Supporting Information for

Regioselective three-component synthesis of 1,2-diarylindoles from cyclohexanones, *α*-hydroxyketones and anilines under transition-metal-free conditions

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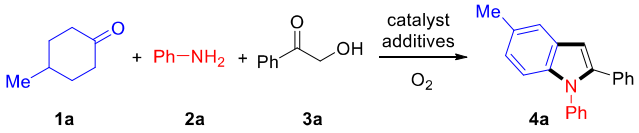
1. General information:

All reactions were carried out under an atmosphere of oxygen unless otherwise noted. Column chromatography was performed using silica gel (200-300 mesh). ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker-AV (400 and 100 MHz, respectively) instrument using $CDCl_3$ as solvent and TMS as an internal standard. Mass spectra were measured on Agilent 5975 GC-MS instrument (EI). High-resolution mass spectra were recorded at Keecloud (Shanghai) Biotechnology co. LTD. HRMS was conducted using electrospraying ionization (ESI) and was performed on a Thermo Scientific LTQ Orbitrap XL. The structures of known compounds were further corroborated by comparing their ^{1}H NMR, ^{13}C NMR data and MS data with those of literature. Reagents were used as received or prepared by our laboratory.

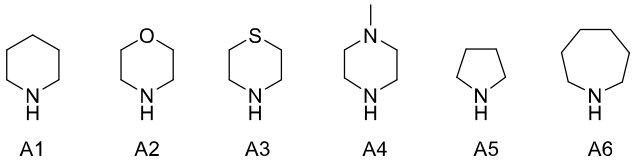
2. Table S1. Optimization of the reaction conditions[a]



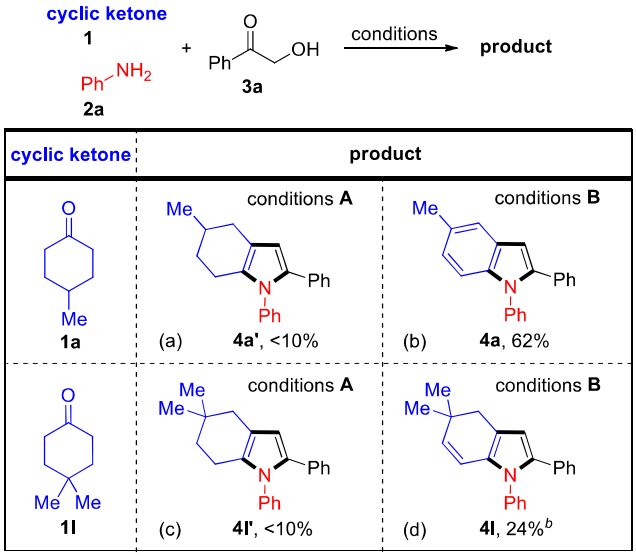
entry	amine catalyst	iodine additive	solvent	yield[b]
1			toluene	0
2		KI	toluene	＜10
3	A1	KI	toluene	55
4	A2	KI	toluene	62
5	A3	KI	toluene	54
6	A4	KI	toluene	27
7	A5	KI	toluene	12
8	A6	KI	toluene	36
9[c]	A2	KI	toluene	45
10	A2	NaI	toluene	60
11	A2	NH_4I	toluene	39
12	A2	I_2	toluene	43
13	A2	NIS	toluene	49
14[d]	A2	KI	toluene	53
15	A2	KI	$PhCF_3$	38
16	A2	KI	1,2-DCE	＜10
17	A2	KI	PhCl	0
18	A2	KI	DMSO	0
19[e]	A2	KI	toluene	39
20[f]	A2	KI	toluene	46
21[g]	A2	KI	toluene	0

22[h]	A2	KI	toluene	62

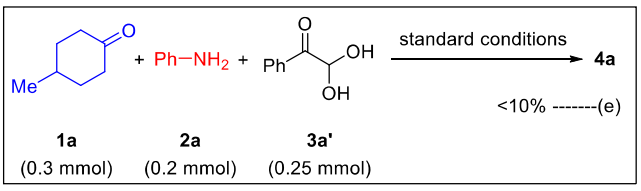
[a] Conditions: **1a** (0.3 mmol), **2a** (0.2 mmol), **3a** (0.25 mmol), Amine cat. (20 mol %), Iodine add. (20 mol %), DMSO (2.0 equiv), solvent (0.1 M), 150 °C, 12 h, under oxygen, in a 20 mL sealed tube. [b] Isolated yields based on **2a**. [c] A2 (10 mol %). [d] KI (10 mol %). [e] DMSO (1.0 equiv.). [f] DMSO (3.0 equiv.). [g] Under argon. [h] 24 h.



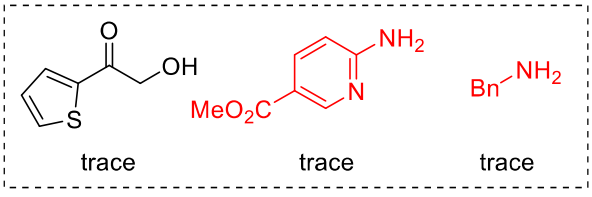
3. Scheme S1.Control experiments



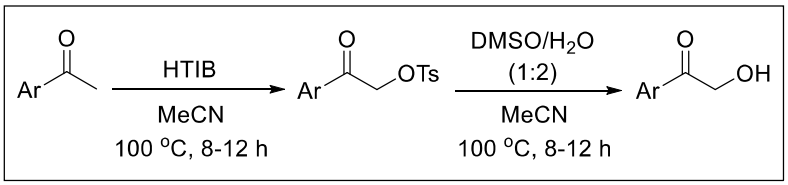
Conditions **A**: **2a** (0.2 mmol), cyclic ketone (0.3 mmol), **3a** (0.25 mmol), morpholine (20 mol %), toluene (0.1 M), 150 °C, 12 h under argon, in a 20 mL sealed tube. Product was determined by GC-MS. conditions **B**: standard conditions. Isolated yields based on **2a**. [b] DMSO (1.0 equiv.).



failed reactants



4. Materials Preparation



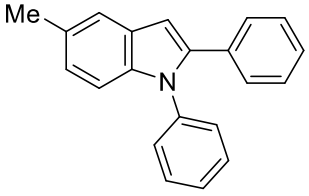
Substrates α-hydroxyketones **3** were prepared according to the literature.[1] the mixture of acetophenone (2.0 mmol) and HTIB (2.4 mmol) in acetonitrile (15 mL) was heated at 100 °C for 10 h. Then 12 mL of DMSO/H_2O (1:2) was added and the mixture was stirred at 100 °C for 10 h. After removal of acetonitrile under reduced pressure, the aqueous phase was extracted with EtOAc. The combined organic extracts were concentrated under reduced pressure. The resulting residue was then dissolved in ethyl acetate, washed with H_2O, and dried over $MgSO_4$. The solvent was evaporated off and the residue was purified by chromatography on silica gel (petroleum ether/ethyl acetate = 10:1) to afforded substrate **3**.

5. General procedure (4a):

A 20 mL oven-dried reaction vessel was charged with KI (6.6 mg, 20 mol %), 4-methylcyclohexanone **1a** (37.6 μL, 0.3 mmol) and α-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol). The reaction vessel was purged with oxygen for three times and was added aniline **2a** (18.2 μL, 0.2 mmol), morpholine (3.5 μL, 20 mol %), DMSO (28.4 μL, 0.4 mmol) and toluene (2.0 mL) by syringe. The sealed vessel was stirred at 150 °C for 12 h. After cooling to room temperature, the volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/Et_3N = 100:0.5, R_f = 0.48) to give the desired product **4a** as a white solid (35.1 mg, 62% yield), mp = 149-151 °C.

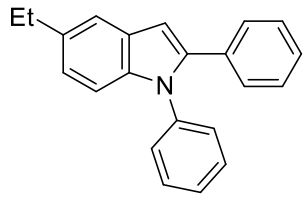
6. Characterization data of products

5-Methyl-1,2-diphenyl-1*H*-indole (4a, Cas: 1131890-87-3) [2].



^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.46 (s, 1H), 7.41-7.37 (m, 2H), 7.34-7.30 (m, 1H), 7.25-7.17 (m, 8H), 7.00 (dd, J = 8.4, 1.3 Hz, 1H), 6.72 (s, 1H), 2.46 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm) δ 140.7, 138.7, 137.5, 132.6, 129.9, 129.2, 128.8, 128.5, 128.1, 127.9, 127.1, 127.0, 123.9, 120.2, 110.3, 103.3, 21.4; MS (EI) m/z (%) 283 (100), 267, 165, 134, 77.

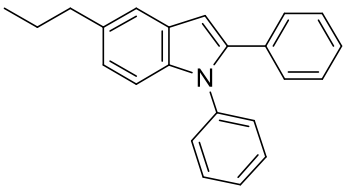
5-Ethyl-1,2-diphenyl-1*H*-indole (4b).



4-Ethylcyclohexanone **1b** (42.3 μL, 0.3 mmol), aniline **2a** (18.2 μL, 0.2 mmol), α-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/Et_3N = 100:0.5, R_f = 0.50) to afford 29.7 mg of **4b** as a white solid in 50% yield, mp = 108-110 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.49 (s, 1H), 7.42-7.36 (m, 2H), 7.34-7.29 (m, 1H), 7.27-7.19 (m, 8H), 7.03 (dd, J = 8.4, 1.6 Hz, 1H), 6.74 (s, 1H), 2.76 (q, J = 7.6 Hz, 2H), 1.30 (t, J = 7.6 Hz, 3H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm) δ 140.7, 138.7, 137.5, 136.8, 132.6, 129.2, 128.8, 128.4, 128.1, 127.9, 127.1, 127.0, 122.9, 118.9, 110.4, 103.4, 29.0, 16.5; HRMS (ESI) calcd for: $C_{22}H_{20}N^+$ $(M+H)^+$ 298.1590, found: 298.1595.

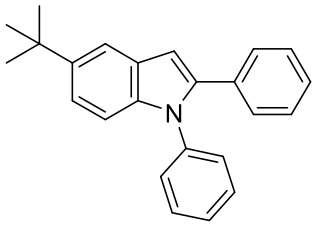
1,2-Diphenyl-5-propyl-1*H*-indole (4c).



4-Propylcyclohexanone **1c** (46.4 μL, 0.3 mmol), aniline **2a** (18.2 μL, 0.2 mmol), α-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/Et_3N = 100:0.5, R_f = 0.70) to afford 31.1 mg of **4c** as a white solid in 50% yield, mp = 84-86 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.47 (s, 1H), 7.41-7.35 (m, 2H), 7.34-7.30 (m, 1H), 7.27-7.19 (m, 8H), 7.01 (dd, J = 8.4, 1.6 Hz, 1H), 6.74 (s, 1H), 2.75-2.64 (m, 2H), 1.75-1.65 (m, 2H), 0.97 (t, J = 7.3 Hz, 3H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm) δ 140.7, 138.7, 137.6, 135.1, 132.7, 129.2, 128.8, 128.4, 128.1, 127.9, 127.1, 127.0, 123.4, 119.6, 110.3, 103.4, 38.1, 25.3, 13.9; HRMS (ESI) calcd for: $C_{23}H_{22}N^+$ $(M+H)^+$ 312.1747, found: 312.1749.

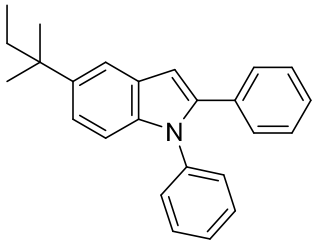
5-(*tert*-Butyl)-1,2-diphenyl-1*H*-indole (4d).



4-*tert*-Butylcyclohexanone **1d** (51.8 μL, 0.3 mmol), aniline **2a** (18.2 μL, 0.2 mmol), α-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/Et_3N = 100:0.5, R_f = 0.55) to afford 33.3 mg of **4d** as a white solid in 51% yield, mp = 134-136 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.69 (s, 1H), 7.42-7.37 (m, 2H), 7.34-7.21 (m, 10H), 6.77 (s, 1H), 1.41 (s, 9H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm) δ 143.7, 140.8, 138.7, 137.2, 132.7, 129.2, 128.8, 128.1, 128.0, 127.9, 127.1, 127.0, 120.6, 116.4, 110.1, 103.8, 34.6, 31.9; HRMS (ESI) calcd for: $C_{24}H_{24}N^+$ $(M+H)^+$ 326.1903, found: 326.1909.

5-(*tert*-Pentyl)-1,2-diphenyl-1*H*-indole (4e).

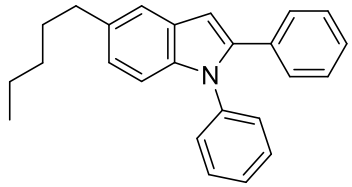


4-*tert*-Pentylcyclohexanone **1e** (54.9 μL, 0.3 mmol), aniline **2a** (18.2 μL, 0.2 mmol), α-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue

was purified by column chromatography on silica gel (petroleum ether/Et_3N = 100:0.5, R_f = 0.65) to afford 37.3 mg of **4e** as a white solid in 55% yield, mp = 125-127 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.63 (s, 1H), 7.42-7.38 (m, 2H), 7.35-7.31 (m, 1H), 7.25-7.18 (m, 9H), 6.77 (s, 1H), 1.72 (q, J = 7.4 Hz, 2H), 1.37 (s, 6H), 0.73 (t, J = 7.4 Hz, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 141.9, 140.6, 138.7, 137.1, 132.7, 129.1, 128.8, 128.1, 128.0, 127.9, 127.1, 126.9, 121.1, 117.4, 110.0, 103.8, 37.8, 37.1, 29.0, 9.3; HRMS (ESI) calcd for: $C_{25}H_{26}N^+$ $(M+H)^+$ 340.2060, found: 340.2062.

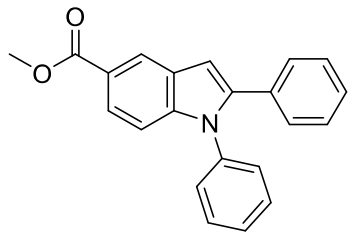
5-*n*-Pentyl-1,2-diphenyl-1*H*-indole (4f).



4-*n*-Pentylcyclohexanone **1f** (56.7 μL, 0.3 mmol), aniline **2a** (18.2 μL, 0.2 mmol), *α*-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/Et_3N = 100:0.5, R_f = 0.50) to afford 33.2 mg of **4f** as a white solid in 49% yield, mp = 67-69 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.51 (s, 1H), 7.44-7.38 (m, 2H), 7.37-7.31 (m, 1H), 7.29-7.22 (m, 8H), 7.05 (dd, J = 8.4, 1.1 Hz, 1H), 6.77 (s, 1H), 2.78-2.69 (m, 2H), 1.75-1.65 (m, 2H), 1.42-1.34 (m, 4H), 0.96-0.89 (m, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 140.7, 138.7, 137.5, 135.3, 132.7, 129.2, 128.8, 128.4, 128.1, 127.9, 127.1, 127.0, 123.4, 119.6, 110.3, 103.4, 36.0, 32.0, 31.6, 22.6, 14.1; HRMS (ESI) calcd for: $C_{25}H_{26}N^+$ $(M+H)^+$ 340.2060, found: 340.2062.

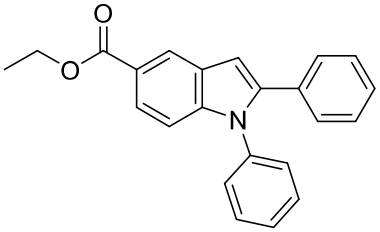
Methyl-1,2-diphenyl-1*H*-indole-5-carboxylate (4g).



Methyl-4-oxocyclohexanecarboxylate **1g** (46.8 mg, 0.3 mmol), aniline **2a** (18.2 μL, 0.2 mmol), *α*-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate/Et_3N = 100:4:0.5, R_f = 0.35) to afford 39.9 mg of **4g** as a yellow solid in 61% yield, mp = 153-155 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 8.45 (d, J = 1.2 Hz, 1H), 7.87 (dd, J = 8.7, 1.6 Hz, 1H), 7.45-7.35 (m, 3H), 7.28-7.19 (m, 8H), 6.87 (d, J = 0.5 Hz, 1H), 3.94 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 168.0, 142.1, 141.2, 137.8, 131.8, 129.4, 128.8, 128.2, 127.9, 127.7, 127.6, 123.6, 123.4, 122.6, 110.2, 104.5, 51.8; HRMS (ESI) calcd for: $C_{22}H_{18}NO_2^+$ $(M+H)^+$ 328.1332, found: 328.1336.

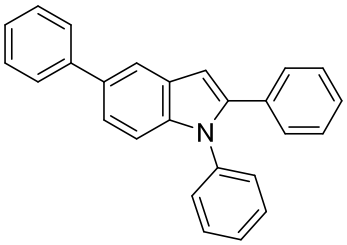
Ethyl-1,2-diphenyl-1*H*-indole-5-carboxylate (4h).



Ethyl-4-oxocyclohexane-carboxylate **1h** (47.8 μL, 0.3 mmol), aniline **2a** (18.2 μL, 0.2 mmol), *α*-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate/Et_3N = 100:4:0.5, R_f = 0.35) to afford 40.9 mg of **4h** as a yellow solid in 60% yield, mp = 105-107 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 8.46-8.45 (m, 1H), 7.89-7.87 (m, 1H), 7.45-7.35 (m, 3H), 7.29-7.23 (m, 8H), 6.89-6.85 (m, 1H), 4.41 (q, J = 7.1 Hz, 2H), 1.43 (t, J = 7.1 Hz, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 167.5, 142.1, 141.3, 137.9, 131.9, 129.4, 128.9, 128.2, 127.9, 127.7, 127.6, 123.6, 123.3, 123.0, 110.2, 104.5, 60.6, 14.4; HRMS (ESI) calcd for: $C_{23}H_{20}NO_2^+$ $(M+H)^+$ 342.1489, found: 342.1494.

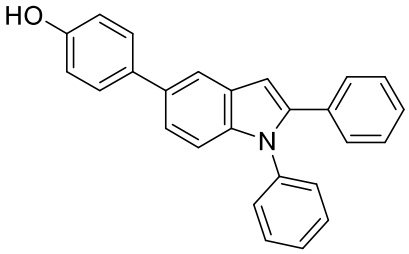
1,2,5-Triphenyl-1*H*-indole (4i).



4-Phenylcyclohexanone **1i** (52.3 mg, 0.3 mmol), aniline **2a** (18.2 μL, 0.2 mmol), *α*-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 2.0 equiv) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate/Et_3N = 100:0.5:0.5, R_f = 0.30) to afford 38.6 mg of **4i** as a light yellow solid in 56% yield, mp = 152-154 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.89 (s, 1H),, 7.68-7.66 (m, 2H), 7.47-7.39 (m, 5H), 7.37-7.31 (m, 3H), 7.30-7.22 (m, 7H), 6.85 (s, 1H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 142.4, 141.4, 138.5, 138.4, 134.3, 132.4, 129.3, 128.9, 128.7, 128.6, 128.2, 127.9, 127.4, 127.2, 126.4, 122.1, 119.0, 110.8, 104.0; HRMS (ESI) calcd for: $C_{26}H_{20}N^+$ $(M+H)^+$ 346.1590, found: 346.1595.

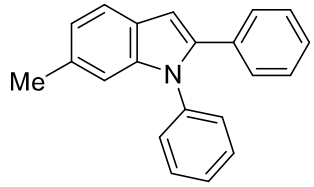
4-(1,2-Diphenyl-1*H*-indol-5-yl)phenol (4j).



4-(4-Hydroxyphenyl)cyclohexanone **1j** (57.1 mg, 0.3 mmol), aniline **2a** (18.2 μL, 0.2 mmol), *α*-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 2.0 equiv) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate/Et_3N = 100:12:0.5, R_f = 0.30) to afford 26.0 mg of **4j** as a light yellow solid in 36% yield, mp = 128-130 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.82 (d, J = 0.9 Hz, 1H), 7.54-7.52 (m, 2H), 7.45-7.39 (m, 2H), 7.38-7.31 (m, 3H), 7.30-7.22 (m, 7H), 6.92-6.90 (m, 2H), 6.83 (s, 1H). The peak of the hydroxyl group did not appeared. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 154.5, 141.3, 138.5, 138.2, 135.1, 133.9, 132.4, 129.3, 128.9, 128.7, 128.5, 128.2, 127.9, 127.3, 127.2, 121.9, 118.5, 115.5, 110.8, 103.9; HRMS (ESI) calcd for: $C_{26}H_{20}NO^+$ $(M+H)^+$ 362.1539, found 362.1541.

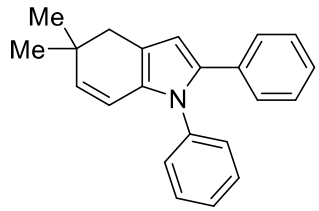
6-Methyl-1,2-diphenyl-1*H*-indole (4k).



3-Methylcyclohexanone **1k** (36.8 μL, 0.3 mmol), aniline **2a** (18.2 μL, 0.2 mmol), α-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/Et_3N = 100:0.5, R_f = 0.50) to afford 28.9 mg of **4k** as a white solid in 51% yield, mp = 134-136 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.56 (d, J = 8.0 Hz, 1H), 7.42-7.39 (m, 2H), 7.35-7.31 (m, 1H), 7.25-7.18 (m, 7H), 7.08 (s, 1H), 7.01 (d, J = 8.0 Hz, 1H), 6.75 (s, 1H), 2.42 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 140.1, 139.4, 138.6, 132.6, 132.2, 129.2, 128.8, 128.7, 128.1, 128.0, 127.0, 126.0, 122.4, 120.2, 110.4, 103.6, 21.9; HRMS (ESI) calcd for: $C21H18N^+$ $(M+H)^+$, 284.1433, found: 284.1434.

5,5-Dimethyl-1,2-diphenyl-4,5-dihydro-1*H*-indole (4l).

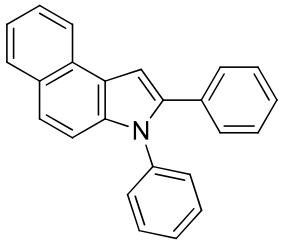


4,4-Dimethylcyclohexanone **1l** (37.8 mg, 0.3 mmol), aniline **2a** (18.2 μL, 0.2 mmol), α-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (14.2 μL, 0.2 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue

was purified by column chromatography on silica gel (petroleum ether/Et_3N = 100:0.5, R_f = 0.65) to afford 14.4 mg of **4l** as a white solid in 24% yield, mp = 138-140 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.37-7.28 (m, 3H), 7.17-7.11 (m, 4H), 7.10-7.03 (m, 3H), 6.27 (s, 1H), 6.02 (d, J = 9.9 Hz, 1H), 5.39 (d, J = 9.9 Hz, 1H), 2.64 (s, 2H), 1.13 (s, 6H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 138.4, 135.0, 133.1, 133.0, 130.6, 128.9, 127.9, 127.8, 127.6, 127.0, 125.6, 117.8, 115.0, 109.5, 36.7, 33.4, 28.6; HRMS (ESI) calcd for: $C_{22}H_{22}N^+$ $(M+H)^+$ 300.1747, found: 300.1747.

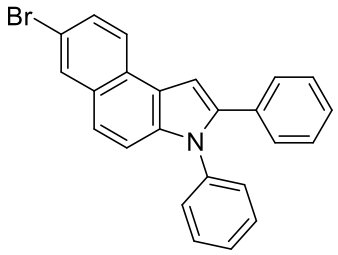
2,3-Diphenyl-3*H*-benzo[*e*]indole (4m).



3,4-Dihydro-1*H*-naphthalen-2-one **1m** (39.6 μL, 0.3 mmol), aniline **2a** (18.2 μL, 0.2 mmol), α-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (14.2 μL, 0.1 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/Et_3N = 100:0.5, R_f = 0.50) to afford 37.7 mg of **4n** as a white solid in 59% yield, mp = 145-147 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 8.31 (d, J = 8.2 Hz, 1H), 7.90 (d, J = 8.1 Hz, 1H), 7.60-7.56 (m, 2H), 7.48-7.36 (m, 5H) , 7.34-7.20 (m, 8H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 139.0, 138.3, 135.4, 132.6, 129.6, 129.3, 128.8, 128.5, 128.2, 127.9, 127.5, 127.0, 125.9, 123.6, 123.3, 123.1, 123.0, 112.2, 102.7; HRMS (ESI) calcd for: $C_{24}H_{18}N^+$ $(M+H)^+$ 320.1434, found: 320.1438.

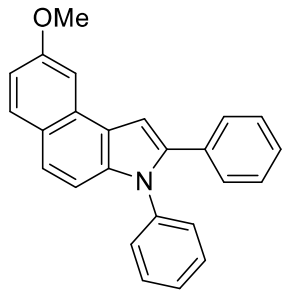
7-Bromo-2,3-diphenyl-3*H*-benzo[*e*]indole (4n).



6-Bromo-2-tetralone **1n** (48.3 μL, 0.3 mmol), aniline **2a** (18.2 μL, 0.2 mmol), *α*-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (14.2 μL, 0.2 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/Et_3N = 100:0.5, R_f = 0.55) to afford 47.6 mg of **4n** as a white solid in 60% yield, mp = 208-210 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 8.17 (d, J = 8.7 Hz, 1H), 8.05 (d, J = 1.9 Hz, 1H), 7.64 (dd, J = 8.7, 1.9 Hz, 1H), 7.48-7.39 (m, 5H), 7.32-7.24 (m, 8H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 139.5, 138.1, 135.5, 132.3, 130.9, 130.5, 129.4, 128.9, 128.8, 128.2, 128.1, 127.7, 127.3, 126.4, 124.8, 123.2, 122.0, 117.1, 113.3, 102.5; HRMS (ESI) calcd for: $C_{24}H_{17}BrN^+$ $(M+H)^+$ 398.0539, found: 398.0540.

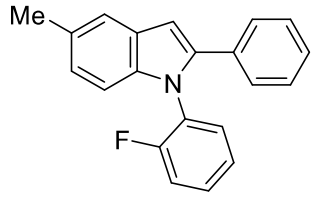
8-Methoxy-2,3-diphenyl-3*H*-benzo[*e*]indole (4o).



7-Methoxy-2-tetralone **1o** (46.8 μL, 0.3 mmol), aniline **2a** (18.2 μL, 0.2 mmol), *α*-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (14.2 μL, 0.2 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate/Et_3N = 100:0.5:0.5, R_f = 0.35) to afford 33.5 mg of **4o** as a light yellow solid in 48% yield, mp = 122-124 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.79 (d, J = 8.9 Hz, 1H), 7.62 (d, J = 2.5 Hz, 1H), 7.49 (d, J = 8.9 Hz, 1H), 7.45-7.36 (m, 3H), 7.32-7.20 (m, 9H), 7.09 (dd, J = 8.8, 2.5 Hz, 1H), 4.00 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 158.0, 138.7, 138.4, 135.9, 132.6, 130.1, 129.3, 129.0, 128.7, 128.1, 127.5, 127.0, 124.5, 123.0, 122.7, 115.1, 109.8, 102.7, 102.7, 55.4; HRMS (ESI) calcd for: $C_{25}H_{20}NO^+$ $(M+H)^+$ 350.1539, found: 350.1539.

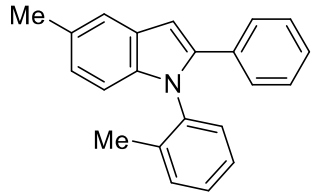
1-(2-Fluorophenyl)-5-methyl-2-phenyl-1*H*-indole (5a).



4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), 2-fluoroaniline **2b** (19.7 μL, 0.2 mmol), *α*-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/Et_3N = 100:0.5, R_f = 0.65) to afford 30.7 mg of **5a** as a white solid in 51% yield, mp = 106-108 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.47 (s, 1H), 7.35-7.31 (m, 1H), 7.30-7.21 (m, 6H), 7.19-7.13 (m, 2H), 7.06-6.95 (m, 2H), 6.74 (s, 1H), 2.46 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 158.0 (d, $J_{C\text{-}F}$ = 251.7 Hz), 141.3, 137.5, 132.4, 130.4, 130.1, 129.3 (d, $J_{C\text{-}F}$ = 7.6 Hz), 128.7, 128.3, 128.2, 127.4, 126.6 (d, $J_{C\text{-}F}$ = 12.7 Hz), 124.5 (d, $J_{C\text{-}F}$ = 3.9 Hz), 124.0, 120.3, 116.8 (d, $J_{C\text{-}F}$ = 19.8 Hz), 110.2 (d, $J_{C\text{-}F}$ = 0.8 Hz), 103.4, 21.4; HRMS (ESI) calcd for: $C_{21}H_{17}NF^+$ $(M+H)^+$ 302.1339, found: 302.1342.

5-Methyl-2-phenyl-1-(*o*-tolyl)-1*H*-indole (5b).

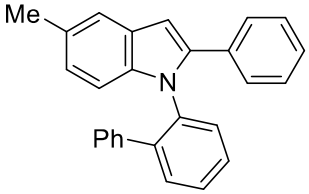


4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), 2-methylaniline **2c** (21.7 μL, 0.2 mmol), *α*-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/Et_3N = 100:0.5, R_f = 0.50) to afford 26.7 mg of **5b** as a white solid in 45% yield, mp = 125-127 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.48 (s, 1H), 7.31-7.24 (m, 6H), 7.22-7.17 (m, 3H), 6.98-6.96 (m, 1H), 6.85-6.82 (m, 1H), 6.76-6.75 (m, 1H), 2.46 (s, 3H), 1.86 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 141.1, 137.7, 137.4, 136.9, 132.8, 131.1, 129.6, 129.5, 128.4, 128.3, 128.2,

128.1, 127.2, 126.8, 123.7, 120.1, 110.4, 102.1, 21.4, 17.5; HRMS (ESI) calcd for: $C22H20N^+$ ($M+H^+$) 298.1590, found: 298.1597.

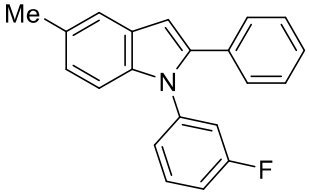
1-([1,1'-Biphenyl]-2-yl)-5-methyl-2-phenyl-1H-indole (5c).



4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), 2-aminodiphenyl **2d** (33.8 mg, 0.2 mmol), *α*-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate/Et_3N = 100:0.5:0.5, R_f = 0.55) to afford 23.0 mg of **5c** as a white solid in 32% yield, mp = 142-144 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.67-7.65 (m, 1H), 7.53 (td, J = 7.6, 1.6 Hz, 1H), 7.46 (td, J = 7.5, 1.3 Hz, 1H), 7.42 (s, 1H), 7.35 (dd, J = 7.6, 1.4 Hz, 1H), 7.20 (d, J = 8.3 Hz, 1H), 7.11-6.99 (m, 5H), 6.93-6.89 (m, 2H), 6.73-6.71 (m, 2H), 6.45 (s, 1H), 6.37-6.32 (m, 2H), 2.48 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 141.1, 140.5, 138.3, 137.5, 136.0, 132.5, 131.3, 129.6, 129.5, 128.5, 128.2, 128.1, 127.9, 127.8, 127.7, 127.6, 126.7, 126.6, 123.7, 120.1, 110.4, 102.2, 21.5; HRMS (ESI) calcd for: $C_{27}H_{22}N^+$ $(M+H)^+$ 360.1747, found 360.1749.

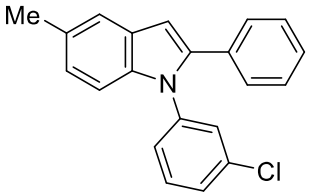
1-(3-Fluorophenyl)-5-methyl-2-phenyl-1*H*-indole (5f).



4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), 3-fluoroaniline **2g** (19.6 μL, 0.2 mmol), *α*-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/Et_3N = 100:0.5, R_f = 0.55) to afford 37.4 mg of **5f** as a white solid in 62% yield, mp = 119-121 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.46 (s, 1H), 7.37-7.31 (m, 1H), 7.26-7.19 (m, 6H), 7.05-6.97 (m, 4H), 6.72 (s, 1H), 2.46 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 162.8 (d, J_{C-F} = 247.8 Hz), 140.6, 140.2 (d, J_{C-F} = 9.9 Hz), 137.2, 132.3, 130.3, 130.3 (d, J_{C-F} = 9.0 Hz), 128.8, 128.6, 128.2, 127.4, 124.2, 123.7 (d, J_{C-F} = 3.1 Hz), 120.3, 115.2 (d, J_{C-F} = 22.8 Hz), 114.0 (d, J_{C-F} = 21.0 Hz), 110.1, 103.9, 21.4; HRMS (ESI) calcd for: $C_{21}H_{17}NF^+$ $(M+H)^+$ 302.1339, found: 302.1342.

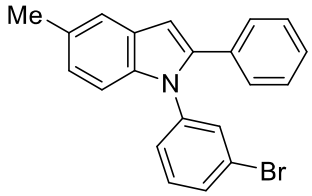
1-(3-Chlorophenyl)-5-methyl-2-phenyl-1*H*-indole (5g).



4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), 3-chloroaniline **2h** (21.6 μL, 0.2 mmol), α-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/Et_3N = 100:0.5, R_f = 0.55) to afford 38.1 mg of **5g** as a white solid in 60% yield, mp = 136-138 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.45 (s, 1H), 7.31-7.27 (m, 3H), 7.25-7.21 (m, 5H), 7.18 (d, J = 8.4 Hz, 1H), 7.06-7.00 (m, 2H), 6.71 (s, 1H), 2.46 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 140.5, 139.9, 137.2, 134.6, 132.2, 130.3, 130.1, 128.8, 128.6, 128.2, 127.9, 127.4, 127.2, 126.2, 124.2, 120.3, 110.0, 104.0, 21.4; HRMS (ESI) calcd for: $C_{21}H_{17}ClN^+$ $(M+H)^+$ 318.1044, found: 318.1047.

1-(3-Bromophenyl)-5-methyl-2-phenyl-1*H*-indole (5h).

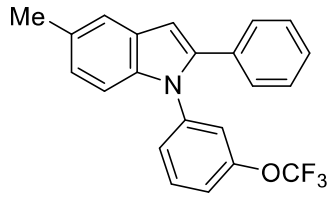


4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), 3-bromoaniline **2i** (22.2 μL, 0.2 mmol), α-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue

was purified by column chromatography on silica gel (petroleum ether/Et_3N = 100:0.5, R_f = 0.55) to afford 44.9 mg of **5h** as a white solid in 62% yield, mp = 124-126 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.48-7.44 (m, 3H), 7.25-7.17 (m, 7H), 7.08 (d, J = 8.0 Hz, 1H), 7.02 (d, J = 8.4 Hz, 1H), 6.71 (s, 1H), 2.46 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 140.6, 140.0, 137.2, 132.2, 130.7, 130.4, 130.4, 130.1, 128.8, 128.6, 128.3, 127.4, 126.7, 124.2, 122.5, 120.3, 110.0, 104.0, 21.4; HRMS (ESI) calcd for: $C_{21}H_{17}BrN^+$ $(M+H)^+$ 362.0539, found: 362.0541.

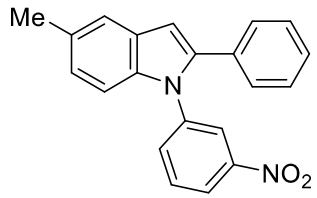
5-Methyl-2-phenyl-1-(3-(trifluoromethoxy)phenyl)-1*H*-indole (5i).



4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), 3-(trifluoromethoxy)-aniline **2j** (27.3 μL, 0.2 mmol), α-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/Et_3N = 100:0.5, R_f = 0.65) to afford 44.8 mg of **5i** as a white solid in 61% yield, mp = 119-121 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.47 (s, 1H), 7.41 (t, J = 8.1 Hz, 1H), 7.25-7.16 (m, 8H), 7.09 (s, 1H), 7.03 (d, J = 8.4 Hz, 1H), 6.73 (s, 1H), 2.47 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 149.5 (q, $J_{C\text{-}F}$ = 2.0 Hz), 140.6, 140.1, 137.0, 132.2, 130.5, 130.2, 128.9, 128.7, 128.3, 127.5, 126.1, 124.3, 120.6, 120.4, 120.3 (q, $J_{C\text{-}F}$ = 258.0 Hz), 119.3, 109.9, 104.2, 21.4; HRMS (ESI) calcd for: $C_{22}H_{17}F_3NO^+$ $(M+H)^+$ 368.1257, found: 368.1257.

5-methyl-1-(3-nitrophenyl)-2-phenyl-1*H*-indole (5j).

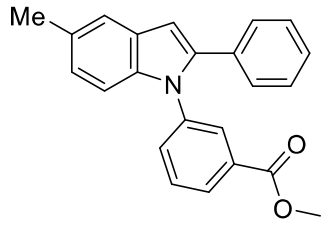


4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), 3-nitroaniline **2k** (27.6 mg, 0.2 mmol), α-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20

mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate/Et_3N = 100:1:0.5, R_f = 0.35) to afford 40.0 mg of **5j** as a yellow solid in 61% yield, mp = 162-164 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 8.19-8.15 (m, 2H), 7.56-7.51 (m, 1H), 7.49-7.45 (m, 2H), 7.27-7.18 (m, 6H), 7.07-7.04 (m, 1H), 6.76 (s, 1H), 2.47 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 148.7, 140.5, 140.0, 137.0, 133.8, 131.8, 130.9, 130.0, 128.9, 128.8, 128.4, 127.7, 124.6, 122.4, 121.6, 120.6, 109.6, 104.9, 21.3; HRMS (ESI) calcd for: $C_{21}H_{17}N_2O_2^+$ $(M+H)^+$ 329.1284, found: 329.1285.

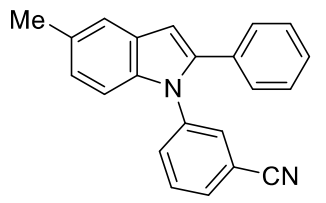
Methyl-3-(5-methyl-2-phenyl-1*H*-indol-1-yl)benzoate (5k).



4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), methyl 3-aminobenzoate **2l** (30.2 mg, 0.2 mmol), α-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate/Et_3N = 100:1:0.5, R_f = 0.30) to afford 39.6 mg of **5k** as a white solid in 58% yield, mp = 150-152 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 8.05 (m, 1H), 8.02-8.00 (m, 1H), 7.44 (m, 2H), 7.30-7.27 (m, 1H), 7.25-7.22 (m, 5H), 7.16 (d, J = 8.4 Hz, 1H), 7.02-7.00 (m, 1H), 6.73 (s, 1H), 3.90 (s, 3H), 2.47 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 166.2, 140.6, 139.0, 137.3, 132.4, 132.2, 131.3, 130.2, 129.3, 128.8, 128.6, 128.6, 128.2, 128.0, 127.3, 124.1, 120.3, 110.0, 103.8, 52.3, 21.3; HRMS (ESI) calcd for: $C_{23}H_{20}NO_2^+$ $(M+H)^+$ 342.1489, found 342.1490.

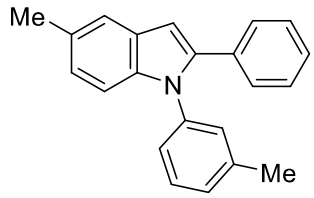
3-(5-Methyl-2-phenyl-1*H*-indol-1-yl)benzonitrile (5l).



4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), 3-aminobenzonitrile **2m** (23.6 mg, 0.2 mmol), *α*-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate/Et_3N = 100:2:0.5, R_f = 0.30) to afford 28.3 mg of **5l** as a white solid in 46% yield, mp = 132-134 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.60 (d, J = 7.6 Hz, 1H), 7.54 (s, 1H), 7.51-7.46 (m, 2H), 7.42 (d, J = 8.2 Hz, 1H), 7.27-7.24 (m, 3H), 7.21-7.18 (m, 2H), 7.15 (d, J = 8.4 Hz, 1H), 7.04 (d, J = 8.4 Hz, 1H), 6.74 (s, 1H), 2.47 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 140.4, 139.7, 136.9, 132.3, 131.8, 130.9, 130.8, 130.4, 130.2, 128.8, 128.7, 128.4, 127.7, 124.5, 120.5, 117.9, 113.4, 109.6, 104.7, 21.3; HRMS (ESI) calcd for: $C_{22}H_{17}N_2^+$ $(M+H)^+$ 309.1386, found: 309.1389.

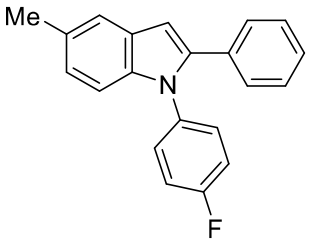
5-Methyl-2-phenyl-1-(*m*-tolyl)-1*H*-indole (5m).



4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), 3-methylaniline **2n** (121.9 μL, 0.2 mmol), *α*-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/Et_3N = 100:0.5, R_f = 0.50) to afford 27.3 mg of **5m** as a white solid in 46% yield, mp = 116-118 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.45 (s, 1H), 7.27-7.15 (m, 7H), 7.13 (d, J = 7.6 Hz, 1H), 7.08 (s, 1H), 7.00-6.98 (m, 2H), 6.71 (s, 1H), 2.46 (s, 3H), 2.33 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 140.7, 139.1, 138.6, 137.5, 132.7, 129.8, 128.9, 128.7, 128.4, 128.1, 127.8, 127.1, 125.1, 123.8, 120.1, 110.4, 103.1, 99.9, 21.4, 21.3; HRMS (ESI) calcd for: $C_{22}H_{20}N^+$ $(M+H^+)$ 298.1590, found: 298.1596.

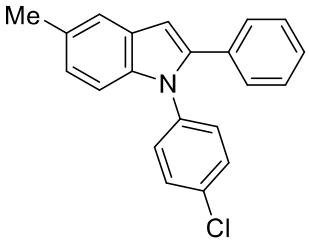
1-(4-Fluorophenyl)-5-methyl-2-phenyl-1*H*-indole (5n).



4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), 4-fluoroaniline **2o** (19.3 μL, 0.2 mmol), *α*-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/Et_3N = 100:0.5, R_f = 0.55) to afford 38.6 mg of **5n** as a white solid in 64% yield, mp = 134-136 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.46 (s, 1H), 7.25-7.18 (m, 7H), 7.14-7.07 (m, 3H), 7.01 (dd, J = 8.4, 1.4 Hz, 1H), 6.71 (s, 1H), 2.46 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm) δ 161.3 (d, $J_{C\text{-}F}$ = 247.1 Hz), 140.7, 137.5, 134.7 (d, $J_{C\text{-}F}$ = 3.0 Hz), 132.4, 130.1, 129.5 (d, $J_{C\text{-}F}$ = 8.5 Hz), 128.8, 128.4, 128.2, 127.3, 124.0, 120.2, 116.1 (d, $J_{C\text{-}F}$ = 22.7 Hz), 110.0, 103.3, 21.4; HRMS (ESI) calcd for: $C_{21}H_{17}NF^+$ $(M+H)^+$ 302.1339, found: 302.1342.

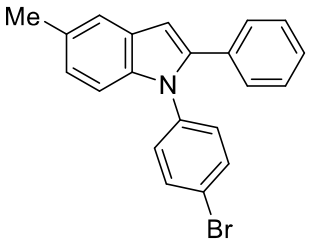
1-(4-Chlorophenyl)-5-methyl-2-phenyl-1*H*-indole (5o) [3].



4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), 4-chloroaniline **2p** (18.2 μL, 0.2 mmol), *α*-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/Et_3N = 100:0.5, R_f = 0.55) to afford 37.5 mg of **5o** as a white solid in 59% yield, mp = 158-160 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.46 (s, 1H), 7.38-7.35 (m, 2H), 7.26-7.23 (m, 5H), 7.18-7.14 (m, 3H), 7.01 (dd, J = 8.4, 1.1 Hz, 1H), 6.72 (s, 1H), 2.46 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm) δ 140.5, 137.2, 132.6, 132.3, 130.2, 129.4, 129.1, 129.0, 128.8, 128.5, 128.2, 127.3, 124.1, 120.3, 110.0, 103.8, 21.4.

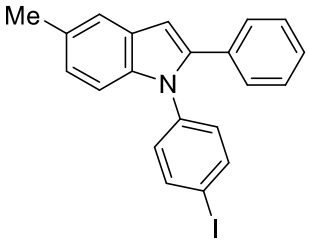
1-(4-Bromophenyl)-5-methyl-2-phenyl-1*H*-indole (5p).



4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), 4-bromoaniline **2q** (23.4 μL, 0.2 mmol), *α*-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.2 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/Et_3N = 100:0.5, R_f = 0.55) to afford 44.9 mg of **5p** as a white solid in 62% yield, mp = 148-150 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.54-7.50 (m, 2H), 7.46 (s, 1H), 7.27-7.23 (m, 5H), 7.16 (d, J = 8.4 Hz, 1H), 7.13-7.08 (m, 2H), 7.02 (m, 1H), 6.72 (s, 1H), 2.46 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 140.5, 137.7, 137.1, 132.4, 132.2, 130.2, 129.3, 128.8, 128.6, 128.2, 127.3, 124.1, 120.5, 120.3, 110.0, 103.8, 21.4; HRMS (ESI) calcd for: $C_{21}H_{17}BrN^+$ $(M+H)^+$ 362.0539, found: 362.0540.

1-(4-Iodophenyl)-5-methyl-2-phenyl-1*H*-indole (5q).

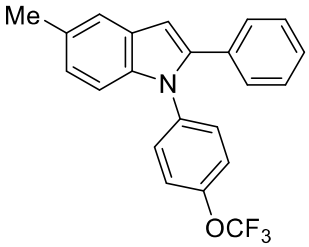


4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), 4-iodoaniline **2r** (24.6 μL, 0.2 mmol), *α*-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/Et_3N = 100:0.5, R_f = 0.55) to afford 50.7 mg of **5q** as a white solid in 62% yield, mp = 164-166 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.71 (d, J = 8.5 Hz, 2H), 7.46 (s, 1H), 7.29-7.24 (m, 5H), 7.17 (d, J = 8.4 Hz, 1H), 7.02-6.97 (m, 3H), 6.71 (s, 1H), 2.46 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 140.4, 138.4, 138.3, 137.1, 132.3, 130.3, 129.6, 128.8, 128.6, 128.3, 127.4, 124.1,

120.3, 110.0, 103.9, 91.9, 21.4; HRMS (ESI) calcd for: $C_{21}H_{17}IN^+$ $(M+H)^+$ 410.0400, found: 410.0402.

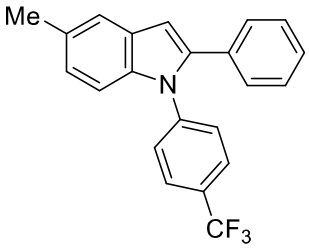
5-Methyl-2-phenyl-1-(4-(trifluoromethoxy)phenyl)-1*H*-indole (5r).



4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), 4-(trifluoromethoxy)aniline **2s** (27.4 μL, 0.2 mmol), *α*-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/Et_3N = 100:0.5, R_f = 0.65) to afford 46.3 mg of **5r** as a white solid in 63% yield, mp = 105-107 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.47 (s, 1H), 7.25-7.22 (m, 9H), 7.17 (d, J = 8.4 Hz, 1H), 7.02 (d, J = 8.4 Hz, 1H), 6.73 (s, 1H), 2.47 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 147.6, 140.6, 137.3, 137.2, 132.3, 130.3, 129.1, 128.8, 128.6, 128.3, 127.4, 124.2, 121.6, 120.4, 120.4 (q, J_{CF} = 257.5 Hz), 110.0, 103.9, 21.3; HRMS (ESI) calcd for: $C_{22}H_{17}F_3NO^+$ $(M+H)^+$ 368.1257, found: 368.1257.

5-Methyl-2-phenyl-1-(4-(trifluoromethyl)phenyl)-1*H*-indole (5s).

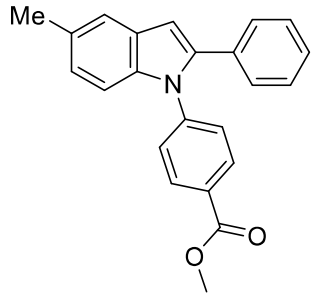


4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), 4-(trifluoromethyl)aniline **2t** (25.6 μL, 0.2 mmol), *α*-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h.

The residue was purified by column chromatography on silica gel (petroleum ether/Et_3N = 100:0.5, R_f = 0.65) to afford 41.5 mg of **5s** as a white solid in 58% yield, mp = 100-102 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.65 (d, J = 8.2 Hz, 2H), 7.47 (s, 1H), 7.35-7.32 (m, 2H), 7.26-7.20 (m, 6H), 7.03 (d, J = 8.4 Hz, 1H), 6.74 (s, 1H), 2.47 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 141.9, 140.5, 137.0, 132.2, 130.6, 128.9, 128.8, 128.6, 128.3, 127.9, 127.5, 126.3 (q, J_{CF} = 3.7 Hz), 124.4, 123.9 (q, J_{CF} = 272.1 Hz), 120.5, 109.9, 104.6, 21.3; HRMS (ESI) calcd for: $C_{22}H_{17}F_3N^+$ $(M+H)^+$ 352.1308, found: 352.1309.

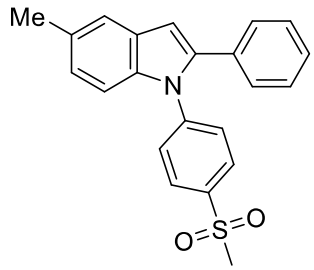
Methyl-4-(5-methyl-2-phenyl-1*H*-indol-1-yl)benzoate (5t).



4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), methyl 4-aminobenzoate **2u** (30.2 mg, 0.2 mmol), α-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate/Et_3N = 100:1:0.5, R_f = 0.35) to afford 39.6 mg of **5t** as a light yellow solid in 58% yield, mp = 148-150 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 8.08-8.05 (m, 2H), 7.47 (s, 1H), 7.31-7.27 (m, 2H), 7.25-7.22 (m, 6H), 7.03 (d, J = 8.3 Hz, 1H), 6.74 (s, 1H), 3.93 (s, 3H), 2.47 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 166.4, 142.8, 140.5, 136.9, 132.2, 130.6, 130.5, 128.8, 128.8, 128.3, 127.4, 127.4, 124.3, 120.4, 110.0, 104.5, 99.9, 52.2, 21.3; HRMS (ESI) calcd for: $C_{23}H_{20}NO_2^+$ $(M+H)^+$ 342.1489, found 342.1490.

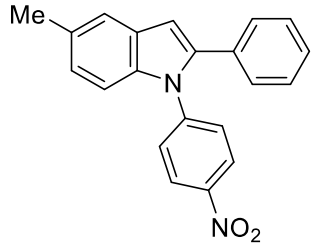
5-Methyl-1-(4-(methylsulfonyl)phenyl)-2-phenyl-1*H*-indole (5u).



4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), 4-methylsulfonylaniline **2v** (34.2 mg, 0.2 mmol), *α*-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate/Et_3N = 100:20:0.5, R_f = 0.35) to afford 41.2 mg of **5u** as a light yellow solid in 57% yield, mp = 138-140 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.98-7.94 (m, 2H), 7.48 (s, 1H), 7.42-7.39 (m, 2H), 7.28-7.19 (m, 6H), 7.05 (d, J = 8.4 Hz, 1H), 6.75 (s, 1H), 3.10 (s, 3H), 2.47 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 143.5, 140.3, 138.2, 136.6, 131.8, 130.8, 128.9, 128.8, 128.5, 128.4, 128.1, 127.6, 124.5, 120.6, 109.7, 105.2, 44.4, 21.3; HRMS (ESI) calcd for: $C_{22}H_{20}NO_2S^+$ $(M+H)^+$ 362.1209, found: 362.1212.

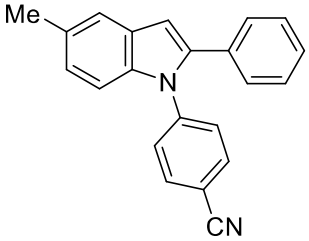
5-Methyl-1-(4-nitrophenyl)-2-phenyl-1*H*-indole (5v).



4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), 4-nitroaniline **2w** (27.6 mg, 0.2 mmol), *α*-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate/Et_3N = 100:1:0.5, R_f = 0.30) to afford 37.4 mg of **5v** as a red solid in 57% yield, mp = 160-162 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.27-8.24 (m, 2H), 7.48 (s, 1H), 7.38-7.35 (m, 2H), 7.30-7.26 (m, 4H), 7.23-7.20 (m, 2H), 7.06 (dd, J = 8.4, 1.0 Hz, 1H), 6.77 (s, 1H), 2.47 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm) δ 145.6, 144.5, 140.3, 136.6, 131.9, 131.1, 129.0, 128.9, 128.5, 128.0, 127.8, 127.8, 124.7, 120.7, 109.8, 105.6, 21.3; HRMS (ESI) calcd for: $C_{21}H_{17}N_2O_2^+$ $(M+H)^+$ 329.1284, found: 329.1286.

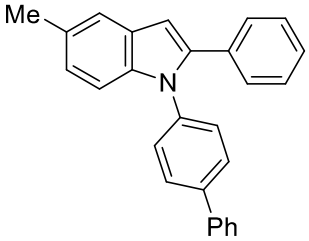
4-(5-methyl-2-phenyl-1*H*-indol-1-yl)benzonitrile (5w).



4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), 4-aminobenzonitrile **2x** (23.6 mg, 0.2 mmol), α-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate/Et_3N = 100:2:0.5, R_f = 0.30) to afford 28.4 mg of **5w** as a white solid in 46% yield, mp = 151-153 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.64-7.62 (m, 2H), 7.45 (s, 1H), 7.28-7.16 (m, 8H), 7.03 (d, J = 8.4 Hz, 1H), 6.73 (s, 1H), 2.45 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm) δ 142.6, 140.2, 136.6, 133.1, 131.9, 130.9, 128.9, 128.8, 128.4, 128.0, 127.6, 124.5, 120.6, 118.3, 110.1, 109.7, 105.2, 21.3; HRMS (ESI) calcd for: $C_{22}H_{17}N_2^+$ $(M+H)^+$ 309.1386, found: 309.1389.

1-([1,1'-Biphenyl]-4-yl)-5-methyl-2-phenyl-1*H*-indole (5x).

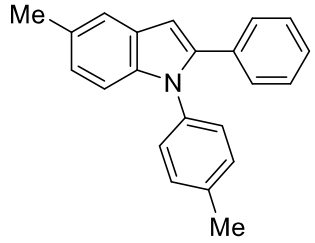


4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), 4-aminobiphenyl **2y** (33.8 mg, 0.2 mmol), α-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue

was purified by column chromatography on silica gel (petroleum ether/ethyl acetate/Et_3N = 100:0.5:0.5, R_f = 0.35) to afford 39.5 mg of **5x** as a white solid in 55% yield, mp = 165-167 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.65-7.61 (m, 4H), 7.49-7.43 (m, 3H), 7.39-7.34 (m, 1H), 7.32-7.28 (m, 4H), 7.26-7.22 (m, 4H), 7.02 (dd, J = 8.4, 1.2 Hz, 1H), 6.74 (s, 1H), 2.48 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 140.7, 140.1, 139.6, 137.9, 137.4, 132.6, 130.0, 128.8, 128.6, 128.2, 128.1, 127.7, 127.5, 127.2, 127.0, 124.0, 122.4, 120.2, 110.3, 103.5, 21.4; HRMS (ESI) calcd for: $C_{27}H_{22}N^+$ $(M+H)^+$ 360.1747, found 360.1749.

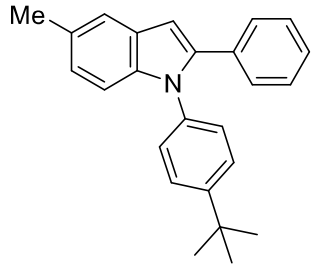
5-Methyl-2-phenyl-1-(p-tolyl)-1*H*-indole (5y) [3].



4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), 4-methylaniline **2z** (22.5 μL, 0.2 mmol), α-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/Et_3N = 100:0.5, R_f = 0.50) to afford 27.4 mg of **5y** as a white solid in 46% yield, mp = 134-136 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.46 (s, 1H), 7.26-7.09 (m, 10H), 7.00-6.98 (m, 1H), 6.70 (s, 1H), 2.46 (s, 3H), 2.39 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 140.8, 137.6, 136.8, 136.1, 132.8, 129.8, 128.8, 128.4, 128.1, 127.7, 127.1, 123.8, 122.2, 120.1, 110.4, 103.0, 21.4, 21.1.

1-(4-(*tert*-Butyl)phenyl)-5-methyl-2-phenyl-1*H*-indole (5z).

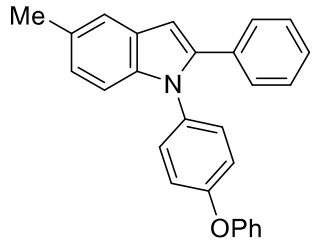


4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), 4-*tert*-butylaniline **2aa** (32.5 μL, 0.2 mmol),

α-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether to petroleum ether/Et_3N = 100:0.5, R_f = 0.55) to afford 30.6 mg of **5z** as a white solid in 45% yield. **5z**: mp = 113-115 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.45 (s, 1H), 7.40 – 7.38 (m, 2H), 7.25 – 7.13 (m, 8H), 6.98 (d, J = 8.4 Hz, 1H), 6.70 (s, 1H), 2.46 (s, 3H), 1.34 (s, 9H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 150.0, 140.7, 137.5, 135.9, 132.8, 129.8, 128.8, 128.4, 128.0, 127.3, 127.0, 126.0, 123.7, 120.0, 110.5, 103.0, 34.6, 31.4, 21.4; HRMS (ESI) calcd for: $C_{25}H_{26}N^+$ $(M+H)^+$ 340.2060, found: 340.2063.

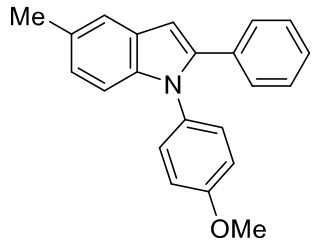
5-methyl-1-(4-phenoxyphenyl)-2-phenyl-1*H*-indole (5aa).



4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), 4-phenoxyaniline **2ab** (37.0 mg, 0.2 mmol), α-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate/Et_3N = 100:0.75:0.5, R_f = 0.45) to afford 35.3 mg of **5aa** as a light yellow solid in 47% yield, mp = 168-170 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.46 (s, 1H), 7.39-7.35 (m, 2H), 7.27-7.23 (m, 5H), 7.19-7.13 (m, 4H), 7.07-7.00 (m, 5H), 6.71 (s, 1H), 2.47 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 156.7, 156.2, 140.8, 137.6, 133.6, 132.6, 129.9, 129.9, 129.2, 128.8, 128.4, 128.1, 127.2, 123.9, 123.7, 120.2, 119.2, 119.0, 110.2, 103.1, 21.4. HRMS (ESI) calcd for: $C_{27}H_{22}NO^+$ $(M+H)^+$ 376.1696, found: 376.1696.

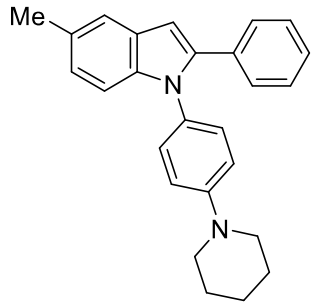
1-(4-Methoxyphenyl)-5-methyl-2-phenyl-1*H*-indole (5ab, Cas: 1131891-07-0) [2].



4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), 4-methoxyaniline **2ac** (24.6 mg, 0.2 mmol), *α*-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate/Et_3N = 100:0.5:0.5, R_f = 0.35) to afford 26.3 mg of **5ab** as a light yellow solid in 42% yield, mp = 178-180 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.45 (s, 1H), 7.27-7.20 (m, 5H), 7.17-7.10 (m, 3H), 6.99 (d, J = 8.5 Hz, 1H), 6.92-6.90 (m, 2H), 6.70 (s, 1H), 3.83 (s, 3H), 2.46 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 158.4, 140.8, 137.8, 132.7, 131.5, 129.7, 129.0, 128.8, 128.3, 128.1, 127.1, 123.7, 120.0, 114.4, 110.3, 102.7, 55.4, 21.4.

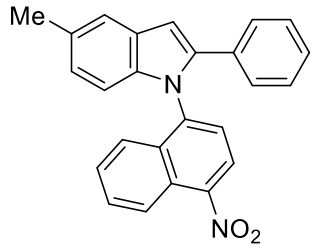
5-Methyl-2-phenyl-1-(4-(piperidin-1-yl)phenyl)-1*H*-indole (5ac).



4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), 4-piperidinoaniline **2ad** (35.2g, 0.2 mmol), *α*-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate/Et_3N = 100:1:0.5, R_f = 0.25) to afford 22.7 mg of **5ac** as a light yellow solid in 31% yield, mp = 157-159 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.44 (s, 1H), 7.31-7.27 (m, 2H), 7.24-7.18 (m, 3H), 7.15-7.07 (m, 3H), 6.97 (dd, J = 8.4, 1.2 Hz, 1H), 6.96-6.88 (m, 2H), 6.68 (s, 1H), 3.22-3.16 (m, 4H), 2.45 (s, 3H), 1.74-1.69 (m, 4H), 1.62-1.56 (m, 2H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm) δ 150.9, 140.8, 137.9, 132.9, 129.8, 129.6, 128.8, 128.5, 128.2, 128.0, 126.9, 123.6, 120.0, 116.4, 110.5, 102.4, 50.3, 25.8, 24.2, 21.4; HRMS (ESI) calcd for: $C_{26}H_{27}N_2^+$ $(M+H)^+$ 367.2169, found: 367.2171.

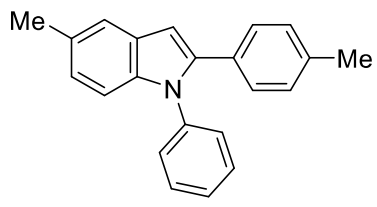
5-Methyl-1-(4-nitronaphthalen-1-yl)-2-phenyl-1*H*-indole (5ad).



4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), 4-nitro-1-naphthylamine **2ae** (37.6 mg, 0.2 mmol), α-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μl, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate/Et_3N = 100:1.5:0.5, R_f = 0.25) to afford 24.2 mg of **5ad** as a light yellow solid in 32% yield, mp = 180-182 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.64 (d, J = 8.8 Hz, 1H), 8.18 (d, J = 8.1 Hz, 1H), 7.77-7.71 (m, 2H), 7.56-7.51 (m, 2H), 7.29 (d, J = 8.1 Hz, 1H), 7.19-7.13 (m, 5H), 6.93 (dd, J = 8.4, 1.1 Hz, 1H), 6.89 (s, 1H), 6.66 (d, J = 8.4 Hz, 1H), 2.47 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm) δ 145.9, 142.1, 141.4, 138.5, 131.9, 131.9, 130.7, 130.0, 128.8, 128.4, 128.4, 128.1, 127.7, 126.1, 125.5, 124.7, 124.4, 123.8, 123.6, 120.5, 110.6, 104.4, 21.4; HRMS (ESI) calcd for: $C_{25}H_{19}N_2O_2^+$ $(M+H)^+$ 379.1441, found: 379.1443.

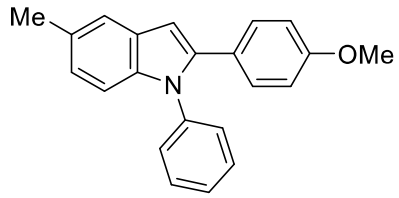
5-Methyl-1-phenyl-2-(*p*-tolyl)-1*H*-indole (6a).



4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), aniline **2a** (18.2 μL, 0.2 mmol), 2-hydroxy-1-(p-tolyl)ethan-1-one **3b** (37.5 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/Et_3N = 100:0.5, R_f = 0.50) to afford 30.9 mg of **6a** as a white solid in 54% yield, mp = 139-141 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.45 (s, 1H), 7.41-7.37 (m, 2H), 7.33-7.29 (m, 1H), 7.24-7.21 (m, 2H), 7.18-7.13 (m, 3H), 7.03 (d, J = 8.0 Hz, 2H), 6.98 (dd, J = 8.4, 0.9 Hz, 1H), 6.68 (s, 1H), 2.45 (s, 3H), 2.29 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 140.8, 138.8, 137.4, 137.0, 129.9, 129.7, 129.2, 128.8, 128.7, 128.5, 128.0, 126.9, 123.7, 120.0, 110.2, 102.9, 21.4, 21.2; HRMS (ESI) calcd for: $C_{22}H_{20}N^+$ $(M+H^+)$ 298.1590, found: 298.1597.

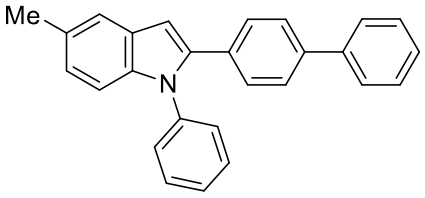
2-(4-Methoxyphenyl)-5-methyl-1-phenyl-1*H*-indole (6b).



4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), aniline **2a** (18.2 μL, 0.2 mmol), 2-hydroxy-1-(4-methoxyphenyl)ethan-1-one **3c** (41.5 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate/Et_3N = 100:1:0.5, R_f = 0.30) to afford 35.1 mg of **6b** as a light yellow solid in 56% yield, mp = 160-162 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.44 (s, 1H), 7.41-7.38 (m, 2H), 7.34-7.30 (m, 1H), 7.24-7.21 (m, 2H), 7.18-7.14 (m, 3H), 6.99-6.96 (m, 1H), 6.78-6.75 (m, 2H), 6.64 (s, 1H), 3.76 (s, 3H), 2.46 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 158.8, 140.6, 138.8, 137.2, 130.0, 129.9, 129.2, 128.6, 128.0, 126.9, 125.2, 123.5, 119.9, 113.6, 110.2, 102.4, 55.2, 21.4; HRMS (ESI) calcd for: $C_{22}H_{20}NO^+$ $(M+H)^+$ 314.1539, found: 314.1541.

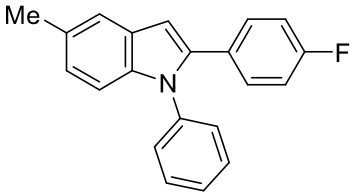
2-([1,1'-Biphenyl]-4-yl)-5-methyl-1-phenyl-1*H*-indole (6c).



4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), aniline **2a** (18.2 μL, 0.2 mmol), 1-([1,1'-biphenyl]-4-yl)-2-hydroxyethan-1-one **3d** (53.1 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate/Et_3N = 100:0.5:0.5, R_f = 0.40) to afford 39.5 mg of **6c** as a light yellow solid in 55% yield, mp = 179-181 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.58-7.54 (m, 2H), 7.48-7.26 (m, 13H), 7.19 (d, J = 8.4 Hz, 1H), 7.01 (dd, J = 8.4, 1.2 Hz, 1H), 6.78 (s, 1H), 2.47 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm) δ 140.4, 140.3, 139.7, 138.7, 137.6, 131.6, 130.0, 129.3, 129.0, 128.7, 128.5, 128.0, 127.3, 127.1, 126.9, 126.8, 124.0, 120.2, 110.3, 103.4, 21.4; HRMS (ESI) calcd for: $C_{27}H_{22}N^+$ $(M+H)^+$ 360.1747, found 360.1749.

2-(4-Fluorophenyl)-5-methyl-1-phenyl-1*H*-indole (6d).

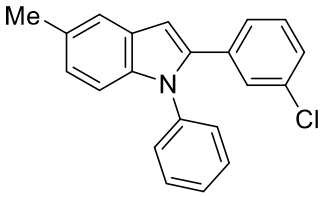


4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), aniline **2a** (18.2 μL, 0.2 mmol), 1-(4-fluorophenyl)-2-hydroxyethan-1-one **3e** (38.5 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/Et_3N = 100:0.5, R_f = 0.55) to afford 36.8 mg of **6d** as a white solid in 61% yield, mp = 155-157 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.46 (s, 1H), 7.42-7.38 (m, 2H), 7.35-7.32 (m, 1H), 7.24-7.15 (m, 5H), 7.02-6.98 (m, 1H), 6.96-6.88 (m, 2H), 6.67 (s, 1H), 2.46 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm) δ 162.0 (d, $J_{C\text{-}F}$ = 247.3 Hz), 139.7, 138.5, 137.4, 130.5 (d, $J_{C\text{-}F}$ = 8.0 Hz),

130.1, 129.3, 128.8 (d, $J_{C\text{-}F}$ = 2.9 Hz), 128.4, 127.9, 127.1, 124.0, 120.1, 115.2 (d, $J_{C\text{-}F}$ = 21.6 Hz), 110.3, 103.2, 21.4; HRMS (ESI) calcd for: $C_{21}H_{17}NF^+$ $(M+H)^+$ 302.1339, found: 302.1342.

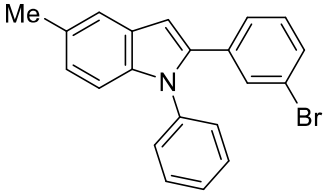
2-(3-Chlorophenyl)-5-methyl-1-phenyl-1*H*-indole (6e).



4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), aniline **2a** (18.2 μL, 0.2 mmol), 1-(3-chlorophenyl)-2-hydroxyethan-1-one **3f** (42.6 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 ^oC for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether to petroleum ether/Et_3N = 100:0.5, R_f = 0.55) to afford 36.9 mg of **6e** as a white solid in 58% yield, mp = 121-123 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.46 (s, 1H), 7.44-7.40 (m, 2H), 7.37-7.33 (m, 1H), 7.32-7.30 (m, 1H), 7.24-7.21 (m, 2H), 7.19-7.16 (m, 2H), 7.12 (t, J = 7.8 Hz, 1H), 7.05-7.00 (m, 2H), 6.74 (s, 1H), 2.46 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 139.0, 138.3, 137.6, 134.4, 134.0, 130.2, 129.3, 129.3, 128.6, 128.3, 127.9, 127.3, 127.1, 126.8, 124.4, 120.3, 110.4, 104.0, 21.4; HRMS (ESI) calcd for: $C_{21}H_{17}ClN^+$ $(M+H)^+$ 318.1044, found: 318.1047.

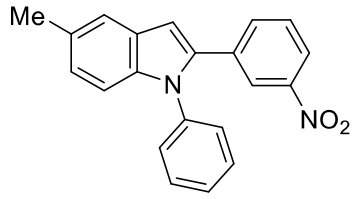
2-(3-Bromophenyl)-5-methyl-1-phenyl-1*H*-indole (6f).



4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), aniline **2a** (18.2 μL, 0.2 mmol), 1-(3-bromophenyl)-2-hydroxyethan-1-one **3g** (53.2 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 ^oC for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/Et_3N = 100:0.5, R_f = 0.55) to afford 43.5 mg of **6f** as a white solid in 60% yield, mp = 102-104 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.48-7.45 (m, 2H), 7.43-7.40 (m, 2H), 7.37-7.30 (m, 2H), 7.23-7.20 (m, 2H), 7.19-7.16 (m, 1H), 7.07-7.00 (m, 3H), 6.73 (s, 1H), 2.46 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm) δ 138.9, 138.3, 137.6, 134.7, 131.5, 130.2, 130.0, 129.5, 129.3, 128.3, 127.9, 127.3, 127.2, 124.4, 122.2, 120.3, 110.4, 104.0, 21.4; HRMS (ESI) calcd for: $C_{21}H_{17}BrN^{+}$ $(M+H)^{+}$ 362.0539, found: 362.0541.

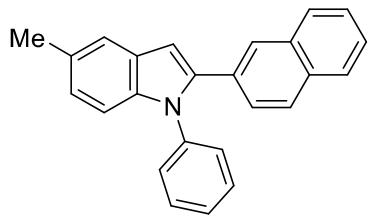
5-Methyl-2-(3-nitrophenyl)-1-phenyl-1*H*-indole (6g).



4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), aniline **2a** (18.2 μL, 0.2 mmol), 2-hydroxy-1-(3-nitrophenyl)ethan-1-one **3h** (45.3 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 ^{o}C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate/Et_3N = 100:1:0.5, R_f = 0.35) to afford 23.0 mg of **6g** as a yellow solid in 35% yield, mp = 146-148 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.19-8.15 (m, 1H), 8.07-8.02 (m, 1H), 7.51-7.47 (m, 2H), 7.46-7.42 (m, 2H), 7.40-7.35 (m, 2H), 7.26-7.22 (m, 2H), 7.21-7.16 (m, 1H), 7.08-7.03 (m, 1H), 6.85 (s, 1H), 2.47 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm) δ 148.1, 138.0, 137.9, 137.7, 134.3, 134.2, 130.5, 129.6, 129.0, 128.1, 127.9, 127.7, 124.9, 123.2, 121.7, 120.5, 110.5, 104.8, 21.4; HRMS (ESI) calcd for: $C_{21}H_{17}N_2O_2^{+}$ $(M+H)^{+}$ 329.1284, found: 329.1285.

5-Methyl-2-(naphthalen-2-yl)-1-phenyl-1*H*-indole (6h).

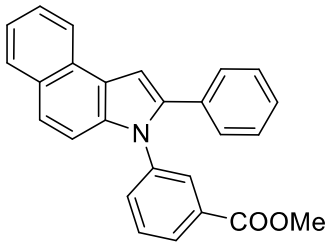


4-Methylcyclohexanone **1a** (37.6 μL, 0.3 mmol), aniline **2a** (18.2 μL, 0.2 mmol),, 2-hydroxy-1-(naphthalen-2-yl)ethan-1-one **3i** (46.6 mg, 0.25 mmol), morpholine (3.5 μL, 20

mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate/Et_3N = 100:0.5:0.5, R_f = 0.40) to afford 34.7 mg of **6h** as a white solid in 52% yield, mp = 172-174 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.77-7.73 (m, 2H), 7.69-7.64 (m, 2H), 7.49 (s, 1H), 7.44-7.36 (m, 4H), 7.34-7.30 (m, 2H), 7.29-7.27 (m, 2H), 7.24-7.20 (m, 1H), 7.02 (dd, J = 8.4, 1.1 Hz, 1H), 6.84 (s, 1H), 2.48 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 140.6, 138.7, 137.6, 133.2, 132.3, 130.1, 130.0, 129.3, 128.6, 128.1, 127.9, 127.7, 127.6, 127.5, 127.1, 126.7, 126.2, 126.0, 124.0, 120.2, 110.3, 103.8, 21.4; HRMS (ESI) calcd for: $C_{25}H_{20}N^+$ $(M+H)^+$ 334.1590, found: 334.1593.

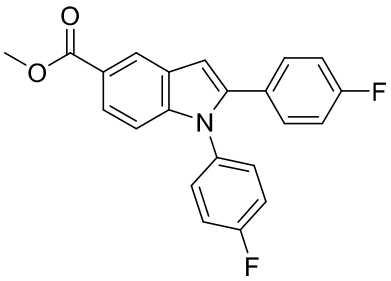
Methyl-3-(2-phenyl-3*H*-benzo[*e*]indol-3-yl)benzoate (7).



3,4-Dihydro-1*H*-naphthalen-2-one **1m** (39.6 μL, 0.3 mmol), 3-aminobenzoate **2n** (30.2 mg, 0.2 mmol), α-hydroxyacetophenone **3a** (34.7 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (14.1 μL, 0.2 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate/Et_3N = 100:5:0.5, R_f = 0.30) to afford 42.3 mg of **7** as a yellow solid in 56% yield, mp = 170-172 °C.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 8.31 (d, J = 8.2 Hz, 1H), 8.12 (t, J = 1.7 Hz, 1H), 8.08 (dt, J = 7.8, 1.3 Hz, 1H), 7.91 (d, J = 8.0 Hz, 1H), 7.61-7.57 (m, 2H), 7.51-7.43 (m, 2H), 7.40-7.33 (m, 3H), 7.31-7.23 (m, 5H), 3.92 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 166.2, 138.9, 138.7, 135.3, 132.7, 132.2, 131.5, 129.6, 129.5, 128.9, 128.6, 128.6, 128.3, 127.8, 127.2, 126.0, 123.8, 123.4, 123.0, 111.8, 103.2, 52.4; HRMS (ESI) calcd for: $C_{26}H_{20}NO_2^+$ $(M+H)^+$ 378.1489, found: 378.1489.

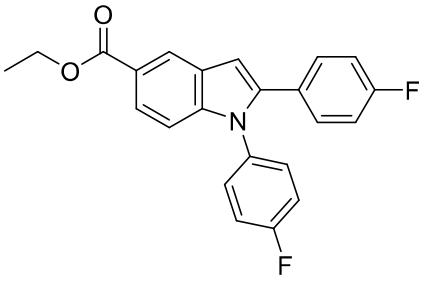
Methyl-1,2-bis(4-fluorophenyl)-1*H*-indole-5-carboxylate (8).



Methyl-4-oxocyclohexanecarboxylate **1g** (46.8 mg, 0.3 mmol), 4-fluoroaniline **2q** (19.3 μL, 0.2 mmol), 1-(4-fluorophenyl)-2-hydroxyethan- 1-one **3e** (38.5 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate/Et_3N = 100:5:0.5, R_f = 0.35) to afford 43.6 mg of **8** as a yellow solid in 60% yield, mp = 126-128 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.43 (d, J = 0.9 Hz, 1H), 7.89 (dd, J = 8.7, 1.5 Hz, 1H), 7.23-7.19 (m, 5H), 7.16-7.11 (m, 2H), 6.99-6.95 (m, 2H), 6.82 (s, 1H), 3.95 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm) δ 168.1, 162.3 (d, $J_{C\text{-}F}$ = 248.5 Hz), 161.7 (d, $J_{C\text{-}F}$ = 248.5 Hz), 141.2, 141.1, 133.6 (d, $J_{C\text{-}F}$ = 3.2 Hz), 130.6 (d, $J_{C\text{-}F}$ = 8.2 Hz), 129.5 (d, $J_{C\text{-}F}$ = 8.6 Hz), 127.8 (d, $J_{C\text{-}F}$ = 3.4 Hz), 127.6, 123.8, 123.4, 122.8, 116.5 (d, $J_{C\text{-}F}$ = 22.8 Hz), 115.4 (d, $J_{C\text{-}F}$ = 21.7 Hz), 110.0, 104.5, 51.9; HRMS (ESI) calcd for: $C_{22}H_{16}F_2NO_2^+$ $(M+H)^+$ 364.1144, found: 364.1150.

Ethyl-1,2-bis(4-fluorophenyl)-1*H*-indole-5-carboxylate (9).



Ethyl-4-oxocyclohexane-carboxylate **1h** (47.8 μL, 0.3 mmol), 4-fluoroaniline **2q** (19.3 μL, 0.2 mmol), 1-(4-fluorophenyl)-2-hydroxyethan- 1-one **3e** (38.5 mg, 0.25 mmol), morpholine (3.5 μL, 20 mol %), KI (6.6 mg, 20 mol%) and DMSO (28.4 μL, 0.4 mmol) reacted in toluene (0.1 M), at 150 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate/Et_3N = 100:5:0.5, R_f = 0.35) to afford 43.8 mg of **9** as a yellow solid in 58% yield, mp = 137-139 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.44 (d, J = 1.2 Hz, 1H), 7.90 (dd, J = 8.7, 1.5 Hz, 1H), 7.23-7.19 (m, 5H), 7.17-7.12 (m, 2H), 7.01-6.95 (m, 2H), 6.83 (s, 1H), 4.41 (q, J = 7.1 Hz, 2H), 1.43 (t, J = 7.1 Hz, 3H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm) δ 167.4, 162.4 (d, $J_{C\text{-}F}$ = 248.5 Hz), 161.7 (d, $J_{C\text{-}F}$ = 248.6 Hz), 141.3, 141.1, 133.7 (d, $J_{C\text{-}F}$ = 3.2 Hz), 130.7 (d, $J_{C\text{-}F}$ = 8.2 Hz), 129.6 (d, $J_{C\text{-}F}$ = 8.6 Hz), 127.8 (d, $J_{C\text{-}F}$ = 3.4 Hz), 127.6, 123.9, 123.4, 123.3, 116.5 (d, $J_{C\text{-}F}$ = 22.8 Hz), 115.4 (d, $J_{C\text{-}F}$ = 21.7 Hz), 110.0, 104.5, 60.7, 14.4; HRMS (ESI) calcd for: $C_{23}H_{18}F_2NO_2^+$ $(M+H)^+$ 378.1300, found: 378.1305.

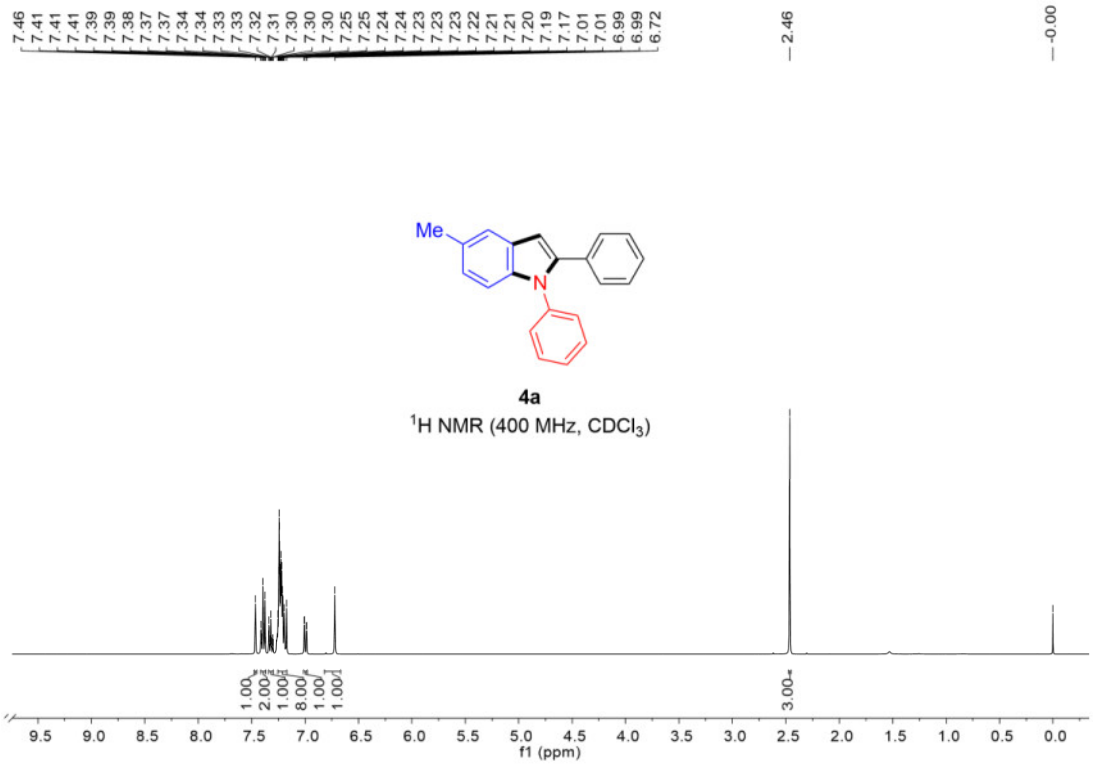
7. Reference

[1] H. Huang, R. Hou, H. Wang and L. Chen, *Org. Prep. Pro. Int.* 2006, **38**, 473.

[2] J. Barluenga, A. Jimenez-Aquino, F. Aznar and C. Valdes, *J. Am. Chem. Soc.*, 2009, **131**, 4031.

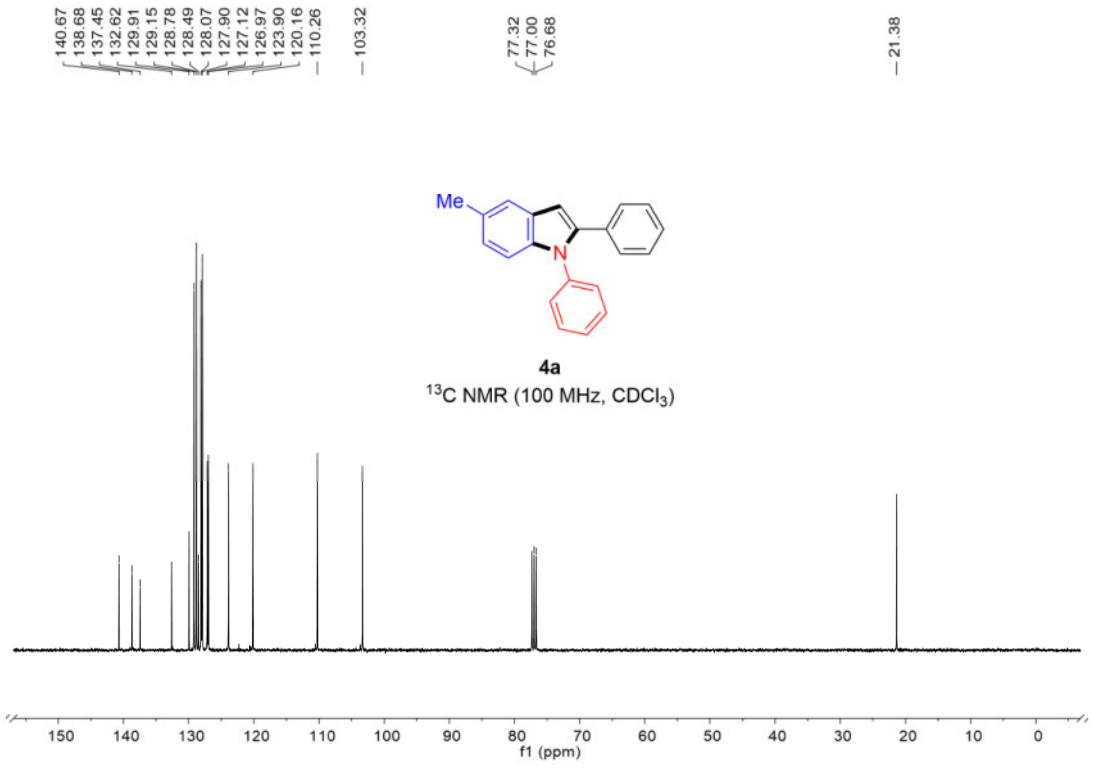
[3] J. Gao, Y. Shao, J. Zhu, J. Zhu, H. Mao, X. Wang and X. Lv, *J. Org. Chem.*, 2014, **79**, 9000.

8. ^{1}H and ^{13}C NMR spectra of products



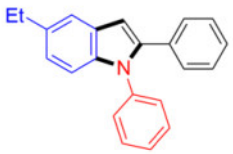
4a

^{1}H NMR (400 MHz, $CDCl_3$)



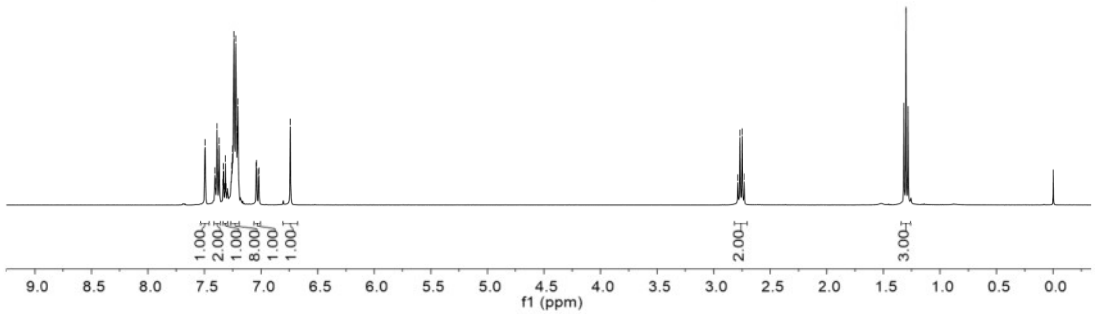
4a

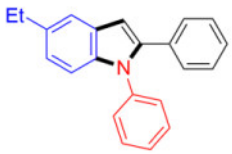
^{13}C NMR (100 MHz, $CDCl_3$)



4b

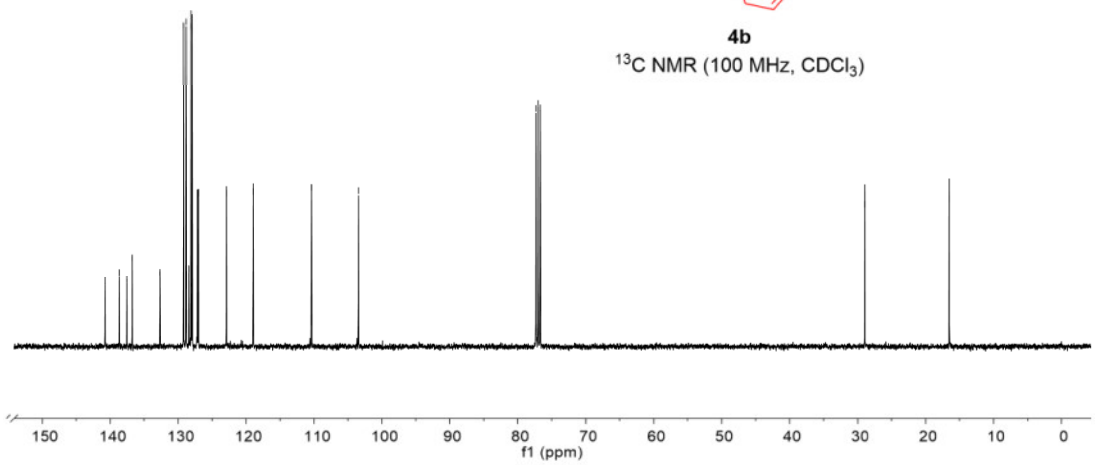
^{1}H NMR (400 MHz, $CDCl_3$)

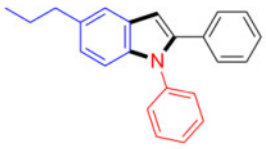




4b

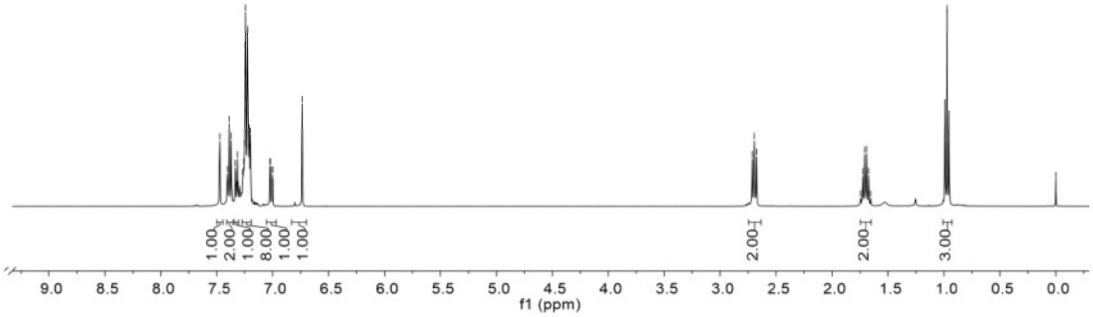
^{13}C NMR (100 MHz, $CDCl_3$)

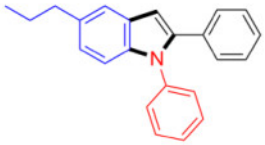




4c

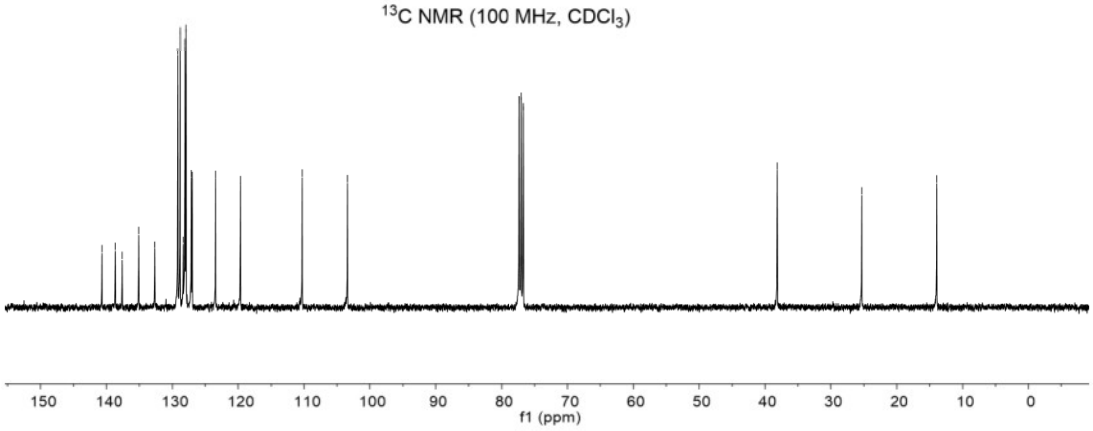
^{1}H NMR (400 MHz, $CDCl_3$)

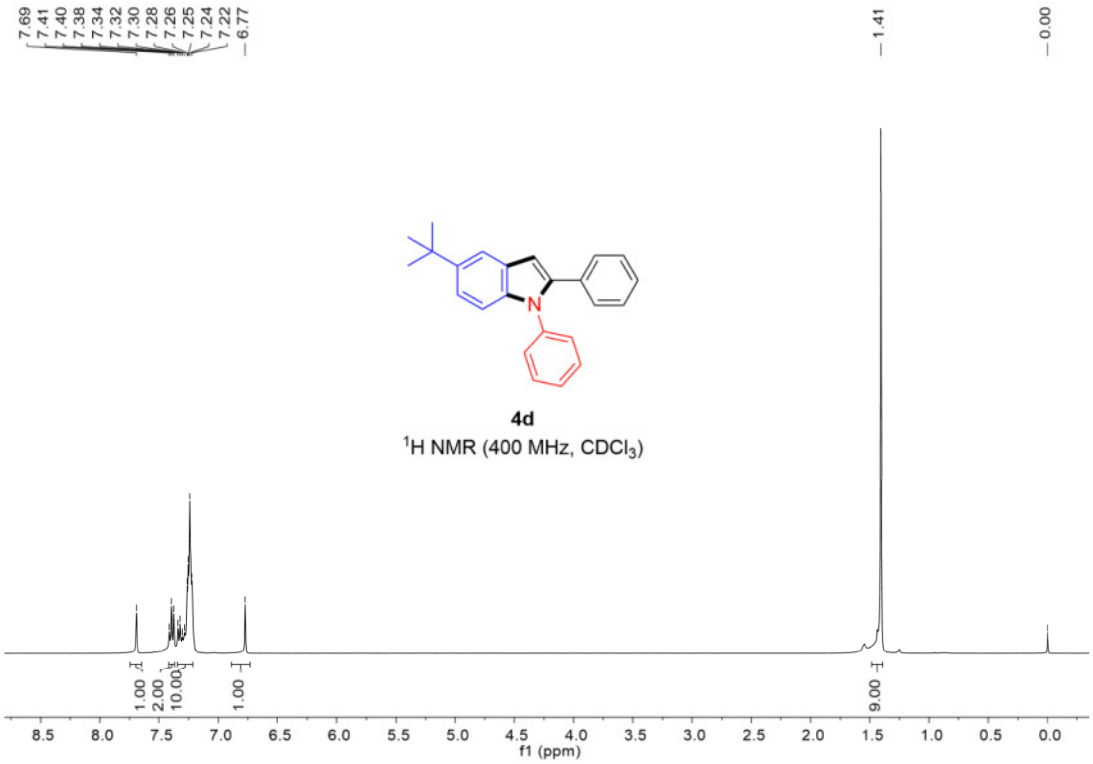


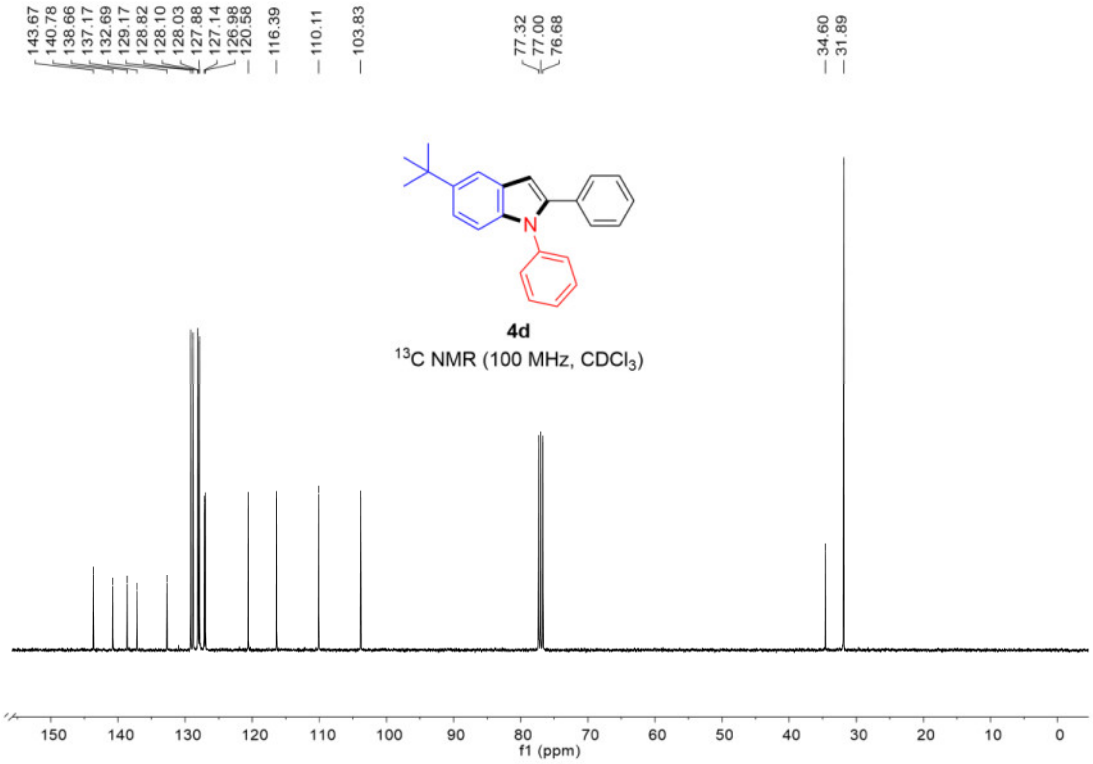


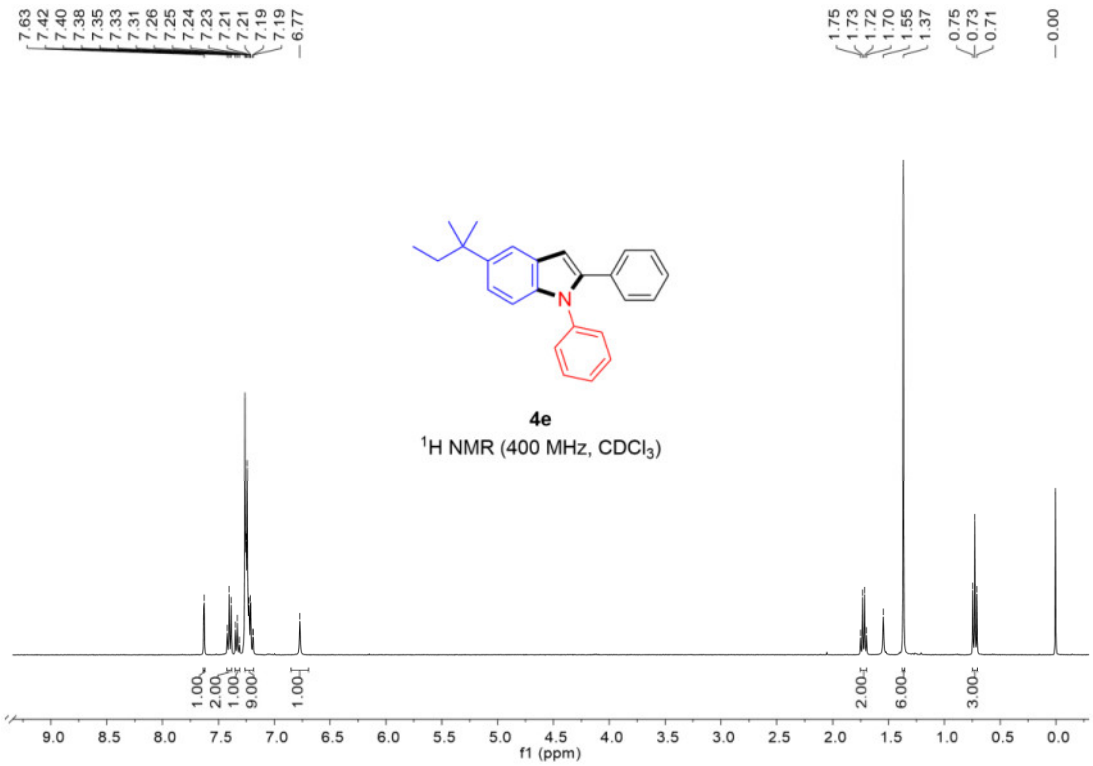
4c

^{13}C NMR (100 MHz, $CDCl_3$)



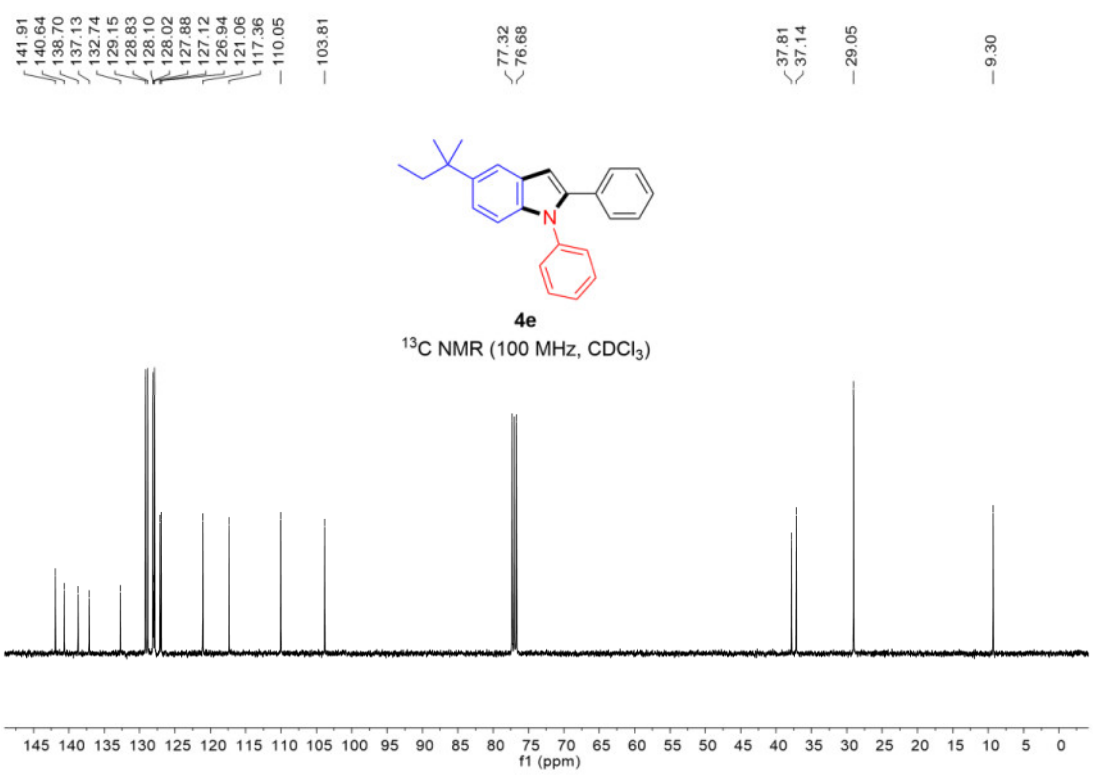

7.69
7.41
7.40
7.38
7.34
7.32
7.30
7.28
7.26
7.25
7.24
7.22
6.77
1.41
0.00
4d
1H NMR (400 MHz, CDCl3)
1.00
2.00
10.00
1.00
9.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


143.67
140.78
138.66
137.17
132.69
129.17
128.82
128.10
128.03
127.88
127.14
126.98
120.58
116.39
110.11
103.83
77.32
77.00
76.68
34.60
31.89
4d
13C NMR (100 MHz, CDCl3)
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



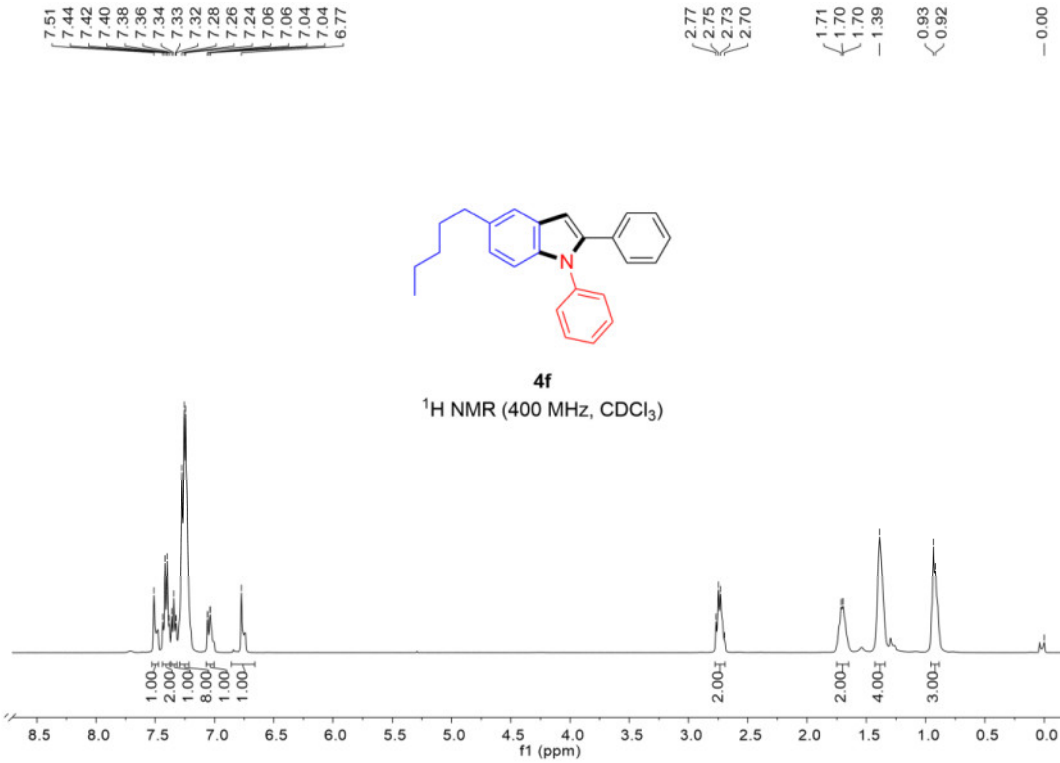
4e

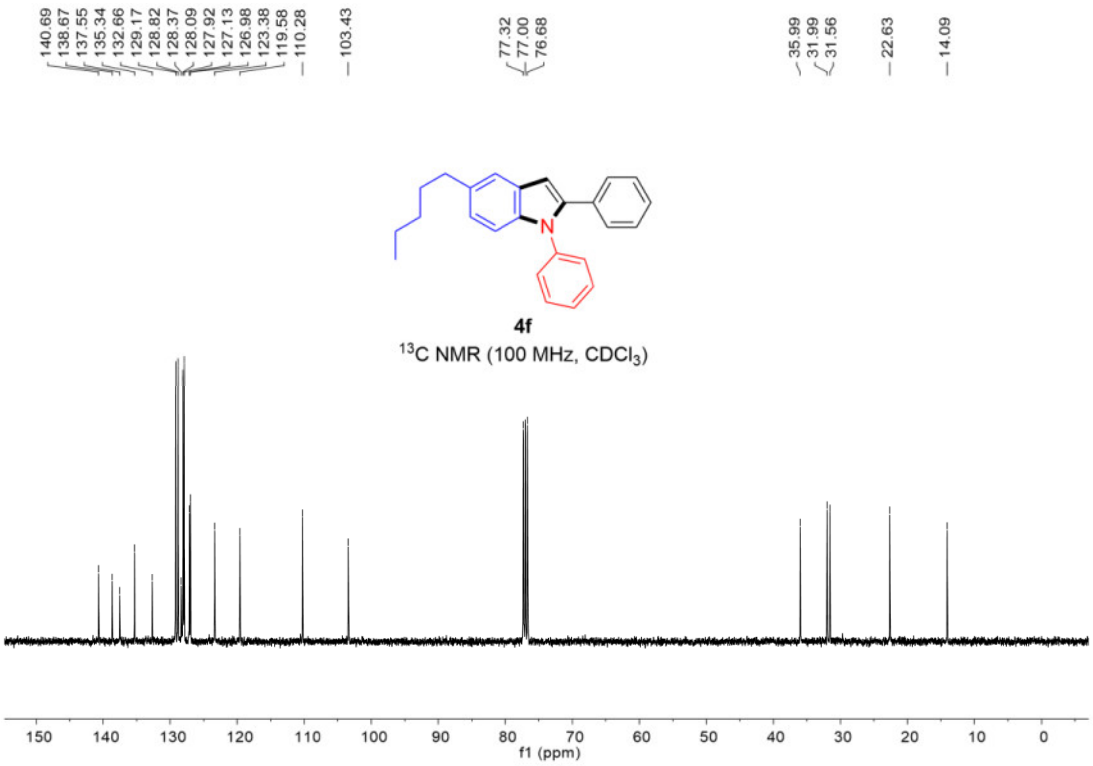
^{1}H NMR (400 MHz, $CDCl_3$)



4e

^{13}C NMR (100 MHz, $CDCl_3$)


7.51
7.44
7.42
7.40
7.38
7.36
7.34
7.33
7.32
7.28
7.26
7.24
7.06
7.06
7.04
7.04
6.77
2.77
2.75
2.73
2.70
1.71
1.70
1.70
1.39
0.93
0.92
0.00
N
4f
^{1}H NMR (400 MHz, $CDCl_3$)
1.00
2.00
1.00
8.00
1.00
1.00
2.00
2.00
4.00
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


140.69
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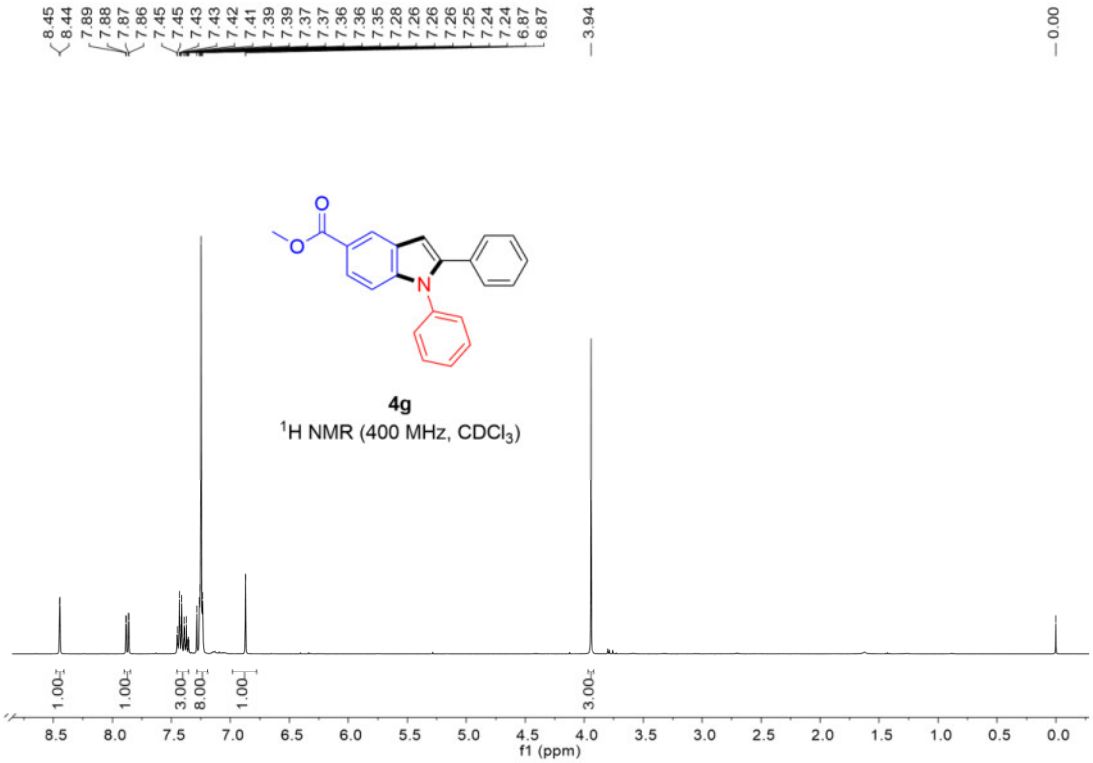
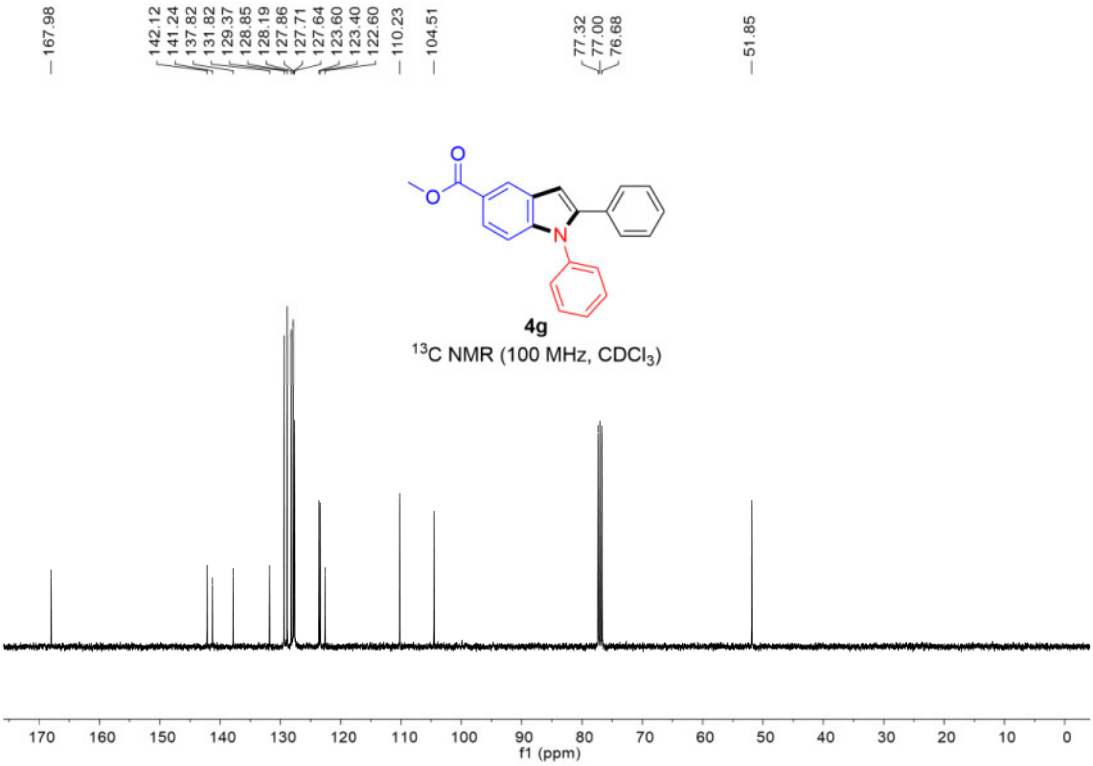
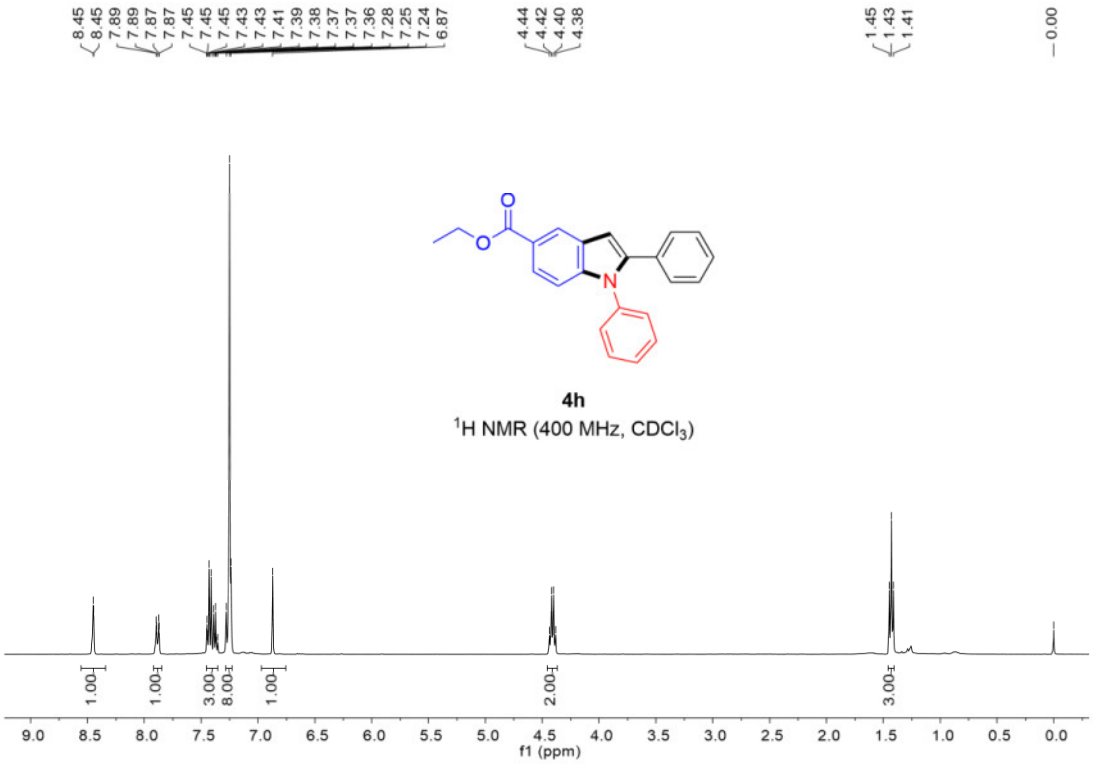
137.55
135.34
132.66
129.17
128.82
128.37
128.09
127.92
127.13
126.98
123.38
119.58
110.28
103.43
77.32
77.00
76.68
35.99
31.99
31.56
22.63
14.09
N
4f
^{13}C NMR (100 MHz, $CDCl_3$)
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.45
8.44
7.89
7.88
7.87
7.86
7.45
7.45
7.43
7.43
7.42
7.41
7.39
7.39
7.37
7.37
7.36
7.36
7.35
7.28
7.26
7.26
7.25
7.24
7.24
6.87
6.87
3.94
0.00
O
O
N
4g
1H NMR (400 MHz, CDCl3)
1.00
1.00
3.00
8.00
1.00
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


167.98
142.12
141.24
137.82
131.82
129.37
128.85
128.19
127.86
127.71
127.64
123.60
123.40
122.60
110.23
104.51
77.32
77.00
76.68
51.85
O
O
N
4g
13C NMR (100 MHz, CDCl3)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.45
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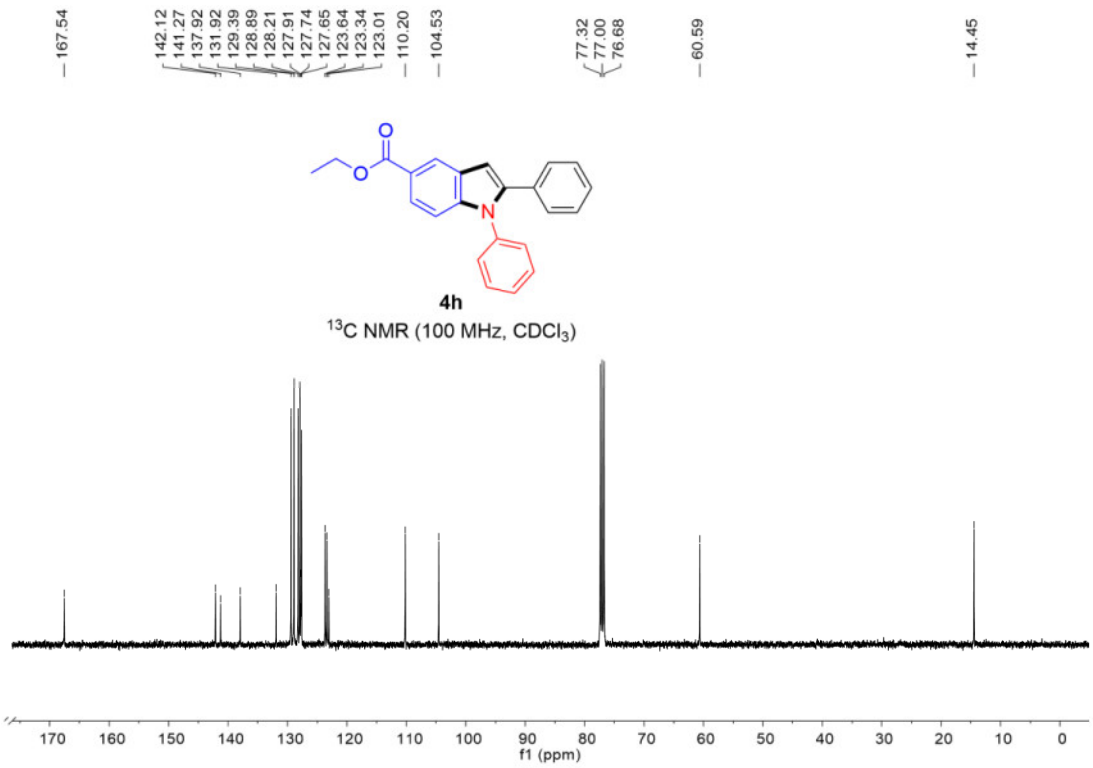
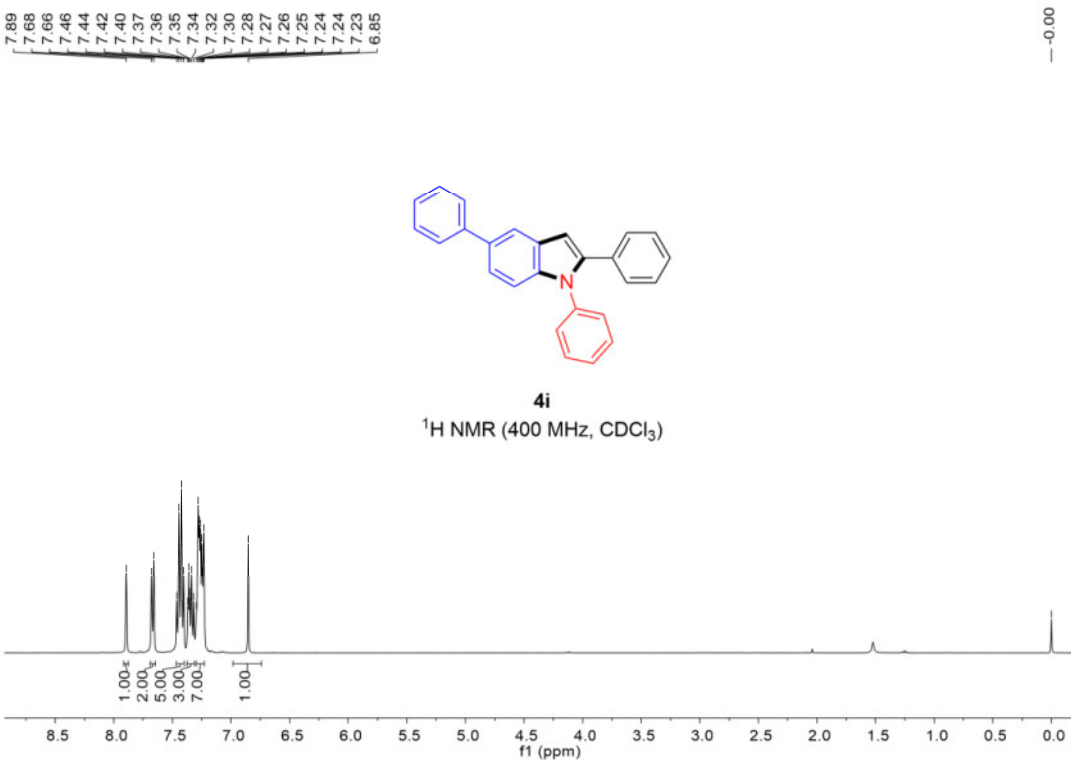
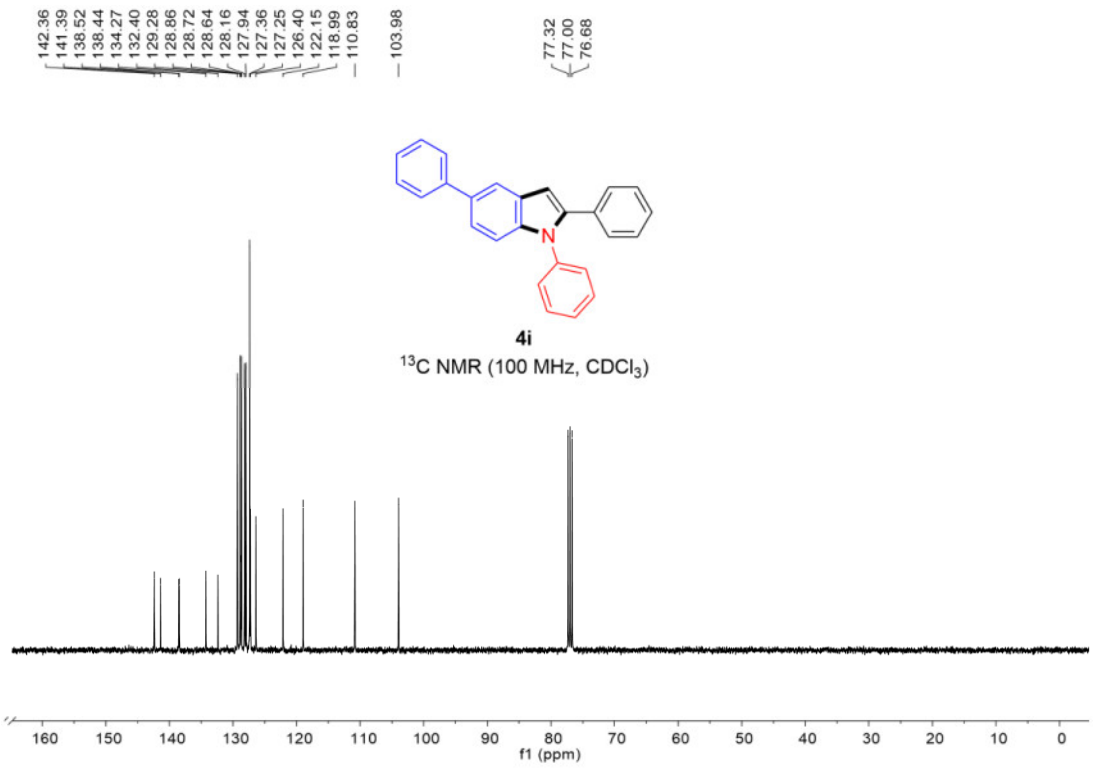
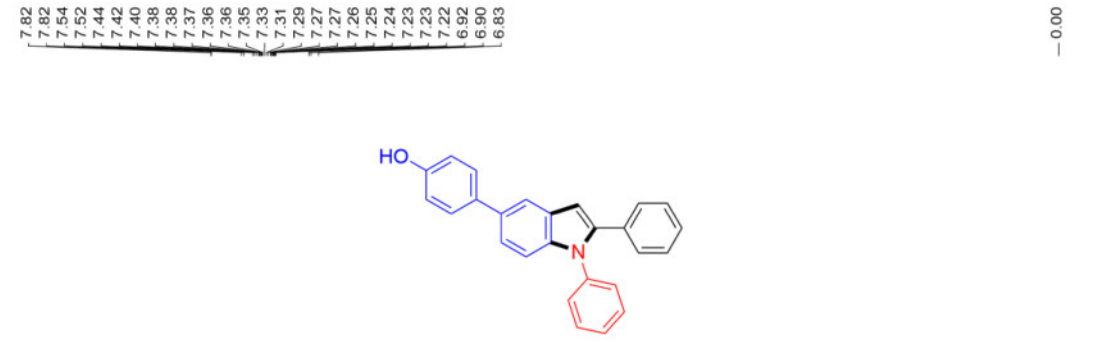
7.89
7.87
7.87
7.45
7.45
7.45
7.43
7.43
7.41
7.39
7.38
7.37
7.37
7.36
7.28
7.25
7.24
6.87
4.44
4.42
4.40
4.38
1.45
1.43
1.41
0.00
O
O
N
4h
^{1}H NMR (400 MHz, CDCl$_3$)
1.00
1.00
3.00
8.00
1.00
2.00
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


167.54
142.12
141.27
137.92
131.92
129.39
128.89
128.21
127.91
127.74
127.65
123.64
123.34
123.01
110.20
104.53
77.32
77.00
76.68
60.59
14.45
O
O
N
4h
^{13}C NMR (100 MHz, CDCl$_3$)
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.89
7.68
7.66
7.46
7.44
7.42
7.40
7.37
7.36
7.35
7.34
7.32
7.30
7.28
7.27
7.26
7.25
7.24
7.24
7.23
6.85
-0.00
N
4i
^{1}H NMR (400 MHz, $CDCl_3$)
1.00
2.00
5.00
3.00
7.00
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

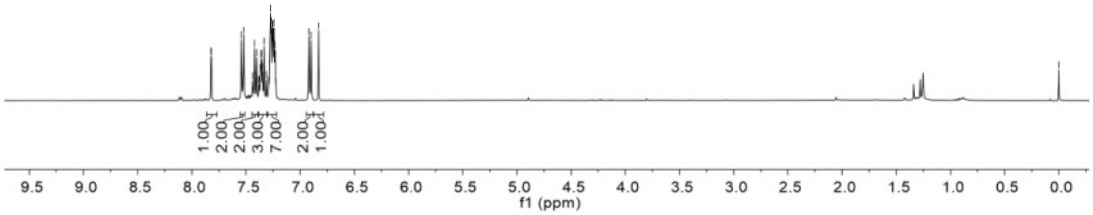

142.36
141.39
138.52
138.44
134.27
132.40
129.28
128.86
128.72
128.64
128.16
127.94
127.36
127.25
126.40
122.15
118.99
110.83
103.98
77.32
77.00
76.68
N
4i
^{13}C NMR (100 MHz, $CDCl_3$)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

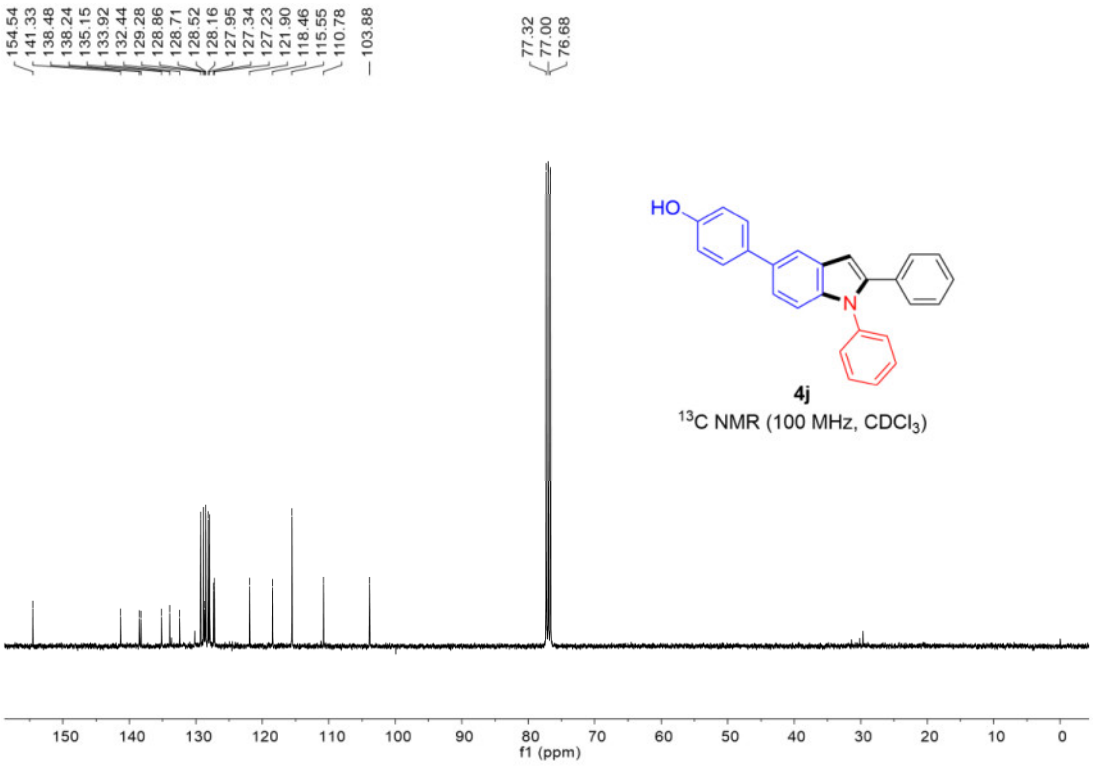


4j

^{1}H NMR (400 MHz, $CDCl_3$)

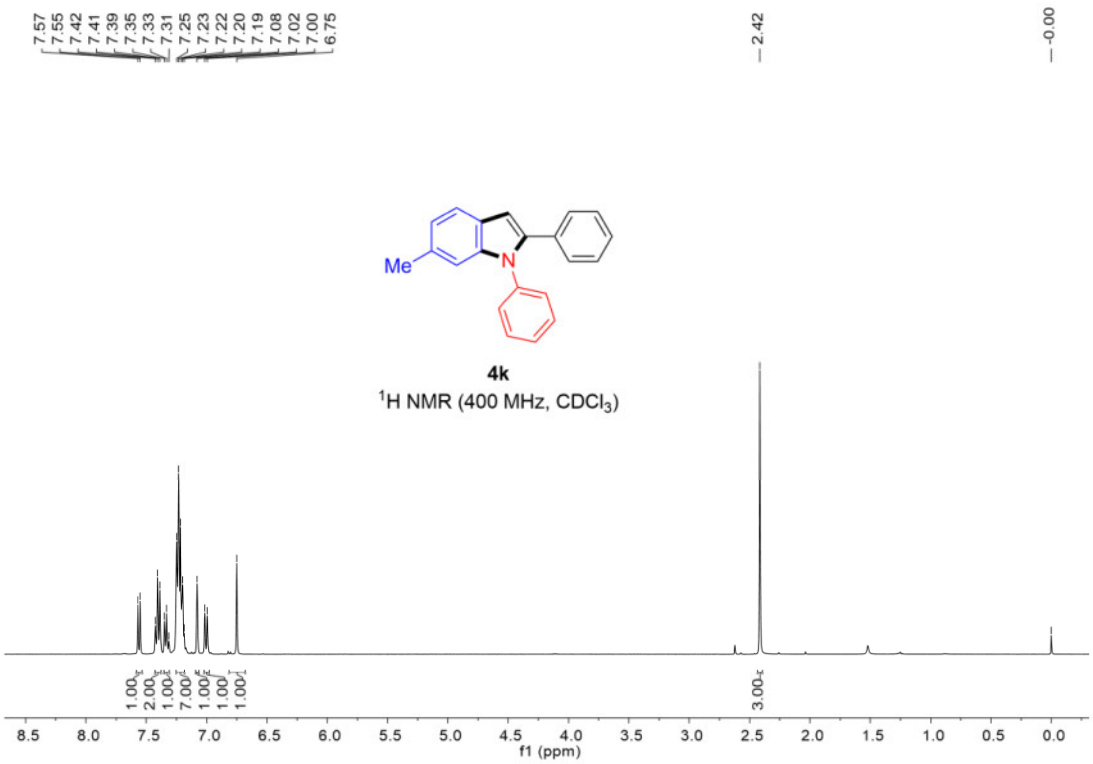
The peak of the hydroxyl group did not appear.

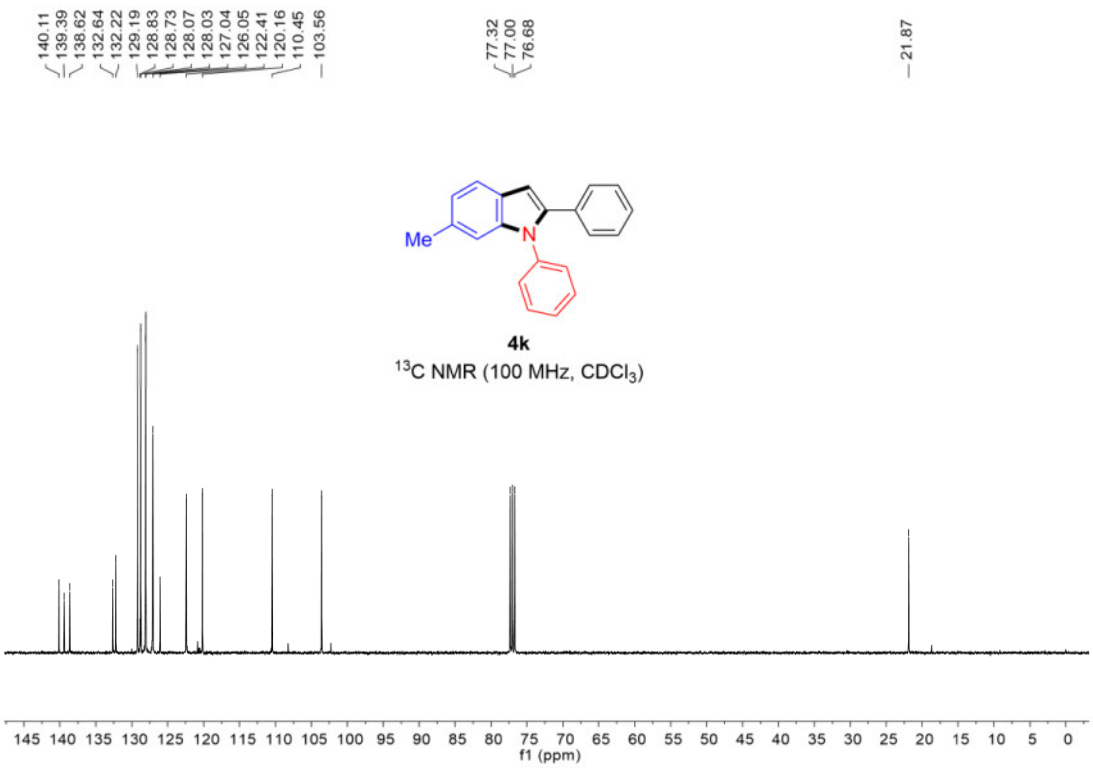


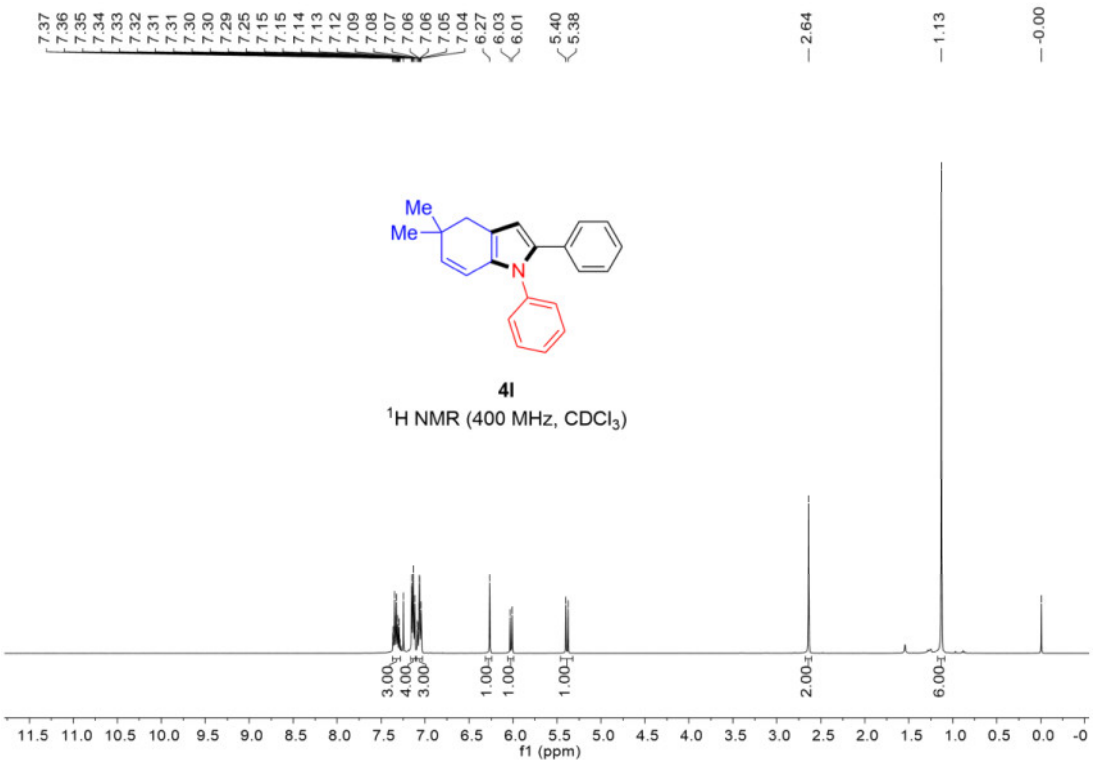


4j

^{13}C NMR (100 MHz, $CDCl_3$)

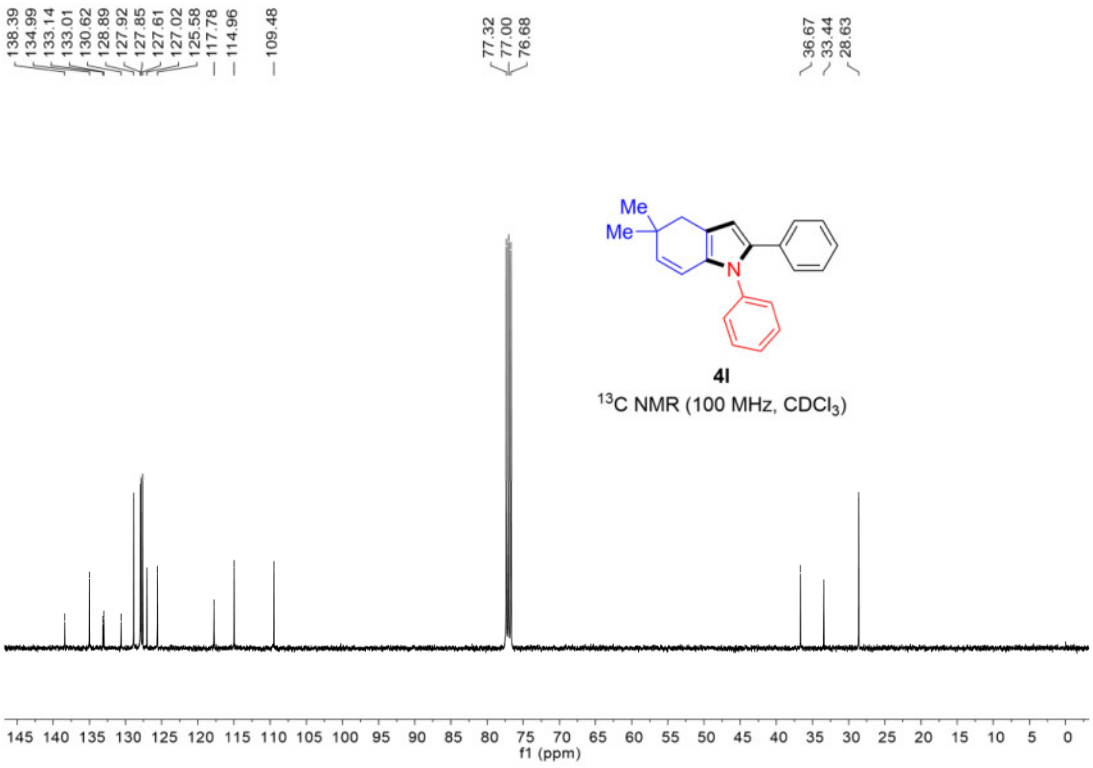

7.57
7.55
7.42
7.41
7.39
7.35
7.33
7.31
7.25
7.23
7.22
7.20
7.19
7.08
7.02
7.00
6.75
2.42
-0.00
Me
N
4k
1H NMR (400 MHz, CDCl3)
1.00
2.00
1.00
7.00
1.00
1.00
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


140.11
139.39
138.62
132.64
132.22
129.19
128.83
128.73
128.07
128.03
127.04
126.05
122.41
120.16
110.45
103.56
77.32
77.00
76.68
21.87
Me
N
4k
13C NMR (100 MHz, CDCl3)
145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)



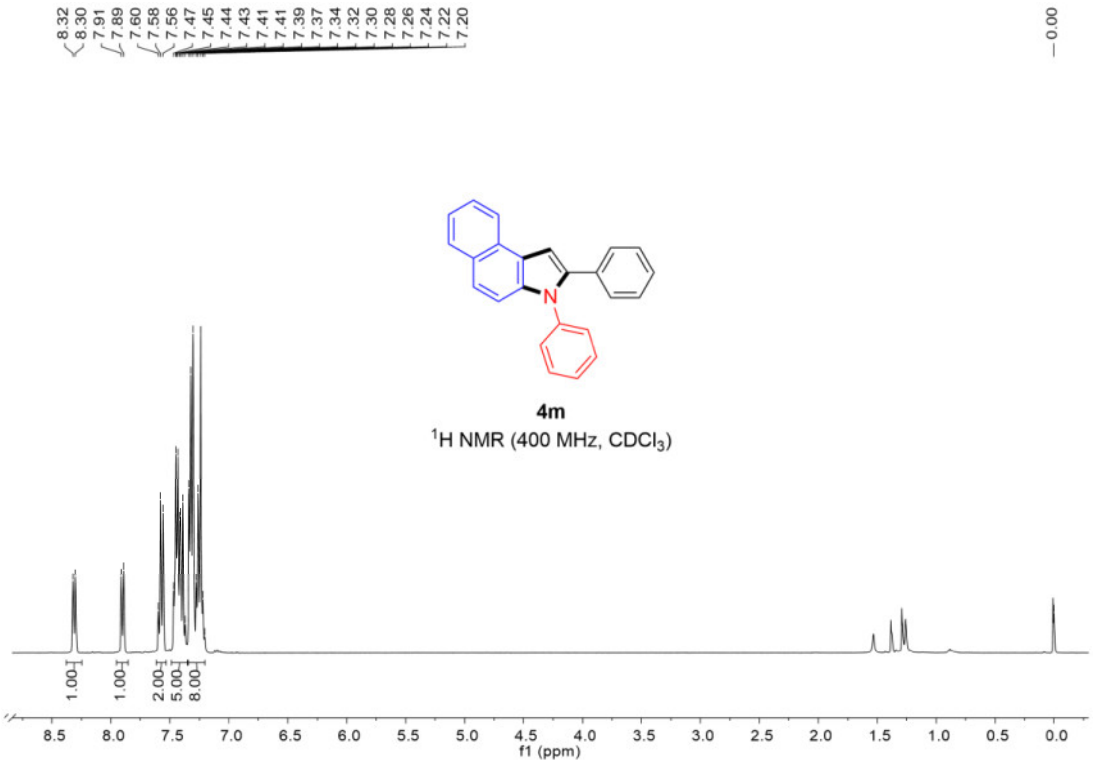
4l

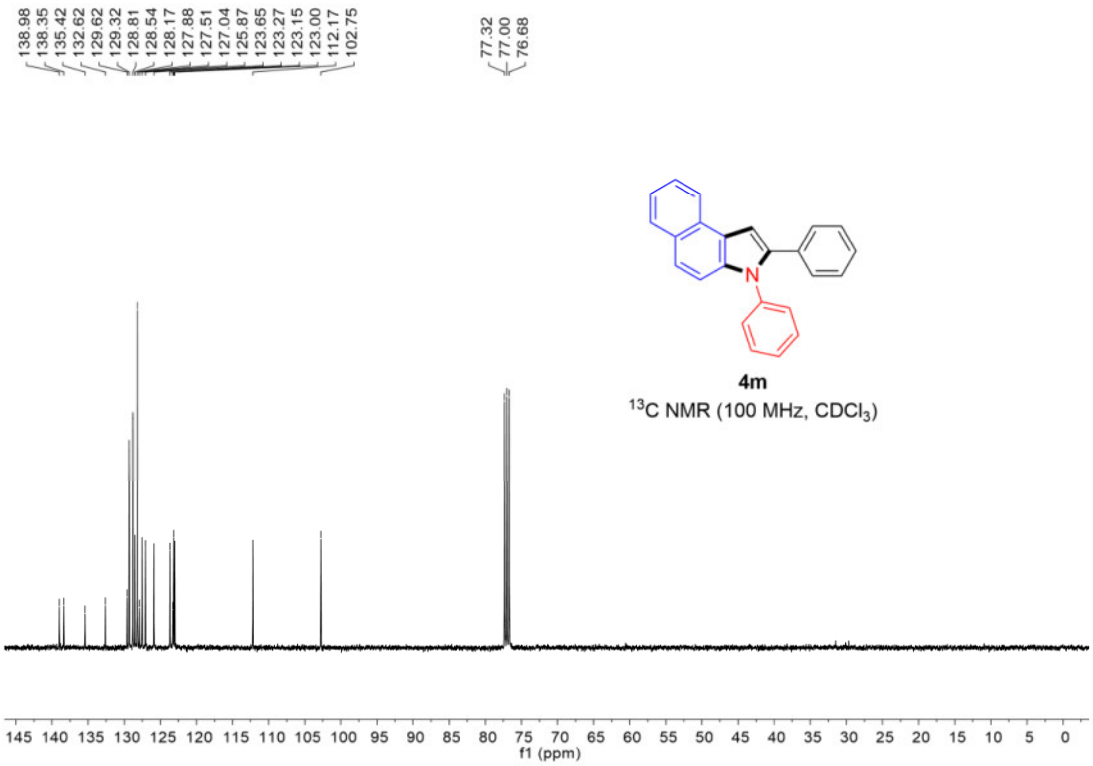
^{1}H NMR (400 MHz, $CDCl_3$)

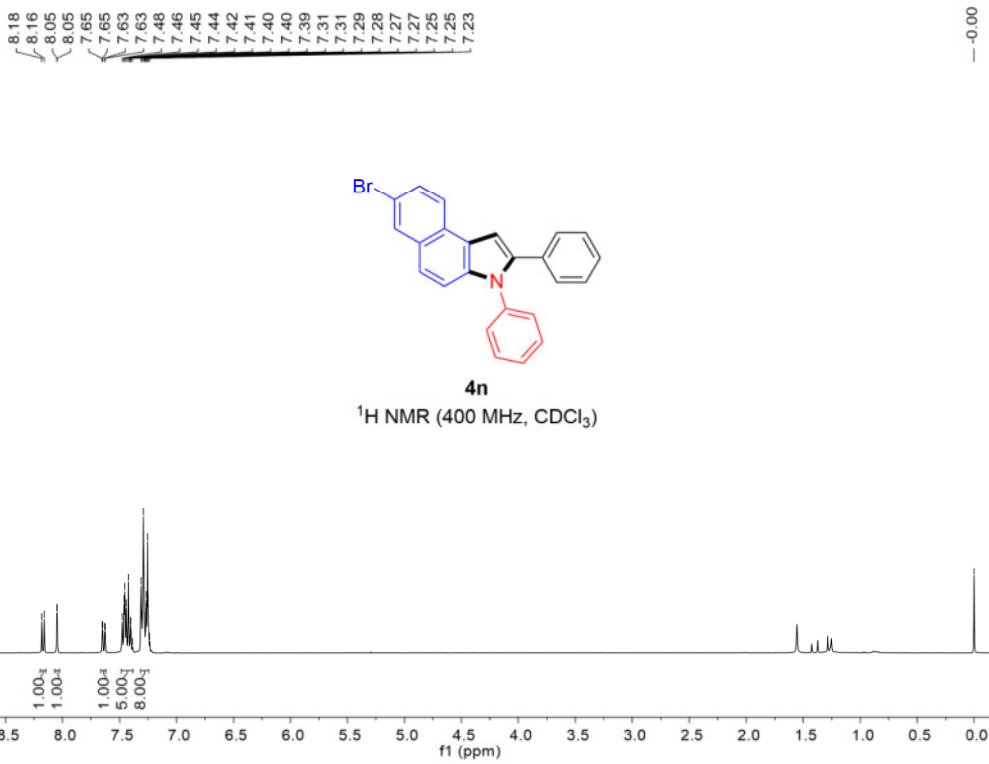


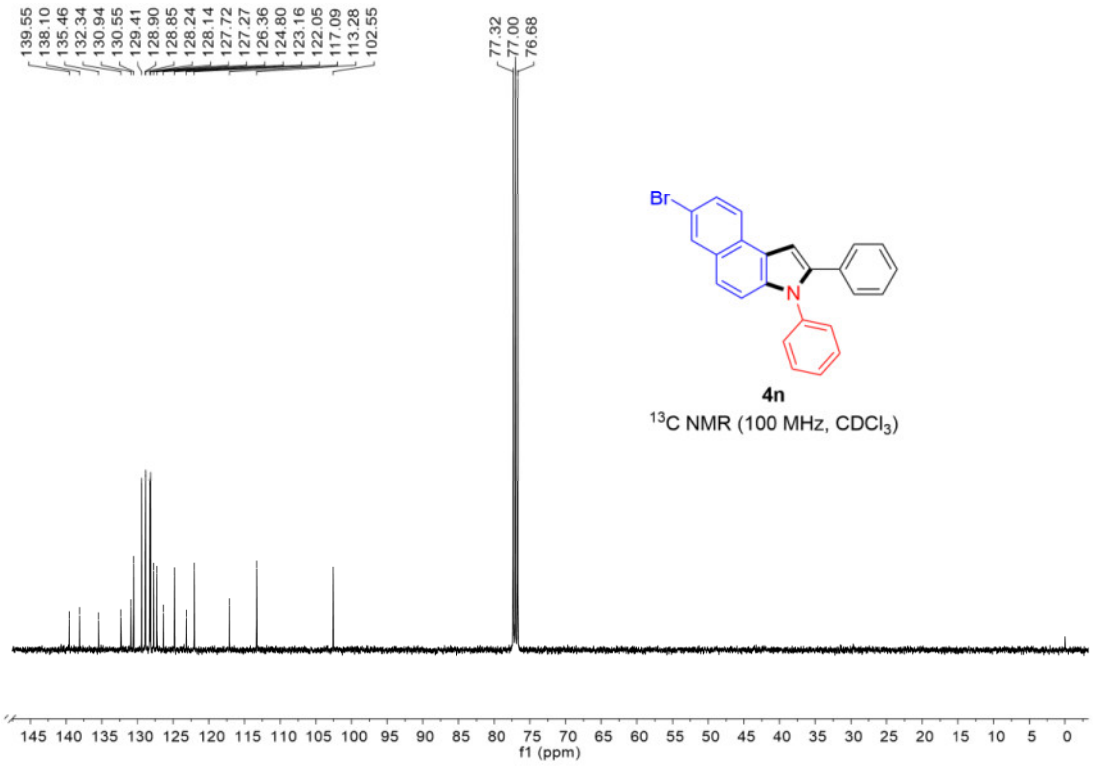
4l

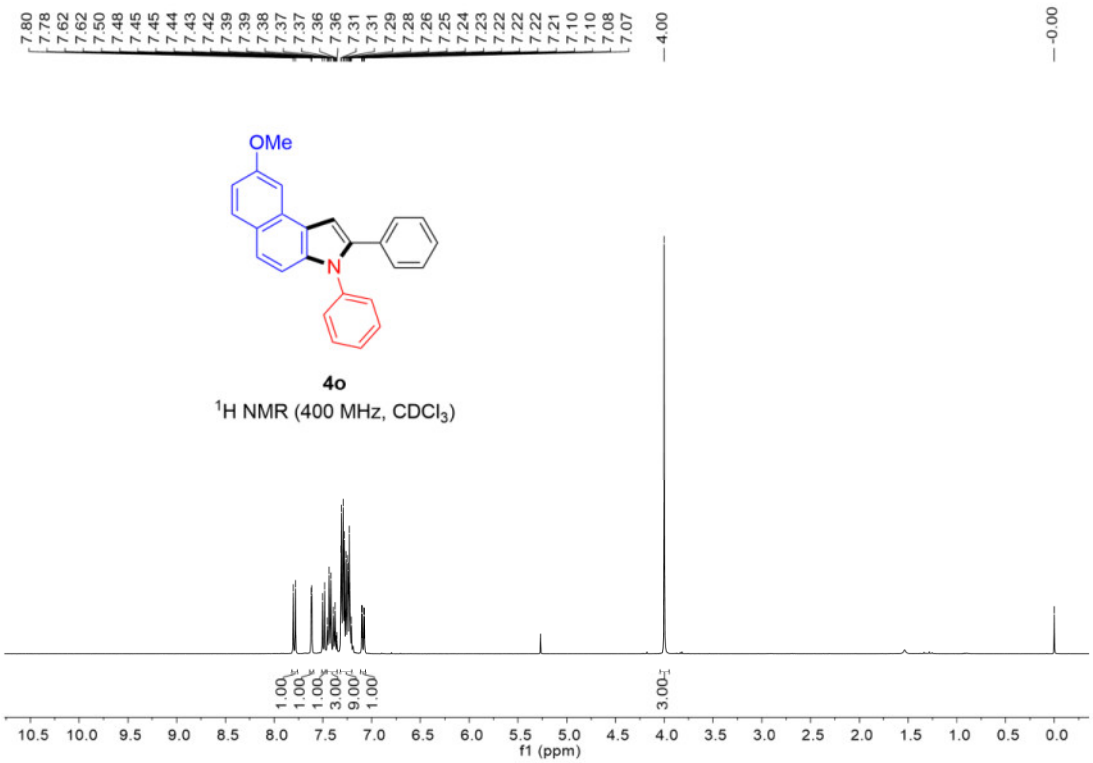
^{13}C NMR (100 MHz, $CDCl_3$)

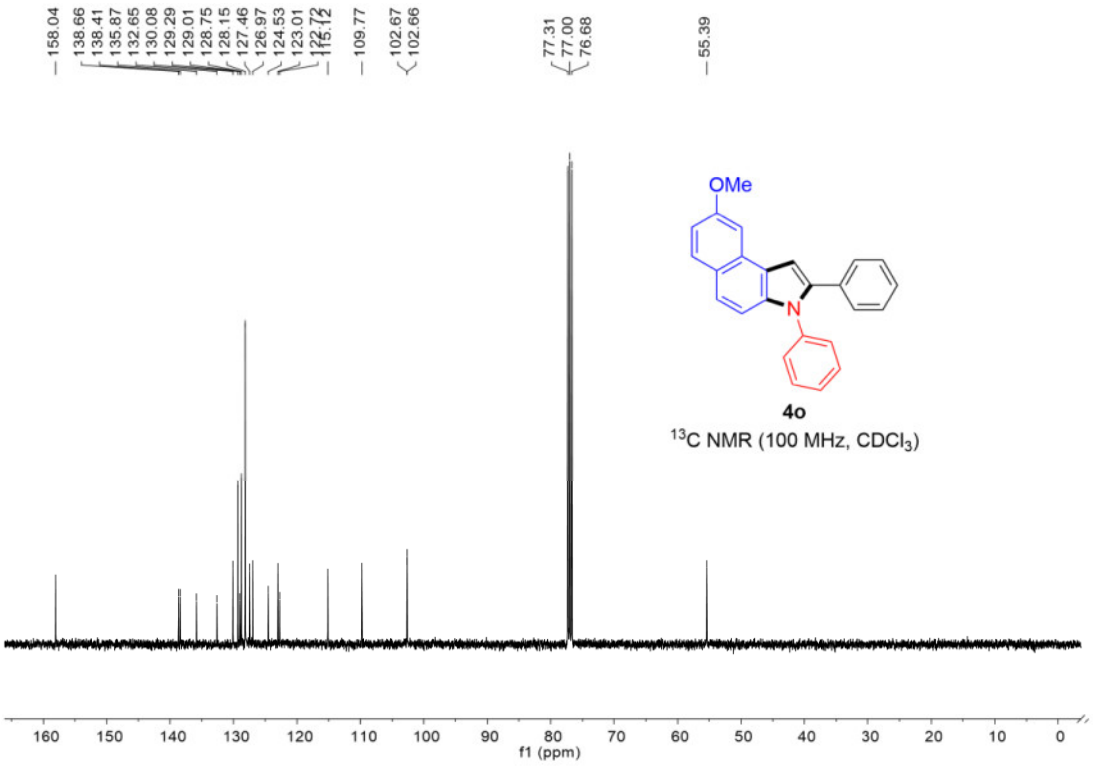

8.32
8.30
7.91
7.89
7.60
7.58
7.56
7.47
7.45
7.44
7.43
7.41
7.41
7.39
7.37
7.34
7.32
7.30
7.28
7.26
7.24
7.22
7.20
0.00
N
4m
1H NMR (400 MHz, CDCl3)
1.00
1.00
2.00
5.00
8.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

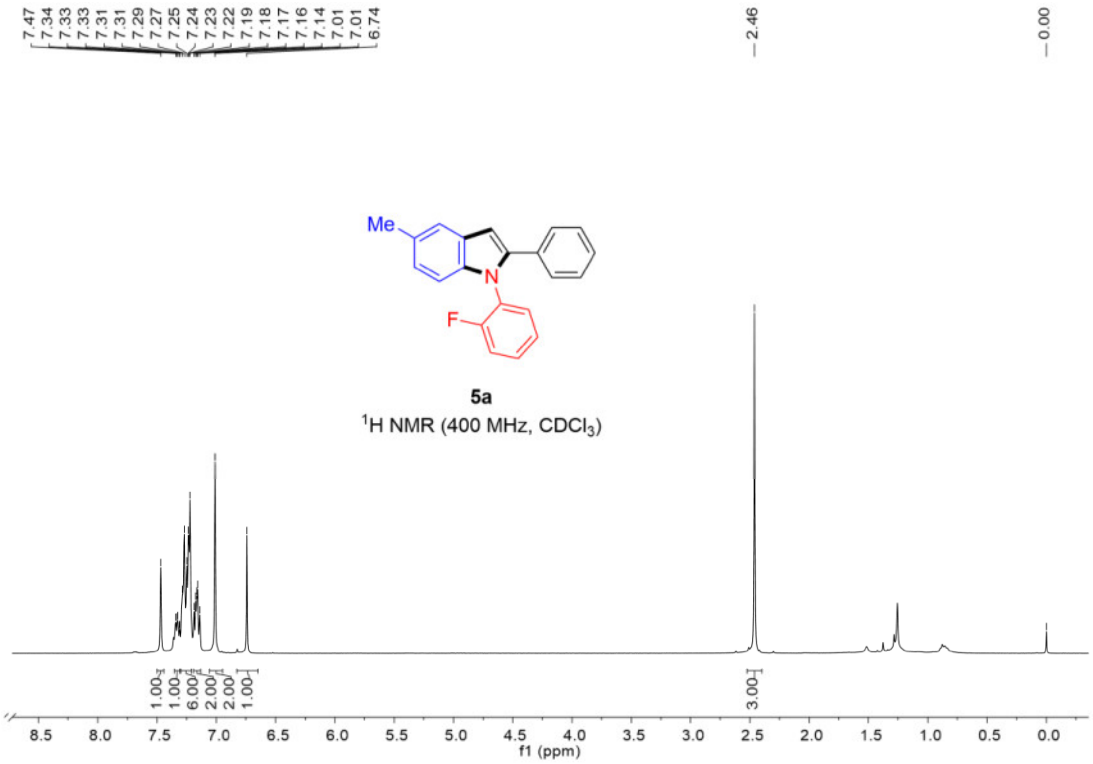

138.98
138.35
135.42
132.62
129.62
129.32
128.81
128.54
128.17
127.88
127.51
127.04
125.87
123.65
123.27
123.15
123.00
112.17
102.75
77.32
77.00
76.68
N
4m
13C NMR (100 MHz, CDCl3)
145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)


8.18
8.16
8.05
8.05
7.65
7.65
7.63
7.63
7.48
7.46
7.45
7.44
7.42
7.41
7.40
7.40
7.39
7.31
7.31
7.29
7.28
7.27
7.27
7.25
7.25
7.23
-0.00
Br
N
4n
1H NMR (400 MHz, CDCl3)
1.00
1.00
1.00
5.00
8.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


139.55
138.10
135.46
132.34
130.94
130.55
129.41
128.90
128.85
128.24
128.14
127.72
127.27
126.36
124.80
123.16
122.05
117.09
113.28
102.55
77.32
77.00
76.68
Br
N
4n
13C NMR (100 MHz, CDCl3)
145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)

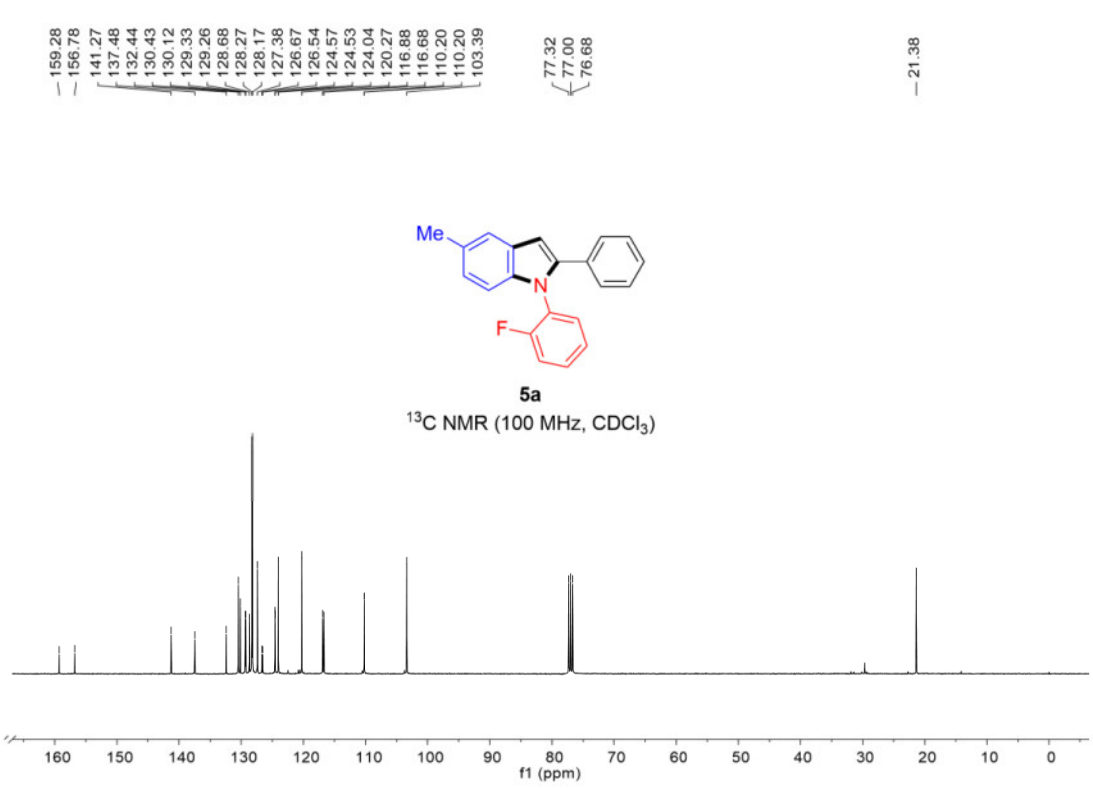

OMe
N
4o
^{1}H NMR (400 MHz, $CDCl_3$)
f1 (ppm)


OMe
N
4o
^{13}C NMR (100 MHz, $CDCl_3$)
f1 (ppm)



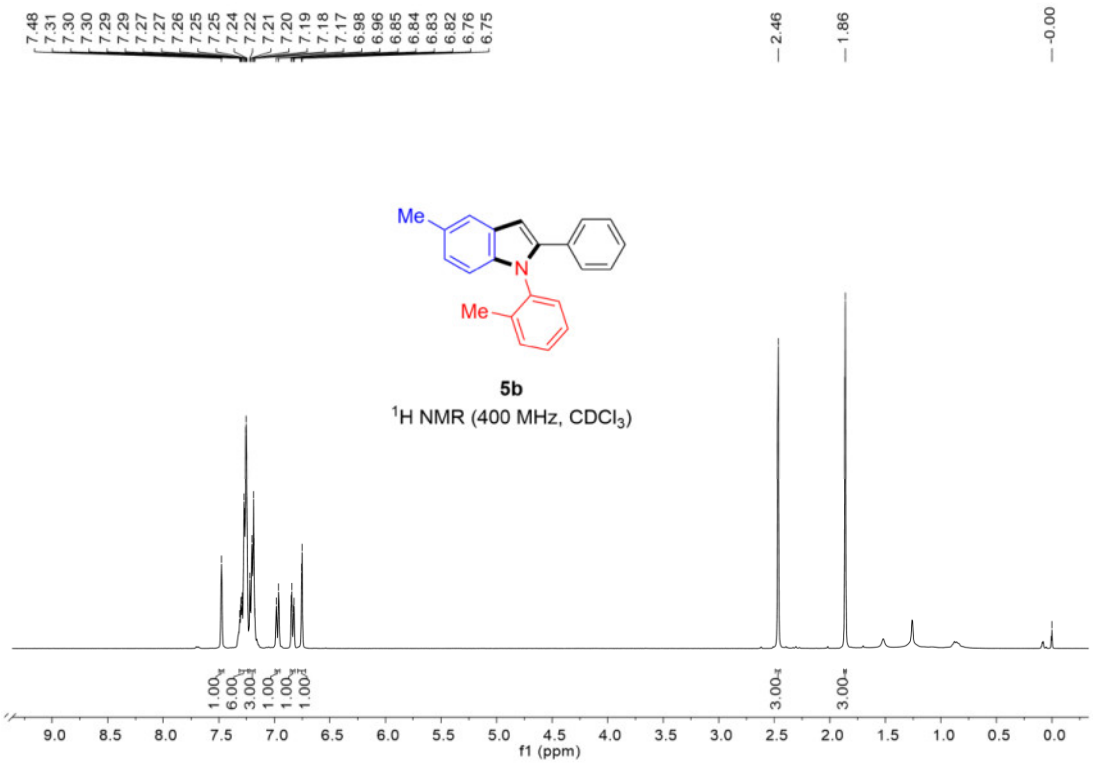
5a

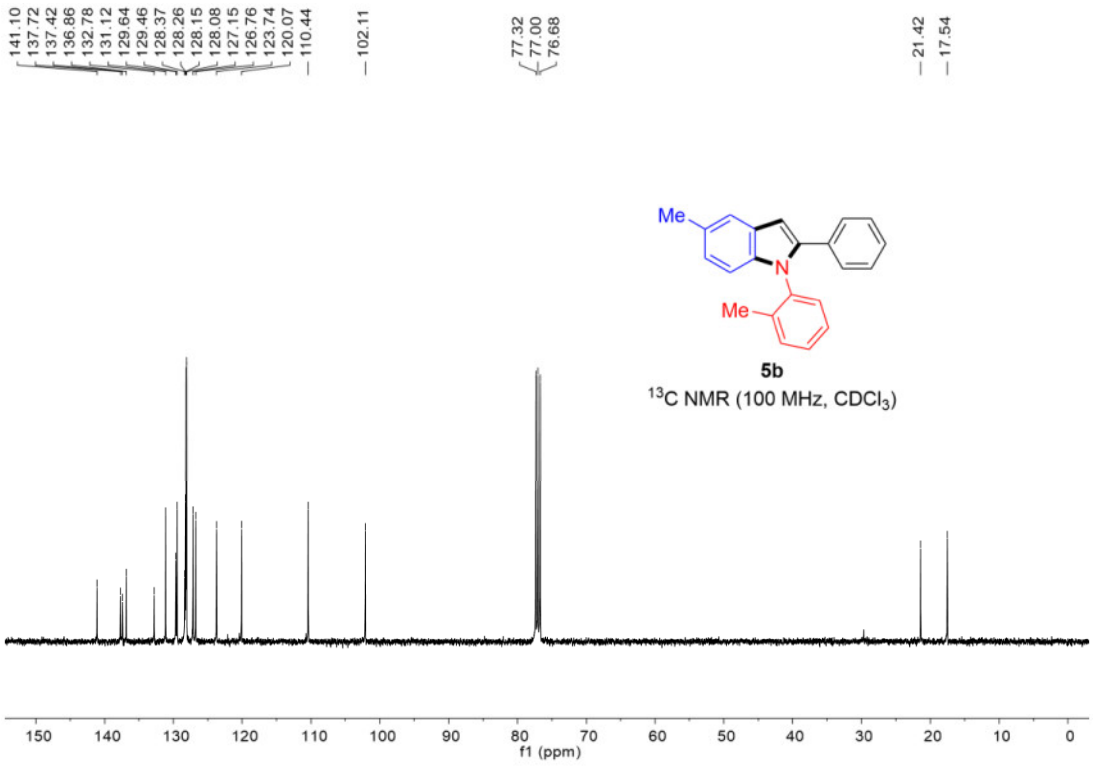
^{1}H NMR (400 MHz, $CDCl_3$)

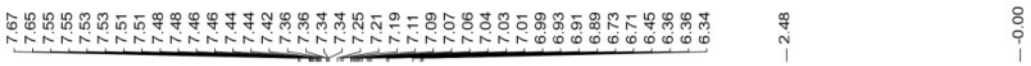


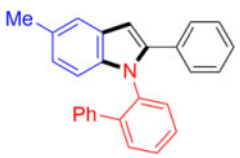
5a

^{13}C NMR (100 MHz, $CDCl_3$)


7.48
7.31
7.30
7.30
7.29
7.29
7.27
7.27
7.26
7.25
7.25
7.24
7.22
7.21
7.20
7.19
7.18
7.17
6.98
6.96
6.85
6.84
6.83
6.82
6.76
6.75
2.46
1.86
0.00
Me
N
Me
5b
1H NMR (400 MHz, CDCl3)
1.00
6.00
3.00
1.00
1.00
1.00
3.00
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

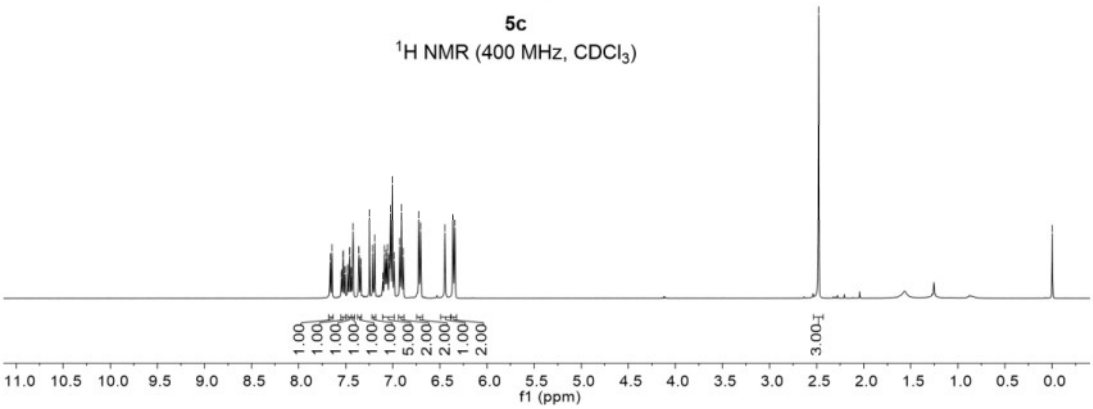

141.10
137.72
137.42
136.86
132.78
131.12
129.64
129.46
128.37
128.26
128.15
128.08
127.15
126.76
123.74
120.07
110.44
102.11
77.32
77.00
76.68
21.42
17.54
Me
N
Me
5b
13C NMR (100 MHz, CDCl3)
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

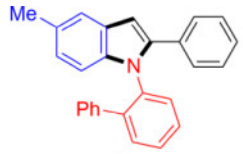




5c

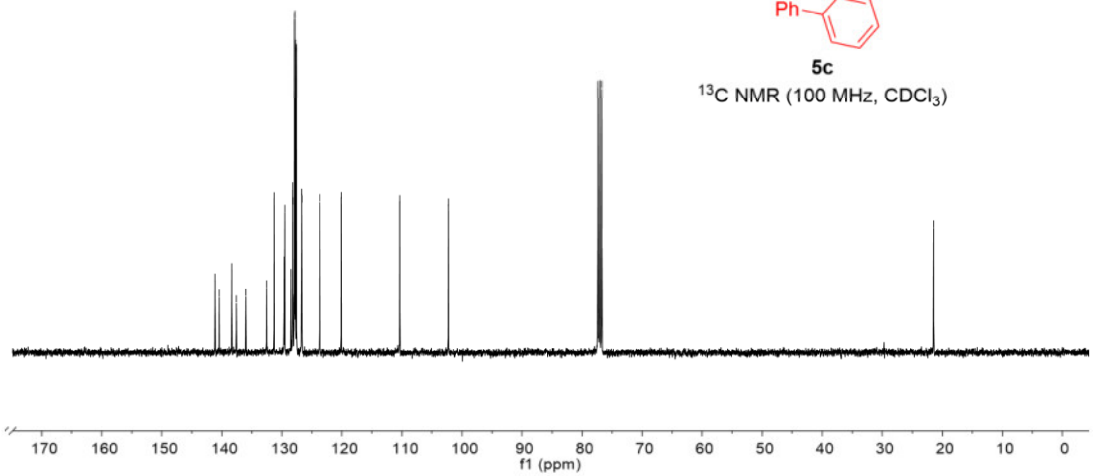
^{1}H NMR (400 MHz, $CDCl_3$)

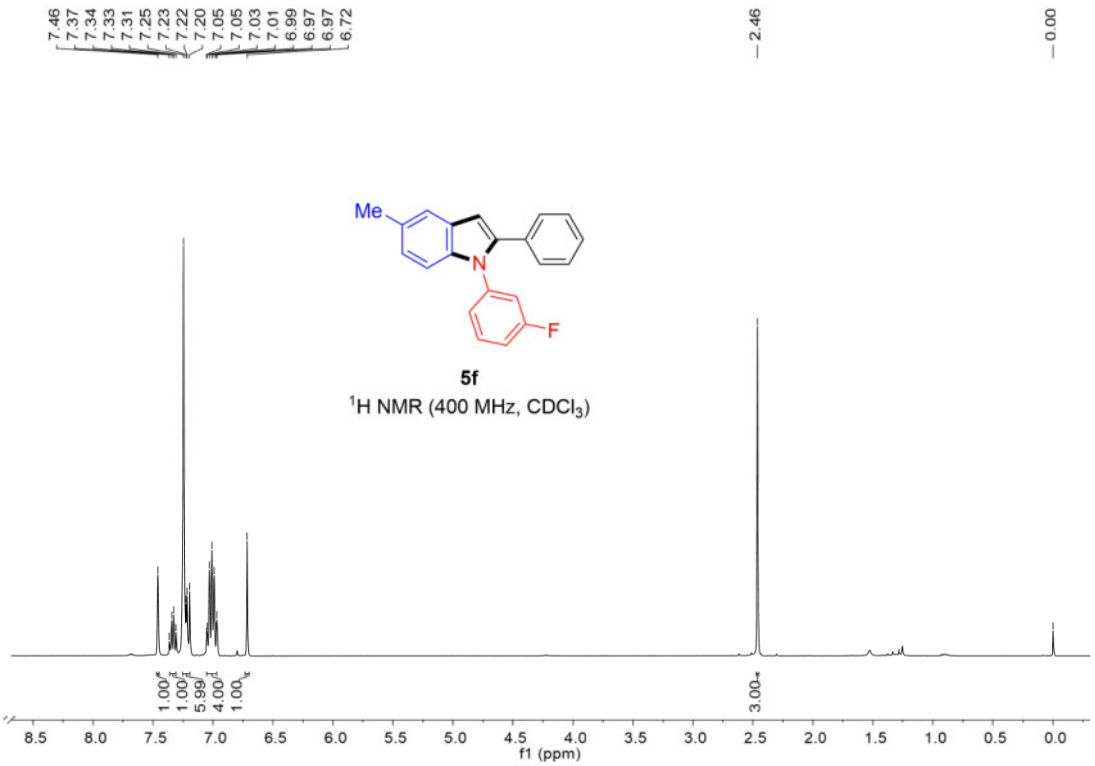


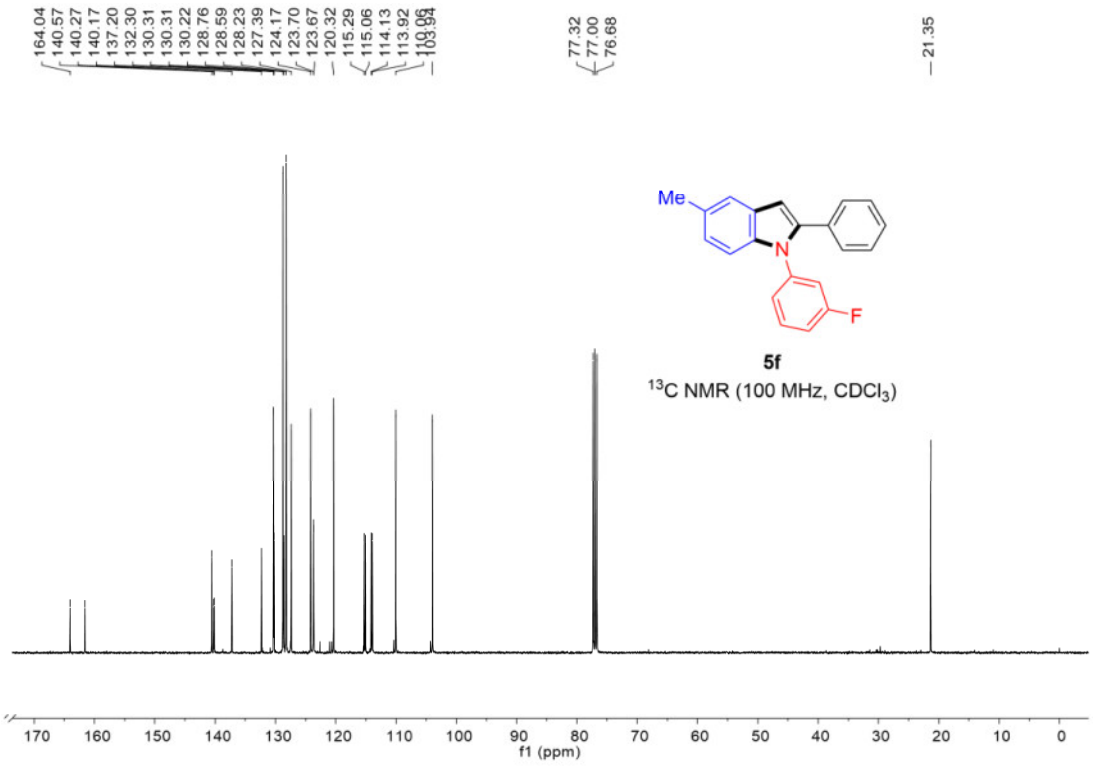


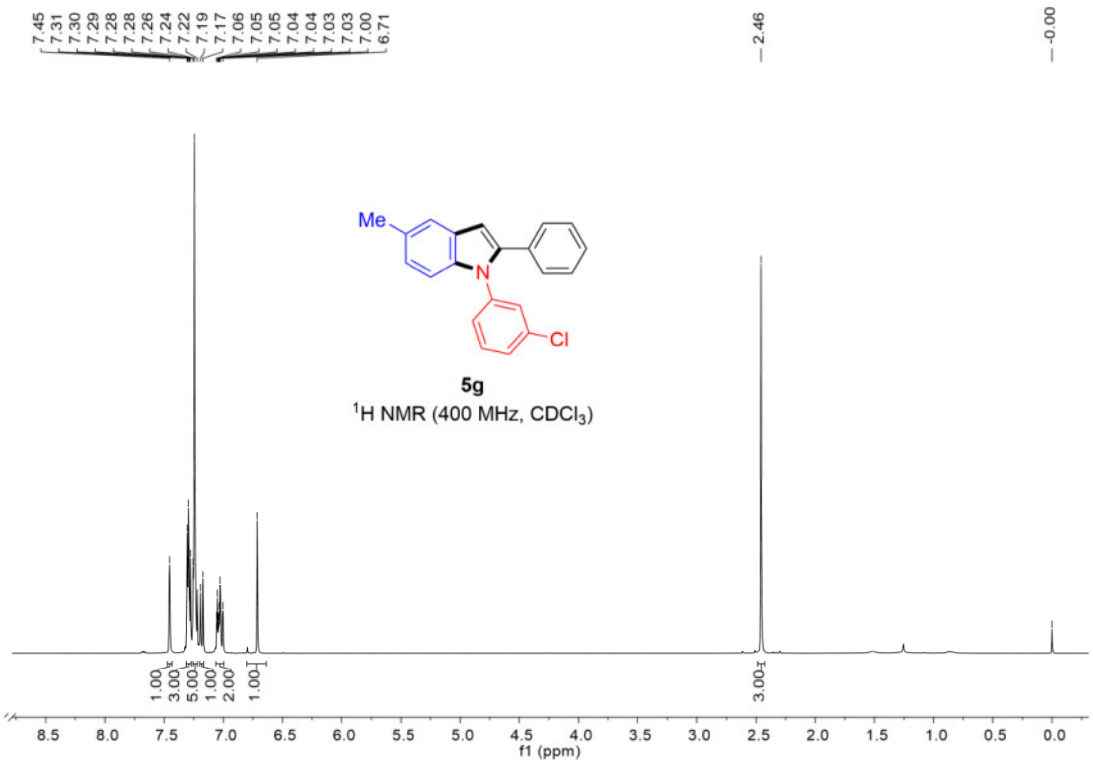
5c

^{13}C NMR (100 MHz, $CDCl_3$)



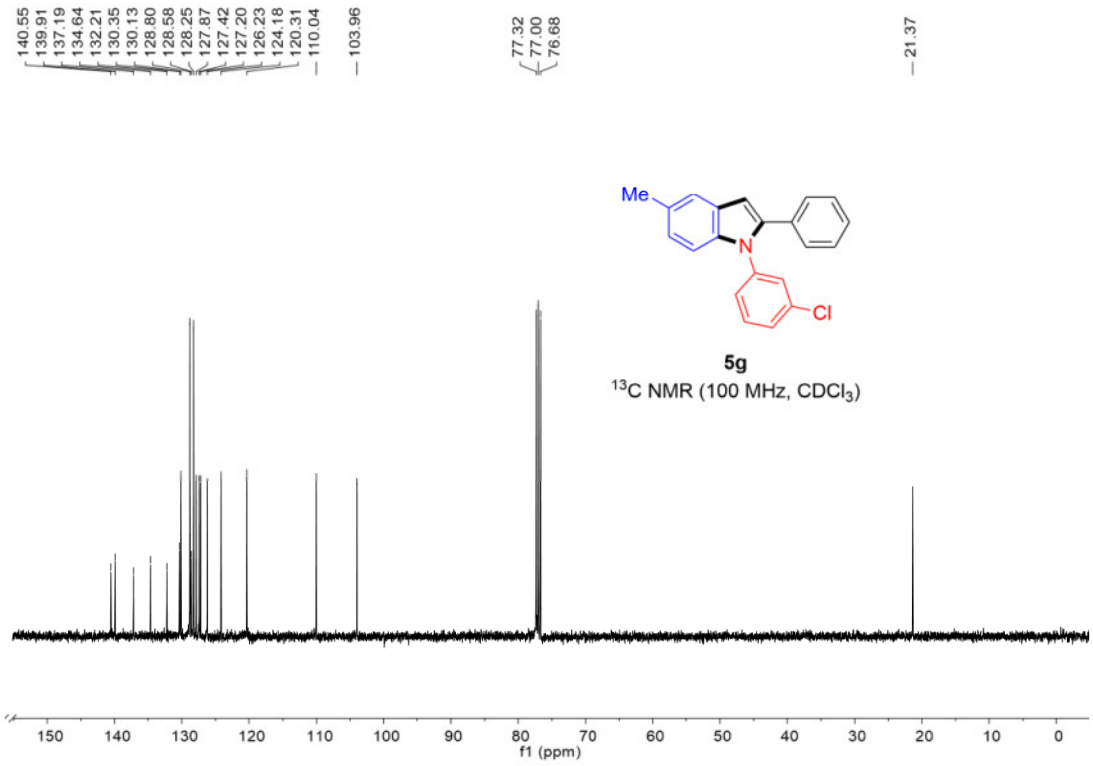

7.46
7.37
7.34
7.33
7.31
7.25
7.23
7.22
7.20
7.05
7.05
7.03
7.01
6.99
6.97
6.97
6.72
2.46
0.00
Me
N
F
5f
1H NMR (400 MHz, CDCl3)
1.00
1.00
5.99
4.00
1.00
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


164.04
140.57
140.27
140.17
137.20
132.30
130.31
130.31
130.22
128.76
128.59
128.23
127.39
124.17
123.70
123.67
120.32
115.29
115.06
114.13
113.92
110.06
103.94
77.32
77.00
76.68
21.35
Me
N
F
5f
13C NMR (100 MHz, CDCl3)
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



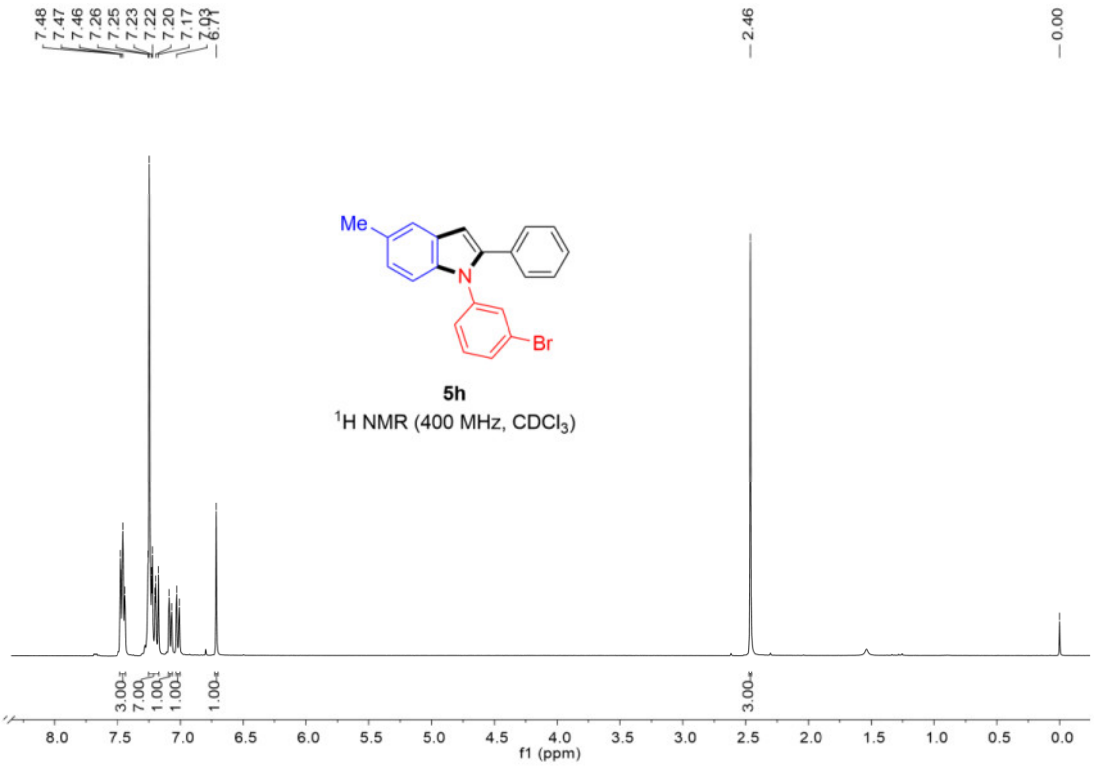
5g

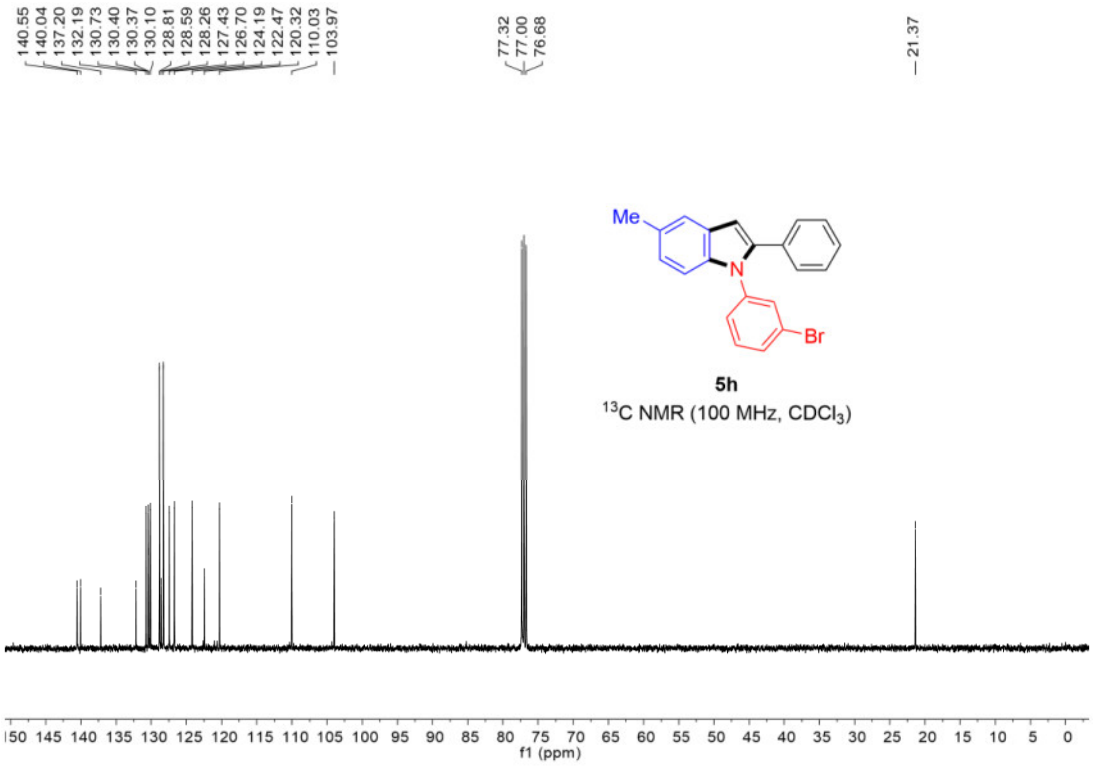
^{1}H NMR (400 MHz, $CDCl_3$)

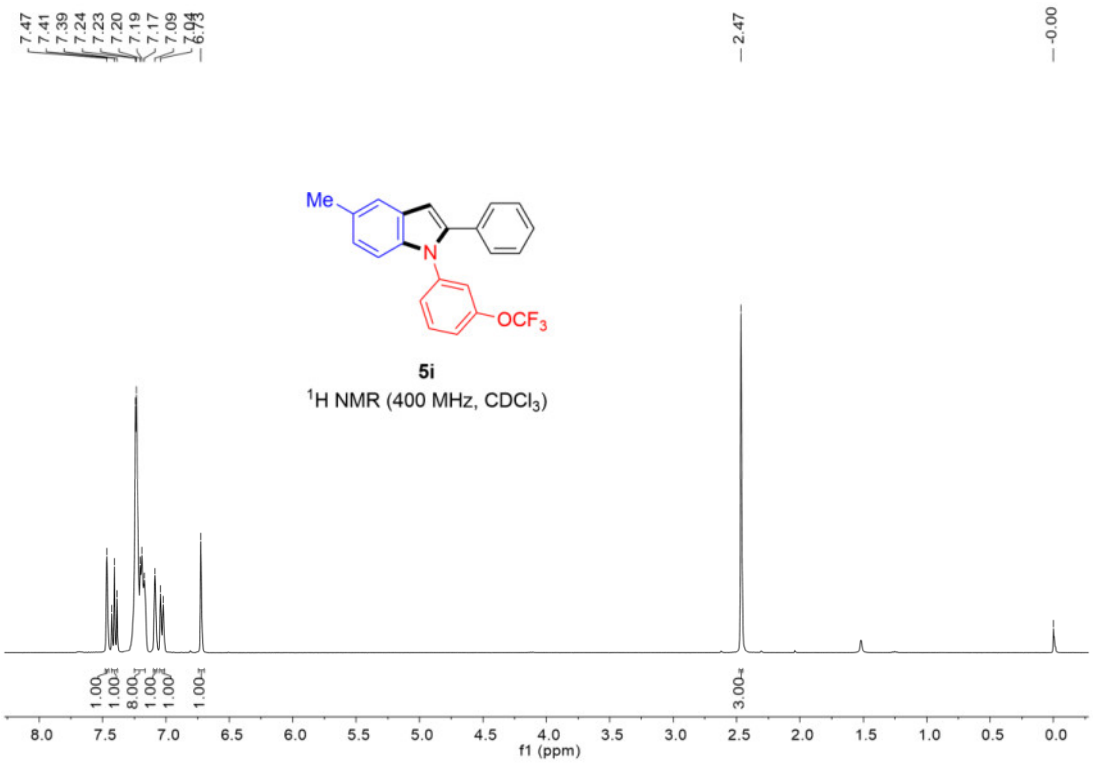


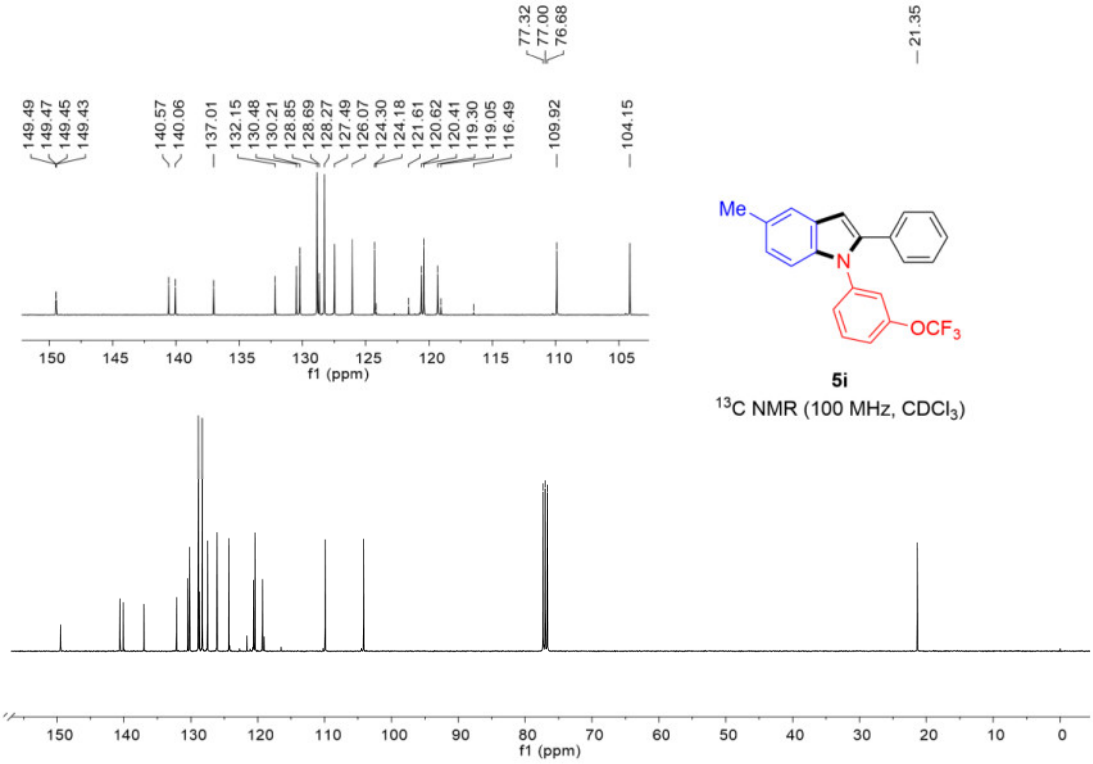
5g

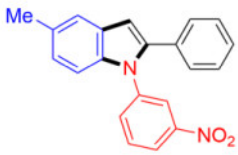
^{13}C NMR (100 MHz, $CDCl_3$)


7.48
7.47
7.46
7.26
7.25
7.23
7.22
7.20
7.17
7.03
6.71
2.46
0.00
Me
N
Br
5h
^{1}H NMR (400 MHz, CDCl$_3$)
3.00
7.00
1.00
1.00
1.00
3.00
f1 (ppm)


140.55
140.04
137.20
132.19
130.73
130.40
130.37
130.10
128.81
128.59
128.26
127.43
126.70
124.19
122.47
120.32
110.03
103.97
77.32
77.00
76.68
21.37
Me
N
Br
5h
^{13}C NMR (100 MHz, CDCl$_3$)
f1 (ppm)


7.47
7.41
7.39
7.24
7.23
7.20
7.19
7.17
7.09
6.93
2.47
-0.00
Me
N
OCF3
5i
1H NMR (400 MHz, CDCl3)
1.00
1.00
8.00
1.00
1.00
1.00
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

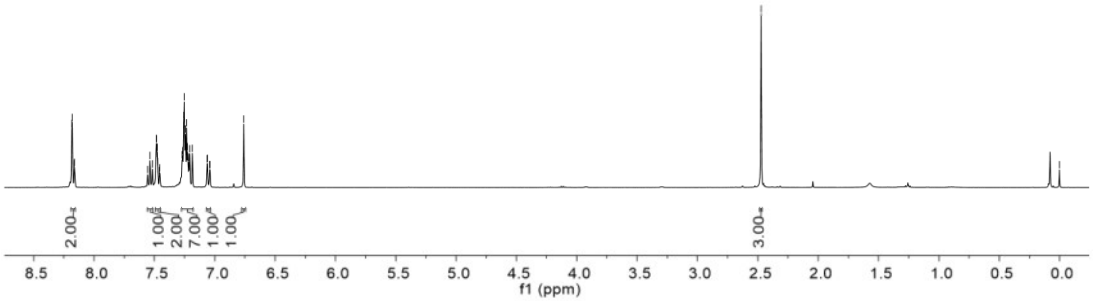

77.32
77.00
76.68
21.35
149.49
149.47
149.45
149.43
140.57
140.06
137.01
132.15
130.48
130.21
128.85
128.69
128.27
127.49
126.07
124.30
124.18
121.61
120.62
120.41
119.30
119.05
116.49
109.92
104.15
Me
N
OCF3
5i
13C NMR (100 MHz, CDCl3)
150
145
140
135
130
125
120
115
110
105
f1 (ppm)
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

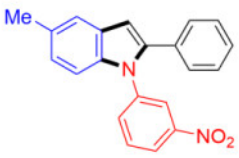


5j

^{1}H NMR (400 MHz, $CDCl_3$)

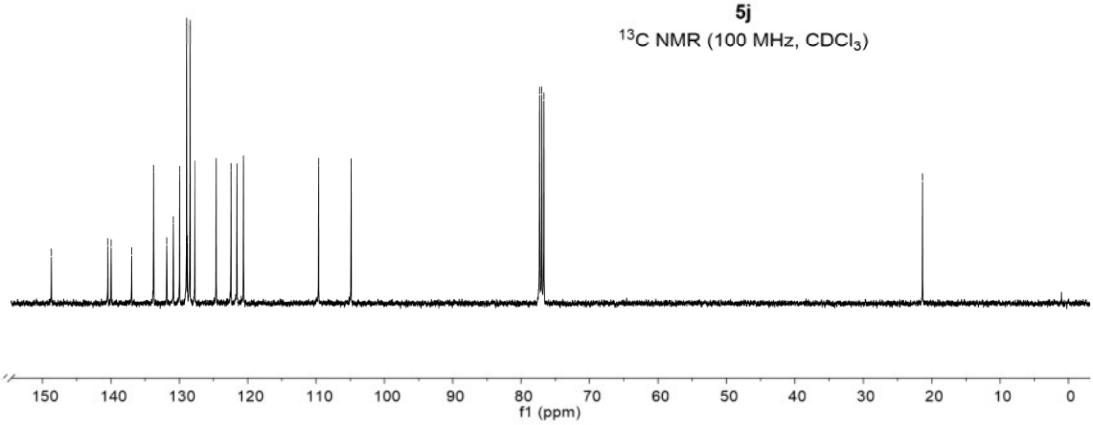
The solvent peak (1H) was contained

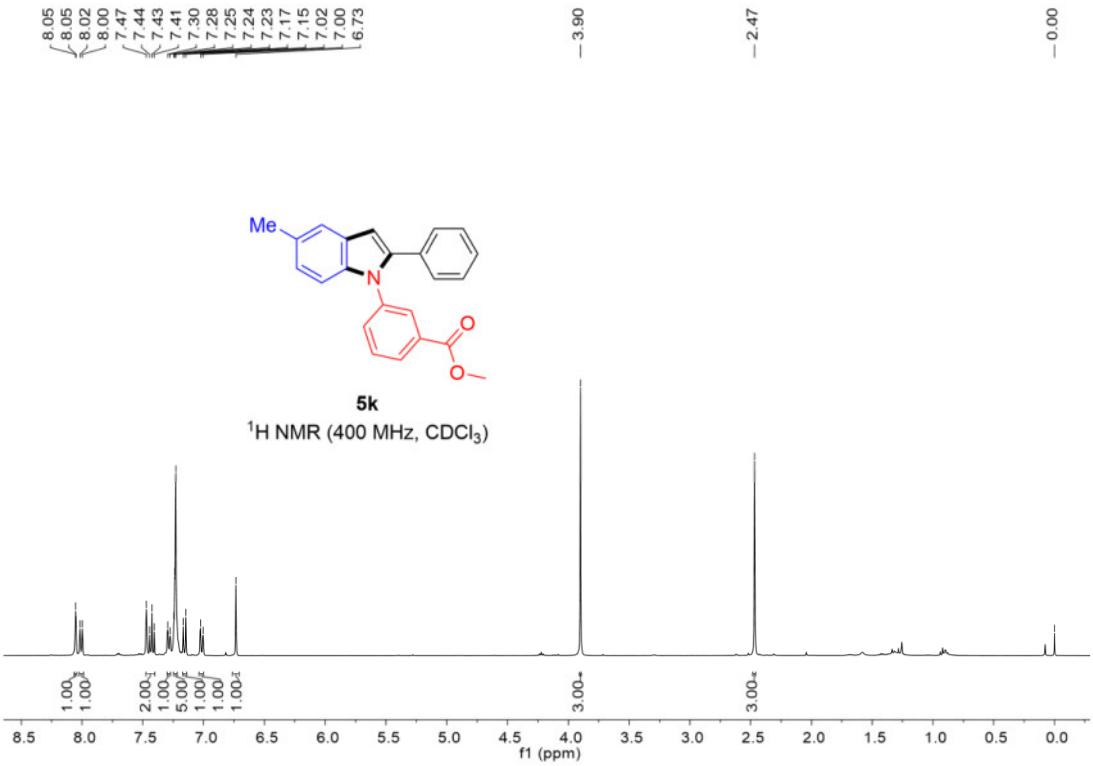


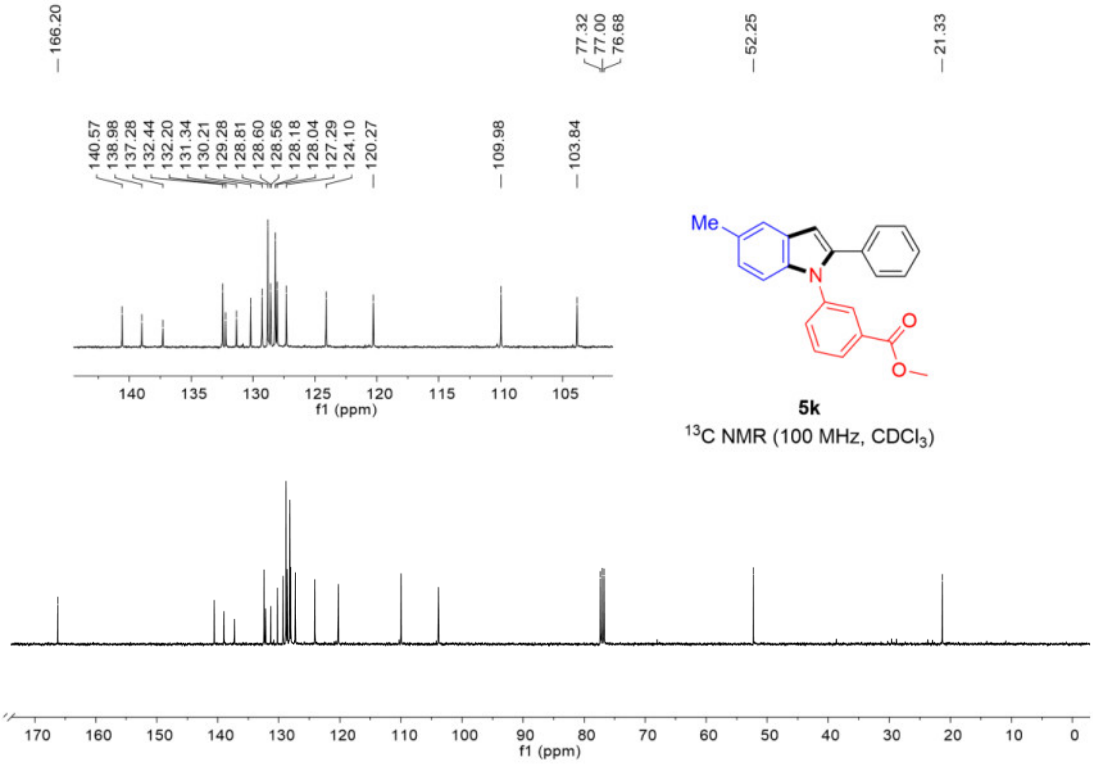


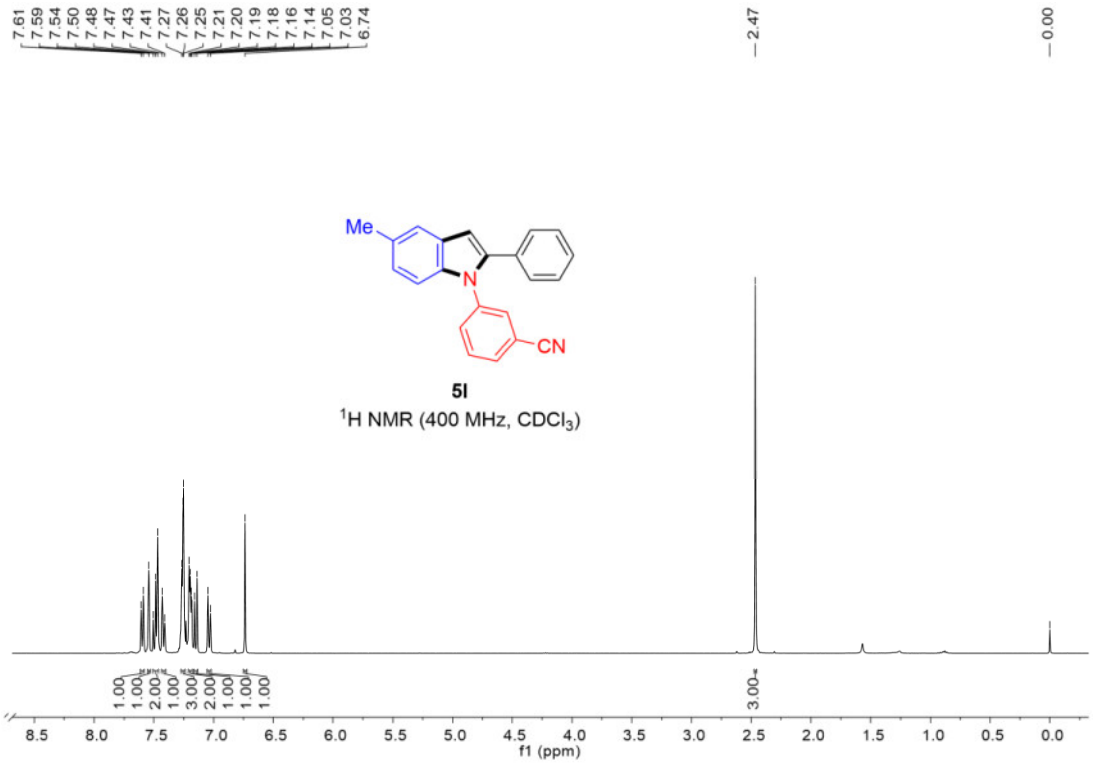
5j

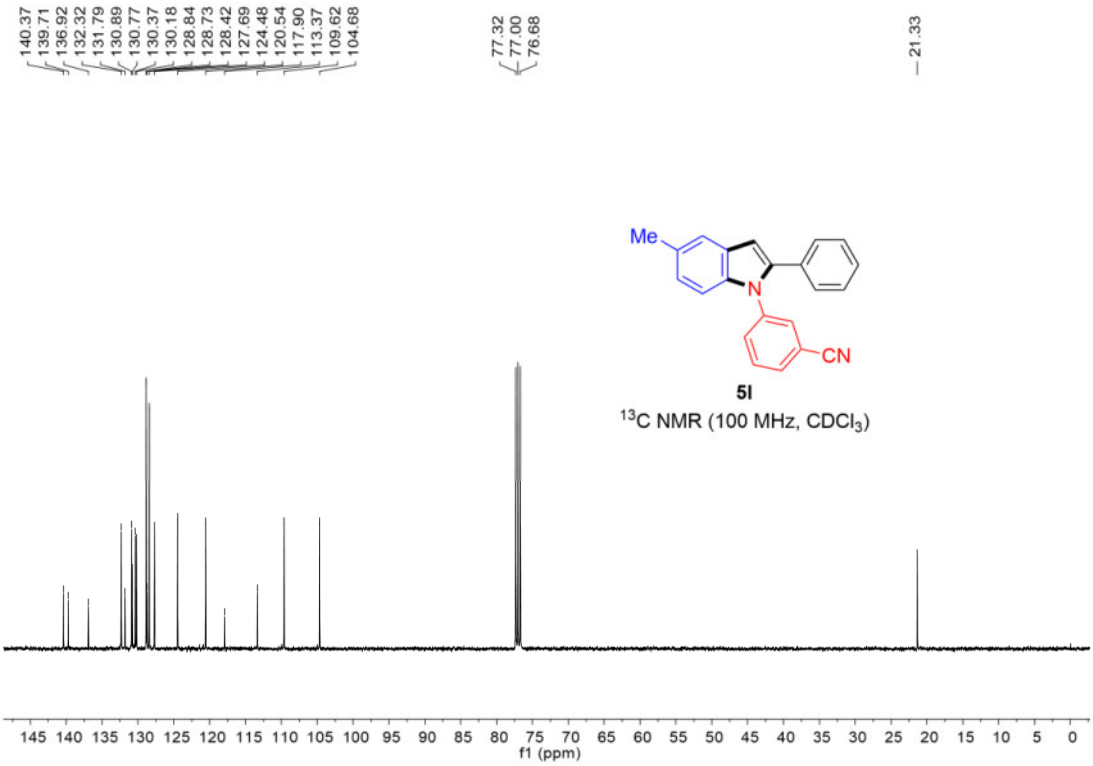
^{13}C NMR (100 MHz, $CDCl_3$)

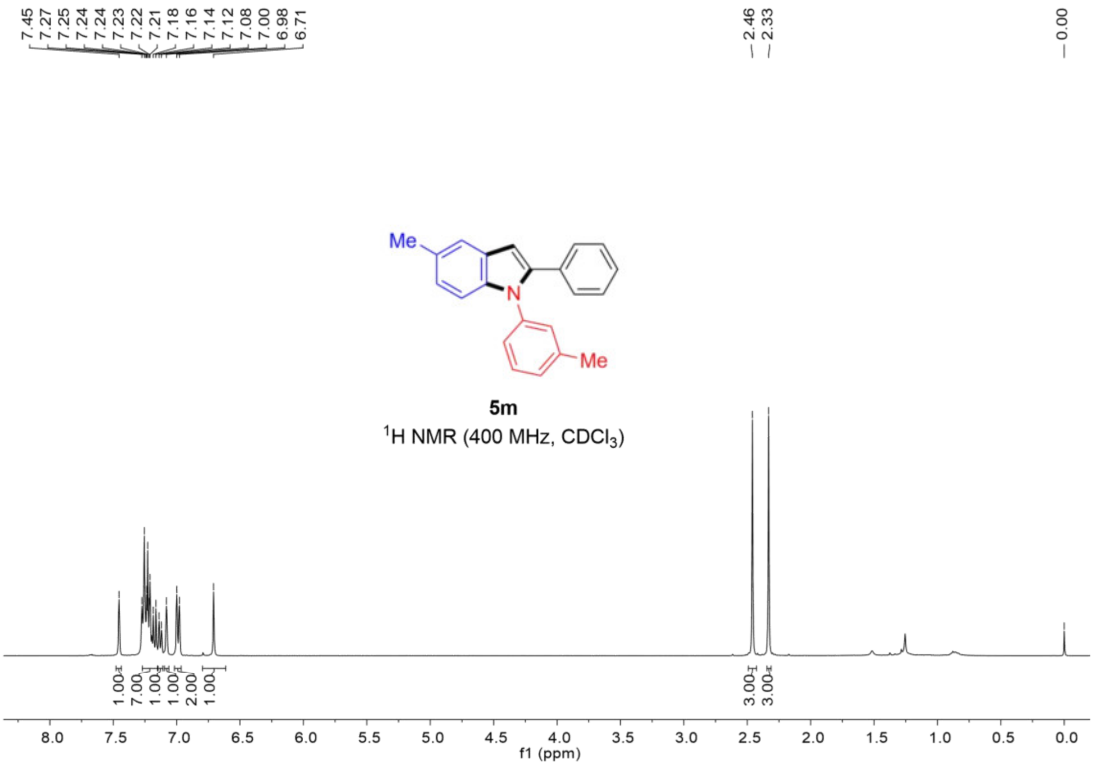


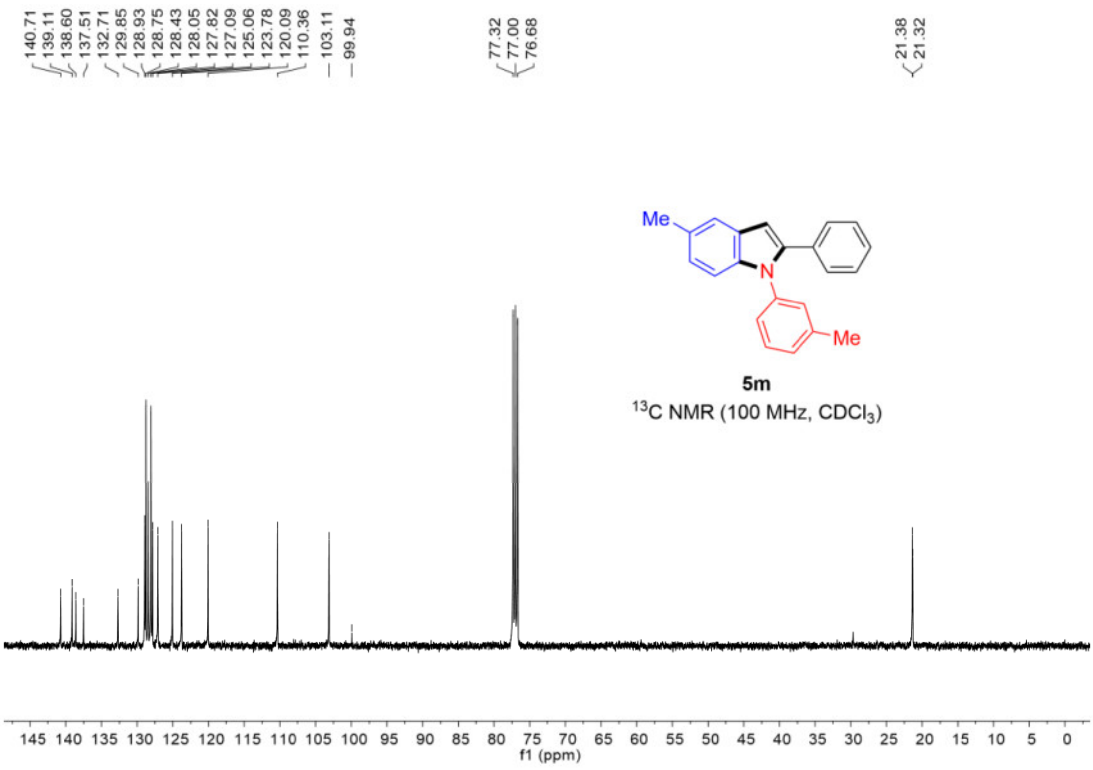

8.05
8.05
8.02
8.00
7.47
7.44
7.43
7.41
7.30
7.28
7.25
7.24
7.23
7.17
7.15
7.02
7.00
6.73
3.90
2.47
0.00
Me
N
O
O
5k
1H NMR (400 MHz, CDCl3)
1.00
1.00
2.00
1.00
5.00
1.00
1.00
1.00
3.00
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

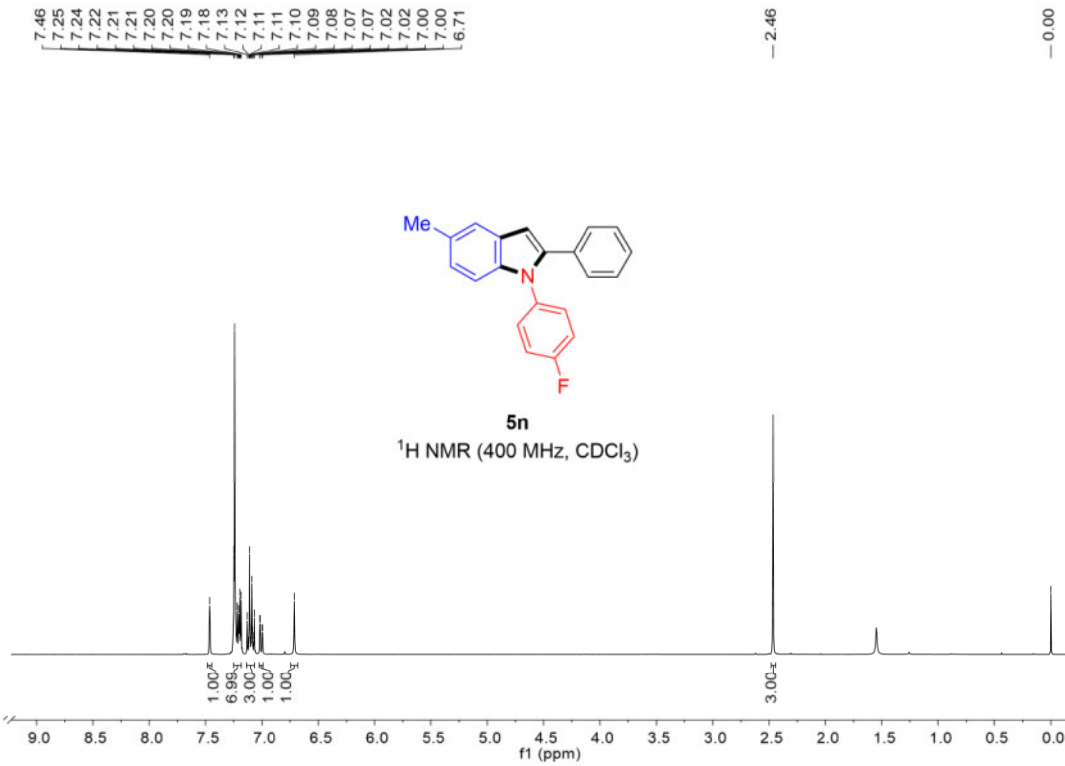

166.20
77.32
77.00
76.68
52.25
21.33
140.57
138.98
137.28
132.44
132.20
131.34
130.21
129.28
128.81
128.60
128.56
128.18
128.04
127.29
124.10
120.27
109.98
103.84
140
135
130
125
120
115
110
105
f1 (ppm)
Me
N
O
O
5k
13C NMR (100 MHz, CDCl3)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.61
7.59
7.54
7.50
7.48
7.47
7.43
7.41
7.27
7.26
7.25
7.21
7.20
7.19
7.18
7.16
7.14
7.05
7.03
6.74
2.47
0.00
Me
N
CN
5l
1H NMR (400 MHz, CDCl3)
1.00
1.00
2.00
1.00
3.00
2.00
1.00
1.00
1.00
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


140.37
139.71
136.92
132.32
131.79
130.89
130.77
130.37
130.18
128.84
128.73
128.42
127.69
124.48
120.54
117.90
113.37
109.62
104.68
77.32
77.00
76.68
21.33
Me
N
CN
5l
13C NMR (100 MHz, CDCl3)
145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)

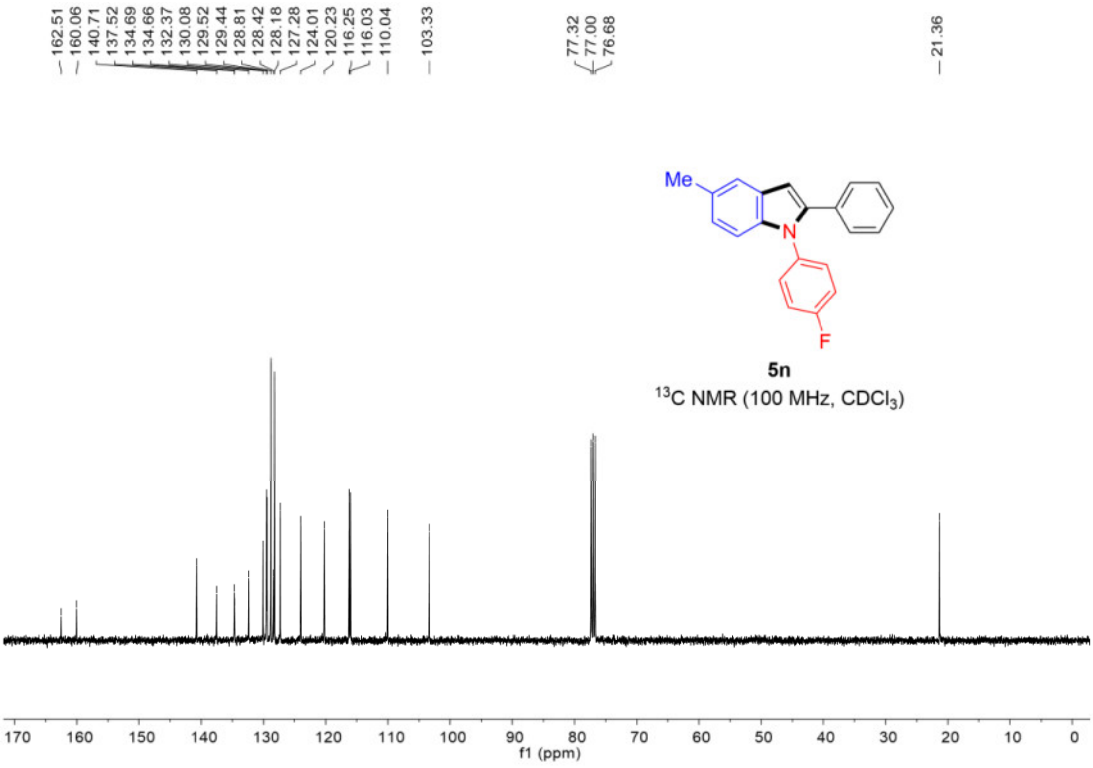

7.45
7.27
7.25
7.24
7.24
7.23
7.22
7.21
7.18
7.16
7.14
7.12
7.08
7.00
6.98
6.71
2.46
2.33
0.00
Me
N
Me
5m
1H NMR (400 MHz, CDCl3)
1.00
7.00
1.00
1.00
2.00
1.00
3.00
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


140.71
139.11
138.60
137.51
132.71
129.85
128.93
128.75
128.43
128.05
127.82
127.09
125.06
123.78
120.09
110.36
103.11
99.94
77.32
77.00
76.68
21.38
21.32
Me
N
Me
5m
13C NMR (100 MHz, CDCl3)
145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)



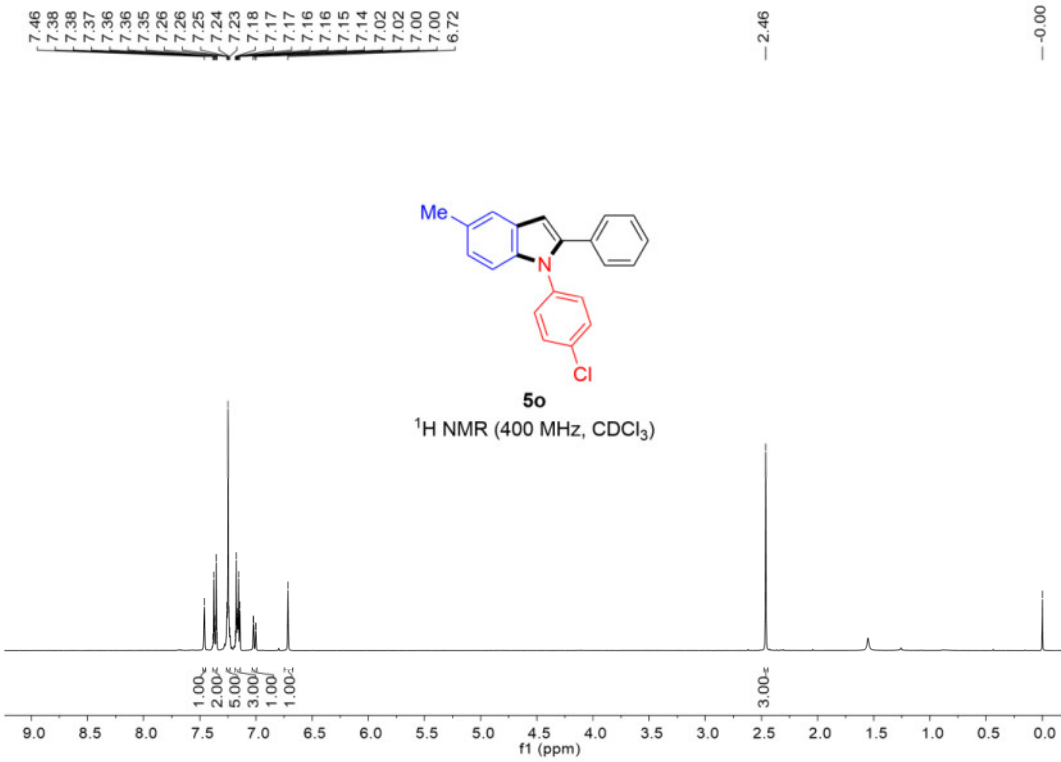
5n

^{1}H NMR (400 MHz, $CDCl_3$)



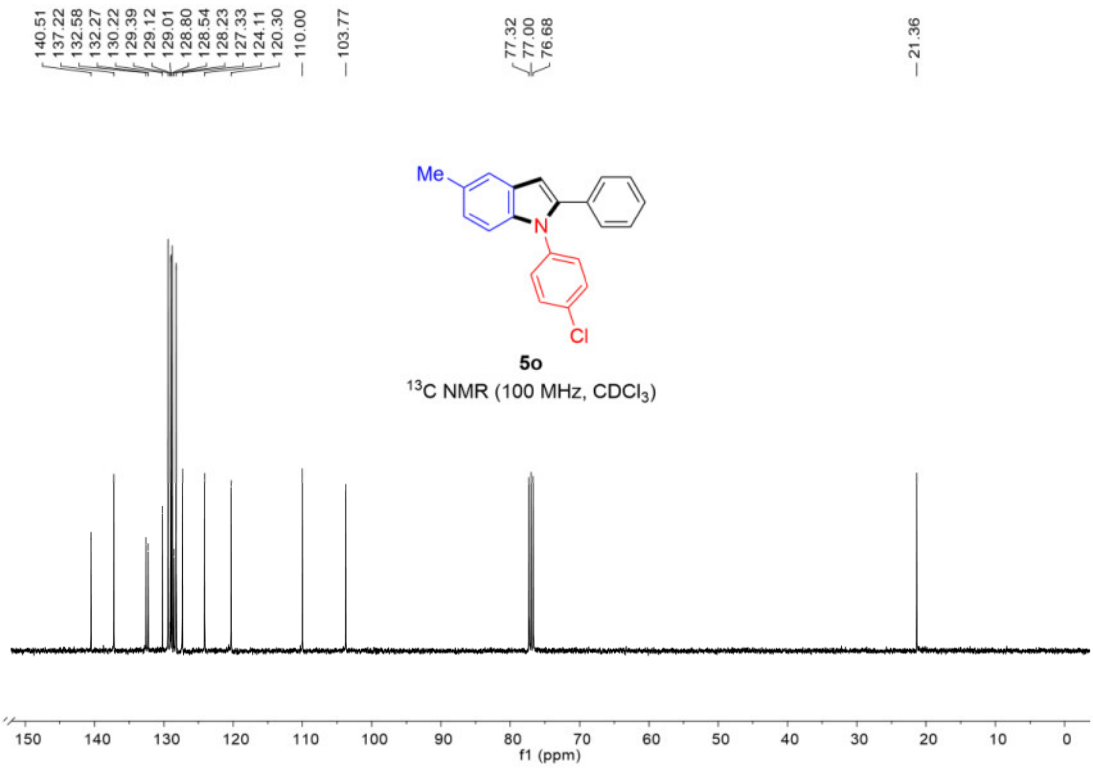
5n

^{13}C NMR (100 MHz, $CDCl_3$)



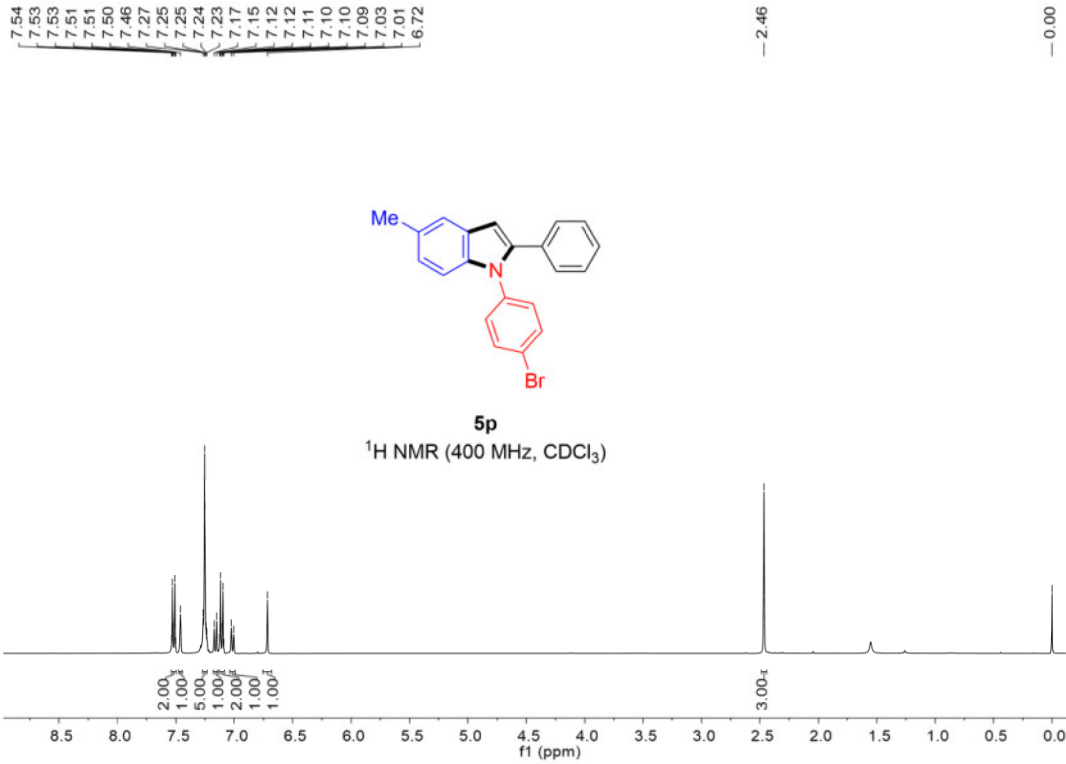
5o

^{1}H NMR (400 MHz, $CDCl_3$)



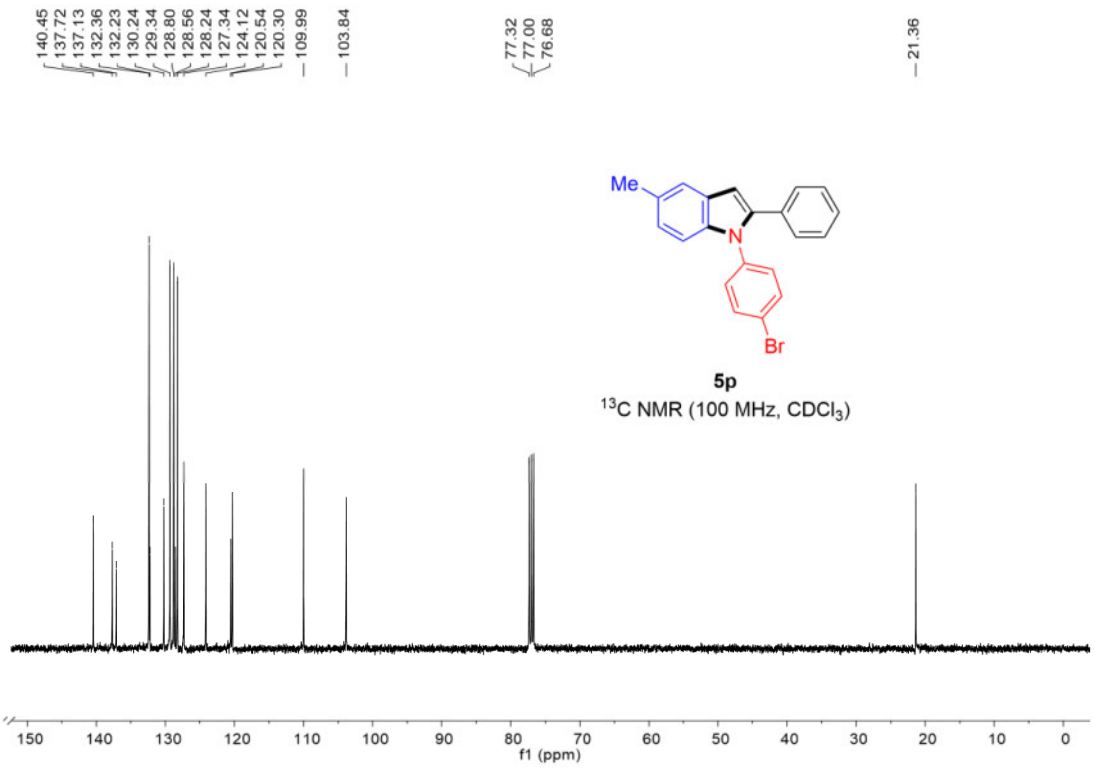
5o

^{13}C NMR (100 MHz, $CDCl_3$)



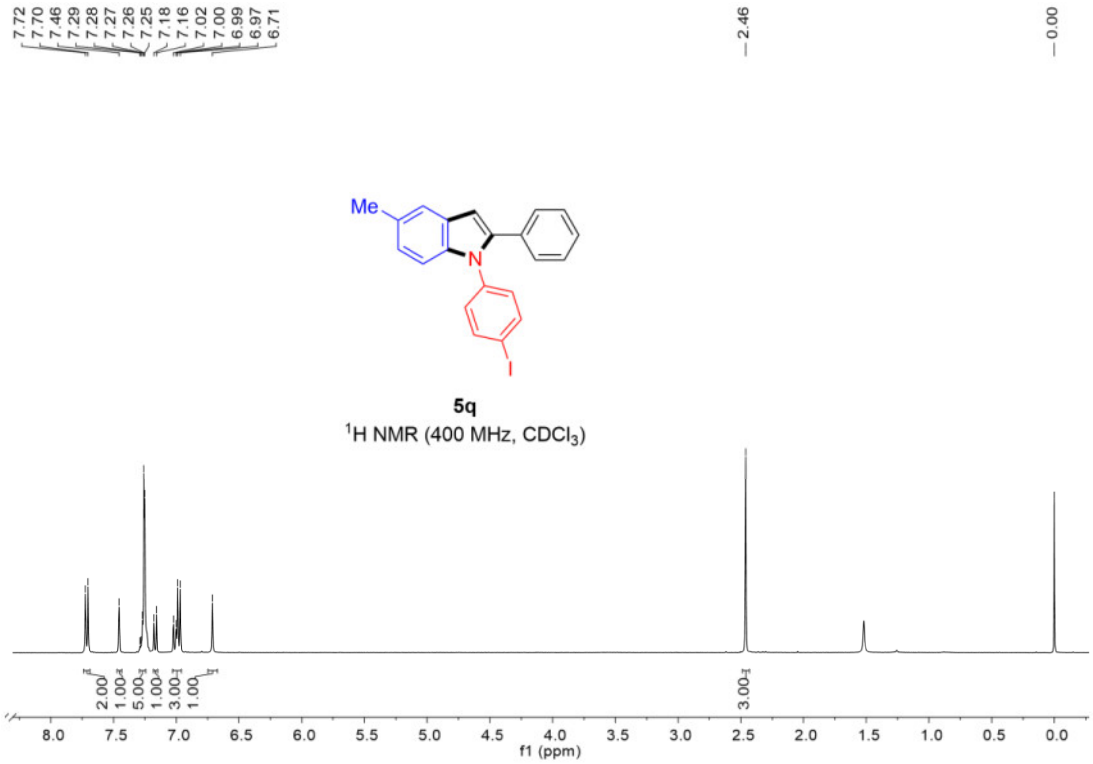
5p

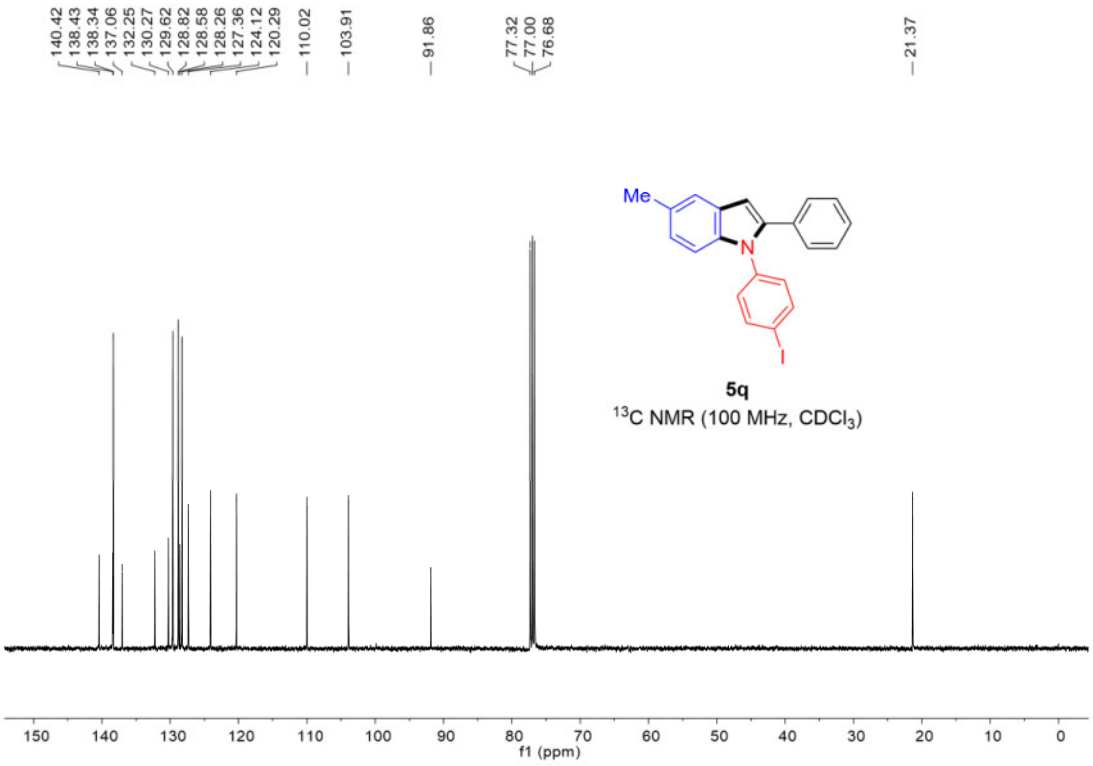
^{1}H NMR (400 MHz, $CDCl_3$)

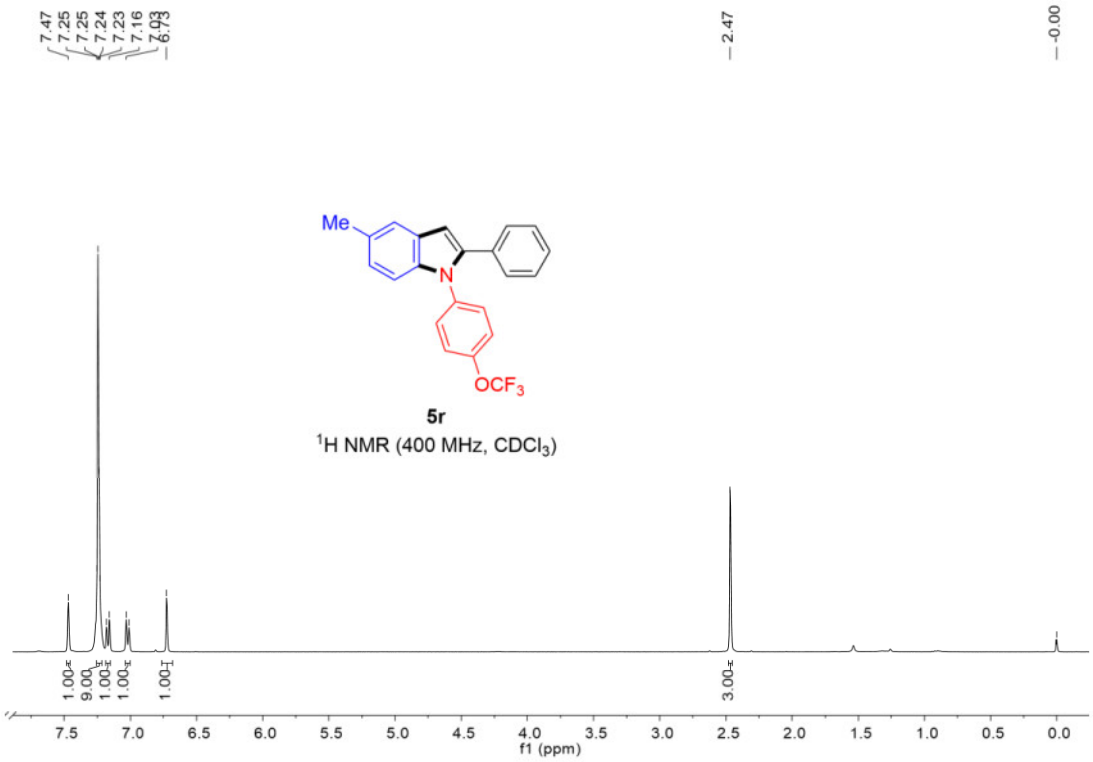


5p

^{13}C NMR (100 MHz, $CDCl_3$)

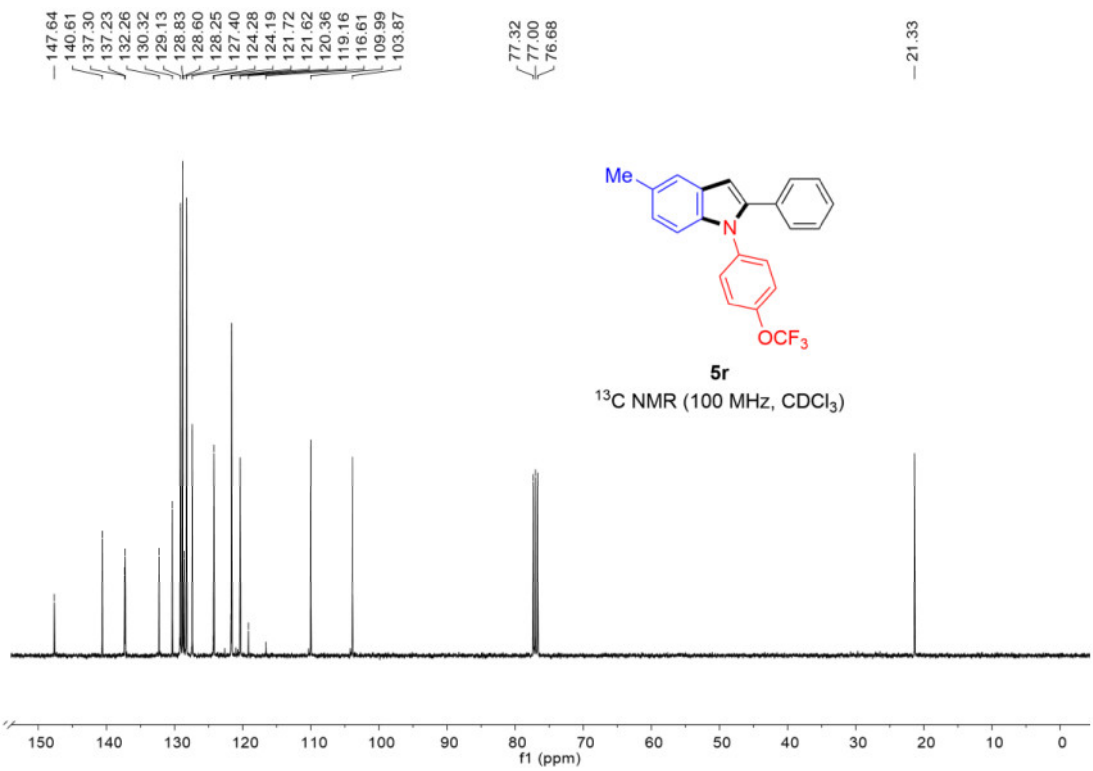

7.72
7.70
7.46
7.29
7.28
7.27
7.26
7.25
7.18
7.16
7.02
7.00
6.99
6.97
6.71
2.46
0.00
Me
N
I
5q
1H NMR (400 MHz, CDCl3)
2.00
1.00
5.00
1.00
3.00
1.00
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


140.42
138.43
138.34
137.06
132.25
130.27
129.62
128.82
128.58
128.26
127.36
124.12
120.29
110.02
103.91
91.86
77.32
77.00
76.68
21.37
Me
N
I
5q
13C NMR (100 MHz, CDCl3)
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



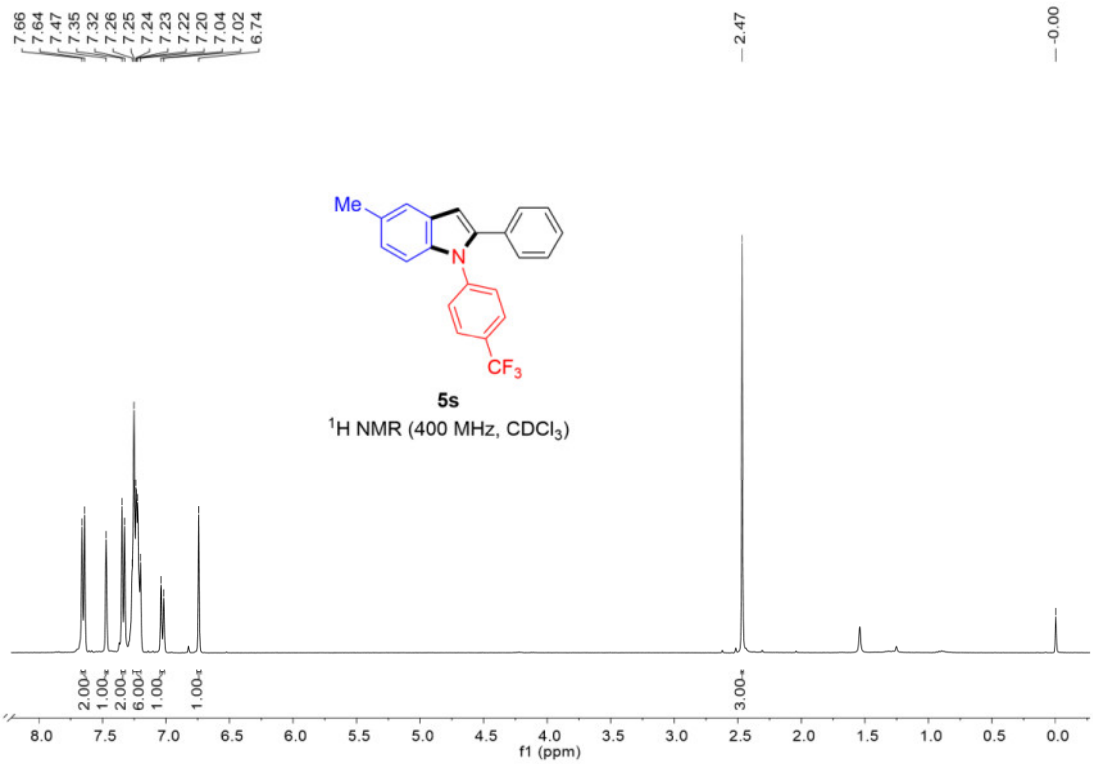
5r

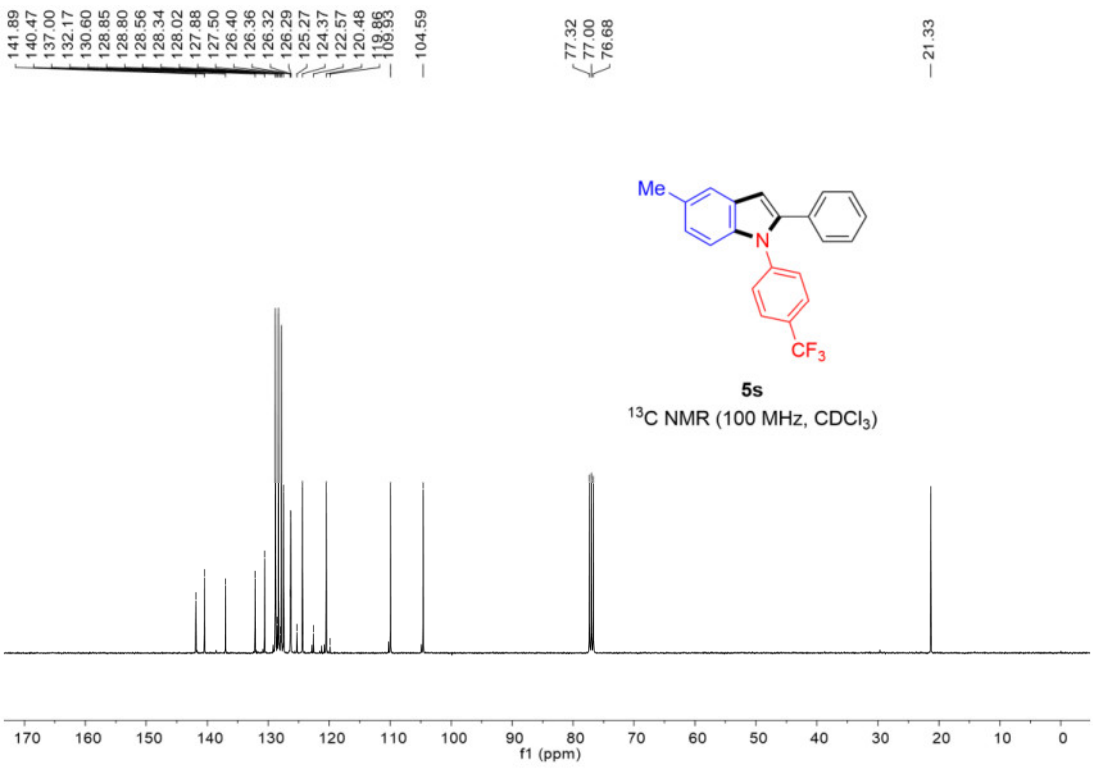
^{1}H NMR (400 MHz, $CDCl_3$)

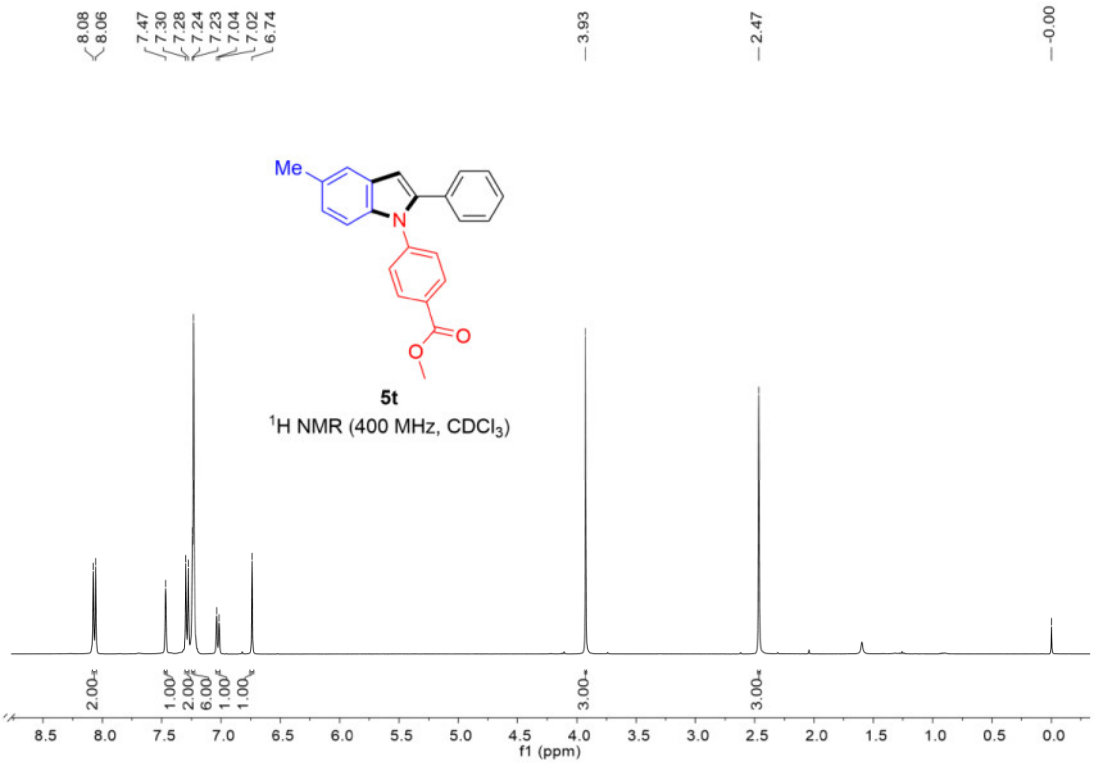


5r

^{13}C NMR (100 MHz, $CDCl_3$)

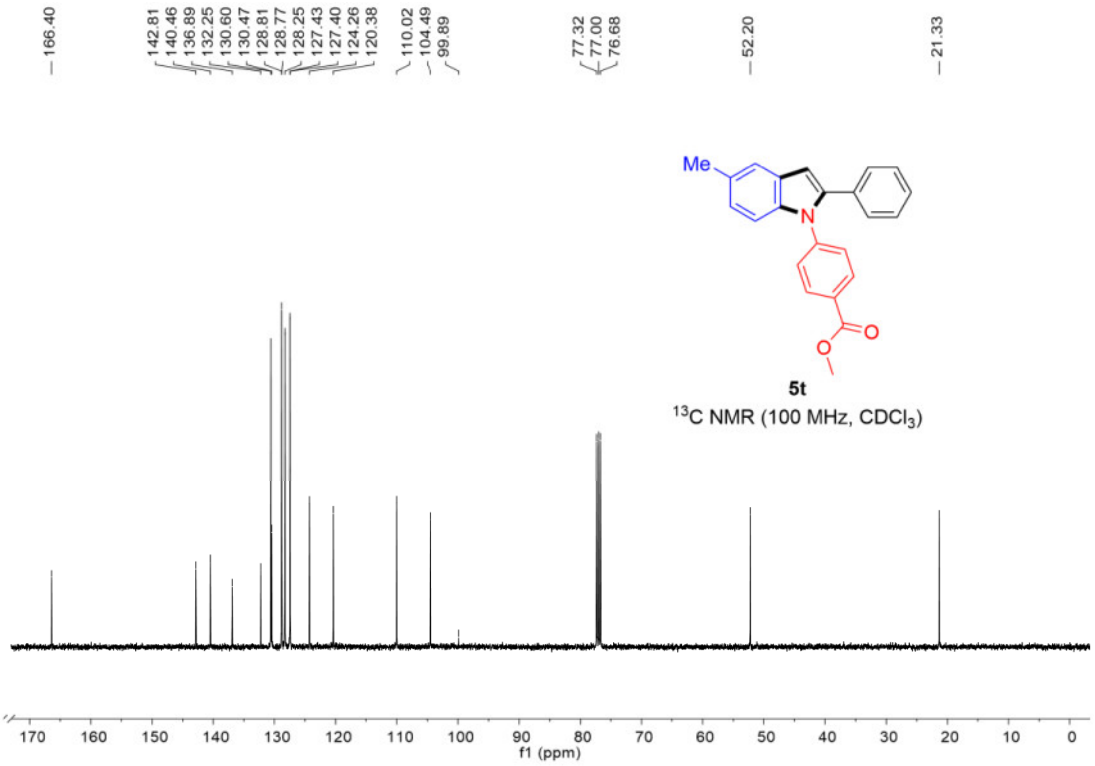

7.66
7.64
7.47
7.35
7.32
7.26
7.25
7.24
7.23
7.22
7.20
7.04
7.02
6.74
2.47
0.00
Me
N
CF3
5s
1H NMR (400 MHz, CDCl3)
2.00
1.00
2.00
6.00
1.00
1.00
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


141.89
140.47
137.00
132.17
130.60
128.85
128.80
128.56
128.34
128.02
127.88
127.50
126.40
126.36
126.32
126.29
125.27
124.37
122.57
120.48
119.86
109.93
104.59
77.32
77.00
76.68
21.33
Me
N
CF3
5s
13C NMR (100 MHz, CDCl3)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



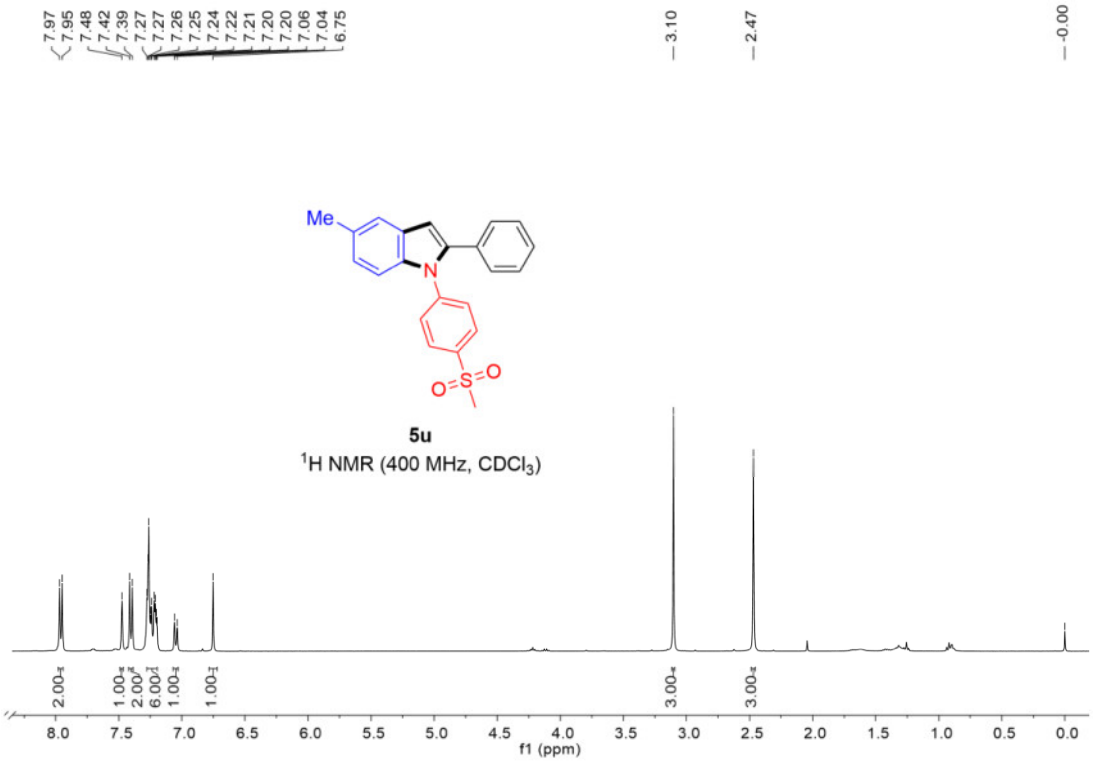
5t

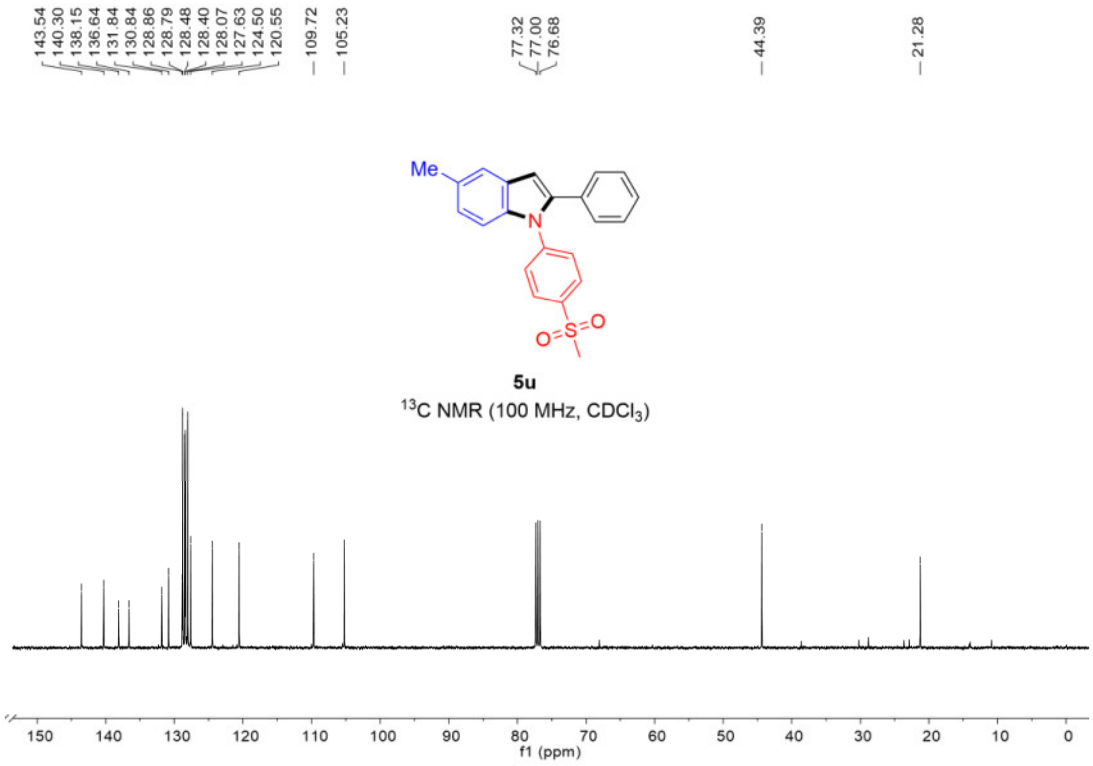
^{1}H NMR (400 MHz, $CDCl_3$)

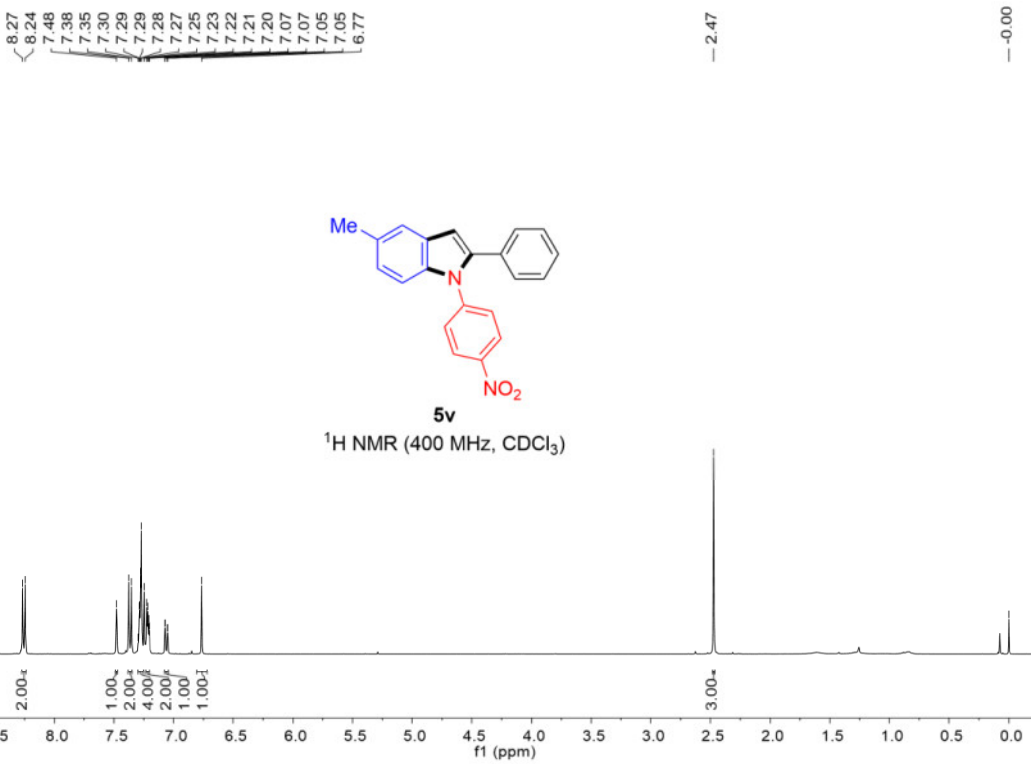


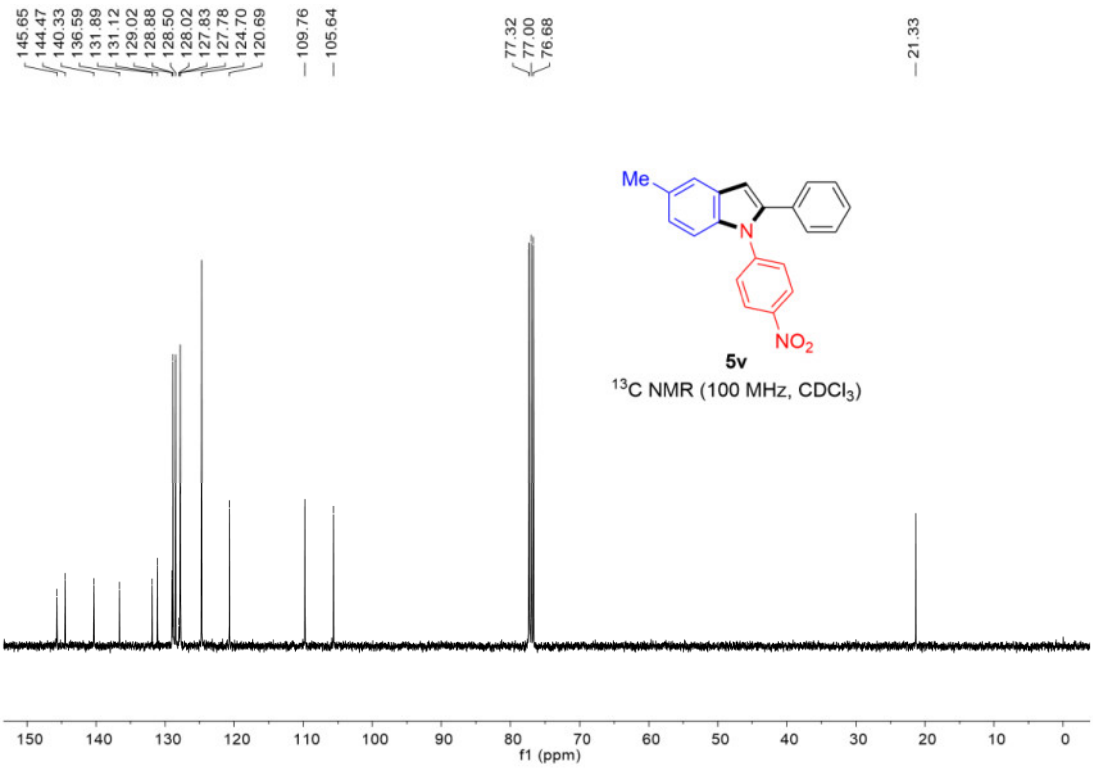
5t

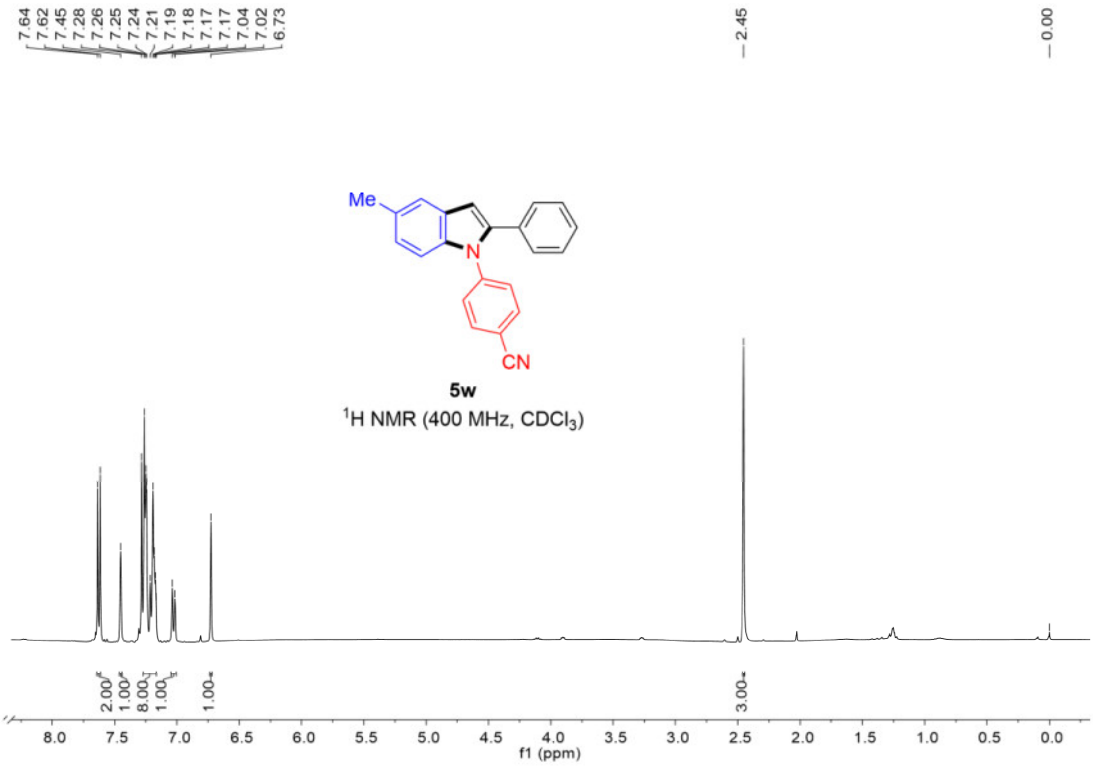
^{13}C NMR (100 MHz, $CDCl_3$)

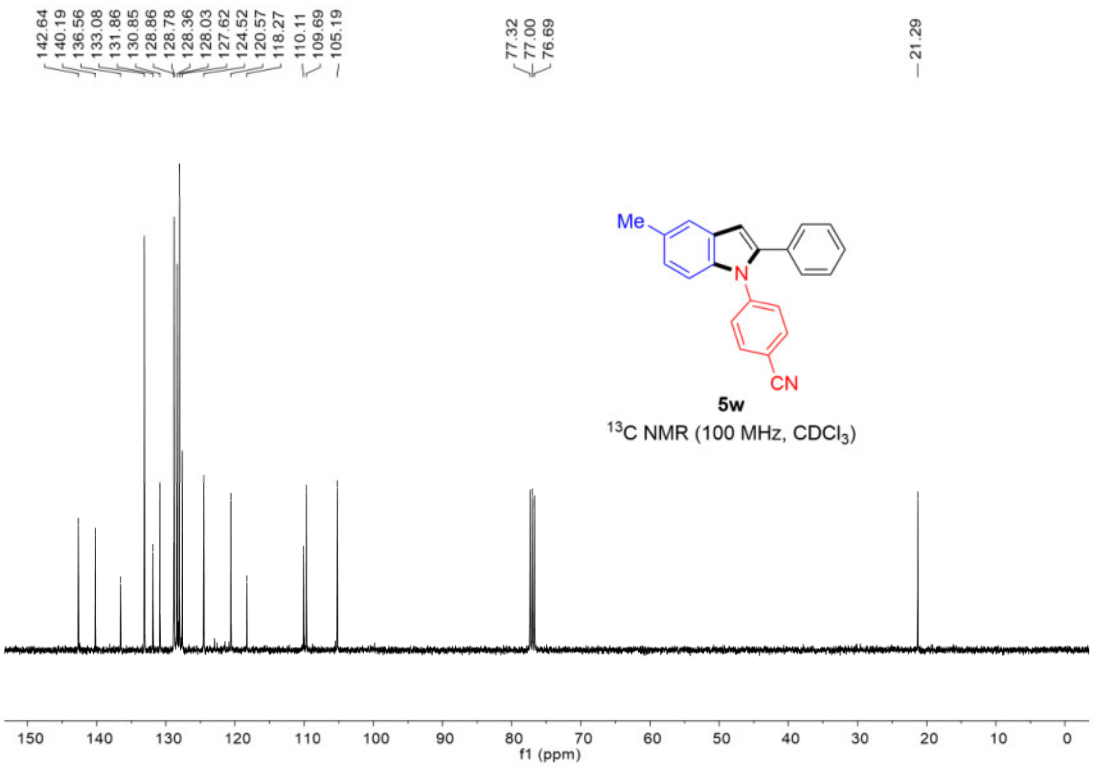

7.97
7.95
7.48
7.42
7.39
7.27
7.27
7.26
7.25
7.24
7.22
7.21
7.20
7.20
7.06
7.04
6.75
3.10
2.47
0.00
Me
N
O=S=O
5u
1H NMR (400 MHz, CDCl3)
2.00
1.00
2.00
6.00
1.00
1.00
3.00
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

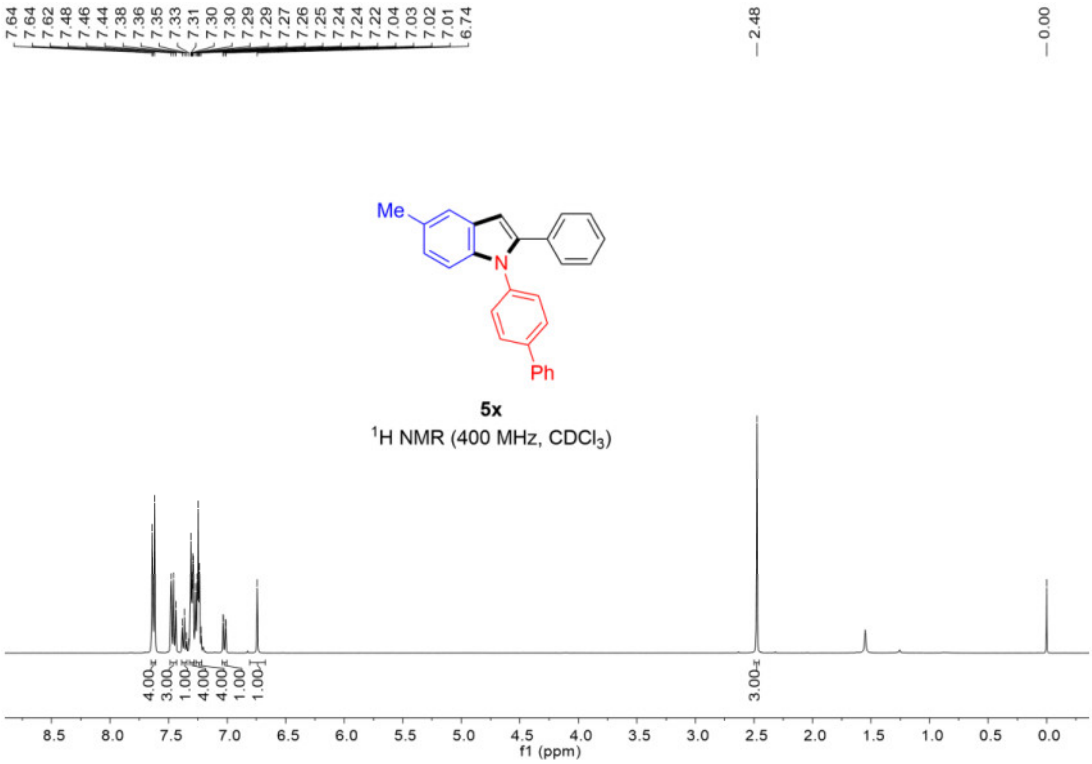

143.54
140.30
138.15
136.64
131.84
130.84
128.86
128.79
128.48
128.40
128.07
127.63
124.50
120.55
109.72
105.23
77.32
77.00
76.68
44.39
21.28
Me
N
O=S=O
5u
13C NMR (100 MHz, CDCl3)
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

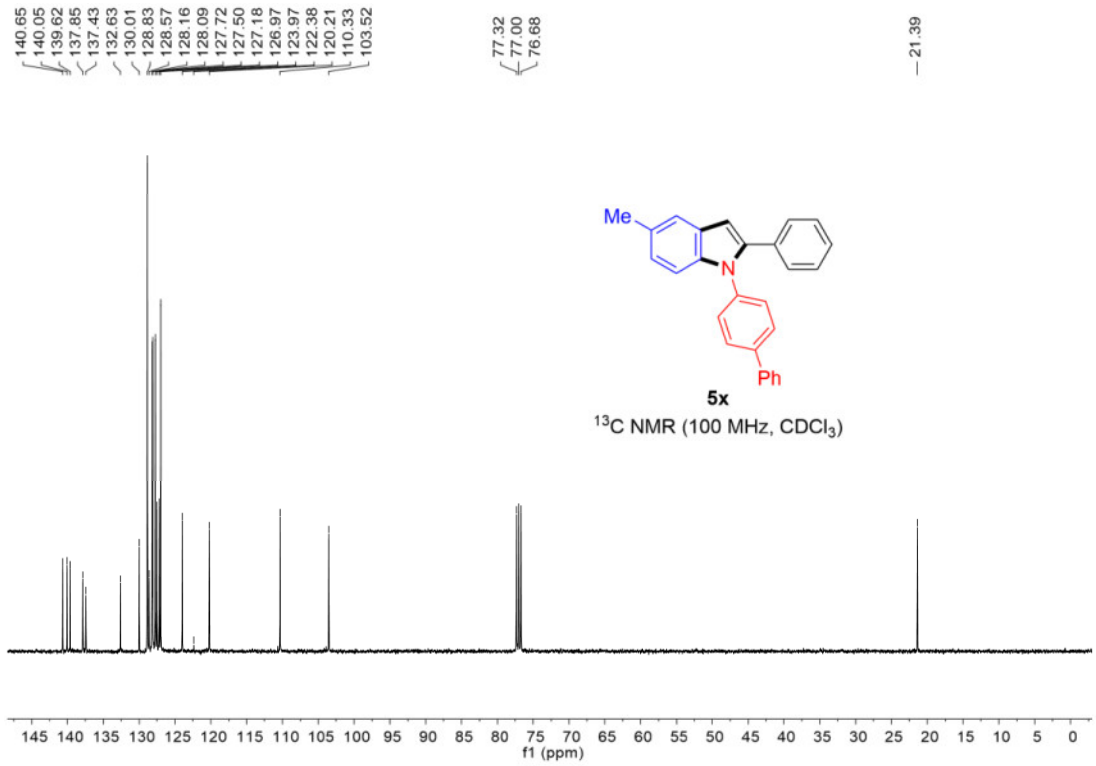

8.27
8.24
7.48
7.38
7.35
7.30
7.29
7.29
7.28
7.27
7.25
7.23
7.22
7.21
7.20
7.07
7.07
7.05
7.05
6.77
2.47
-0.00
Me
N
NO2
5v
1H NMR (400 MHz, CDCl3)
2.00
1.00
2.00
4.00
2.00
1.00
1.00
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

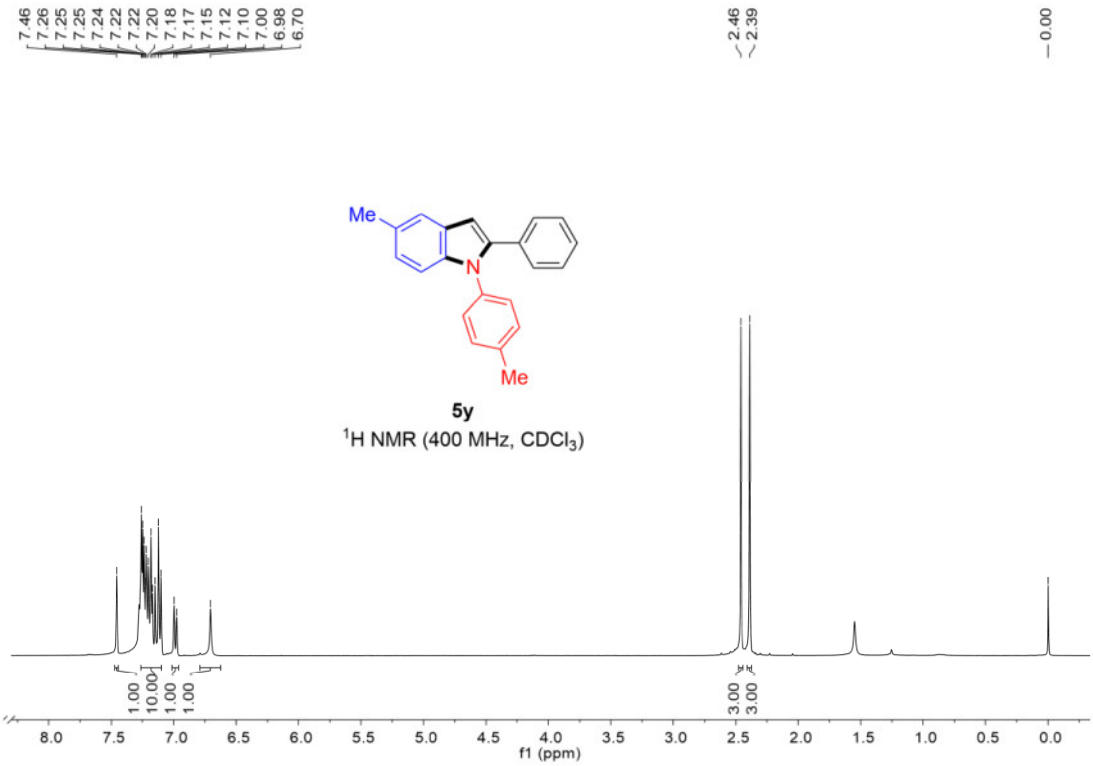

145.65
144.47
140.33
136.59
131.89
131.12
129.02
128.88
128.50
128.02
127.83
127.78
124.70
120.69
109.76
105.64
77.32
77.00
76.68
21.33
Me
N
NO2
5v
13C NMR (100 MHz, CDCl3)
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

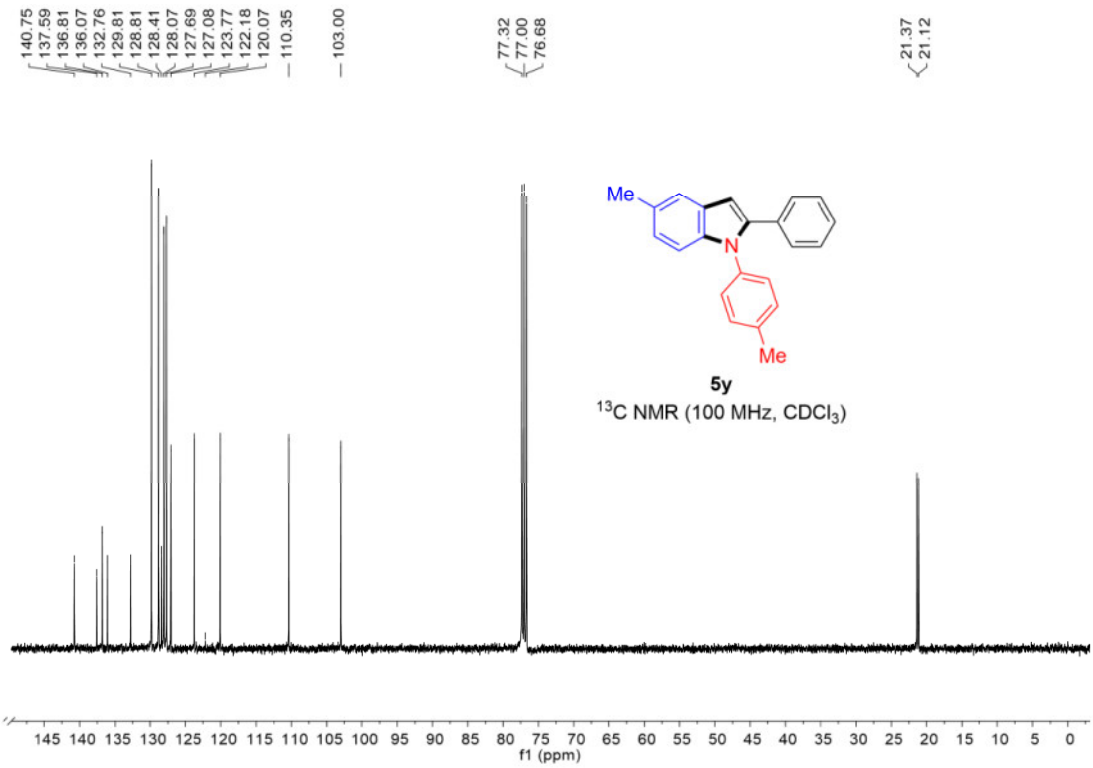

7.64
7.62
7.45
7.28
7.26
7.25
7.24
7.21
7.19
7.18
7.17
7.17
7.04
7.02
6.73
2.45
0.00
Me
N
CN
5w
1H NMR (400 MHz, CDCl3)
2.00
1.00
8.00
1.00
1.00
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

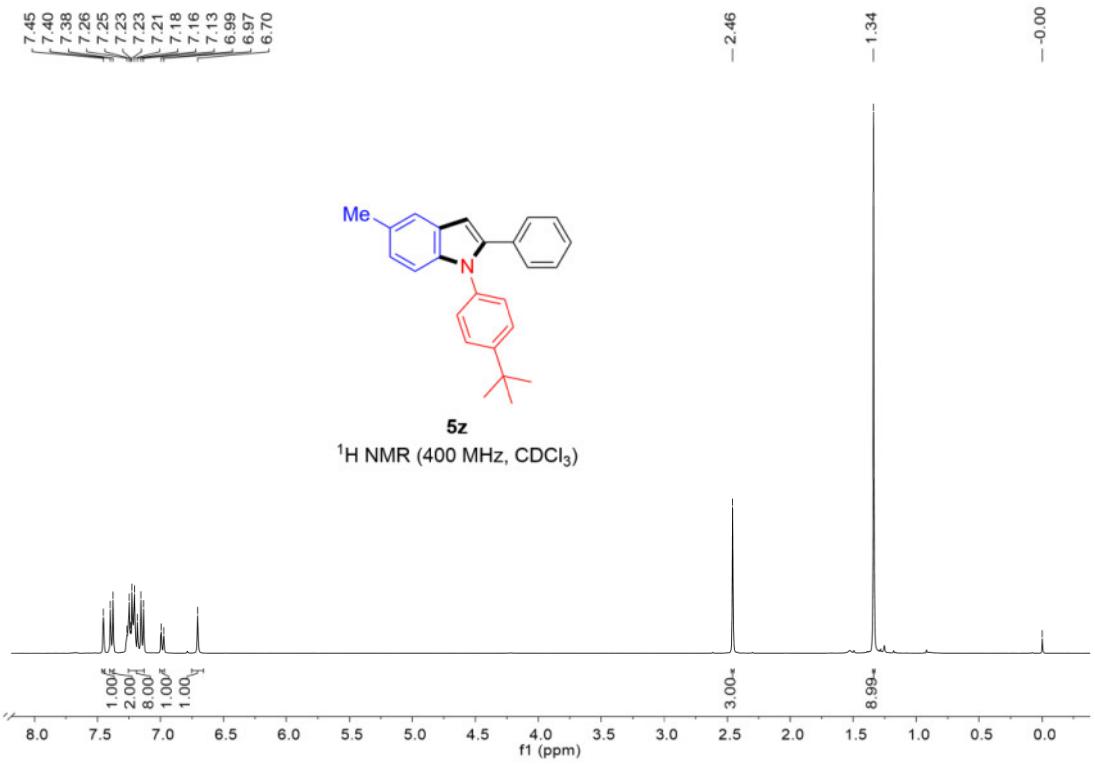

142.64
140.19
136.56
133.08
131.86
130.85
128.86
128.78
128.36
128.03
127.62
124.52
120.57
118.27
110.11
109.69
105.19
77.32
77.00
76.69
21.29
Me
N
CN
5w
13C NMR (100 MHz, CDCl3)
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.64
7.64
7.62
7.48
7.46
7.44
7.38
7.36
7.35
7.33
7.31
7.30
7.30
7.29
7.29
7.27
7.26
7.25
7.24
7.24
7.22
7.04
7.03
7.02
7.01
6.74
2.48
0.00
Me
N
Ph
5x
1H NMR (400 MHz, CDCl3)
4.00
3.00
1.00
4.00
4.00
1.00
1.00
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


140.65
140.05
139.62
137.85
137.43
132.63
130.01
128.83
128.57
128.16
128.09
127.72
127.50
127.18
126.97
123.97
122.38
120.21
110.33
103.52
77.32
77.00
76.68
21.39
Me
N
Ph
5x
13C NMR (100 MHz, CDCl3)
145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)

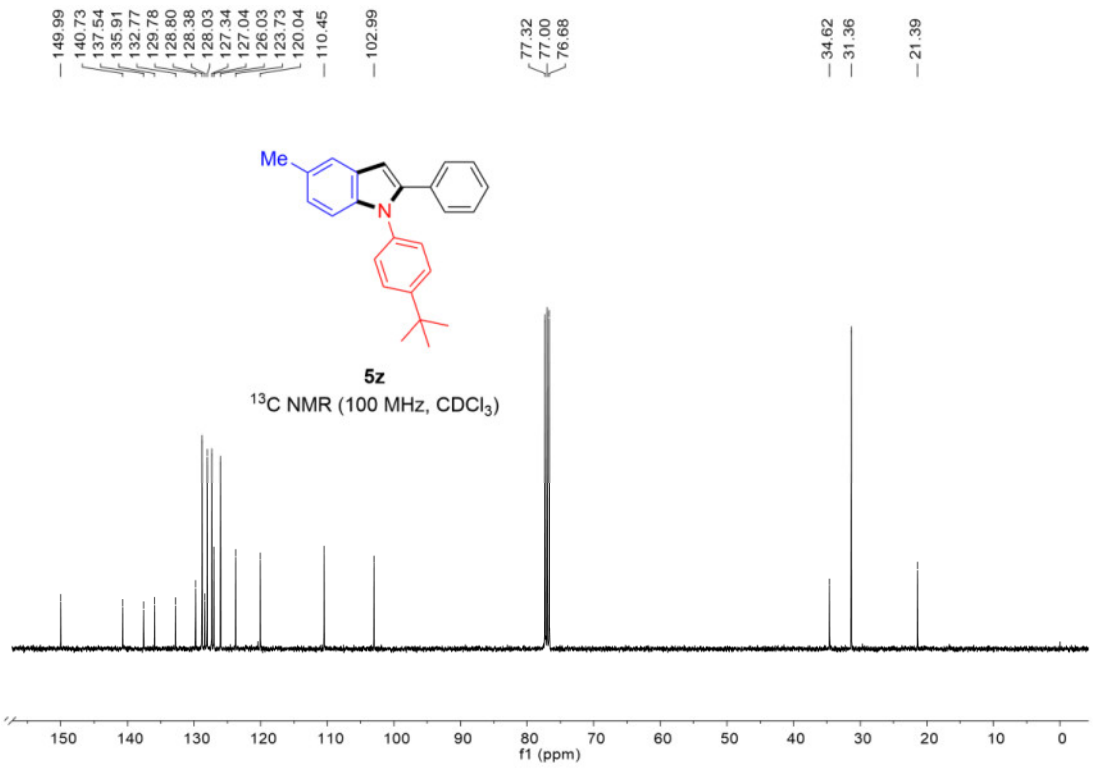

7.46
7.26
7.25
7.25
7.24
7.22
7.22
7.20
7.18
7.17
7.15
7.12
7.10
7.00
6.98
6.70
2.46
2.39
0.00
Me
N
Me
5y
1H NMR (400 MHz, CDCl3)
1.00
10.00
1.00
1.00
3.00
3.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


140.75
137.59
136.81
136.07
132.76
129.81
128.81
128.41
128.07
127.69
127.08
123.77
122.18
120.07
110.35
103.00
77.32
77.00
76.68
21.37
21.12
Me
N
Me
5y
13C NMR (100 MHz, CDCl3)
145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)



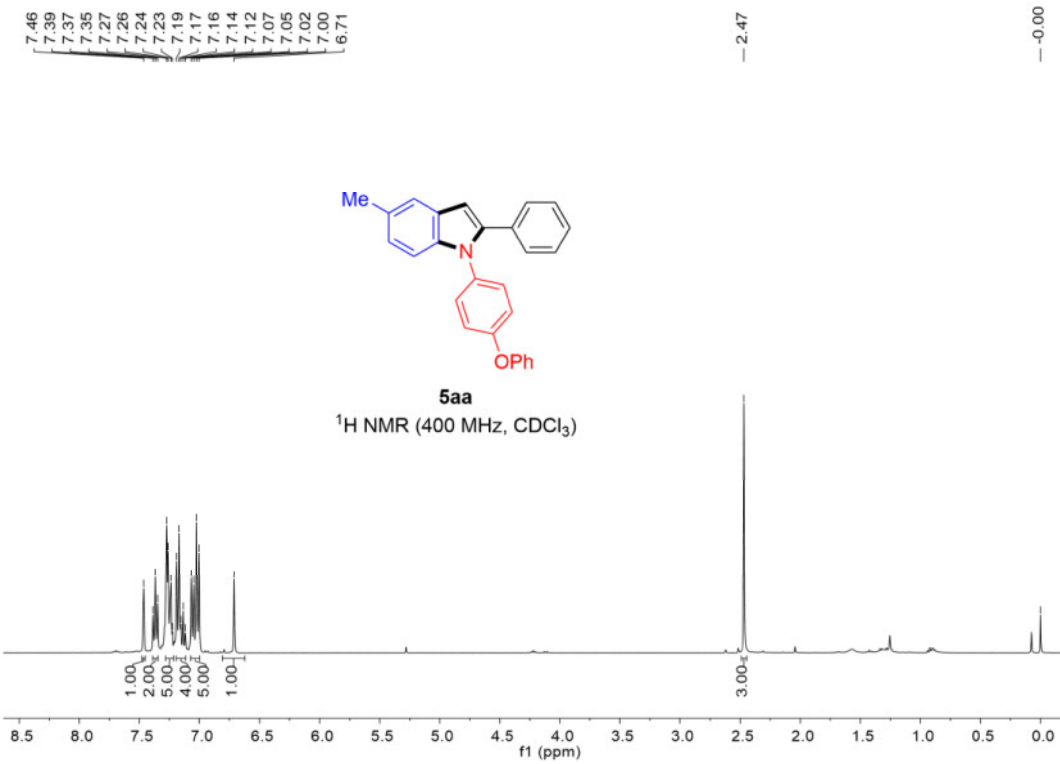
5z

^{1}H NMR (400 MHz, $CDCl_3$)



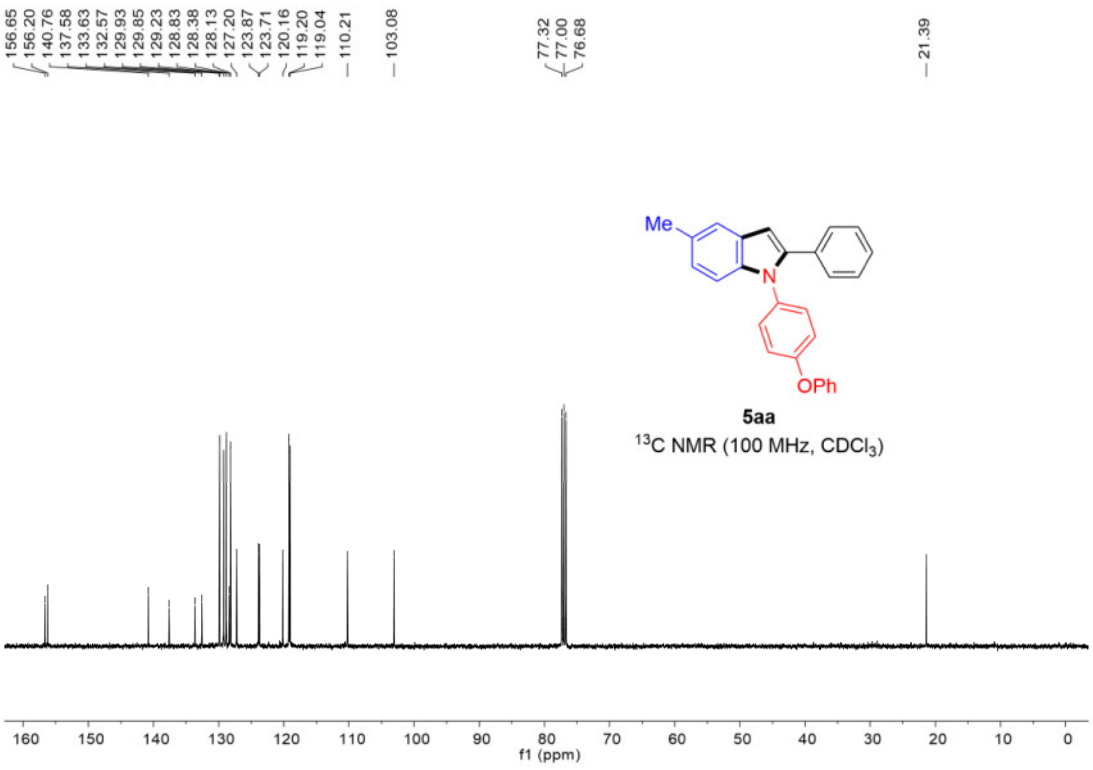
5z

^{13}C NMR (100 MHz, $CDCl_3$)



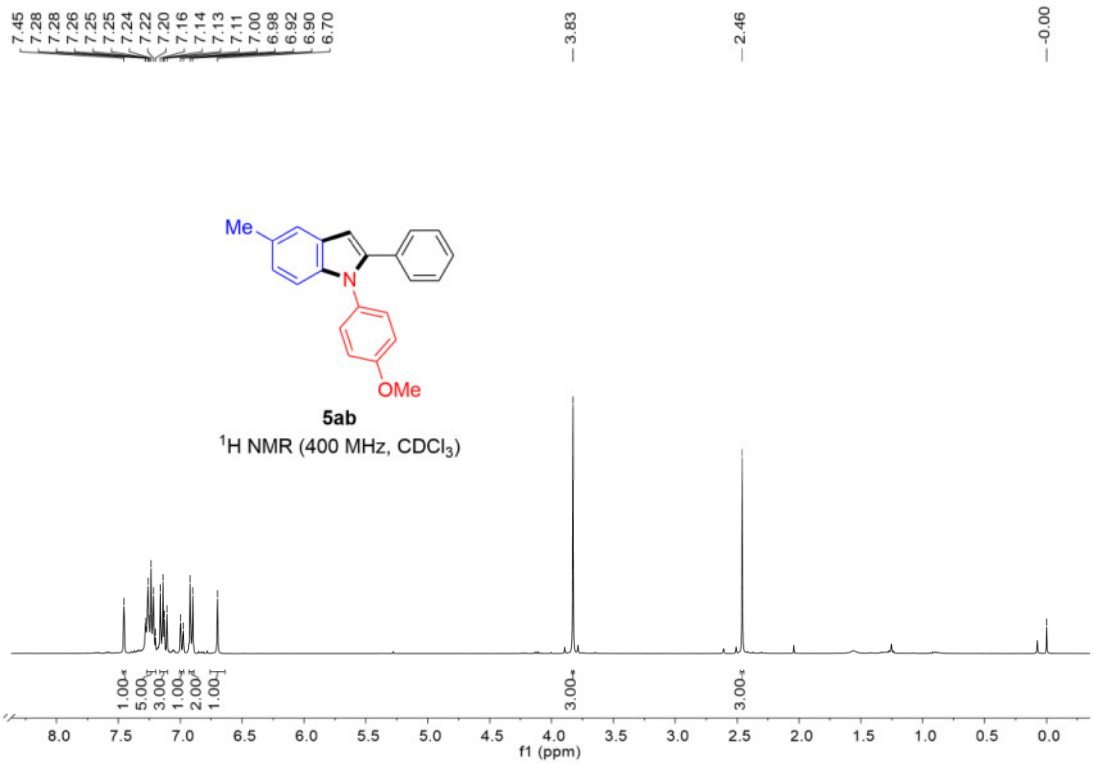
5aa

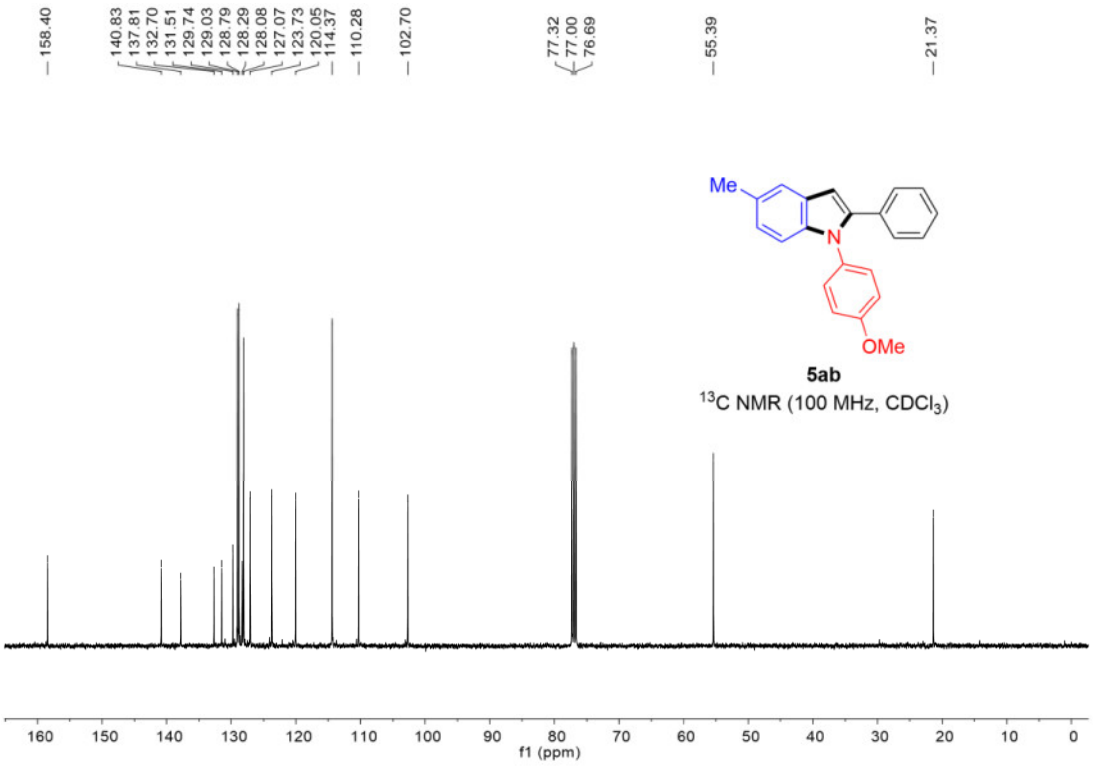
^{1}H NMR (400 MHz, $CDCl_3$)

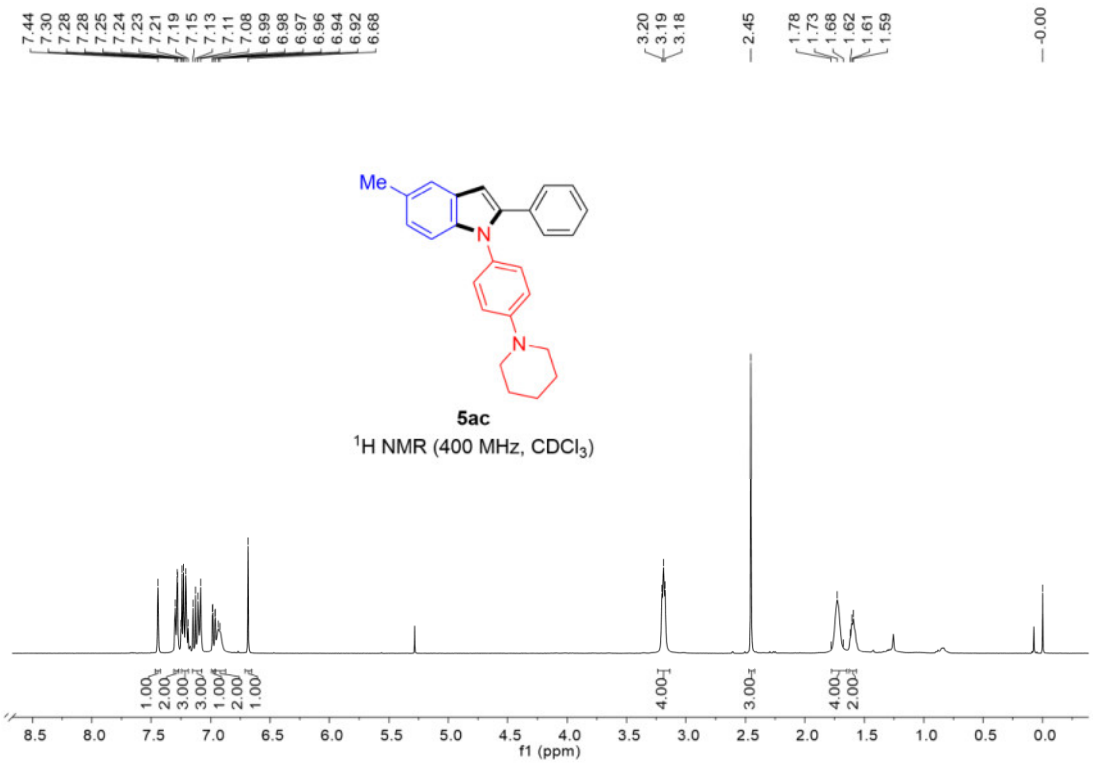


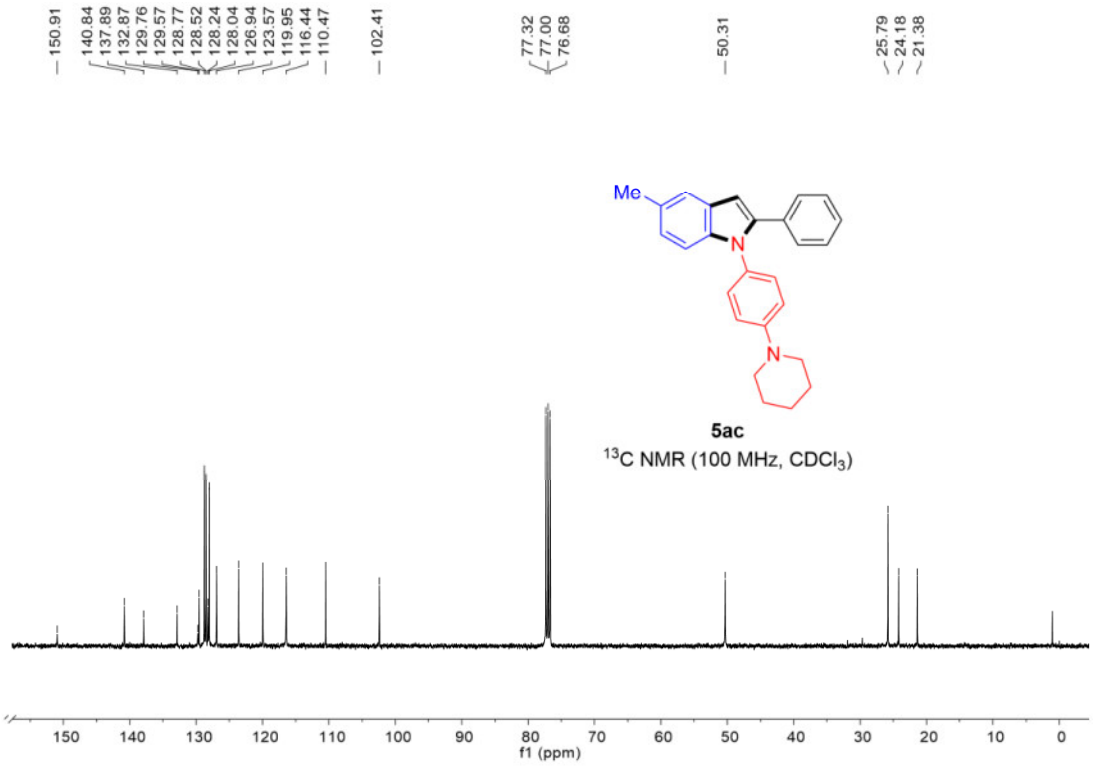
5aa

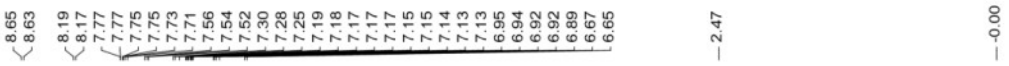
^{13}C NMR (100 MHz, $CDCl_3$)

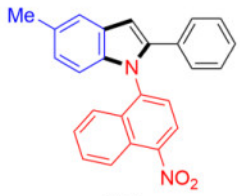

7.45
7.28
7.28
7.26
7.25
7.25
7.24
7.22
7.20
7.16
7.14
7.13
7.11
7.00
6.98
6.92
6.90
6.70
3.83
2.46
-0.00
Me
N
OMe
5ab
1H NMR (400 MHz, CDCl3)
1.00
5.00
3.00
1.00
2.00
1.00
3.00
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


158.40
140.83
137.81
132.70
131.51
129.74
129.03
128.79
128.29
128.08
127.07
123.73
120.05
114.37
110.28
102.70
77.32
77.00
76.69
55.39
21.37
Me
N
OMe
5ab
13C NMR (100 MHz, CDCl3)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.44
7.30
7.28
7.28
7.25
7.24
7.23
7.21
7.19
7.15
7.13
7.11
7.08
6.99
6.98
6.97
6.96
6.94
6.92
6.68
3.20
3.19
3.18
2.45
1.78
1.73
1.68
1.62
1.61
1.59
0.00
Me
N
N
5ac
1H NMR (400 MHz, CDCl3)
1.00
2.00
3.00
3.00
1.00
2.00
1.00
4.00
3.00
4.00
2.00
f1 (ppm)

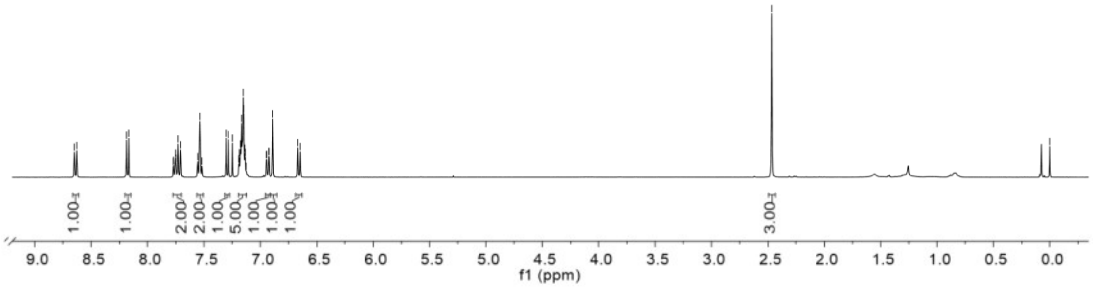

150.91
140.84
137.89
132.87
129.76
129.57
128.77
128.52
128.24
128.04
126.94
123.57
119.95
116.44
110.47
102.41
77.32
77.00
76.68
50.31
25.79
24.18
21.38
Me
N
N
5ac
13C NMR (100 MHz, CDCl3)
f1 (ppm)

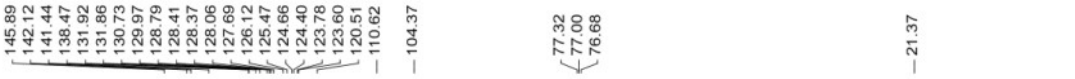


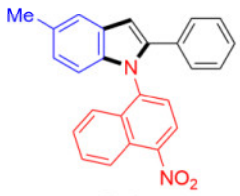


5ad

^{1}H NMR (400 MHz, $CDCl_3$)

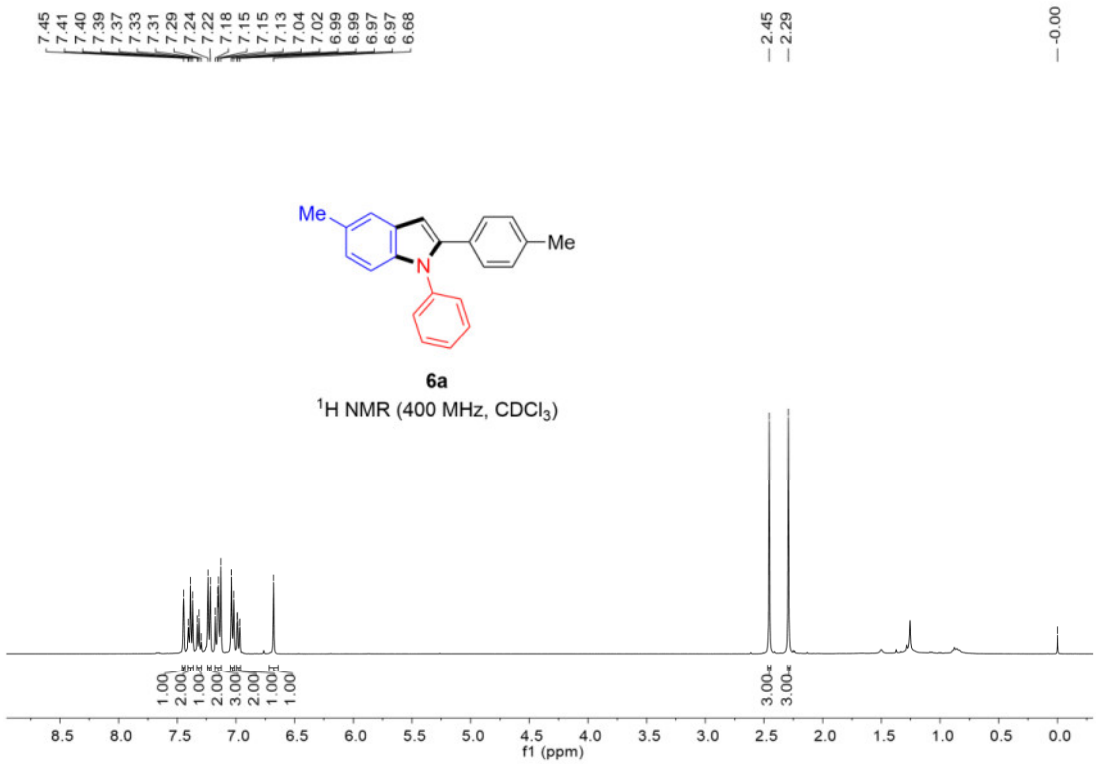


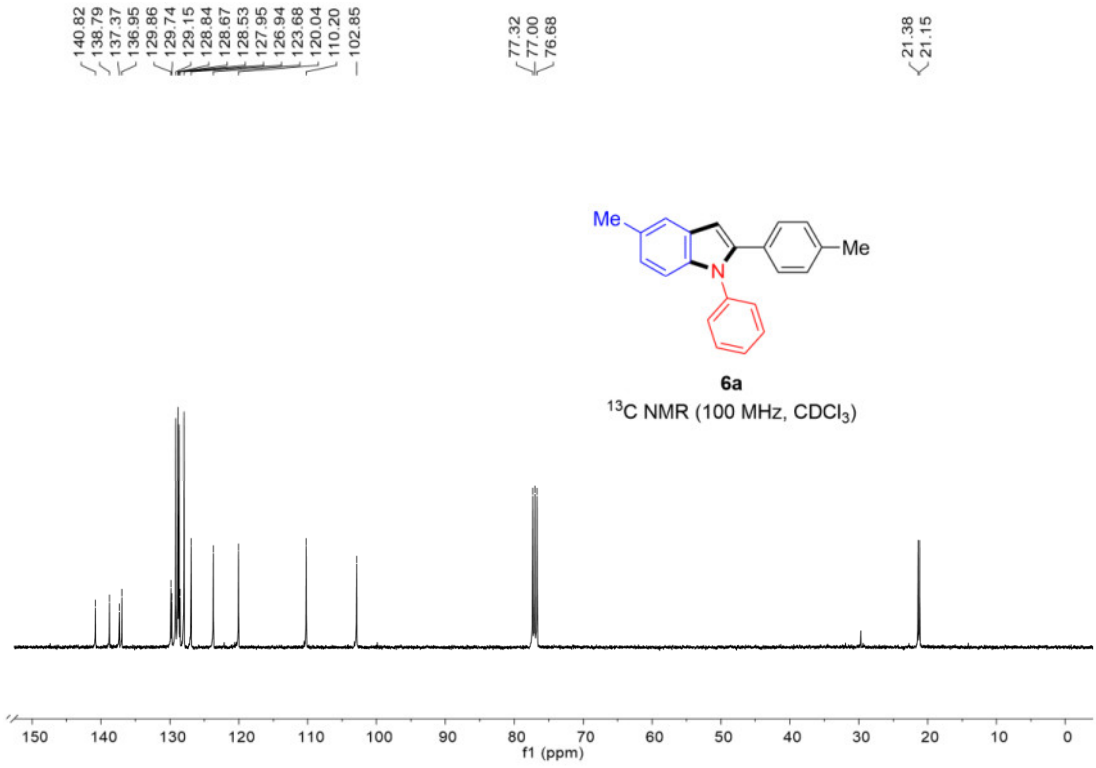


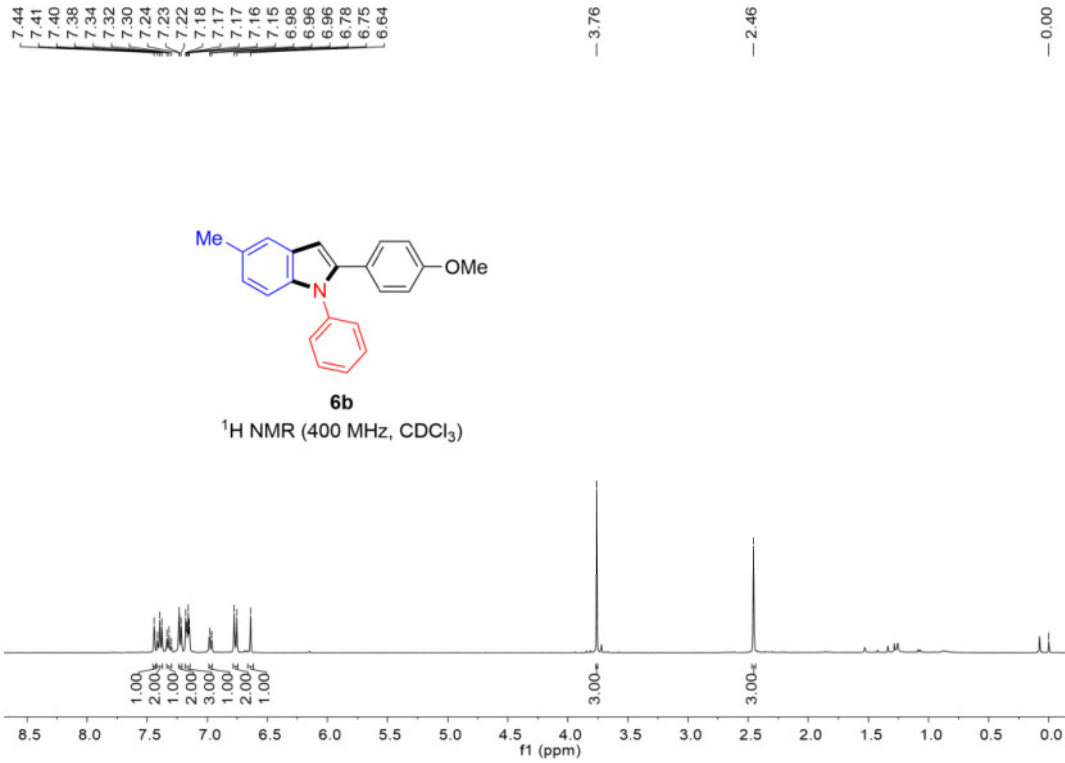


5ad

^{13}C NMR (100 MHz, $CDCl_3$)

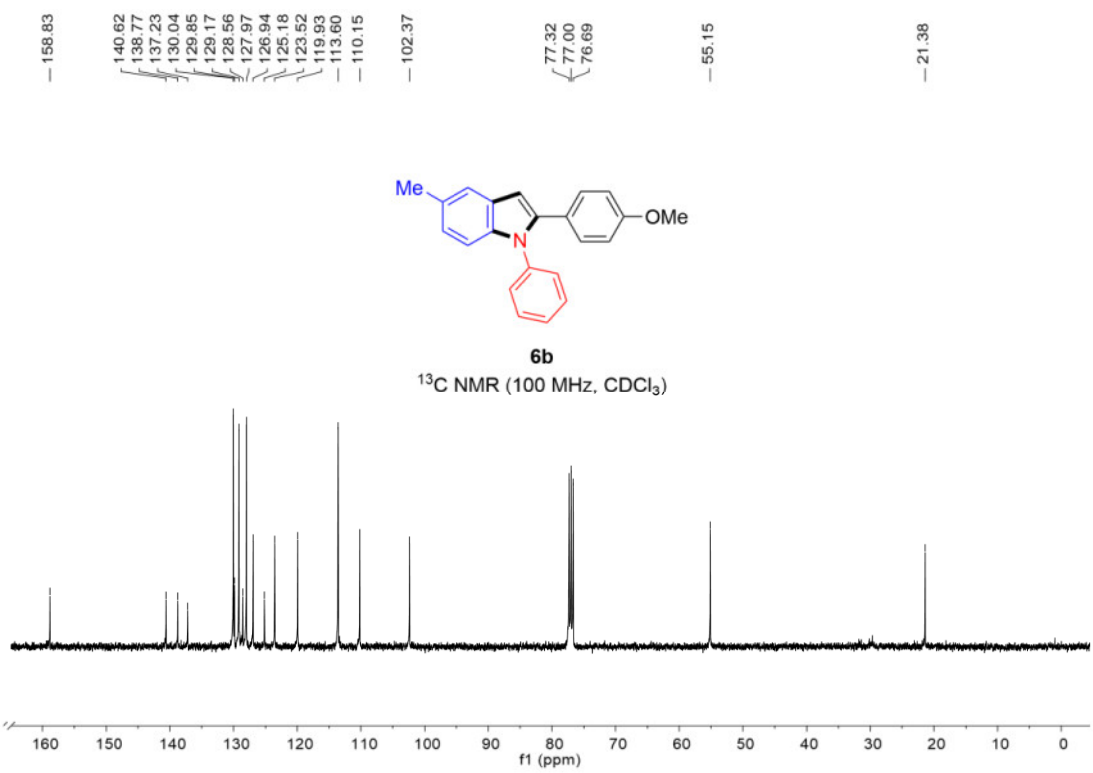

7.45
7.41
7.40
7.39
7.37
7.33
7.31
7.29
7.24
7.22
7.18
7.15
7.15
7.13
7.04
7.02
6.99
6.99
6.97
6.97
6.68
2.45
2.29
-0.00
Me
Me
N
6a
^{1}H NMR (400 MHz, $CDCl_3$)
1.00
2.00
1.00
2.00
3.00
2.00
1.00
1.00
3.00
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


140.82
138.79
137.37
136.95
129.86
129.74
129.15
128.84
128.67
128.53
127.95
126.94
123.68
120.04
110.20
102.85
77.32
77.00
76.68
21.38
21.15
Me
Me
N
6a
^{13}C NMR (100 MHz, $CDCl_3$)
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



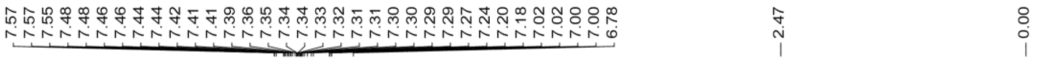
6b

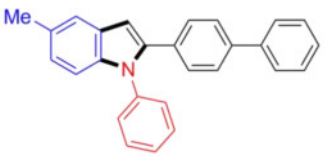
^{1}H NMR (400 MHz, $CDCl_3$)



6b

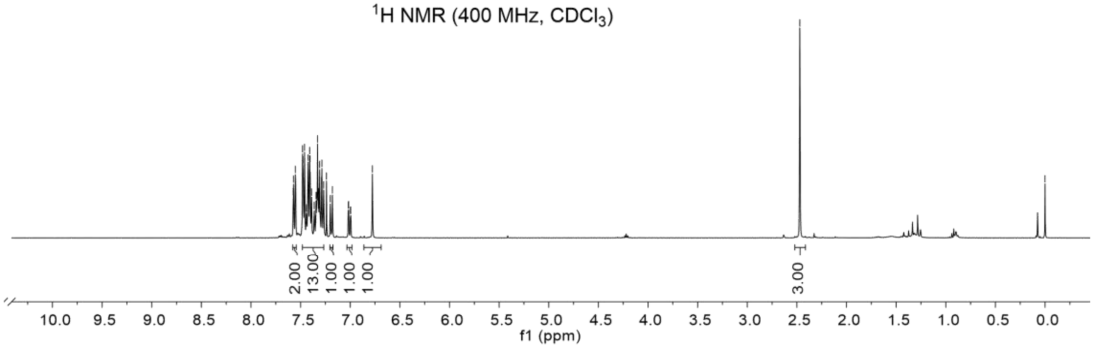
^{13}C NMR (100 MHz, $CDCl_3$)

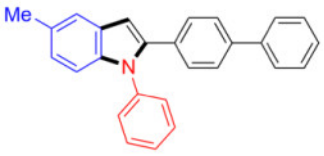




6c

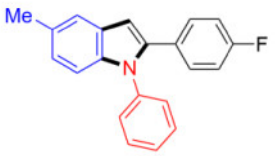
^{1}H NMR (400 MHz, $CDCl_3$)





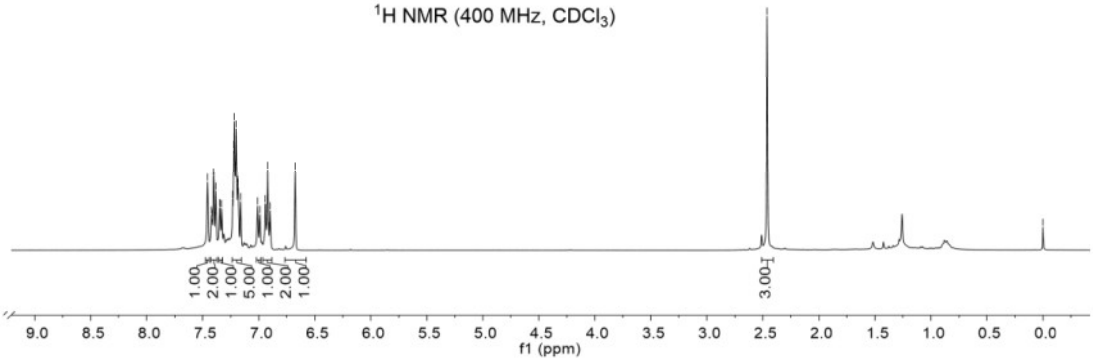
6c

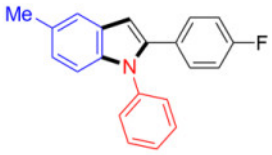
^{13}C NMR (100 MHz, $CDCl_3$)



6d

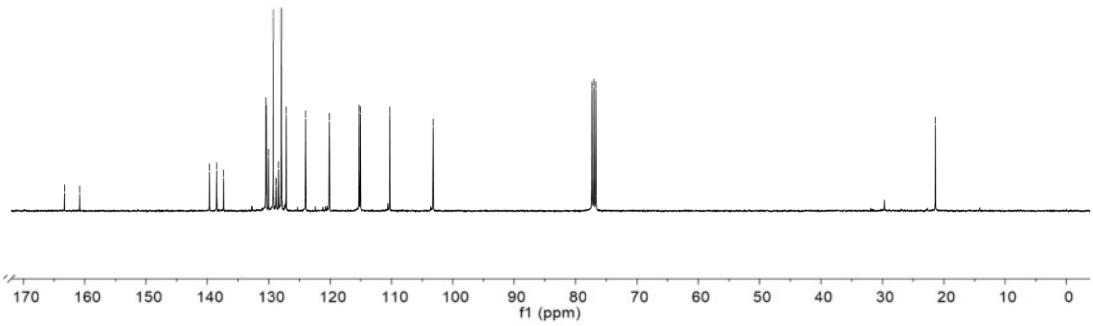
^{1}H NMR (400 MHz, $CDCl_3$)

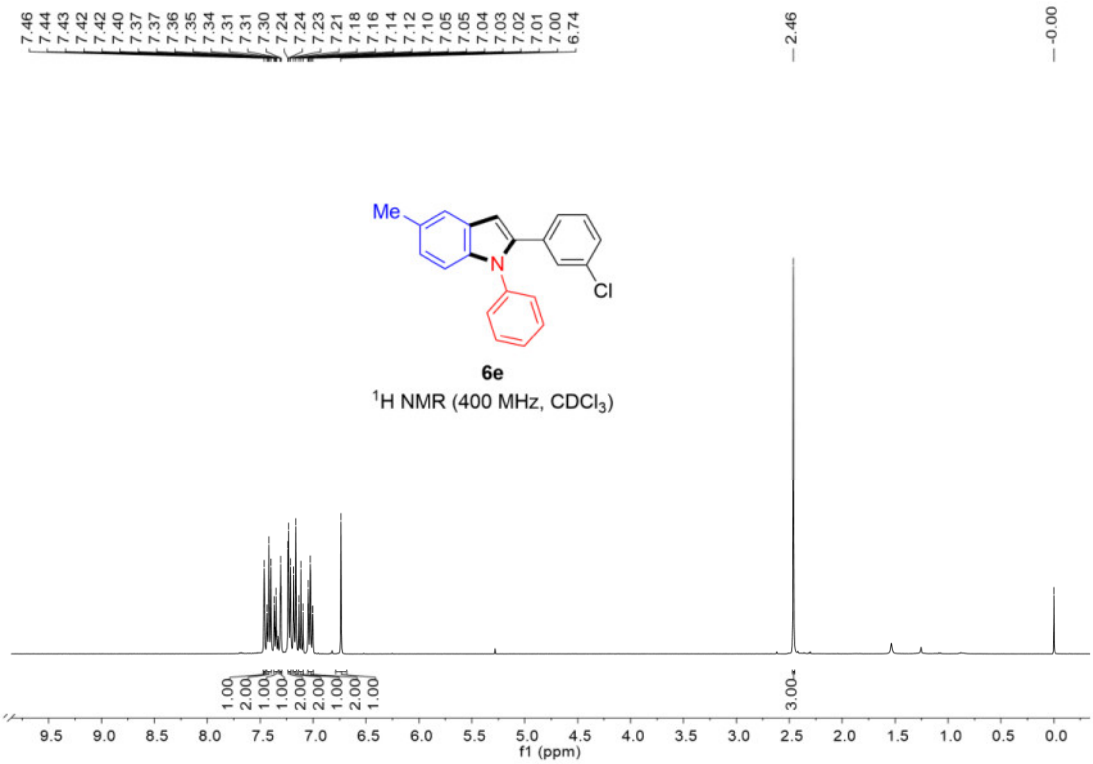


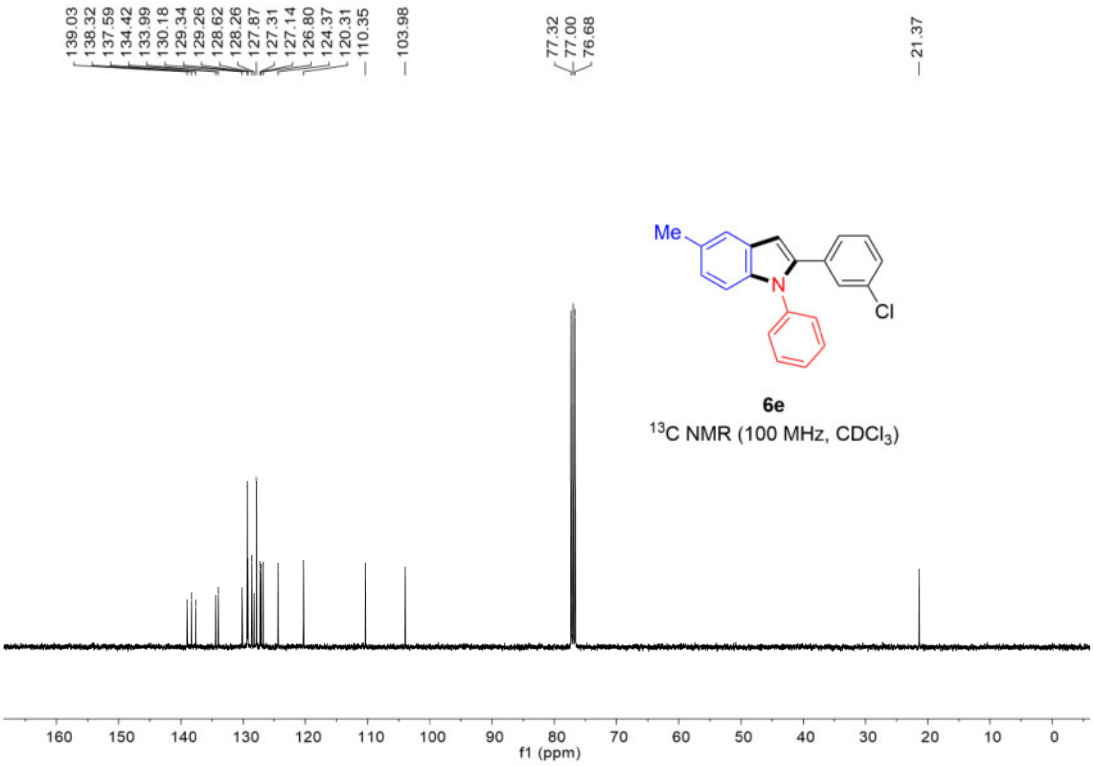


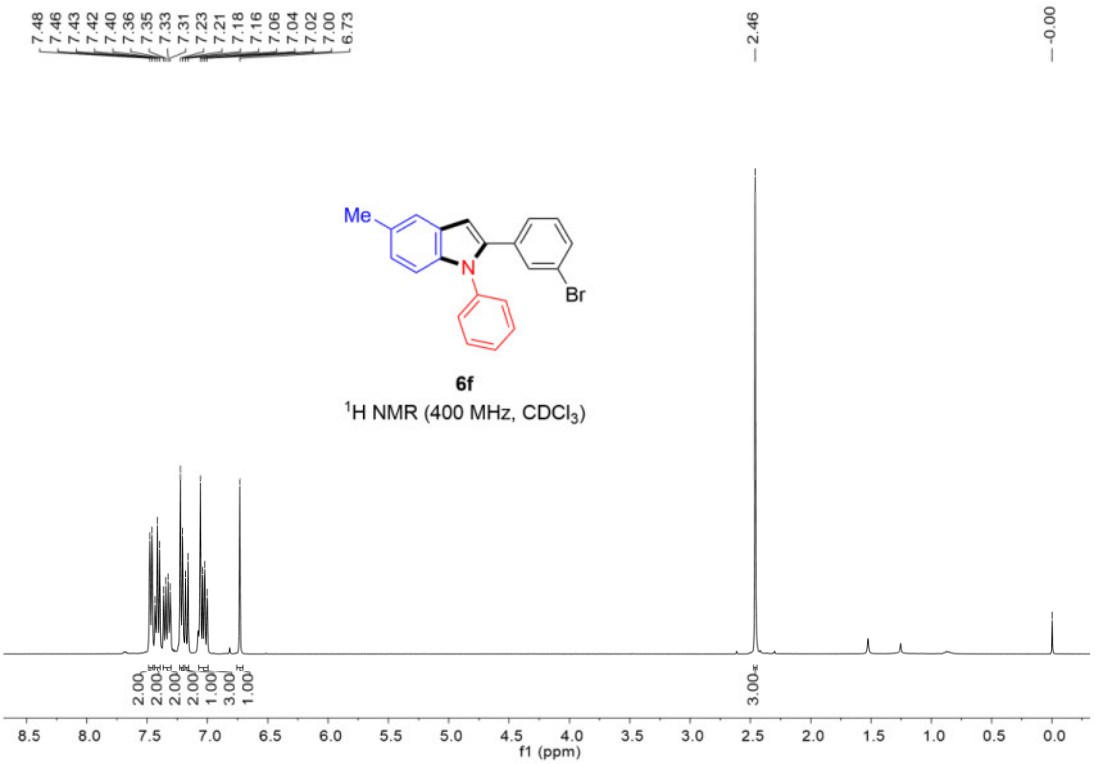
6d

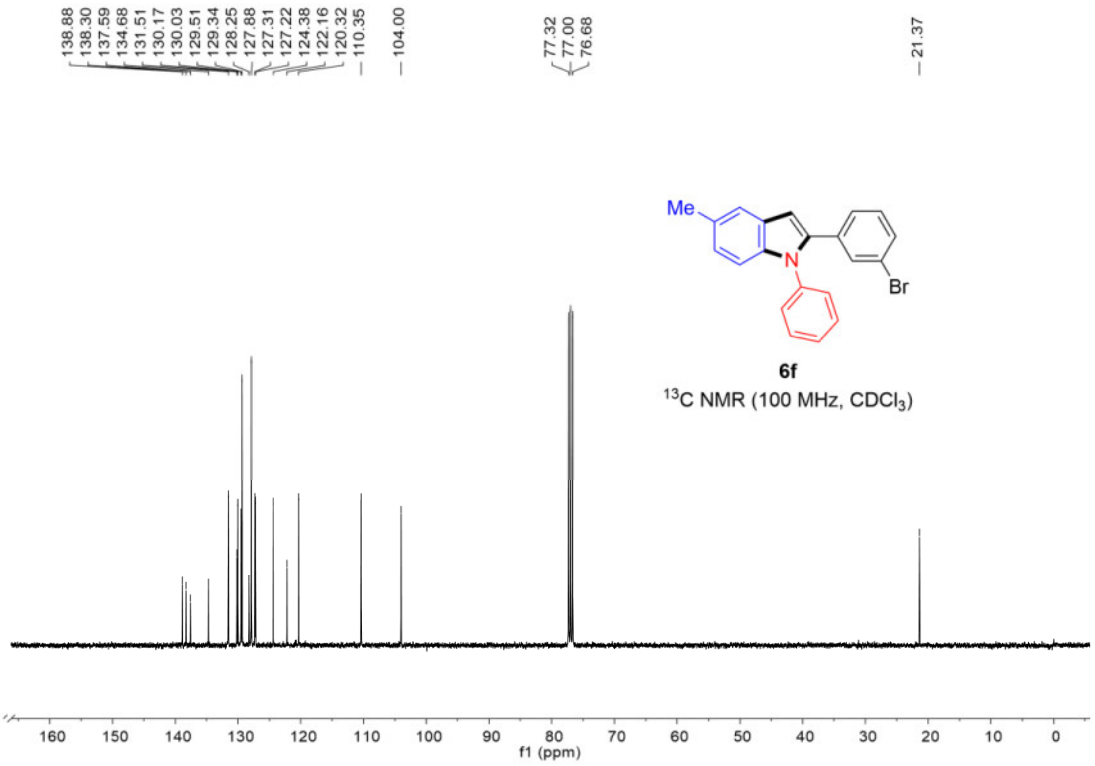
^{13}C NMR (100 MHz, $CDCl_3$)

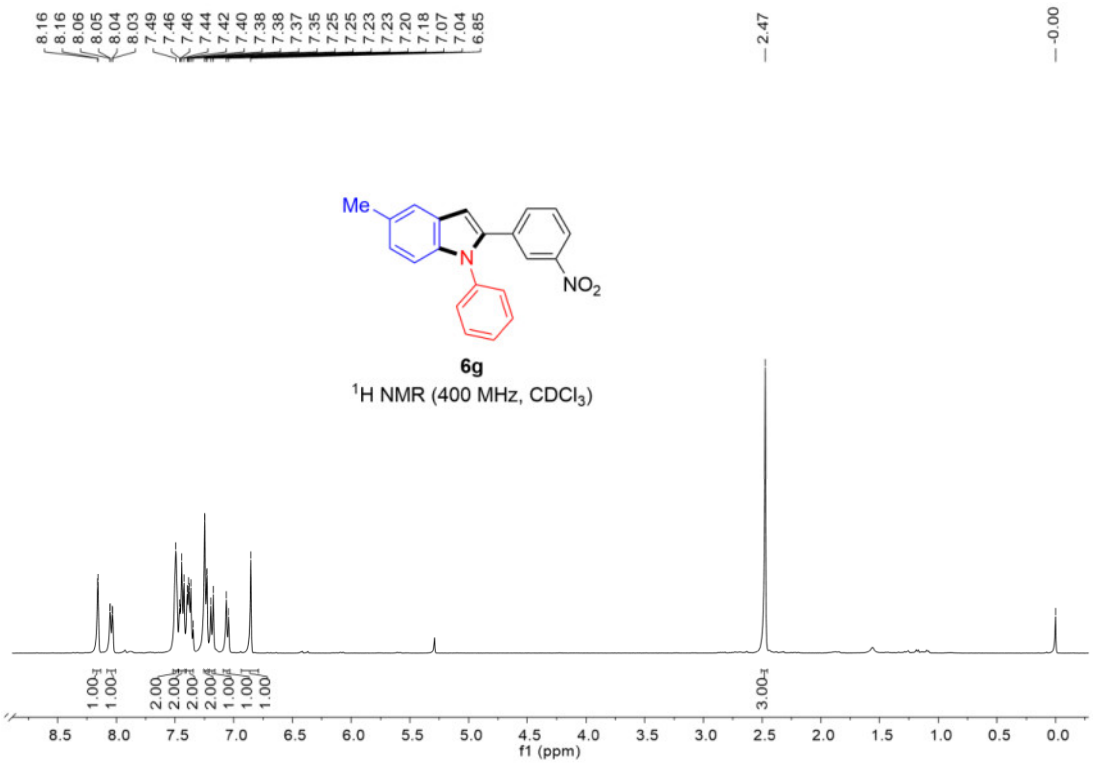


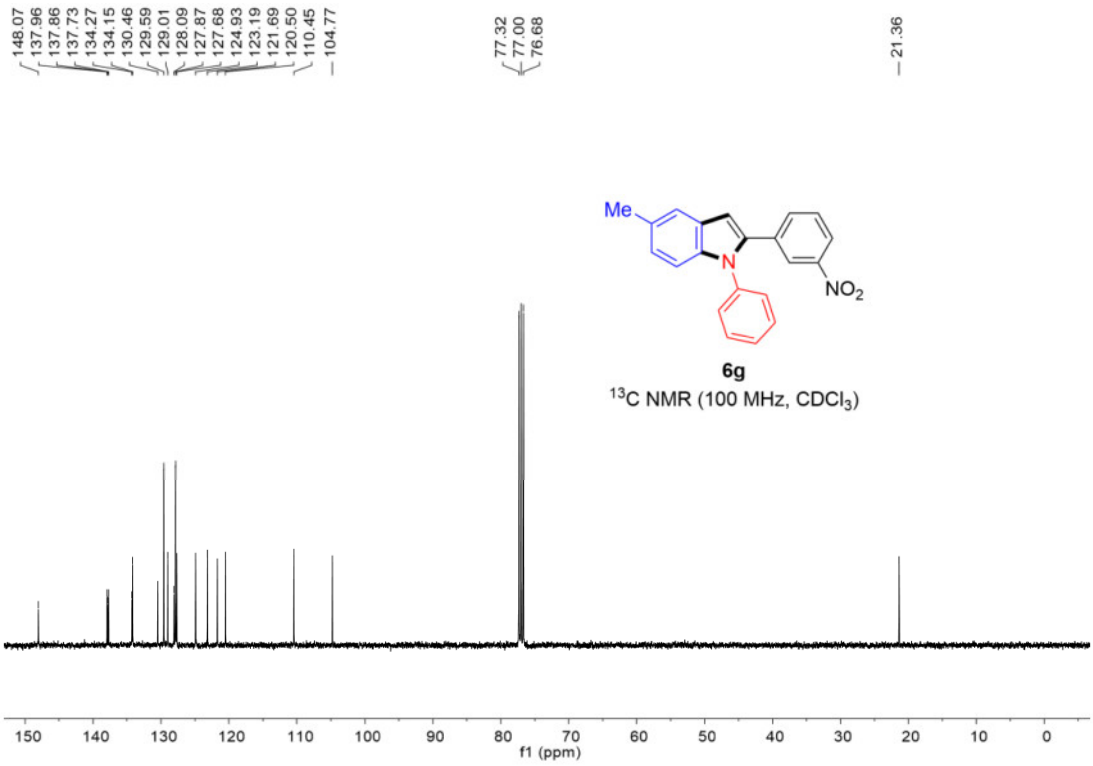

7.46
7.44
7.43
7.42
7.42
7.40
7.37
7.37
7.36
7.35
7.34
7.31
7.31
7.30
7.24
7.24
7.23
7.21
7.18
7.16
7.14
7.12
7.10
7.05
7.05
7.04
7.03
7.02
7.01
7.00
6.74
2.46
-0.00
Me
N
Cl
6e
1H NMR (400 MHz, CDCl3)
1.00
2.00
1.00
1.00
2.00
2.00
1.00
2.00
1.00
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

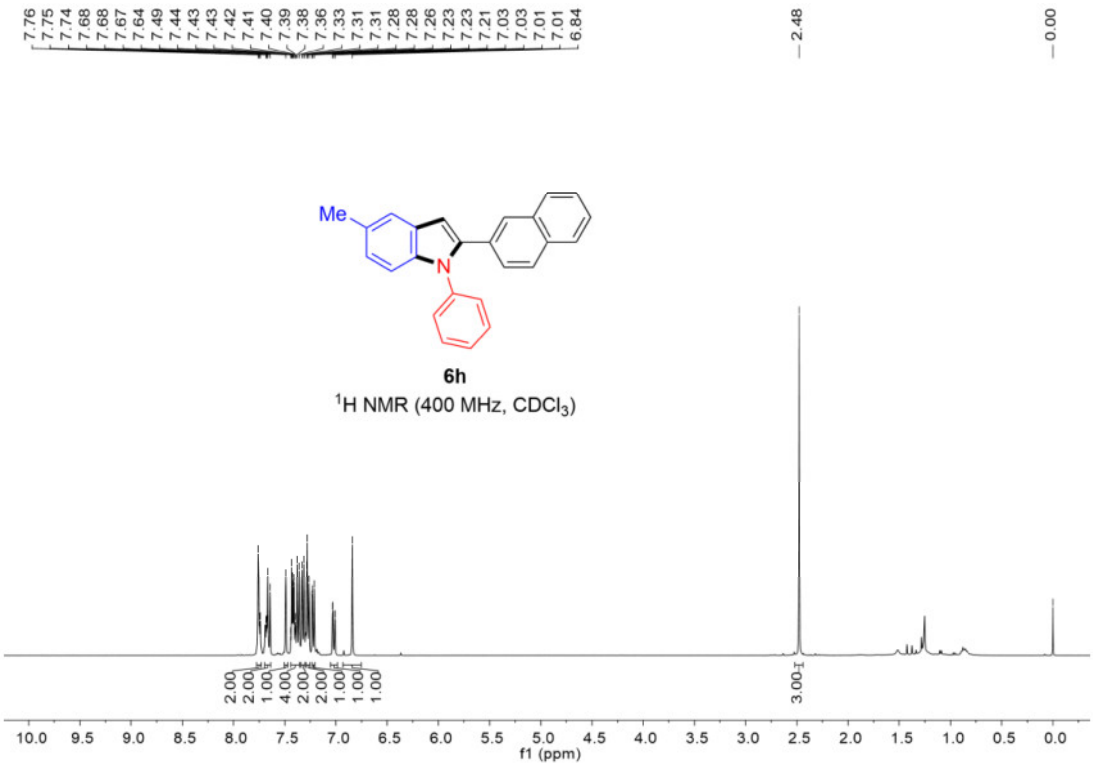

139.03
138.32
137.59
134.42
133.99
130.18
129.34
129.26
128.62
128.26
127.87
127.31
127.14
126.80
124.37
120.31
110.35
103.98
77.32
77.00
76.68
21.37
Me
N
Cl
6e
13C NMR (100 MHz, CDCl3)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.48
7.46
7.43
7.42
7.40
7.36
7.35
7.33
7.31
7.23
7.21
7.18
7.16
7.06
7.04
7.02
7.00
6.73
2.46
-0.00
Me
N
Br
6f
1H NMR (400 MHz, CDCl3)
2.00
2.00
2.00
2.00
1.00
1.00
3.00
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


138.88
138.30
137.59
134.68
131.51
130.17
130.03
129.51
129.34
128.25
127.88
127.31
127.22
124.38
122.16
120.32
110.35
104.00
77.32
77.00
76.68
21.37
Me
N
Br
6f
13C NMR (100 MHz, CDCl3)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

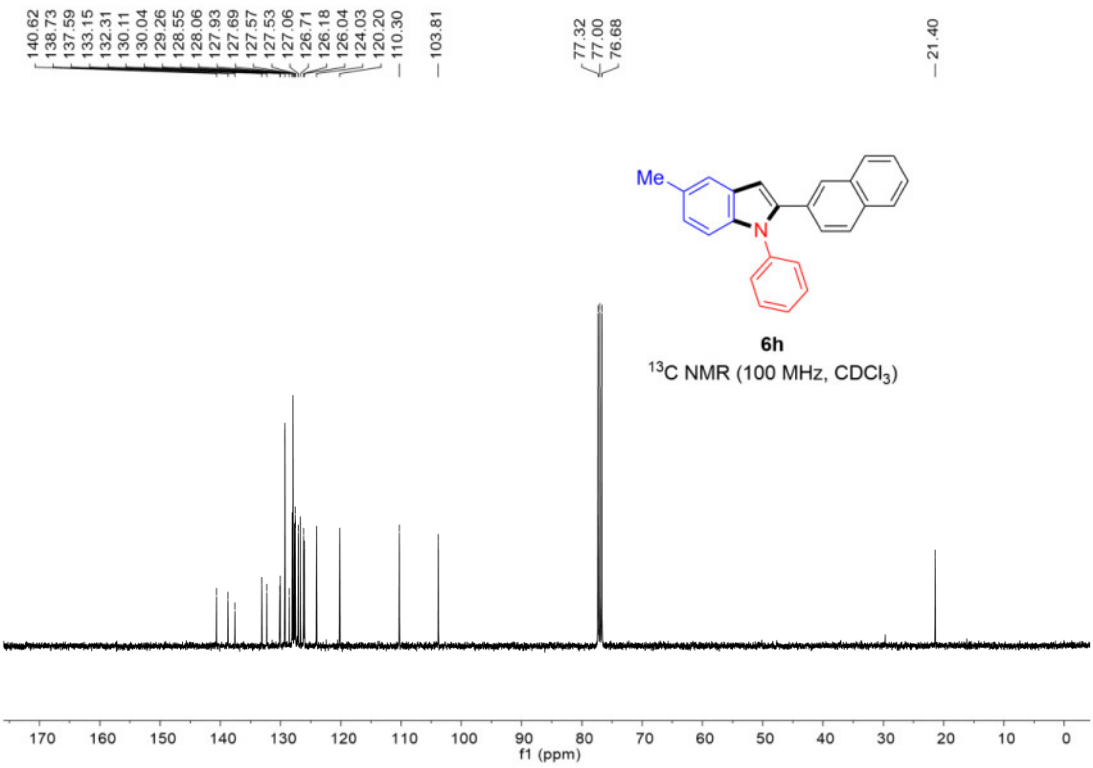

8.16
8.16
8.06
8.05
8.04
8.03
7.49
7.46
7.46
7.44
7.42
7.40
7.38
7.38
7.37
7.35
7.25
7.25
7.23
7.23
7.20
7.18
7.07
7.04
6.85
2.47
-0.00
Me
N
NO2
6g
1H NMR (400 MHz, CDCl3)
1.00
1.00
2.00
2.00
2.00
2.00
1.00
1.00
1.00
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


148.07
137.96
137.86
137.73
134.27
134.15
130.46
129.59
129.01
128.09
127.87
127.68
124.93
123.19
121.69
120.50
110.45
104.77
77.32
77.00
76.68
21.36
Me
N
NO2
6g
13C NMR (100 MHz, CDCl3)
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



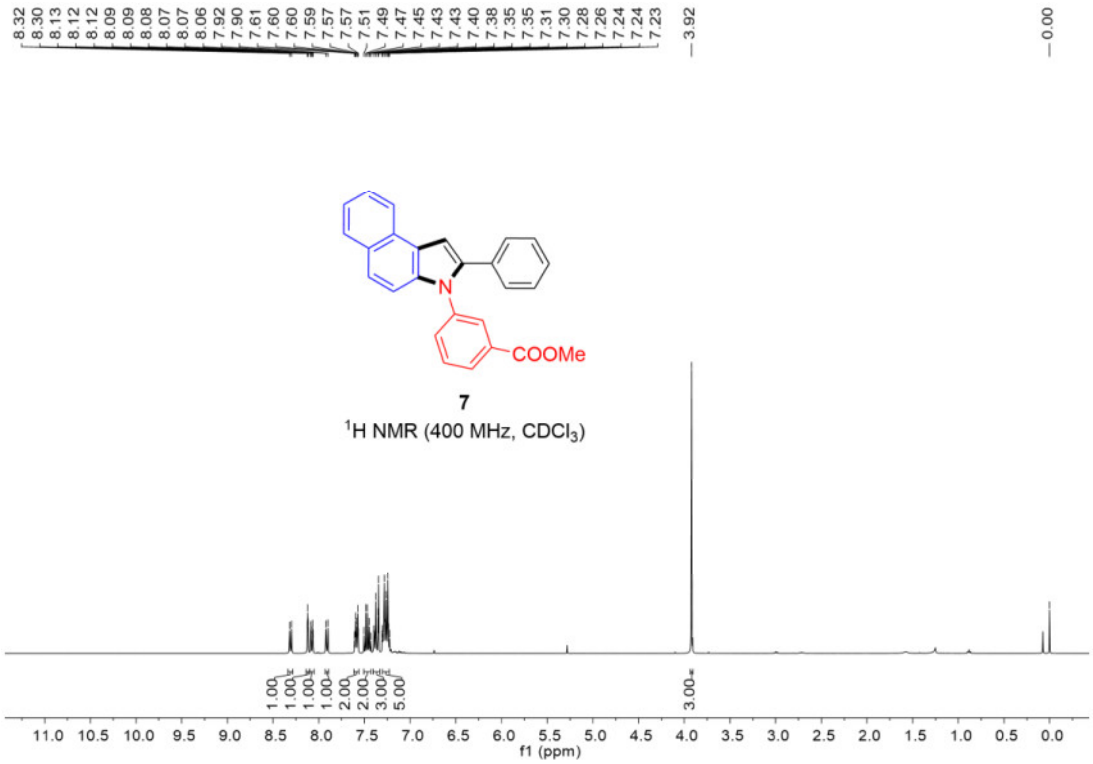
6h

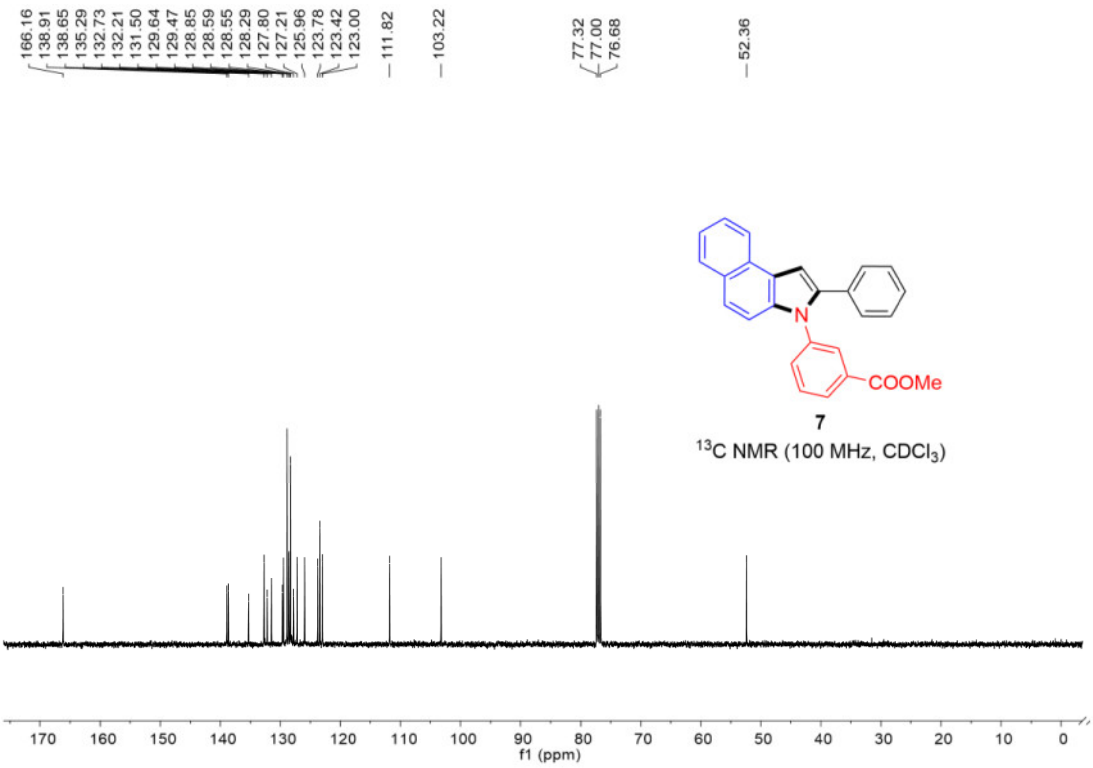
^{1}H NMR (400 MHz, $CDCl_3$)

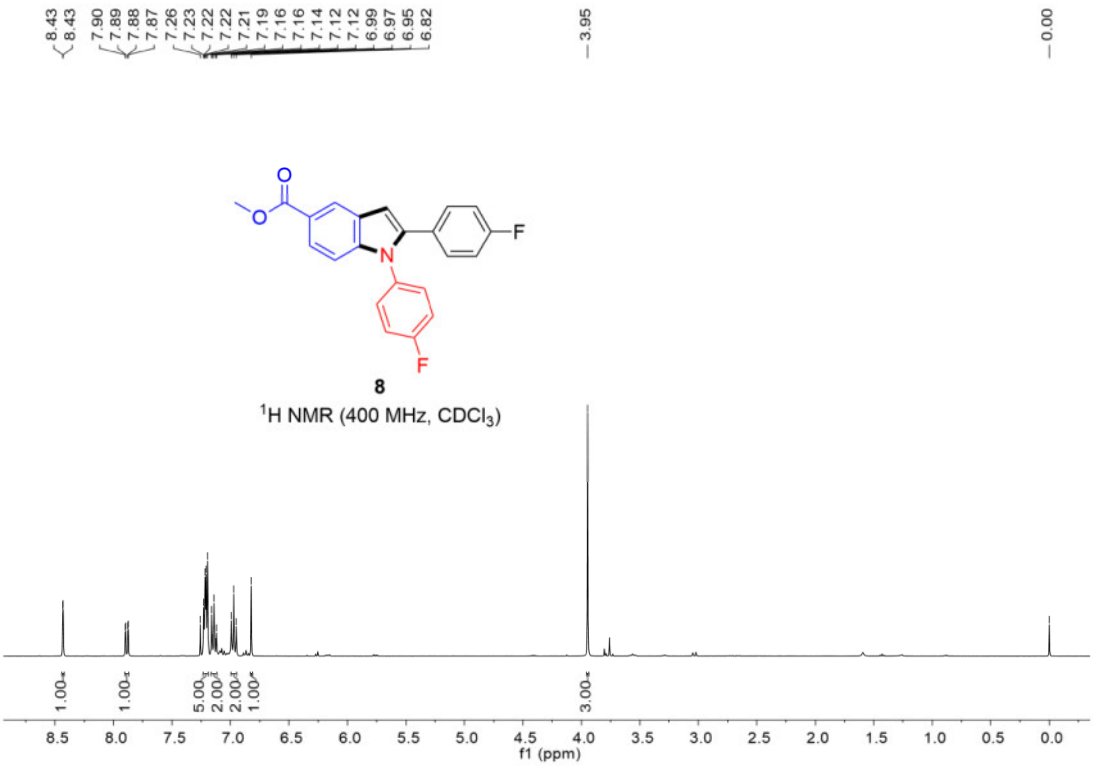


6h

^{13}C NMR (100 MHz, $CDCl_3$)

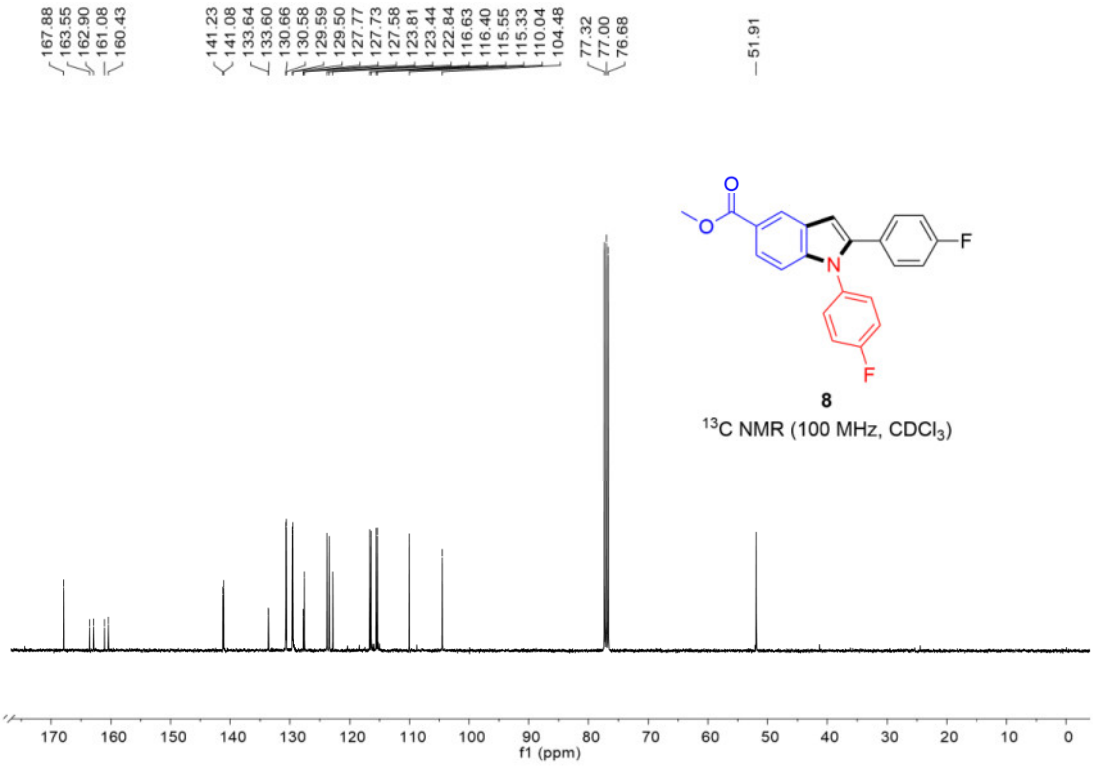

8.32
8.30
8.13
8.12
8.12
8.09
8.09
8.08
8.07
8.07
8.06
7.92
7.90
7.61
7.60
7.60
7.59
7.57
7.57
7.51
7.49
7.47
7.45
7.43
7.40
7.38
7.35
7.35
7.31
7.30
7.28
7.26
7.24
7.24
7.23
3.92
0.00
N
COOMe
7
1H NMR (400 MHz, CDCl3)
1.00
1.00
1.00
1.00
2.00
2.00
3.00
5.00
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


166.16
138.91
138.65
135.29
132.73
132.21
131.50
129.64
129.47
128.85
128.59
128.55
128.29
127.80
127.21
125.96
123.78
123.42
123.00
111.82
103.22
77.32
77.00
76.68
52.36
N
COOMe
7
13C NMR (100 MHz, CDCl3)
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



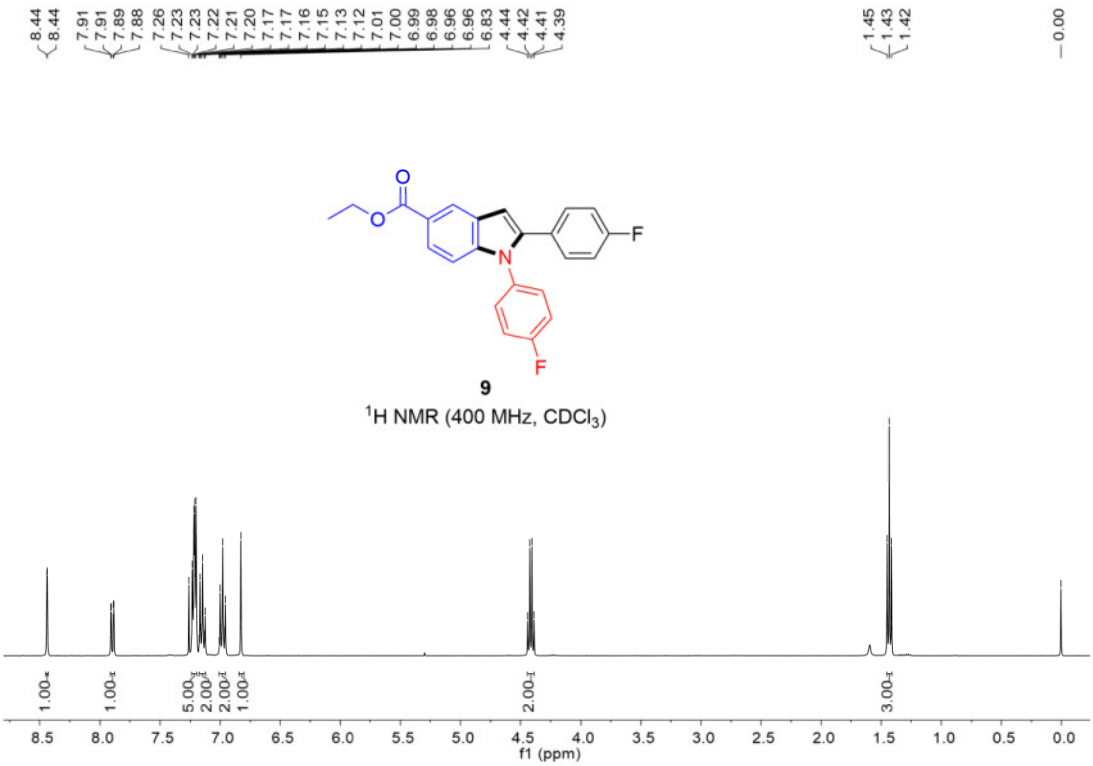
8

^{1}H NMR (400 MHz, $CDCl_3$)



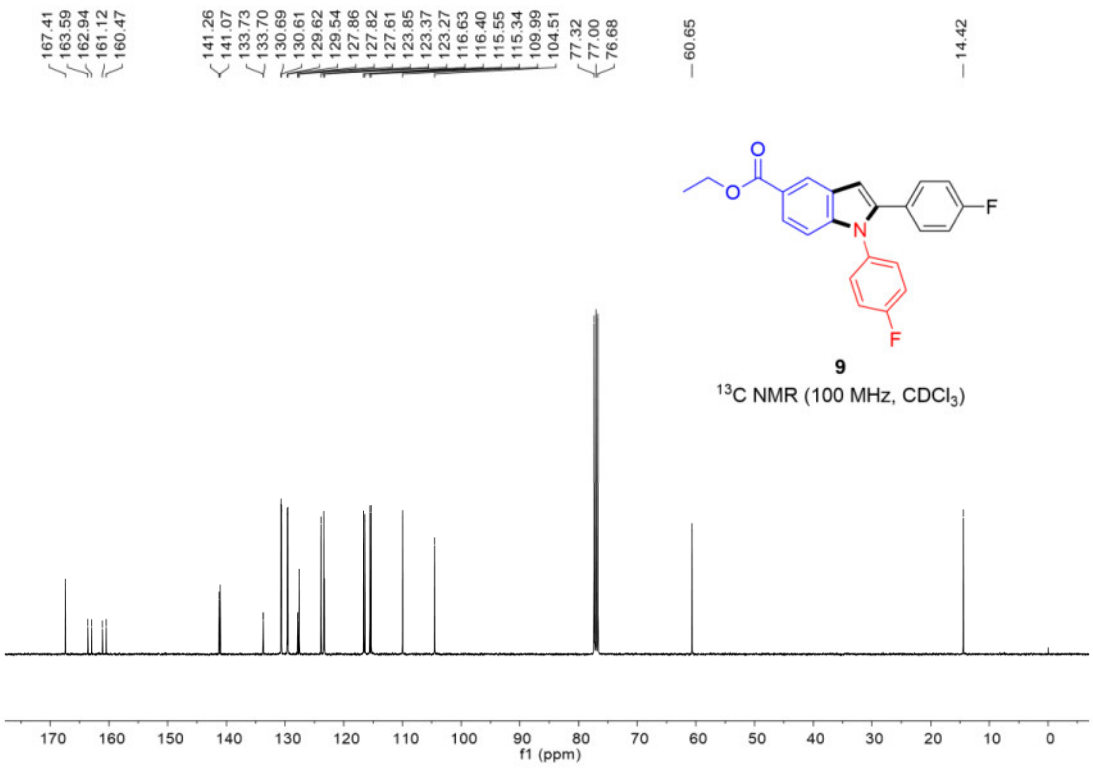
8

^{13}C NMR (100 MHz, $CDCl_3$)



9

^{1}H NMR (400 MHz, $CDCl_3$)



9

^{13}C NMR (100 MHz, $CDCl_3$)