylmethyl)-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethyl)carbamate (4ia): Preparative thin layer chromatography: petroleum ether/ethyl acetate = 10/1; reaction time = 12 h; yield: 73% (41.6 mg); yellow solid; m.p. 101-102 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.72 (d, *J* = 7.3 Hz, 1H), 7.61 (s, 1H), 7.44 (d, *J* = 7.8 Hz, 1H), 7.35 (d, *J* = 8.1 Hz, 1H), 7.28 – 7.09 (m, 11H), 6.96 (s, 2H), 5.63 (s, 1H), 4.28 (s, 1H), 3.25 (s, 2H), 2.87 (t, *J* = 7.4 Hz, 2H), 2.31 (s, 6H), 1.37 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.7, 139.0, 138.6, 135.9, 135.3, 129.5, 128.8, 128.6, 127.9, 125.8, 122.2, 121.6, 120.5, 119.6, 119.3, 119.1, 112.1, 111.1, 110.6, 105.9, 78.7, 48.6, 41.0, 28.4, 25.5, 21.5, 18.4; IR (KBr): 3126, 1696, 1521, 1457, 1399, 742, 668, 457 cm^{-1}; ESI FTMS exact mass calcd for ($C_{38}H_{39}N_3O_2$+Na)$^+$ requires m/z 592.2940, found m/z 592.2943.

***tert*-butyl**

(2-(2'-(bis(3-methoxyphenyl)methyl)-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethyl)carbamate (4ja): Preparative thin layer chromatography: petroleum ether/ethyl acetate = 10/1; reaction time = 12 h; yield: 70% (42.1 mg); yellow solid; m.p. 89-90 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (s, 1H), 7.76 – 7.61 (m, 2H), 7.42 (d, *J* = 7.8 Hz, 1H), 7.33 (d, *J* = 8.1 Hz, 1H), 7.27 (s, 1H), 7.26 – 7.09 (m, 7H), 6.85 – 6.67 (m, 6H), 5.63 (s, 1H), 4.36 (s, 1H), 3.74 (s, 6H), 3.24 (s, 2H), 2.87 (t, *J* = 6.3 Hz, 2H), 1.36 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 155.7, 138.4, 135.9, 135.3, 129.9, 128.6, 128.4, 122.3, 121.6, 121.1, 120.5, 119.6, 119.3, 119.1, 115.0, 112.2, 112.0, 111.1, 110.6, 106.1, 78.7, 55.2, 48.6, 41.0, 28.3, 25.5; IR (KBr): 3126, 1696, 1521, 1399, 1168, 745, 668, 649 cm^{-1}; ESI FTMS exact mass calcd for ($C_{38}H_{39}N_3O_4$+Na)$^+$ requires m/z 624.2839, found m/z 624.2841.

***tert*-butyl**

(2-(2'-(bis(4-fluorophenyl)methyl)-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethyl)carbamate (4ka): Preparative thin layer chromatography: petroleum ether/ethyl acetate = 10/1; reaction time = 12 h; yield: 63% (36.4 mg); yellow solid; m.p. 110-111 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.69 (d, *J* = 7.9 Hz, 2H), 7.43 (d, *J* = 7.8 Hz, 1H), 7.35 (d, *J* = 8.1 Hz, 1H), 7.25 – 6.99 (m, 14H), 5.69 (s, 1H), 4.34 (s, 1H), 3.25 (s, 2H),

2.84 (t, *J* = 6.5 Hz, 2H), 1.34 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.8 (d, *J* = 247.0 Hz), 155.7, 138.2, 136.0, 135.5, 130.3, 130.2, 128.5, 128.3, 122.6, 121.9, 120.8, 119.5, 119.0, 115.8 (d, *J* = 21.4 Hz), 112.2, 111.2, 110.7, 106.3, 78.9, 47.1, 40.9, 28.3, 25.4; IR (KBr): 3122, 1694, 1507, 1398, 1158, 744, 711, 565 cm^{-1}; ESI FTMS exact mass calcd for ($C_{36}H_{33}F_2N_3O_2$+Na)$^+$ requires m/z 600.2439, found m/z 600.2442.

***tert*-butyl (2-(2'-benzhydryl-4-methyl-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethyl)carbamate (4ab):** Preparative thin layer chromatography: petroleum ether/ethyl acetate = 10/1; reaction time = 12 h; yield: 65% (36.1 mg); brown solid; m.p. 107-108 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (s, 1H), 7.58 (s, 1H), 7.43 (d, *J* = 7.8 Hz, 1H), 7.37 – 7.28 (m, 7H), 7.23 – 7.11 (m, 6H), 7.08 – 6.99 (m, 2H), 6.89 (d, *J* = 6.9 Hz, 1H), 5.70 (s, 1H), 4.31 (s, 1H), 3.18 (d, *J* = 40.4 Hz, 2H), 3.00 (s, 2H), 2.79 (s, 3H), 1.33 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.7, 138.9, 136.3, 135.4, 130.6, 128.9, 128.7, 128.5, 127.2, 126.8, 122.3, 121.6, 121.3, 120.6, 119.6, 112.8, 111.1, 108.6, 106.1, 78.7, 48.7, 42.7, 28.3, 26.5, 20.4; IR (KBr): 3122, 1716, 1516, 1398, 1168, 745, 700, 668 cm^{-1}; ESI FTMS exact mass calcd for ($C_{37}H_{37}N_3O_2$+Na)$^+$ requires m/z 578.2784, found m/z 578.2788.

***tert*-butyl (2-(2'-benzhydryl-4-fluoro-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethyl)carbamate (4ac):** Preparative thin layer chromatography: petroleum ether/ethyl acetate = 10/1; reaction time = 12 h; yield: 62% (34.7 mg); yellow solid; m.p. 94-95 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.56 (s, 1H), 7.43 (d, *J* = 7.8 Hz, 1H), 7.38 – 7.28 (m, 7H), 7.24 – 7.10 (m, 6H), 7.08 – 6.99 (m, 1H), 6.90 (d, *J* = 7.7 Hz, 1H), 6.80 – 6.72 (m, 1H), 5.73 (s, 1H), 4.35 (s, 1H), 3.30 (s, 2H), 2.92 (s, 2H), 1.28 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.6, 139.2, 138.5 (d, *J* = 11.9 Hz), 135.2, 130.0, 129.0, 128.0, 128.2, 127.2, 122.3, 122.0, 120.7, 119.4, 111.1, 106.7, 105.3, 104.6 (d, *J* = 20.5 Hz), 78.6, 48.7, 41.6, 28.2, 26.2; IR (KBr): 3123, 1697, 1521, 1457, 1399, 746, 668, 649 cm^{-1}; ESI FTMS exact mass calcd for ($C_{36}H_{34}FN_3O_2$+Na)$^+$ requires m/z 582.2533, found m/z 582.2536.

***tert*-butyl (2-(2'-benzhydryl-5-methyl-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethyl)carbamate (4ad):** Preparative thin layer chromatography: petroleum ether/ethyl acetate = 10/1; reaction time = 12 h; yield: 93% (51.6 mg); yellow solid; m.p. 114-115 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.49 (s, 1H), 7.42 (d, *J* = 7.9 Hz, 1H), 7.38 – 7.27 (m, 7H), 7.23 – 7.06 (m, 7H), 7.00 (t, *J* = 9.0 Hz, 1H), 5.71 (s, 1H), 4.31 (s, 1H), 3.25 (s, 2H), 2.84 (t, *J* = 6.5 Hz, 2H), 2.50 (s, 3H), 1.36 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.8, 138.8, 138.7, 136.4, 135.4, 134.3, 131.6, 128.9, 128.8, 128.6, 128.5, 127.8, 127.2, 126.3, 123.2, 122.3, 121.0, 120.6, 119.6, 118.7, 111.9, 111.7, 111.1, 110.6, 110.3, 106.2, 78.7, 48.6, 41.0, 28.4, 25.4, 21.7; IR (KBr): 3126, 1696, 1521, 1399, 1168, 745, 668, 649 cm^{-1}; ESI FTMS exact mass calcd for ($C_{37}H_{37}N_3O_2$+Na)$^+$ requires m/z 578.2784, found m/z 578.2785.

***tert*-butyl (2-(2'-benzhydryl-5-methoxy-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethyl)carbamate (4ae):** Preparative thin layer chromatography: petroleum ether/ethyl acetate = 10/1; reaction time = 12 h; yield: 96% (54.8 mg); brown solid; m.p. 70-71 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (s, 1H), 7.60 (s, 1H), 7.45 (d, *J* = 7.8 Hz, 1H), 7.39 – 7.27 (m, 8H), 7.23 – 7.09 (m, 8H), 6.89 – 6.84 (m, 1H), 5.74 (s, 1H), 4.37 (s, 1H), 3.91 (s, 3H), 3.25 (s, 2H), 2.85 (t, *J* = 6.6 Hz, 2H), 1.38 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.8, 154.0, 138.7, 135.4, 131.2, 129.5, 128.9, 128.8, 128.4, 127.2, 122.3, 120.6, 119.6, 111.8, 111.4, 111.1, 106.2, 100.9, 77.8, 56.1, 48.7, 40.8, 28.4, 25.4; IR (KBr): 3126, 1696, 1507, 1399, 1170, 745, 668, 649 cm^{-1}; ESI FTMS exact mass calcd for ($C_{37}H_{37}N_3O_3$+Na)$^+$ requires m/z 594.2733, found m/z 594.2736.

***tert*-butyl (2-(2'-benzhydryl-5-fluoro-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethyl)carbamate (4af):** Preparative thin layer chromatography: petroleum ether/ethyl acetate = 10/1; reaction time = 12 h; yield: 63% (35.3 mg); yellow solid; m.p. 106-107 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.54 (s, 1H), 7.42 (d, *J* = 7.8 Hz, 1H), 7.39 – 7.27 (m, 8H), 7.24 – 7.03 (m, 7H), 6.95 – 6.85 (m, 1H), 5.70 (s, 1H), 4.30 (s, 1H), 3.19 (s, 2H), 2.81 (t, *J* = 7.0 Hz, 2H), 1.36 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ157.7 (d, *J* =

234.7 Hz), 155.7, 138.8, 135.3, 132.4, 130.4, 129.0, 128.8, 128.3, 127.2, 122.4, 120.7, 119.5, 111.2, 109.8 (d, J = 26.9 Hz), 105.8, 78.9, 48.7, 40.9, 28.3, 25.4; IR (KBr): 3126, 1684, 1521, 1472, 1399, 1172, 745, 668 cm^{-1}; ESI FTMS exact mass calcd for ($C_{36}H_{34}FN_3O_2$+Na)$^+$ requires m/z 582.2533, found m/z 582.2534.

***tert*-butyl (2-(2'-benzhydryl-5-bromo-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethyl)carbamate (4ag):** Preparative thin layer chromatography: petroleum ether/ethyl acetate = 10/1; reaction time = 12 h; yield: 62% (38.4 mg); brown solid; m.p. 112-113 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (s, 1H), 7.78 (s, 1H), 7.62 (s, 1H), 7.45 – 7.26 (m, 9H), 7.24 – 7.10 (m, 7H), 7.03 (d, J = 8.4 Hz, 1H), 5.69 (s, 1H), 4.31 (s, 1H), 3.18 (s, 2H), 2.80 (t, J = 6.8 Hz, 2H), 1.37 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.7, 139.0, 135.3, 134.5, 130.3, 129.9, 129.0, 128.8, 128.3, 127.3, 124.4, 122.4, 121.4, 120.7, 119.4, 112.6, 112.0, 111.2, 105.5, 78.9, 48.7, 41.0, 28.3, 25.3; IR (KBr): 3123, 1696, 1521, 1398, 1363, 1168, 745, 668 cm^{-1}; ESI FTMS exact mass calcd for ($C_{36}H_{34}BrN_3O_2$+Na)$^+$ requires m/z 642.1732, found m/z 642.1735.

***tert*-butyl (2-(2'-benzhydryl-6-methyl-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethyl)carbamate (4ah):** Preparative thin layer chromatography: petroleum ether/ethyl acetate = 10/1; reaction time = 12 h; yield: 71% (39.4 mg); yellow solid; m.p. 107-108 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (s, 1H), 7.60 (d, J = 7.8 Hz, 1H), 7.51 (s, 1H), 7.43 (d, J = 7.8 Hz, 1H), 7.37 – 7.28 (m, 7H), 7.23 – 7.12 (m, 6H), 7.00 (d, J = 7.8 Hz, 2H), 5.72 (s, 1H), 4.32 (s, 1H), 3.26 (s, 2H), 2.84 (t, J = 6.7 Hz, 2H), 2.48 (s, 3H), 1.37 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.8, 138.7, 136.4, 135.4, 131.6, 128.9, 128.8, 128.5, 127.8, 127.2, 126.3, 122.3, 121.0, 120.5, 119.6, 118.7, 111.9, 111.1, 110.6, 106.3, 78.8, 48.6, 40.9, 28.4, 25.5, 21.7; IR (KBr): 3126, 1696, 1576, 1399, 1168, 745, 668, 649 cm^{-1}; ESI FTMS exact mass calcd for ($C_{37}H_{37}N_3O_2$+Na)$^+$ requires m/z 578.2784, found m/z 578.2785.

***tert*-butyl (2-(2'-benzhydryl-6-chloro-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethyl)carbamate (4ai):** Preparative thin layer chromatography: petroleum ether/ethyl acetate = 10/1; reaction

time = 12 h; yield: 81% (46.6 mg); yellow solid; m.p. 87-88 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.61 – 7.52 (m, 2H), 7.41 – 7.30 (m, 9H), 7.23 – 7.08 (m, 8H), 5.69 (s, 1H), 4.28 (s, 1H), 3.20 (s, 2H), 2.83 (t, *J* = 7.0 Hz, 2H), 1.36 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.9, 138.9, 136.2, 135.3, 129.0, 128.8, 128.2, 128.1, 127.7 127.5, 127.3, 127.2, 122.4, 122.2, 120.7, 120.0, 119.8, 119.4, 111.2, 110.5, 105.6, 103.1, 78.9, 48.7, 28.3, 25.4; IR (KBr): 3126, 1670, 1521, 1399, 1339, 747, 668, 649 cm^{-1}; ESI FTMS exact mass calcd for ($C_{36}H_{34}ClN_3O_2$+Na)$^+$ requires m/z 598.2238, found m/z 598.2242.

***tert*-butyl (2-(2'-benzhydryl-7-methyl-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethyl)carbamate (4aj):** Preparative thin layer chromatography: petroleum ether/ethyl acetate = 10/1; reaction time = 12 h; yield: 65% (36.1 mg); brown solid; m.p. 90-91 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (s, 1H), 7.57 (d, *J* = 7.6 Hz, 1H), 7.46 (d, *J* = 7.5 Hz, 2H), 7.41 – 7.29 (m, 7H), 7.24 – 7.12 (m, 6H), 7.07 (t, *J* = 7.5 Hz, 1H), 6.97 (d, *J* = 7.1 Hz, 1H), 5.74 (s, 1H), 4.37 (s, 1H), 3.32 (s, 2H), 2.93 (s, 2H), 2.16 (s, 3H), 1.37 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.8, 138.7, 135.4, 135.3, 129.0, 128.8, 128.3, 127.9, 127.3, 122.3, 122.2, 120.6, 119.7, 119.6, 116.7, 112.2, 111.2, 106.2, 78.8, 48.8, 40.9, 28.4, 25.6, 16.1; IR (KBr): 3126, 1695, 1507, 1399, 1167, 745, 668, 648 cm^{-1}; ESI FTMS exact mass calcd for ($C_{37}H_{37}N_3O_2$+Na)$^+$ requires m/z 578.2784, found m/z 578.2786.

***N*-(2-(2'-benzhydryl-5-methoxy-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethyl)acetamide (4ak):** Preparative thin layer chromatography: Dichloromethane / Methanol = 40/1; reaction time = 12 h; yield: 62% (31.8 mg); yellow solid; m.p. 46-47 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.63 (s, 1H), 7.44 (s, 1H), 7.36 – 7.28 (m, 7H), 7.21 (t, *J* = 7.6 Hz, 2H), 7.16 – 7.11 (m, 6H), 6.88 – 6.84 (m, 1H), 5.71 (s, 1H), 5.14 (s, 1H), 3.89 (s, 3H), 3.37 – 3.23 (m, 2H), 2.80 (t, *J* = 6.9 Hz, 2H), 1.62 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.8, 154.1, 138.6, 135.4, 131.1, 129.8, 129.2, 128.9, 128.8, 128.7, 128.5, 128.3, 127.2, 122.5, 120.7, 119.3, 112.1, 112.0, 111.5, 111.3, 106.1, 100.5, 56.0, 48.6, 39.9, 24.8, 23.1 cm^{-1}; ESI FTMS exact mass calcd for ($C_{34}H_{31}N_3O_2$ -H)$^-$ requires m/z 512.2333, found m/z 512.2341.

***N*-(2-(2'-benzhydryl-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethyl)-4-methylbenzenesulfo namide (4al):** Preparative thin layer chromatography: Toluene/ ethyl acetate = 10/1; reaction time = 12 h; yield: 76% (45.2 mg); yellow solid; m.p. 57-58 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.55 (s, 1H), 7.49 – 7.41 (m, 3H), 7.37 – 7.30 (m, 8H), 7.23 (t, *J* = 7.4 Hz, 2H), 7.17 – 7.10 (m, 7H), 7.06 (d, *J* = 8.0 Hz, 2H), 5.66 (s, 1H), 4.07 (t, *J* = 6.0 Hz, 1H), 3.08 (s, 2H), 2.79 (t, *J* = 7.1 Hz, 2H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.9, 138.9, 136.7, 135.9, 135.3, 129.4, 129.0, 128.9, 128.8, 128.2, 128.0, 127.3, 126.9, 122.4, 121.9, 120.7, 119.5, 119.4, 118.4, 111.2, 110.8, 110.5, 105.6, 48.7, 43.1, 25.2, 21.5; IR (KBr): 3358, 3056, 1598, 1456, 1324, 1156, 908, 744 cm^{-1}; ESI FTMS exact mass calcd for $(C_{38}H_{33}N_3O_2S$ -H)$^-$ requires m/z 594.2210, found m/z 594.2223.

benzyl (2-(2'-benzhydryl-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethyl)carbamate (4am): Preparative thin layer chromatography: petroleum ether / ethyl acetate = 3/1; reaction time = 12 h; yield: 65% (37.4 mg); white solid; m.p. 58-59 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (s, 1H), 7.71 (d, *J* = 7.6 Hz, 1H), 7.62 (s, 1H), 7.43 (d, *J* = 7.9 Hz, 1H), 7.37 – 7.27 (m, 11H), 7.25 – 7.04 (m, 10H), 5.72 (s, 1H), 5.00 (s, 2H), 4.52 (s, 1H), 3.33 (s, 2H), 2.90 (t, *J* = 7.2 Hz, 2H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.1, 138.8, 136.7, 135.9, 135.3, 128.9, 128.8, 128.5, 128.4, 128.4, 127.9, 127.9, 127.2, 122.4, 121.8, 120.6, 119.5, 119.4, 118.8, 111.8, 111.2, 110.7, 106.0, 66.3, 48.7, 41.4, 25.3; IR (KBr): 3000, 1700, 1457, 1233, 1028, 907, 744, 698 cm^{-1}; ESI FTMS exact mass calcd for $(C_{39}H_{33}N_3O_2$ -H)$^-$ requires m/z 574.2489, found m/z 574.2495.

2-(2'-benzhydryl-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethanol (5aa): Preparative thin layer chromatography: petroleum ether/ethyl acetate = 5/1; reaction time = 12 h; yield: 67% (29.6 mg); yellow solid; m.p. 111-112 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.69 (d, *J* = 7.1 Hz, 1H), 7.58 (s, 1H), 7.44 (d, *J* = 7.8 Hz, 1H), 7.39 – 7.27 (m, 7H), 7.24 – 7.09 (m, 9H), 5.72 (s, 1H), 3.72 (t, *J* = 6.8 Hz, 2H), 2.99 (t, *J* = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.8, 136.0, 135.4, 129.0, 128.9, 128.8, 128.7, 128.6, 128.3, 127.2, 122.3, 121.7, 120.6, 119.6, 119.4, 118.7, 111.2, 111.1, 110.7,

106.2, 63.0, 48.7, 28.6; IR (KBr): 3056, 1598, 1453, 1326, 1234, 1041, 744, 701, 486 cm^{-1}; ESI FTMS exact mass calcd for ($C_{31}H_{26}N_2O+Na)^+$ requires m/z 465.1943, found m/z 465.1930.

2-(2'-benzhydryl-5'-chloro-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethanol (5ca): Preparative thin layer chromatography: petroleum ether/ethyl acetate = 5/1; reaction time = 12 h; yield: 80% (38.1 mg); yellow solid; m.p. 98-99 ºC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.09 (s, 1H), 7.68 (d, *J* = 7.4 Hz, 1H), 7.57 (s, 1H), 7.43 – 7.28 (m, 7H), 7.25 – 7.10 (m, 9H), 5.71 (s, 1H), 3.71 (t, *J* = 6.8 Hz, 2H), 2.97 (t, *J* = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.3, 136.0, 133.6, 129.5, 129.0, 128.7, 128.5, 128.1, 127.3, 126.4, 122.6, 121.9, 119.5, 119.0, 118.8, 112.2, 111.4, 110.8, 105.9, 62.9, 48.7, 28.6; IR (KBr): 3056, 2924, 1463, 1296, 1008, 1041, 799, 745, 492 cm^{-1}; ESI FTMS exact mass calcd for ($C_{31}H_{25}ClN_2O+Na)^+$ requires m/z 499.1553, found m/z 499.1551.

2-(2'-benzhydryl-6'-chloro-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethanol (5fa): Preparative thin layer chromatography: petroleum ether/ethyl acetate = 5/1; reaction time = 12 h; yield: 79% (37.6 mg); yellow solid; m.p. 90-91 ºC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.67 (d, *J* = 7.4 Hz, 1H), 7.60 (s, 1H), 7.42 – 7.27 (m, 8H), 7.24 – 7.07 (m, 8H), 5.70 (s, 1H), 3.70 (t, *J* = 6.8 Hz, 2H), 2.96 (t, *J* = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.5, 136.0, 135.7, 129.0, 128.7, 128.5, 128.3, 128.2, 127.3, 126.9, 121.9, 121.3, 120.4, 119.5, 118.8, 111.3, 111.2, 110.8, 106.3, 62.9, 48.7, 28.5; IR (KBr): 3427, 2924, 1599, 1451, 1323, 1007, 807, 744, 518 cm^{-1}; ESI FTMS exact mass calcd for ($C_{31}H_{25}ClN_2O+Na)^+$ requires m/z 499.1553, found m/z 499.1549.

2-(2'-benzhydryl-6'-bromo-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethanol (5ga): Preparative thin layer chromatography: petroleum ether/ethyl acetate = 5/1; reaction time = 12 h; yield: 72% (37.4 mg); brown solid; m.p. 60-61 ºC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.67 (d, *J* = 7.4 Hz, 1H), 7.60 (s, 1H), 7.46 (d, *J* = 1.5 Hz, 1H), 7.39 – 7.27 (m, 7H), 7.25 – 7.09 (m, 8H), 5.70 (s, 1H), 3.69 (t, *J* = 6.8 Hz, 2H), 2.95 (t, *J* = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.5, 136.1, 136.0, 129.0, 128.7, 128.5, 128.2, 127.8, 127.2, 123.9, 121.9, 120.8, 119.5, 118.8, 115.7, 114.1, 111.4,

110.8, 106.4, 62.9, 48.6, 28.5; IR (KBr): 3056, 2340, 1598, 1451, 1324, 1282, 744, 700, 489 cm^{-1}; ESI FTMS exact mass calcd for ($C_{31}H_{25}BrN_2O+Na)^+$ requires m/z 543.1048, found m/z 543.1043.

2-(2'-benzhydryl-7'-bromo-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethanol (5ha): Preparative thin layer chromatography: petroleum ether/ethyl acetate = 5/1; reaction time = 12 h; yield: 60% (31.2 mg); brown solid; m.p. 82-83 ºC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.11 (s, 1H), 7.70 (d, *J* = 7.3 Hz, 1H), 7.61 (s, 1H), 7.40 – 7.29 (m, 8H), 7.22 – 7.00 (m, 8H), 5.73 (s, 1H), 3.72 (t, *J* = 6.8 Hz, 2H), 2.97 (t, *J* = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.5, 136.0, 134.1, 129.5, 129.1, 128.7, 128.5, 128.3, 127.4, 124.7, 122.0, 121.8, 119.5, 118.8, 111.5, 110.8, 107.5, 104.7, 63.0, 48.7, 28.6; IR (KBr): 3425, 3057, 1518, 1446, 1323, 1031, 780, 700, 487 cm^{-1}; ESI FTMS exact mass calcd for ($C_{31}H_{25}BrN_2O+Na)^+$ requires m/z 543.1048, found m/z 543.1040.

2-(2'-(bis(3-fluorophenyl)methyl)-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethanol (5la): Preparative thin layer chromatography: petroleum ether/ethyl acetate = 5/1; reaction time = 12 h; yield: 72% (34.4 mg); yellow solid; m.p. 105-106 ºC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.75 – 7.64 (m, 2H), 7.45 (d, *J* = 7.9 Hz, 1H), 7.41 – 7.26 (m, 4H), 7.24 – 6.80 (m, 10H), 5.73 (s, 1H), 3.72 (t, *J* = 6.8 Hz, 2H), 2.96 (t, *J* = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.1 (d, *J* = 247.6 Hz), 137.3, 136.1, 135.5, 130.5 (d, *J* = 8.3 Hz), 128.6 (d, *J* = 9.1 Hz), 128.3, 124.4, 122.8, 122.0, 120.8, 119.7, 119.5, 118.8, 115.7 (d, *J* = 22.1 Hz), 114.4 (d, *J* = 21.0 Hz), 111.5, 111.3, 110.8, 106.8, 62.9, 48.0, 28.5; IR (KBr): 3446, 3057, 2921, 1588, 1485, 1238, 1041, 787, 743, 522 cm^{-1}; ESI FTMS exact mass calcd for ($C_{31}H_{24}F_2N_2O+Na)^+$ requires m/z 501.1755, found m/z 501.1755.

2-(2'-benzhydryl-5-fluoro-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethanol (5ab): Preparative thin layer chromatography: petroleum ether/ethyl acetate = 5/1; reaction time = 12 h; yield: 67% (30.8 mg); gray solid; m.p. 100-101 ºC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.31 (s, 1H), 7.99 (s, 1H), 7.57 (d, *J* = 7.8 Hz, 1H), 7.38 – 7.27 (m, 11H), 7.25 – 7.09 (m, 4H), 6.95 – 6.87 (m, 1H), 6.41 (d, *J* = 1.5 Hz, 1H), 3.23 (t, *J* = 7.1 Hz, 2H), 2.52 (t, *J* = 7.1 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.8 (d, *J* = 233 Hz), 138.9, 135.3, 132.4, 130.9, 129.8, 129.0, 128.7, 128.3, 128.2, 127.5, 127.2, 122.4,

120.7, 120.1, 119.5, 111.2, 109.9 (d, J = 26.3 Hz), 105.9, 103.6, 62.8, 48.7, 28.5; IR (KBr): 3125, 1716, 1487, 1399, 1261, 1177, 792, 746, 701 cm^{-1}; ESI FTMS exact mass calcd for ($C_{31}H_{25}FN_2O+Na)^+$ requires m/z 483.1849, found m/z 483.1840.

2-(2'-benzhydryl-5-methyl-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethanol (5ac): Preparative thin layer chromatography: petroleum ether/ethyl acetate = 5/1; reaction time = 12 h; yield: 74% (33.8 mg); yellow solid; m.p. 108-109 ºC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.03 (s, 1H), 7.54 – 7.42 (m, 3H), 7.40 – 7.27 (m, 7H), 7.25 – 7.00 (m, 8H), 5.72 (s, 1H), 3.71 (t, J = 6.8 Hz, 2H), 2.97 (t, J = 6.8 Hz, 2H), 2.50 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.8, 135.4, 134.3, 129.1, 129.0, 128.9, 128.8, 128.7, 128.3, 127.2, 123.3, 122.3, 120.6, 119.6, 118.4, 111.1, 110.6, 110.4, 106.3, 63.0, 48.7, 28.5, 21.5; IR (KBr): 3132, 2921, 1453, 1399, 1233, 1017, 745, 700, 601 cm^{-1}; ESI FTMS exact mass calcd for ($C_{32}H_{28}N_2O+Na)^+$ requires m/z 479.2100, found m/z 479.2101.

2-(2'-benzhydryl-5-methoxy-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethanol (5ad): Preparative thin layer chromatography: petroleum ether/ethyl acetate = 5/1; reaction time = 12 h; yield: 88% (41.6 mg); brown solid; m.p. 88-89 ºC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.52 – 7.40 (m, 2H), 7.37 – 7.27 (m, 7H), 7.23 – 7.05 (m, 8H), 6.89 – 6.80 (m, 1H), 5.72 (s, 1H), 3.89 (s, 3H), 3.70 (t, J = 6.8 Hz, 2H), 2.96 (t, J = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.0, 138.8, 135.4, 131.1, 129.9, 129.8, 129.0, 128.9, 128.8, 128.4, 128.3, 127.4, 127.2, 122.3, 120.6, 119.6, 111.8, 111.5, 111.1, 110.9, 106.3, 100.7, 63.0, 56.0, 48.7, 28.6; IR (KBr): 3058, 2938, 1598, 1452, 1215, 1030, 745, 701, 486 cm^{-1}; ESI FTMS exact mass calcd for ($C_{32}H_{28}N_2O_2+Na)^+$ requires m/z 495.2049, found m/z 495.2039.

2-(2'-benzhydryl-6-fluoro-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethanol (5ae): Preparative thin layer chromatography: petroleum ether/ethyl acetate = 5/1; reaction time = 12 h; yield: 60% (27.6 mg); brown solid; m.p. 87-88 ºC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.03 (s, 1H), 7.62 – 7.51 (m, 2H), 7.43 (d, J = 7.8 Hz, 1H), 7.39 – 7.27 (m, 7H), 7.24 – 7.10 (m, 6H), 6.95 – 6.82 (m, 2H), 5.71 (s, 1H), 3.69 (t, J = 6.8 Hz, 2H), 2.95 (t, J = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8 (d, J = 237.6 Hz), 138.9, 135.3, 129.0, 128.7, 128.3, 127.2, 122.4, 120.6, 119.6, 119.5, 119.4, 111.3,

111.2, 108.0 (d, J = 24.3 Hz), 105.9, 97.1 (d, J = 25.9 Hz), 63.0, 48.7, 28.5; IR (KBr): 3126, 1623, 1399, 1261, 1030, 746, 700, 485 cm^{-1}; ESI FTMS exact mass calcd for ($C_{31}H_{25}FN_2O+Na)^+$ requires m/z 483.1849, found m/z 483.1840.

2-(2'-benzhydryl-6-chloro-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethanol (5af): Preparative thin layer chromatography: petroleum ether/ethyl acetate = 5/1; reaction time = 12 h; yield: 60% (28.6 mg); yellow solid; m.p. 112-113 ºC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.61 – 7.50 (m, 2H), 7.42 (d, J = 7.9 Hz, 1H), 7.37 – 7.27 (m, 7H), 7.24 – 7.09 (m, 8H), 5.70 (s, 1H), 3.69 (t, J = 6.8 Hz, 2H), 2.95 (t, J = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.0, 136.2, 135.3, 129.6, 129.0, 128.7, 128.2, 127.6, 127.3, 127.2, 122.4, 120.7, 120.0, 119.6, 119.5, 111.3, 111.2, 110.6, 105.7, 62.9, 48.7, 28.5; IR (KBr): 3127, 1455, 1326, 1231, 917, 746, 701, 486 cm^{-1}; ESI FTMS exact mass calcd for ($C_{31}H_{25}ClN_2O+Na)^+$ requires m/z 499.1553, found m/z 499.1559.

2-(2'-benzhydryl-6-methyl-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethanol (5ag): Preparative thin layer chromatography: petroleum ether/ethyl acetate = 5/1; reaction time = 12 h; yield: 60% (27.4 mg); brown solid; m.p. 114-115 ºC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.57 (d, J = 8.5 Hz, 1H), 7.51 – 7.41 (m, 2H), 7.40 – 7.27 (m, 7H), 7.24 – 7.06 (m, 6H), 7.00 (d, J = 6.9 Hz, 2H), 5.72 (s, 1H), 3.71 (t, J = 6.8 Hz, 2H), 2.97 (t, J = 6.8 Hz, 2H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.7, 136.4, 135.4, 131.6, 128.9, 128.8, 128.4, 128.2, 127.2, 126.5, 122.3, 121.1, 120.5, 119.6, 118.4, 111.1, 110.9, 110.7, 106.3, 63.0, 48.6, 28.6, 21.6; IR (KBr): 3123, 1399, 1261, 1030, 746, 700, 668 cm^{-1}; ESI FTMS exact mass calcd for ($C_{32}H_{28}N_2O+Na)^+$ requires m/z 479.2100, found m/z 479.2090.

2-(2'-benzhydryl-7-bromo-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethanol (5ah): Preparative thin layer chromatography: petroleum ether/ethyl acetate = 5/1; reaction time = 12 h; yield: 79% (40.1 mg); yellow solid; m.p. 102-103 ºC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.74 – 7.64 (m, 1H), 7.59 (s, 1H), 7.45 (d, J = 7.9 Hz, 1H), 7.37 – 7.28 (m, 6H), 7.25 – 7.07 (m, 9H), 5.72 (s, 1H), 3.72 (t, J = 6.8 Hz, 2H), 2.99 (t, J = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.8, 136.0, 135.4, 128.9, 128.8, 128.6, 128.3, 127.2, 122.3, 121.7, 120.6, 119.6, 119.4, 118.7, 111.1, 110.7,

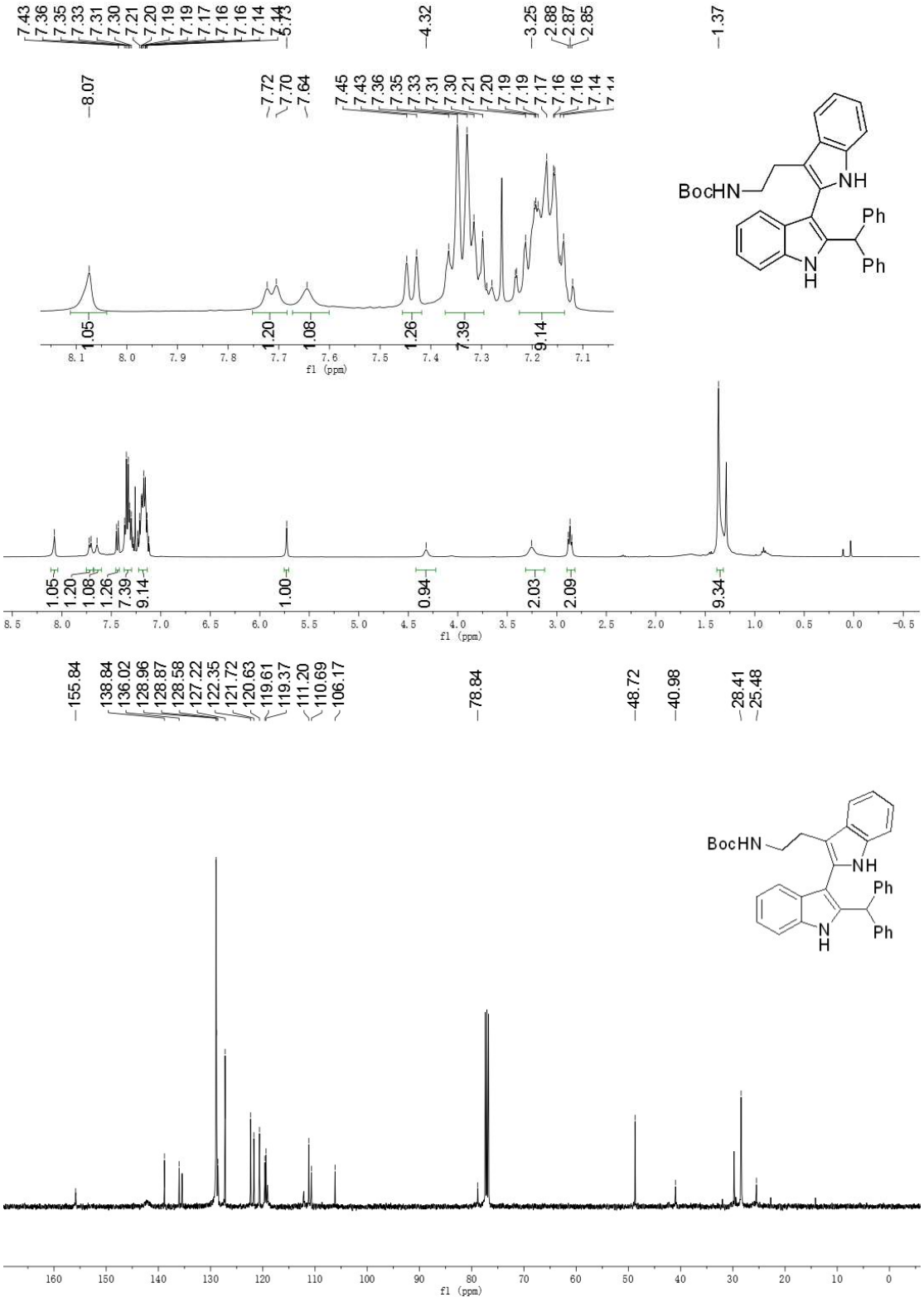
106.2, 63.0, 48.7, 28.6; IR (KBr): 3126, 1399, 1234, 1031, 745, 701, 471 cm^{-1}; ESI FTMS exact mass calcd for ($C_{31}H_{25}BrN_2O+Na)^+$ requires m/z 543.1048, found m/z 543.1044.

2-(2'-benzhydryl-7-methyl-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethanol (5ai): Preparative thin layer chromatography: petroleum ether/ethyl acetate = 5/1; reaction time = 12 h; yield: 70% (31.9 mg); brown solid; m.p. 66-67 ºC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.03 (s, 1H), 7.55 (d, *J* = 7.9 Hz, 1H), 7.52 – 7.43 (m, 2H), 7.41 – 7.28 (m, 7H), 7.25 – 7.05 (m, 7H), 6.98 (d, *J* = 7.1 Hz, 1H), 5.75 (s, 1H), 3.77 (t, *J* = 6.8 Hz, 2H), 3.06 (t, *J* = 6.8 Hz, 2H), 2.17 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.8, 135.4, 135.3, 129.0, 128.8, 128.7, 128.1, 128.0, 127.3, 122.3, 122.2, 120.6, 119.9, 119.7, 119.6, 116.4, 111.3, 111.2, 106.2, 63.1, 48.8, 28.7, 16.1; IR (KBr): 3057, 1597, 1455, 1232, 745, 701, 485 cm^{-1}; ESI FTMS exact mass calcd for ($C_{32}H_{28}N_2O+Na)^+$ requires m/z 479.2100, found m/z 479.2088.

2-(2'-benzhydryl-7-methoxy-1*H*,1'*H*-[2,3'-biindol]-3-yl)ethanol (5aj): Preparative thin layer chromatography: petroleum ether/ethyl acetate = 5/1; reaction time = 12 h; yield: 68% (32.1 mg); brown solid; m.p. 108-109 ºC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.06 (s, 2H), 7.96 (s, 2H), 7.46 (d, *J* = 7.8 Hz, 1H), 7.38 – 7.26 (m, 8H), 7.25 – 7.05 (m, 7H), 6.67 (d, *J* = 7.7 Hz, 1H), 5.76 (s, 1H), 3.92 (s, 3H), 3.67 (t, *J* = 6.7 Hz, 2H), 2.94 (t, *J* = 6.7 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.9, 138.8, 135.4, 129.9, 128.9, 128.8, 128.6, 128.5, 127.1, 126.6, 122.3, 120.5, 119.8, 119.6, 111.6, 111.5, 111.1, 106.3, 101.9, 63.1, 55.3, 48.6, 28.8; IR (KBr): 3130, 1576, 1400, 1255, 1099, 745, 701 cm^{-1}; ESI FTMS exact mass calcd for ($C_{32}H_{28}N_2O_2+Na)^+$ requires m/z 495.2049, found m/z 495.2046.

5. NMR Spectra of products 4 and 5

4aa



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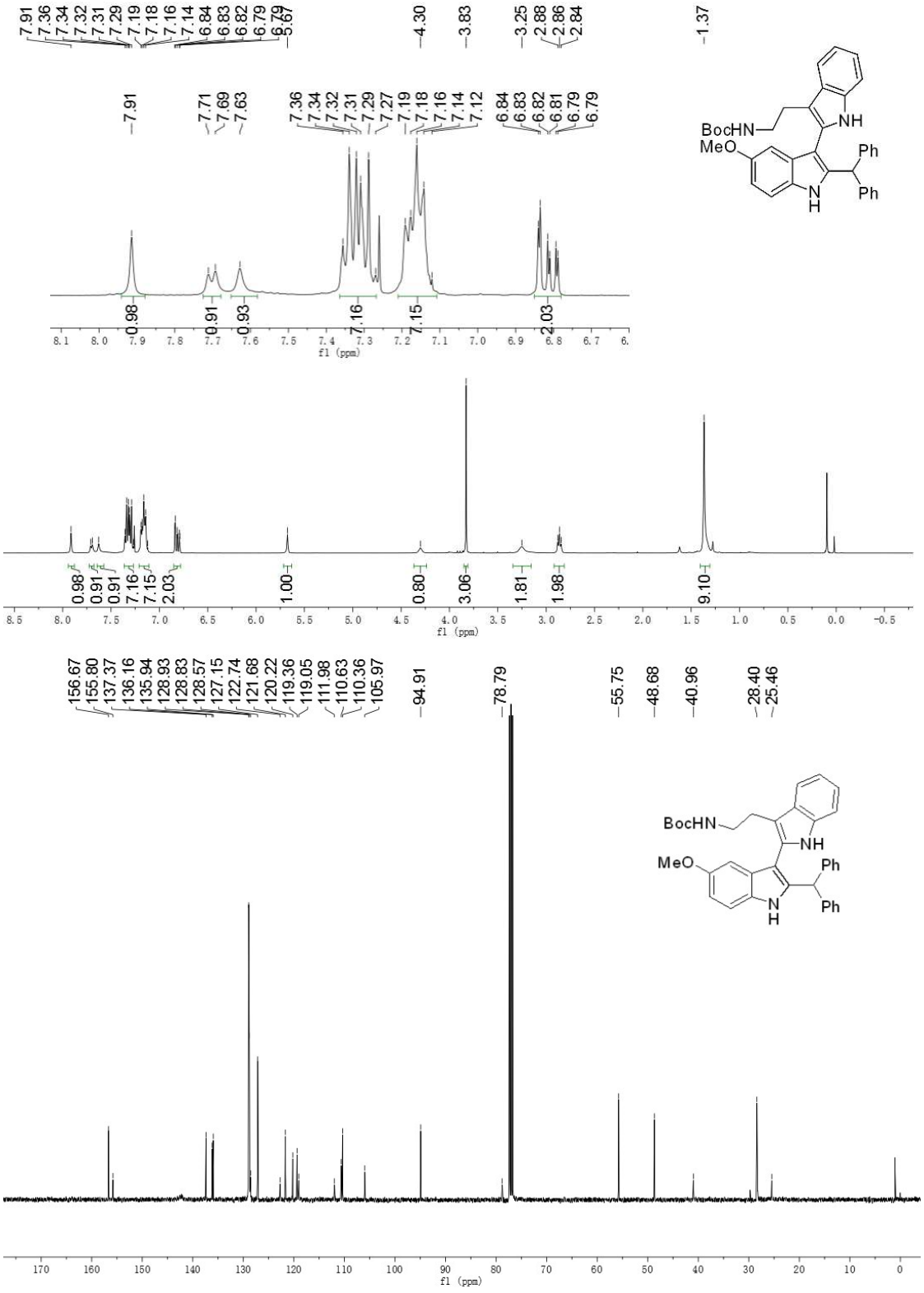
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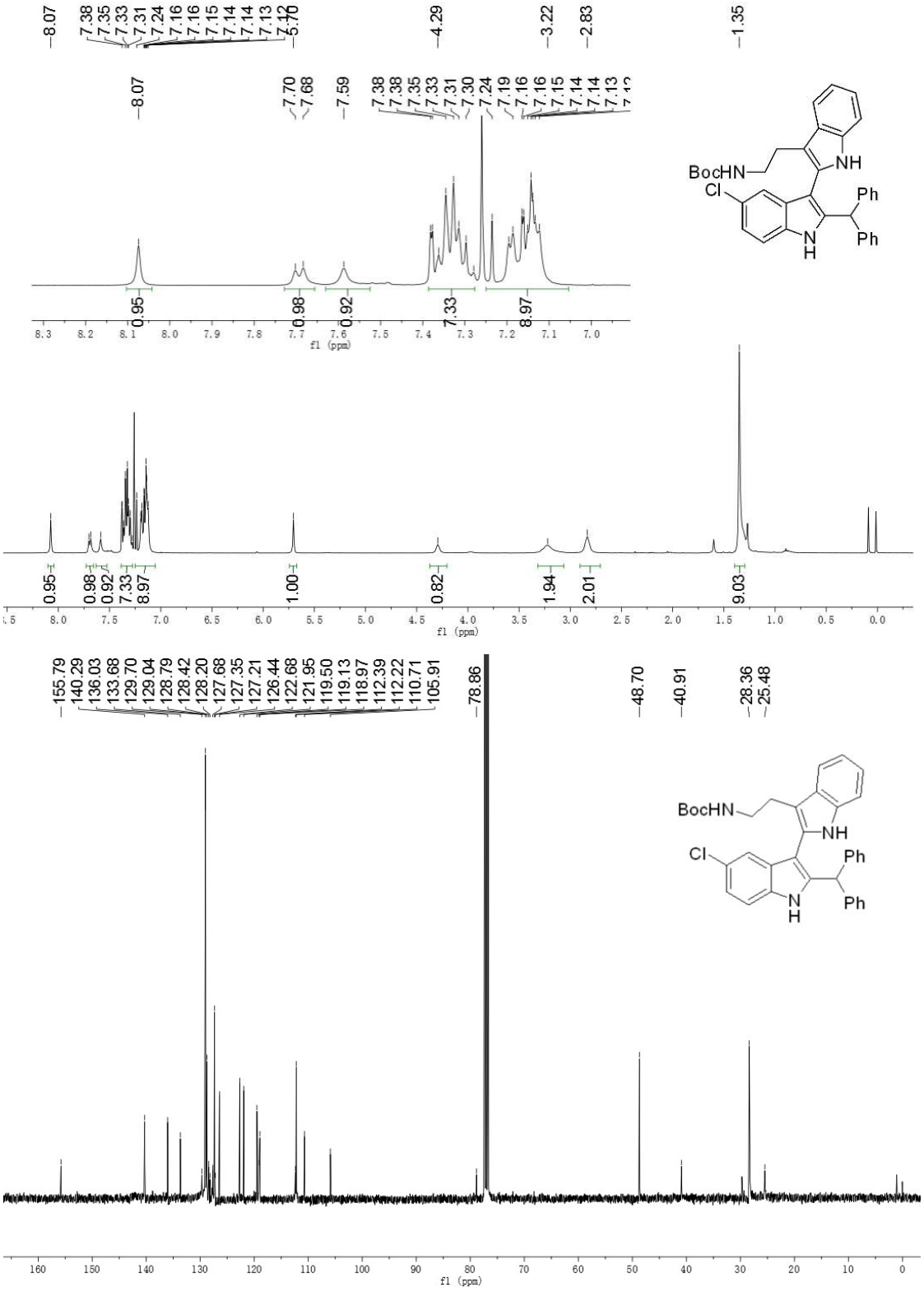
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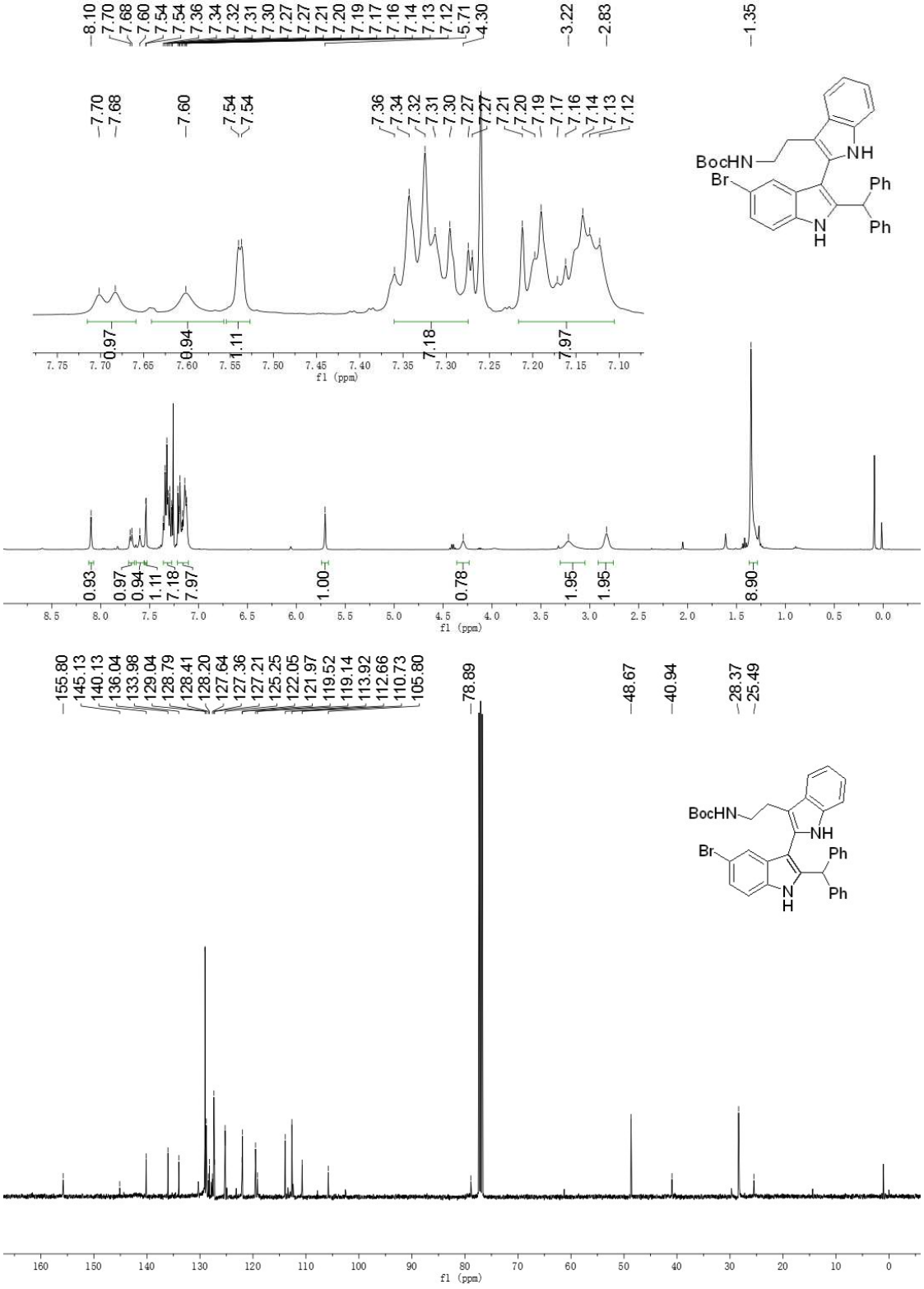
4da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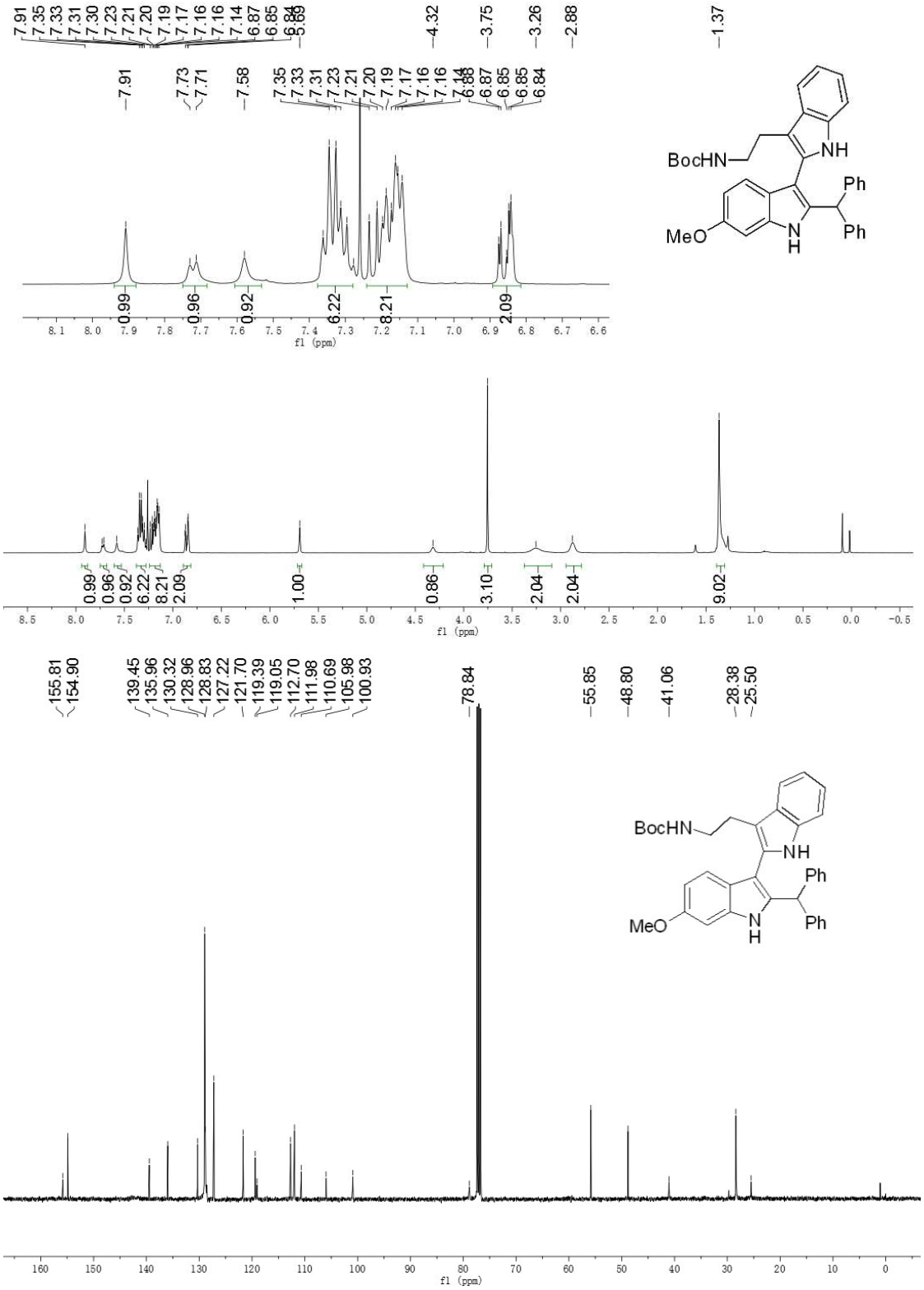
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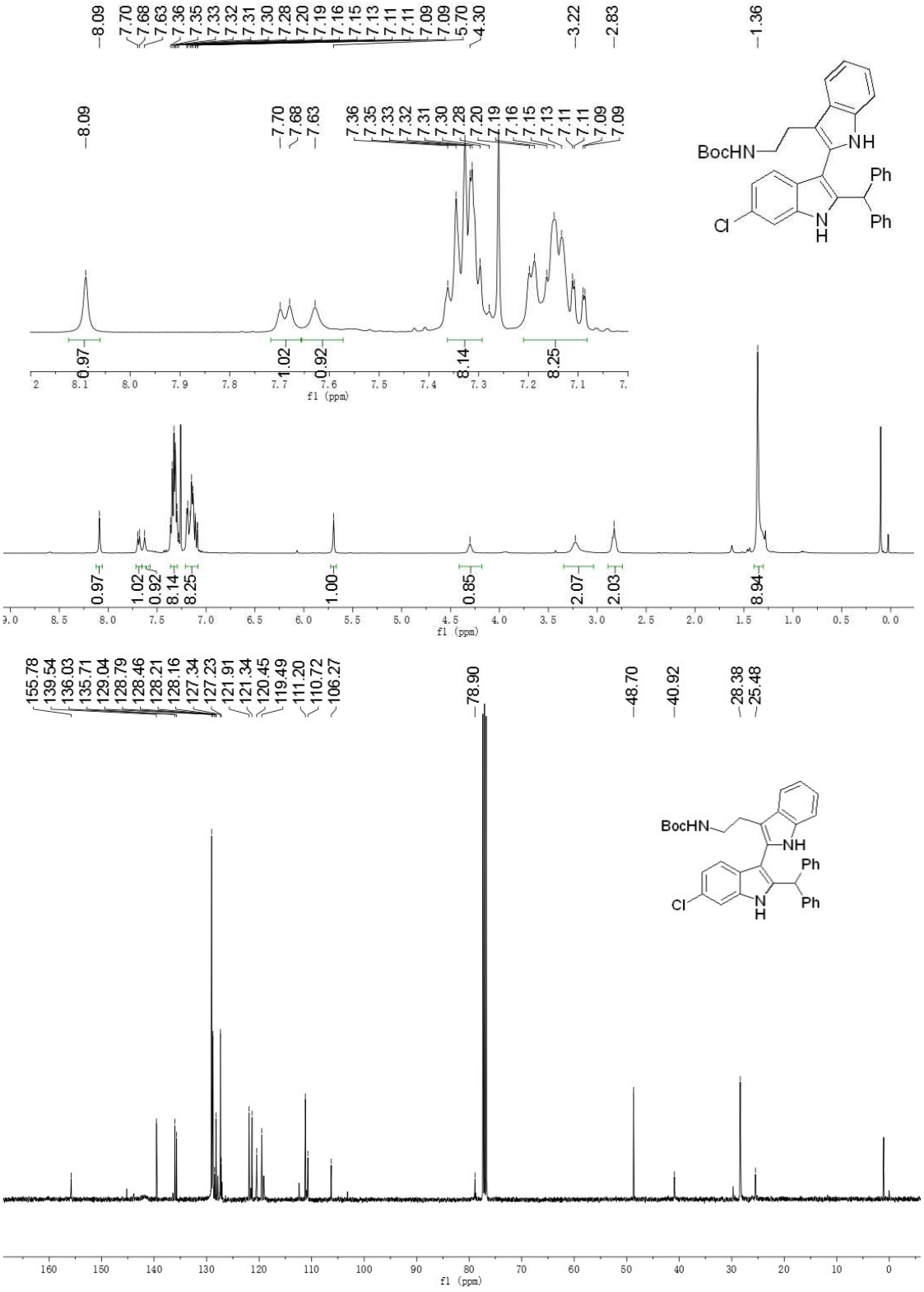
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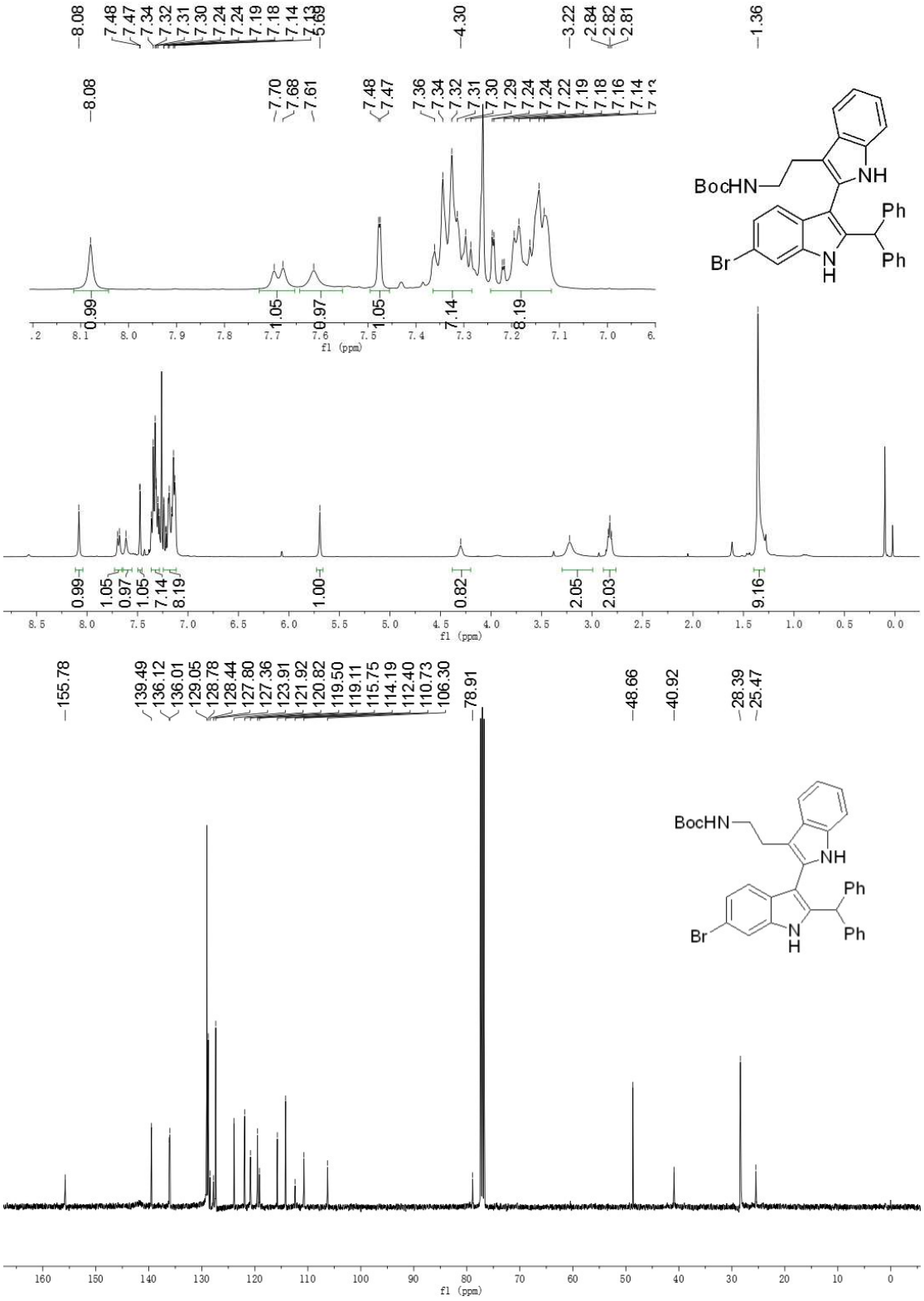
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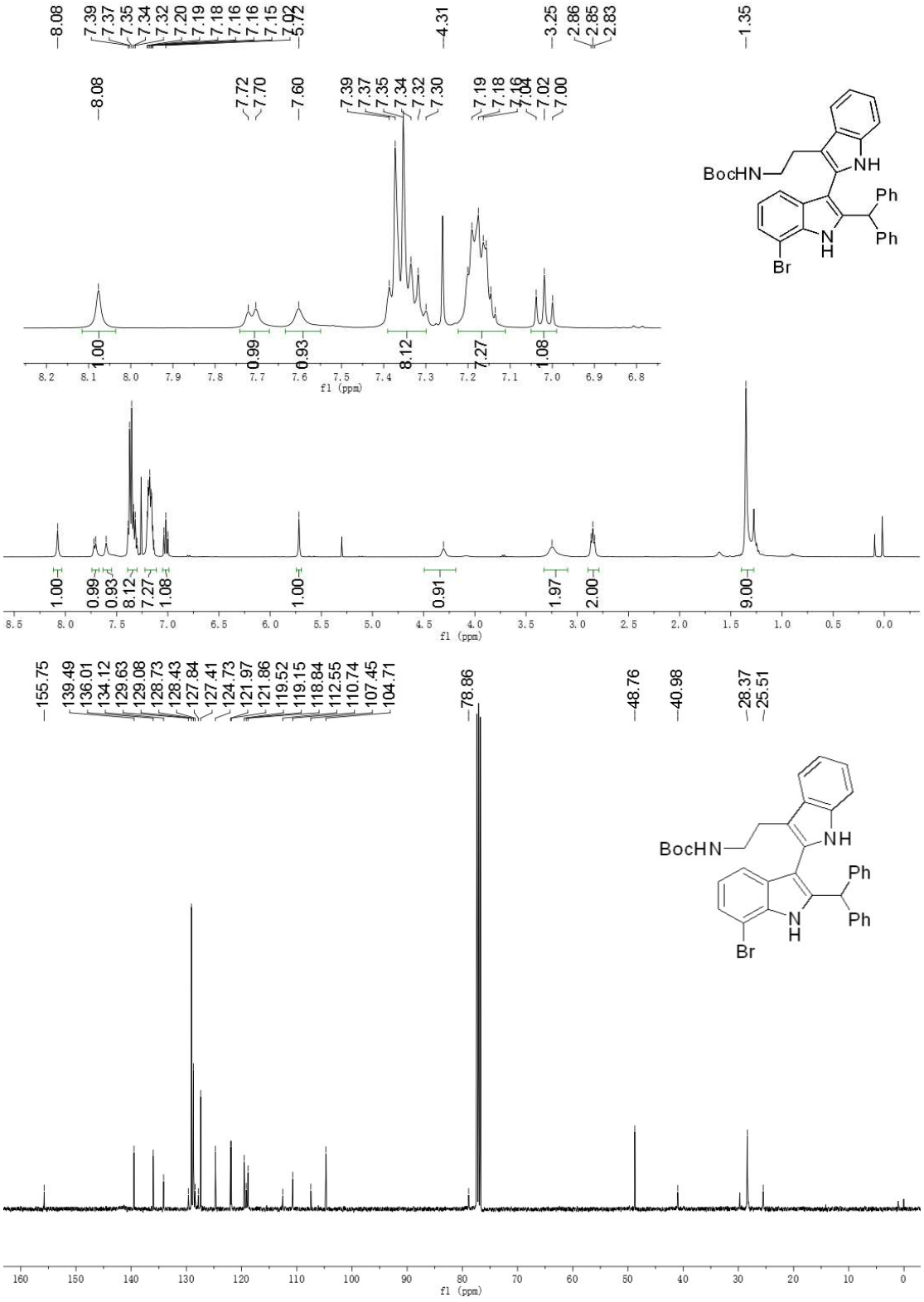
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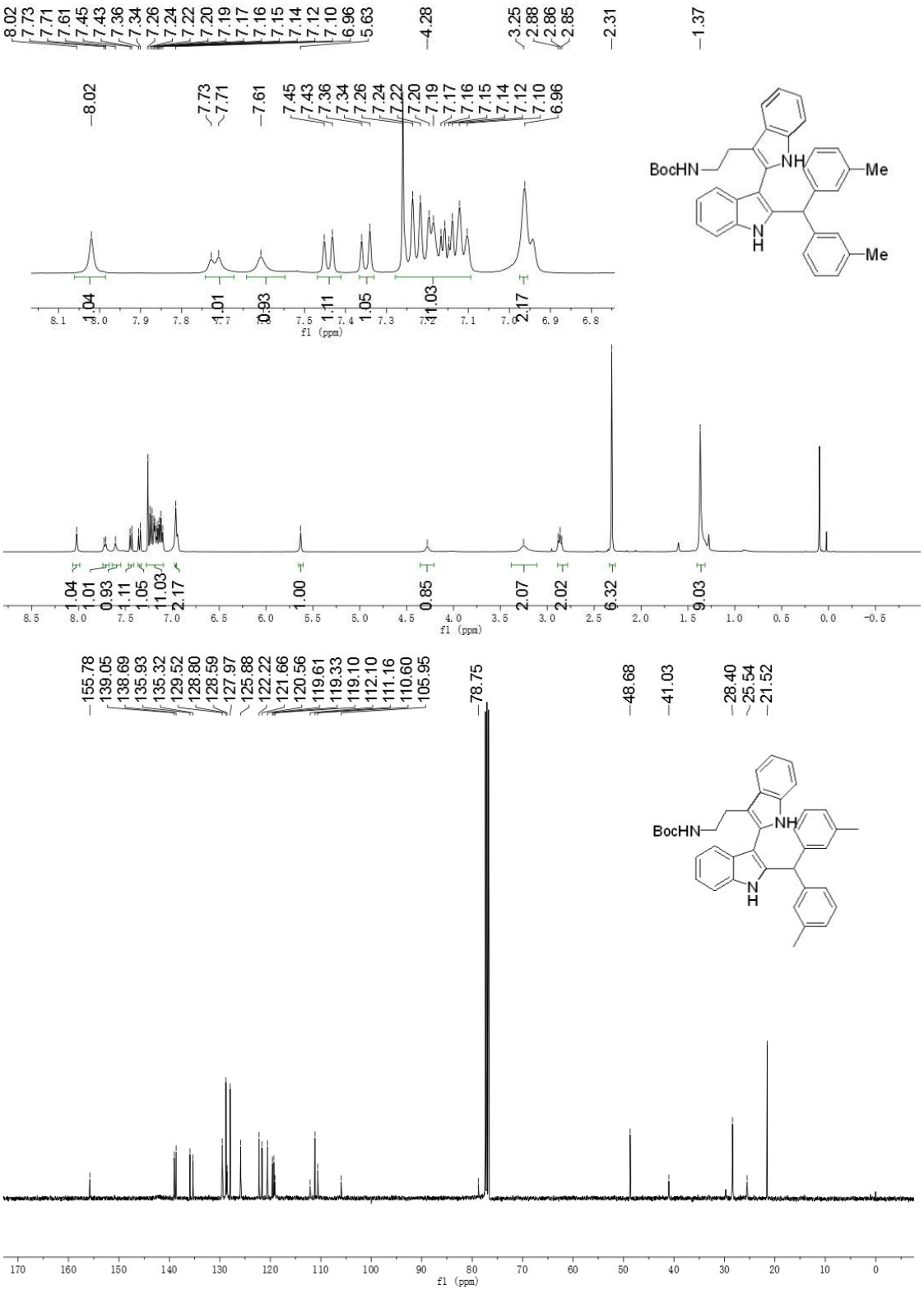
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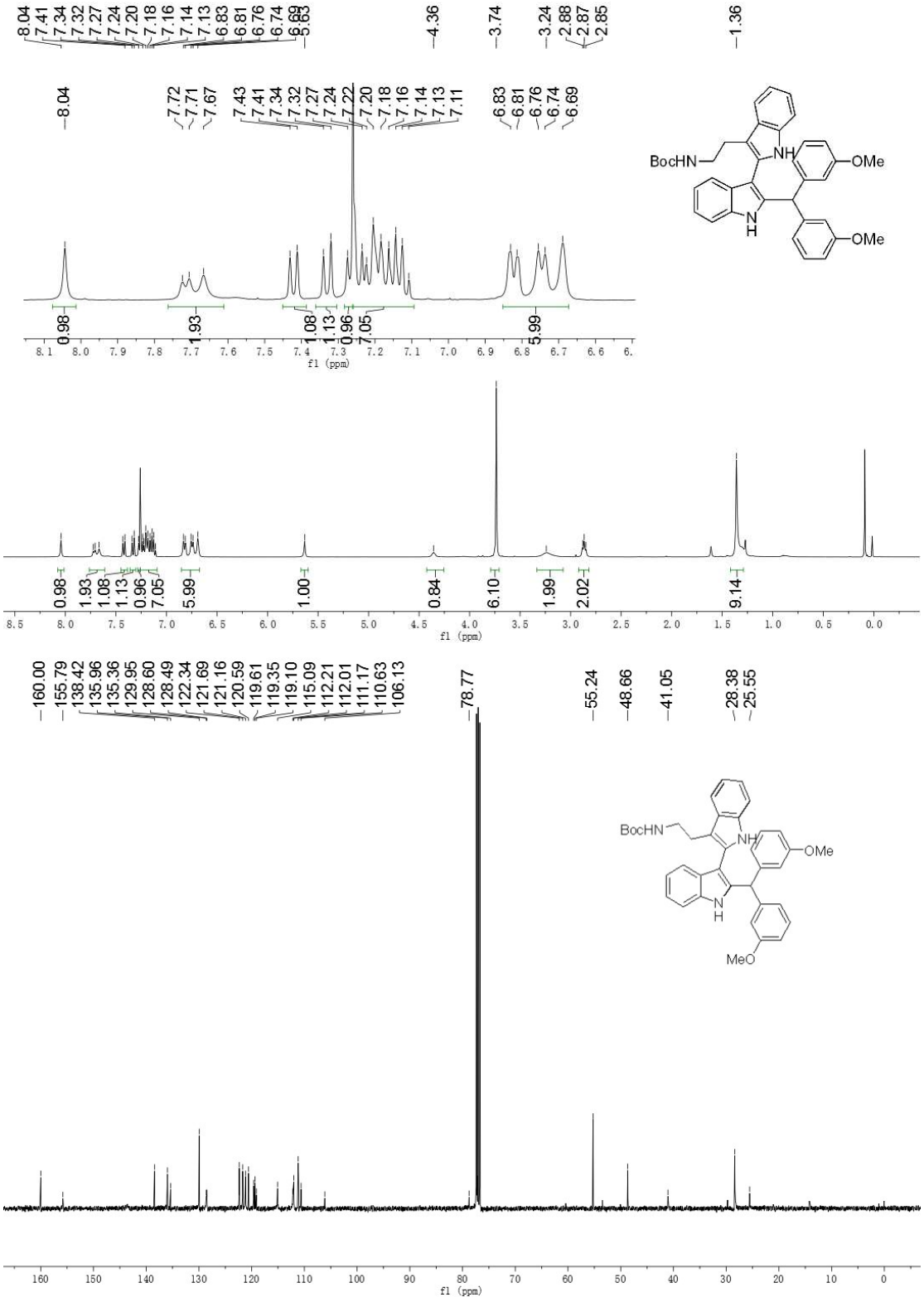
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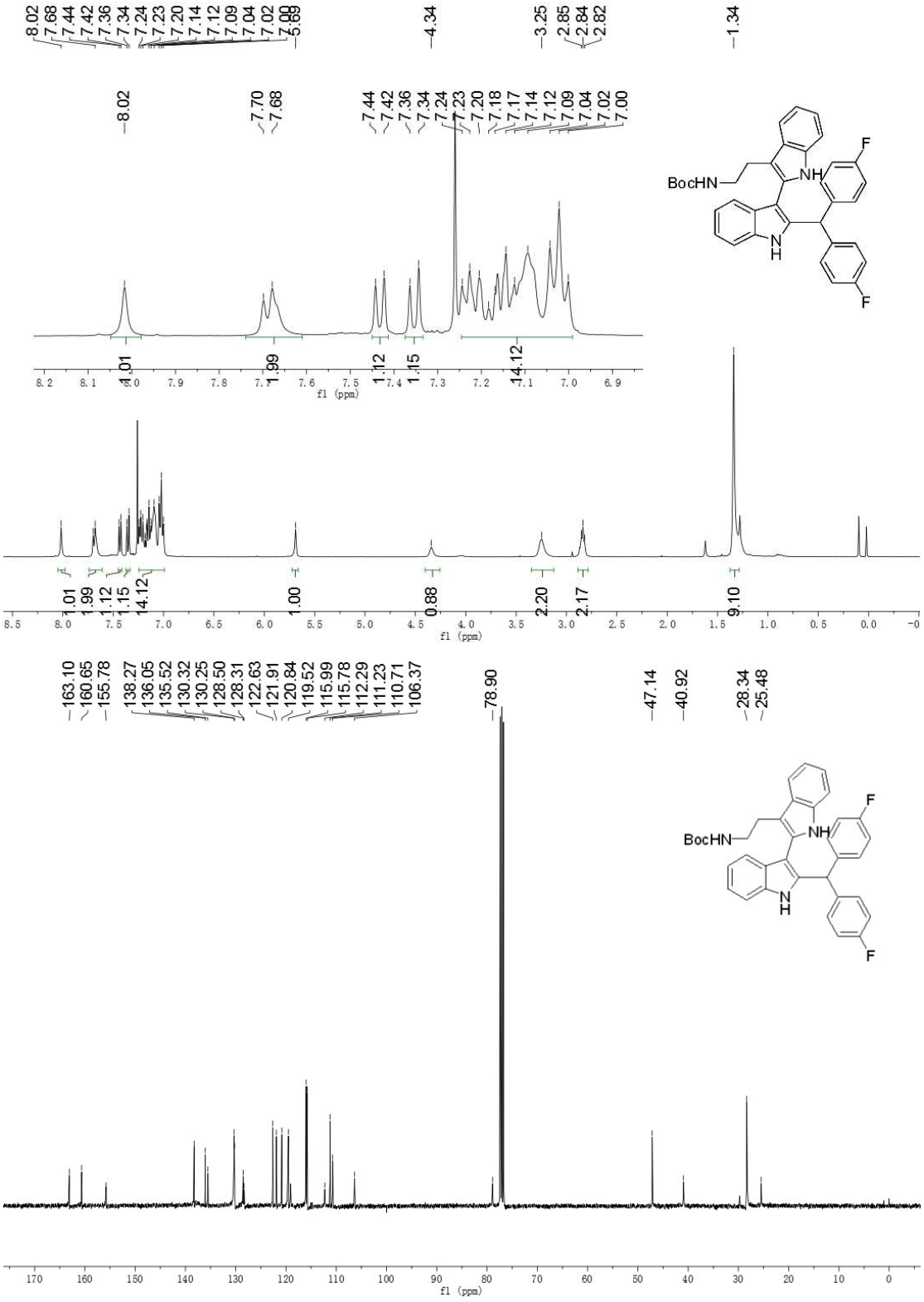
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F
F
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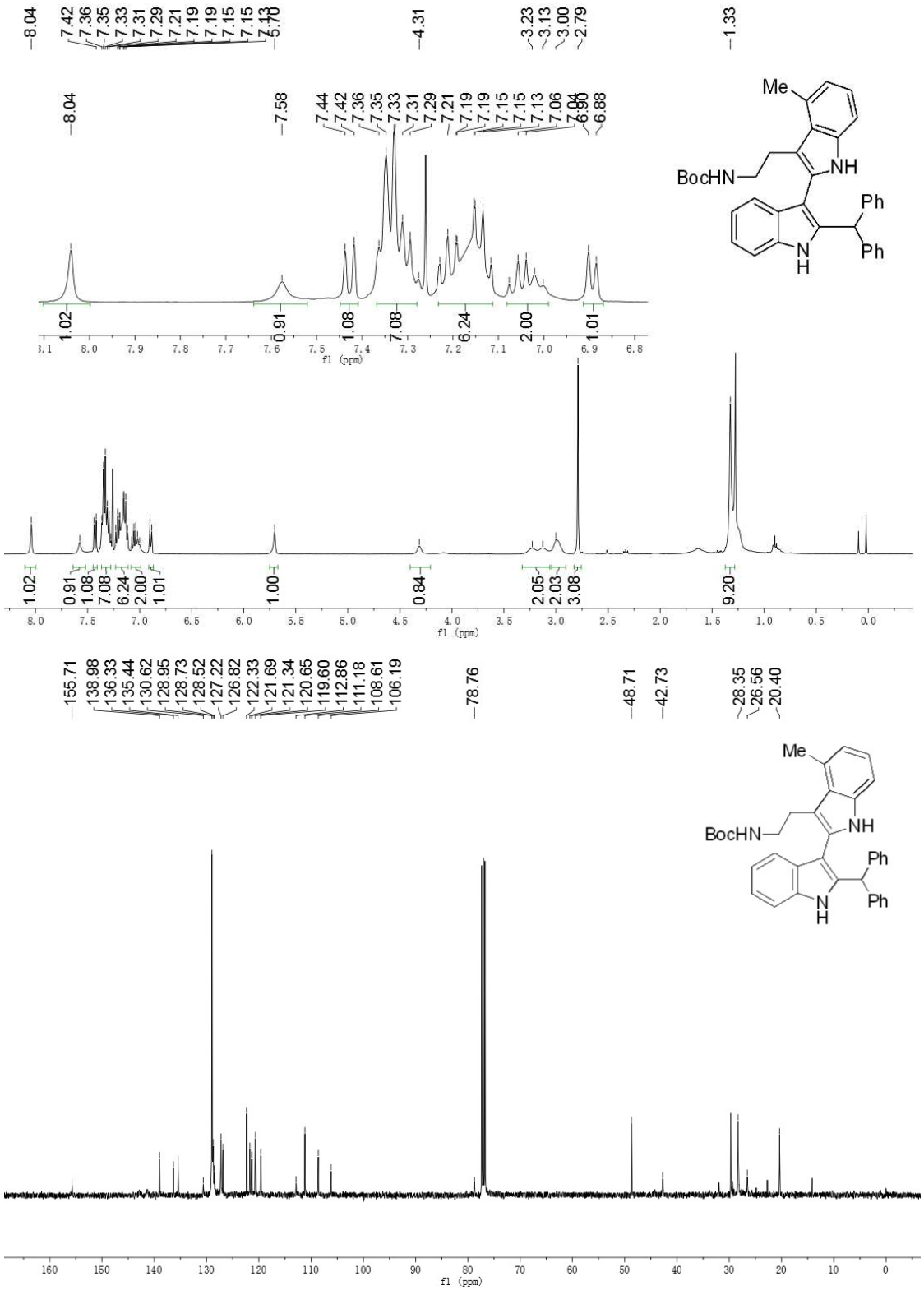
25.48

4ab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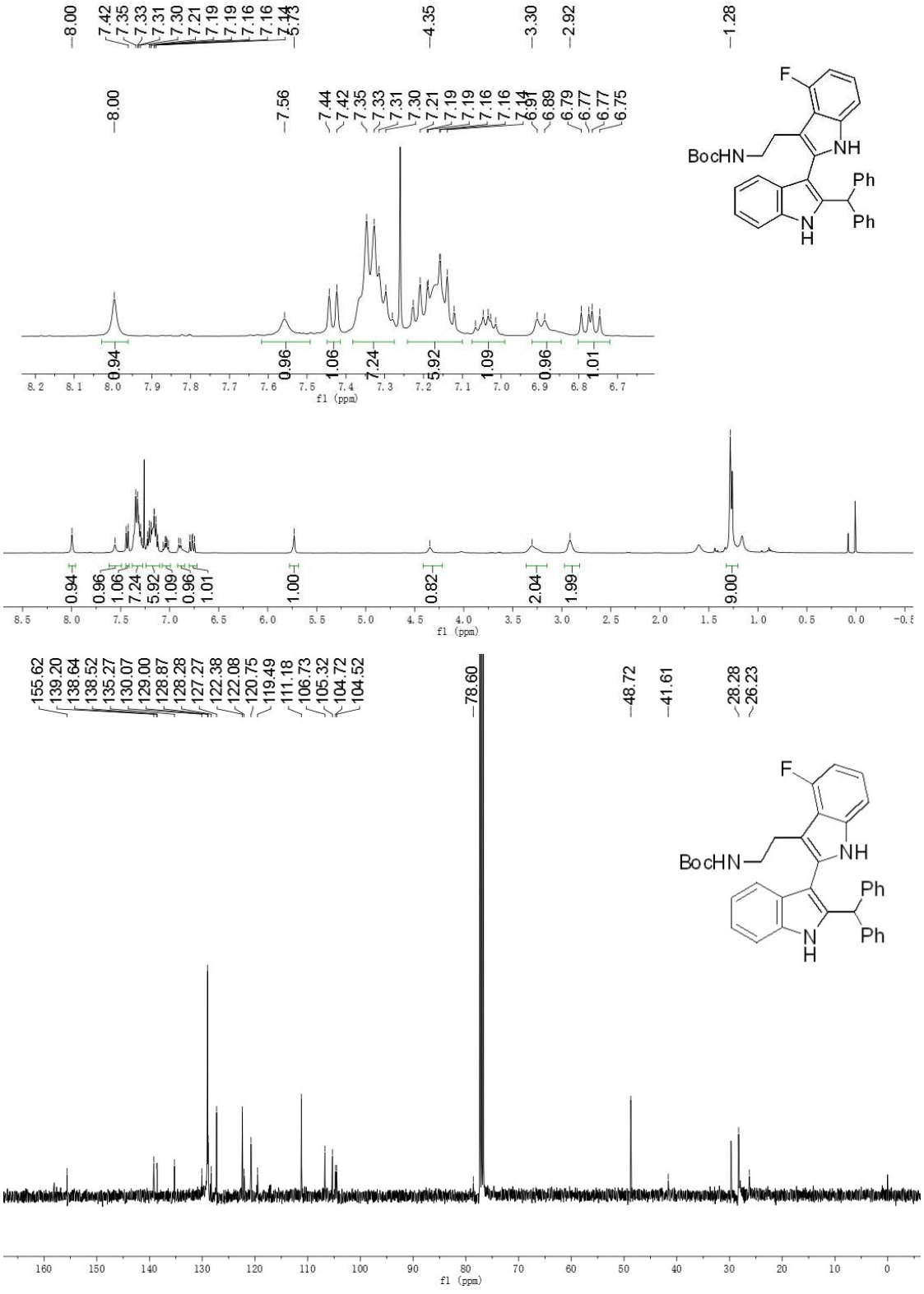
7.42
7.36
7.35
7.33
7.31
7.29
7.21
7.19
7.19
7.15
7.15
7.13
5.10
4.31
3.23
3.13
3.00
2.79
1.33
Me
BocHN
NH
Ph
Ph
N
H
1.02
0.91
1.08
7.08
6.24
2.00
1.01
1.00
0.84
2.05
2.03
3.08
9.20
f1 (ppm)
155.71
138.98
136.33
135.44
130.62
128.95
128.73
128.52
127.22
126.82
122.33
121.69
121.34
120.65
119.60
112.86
111.18
108.61
106.19
78.76
48.71
42.73
28.35
26.56
20.40

4ac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7.42
7.35
7.33
7.31
7.30
7.21
7.19
7.19
7.16
7.16
7.14
5.73
4.35
3.30
2.92
1.28
F
BocHN
NH
Ph
Ph
N
H
0.94
0.96
1.06
7.24
5.92
1.09
0.96
1.01
1.00
0.82
2.04
1.99
9.00
f1 (ppm)
155.62
139.20
138.64
138.52
135.27
130.07
129.00
128.87
128.28
127.27
122.38
122.08
120.75
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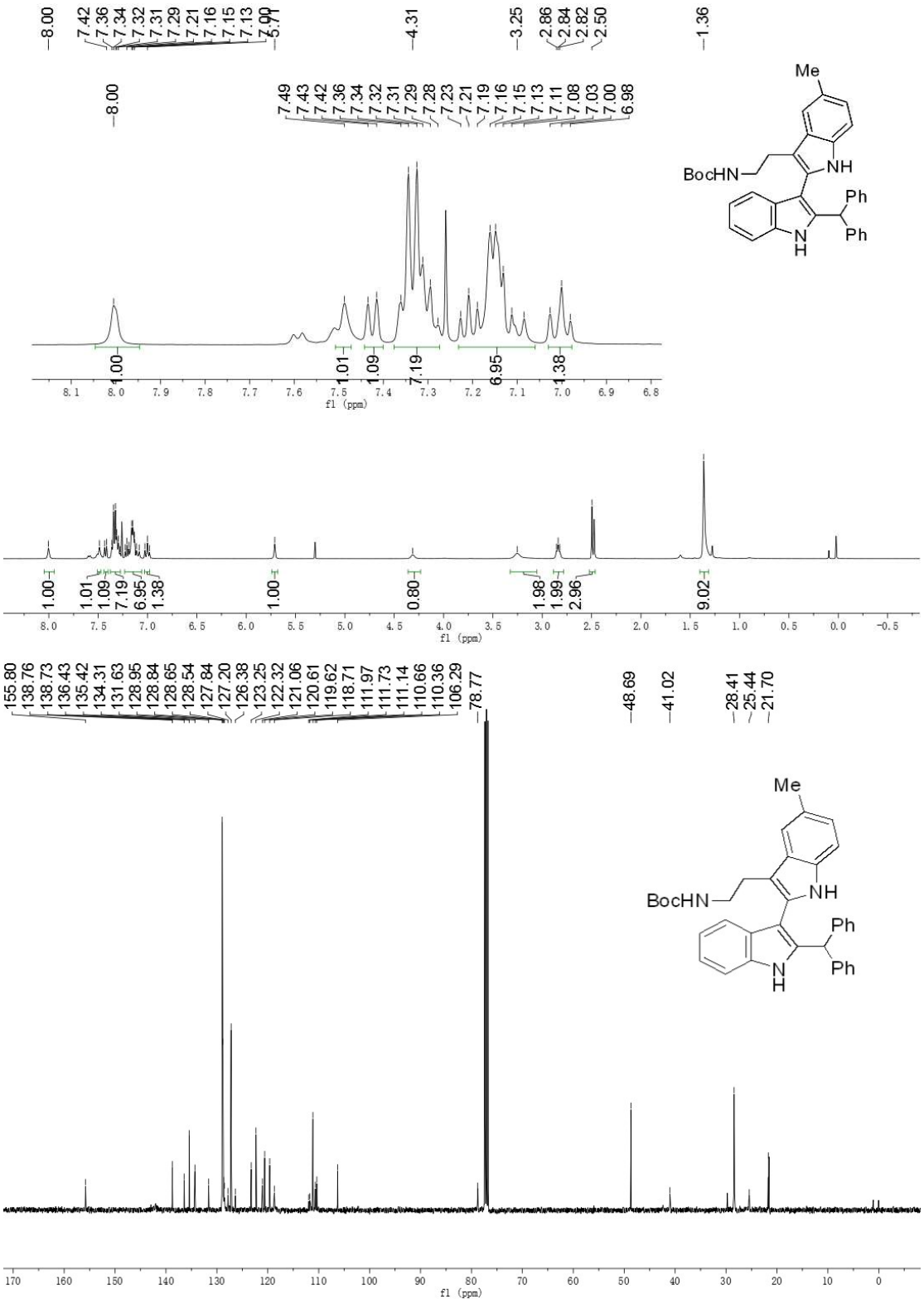
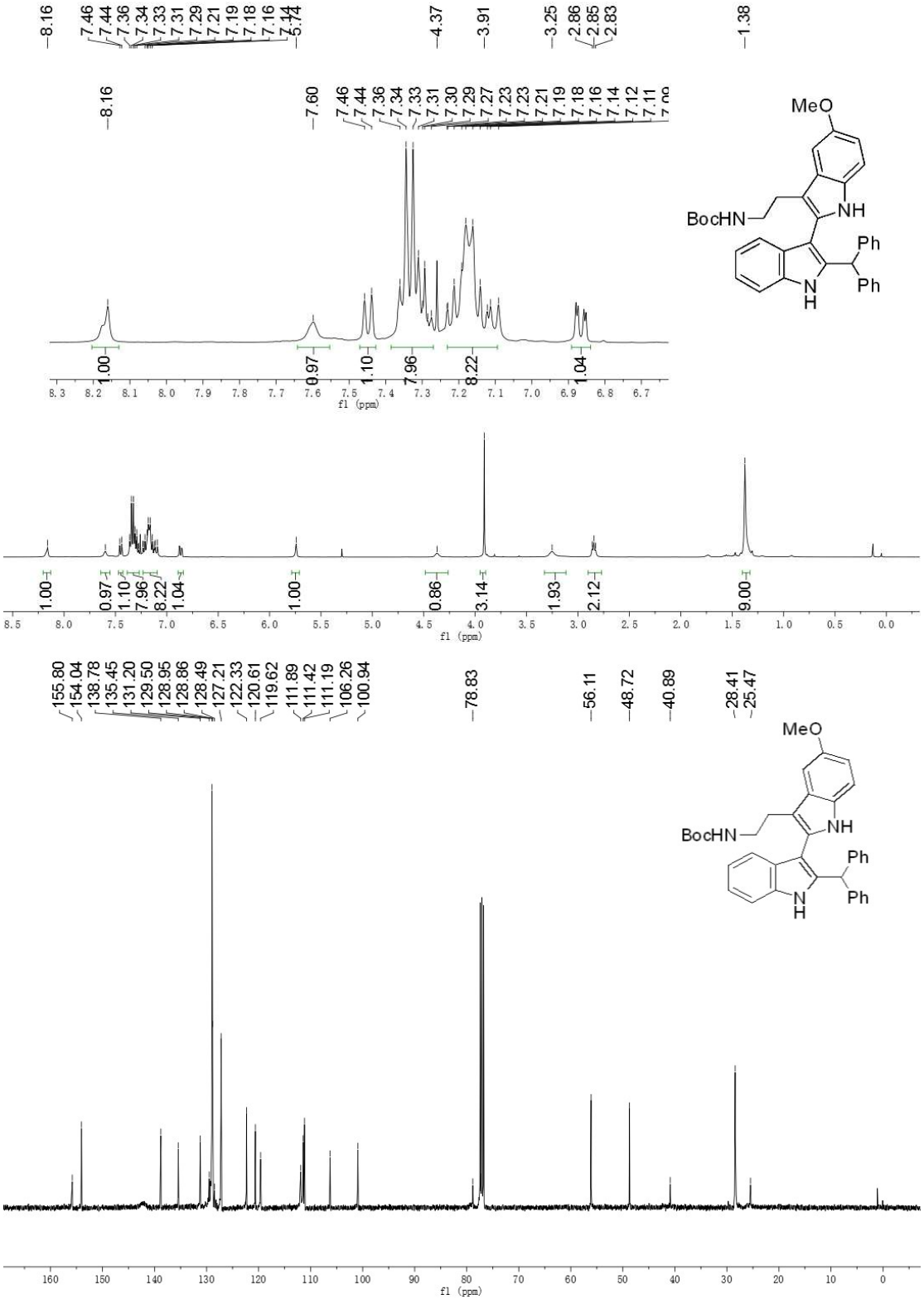
111.18
106.73
105.32
104.72
104.52
78.60
48.72
41.61
28.28
26.23

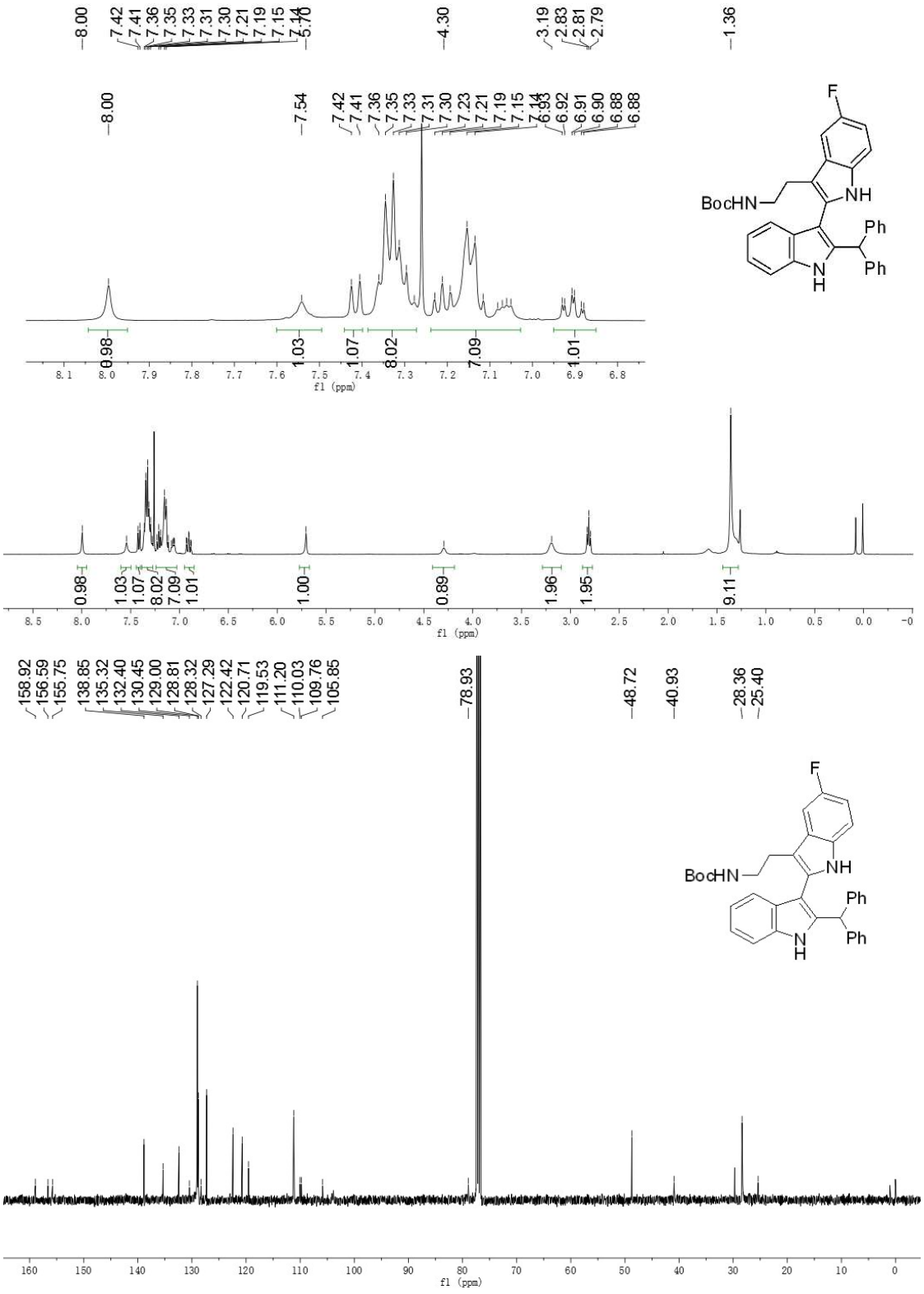
4ad


8.00
7.42
7.36
7.34
7.32
7.31
7.29
7.21
7.16
7.15
7.13
5.11
4.31
3.25
2.86
2.84
2.82
2.50
1.36
Me
BocHN
NH
Ph
Ph
N
H
1.00
1.01
1.09
7.19
6.95
1.38
1.00
0.80
1.98
1.99
2.96
9.02
f1 (ppm)
155.80
138.76
138.73
136.43
135.42
134.31
131.63
128.95
128.84
128.65
128.54
127.84
127.20
126.38
123.25
122.32
121.06
120.61
119.62
118.71
111.97
111.73
111.14
110.66
110.36
106.29
78.77
48.69
41.02
28.41
25.44
21.70

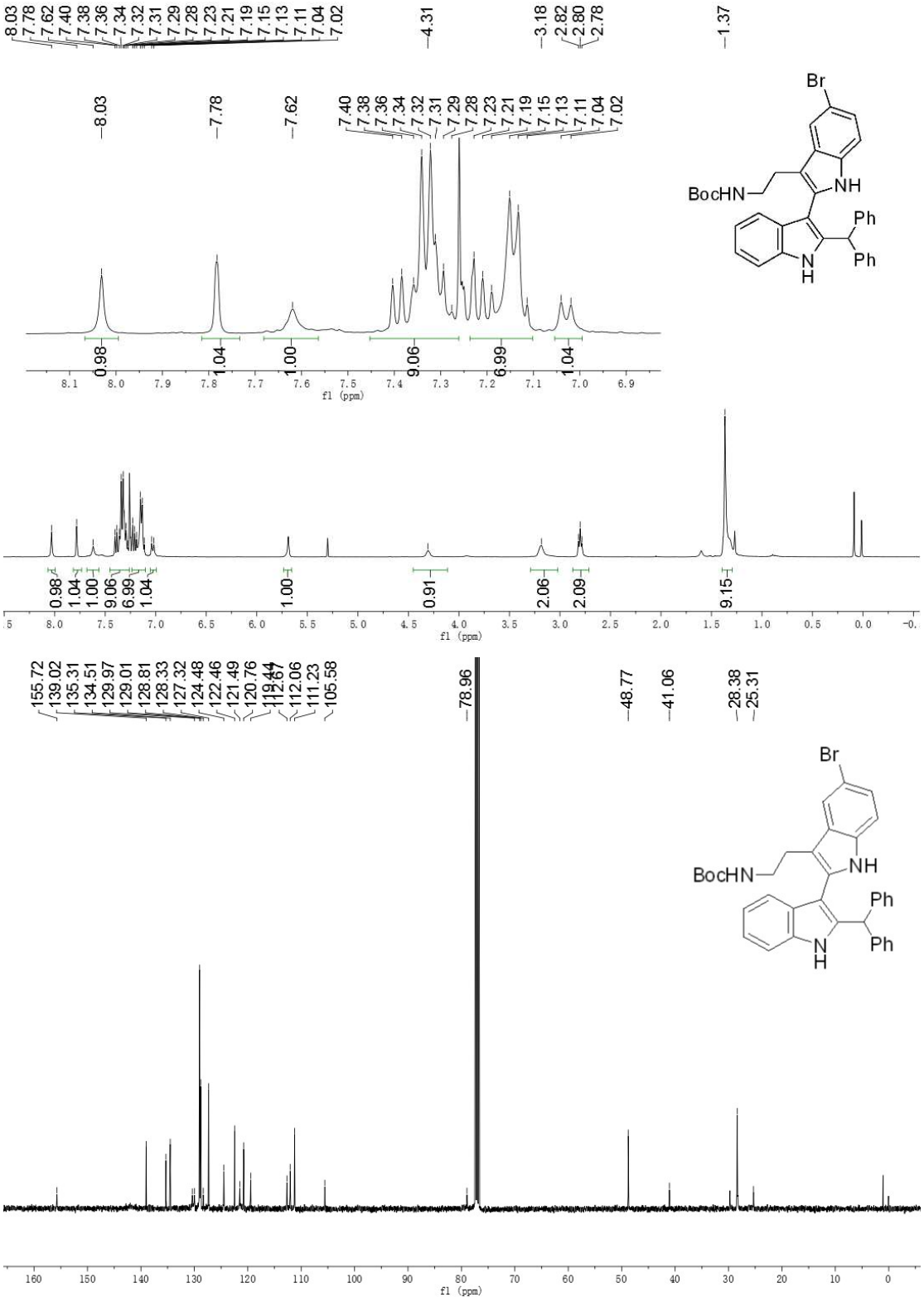
4ae



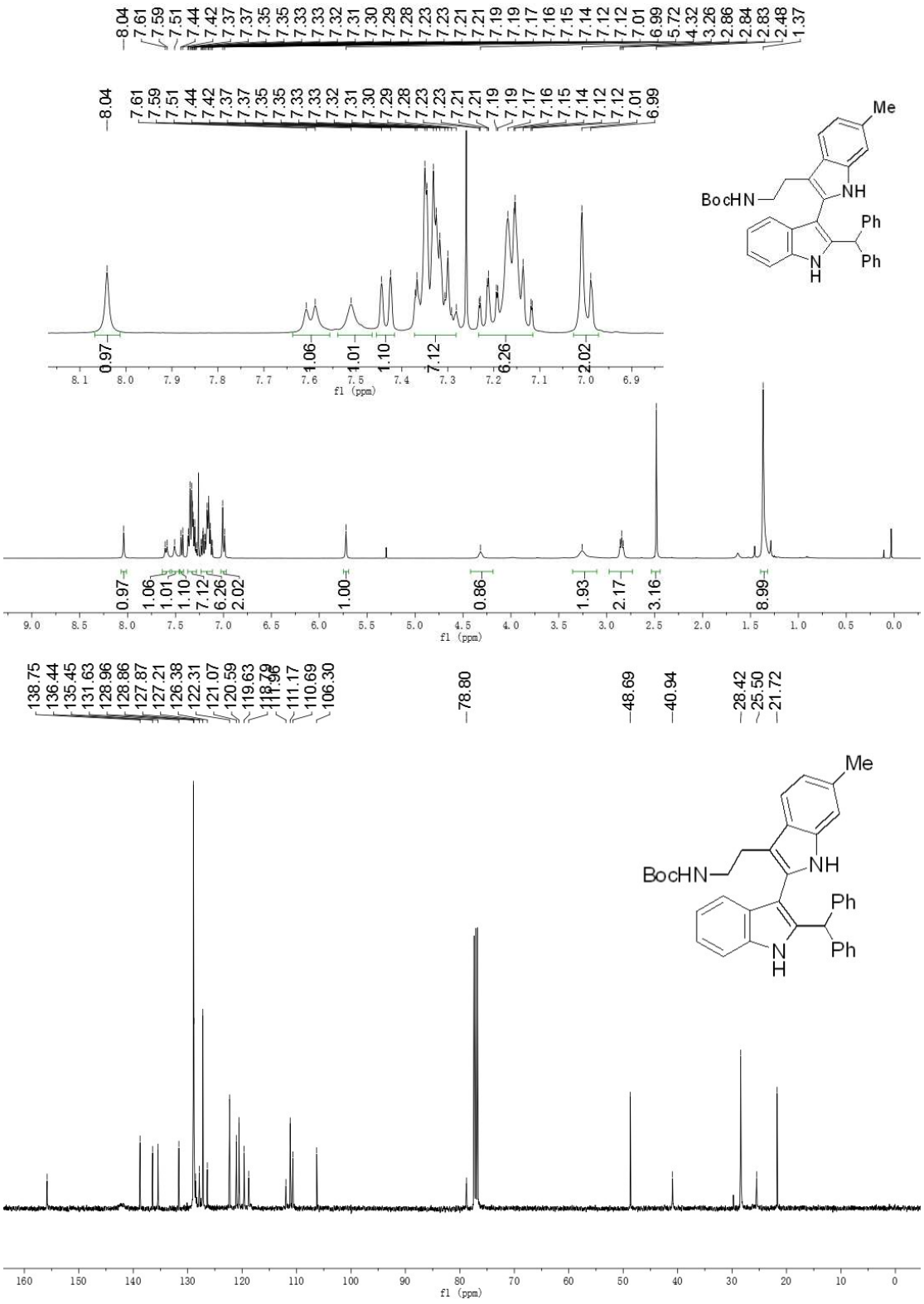
4af


8.00
7.42
7.41
7.36
7.35
7.33
7.31
7.30
7.21
7.19
7.15
5.10
4.30
3.19
2.83
2.81
2.79
1.36
7.54
7.23
6.92
6.91
6.90
6.88
6.88
BocHN
NH
Ph
Ph
F
0.98
1.03
1.07
8.02
7.09
1.01
1.00
0.89
1.96
1.95
9.11
f1 (ppm)
158.92
156.59
155.75
138.85
135.32
132.40
130.45
129.00
128.81
128.32
127.29
122.42
120.71
119.53
111.20
110.03
109.76
105.85
78.93
48.72
40.93
28.36
25.40

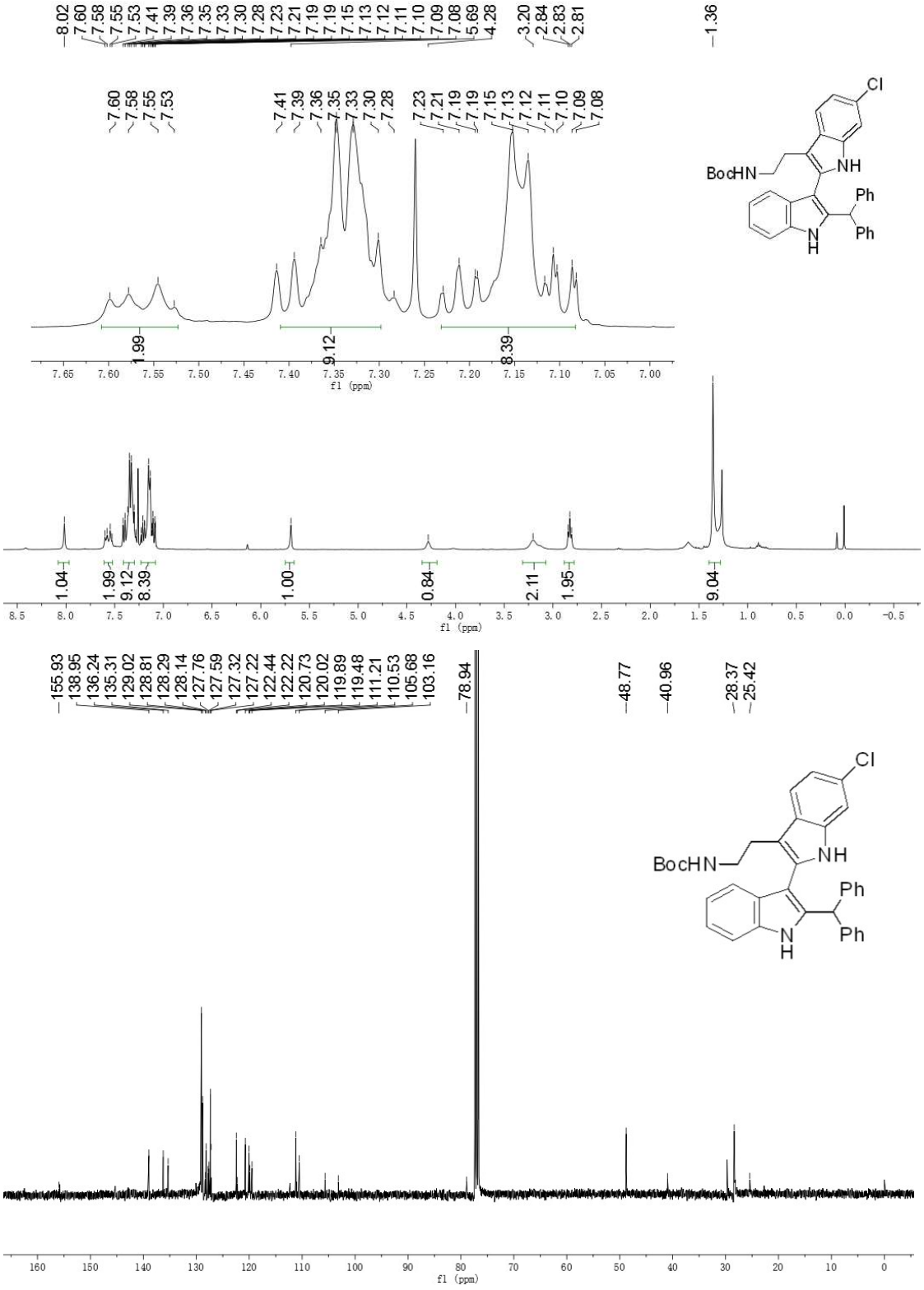
4ag


8.03
7.78
7.62
7.40
7.38
7.36
7.34
7.32
7.31
7.29
7.28
7.23
7.21
7.19
7.15
7.13
7.11
7.04
7.02
4.31
3.18
2.82
2.80
2.78
1.37
Br
BocHN
NH
Ph
Ph
N
H
0.98
1.04
1.00
9.06
6.99
1.04
1.00
0.91
2.06
2.09
9.15
f1 (ppm)
155.72
139.02
135.31
134.51
129.97
129.01
128.81
128.33
127.32
124.48
122.46
121.49
120.76
112.06
111.23
105.58
78.96
48.77
41.06
28.38
25.31

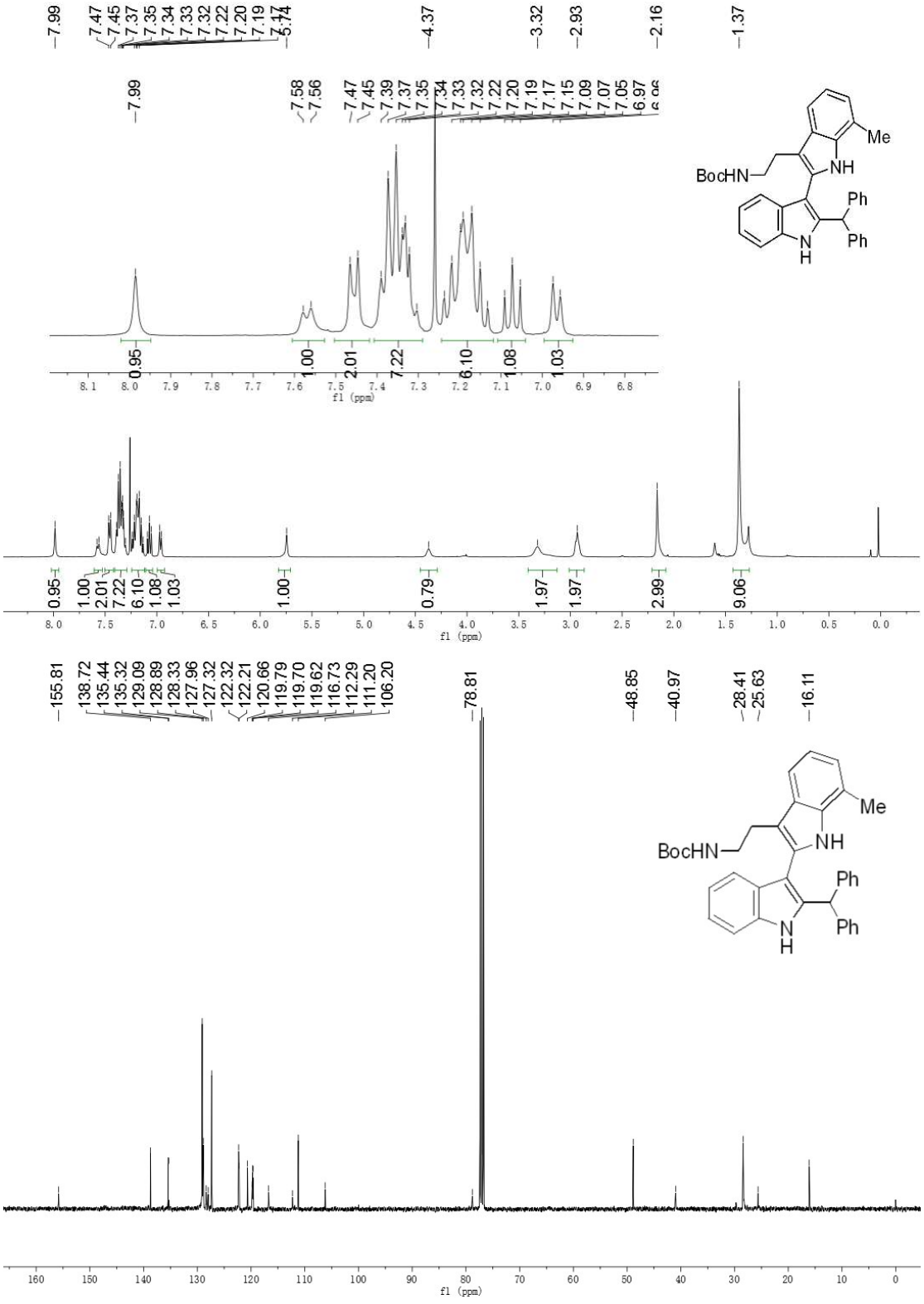
4ah


8.04 7.61 7.59 7.51 7.44 7.42 7.37 7.37 7.35 7.35 7.33 7.33 7.32 7.31 7.30 7.29 7.28 7.23 7.23 7.21 7.21 7.19 7.19 7.17 7.16 7.15 7.14 7.12 7.12 7.01 6.99 5.72 4.32 3.26 2.86 2.84 2.83 2.48 1.37
0.97 1.06 1.01 1.10 7.12 6.26 2.02
f1 (ppm)
Me
BocHN
NH
Ph
Ph
N
H
0.97 1.06 1.01 1.10 7.12 6.26 2.02 1.00 0.86 1.93 2.17 3.16 8.99
f1 (ppm)
138.75 136.44 135.45 131.63 128.96 128.86 127.87 127.21 126.38 122.31 121.07 120.59 119.63 111.17 110.69 106.30
78.80
48.69
40.94
28.42 25.50 21.72
f1 (ppm)

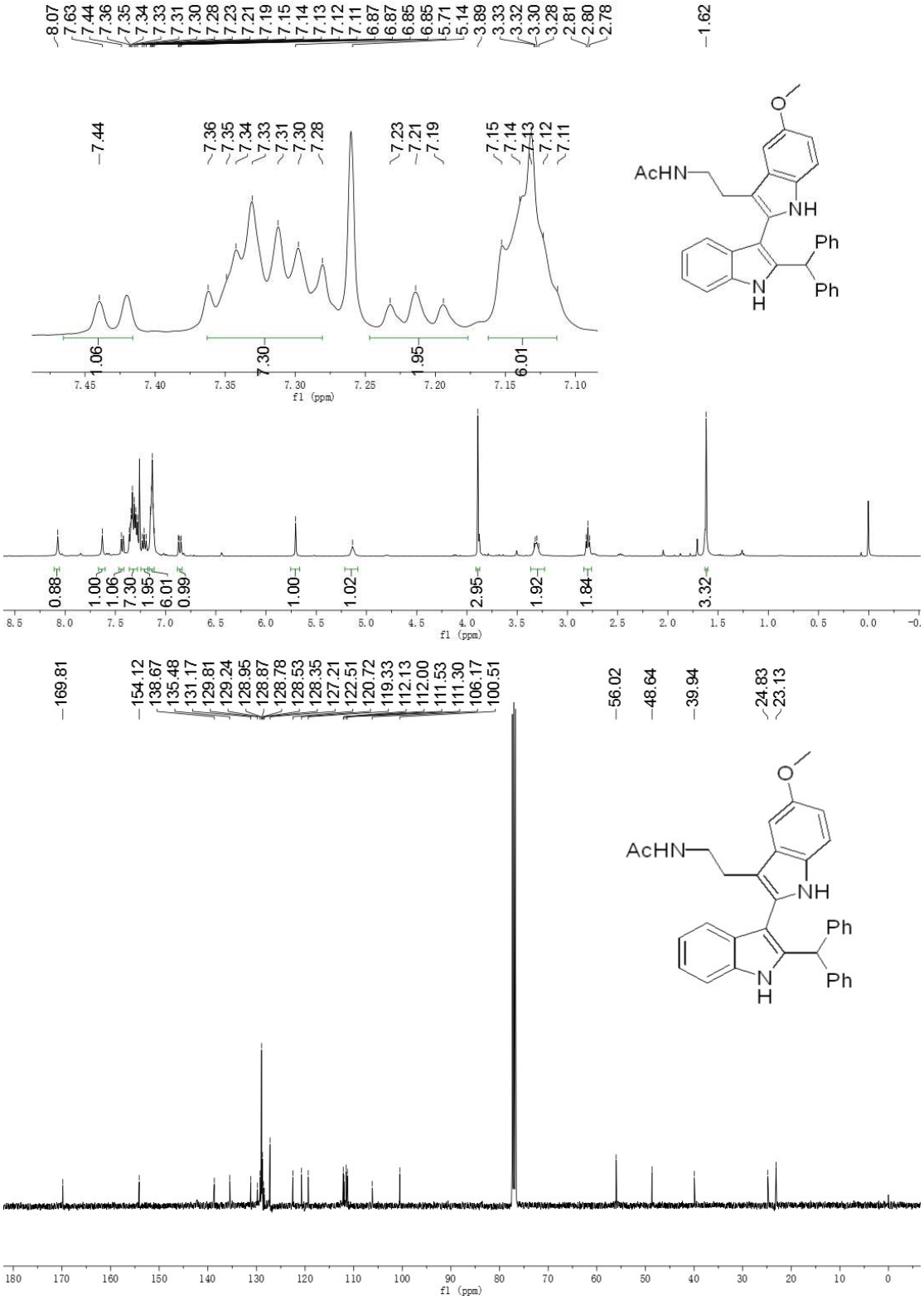
4ai


8.02
7.60
7.58
7.55
7.53
7.41
7.39
7.36
7.35
7.33
7.30
7.28
7.23
7.21
7.19
7.19
7.15
7.13
7.12
7.11
7.10
7.09
7.08
5.69
4.28
3.20
2.84
2.83
2.81
1.36
Cl
BocHN
NH
Ph
Ph
N
H
1.99
9.12
8.39
1.04
1.99
9.12
8.39
1.00
0.84
2.11
1.95
9.04
f1 (ppm)
155.93
138.95
136.24
135.31
129.02
128.81
128.29
128.14
127.76
127.59
127.32
127.22
122.44
122.22
120.73
120.02
119.89
119.48
111.21
110.53
105.68
103.16
78.94
48.77
40.96
28.37
25.42

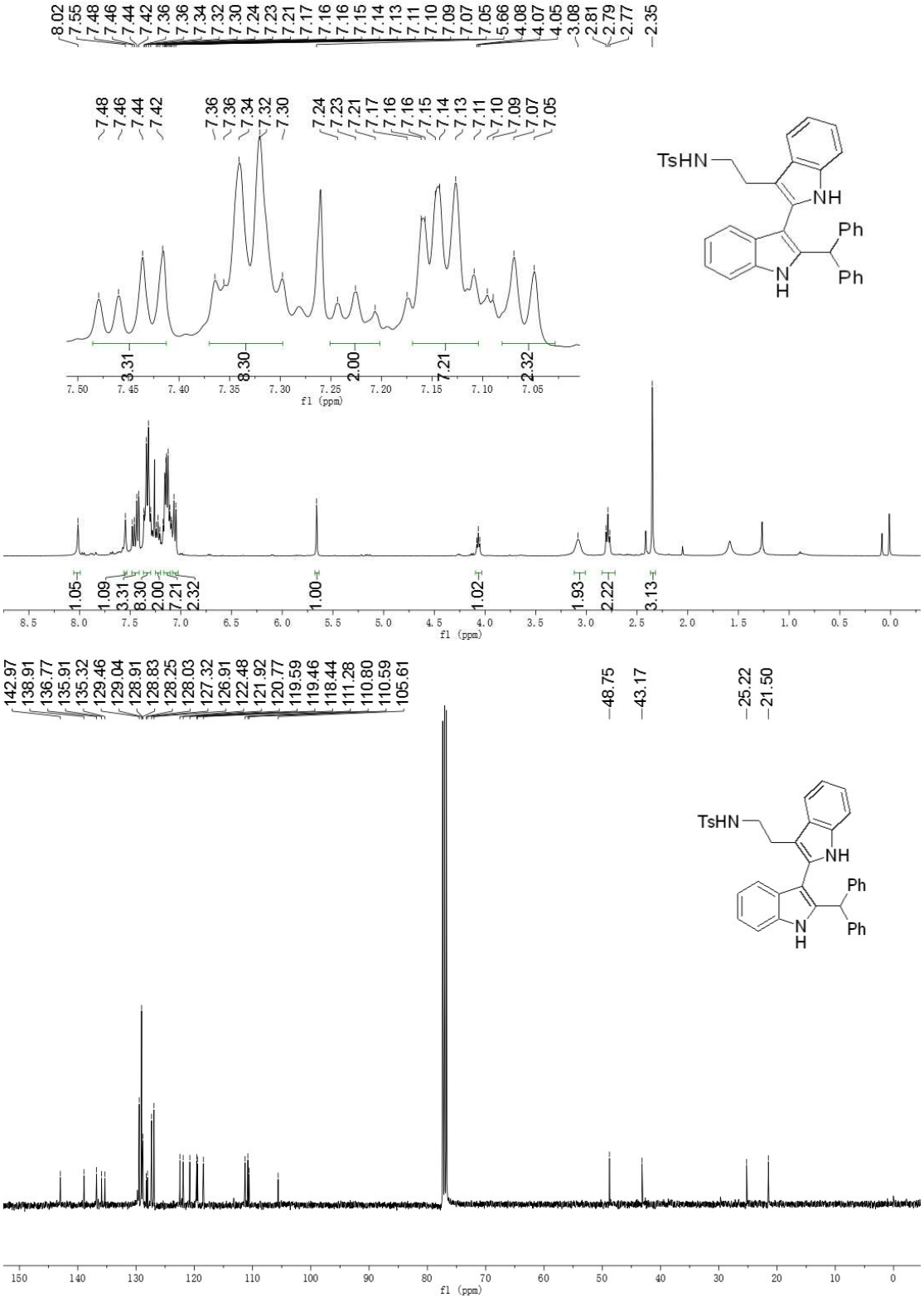
4aj


7.99
7.47
7.45
7.37
7.35
7.34
7.33
7.32
7.22
7.20
7.19
5.14
4.37
3.32
2.93
2.16
1.37
Me
BocHN
NH
Ph
Ph
N
H
0.95
1.00
2.01
7.22
6.10
1.08
1.03
0.79
1.97
2.99
9.06
f1 (ppm)
155.81
138.72
135.44
135.32
129.09
128.89
128.33
127.96
127.32
122.32
122.21
120.66
119.79
119.70
119.62
116.73
112.29
111.20
106.20
78.81
48.85
40.97
28.41
25.63
16.11

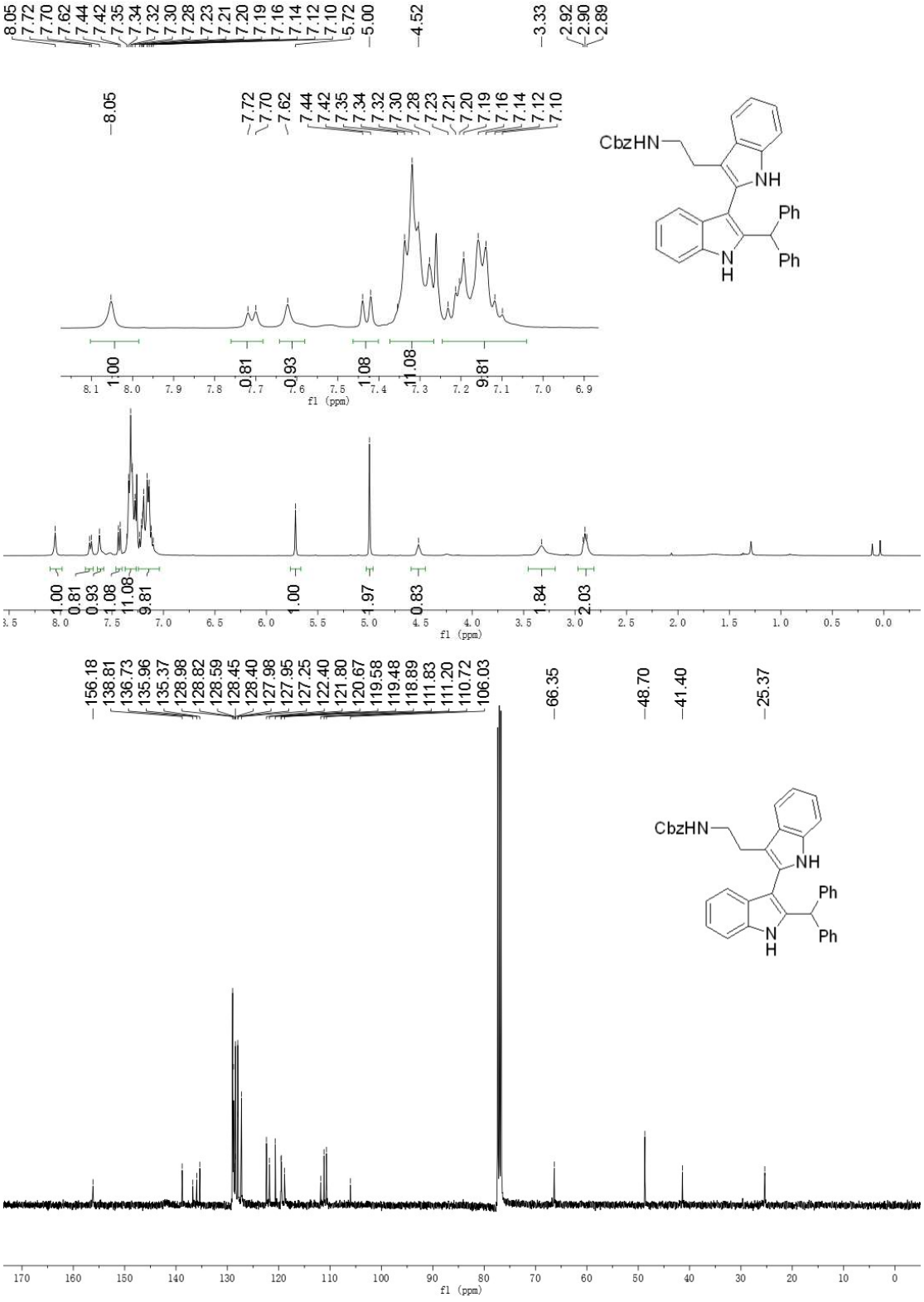
4ak


8.07
7.63
7.44
7.36
7.35
7.34
7.33
7.31
7.30
7.28
7.23
7.21
7.19
7.15
7.14
7.13
7.12
7.11
6.87
6.87
6.85
6.85
5.71
5.14
3.89
3.33
3.32
3.30
3.28
2.81
2.80
2.78
1.62
AcHN
NH
Ph
Ph
N
H
1.06
7.30
1.95
6.01
f1 (ppm)
0.88
1.00
1.06
7.30
1.95
6.01
0.99
1.00
1.02
2.95
1.92
1.84
3.32
f1 (ppm)
169.81
154.12
138.67
135.48
131.17
129.81
129.24
128.95
128.87
128.78
128.53
128.35
127.21
122.51
120.72
119.33
112.13
112.00
111.53
111.30
106.17
100.51
56.02
48.64
39.94
24.83
23.13
AcHN
NH
Ph
Ph
N
H
f1 (ppm)

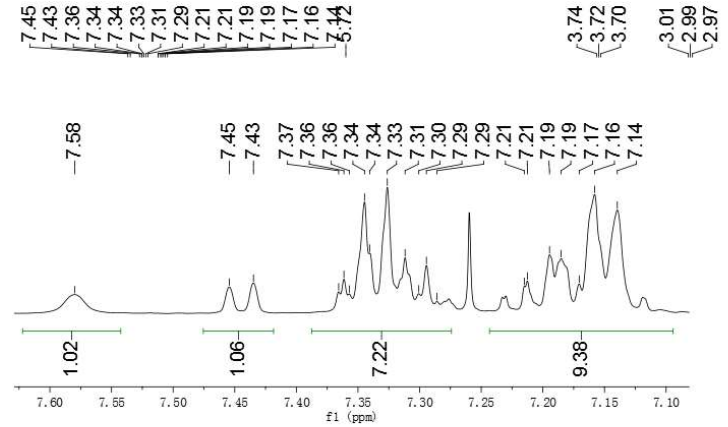
4al

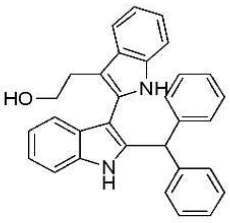

8.02
7.55
7.48
7.46
7.44
7.42
7.36
7.36
7.34
7.32
7.30
7.24
7.23
7.21
7.17
7.16
7.16
7.15
7.14
7.13
7.11
7.10
7.09
7.07
7.05
5.66
4.08
4.07
4.05
3.08
2.81
2.79
2.77
2.35
TsHN
NH
Ph
Ph
N
H
3.31
8.30
2.00
7.21
2.32
f1 (ppm)
1.05
1.09
3.31
8.30
2.00
7.21
2.32
1.00
1.02
1.93
2.22
3.13
f1 (ppm)
142.97
138.91
136.77
135.91
135.32
129.46
129.04
128.91
128.83
128.25
128.03
127.32
126.91
122.48
121.92
120.77
119.59
119.46
118.44
111.28
110.80
110.59
105.61
48.75
43.17
25.22
21.50
TsHN
NH
Ph
Ph
N
H
f1 (ppm)

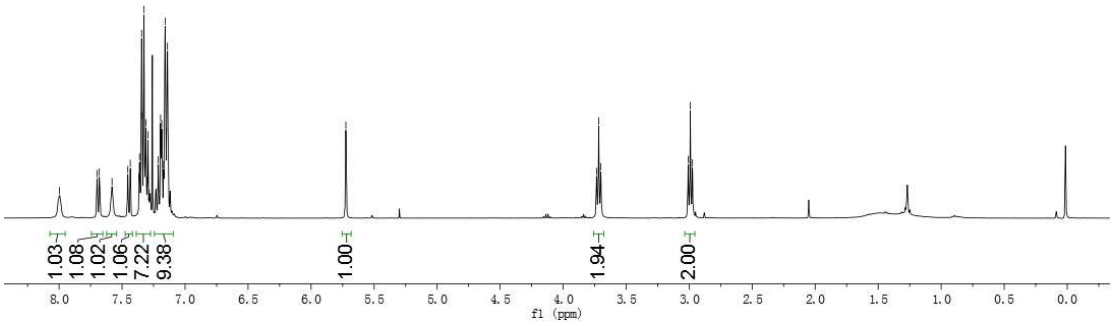
4am

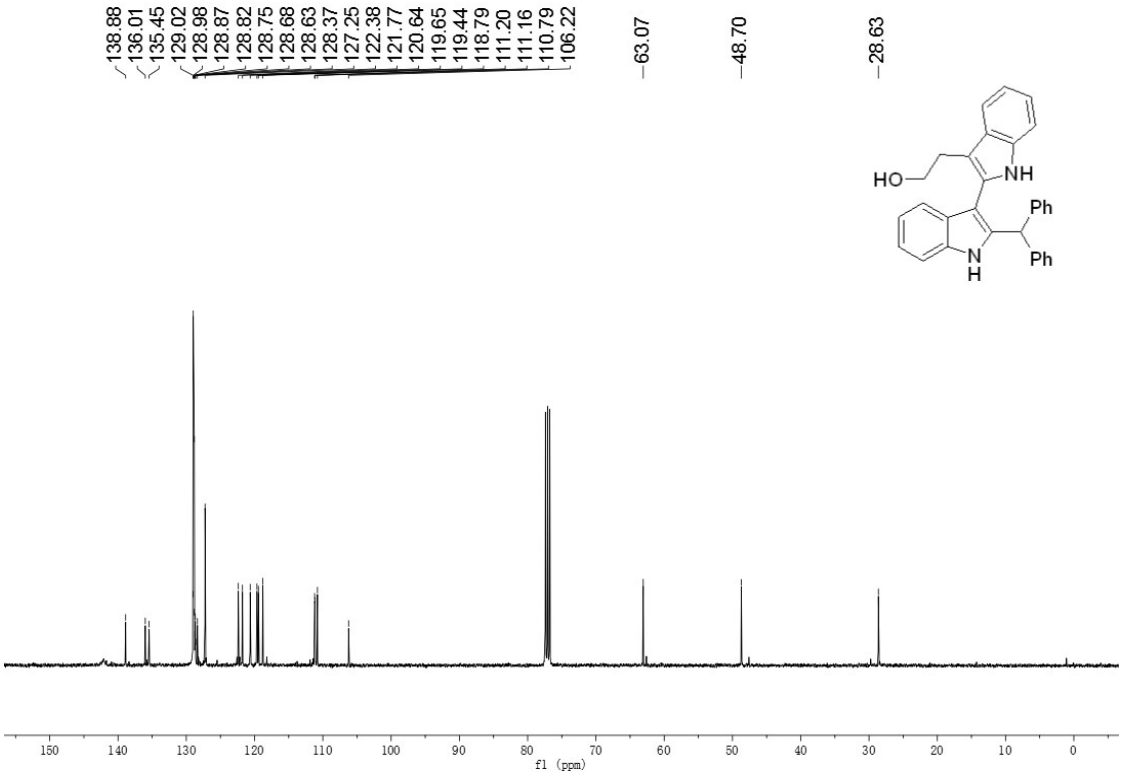

8.05
7.72
7.70
7.62
7.44
7.42
7.35
7.34
7.32
7.30
7.28
7.23
7.21
7.20
7.19
7.16
7.14
7.12
7.10
5.72
5.00
4.52
3.33
2.92
2.90
2.89
CbzHN
NH
Ph
Ph
N
H
1.00
0.81
0.93
1.08
11.08
9.81
f1 (ppm)
1.00
0.81
0.93
1.08
11.08
9.81
1.00
1.97
0.83
1.84
2.03
f1 (ppm)
156.18
138.81
136.73
135.96
135.37
128.98
128.82
128.59
128.45
128.40
127.98
127.95
127.25
122.40
121.80
120.67
119.58
119.48
118.89
111.83
111.20
110.72
106.03
66.35
48.70
41.40
25.37
CbzHN
NH
Ph
Ph
N
H
f1 (ppm)

5aa


7.45
7.43
7.36
7.34
7.34
7.33
7.31
7.29
7.21
7.21
7.19
7.19
7.17
7.16
3.74
3.72
3.70
3.01
2.99
2.97
7.58
7.45
7.43
7.37
7.36
7.36
7.34
7.34
7.33
7.31
7.30
7.29
7.29
7.21
7.21
7.19
7.19
7.17
7.16
7.14
1.02
1.06
7.22
9.38
f1 (ppm)

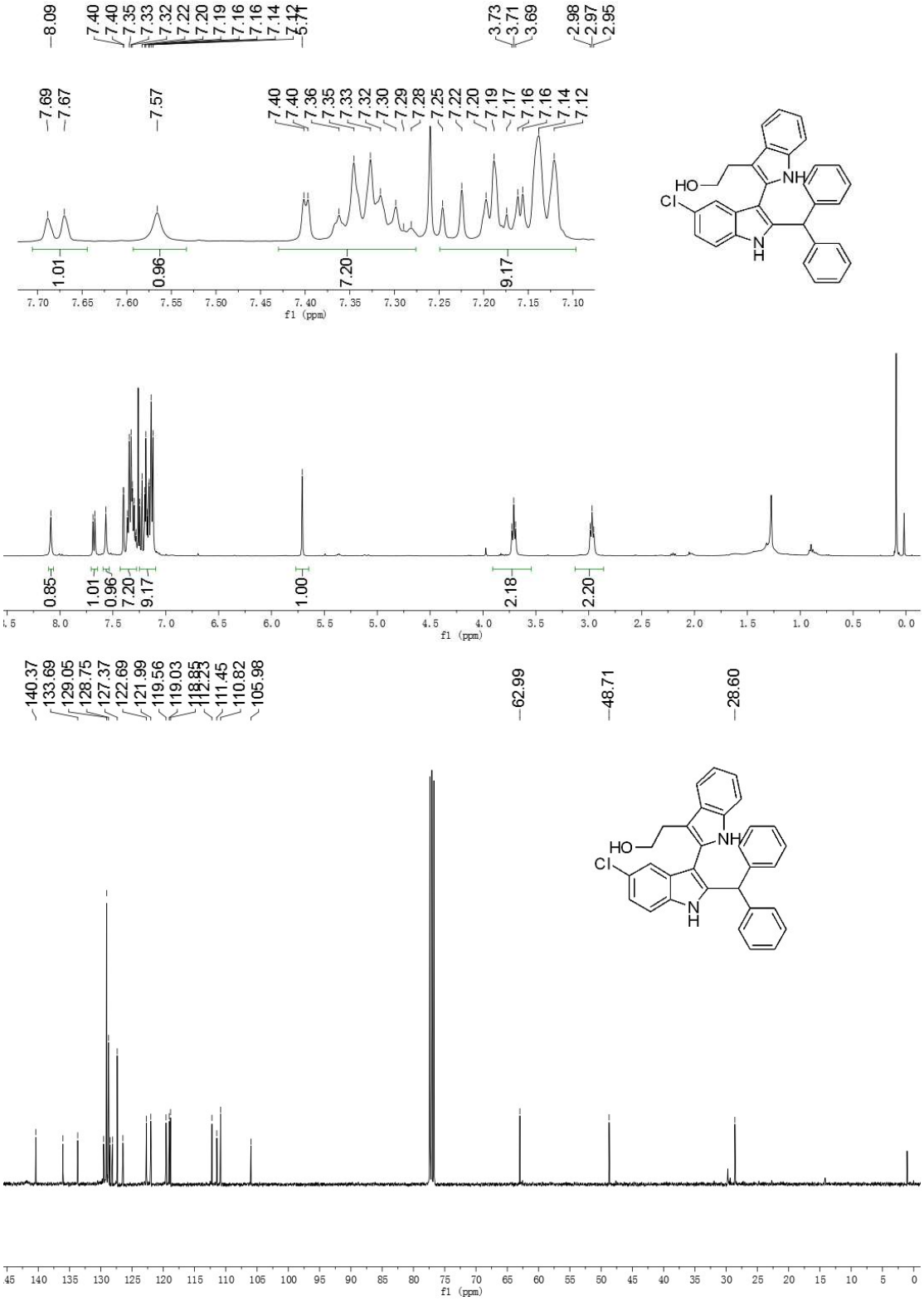

HO
NH
N
H


1.03
1.08
1.02
1.06
7.22
9.38
1.00
1.94
2.00
f1 (ppm)

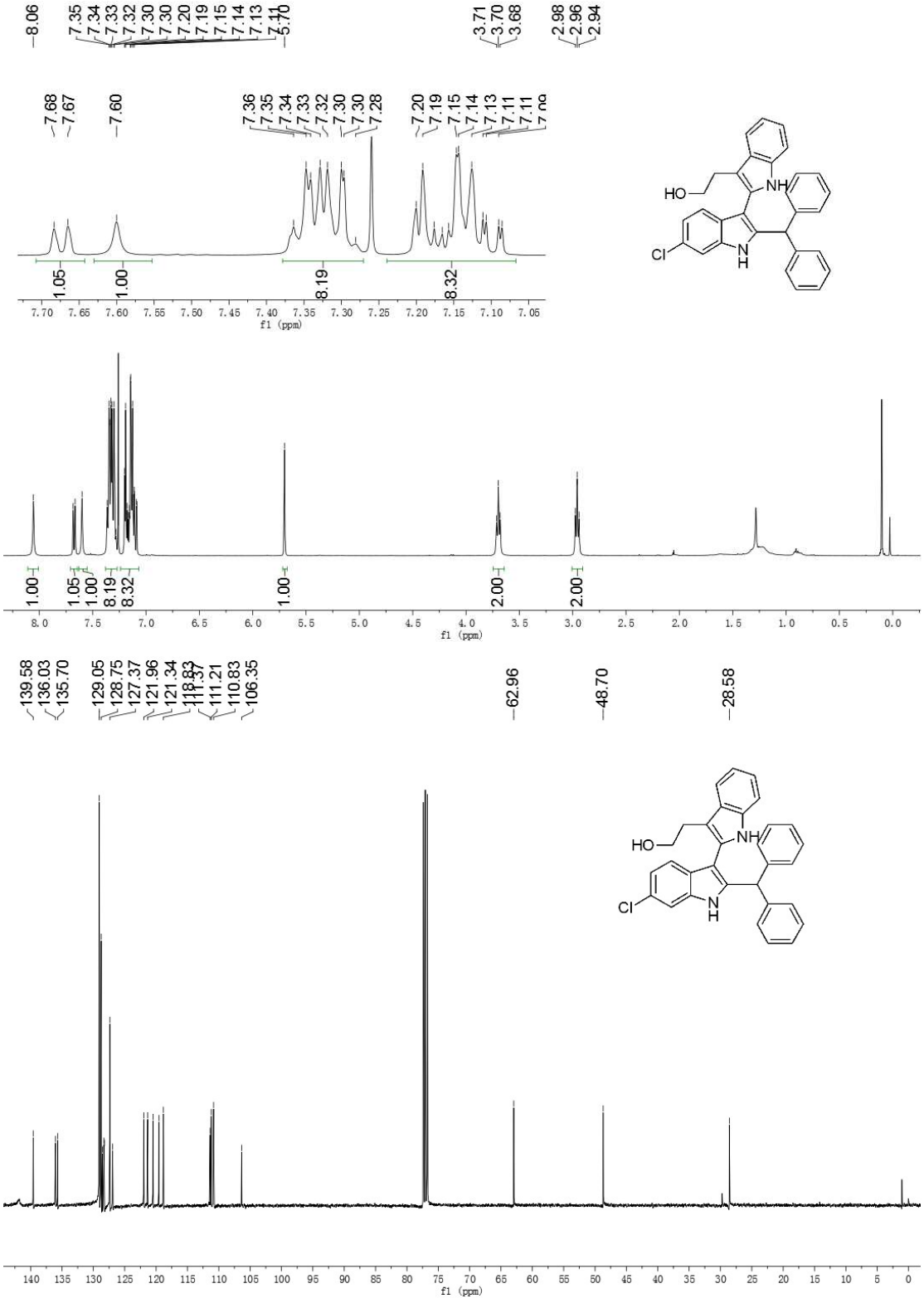

138.88
136.01
135.45
129.02
128.98
128.87
128.82
128.75
128.68
128.63
128.37
127.25
122.38
121.77
120.64
119.65
119.44
118.79
111.20
111.16
110.79
106.22
63.07
48.70
28.63
f1 (ppm)

HO
NH
Ph
Ph
N
H

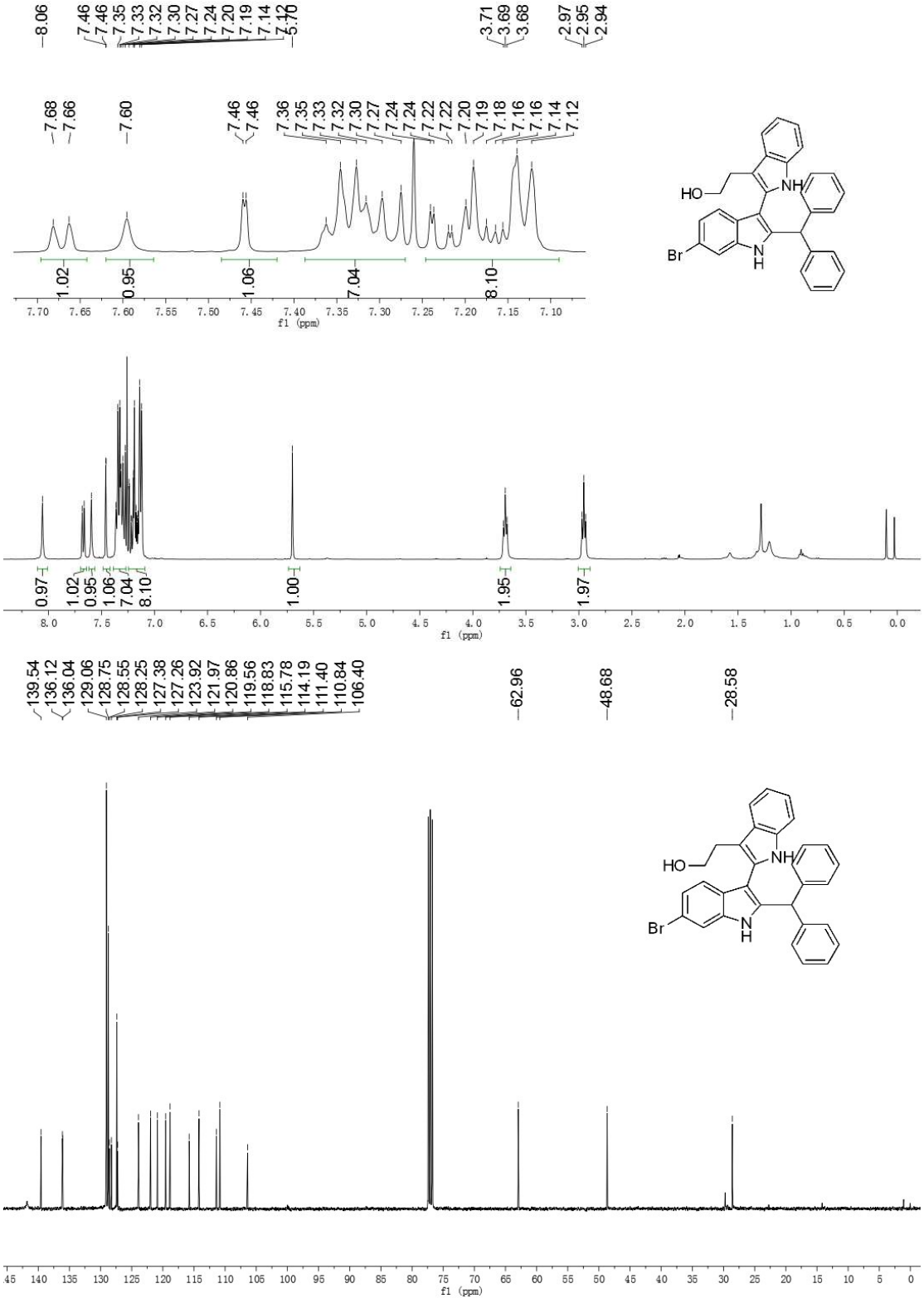
5ca


8.09
7.40
7.40
7.35
7.33
7.32
7.22
7.20
7.19
7.16
7.16
7.14
7.12
3.73
3.71
3.69
2.98
2.97
2.95
7.69
7.67
7.57
7.40
7.40
7.36
7.35
7.33
7.32
7.30
7.29
7.28
7.25
7.22
7.20
7.19
7.17
7.16
7.16
7.14
7.12
1.01
0.96
7.20
9.17
f1 (ppm)
HO
Cl
NH
N
H
0.85
1.01
0.96
7.20
9.17
1.00
2.18
2.20
f1 (ppm)
140.37
133.69
129.05
128.75
127.37
122.69
121.99
119.56
119.03
118.85
112.23
111.45
110.82
105.98
62.99
48.71
28.60
HO
Cl
NH
N
H
f1 (ppm)

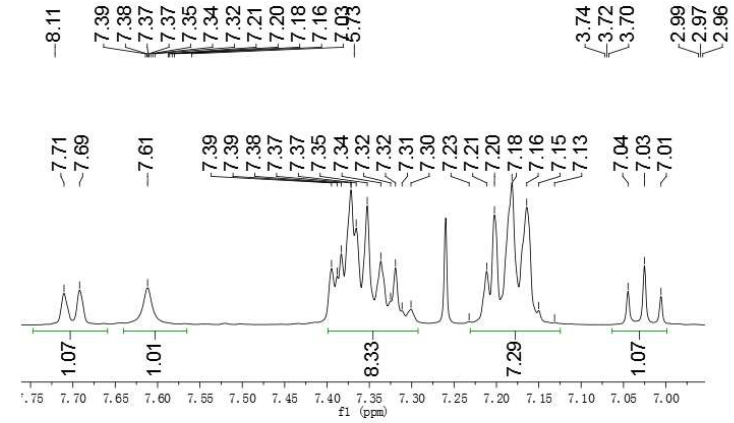
5fa


8.06
7.35
7.34
7.33
7.32
7.30
7.30
7.20
7.19
7.15
7.14
7.13
7.11
5.70
3.71
3.70
3.68
2.98
2.96
2.94
7.68
7.67
7.60
7.36
7.35
7.34
7.33
7.32
7.30
7.30
7.28
7.20
7.19
7.15
7.14
7.13
7.11
7.11
1.05
1.00
8.19
8.32
f1 (ppm)
HO
NH
Cl
N
H
1.00
1.05
1.00
8.19
8.32
1.00
2.00
2.00
f1 (ppm)
139.58
136.03
135.70
129.05
128.75
127.37
121.96
121.34
118.83
111.37
111.21
110.83
106.35
62.96
48.70
28.58
HO
NH
Cl
N
H
f1 (ppm)

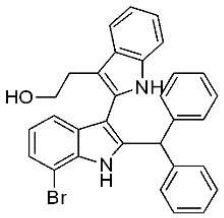
5ga

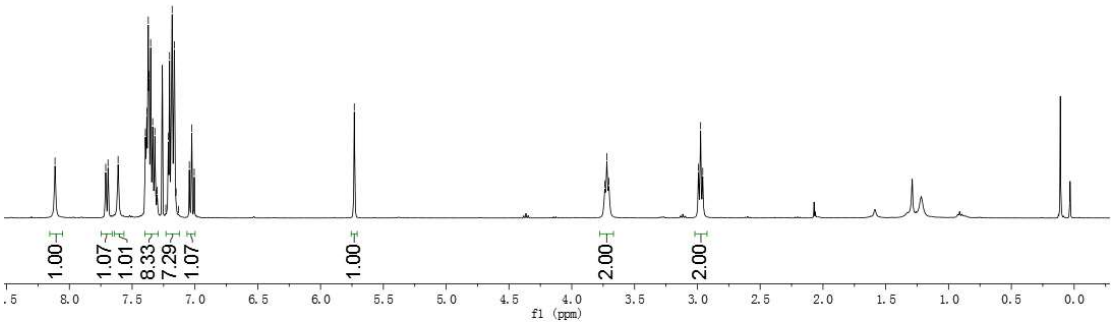

8.06
7.46
7.46
7.35
7.33
7.32
7.30
7.27
7.24
7.20
7.19
7.14
5.10
3.71
3.69
3.68
2.97
2.95
2.94
7.68
7.66
7.60
7.46
7.46
7.36
7.35
7.33
7.32
7.30
7.27
7.24
7.24
7.22
7.22
7.20
7.19
7.18
7.16
7.16
7.14
7.12
1.02
0.95
1.06
7.04
8.10
f1 (ppm)
HO
NH
Br
N
H
0.97
1.02
0.95
1.06
7.04
8.10
1.00
1.95
1.97
f1 (ppm)
139.54
136.12
136.04
129.06
128.75
128.55
128.25
127.38
127.26
123.92
121.97
120.86
119.56
118.83
115.78
114.19
111.40
110.84
106.40
62.96
48.68
28.58
f1 (ppm)

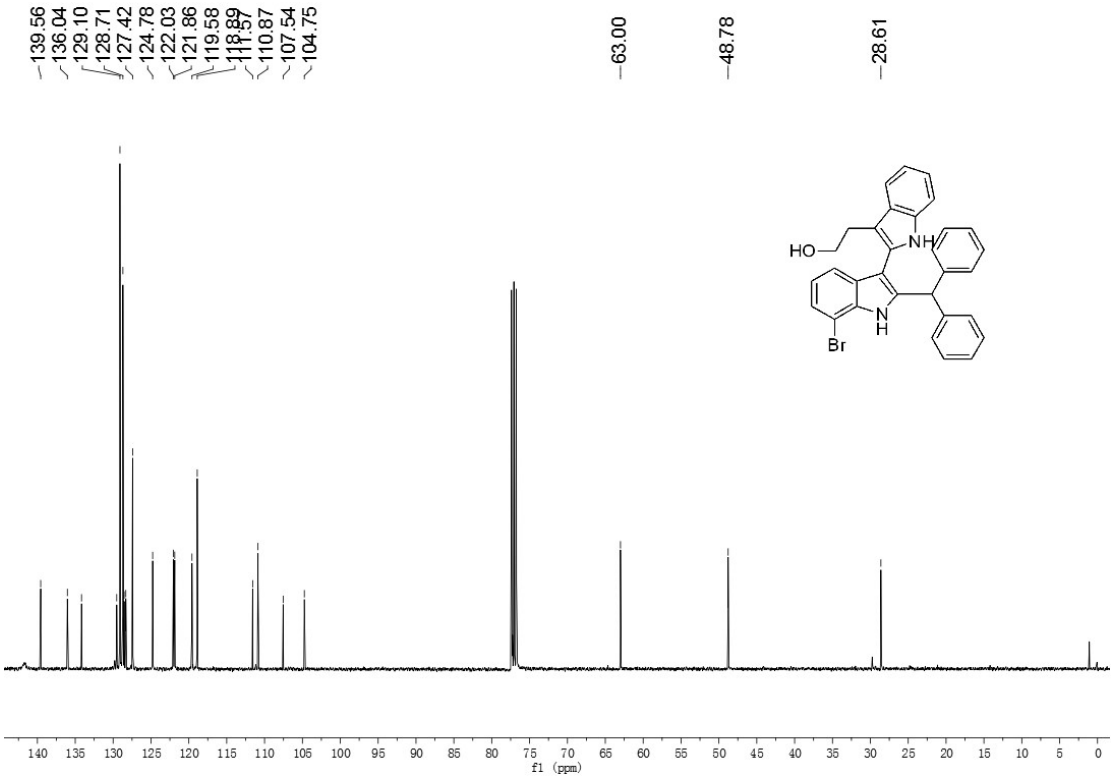
5ha


8.11
7.39
7.38
7.37
7.37
7.35
7.34
7.32
7.21
7.20
7.18
7.16
7.03
5.73
3.74
3.72
3.70
2.99
2.97
2.96

7.71
7.69
7.61
7.39
7.39
7.38
7.37
7.37
7.35
7.34
7.32
7.32
7.31
7.30
7.23
7.21
7.20
7.18
7.16
7.15
7.13
7.04
7.03
7.01
1.07
1.01
8.33
7.29
1.07
f1 (ppm)

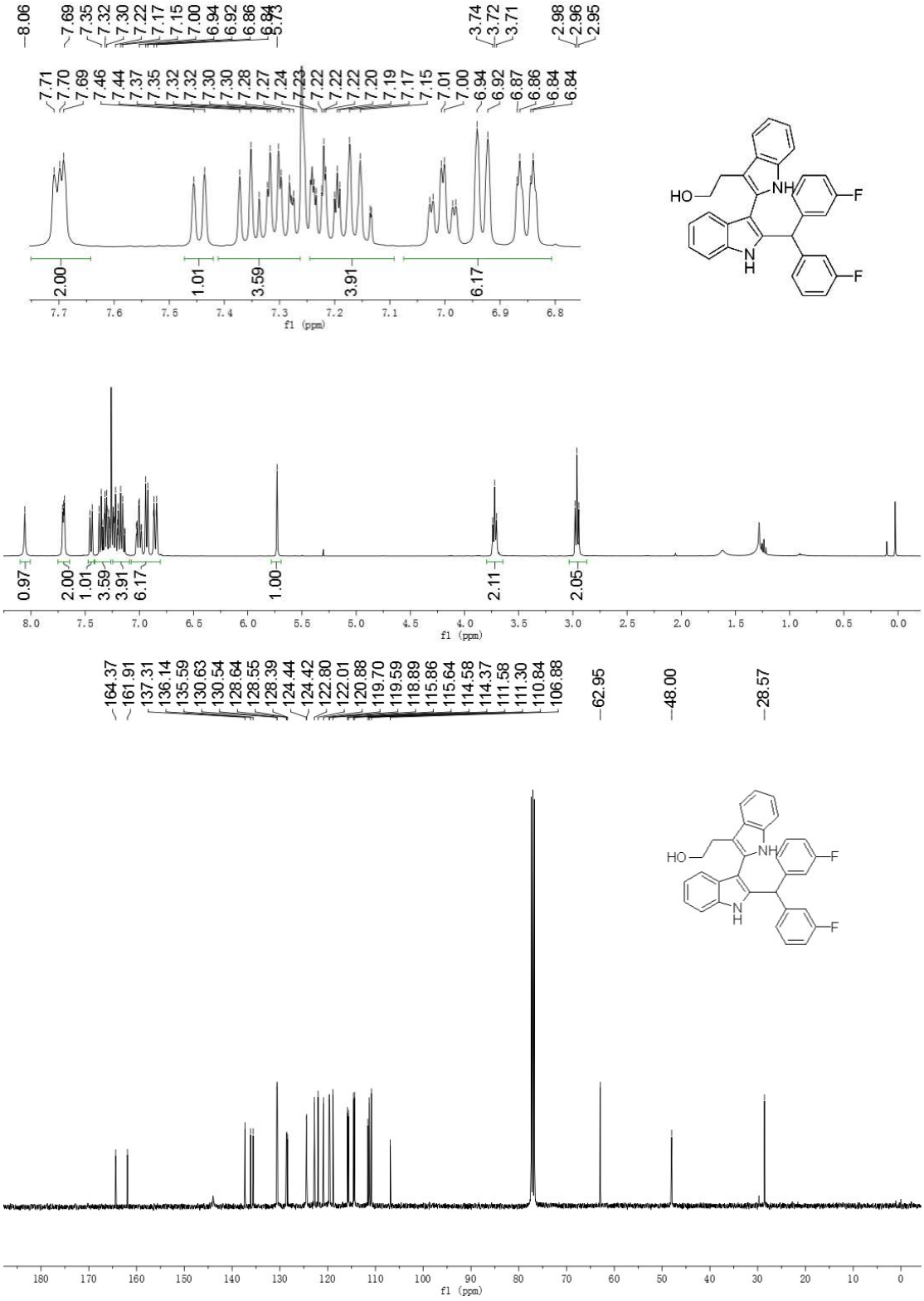

HO
NH
N
H
Br


1.00
1.07
1.01
8.33
7.29
1.07
1.00
2.00
2.00
f1 (ppm)

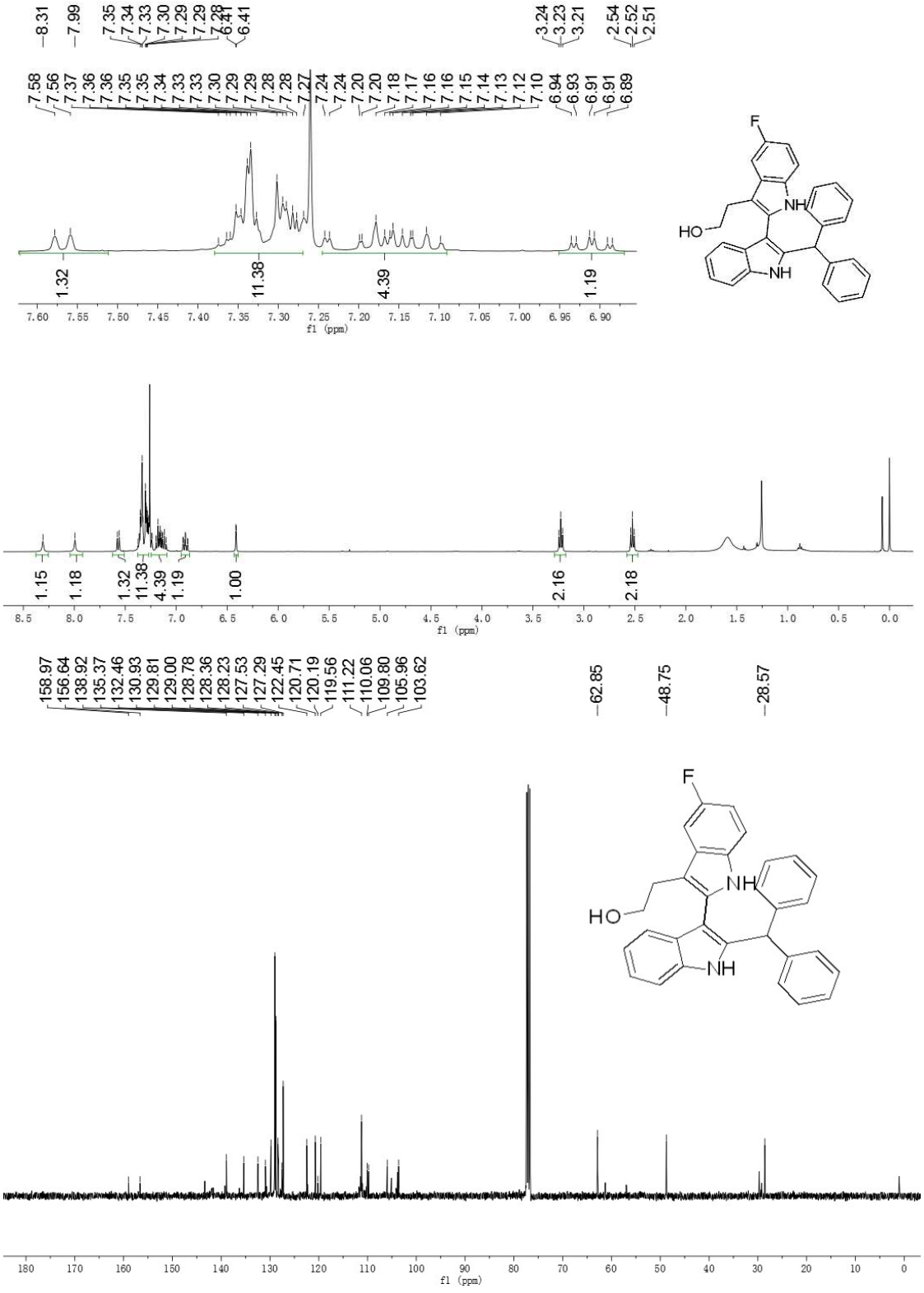

139.56
136.04
129.10
128.71
127.42
124.78
122.03
121.86
119.58
118.89
111.57
110.87
107.54
104.75
63.00
48.78
28.61
f1 (ppm)

HO
NH
N
H
Br

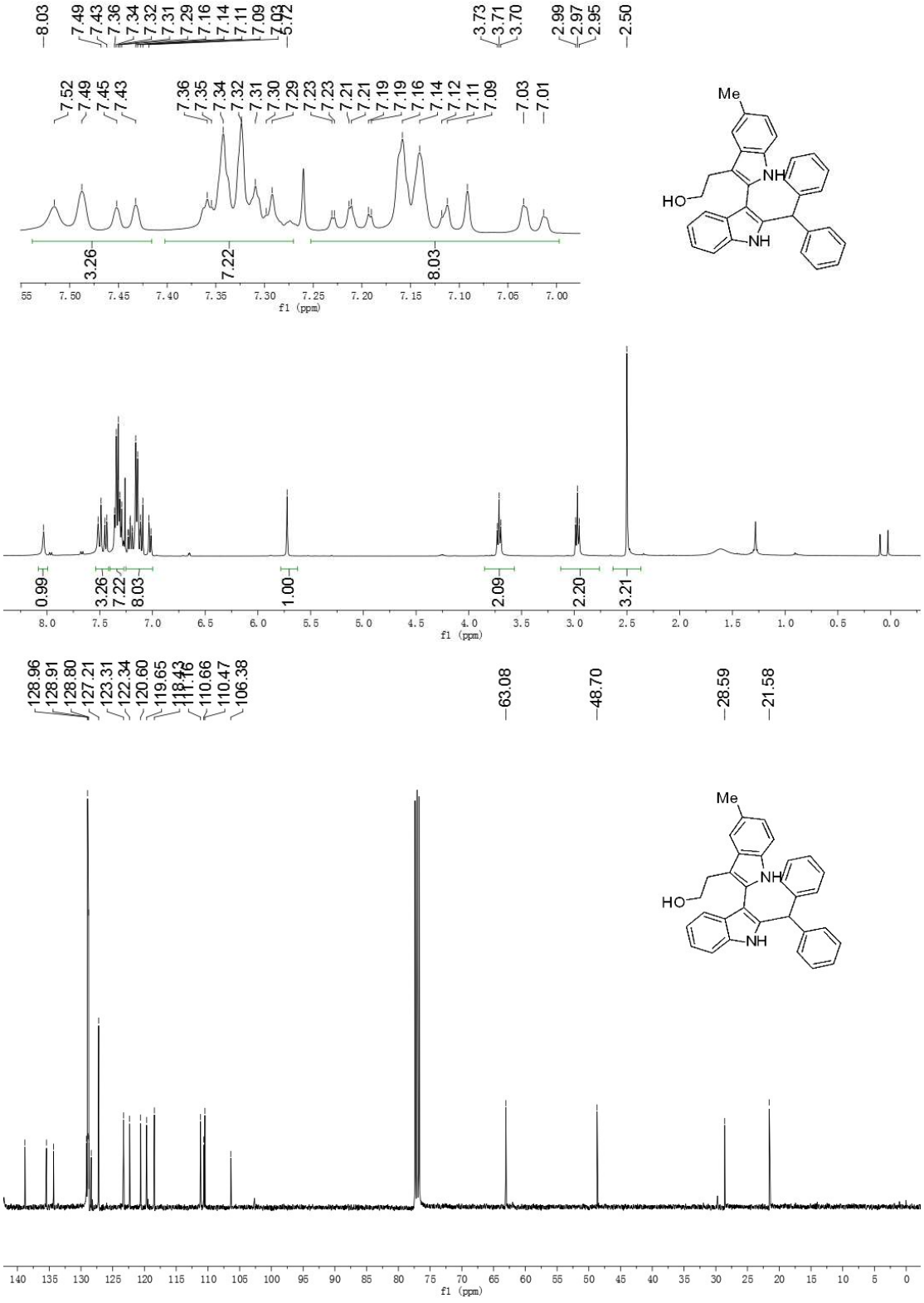
5la


8.06
7.69
7.35
7.32
7.30
7.22
7.17
7.15
7.00
6.94
6.92
6.86
6.84
5.13
3.74
3.72
3.71
2.98
2.96
2.95
7.71
7.70
7.69
7.46
7.44
7.37
7.35
7.32
7.32
7.30
7.30
7.28
7.27
7.24
7.23
7.22
7.22
7.22
7.20
7.19
7.17
7.15
7.01
7.00
6.94
6.92
6.87
6.86
6.84
6.84
2.00
1.01
3.59
3.91
6.17
f1 (ppm)
HO
NH
F
N
H
F
0.97
2.00
1.01
3.59
3.91
6.17
1.00
2.11
2.05
f1 (ppm)
164.37
161.91
137.31
136.14
135.59
130.63
130.54
128.64
128.55
128.39
124.44
124.42
122.80
122.01
120.88
119.70
119.59
118.89
115.86
115.64
114.58
114.37
111.58
111.30
110.84
106.88
62.95
48.00
28.57
HO
NH
F
N
H
F
f1 (ppm)

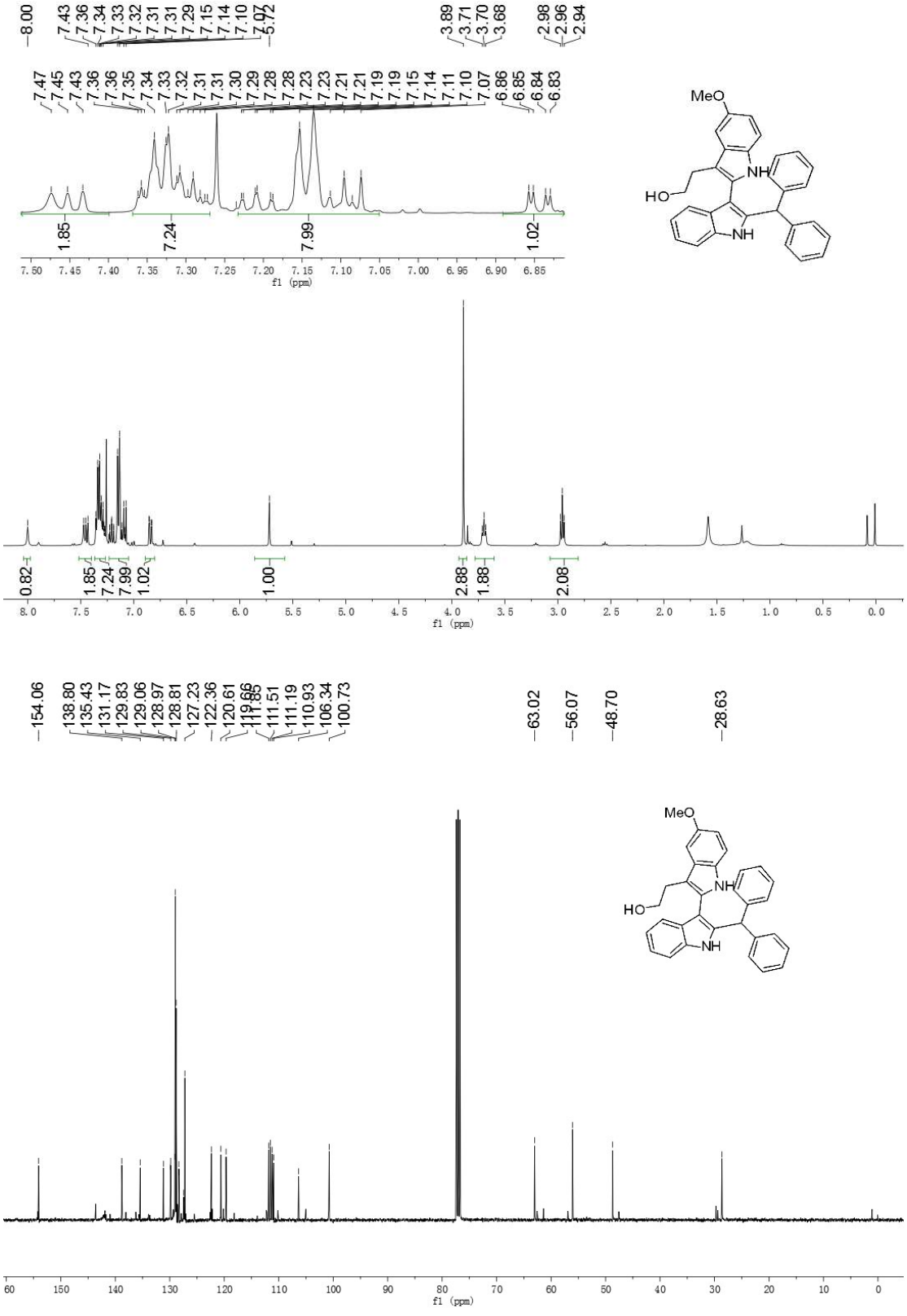
5ab


8.31
7.99
7.35
7.34
7.33
7.30
7.29
7.29
7.28
6.41
6.41
3.24
3.23
3.21
2.54
2.52
2.51
7.58
7.56
7.37
7.36
7.36
7.35
7.35
7.34
7.33
7.33
7.30
7.29
7.29
7.28
7.28
7.27
7.24
7.24
7.20
7.20
7.18
7.17
7.16
7.16
7.15
7.14
7.13
7.12
7.10
6.94
6.93
6.91
6.91
6.89
1.32
11.38
4.39
1.19
f1 (ppm)
F
NH
HO
NH
1.15
1.18
1.32
11.38
4.39
1.19
1.00
2.16
2.18
f1 (ppm)
158.97
156.64
138.92
135.37
132.46
130.93
129.81
129.00
128.78
128.36
128.23
127.53
127.29
122.45
120.71
120.19
119.56
111.22
110.06
109.80
105.96
103.62
62.85
48.75
28.57
F
NH
HO
NH
f1 (ppm)

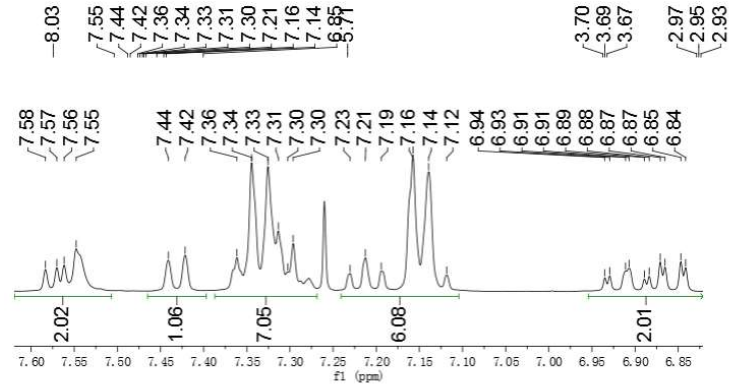
5ac

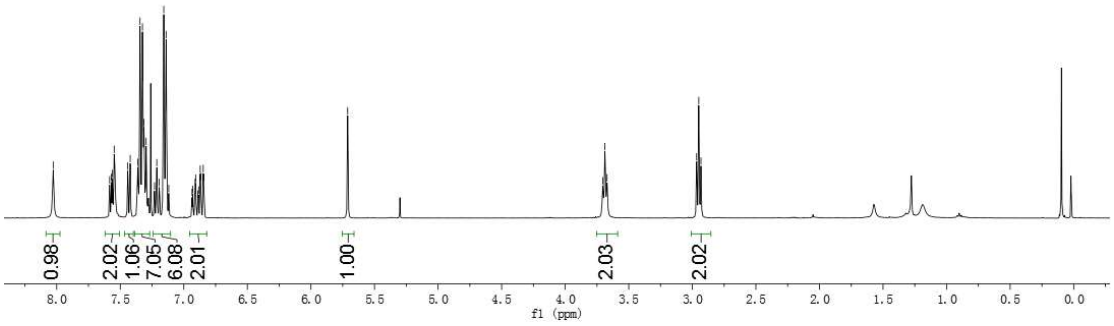

8.03
7.49
7.43
7.36
7.34
7.32
7.31
7.29
7.16
7.14
7.11
7.09
7.03
5.72
3.73
3.71
3.70
2.99
2.97
2.95
2.50
7.52
7.49
7.45
7.43
7.36
7.35
7.34
7.32
7.31
7.30
7.29
7.23
7.23
7.21
7.21
7.19
7.19
7.16
7.14
7.12
7.11
7.09
7.03
7.01
3.26
7.22
8.03
f1 (ppm)
Me
NH
HO
NH
0.99
3.26
7.22
8.03
1.00
2.09
2.20
3.21
f1 (ppm)
128.96
128.91
128.80
127.21
123.31
122.34
120.60
119.65
118.43
111.16
110.66
110.47
106.38
63.08
48.70
28.59
21.58
Me
NH
HO
NH
f1 (ppm)

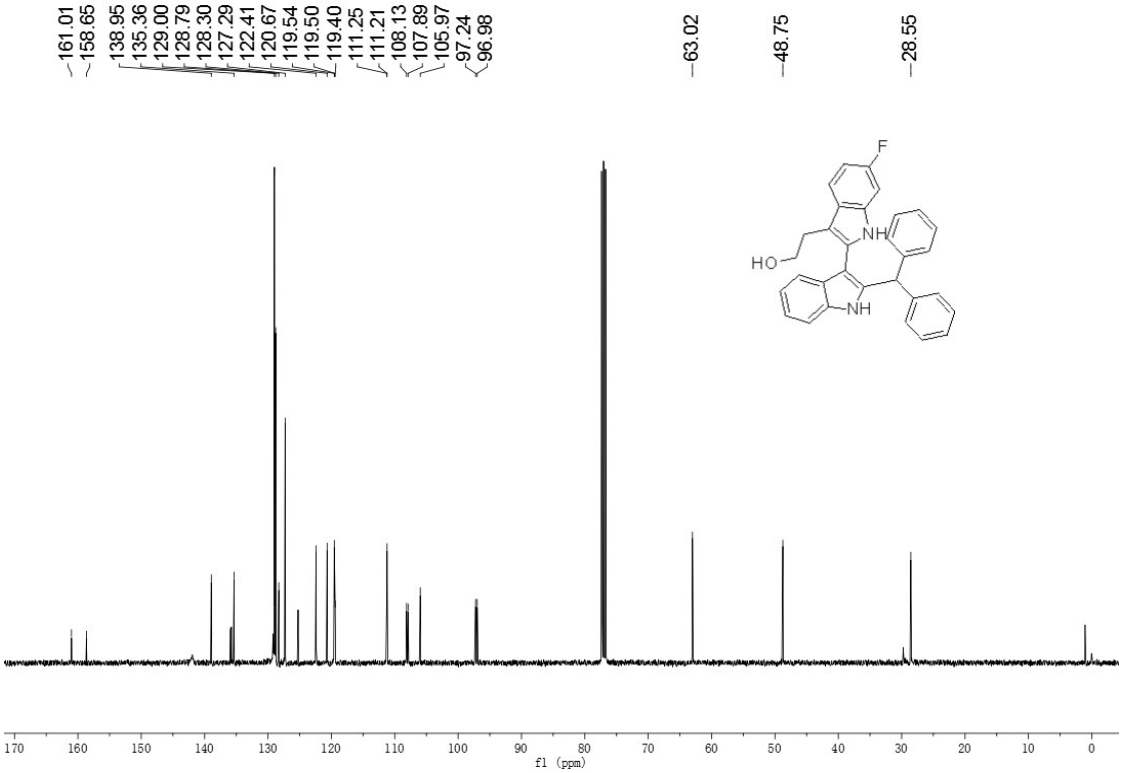
5ad


8.00
7.43
7.36
7.34
7.33
7.32
7.31
7.31
7.29
7.15
7.14
7.10
7.07
5.72
3.89
3.71
3.70
3.68
2.98
2.96
2.94
7.47
7.45
7.43
7.36
7.36
7.35
7.34
7.33
7.32
7.31
7.31
7.30
7.29
7.28
7.28
7.23
7.23
7.21
7.21
7.19
7.19
7.15
7.14
7.11
7.10
7.07
6.86
6.85
6.84
6.83
1.85
7.24
7.99
1.02
f1 (ppm)
MeO
NH
HO
NH
0.82
1.85
7.24
7.99
1.02
1.00
2.88
1.88
2.08
f1 (ppm)
154.06
138.80
135.43
131.17
129.83
129.06
128.97
128.81
127.23
122.36
120.61
119.66
111.85
111.51
111.19
110.93
106.34
100.73
63.02
56.07
48.70
28.63
MeO
NH
HO
NH
f1 (ppm)

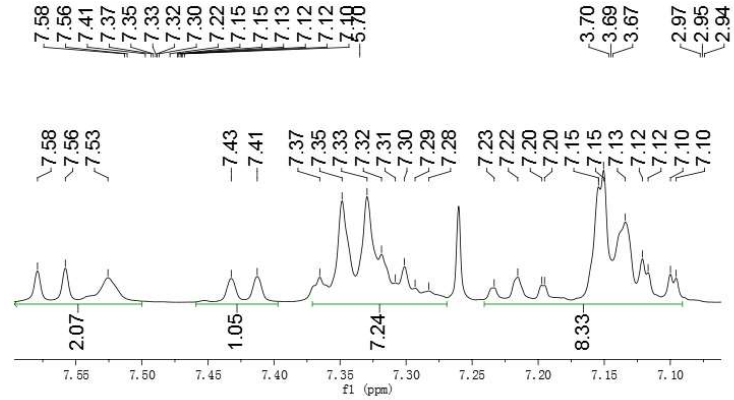
5ae


8.03
7.55
7.44
7.42
7.36
7.34
7.33
7.31
7.30
7.21
7.16
7.14
6.85
5.71
3.70
3.69
3.67
2.97
2.95
2.93
7.58
7.57
7.56
7.55
7.44
7.42
7.36
7.34
7.33
7.31
7.30
7.30
7.23
7.21
7.19
7.16
7.14
7.12
6.94
6.93
6.91
6.91
6.89
6.88
6.87
6.87
6.85
6.84
2.02
1.06
7.05
6.08
2.01
f1 (ppm)
F
NH
HO
NH

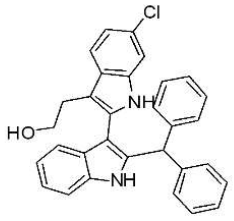

0.98
2.02
1.06
7.05
6.08
2.01
1.00
2.03
2.02
f1 (ppm)

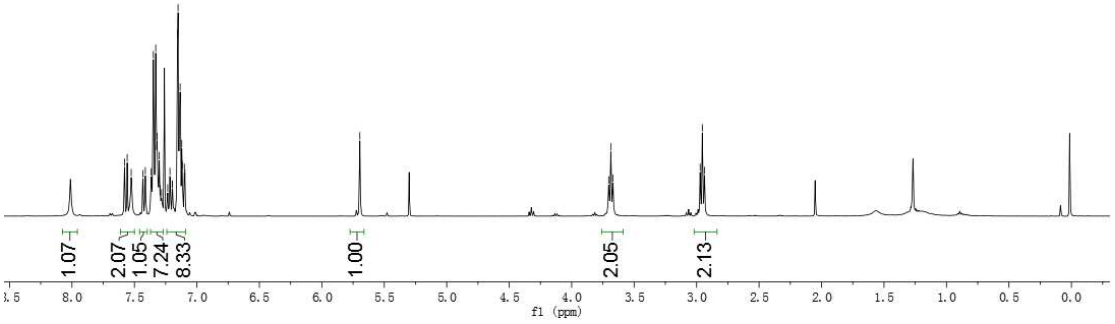

161.01
158.65
138.95
135.36
129.00
128.79
128.30
127.29
122.41
120.67
119.54
119.50
119.40
111.25
111.21
108.13
107.89
105.97
97.24
96.98
63.02
48.75
28.55
F
NH
HO
NH
f1 (ppm)

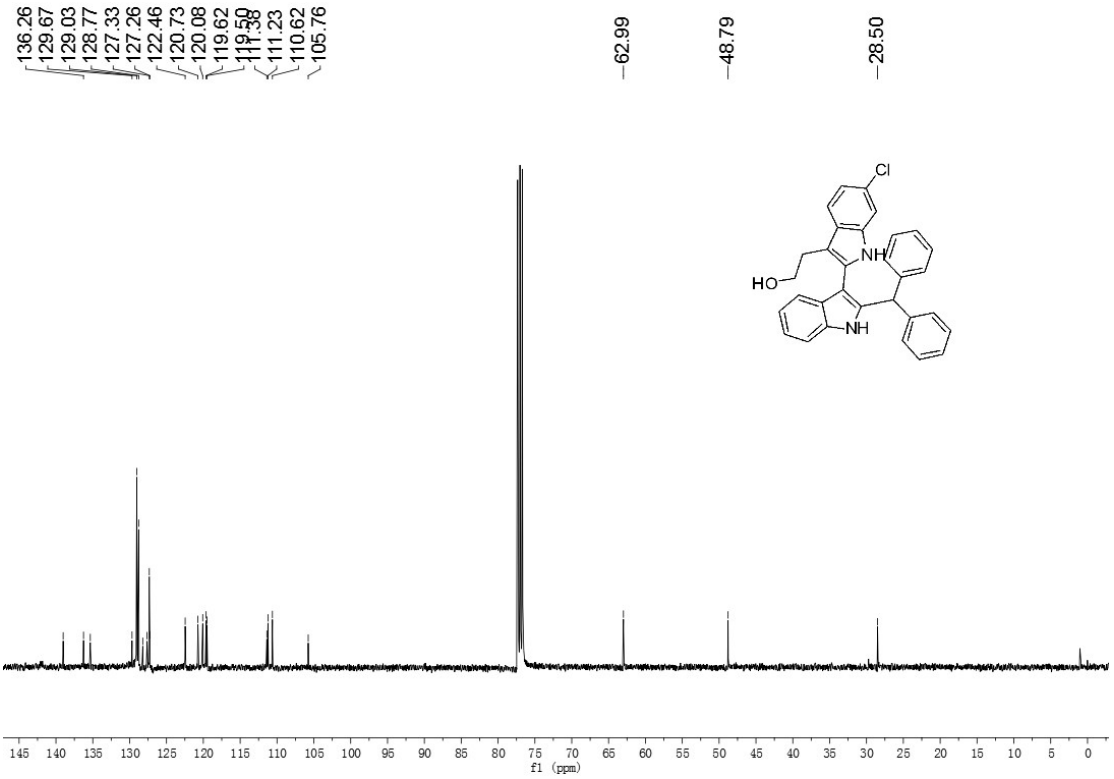
5af


7.58
7.56
7.41
7.37
7.35
7.33
7.32
7.30
7.22
7.15
7.15
7.13
7.12
7.12
5.10
3.70
3.69
3.67
2.97
2.95
2.94

7.58
7.56
7.53
7.43
7.41
7.37
7.35
7.33
7.32
7.31
7.30
7.29
7.28
7.23
7.22
7.20
7.20
7.15
7.15
7.13
7.12
7.12
7.10
7.10
2.07
1.05
7.24
8.33
f1 (ppm)

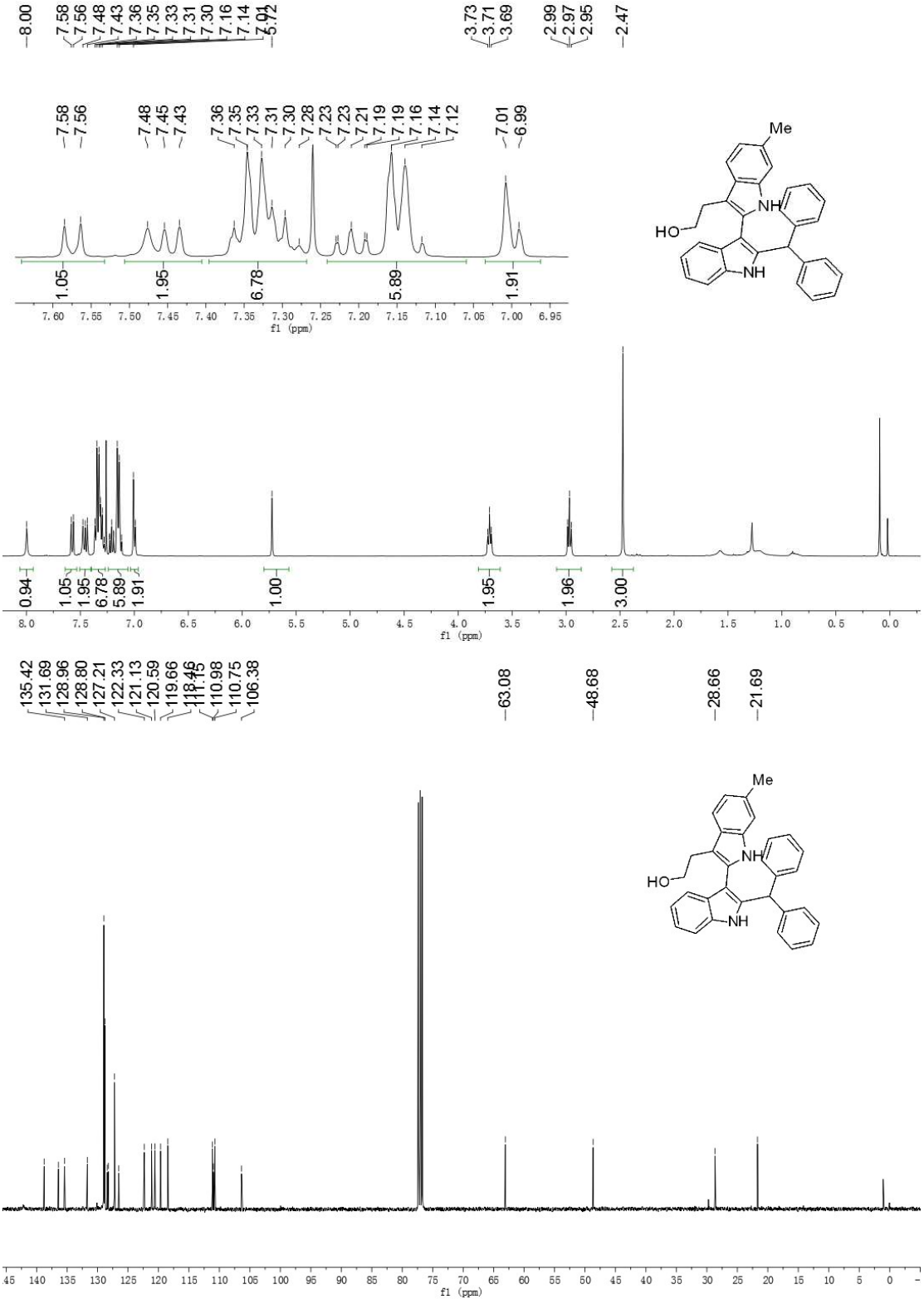

Cl
NH
HO
NH


1.07
2.07
1.05
7.24
8.33
1.00
2.05
2.13
f1 (ppm)

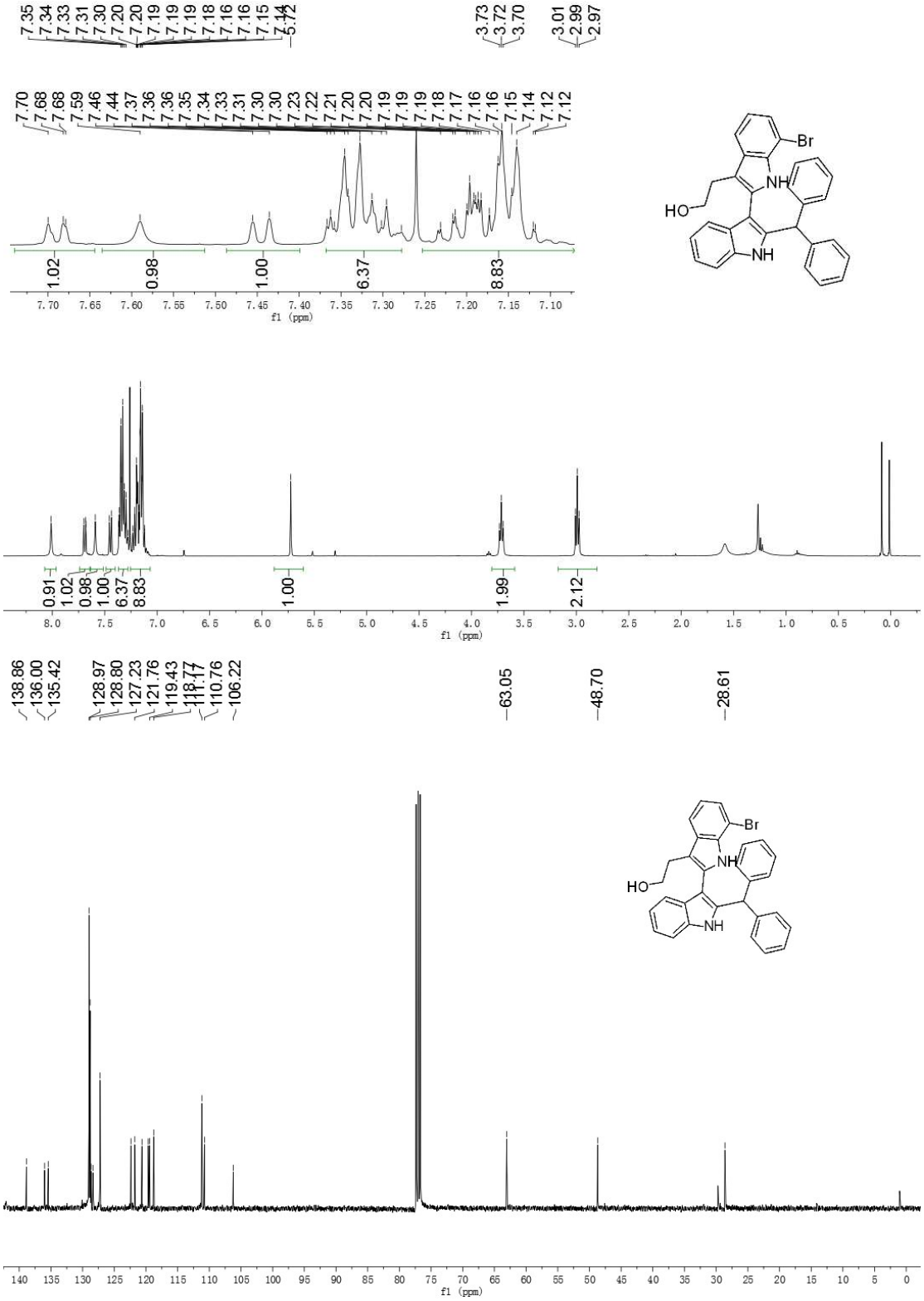

136.26
129.67
129.03
128.77
127.33
127.26
122.46
120.73
120.08
119.62
111.38
111.23
110.62
105.76
62.99
48.79
28.50
f1 (ppm)

Cl
NH
HO
NH

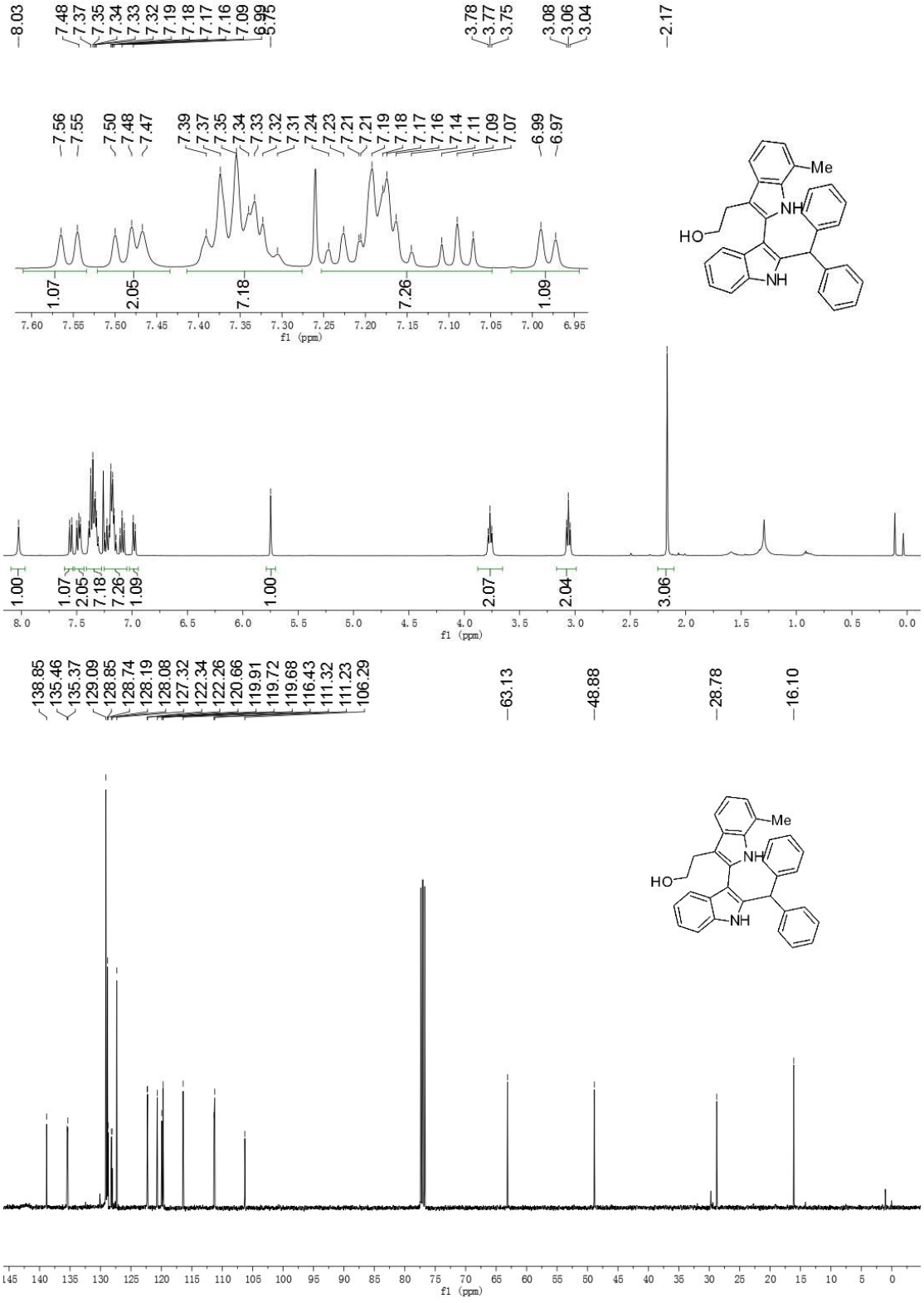
5ag


8.00
7.58
7.56
7.48
7.43
7.36
7.35
7.33
7.31
7.30
7.16
7.14
5.72
3.73
3.71
3.69
2.99
2.97
2.95
2.47
7.58
7.56
7.48
7.45
7.43
7.36
7.35
7.33
7.31
7.30
7.28
7.23
7.23
7.21
7.19
7.19
7.16
7.14
7.12
7.01
6.99
1.05
1.95
6.78
5.89
1.91
f1 (ppm)
Me
NH
HO
NH
0.94
1.05
1.95
6.78
5.89
1.91
1.00
1.95
1.96
3.00
f1 (ppm)
135.42
131.69
128.96
128.80
127.21
122.33
121.13
120.59
119.66
118.46
111.15
110.98
110.75
106.38
63.08
48.68
28.66
21.69
Me
NH
HO
NH
f1 (ppm)

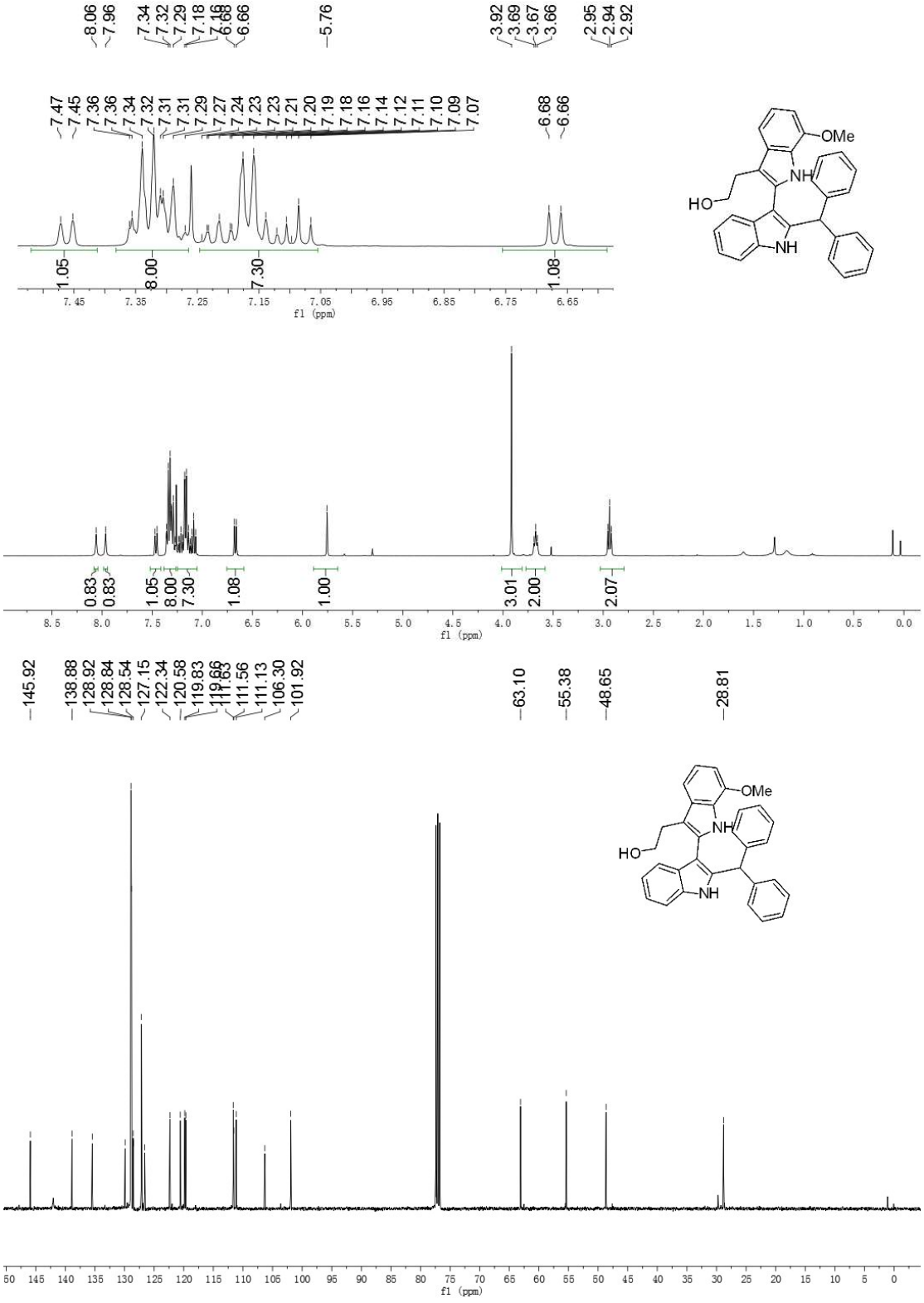
5ah


7.35
7.34
7.33
7.31
7.30
7.20
7.20
7.19
7.19
7.19
7.18
7.16
7.16
7.15
7.14
5.12
3.73
3.72
3.70
3.01
2.99
2.97
7.70
7.68
7.68
7.59
7.46
7.44
7.37
7.36
7.36
7.35
7.34
7.33
7.31
7.30
7.30
7.23
7.22
7.21
7.20
7.20
7.19
7.19
7.19
7.18
7.17
7.16
7.16
7.15
7.14
7.12
7.12
1.02
0.98
1.00
6.37
8.83
f1 (ppm)
Br
NH
HO
NH
0.91
1.02
0.98
1.00
6.37
8.83
1.00
1.99
2.12
f1 (ppm)
138.86
136.00
135.42
128.97
128.80
127.23
121.76
119.43
118.77
111.17
110.76
106.22
63.05
48.70
28.61
Br
NH
HO
NH
f1 (ppm)

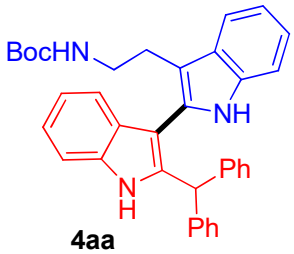
5ai


8.03
7.48
7.37
7.35
7.34
7.33
7.32
7.19
7.18
7.17
7.16
7.09
6.99
6.95
3.78
3.77
3.75
3.08
3.06
3.04
2.17
7.56
7.55
7.50
7.48
7.47
7.39
7.37
7.35
7.34
7.33
7.32
7.31
7.24
7.23
7.21
7.21
7.19
7.18
7.17
7.16
7.14
7.11
7.09
7.07
6.99
6.97
1.07
2.05
7.18
7.26
1.09
f1 (ppm)
Me
NH
HO
NH
1.00
1.07
2.05
7.18
7.26
1.09
1.00
2.07
2.04
3.06
f1 (ppm)
138.85
135.46
135.37
129.09
128.85
128.74
128.19
128.08
127.32
122.34
122.26
120.66
119.91
119.72
119.68
116.43
111.32
111.23
106.29
63.13
48.88
28.78
16.10
Me
NH
HO
NH
f1 (ppm)

5aj


8.06
7.96
7.34
7.32
7.29
7.18
6.68
6.66
5.76
3.92
3.69
3.67
3.66
2.95
2.94
2.92
7.47
7.45
7.36
7.34
7.32
7.31
7.29
7.27
7.24
7.23
7.21
7.20
7.19
7.18
7.16
7.14
7.12
7.11
7.10
7.09
7.07
6.68
6.66
1.05
8.00
7.30
1.08
f1 (ppm)
OMe
NH
HO
NH
0.83
0.83
1.05
8.00
7.30
1.08
1.00
3.01
2.00
2.07
f1 (ppm)
145.92
138.88
128.92
128.84
128.54
127.15
122.34
120.58
119.83
111.56
111.13
106.30
101.92
63.10
55.38
48.65
28.81
OMe
NH
HO
NH
f1 (ppm)

6. X-ray single crystal data for compounds 4aa and 5aj:

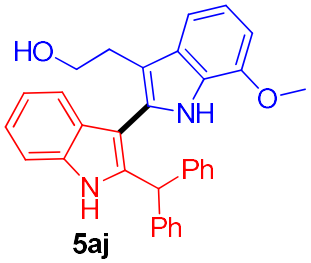


4aa

The thermal ellipsoid was drawn at the 30% probability level.

Identification code	mo_dm16248_0m
Empirical formula	C36 H35 N3 O2
Formula weight	541.67
Temperature	273(2) K

Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C c	
Unit cell dimensions	a = 14.9636(17) Å	α= 90°.
	b = 12.2439(14) Å	β= 96.500(2)°.
	c = 33.362(4) Å	γ = 90°.
Volume	6073.1(12) $Å^3$	
Z	8	
Density (calculated)	1.185 Mg/m^3	
Absorption coefficient	0.074 mm^{-1}	
F(000)	2304	
Crystal size	0.200 x 0.170 x 0.110 mm^3	
Theta range for data collection	1.229 to 25.500°.	
Index ranges	-17<=h<=18, -14<=k<=14, -40<=l<=38	
Reflections collected	20737	
Independent reflections	8659 [R(int) = 0.0715]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6720	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8659 / 44 / 770	
Goodness-of-fit on F^2	0.969	
Final R indices [I>2sigma(I)]	R1 = 0.0480, wR2 = 0.0830	
R indices (all data)	R1 = 0.1250, wR2 = 0.1171	
Absolute structure parameter	4.5(10)	
Extinction coefficient	0.00051(10)	
Largest diff. peak and hole	0.142 and -0.142 $e.Å^{-3}$	



5aj

The thermal ellipsoid was drawn at the 30% probability level.

Identification code	sf20170406_xmm_0m	
Empirical formula	C32 H28 N2 O2	
Formula weight	472.56	
Temperature	296.15 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21/n 1	
Unit cell dimensions	a = 13.672(3) Å	α= 90°.
	b = 17.459(4) Å	β= 92.451(3)°.
	c = 23.660(5) Å	γ = 90°.

Volume	5642(2) $Å^3$
Z	8
Density (calculated)	1.113 Mg/m^3
Absorption coefficient	0.069 mm^{-1}
F(000)	2000
Crystal size	0.6 x 0.5 x 0.1 mm^3
Theta range for data collection	2.487 to 25.000°.
Index ranges	-16<=h<=15, -20<=k<=20, -28<=l<=24
Reflections collected	27698
Independent reflections	9858 [R(int) = 0.0320]
Completeness to theta = 25.000°	99.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.6626
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9858 / 50 / 672
Goodness-of-fit on F^2	1.013
Final R indices [I>2sigma(I)]	R1 = 0.0721, wR2 = 0.2058
R indices (all data)	R1 = 0.1154, wR2 = 0.2453
Extinction coefficient	n/a
Largest diff. peak and hole	0.896 and -0.252 $e.Å^{-3}$