Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Ligand-Controlled Regiodivergent Direct Arylation of Indoles via Oxidative Boron Heck Reaction

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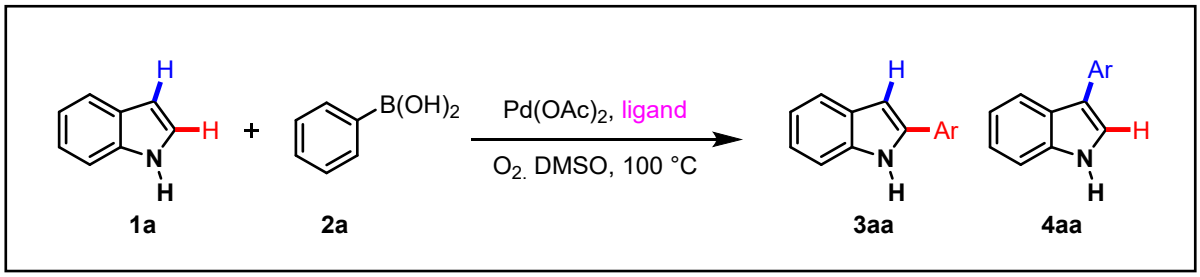
1. General Information

General: Unless noted otherwise, all starting materials and reagents were obtained from commercial suppliers (Strem chemicals, Aldrich, Acros Organics, Alfa Aesar, and TCI) and were used without further purification. All solvents used for routine isolation of products and chromatography were reagent grade. Reaction flasks were dried at 80 °C. Analytical thin-layer chromatography (TLC) was performed using Merck silica gel glass plates with F-254 indicator, visualized by UV light (254 nm and 365 nm), in some cases stained with ninhydrin or Hanessian's stain followed by heating. Flash column chromatography was performed with a Biotage Isolera One purification system equipped with 5, 10, and 25 g Biotage® Sfär Silica 60 µm columns with the indicated solvents. NMR spectra were recorded and obtained using a Varian VNMRS500 (500 MHz for ^{1}H NMR, 126 MHz for ^{13}C NMR, and 471 MHz for ^{19}F NMR) spectrometer, respectively. ^{1}H, ^{13}C, and ^{19}F NMR chemical shifts are reported in parts per million (ppm) relative to TMS (tetramethylsilane), with the residual solvent peak used as an internal reference. Signals are reported as m (multiplet), s (singlet), bs (broad singlet), d (doublet), dd (doublet of doublet), td (triplet of doublet), t (triplet), and q (quartet); the coupling constants (*J*) are reported in Hertz (Hz). High-resolution mass spectrometry (HRMS) data were obtained with a Jeol AccuTOF (JMS-T100TD) equipped with a DART (direct analysis in real-time) ion source from Ionsens, (Tokyo, Japan) in the ESI mode.

2. Optimization for Regioselective Arylation

Table S1. Ligand Screening



entry[a]	ligand	yield (%)[b]	**3aa**:**4aa**[c]
1	none	0	-
2	L1	50	1:>20
3	L2	54	1:>20
4	L3	60	1:>20
5	**L4**	**80**	**1:>20**
6	L5	29	1:>20
7	**L6**	**34**	**>20:1**
8	L7	33	2:1
9	L8	36	1:3
10	L9	34	1:1
11	L10	40	3:2
12	L11	53	1:>20

[a]Reaction conditions: **1a** (0.3 mmol, 1 equiv.), **2a** (0.6 mmol, 2 equiv.), $Pd(OAc)_2$ (10 mol%), ligand (20 mol%), solvent (1.0 mL), 100 °C, 24 h. [b]Yields were determined by ^1H NMR with internal standard 1,3,5-trimethoxybenzene. [c]Ratio was determined by ^1H-NMR.

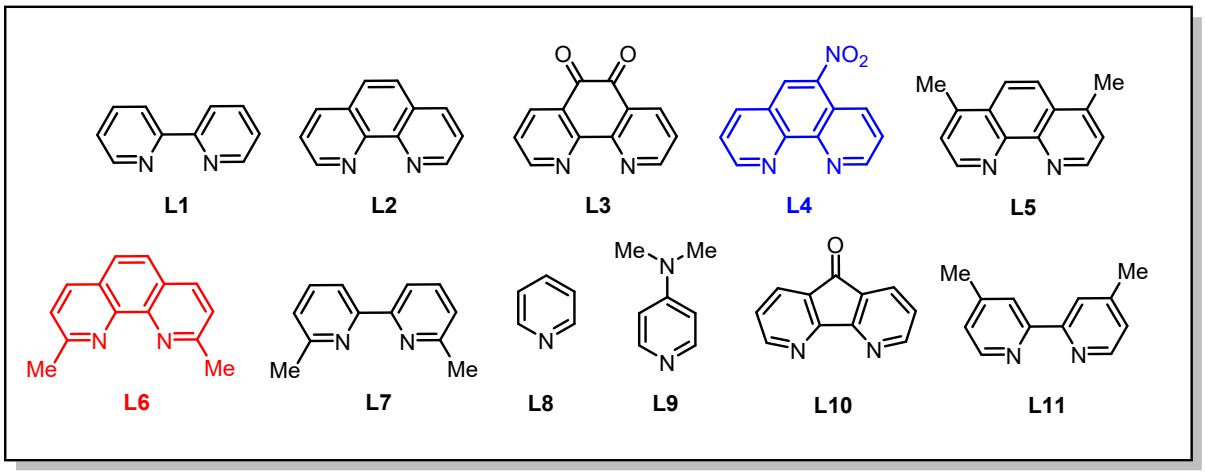
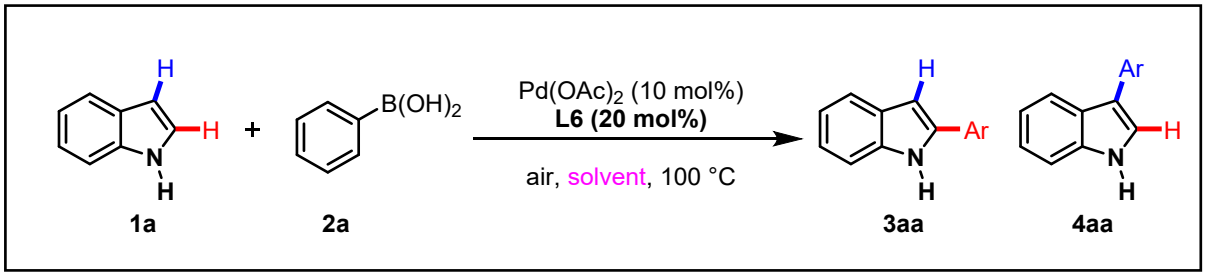


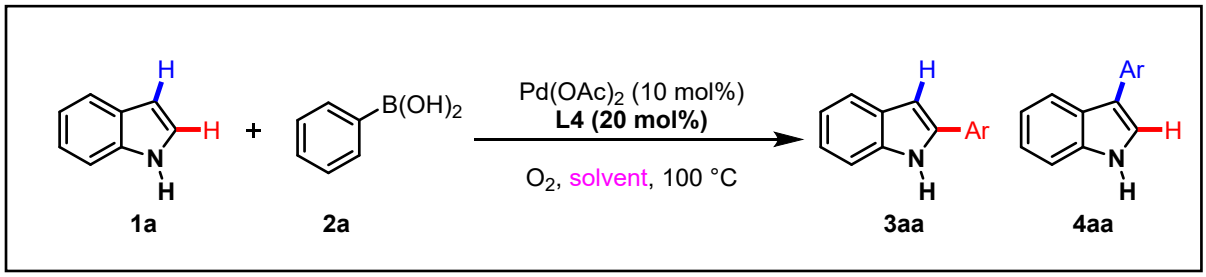
Table S2. Solvent Screening for C2-Selective Arylation



entry[a]	solvent	yield (%)[b]	**3aa**:**4aa**[c]
1	DMSO	34	>20:1
2	DMF	22	>20:1
3	chlorobenzene	43	>20:1
4	toluene	43	5:1
5	*o*-xylene	40	10:1
6	H_2O	34	>20:1
7	DCE	100	>20:1
8[d]	DCE	91	>20:1
9[e]	**DCE**	**100**	**>20:1**
10[f]	DCE	86	>20:1
11[g]	DCE	91	>20:1

[a]Reaction conditions: **1a** (0.3 mmol, 1 equiv,), **2a** (0.6 mmol, 2 equiv.), $Pd(OAc)_2$ (10 mol%), **Ligand 6** (20 mol%), solvent (1.0 mL), 100 °C under air, 24 h. [b]Yields were determined by ^{1}H NMR with internal standard 1,3,5-trimethoxybenzene. [c]Ratio was determined by ^{1}H-NMR. [d]O_2 was used instead of Air. [e]The reaction was done at 80 °C. [f]The reaction was done at 60 °C. [g]$Pd(OAc)_2$ (5 mol%) and Ligand 6 (10 mol%).

Table S3. Solvent Screening for C3-Selective Arylation

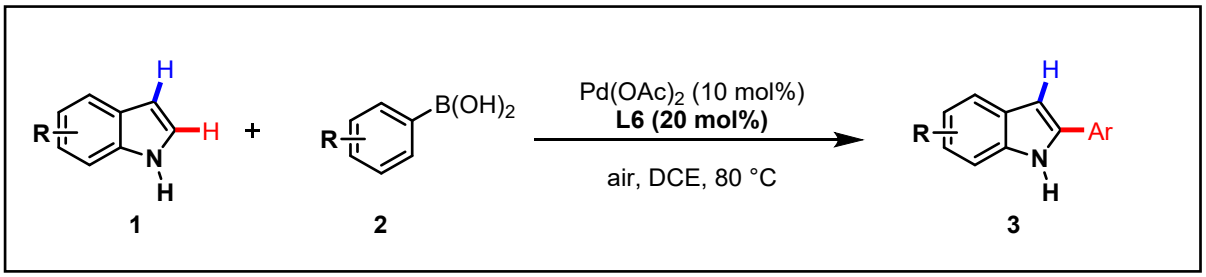


entry[a]	solvent	yield (%)[b]	**3aa**:**4aa**[c]
1	DMSO	80	1:>20
2	chlorobenzene	32	1:>20
3	DCE	34	1:>20
4	AcOH	11	1:>20
5	H_2O	43	1:>20
6	DMF	91	1:>20
7[d]	DMF	82	1:>20
8[e]	DMF	54	1:>20
9[f]	**DMF**	**93**	**1:>20**

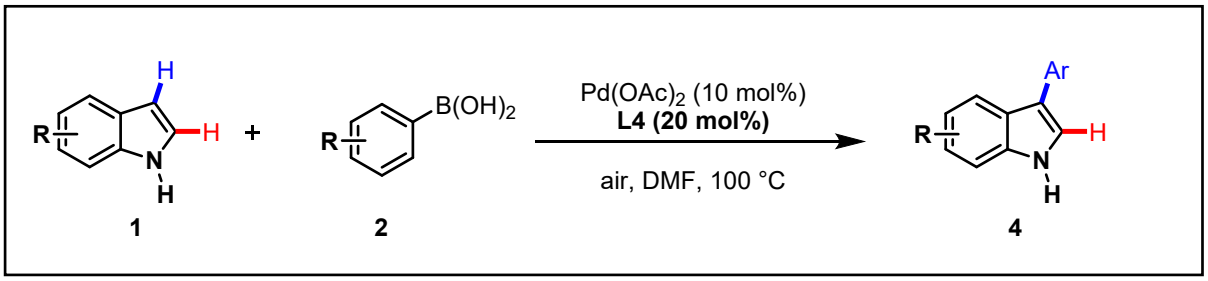
[a]Reaction conditions: **1a** (0.3 mmol, 1 equiv.), **2a** (0.6 mmol, 2 equiv.), $Pd(OAc)_2$ (10 mol%), **Ligand 4** (20 mol%), solvent (1.0

mL), 100 °C under O_2 atmosphere, 24 h. [b]Yields were determined by ^{1}H NMR with internal standard 1,3,5-trimethoxybenzene. [c]Ratio was determined by ^{1}H-NMR. [d]$Pd(OAc)_2$ (5 mol%) and Ligand 4 (10 mol%). [e]The reaction was done at 80 °C. [f]Air instead of O_2.

3. General Procedure for Regioselective Arylation



Procedure for C2-Selective Arylation of 1*H*-Indoles (3aa-3an): To a 10 mL round bottom flask, 1*H*-indole **1** (0.30 mmol, 1.0 equiv.), phenylboronic acid **2** (0.60 mmol, 2.0 equiv.) $Pd(OAc)_2$ (10.0 mol%), and neocuproine (**Ligand 6**, 20.0 mol%) were added, and then dissolved with DCE (1.0 mL). Under air, the reaction mixture was stirred at 80 °C in an oil bath until the complete conversion of the starting material on TLC. Then, the reaction mixture was cooled to room temperature, and added water. The resulting mixture was extracted with EtOAc. The combined organic layers were dried with Na_2SO_4, filtered, and concentrated in vacuo. The residue was purified by column chromatography.

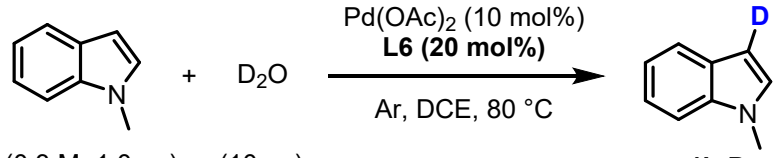


Procedure for C3-Selective Arylation of Indoles (4aa-4ao): To a 10 mL round bottom flask, 1*H*-indole **1** (0.30 mmol, 1.0 equiv.), phenylboronic acid **2** (0.60 mmol, 2.0 equiv.) $Pd(OAc)_2$ (10.0 mol%), and 5-nitro-1,10-phenanthroline (**Ligand 4**, 20.0 mol%) were added, and then dissolved with DMF (1.0 mL). Under air, the reaction mixture was stirred at 100 °C in an oil bath until the complete conversion of the starting material on TLC. Then, the reaction mixture was cooled to room temperature, and added water. The resulting mixture was extracted with EtOAc. The combined organic layers were dried with Na_2SO_4, filtered, and concentrated in vacuo. The residue was purified by column chromatography.

4. Mechanism Study

(1) Experiment for Monitoring the Deuteration Progress of *N*-Methylindole

a. The Pd(II)/L6 System

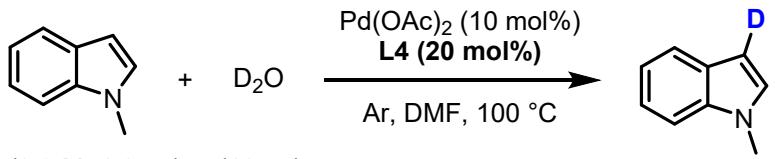


(0.3 M, 1.0 eq) (10 eq) **1b-D**

	0.5 h	1 h	2 h	4 h	24 h
C2 (D)	0 %	0 %	0 %	0 %	0 %
C3 (D)	2 %	2.7 %	6 %	6 %	8 %

To a 10 mL round bottom flask, *N*-methylindole (0.30 mmol, 1.0 equiv.), D_2O (3.0 mmol, 10.0 equiv.) $Pd(OAc)_2$ (0.03 mmol, 10.0 mol%), and Ligand 6 (0.06 mmol, 20.0 mol%) were added, and then dissolved with DCE (1.0 mL). Under Ar, the reaction mixture was stirred at 80 °C in an oil bath and aliquots of the reaction mixture (ca. 0.1 mL each) were sampled by a syringe at 0.5 h, 1 h, 2 h, 4 h, and 24 h, respectively. The aliquots were immediately quenched by brine (5.0 mL) and extracted with EA (1.0 mL), and the organic layer was separated and submitted to 1H analysis for determining the deuterium incorporation at C2- and C3- positions.

b. The Pd(II)/L4 System:



(0.3 M, 1.0 eq) (10 eq) **1b-D**

	0.5 h	1 h	2 h	4 h	24 h
C2 (D)	0 %	0 %	0 %	0 %	0 %
C3 (D)	21 %	32 %	47 %	64 %	96 %

To a 10 mL round bottom flask, *N*-methylindole (0.30 mmol, 1.0 equiv.), D_2O (3.0 mmol, 10.0 equiv.)

$Pd(OAc)_2$ (0.03 mmol, 10.0 mol%), and Ligand 4 (0.06 mmol, 20.0 mol%) were added, and then dissolved with DMF (1.0 mL). Under Ar, the reaction mixture was stirred at 100 °C in an oil bath and aliquots of the reaction mixture (ca. 0.1 mL each) were sampled by a syringe at 0.5 h, 1 h, 2 h, 4 h, and 24 h, respectively. The aliquots were immediately quenched by brine (5.0 mL) and extracted with EA (1.0 mL), and the organic layer was separated and submitted to 1H analysis for determining the deuterium incorporation at C2- and C3-positions.

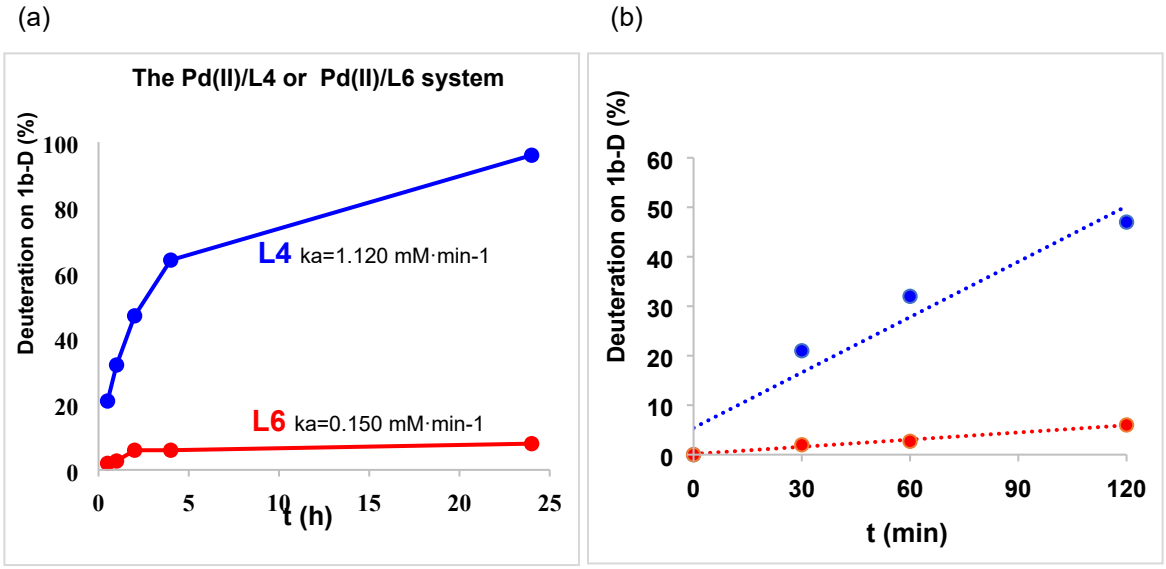
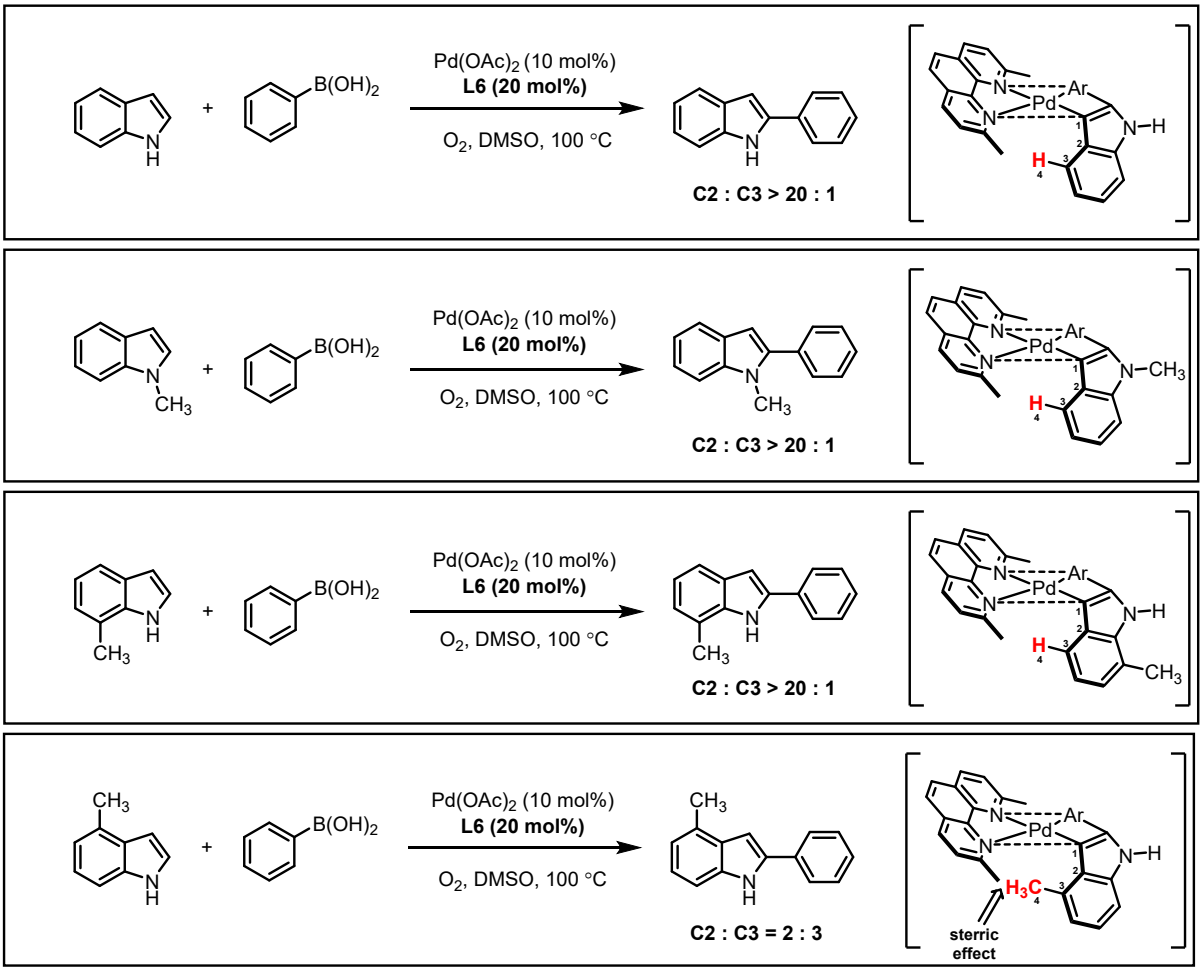


Figure S1. (a) Plots of the yields of products 1b-D. (b) Initial rates for the formation of 1b-D (**Ligand 4**) 1.120 $mM \cdot min^{-1}$; (**Ligand 6**) 0.150 mM·min-1.

(2) Experiment for Elucidating Steric Effect by Ligand 6 (L6)



To a 10 mL round bottom flask, indoles (0.30 mmol, 1.0 equiv.), phenylboronic acid (0.60 mmol, 2.0 equiv.) $Pd(OAc)_2$ (10.0 mol%), and Ligand 6 (20.0 mol%) were added, and then dissolved with DMSO (1.0 mL). Under O_2, the reaction mixture was stirred at 100 °C in an oil bath for 24h. Then, Ratio was determined by ^{1}H-NMR with internal standard 1,3,5-trimethoxybenzene.

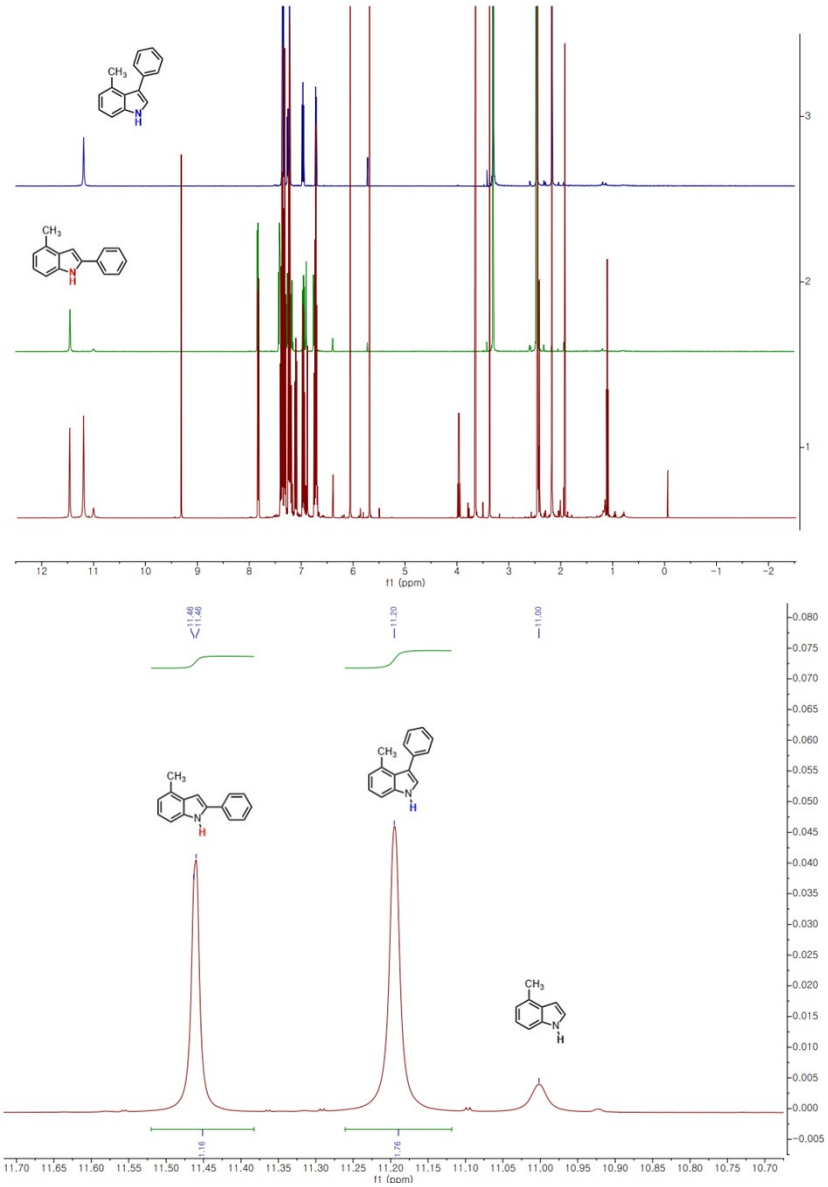
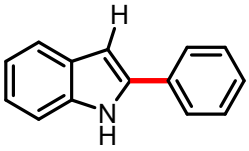


Figure S2. C2 to C3 arylated ratio of 4-methyl indole in Ligand 6 system by ^{1}H-NMR in DMSO-d_6

5. Compound Characterization Data

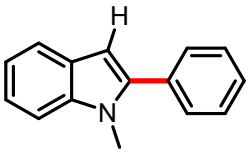


2-Phenyl-1*H*-indole (3aa)[1]; white solid (53.9 mg, 93%), mp 186-188°C.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.32 (s, 1H), 7.70 – 7.64 (m, 3H), 7.49 – 7.44 (m, 2H), 7.41 (dd, *J* = 8.1, 0.9 Hz, 1H), 7.35 (m, 1H), 7.23 (ddd, *J* = 8.2, 7.1, 1.2 Hz, 1H), 7.16 (ddd, *J* = 8.0, 7.1, 1.0 Hz, 1H), 6.86 (dd, *J* = 2.2, 0.9 Hz, 1H).

^{13}C{^{1}H} NMR (126 MHz, Chloroform-*d*) δ 138.00, 136.92, 132.46, 129.37, 129.15, 127.84, 125.27, 122.48, 120.80, 120.40, 111.04, 100.09.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{14}H_{11}N$, 194.0964; found, 194.1005.

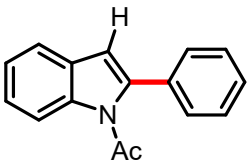


1-Methyl-2-phenyl-1*H*-indole (3ba)[1]; white solid (60.9 mg, 98%), mp 100-101 °C.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.66 (dt, *J* = 7.8, 1.0 Hz, 1H), 7.56 – 7.52 (m, 2H), 7.51 – 7.46 (m, 2H), 7.42 (m, 1H), 7.39 (dq, *J* = 8.2, 0.9 Hz, 1H), 7.27 (m, 1H), 7.17 (ddd, *J* = 7.9, 7.0, 1.0 Hz, 1H), 6.59 (d, *J* = 0.9 Hz, 1H), 3.77 (s, 3H).

^{13}C{^{1}H} NMR (126 MHz, Chloroform-*d*) δ 141.70, 138.46, 132.96, 129.52, 128.63, 128.07, 128.00, 121.79, 120.60, 119.99, 109.75, 101.76, 31.32.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{15}H_{13}N$, 208.1121; found, 208.1160.

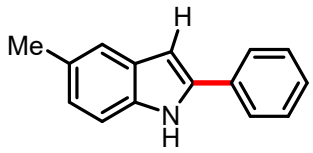


1-(2-Phenyl-1*H*-indol-1-yl)ethan-1-one (3ca)[2]; colorless oil (C2 condition 27.5 mg, 39% / C3 condition 31.1 mg, 44%).

^{1}H NMR (500 MHz, DMSO-d_6) δ 8.22 (dq, *J* = 8.3, 0.9 Hz, 1H), 7.62 (ddd, *J* = 7.6, 1.4, 0.7 Hz, 1H), 7.57 – 7.53 (m, 2H), 7.52 – 7.48 (m, 2H), 7.46 (m, 1H), 7.34 (ddd, *J* = 8.4, 7.2, 1.4 Hz, 1H), 7.28 (td, *J* = 7.4, 1.1 Hz, 1H), 6.78 (d, *J* = 0.8 Hz, 1H), 2.09 (s, 3H).

^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 171.05, 139.80, 136.98, 133.60, 128.93, 128.80, 128.71, 128.59, 124.76, 123.47, 120.60, 115.41, 110.95, 27.59.

HR-MS (EI) *m*/*z*: [M] calcd for $C_{16}H_{13}NO$, 235.0997; found, 235.0997.

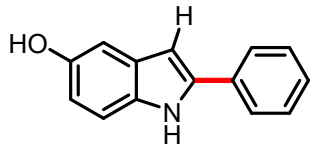


5-Methyl-2-phenyl-1*H*-indole (3da)[1]; white solid (57.2 mg, 92%), mp 218-219 ℃.

^{1}H NMR (500 MHz, Chloroform-*d*) ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.22 (s, 1H), 7.72 – 7.61 (m, 2H), 7.50 – 7.39 (m, 3H), 7.34 (m, 1H), 7.30 (d, *J* = 8.3 Hz, 1H), 7.05 (dd, *J* = 8.2, 1.7 Hz, 1H), 6.77 (dd, *J* = 2.1, 0.9 Hz, 1H), 2.48 (s, 3H).

^{13}C{^{1}H} NMR (126 MHz, Chloroform-*d*) δ 138.06, 135.27, 132.61, 129.66, 129.61, 129.12, 127.70, 125.18, 124.11, 120.43, 110.68, 99.66, 21.61.

HR-MS (ESI+) *m*/*z*: $[M+H]^+$ calcd for $C_{15}H_{13}N$, 208.1121; found, 208.1170.

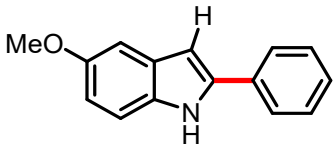


2-Phenyl-1*H*-indol-5-ol (3ea)[3]; white solid (57.8 mg, 92%), mp 246-251 °C.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.21 (d, *J* = 2.2 Hz, 1H), 8.69 (s, 1H), 7.85 – 7.75 (m, 2H), 7.47 – 7.39 (m, 2H), 7.27 (m, 1H), 7.19 (d, *J* = 8.6 Hz, 1H), 6.84 (d, *J* = 2.3 Hz, 1H), 6.71 (dd, *J* = 2.2, 0.9 Hz, 1H), 6.62 (dd, *J* = 8.6, 2.3 Hz, 1H).

^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 150.93, 137.85, 132.47, 131.72, 129.39, 128.86, 127.14, 124.77, 112.01, 111.64, 103.75, 98.02.

HR-MS (EI) *m/z*: [M] calcd for $C_{14}H_{11}NO$, 209.0841; found, 209.0841.

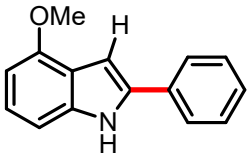


5-Methoxy-2-phenyl-1*H*-indole (3fa)[1]; white solid (60.9 mg, 91%), mp 170-171°C.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.37 (s, 1H), 7.88 – 7.78 (m, 2H), 7.49 – 7.40 (m, 2H), 7.34 – 7.25 (m, 2H), 7.02 (d, *J* = 2.4 Hz, 1H), 6.81 (dd, *J* = 2.2, 0.9 Hz, 1H), 6.74 (dd, *J* = 8.7, 2.5 Hz, 1H), 3.76 (s, 3H).

^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 153.62, 138.10, 132.33, 132.28, 129.03, 128.91, 127.29, 124.85, 111.99, 111.85, 101.53, 98.58, 55.26.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{15}H_{13}NO$, 224.1070; found, 224.1119.

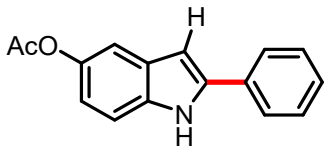


4-Methoxy-2-phenyl-1*H*-indole (3ga)[4]; colorless oil (50.2 mg, 75%)

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.52 (s, 1H), 7.90 – 7.82 (m, 2H), 7.48 – 7.40 (m, 2H), 7.28 (m, 1H), 7.06 – 6.99 (m, 2H), 6.91 (d, *J* = 2.2 Hz, 1H), 6.50 (m, 1H), 3.88 (s, 3H).

^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 152.74, 138.39, 136.09, 132.24, 128.90, 127.16, 124.82, 122.53, 119.22, 104.72, 99.38, 96.02, 54.92.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{15}H_{13}NO$, 224.1070; found, 224.1120.

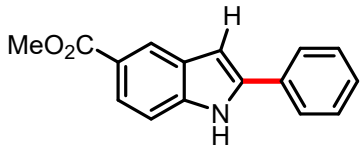


2-Phenyl-1*H*-indol-5-yl acetate (3ha)[1]; light orange solid (67.8 mg, 90%), mp 170-175 ºC.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.64 (s, 1H), 7.91 – 7.82 (m, 2H), 7.50 – 7.44 (m, 2H), 7.39 (dt, *J* = 8.7, 0.7 Hz, 1H), 7.32 (m, 1H), 7.24 (d, *J* = 2.2 Hz, 1H), 6.90 (dd, *J* = 2.3, 0.9 Hz, 1H), 6.84 (dd, *J* = 8.7, 2.3 Hz, 1H), 2.27 (s, 3H).

^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 169.89, 144.02, 139.02, 134.89, 131.97, 128.98, 128.69, 127.67, 125.08, 116.00, 112.09, 111.61, 98.84, 20.96.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{16}H_{13}NO_2$, 252.1019; found, 252.1018.

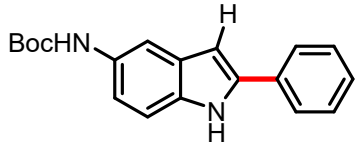


Methyl 2-phenyl-1*H*-indole-5-carboxylate (3ia)[5]; white solid (67.8 mg, 90%), mp 185-190 °C.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.95 (s, 1H), 8.25 (s, 1H), 7.88 (d, *J* = 7.4 Hz, 2H), 7.75 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.52 – 7.44 (m, 3H), 7.35 (t, *J* = 7.3 Hz, 1H), 7.05 (m, 1H), 3.85 (s, 3H).

^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 167.22, 139.74, 139.51, 131.60, 129.02, 128.25, 127.97, 125.23, 122.61, 122.57, 120.90, 111.26, 99.94, 51.71.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{16}H_{13}NO_2$, 252.1019; found, 252.1066.

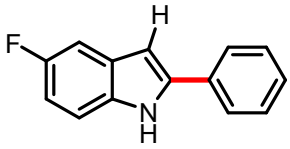


***tert*-Butyl (2-phenyl-1*H*-indol-5-yl)carbamate (3ja)[6];** white solid (87.0 mg, 90%), mp 165-170 °C.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.37 (s, 1H), 9.07 (s, 1H), 7.83 (dd, *J* = 8.3, 1.1 Hz, 2H), 7.67 (s, 1H), 7.44 (t, *J* = 7.8 Hz, 2H), 7.29 (t, *J* = 7.4 Hz, 1H), 7.26 (d, *J* = 8.7 Hz, 1H), 7.14 (d, *J* = 7.9 Hz, 1H), 6.82 (d, *J* = 1.5 Hz, 1H), 1.49 (s, 9H).

^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 153.19, 138.04, 133.46, 132.28, 131.89, 128.88, 128.60, 127.30, 124.88, 111.03, 98.61, 78.36, 28.28.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{19}H_{20}N_2O_2$, 309.1598; found, 309.1625.



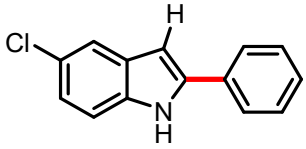
5-Fluoro-2-phenyl-1*H*-indole (3ka)[3]; white solid (48.8 mg, 77%), mp 175-180 °C.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.64 (s, 1H), 7.89 – 7.82 (m, 2H), 7.52 – 7.43 (m, 2H), 7.38 (m, 1H), 7.33 (m, 1H), 7.28 (dd, *J* = 10.0, 2.6 Hz, 1H), 6.94 (ddd, *J* = 9.6, 8.7, 2.6 Hz, 1H), 6.89 (dd, *J* = 2.3, 0.9 Hz, 1H).

^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 157.18, 139.57, 133.82, 131.89, 128.97, 128.86, 127.75, 125.11, 112.22, 109.65, 104.51, 98.85.

^{19}F NMR (471 MHz, DMSO-D_6) δ -124.53.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{14}H_{10}FN$, 212.0870; found, 212.0900.

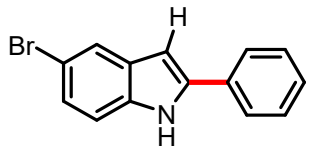


5-Chloro-2-phenyl-1*H*-indole (3la)[3]; white solid (49.0 mg, 72%), mp 190°C.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.35 (s, 1H), 7.69 – 7.62 (m, 2H), 7.59 (d, *J* = 2.0 Hz, 1H), 7.46 (dd, *J* = 8.4, 7.0 Hz, 2H), 7.35 (m, 1H), 7.30 (d, *J* = 8.5 Hz, 1H), 7.15 (dd, *J* = 8.5, 2.0 Hz, 1H), 6.76 (m, 1H).

$^{13}C\{^1H\}$ NMR (126 MHz, Chloroform-*d*) δ 139.42, 135.25, 131.98, 130.45, 129.24, 128.27, 125.97, 125.37, 122.70, 120.12, 112.00, 99.68.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{14}H_{10}ClN$, 228.0575; found, 228.0605.

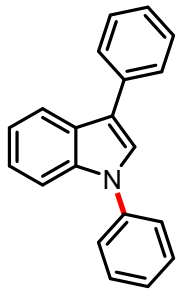


5-Bromo-2-phenyl-1*H*-indole (3ma)[1]; white solid (60.4 mg, 74%), mp 195 °C.

^1H NMR (500 MHz, DMSO-d_6) δ 11.75 (s, 1H), 7.89 – 7.82 (m, 2H), 7.71 (d, *J* = 1.9 Hz, 1H), 7.47 (t, *J* = 7.8 Hz, 2H), 7.39 – 7.30 (m, 2H), 7.20 (dd, *J* = 8.5, 2.0 Hz, 1H), 6.89 (dd, *J* = 2.2, 0.9 Hz, 1H).

$^{13}C\{^1H\}$ NMR (126 MHz, DMSO-D_6) δ 139.17, 135.79, 131.65, 130.51, 129.00, 127.90, 125.20, 123.99, 122.13, 113.26, 111.87, 98.27.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{14}H_{10}BrN$, 272.0069; found, 272.0060.

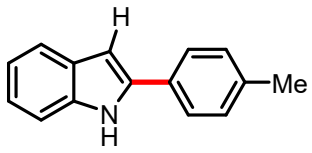


1,3-Diphenyl-1H-indole(3na'); yellow oil (37.8 mg, 46%)

^1H NMR (500 MHz, Chloroform-*d*) δ 8.02 (m, 1H), 7.78 – 7.71 (m, 2H), 7.64 (m, 1H), 7.61 – 7.53 (m, 5H), 7.53 – 7.47 (m, 2H), 7.41 (tt, *J* = 6.4, 1.9 Hz, 1H), 7.35 (m, 1H), 7.33 – 7.25 (m, 2H).

$^{13}C\{^1H\}$ NMR (126 MHz, Chloroform-*d*) δ 139.62, 136.75, 135.22, 129.81, 128.97, 127.73, 127.24, 126.79, 126.35, 125.65, 124.59, 122.93, 121.01, 120.26, 119.22, 110.96,

HR-MS (EI) *m/z*: [M] calcd for $C_{20}H_{15}N$, 270.1277; found, 270.1233.

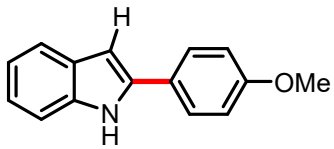


2-(*p*-Tolyl)-1*H*-indole (3ab)[3]; white solid (46.0 mg, 74%), mp 215 °C.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.29 (s, 1H), 7.64 (d, *J* = 7.9 Hz, 1H), 7.57 (d, *J* = 8.2 Hz, 2H), 7.40 (dd, *J* = 8.0, 0.9 Hz, 1H), 7.27 (s, 1H), 7.25 (m, 1H), 7.20 (ddd, *J* = 8.1, 7.1, 1.2 Hz, 1H), 7.13 (m, 1H), 6.80 (dd, *J* = 2.1, 0.8 Hz, 1H), 2.41 (s, 3H).

^{13}C{^{1}H} NMR (126 MHz, Chloroform-*d*) δ 138.18, 137.78, 136.82, 129.84, 129.68, 129.46, 125.20, 122.24, 120.65, 120.32, 110.96, 99.50, 21.37.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{15}H_{13}N$, 208.1121; found, 208.1160.

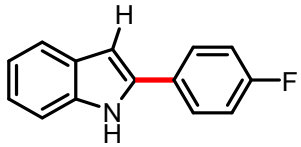


2-(4-Methoxyphenyl)-1*H*-indole (3ac)[3]; white solid (37.5 mg, 56%), mp 227-230 °C.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.40 (s, 1H), 7.83 – 7.73 (m, 2H), 7.49 (d, *J* = 7.8 Hz, 1H), 7.37 (d, *J* = 8.0 Hz, 1H), 7.10 – 6.98 (m, 3H), 6.96 (m, 1H), 6.76 (dd, *J* = 2.2, 0.9 Hz, 1H), 3.80 (s, 3H).

^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 158.79, 137.78, 136.93, 128.83, 126.36, 124.90, 121.04, 119.67, 119.23, 114.36, 111.07, 97.33, 55.21.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{15}H_{13}NO$, 224.1070; found, 224.1111.



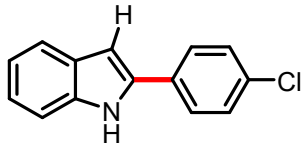
2-(4-Fluorophenyl)-1*H*-indole (3ad)[4]; white solid (55.1 mg, 87%), mp 185 °C.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.52 (s, 1H), 7.93 – 7.86 (m, 2H), 7.52 (d, *J* = 7.8 Hz, 1H), 7.39 (dq, *J* = 8.3, 1.0 Hz, 1H), 7.34 – 7.26 (m, 2H), 7.09 (ddd, *J* = 8.2, 7.0, 1.2 Hz, 1H), 6.99 (ddd, *J* = 8.0, 7.0, 1.1 Hz, 1H), 6.87 (dd, *J* = 2.2, 0.9 Hz, 1H).

^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 162.59 (d, *J* = 244.7 Hz), 137.46 (d, *J* = 50.7 Hz), 128.92 (d, *J* = 3.0 Hz), 128.69, 127.01 (d, *J* = 7.9 Hz), 121.62, 119.77 (d, *J* = 77.0 Hz), 115.84 (d, *J* = 21.6 Hz), 111.32, 98.69.

^{19}F NMR (471 MHz, DMSO-d_6) δ -114.51.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{14}H_{10}FN$, 212.0870; found, 212.0886.

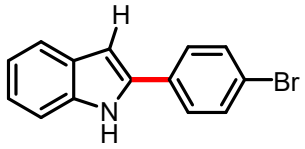


2-(4-Chlorophenyl)-1*H*-indole (3ae)[3]; white solid (60.1 mg, 88%), mp 190-195 °C.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.28 (s, 1H), 7.63 (d, *J* = 7.9 Hz, 1H), 7.61 – 7.56 (m, 2H), 7.45 – 7.38 (m, 3H), 7.21 (ddd, *J* = 8.2, 7.1, 1.1 Hz, 1H), 7.14 (m, 1H), 6.82 (dd, *J* = 2.1, 0.8 Hz, 1H).

^{13}C{^{1}H} NMR (126 MHz, Chloroform-*d*) δ 137.02, 136.81, 133.58, 131.01, 129.37, 129.29, 126.45, 122.83, 120.90, 120.61, 111.08, 100.60.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{14}H_{10}ClN$, 228.0575; found, 228.0574.

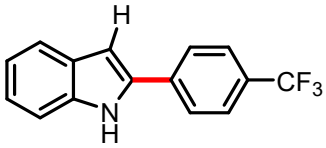


2-(4-Bromophenyl)-1*H*-indole (3af)[1]; white solid (63.7 mg, 78%), mp 210 °C.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.59 (s, 1H), 7.84 – 7.79 (m, 2H), 7.68 – 7.62 (m, 2H), 7.53 (d, *J* = 7.9 Hz, 1H), 7.39 (dd, *J* = 8.1, 0.8 Hz, 1H), 7.11 (ddd, *J* = 8.2, 7.0, 1.2 Hz, 1H), 7.00 (ddd, *J* = 7.9, 7.0, 1.0 Hz, 1H), 6.95 (dd, *J* = 2.1, 0.8 Hz, 1H).

$^{13}C\{^1H\}$ NMR (126 MHz, DMSO-d_6) δ 137.24, 136.39, 131.82, 131.49, 128.54, 126.91, 121.93, 120.32, 120.20, 119.55, 111.39, 99.38.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{14}H_{10}BrN$, 272.0069; found, 272.0025.



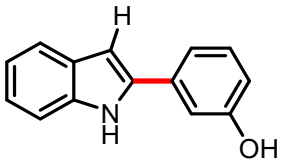
2-(4-(Trifluoromethyl)phenyl)-1*H*-indole (3ag)[7]; white solid (70.5 mg, 90%), mp 235 °C.

^1H NMR (500 MHz, DMSO-d_6) δ 11.74 (s, 1H), 8.07 (d, *J* = 8.1 Hz, 2H), 7.81 (d, *J* = 8.3 Hz, 2H), 7.57 (d, *J* = 7.9 Hz, 1H), 7.44 (dd, *J* = 8.1, 0.8 Hz, 1H), 7.15 (ddd, *J* = 8.1, 7.0, 1.1 Hz, 1H), 7.07 (d, *J* = 1.6 Hz, 1H), 7.03 (ddd, *J* = 7.9, 7.1, 0.9 Hz, 1H).

$^{13}C\{^1H\}$ NMR (126 MHz, DMSO-d_6) δ 137.54, 136.13, 135.87, 128.43, 127.28, 125.88, 125.38, 123.31, 122.47, 120.55, 119.74, 111.60, 100.77.

^{19}F NMR (471 MHz, DMSO-d_6) δ -60.79.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{15}H_{10}F_3N$, 262.0838; found, 262.0814.

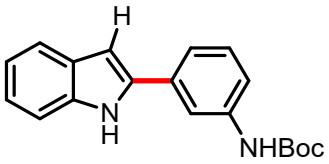


3-(1*H*-Indol-2-yl)phenol (3ah)[8]; white solid (55.8 mg, 89%), mp 170 °C.

^1H NMR (500 MHz, DMSO-d_6) δ 11.46 (s, 1H), 9.56 (s, 1H), 7.52 (d, *J* = 7.9 Hz, 1H), 7.38 (dd, *J* = 8.1, 0.8 Hz, 1H), 7.31 – 7.21 (m, 3H), 7.08 (ddd, *J* = 8.2, 7.0, 1.2 Hz, 1H), 6.98 (ddd, *J* = 8.0, 7.0, 1.0 Hz, 1H), 6.80 (dd, *J* = 2.1, 0.7 Hz, 1H), 6.74 (ddd, *J* = 7.8, 2.4, 1.1 Hz, 1H).

$^{13}C\{^1H\}$ NMR (126 MHz, DMSO-d_6) δ 157.79, 137.85, 137.04, 133.55, 129.91, 128.59, 121.48, 120.01, 119.33, 116.04, 114.57, 111.92, 111.32, 98.52.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{14}H_{11}NO$, 210.0913; found, 210.0937.

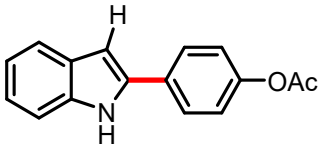


***tert*-Butyl(3-(1*H*-indol-2-yl)phenyl)carbamate (3ai)[9];** white solid (86.9 mg, 96%), mp 70-75 °C.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.48 (s, 1H), 9.44 (s, 1H), 8.01 (s, 1H), 7.54 (dt, *J* = 7.7, 0.9 Hz, 1H), 7.44 (dt, *J* = 7.0, 1.8 Hz, 1H), 7.40 (m, 1H), 7.33 (q, *J* = 8.3 Hz, 2H), 7.09 (ddd, *J* = 8.1, 7.1, 1.1 Hz, 1H), 6.99 (ddd, *J* = 7.9, 7.1, 1.0 Hz, 1H), 6.75 (m, 1H), 1.50 (s, 9H).

^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 152.89, 140.08, 137.89, 137.15, 132.76, 129.19, 128.58, 121.54, 120.06, 119.37, 119.02, 117.65, 115.01, 111.41, 98.60, 79.17, 28.18.

HR-MS (ESI+) *m*/*z*: $[M+H]^+$ calcd for $C_{19}H_{20}N_2O_2$, 309.1598; found, 309.1565.

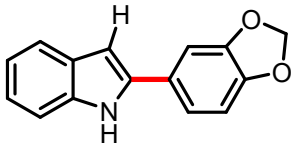


4-(1*H*-Indol-2-yl)phenyl acetate (3aj); white solid (57.3 mg, 76%), mp 200 °C.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.54 (s, 1H), 7.93 – 7.84 (m, 2H), 7.53 (d, *J* = 7.8 Hz, 1H), 7.39 (m, 1H), 7.27 – 7.18 (m, 2H), 7.10 (ddd, *J* = 8.1, 6.9, 1.2 Hz, 1H), 7.01 (m, 1H), 6.89 (d, *J* = 2.1 Hz, 1H), 2.29 (s, 3H).

^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 169.29, 149.76, 137.17, 136.95, 129.96, 128.66, 126.07, 122.38, 121.65, 120.09, 119.45, 111.33, 98.83, 20.91.

HR-MS (ESI+) *m*/*z*: $[M+H]^+$ calcd for $C_{16}H_{13}NO_2$, 252.1019; found, 252.1012.

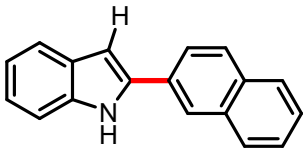


2-(Benzo[d][1,3]dioxol-5-yl)-1*H*-indole (3ak)[7]; white solid (62.6 mg, 88%), mp 155-160 ℃.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.39 (s, 1H), 7.49 (d, *J* = 7.9 Hz, 1H), 7.45 (d, *J* = 1.7 Hz, 1H), 7.37 (dt, *J* = 8.1, 1.3 Hz, 2H), 7.07 (ddd, *J* = 8.1, 7.1, 1.2 Hz, 1H), 7.01 (d, *J* = 8.1 Hz, 1H), 6.98 (ddd, *J* = 7.9, 7.1, 1.0 Hz, 1H), 6.79 (dd, *J* = 2.1, 0.8 Hz, 1H), 6.07 (s, 2H).

^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 147.91, 146.74, 137.67, 136.91, 128.71, 126.56, 121.27, 119.78, 119.32, 118.73, 111.11, 108.75, 105.58, 101.19, 97.99.

HR-MS (ESI+) *m/z*: [M+H]$^+$ calcd for $C_{15}H_{11}NO_2$, 238.0863; found, 238.0899.

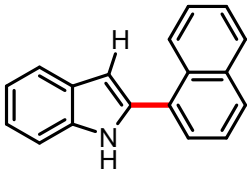


2-(Naphthalen-2-yl)-1*H*-indole (3al)[10]; pale yellow solid (70.0 mg, 96%), mp 196-197 °C.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.72 (s, 1H), 8.39 (s, 1H), 8.04 (m, 1H), 7.99 (d, *J* = 8.6 Hz, 1H), 7.96 – 7.88 (m, 2H), 7.61 – 7.48 (m, 3H), 7.45 (d, *J* = 8.1 Hz, 1H), 7.13 (ddt, *J* = 8.2, 7.0, 1.3 Hz, 1H), 7.08 – 6.94 (m, 2H).

^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 137.57, 137.40, 133.28, 132.30, 129.70, 128.70, 128.44, 127.90, 127.72, 126.74, 126.05, 123.85, 122.82, 121.84, 120.17, 119.48, 111.35, 99.58.

HR-MS (ESI+) *m/z*: [M+H]$^+$ calcd for $C_{18}H_{13}N$, 244.1121; found, 244.1119.

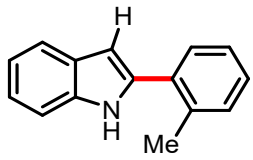


2-(Naphthalen-1-yl)-1*H*-indole (3am)[1]; white solid (31.4 mg, 43%), mp 95-100 °C.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.58 (s, 1H), 8.32 (m, 1H), 8.03 (m, 1H), 7.99 (d, *J* = 8.2 Hz, 1H), 7.72 (dd, *J* = 7.1, 1.2 Hz, 1H), 7.66 – 7.54 (m, 4H), 7.44 (m, 1H), 7.15 (ddd, *J* = 8.1, 7.1, 1.2 Hz, 1H), 7.05 (m, 1H), 6.74 (dd, *J* = 2.0, 0.7 Hz, 1H).

^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 136.70, 136.48, 133.59, 130.91, 130.79, 128.47, 128.37, 128.17, 127.30, 126.76, 126.16, 125.55, 125.49, 121.43, 120.06, 119.30, 111.38, 102.48.

HR-MS (EI) *m*/*z*: [M] calcd for $C_{18}H_{13}N$, 243.1048; found, 243.1048.

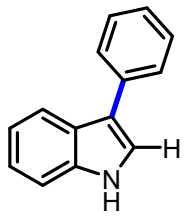


2-(*o*-Tolyl)-1*H*-indole (3an)[7]; white solid (36.7 mg, 59%), mp 95 °C.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.28 (s, 1H), 7.57 – 7.52 (m, 2H), 7.39 (dd, *J* = 8.1, 0.9 Hz, 1H), 7.36 – 7.26 (m, 3H), 7.10 (ddd, *J* = 8.1, 7.1, 1.2 Hz, 1H), 7.00 (ddd, *J* = 7.9, 7.1, 1.0 Hz, 1H), 6.57 (dd, *J* = 2.2, 0.8 Hz, 1H), 2.47 (s, 3H).

^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 137.34, 136.40, 135.48, 132.51, 130.95, 129.01, 128.36, 127.60, 126.02, 121.26, 119.95, 119.12, 111.22, 101.74, 21.08.

HR-MS (EI) *m*/*z*: [M] calcd for $C_{15}H_{13}N$, 207.1048; found, 207.1048.

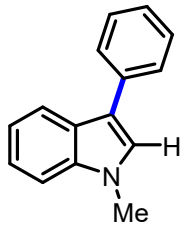


3-Phenyl-1*H*-indole (4aa)[5]; white solid (53.9 mg, 93%), mp 85 ℃.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.19 (s, 1H), 7.98 (d, *J* = 8.0 Hz, 1H), 7.71 (dd, *J* = 8.2, 1.2 Hz, 2H), 7.53 – 7.41 (m, 3H), 7.37 (d, *J* = 2.5 Hz, 1H), 7.34 – 7.20 (m, 3H).

$^{13}C\{^1H\}$ NMR (126 MHz, Chloroform-*d*) δ 136.75, 135.66, 128.91, 127.61, 126.12, 125.83, 122.54, 121.92, 120.44, 119.94, 118.42, 111.54.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{14}H_{11}N$, 194.0964; found, 194.0968.

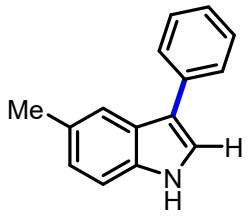


1-Methyl-3-phenyl-1*H*-indole (4ba)[11]; colorless oil (33.6 mg, 54%).

^1H NMR (500 MHz, Chloroform-*d*) δ 7.97 (dt, *J* = 8.0, 0.9 Hz, 1H), 7.69 – 7.65 (m, 2H), 7.48 – 7.43 (m, 2H), 7.38 (dt, *J* = 8.2, 0.8 Hz, 1H), 7.33 – 7.27 (m, 2H), 7.25 (s, 1H), 7.21 (ddd, *J* = 8.0, 7.0, 1.1 Hz, 1H), 3.85 (s, 3H).

$^{13}C\{^1H\}$ NMR (126 MHz, Chloroform-*d*) δ 137.58, 135.79, 128.88, 127.45, 126.69, 126.25, 125.83, 122.10, 120.06, 120.01, 116.82, 109.67, 33.03.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{15}H_{13}N$, 208.1121; found, 208.1119.

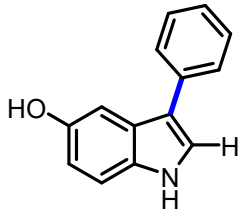


5-Methyl-3-phenyl-1*H*-indole (4da)[12]; white solid (47.9 mg, 77%), mp 95 ℃.

^1H NMR (500 MHz, Chloroform-*d*) δ 8.07 (s, 1H), 7.78 (s, 1H), 7.75 – 7.67 (m, 2H), 7.49 (t, *J* = 7.8 Hz, 2H), 7.37 – 7.30 (m, 3H), 7.12 (d, *J* = 8.3 Hz, 1H), 2.52 (s, 3H).

$^{13}C\{^1H\}$ NMR (126 MHz, Chloroform-*d*) δ 135.83, 135.06, 129.74, 128.87, 127.61, 126.06, 126.00, 124.13, 122.07, 119.51, 117.94, 111.18, 21.76.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{15}H_{13}N$, 208.1121; found, 208.1129.

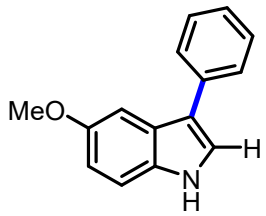


3-Phenyl-1*H*-indol-5-ol (4ea)[3]; white solid (43.3 mg, 77%), mp 120 °C.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.06 (s, 1H), 8.75 (s, 1H), 7.62 (dd, *J* = 8.3, 1.2 Hz, 2H), 7.57 (d, *J* = 2.6 Hz, 1H), 7.44 – 7.37 (m, 2H), 7.28 – 7.15 (m, 3H), 6.67 (dd, *J* = 8.6, 2.3 Hz, 1H).

^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 151.34, 136.33, 131.40, 128.72, 126.15, 125.66, 124.94, 123.80, 114.81, 112.34, 111.72, 102.90.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{14}H_{11}NO$, 210.0913; found, 210.0920

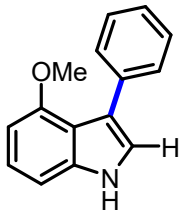


5-Methoxy-3-phenyl-1*H*-indole (4fa)[5]; light yellow solid (56.2 mg, 84%), mp 65 ℃.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.14 (s, 1H), 7.72 – 7.64 (m, 2H), 7.52 – 7.45 (m, 2H), 7.41 (d, *J* = 2.4 Hz, 1H), 7.37 – 7.29 (m, 3H), 6.94 (dd, *J* = 8.8, 2.4 Hz, 1H), 3.89 (s, 3H).

^{13}C{^{1}H} NMR (126 MHz, Chloroform-*d*) δ 154.82, 135.81, 131.88, 128.95, 127.50, 126.23, 126.05, 122.74, 118.24, 112.81, 112.25, 101.63, 56.10.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{15}H_{13}NO$, 224.1070; found, 224.1071.

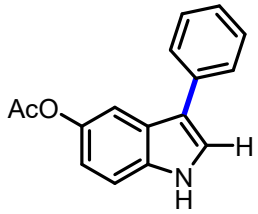


4-Methoxy-3-phenyl-1*H*-indole (4ga)[5]; colorless oil (53.5 mg, 80%)

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.16 (s, 1H), 7.69 – 7.65 (m, 2H), 7.44 – 7.39 (m, 2H), 7.31 (m, 1H), 7.19 (t, *J* = 8.0 Hz, 1H), 7.11 (d, *J* = 2.5 Hz, 1H), 7.03 (dd, *J* = 8.2, 0.7 Hz, 1H), 6.61 (d, *J* = 7.7 Hz, 1H), 3.85 (s, 3H).

^{13}C{^{1}H} NMR (126 MHz, Chloroform-*d*) δ 154.73, 138.35, 136.21, 129.79, 127.70, 125.85, 123.25, 122.04, 119.00, 115.76, 104.73, 100.61, 55.24.

HR-MS (ESI+) *m/z*: [M+H]$^+$ calcd for $C_{15}H_{13}NO$, 224.1070; found, 224.1072.

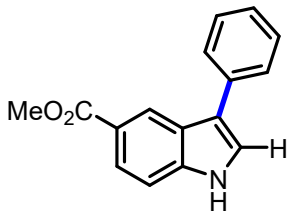


3-Phenyl-1*H*-indol-5-yl acetate (4ha); white solid (57.3 mg, 76%), mp 173 °C.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.30 (s, 1H), 7.63 – 7.59 (m, 3H), 7.47 – 7.41 (m, 2H), 7.37 – 7.33 (m, 2H), 7.29 (m, 1H), 6.96 (dd, *J* = 8.7, 2.2 Hz, 1H), 2.34 (s, 3H).

^{13}C{^{1}H} NMR (126 MHz, Chloroform-*d*) δ 170.78, 144.97, 135.27, 134.64, 128.92, 127.54, 126.24, 126.22, 123.26, 118.73, 116.67, 112.05, 112.02, 21.33.

HR-MS (ESI+) *m/z*: [M+H]$^+$ calcd for $C_{16}H_{13}NO_2$, 252.1019; found, 252.1009.

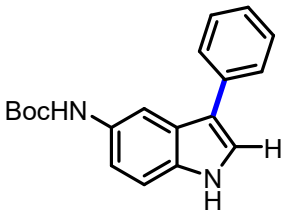


Methyl 3-phenyl-1*H*-indole-5-carboxylate (4ia)[13]; white solid (57.3 mg, 76%), mp 158-160 °C.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.77 (s, 1H), 8.51 (d, *J* = 1.7 Hz, 1H), 7.85 – 7.76 (m, 2H), 7.70 – 7.63 (m, 2H), 7.54 (d, *J* = 8.6 Hz, 1H), 7.53 – 7.43 (m, 2H), 7.29 (m, 1H), 3.85 (s, 3H).

$^{13}C\{^1H\}$ NMR (126 MHz, DMSO-d_6) δ 167.24, 139.44, 134.97, 128.99, 126.85, 125.93, 125.26, 124.69, 122.45, 121.44, 121.07, 117.17, 112.04, 51.80.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{16}H_{13}NO_2$, 252.1019; found, 252.1015.

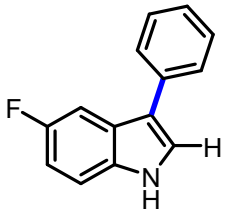


***tert*-Butyl (3-phenyl-1*H*-indol-5-yl)carbamate (4ja);** a light yellow solid (60.1 mg, 65%), mp 205 °C.

^1H NMR (500 MHz, DMSO-d_6) δ 11.17 (d, *J* = 2.6 Hz, 1H), 9.07 (s, 1H), 8.01 (s, 1H), 7.62 – 7.56 (m, 3H), 7.41 – 7.36 (m, 2H), 7.27 (m, 1H), 7.23 – 7.14 (m, 2H), 1.44 (s, 9H).

$^{13}C\{^1H\}$ NMR (126 MHz, DMSO-d_6) δ 153.21, 136.05, 133.12, 132.27, 128.75, 126.36, 125.17, 124.90, 123.92, 115.52, 114.69, 111.68, 108.31, 78.38, 28.27.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{19}H_{20}N_2O_2$, 309.1598; found, 306.1603.



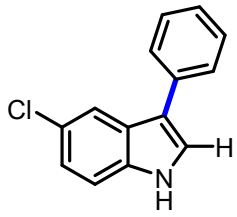
5-Fluoro-3-phenyl-1*H*-indole (4ka)[4]; white solid (38.0 mg, 60%), mp 50 ℃.

^1H NMR (500 MHz, Chloroform-*d*) δ 8.25 (s, 1H), 7.65 – 7.61 (m, 2H), 7.58 (m, 1H), 7.49 – 7.43 (m, 2H), 7.42 (d, *J* = 2.6 Hz, 1H), 7.35 (ddd, *J* = 8.9, 4.4, 0.5 Hz, 1H), 7.30 (m, 1H), 7.01 (td, *J* = 9.0, 2.5 Hz, 1H).

$^{13}C\{^1H\}$ NMR (126 MHz, Chloroform-*d*) δ 158.56 (d, *J* = 234.9 Hz), 135.20, 133.27, 129.01, 127.41, 126.33, 126.25 (d, *J* = 9.9 Hz), 123.56, 118.71 (d, *J* = 4.6 Hz), 112.14 (d, *J* = 9.7 Hz), 111.01 (d, *J* = 26.3 Hz), 104.95 (d, *J* = 24.2 Hz).

^{19}F NMR (471 MHz, Chloroform-*d*) δ -123.69.

HR-MS (ESI+) *m*/*z*: [M+H]$^+$ calcd for $C_{14}H_{10}FN$, 212.0870; found, 212.0876.

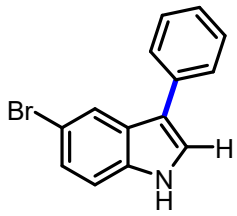


5-Chloro-3-phenyl-1*H*-indole (4la)[4]; white solid (43.7 mg, 64%), mp 90-95 ℃.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.22 (s, 1H), 7.92 (d, *J* = 2.0 Hz, 1H), 7.67 – 7.61 (m, 2H), 7.48 (tt, *J* = 8.0, 1.5 Hz, 2H), 7.37 (d, *J* = 2.5 Hz, 1H), 7.35 – 7.31 (m, 2H), 7.22 (dd, *J* = 8.6, 2.0 Hz, 1H).

^{13}C{^{1}H} NMR (126 MHz, Chloroform-*d*) δ 135.05, 134.92, 129.02, 127.57, 126.94, 126.46, 126.24, 123.13, 122.87, 119.43, 118.30, 112.52.

HR-MS (ESI+) *m*/*z*: [M+H]$^+$ calcd for $C_{14}H_{10}ClN$, 228.0575; found, 228.0578.

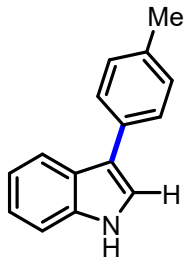


5-Bromo-3-phenyl-1*H*-indole (4ma)[11]; colorless oil (49.0 mg, 60%).

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.45 (s, 1H), 7.85 (d, *J* = 7.9 Hz, 1H), 7.75 (s, 1H), 7.71 – 7.63 (m, 2H), 7.62 – 7.53 (m, 2H), 7.45 (d, *J* = 8.0 Hz, 1H), 7.16 (t, *J* = 7.5 Hz, 1H), 7.10 (t, *J* = 7.4 Hz, 1H).

^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 137.11, 135.37, 131.79, 128.52, 124.86, 124.15, 121.78, 120.02, 119.07, 118.04, 114.53, 112.27.

HR-MS (ESI+) *m*/*z*: [M+H]$^+$ calcd for $C_{14}H_{10}BrN$, 272.0069; found, 272.0071.

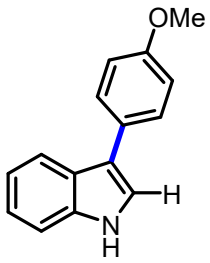


3-(*p*-Tolyl)-1*H*-indole (4ab)[11]; white solid (50.3 mg, 81%), mp 90 ℃.

^{1}H NMR ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.30 (s, 1H), 7.83 (d, *J* = 7.9 Hz, 1H), 7.63 (d, *J* = 2.5 Hz, 1H), 7.57 (d, *J* = 8.1 Hz, 2H), 7.43 (d, *J* = 8.1 Hz, 1H), 7.23 (d, *J* = 7.9 Hz, 2H), 7.14 (m, 1H), 7.07 (td, *J* = 7.5, 7.1, 1.0 Hz, 1H), 2.33 (s, 3H).

^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 137.03, 134.42, 133.14, 129.54, 126.60, 125.20, 123.18, 121.51, 119.65, 119.19, 115.82, 112.10, 20.91.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{15}H_{13}N$, 208.1121; found, 208.1120.

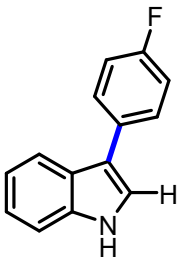


3-(4-Methoxyphenyl)-1*H*-indole (4ac)[5]; white solid (42.8 mg, 64%), mp 130 °C.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.17 (s, 1H), 7.92 (m, 1H), 7.65 – 7.57 (m, 2H), 7.42 (d, *J* = 8.1 Hz, 1H), 7.32 – 7.24 (m, 2H), 7.21 (ddd, *J* = 8.0, 7.0, 1.1 Hz, 1H), 7.06 – 6.98 (m, 2H), 3.88 (s, 3H).

^{13}C{^{1}H} NMR (126 MHz, Chloroform-*d*) δ 158.21, 136.69, 128.75, 128.23, 126.01, 122.43, 121.29, 120.27, 119.86, 118.12, 114.38, 111.48, 55.49.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{15}H_{13}NO$, 224.1070; found, 224.1071.



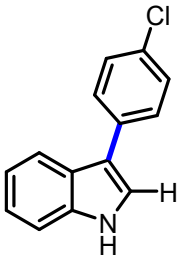
3-(4-Fluorophenyl)-1*H*-indole (4ad)[3]; white solid (46.3 mg, 73%), mp 100 ℃.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.20 (s, 1H), 7.90 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.66 – 7.59 (m, 2H), 7.44 (dt, *J* = 8.1, 0.9 Hz, 1H), 7.32 (d, *J* = 2.5 Hz, 1H), 7.28 (ddd, *J* = 8.2, 7.1, 1.2 Hz, 1H), 7.22 (ddd, *J* = 8.0, 7.1, 1.1 Hz, 1H), 7.19 – 7.12 (m, 2H).

^{13}C{^{1}H} NMR (126 MHz, Chloroform-*d*) δ 161.61 (d, *J* = 244.4 Hz), 136.68, 131.66, 129.05, 125.82, 122.19, 120.09, 117.56, 115.73, 111.58.

^{19}F NMR (471 MHz, Chloroform-*d*) δ -116.84.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{14}H_{10}FN$, 212.0870; found, 212.0876.

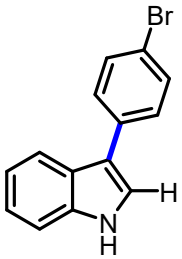


3-(4-Chlorophenyl)-1*H*-indole (4ae)[5]; white solid (49.2 mg, 72%), mp 135 °C.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.44 (s, 1H), 7.85 (d, *J* = 7.9 Hz, 1H), 7.75 (d, *J* = 2.2 Hz, 1H), 7.74 – 7.68 (m, 2H), 7.50 – 7.41 (m, 3H), 7.16 (ddd, *J* = 8.1, 7.1, 1.1 Hz, 1H), 7.10 (ddd, *J* = 8.0, 7.0, 1.1 Hz, 1H).

^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 136.93, 134.83, 129.52, 128.72, 127.98, 124.74, 123.95, 121.59, 119.82, 118.89, 114.36, 112.08.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{14}H_{10}ClN$, 228.0575; found, 228.0580.

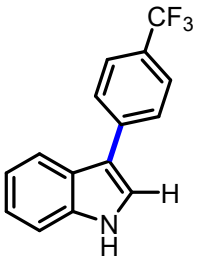


3-(4-Bromophenyl)-1*H*-indole (4af)[4]; white solid (51.4 mg, 63%), mp 135 °C.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.26 (s, 1H), 7.89 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.59 – 7.53 (m, 4H), 7.44 (dt, *J* = 8.1, 0.9 Hz, 1H), 7.37 (d, *J* = 2.6 Hz, 1H), 7.27 (m, 1H), 7.22 (ddd, *J* = 8.1, 7.1, 1.1 Hz, 1H).

^{13}C{^{1}H} NMR (126 MHz, Chloroform-*d*) δ 136.76, 134.63, 131.96, 129.09, 125.57, 122.77, 122.00, 120.70, 119.75, 119.69, 117.35, 111.65.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{14}H_{10}BrN$, 272.0069; found, 272.0071.



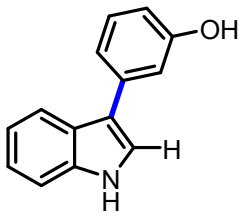
3-(4-(Trifluoromethyl)phenyl)-1*H*-indole (4ag)[5]; white solid (29.8 mg, 38%), mp 130 ℃.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.32 (s, 1H), 7.95 (d, *J* = 7.9 Hz, 1H), 7.79 (d, *J* = 8.3 Hz, 2H), 7.70 (d, *J* = 8.2 Hz, 2H), 7.50 – 7.41 (m, 2H), 7.30 (t, *J* = 7.5 Hz, 1H), 7.25 (m, 1H).

^{13}C{^{1}H} NMR (126 MHz, Chloroform-*d*) δ 139.43, 136.84, 127.92 (d, *J* = 32.4 Hz), 127.45, 125.85 (q, *J* = 3.8 Hz), 125.71, 125.54, 123.55, 122.97, 122.69, 120.97, 119.69, 117.24, 111.76.

^{19}F NMR (471 MHz, Chloroform-*d*) δ -62.06.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{15}H_{10}F_3N$, 262.0838; found, 262.0845.

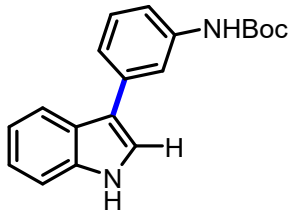


3-(1*H*-Indol-3-yl)phenol (4ah)[14]; white solid (42.7 mg, 68%), mp 135-140 °C.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.31 (s, 1H), 9.35 (s, 1H), 7.83 (d, *J* = 7.9 Hz, 1H), 7.62 (d, *J* = 2.6 Hz, 1H), 7.44 (d, *J* = 8.0 Hz, 1H), 7.21 (t, *J* = 7.8 Hz, 1H), 7.16 – 7.04 (m, 4H), 6.63 (ddd, *J* = 8.0, 2.3, 1.0 Hz, 1H).

^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 157.68, 137.09, 136.89, 129.70, 125.01, 123.31, 121.38, 119.53, 119.05, 117.43, 115.81, 113.33, 112.37, 111.99.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{14}H_{11}NO$, 210.0913; found, 210.0885.

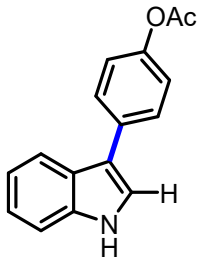


***tert*-Butyl(3-(1*H*-indol-3-yl)phenyl)carbamate (4ai);** colorless oil (57.4 mg, 62%).

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.34 (s, 1H), 9.38 (s, 1H), 7.90 (dt, *J* = 8.0, 0.9 Hz, 1H), 7.83 (d, *J* = 2.2 Hz, 1H), 7.63 (d, *J* = 2.6 Hz, 1H), 7.44 (dt, *J* = 8.1, 1.0 Hz, 1H), 7.37 (m, 1H), 7.31 – 7.24 (m, 2H), 7.15 (ddd, *J* = 8.2, 7.0, 1.2 Hz, 1H), 7.09 (ddd, *J* = 8.0, 7.0, 1.2 Hz, 1H), 1.49 (s, 9H).

^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 152.88, 139.91, 136.91, 136.18, 128.99, 124.96, 123.34, 121.43, 120.34, 119.56, 119.18, 116.20, 115.69, 115.07, 111.98, 78.93, 28.19.

HR-MS (ESI+) *m/z*: $[M+H]^+$ calcd for $C_{19}H_{20}N_2O_2$, 309.1598; found, 309.1544.

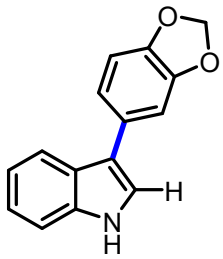


4-(1*H*-Indol-3-yl)phenyl acetate (4aj); white solid (58.8 mg, 78%), mp 226 °C.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.38 (s, 1H), 7.86 (d, *J* = 7.9 Hz, 1H), 7.73 – 7.68 (m, 3H), 7.46 (d, *J* = 8.0 Hz, 1H), 7.21 – 7.14 (m, 3H), 7.10 (ddd, *J* = 8.0, 7.1, 1.0 Hz, 1H), 2.29 (s, 3H).

^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 169.45, 148.18, 136.87, 133.53, 127.29, 124.89, 123.58, 122.16, 121.49, 119.68, 118.90, 114.89, 112.02, 20.92.

HR-MS (ESI+) *m*/*z*: $[M+H]^+$ calcd for $C_{16}H_{13}NO_2$, 252.1019; found, 252.0966.

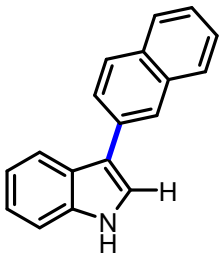


3-(Benzo[*d*][1,3]dioxol-5-yl)-1*H*-indole (4ak)[3]; white solid (37.0 mg, 52%), mp 155 °C.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.17 (s, 1H), 7.90 (d, *J* = 7.9 Hz, 1H), 7.42 (d, *J* = 8.1 Hz, 1H), 7.30 – 7.23 (m, 2H), 7.20 (t, *J* = 7.5 Hz, 1H), 7.17 – 7.13 (m, 2H), 6.92 (d, *J* = 7.8 Hz, 1H), 6.01 (s, 2H).

^{13}C{^{1}H} NMR (126 MHz, Chloroform-*d*) δ 148.07, 146.08, 136.66, 129.68, 125.88, 122.54, 121.49, 120.85, 120.38, 119.79, 118.30, 111.51, 108.83, 108.35, 101.06.

HR-MS (ESI+) *m*/*z*: $[M+H]^+$ calcd for $C_{15}H_{11}NO_2$, 238.0863; found, 238.0869.

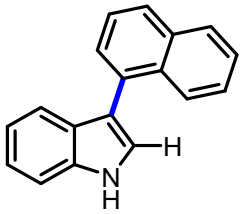


3-(Naphthalen-2-yl)-1*H*-indole (4al)[15]; white solid (56.2 mg, 77%), mp 140-145 °C.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.48 (s, 1H), 8.22 (m, 1H), 8.07 (d, *J* = 7.6 Hz, 1H), 8.01 – 7.92 (m, 2H), 7.92 – 7.85 (m, 3H), 7.54 – 7.41 (m, 3H), 7.23 – 7.12 (m, 2H).

^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 137.11, 133.78, 133.54, 131.27, 128.15, 127.67, 127.51, 126.18, 125.98, 125.06, 125.03, 124.24, 123.45, 121.63, 119.84, 119.36, 115.48, 112.10.

HR-MS (ESI+) *m*/*z*: $[M+H]^+$ calcd for $C_{18}H_{13}N$, 244.1121; found, 244.1097.

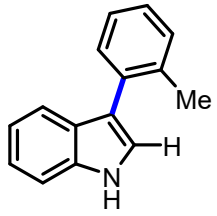


3-(Naphthalen-1-yl)-1*H*-indole (4am)[12]; colorless oil (59.8 mg, 82%)

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.46 (s, 1H), 8.03 – 7.96 (m, 2H), 7.90 (m, 1H), 7.62 – 7.49 (m, 5H), 7.45 (ddd, *J* = 8.3, 6.7, 1.4 Hz, 1H), 7.31 (m, 1H), 7.17 (ddd, *J* = 8.1, 6.9, 1.2 Hz, 1H), 7.01 (ddd, *J* = 7.9, 6.9, 1.0 Hz, 1H).

^{13}C{^{1}H} NMR (126 MHz, Chloroform-*d*) δ 136.17, 134.09, 133.06, 132.66, 128.38, 127.86, 127.80, 127.28, 126.68, 125.85, 125.83, 125.73, 123.68, 122.50, 120.45, 120.15, 116.67, 111.40.

HR-MS (ESI+) *m*/*z*: $[M+H]^+$ calcd for $C_{18}H_{13}N$, 244.1121; found, 244.1127.

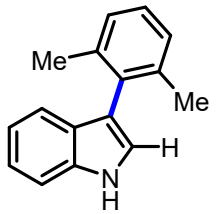


3-(*o*-Tolyl)-1*H*-indole (4an)[3]; a light yellow oil (57.2 mg, 92%)

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.15 (s, 1H), 7.59 (m, 1H), 7.49 (m, 1H), 7.46 (dt, *J* = 8.2, 0.8 Hz, 1H), 7.38 (m, 1H), 7.34 – 7.27 (m, 3H), 7.22 – 7.18 (m, 2H), 2.38 (s, 3H).

^{13}C{^{1}H} NMR (126 MHz, Chloroform-*d*) δ 137.00, 135.96, 134.56, 131.00, 130.48, 127.24, 126.89, 125.76, 122.92, 122.29, 120.23, 120.04, 117.57, 111.32, 20.85.

H-MS (EI) *m*/*z*: [M] calcd for $C_{15}H_{13}N$, 207.1048; found, 207.1048.



3-(2,6-Dimethylphenyl)-1*H*-indole (4ao); white solid (21.2 mg, 32%), mp 115 °C.

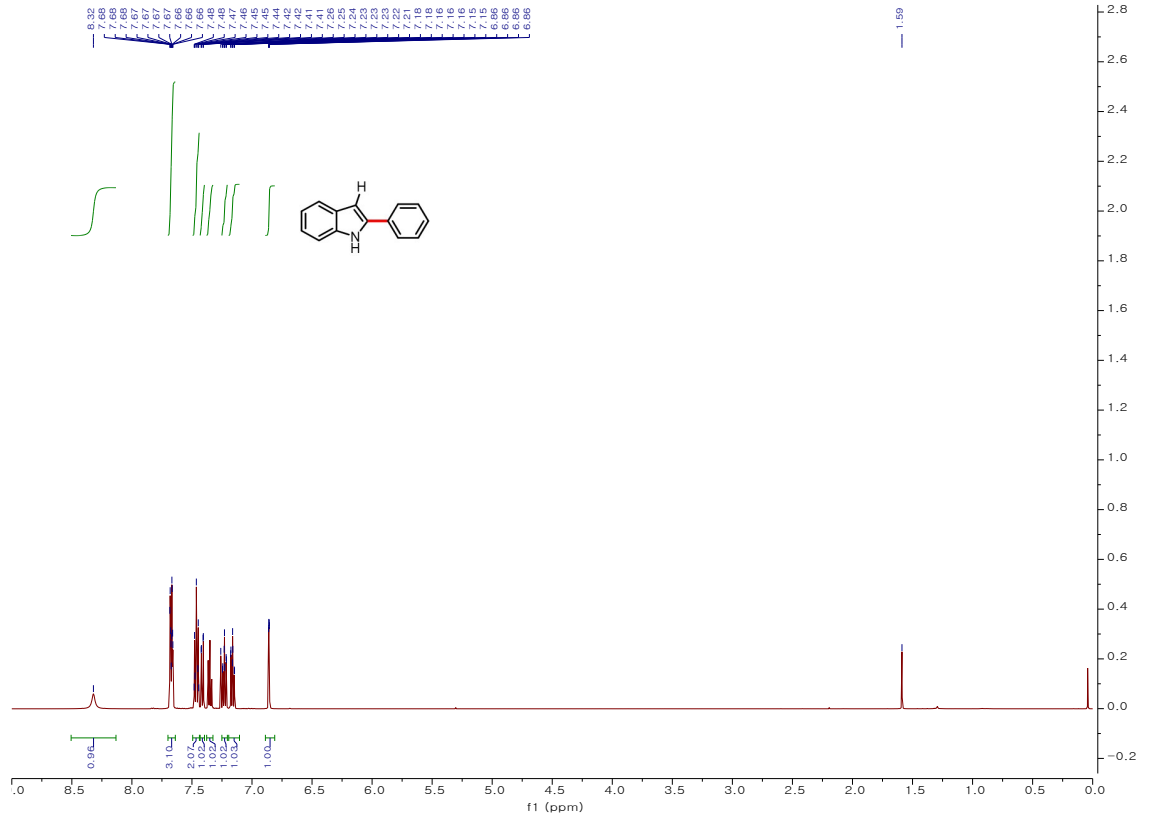
^{1}H NMR (500 MHz, DMSO-d_6) δ 11.20 (s, 1H), 7.44 (dt, *J* = 8.1, 0.8 Hz, 1H), 7.25 (d, *J* = 2.4 Hz, 1H), 7.18 – 7.07 (m, 4H), 7.02 (d, *J* = 7.4 Hz, 1H), 6.95 (ddd, *J* = 7.9, 6.9, 1.0 Hz, 1H), 2.01 (s, 6H).

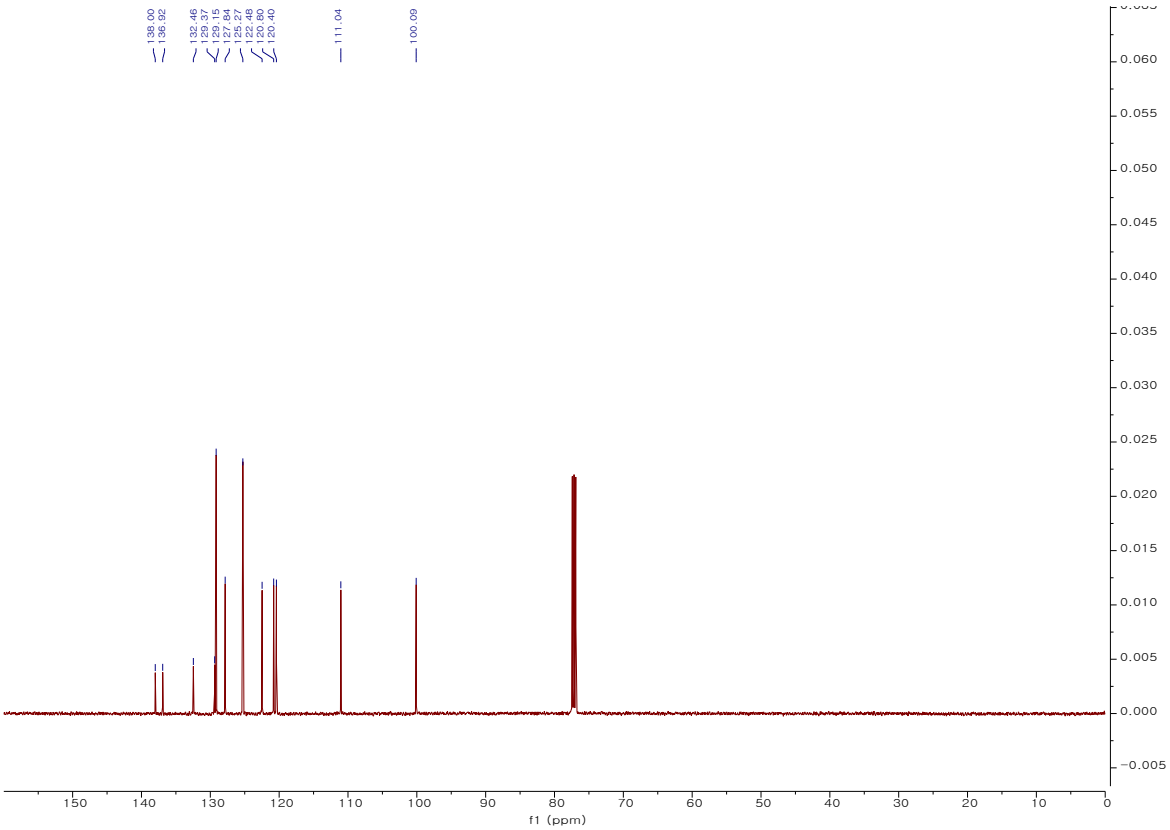
^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 137.57, 136.09, 134.30, 127.14, 126.66, 126.53, 123.58, 120.97, 118.86, 118.69, 113.50, 111.69, 20.74.

HR-MS (ESI+) *m*/*z*: $[M+H]^+$ calcd for $C_{16}H_{15}N$, 222.1277; found, 222.1250.

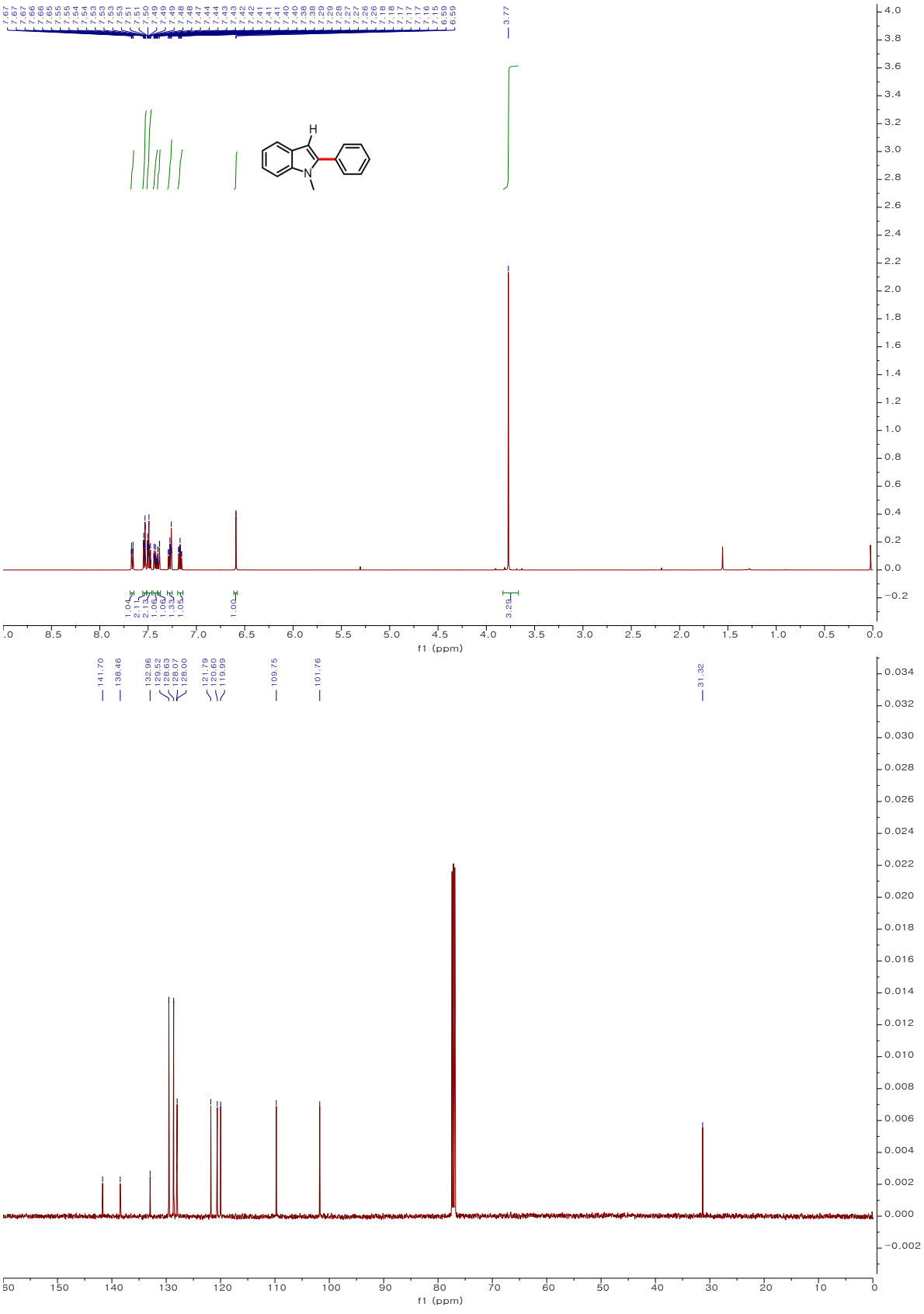
6. Compounds Characterization Data

2-Phenyl-1*H*-indole (3aa);

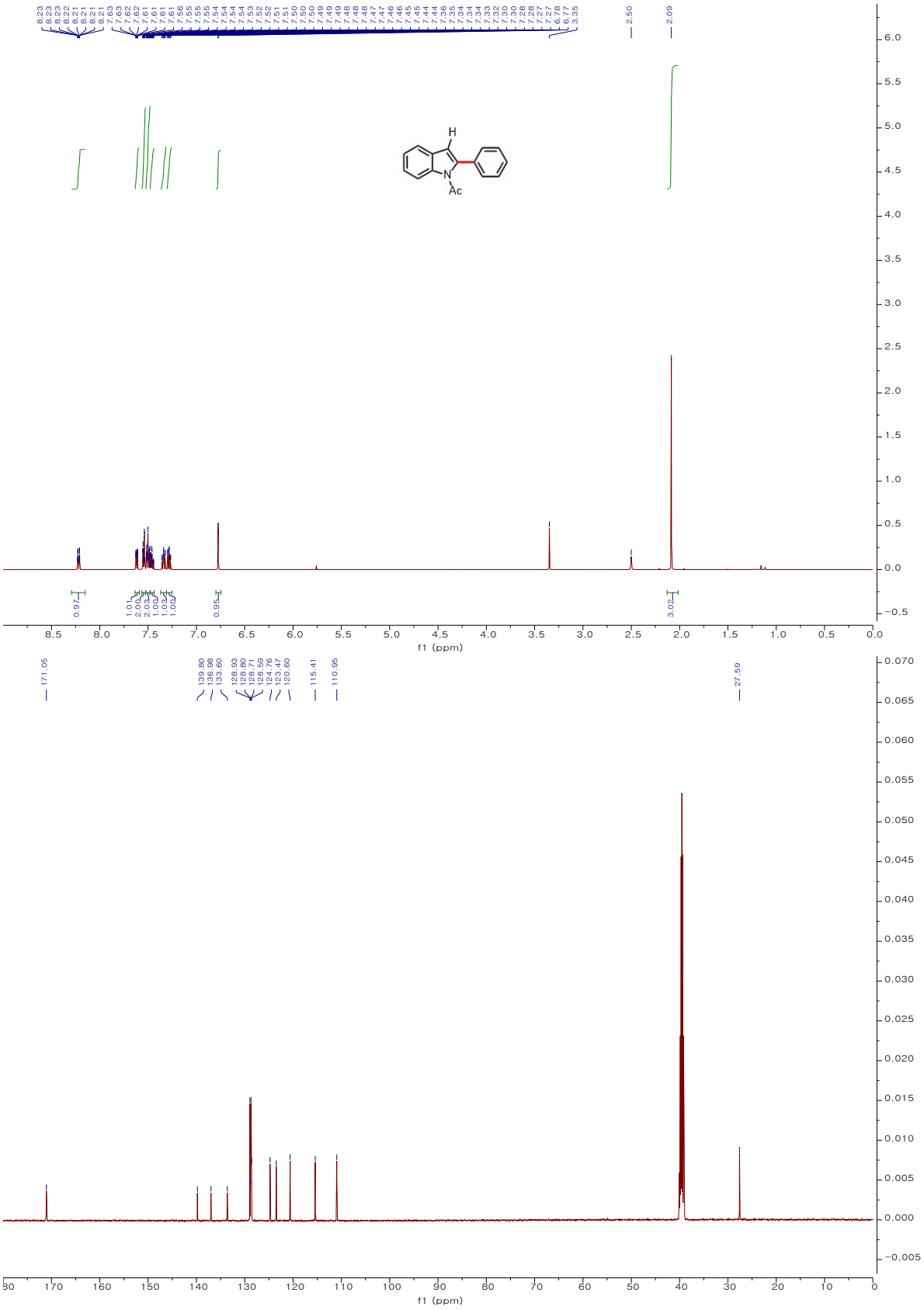




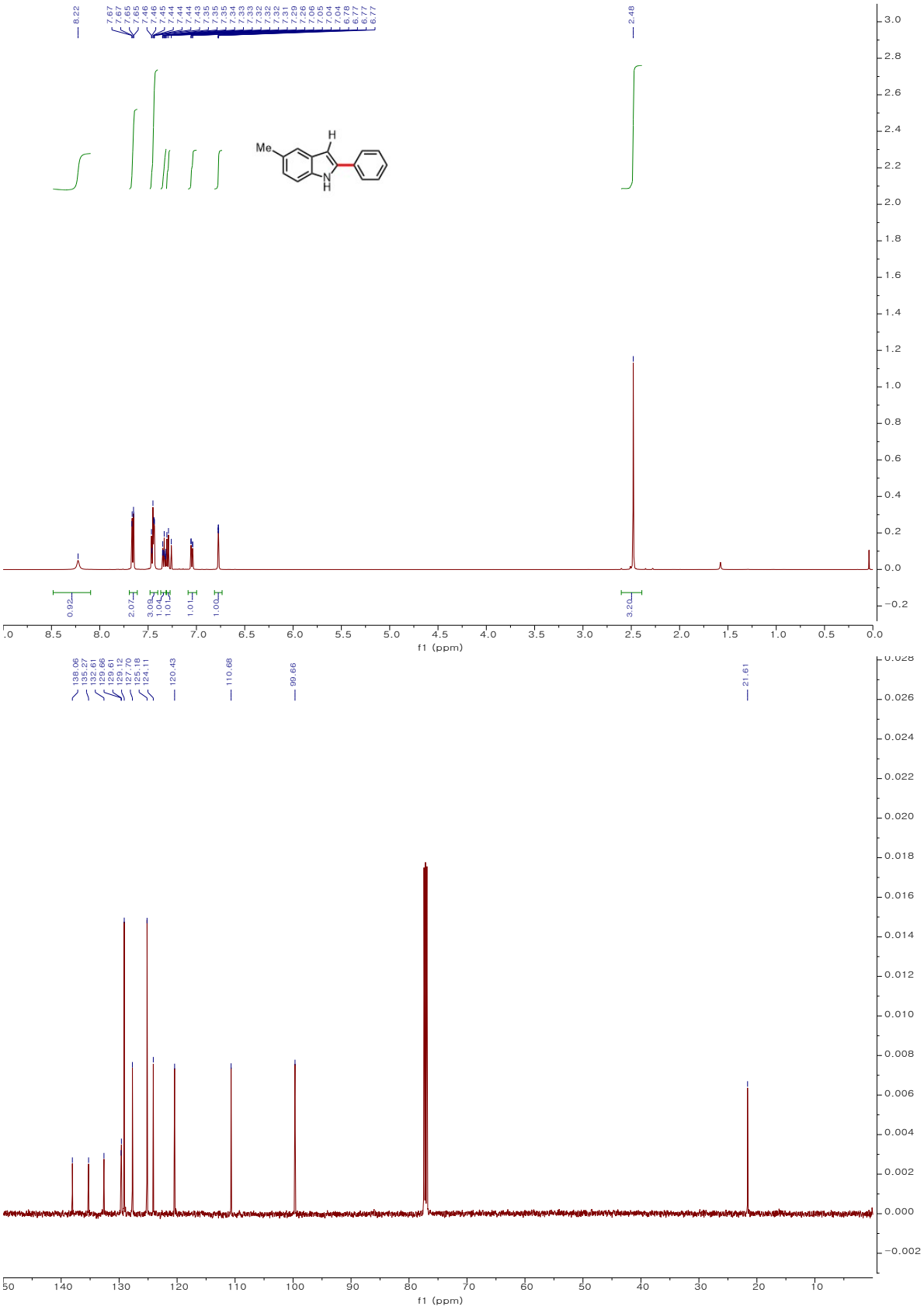
1-Methyl-2-phenyl-1*H*-indole (3ba);



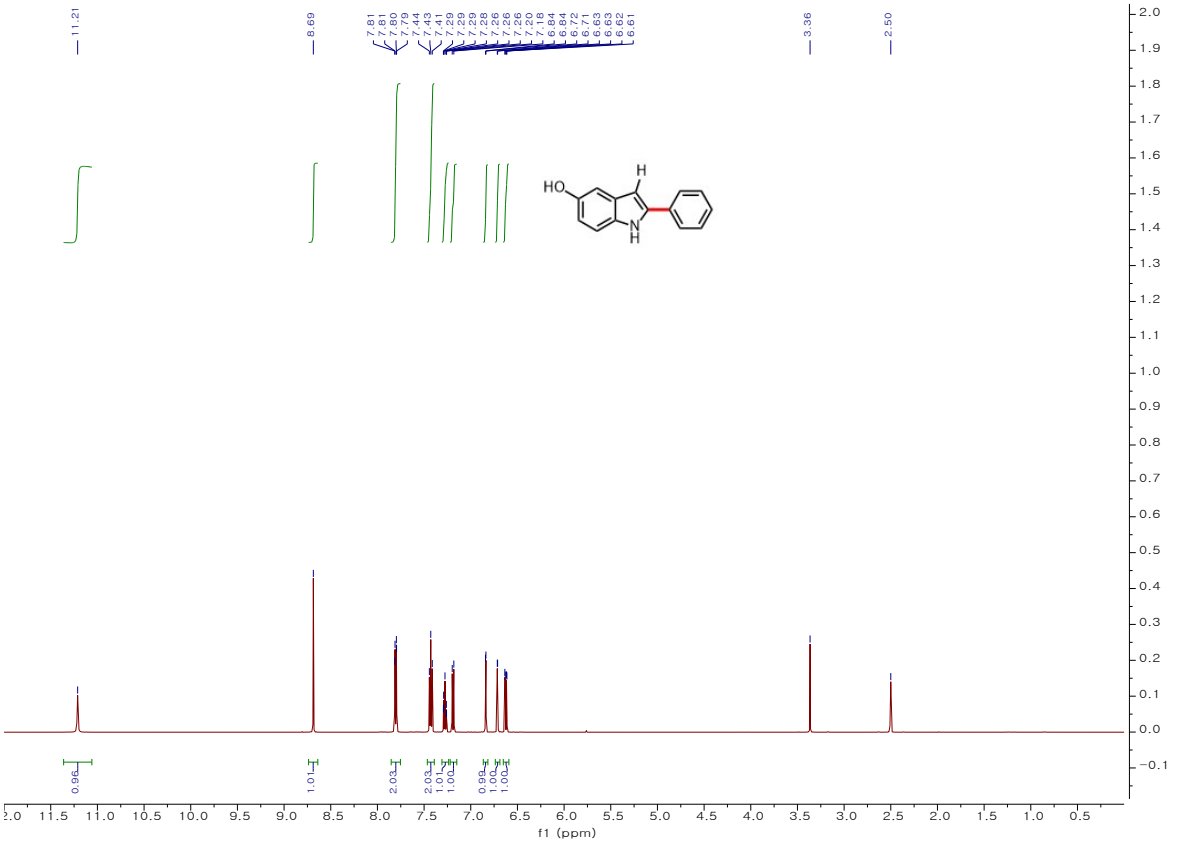
1-(2-Phenyl-1*H*-indol-1-yl)ethan-1-one (3ca);

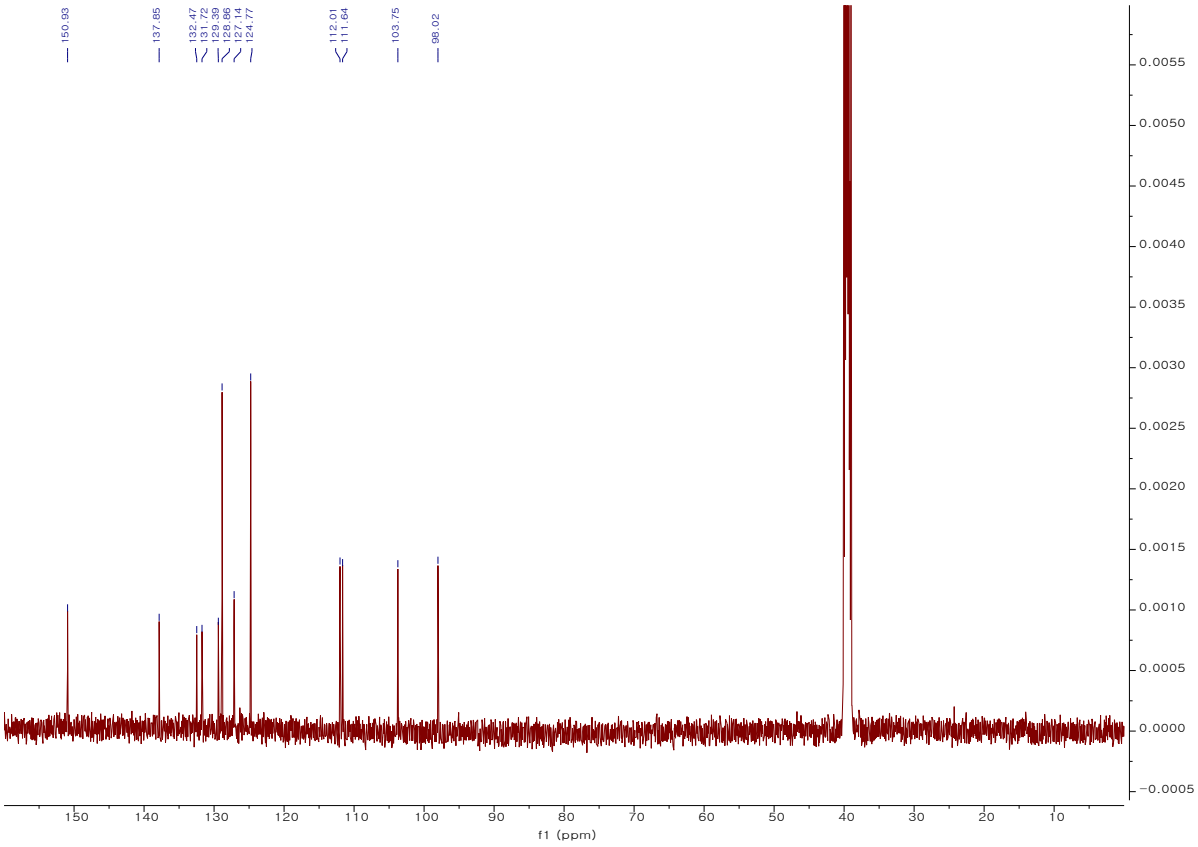


5-Methyl-2-phenyl-1*H*-indole (3da);

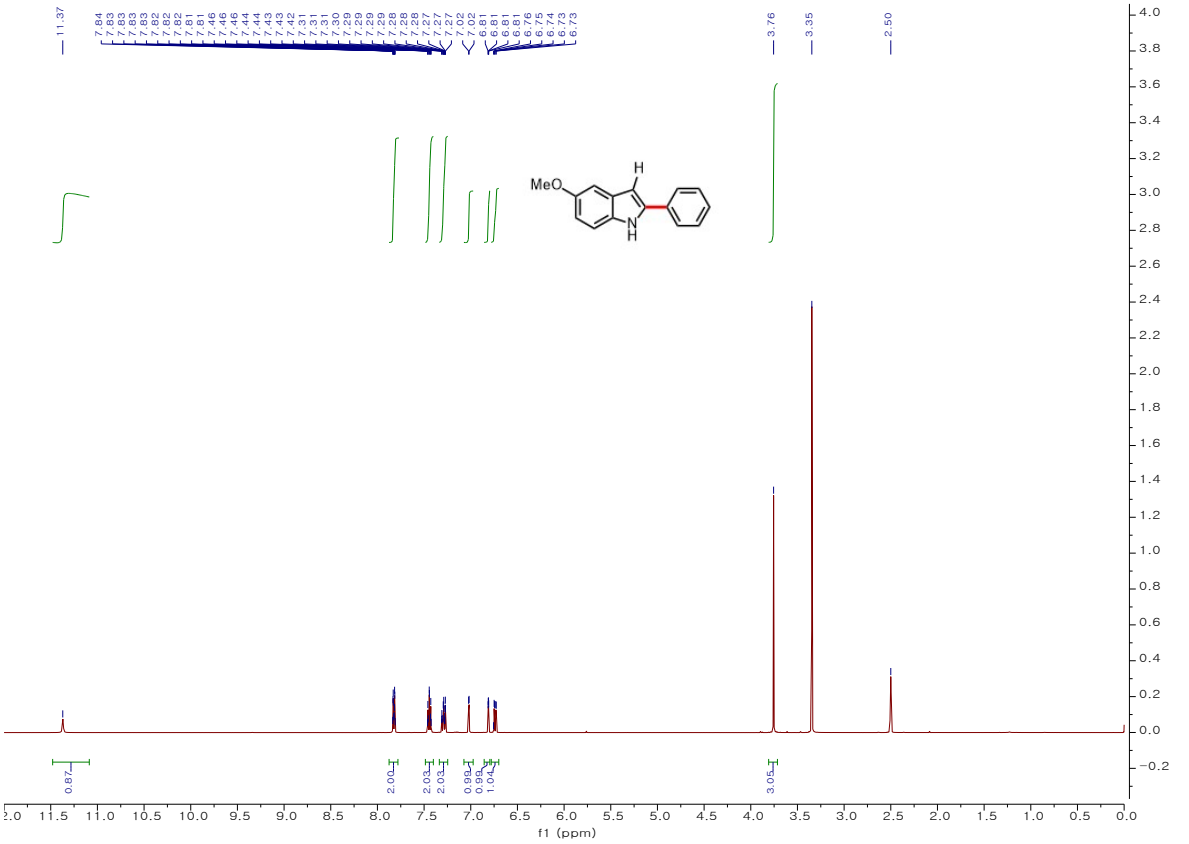


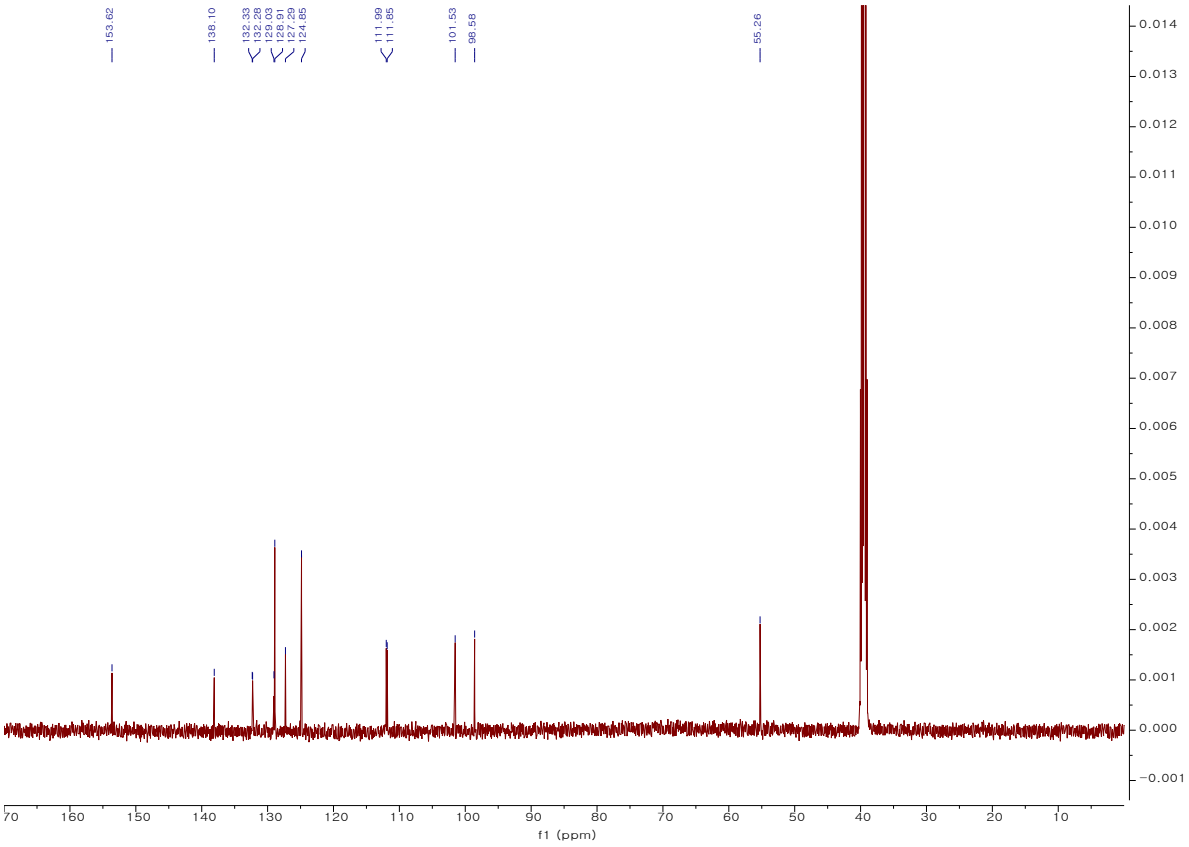
2-Phenyl-1*H*-indol-5-ol (3ea);



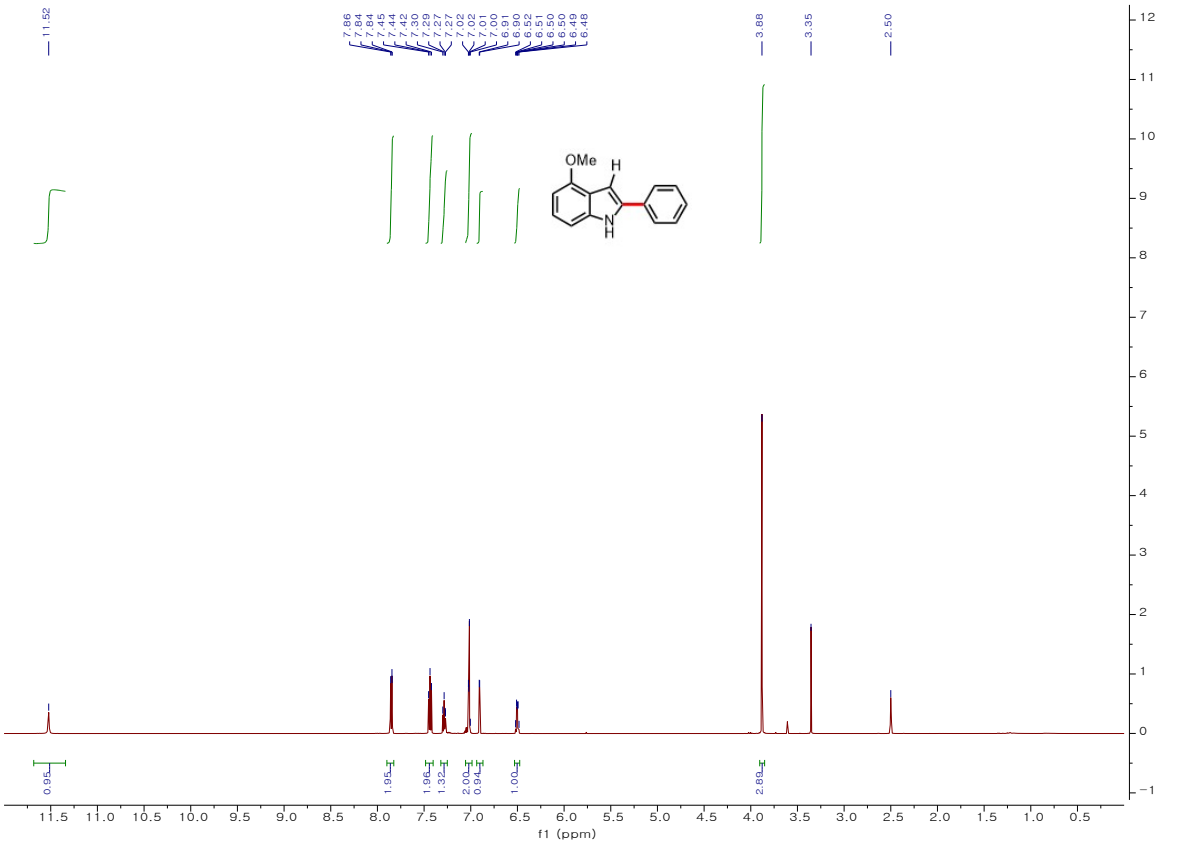


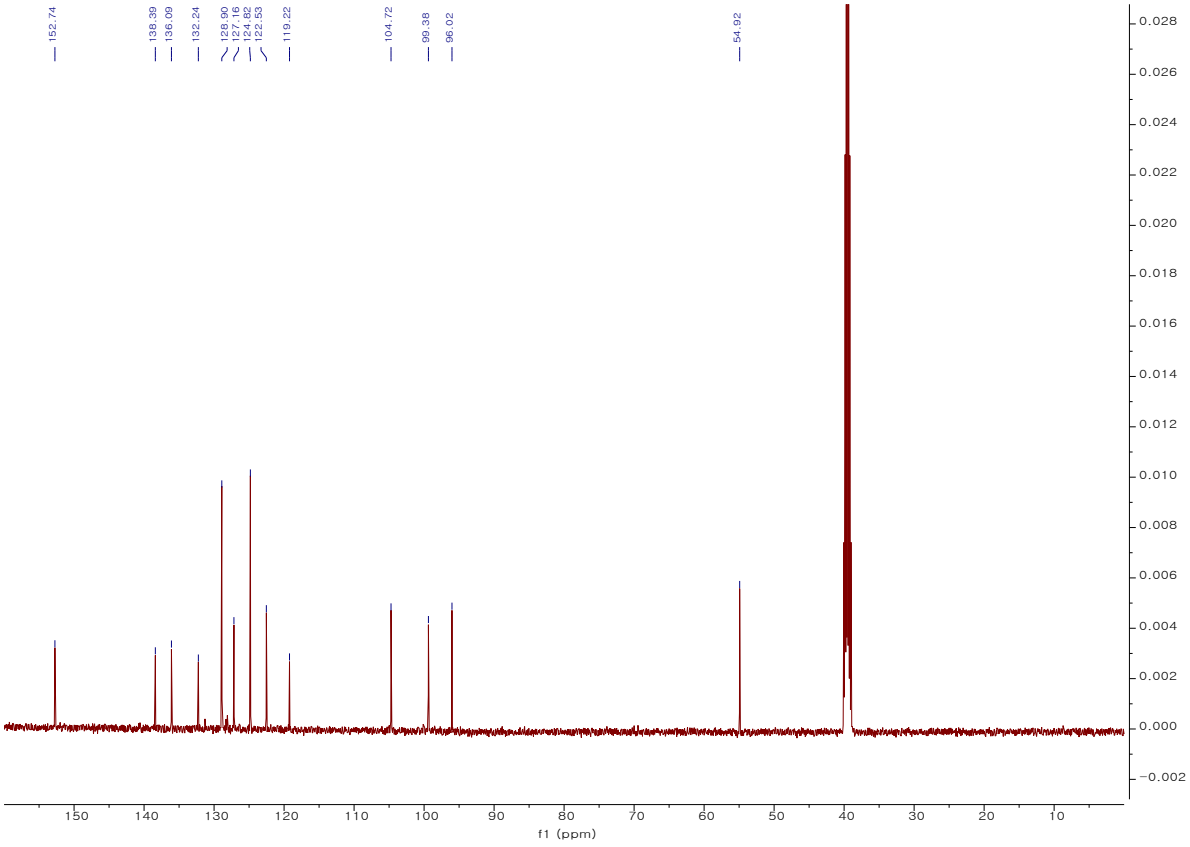
5-Methoxy-2-phenyl-1*H*-indole (3fa);



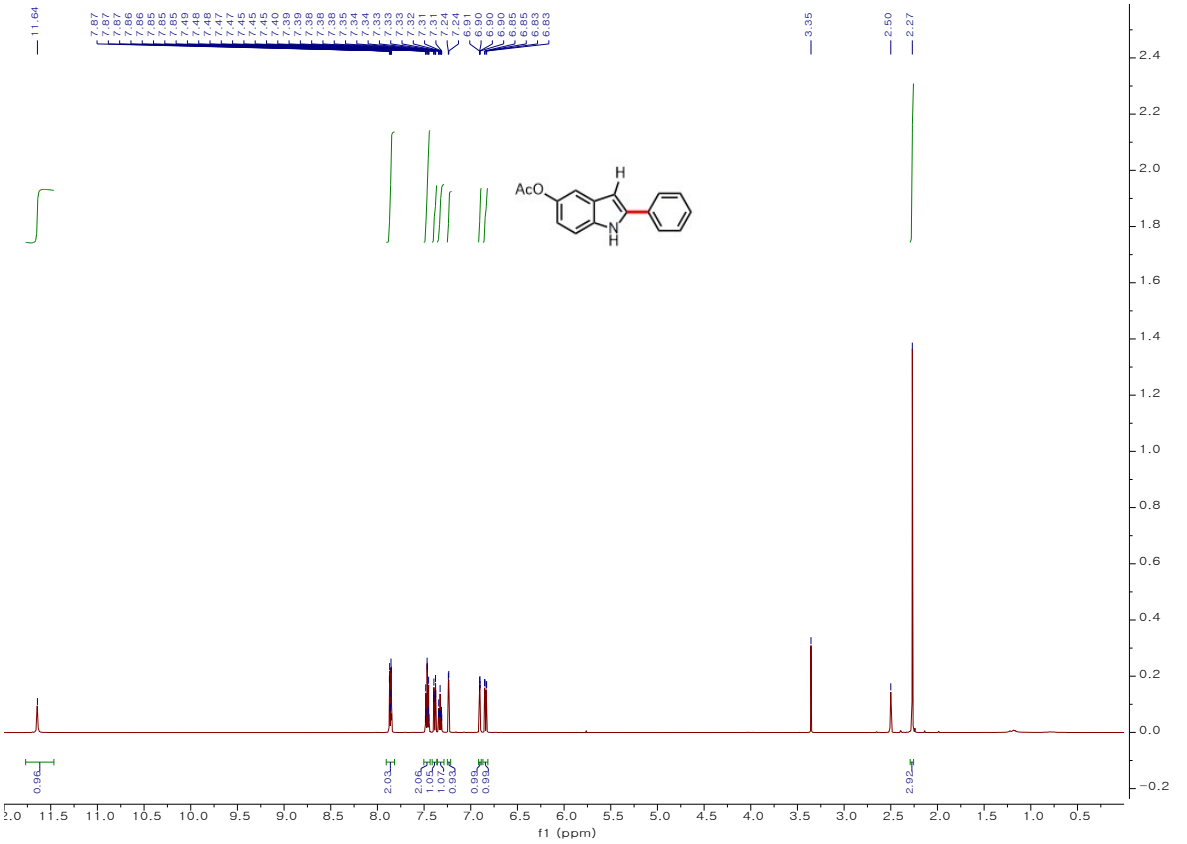


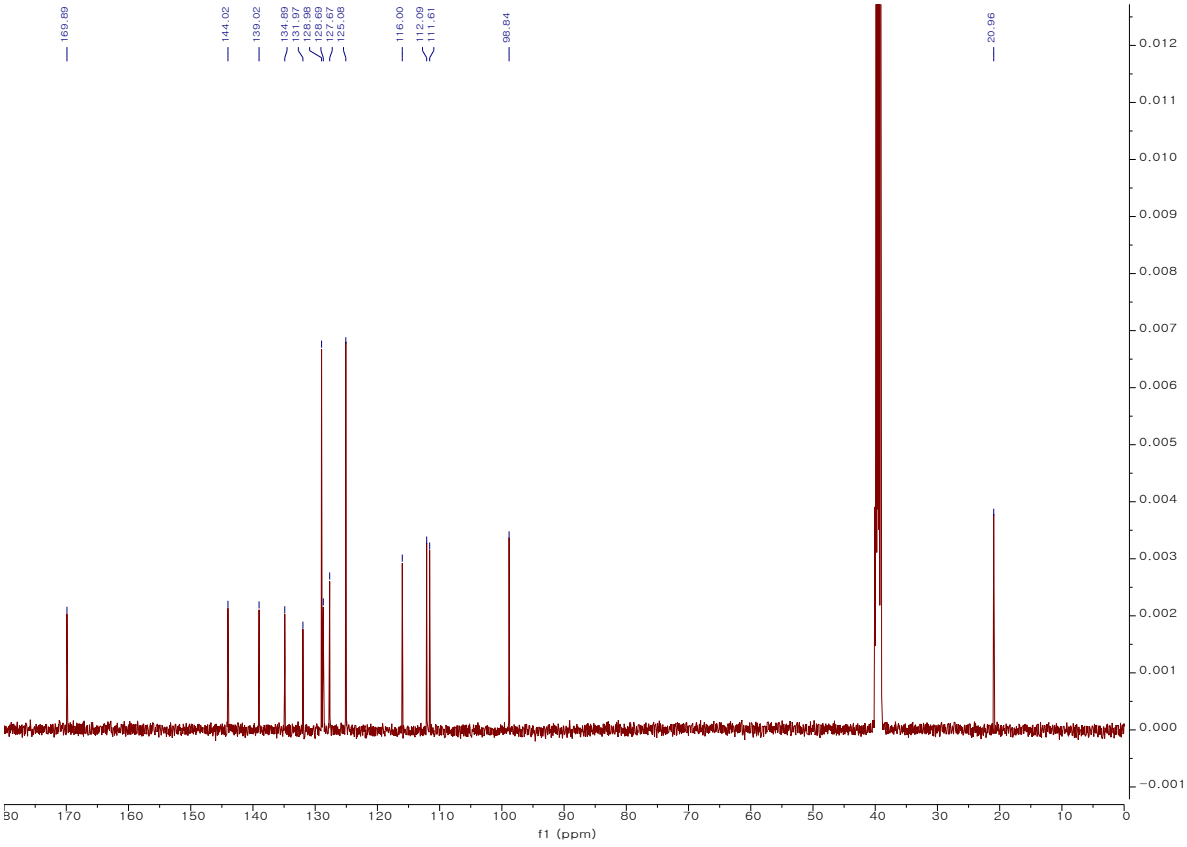
4-Methoxy-2-phenyl-1*H*-indole (3ga);



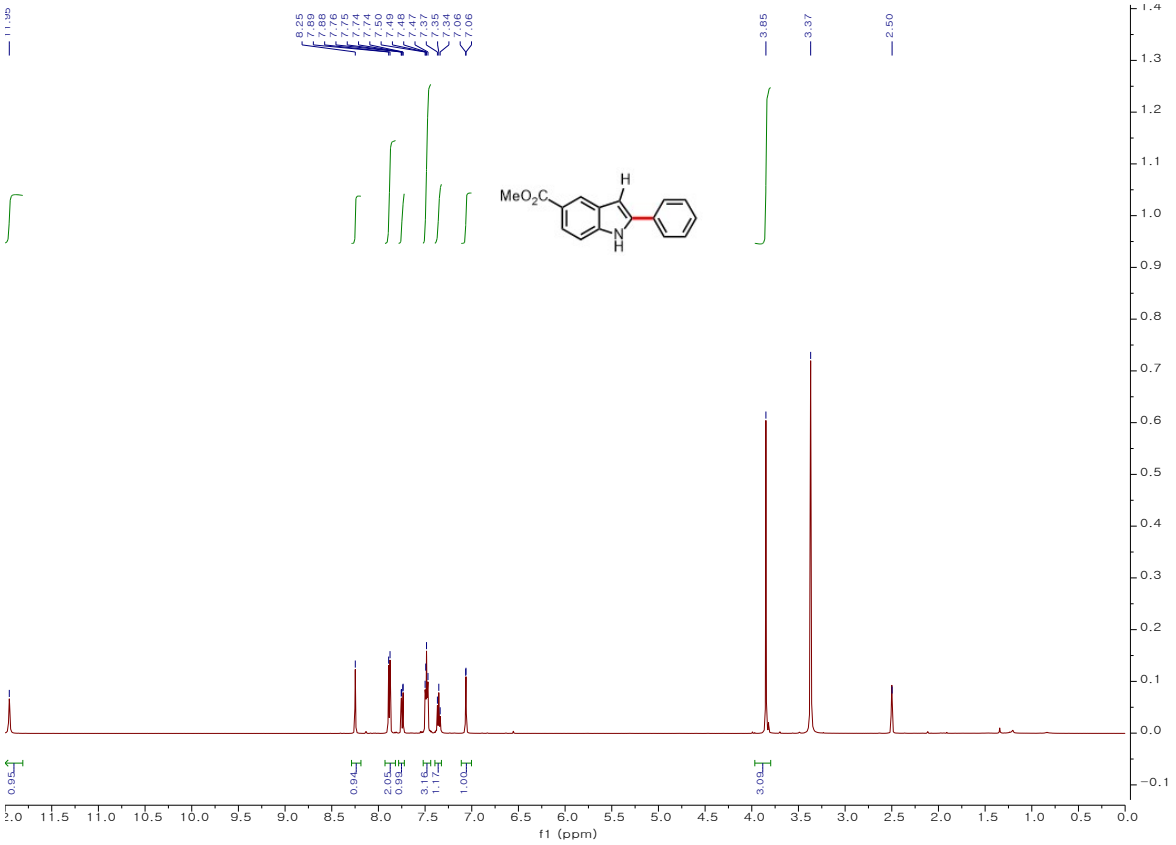


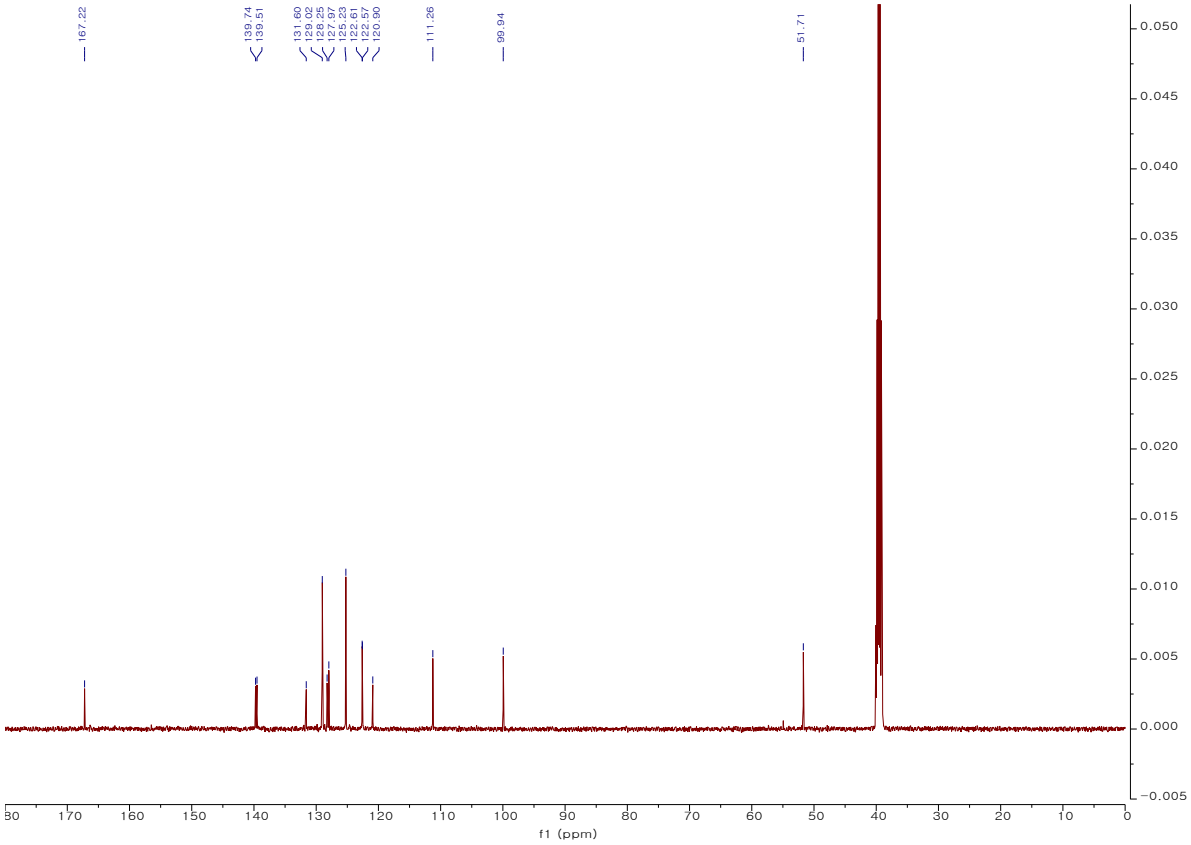
2-Phenyl-1*H*-indol-5-yl acetate (3ha);



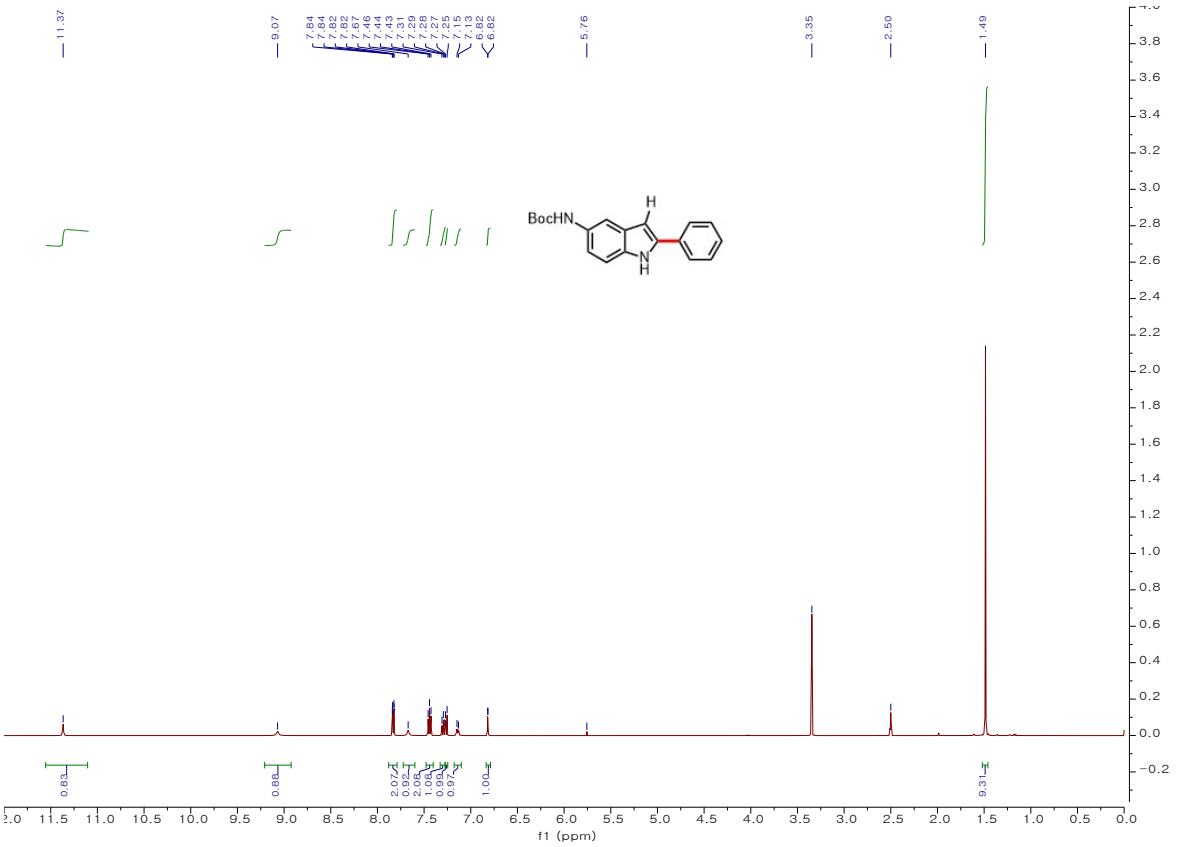


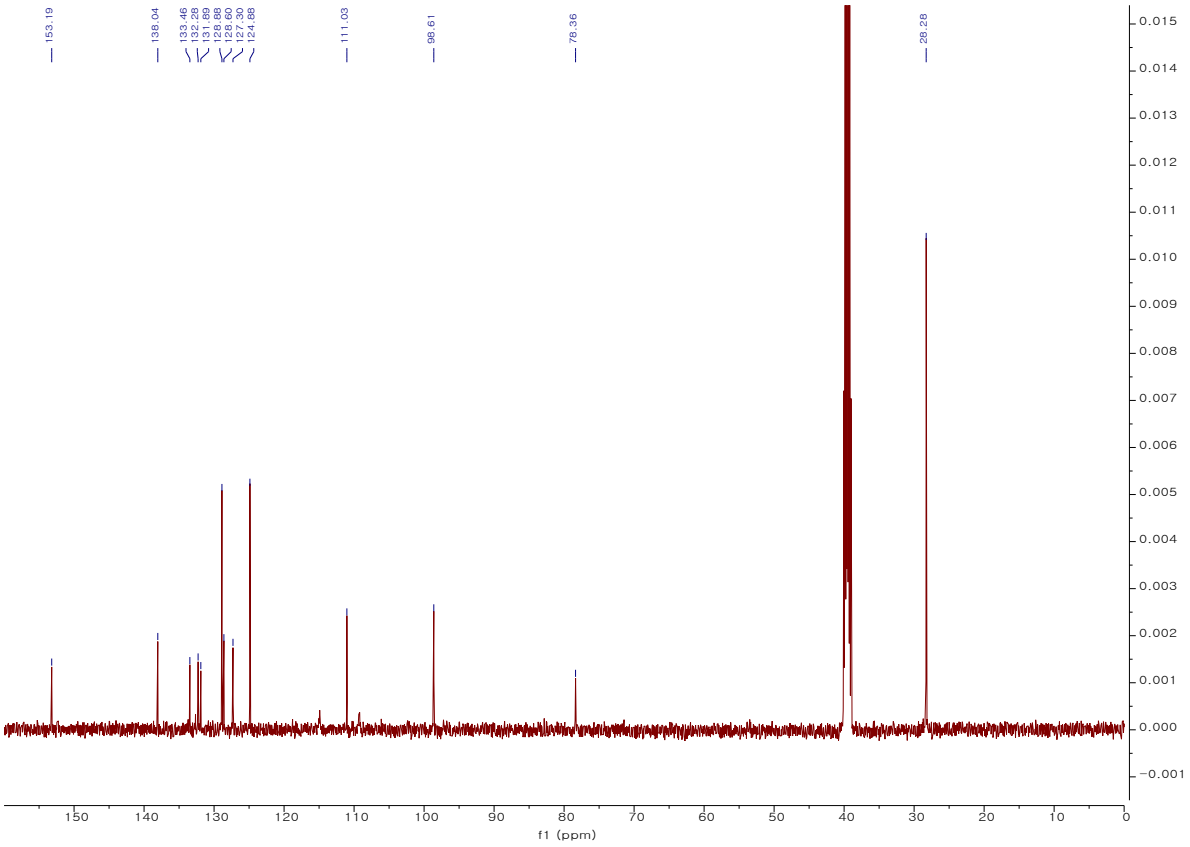
Methyl 2-phenyl-1*H*-indole-5-carboxylate (3ia);



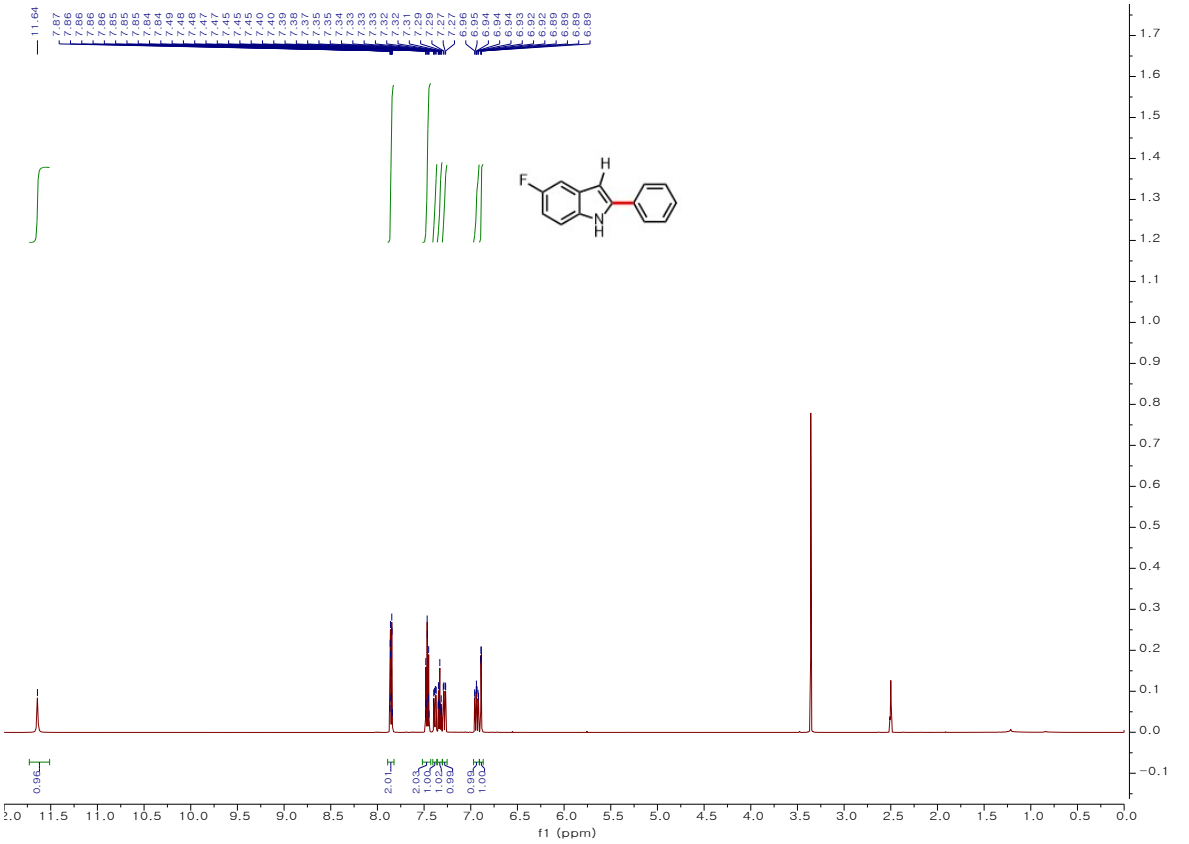


***tert*-Butyl (2-phenyl-1*H*-indol-5-yl)carbamate (3ja);**





5-Fluoro-2-phenyl-1*H*-indole (3ka);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6.92
6.89
6.89
6.89
6.89
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H
N
H
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2.03
1.00
1.02
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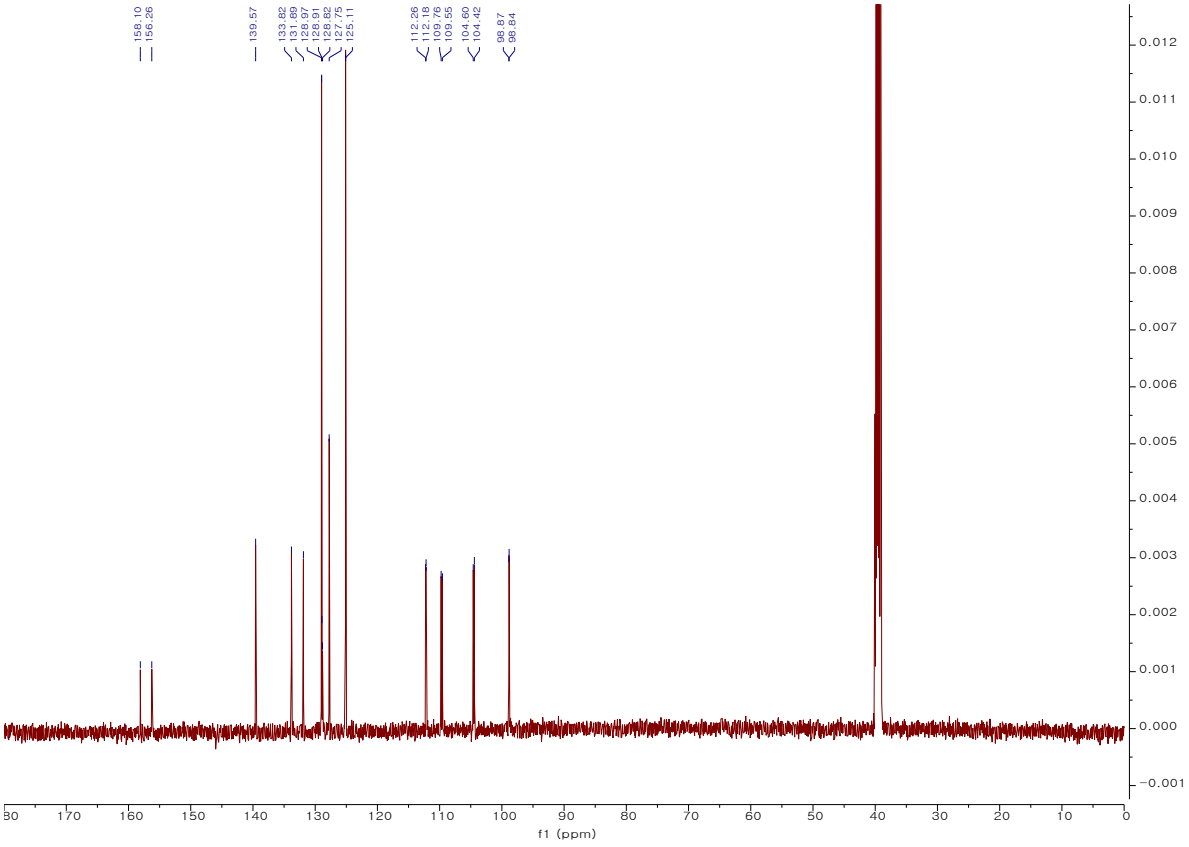
1.00
f1 (ppm)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128.91
128.82
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125.11
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112.18
109.76
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104.60
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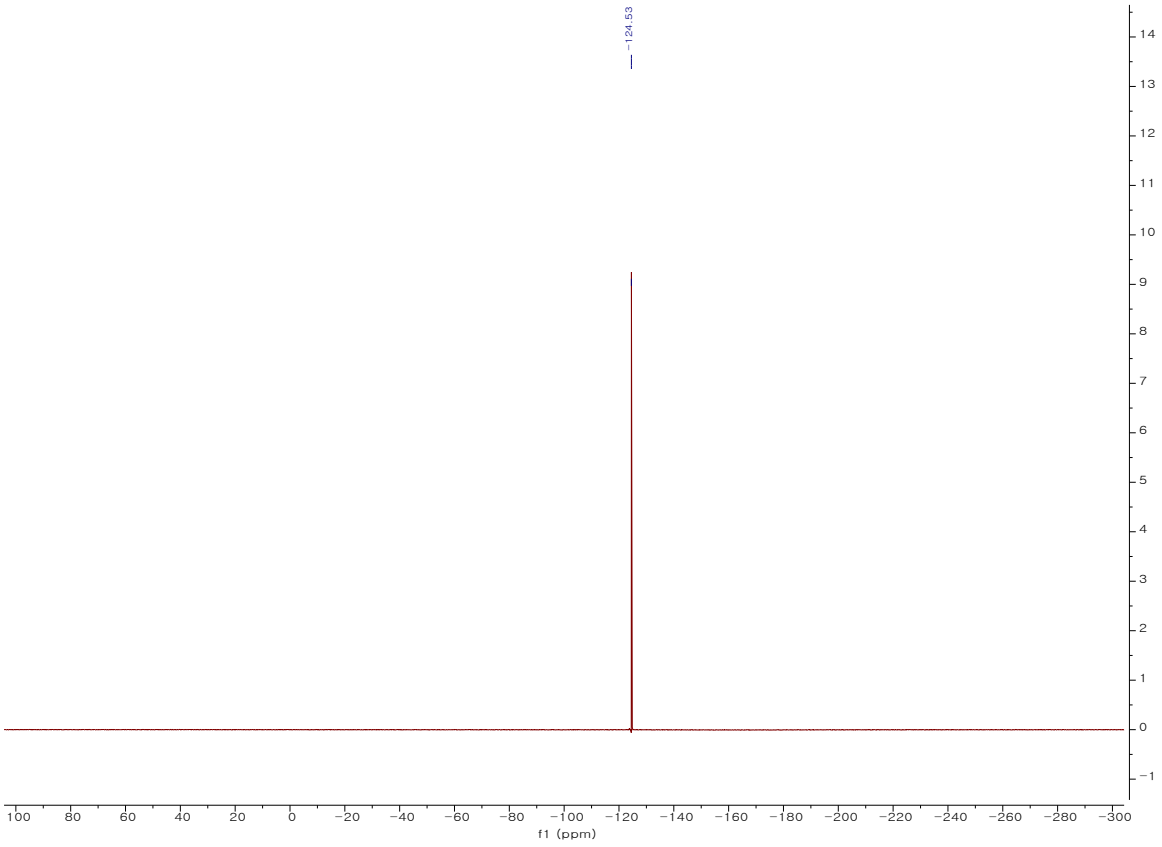
98.84
f1 (ppm)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4
3
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0
-1
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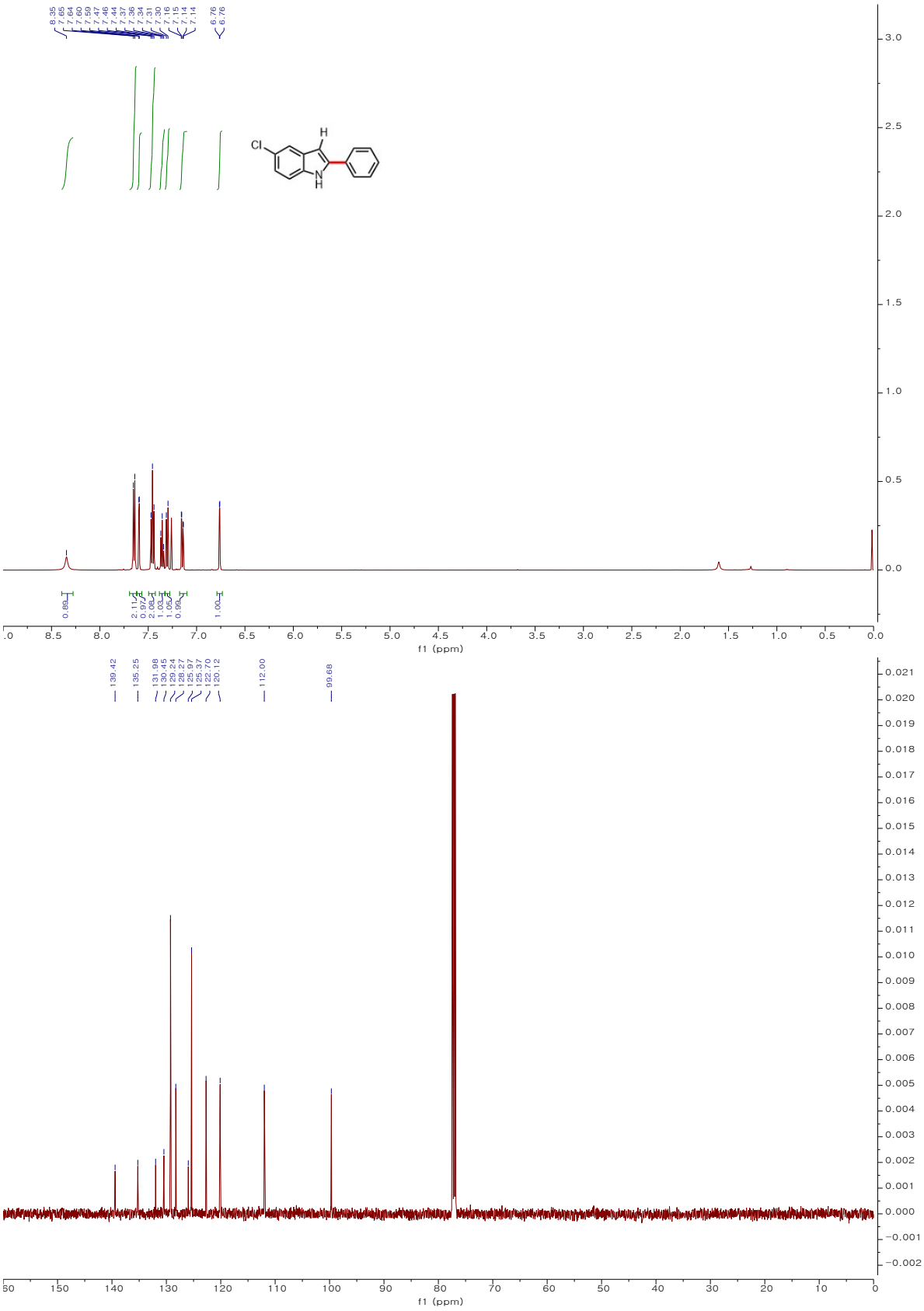
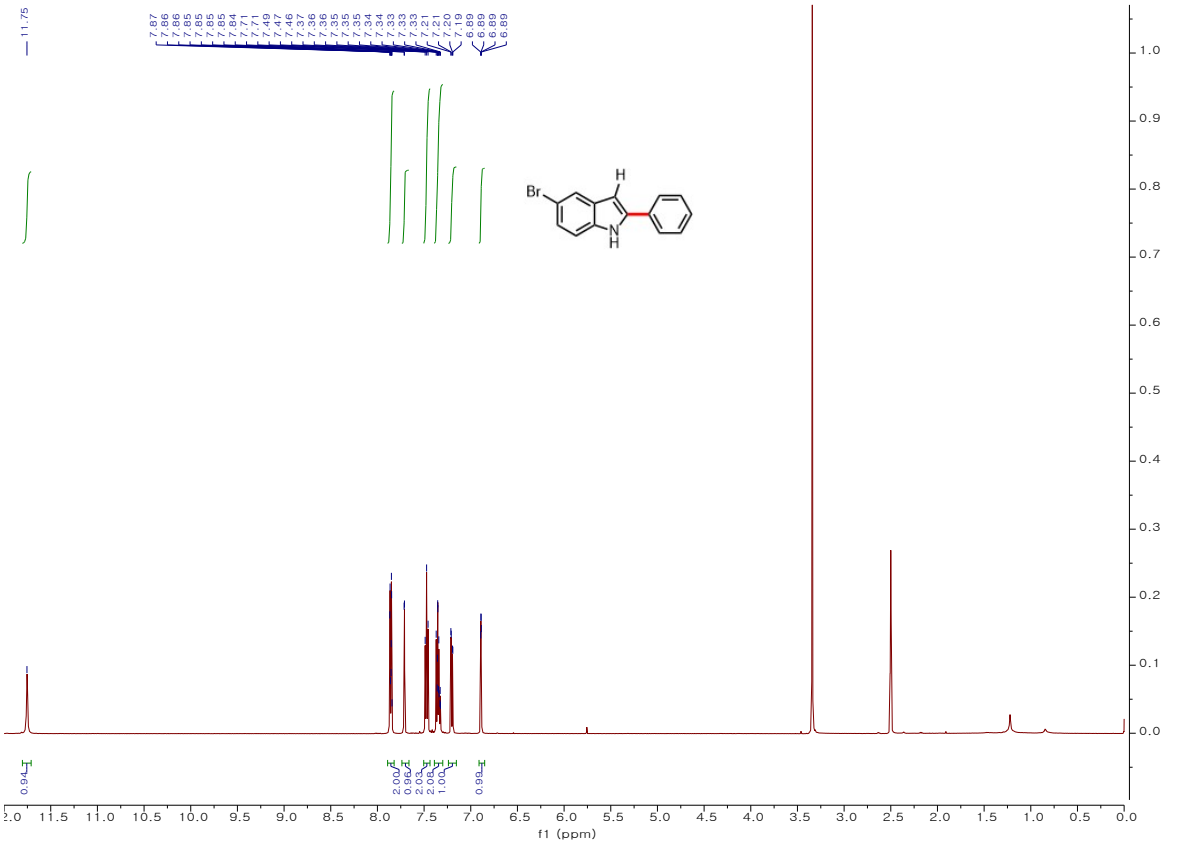
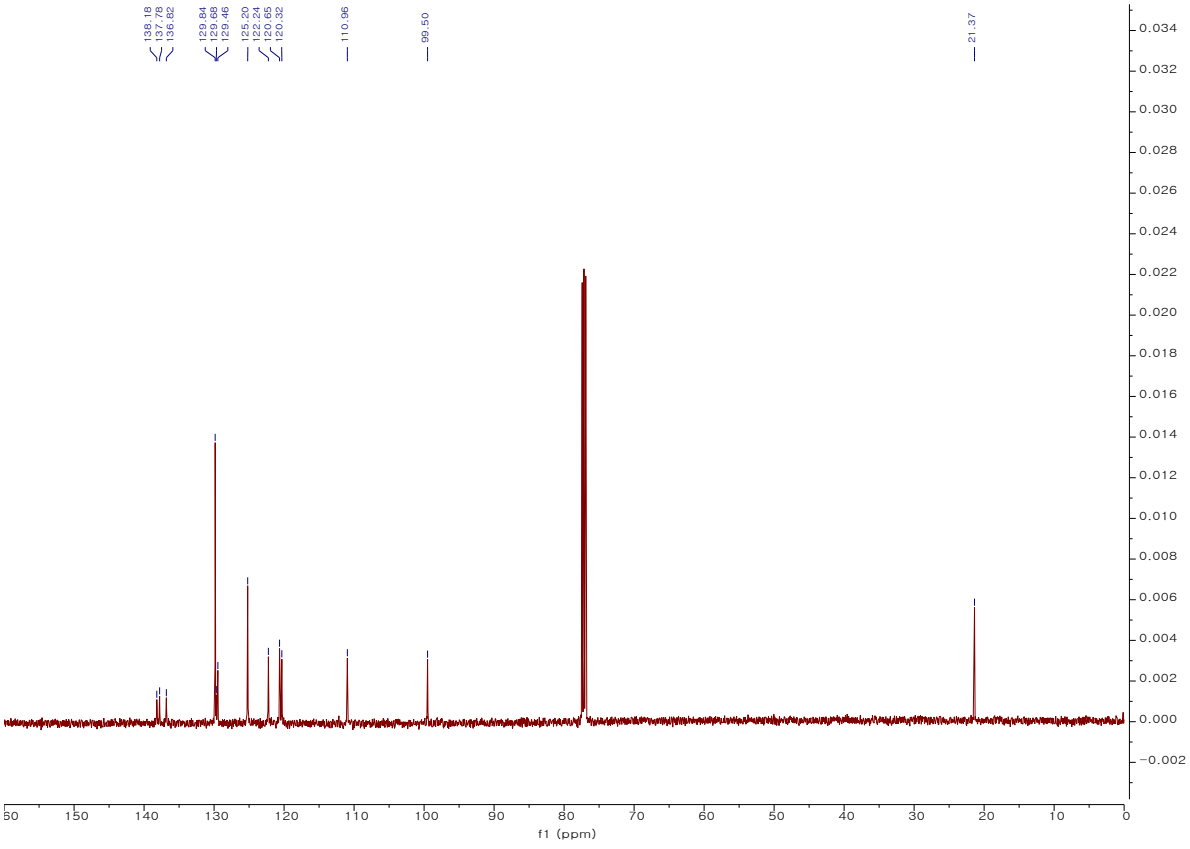
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
-240
-260
-280
-300
f1 (ppm)

5-Chloro-2-phenyl-1*H*-indole (3la);

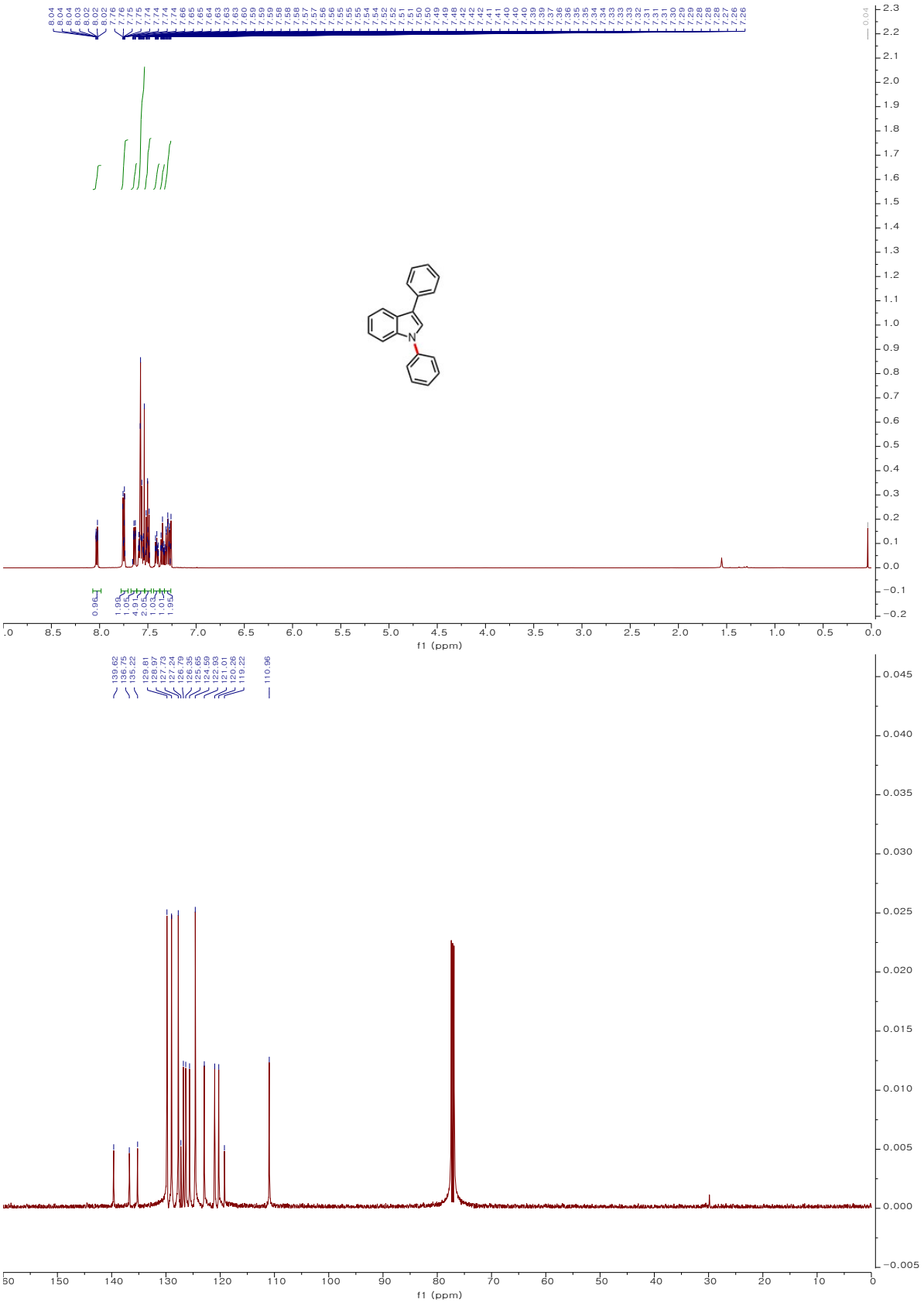


5-Bromo-2-phenyl-1*H*-indole (3ma);

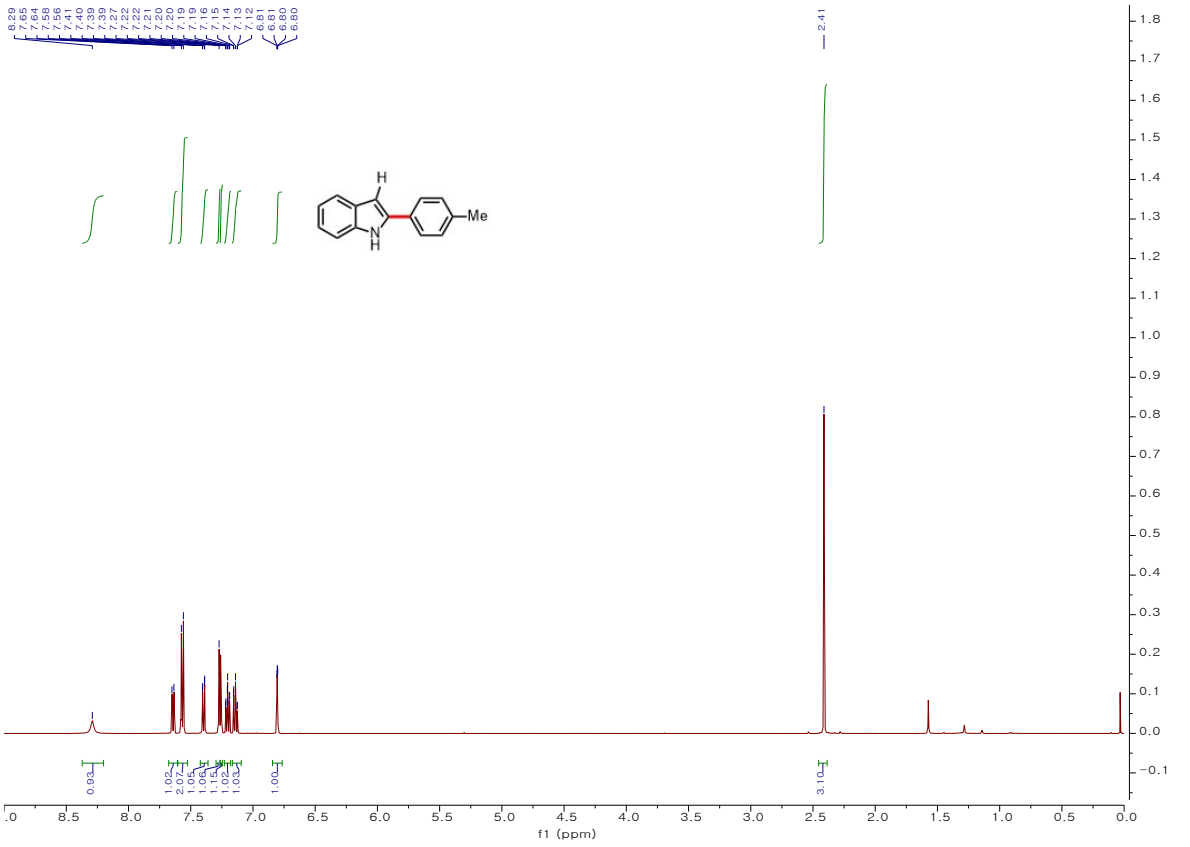


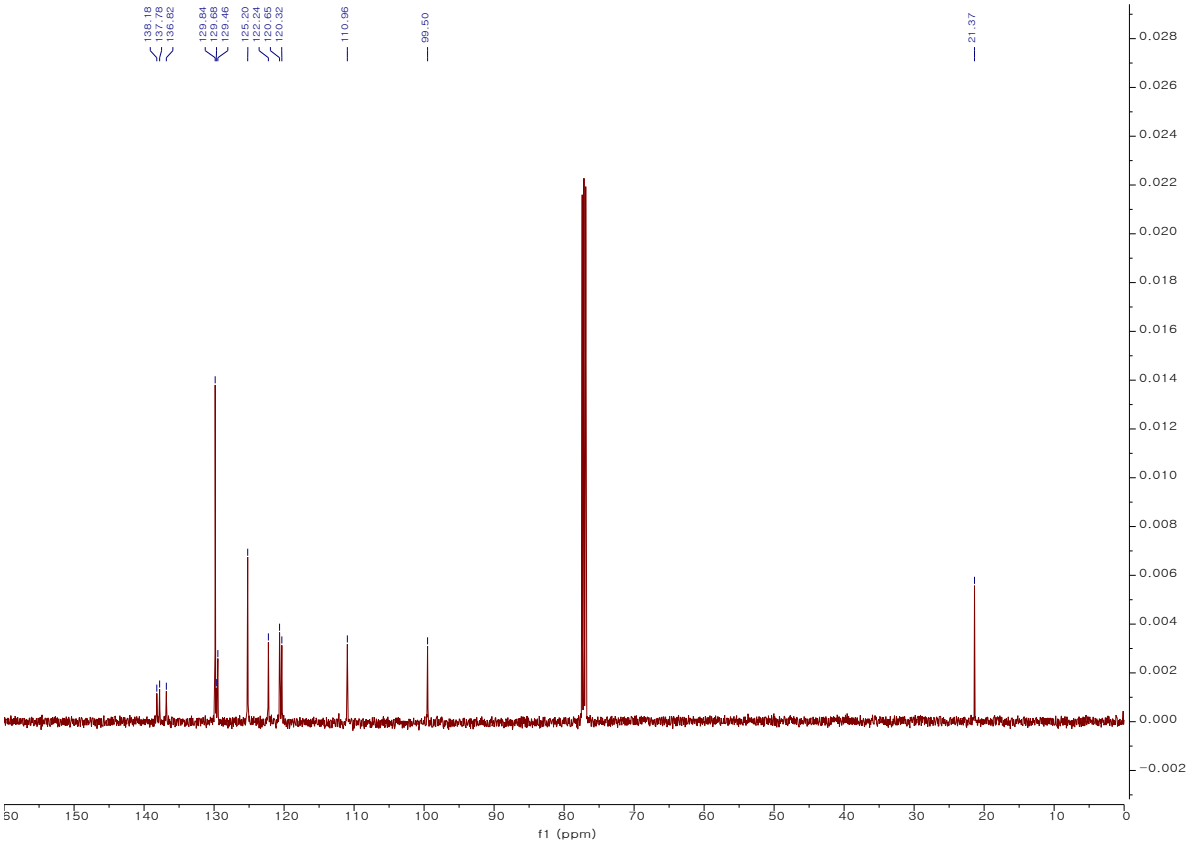


1,3-Diphenyl-1H-indole(3na');

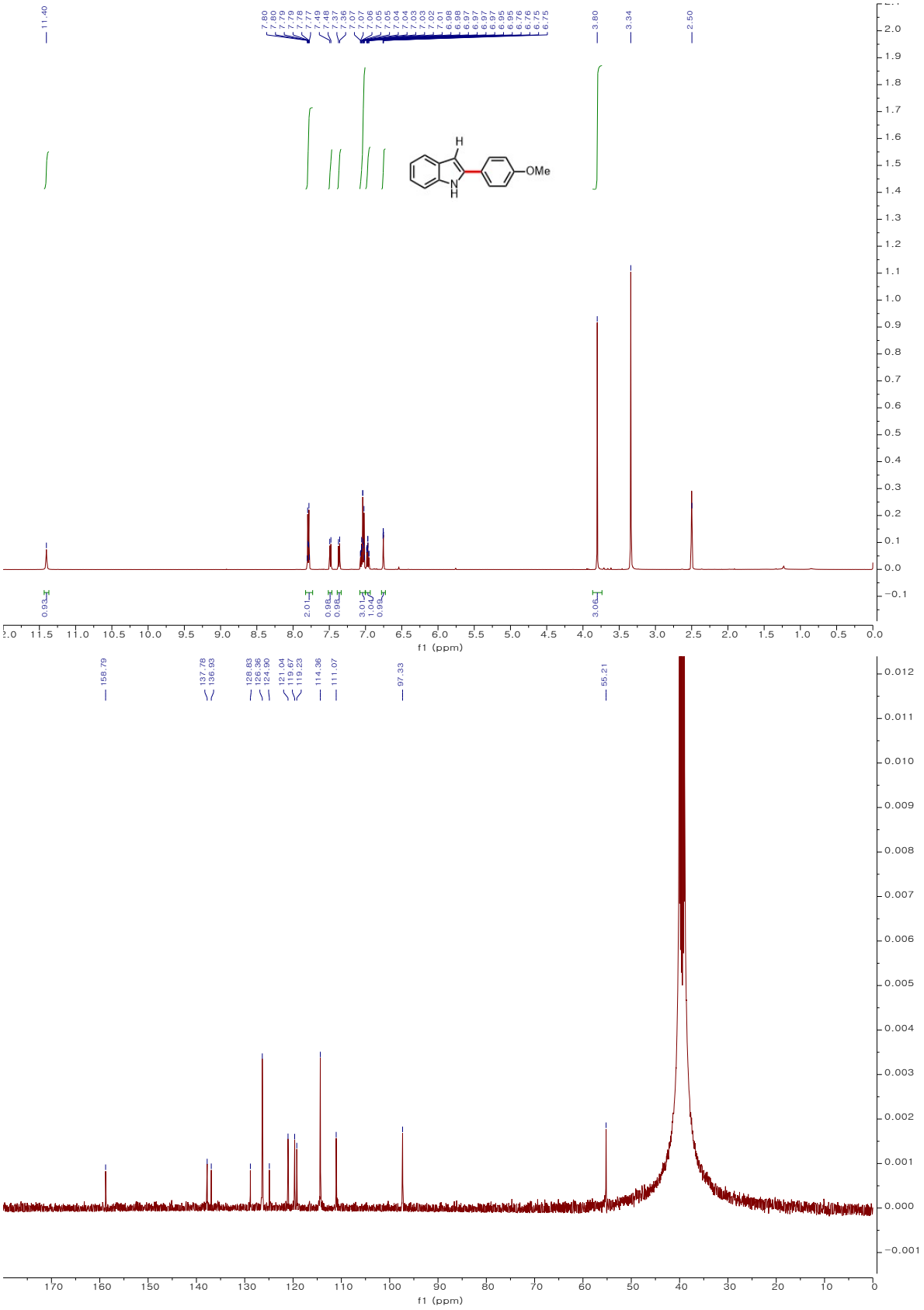


2-(*p*-Tolyl)-1*H*-indole (3ab);

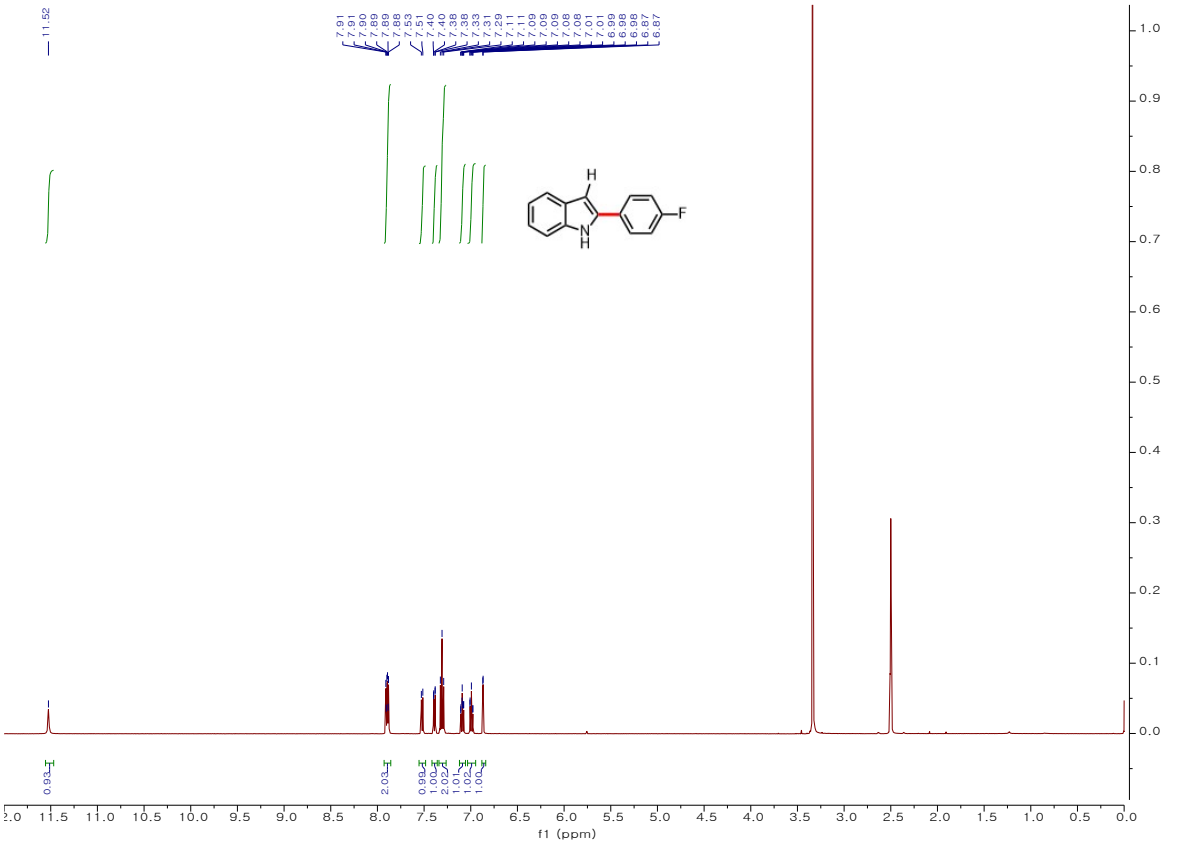


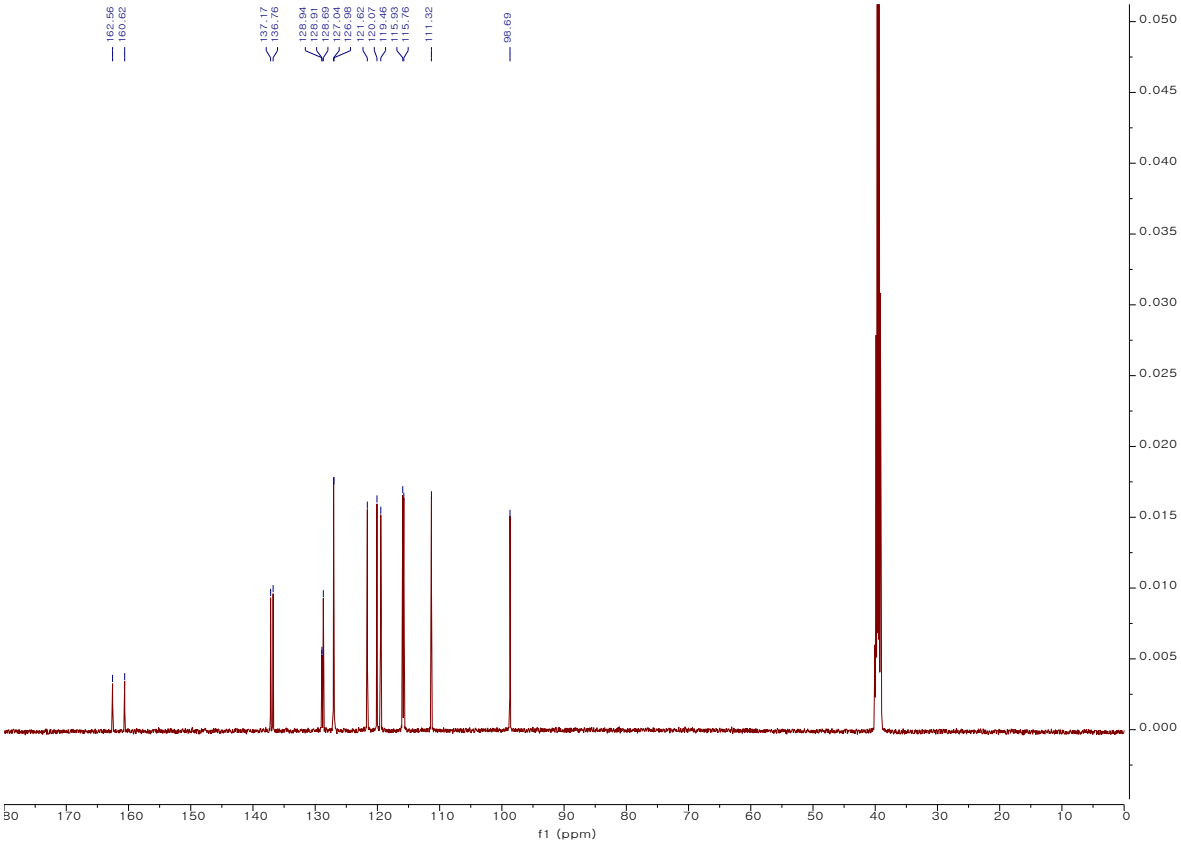


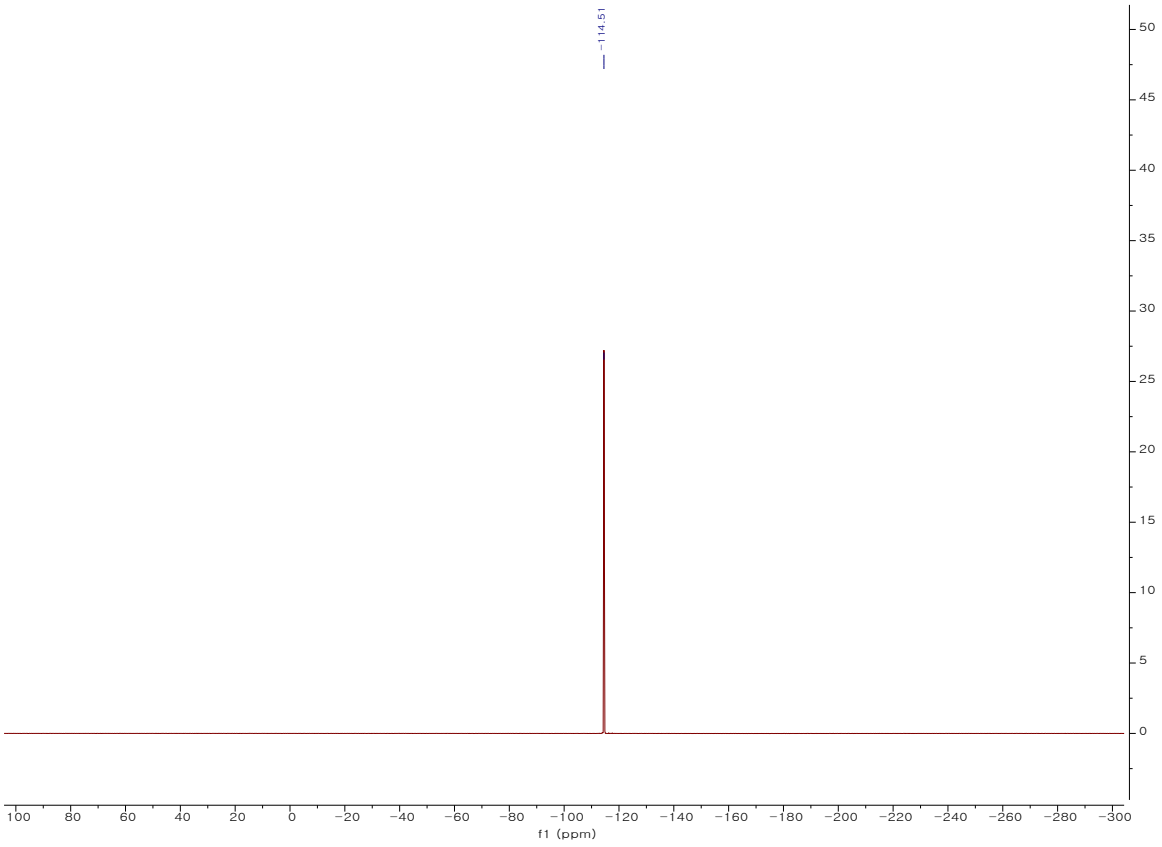
2-(4-Methoxyphenyl)-1*H*-indole (3ac);



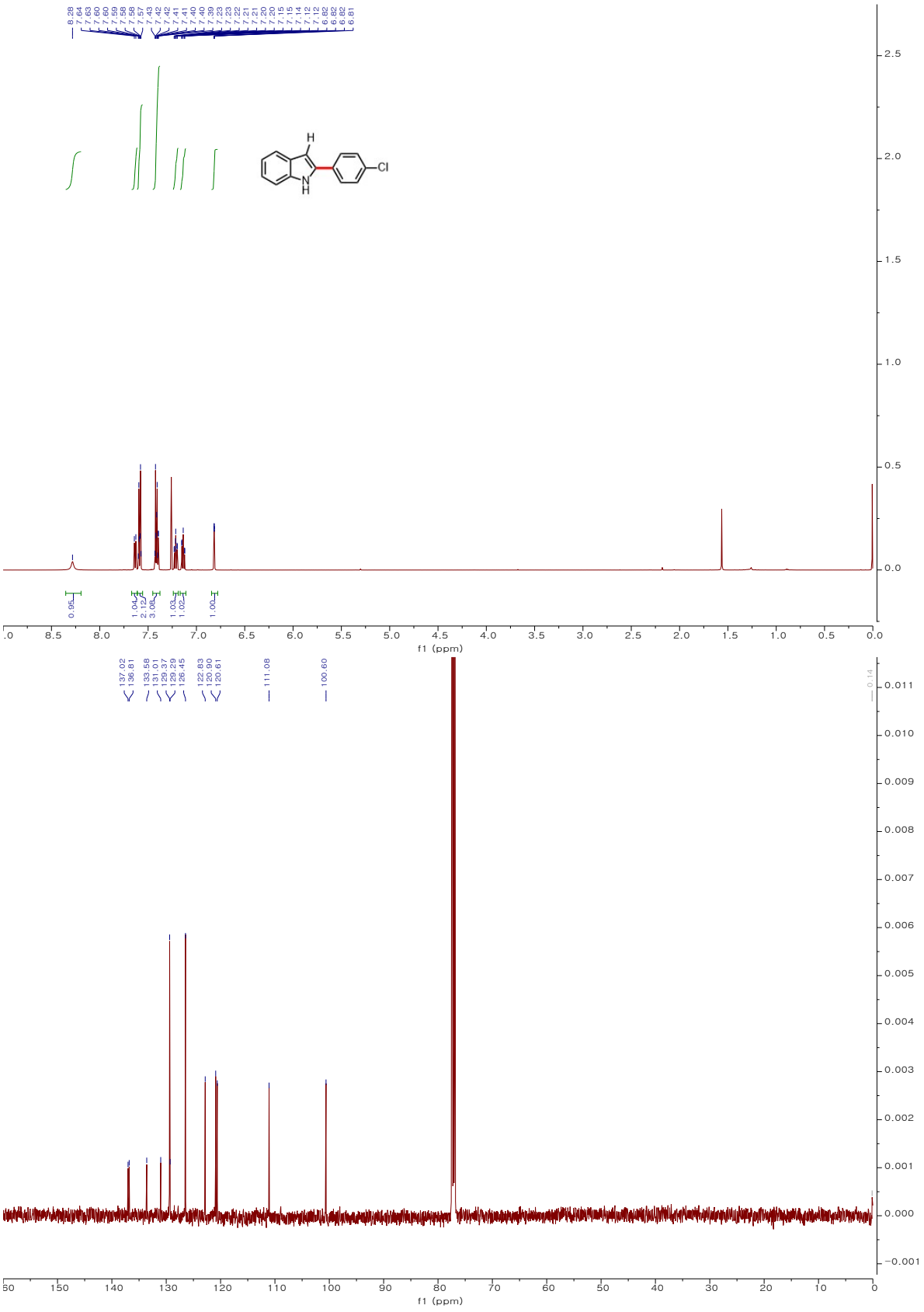
2-(4-Fluorophenyl)-1*H*-indole (3ad);


11.52
7.91
7.90
7.89
7.88
7.53
7.51
7.40
7.38
7.33
7.31
7.29
7.11
7.09
7.08
7.01
6.99
6.88
6.87
H
N
H
F
f1 (ppm)

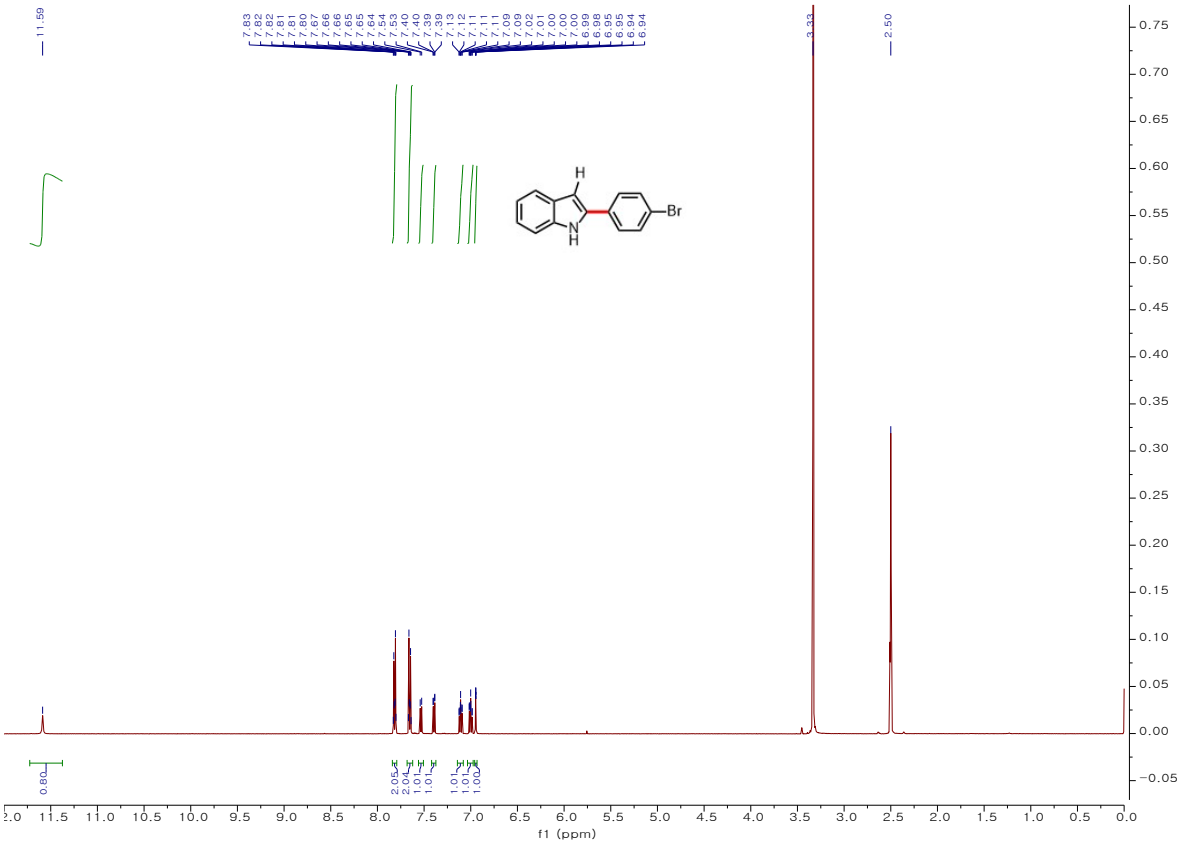

162.56
160.62
137.17
136.76
128.94
128.91
128.69
127.04
126.98
121.62
120.07
119.46
115.93
115.76
111.32
98.69
f1 (ppm)

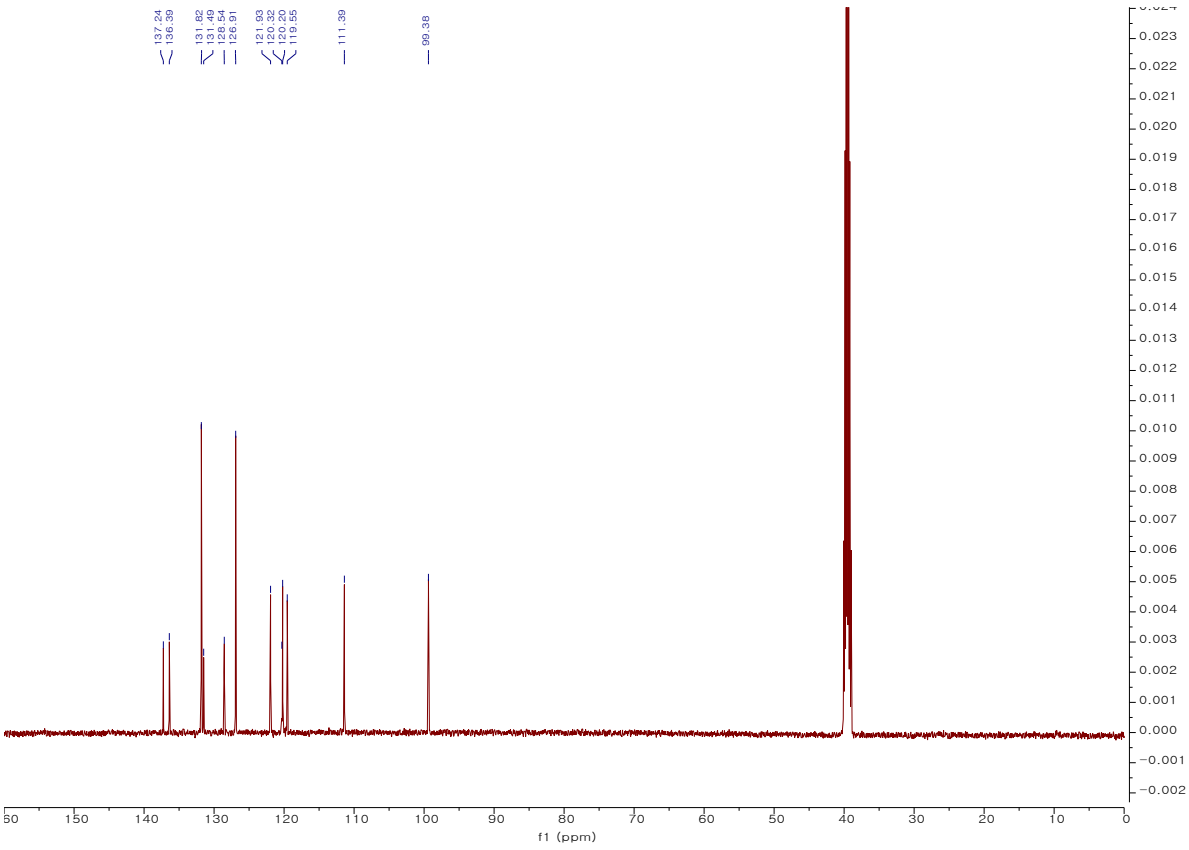

−114.51
50
45
40
35
30
25
20
15
10
5
0
100
80
60
40
20
0
−20
−40
−60
−80
−100
−120
−140
−160
−180
−200
−220
−240
−260
−280
−300
f1 (ppm)

2-(4-Chlorophenyl)-1*H*-indole (3ae);

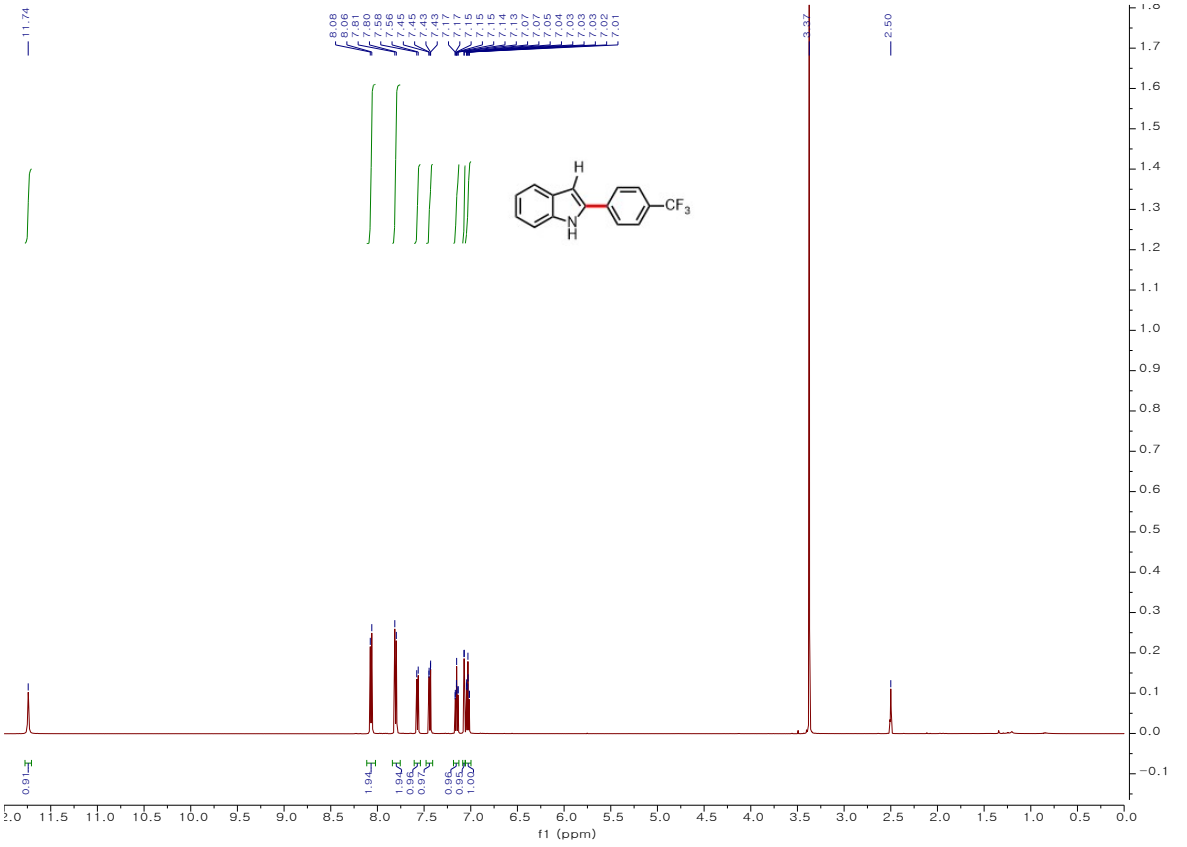


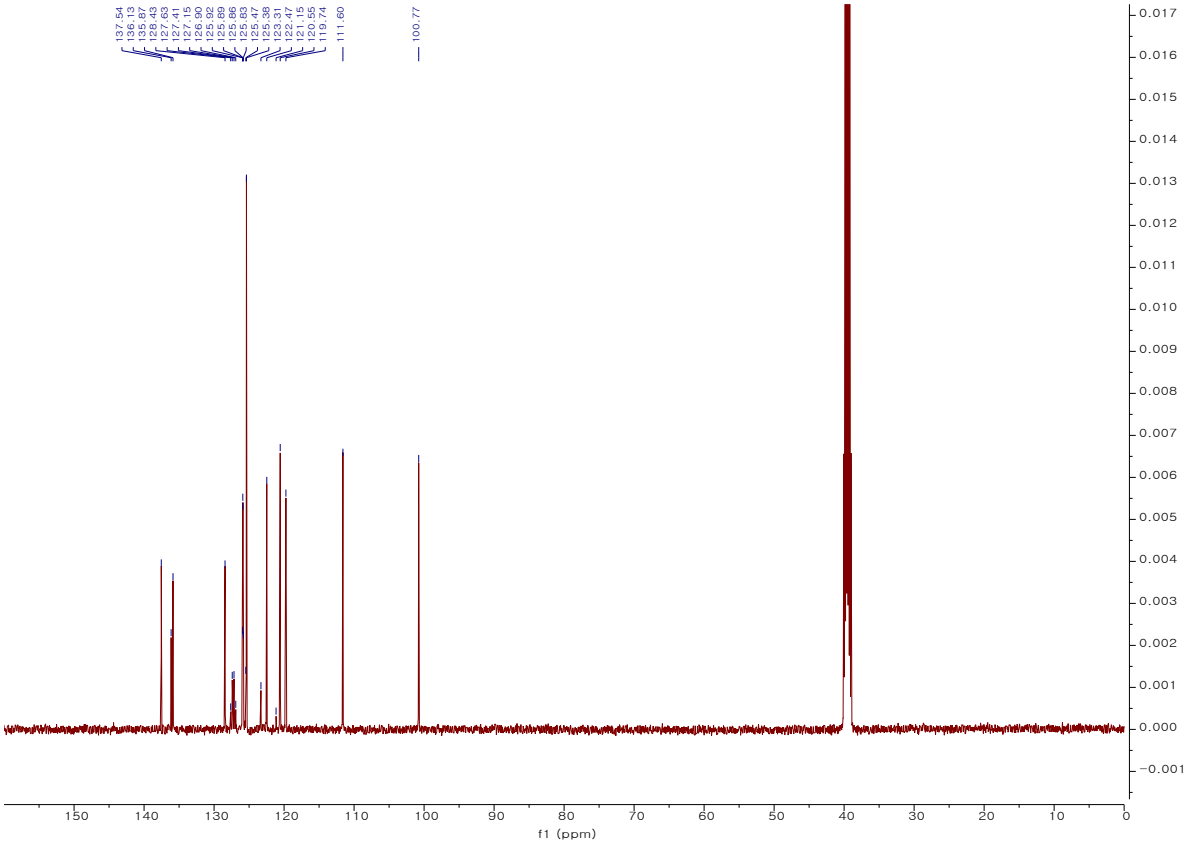
2-(4-Bromophenyl)-1*H*-indole (3af);

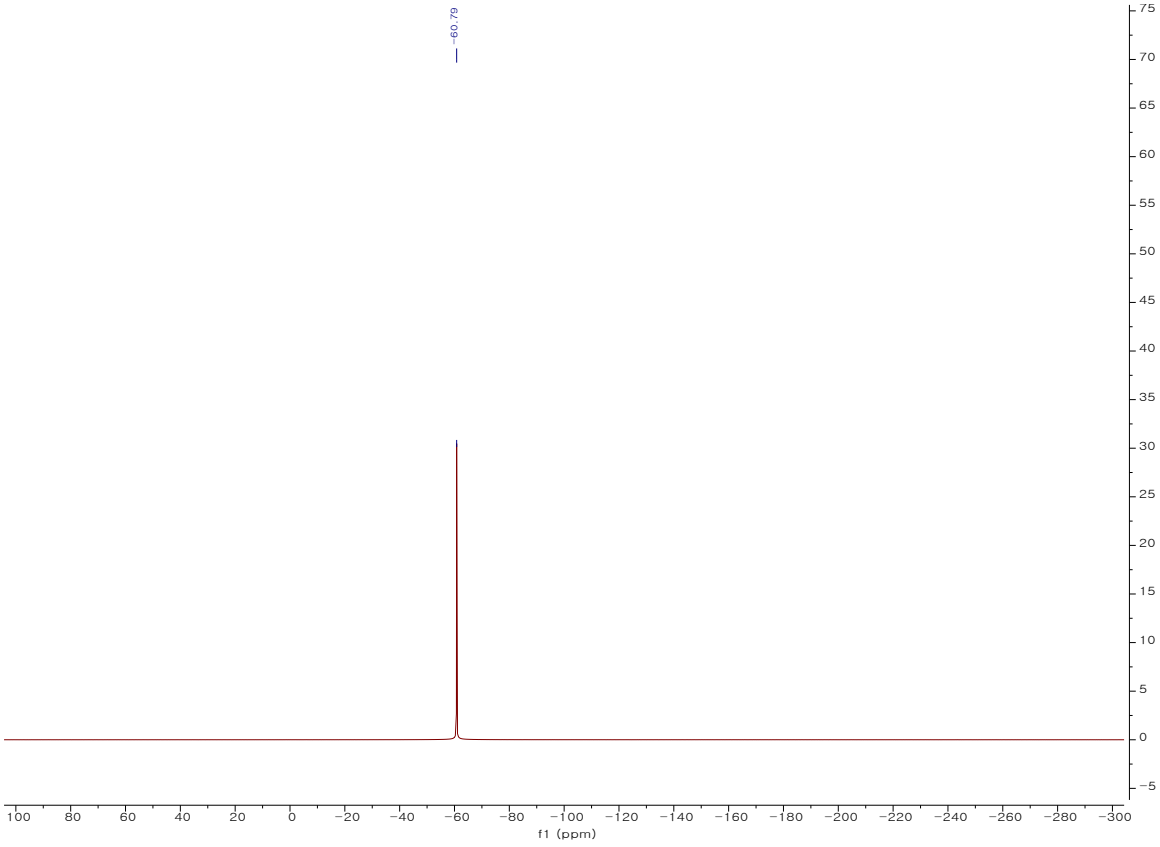




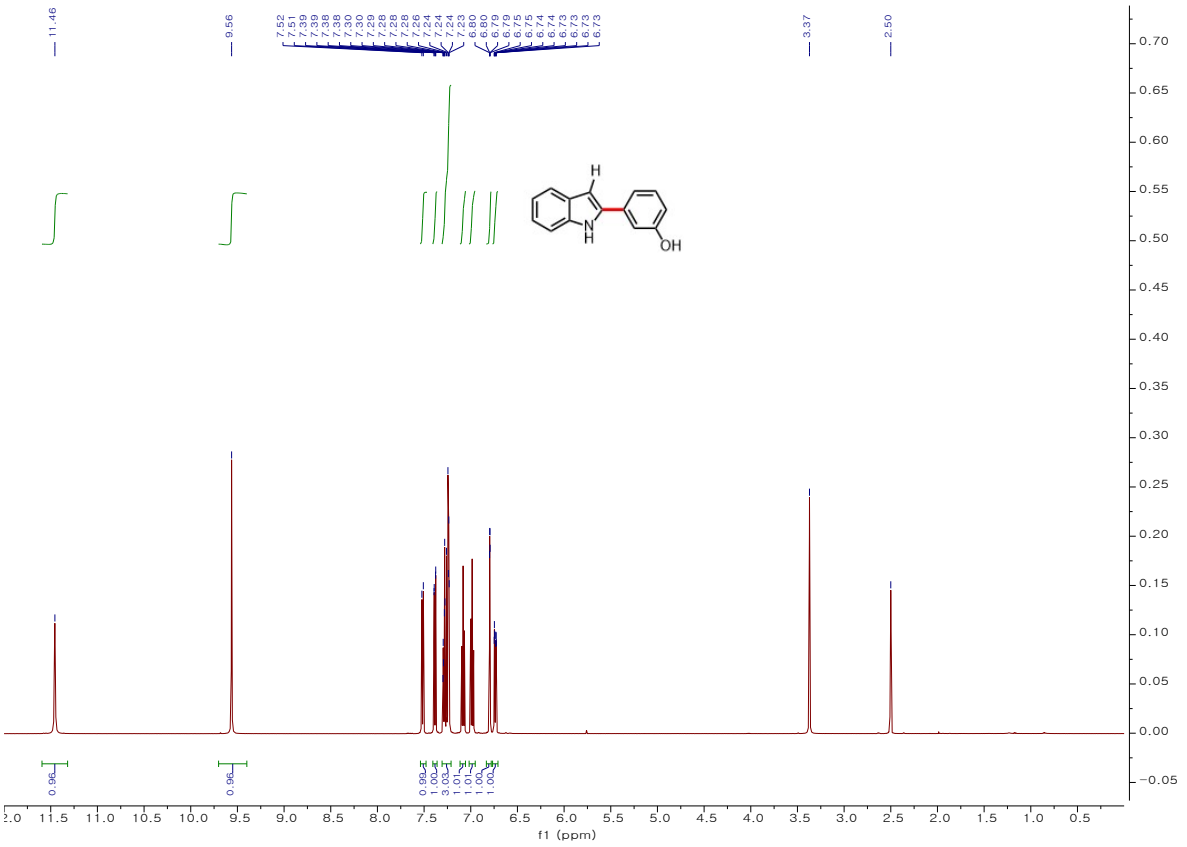
2-(4-(Trifluoromethyl)phenyl)-1*H*-indole (3ag);

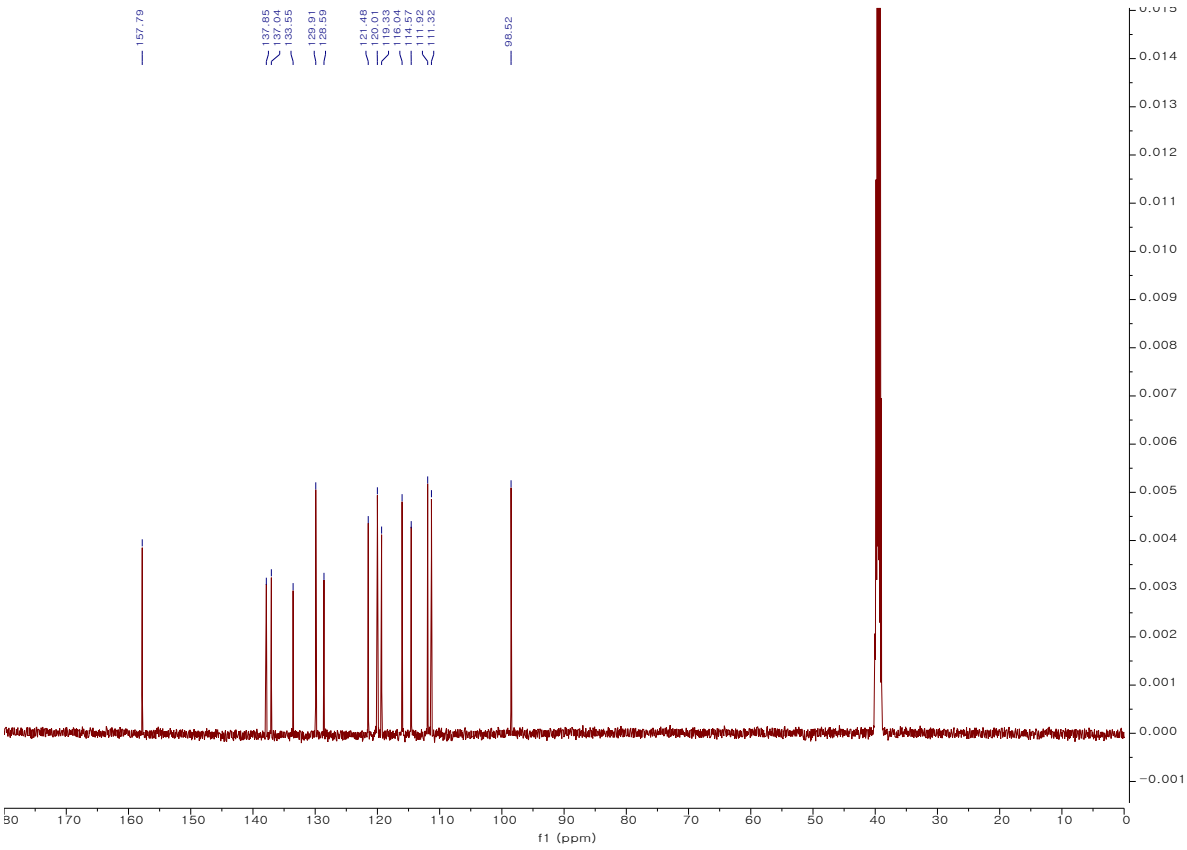

11.74
8.08
8.06
7.81
7.80
7.58
7.56
7.45
7.45
7.43
7.43
7.17
7.17
7.15
7.15
7.14
7.13
7.07
7.07
7.05
7.04
7.03
7.03
7.03
7.02
7.01
3.37
2.50
H
N
H
CF3
0.91
1.94
1.94
0.96
0.97
0.96
0.95
1.00
f1 (ppm)


137.54
136.13
135.87
128.43
127.63
127.41
127.15
126.90
125.92
125.89
125.86
125.83
125.47
125.38
123.31
121.47
121.15
120.55
119.74
111.60
100.77
f1 (ppm)

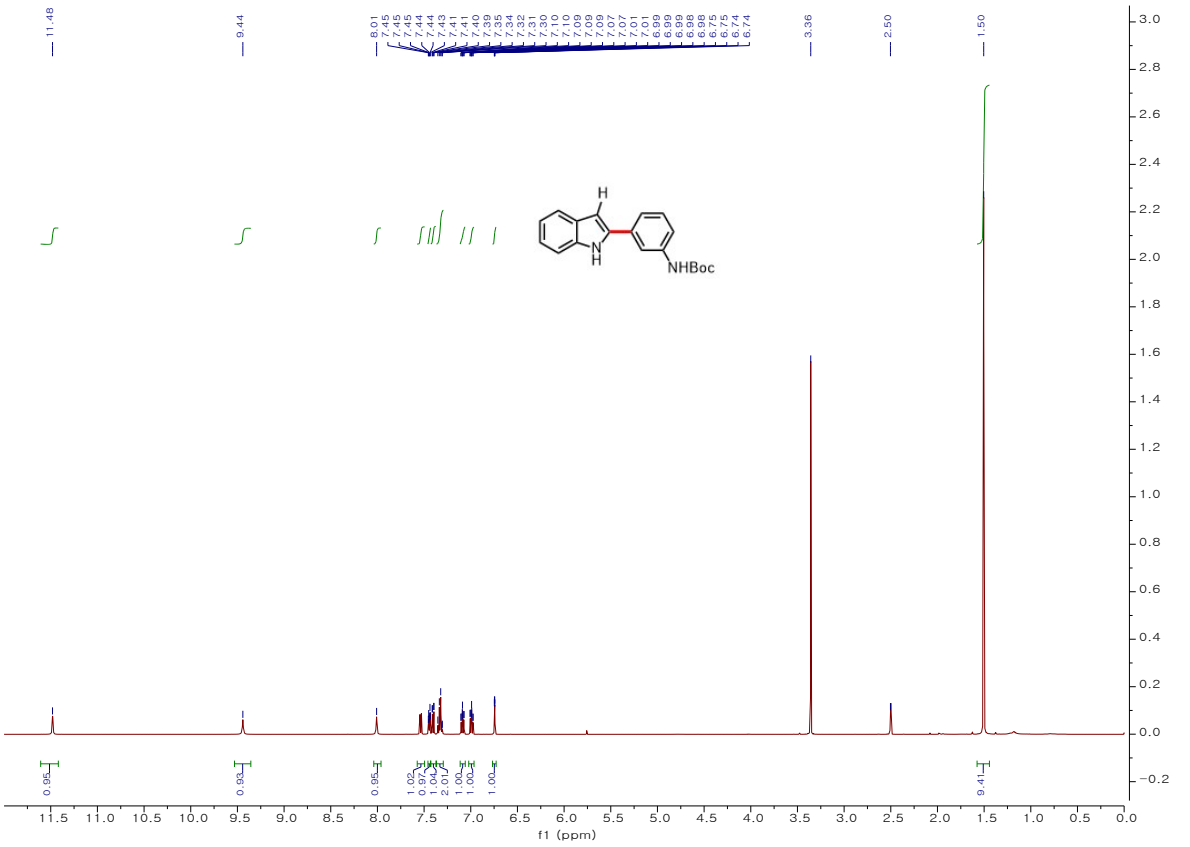

−60.79
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
−5
100
80
60
40
20
0
−20
−40
−60
−80
−100
−120
−140
−160
−180
−200
−220
−240
−260
−280
−300
f1 (ppm)

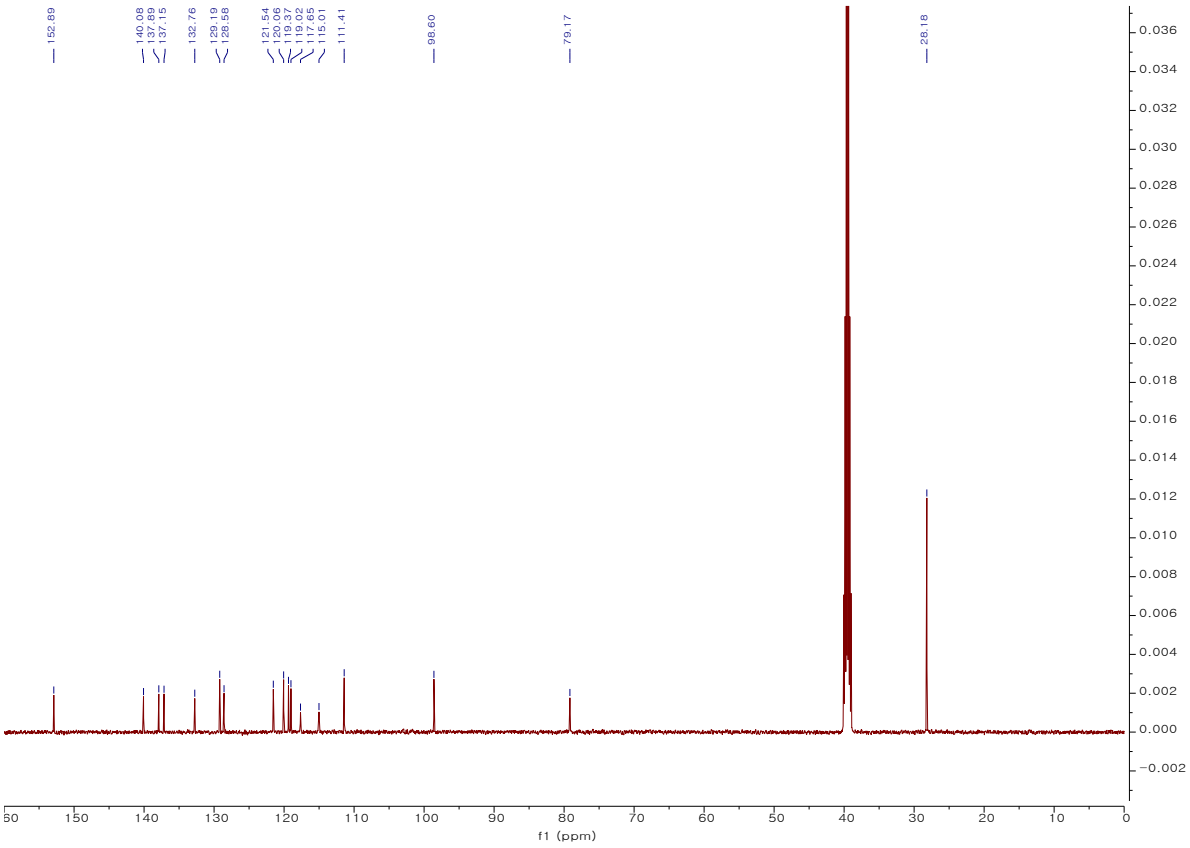
3-(1*H*-Indol-2-yl)phenol (3ah);



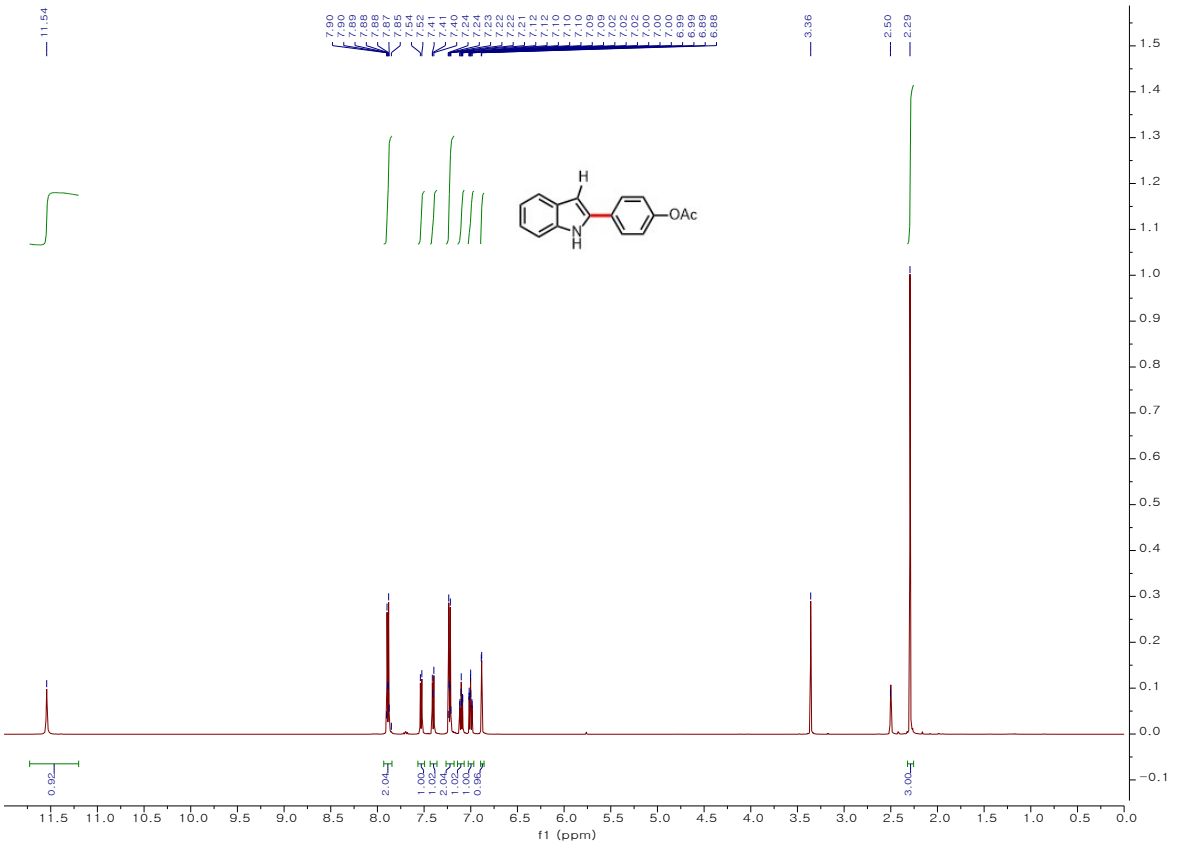


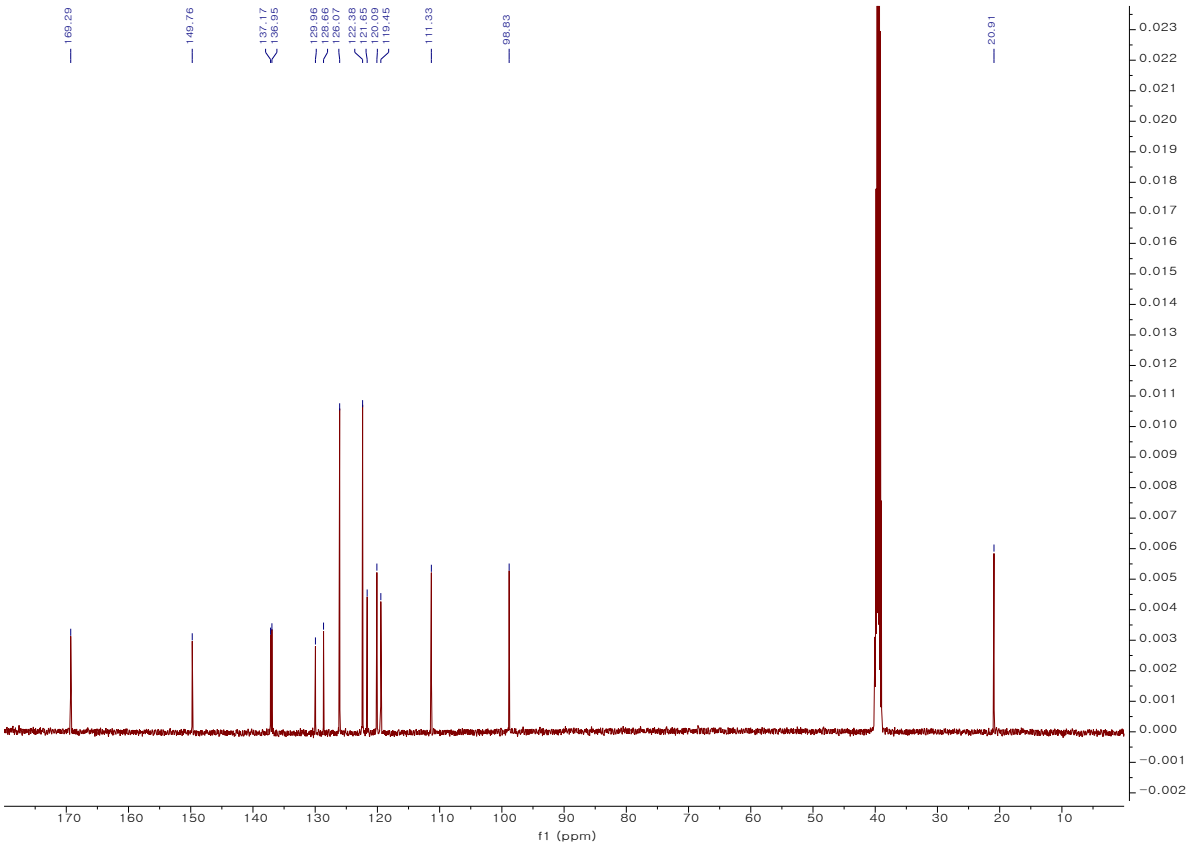
***tert*-Butyl (3-(1*H*-indol-2-yl)phenyl)carbamate (3ai);**



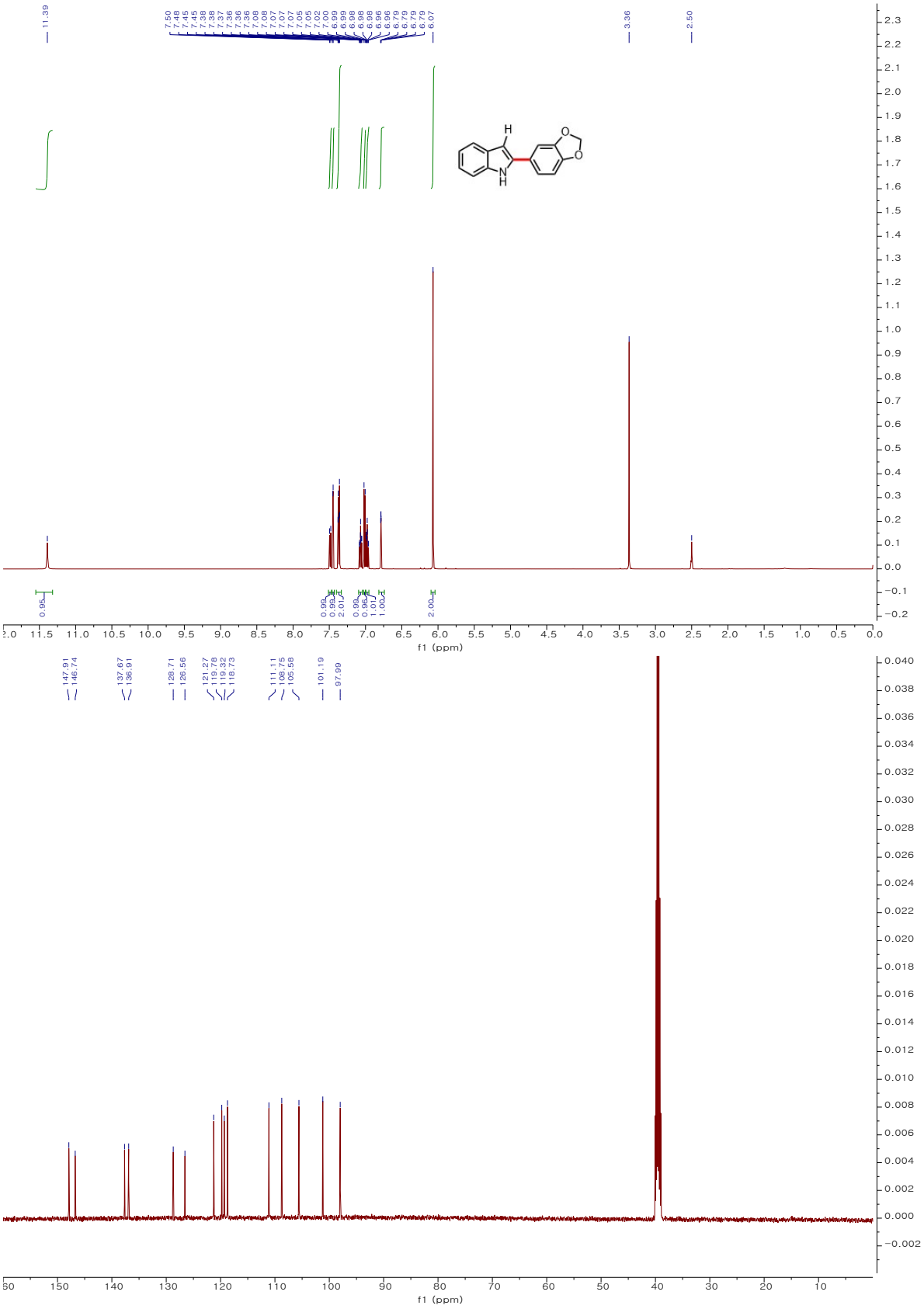


4-(1*H*-Indol-2-yl)phenyl acetate (3aj);

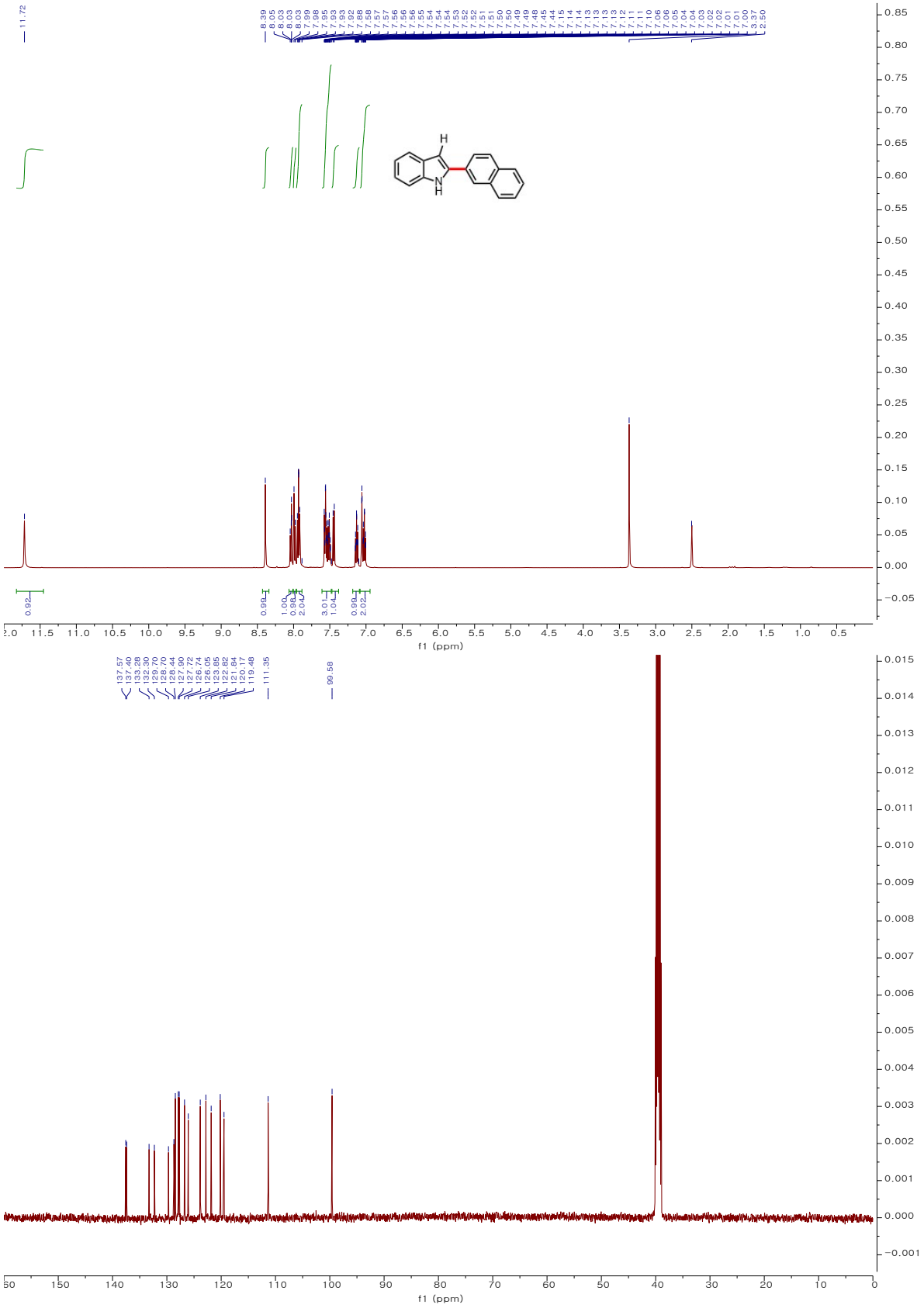




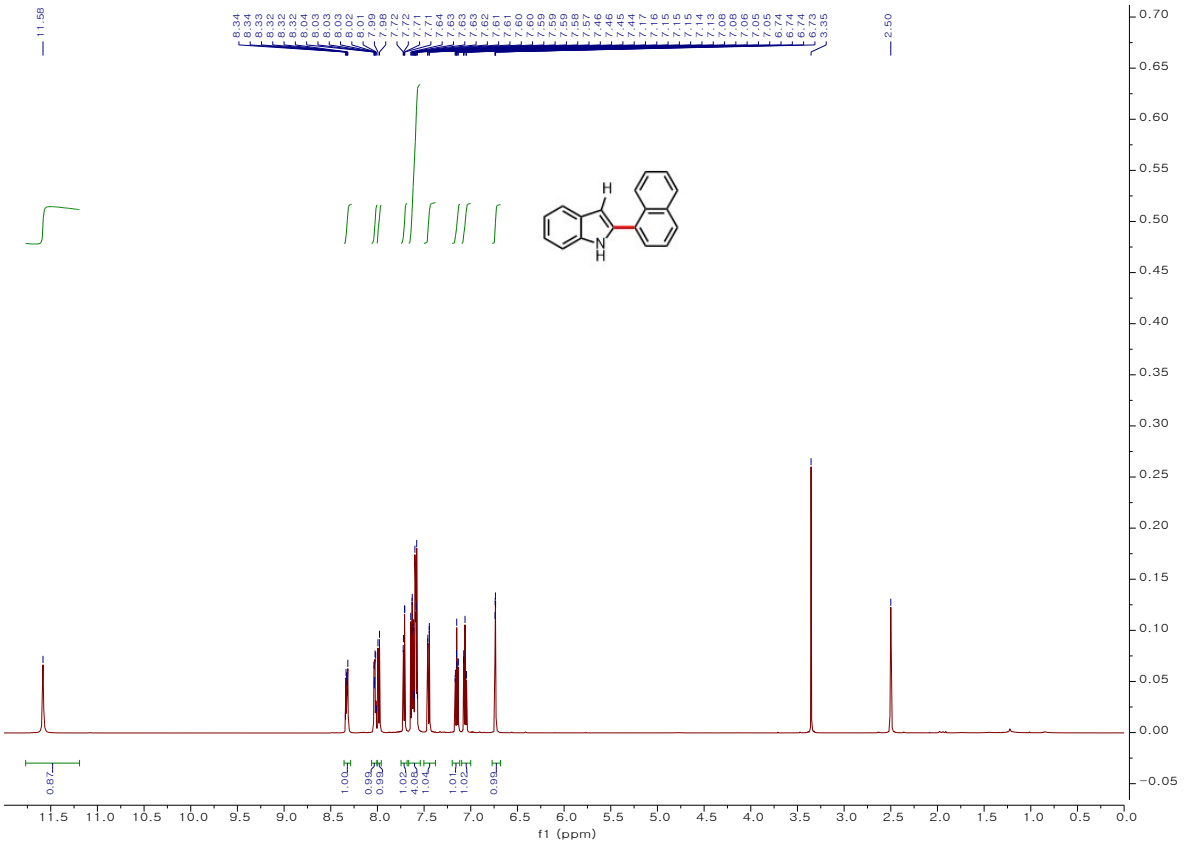
2-(Benzo[d][1,3]dioxol-5-yl)-1*H*-indole (3ak);

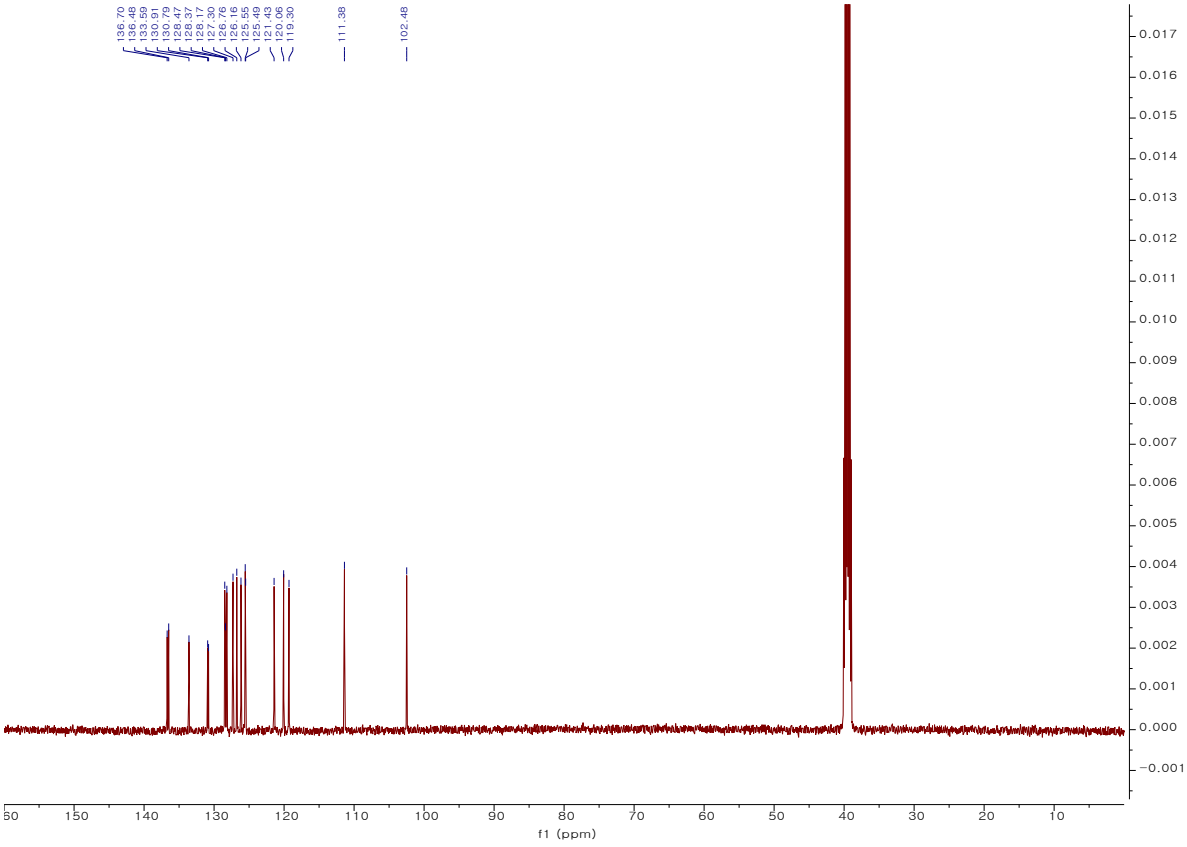


2-(Naphthalen-2-yl)-1*H*-indole (3al);

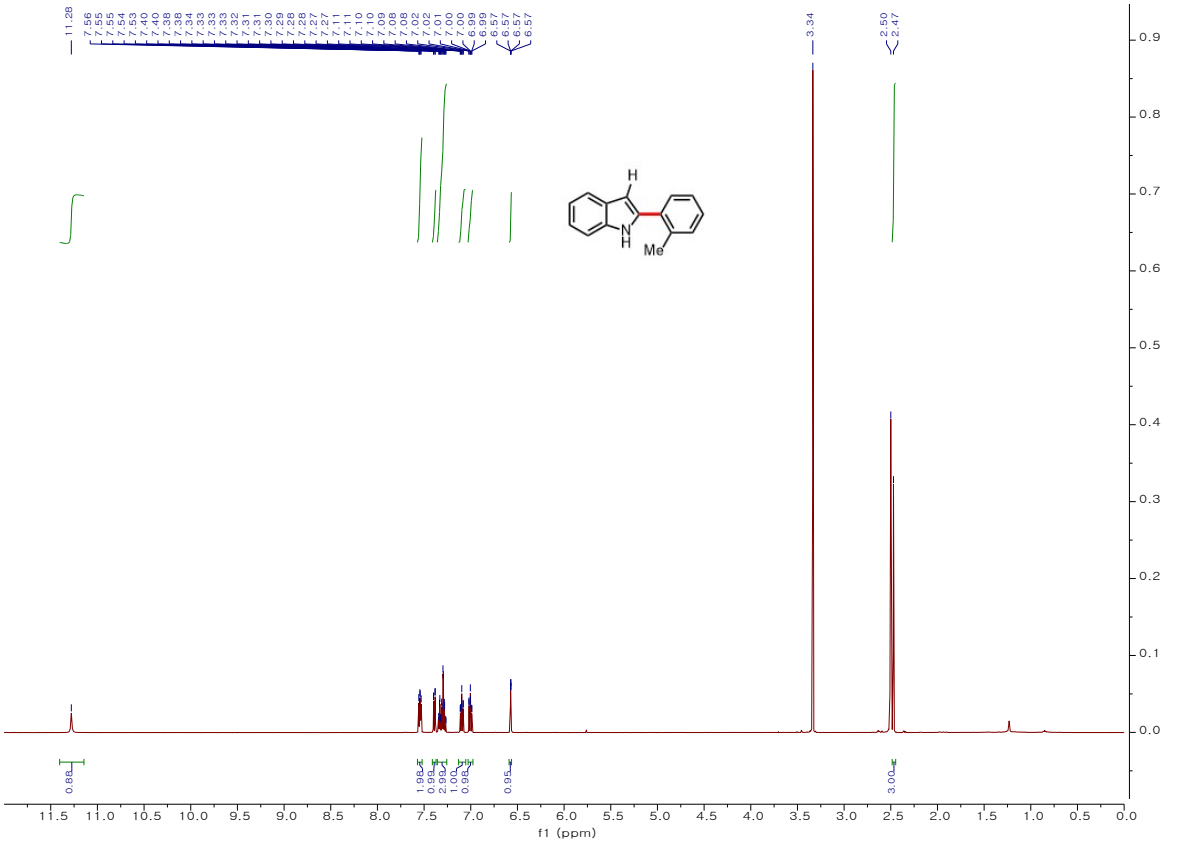


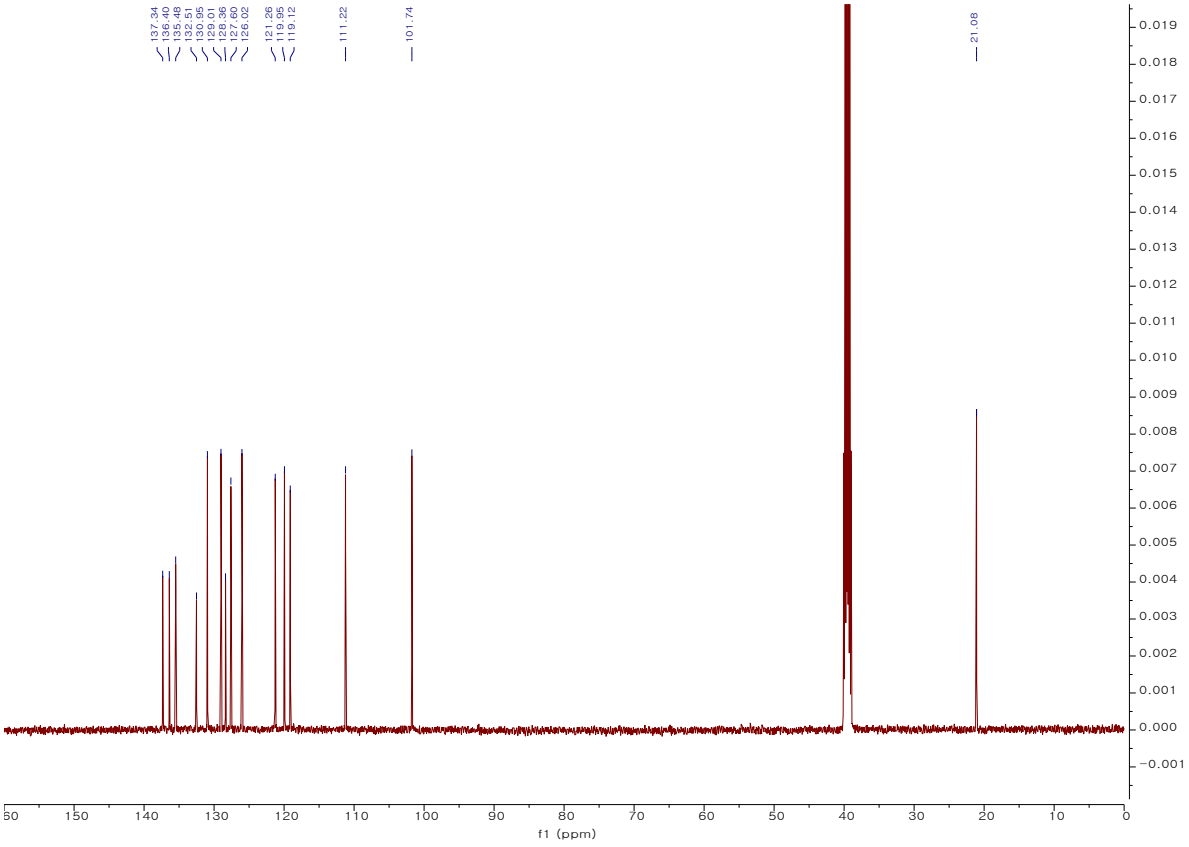
2-(Naphthalen-1-yl)-1*H*-indole (3am);



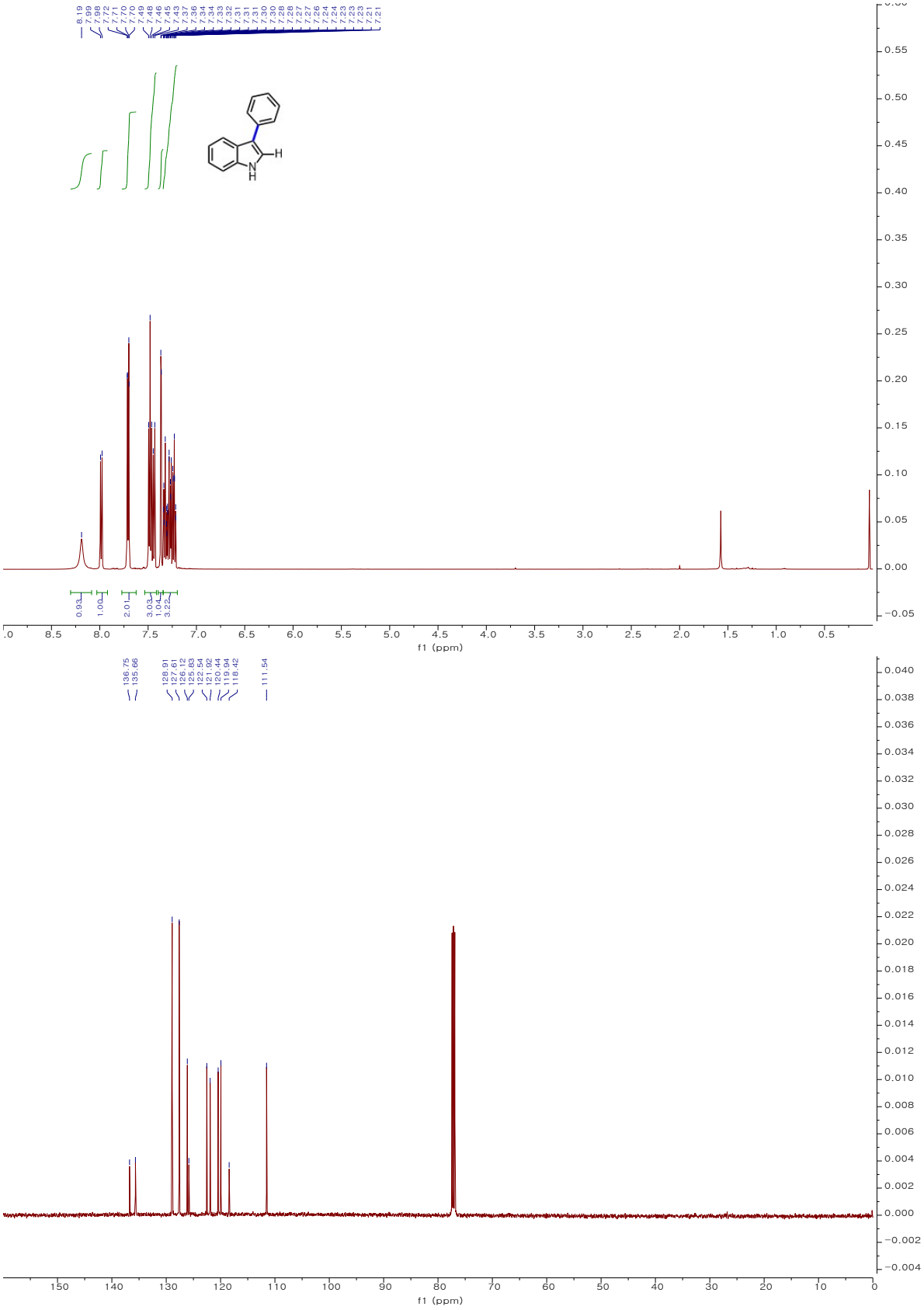


2-(*o*-Tolyl)-1*H*-indole (3an);

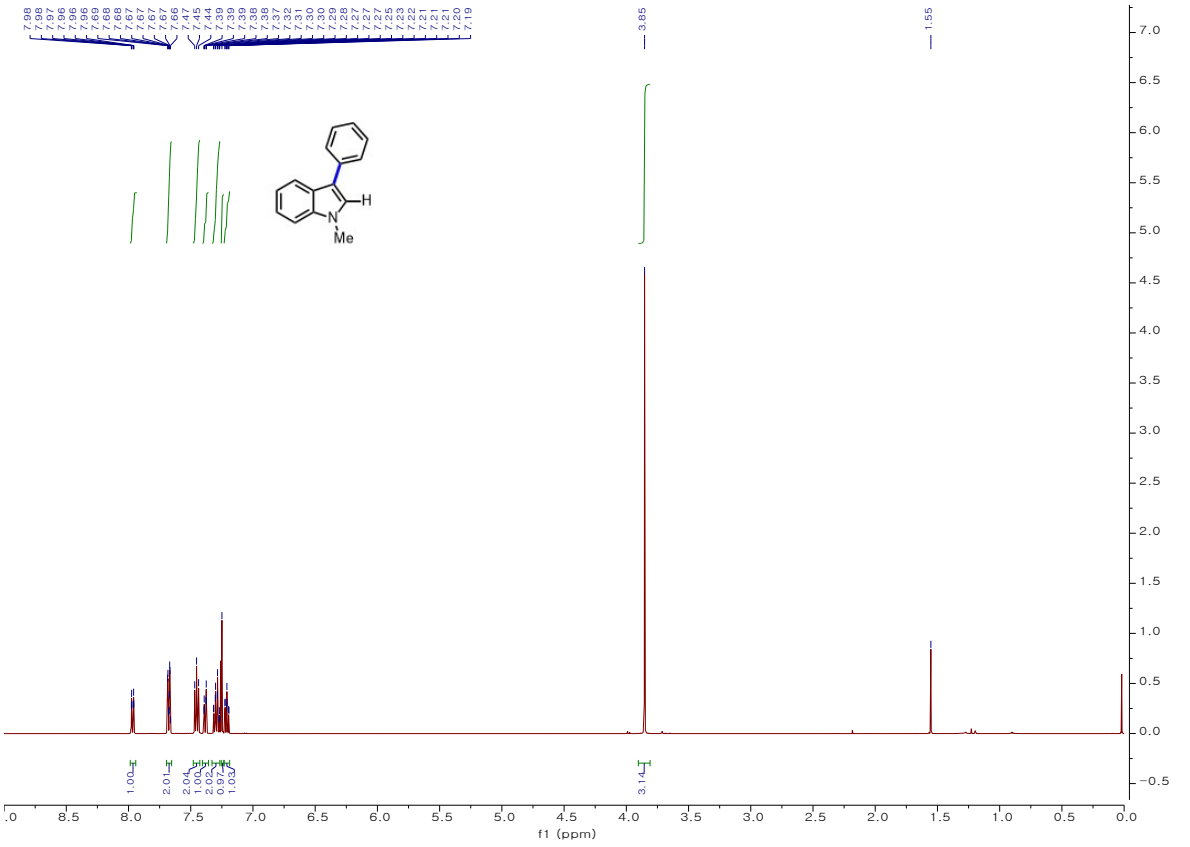


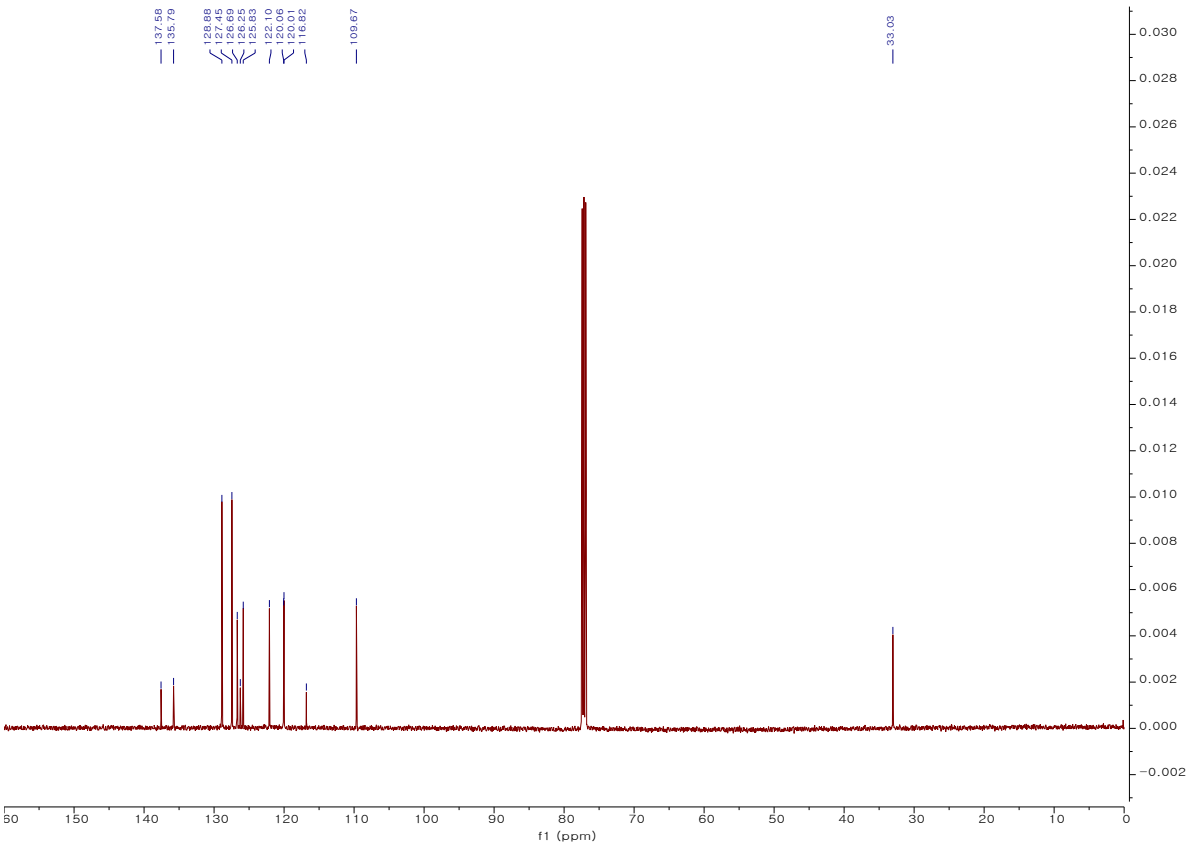


3-Phenyl-1*H*-indole (4aa);

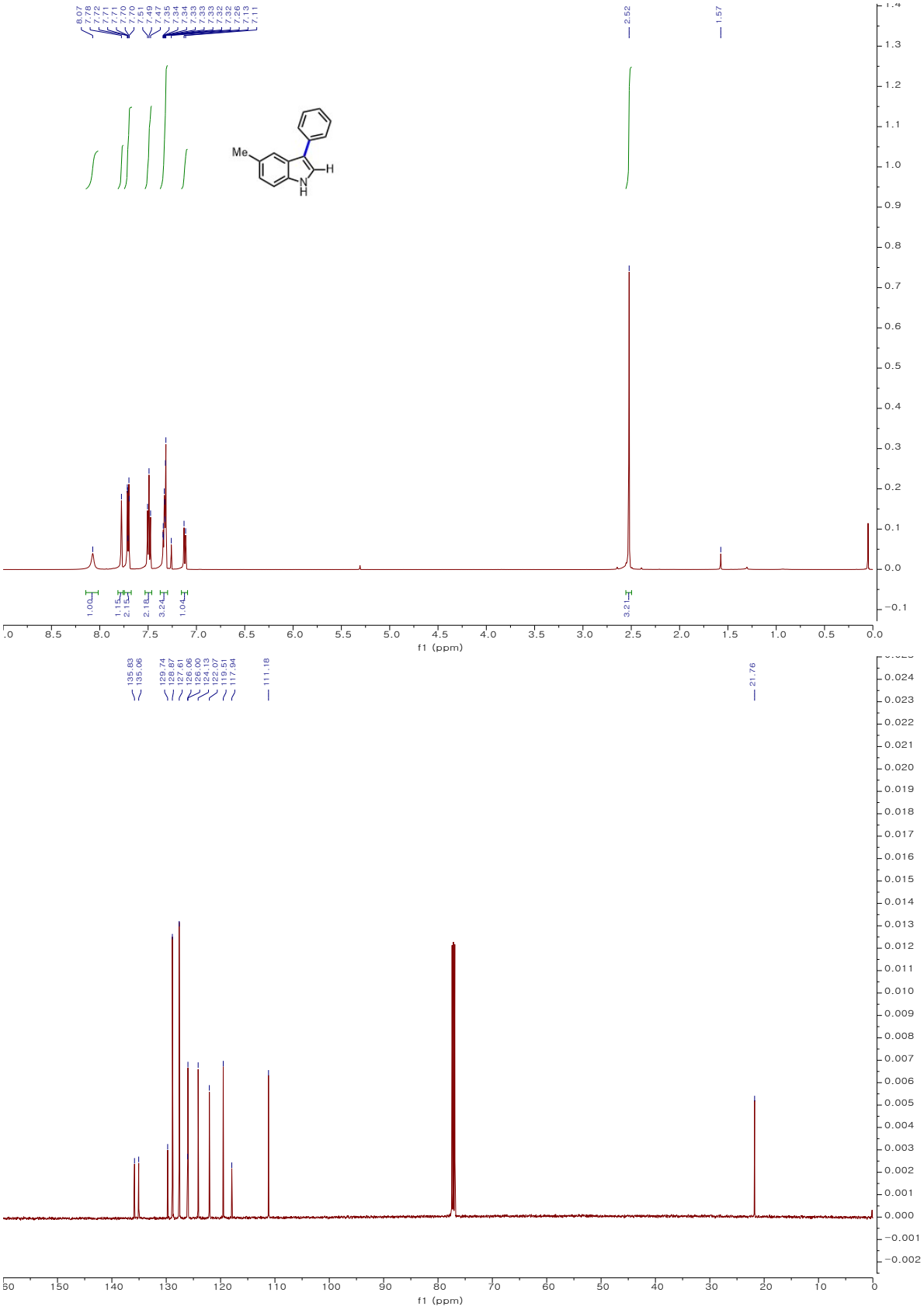


1-Methyl-3-phenyl-1*H*-indole (4ba);

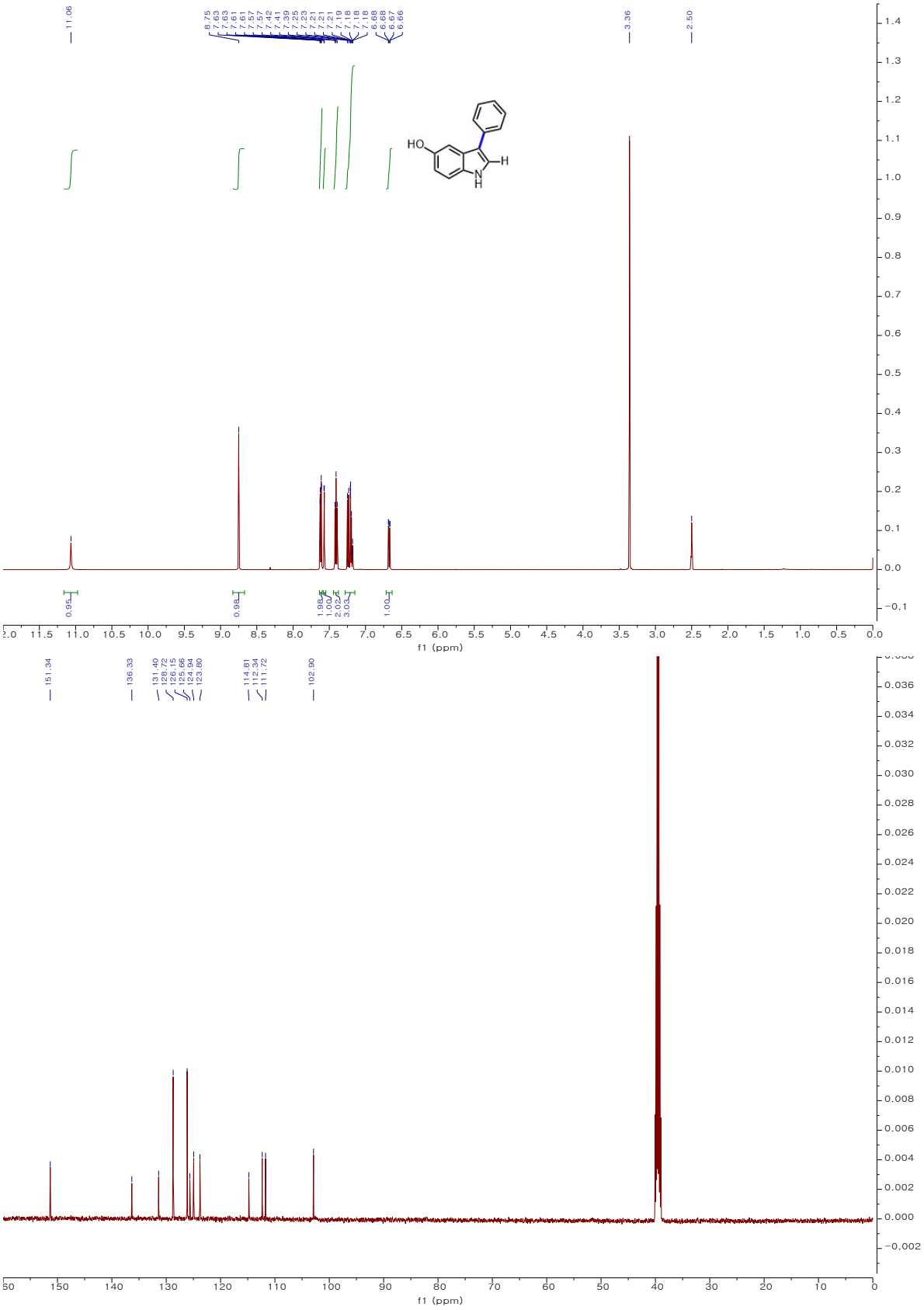




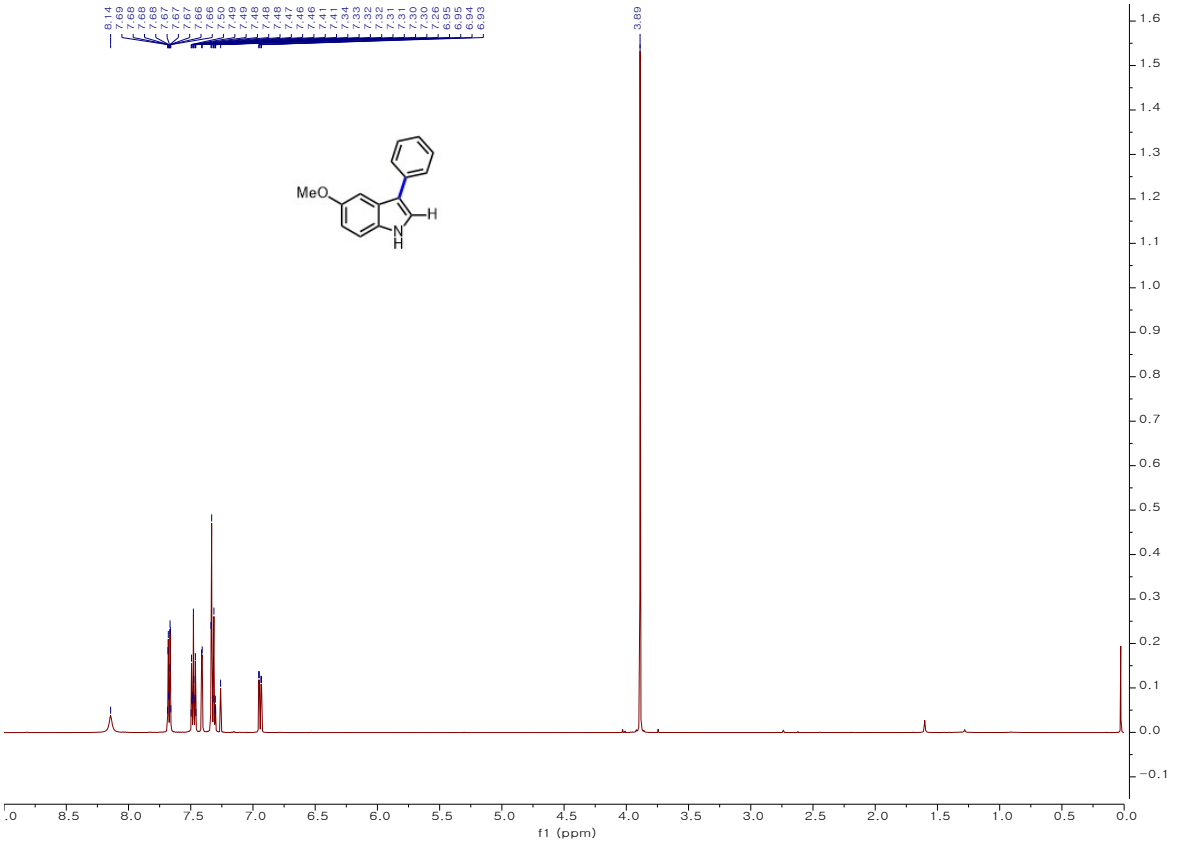
5-Methyl-3-phenyl-1*H*-indole (4da);

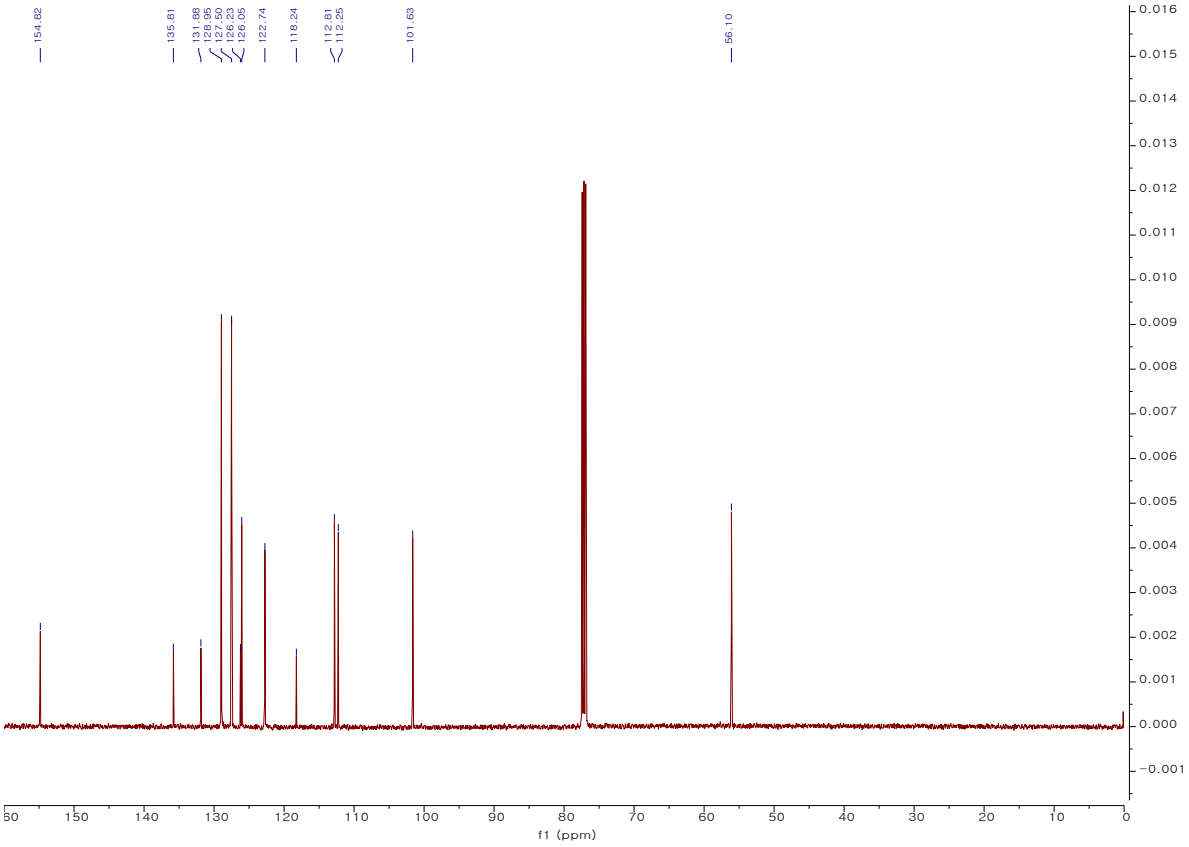


3-Phenyl-1*H*-indol-5-ol (4ea);

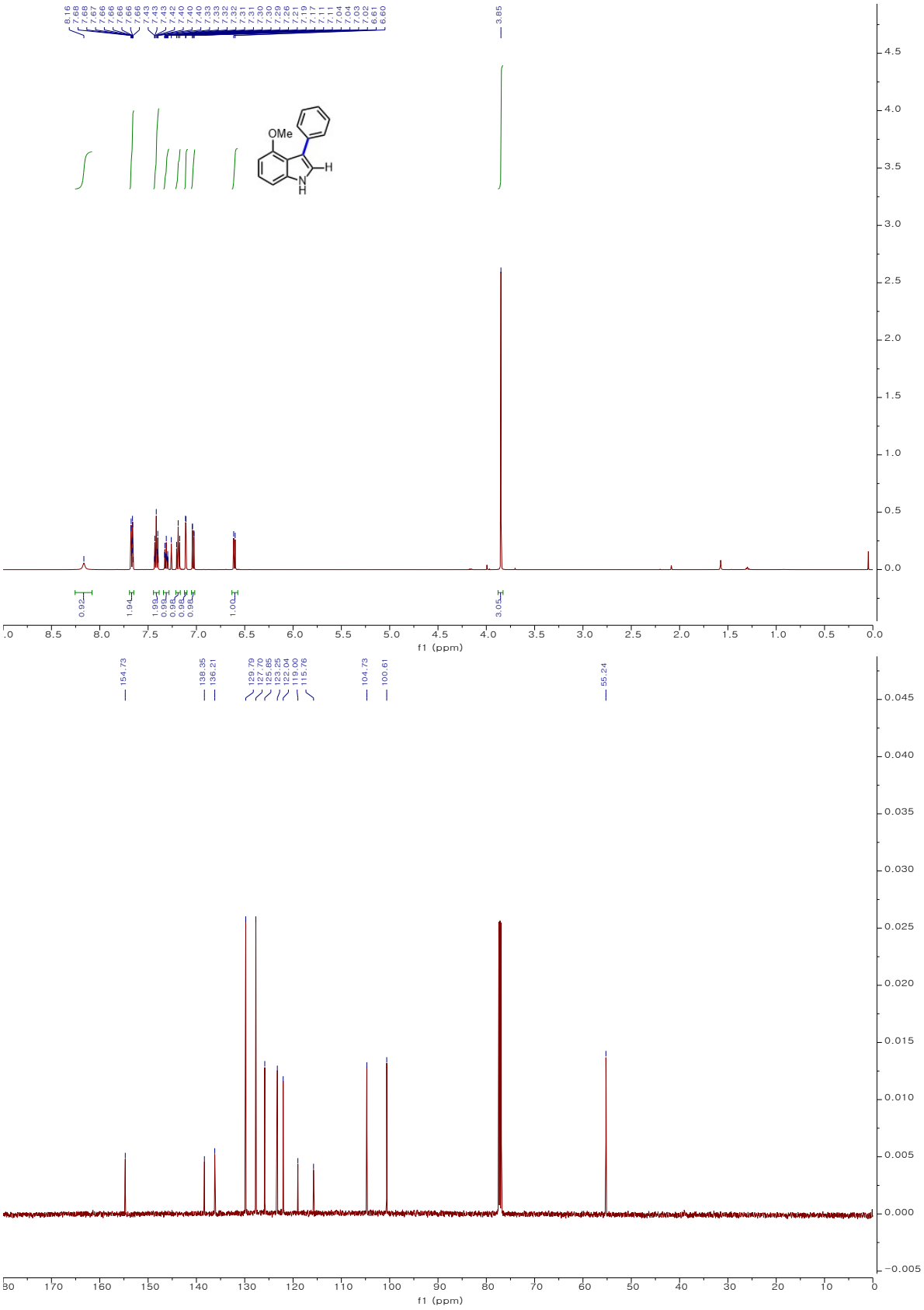


5-Methoxy-3-phenyl-1*H*-indole (4fa);

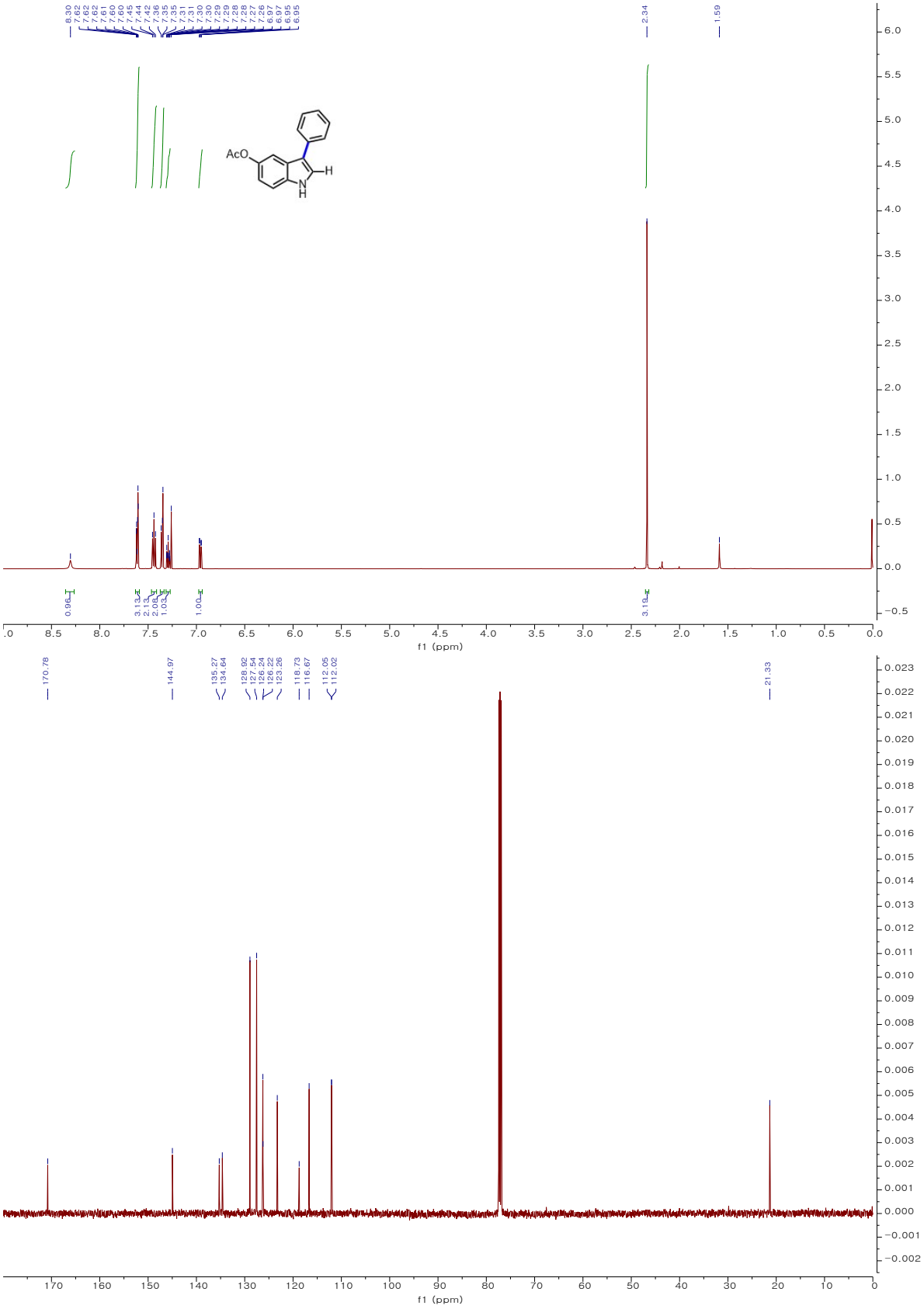




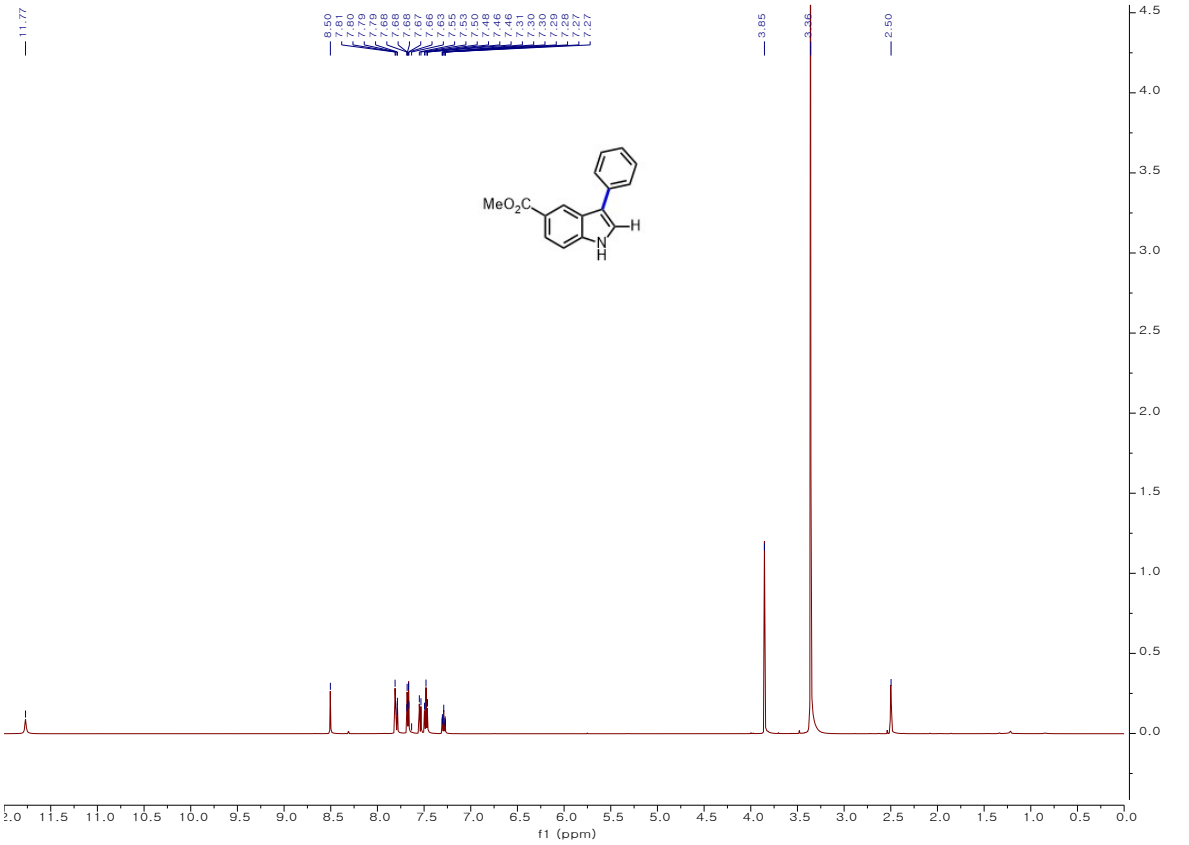
4-Methoxy-3-phenyl-1*H*-indole (4ga);

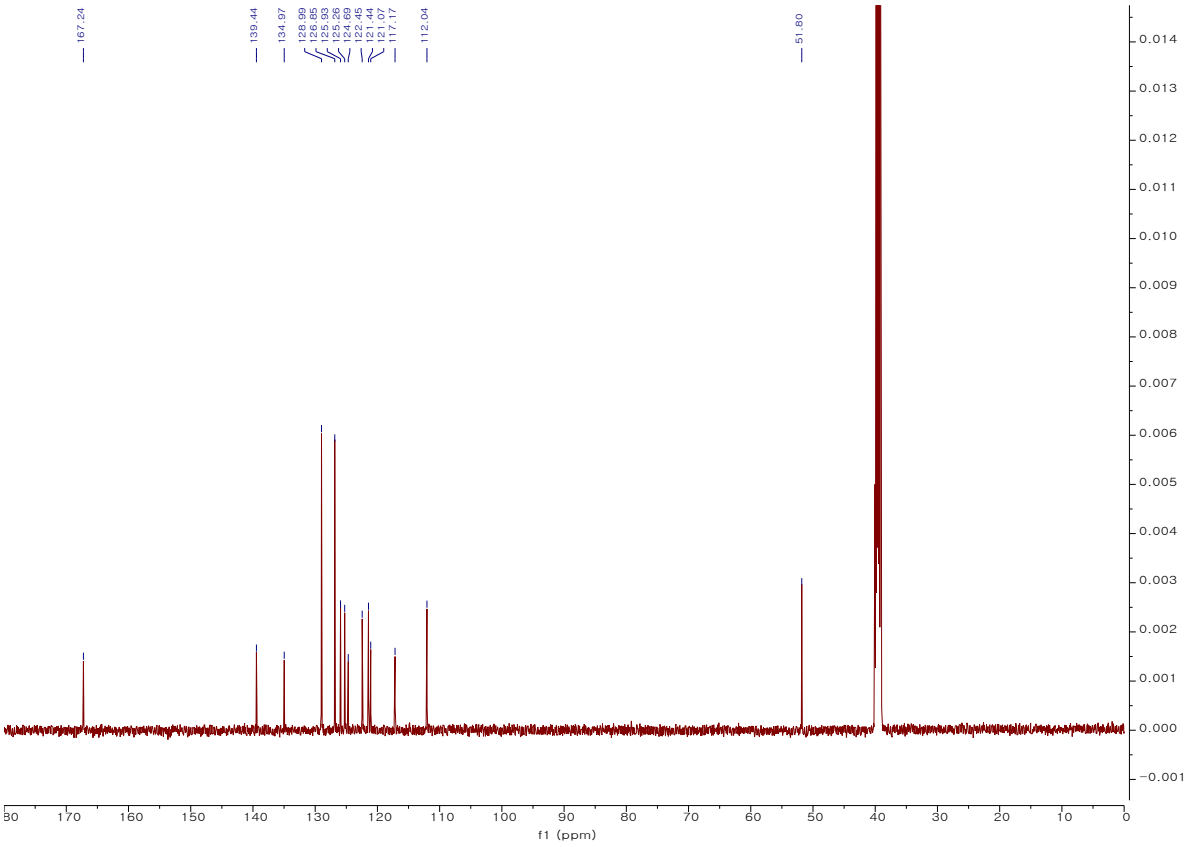


3-Phenyl-1*H*-indol-5-yl acetate (4ha);

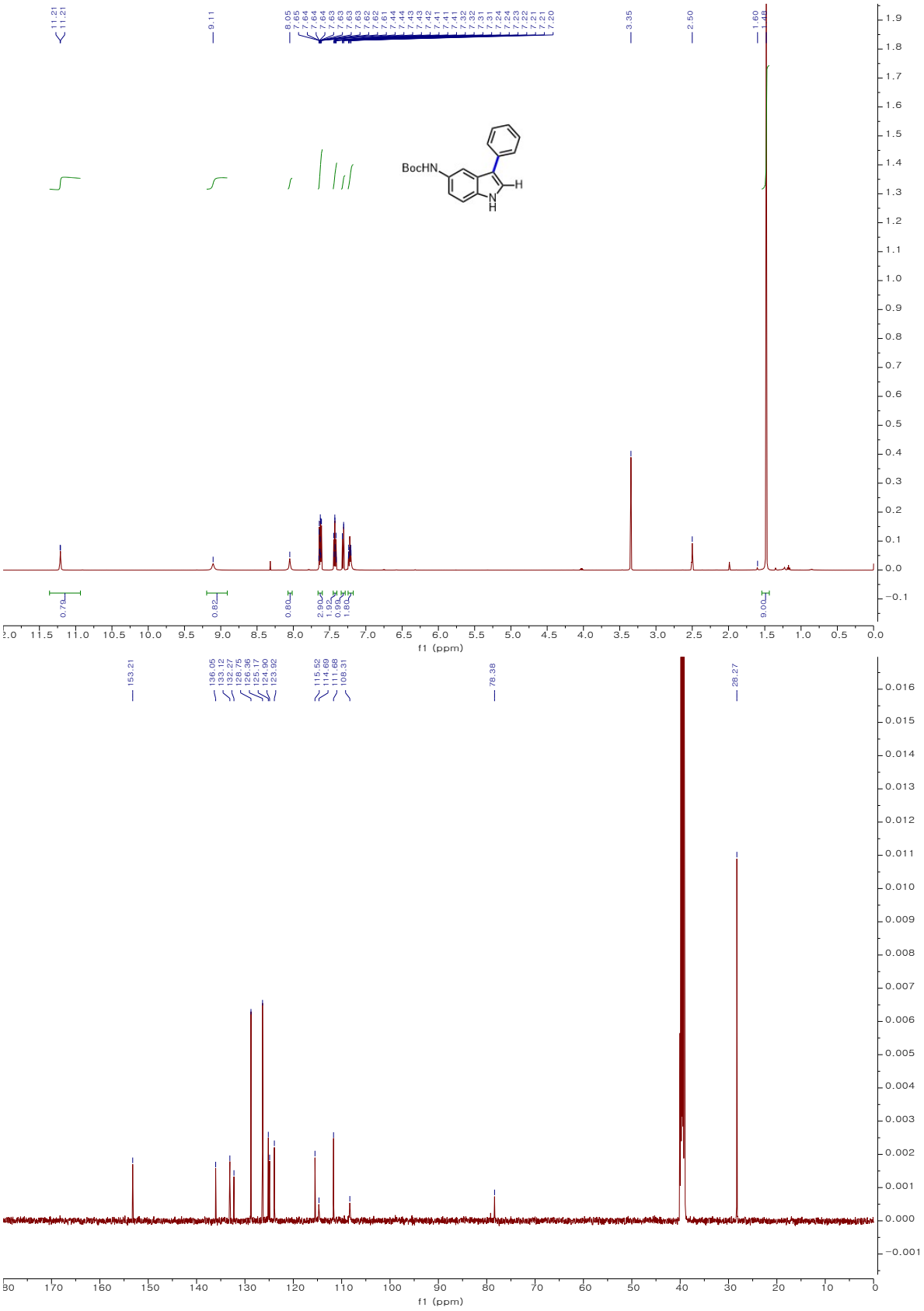


Methyl 3-phenyl-1*H*-indole-5-carboxylate (4ia);

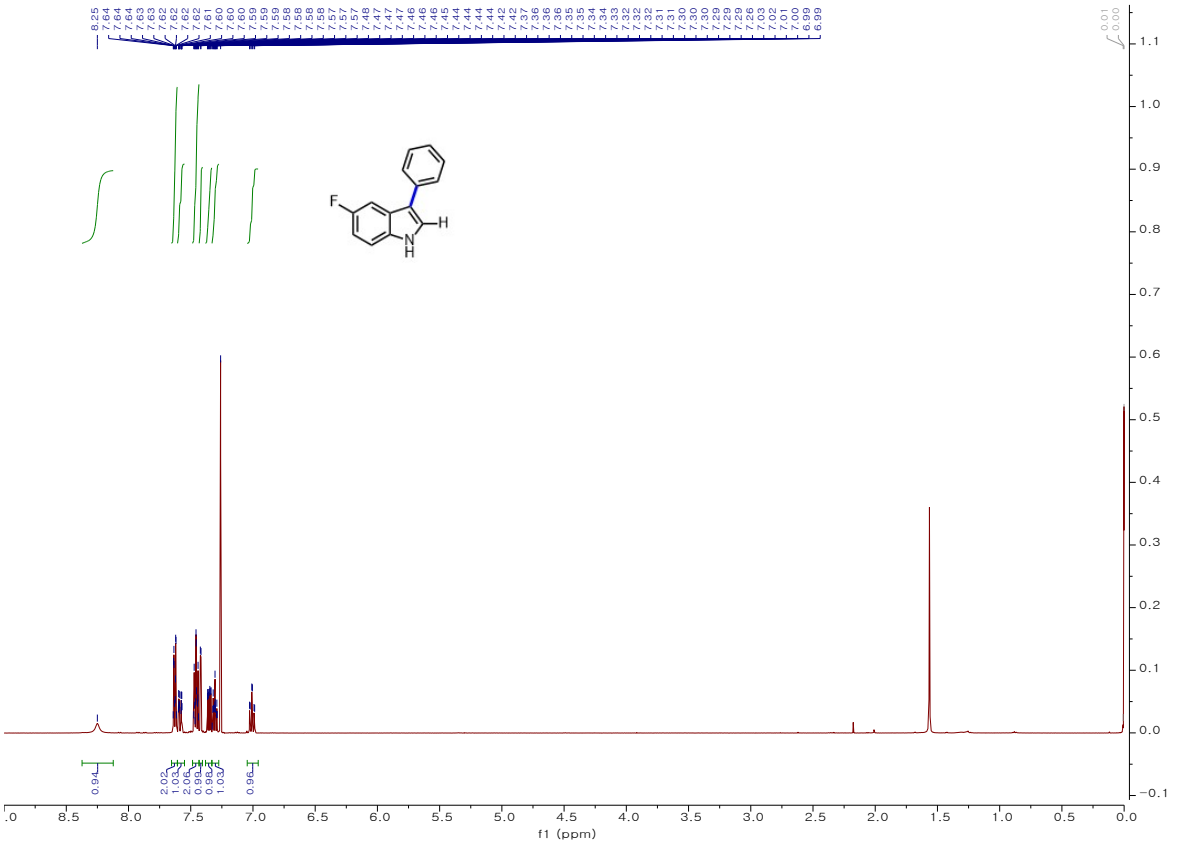


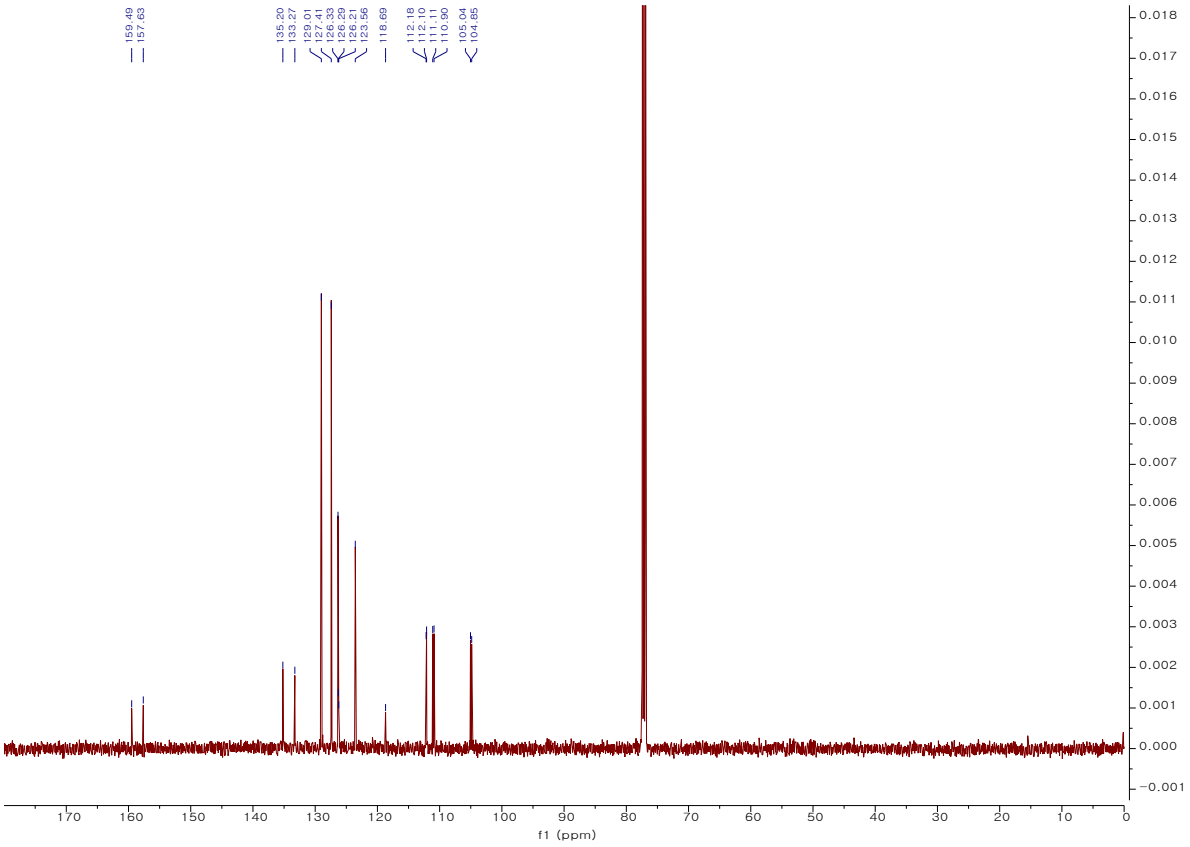


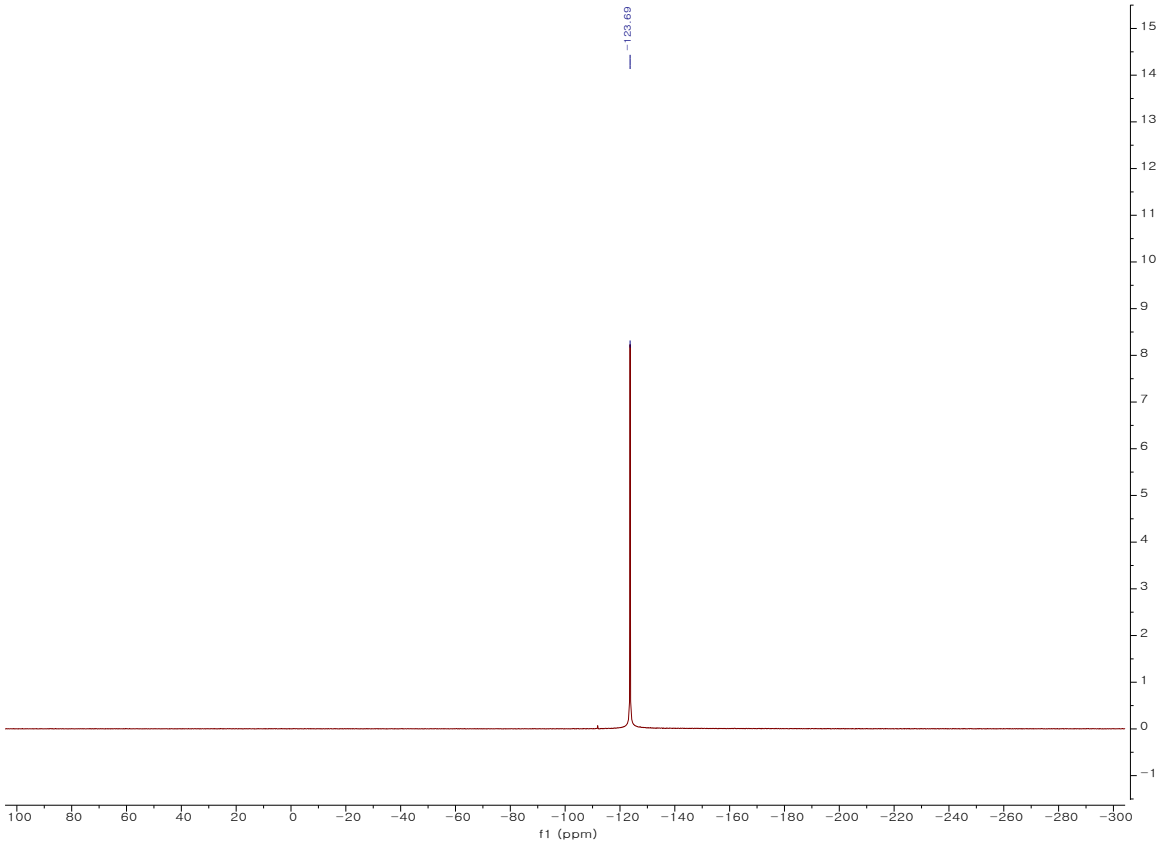
***tert*-Butyl (3-phenyl-1*H*-indol-5-yl)carbamate (4ja);**



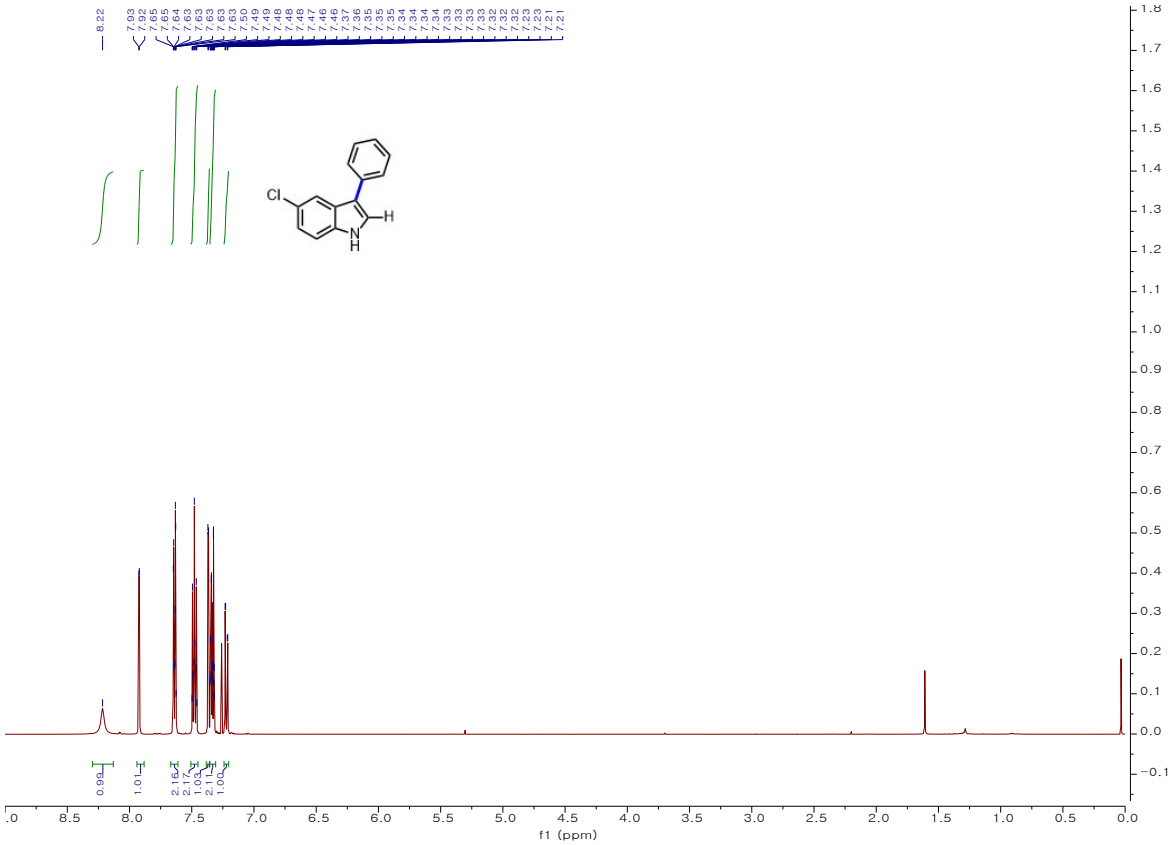
5-Fluoro-3-phenyl-1*H*-indole (4ka);

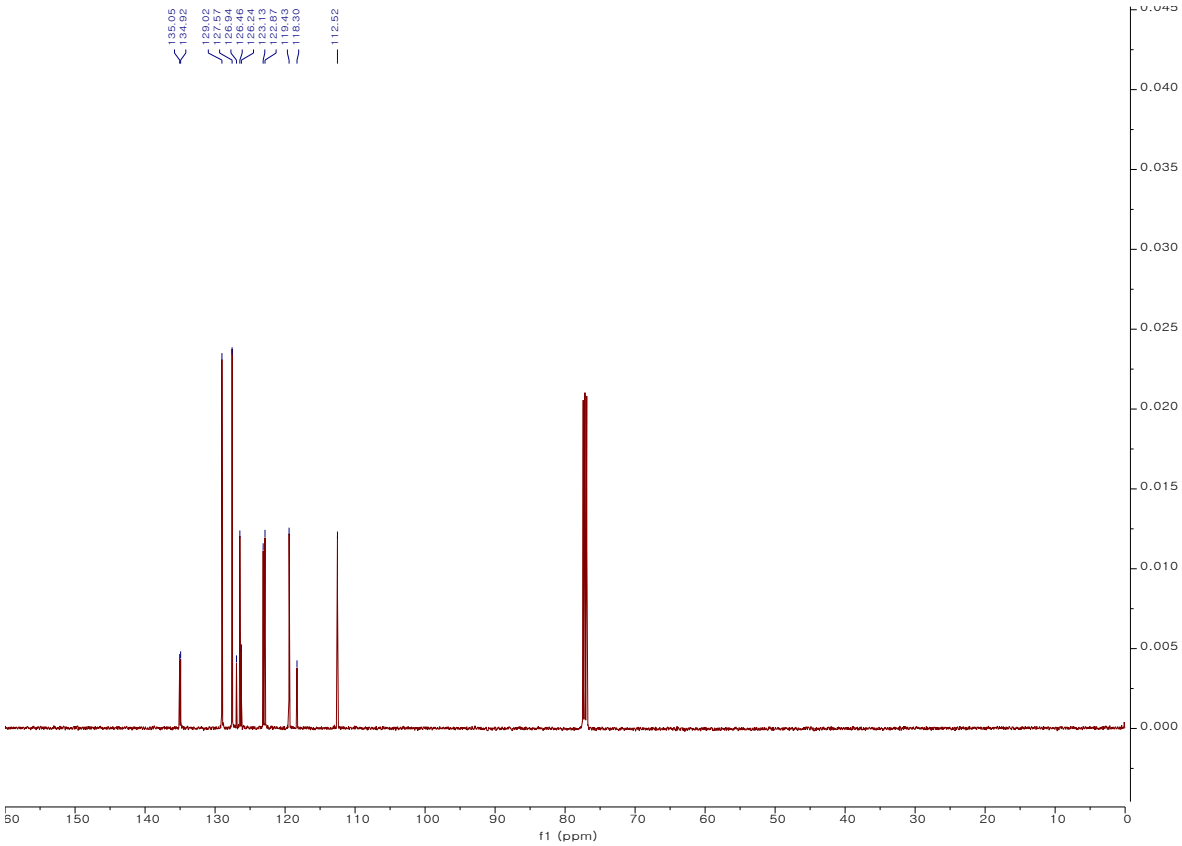

F
H
N
H
f1 (ppm)


159.49
157.63
135.20
133.27
129.01
127.41
125.83
125.29
123.56
118.69
112.18
112.10
111.11
110.90
105.04
104.85
f1 (ppm)

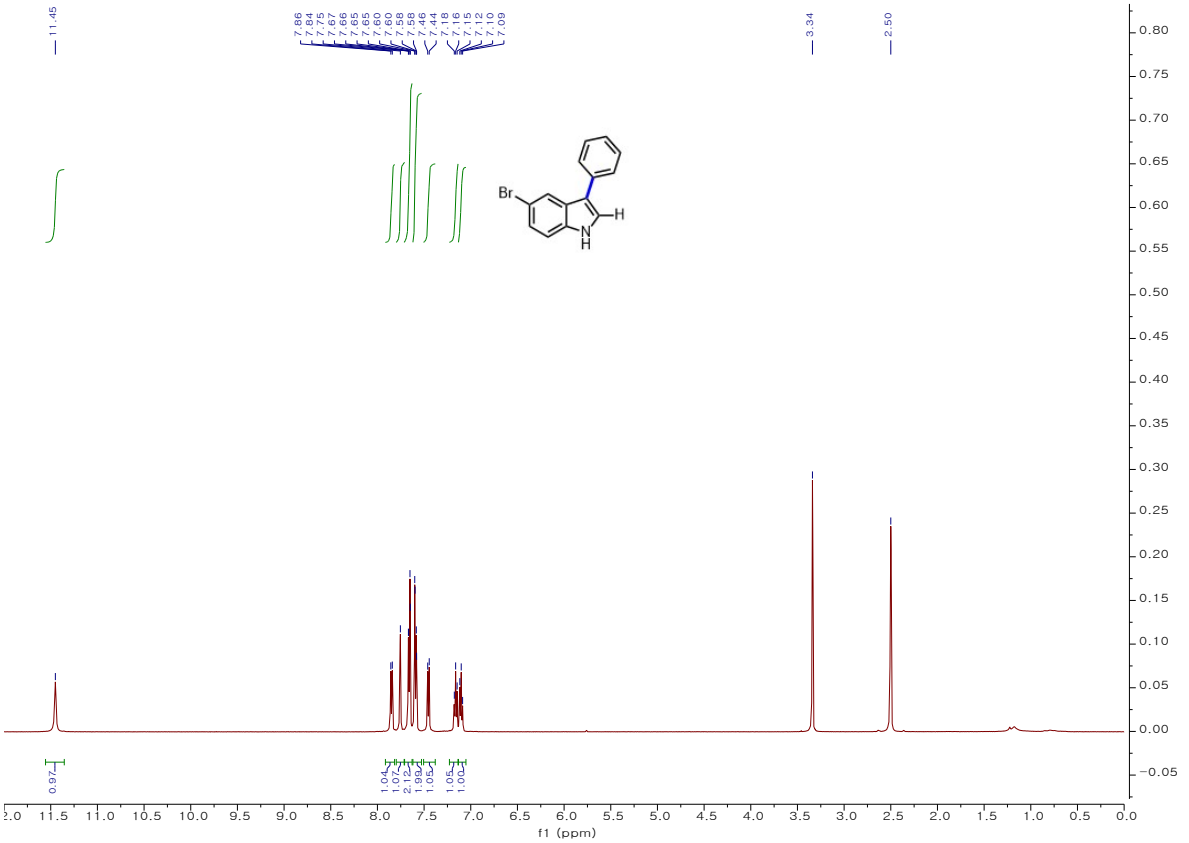

−123.69
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
100
80
60
40
20
0
−20
−40
−60
−80
−100
−120
−140
−160
−180
−200
−220
−240
−260
−280
−300
f1 (ppm)

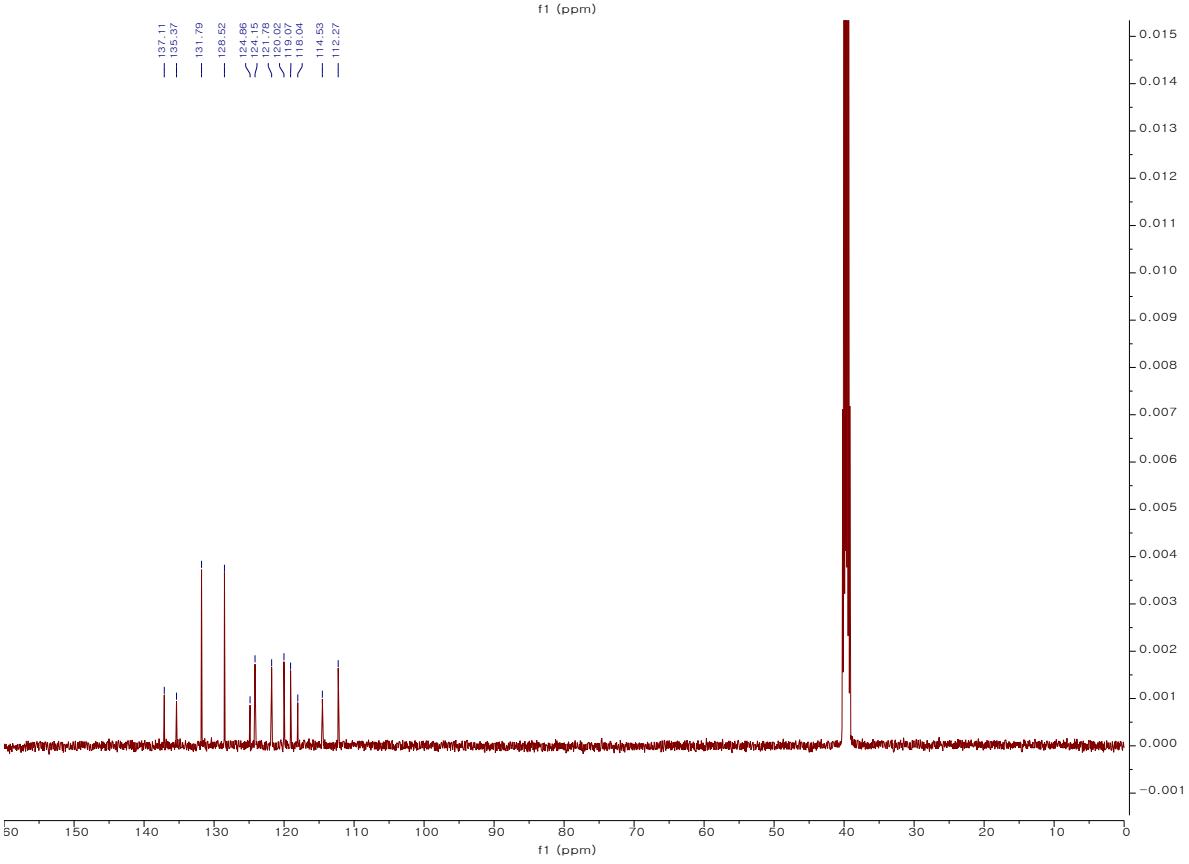
5-Chloro-3-phenyl-1*H*-indole (4la);



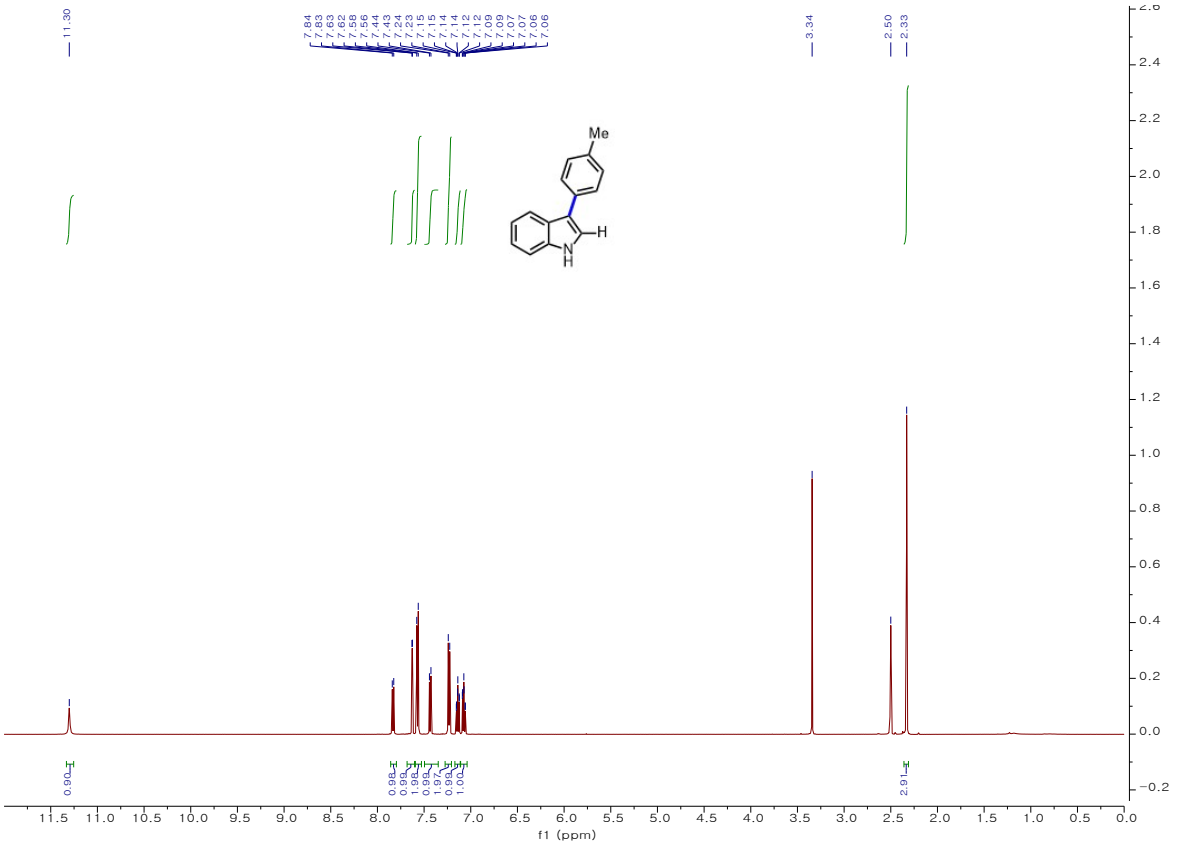


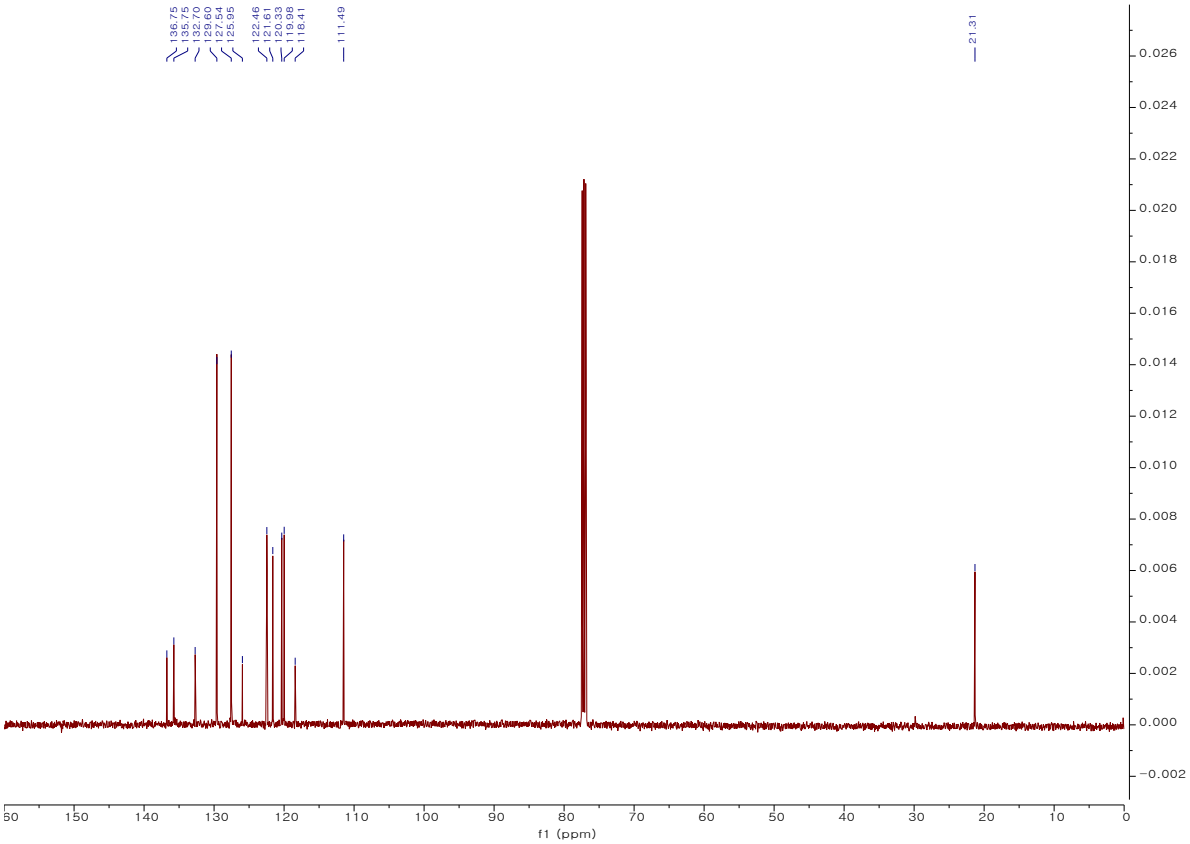
5-Bromo-3-phenyl-1*H*-indole (4ma);



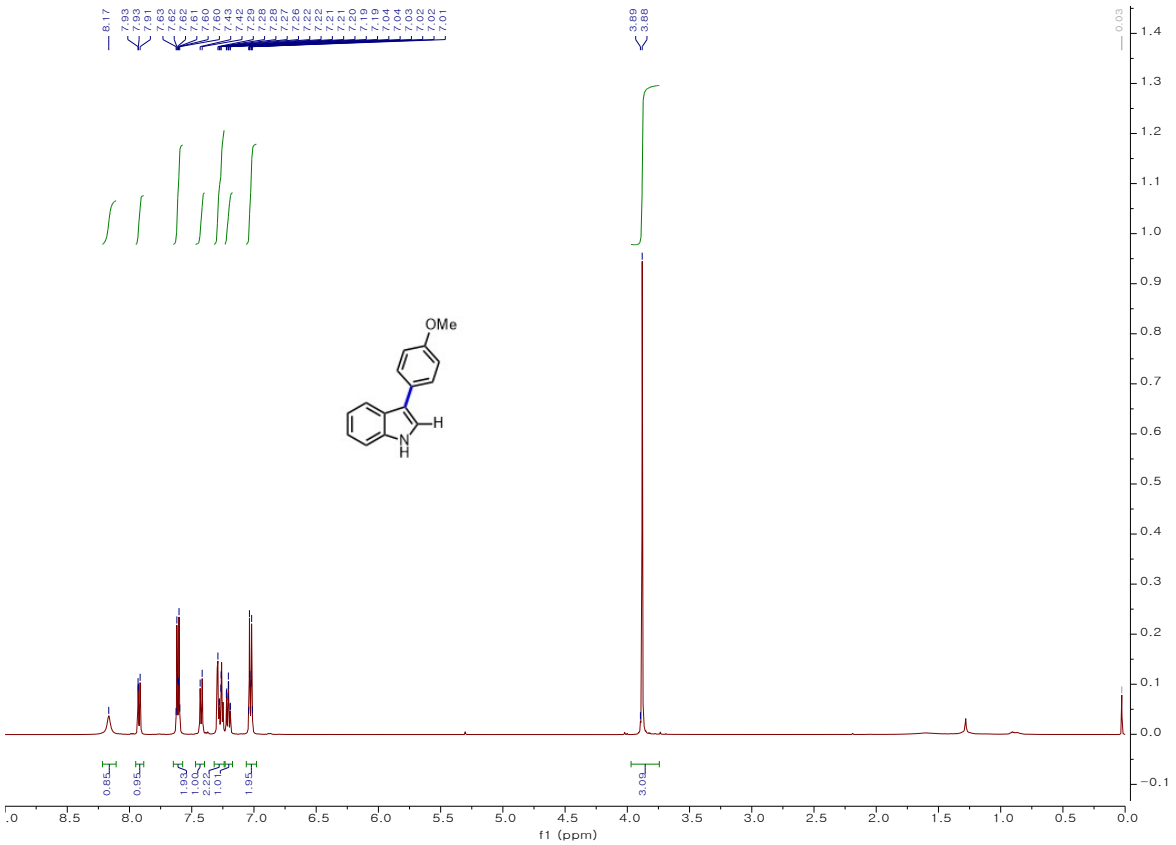


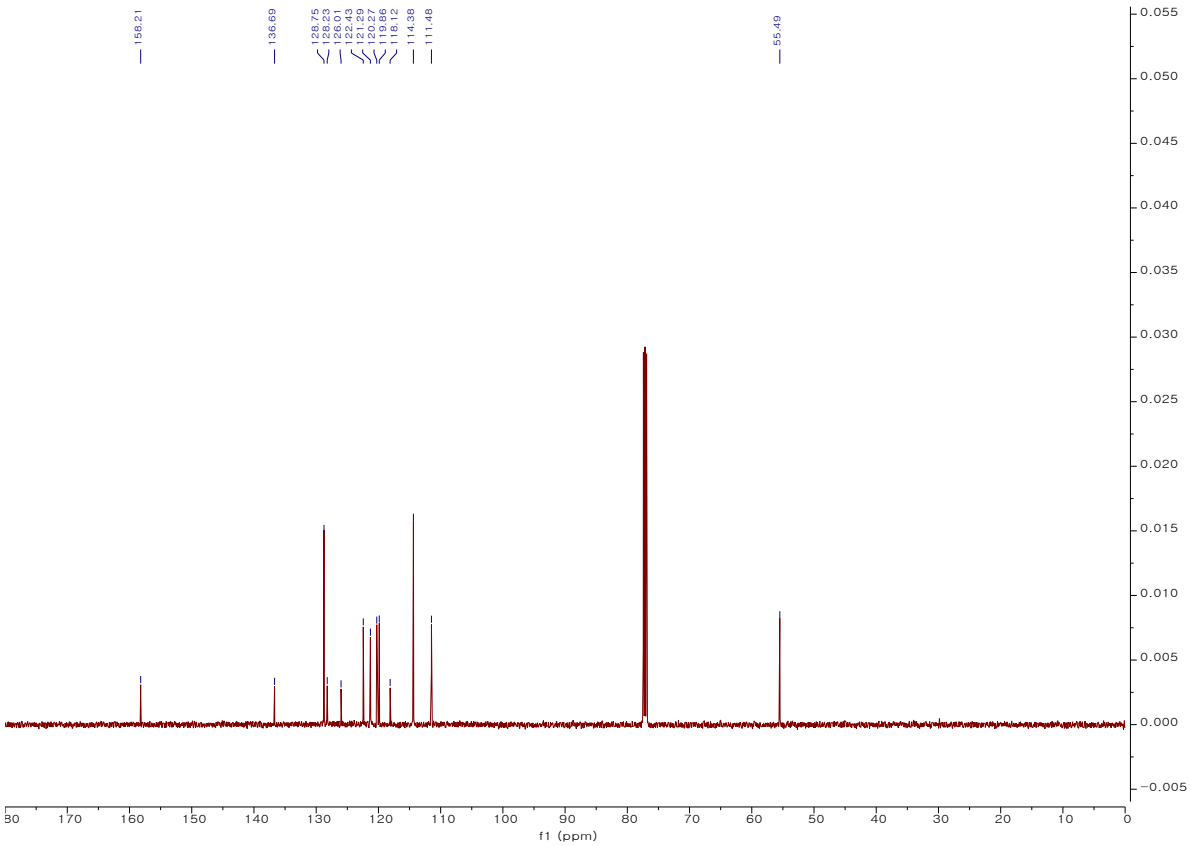
3-(*p*-Tolyl)-1*H*-indole (4ab);



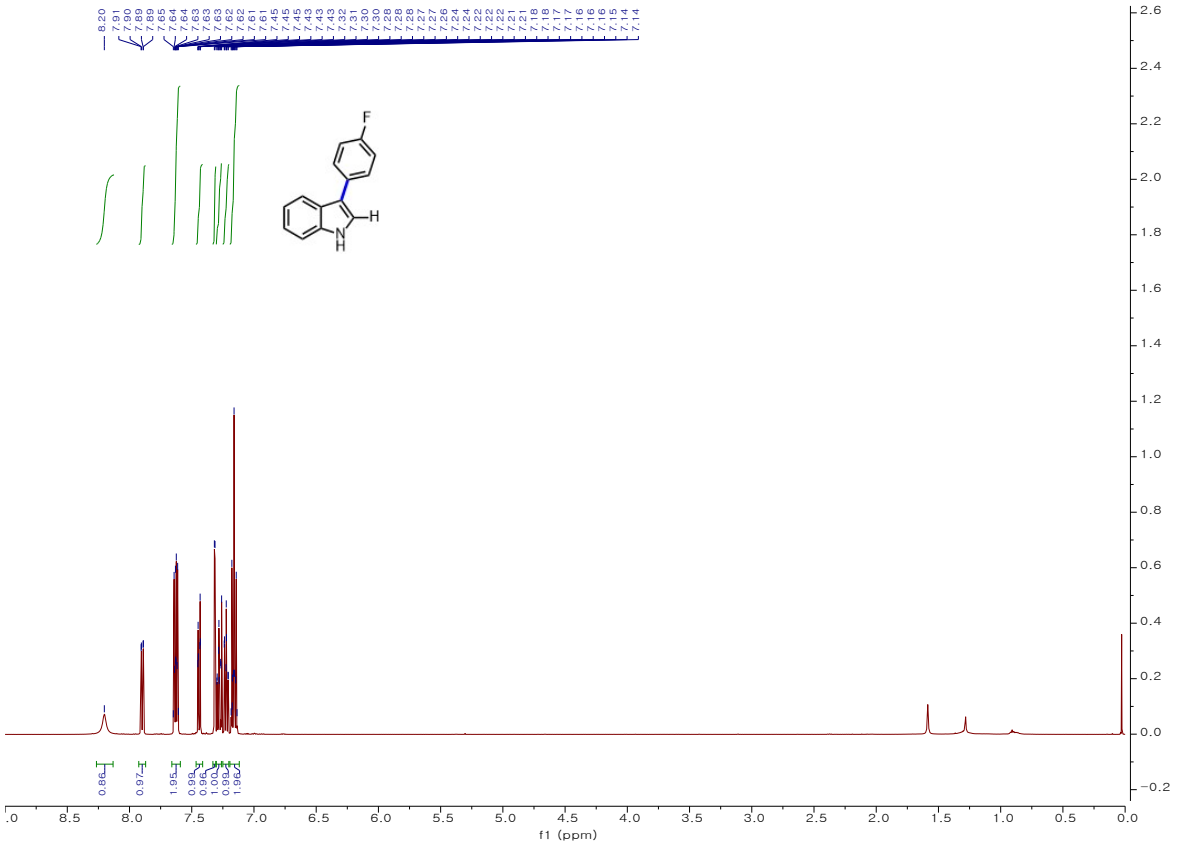


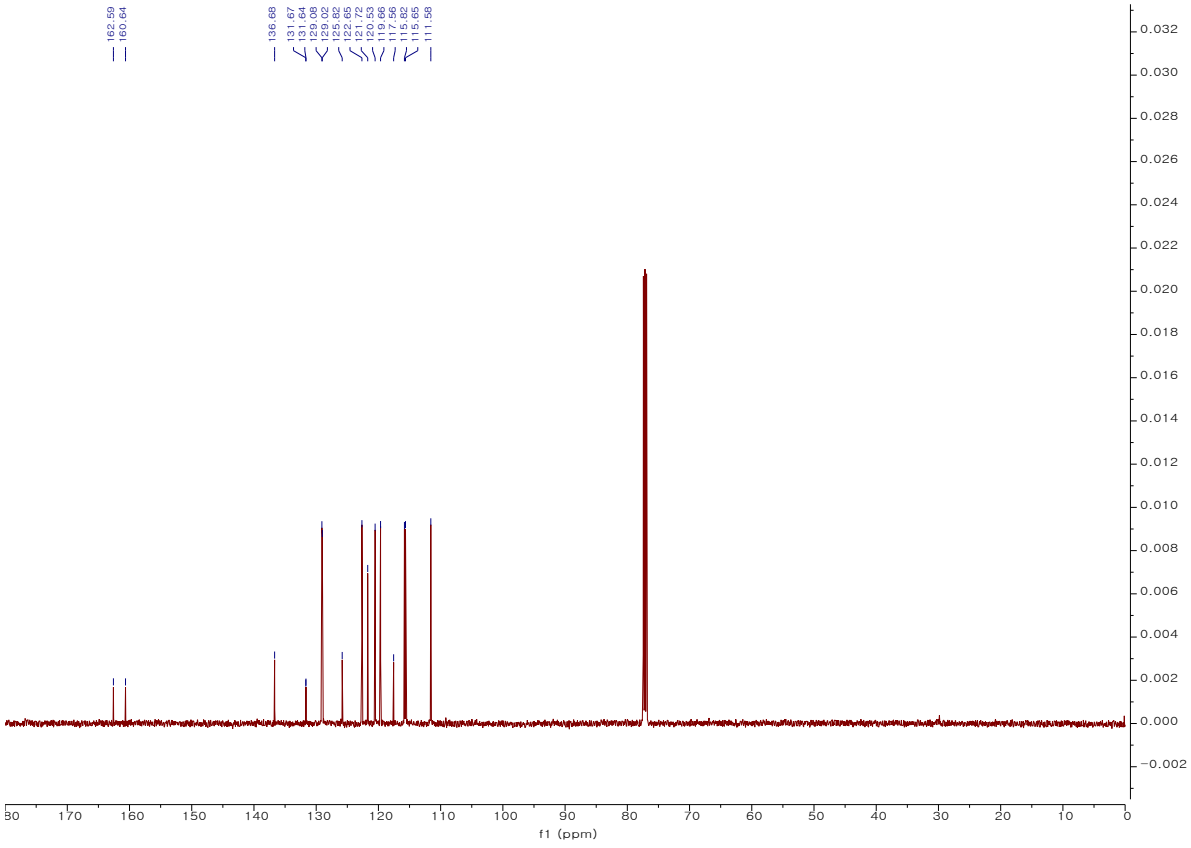
3-(4-Methoxyphenyl)-1*H*-indole (4ac);

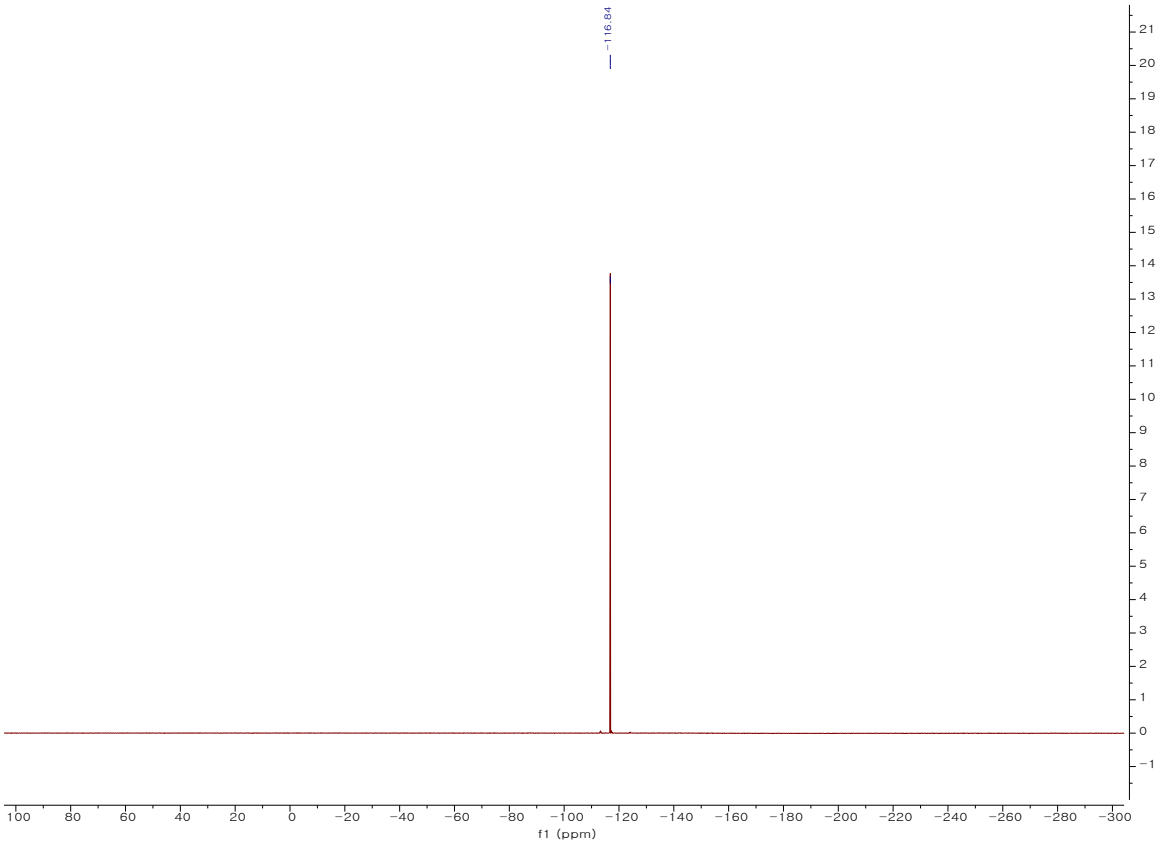




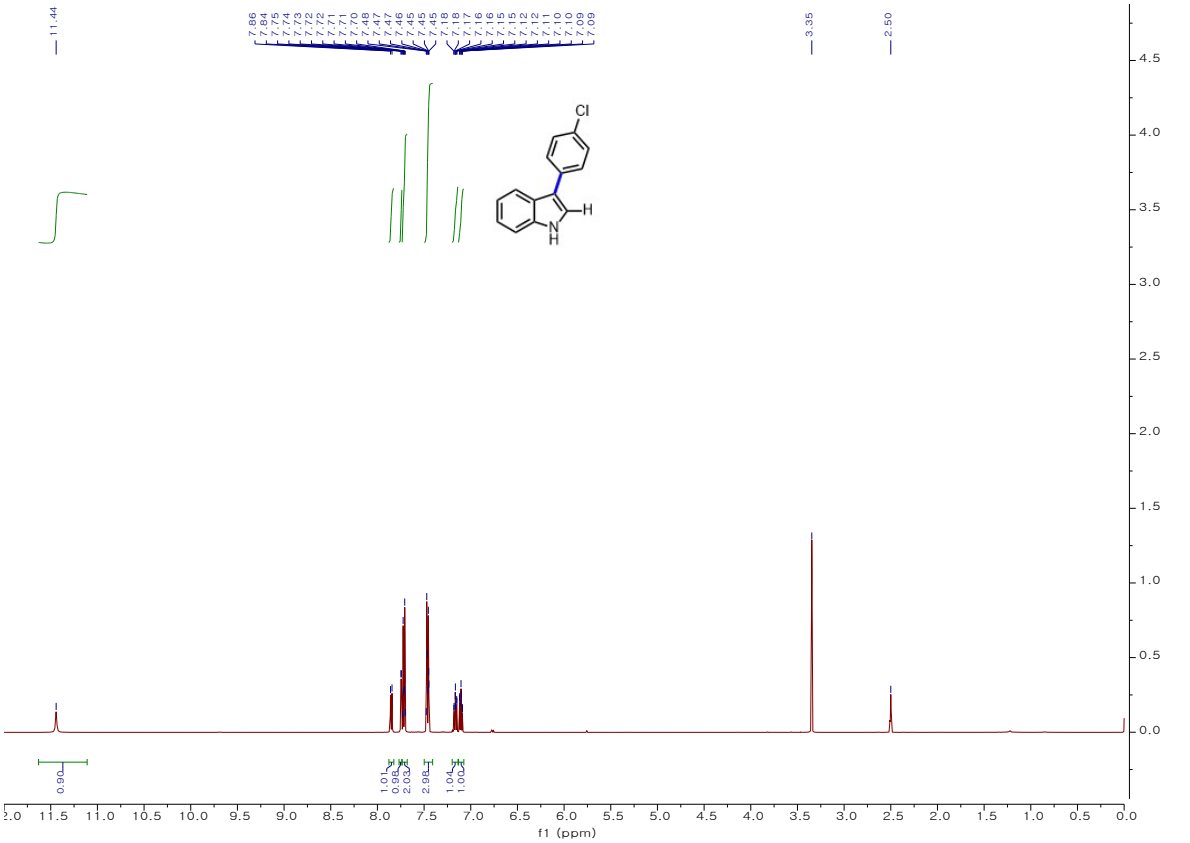
3-(4-Fluorophenyl)-1*H*-indole (4ad);

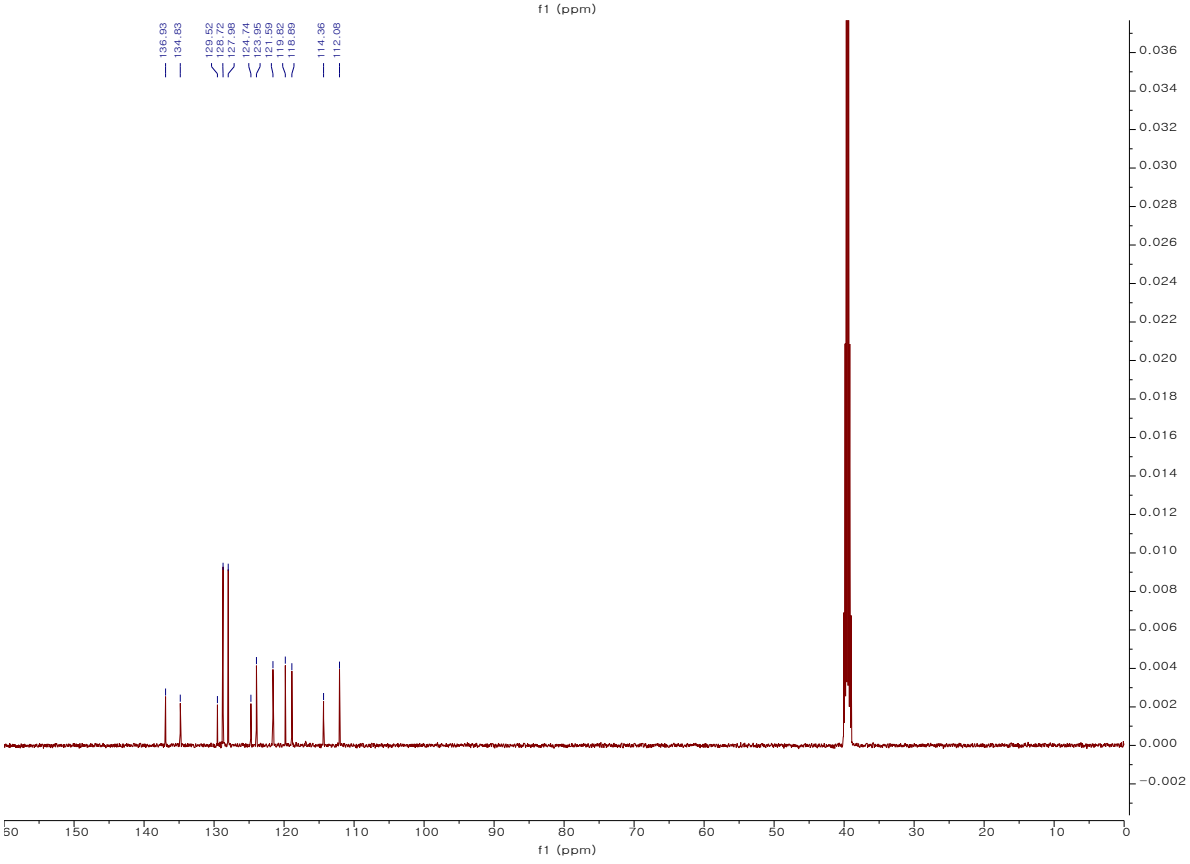




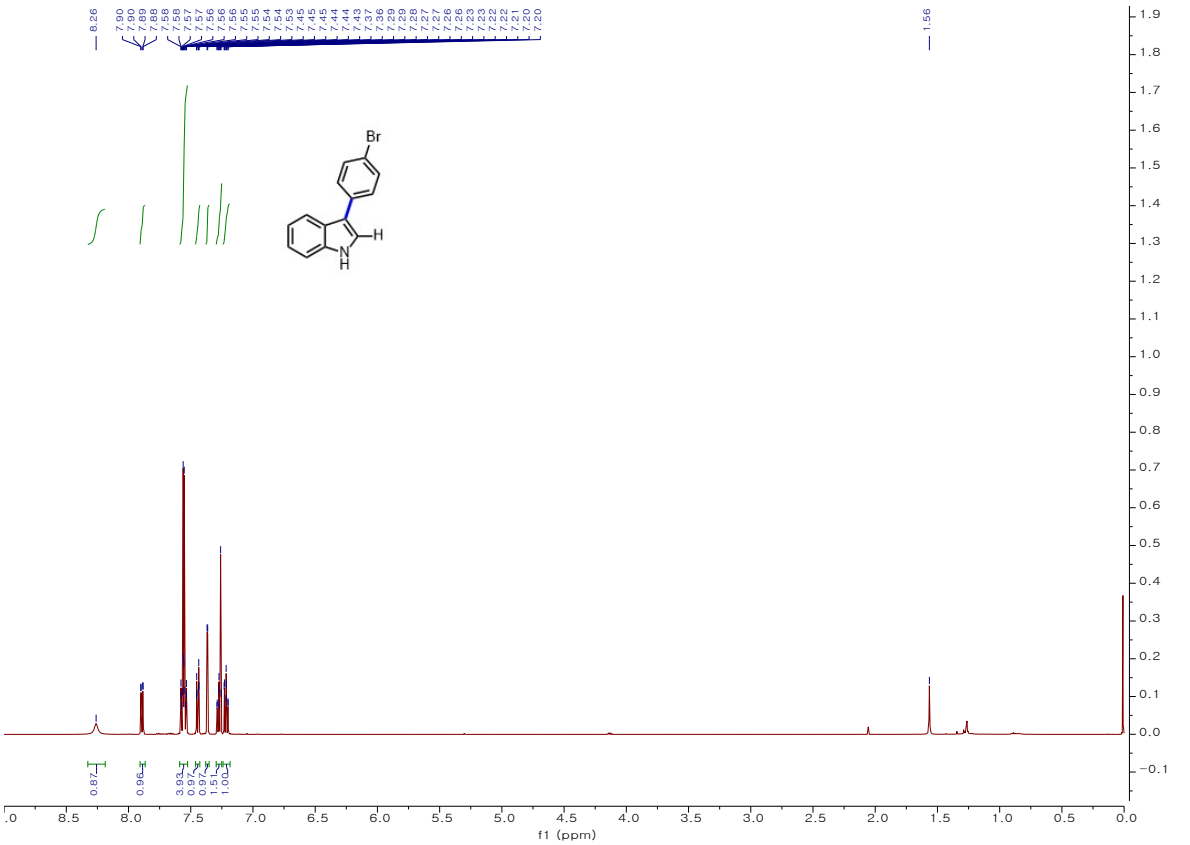

−116.84
21
20
19
18
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
100
80
60
40
20
0
−20
−40
−60
−80
−100
−120
−140
−160
−180
−200
−220
−240
−260
−280
−300
f1 (ppm)

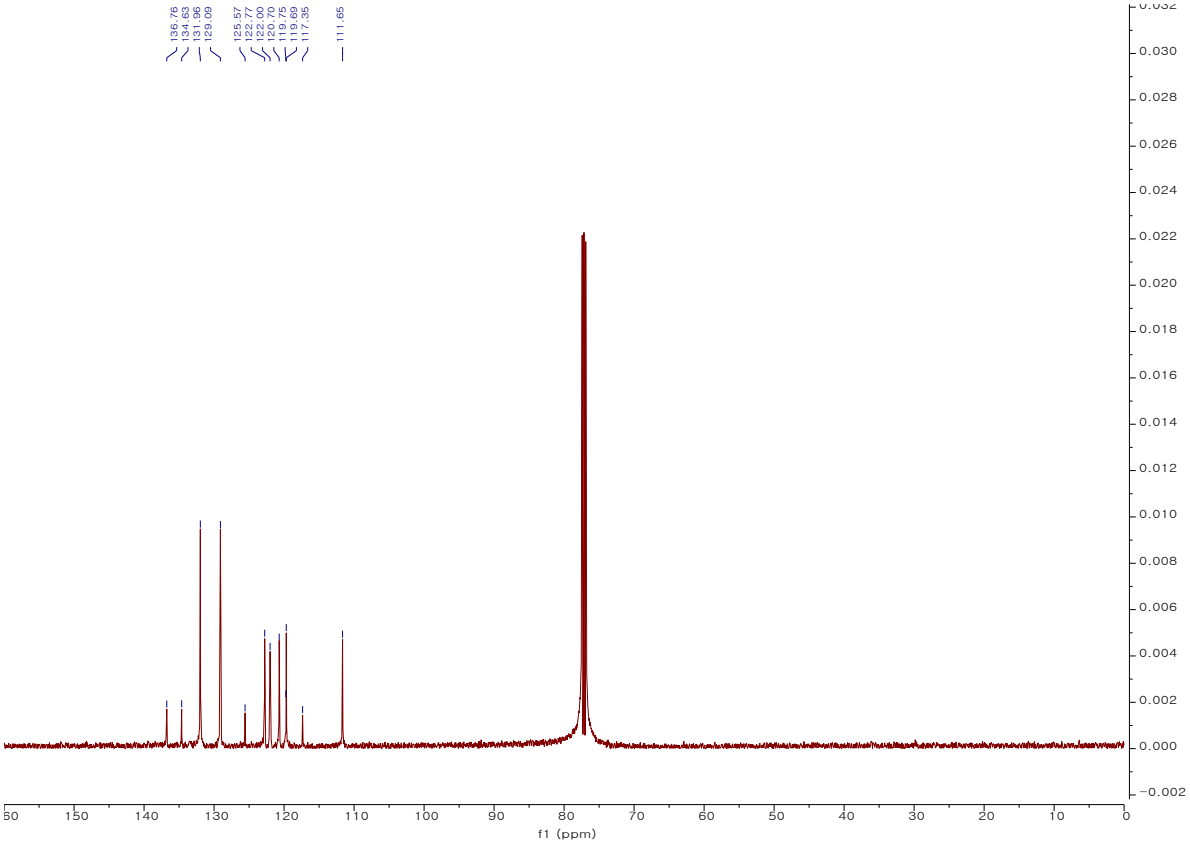
3-(4-Chlorophenyl)-1*H*-indole (4ae);



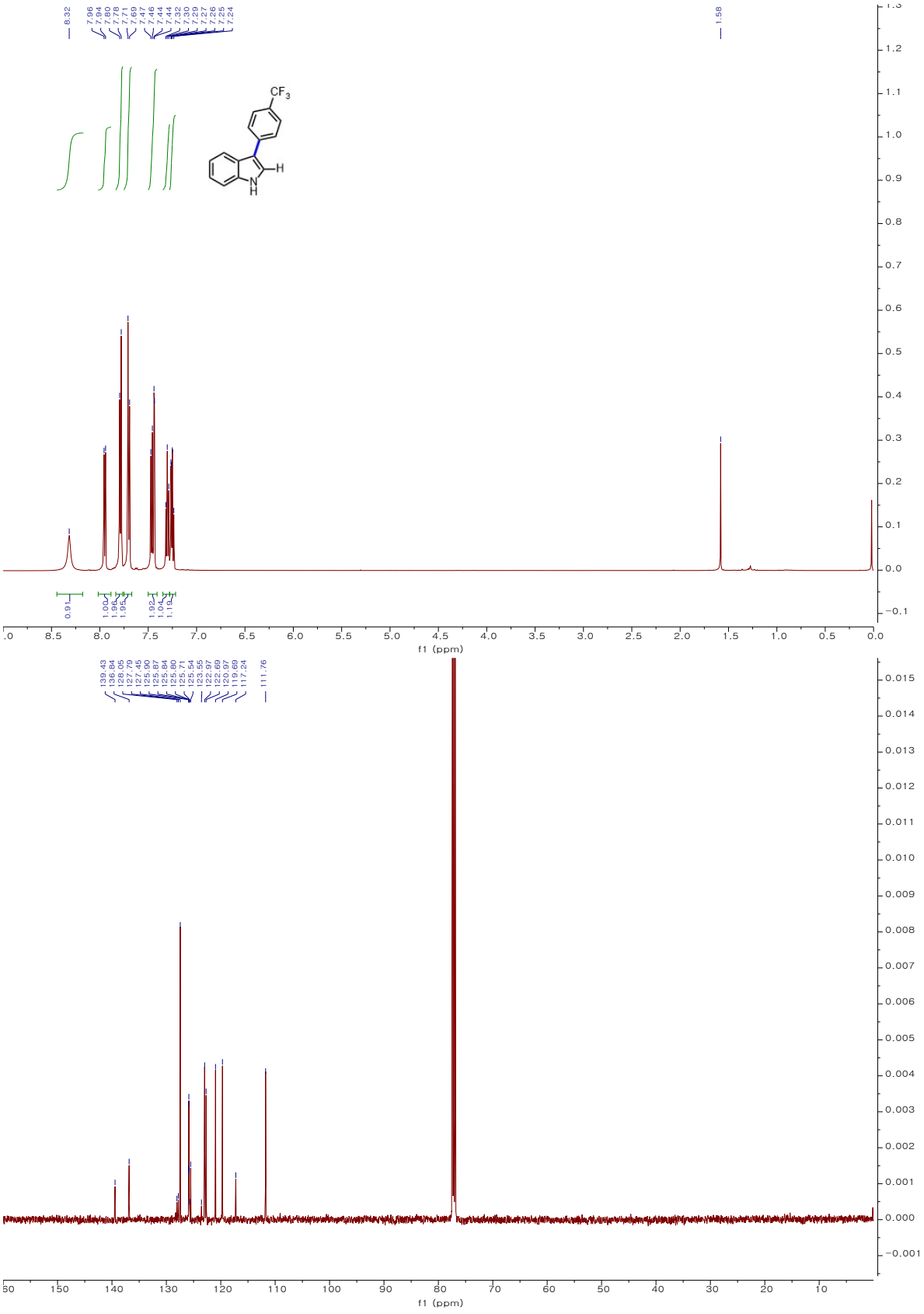


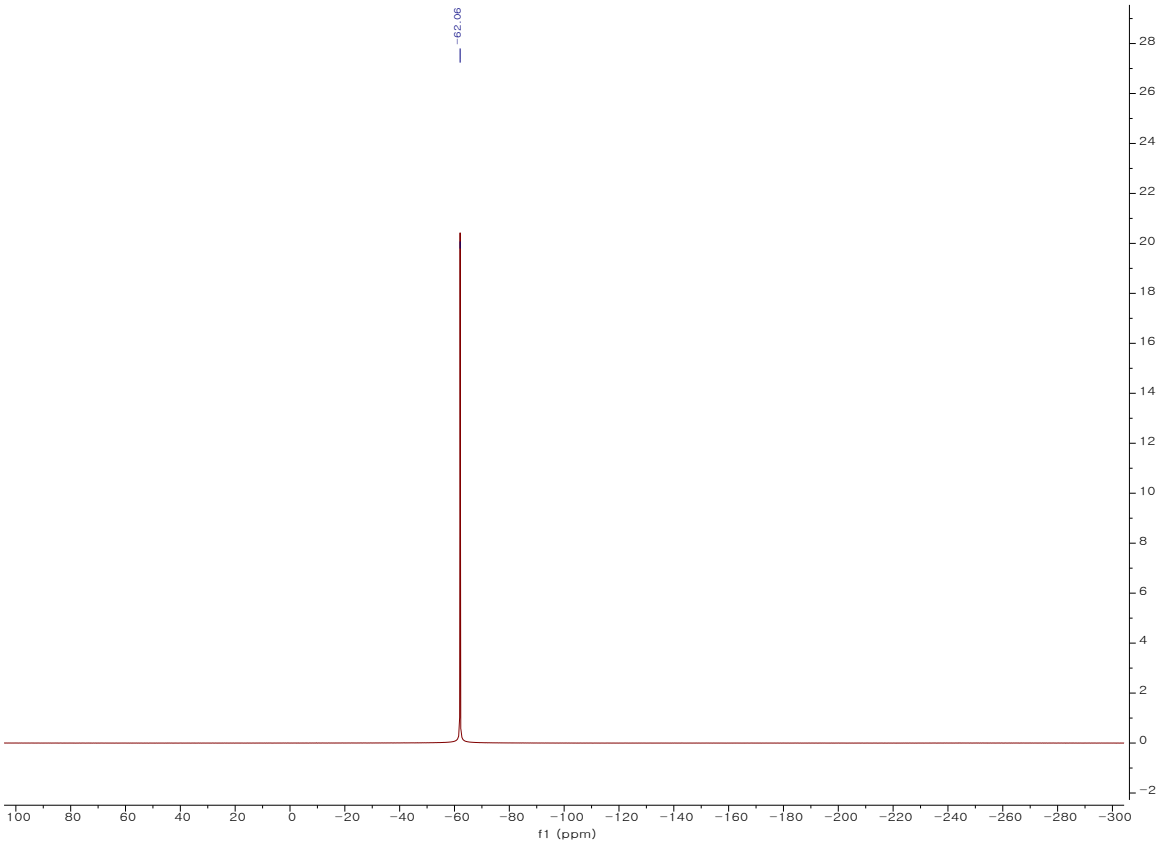
3-(4-Bromophenyl)-1*H*-indole (4af);



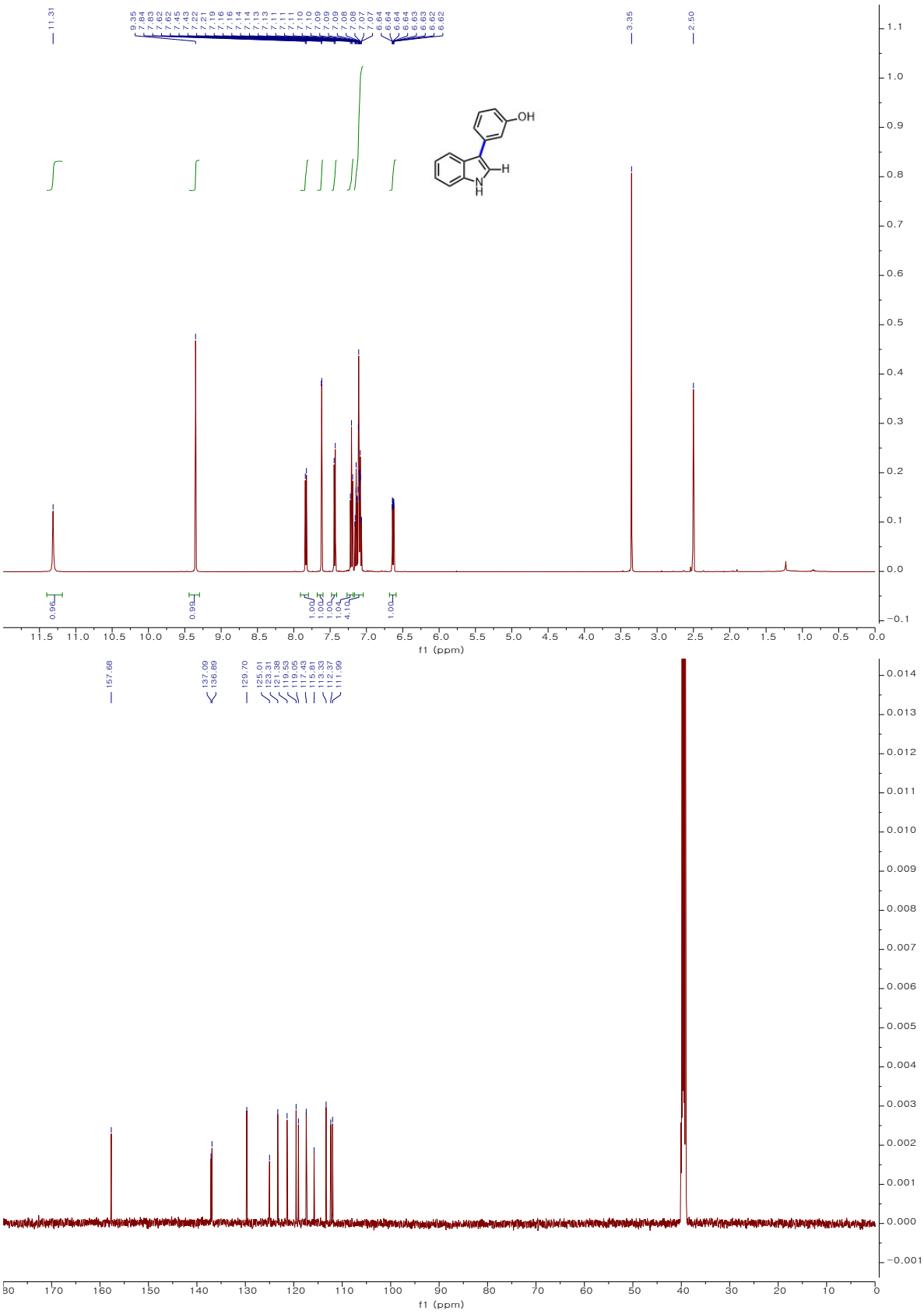


3-(4-(Trifluoromethyl)phenyl)-1*H*-indole (4ag);

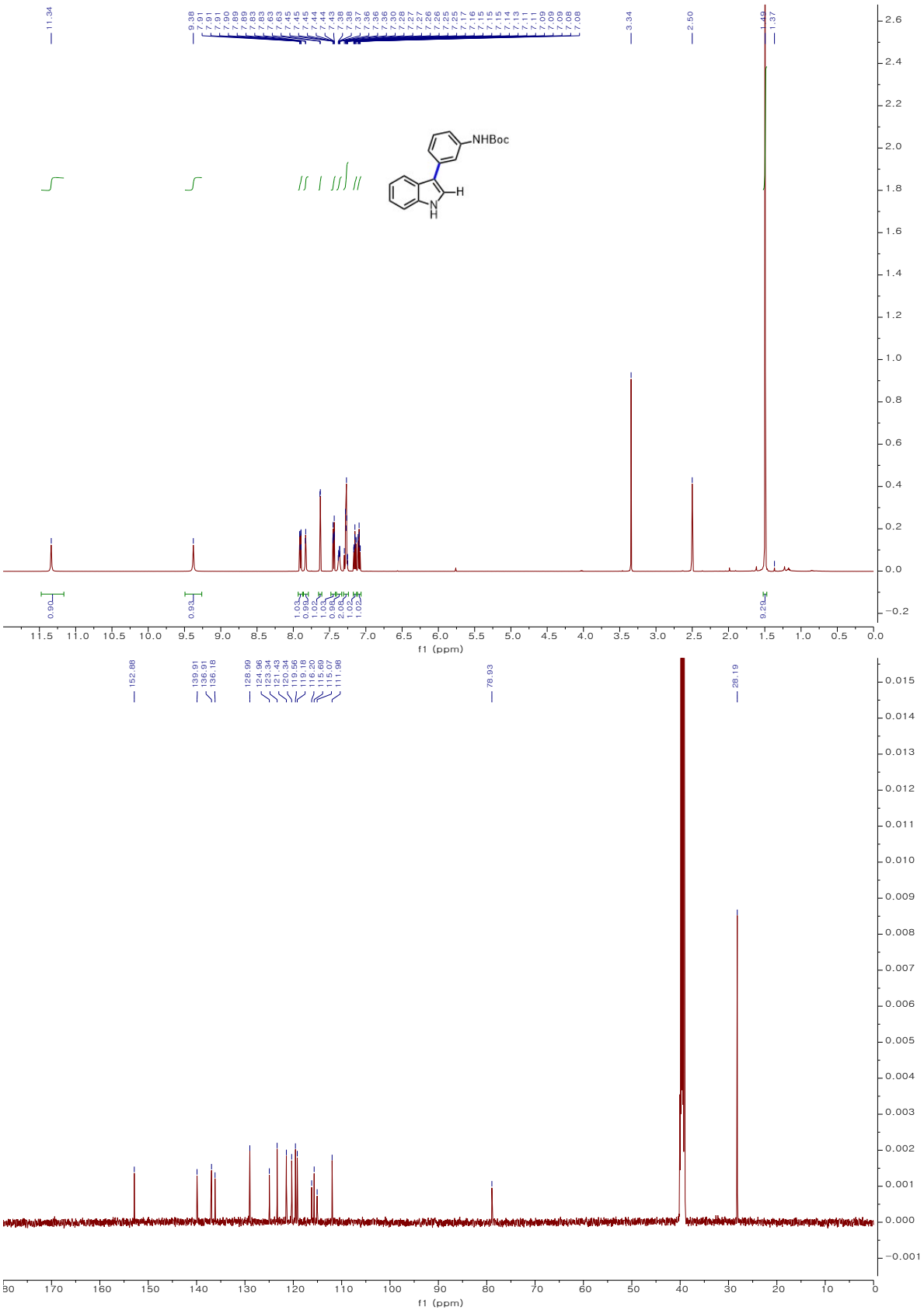



-62.06
28
26
24
22
20
18
16
14
12
10
8
6
4
2
0
-2
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
-240
-260
-280
-300
f1 (ppm)

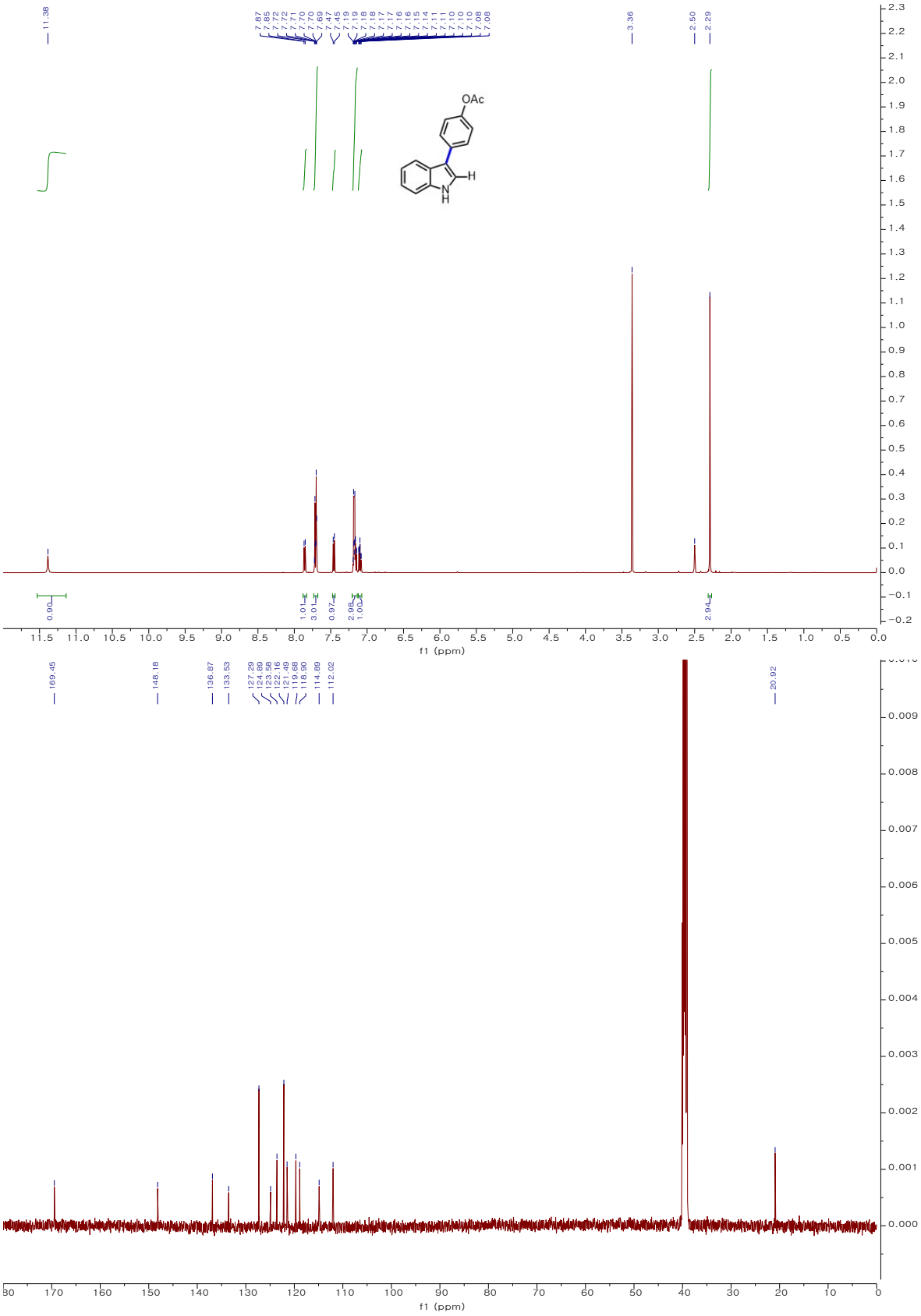
3-(1*H*-Indol-3-yl)phenol (4ah);



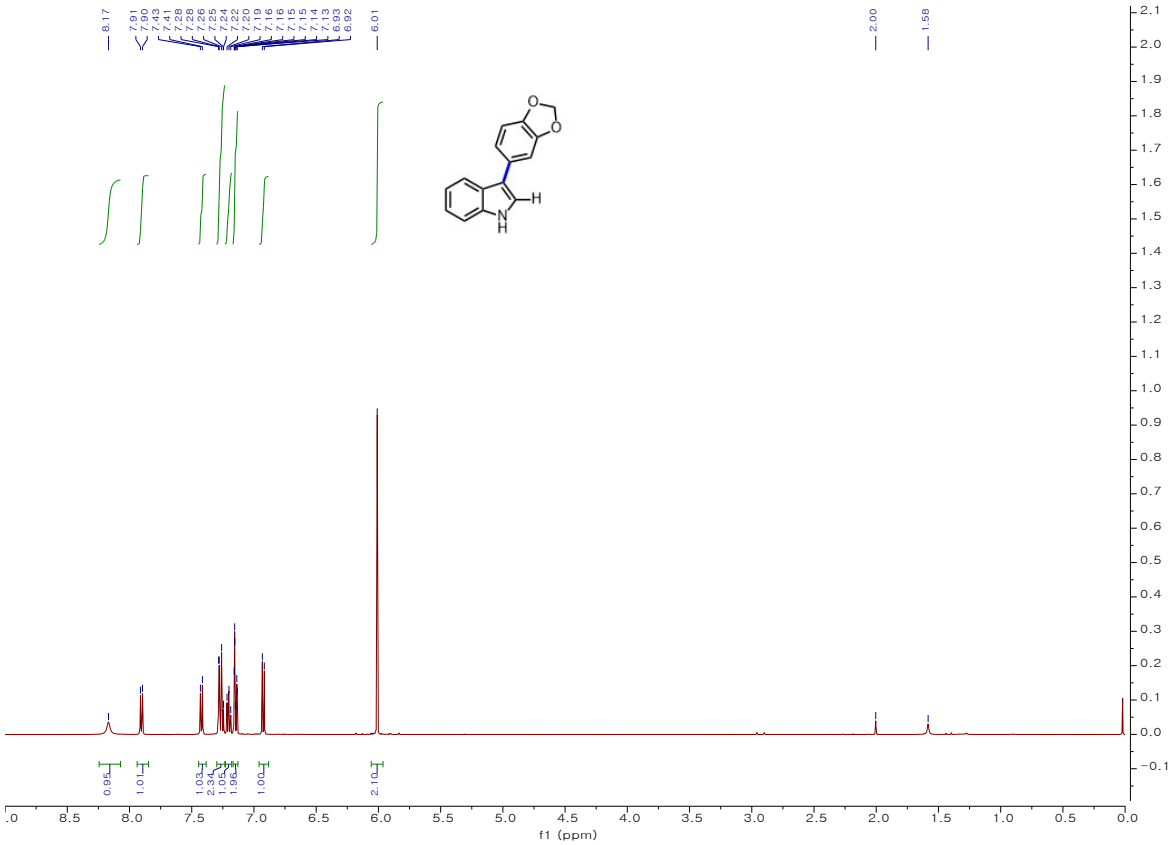
***tert*-Butyl (3-(1*H*-indol-3-yl)phenyl)carbamate (4ai);**

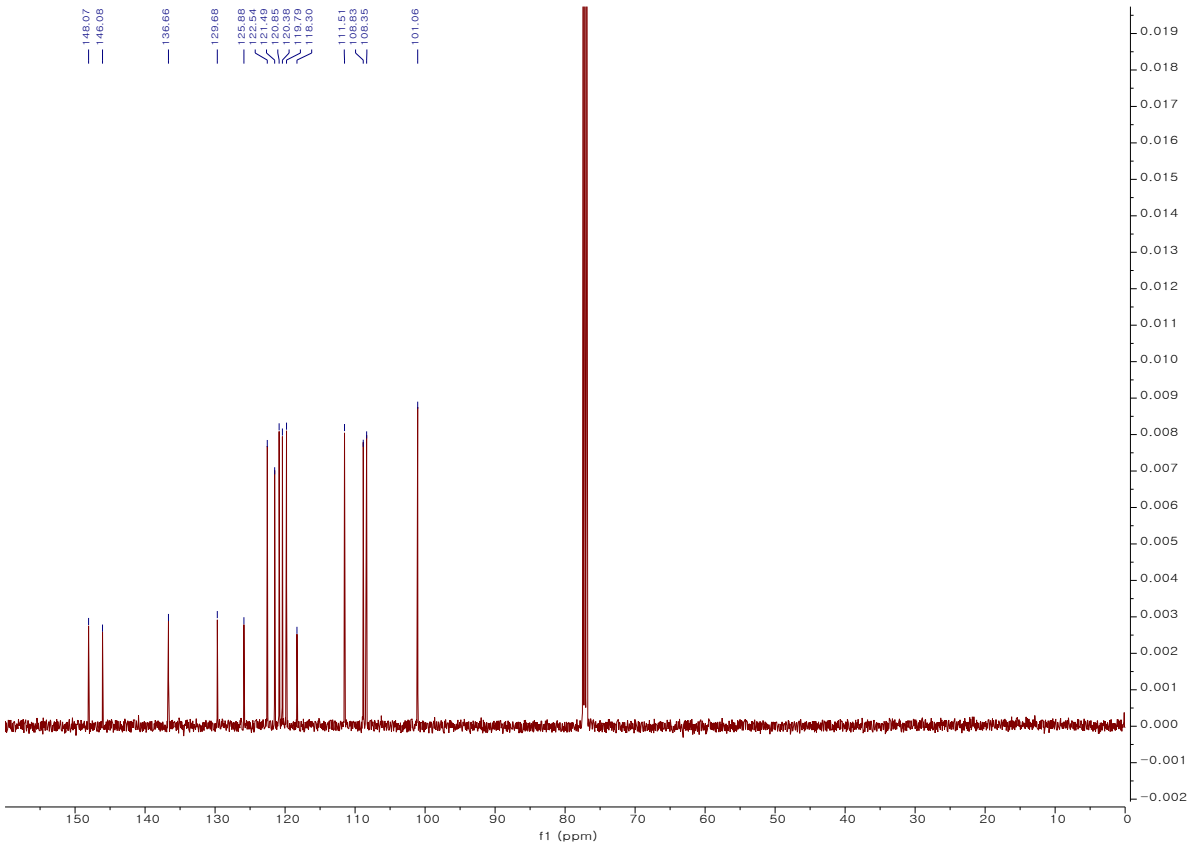


4-(1*H*-Indol-3-yl)phenyl acetate (4aj);

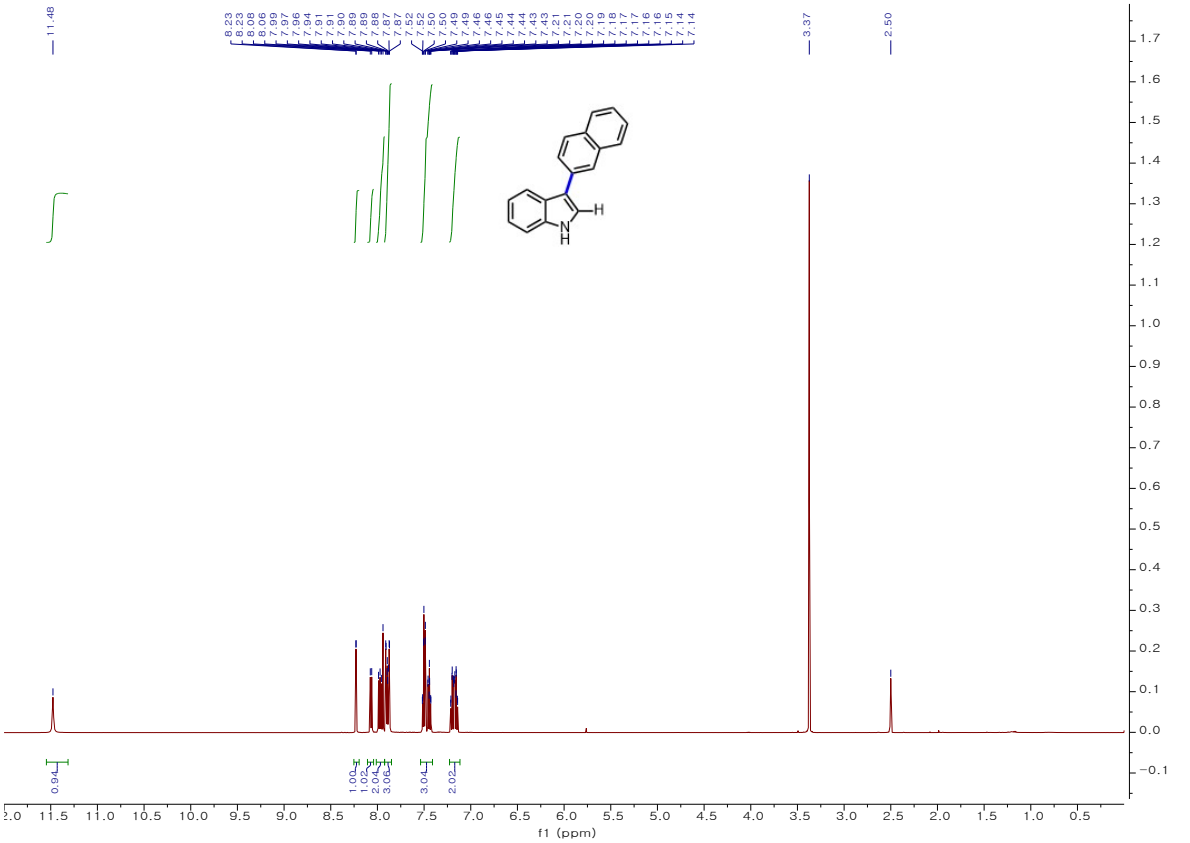


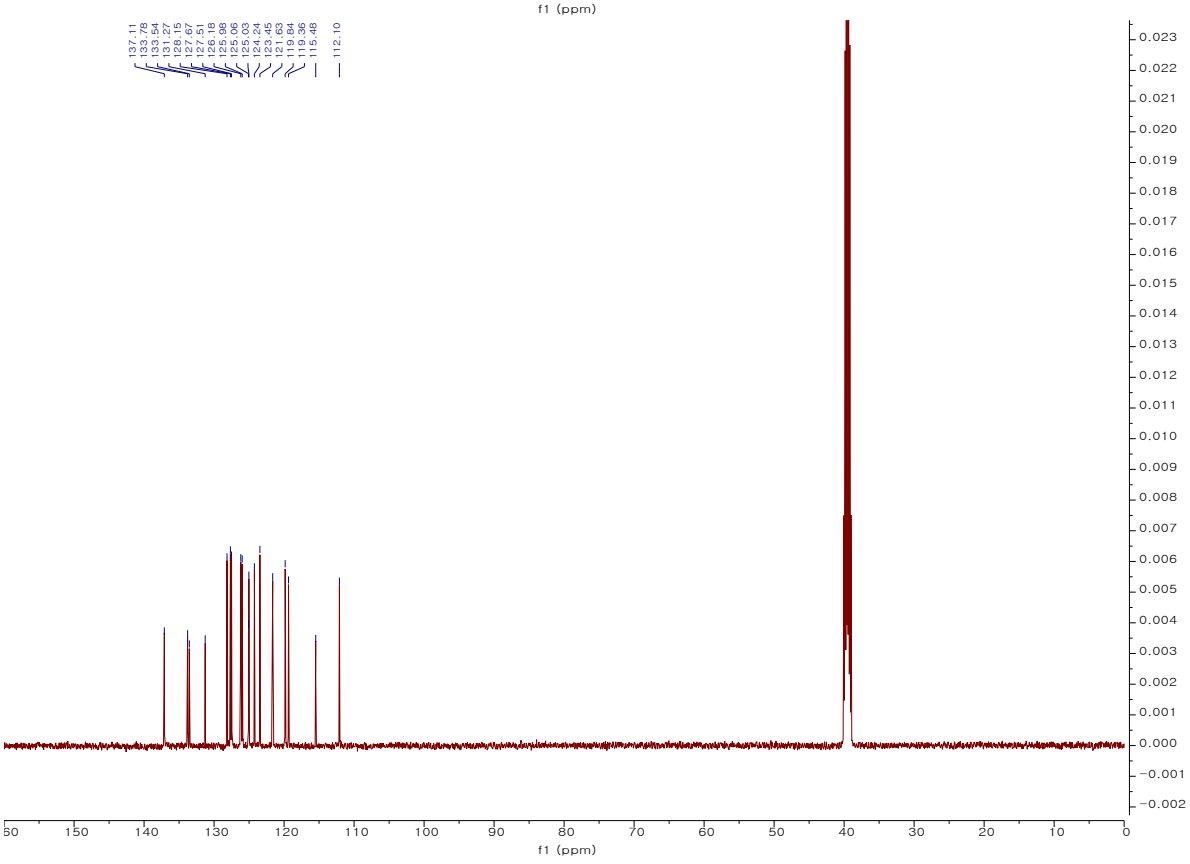
3-(Benzo[*d*][1,3]dioxol-5-yl)-1*H*-indole (4ak);



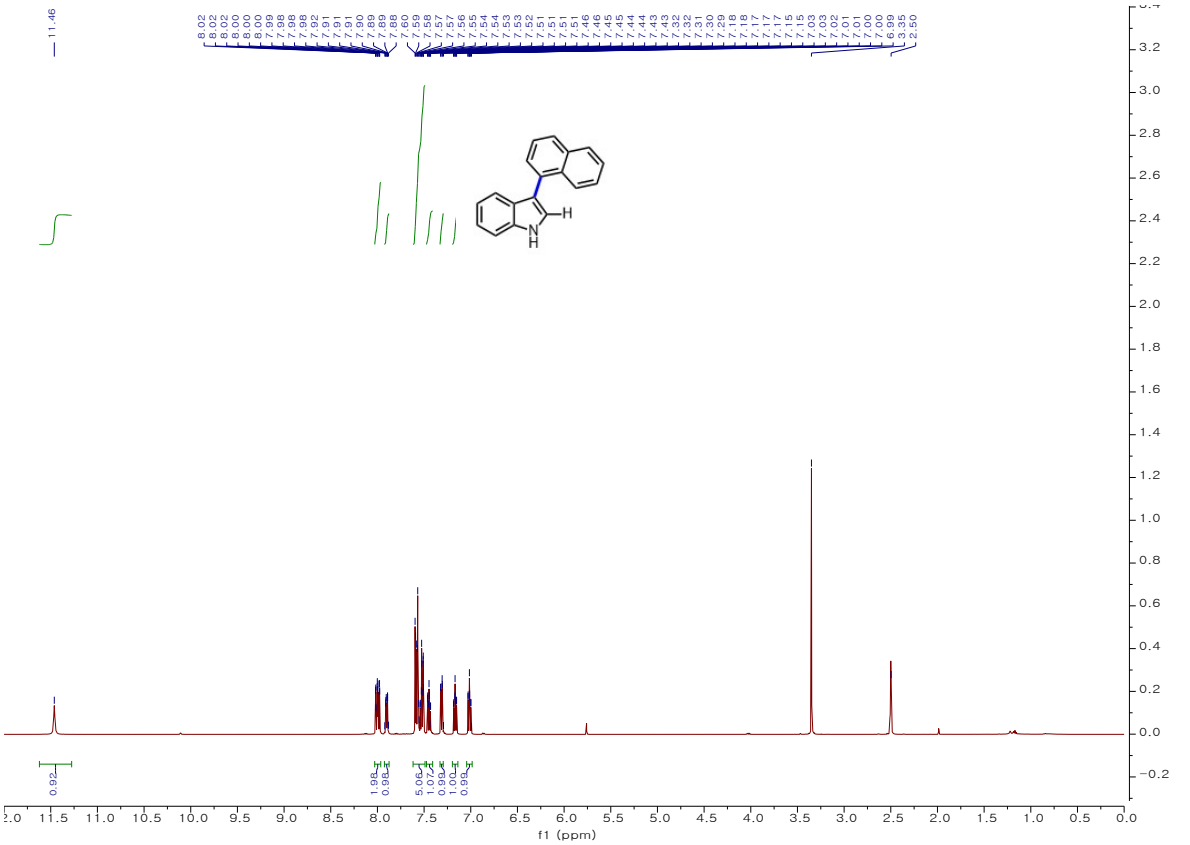


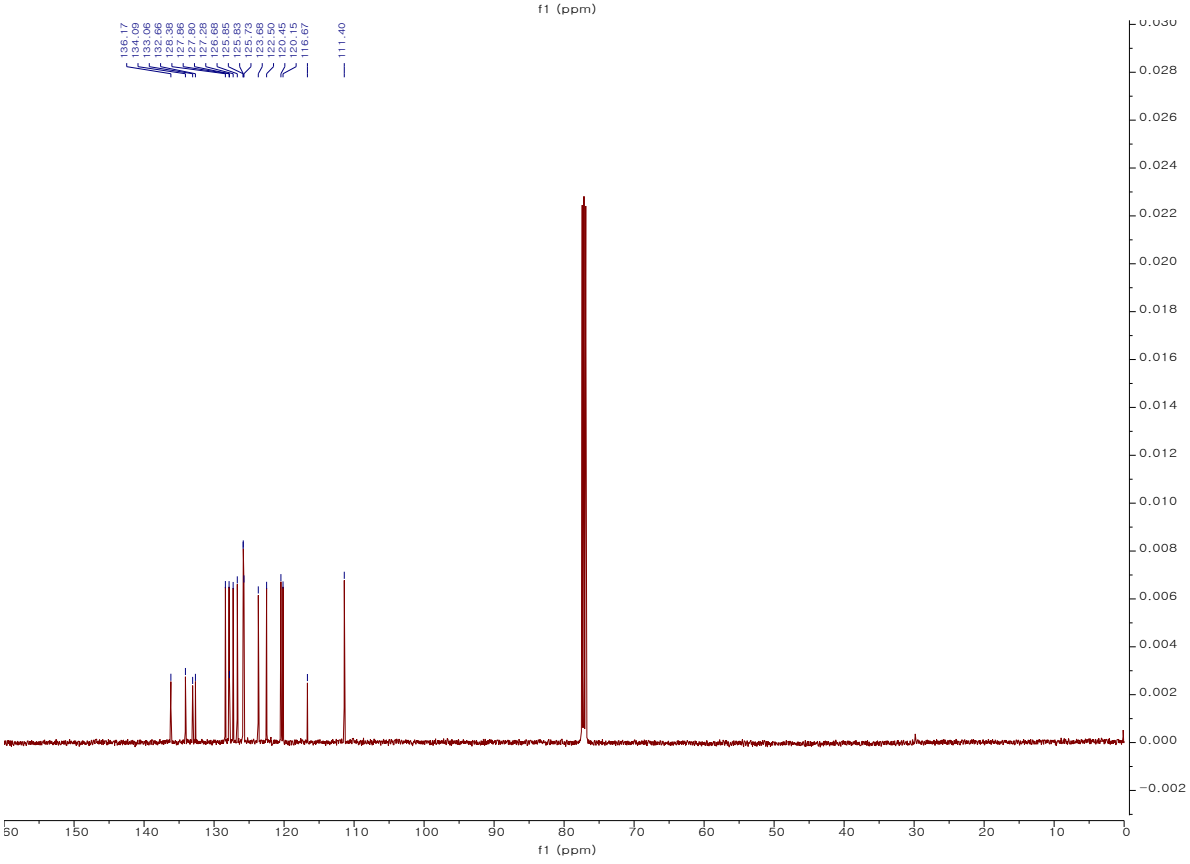
3-(Naphthalen-2-yl)-1*H*-indole (4al);



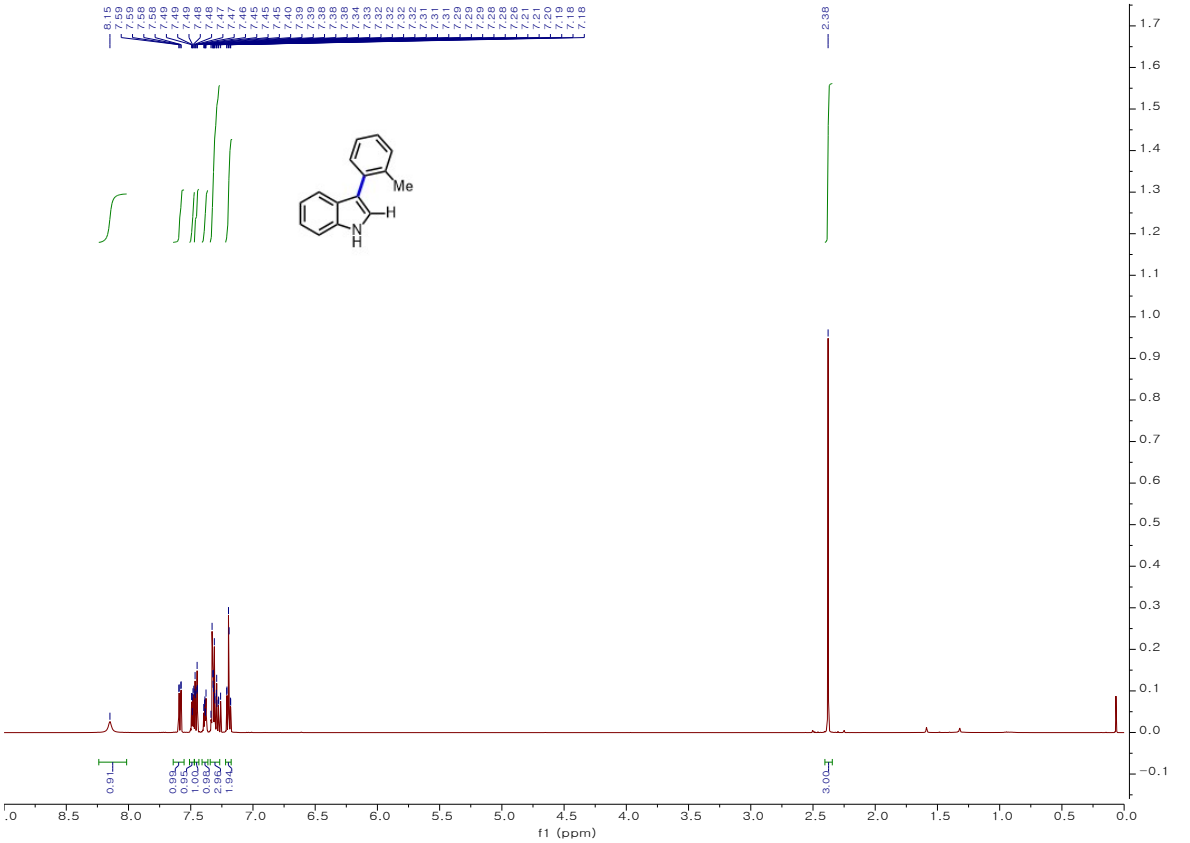


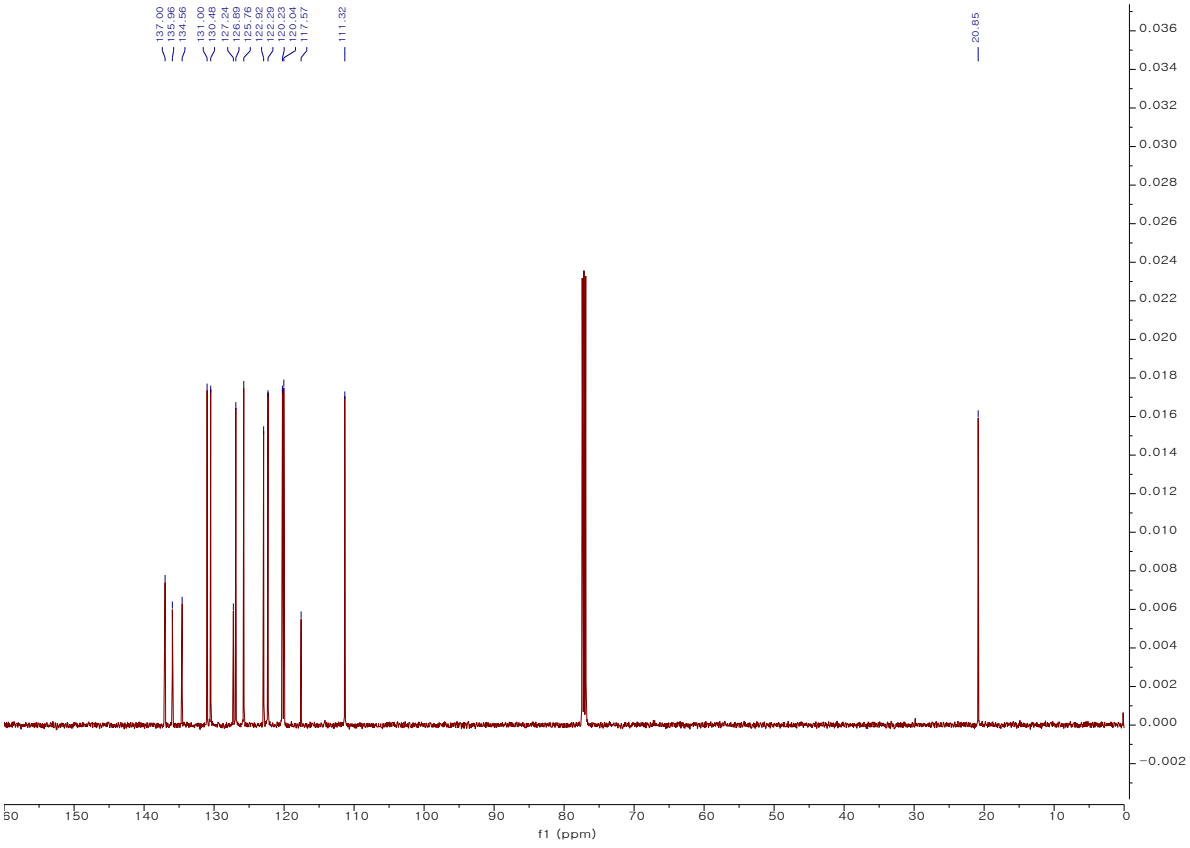
3-(Naphthalen-1-yl)-1*H*-indole (4am);



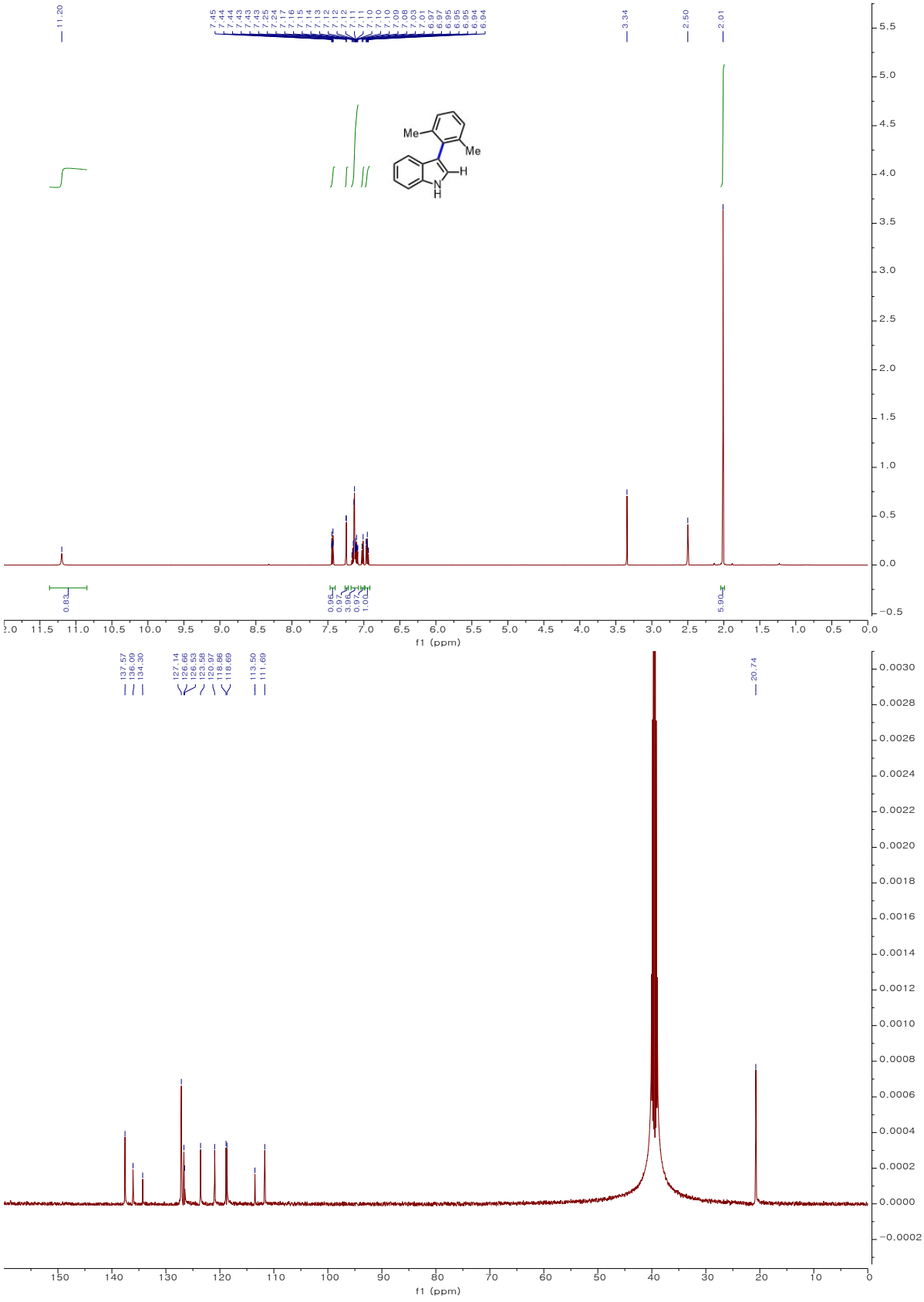


3-(*o*-Tolyl)-1*H*-indole (4an);





3-(2,6-Dimethylphenyl)-1*H*-indole (4ao);



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